

Supplementary Information

**Enantioselective Synthesis of Unsymmetrical  $\alpha,\alpha$ -Diarylacetates  
via Organocatalyzed Formal C–H Insertion Reactions of  
Sulfoxonium Ylides with Indoles and Pyrroles**

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## I. General Information

Flash column chromatography was performed over silica gel (200–300 mesh) purchased from Qindao Puke Co., China. All air or moisture sensitive reactions were conducted in oven-dried glassware under nitrogen atmosphere using anhydrous solvents. Anhydrous acetonitrile was purified by the Innovative® solvent purification system or purchased from J&K Scientific Ltd. Trimethylsulfoxonium iodide, KO<sup>t</sup>Bu, aryl bromides, aryl acyl chloride used in this study were purchased from Energy Chemical, and used as received. XPhos and anilines used in this study were purchased from Shanghai Haohong Scientific Co., Ltd (Leyan). Other solvents (such as DCM, MeOH, THF, EA, and *n*-hexane) used in this study all were purchased from Energy Chemical, and directly used without further purification. <sup>1</sup>H, <sup>13</sup>C and <sup>19</sup>F NMR spectra were collected on a Bruker AV 400 or 300 MHz NMR spectrometer using residue solvent peaks as an internal standard (<sup>1</sup>H NMR: CDCl<sub>3</sub> at 7.26 ppm; <sup>13</sup>C NMR: CDCl<sub>3</sub> at 77.0 ppm). Mass spectra were collected on an Agilent GC/MS 5975C system, a MALDI Micro MX mass spectrometer, or an API QSTAR XL System with TOF as mass analyzer. Optical rotations were measured on Shanghai Shengguang polarimeter with [α]<sub>D</sub> values reported in degrees. The enantiomeric excess values were determined by chiral HPLC using an Agilent 1260 LC system with a Daicel CHIRALCEL OD-H column, or a Daicel CHIRALPAK AD-H, IC and AS-H column. Unless otherwise noted, the racemic samples in this study were prepared using the racemic catalyst 1,1'-binaphthyl-2,2'-diyl hydrogenphosphate (10 mol%). The optimal catalysts (*S*)-**HA-10** and (*R*)-**HA-10** were synthesized according to the literature procedure.<sup>1</sup>

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(1) H. Ishihara, J. Huang, T. Mochizuki, M. Hatano, K. Ishihara, *ACS Catal.*, 2021, **11**, 6121–6127.

## II. Synthesis of Sulfoxonium Ylide

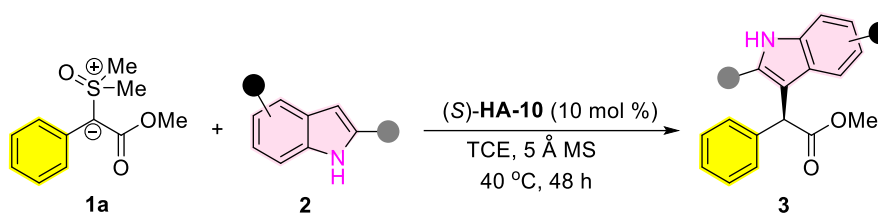
All the sulfoxonium ylides used in this work are known compounds and were synthesized according to the literature procedure.<sup>2-3</sup>

## III. Synthesis of $\alpha$ -substituted pyrrole

$\alpha$ -Substituted pyrrole used in this work are known compounds and were synthesized according to the literature procedure.<sup>4</sup>

## IV. Catalytic Asymmetric Synthesis of $\alpha,\alpha$ -Heterodiaryl Acetates

### General Procedure A.



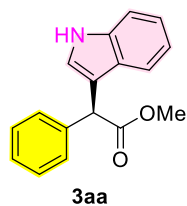
In an oven-dried 4-mL vial equipped with a magnetic stirring bar, sulfoxonium ylide **1a** (0.2 mmol, 1.0 equiv), CPA catalyst (S)-HA-10 (14.6 mg, 10 mol %), and 5 Å molecular sieves (100 mg) were combined. Subsequently, 1.0 mL of TCE was added, followed by the addition of indole **2** (0.22 mmol, 1.1 equiv). The resulting mixture was stirred at 40 °C and monitored by TLC. After completion (48 h), the mixture was directly subjected to flash column chromatography on silica gel (eluent: hexanes/ethyl acetate = 10:1 to 5:1) to afford the desired product **3**.

(2) C. Janot, P. Palamini, B. C. Dobson, J. Muir, C. Aïssa, *Org. Lett.*, 2019, **21**, 296–299.

(3) J. Lu, L. Li, X.-K. He, G.-Y. Xu, J. Xuan, *Chin. J. Chem.*, 2021, **39**, 1646–1650.

(4) S. J. Mishra, S. Ghosh, A. R. Stothert, C. A. Dickey, B. S. J. Blagg, *ACS Chem. Biol.*, 2017, **12**, 244–253.





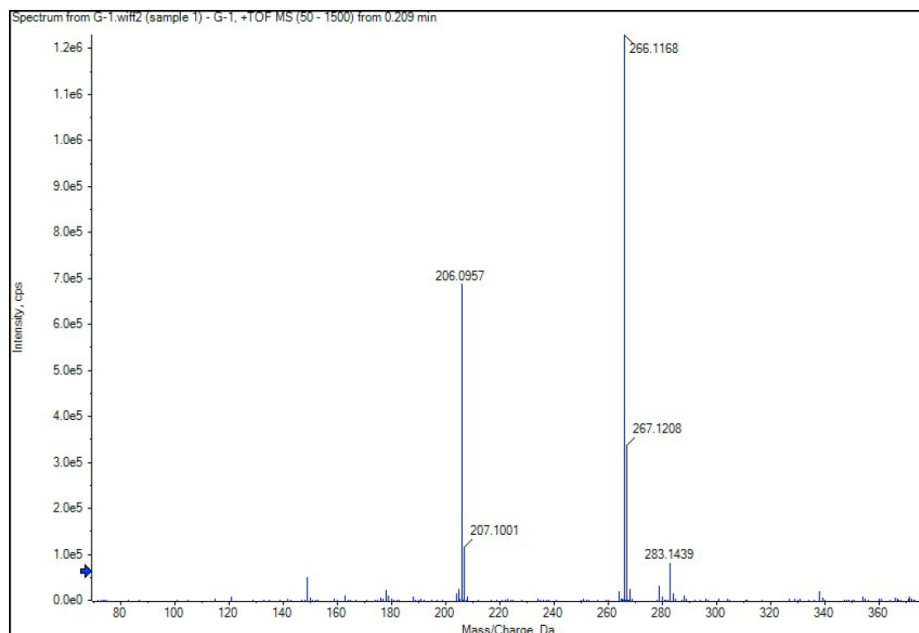
**Methyl (S)-2-(1H-indol-3-yl)-2-phenylacetate (3aa)** was prepared as a colorless oil according to the General Procedure A (eluent: hexanes/EtOAc = 10:1, 38.0 mg, 71% yield, 89% ee).

$[\alpha]_D^{25}$ : +12.1 ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK<sup>®</sup> IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 8.5 min (major), 14.0 min (minor).

<sup>1</sup>H NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.03 (s, 1H), 7.37 – 7.32 (m, 3H), 7.24 – 7.16 (m, 4H), 7.10 – 6.95 (m, 3H), 5.18 (s, 1H), 3.65 (s, 3H) ppm.

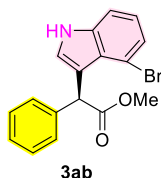
<sup>13</sup>C NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  173.6, 138.6, 136.3, 128.6, 128.5, 127.3, 126.6, 123.3, 122.3, 119.8, 119.0, 113.6, 111.3, 52.3, 48.9 ppm.

HRMS (ESI+) Calcd for  $\text{C}_{17}\text{H}_{16}\text{NO}_2$   $[\text{M}+\text{H}]^+$ : 266.1176, found: 266.1168.



Note: It is a known compound, the spectroscopy data were in good agreement with the literature.<sup>5</sup>

(5) J. M. Fraile, K. L. Jeune, J. A. Mayoral, N. Ravasio, F. Zaccheria, *Org. Biomol. Chem.*, 2013, **11**, 4327–4332.



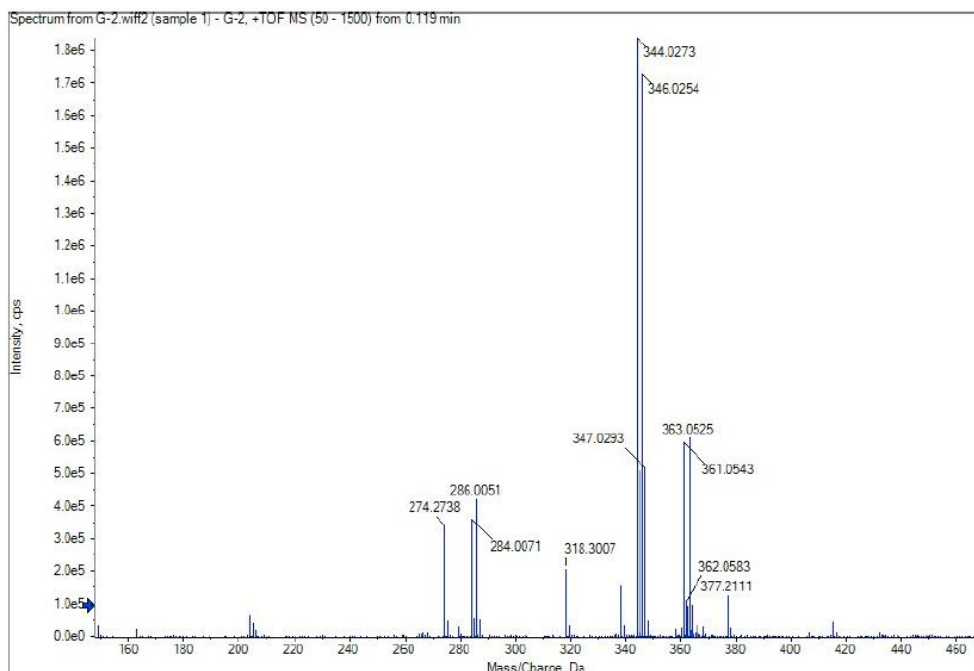
**Methyl (S)-2-(4-bromo-1H-indol-3-yl)-2-phenylacetate (3ab)** was prepared as a brown solid according to the General Procedure A (eluent: hexanes/EtOAc = 10:1, 38.2 mg, 55% yield, 88% ee).

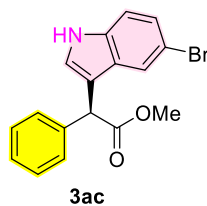
$[\alpha]_D^{25}$ :  $-56.6$  ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK<sup>®</sup> IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 7.8 min (major), 18.0 min (minor).

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.34 (s, 1H), 7.35 – 7.34 (m, 4H), 7.32 – 7.28 (m, 1H), 7.24 – 7.21 (m, 1H), 7.13 – 7.11 (m, 1H), 6.95 – 6.90 (m, 1H), 6.753 – 6.747 (m, 1H), 5.94 (s, 1H), 3.75 (s, 3H) ppm.

$^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  174.5, 138.7, 137.7, 128.7, 128.6, 127.3, 125.9, 124.7, 124.3, 123.1, 114.8, 113.7, 110.8, 52.6, 48.9 ppm.

**HRMS** (ESI+) Calcd for  $\text{C}_{17}\text{H}_{15}\text{BrNO}_2$   $[\text{M}+\text{H}]^+$ : 344.0281, found: 344.0273.





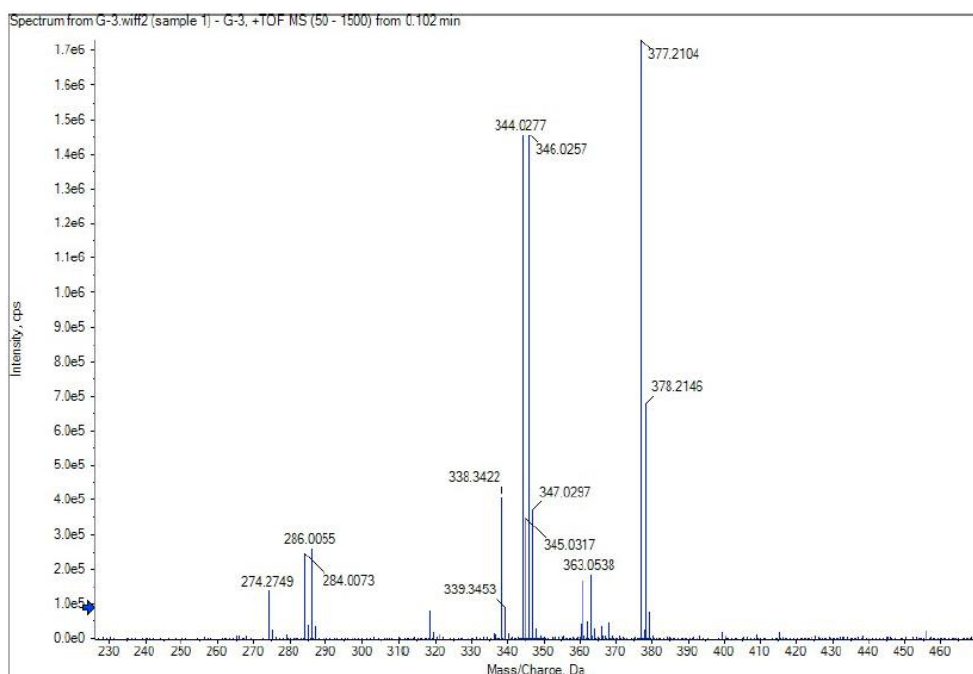
**Methyl (S)-2-(5-bromo-1H-indol-3-yl)-2-phenylacetate (3ac)** was prepared as a white solid according to the General Procedure A (eluent: hexanes/EtOAc = 10:1, 47.0 mg, 68% yield, 92% ee).

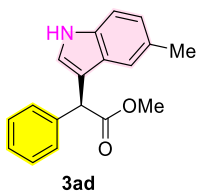
$[\alpha]_D^{25}$ :  $-47.2$  ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK<sup>®</sup> IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 5.7 min (major), 6.6 min (minor).

<sup>1</sup>H NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.20 (s, 1H), 7.56 – 7.55 (m, 1H), 7.39 – 7.37 (m, 2H), 7.34 – 7.30 (m, 2H), 7.29 – 7.27 (m, 1H), 7.25 – 7.22 (m, 1H), 7.18 – 7.13 (m, 2H), 5.18 (s, 1H), 3.75 (s, 3H) ppm.

<sup>13</sup>C NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  173.3, 138.1, 134.9, 128.7, 128.33, 128.28, 127.5, 125.2, 124.6, 121.5, 113.3, 113.1, 112.8, 52.5, 48.6 ppm.

HRMS (ESI+) Calcd for  $\text{C}_{17}\text{H}_{15}\text{BrNO}_2$   $[\text{M}+\text{H}]^+$ : 344.0281, found: 344.0277.





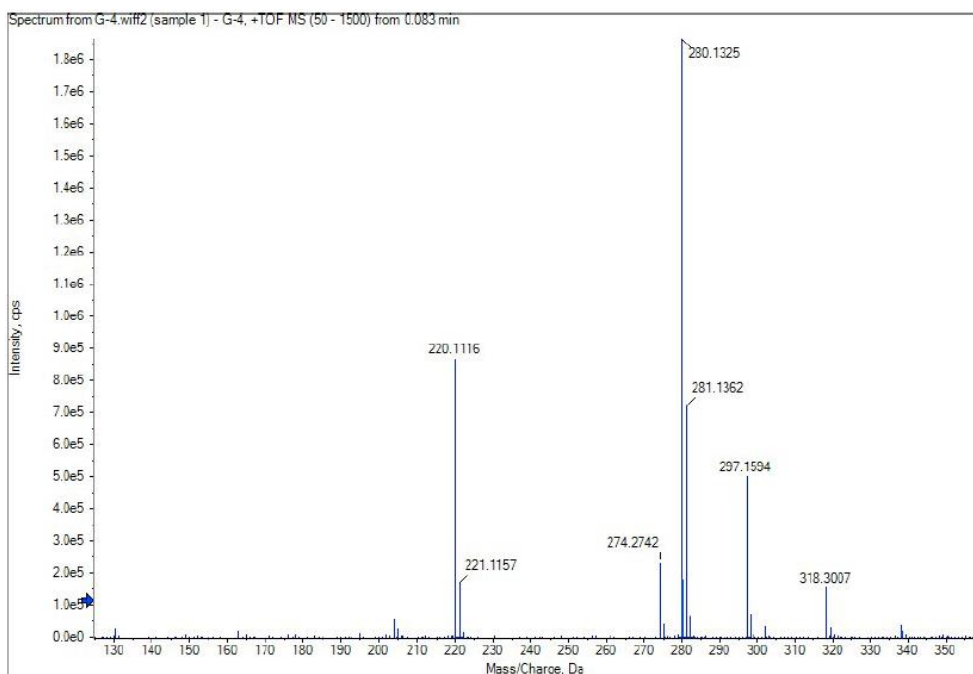
**Methyl (S)-2-(5-methyl-1H-indol-3-yl)-2-phenylacetate (3ad)** was prepared as a yellow solid according to the General Procedure A (eluent: hexanes/EtOAc = 10:1, 42.1 mg, 75% yield, 88% ee).

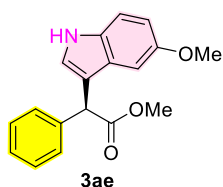
$[\alpha]_D^{25}$ : +1.5 ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 8.1 min (major), 10.0 min (minor).

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.02 (s, 1H), 7.42 – 7.40 (m, 2H), 7.32 – 7.29 (m, 2H), 7.27 – 7.19 (m, 3H), 7.090 – 7.085 (m, 1H), 7.00 – 6.98 (m, 1H), 5.24 (s, 1H), 3.73 (s, 3H), 2.39 (s, 3H) ppm.

$^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  173.7, 138.6, 134.6, 129.0, 128.6, 128.4, 127.3, 126.8, 124.0, 123.4, 118.5, 113.1, 111.0, 52.4, 48.8, 21.6 ppm.

**HRMS (ESI+)** Calcd for  $\text{C}_{18}\text{H}_{18}\text{NO}_2$   $[\text{M}+\text{H}]^+$ : 280.1332, found: 280.1325.





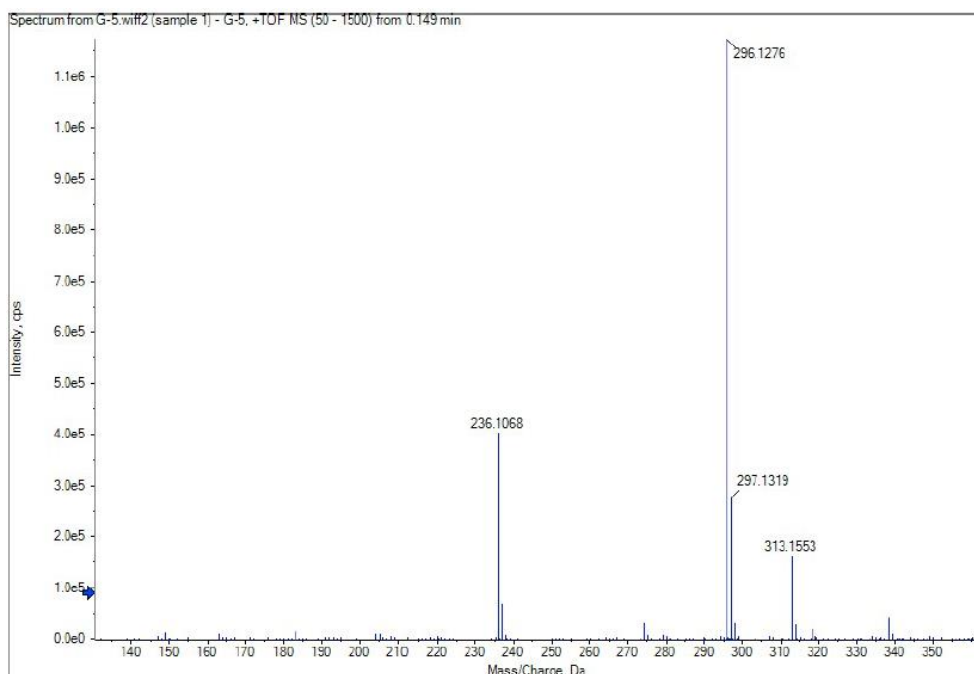
**Methyl (S)-2-(5-methoxy-1H-indol-3-yl)-2-phenylacetate (3ae)** was prepared as a yellow oil according to the General Procedure A (eluent: hexanes/EtOAc = 10:1, 42.8 mg, 72% yield, 89% ee).

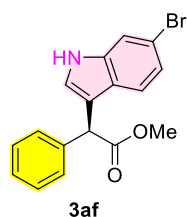
$[\alpha]_{\text{D}}^{25}$ :  $-12.5$  ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 13.9 min (major), 24.7 min (minor).

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.04 (s, 1H), 7.42 – 7.40 (m, 2H), 7.33 – 7.29 (m, 2H), 7.27 – 7.20 (m, 2H), 7.13 – 7.12 (m, 1H), 6.87 – 6.82 (m, 2H), 5.22 (s, 1H), 3.77 (s, 3H), 3.75 (s, 3H) ppm.

$^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  173.5, 154.1, 138.5, 131.4, 128.6, 128.4, 127.3, 127.0, 124.0, 113.3, 112.4, 112.0, 100.9, 55.8, 52.4, 48.9 ppm.

**HRMS (ESI+)** Calcd for  $\text{C}_{18}\text{H}_{18}\text{NO}_3$   $[\text{M}+\text{H}]^+$ : 296.1281, found: 296.1276.





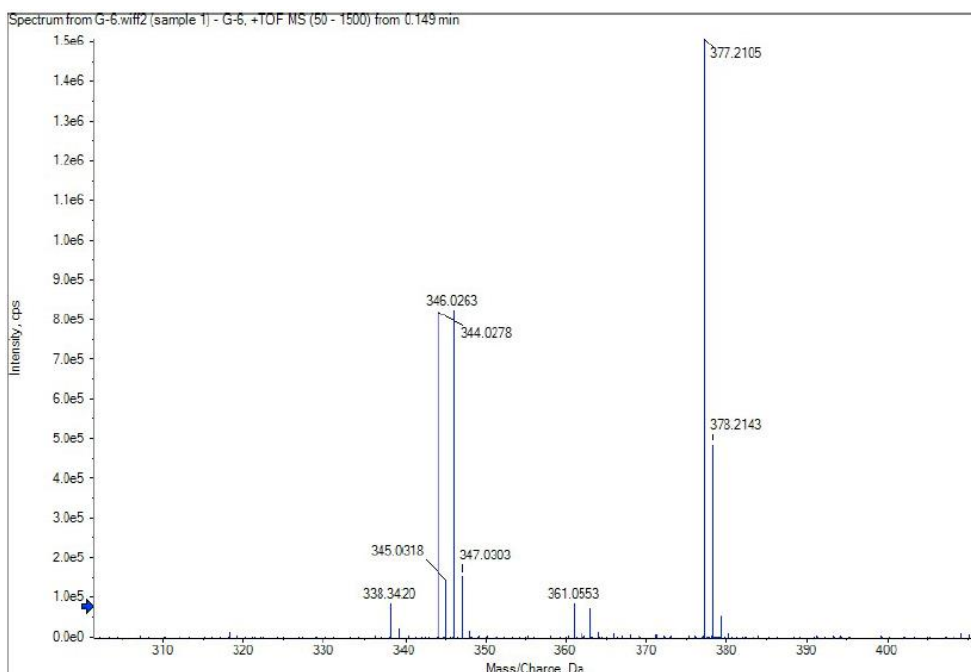
**Methyl (S)-2-(6-bromo-1H-indol-3-yl)-2-phenylacetate (3af)** was prepared as a brown oil according to the General Procedure A (eluent: hexanes/EtOAc = 10:1, 42.0 mg, 61% yield, 89% ee).

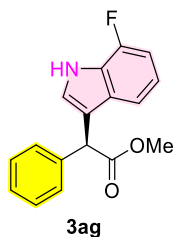
$[\alpha]_{D^{25}}$ : +2.7 ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK® AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 25.0 min (major), 28.5 min (minor).

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.16 (s, 1H), 7.46 – 7.45 (m, 1H), 7.39 – 7.37 (m, 2H), 7.33 – 7.29 (m, 2H), 7.28 – 7.25 (m, 2H), 7.16 – 7.11 (m, 2H), 5.21 (s, 1H), 3.75 (s, 3H) ppm.

$^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  173.3, 138.2, 137.1, 128.7, 128.4, 127.5, 125.5, 123.9, 123.1, 120.3, 115.9, 114.2, 113.9, 52.5, 48.7 ppm.

**HRMS (ESI+)** Calcd for  $\text{C}_{17}\text{H}_{15}\text{BrNO}_2$   $[\text{M}+\text{H}]^+$ : 344.0281, found: 344.0278.





**Methyl (S)-2-(7-fluoro-1H-indol-3-yl)-2-phenylacetate (3ag)** was prepared as a yellow oil according to the General Procedure A (eluent: hexanes/EtOAc = 10:1, 40.0 mg, 70% yield, 94% ee).

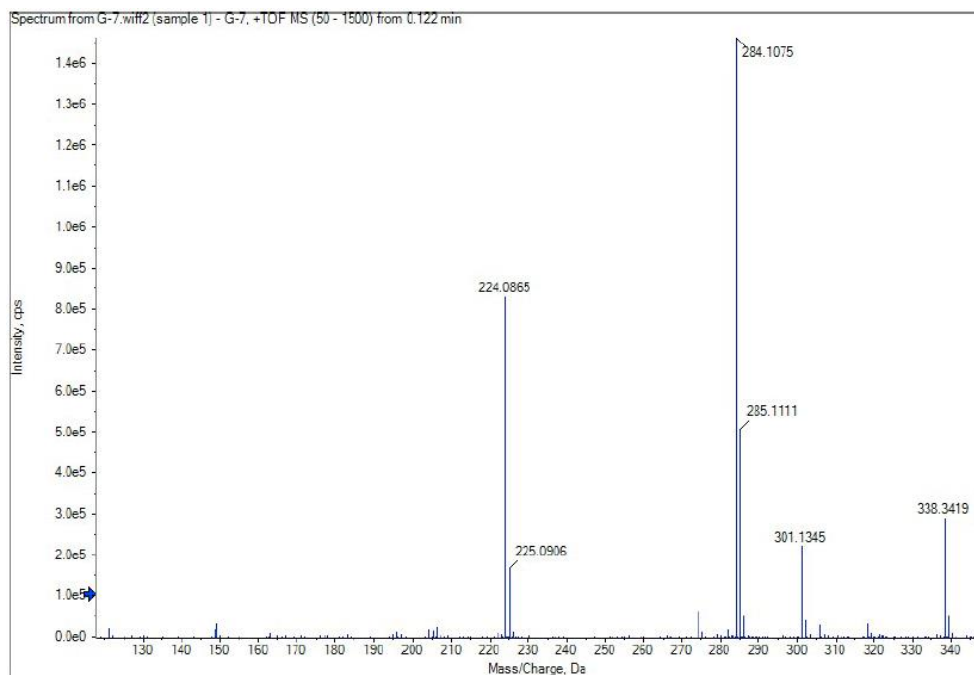
$[\alpha]_D^{25}$ : +3.4 ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK® AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 14.4 min (major), 17.8 min (minor).

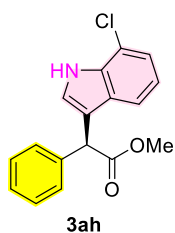
$^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.27 (s, 1H), 7.33 – 7.30 (m, 2H), 7.25 – 7.15 (m, 3H), 7.12 – 7.09 (m, 2H), 6.91 – 6.76 (m, 2H), 5.15 (s, 1H), 3.66 (s, 3H) ppm.

$^{13}\text{C NMR}$  (75 MHz,  $\text{CDCl}_3$ )  $\delta$  173.3, 149.6 (d,  $^1J_{\text{C-F}} = 242.4$  Hz), 138.3, 130.3 (d,  $^3J_{\text{C-F}} = 5.2$  Hz), 128.7, 128.4, 127.4, 124.7 (d,  $^2J_{\text{C-F}} = 13.5$  Hz), 124.0, 120.0 (d,  $^3J_{\text{C-F}} = 6.2$  Hz), 114.8 (d,  $^4J_{\text{C-F}} = 3.0$  Hz), 114.6 (d,  $^4J_{\text{C-F}} = 2.2$  Hz), 107.1 (d,  $^2J_{\text{C-F}} = 15.9$  Hz), 52.4, 48.9 ppm.

$^{19}\text{F NMR}$  (282 MHz,  $\text{CDCl}_3$ )  $\delta$  -135.3 ppm.

**HRMS** (ESI+) Calcd for  $\text{C}_{17}\text{H}_{15}\text{FNO}_2$   $[\text{M}+\text{H}]^+$ : 284.1081, found: 284.1075.





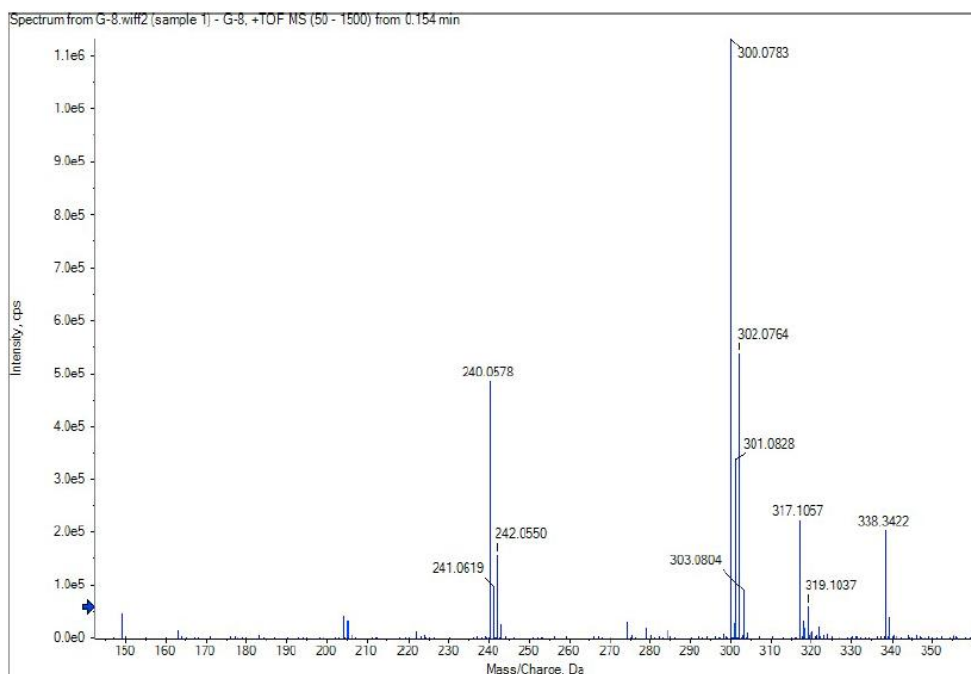
**Methyl (S)-2-(7-chloro-1H-indol-3-yl)-2-phenylacetate (3ah)** was prepared as a yellow solid according to the General Procedure A (eluent: hexanes/EtOAc = 10:1, 41.2 mg, 68% yield, 96% ee).

$[\alpha]_D^{25}$ : +21.8 ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK® AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 17.5 min (major), 21.3 min (minor).

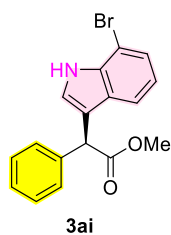
$^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.29 (s, 1H), 7.32 – 7.29 (m, 2H), 7.25 – 7.06 (m, 6H), 6.89 (t,  $J = 7.8$  Hz, 1H), 5.15 (s, 1H), 3.66 (s, 3H) ppm.

$^{13}\text{C NMR}$  (75 MHz,  $\text{CDCl}_3$ )  $\delta$  173.2, 138.2, 133.6, 128.7, 128.4, 128.1, 127.5, 124.0, 121.7, 120.6, 117.7, 116.8, 114.8, 52.4, 48.9 ppm.

**HRMS** (ESI+) Calcd for  $\text{C}_{17}\text{H}_{15}\text{ClNO}_2$   $[\text{M}+\text{H}]^+$ : 300.0786, found: 300.0783.







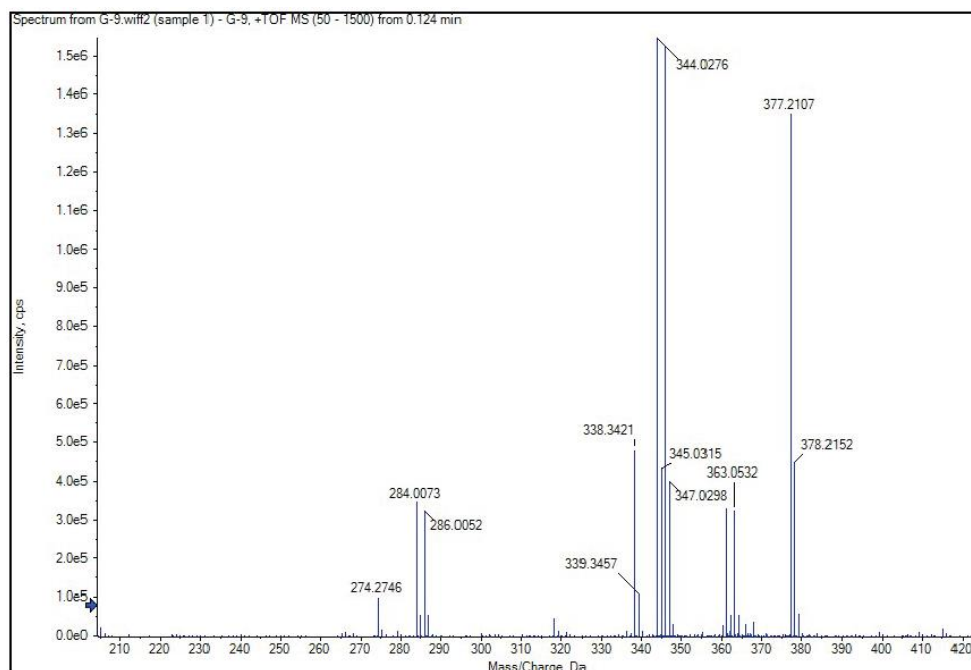
**Methyl (S)-2-(7-bromo-1H-indol-3-yl)-2-phenylacetate (3ai)** was prepared as a white solid according to the General Procedure A (eluent: hexanes/EtOAc = 10:1, 47.0 mg, 68% yield, 96% ee).

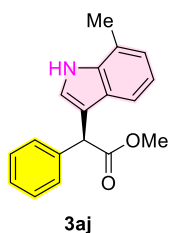
$[\alpha]_D^{25}$ : +34.7 ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK<sup>®</sup> IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 6.4 min (major), 7.0 min (minor).

<sup>1</sup>H NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.31 (s, 1H), 7.40 – 7.38 (m, 2H), 7.36 – 7.31 (m, 3H), 7.29 – 7.24 (m, 3H), 6.94 (t,  $J = 7.8$  Hz, 1H), 5.23 (s, 1H), 3.75 (s, 3H) ppm.

<sup>13</sup>C NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  173.2, 138.2, 135.0, 128.7, 128.4, 127.7, 127.5, 124.7, 123.9, 121.0, 118.4, 114.9, 104.9, 52.5, 49.0 ppm.

HRMS (ESI+) Calcd for  $\text{C}_{17}\text{H}_{15}\text{BrNO}_2$   $[\text{M}+\text{H}]^+$ : 344.0281, found: 344.0276.





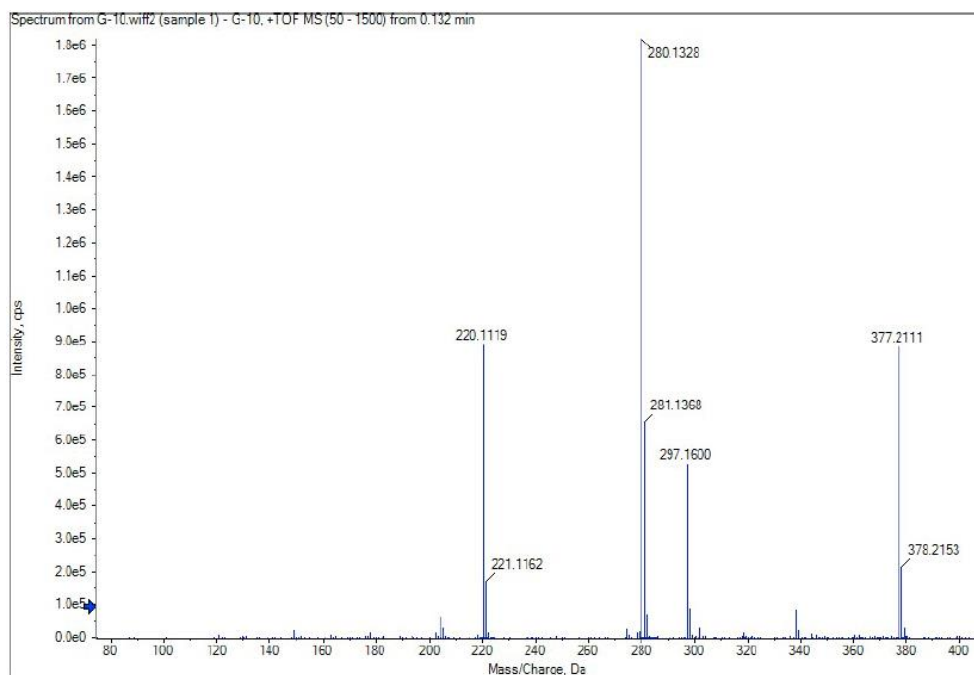
**Methyl (S)-2-(7-methyl-1H-indol-3-yl)-2-phenylacetate (3aj)** was prepared as a red solid according to the General Procedure A (eluent: hexanes/EtOAc = 10:1, 36.0 mg, 65% yield, 93% ee).

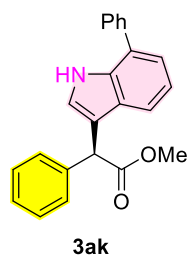
$[\alpha]_D^{25}$ : +13.7 ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK<sup>®</sup> IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 7.7 min (major), 17.4 min (minor).

<sup>1</sup>H NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.00 (s, 1H), 7.33 – 7.31 (m, 2H), 7.23 – 7.13 (m, 4H), 7.03 – 7.02 (m, 1H), 6.92 – 6.87 (m, 2H), 5.17 (s, 1H), 3.65 (s, 3H), 2.33 (s, 3H) ppm.

<sup>13</sup>C NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  173.7, 138.6, 135.9, 128.6, 128.5, 127.3, 126.1, 123.1, 122.9, 120.5, 120.0, 116.7, 114.1, 52.4, 49.0, 16.6 ppm.

HRMS (ESI+) Calcd for  $\text{C}_{18}\text{H}_{18}\text{NO}_2$   $[\text{M}+\text{H}]^+$ : 280.1332, found: 280.1328.





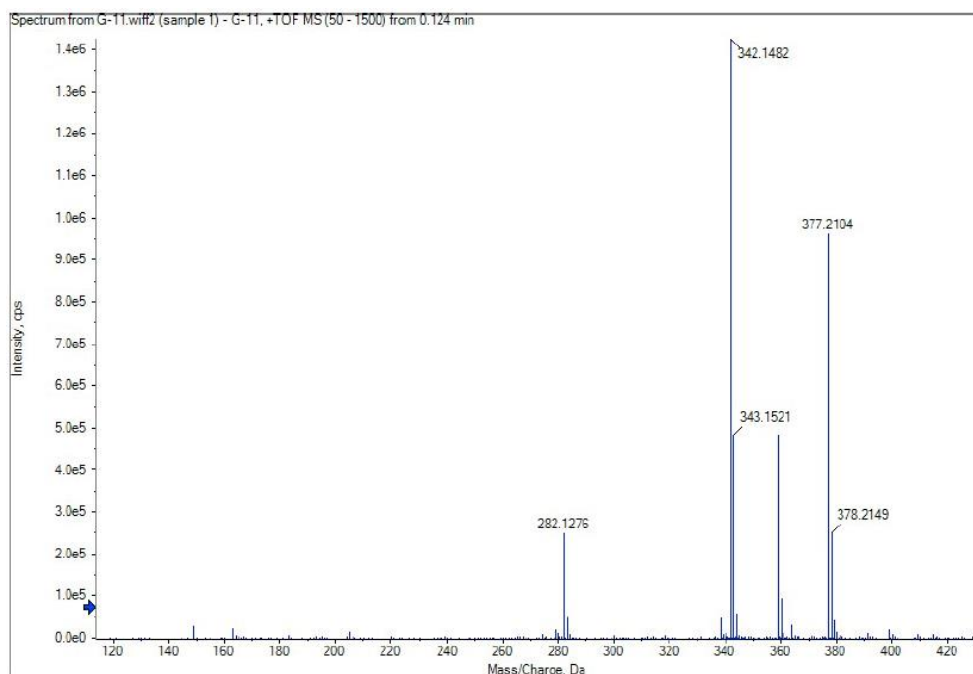
**Methyl (S)-2-phenyl-2-(7-phenyl-1H-indol-3-yl)acetate (3ak)** was prepared as a brown oil according to the General Procedure A (eluent: hexanes/EtOAc = 10:1, 50.0 mg, 73% yield, 87% ee).

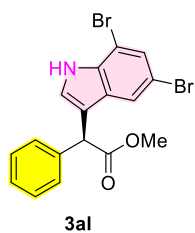
$[\alpha]_D^{25}$ : +16.9 ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK<sup>®</sup> IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 6.4 min (major), 9.4 min (minor).

<sup>1</sup>H NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.25 (s, 1H), 7.53 – 7.50 (m, 2H), 7.43 – 7.31(m, 6H), 7.28 – 7.16 (m, 3H), 7.13 – 7.04 (m, 3H), 5.21 (s, 1H), 3.67 (s, 3H) ppm.

<sup>13</sup>C NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  173.4, 139.0, 138.5, 134.1, 129.2, 128.6, 128.5, 128.3, 127.5, 127.3, 127.0, 125.8, 123.5, 122.3, 120.3, 118.3, 114.1, 52.4, 49.0 ppm.

**HRMS (ESI+)** Calcd for  $\text{C}_{23}\text{H}_{20}\text{NO}_2$   $[\text{M}+\text{H}]^+$ : 342.1489, found: 342.1482.





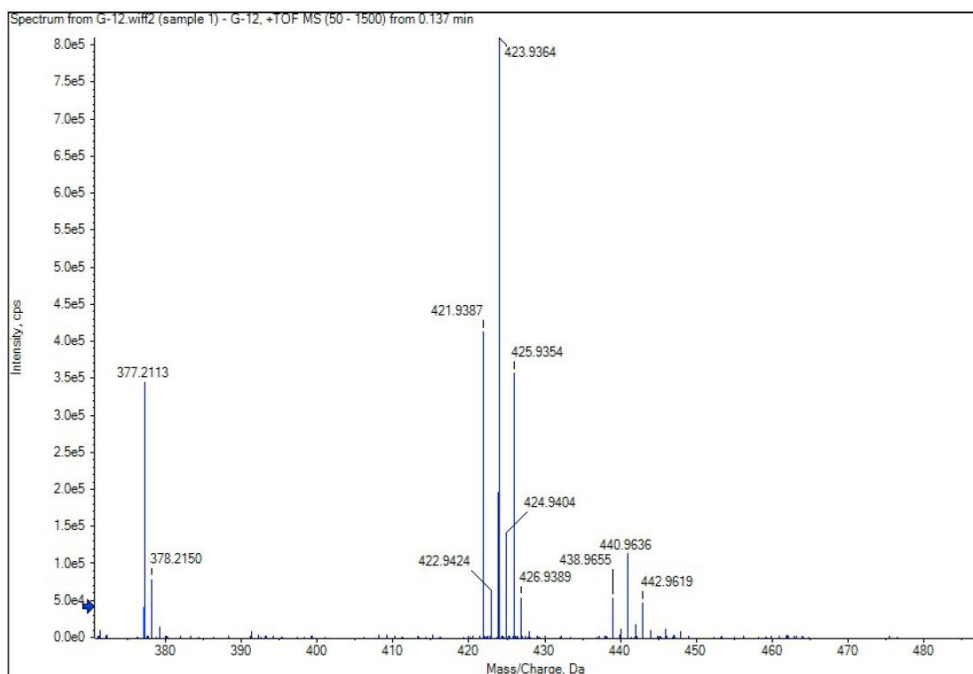
**Methyl (S)-2-(5,7-dibromo-1H-indol-3-yl)-2-phenylacetate (3al)** was prepared as a yellow solid according to the General Procedure A (eluent: hexanes/EtOAc = 10:1, 61.0 mg, 72% yield, 97% ee).

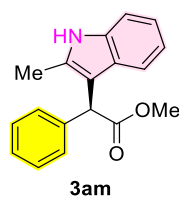
$[\alpha]_D^{25}$ :  $-13.2$  ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK® AD-H column; 15% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 6.1 min (major), 8.5 min (minor).

$^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.31 (s, 1H), 7.41 (s, 1H), 7.33 (s, 1H), 7.29 – 7.13 (m, 6H), 5.07 (s, 1H), 3.66 (s, 3H) ppm.

$^{13}\text{C NMR}$  (75 MHz,  $\text{CDCl}_3$ )  $\delta$  173.0, 137.8, 133.9, 128.8 (two C), 128.3, 127.6, 127.0, 125.2, 121.0, 114.6, 112.8, 105.3, 52.6, 48.7 ppm.

**HRMS (ESI+)** Calcd for  $\text{C}_{17}\text{H}_{14}\text{Br}_2\text{NO}_2$   $[\text{M}+\text{H}]^+$ : 421.9386, found: 421.9387.





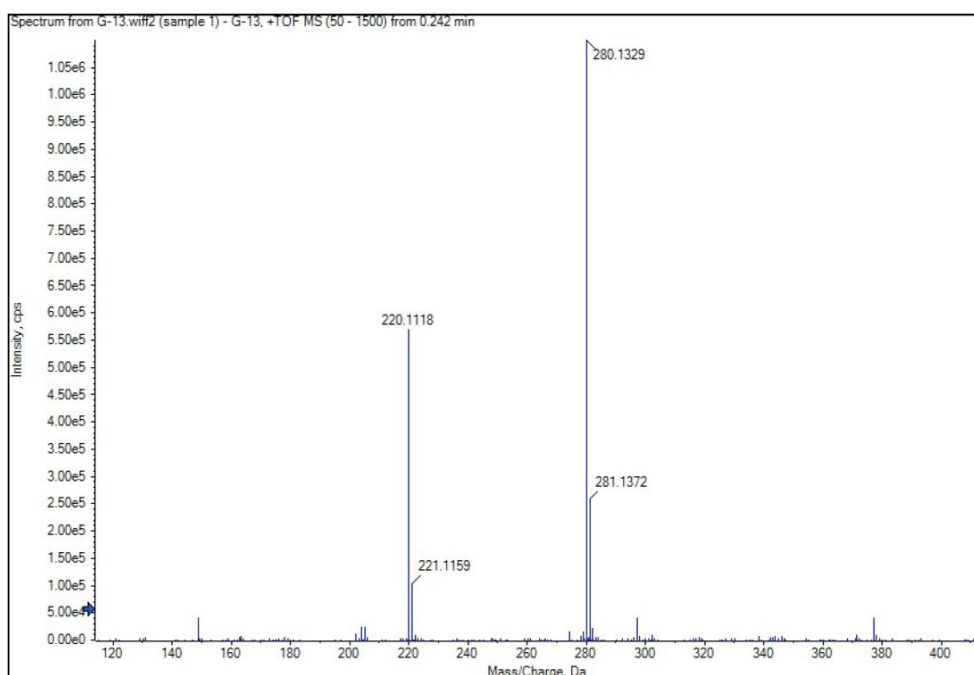
**Methyl (S)-2-(2-methyl-1H-indol-3-yl)-2-phenylacetate (3am)** was prepared as a colorless solid according to the General Procedure A (eluent: hexanes/EtOAc = 10:1, 42.0 mg, 75% yield, 54% ee).

$[\alpha]_D^{25}$ : +25.2 ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK<sup>®</sup> IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 7.6 min (major), 9.5 min (minor).

<sup>1</sup>H NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  7.81 (s, 1H), 7.37 (d,  $J = 7.8$  Hz, 1H), 7.19 – 7.11 (m, 6H), 7.03 – 6.91 (m, 2H), 5.19 (s, 1H), 3.63 (s, 3H), 2.19 (s, 3H) ppm.

<sup>13</sup>C NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  173.8, 138.7, 135.2, 133.1, 128.4 (two C), 127.8, 126.9, 121.2, 119.7, 119.3, 110.4, 108.5, 52.2, 48.0, 12.1 ppm.

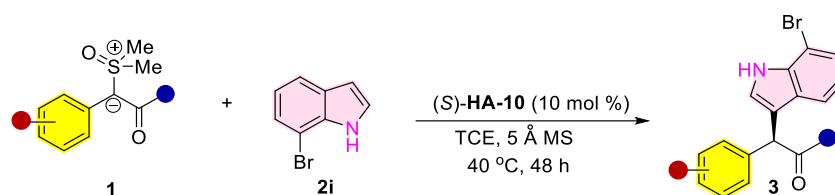
HRMS (ESI+) Calcd for  $\text{C}_{18}\text{H}_{18}\text{NO}_2$   $[\text{M}+\text{H}]^+$ : 280.1332, found: 280.1329.



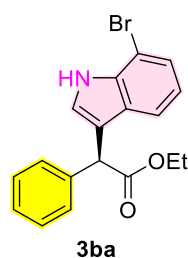
Note: It is a known compound, the spectroscopy data were in good agreement with the literature.<sup>6</sup>

(6) A. N. Leveille, R. Echemendía, A. E. Mattson, A. C. B. Burtoloso, *Org. Lett.*, 2021, **23**, 9446–9450.

## General Procedure B.



In an oven-dried 4-mL vial equipped with a magnetic stirring bar, sulfoxonium ylide **1** (0.2 mmol, 1.0 equiv), CPA catalyst (S)-HA-10 (14.6 mg, 10 mol %), and 5 Å molecular sieves (100 mg) were combined. Subsequently, 1.0 mL of TCE was added, followed by the addition of indole **2i** (43.1 mg, 0.22 mmol, 1.1 equiv). The resulting mixture was stirred at 40 °C and monitored by TLC. After completion (48 h), the mixture was directly subjected to flash column chromatography on silica gel (eluent: hexanes/ethyl acetate = 10:1 to 5:1) to afford the desired product **3**.



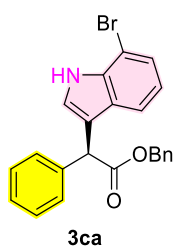
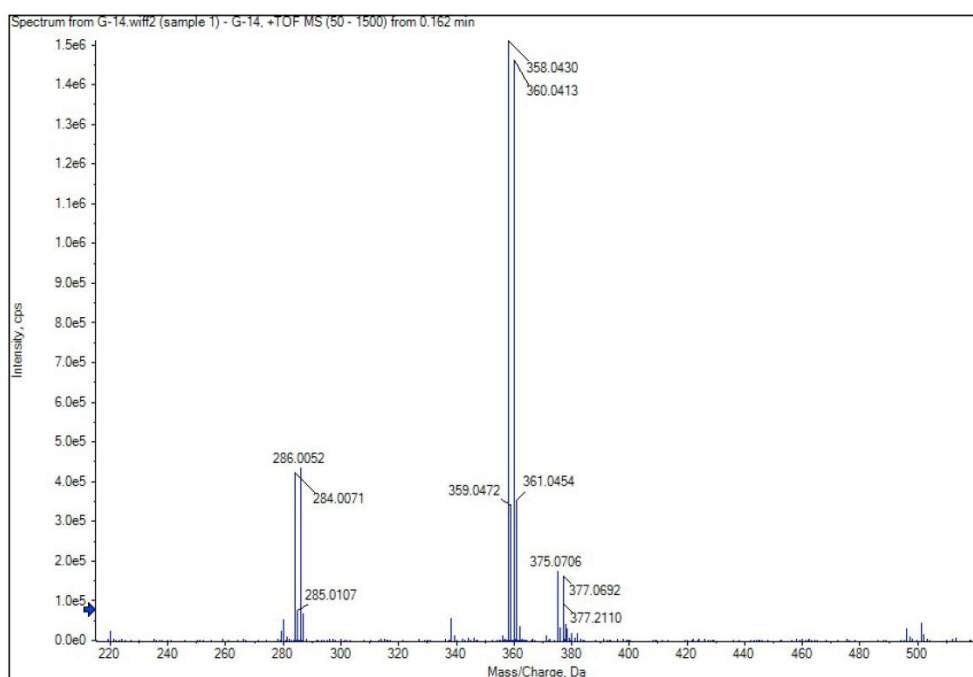
Ethyl (S)-2-(7-bromo-1H-indol-3-yl)-2-phenylacetate (**3ba**) was prepared as a colorless oil according to the General Procedure B (eluent: hexanes/EtOAc = 10:1, 53.2 mg, 74% yield, 93% ee).

$[\alpha]_{\text{D}}^{25}$ : +28.3 ( $c = 1.5$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 6.0 min (major), 6.6 min (minor).

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.32 (s, 1H), 7.41 – 7.37 (m, 3H), 7.32 – 7.23 (m, 5H), 6.93 (t,  $J = 7.8$  Hz, 1H), 5.20 (s, 1H), 4.25 – 4.17 (m, 2H), 1.25 (t,  $J = 7.0$  Hz, 3H) ppm.

$^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  172.7, 138.3, 135.0, 128.6, 128.4, 127.8, 127.4, 124.7, 123.9, 120.9, 118.4, 115.1, 104.9, 61.3, 49.1, 14.2 ppm.

HRMS (ESI+) Calcd for C<sub>18</sub>H<sub>17</sub>BrNO<sub>2</sub> [M+H]<sup>+</sup>: 358.0437, found: 358.0430.



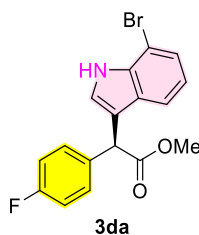
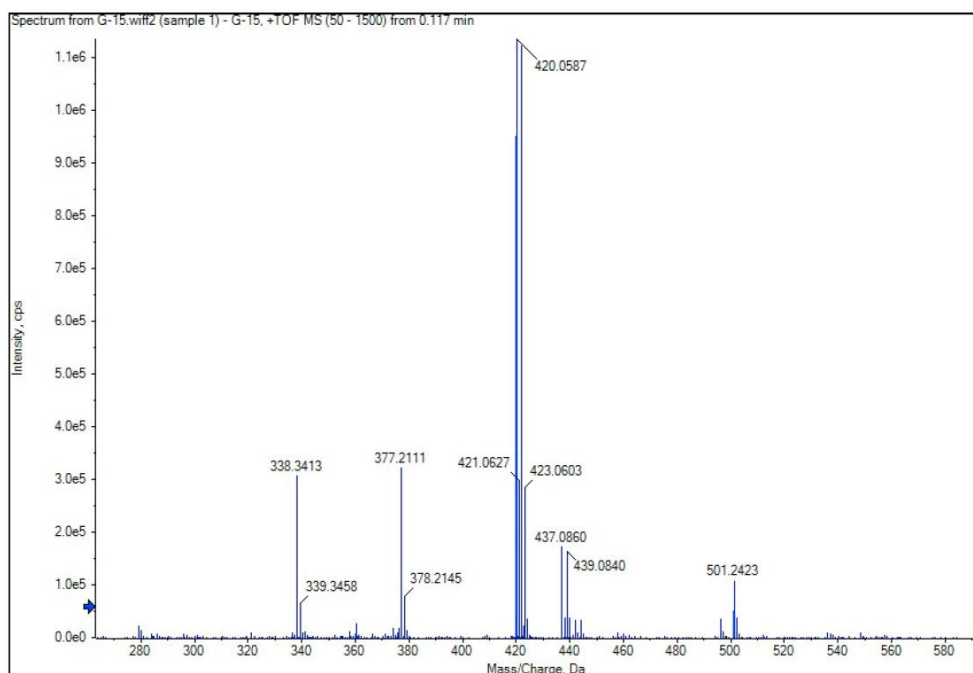
**Benzyl (S)-2-(7-bromo-1H-indol-3-yl)-2-phenylacetate (3ca)** was prepared as a colorless oil according to the General Procedure B (eluent: hexanes/ EtOAc = 10:1, 55.8 mg, 67% yield, 95% ee).

$[\alpha]_D^{25}$ : +26.9 ( $c = 1.5$ , CH<sub>2</sub>Cl<sub>2</sub>). HPLC analysis of the product: Daicel CHIRALPAK<sup>®</sup> IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 5.9 min (major), 6.9 min (minor).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.27 (s, 1H), 7.39 – 7.37 (m, 2H), 7.32 – 7.21 (m, 10H), 7.20 – 7.19 (m, 1H), 6.88 (t,  $J = 7.8$  Hz, 1H), 5.26 (s, 1H), 5.18 (q,  $J = 12.4$  Hz, 2H) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  172.5, 138.1, 135.7, 135.0, 128.7, 128.6, 128.5, 128.32, 128.26, 127.8, 127.5, 124.7, 123.9, 121.0, 118.4, 114.8, 104.8, 67.0, 49.1 ppm.

HRMS (ESI+) Calcd for C<sub>23</sub>H<sub>19</sub>BrNO<sub>2</sub> [M+H]<sup>+</sup>: 420.0594, found: 420.0587.



**Methyl (S)-2-(7-bromo-1H-indol-3-yl)-2-(4-fluorophenyl)acetate (3da)** was prepared as a yellow oil according to the General Procedure B (eluent: hexanes/EtOAc = 10:1, 51.4 mg, 71% yield, 96% ee).

$[\alpha]_D^{25}$ : +27.7 ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK® AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 22.2 min (major), 24.7 min (minor).

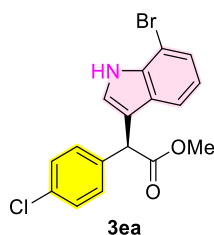
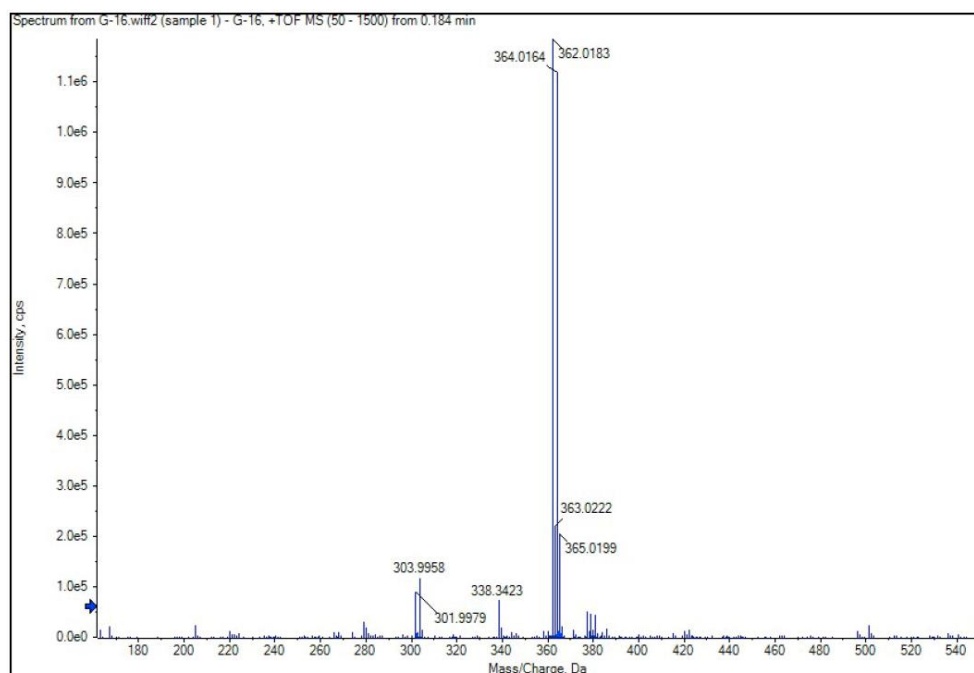
$^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.27 (s, 1H), 7.28 – 7.15 (m, 5H), 6.93 – 6.82 (m, 3H), 5.12 (s, 1H), 3.66 (s, 3H) ppm.

$^{13}\text{C NMR}$  (75 MHz,  $\text{CDCl}_3$ )  $\delta$  173.0, 162.1 (d,  $^1J_{\text{C-F}} = 244.5$  Hz), 135.0, 134.0 (d,  $^4J_{\text{C-F}} = 3.2$  Hz), 130.0 (d,  $^3J_{\text{C-F}} = 8.0$  Hz), 127.6, 124.8, 123.8, 121.1, 118.3, 115.5 (d,  $^2J_{\text{C-F}} = 21.3$  Hz), 114.7, 104.9, 52.5, 48.2 ppm.

$^{19}\text{F NMR}$  (282 MHz,  $\text{CDCl}_3$ )  $\delta$  -115.1 ppm.

**HRMS** (ESI+) Calcd for  $\text{C}_{17}\text{H}_{14}\text{BrFNO}_2$   $[\text{M}+\text{H}]^+$ : 362.0186, found: 362.0183.





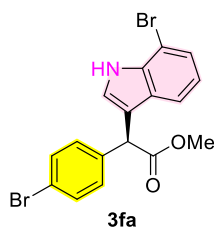
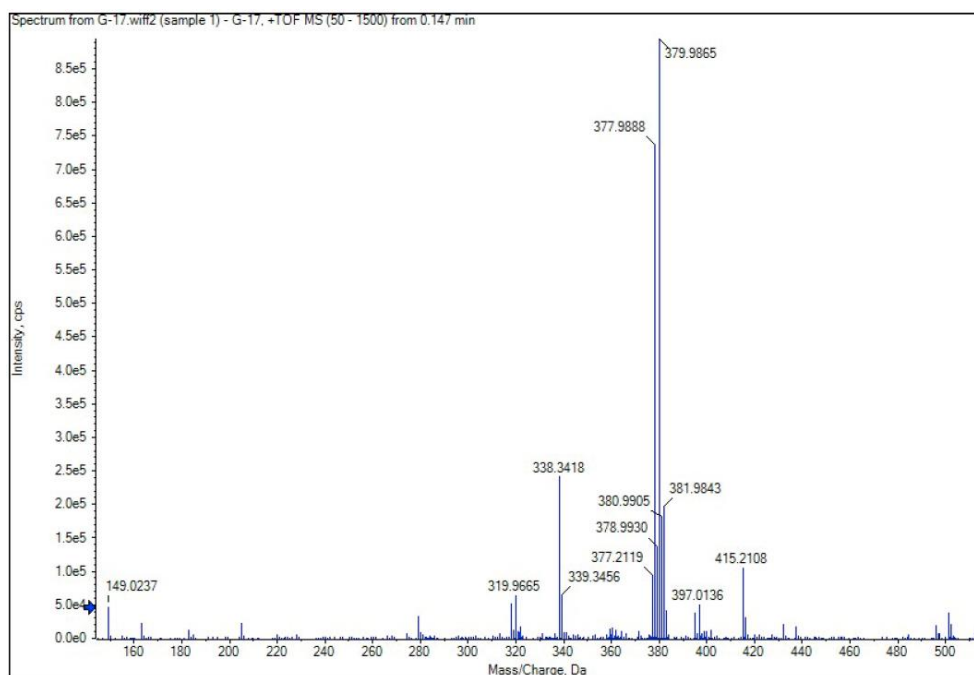
**Methyl (S)-2-(7-bromo-1H-indol-3-yl)-2-(4-chlorophenyl)acetate (3ea)** was prepared as a colorless oil according to the General Procedure B (eluent: hexanes/EtOAc = 10:1, 56.6 mg, 75% yield, 96% ee).

$[\alpha]_{\text{D}}^{25}$ : +26.6 ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK<sup>®</sup> AD-H column; 15% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 14.8 min (major), 16.3 min (minor).

<sup>1</sup>H NMR (300MHz,  $\text{CDCl}_3$ )  $\delta$  8.26 (s, 1H), 7.26 – 7.17 (m, 7H), 6.85 (t,  $J = 7.8$  Hz, 1H), 5.11 (s, 1H), 3.67 (s, 3H) ppm.

<sup>13</sup>C NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  172.8, 136.7, 135.0, 133.4, 129.8, 128.8, 127.5, 124.9, 123.8, 121.1, 118.3, 114.4, 104.9, 52.6, 48.3 ppm.

HRMS (ESI+) Calcd for  $\text{C}_{17}\text{H}_{14}\text{BrClNO}_2$   $[\text{M}+\text{H}]^+$ : 377.9891, found: 377.9888.



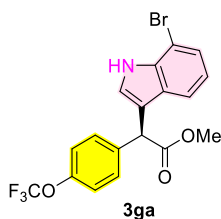
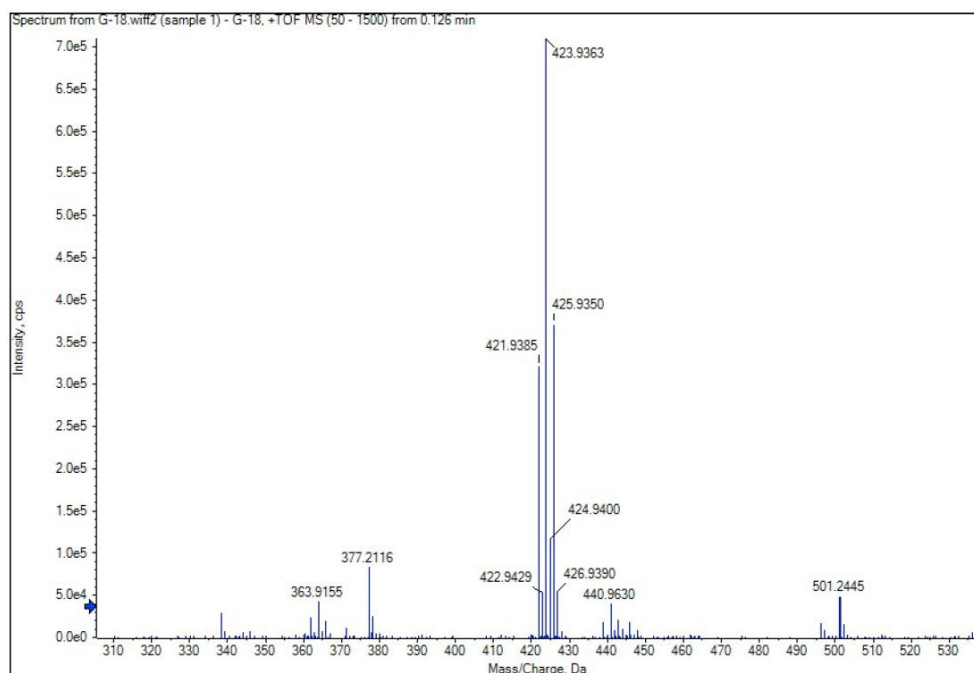
**Methyl (S)-2-(7-bromo-1H-indol-3-yl)-2-(4-bromophenyl)acetate (3fa)** was prepared as a white solid according to the General Procedure B (eluent: hexanes/EtOAc = 10:1, 66.8 mg, 79% yield, 94% ee).

$[\alpha]_{\text{D}}^{25}$ : +23.9 ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK<sup>®</sup> AD-H column; 15% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 15.9 min (major), 17.2 min (minor).

<sup>1</sup>H NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.28 (s, 1H), 7.33 (d,  $J = 7.8$  Hz, 2H), 7.24 (d,  $J = 7.8$  Hz, 2H), 7.16 (d,  $J = 8.6$  Hz, 3H), 6.85 (t,  $J = 7.8$  Hz, 1H), 5.09 (s, 1H), 3.66 (s, 3H) ppm.

<sup>13</sup>C NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  172.7, 137.2, 135.0, 131.8, 130.2, 127.5, 124.9, 123.9, 121.5, 121.1, 118.3, 114.3, 104.9, 52.6, 48.4 ppm.

HRMS (ESI+) Calcd for  $\text{C}_{17}\text{H}_{14}\text{Br}_2\text{NO}_2$   $[\text{M}+\text{H}]^+$ : 421.9386, found: 421.9385.



**Methyl (S)-2-(7-bromo-1H-indol-3-yl)-2-(4-(trifluoromethoxy)phenyl)acetate (3ga)** was prepared as a colorless oil according to the General Procedure B (eluent: hexanes/EtOAc = 10:1, 58.2 mg, 68% yield, 97% ee).

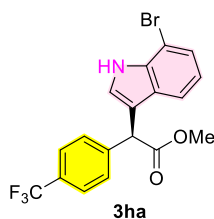
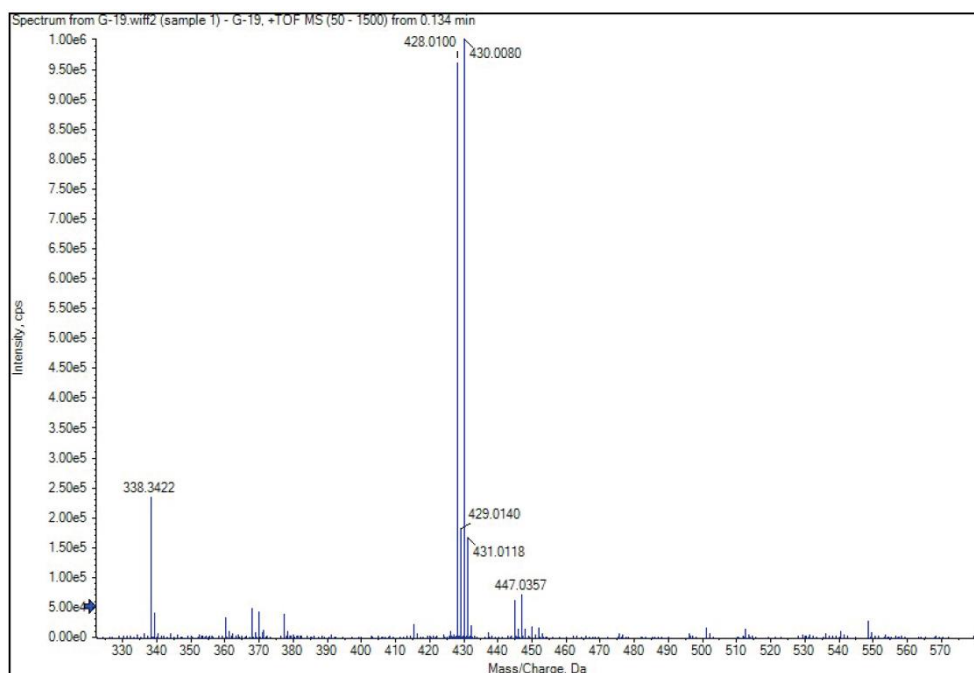
$[\alpha]_D^{25}$ : +38.8 ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK® AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 12.6 min (major), 16.8 min (minor).

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.30 (s, 1H), 7.34 – 7.32 (m, 2H), 7.27 – 7.25 (m, 2H), 7.190 – 7.185 (m, 1H), 7.08 – 7.06 (m, 2H), 6.88 (t,  $J = 7.8$  Hz, 1H), 5.15 (s, 1H), 3.67 (s, 3H) ppm.

$^{13}\text{C NMR}$  (100 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  172.8, 148.5, 136.9, 135.0, 129.8, 127.5, 124.9, 123.9, 121.14, 121.08, 120.5 (q,  $^1J_{\text{C-F}} = 266.6$  Hz), 118.2, 114.3, 105.0, 52.6, 48.3 ppm.

$^{19}\text{F NMR}$  (376 MHz,  $\text{CDCl}_3$ )  $\delta$  –57.8 ppm.

**HRMS** (ESI+) Calcd for  $\text{C}_{18}\text{H}_{14}\text{BrF}_3\text{NO}_3$   $[\text{M}+\text{H}]^+$ : 428.0104, found: 428.0100.



**Methyl (S)-2-(7-bromo-1H-indol-3-yl)-2-(4-(trifluoromethyl)phenyl)acetate (3ha)** was prepared as a yellow solid according to the General Procedure B (eluent: hexane /EtOAc = 10:1, 42.8 mg, 52% yield, 96% ee).

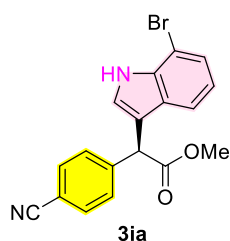
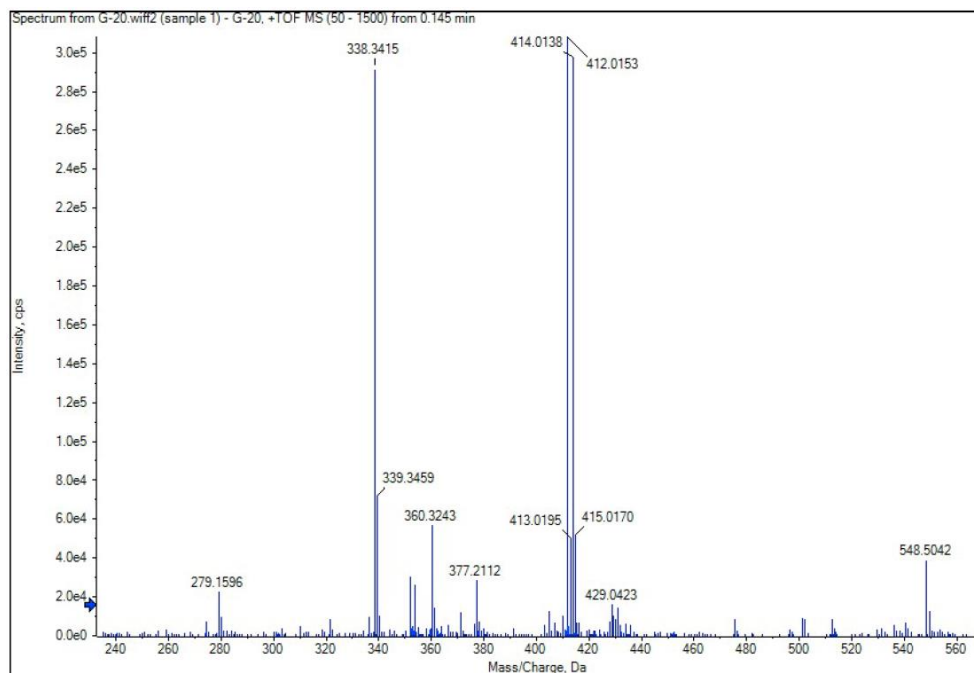
$[\alpha]_{\text{D}}^{25}$ : +18.2 ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK<sup>®</sup> AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 14.2 min (major), 17.9 min (minor).

<sup>1</sup>H NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.29 (s, 1H), 7.50 – 7.41 (m, 4H), 7.27 – 7.22 (m, 3H), 6.87 (t,  $J = 7.7$  Hz, 1H), 5.21 (s, 1H), 3.68 (s, 3H) ppm.

<sup>13</sup>C NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  172.5, 142.2, 135.0, 129.7 ( $q$ ,  $^2J_{\text{C-F}} = 32.3$  Hz), 128.8, 127.5, 125.6 ( $q$ ,  $^4J_{\text{C-F}} = 3.8$  Hz), 124.9, 124.1 ( $q$ ,  $^1J_{\text{C-F}} = 270.2$  Hz), 123.9, 121.2, 118.2, 114.0, 105.0, 52.6, 48.7 ppm.

<sup>19</sup>F NMR (282 MHz,  $\text{CDCl}_3$ )  $\delta$  –62.5 ppm.

HRMS (ESI+) Calcd for  $\text{C}_{18}\text{H}_{14}\text{BrF}_3\text{NO}_2$   $[\text{M}+\text{H}]^+$ : 412.0155, found: 412.0153.



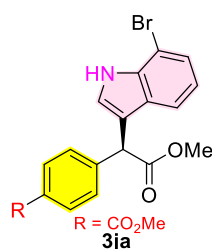
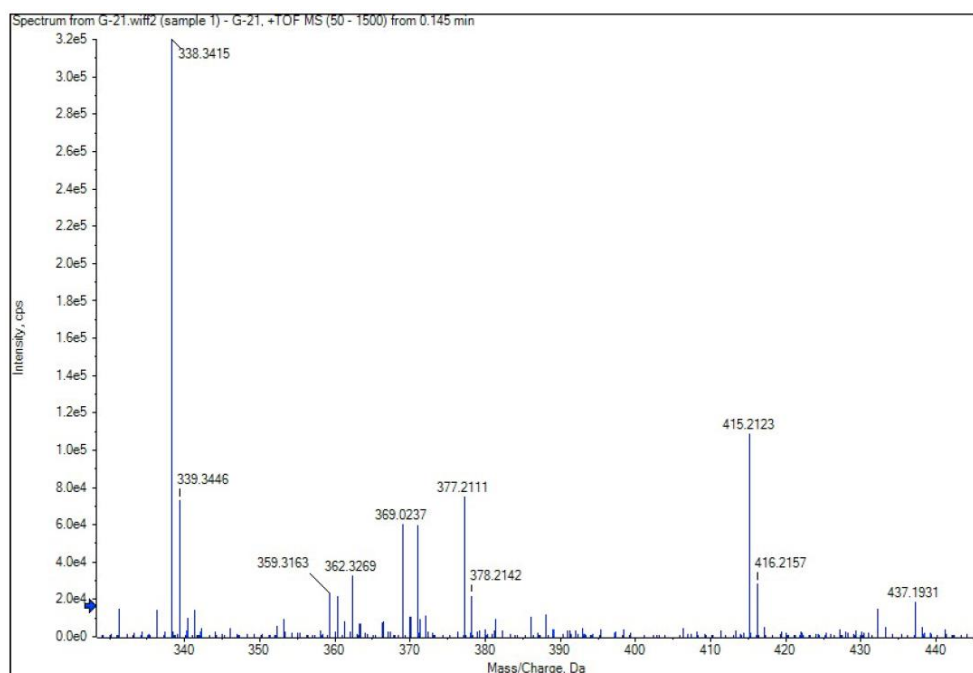
**Methyl (S)-2-(7-bromo-1H-indol-3-yl)-2-(4-cyanophenyl)acetate (3ia)** was prepared as a yellow solid according to the General Procedure B (eluent: hexanes/EtOAc = 5:1, 44.2 mg, 60% yield, 94% ee).

$[\alpha]_{\text{D}}^{25}$ : +62.5 ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK® AD-H column; 15% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 26.7 min (minor), 33.1 min (major).

$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.38 (s, 1H), 7.52 – 7.50 (m, 2H), 7.42 – 7.39 (m, 2H), 7.28 – 7.17 (m, 3H), 6.87 (t,  $J = 7.8$  Hz, 1H), 5.20 (s, 1H), 3.69 (s, 3H) ppm.

$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  172.1, 143.6, 135.0, 132.4, 129.3, 127.3, 125.0, 124.0, 121.3, 118.7, 118.1, 113.4, 111.4, 105.0, 52.7, 48.9 ppm.

HRMS (ESI+) Calcd for  $\text{C}_{18}\text{H}_{14}\text{BrN}_2\text{O}_2$   $[\text{M}+\text{H}]^+$ : 369.0233, found: 369.0237.



**Methyl (S)-4-(1-(7-bromo-1H-indol-3-yl)-2-methoxy-2-oxoethyl)benzoate (3ja)**

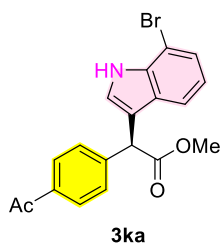
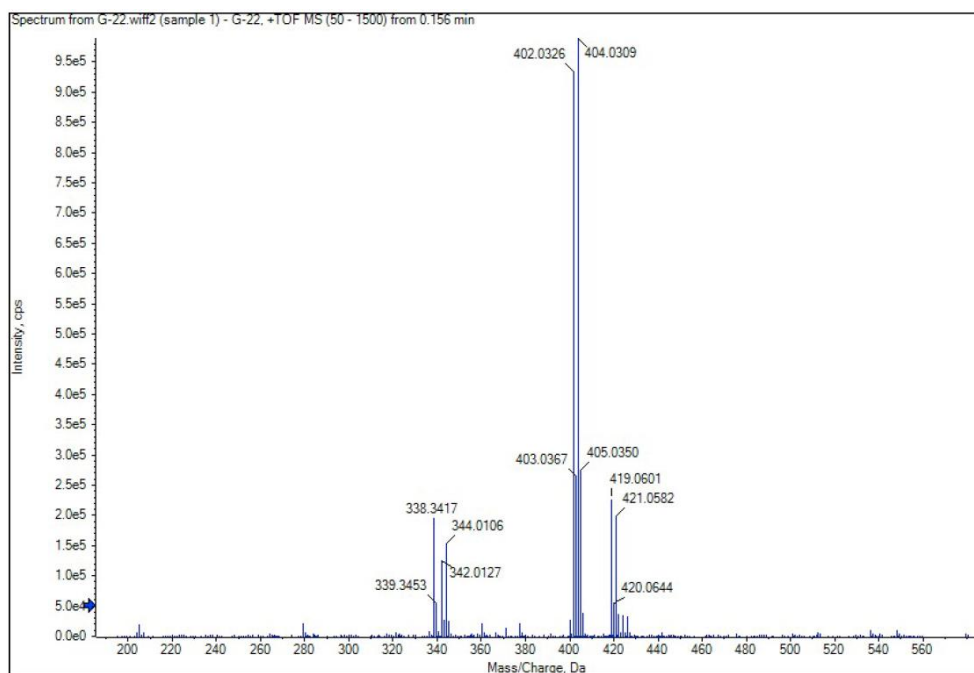
was prepared as a yellow oil according to the General Procedure B (eluent: hexanes/EtOAc = 5:1, 46.7 mg, 58% yield, 96% ee).

$[\alpha]_D^{25}$ : +13.2 ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK<sup>®</sup> IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 17.3 min (major), 20.4 min (minor).

<sup>1</sup>H NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.43 (s, 1H), 7.98 (d,  $J = 8.1$  Hz, 2H), 7.46 (d,  $J = 8.1$  Hz, 2H), 7.34 – 7.25 (m, 3H), 6.93 (t,  $J = 7.8$  Hz, 1H), 5.28 (s, 1H), 3.89 (s, 3H), 3.75 (s, 3H) ppm.

<sup>13</sup>C NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  172.5, 166.9, 143.3, 135.0, 130.0, 129.3, 128.5, 127.5, 124.9, 124.0, 121.1, 118.2, 114.1, 104.9, 52.6, 52.2, 48.9 ppm.

HRMS (CI+) Calcd for  $\text{C}_{19}\text{H}_{17}\text{BrNO}_4$   $[\text{M}+\text{H}]^+$ : 402.0335, found: 402.0326.



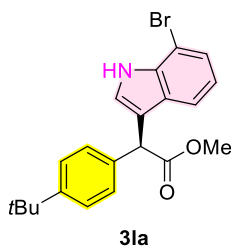
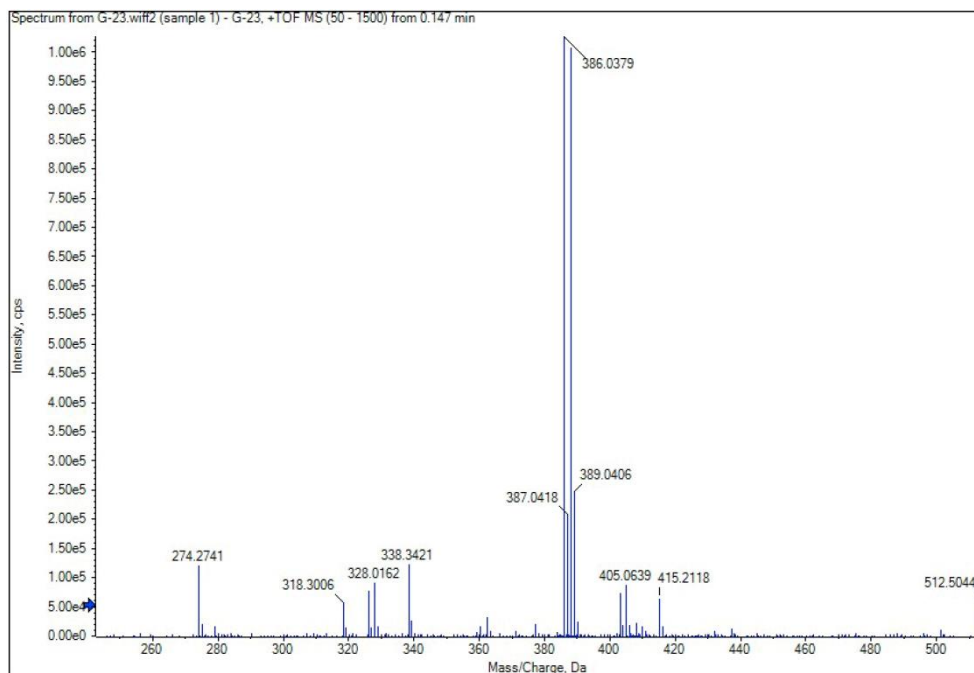
**Methyl (S)-2-(4-acetylphenyl)-2-(7-bromo-1H-indol-3-yl)acetate (3ka)** was prepared as a yellow solid according to the General Procedure B (eluent: hexanes/EtOAc = 5:1, 43.8 mg, 57% yield, 92% ee).

$[\alpha]_D^{25}$ : +12.6 ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK<sup>®</sup> IC column; 15% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 20.4 min (major), 24.5 min (minor).

<sup>1</sup>H NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.42 (s, 1H), 7.82 (d,  $J = 8.1$  Hz, 2H), 7.40 (d,  $J = 8.1$  Hz, 2H), 7.26 – 7.17 (m, 3H), 6.85 (t,  $J = 7.7$  Hz, 1H), 5.21 (s, 1H), 3.68 (s, 3H), 2.48 (s, 3H) ppm.

<sup>13</sup>C NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  197.8, 172.5, 143.5, 136.3, 135.0, 128.73, 128.70, 127.5, 124.9, 124.0, 121.1, 118.2, 114.0, 105.0, 52.6, 48.9, 26.7 ppm.

HRMS (ESI+) Calcd for  $\text{C}_{19}\text{H}_{17}\text{BrNO}_3$   $[\text{M}+\text{H}]^+$ : 386.0386, found: 386.0379.



**Methyl (S)-2-(7-bromo-1H-indol-3-yl)-2-(4-(tert-butyl)phenyl)acetate (3a)**

was prepared as a yellow oil according to the General Procedure B (eluent: hexanes/EtOAc = 10:1, 52.2 mg, 65% yield, 85% ee).

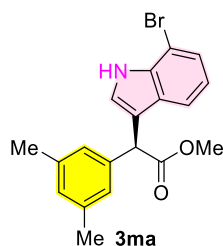
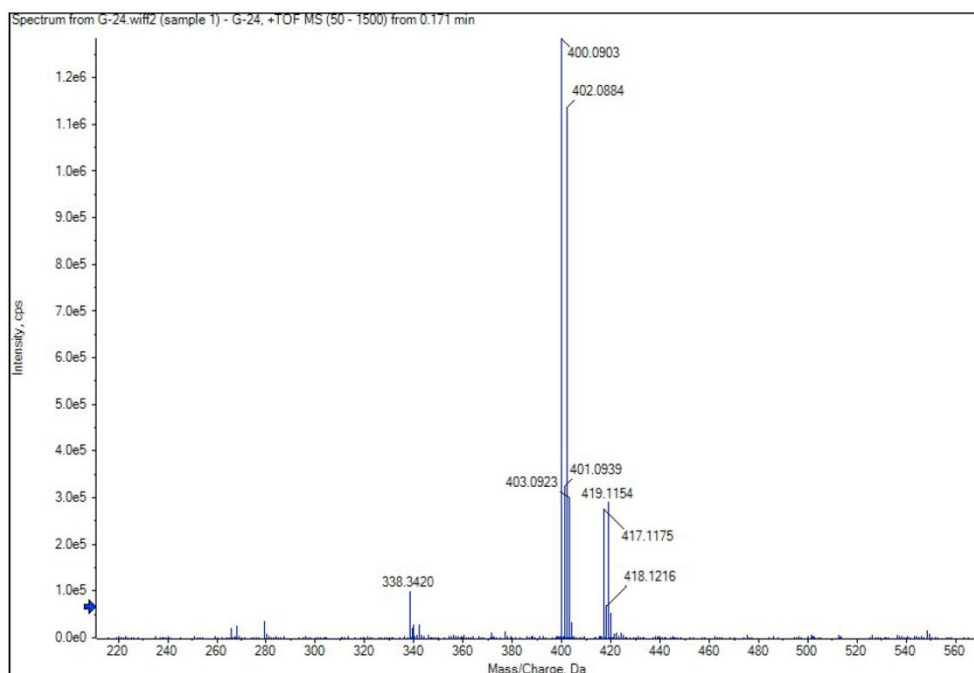
$[\alpha]_D^{25}$ : +4.5 ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK® AD-H column; 15% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 8.3 min (major), 14.8 min (minor).

$^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.21 (s, 1H), 7.33 (d,  $J = 7.9$  Hz, 1H), 7.24 – 7.14 (m, 6H), 6.86 (t,  $J = 7.8$  Hz, 1H), 5.12 (s, 1H), 3.65 (s, 3H), 1.20 (s, 9H) ppm.

$^{13}\text{C NMR}$  (75 MHz,  $\text{CDCl}_3$ )  $\delta$  173.4, 150.2, 135.1, 135.0, 128.0, 127.8, 125.6, 124.6, 123.9, 120.9, 118.4, 115.2, 104.9, 52.4, 48.5, 34.5, 31.4 ppm.

**HRMS** (ESI+) Calcd for  $\text{C}_{21}\text{H}_{23}\text{BrNO}_2$   $[\text{M}+\text{H}]^+$ : 400.0907, found: 400.0903.





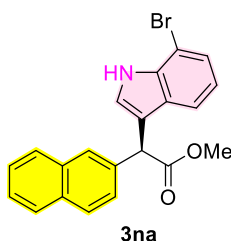
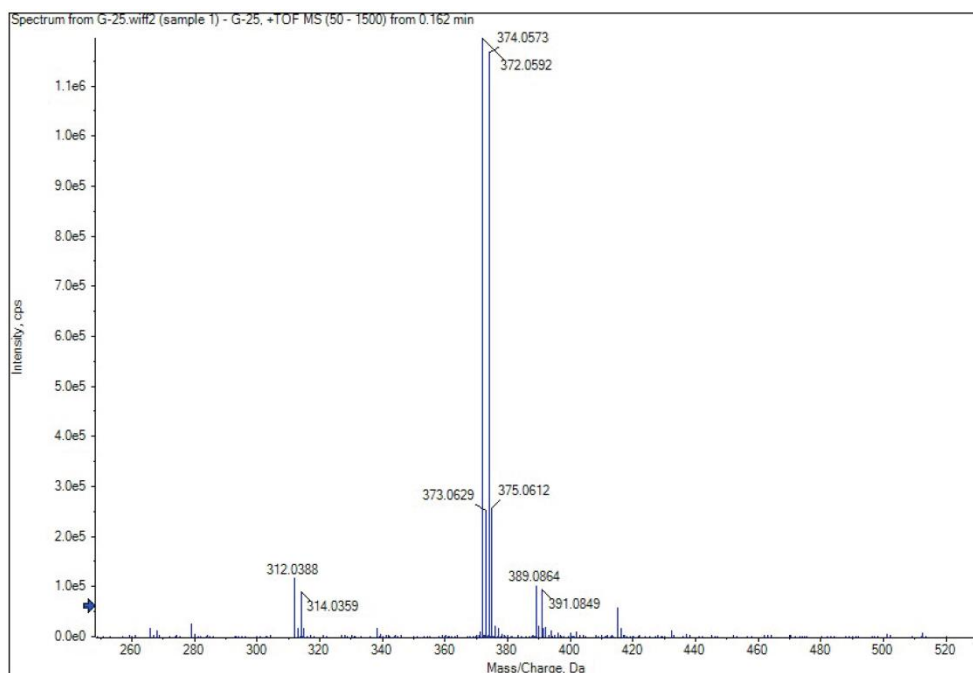
**Methyl (S)-2-(7-bromo-1H-indol-3-yl)-2-(3,5-dimethylphenyl)acetate (3ma)** was prepared as a yellow oil according to the General Procedure B (eluent: hexanes/EtOAc = 10:1, 54.7 mg, 74% yield, 95% ee).

$[\alpha]_{\text{D}}^{25}$ : +15.3 ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK<sup>®</sup> AD-H column; 15% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 10.7 min (major), 15.7 min (minor).

<sup>1</sup>H NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.21 (s, 1H), 7.32 – 7.15 (m, 3H), 6.92 – 6.81 (m, 4H), 5.06 (s, 1H), 3.65 (s, 3H), 2.18 (s, 6H) ppm.

<sup>13</sup>C NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  173.4, 138.2, 138.0, 134.9, 129.2, 127.9, 126.1, 124.6, 123.9, 120.9, 118.3, 115.1, 104.8, 52.4, 48.8, 21.4 ppm.

HRMS (ESI+) Calcd for  $\text{C}_{19}\text{H}_{19}\text{BrNO}_2$   $[\text{M}+\text{H}]^+$ : 372.0594, found: 372.0592.



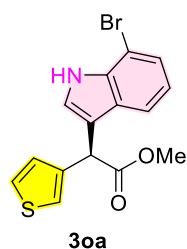
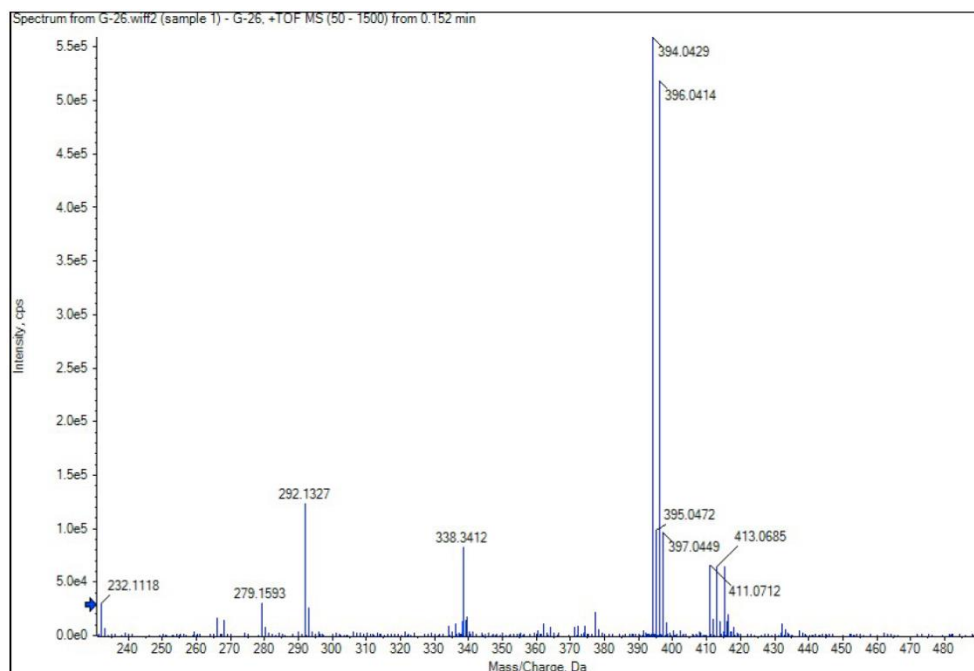
**Methyl (S)-2-(7-bromo-1H-indol-3-yl)-2-(naphthalen-2-yl)acetate (3na)** was prepared as a yellow solid according to the General Procedure B (eluent: hexanes/EtOAc = 10:1, 52.8 mg, 67% yield, 93% ee).

$[\alpha]_D^{25}$ : +24.2 ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK<sup>®</sup> IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 7.4 min (major), 10.0 min (minor).

<sup>1</sup>H NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.23 (s, 1H), 7.75 – 7.68 (m, 4H), 7.44 – 7.19 (m, 6H), 6.82 (t,  $J = 7.8$  Hz, 1H), 5.30 (s, 1H), 3.67 (s, 3H) ppm.

<sup>13</sup>C NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  173.1, 135.6, 135.0, 133.4, 132.7, 128.4, 128.0, 127.8, 127.7, 127.2, 126.5, 126.2, 126.0, 124.7, 124.1, 121.0, 118.4, 114.9, 104.9, 52.5, 49.1 ppm.

HRMS (ESI+) Calcd for  $\text{C}_{21}\text{H}_{17}\text{BrNO}_2$   $[\text{M}+\text{H}]^+$ : 394.0437, found: 394.0429.



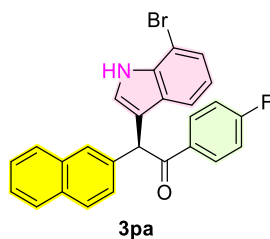
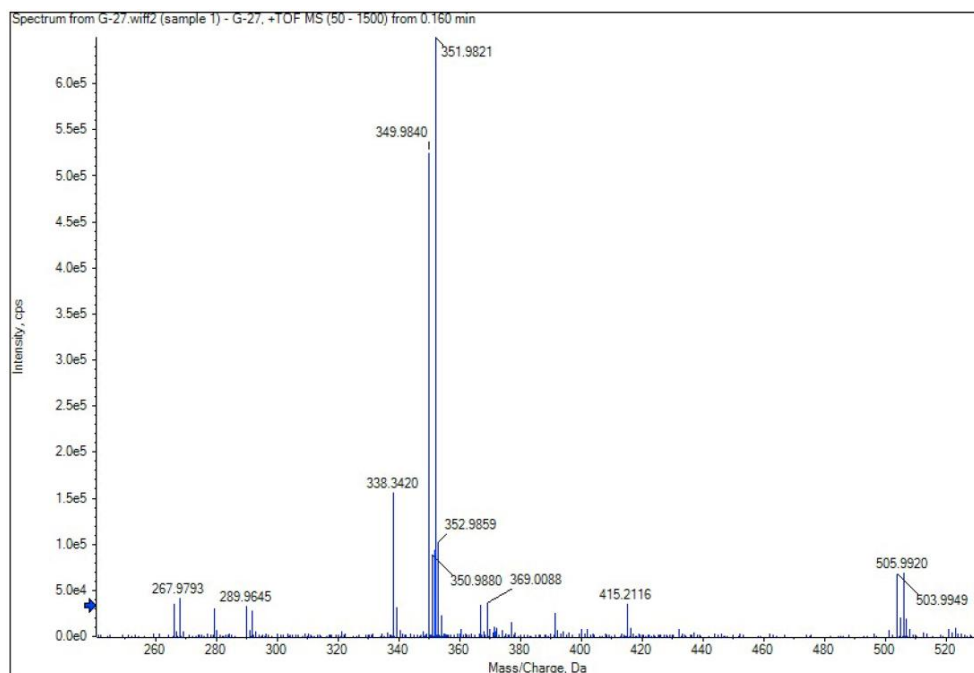
**Methyl 2-(7-bromo-1H-indol-3-yl)-2-(thiophen-3-yl)acetate (3oa)** was prepared as a yellow solid according to the General Procedure B (eluent: hexanes/EtOAc = 10:1, 49.2 mg, 70% yield, 92% ee).

$[\alpha]_D^{25}$ : +8.2 ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK® AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 21.1 min (major), 23.2 min (minor).

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.25 (s, 1H), 7.38 (d,  $J = 8.0$  Hz, 1H), 7.26 (d,  $J = 7.5$  Hz, 1H), 7.20 – 7.18 (m, 1H), 7.112 – 7.107 (m, 2H), 7.01 – 7.00 (m, 1H), 6.89 (t,  $J = 7.8$  Hz, 1H), 5.22 (s, 1H), 3.67 (s, 3H) ppm.

$^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  172.9, 138.4, 135.0, 127.9, 127.6, 125.9, 124.7, 123.8, 122.7, 121.1, 118.5, 114.8, 104.9, 52.5, 44.5 ppm.

**HRMS** (ESI+) Calcd for  $\text{C}_{15}\text{H}_{13}\text{BrNO}_2\text{S}$   $[\text{M}+\text{H}]^+$ : 349.9845, found: 349.9840.



**(S)-2-(7-Bromo-1H-indol-3-yl)-1-(4-fluorophenyl)-2-(naphthalen-2-yl)ethan-1-one (3pa)** was prepared as a yellow oil according to the General Procedure B (eluent: hexanes/EtOAc = 5:1, 60.7 mg, 66% yield, 86% ee).

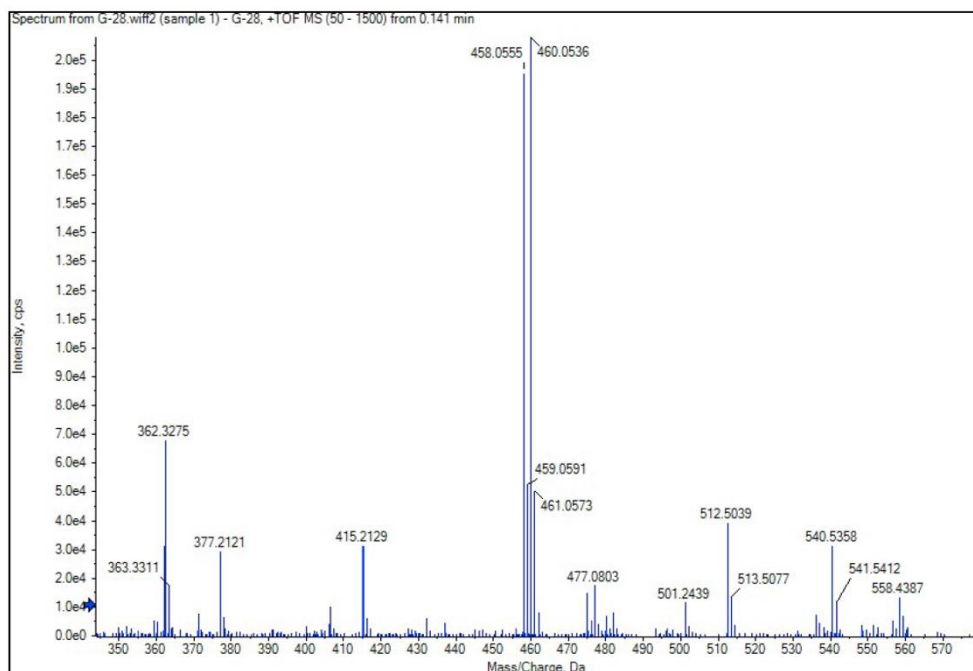
$[\alpha]_{\text{D}}^{25}$ : +185.3 ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK<sup>®</sup> IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 8.3 min (major), 9.2 min (minor).

<sup>1</sup>H NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.58 (s, 1H), 8.36 (s, 1H), 8.07 – 8.04 (m, 1H), 7.88 – 7.80 (m, 3H), 7.57 – 7.43 (m, 3H), 7.34 – 7.31 (m, 3H), 7.04 – 6.94 (m, 4H), 6.37 (s, 1H) ppm.

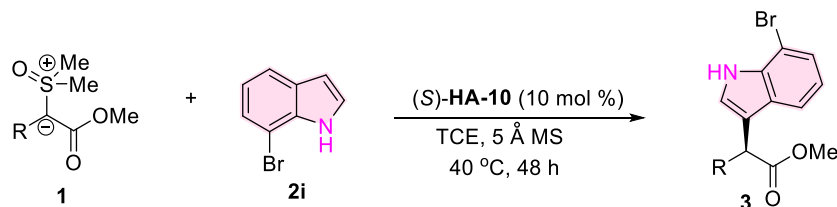
<sup>13</sup>C NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  198.1, 162.1 (d,  $^1J_{\text{C-F}} = 244.1$  Hz), 135.6, 135.2, 134.4 (d,  $^4J_{\text{C-F}} = 3.1$  Hz), 133.8, 132.5, 130.64 (d,  $^3J_{\text{C-F}} = 8.1$  Hz), 130.60, 129.8, 128.8, 128.7, 127.8, 127.6, 126.9, 125.0, 124.5, 124.4, 121.2, 118.2, 115.6 (d,  $^2J_{\text{C-F}} = 21.1$  Hz), 115.5, 105.1, 50.1 ppm.

$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -115.4 ppm.

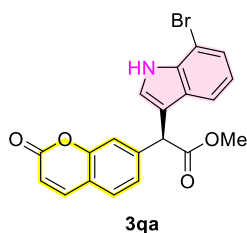
HRMS (ESI+) Calcd for  $\text{C}_{26}\text{H}_{18}\text{BrFNO}$   $[\text{M}+\text{H}]^+$ : 458.0550, found: 458.0555.



### General Procedure C.



In an oven-dried 4-mL vial equipped with a magnetic stirring bar, bioactive molecule derived sulfoxonium ylide **1** (0.2 mmol, 1.0 equiv), CPA catalyst (*S*)-**HA-10** (14.6 mg, 10 mol %), and 5 Å molecular sieves (100 mg) were combined. Subsequently, 1.0 mL of TCE was added, followed by the addition of indole **2i** (43.1 mg, 0.22 mmol, 1.1 equiv). The resulting mixture was stirred at 40 °C and monitored by TLC. After completion (48 h), the mixture was directly subjected to flash column chromatography on silica gel (eluent: hexanes/ethyl acetate = 10:1 to 5:1) to afford the desired product **3**.



**Methyl (S)-2-(7-bromo-1H-indol-3-yl)-2-(2-oxo-2H-chromen-7-yl)acetate (3qa)**

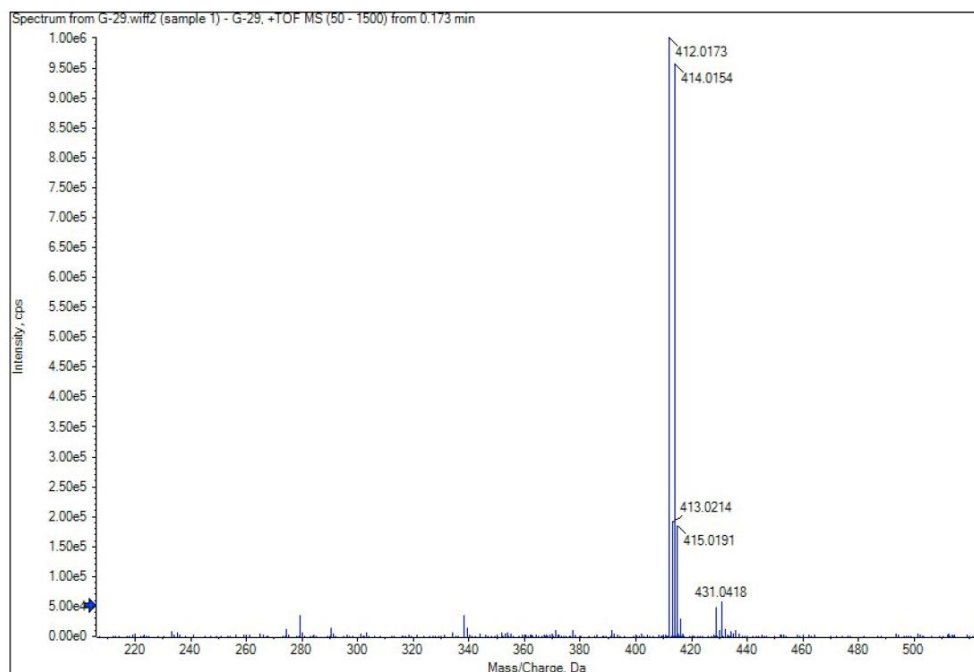
was prepared as a yellow oil according to the General Procedure C (eluent: hexanes/EtOAc = 3:1, 42.3 mg, 51% yield, 92% ee).

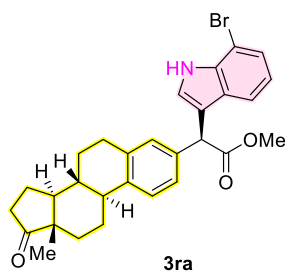
$[\alpha]_D^{25}$ : +27.6 ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK<sup>®</sup> IC column; 25% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 27.5 min (major), 31.8 min (minor).

<sup>1</sup>H NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.45 (s, 1H), 7.56 (d,  $J = 9.5$  Hz, 1H), 7.33 – 7.18 (m, 6H), 6.86 (t,  $J = 7.8$  Hz, 1H), 6.30 (d,  $J = 9.5$  Hz, 1H), 5.23 (s, 1H), 3.69 (s, 3H) ppm.

<sup>13</sup>C NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  172.2, 160.7, 154.1, 143.1, 142.9, 135.0, 128.0, 127.4, 125.0, 124.7, 124.0, 121.2, 118.1, 118.0, 116.8, 116.6, 113.5, 105.0, 52.7, 48.8 ppm.

HRMS (ESI+) Calcd for  $\text{C}_{20}\text{H}_{15}\text{BrNO}_4$   $[\text{M}+\text{H}]^+$ : 412.0179, found: 412.0173.



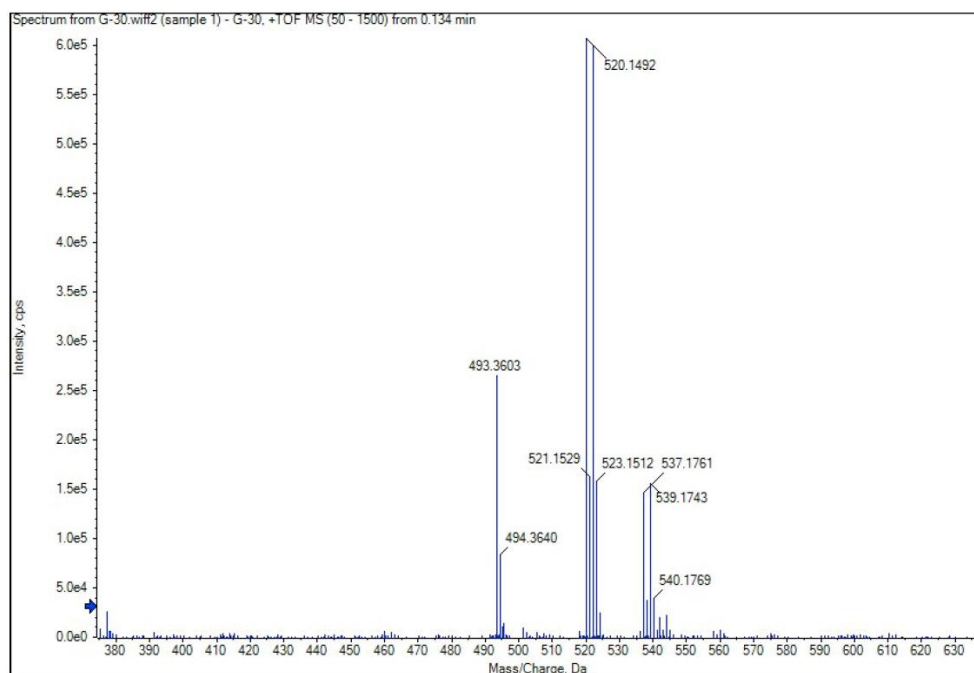


**Methyl (S)-2-(7-bromo-1H-indol-3-yl)-2-((8R,9S,13S,14S)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-3-yl)acetate (3ra)** was prepared as a yellow solid according to the General Procedure C (eluent: hexanes/EtOAc = 5:1, 52 mg, 50% yield, >20 : 1 d.r.).

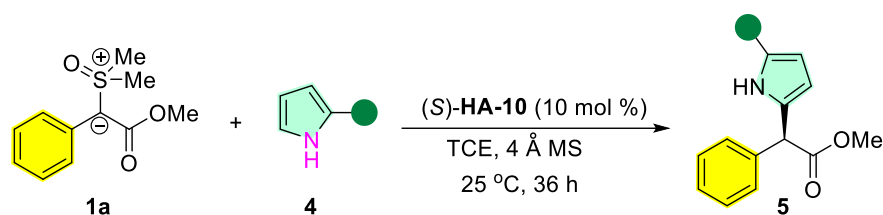
$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.39 (s, 1H), 7.41 (d,  $J = 8.0$  Hz, 1H), 7.32 – 7.29 (m, 2H), 7.25 – 7.16 (m, 2H), 7.11 (s, 1H), 6.94 (t,  $J = 7.8$  Hz, 1H), 5.17 (s, 1H), 3.74 (s, 3H), 2.87 – 2.84 (m, 2H), 2.53 – 2.46 (m, 1H), 2.40 – 2.36 (m, 1H), 2.28 – 2.22 (m, 1H), 2.17 – 1.93 (m, 4H), 1.63 – 1.37 (m, 6H), 0.88 (s, 3H) ppm.

$^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  221.1, 173.3, 138.9, 136.8, 135.6, 134.9, 128.8, 127.8, 125.74, 125.66, 124.6, 123.9, 120.9, 118.3, 115.0, 104.9, 52.4, 50.5, 48.4, 48.0, 44.3, 38.0, 35.9, 31.6, 29.4, 26.5, 25.6, 21.6, 13.9 ppm.

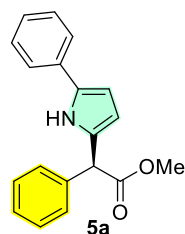
**HRMS** (ESI+) Calcd for  $\text{C}_{29}\text{H}_{31}\text{BrNO}_3$   $[\text{M}+\text{H}]^+$ : 520.1482, found: 520.1492.



### General Procedure D.



In an oven-dried 4-mL vial equipped with a magnetic stirring bar, sulfoxonium ylide **1a** (45.3 mg, 0.2 mmol, 1.0 equiv), CPA catalyst (S)-HA-10 (14.6 mg, 10 mol %), and 4 Å molecular sieves (100 mg) were combined. Subsequently, 1.0 mL of TCE was added, followed by the addition of pyrrole derivative **4** (0.22 mmol, 1.1 equiv). The resulting mixture was stirred at 25 °C and monitored by TLC. After completion (36 h), the mixture was directly subjected to flash column chromatography on silica gel (eluent: hexanes/ethyl acetate = 10:1) to afford the desired product **5**.



**Methyl (S)-2-phenyl-2-(5-phenyl-1H-pyrrol-2-yl)acetate (5a)** was prepared as a colorless oil according to the General Procedure D (eluent: hexanes/EtOAc = 10:1, 50.3 mg, 86% yield, 95% ee).

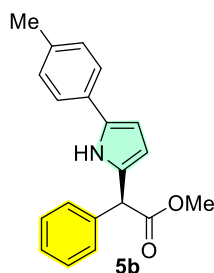
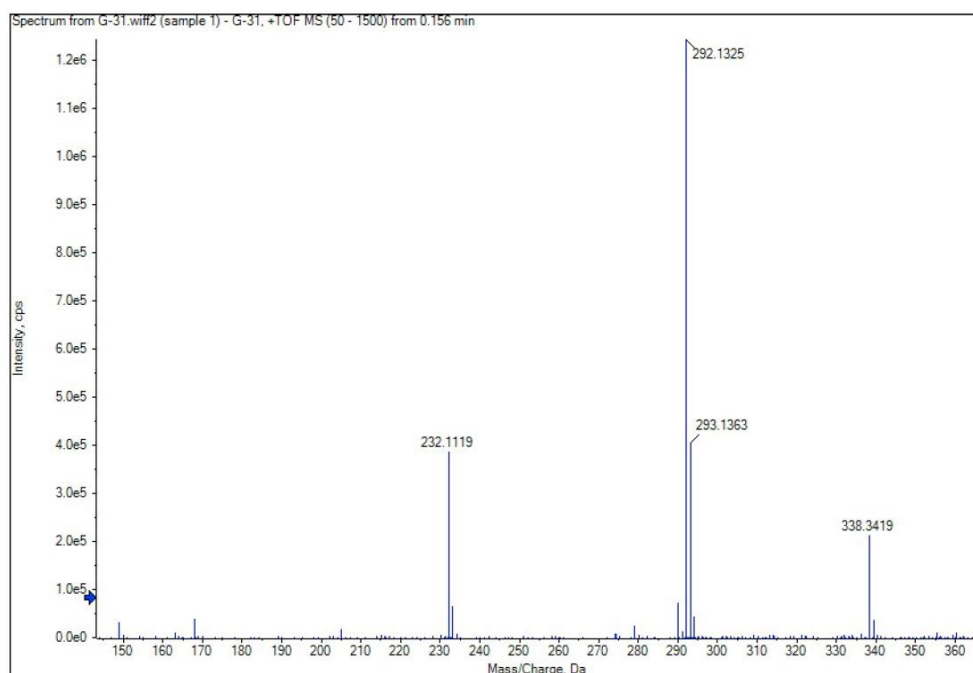
$[\alpha]_{\text{D}}^{25}$ : +107.8 ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK® AD-H column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 12.0 min (major), 14.0 min (minor).

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.05 (s, 1H), 7.39 – 7.36 (m, 2H), 7.27 – 7.18 (m, 7H), 7.13 – 7.07 (m, 1H), 6.37 – 6.35 (m, 1H), 6.01 – 6.00 (m, 1H), 5.01 (s, 1H), 3.67 (s, 3H) ppm.

$^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  173.0, 138.2, 132.7, 132.3, 128.9 (two C), 128.6, 127.9, 127.7, 126.2, 123.8, 109.7, 106.1, 52.7, 50.1 ppm.



HRMS (ESI+) Calcd for C<sub>19</sub>H<sub>18</sub>NO<sub>2</sub> [M+H]<sup>+</sup>: 292.1332, found: 292.1325.



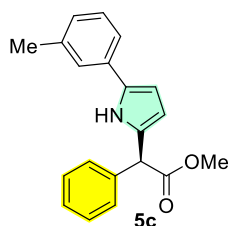
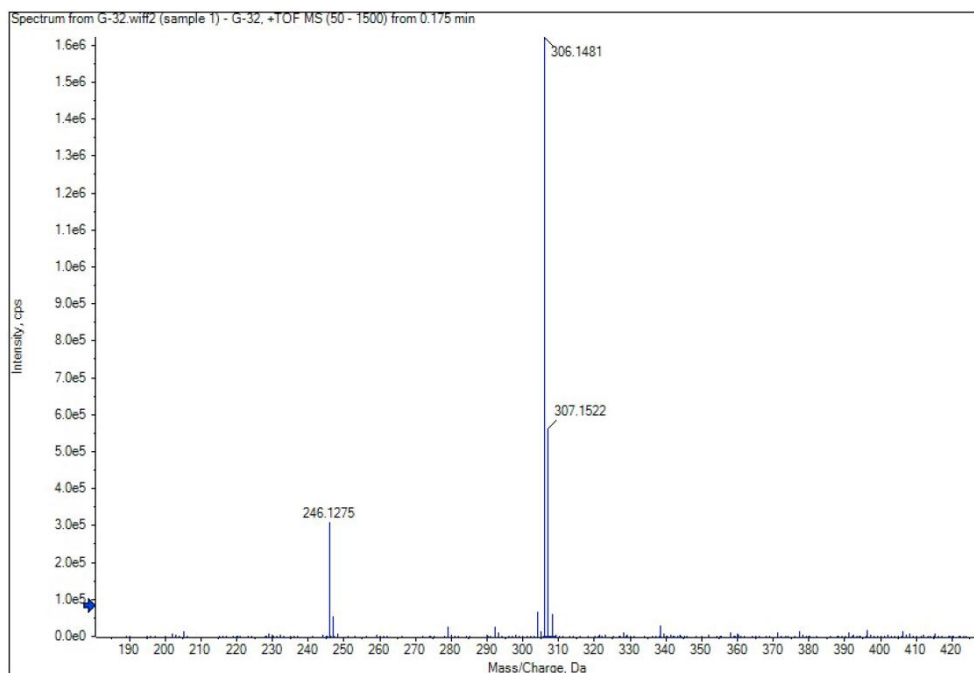
**Methyl (S)-2-phenyl-2-(5-(p-tolyl)-1H-pyrrol-2-yl)acetate (5b)** was prepared as a brown solid according to the General Procedure D (eluent: hexanes/EtOAc = 10:1, 52.7 mg, 87% yield, 93% ee).

$[\alpha]_{\text{D}}^{25}$ : +51.1 ( $c = 1.5$ , CH<sub>2</sub>Cl<sub>2</sub>). HPLC analysis of the product: Daicel CHIRALPAK<sup>®</sup> AD-H column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 13.8 min (major), 17.1 min (minor).

<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$  9.06 (s, 1H), 7.37 – 7.25 (m, 7H), 7.15 – 7.13 (m, 2H), 6.40 – 6.38 (m, 1H), 6.07 (s, 1H), 5.08 (s, 1H), 3.75 (s, 3H), 2.32 (s, 3H) ppm.

<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)  $\delta$  173.0, 138.3, 135.9, 132.5, 130.0, 129.5, 128.9, 128.1, 127.9, 127.6, 123.8, 109.6, 105.5, 52.6, 50.1, 21.2 ppm.

HRMS (ESI+) Calcd for C<sub>20</sub>H<sub>20</sub>NO<sub>2</sub> [M+H]<sup>+</sup>: 306.1489, found: 306.1481.



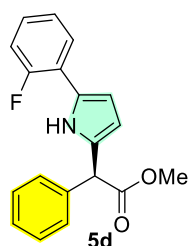
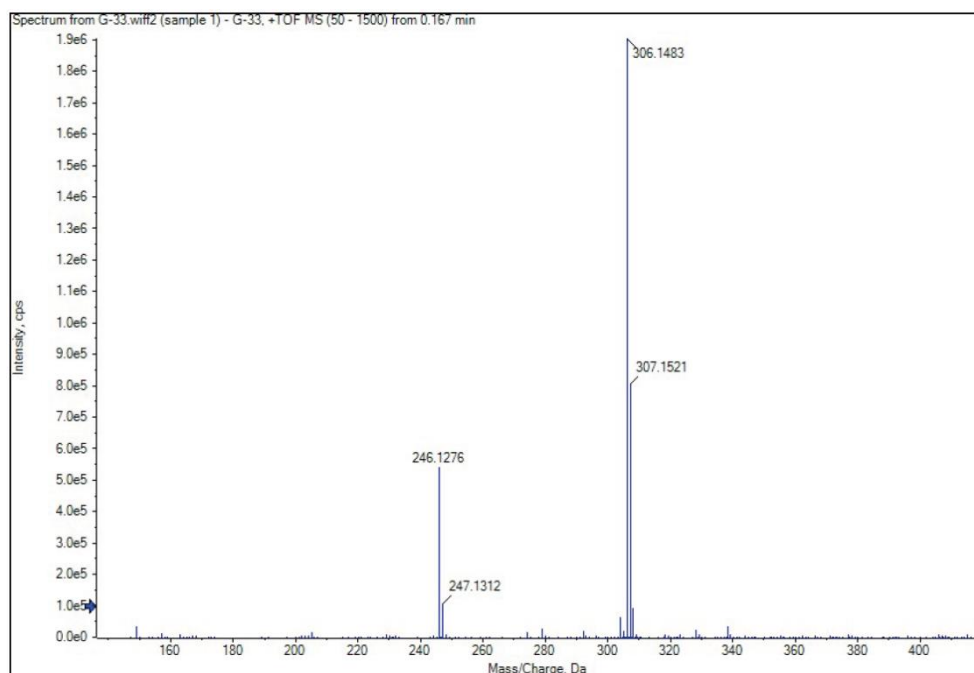
**Methyl (S)-2-phenyl-2-(5-(m-tolyl)-1H-pyrrol-2-yl)acetate (5c)** was prepared as a brown oil according to the General Procedure D (eluent: hexanes/EtOAc = 10:1, 56.1 mg, 92% yield, 93% ee).

$[\alpha]_D^{25}$ : +52.3 ( $c = 1.5$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK® AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 7.4 min (major), 7.9 min (minor).

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.11 (s, 1H), 7.33 – 7.20 (m, 8H), 7.00 – 6.98 (m, 1H), 6.43 – 6.42 (m, 1H), 6.08 – 6.07 (m, 1H), 5.09 (s, 1H), 3.75 (s, 3H), 2.35 (s, 3H) ppm.

$^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  173.1, 138.5, 138.3, 132.6, 132.5, 128.9, 128.8, 128.4, 127.9, 127.7, 127.0, 124.5, 121.0, 109.7, 106.0, 52.7, 50.1, 21.6 ppm.

**HRMS** (ESI+) Calcd for  $\text{C}_{20}\text{H}_{20}\text{NO}_2$   $[\text{M}+\text{H}]^+$ : 306.1489, found: 306.1483.



**Methyl (S)-2-(5-(2-fluorophenyl)-1H-pyrrol-2-yl)-2-phenylacetate (5d)** was prepared as a brown solid according to the General Procedure D (eluent: hexanes/EtOAc = 10:1, 47.6 mg, 77% yield, 96% ee).

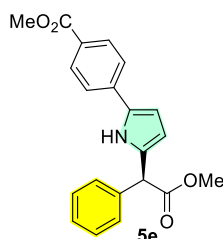
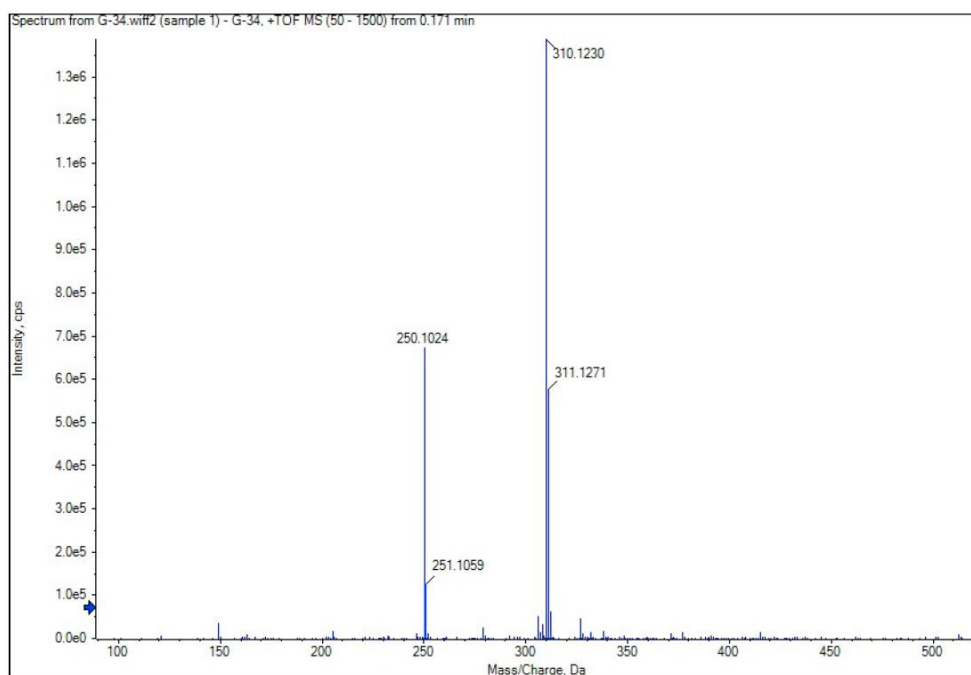
$[\alpha]_{\text{D}}^{25}$ : +37.5 ( $c = 1.5$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK<sup>®</sup> AD-H column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 9.8 min (major), 11.3 min (minor).

<sup>1</sup>H NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  9.59 (s, 1H), 7.59 – 7.53 (m, 1H), 7.32 – 7.26 (m, 5H), 7.11 – 7.04 (m, 3H), 6.57 (s, 1H), 6.10 (s, 1H), 5.09 (s, 1H), 3.76 (s, 3H) ppm.

<sup>13</sup>C NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  172.6, 158.5 (d,  $^1J_{\text{C-F}} = 243.1$  Hz), 138.0, 129.0 (d,  $^3J_{\text{C-F}} = 3.3$  Hz), 128.9, 127.9, 127.7, 127.0 (d,  $^3J_{\text{C-F}} = 8.6$  Hz), 126.8 (d,  $^5J_{\text{C-F}} = 2.0$  Hz), 126.4 (d,  $^3J_{\text{C-F}} = 4.4$  Hz), 124.6 (d,  $^4J_{\text{C-F}} = 3.1$  Hz), 120.3 (d,  $^2J_{\text{C-F}} = 11.3$  Hz), 116.3 (d,  $^2J_{\text{C-F}} = 23.0$  Hz), 109.1, 107.9 (d,  $^4J_{\text{C-F}} = 2.8$  Hz), 52.7, 50.2 ppm.

<sup>19</sup>F NMR (282 MHz,  $\text{CDCl}_3$ )  $\delta$  -118.6 ppm.

HRMS (ESI+) Calcd for C<sub>19</sub>H<sub>17</sub>FNO<sub>2</sub> [M+H]<sup>+</sup>: 310.1238, found: 310.1230.



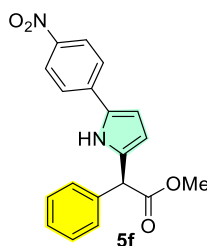
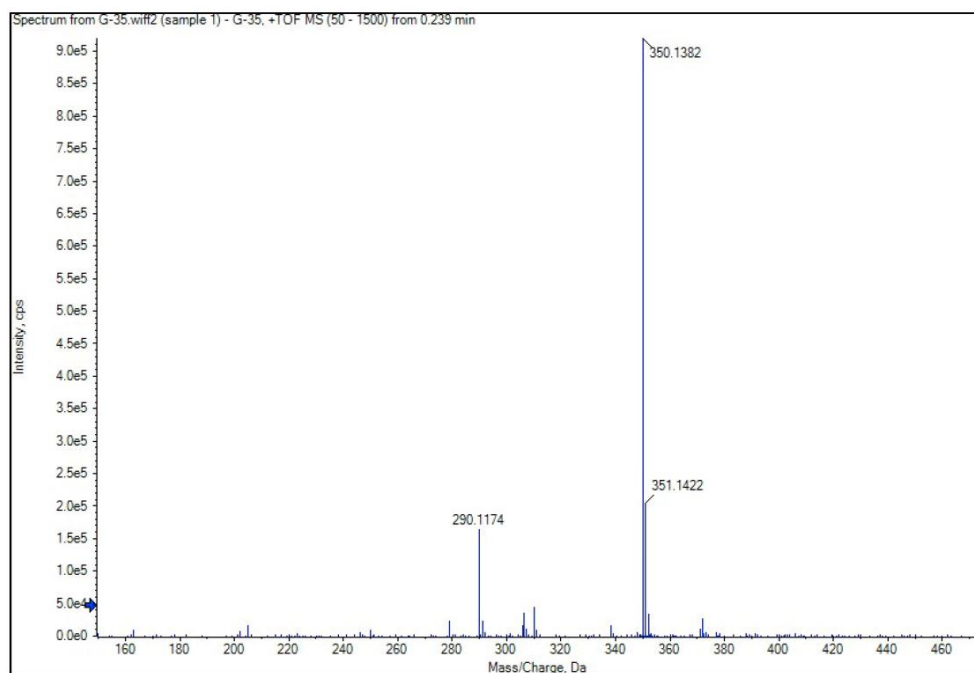
**Methyl (S)-4-(5-(2-methoxy-2-oxo-1-phenylethyl)-1H-pyrrol-2-yl)benzoate (5e)** was prepared as a yellow oil according to the General Procedure D (eluent: hexanes/EtOAc = 10:1, 66.4 mg, 95% yield, 96% ee).

$[\alpha]_D^{25}$ : +195.2 ( $c = 1.5$ , CH<sub>2</sub>Cl<sub>2</sub>). HPLC analysis of the product: Daicel CHIRALPAK<sup>®</sup> IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 12.7 min (major), 14.1 min (minor).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  9.39 (s, 1H), 7.99 (d,  $J = 8.4$  Hz, 2H), 7.50 (d,  $J = 8.4$  Hz, 2H), 7.34 – 7.25 (m, 5H), 6.58 – 6.56 (m, 1H), 6.12 – 6.11 (m, 1H), 5.10 (s, 1H), 3.89 (s, 3H), 3.76 (s, 3H) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  172.9, 167.0, 137.9, 136.7, 131.1, 130.3, 130.2, 128.9, 127.84, 127.76, 127.2, 123.0, 110.3, 108.1, 52.8, 52.1, 50.0 ppm.

HRMS (ESI+) Calcd for C<sub>21</sub>H<sub>20</sub>NO<sub>4</sub> [M+H]<sup>+</sup>: 350.1387, found: 350.1382.



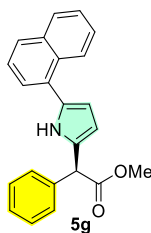
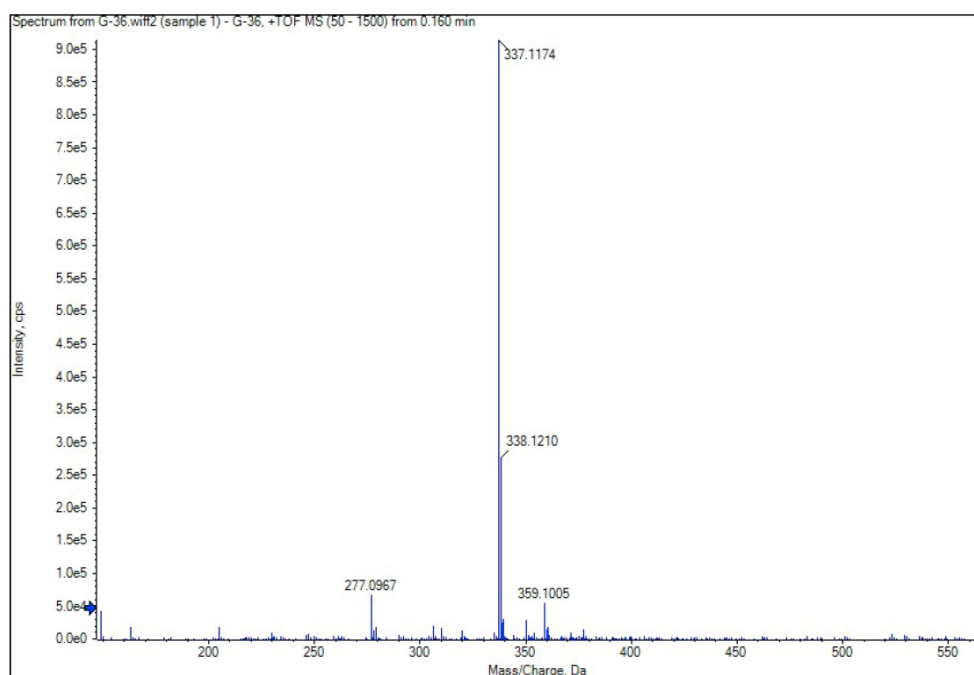
**Methyl (S)-2-(5-(4-nitrophenyl)-1H-pyrrol-2-yl)-2-phenylacetate (5f)** was prepared as a yellow oil according to the General Procedure D (eluent: hexanes/DCM = 3:1, 57.9 mg, 86% yield, 91% ee).

$[\alpha]_D^{25}$ : +154.0 ( $c = 1.5$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK<sup>®</sup> IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 12.8 min (minor), 13.5 min (major).

<sup>1</sup>H NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.52 (s, 1H), 8.17 (d,  $J = 8.9$  Hz, 2H), 7.53 (d,  $J = 8.9$  Hz, 2H), 7.36 – 7.28 (m, 5H), 6.65 – 6.63 (m, 1H), 6.15 – 6.13 (m, 1H), 5.12 (s, 1H), 3.79 (s, 3H) ppm.

<sup>13</sup>C NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  172.9, 145.2, 138.5, 137.6, 131.8, 129.9, 129.0, 127.9, 127.8, 124.6, 123.2, 110.8, 109.9, 52.9, 49.9 ppm.

HRMS (ESI+) Calcd for  $\text{C}_{19}\text{H}_{17}\text{N}_2\text{O}_4$   $[\text{M}+\text{H}]^+$ : 337.1183, found: 337.1174.



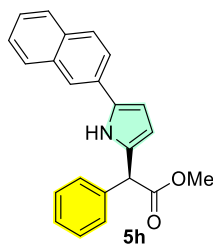
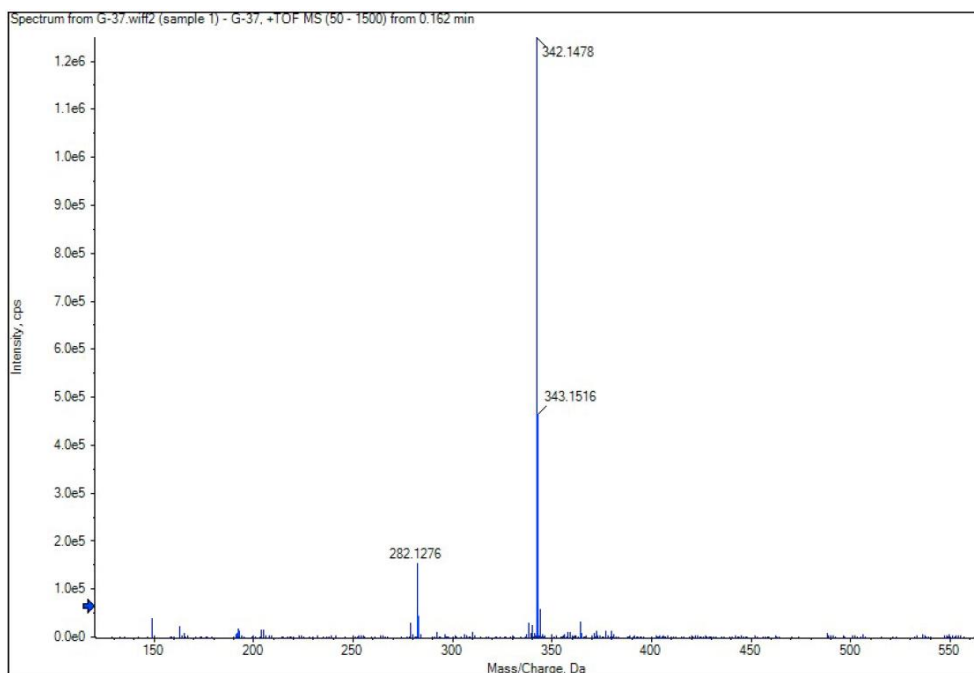
**Methyl (S)-2-(5-(naphthalen-1-yl)-1H-pyrrol-2-yl)-2-phenylacetate (5g)** was prepared as a brown oil according to the General Procedure D (eluent: hexanes/EtOAc = 10:1, 53.3 mg, 78% yield, 87% ee).

$[\alpha]_{\text{D}}^{25}$ : +38.0 ( $c = 1.5$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK<sup>®</sup> AD-H column; 1% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 22.9 min (minor), 25.4 min (major).

<sup>1</sup>H NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.02 (s, 1H), 8.34 – 8.31 (m, 1H), 7.86 – 7.84 (m, 1H), 7.77 – 7.75 (m, 1H), 7.49 – 7.44 (m, 4H), 7.36 – 7.24 (m, 5H), 6.44 – 6.43 (m, 1H), 6.20 – 6.19 (m, 1H), 5.14 (s, 1H), 3.74 (s, 3H) ppm.

<sup>13</sup>C NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  172.9, 138.3, 134.1, 131.5, 131.3, 130.8, 128.9, 128.5, 128.3, 128.0, 127.7, 127.5, 126.4, 126.03, 126.0, 125.8, 125.5, 109.7, 109.1, 52.7, 50.3 ppm.

**HRMS** (ESI+) Calcd for  $\text{C}_{23}\text{H}_{20}\text{NO}_2$   $[\text{M}+\text{H}]^+$ : 342.1489, found: 342.1478.



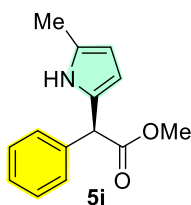
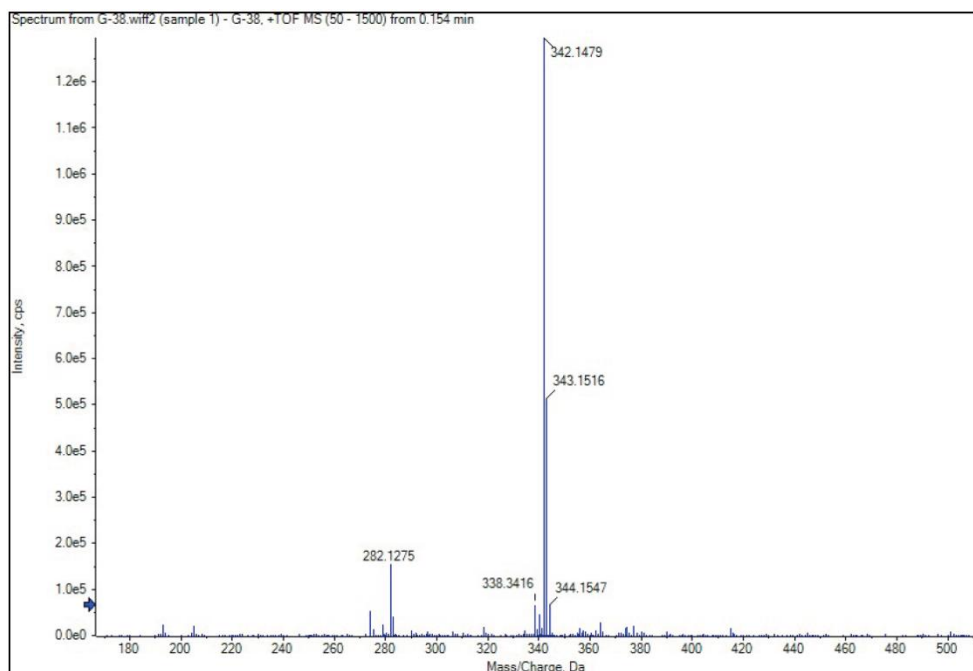
**Methyl (S)-2-(5-(naphthalen-2-yl)-1H-pyrrol-2-yl)-2-phenylacetate (5h)** was prepared as a brown solid according to the General Procedure D (eluent: hexanes/EtOAc = 10:1, 61.6 mg, 90% yield, 95% ee).

$[\alpha]_D^{25}$ : +92.6 ( $c = 1.5$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK® AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 12.2 min (major), 14.1 min (minor).

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.31 (s, 1H), 7.82 – 7.74 (m, 4H), 7.64 – 7.61 (m, 1H), 7.44 – 7.25 (m, 7H), 6.57 – 6.56 (m, 1H), 6.14 – 6.12 (m, 1H), 5.11 (s, 1H), 3.74 (s, 3H) ppm.

$^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  173.1, 138.2, 133.9, 132.4, 132.2, 130.1, 129.1, 129.0, 128.6, 127.9, 127.81, 127.78, 127.7, 126.5, 125.4, 123.2, 120.9, 110.0, 106.9, 52.8, 50.2 ppm.

**HRMS** (ESI+) Calcd for  $\text{C}_{23}\text{H}_{20}\text{NO}_2$   $[\text{M}+\text{H}]^+$ : 342.1489, found: 342.1479.



**Methyl (S)-2-(5-methyl-1H-pyrrol-2-yl)-2-phenylacetate (5i)** was prepared as a colorless oil according to the General Procedure D (eluent: hexanes/EtOAc = 10:1, 38.2 mg, 83% yield, 92% ee).

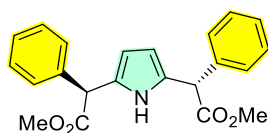
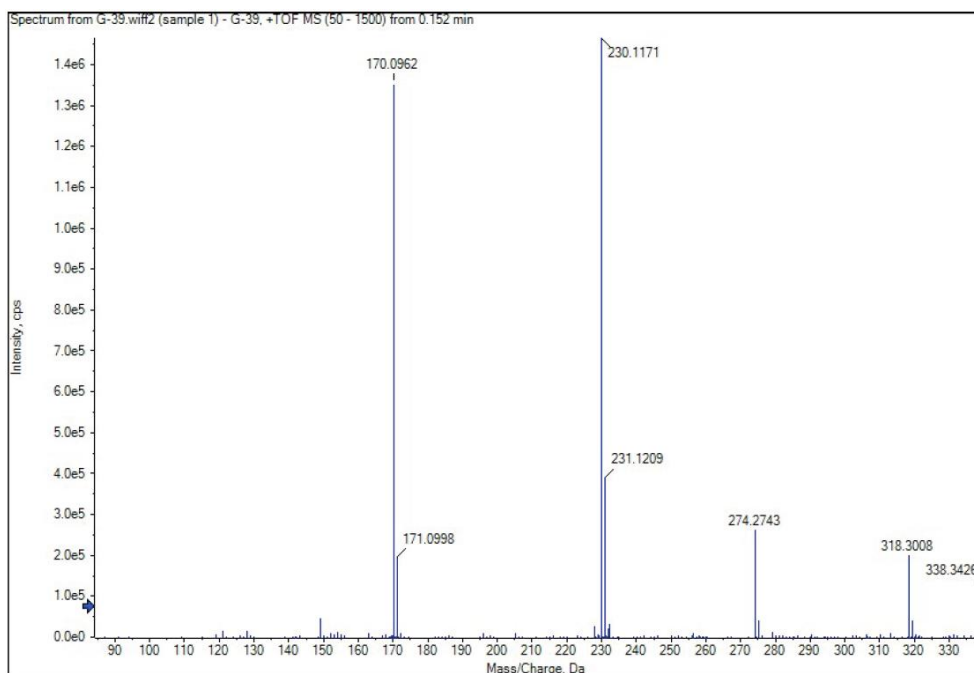
$[\alpha]_D^{25}$ : +9.8 ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK<sup>®</sup> IC column; 1% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 9.9 min (minor), 11.5 min (major).

<sup>1</sup>H NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.41 (s, 1H), 7.33 – 7.22 (m, 5H), 5.90 (s, 1H), 5.79 (s, 1H), 5.00 (s, 1H), 3.73 (s, 3H), 2.23 (s, 3H) ppm.

<sup>13</sup>C NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  173.1, 138.5, 128.7, 128.1, 127.8, 127.4, 125.9, 108.0, 106.0, 52.5, 50.2, 13.1 ppm.

HRMS (ESI+) Calcd for  $\text{C}_{14}\text{H}_{16}\text{NO}_2$   $[\text{M}+\text{H}]^+$ : 230.1176, found: 230.1171.





**5j**

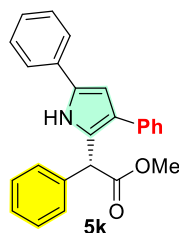
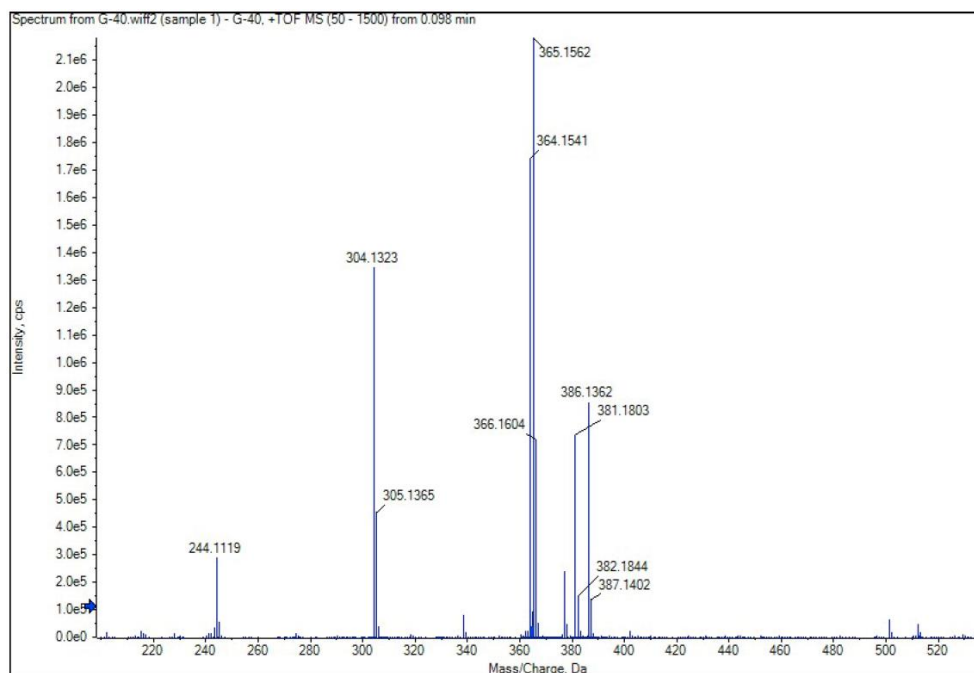
**Methyl (S)-2-(5-((R)-2-methoxy-2-oxo-1-phenylethyl)-1H-pyrrol-2-yl)-2-phenylacetate (5j)** was prepared as a yellow oil according to the General Procedure D (eluent: hexanes/EtOAc = 10:1, 56.0 mg, 77% yield, 96% ee, C<sub>2</sub>: *meso* = 2:1 by crude <sup>1</sup>H NMR analysis).

[α]<sub>D</sub><sup>25</sup>: +38.5 (c = 1.0, CH<sub>2</sub>Cl<sub>2</sub>). HPLC analysis of the product: Daicel CHIRALPAK<sup>®</sup> IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 7.8 min (major), 8.5 min (minor).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 9.28 – 9.24 (m, 1H), 7.34 – 7.24 (m, 10H), 5.95 – 5.91 (m, 2H), 5.021 – 5.015 (m, 2H), 3.73 (s, 6H) ppm.

<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) δ 172.6, 138.1, 128.7, 128.0, 127.7, 127.5, 107.9, 52.5, 50.3 ppm.

HRMS (ESI+) Calcd for C<sub>22</sub>H<sub>22</sub>NO<sub>4</sub> [M+H]<sup>+</sup>: 364.1543, found: 364.1541.



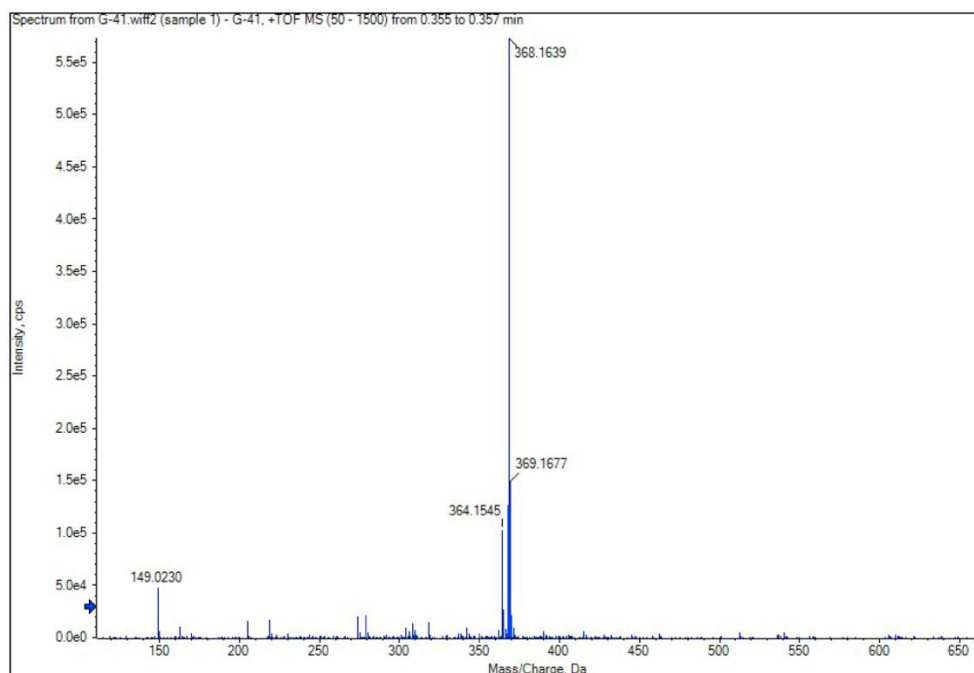
**Methyl (R)-2-(3,5-diphenyl-1H-pyrrol-2-yl)-2-phenylacetate (5k)** was prepared as a yellow oil according to the General Procedure D (eluent: hexanes/EtOAc = 10:1, 58.6 mg, 80% yield,  $-78\%$  ee).

$[\alpha]_D^{25}$ :  $-52.7$  ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK® AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 7.8 min (minor), 13.9 min (major).

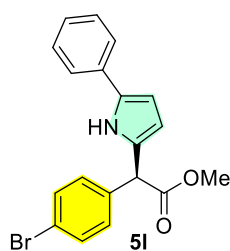
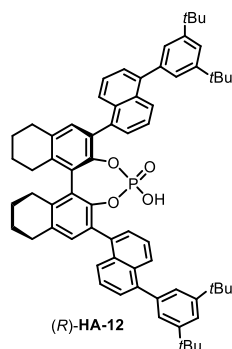
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.54 (s, 1H), 7.55 – 7.53 (m, 2H), 7.39 – 7.20 (m, 13H), 6.65 – 6.64 (m, 1H), 5.33 (s, 1H), 3.74 (s, 3H) ppm.

$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  173.6, 138.7, 136.0, 132.4, 132.0, 129.1, 129.0, 128.6, 128.2, 127.7, 127.6, 126.5, 126.2, 125.4, 123.9, 123.8, 106.6, 52.8, 47.8 ppm.

HRMS (ESI+) Calcd for  $\text{C}_{25}\text{H}_{22}\text{NO}_2$   $[\text{M}+\text{H}]^+$ : 368.1645, found: 368.1639.



Note: the structure of optimal CPA for this case:



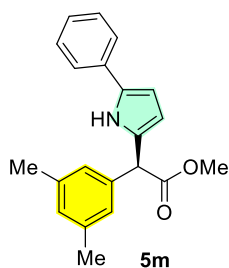
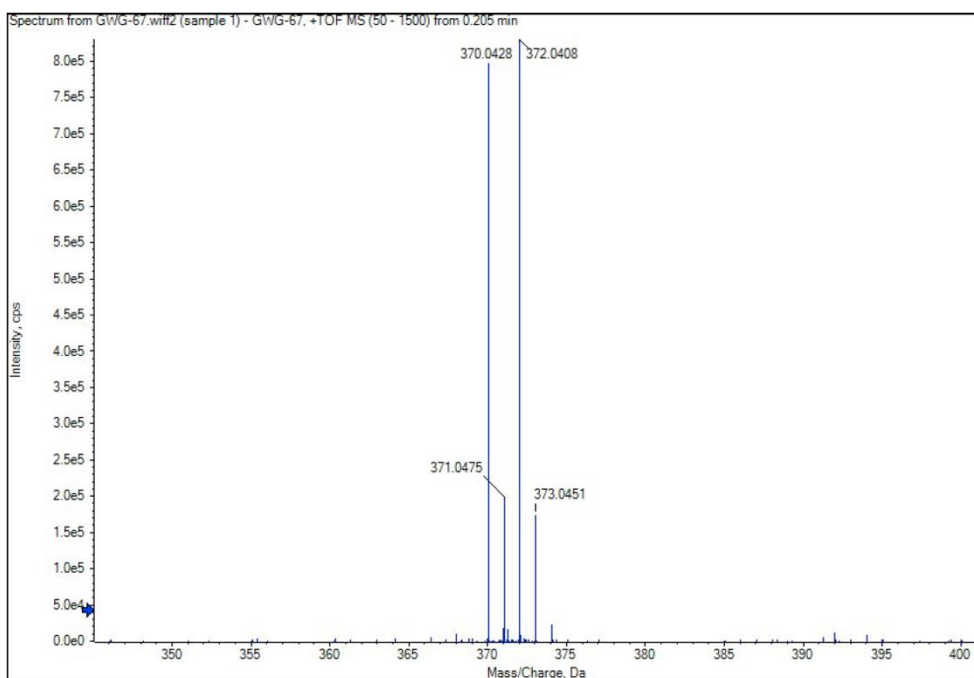
**Methyl (S)-2-(4-bromophenyl)-2-(5-phenyl-1H-pyrrol-2-yl) acetate (51)** was prepared as a colorless oil according to the General Procedure D (eluent: hexanes/EtOAc = 10:1, 66 mg, 89% yield, 96% ee).

$[\alpha]_D^{25}$ : +151.0 ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK® AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 10.3 min (major), 12.1 min (minor).

$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  9.11 (s, 1H), 7.47 – 7.42 (m, 4H), 7.37 – 7.32 (m, 2H), 7.21 – 7.16 (m, 3H), 6.44 (t,  $J = 3.0$  Hz, 1H), 6.06 (t,  $J = 3.0$  Hz, 1H), 5.03 (s, 1H), 3.76 (s, 3H) ppm.

$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  172.5, 137.2, 132.5, 131.9, 129.7 (two C), 128.9, 127.9, 126.3, 123.8, 121.7, 109.9, 106.1, 52.8, 49.5 ppm.

HRMS (ESI+) Calcd for  $\text{C}_{19}\text{H}_{17}\text{BrNO}_2$   $[\text{M}+\text{H}]^+$ : 370.0437, found: 370.0428.



**Methyl (S)-2-(3,5-dimethylphenyl)-2-(5-phenyl-1H-pyrrol-2-yl) acetate (5m)**

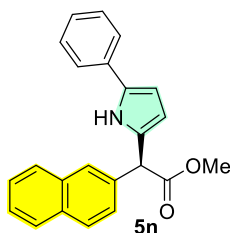
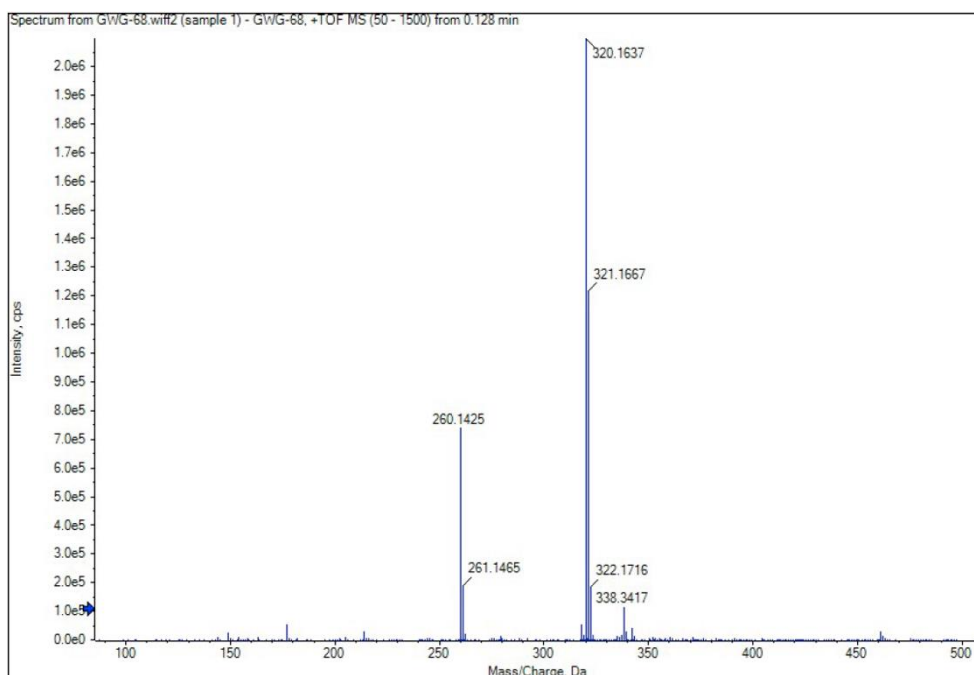
was prepared as a colorless oil according to the General Procedure D (eluent: hexanes/EtOAc = 10:1, 56 mg, 88% yield, 97% ee).

$[\alpha]_{\text{D}}^{25}$ : +161.6 ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK<sup>®</sup> AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 5.9 min (major), 6.5 min (minor).

$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  9.11 (s, 1H), 7.47 – 7.44 (m, 2H), 7.35 – 7.30 (m, 2H), 7.18 – 7.13 (m, 1H), 6.91 – 6.89 (m, 3H), 6.44 (t,  $J$  = 3.0 Hz, 1H), 6.08 (t,  $J$  = 3.0 Hz, 1H), 5.01 (s, 1H), 3.74 (s, 3H), 2.27 (s, 6H) ppm.

$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  173.2, 138.5, 138.0, 132.8, 132.2, 129.4, 128.92, 128.90, 126.1, 125.6, 123.8, 109.5, 106.1, 52.7, 50.0, 21.4 ppm.

HRMS (ESI+) Calcd for  $\text{C}_{21}\text{H}_{22}\text{NO}_2$   $[\text{M}+\text{H}]^+$ : 320.1645, found: 320.1637.



**Methyl (S)-2-(naphthalen-2-yl)-2-(5-phenyl-1H-pyrrol-2-yl) acetate (5n)** was prepared as a colorless oil according to the General Procedure D (eluent: hexanes/EtOAc = 10:1, 47 mg, 69% yield, 96% ee).

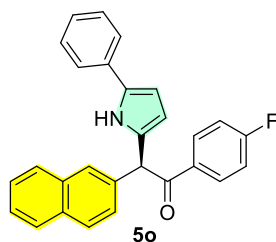
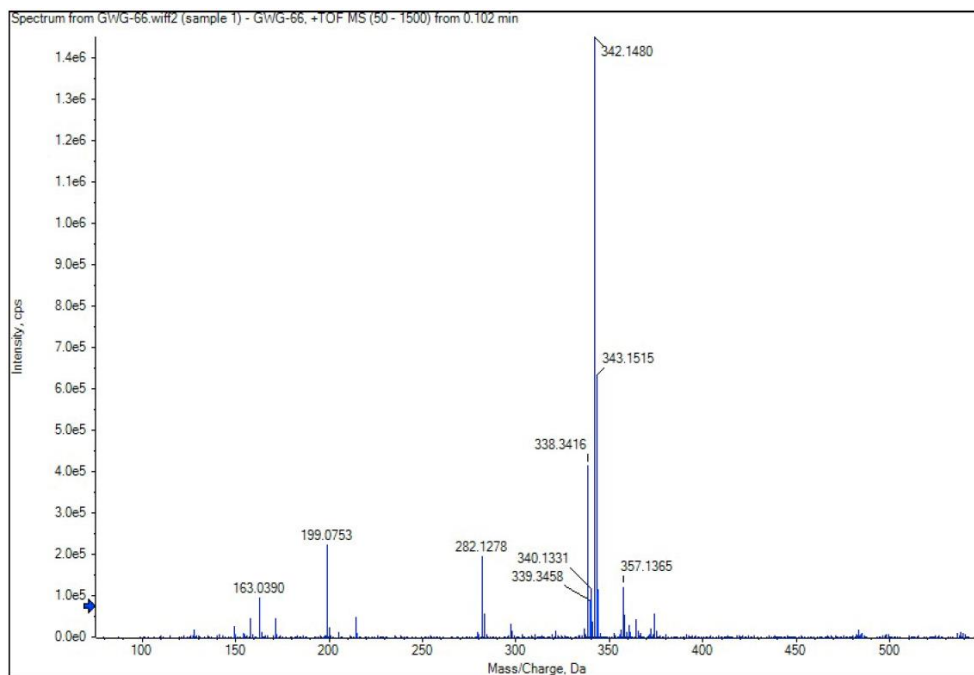
$[\alpha]_{\text{D}}^{25}$ : +262.4 ( $c$  = 1.0,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK<sup>®</sup> AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 12.7 min (major), 16.2 min (minor).

$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  9.17 (s, 1H), 7.79 – 7.73 (m, 4H), 7.47 – 7.42 (m,

5H), 7.34 – 7.29 (m, 2H), 7.18 – 7.13 (m, 1H), 6.46 (t,  $J = 3.0$  Hz, 1H), 6.12 (t,  $J = 3.0$  Hz, 1H), 5.24 (s, 1H), 3.75 (s, 3H) ppm.

$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  173.0, 135.6, 133.5, 132.8, 132.7, 132.4, 128.9, 128.7, 128.6, 128.1, 127.7, 126.8, 126.4, 126.3, 126.2, 125.9, 123.8, 109.9, 106.2, 52.8, 50.3 ppm.

HRMS (ESI+) Calcd for  $\text{C}_{23}\text{H}_{20}\text{NO}_2$   $[\text{M}+\text{H}]^+$ : 342.1489, found: 342.1480.



**(S)-1-(4-Fluorophenyl)-2-(naphthalen-2-yl)-2-(5-phenyl-1H-pyrrol-2-yl)ethan-1-one (5o)** was prepared as a yellow oil according to the General Procedure D (eluent: hexanes/EtOAc = 10:1, 51 mg, 63% yield, 90% ee).

$[\alpha]_{\text{D}}^{25}$ :  $-87.5$  ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK<sup>®</sup> AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 31.1 min (minor), 42.9 min (major).

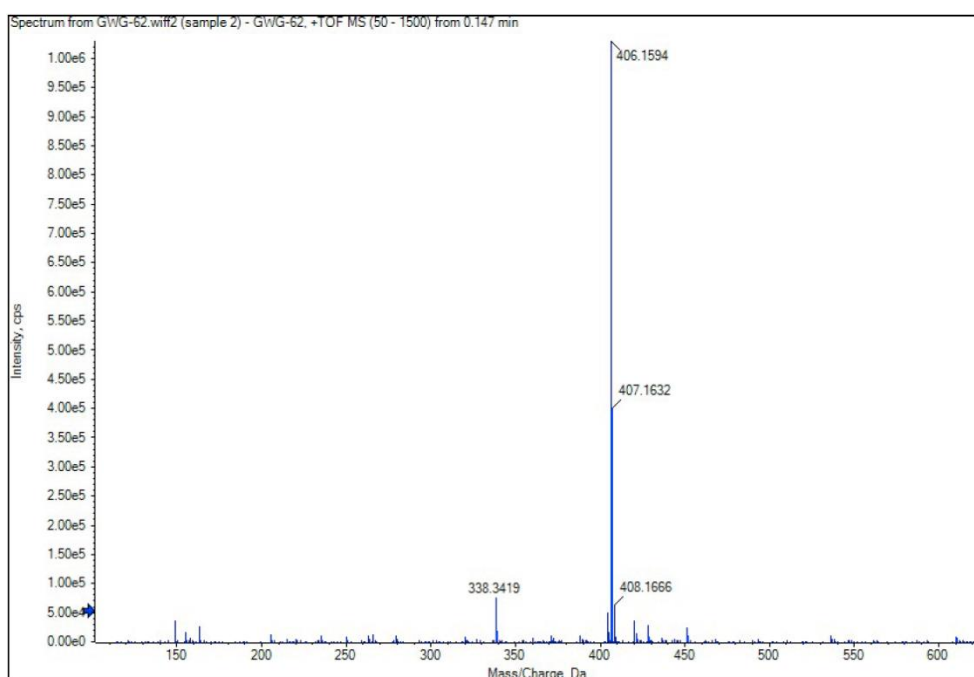
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  9.26 (s, 1H), 8.65 (s, 1H), 8.14 – 8.12 (m, 1H), 8.01

– 7.89 (m, 3H), 7.68 – 7.53 (m, 4H), 7.42 – 7.36 (m, 4H), 7.28 – 7.22 (m, 1H), 7.08 – 7.02 (m, 2H), 6.53 (s, 1H), 6.35 (s, 1H), 6.25 (s, 1H) ppm.

$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  198.9, 158.5 (d,  $^1J_{\text{C-F}} = 245.1$  Hz), 135.8, 134.9 (d,  $^4J_{\text{C-F}} = 3.1$  Hz), 133.7, 132.9, 132.6 (d,  $^3J_{\text{C-F}} = 10.6$  Hz), 131.0, 130.0, 129.9, 129.8, 129.5, 129.0, 128.89, 128.86, 127.8, 127.1, 126.3, 124.4, 123.8, 115.9 (d,  $^2J_{\text{C-F}} = 21.4$  Hz), 110.1, 106.2, 50.7 ppm.

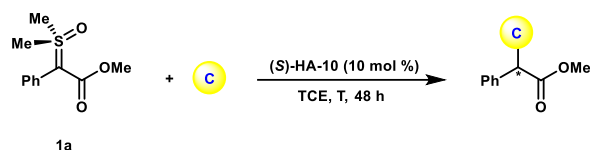
$^{19}\text{F}$  NMR (282 MHz,  $\text{CDCl}_3$ )  $\delta$  –114.9 ppm.

HRMS (ESI+) Calcd for  $\text{C}_{28}\text{H}_{21}\text{FNO}$   $[\text{M}+\text{H}]^+$ : 406.1602, found: 406.1594.



## V. Unsuccessful Carbon Nucleophiles

**Table S1** The selected unsuccessful nucleophiles.<sup>a</sup>



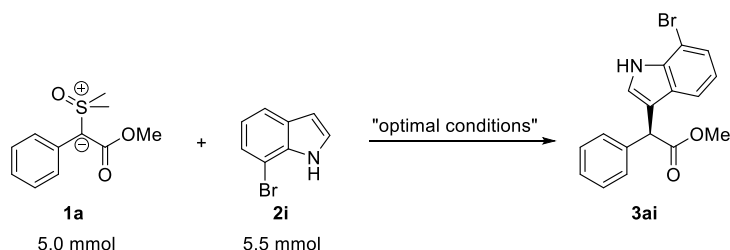
	T(40 °C)	T(90 °C)
	N. R.	N. R.
	N. R.	N. R.
	N. R.	N. R.
	N. R.	N. R.
	N. R.	N. R.
	N. R.	N. R.
	N. R.	messy
	N. R.	N. R.
TMSCN	N. R.	N. R.
	N. R.	N. R.
	N. R.	N. R.
	no desired product <sup>b</sup>	
	no desired product <sup>c</sup>	
	no desired product <sup>d</sup>	

<sup>a</sup> all reactions were carried out with **1a** (0.1 mmol), carbon nucleophile (0.11 mmol), and (S)-**HA-10** (10 mol %) in 1,1,2,2-tetrachloroethane (TCE) (0.5 mL) at the specified temperature for 48 h. <sup>b</sup> N–H insertion products were identified in 86% yield and 22% ee at 40 °C. <sup>c</sup> N–H insertion products were identified in 88% yield and 63% ee at 40 °C. <sup>d</sup> Trace amount of racemic N–H insertion products were identified at 40 °C.



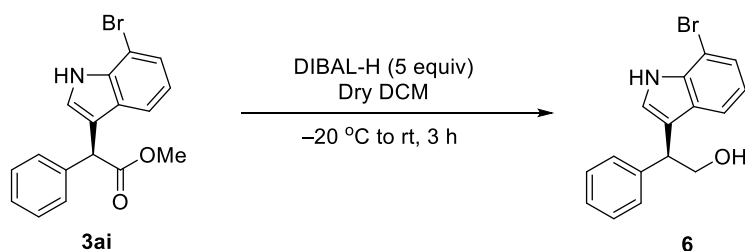
## VI. The Procedure for Gram-Scale Synthesis and Synthetic Transformation

### Gram-Scale Synthesis of 3ai:



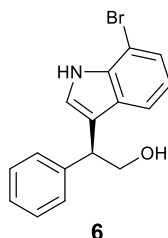
In an oven-dried 100-mL round-bottomed flask equipped with a magnetic stirring bar, sulfoxonium ylide **1a** (1.1 g, 5.0 mmol, 1.0 equiv), CPA catalyst (*S*)-**HA-10** (365 mg, 10 mol %), and 5 Å molecular sieves (2.5 g) were combined. Subsequently, 25.0 mL of TCE was added, followed by the addition of indole **2i** (1.1 g, 5.5 mmol, 1.1 equiv). The resulting mixture was stirred at 40 °C and monitored by TLC. After completion (48 h), the mixture was directly subjected to flash column chromatography on silica gel (eluent: hexanes/ethyl acetate = 10:1 to 5:1) to afford the desired product **3ai** (1.2 g, 70% yield, 96% ee). At the same time, the optimized catalyst (*S*)-**HA-10** could also be recovered in 90% yield (eluent: DCM/MeOH = 50:1, 328.5 mg). After fully acidified with 4 M HCl, the recovered catalyst could be used for the next batch reaction without adverse effect on reactivity and selectivity.

### Synthetic Transformations: Synthesis of Chiral Tryptophol 6



Under a nitrogen atmosphere, enantioenriched **3ai** (490.0 mg, 1.4 mmol, 1.0 equiv) and anhydrous DCM (10.0 mL) were introduced to an oven-dried 100-mL round-bottomed flask equipped with a magnetic stirring bar. The resulting

clear solution was cooled to  $-20\text{ }^{\circ}\text{C}$ , and DIBAL-H (7.0 mL, 7.0 mmol, 5 equiv, 1.0 M in *n*-hexane) was added dropwise. After completion (15 min), the reaction mixture was slowly warmed to room temperature and stirred for 3 h. Then, the reaction mixture was quenched employing 1.0 M HCl (5 mL), and extracted with DCM ( $3 \times 20\text{ mL}$ ). The combined organic phases were washed with brine, dried over  $\text{Na}_2\text{SO}_4$ , filtered, and concentrated under reduced pressure. The residue was purified on column chromatography on silica gel (eluent: hexanes/EtOAc = 5:1) to obtain the desired product **6**.



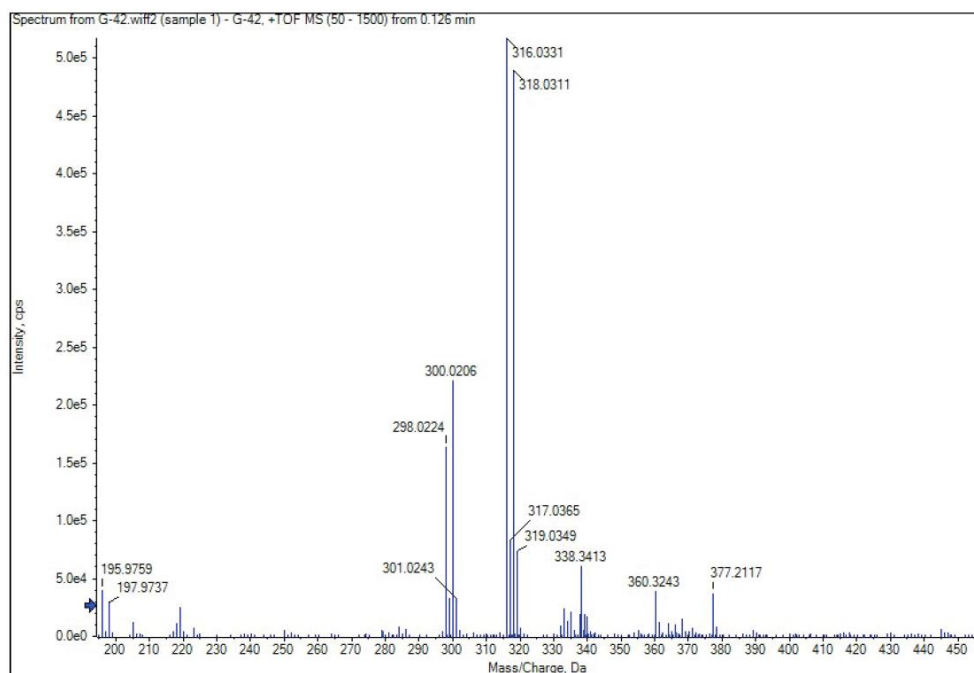
**(S)-2-(7-Bromo-1H-indol-3-yl)-2-phenylethan-1-ol (6)** was prepared as a white solid (420.5 mg, 95% yield, 96% ee).

$[\alpha]_{\text{D}}^{25}$ : +62.6 ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK<sup>®</sup> AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 32.0 min (minor), 34.2 min (major).

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ) 8.27 (s, 1H), 7.26 – 7.19 (m, 6H), 7.14 – 7.11 (m, 1H), 7.032 – 7.028 (m, 1H), 6.80 (t,  $J = 7.8\text{ Hz}$ , 1H), 4.32 (t,  $J = 6.8\text{ Hz}$ , 1H), 4.12 – 4.01 (m, 2H), 1.71 (br, 1H) ppm.

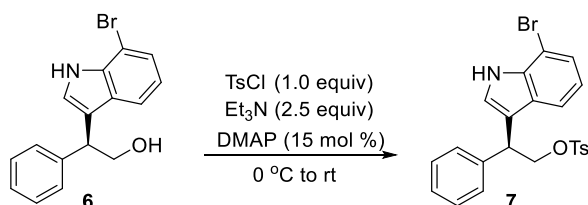
$^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  141.3, 135.2, 128.7, 128.34, 128.28, 127.0, 124.7, 122.5, 120.8, 118.7, 117.4, 104.9, 66.4, 45.7 ppm.

**HRMS** (ESI+) Calcd for  $\text{C}_{16}\text{H}_{15}\text{NO}$   $[\text{M}+\text{H}]^+$ : 316.0332, found: 316.0331.



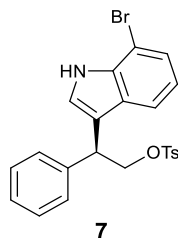
## Synthetic Transformations: Synthesis of O-Tosylated Tryptophol Derivative

7



Under a nitrogen atmosphere, a solution of **6** (63.2 mg, 0.2 mmol, 96% ee) and DMAP (3.7 mg, 0.03 mmol, 15 mol%) in anhydrous DCM (10.0 mL) was treated with Et<sub>3</sub>N (69.5  $\mu$ L, 0.5 mmol, 2.5 equiv). The resulting colorless solution was cooled to 0 °C, and TsCl (38.1 mg, 0.2 mmol, 1.0 equiv) in anhydrous DCM (1.0 mL) was added dropwise. After completion (20 min), the reaction mixture was allowed to warm to room temperature. Following 24 h of stirring, the reaction mixture was diluted with DCM. The organic layer was subsequently washed with water and brine. The combined organic layers were dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under reduced pressure. The resulting

residue was purified by column chromatography on silica gel (eluent: hexanes/EtOAc = 5:1) to yield the desired product **7**.



**(S)-2-(7-Bromo-1H-indol-3-yl)-2-phenylethyl 4-methylbenzenesulfonate (7)** was prepared as a colorless oil (60.2 mg, 64% yield, 96% ee).

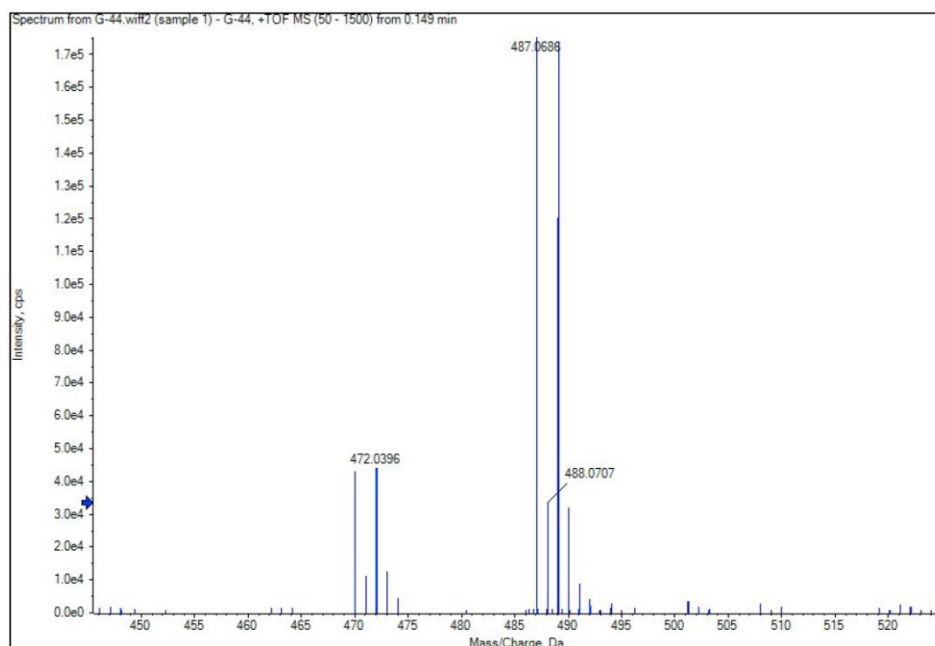
$[\alpha]_D^{25}$ : +25.2 ( $c = 2.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel CHIRALPAK® AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 26.3 min (major), 37.0 min (minor).

$^1\text{H NMR}$  (400 MHz,  $\text{CD}_2\text{Cl}_2$ ) 8.36 (s, 1H), 7.58 – 7.55 (m, 2H), 7.28 – 7.16 (m, 9H), 7.07 – 7.06 (m, 1H), 6.84 (t,  $J = 7.8$  Hz 1H), 4.58 – 4.44 (m, 3H), 2.38 (s, 3H) ppm.

$^{13}\text{C NMR}$  (100 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  145.4, 140.1, 135.4, 132.9, 130.2, 129.0, 128.5, 128.1 (two C), 127.6, 124.9, 123.2, 121.1, 118.7, 116.4, 105.0, 72.7, 42.7, 21.8 ppm.

**HRMS** (ESI+) Calcd for  $\text{C}_{23}\text{H}_{21}\text{BrNO}_3\text{S}$   $[\text{M}+\text{H}]^+$ : 470.0400, found: 472.0396.

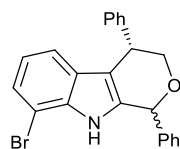
**Note: this compound has been observed to exhibit low stability at room temperature.**



### Synthetic Transformations: Synthesis of **8** via Pictet-Spengler Reaction



Under a nitrogen atmosphere, a solution of **6** (158.1 mg, 0.5 mmol, 96% ee) and benzaldehyde (76.5  $\mu\text{L}$ , 0.75 mmol, 1.5 equiv) in anhydrous DCM (10.0 mL) at 0  $^\circ\text{C}$  was treated with  $\text{BF}_3 \cdot \text{Et}_2\text{O}$  (0.05 mmol, 10 mol %). The resulted mixture was allowed to stirred at room temperature for 4 h, then concentrated at reduced pressure. The residue was purified by column chromatography on silica gel (eluent: hexanes/ethyl acetate = 20:1) to afford the desired product **8**.



**8A**

**Isomer (8A)** was prepared as a white solid (32% yield, 95% ee).

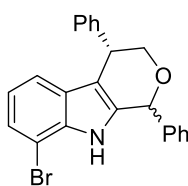
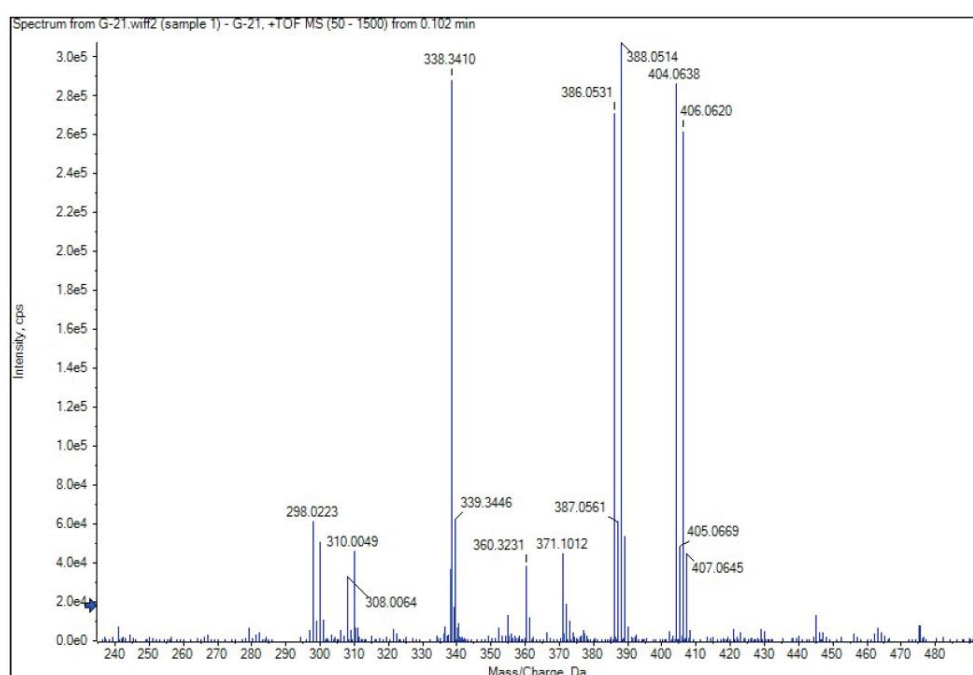
$[\alpha]_{\text{D}}^{25}$ :  $-48.9$  ( $c = 2.0$ ,  $\text{CH}_2\text{Cl}_2$ ). HPLC analysis of the product: Daicel

CHIRALPAK® AS-H column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 7.0 min (major), 9.8 min (minor).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) 7.69 (s, 1H), 7.42 (s, 5H), 7.33 – 7.22 (m, 6H), 6.80 – 6.75 (m, 2H), 5.923 – 5.919 (m, 1H), 4.53 – 4.50 (m, 1H), 4.39 – 4.35 (m, 1H), 3.81 – 3.76 (m, 1H) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 140.4, 138.7, 135.4, 134.9, 129.3, 129.1, 128.61 (two C), 128.55, 127.5, 127.1, 124.3, 120.9, 119.2, 113.0, 104.6, 76.4, 72.6, 41.3 ppm.

HRMS (ESI+) Calcd for C<sub>22</sub>H<sub>19</sub>BrNO [M+H]<sup>+</sup>: 404.0645, found: 404.0638.



**8B**

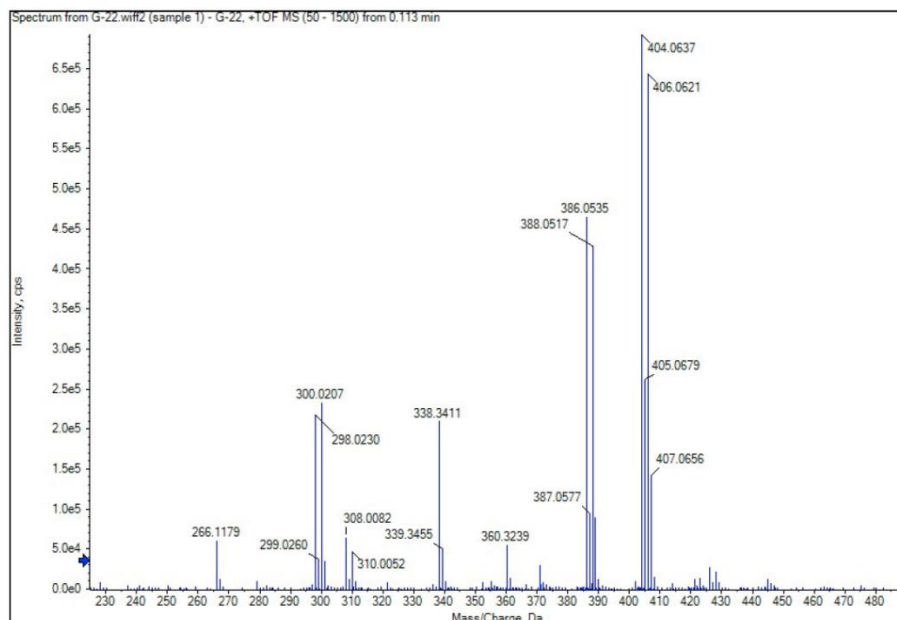
**Isomer (8B)** was prepared as a colorless oil (55% yield, 95% ee).

[α]<sub>D</sub><sup>25</sup>: +28.8 (c = 3.0, CH<sub>2</sub>Cl<sub>2</sub>). HPLC analysis of the product: Daicel CHIRALPAK® AS-H column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 9.7 min (minor), 13.9 min (major).

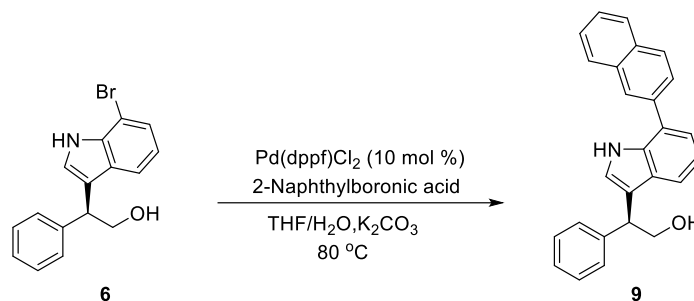
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) 7.81 (s, 1H), 7.44 – 7.19 (m, 11H), 7.06 (d, *J* = 8.1 Hz, 1H), 6.83 (t, *J* = 7.8 Hz, 1H), 5.84 (s, 1H), 4.27 – 4.05 (m, 3H) ppm.

$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  142.4, 138.9, 135.0, 134.9, 129.2, 129.1, 128.63, 128.58, 128.4, 127.9, 126.8, 124.6, 121.1, 118.7, 112.6, 104.7, 75.7, 70.8, 40.2 ppm.

HRMS (ESI+) Calcd for  $\text{C}_{22}\text{H}_{19}\text{BrNO}$   $[\text{M}+\text{H}]^+$ : 404.0645, found: 404.0637.

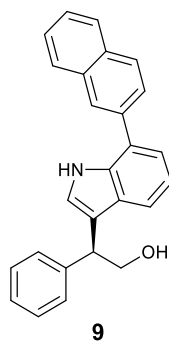


### Synthetic Transformations: Synthesis of 9



To a suspension of **6** (63.2 mg, 0.2 mmol, 1.0 equiv, 96% ee), 2-naphthylboronic acid (41.3 mg, 0.24 mmol, 1.2 equiv), and  $\text{K}_2\text{CO}_3$  (82.8 mg, 0.6 mmol, 3.0 equiv) in a mixture solvent of THF and water (5 mL,  $v/v = 4:1$ ) was added  $\text{Pd}(\text{dppf})\text{Cl}_2$  (14.6 mg, 0.02 mmol, 10 mol %). The mixture was degassed using freeze-pump-thaw cycles (3 times) (freeze-pump-thaw: cooled to  $-78\text{ }^\circ\text{C}$  and degassed *via* vacuum evacuation for 5 min, backfilled with nitrogen, and warm to room temperature) and then stirred for 12 h at  $80\text{ }^\circ\text{C}$ . After cooling to room temperature, the mixture was diluted with EtOAc (20 mL), and washed successively with water and brine. The combined organic layers were dried

over anhydrous Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated in reduced pressure. The residue was purified by column chromatography on silica gel (eluent: hexanes/ethyl acetate = 5:1) to afford the desired product **9**.



**(S)-2-(7-(Naphthalen-2-yl)-1H-indol-3-yl)-2-phenylethan-1-ol (9)** was prepared as a colorless oil (55.2 mg, 76% yield, 96% ee).

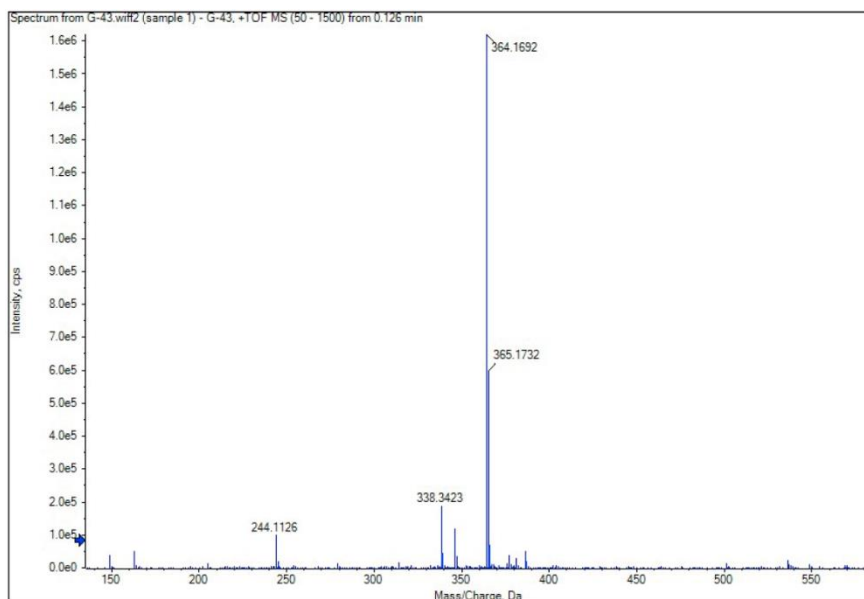
[ $\alpha$ ]<sub>D</sub><sup>25</sup>: +100.5 (*c* = 2.0, CH<sub>2</sub>Cl<sub>2</sub>). HPLC analysis of the product: Daicel CHIRALPAK® AD-H column; 15% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 30.0 min (minor), 61.3 min (major).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) 8.26 (s, 1H), 7.90 (s, 1H), 7.82 – 7.72 (m, 3H), 7.58 – 7.56 (m, 1H), 7.41 – 7.32 (m, 3H), 7.22 – 7.15 (m, 5H), 7.11 – 7.01 (m, 2H), 6.871 – 6.866 (m, 1H), 4.34 (t, *J* = 6.8 Hz 1H), 4.09 – 3.97 (m, 2H), 1.64 (br, 1H) ppm.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  141.7, 136.6, 134.6, 133.8, 132.7, 128.9, 128.7, 128.4, 128.1, 127.9, 127.6, 126.91, 126.86, 126.7, 126.6, 126.2, 125.7, 122.6, 122.3, 120.2, 118.8, 116.5, 66.5, 45.7 ppm.

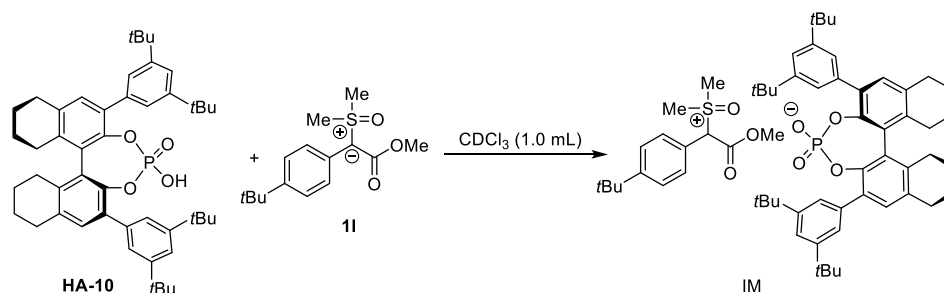
HRMS (ESI+) Calcd for C<sub>26</sub>H<sub>22</sub>NO [M+H]<sup>+</sup>: 364.1696, found: 364.1692.



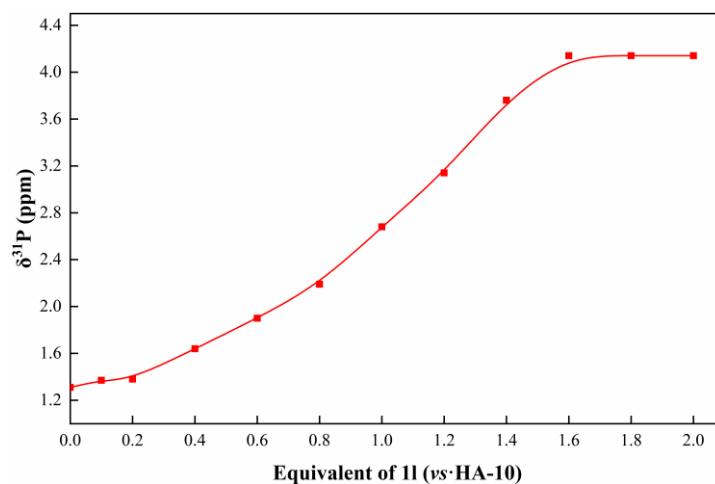


## VII. Mechanistic Study

### NMR Titration Experiment



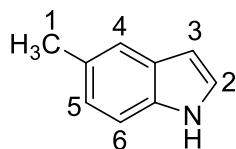
entry	CPA [M]	Ylide [M]	$\Delta m$ (mg)	Ylide/CPA	$\delta(^{31}\text{P NMR})$ ppm
1	0.05	0	-	0	1.31
2	0.05	0.005 (1.4 mg)	0	0.1	1.37
3	0.05	0.01 (2.8 mg)	1.4 mg	0.2	1.38
4	0.05	0.02 (5.6 mg)	2.8 mg	0.4	1.64
5	0.05	0.03 (8.5 mg)	2.8 mg	0.6	1.9
6	0.05	0.04 (11.3 mg)	2.8 mg	0.8	2.19
7	0.05	0.05 (14.1 mg)	2.8 mg	1.0	2.68
8	0.05	0.06 (16.9 mg)	2.8 mg	1.2	3.14
9	0.05	0.07 (19.8 mg)	2.8 mg	1.4	3.76
10	0.05	0.08 (22.6 mg)	2.8 mg	1.6	4.14
11	0.05	0.09 (25.4 mg)	2.8 mg	1.8	4.14
12	0.05	0.1 (28.2 mg)	2.8 mg	2.0	4.14



### Kinetic Isotope Effects at Natural Abundance

The  $^{13}\text{C}$  NMR analysis of the virgin and recovered samples of 5-methyl indole (**2d**) was performed following Singleton's method at natural abundance.<sup>7</sup> The NMR samples were prepared in an identical fashion by weighing out 20 mg of **2d** in a 5 mm high precision NMR tube and adding 0.5 mL  $\text{CDCl}_3$ . A T1 determination by the inverse-recovery method was performed on each sample before analysis and any sample that showed significantly different T1 values was omitted. The  $^{13}\text{C}$  NMR spectra were recorded with inverse gated decoupling and calibrated  $45^\circ$  pulses. A 60 s delay time between pulses was used to minimize any T1 variations ( $d_1 = 60$  s,  $at = 5.0$  s,  $np = 255170$ ,  $nt = 720$ ). All NMR data is summarized below in Table S2. Only a zero-order baseline correction was applied to each spectrum and the integration region for each peak was five times the peak width at half height.

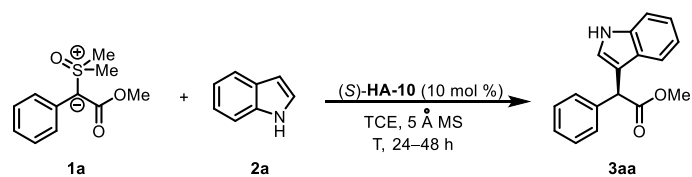
(7) D. A. Singleton, A. A. Thomas, *J. Am. Chem. Soc.*, 1995, **117**, 9357–9358.



**Table S2 <sup>13</sup>C Integrations of Recovered and Virgin Samples of 5-Methyl Indole (2d).**

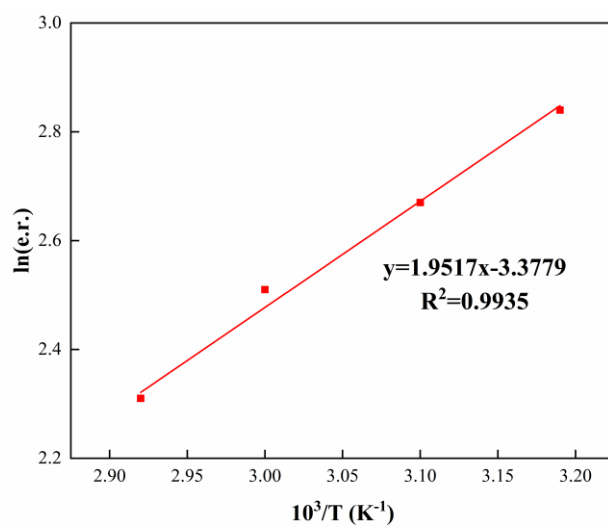
<b>Run 1</b>				
C#	Virgin	Recovered (69%)	R/R <sub>0</sub>	% Change
1	1.000	1.000	1.000	0.00
2	0.998	1.002	1.004	0.40
3	1.001	1.023	1.022	2.20
4	0.998	1.002	1.004	0.40
5	0.994	1.001	1.007	0.70
6	1.004	1.003	0.999	-0.10
<b>Run 2</b>				
C#	Virgin	Recovered (73%)	R/R <sub>0</sub>	% Change
1	1.000	1.000	1.000	0.00
2	0.998	1.003	1.005	0.50
3	1.001	1.029	1.028	2.80
4	0.998	0.996	0.998	-0.20
5	0.994	1.002	1.008	0.80
6	1.004	1.001	0.997	-0.30
<b>Run 3</b>				
C#	Virgin	Recovered (71%)	R/R <sub>0</sub>	% Change
1	1.000	1.000	1.000	0.00
2	0.998	1.004	1.006	0.60
3	1.001	1.038	1.037	3.70
4	0.998	0.998	1.000	0.00
5	0.994	1.001	1.007	0.70
6	1.004	0.998	0.994	-0.60

## Eyring Plot Analysis



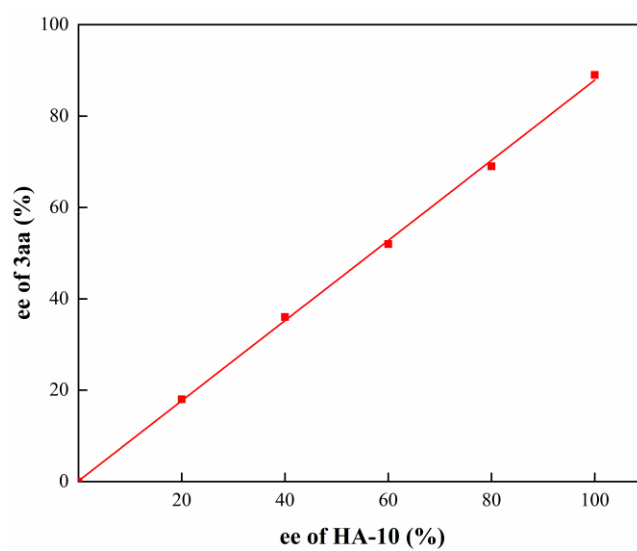
T/K	T/°C	ee (%)	e.r.	10 <sup>3</sup> /T (K <sup>-1</sup> )	ln(e.r.)
313	40	89	94.5:5.5	3.19	2.84
323	50	87	93.5:6.5	3.10	2.67
333	60	85	92.5:7.5	3.00	2.51
343	70	82	91:9	2.92	2.31

Note: Apart from the temperature variation, all other parameters are maintained in accordance with the optimal reaction conditions.



## Nonlinear Effect Study

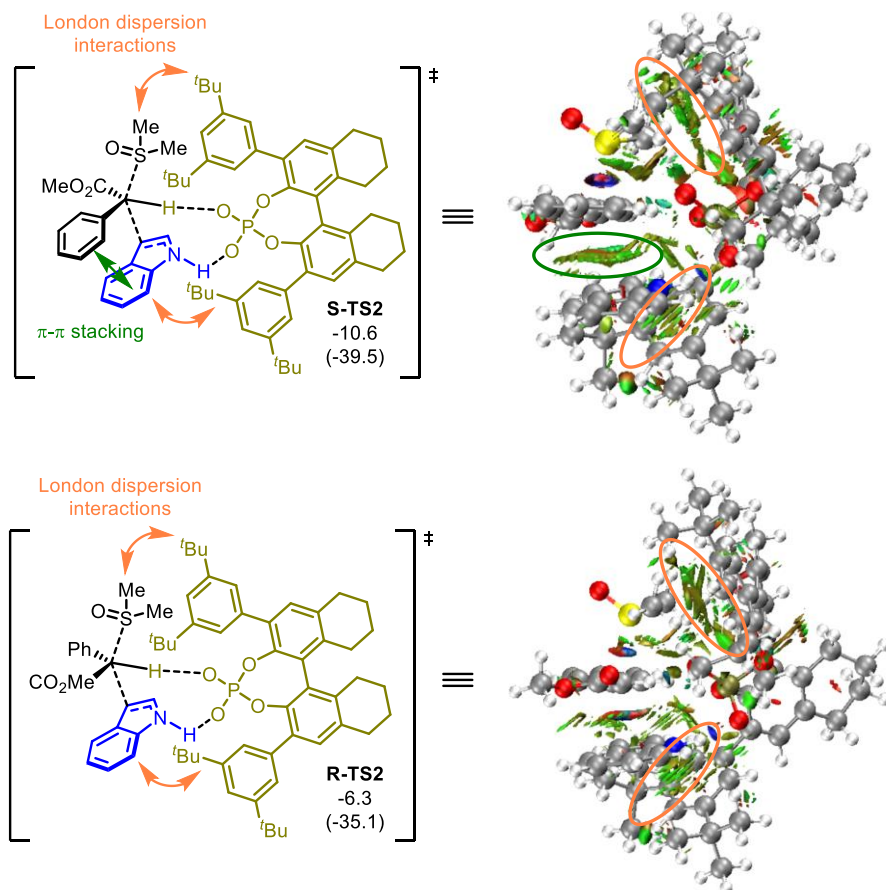
ee of (S)-HA-10 (%)	ee of 3aa (%)
100	89
80	69
60	52
40	36
20	18
0	0



## VIII. DFT Calculations

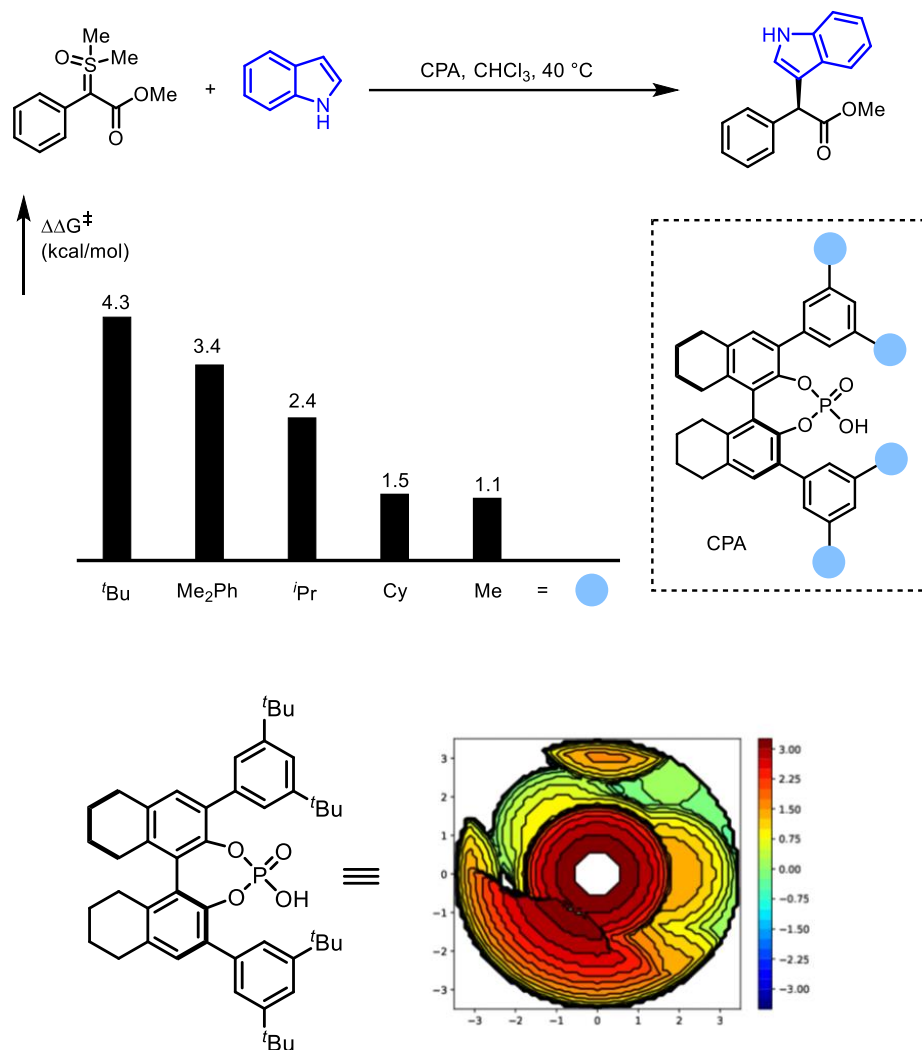
All DFT calculations were carried out with the Gaussian 16 package.<sup>8</sup> All molecular geometries were optimized with the B3LYP-D3(BJ) method and the 6-31G(d) basis set was used for all atoms involved.<sup>9</sup> Single point energies were calculated at B3LYP-D3(BJ)/6-311++G(d,p)/SMD(CHCl<sub>3</sub>) level of theory with the optimized structure.<sup>10</sup> The reported free energies and electronic energies were obtained from the above-mentioned single-point calculations combined with the liquid-phase free-energy and ZPE corrections, respectively. Frequency analysis was then performed on the optimized structure. Intrinsic reaction coordinate (IRC) calculation was carried out on the transition state geometries to verify that they are connected to the expected minima.<sup>11</sup> The conformational search was employed with CREST.<sup>12</sup> All energies discussed are Gibbs free relative energies at 313 K and 1 atm in kcal mol<sup>-1</sup>. 3D structures shown in figures were generated by CYLview<sup>13</sup> and VMD.<sup>14</sup> The buried value calculations were performed by Cavallo's SambVca 2.0.<sup>15</sup> The NCI analysis was calculated by Multiwfn.<sup>16</sup>

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**Fig. S1.** NCI plots of interactions for enantioselective transition states. Isosurfaces are color-coded red (indicating strong repulsion), blue (strong attractive interactions), and green (corresponding to weak interactions).

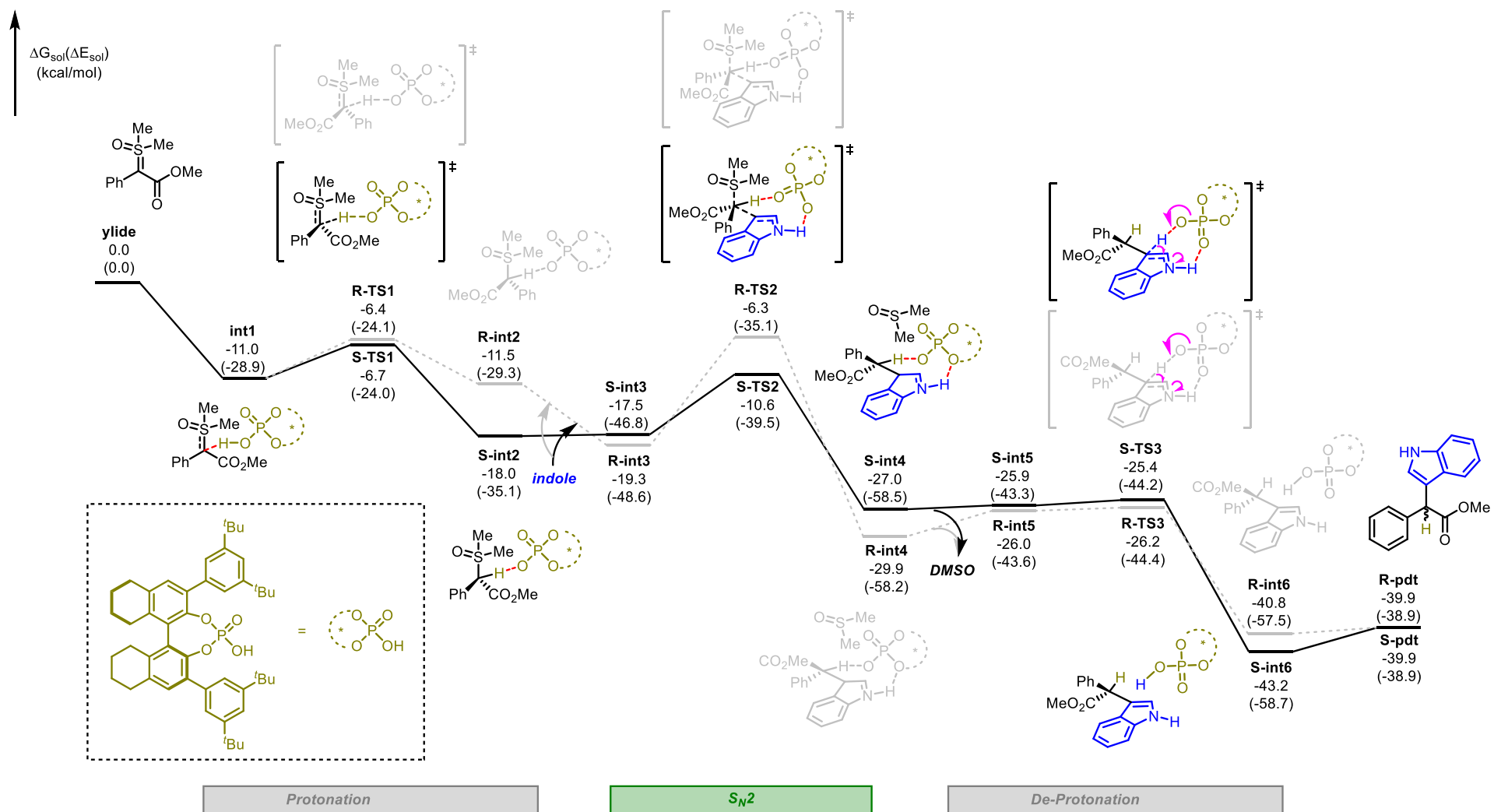
**Table S3 Enantioselectivities for the S<sub>N</sub>2 Step of *H*<sub>8</sub>-BINOL-Derived Phosphoric Acid Catalyst with Various Substituents.**



**Fig. S2.** Buried volume for *H*<sub>8</sub>-BINOL-derived phosphoric acid catalyst

The corresponding buried volume calculations were performed by Cavallo's SambVca 2.0 web tool (<https://www.molnac.unisa.it/OMtools/sambvca2.0/>). The parameter settings are shown as following: cartesian coordinate was generated from Gaussian .log output file and exported as .xyz file; atom coordinated to center of sphere: P; atom for z-axis definition: P=O; atom for x-z plane definition: The plane of P-OH; atom to be deleted: NA; bond radii scaled by 1.17; sphere radius set: 3.5 Å; distance of the coordination point from the center of the sphere: 0.0 Å; mesh spacing for numerical integration: 0.10; no H atom was included in calculation.





**Fig. S3.** Complete energy profile in the level of B3LYP-D3(BJ)/6-311++G(d,p)/SMD(CHCl<sub>3</sub>)/313K//B3LYP-D3(BJ)/6-31G(d) theory.

## Energies

**Table S4 Absolute Electronic Energies, Thermal Corrections to Energies and Free Energies at 313 K (in Hartree) of all Stationary Points. Geometries were Optimized in the Level of B3LYP-D3(BJ)/6-31G(d). Free Energies were Obtained from the Single Point SMD Calculation in Trichloromethane by SMD Model at the Level of B3LYP-D3(BJ)/6-311++G(d,p)/313K Combined with the Gas-Phase Free-Energy Correction Mentioned Above.**

	<b>E+ZPE</b>	<b>E</b>	<b>G</b>
<b>Indole</b>	-363.8289359	-363.8226049	-363.8592799
<b>Ylide</b>	-1051.424449	-1051.408513	-1051.468599
<b>DMSO</b>	-553.2127203	-553.2070723	-553.2410583
<b>S-cat</b>	-2508.173561	-2508.120995	-2508.260801
<b>Int1</b>	-3559.644227	-3559.575602	-3559.746894
<b>S-int2</b>	-3559.654319	-3559.585364	-3559.758161
<b>R-int2</b>	-3559.645147	-3559.5762	-3559.747723
<b>S-int3</b>	-3923.503685	-3923.426763	-3923.616522
<b>R-int3</b>	-3923.506288	-3923.429515	-3923.619462
<b>S-int4</b>	-3923.520036	-3923.443418	-3923.631765
<b>R-int4</b>	-3923.521758	-3923.444815	-3923.636389
<b>S-int5</b>	-3370.283715	-3370.214121	-3370.388912
<b>R-int5</b>	-3370.284217	-3370.214528	-3370.389075
<b>S-int6</b>	-3370.30893	-3370.238664	-3370.416419
<b>R-int6</b>	-3370.306984	-3370.236743	-3370.412693
<b>S-TS1</b>	-3559.636521	-3559.567828	-3559.740061
<b>R-TS1</b>	-3559.636746	-3559.567944	-3559.739678
<b>S-TS2</b>	-3923.49211	-3923.415125	-3923.605495
<b>R-TS2</b>	-3923.484959	-3923.408038	-3923.598777
<b>S-TS3</b>	-3370.284342	-3370.215405	-3370.388026
<b>R-TS3</b>	-3370.285067	-3370.215724	-3370.389339
<b>S-pdt</b>	-862.1030573	-862.0860803	-862.1504793
<b>R-pdt</b>	-862.1030582	-862.0860812	-862.1504812
<b>S-Me-cat</b>	-2036.553807	-2036.515795	-2036.627842
<b>Me-R-TS2</b>	-3451.859698	-3451.797434	-3451.960633

<b>Me-S-TS2</b>	-3451.859648	-3451.797244	-3451.962402
<b>S-Cy-cat</b>	-2817.840589	-2817.7861	-2817.934818
<b>Cy-R-TS2</b>	-4233.156407	-4233.077734	-4233.275349
<b>Cy-S-TS2</b>	-4233.158849	-4233.080043	-4233.277773
<b>S-<i>i</i>Pr-cat</b>	-2350.968783	-2350.920787	-2351.053626
<b><i>i</i>Pr-R-TS2</b>	-3766.280741	-3766.208739	-3766.390505
<b><i>i</i>Pr-S-TS2</b>	-3766.283134	-3766.210967	-3766.394256
<b>S-Me<sub>2</sub>Ph-cat</b>	-3275.190977	-3275.125785	-3275.299016
<b>Me<sub>2</sub>Ph-R-TS2</b>	-4690.503501	-4690.413989	-4690.63596
<b>Me<sub>2</sub>Ph-S-TS2</b>	-4690.512827	-4690.42373	-4690.641353

**Table S5 Relative Electronic Energies, Thermal Corrections to Energies and Free Energies at 313 K (in kcal/mol) of all Stationary Points. Geometries were Optimized in the Level of B3LYP-D3(BJ)/6-31G(d). Free Energies were Obtained from the Single Point SMD Calculation in Trichloromethane by SMD Model at the Level of B3LYP-D3(BJ)/6-311++G(d,p)/313K Combined with the Gas-Phase Free-Energy Correction Mentioned Above.**

	<b>E+ZPE</b>	<b>E</b>	<b>G</b>
<b>Int1</b>	-29.0	-28.9	-11.0
<b>S-int2</b>	-35.3	-35.1	-18.0
<b>R-int2</b>	-29.6	-29.3	-11.5
<b>S-int3</b>	-48.2	-46.8	-17.5
<b>R-int3</b>	-49.8	-48.6	-19.3
<b>S-int4</b>	-58.4	-57.3	-27.0
<b>R-int4</b>	-59.5	-58.2	-29.9
<b>S-int5</b>	-43.6	-43.3	-25.9
<b>R-int5</b>	-43.9	-43.6	-26.0
<b>S-int6</b>	-59.4	-58.7	-43.2
<b>R-int6</b>	-58.2	-57.5	-40.8
<b>S-TS1</b>	-24.2	-24.0	-6.7
<b>R-TS1</b>	-24.3	-24.1	-6.4
<b>S-TS2</b>	-40.9	-39.5	-10.6
<b>R-TS2</b>	-36.4	-35.1	-6.3

<b>S-TS3</b>	-44.0	-44.2	-25.4
<b>R-TS3</b>	-44.5	-44.4	-26.2
<b>S-pdt</b>	-39.2	-38.9	-39.9
<b>R-pdt</b>	-39.2	-38.9	-39.9
<b>Me-R-TS2</b>	-32.9	-31.7	-3.1
<b>Me-S-TS2</b>	-32.9	-31.6	-4.2
<b>Cy-R-TS2</b>	-39.2	-38.0	-7.9
<b>Cy-S-TS2</b>	-40.7	-39.4	-9.5
<b><i>i</i>Pr-R-TS2</b>	-36.8	-35.7	-5.6
<b><i>i</i>Pr-S-TS2</b>	-38.3	-37.1	-8.0
<b>Me<sub>2</sub>Ph-R-TS2</b>	-37.1	-35.8	-5.7
<b>Me<sub>2</sub>Ph-S-TS2</b>	-43.0	-41.9	-9.1

### Cartesian Coordinates (Å)

#### Indole

C	0.24946700	0.75180000	-0.00008300
C	0.24701800	-0.67250300	-0.00011900
C	-0.93513900	-1.41857700	-0.00010800
C	-2.13542700	-0.71813300	0.00003800
C	-2.15843500	0.69167800	0.00026200
C	-0.98186700	1.42875800	-0.00019800
C	1.62556900	1.16682500	-0.00011400
C	2.39082200	0.03041300	0.00019800
H	-0.91734600	-2.50519000	-0.00068000
H	-3.07272500	-1.26711400	-0.00036700
H	-3.11518100	1.20612900	0.00071500
H	-1.00947600	2.51512800	0.00018700
H	1.99624100	2.18230700	-0.00026200
H	3.46528900	-0.08716800	-0.00014400
N	1.56599700	-1.08101300	0.00003400
H	1.87916600	-2.03855800	0.00106500

**Ylide**

C	1.19894600	1.32103100	0.11606500
C	0.41935300	0.12005700	-0.05348300
O	2.42064800	1.39961500	0.24435000
S	1.25584000	-1.34544300	0.04586500
O	1.51088000	-2.03692200	1.34119300
C	0.33602000	-2.48702500	-1.01871800
H	0.27528000	-2.07699600	-2.02772800
H	0.87168400	-3.43779700	-0.99570500
H	-0.66097000	-2.60142300	-0.59503100
C	2.83054300	-1.20302600	-0.83466800
H	3.25666200	-2.20826000	-0.85445300
H	2.65072900	-0.81407000	-1.83770100
H	3.44120100	-0.50694900	-0.26474500
C	-1.06067700	0.05017000	-0.00194000
C	-1.83764300	0.75655900	-0.93635500
C	-1.72637900	-0.73792800	0.95398500
C	-3.22736500	0.67791500	-0.91396200
H	-1.33614400	1.37512400	-1.67292800
C	-3.11807300	-0.84304600	0.95326800
H	-1.14243800	-1.26080700	1.70662700
C	-3.87501100	-0.13193600	0.02276400
H	-3.80852500	1.23909600	-1.64095700
H	-3.60965600	-1.46398700	1.69738700
H	-4.95911600	-0.20124700	0.02996100
O	0.41317000	2.43459900	0.09976500
C	1.11596000	3.66922000	0.26601800
H	0.34818900	4.44405400	0.24515800
H	1.65194100	3.68741300	1.21892700
H	1.83609500	3.82266500	-0.54297100

**DMSO**

S	-0.25814200	0.43272000	0.00000000
O	1.09424300	1.10685400	0.00000000
C	-0.25814200	-0.80146400	1.35869600
H	-1.17707400	-1.39438000	1.32367900
H	0.62445200	-1.44112900	1.26650700
H	-0.21036000	-0.24488400	2.29741700
C	-0.25814200	-0.80146400	-1.35869600
H	0.62445200	-1.44112900	-1.26650700
H	-1.17707400	-1.39438000	-1.32367900
H	-0.21036000	-0.24488400	-2.29741700

**S-cat**

C	-1.94425200	-1.05459700	1.49681400
C	-2.75492500	0.09366100	1.48251200
H	-0.60587000	-2.30695600	0.37956500
C	-1.24540700	-1.42909200	0.35531600
C	-2.86644900	0.85634200	0.30386800
C	-2.22990100	0.37551800	-0.85804800
C	-1.38502200	-0.74105400	-0.85778700
C	-3.63031100	2.14029100	0.25075200
C	-3.32734100	3.25408900	1.05874500
C	-4.63660200	2.29055200	-0.71134700
C	-2.18683800	3.31528600	2.04561000
C	-4.06175200	4.44545000	0.90519100
C	-5.34811700	3.47725500	-0.92166500
C	-2.61204000	3.91785600	3.40579500
H	-1.41079000	3.96209100	1.61040600
C	-3.70419100	5.59864000	1.80917100
C	-5.05768800	4.54319900	-0.06150100

C	-3.58734000	5.11548500	3.26581300
H	-3.08514100	3.13933000	4.01189100
H	-2.74300600	6.03237100	1.49406500
H	-5.60524900	5.47489000	-0.17535900
H	-4.58679600	4.81722600	3.60208400
H	-4.44909400	6.39728500	1.72561300
H	-3.27423700	5.94468800	3.90947100
H	-1.70684100	4.22020100	3.94403100
H	-1.71856800	2.34032800	2.18653800
C	-3.54225200	0.36217700	2.74383500
H	-4.04776400	1.32883500	2.70640800
H	-4.34240400	-0.39146900	2.78709500
C	-2.69700700	0.23889500	4.03604700
H	-3.38000600	0.04311700	4.87025500
H	-2.21702300	1.19798100	4.25216700
C	-1.61177900	-0.86321400	3.95825000
H	-1.55956800	-1.41721400	4.90194600
H	-0.62860500	-0.40173000	3.80950600
C	-1.85700300	-1.82995300	2.78710300
H	-2.79493200	-2.37956900	2.95933200
H	-1.06104300	-2.58017900	2.72982800
C	-0.61571300	-1.19138700	-2.04694600
C	-1.22779800	-1.41605000	-3.28288700
C	0.75601800	-1.43577100	-1.91115300
C	-0.49141200	-1.86734900	-4.38228300
H	-2.29109300	-1.24883400	-3.38445800
C	1.52413500	-1.89247600	-2.98674000
H	1.22404100	-1.24486100	-0.95013000
C	0.87949000	-2.09939400	-4.21278000
H	1.45869900	-2.44938200	-5.05531300

C	-6.23891000	3.64234800	-2.09630500
C	-6.12333400	4.80711800	-2.87610800
C	-7.11000000	2.63350500	-2.51362700
C	-6.84827000	4.96282500	-4.05720900
H	-5.42007600	5.56713100	-2.55975600
C	-7.83478000	2.74166300	-3.70879200
H	-7.19708100	1.73819200	-1.91261900
C	-7.69021800	3.91066300	-4.45866500
H	-8.23685100	4.01195000	-5.38783900
C	-8.70267200	1.56027100	-4.16210600
C	-7.78614200	0.33671500	-4.39032600
H	-7.22966100	0.06326900	-3.48939200
H	-8.38044200	-0.53145200	-4.69931800
H	-7.04954600	0.54043200	-5.17537700
C	-9.45571600	1.85498100	-5.46931300
H	-10.06454500	0.98765900	-5.74597800
H	-10.12740400	2.71493100	-5.36665000
H	-8.76792900	2.05221800	-6.29901400
C	-9.74238900	1.23124800	-3.06964500
H	-9.26608500	0.96353100	-2.12160100
H	-10.40064400	2.08791200	-2.88615500
H	-10.36283400	0.38306800	-3.38162500
C	-6.73051800	6.21295500	-4.94039100
C	-6.19230100	5.80656400	-6.32960200
H	-6.85190800	5.08797300	-6.82622800
H	-6.10575500	6.68633700	-6.97809200
H	-5.20034300	5.34870300	-6.24318400
C	-5.77828300	7.26214400	-4.34363800
H	-6.11486600	7.59913600	-3.35698000
H	-4.75784100	6.87607800	-4.24519700



H	-5.73885600	8.13861200	-4.99932400
C	-8.12405700	6.85918000	-5.09734400
H	-8.06019700	7.75212000	-5.73032000
H	-8.84088600	6.17255000	-5.55841400
H	-8.52554500	7.15809800	-4.12281400
C	3.02724100	-2.13992000	-2.79066500
C	3.71132300	-2.64681400	-4.07086300
H	3.62908800	-1.92237000	-4.88844900
H	4.77727500	-2.81143300	-3.87843900
H	3.28371500	-3.59654700	-4.41044800
C	3.71125500	-0.82140500	-2.36897500
H	3.58018200	-0.05340600	-3.13917400
H	3.29572500	-0.43115900	-1.43455800
H	4.78651800	-0.97833900	-2.21972400
C	3.23045800	-3.19884400	-1.68533900
H	2.80153800	-2.87488000	-0.73172700
H	2.75353400	-4.14544100	-1.96274300
H	4.29926600	-3.38673800	-1.52628100
C	-1.20647500	-2.06930300	-5.72600400
C	-2.41439800	-3.01275600	-5.53709600
H	-2.09413000	-3.98461400	-5.14431200
H	-3.15211500	-2.58911500	-4.85007500
H	-2.91388600	-3.18077500	-6.49896000
C	-1.71433400	-0.69934300	-6.22946900
H	-0.88244700	0.00449300	-6.34712400
H	-2.20727300	-0.81272400	-7.20318700
H	-2.43792800	-0.26662300	-5.53333800
C	-0.28163800	-2.67282500	-6.79528300
H	0.56631800	-2.01589500	-7.01944800
H	0.11236700	-3.64828400	-6.48752700

H	-0.84125100	-2.81734200	-7.72591300
O	-2.39639300	1.08138100	-2.06345000
O	-4.87591500	1.20734700	-1.56777300
P	-3.83613700	1.02548400	-2.79858700
O	-4.19889500	-0.15037000	-3.61399400
O	-3.73362900	2.43795600	-3.55686200
H	-4.55930600	2.64491500	-4.02943400

### **Int1**

C	2.03403500	2.47302300	2.91051300
C	0.74707500	2.64661500	2.37439800
H	3.74076400	1.17542000	3.04043000
C	2.75682400	1.31979900	2.60152200
C	0.25400100	1.70640300	1.43792000
C	0.98160900	0.52940200	1.21879200
C	2.23602600	0.30134300	1.80111400
C	-1.02531500	1.95767700	0.71010900
C	-1.21186900	3.12766200	-0.06703800
C	-2.05807500	1.02072900	0.78041800
C	-0.03446000	4.03106900	-0.38969000
C	-2.48852700	3.39397200	-0.58715000
C	-3.32645100	1.23276400	0.21691900
C	-0.31157800	4.95293900	-1.57820000
H	0.84276600	3.41139300	-0.58758100
C	-2.78167500	4.63918200	-1.40638700
C	-3.51979700	2.46656700	-0.40909700
C	-1.64882900	5.66698200	-1.38417700
H	0.51259100	5.66591700	-1.68326000
H	-2.96333900	4.33794500	-2.44963900
H	-4.50117700	2.69044100	-0.81947900

H	-1.64138800	6.19455700	-0.41990100
H	-3.72187400	5.08620000	-1.05903700
H	-1.81734400	6.42342600	-2.15952000
H	-0.33625800	4.35908300	-2.50098200
H	0.22581700	4.65386100	0.47545800
C	-0.14527900	3.75307000	2.91345300
H	-0.86688900	4.08573000	2.16824200
H	-0.74838800	3.31033000	3.72134400
C	0.63506300	4.93868100	3.48398800
H	-0.05929100	5.64578900	3.95253000
H	1.13982500	5.47765800	2.66928300
C	1.67464500	4.44653300	4.49243000
H	1.16289600	3.90391400	5.29901000
H	2.20269800	5.28678200	4.95812700
C	2.67842900	3.51965800	3.80276000
H	3.31946100	3.02674800	4.54318600
H	3.35083400	4.12976600	3.18012300
C	3.02237400	-0.93622200	1.56733500
C	2.47625400	-2.19433000	1.83029300
C	4.33293900	-0.84028000	1.07485400
C	3.21175100	-3.36477500	1.59545100
H	1.46087300	-2.25952200	2.19640000
C	5.09141600	-1.98311400	0.81963900
H	4.73825700	0.14142400	0.86612200
C	4.50972100	-3.23194400	1.09263400
H	5.09389900	-4.12356900	0.90066700
C	-4.37151500	0.18192300	0.18662700
C	-5.14421000	0.02321900	-0.97691200
C	-4.58373000	-0.68479000	1.25970300
C	-6.10596900	-0.97927000	-1.07766900

H	-4.95252400	0.68073000	-1.81570200
C	-5.52430600	-1.71995200	1.18674300
H	-3.99002700	-0.56402500	2.15526100
C	-6.27619700	-1.84258800	0.01758100
H	-7.00723200	-2.63797300	-0.05920700
C	-5.64591600	-2.69604500	2.36441700
C	-6.75900400	-3.73466100	2.15121900
H	-6.56927600	-4.35740200	1.27010200
H	-6.81281400	-4.40010500	3.01971000
H	-7.74002600	-3.26023300	2.03254000
C	-5.95775100	-1.91669000	3.65971900
H	-6.04156200	-2.60802200	4.50660900
H	-5.17260400	-1.19315100	3.89875700
H	-6.90347600	-1.37029100	3.56884600
C	-4.30224000	-3.44439100	2.52012100
H	-4.07576500	-4.02252100	1.61767700
H	-3.46394500	-2.76120300	2.68490000
H	-4.34883300	-4.13783100	3.36884400
C	-6.95228300	-1.18769100	-2.34131800
C	-6.68259600	-2.59795200	-2.90951700
H	-5.62403500	-2.71609400	-3.16556700
H	-6.94074100	-3.38046100	-2.18926700
H	-7.27744400	-2.76556900	-3.81561600
C	-6.62853300	-0.15968400	-3.43789300
H	-6.81525700	0.86570600	-3.09974400
H	-5.58431900	-0.22973900	-3.76244500
H	-7.26129700	-0.34205400	-4.31338600
C	-8.44797300	-1.05477100	-1.98226400
H	-9.07042500	-1.21057000	-2.87168900
H	-8.74964400	-1.78919800	-1.22895300

H	-8.66427600	-0.05771200	-1.58273100
C	6.51639000	-1.91575800	0.25341000
C	6.95218200	-0.47249700	-0.05019600
H	6.97142500	0.14347200	0.85622100
H	7.96561100	-0.47581100	-0.46659000
H	6.28799100	-0.00116600	-0.78097800
C	7.49507200	-2.52209800	1.28189300
H	7.46352400	-1.96426200	2.22452200
H	7.25313300	-3.56679300	1.50343700
H	8.52165900	-2.48792800	0.89776900
C	6.58728000	-2.72006500	-1.06332800
H	6.31082400	-3.76934600	-0.91511400
H	5.91769300	-2.28311700	-1.81007000
H	7.60819700	-2.69943500	-1.46328000
C	2.55425100	-4.73338800	1.82365100
C	1.77313100	-4.74333800	3.15501200
H	2.42616900	-4.48563800	3.99662800
H	0.93330300	-4.04429600	3.13677100
H	1.36301100	-5.74374400	3.33571000
C	1.56226900	-4.99270300	0.66642300
H	1.08237800	-5.97148800	0.78919400
H	0.77730000	-4.23144100	0.64743900
H	2.08319600	-4.99246000	-0.29918700
C	3.58765900	-5.87227200	1.85803100
H	4.34885500	-5.70325600	2.62838900
H	3.08403800	-6.81858000	2.08281100
H	4.09669200	-5.99657000	0.89576400
O	0.47667700	-0.42536100	0.32741300
O	-1.80197200	-0.18944900	1.42994300
P	-0.86269200	-1.29339300	0.70014700

O	-0.68359200	-2.45767600	1.59094200
O	-1.45180600	-1.57798300	-0.73764100
H	-0.90784200	-1.27444400	-1.53151800
C	0.48330700	0.30807200	-2.66925000
C	1.85255300	0.57184900	-2.49284900
O	-0.00551100	-0.84733800	-2.81916700
S	2.87768500	-0.79542200	-2.64693500
O	4.30532300	-0.46992400	-2.42467200
C	2.38144400	-2.19260000	-1.62289000
H	3.13459300	-2.96746600	-1.77402500
H	2.38428400	-1.84918300	-0.59154800
H	1.38411700	-2.50515400	-1.92356900
C	2.66882500	-1.47338000	-4.31391100
H	3.06229000	-0.71745400	-4.99566700
H	3.24171000	-2.40080100	-4.38802900
H	1.60237800	-1.64094200	-4.47219600
C	2.47781000	1.88948400	-2.24537200
C	3.21587600	2.12623300	-1.07612900
C	2.30631600	2.94443300	-3.15418200
C	3.76218000	3.38061400	-0.81686500
H	3.33693700	1.32461700	-0.36119600
C	2.83987500	4.20434700	-2.88904900
H	1.73420000	2.77239100	-4.06020600
C	3.57120900	4.42721300	-1.72056700
H	4.31960500	3.54210100	0.10169600
H	2.68651100	5.01335300	-3.59792400
H	3.98727900	5.40987500	-1.51650100
O	-0.31458800	1.39769000	-2.68777900
C	-1.69625700	1.14737600	-2.99281700
H	-2.14772400	2.13289400	-3.08793200

H	-1.78616000	0.58598600	-3.92606800
H	-2.18135400	0.59640100	-2.18654100

**R-int2**

C	-1.64285700	-0.56147700	1.95509600
C	-2.49152400	0.53599200	1.72721200
H	-0.27930000	-1.97745300	1.07814700
C	-0.94875200	-1.14057300	0.89559000
C	-2.64176900	1.05386100	0.42690200
C	-2.03070200	0.35667500	-0.63304700
C	-1.15053500	-0.71222700	-0.42054600
C	-3.36982500	2.32331000	0.13369400
C	-3.00296500	3.54053200	0.75880900
C	-4.36244400	2.32763700	-0.85943200
C	-1.81360100	3.60895700	1.70053200
C	-3.72719900	4.70545900	0.45156900
C	-5.01020100	3.50949900	-1.26993800
C	-1.28527500	5.03301900	1.89096300
H	-1.02287100	2.94572500	1.33380800
C	-3.43442400	6.04411400	1.11015600
C	-4.70724100	4.66463200	-0.54113200
C	-2.44086500	5.95893200	2.27106000
H	-0.50609200	5.03639100	2.66202000
H	-3.02954000	6.73240200	0.35196600
H	-5.24372100	5.58087800	-0.77403900
H	-2.94055200	5.55580600	3.16263400
H	-4.37687900	6.49669300	1.44380900
H	-2.08349500	6.96175900	2.53250200
H	-0.81547400	5.39251700	0.96352600
H	-2.09041600	3.22306400	2.68831100

C	-3.29785500	0.99788100	2.91692400
H	-2.64636300	1.46814300	3.66794200
H	-4.03998200	1.74442100	2.62308400
C	-3.98914000	-0.22216000	3.56250500
H	-4.72420900	-0.60675800	2.84776000
H	-4.54854900	0.10345300	4.44675700
C	-2.98252300	-1.34340500	3.93676900
H	-3.34402600	-2.30215500	3.55043200
H	-2.91154600	-1.45037700	5.02526000
C	-1.56762200	-1.08099400	3.36766200
H	-0.96131400	-1.99174400	3.41647000
H	-1.06541800	-0.33777100	4.00459200
C	-0.42649600	-1.33949600	-1.55998900
C	-1.12118000	-1.98406600	-2.58327500
C	0.97252900	-1.23936700	-1.62632000
C	-0.44569500	-2.51677300	-3.69125100
H	-2.20186800	-2.04068900	-2.51877000
C	1.67838700	-1.75778000	-2.71386000
H	1.48818300	-0.72960200	-0.82059900
C	0.94573200	-2.38740600	-3.73644500
H	1.48493600	-2.79027700	-4.58554600
C	-5.86004500	3.58403300	-2.48534200
C	-5.84166200	4.75600100	-3.24911100
C	-6.61054000	2.49499800	-2.95587900
C	-6.53167600	4.86270700	-4.46142600
H	-5.24488300	5.59284200	-2.90740000
C	-7.24883900	2.53655000	-4.19198800
H	-6.64688100	1.59843100	-2.36115800
C	-7.20659600	3.73243700	-4.92764700
H	-7.70223900	3.76977700	-5.89003700



C	-7.90905200	1.28791100	-4.79307600
C	-7.95383000	0.11222600	-3.80088900
H	-8.45843300	-0.74012200	-4.26959100
H	-6.95239700	-0.21933400	-3.50767300
H	-8.51151300	0.37144500	-2.89378100
C	-7.06593100	0.84641000	-6.01087600
H	-7.49580900	-0.05142200	-6.47162700
H	-7.02891500	1.63134000	-6.77525900
H	-6.04212400	0.61725100	-5.69724300
C	-9.35072300	1.60301300	-5.24084300
H	-9.96210600	1.92025300	-4.38844100
H	-9.38420100	2.39939300	-5.99168100
H	-9.81510600	0.71256600	-5.68100900
C	-6.53308300	6.20499900	-5.20729500
C	-5.09042900	6.72274600	-5.38438000
H	-4.48353100	6.00348500	-5.93660200
H	-5.09415400	7.66992200	-5.93780700
H	-4.59961100	6.90456500	-4.42323400
C	-7.33929600	7.22491600	-4.37330600
H	-8.37265300	6.88674800	-4.23879500
H	-6.90019600	7.35795900	-3.37880500
H	-7.35892500	8.20266700	-4.87096900
C	-7.17764900	6.09976300	-6.59909300
H	-8.22888100	5.79863400	-6.53776000
H	-7.14184300	7.07478100	-7.09809000
H	-6.64863300	5.37926100	-7.23090000
C	3.20507300	-1.64607800	-2.84037400
C	3.84274000	-0.94420900	-1.63044500
H	3.64407900	-1.48586100	-0.69960200
H	4.92922100	-0.89302700	-1.76187900

H	3.47284600	0.08059300	-1.51367400
C	3.81652800	-3.05900800	-2.95595600
H	3.57891400	-3.65534600	-2.06849400
H	3.43535000	-3.59555300	-3.83018700
H	4.90780200	-2.99855900	-3.04701100
C	3.55596900	-0.83356500	-4.10649800
H	3.14600900	-1.29590800	-5.01024100
H	3.15677500	0.18590500	-4.03433000
H	4.64318100	-0.76048400	-4.22955100
C	-1.25543400	-3.21482400	-4.79200900
C	-0.36983000	-3.68689800	-5.95601000
H	0.38285900	-4.41542700	-5.63215400
H	-0.99200100	-4.16970300	-6.71713300
H	0.14665000	-2.84731900	-6.43622100
C	-1.96149300	-4.44483400	-4.18059300
H	-2.64515500	-4.15059400	-3.37899500
H	-2.54716900	-4.96450500	-4.94837500
H	-1.23260900	-5.15198000	-3.76734100
C	-2.32103200	-2.24378800	-5.34754900
H	-3.02029500	-1.91575600	-4.57407900
H	-1.85561800	-1.35415300	-5.78361700
H	-2.89939800	-2.74222800	-6.13549300
O	-2.27866200	0.76787500	-1.93171600
O	-4.71452000	1.11871800	-1.41757500
P	-3.79391100	0.40311300	-2.59666800
O	-4.11410700	-1.04877900	-2.56312800
O	-3.78798200	1.20269700	-3.87503200
H	-2.68695300	2.42612200	-4.22853300
C	-1.39114200	4.09383700	-3.78543600
C	-1.97924700	3.11230000	-4.77057100

O	-0.22475500	4.12321500	-3.42764400
S	-0.70079200	1.90539800	-5.34343200
O	-1.25833300	0.97838400	-6.34289000
C	0.66795100	2.83529400	-6.05644200
H	0.27276300	3.34233900	-6.93810400
H	1.03771400	3.53915900	-5.31110600
H	1.42385800	2.10086400	-6.34315600
C	-0.01836700	1.08074600	-3.91388300
H	0.57528000	0.24200800	-4.28367300
H	0.57074000	1.80609800	-3.35359500
H	-0.85837600	0.72270900	-3.31130300
C	-2.66875500	3.67494800	-5.98140100
C	-2.12009900	4.74301200	-6.70582100
C	-3.85006600	3.06382600	-6.41574800
C	-2.74077400	5.18653700	-7.87103900
H	-1.22165200	5.24076100	-6.34746900
C	-4.46798400	3.51594400	-7.58085600
H	-4.26919400	2.25243300	-5.83144600
C	-3.91234900	4.56566000	-8.31307300
H	-2.31974100	6.01904300	-8.42675000
H	-5.38599700	3.04235100	-7.91360800
H	-4.39774200	4.91223300	-9.22077700
O	-2.34264200	4.90312600	-3.33886800
C	-1.94697800	5.84009200	-2.31532500
H	-1.12637100	6.46466400	-2.67475500
H	-2.83752700	6.43178300	-2.11619100
H	-1.64645400	5.29701400	-1.41853500

### S-int2

C	0.78894900	-2.68086100	3.68169900
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C	-0.12588700	-1.62381500	3.54016900
H	2.34100100	-3.83186700	2.73344900
C	1.62613900	-3.02130400	2.61142400
C	-0.15772700	-0.89583000	2.32565800
C	0.59831500	-1.35958000	1.24369800
C	1.52531200	-2.40445400	1.36574000
C	-0.97003000	0.35044000	2.17360500
C	-0.77969200	1.46645400	3.01571400
C	-1.93673100	0.43222000	1.15057400
C	0.35434800	1.60973800	4.00688200
C	-1.61140100	2.59129700	2.87360300
C	-2.82311900	1.51934200	1.04151200
C	-0.06298500	2.23360600	5.36388900
H	1.09199500	2.27237300	3.53772800
C	-1.37356600	3.75985100	3.79814500
C	-2.63738500	2.58528700	1.93368400
C	-1.22393000	3.24666000	5.24023200
H	-0.34753400	1.44442200	6.06812100
H	-0.45699000	4.29737700	3.50904900
H	-3.29748200	3.44554000	1.85791400
H	-2.16730100	2.76381500	5.52091400
H	-2.19685800	4.47892400	3.72410600
H	-1.07780200	4.08359700	5.93225800
H	0.81920200	2.72175000	5.79386700
H	0.86676000	0.66042700	4.16883400
C	-1.11394700	-1.29782000	4.64727100
H	-0.79266500	-0.40272000	5.19122700
H	-2.07947100	-1.03984500	4.19877800
C	-1.27296100	-2.43611600	5.65860800
H	-1.80674000	-3.27746900	5.19608200

H	-1.88354900	-2.09452700	6.50249100
C	0.10436600	-2.90607300	6.12856900
H	0.02068500	-3.64044100	6.93795700
H	0.65942600	-2.04713000	6.53226700
C	0.86711200	-3.51372200	4.94942900
H	0.45435100	-4.51098800	4.73731300
H	1.92016300	-3.67710900	5.21286700
C	2.39790700	-2.78706800	0.22561800
C	1.85085300	-3.21138500	-0.98955500
C	3.78560500	-2.69619900	0.35875400
C	2.67478600	-3.56489400	-2.06398100
H	0.77293900	-3.24784300	-1.09268900
C	4.63909100	-2.99800500	-0.70676800
H	4.19328000	-2.35171400	1.30388100
C	4.06246100	-3.44939800	-1.90024300
H	4.70964700	-3.70481200	-2.72740700
C	-3.96225000	1.55634200	0.08604300
C	-3.81870700	1.22348900	-1.26979100
C	-5.21689800	1.95469400	0.55587000
C	-4.90702900	1.26721300	-2.13868400
H	-2.84343100	0.94206100	-1.63449400
C	-6.33063800	2.02569800	-0.29256600
H	-5.32607600	2.18709200	1.61073900
C	-6.15188600	1.67539400	-1.63165600
H	-6.99911700	1.71107800	-2.30549100
C	-7.68704600	2.46440400	0.27794300
C	-7.55497000	3.88203100	0.87557500
H	-7.25188000	4.60070100	0.10587700
H	-8.51311700	4.21238400	1.29475900
H	-6.80962500	3.91492000	1.67665100

C	-8.11805400	1.47910900	1.38585200
H	-9.08489400	1.77772600	1.80911100
H	-8.21732600	0.46470500	0.98449000
H	-7.38989800	1.44482000	2.20228300
C	-8.79052000	2.49648300	-0.79198400
H	-8.55065900	3.19591100	-1.60051700
H	-8.95628400	1.50731500	-1.23247400
H	-9.73397600	2.82112900	-0.33938600
C	-4.78067400	0.87623600	-3.61797900
C	-5.74012900	-0.29664000	-3.91564500
H	-5.66475300	-0.59187800	-4.96919900
H	-5.48854400	-1.16522500	-3.29799600
H	-6.78344200	-0.03098300	-3.71576100
C	-3.35501000	0.43048100	-3.98495200
H	-2.62261800	1.22612100	-3.81425000
H	-3.03178000	-0.44114900	-3.40787300
H	-3.31937700	0.16300600	-5.04731900
C	-5.15791500	2.08496000	-4.50108200
H	-5.08335500	1.82137000	-5.56310400
H	-6.18147200	2.42454500	-4.31074800
H	-4.48496200	2.92909000	-4.31066200
C	6.15159600	-2.79548200	-0.54039800
C	6.92873000	-3.09221400	-1.83326400
H	6.60936700	-2.43763800	-2.65153100
H	7.99856100	-2.92292600	-1.66812200
H	6.80312600	-4.13174800	-2.15494600
C	6.42595200	-1.32623800	-0.14782100
H	7.50420200	-1.15563600	-0.03992600
H	6.04056600	-0.63990600	-0.90759600
H	5.95088000	-1.06787400	0.80360900

C	6.67592100	-3.73094100	0.56941100
H	6.17726000	-3.53867000	1.52506500
H	6.50121300	-4.78028400	0.30722000
H	7.75356100	-3.58863600	0.71671200
C	2.03353900	-4.03929400	-3.37737400
C	1.07368500	-5.21289900	-3.08330000
H	1.60526800	-6.04318200	-2.60430300
H	0.25489700	-4.90439400	-2.42778300
H	0.63210300	-5.58136100	-4.01697500
C	1.22300800	-2.88126400	-4.00224800
H	1.87664200	-2.03779800	-4.25628300
H	0.74291000	-3.21757600	-4.92973400
H	0.44093900	-2.52600500	-3.32513100
C	3.07885400	-4.51631000	-4.39887700
H	3.75566000	-3.70878100	-4.70313900
H	3.68664200	-5.33968300	-4.00642200
H	2.57268200	-4.87398900	-5.30203000
O	0.50488900	-0.70236700	0.03770900
O	-2.03620200	-0.61722400	0.25773100
P	-0.87430900	-0.77043700	-0.91913900
O	-1.06956500	-2.09132300	-1.57082300
O	-0.72126500	0.52038100	-1.69797900
H	1.34527000	0.81787500	-0.89512900
C	2.50829500	1.65738000	0.65638400
C	2.15415200	1.55540200	-0.82107300
O	2.11799100	2.53838500	1.39581000
S	1.31785800	3.10405200	-1.35308500
O	2.15296500	4.32223800	-1.30110000
C	0.79801200	2.69855900	-3.02314600
H	0.17579500	1.79773400	-2.95167900

H	0.24181900	3.56301500	-3.39223600
H	1.70398800	2.53747500	-3.60883500
C	-0.21667800	3.21422400	-0.42780700
H	-0.74715700	4.08825500	-0.81205300
H	-0.75433700	2.28099800	-0.63012300
H	0.04240300	3.32494000	0.62326600
C	3.27846800	1.20010200	-1.75395700
C	3.20157000	-0.00713300	-2.45485500
C	4.39062000	2.03904700	-1.91059000
C	4.23069200	-0.36793400	-3.32308300
H	2.35767200	-0.67022700	-2.29927700
C	5.41213100	1.67412900	-2.78489000
H	4.44741400	2.97331800	-1.36069300
C	5.33079400	0.47282000	-3.49444400
H	4.17198300	-1.31176600	-3.85288700
H	6.27247400	2.32479700	-2.90940500
H	6.13054800	0.18902900	-4.17244100
O	3.25442200	0.61639800	1.00224200
C	3.52962000	0.44008400	2.40824800
H	3.68402100	1.40656100	2.88907400
H	2.68991900	-0.08747400	2.86340600
H	4.42977400	-0.17072500	2.45099600

### **R-int3**

C	-0.50054700	-3.48822800	3.77567000
C	-1.35308600	-2.40062100	3.51729200
H	1.33937000	-4.45756800	3.31245700
C	0.68602900	-3.62562500	3.06921900
C	-0.97510300	-1.43348300	2.57318900
C	0.20212200	-1.63993200	1.82383900



C	1.05949500	-2.73734900	2.04367100
C	-1.81550100	-0.23026400	2.29957000
C	-2.12383900	0.72691900	3.29388200
C	-2.28753700	-0.02926500	0.99857300
C	-1.51657300	0.61150200	4.68084200
C	-2.95430400	1.81330300	2.96468800
C	-3.14034700	1.02366000	0.65869400
C	-1.51730300	1.93754700	5.44597600
H	-0.50021600	0.21180000	4.59954100
C	-3.28490500	2.90737800	3.96578400
C	-3.46429900	1.92997100	1.66645600
C	-2.91590800	2.55460500	5.40841300
H	-1.18871700	1.76687200	6.47785500
H	-2.74146400	3.81864000	3.67479000
H	-4.12101600	2.76297900	1.42621300
H	-3.63833900	1.83215700	5.81392300
H	-4.35049000	3.15903800	3.89176000
H	-2.97336300	3.45015400	6.03797500
H	-0.79856100	2.63274200	4.99087400
H	-2.08017700	-0.12212600	5.27199800
C	-2.69410700	-2.43655600	4.20799100
H	-2.57888300	-2.25313700	5.28611500
H	-3.35610900	-1.65772400	3.82206400
C	-3.32600800	-3.83009700	4.00347600
H	-3.53110700	-3.94890100	2.93355300
H	-4.29256000	-3.87343100	4.51788200
C	-2.40039000	-4.97965200	4.48441800
H	-2.34820900	-5.75297100	3.70999100
H	-2.81494800	-5.45959900	5.37808900
C	-0.96633100	-4.49031800	4.80015200

H	-0.27678900	-5.33924100	4.85927300
H	-0.96748400	-4.02075400	5.79436500
C	2.25092600	-3.03218900	1.20132300
C	2.68573700	-4.36316900	1.06144500
C	2.93495600	-2.03834600	0.48692200
C	3.73330100	-4.71463200	0.20818600
H	2.15706000	-5.14183300	1.59465700
C	3.98113400	-2.35079500	-0.38516600
H	2.62372800	-1.01443400	0.60311400
C	4.36287500	-3.69091000	-0.51204400
H	5.17322400	-3.94632300	-1.18659000
C	-3.65698400	1.16054700	-0.72855600
C	-3.26916100	2.24661700	-1.51696400
C	-4.53140400	0.20065100	-1.25080800
C	-3.75176400	2.39742800	-2.82120900
H	-2.55847600	2.94928100	-1.10150400
C	-5.04705000	0.32359200	-2.54425900
H	-4.80556900	-0.63973100	-0.62465200
C	-4.64556700	1.43226700	-3.30267700
H	-5.02403000	1.53524300	-4.31463000
C	-6.00403200	-0.71054100	-3.15716000
C	-7.28273000	-0.00221200	-3.65274900
H	-7.97840800	-0.73198600	-4.08411300
H	-7.78992400	0.50655600	-2.82553200
H	-7.06524300	0.74523400	-4.42192300
C	-6.41759800	-1.79430800	-2.14829300
H	-7.11844300	-2.49023500	-2.62295300
H	-5.55927700	-2.37748300	-1.80248900
H	-6.91693300	-1.36188500	-1.27393000
C	-5.30564700	-1.40573700	-4.34699800

H	-4.98602700	-0.68287900	-5.10504500
H	-4.42260400	-1.95946800	-4.01371200
H	-5.99085900	-2.11717800	-4.82556800
C	-3.32395800	3.55838000	-3.73022200
C	-2.32543300	4.49895100	-3.03585200
H	-1.41102300	3.97117100	-2.74494100
H	-2.04303800	5.30573000	-3.72111300
H	-2.75657100	4.95920800	-2.13979700
C	-4.57034300	4.37746100	-4.12874000
H	-5.30132800	3.76622800	-4.66810000
H	-5.06632300	4.78819800	-3.24207600
H	-4.28569100	5.21252500	-4.78003200
C	-2.64739400	2.99644500	-4.99959400
H	-3.31462700	2.33191500	-5.55767900
H	-2.35608200	3.81668800	-5.66670800
H	-1.74980900	2.42494700	-4.74422300
C	4.71286800	-1.26342900	-1.18437300
C	3.98943700	0.09371800	-1.11253300
H	3.98822800	0.50231100	-0.09673600
H	4.50484700	0.81723500	-1.75394600
H	2.94792700	0.02612800	-1.44502200
C	6.13672500	-1.09978000	-0.61040100
H	6.09906300	-0.79782000	0.44204900
H	6.70047300	-2.03730200	-0.67090200
H	6.68988800	-0.33374500	-1.16719800
C	4.80591500	-1.67815000	-2.66745900
H	5.39567800	-2.58991100	-2.80705000
H	3.81157100	-1.84808800	-3.08904000
H	5.28888100	-0.88477200	-3.25020200
C	4.18297400	-6.17048100	0.00829900

C	3.95344300	-6.58151400	-1.46351600
H	4.48056300	-5.91632200	-2.15509200
H	4.31646000	-7.60112500	-1.63850800
H	2.88734500	-6.56489100	-1.72169600
C	5.68506700	-6.29228700	0.34404300
H	5.87393400	-6.00143700	1.38311000
H	6.02412500	-7.32623900	0.20943000
H	6.29805300	-5.65289800	-0.29848500
C	3.41253600	-7.15384900	0.90500600
H	3.54025400	-6.91807400	1.96708800
H	2.33942500	-7.15915600	0.68182500
H	3.78449500	-8.17086000	0.74099600
O	0.50189200	-0.70631200	0.85044000
O	-1.87562100	-0.89827400	0.00423100
P	-0.32990800	-0.70255100	-0.58514200
O	-0.09225400	-1.97041300	-1.36488200
O	-0.10543800	0.64731300	-1.19043000
H	-1.34191400	-2.99805200	-2.90861800
C	-1.59451300	-4.06103500	-3.01928700
S	0.01145100	-4.91472500	-2.59835700
O	0.08642300	-6.31981600	-3.05482100
C	1.32522200	-3.85633500	-3.21121100
H	1.23022300	-3.81568600	-4.29781600
H	1.17275400	-2.87923400	-2.74200600
H	2.26434400	-4.31509100	-2.89380700
C	0.09832900	-4.82298700	-0.81814400
H	1.09134400	-5.18188500	-0.55005300
H	-0.03096700	-3.77379700	-0.53733900
H	-0.68535200	-5.47342200	-0.42999200
C	-0.28788700	-1.45129500	-5.56943800

C	0.40358500	-0.63570700	-4.62308100
C	1.80009500	-0.57273200	-4.57472900
C	2.51223500	-1.33552300	-5.49435600
C	1.84918100	-2.14577600	-6.44104000
C	0.46127100	-2.20700000	-6.48824100
C	-1.68903500	-1.29324100	-5.28960700
C	-1.78934500	-0.42757600	-4.22274500
H	2.30408300	0.05126200	-3.84334600
H	3.59771400	-1.30495200	-5.48599200
H	2.43636300	-2.72799800	-7.14595100
H	-0.03740300	-2.84724800	-7.20951400
H	-2.51770200	-1.72423400	-5.83179700
H	-2.66101700	-0.06174500	-3.70313200
N	-0.53798600	-0.00370300	-3.84370300
H	-0.34060600	0.44239100	-2.93676400
C	-1.87221800	-4.36765800	-4.48690500
O	-1.01849700	-4.66679300	-5.29096400
O	-3.17554300	-4.25020400	-4.75502100
C	-3.54468200	-4.46055600	-6.13127500
H	-4.61928700	-4.28844900	-6.16726200
H	-3.01593400	-3.75504100	-6.77537100
H	-3.29886000	-5.48119700	-6.43311900
C	-2.64446800	-4.47047800	-2.02576800
C	-3.16422300	-5.77260800	-2.01616000
C	-3.04358000	-3.55085200	-1.05253000
C	-4.07734700	-6.14672700	-1.03284600
H	-2.84570900	-6.48980300	-2.76722500
C	-3.96104300	-3.93002100	-0.07275300
H	-2.62376800	-2.55393600	-1.04056000
C	-4.47681500	-5.22620600	-0.05881600

H	-4.47786800	-7.15609400	-1.02582100
H	-4.26028800	-3.20770900	0.68090600
H	-5.18746800	-5.52199000	0.70762600

**S-int3**

C	0.73633500	-1.75656500	4.57832800
C	-0.21695800	-0.74072600	4.38240800
H	2.64572300	-2.54150900	4.04687500
C	1.92036000	-1.75834800	3.84964000
C	0.05785200	0.29333700	3.47041900
C	1.24256200	0.22732100	2.70970000
C	2.19987400	-0.79695700	2.86049600
C	-0.88428600	1.42974500	3.24193700
C	-1.26951100	2.29519200	4.29334700
C	-1.37567300	1.66614800	1.94802500
C	-0.60287600	2.19305600	5.65491800
C	-2.22907600	3.29190800	4.04668100
C	-2.32923300	2.65545100	1.68734700
C	-0.72740900	3.47966500	6.47537400
H	0.44898700	1.91827400	5.52302200
C	-2.66694100	4.27962900	5.11492500
C	-2.76105500	3.43183000	2.76133100
C	-2.19175800	3.91717200	6.52371000
H	-0.33197200	3.31153300	7.48386300
H	-2.26983500	5.27100600	4.85172100
H	-3.50127400	4.20629400	2.57431000
H	-2.79899700	3.09326600	6.92463300
H	-3.75957100	4.38056100	5.09084500
H	-2.33131100	4.77163400	7.19586200
H	-0.12142900	4.27527800	6.02083700

H	-1.05547500	1.38036000	6.23625700
C	-1.51265100	-0.89897900	5.13976100
H	-1.33714800	-0.71652500	6.20941900
H	-2.25263800	-0.16461000	4.81348000
C	-2.07647500	-2.32913300	4.98174100
H	-2.50439600	-2.42426300	3.97731600
H	-2.91076200	-2.45581500	5.68004100
C	-1.00739400	-3.43429800	5.20706300
H	-0.90499200	-4.04236400	4.29969400
H	-1.32314900	-4.11971700	6.00095100
C	0.37830200	-2.84829200	5.55411400
H	1.13786900	-3.63742300	5.55361000
H	0.34818100	-2.44270300	6.57572000
C	3.36776800	-0.96519400	1.95110100
C	3.90187900	-2.25007200	1.74403300
C	3.89406800	0.09374900	1.19618500
C	4.88436600	-2.49816900	0.78446800
H	3.50689800	-3.08099100	2.31174500
C	4.84509300	-0.12190400	0.19742200
H	3.51932700	1.08797500	1.36497700
C	5.32883600	-1.42053400	0.01015900
H	6.06025300	-1.60159200	-0.77083300
C	-2.84977000	2.91164100	0.31378000
C	-2.08734900	3.66018800	-0.58804600
C	-4.12004200	2.45881900	-0.05683400
C	-2.58486200	3.98268700	-1.85587000
H	-1.09546600	3.96850700	-0.28627900
C	-4.64425500	2.75004000	-1.32173600
H	-4.68760000	1.87637100	0.65959300
C	-3.86431100	3.52332600	-2.19068500

H	-4.26173600	3.76470600	-3.17091000
C	-6.01853500	2.24628600	-1.78621800
C	-6.92195700	3.45258700	-2.12032900
H	-7.90800900	3.11169700	-2.45835200
H	-7.06190700	4.08755800	-1.23859000
H	-6.49088600	4.07184700	-2.91295700
C	-6.72289700	1.39935500	-0.71391500
H	-7.69145800	1.05379300	-1.09163000
H	-6.13331200	0.51427500	-0.44729200
H	-6.90700100	1.97282800	0.20097000
C	-5.84296700	1.37294000	-3.04797900
H	-5.35557800	1.92091800	-3.85941000
H	-5.22586800	0.49456400	-2.82873700
H	-6.81711800	1.02358700	-3.41099100
C	-1.79412500	4.84341800	-2.85254300
C	-0.36314000	5.12569400	-2.36227500
H	0.19358100	4.20582600	-2.15998800
H	0.17924600	5.69210100	-3.12737500
H	-0.36129900	5.72535900	-1.44530300
C	-2.53199800	6.19048400	-3.01913200
H	-3.54530700	6.04703000	-3.40998900
H	-2.61305600	6.71201200	-2.05877400
H	-1.98903900	6.83924400	-3.71702600
C	-1.70481000	4.14283000	-4.22572900
H	-2.69361600	3.92883100	-4.64367200
H	-1.17872200	4.79014400	-4.93721900
H	-1.15921700	3.19925100	-4.15357900
C	5.30490500	1.00530700	-0.73733600
C	4.64511600	2.35377400	-0.40022300
H	4.90031200	2.68572300	0.61252600



H	5.00563900	3.11825600	-1.09755700
H	3.55386400	2.31528700	-0.48367900
C	6.83618900	1.16857600	-0.64750100
H	7.13848200	1.44440500	0.36900100
H	7.36110500	0.24502400	-0.91415700
H	7.17639500	1.95614200	-1.33028100
C	4.90515300	0.62683400	-2.18145100
H	5.39814200	-0.29461800	-2.51070700
H	3.82382200	0.47735800	-2.25476000
H	5.18915300	1.42509600	-2.87795400
C	5.44813400	-3.90283200	0.52407100
C	5.14412900	-4.31413800	-0.93263200
H	5.59026100	-3.61997000	-1.65120400
H	5.54229500	-5.31485400	-1.13950400
H	4.06620000	-4.32915700	-1.12398500
C	6.97600200	-3.88627100	0.74510700
H	7.21602700	-3.60399600	1.77611200
H	7.40218600	-4.87811000	0.55214600
H	7.47148700	-3.17241900	0.07986500
C	4.84156300	-4.96393000	1.45705100
H	5.02920700	-4.73279800	2.51140200
H	3.75912900	-5.06218100	1.31465400
H	5.28932200	-5.94079400	1.24525800
O	1.41490800	1.21728900	1.75928300
O	-0.94670200	0.86882600	0.90036800
P	0.62288500	1.01306100	0.31794800
O	0.89472000	-0.35335500	-0.25154800
O	0.79987500	2.27186200	-0.46864700
H	-0.42250800	-1.40859500	-1.47257800
C	-0.56959800	-2.47128400	-1.70023200

S	-0.49755500	-3.26383100	-0.00566800
O	-1.04955200	-4.63874800	-0.00160900
C	1.22650300	-3.20551600	0.46123100
H	1.76807300	-3.87982400	-0.20057900
H	1.54893800	-2.16646700	0.35036500
H	1.26955500	-3.53596800	1.49996200
C	-1.31194800	-2.20615400	1.19454900
H	-0.94162200	-2.50667000	2.17664800
H	-1.06198100	-1.16384300	0.98512000
H	-2.37936200	-2.39210900	1.08946100
C	-0.61651700	-0.09597100	-4.41862600
C	0.08861500	0.78830600	-3.55099900
C	1.44152000	1.09791900	-3.72360400
C	2.09932500	0.49668000	-4.78966300
C	1.42727700	-0.39282400	-5.65640800
C	0.08293800	-0.69333300	-5.48214100
C	-1.96862900	-0.15379100	-3.92870600
C	-2.03151700	0.65758300	-2.81743400
H	1.94271600	1.77158400	-3.03669800
H	3.15191700	0.70980900	-4.95480000
H	1.97731000	-0.85419200	-6.47191600
H	-0.42087900	-1.38568500	-6.15105300
H	-2.78401800	-0.71841200	-4.35805500
H	-2.85313900	0.88707700	-2.15723900
N	-0.80011900	1.22732500	-2.59641300
H	-0.53203500	1.82833600	-1.82042000
C	-1.98221500	-2.72056800	-2.22747600
O	-2.26530100	-3.30662400	-3.24032200
O	-2.87753700	-2.19483000	-1.36738700
C	-4.25595700	-2.30424600	-1.76587800

H	-4.82675200	-1.82505400	-0.97096800
H	-4.40786900	-1.78394800	-2.71345200
H	-4.53719200	-3.35405400	-1.87450700
C	0.56662400	-3.01852800	-2.50966300
C	1.70721800	-2.22146600	-2.66646400
C	0.53779900	-4.31851700	-3.03444000
C	2.80531400	-2.71402100	-3.36621500
H	1.72493600	-1.22782500	-2.23604300
C	1.64469800	-4.80612800	-3.72580300
H	-0.34456700	-4.93420400	-2.90875200
C	2.77708800	-4.00500300	-3.89464100
H	3.67789500	-2.08250100	-3.49594400
H	1.62154800	-5.81121500	-4.13647700
H	3.63615800	-4.38954900	-4.43734600

**R-int4**

C	-0.16020500	-3.38714600	3.99721400
C	-1.11627900	-2.40156000	3.69807500
H	1.74725100	-4.21533200	3.55023200
C	1.02842100	-3.44823500	3.28384900
C	-0.83028800	-1.44426100	2.71227600
C	0.35979800	-1.57716200	1.96905100
C	1.30994100	-2.58969000	2.20475100
C	-1.77236200	-0.32802300	2.40053100
C	-2.16663800	0.61798600	3.37622300
C	-2.25106100	-0.18686700	1.09187000
C	-1.54796800	0.58987000	4.76287800
C	-3.09227300	1.61884900	3.03075100
C	-3.16656500	0.80336200	0.72955000
C	-1.67076800	1.92621100	5.49940400

H	-0.49932700	0.28479700	4.68451700
C	-3.53279400	2.68906900	4.01558200
C	-3.58871300	1.68238900	1.72452500
C	-3.12297300	2.40314300	5.46189800
H	-1.32002300	1.80987500	6.53138500
H	-3.09052200	3.64749400	3.70557300
H	-4.29888300	2.46364600	1.46343600
H	-3.76852500	1.62177000	5.88697200
H	-4.61946100	2.82460100	3.94299200
H	-3.26455500	3.30134200	6.07402400
H	-1.02579900	2.67790700	5.02389300
H	-2.03845900	-0.17924800	5.37250900
C	-2.44802300	-2.54375800	4.39247800
H	-2.35156100	-2.31435400	5.46365000
H	-3.18383600	-1.84755800	3.98274500
C	-2.94209100	-3.99861200	4.23974100
H	-3.15311600	-4.16986300	3.17765900
H	-3.89225000	-4.11847500	4.77217700
C	-1.90116500	-5.03683100	4.73999000
H	-1.75780600	-5.80791300	3.97556200
H	-2.26830000	-5.54840400	5.63675200
C	-0.53024800	-4.39260200	5.05642100
H	0.24104600	-5.16411600	5.15027200
H	-0.59270600	-3.89129100	6.03309300
C	2.46626200	-2.87121300	1.30725900
C	3.00253200	-4.16682800	1.26218900
C	2.98210000	-1.91982300	0.41109400
C	3.97980800	-4.54234500	0.33451500
H	2.61533700	-4.92275200	1.93134300
C	3.91022200	-2.26825200	-0.56712400

H	2.61697400	-0.90981300	0.45930600
C	4.40435400	-3.58033200	-0.58647100
H	5.11201500	-3.86034600	-1.35648100
C	-3.62435600	0.95556600	-0.68179400
C	-2.99202900	1.89217500	-1.50588900
C	-4.68959200	0.19811600	-1.18197900
C	-3.41063900	2.09234100	-2.82609400
H	-2.15086700	2.43637000	-1.09865000
C	-5.14731900	0.38146100	-2.49304000
H	-5.15676200	-0.52880000	-0.52904400
C	-4.49003500	1.32983600	-3.28977000
H	-4.84175400	1.48649400	-4.30415900
C	-6.33799000	-0.39492800	-3.07382600
C	-7.42735300	0.60473500	-3.51937000
H	-8.29175900	0.06681200	-3.92624800
H	-7.76842100	1.20963700	-2.67214300
H	-7.06380600	1.28785000	-4.29363000
C	-6.95786300	-1.35859200	-2.04982100
H	-7.79691900	-1.89295200	-2.50904300
H	-6.23673600	-2.10633500	-1.70872100
H	-7.34364400	-0.82190600	-1.17598400
C	-5.86830900	-1.21838400	-4.29224000
H	-5.42032200	-0.58133400	-5.06280800
H	-5.13200500	-1.96894600	-3.98932600
H	-6.71535500	-1.74672900	-4.74575100
C	-2.76322500	3.14621400	-3.73737600
C	-1.46590400	3.71184400	-3.13328100
H	-0.74120900	2.92193800	-2.90779500
H	-1.00239300	4.40739700	-3.84138800
H	-1.65546200	4.26365900	-2.20702900

C	-3.76845500	4.30448200	-3.92357100
H	-4.69449600	3.95567400	-4.39313100
H	-4.02954900	4.74975900	-2.95748700
H	-3.33883200	5.08857300	-4.55871000
C	-2.42521100	2.55005100	-5.12050900
H	-3.30636300	2.13691400	-5.62090800
H	-2.01385000	3.32993300	-5.77147600
H	-1.67827800	1.75518800	-5.04067000
C	4.30030900	-1.28568000	-1.68106100
C	3.79283700	0.14282700	-1.41340800
H	4.18221600	0.54054600	-0.46949800
H	4.13356100	0.80553800	-2.21798200
H	2.69979000	0.19719800	-1.38070000
C	5.83205200	-1.23000500	-1.84810400
H	6.31209600	-0.88481600	-0.92546600
H	6.25495900	-2.20731900	-2.10066300
H	6.10149100	-0.53559900	-2.65304800
C	3.64690200	-1.78475500	-2.99020500
H	3.99054000	-2.79107900	-3.25202400
H	2.55802100	-1.81827000	-2.88098200
H	3.89232700	-1.11434000	-3.82378200
C	4.55370500	-5.96918600	0.35700200
C	5.27641900	-6.31916000	-0.95616000
H	6.15387100	-5.68583600	-1.12585900
H	5.62541500	-7.35665500	-0.91796700
H	4.60793700	-6.22238700	-1.81876400
C	5.57068100	-6.04962900	1.51758600
H	5.08733100	-5.83566400	2.47725900
H	6.01390600	-7.05151400	1.57434500
H	6.37902500	-5.32240700	1.38023600

C	3.45047800	-7.02671400	0.58267900
H	2.95926200	-6.90814800	1.55406000
H	2.67455300	-7.00722400	-0.19015300
H	3.90013700	-8.02658400	0.57668400
O	0.56485300	-0.64317200	0.95683300
O	-1.78849400	-1.04999500	0.11020600
P	-0.24587600	-0.80281500	-0.45597600
O	0.07030300	-2.03228700	-1.24822700
O	-0.13887900	0.56098700	-1.12594000
H	-0.89335900	-3.31516500	-3.21861200
C	-1.78464700	-3.38148200	-3.84374800
S	-0.08969000	-5.80682700	-1.53580000
O	0.39095100	-7.24354100	-1.38832600
C	1.33099800	-4.81499100	-2.10905800
H	1.48051600	-5.06871200	-3.16001300
H	1.10541800	-3.75422600	-1.98588400
H	2.20911900	-5.07764500	-1.51878300
C	-0.19060000	-5.09391200	0.14711700
H	0.70106100	-5.38697400	0.70209100
H	-0.25561400	-4.00686900	0.08093800
H	-1.08204700	-5.50933300	0.62384800
C	-0.74962600	-1.50856300	-5.24868300
C	-0.15524700	-0.48330200	-4.50082300
C	1.05195500	0.11188600	-4.83020400
C	1.67822300	-0.35253300	-5.99056900
C	1.09696200	-1.36132600	-6.76644000
C	-0.12061600	-1.95286700	-6.40358300
C	-1.98743000	-1.95947100	-4.49962900
C	-2.03309000	-0.96126900	-3.38034400
H	1.48955800	0.88429400	-4.20733000

H	2.62938100	0.07504100	-6.29076600
H	1.60328000	-1.69930500	-7.66527300
H	-0.55602600	-2.73696500	-7.01200500
H	-2.90566100	-1.96998000	-5.09316000
H	-2.75073200	-0.91673800	-2.57104600
N	-0.99345500	-0.19102100	-3.39842300
H	-0.66057800	0.34761400	-2.50094800
C	-1.46685800	-4.41673000	-4.91075600
O	-0.57516200	-5.22808200	-4.84356200
O	-2.31390300	-4.33277300	-5.96807800
C	-2.11104200	-5.33006700	-6.98712300
H	-2.86971900	-5.13172200	-7.74380400
H	-1.10709400	-5.24225500	-7.40992300
H	-2.23181600	-6.33023300	-6.56530300
C	-2.95412000	-3.79298800	-2.95800700
C	-4.10757200	-4.40853500	-3.45737100
C	-2.86076500	-3.52613200	-1.58676100
C	-5.14382700	-4.76266500	-2.59161900
H	-4.19631400	-4.61725000	-4.51793500
C	-3.90324400	-3.86364700	-0.72712800
H	-1.97134900	-3.04653700	-1.19857100
C	-5.04541200	-4.49314700	-1.22588900
H	-6.03091300	-5.24817200	-2.98822600
H	-3.81095600	-3.63769000	0.33151500
H	-5.85549600	-4.76949100	-0.55688600

#### **S-int4**

C	0.21445800	-3.50869300	3.59765600
C	-0.85014800	-2.61889800	3.35585500
H	2.20912000	-4.10392500	3.05986800



C	1.41023100	-3.38529800	2.89292800
C	-0.67876300	-1.55770700	2.44497000
C	0.54024400	-1.47412400	1.75269000
C	1.58823800	-2.38903300	1.92551500
C	-1.74193900	-0.55297400	2.14440800
C	-2.31486700	0.24372700	3.16611000
C	-2.14230200	-0.34170500	0.81164300
C	-1.75327600	0.20220600	4.57722100
C	-3.36063300	1.12849700	2.85174900
C	-3.16140500	0.56052200	0.48504700
C	-2.09352300	1.45402500	5.39003700
H	-0.66957300	0.05287900	4.52943300
C	-4.00938500	2.02786000	3.89102800
C	-3.77972200	1.25169800	1.52480700
C	-3.60009300	1.70707300	5.33018200
H	-1.75632500	1.32179900	6.42469000
H	-3.73222600	3.06865500	3.66771400
H	-4.57309700	1.95458500	1.28084900
H	-4.12770400	0.80853300	5.67957100
H	-5.10056100	1.98031700	3.78160400
H	-3.89556800	2.52808800	5.99367500
H	-1.55814000	2.32422100	4.98578500
H	-2.15207100	-0.66485500	5.11594200
C	-2.15524600	-2.95746000	4.03485200
H	-2.07637500	-2.75903900	5.11408600
H	-2.96638400	-2.33034100	3.65637300
C	-2.49643100	-4.44775800	3.82886700
H	-2.73057900	-4.62052900	2.77526300
H	-3.40236100	-4.68552100	4.39797600
C	-1.33719600	-5.39279100	4.23521400

H	-1.15041700	-6.08254300	3.40564900
H	-1.61817700	-6.00894000	5.09698400
C	-0.03798100	-4.62635100	4.57780000
H	0.81647600	-5.31163700	4.61002300
H	-0.13463600	-4.20445900	5.58908200
C	2.72561100	-2.38331700	0.97346700
C	3.04033900	-3.56167800	0.28691200
C	3.36058500	-1.19112700	0.61264500
C	3.92714300	-3.55276700	-0.79190200
H	2.51932200	-4.46931100	0.56391700
C	4.23986100	-1.14016700	-0.46921600
H	3.10475800	-0.29004200	1.15023700
C	4.50724500	-2.33145000	-1.15369700
H	5.16386800	-2.30217000	-2.01721100
C	-3.52418000	0.86912900	-0.92840600
C	-2.73953500	1.78742400	-1.63767000
C	-4.66140600	0.31895800	-1.52875500
C	-3.07616200	2.16820300	-2.94036000
H	-1.85545200	2.17854500	-1.15446200
C	-5.03001000	0.67398900	-2.83397900
H	-5.25320300	-0.39083300	-0.96404900
C	-4.22156900	1.59626600	-3.51221600
H	-4.50111500	1.88685600	-4.51973200
C	-6.27782300	0.10907100	-3.52795700
C	-7.22912600	1.27442500	-3.87680300
H	-8.13116600	0.89280300	-4.36967000
H	-7.53494100	1.81136100	-2.97192800
H	-6.75878800	1.99697300	-4.55173300
C	-7.03728600	-0.88898900	-2.63822000
H	-7.91730200	-1.26002500	-3.17533100

H	-6.41121400	-1.74816800	-2.38283700
H	-7.39001600	-0.41777600	-1.71368900
C	-5.85959200	-0.62169200	-4.82295100
H	-5.32696300	0.04429500	-5.51036600
H	-5.21330800	-1.47157400	-4.58633800
H	-6.74620400	-0.99969900	-5.34608300
C	-2.26399500	3.20926100	-3.72621600
C	-1.00488900	3.65764700	-2.96383500
H	-0.35091600	2.81745200	-2.70975300
H	-0.43464200	4.36129500	-3.58046000
H	-1.26251200	4.17046400	-2.03100600
C	-3.15682800	4.44661400	-3.96728600
H	-4.04725800	4.19345800	-4.55236900
H	-3.49106900	4.87363600	-3.01556500
H	-2.60116800	5.21838200	-4.51338700
C	-1.82560400	2.63407600	-5.09032200
H	-2.67842600	2.29155900	-5.68510000
H	-1.30224800	3.40256100	-5.67089200
H	-1.14379800	1.78750500	-4.96345600
C	4.79509200	0.19070800	-0.99413500
C	4.55512600	1.35082300	-0.01277400
H	5.00714100	1.15045500	0.96523900
H	5.00512100	2.26762400	-0.40992400
H	3.48745400	1.54301900	0.13259900
C	6.31027400	0.08676100	-1.25866700
H	6.85046300	-0.15890100	-0.33746700
H	6.54860500	-0.68110500	-2.00140000
H	6.69561100	1.04137200	-1.63604200
C	4.05264300	0.51719400	-2.31099700
H	4.20494000	-0.27313100	-3.05463200

H	2.97634600	0.60669900	-2.12490800
H	4.41548100	1.46266900	-2.73418300
C	4.22222700	-4.80512700	-1.62896900
C	3.81494400	-4.54105500	-3.09613100
H	4.39885000	-3.72736500	-3.53714300
H	3.97783800	-5.43783100	-3.70738600
H	2.76049400	-4.25777500	-3.16654500
C	5.72977900	-5.12770500	-1.56403900
H	6.03839400	-5.33314700	-0.53304900
H	5.96322300	-6.00886000	-2.17445300
H	6.33392200	-4.29261600	-1.93259800
C	3.44391300	-6.03362100	-1.12953400
H	3.70252500	-6.28579000	-0.09543100
H	2.36209200	-5.87021500	-1.17854800
H	3.68143600	-6.90296000	-1.75340900
O	0.67943800	-0.45889100	0.81292700
O	-1.54790100	-1.05512700	-0.21716900
P	0.03560700	-0.73731800	-0.66795100
O	0.48956200	-1.99008600	-1.34603500
O	0.12222800	0.59743500	-1.39558500
H	-1.18667100	-2.91483400	-2.17996500
C	-1.90343900	-3.30037400	-2.91282500
S	-1.58544500	-6.09492500	-0.08656900
O	-2.63072400	-6.20271900	1.02197800
C	-0.31927600	-7.37134100	0.26620500
H	-0.80252300	-8.34576700	0.16538400
H	0.49365600	-7.28203100	-0.45957000
H	0.05319000	-7.24569700	1.28704900
C	-0.53290800	-4.66919500	0.32357900
H	-0.16234000	-4.78263000	1.34200600

H	0.29260900	-4.58396600	-0.38239700
H	-1.14550100	-3.77257700	0.25172300
C	-0.51892000	-2.29025500	-4.80159200
C	0.12997900	-1.13047400	-4.36335900
C	1.45221200	-0.83219100	-4.64816400
C	2.14035200	-1.75735800	-5.43719500
C	1.50845500	-2.91451900	-5.90892200
C	0.17357300	-3.19773200	-5.59236100
C	-1.88191900	-2.31598500	-4.15549700
C	-1.93790900	-0.96702600	-3.51072600
H	1.92912500	0.05904400	-4.25839400
H	3.18173800	-1.57614300	-5.68388000
H	2.06891700	-3.61525900	-6.52003200
H	-0.29496100	-4.11292600	-5.93663400
H	-2.73149600	-2.54463600	-4.80199200
H	-2.73490800	-0.58268300	-2.88962200
N	-0.78591700	-0.37485000	-3.58600900
H	-0.45039300	0.31517400	-2.82680100
C	-3.28363600	-3.28271100	-2.27703500
O	-4.30191100	-2.92749700	-2.84318600
O	-3.22623800	-3.72161600	-1.02202900
C	-4.44900800	-3.77908300	-0.25818700
H	-4.64655200	-2.78860800	0.16072100
H	-5.27785100	-4.08753900	-0.89725100
H	-4.24838300	-4.51310400	0.52121500
C	-1.46344200	-4.69617700	-3.29226900
C	-0.12635100	-5.05373300	-3.08228600
C	-2.34424300	-5.61678700	-3.86483800
C	0.32018200	-6.32783600	-3.42798500
H	0.54825100	-4.31982000	-2.65136800

C	-1.89830700	-6.89490200	-4.20293400
H	-3.38202400	-5.33898700	-4.03041200
C	-0.56705800	-7.25298900	-3.98312300
H	1.36009200	-6.59525700	-3.26778400
H	-2.59126700	-7.61121900	-4.63482900
H	-0.22137800	-8.24843900	-4.24718400

**R-int5**

C	-0.00027800	-2.67237900	4.82772400
C	-0.93115300	-1.69980800	4.41967400
H	1.77793600	-3.77573000	4.31061300
C	1.03787800	-3.05233100	3.97755600
C	-0.83046200	-1.11441700	3.14329500
C	0.11948200	-1.65226500	2.25636000
C	1.09917200	-2.56754900	2.66899700
C	-1.58912400	0.09672300	2.71389200
C	-1.49955200	1.29977800	3.45802200
C	-2.26124300	0.08924200	1.47851400
C	-0.65190400	1.38657500	4.71598300
C	-2.17670000	2.43638000	2.98854700
C	-2.84158200	1.25409600	0.93758000
C	-0.35003600	2.82223400	5.15600600
H	0.27752900	0.82433100	4.56783300
C	-2.17701100	3.75526300	3.74094100
C	-2.82654400	2.38773200	1.75806800
C	-1.63784900	3.64501800	5.16730700
H	0.12130300	2.80849500	6.14592000
H	-1.56074000	4.47559700	3.18278900
H	-3.33403600	3.28409900	1.41467000
H	-2.37719700	3.14917400	5.81144900

H	-3.19323700	4.16927300	3.74420200
H	-1.46908300	4.64440000	5.58536700
H	0.36492200	3.28949600	4.46660700
H	-1.16449600	0.88965700	5.54663500
C	-2.07611200	-1.44752600	5.36973600
H	-1.72151900	-0.94841700	6.28320000
H	-2.82433600	-0.79309800	4.91493300
C	-2.70697100	-2.79977400	5.76577500
H	-3.16692400	-3.23035700	4.87030300
H	-3.51567100	-2.62598700	6.48439400
C	-1.66242800	-3.78981600	6.34945400
H	-1.75174500	-4.75583100	5.84167600
H	-1.85769600	-3.97438600	7.41195000
C	-0.20985300	-3.27960900	6.19091100
H	0.50205000	-4.09235400	6.37001300
H	-0.01792300	-2.52085400	6.96410800
C	2.17939300	-2.90614400	1.70494500
C	1.85862800	-3.53489400	0.49578500
C	3.47856700	-2.43634400	1.91534800
C	2.80136400	-3.65112900	-0.52628400
H	0.83927500	-3.86889100	0.35289300
C	4.44909600	-2.51186100	0.90237100
H	3.71284900	-1.96550800	2.86705200
C	4.08236800	-3.11138700	-0.30802300
H	4.80720900	-3.15654200	-1.10945500
C	-3.35733400	1.35805100	-0.45163600
C	-3.29037200	2.59482900	-1.10652100
C	-3.86721600	0.25960000	-1.16004400
C	-3.72692000	2.76217400	-2.42486200
H	-2.87042500	3.44225100	-0.57918100

C	-4.23622600	0.36746000	-2.49853300
H	-3.94053900	-0.68847900	-0.65612200
C	-4.17354800	1.62956700	-3.11107700
H	-4.47432300	1.72134000	-4.14767300
C	-4.62292200	-0.87127700	-3.31865600
C	-4.82067200	-2.11774500	-2.43753900
H	-5.13183600	-2.96122000	-3.06397500
H	-3.89824800	-2.41131900	-1.92651500
H	-5.59775300	-1.95784300	-1.68157900
C	-3.46631300	-1.16333700	-4.30119200
H	-3.68536700	-2.05623400	-4.89981500
H	-3.30722800	-0.32699000	-4.99143100
H	-2.53777800	-1.33609500	-3.74705200
C	-5.92674100	-0.62222800	-4.10340200
H	-6.75610000	-0.40208800	-3.42168000
H	-5.83577900	0.21525000	-4.80272200
H	-6.19229000	-1.51126900	-4.68746000
C	-3.76031200	4.17295400	-3.03378300
C	-2.42232900	4.90841300	-2.80781900
H	-1.59130900	4.36383200	-3.26373500
H	-2.46277300	5.90844000	-3.25623300
H	-2.20408500	5.03866900	-1.74307700
C	-4.88920700	4.96529200	-2.33620100
H	-5.85657500	4.47260100	-2.48290500
H	-4.71149100	5.03660100	-1.25790200
H	-4.95558100	5.98324400	-2.74047700
C	-4.04847000	4.15464100	-4.54432700
H	-5.03212200	3.72721100	-4.76501700
H	-4.03964900	5.17825400	-4.93517400
H	-3.29527900	3.57995300	-5.09236000



C	5.84379600	-1.91309000	1.13780000
C	6.55525200	-2.72026100	2.24393300
H	6.67036500	-3.76812900	1.94611300
H	7.55186200	-2.30749000	2.44160800
H	5.98840100	-2.69992700	3.18068000
C	6.71054400	-1.93888900	-0.13208600
H	6.88746400	-2.95996500	-0.48612000
H	6.24265800	-1.36364700	-0.93898700
H	7.68626400	-1.48791600	0.07893100
C	5.71426800	-0.43720300	1.57761100
H	5.22239600	0.15715900	0.80064500
H	5.14879800	-0.33924100	2.51144300
H	6.70677200	-0.00706100	1.75575800
C	2.41481000	-4.25351400	-1.88532500
C	3.58822600	-5.04327800	-2.49775800
H	3.92649700	-5.83527300	-1.82029500
H	3.26981900	-5.51141300	-3.43572200
H	4.44786100	-4.40570700	-2.73029300
C	1.20315900	-5.19833600	-1.76247200
H	0.29693100	-4.67072800	-1.45215500
H	1.00338600	-5.66031300	-2.73598700
H	1.40036200	-6.00090400	-1.04252700
C	2.02966800	-3.09424900	-2.83161300
H	1.16917800	-2.54411200	-2.43423500
H	2.86918300	-2.40031400	-2.96688100
H	1.75407900	-3.48044500	-3.82030700
O	0.13170800	-1.22383500	0.94547700
O	-2.36918500	-1.11695700	0.81347000
P	-1.11677200	-1.74065600	-0.07725100
O	-1.26406200	-3.22018900	-0.08876700

O	-0.86590800	-0.93911200	-1.33317700
H	1.65166700	-0.44838000	-2.71144800
C	1.87306100	0.58696200	-2.42869500
C	1.12815300	2.06534100	-0.32005800
C	1.67505800	1.99772000	0.97081200
C	1.56138200	3.01202400	1.90816000
C	0.85269800	4.14958100	1.51427400
C	0.27610300	4.23283300	0.24120000
C	0.39798100	3.19177200	-0.68492800
C	1.35762800	0.73594000	-0.98289200
C	2.15638400	0.01121200	0.01706100
H	1.99238400	2.92569300	2.89993900
H	0.73908900	4.97260800	2.21261800
H	-0.28322900	5.12202700	-0.03336300
H	-0.07674700	3.25471500	-1.65562900
H	0.36936700	0.18559000	-1.00763900
H	2.56708700	-0.98241400	-0.06467300
N	2.29882000	0.73033100	1.10126100
H	2.74970200	0.37866800	1.93828900
C	3.39126700	0.67065200	-2.47304800
O	4.10529100	0.76669300	-1.49019300
O	3.86674700	0.52904600	-3.71568400
C	5.30043700	0.49450400	-3.83674100
H	5.70295900	-0.37347500	-3.30810200
H	5.49770600	0.41989400	-4.90545300
H	5.74049300	1.40411400	-3.42177400
C	1.13103300	1.47627200	-3.40872700
C	-0.17862600	1.12245500	-3.75759600
C	1.69163600	2.64422600	-3.93316800
C	-0.89826800	1.91028300	-4.65284200

H	-0.63672600	0.24838000	-3.30401300
C	0.96829600	3.43145000	-4.82922400
H	2.69875400	2.93947100	-3.65435000
C	-0.32401500	3.05903000	-5.20057400
H	-1.91250100	1.62603600	-4.90933100
H	1.41634800	4.33291700	-5.23758800
H	-0.88594300	3.66945300	-5.90176600

**S-int5**

C	0.09166500	-3.31562700	4.52104700
C	-0.83485600	-2.32085200	4.15790600
H	1.87228200	-4.38973200	3.96126100
C	1.14553500	-3.63597200	3.66827600
C	-0.70312300	-1.64165700	2.93241000
C	0.27646500	-2.10577200	2.03090200
C	1.23827300	-3.05977400	2.39739600
C	-1.48206200	-0.42078600	2.56639300
C	-1.45214100	0.74255100	3.37711100
C	-2.12291800	-0.37153200	1.31922400
C	-0.68446000	0.75902300	4.68783500
C	-2.11328700	1.89889900	2.93054000
C	-2.70802600	0.80321300	0.81849500
C	-0.42523400	2.16192800	5.24373500
H	0.25835700	0.21416300	4.56365700
C	-2.14560000	3.17915200	3.74661700
C	-2.71439600	1.90949400	1.67125000
C	-1.70962000	2.98924100	5.19997700
H	-0.04283000	2.08135700	6.26825700
H	-1.48335300	3.91817500	3.27066200
H	-3.20051600	2.82102400	1.33256400

H	-2.49576400	2.46356800	5.75951100
H	-3.15319700	3.61095600	3.70200100
H	-1.57175000	3.96394100	5.68267800
H	0.35034200	2.66655700	4.65478100
H	-1.24601800	0.20513500	5.44776400
C	-2.01238500	-2.15273600	5.08697800
H	-1.69414500	-1.71689600	6.04493000
H	-2.75623100	-1.47739600	4.65624100
C	-2.63558400	-3.53799400	5.36253400
H	-3.05390800	-3.91041900	4.42162400
H	-3.47402400	-3.42660200	6.05906000
C	-1.59839700	-4.55215500	5.91605600
H	-1.66293200	-5.48658400	5.34881700
H	-1.82242700	-4.80220000	6.95930100
C	-0.14758800	-4.01938000	5.83188700
H	0.56810900	-4.83631900	5.97281300
H	0.01602900	-3.31501200	6.66087100
C	2.33021200	-3.39365200	1.44507900
C	2.02341900	-3.90238000	0.18231800
C	3.66454600	-3.09616800	1.76658300
C	3.01815800	-4.09584600	-0.78454400
H	0.98551500	-4.10228600	-0.05017600
C	4.68440000	-3.25584400	0.82067000
H	3.88330600	-2.72132000	2.76198800
C	4.33483100	-3.75660500	-0.44595100
H	5.11705400	-3.87899000	-1.18576300
C	-3.20656600	0.91498200	-0.57344400
C	-2.94249900	2.08797400	-1.29398400
C	-3.89444500	-0.12889600	-1.20347100
C	-3.35154400	2.23770600	-2.62126300

H	-2.38082000	2.87399300	-0.80591100
C	-4.28736000	-0.03103900	-2.53857800
H	-4.09333600	-1.02809300	-0.64178300
C	-4.01554400	1.16128200	-3.22260500
H	-4.32591800	1.25199900	-4.25884800
C	-4.96761100	-1.19542000	-3.27228500
C	-5.19178000	-2.41026000	-2.35593200
H	-5.67203600	-3.21455400	-2.92446100
H	-4.24803200	-2.79891000	-1.95862700
H	-5.84492300	-2.16463300	-1.51124300
C	-4.06117600	-1.64447900	-4.43944900
H	-4.52801400	-2.46941300	-4.99124800
H	-3.87745800	-0.82826700	-5.14658600
H	-3.09471400	-1.98986500	-4.05787500
C	-6.33418800	-0.73816600	-3.82371800
H	-6.99245500	-0.41533800	-3.00938100
H	-6.23211400	0.09844000	-4.52273000
H	-6.82655500	-1.56101500	-4.35592600
C	-3.12139500	3.53259500	-3.41495600
C	-2.27657800	4.55355500	-2.63438900
H	-1.28216900	4.15526400	-2.40591000
H	-2.14109500	5.45746800	-3.23858800
H	-2.75860200	4.85154400	-1.69657300
C	-4.49453200	4.16886900	-3.72272900
H	-5.12354400	3.49370500	-4.31211100
H	-5.03215000	4.40230100	-2.79673000
H	-4.36921500	5.09836100	-4.29173200
C	-2.38539100	3.22865500	-4.73697000
H	-2.94679200	2.52699400	-5.36255800
H	-2.25309500	4.15181800	-5.31466200

H	-1.39956500	2.80173300	-4.53476500
C	6.14309600	-2.86396400	1.09793100
C	6.34053900	-2.30898000	2.51787900
H	6.06069500	-3.04085500	3.28290600
H	7.39378000	-2.05149900	2.67140000
H	5.75362500	-1.39777200	2.68599800
C	7.04950400	-4.10252500	0.93287100
H	6.76491200	-4.88749100	1.64178700
H	6.98033300	-4.52189000	-0.07542600
H	8.09738300	-3.83733600	1.11651300
C	6.57535300	-1.77279300	0.09153900
H	6.50549700	-2.12567700	-0.94225600
H	5.94677900	-0.87865300	0.18264600
H	7.61438000	-1.47402400	0.27309200
C	2.63156200	-4.55799900	-2.19700500
C	3.80703200	-5.25047100	-2.91056200
H	4.18373500	-6.09883900	-2.32785900
H	3.47601300	-5.62827200	-3.88374900
H	4.64271300	-4.56730800	-3.09900900
C	1.43779800	-5.53471200	-2.15388300
H	0.52523400	-5.04987900	-1.79763600
H	1.24029600	-5.91169300	-3.16388000
H	1.65470400	-6.39371100	-1.50853400
C	2.21438300	-3.30937700	-3.00761600
H	1.36493700	-2.79493900	-2.54801900
H	3.05332300	-2.60629700	-3.09066400
H	1.92045700	-3.59273100	-4.02510600
O	0.33735400	-1.56554700	0.76528400
O	-2.16790400	-1.53275200	0.56913700
P	-0.86715200	-1.94822300	-0.35829300

O	-0.95633600	-3.40827800	-0.63214500
O	-0.60109500	-0.93282100	-1.45040900
H	2.69594200	-0.46474600	-2.94096100
C	2.34803200	0.50145500	-2.57044900
C	1.50354100	1.37993800	-0.20067300
C	2.09230800	1.11949800	1.04604400
C	1.92662600	1.93123000	2.15998400
C	1.12832300	3.06174400	1.98663600
C	0.50775500	3.32960400	0.75925000
C	0.67820200	2.49053500	-0.34283500
C	1.85718000	0.24898900	-1.11755100
C	2.72988600	-0.57915100	-0.29433700
H	2.38432300	1.69900700	3.11623300
H	0.97569800	3.73779500	2.82047800
H	-0.12639800	4.20582800	0.66573200
H	0.18483100	2.68508100	-1.28581400
H	0.88170800	-0.37465300	-1.21774800
H	3.20824000	-1.51265200	-0.55773400
N	2.83536500	-0.07807400	0.91366700
H	3.26466000	-0.59631900	1.67471700
C	1.11970300	0.85254500	-3.40148200
O	0.57180900	1.93885600	-3.42893000
O	0.67687800	-0.23450900	-4.03106000
C	-0.67251900	-0.16693800	-4.54097900
H	-0.75071300	0.60249300	-5.31166700
H	-0.86656500	-1.15458300	-4.95584600
H	-1.35415300	0.04147600	-3.71597300
C	3.50968200	1.47542100	-2.58799800
C	4.79913000	0.94811300	-2.43822000
C	3.34905200	2.86339600	-2.65497300

C	5.90941100	1.78568900	-2.34919300
H	4.93494800	-0.13075000	-2.39232800
C	4.46218400	3.70158700	-2.57481400
H	2.35665400	3.27767000	-2.77959200
C	5.74206600	3.16977500	-2.41694200
H	6.90140700	1.35746700	-2.23523000
H	4.32482200	4.77776100	-2.63297100
H	6.60373300	3.82799300	-2.35091000

**R-int6**

C	0.00684600	-2.47236600	4.88781000
C	-1.00255700	-1.56645500	4.51705500
H	1.86231300	-3.40722400	4.32745000
C	1.07179000	-2.72451200	4.02735100
C	-0.94277100	-0.91425700	3.27090400
C	0.06868900	-1.31509300	2.37722100
C	1.11235900	-2.17254100	2.74123400
C	-1.84382100	0.21773300	2.90011900
C	-1.91650000	1.38900900	3.69490000
C	-2.51524400	0.19075900	1.67291500
C	-1.06905800	1.53643000	4.94623100
C	-2.73717200	2.44738800	3.26778300
C	-3.23033000	1.28635200	1.16252200
C	-0.93858000	2.98415600	5.42885000
H	-0.08141400	1.09946400	4.76271900
C	-2.89618300	3.72628400	4.07316200
C	-3.36902800	2.37713100	2.02603300
C	-2.31892200	3.63746000	5.48625400
H	-0.45220100	2.99674100	6.41098600
H	-2.39199200	4.54264300	3.53485800



H	-3.96272400	3.22563500	1.69631200
H	-2.97828100	3.03222000	6.12379700
H	-3.95791900	4.00113100	4.10606800
H	-2.26991900	4.63635600	5.93428500
H	-0.29416200	3.55908200	4.74949700
H	-1.50656100	0.95384900	5.76419500
C	-2.17240300	-1.46404400	5.46492100
H	-1.86878600	-0.97717000	6.40261100
H	-2.97570200	-0.86039400	5.03499600
C	-2.68031800	-2.88451800	5.79355000
H	-3.09382100	-3.31454600	4.87518900
H	-3.50666200	-2.81610200	6.50954700
C	-1.55528400	-3.80160600	6.34499300
H	-1.55684200	-4.75051900	5.79860500
H	-1.73813900	-4.04555700	7.39739900
C	-0.15304700	-3.15892900	6.21945700
H	0.62770700	-3.91246500	6.36607100
H	-0.03032800	-2.42138400	7.02602600
C	2.24834700	-2.44753500	1.82189100
C	2.04317100	-2.98792500	0.54928700
C	3.54954400	-2.13658700	2.23329200
C	3.11058200	-3.19169000	-0.33068300
H	1.03548200	-3.24590200	0.24980900
C	4.64676200	-2.33220000	1.38230200
H	3.69309900	-1.71770700	3.22515200
C	4.40016100	-2.85247400	0.10397900
H	5.23258000	-2.99695300	-0.56986900
C	-3.63335600	1.38720400	-0.26374500
C	-3.45851100	2.61477200	-0.91319800
C	-4.03955300	0.27792000	-1.02313800

C	-3.65408300	2.75709300	-2.29272800
H	-3.11993900	3.46762700	-0.33620900
C	-4.17269800	0.36372400	-2.40643000
H	-4.19273800	-0.66532000	-0.52349300
C	-3.98851100	1.61389700	-3.01983800
H	-4.09196400	1.68281100	-4.09546900
C	-4.41772400	-0.87577900	-3.27702500
C	-4.59598400	-2.15417700	-2.44026900
H	-4.78045500	-3.00356400	-3.10722200
H	-3.70255100	-2.38637600	-1.85093000
H	-5.45076100	-2.07652400	-1.75882200
C	-3.18175000	-1.07146900	-4.18603500
H	-3.30563200	-1.96370800	-4.81153500
H	-3.02994800	-0.21357400	-4.85029400
H	-2.27754300	-1.19573900	-3.58105300
C	-5.67789400	-0.67652000	-4.14377100
H	-6.56546600	-0.54390900	-3.51482200
H	-5.59303200	0.20142000	-4.79255600
H	-5.84144800	-1.55073000	-4.78504200
C	-3.47361500	4.13747000	-2.94138800
C	-2.04851200	4.66585700	-2.67036800
H	-1.29568400	4.00148200	-3.10297400
H	-1.91806000	5.65578000	-3.12340000
H	-1.84558300	4.76344600	-1.59912100
C	-4.50528200	5.11202700	-2.33281800
H	-5.52721300	4.76129600	-2.51494700
H	-4.37385100	5.21188400	-1.25034400
H	-4.39929900	6.10859000	-2.77815500
C	-3.68697700	4.09608000	-4.46299600
H	-4.69809600	3.76307500	-4.72199400

H	-3.54797500	5.09870700	-4.88200100
H	-2.96708700	3.43084700	-4.94970500
C	6.05853900	-1.96945200	1.86978200
C	6.39465100	-2.81763600	3.11535600
H	6.36306000	-3.88615600	2.87602500
H	7.39972600	-2.57764300	3.48212300
H	5.68691700	-2.63599100	3.93046200
C	7.13247000	-2.23150800	0.80148000
H	7.17163200	-3.28842500	0.51685900
H	6.95815900	-1.63886900	-0.10329700
H	8.11719600	-1.95618700	1.19425700
C	6.11060100	-0.47137700	2.24329400
H	5.90156900	0.15929500	1.37108400
H	5.38527400	-0.22126600	3.02460000
H	7.10618600	-0.20446300	2.61644400
C	2.84267200	-3.81060300	-1.71104400
C	4.04020200	-3.65886500	-2.66542500
H	4.93682900	-4.16636700	-2.29319600
H	3.79149200	-4.11379800	-3.63095100
H	4.28493600	-2.60757500	-2.85188100
C	2.55350200	-5.31505600	-1.51353500
H	1.69133300	-5.46542600	-0.85585900
H	2.33341500	-5.79137200	-2.47672500
H	3.41497200	-5.82524900	-1.06721100
C	1.61569000	-3.14288600	-2.36885500
H	0.68575300	-3.34886700	-1.83522700
H	1.73805300	-2.05767200	-2.40025800
H	1.49881500	-3.50624900	-3.39639800
O	0.06362600	-0.81312600	1.07216600
O	-2.44086100	-0.98605300	0.92196200

P	-1.10788100	-1.33526500	0.06814300
O	-1.12111900	-2.74545900	-0.35944400
O	-0.96331500	-0.29448600	-1.12305100
H	0.46044700	0.19481900	-3.11502500
C	1.42174400	0.71526400	-3.20018700
C	1.39961400	1.59618900	-0.74177700
C	2.14326600	1.30319300	0.43822400
C	1.78496900	1.80824600	1.68766400
C	0.65033900	2.61000500	1.76002100
C	-0.10075800	2.91442000	0.61068000
C	0.26567600	2.42578100	-0.64188800
C	2.00324400	0.84902100	-1.82001300
C	3.06540700	0.17070500	-1.27082700
H	2.35863100	1.56195100	2.57672800
H	0.33634300	3.00585400	2.71888200
H	-0.98028600	3.54185600	0.70419200
H	-0.30516400	2.69375000	-1.52516800
H	-0.68625600	0.60220000	-0.82290500
H	3.76740200	-0.49740000	-1.73949200
N	3.17293300	0.46247800	0.07380800
H	3.70217400	-0.10929800	0.71817700
C	2.28119000	-0.14266700	-4.12565200
O	3.49135200	-0.22034600	-4.12130000
O	1.50000800	-0.80219200	-5.00564500
C	2.20333700	-1.60407400	-5.96677400
H	2.77696300	-2.38442200	-5.46046100
H	1.43205100	-2.04318500	-6.59949500
H	2.88376700	-0.98533700	-6.55725600
C	1.15389700	2.03733000	-3.92113700
C	0.11753900	2.11161400	-4.85968600

C	1.95538100	3.15987200	-3.69904600
C	-0.10849300	3.28961200	-5.57039200
H	-0.50483100	1.23832500	-5.03445800
C	1.71872400	4.34387900	-4.39835600
H	2.75662400	3.10118000	-2.96933800
C	0.68980200	4.41151500	-5.33835800
H	-0.91233100	3.33455000	-6.29966600
H	2.34251400	5.21328000	-4.21015500
H	0.50737800	5.33305500	-5.88389100

**S-int6**

C	-0.14382400	-3.40012300	4.52738800
C	-1.01356100	-2.34658100	4.19267000
H	1.60433700	-4.52156900	3.96374700
C	0.92501100	-3.71732300	3.69392700
C	-0.80308300	-1.60197700	3.01689500
C	0.20776000	-2.04476100	2.14089100
C	1.10670600	-3.06473000	2.46905400
C	-1.56474500	-0.35980100	2.68889900
C	-1.57736200	0.76748900	3.54894800
C	-2.16820100	-0.25113900	1.43302300
C	-0.84393200	0.73763100	4.87855600
C	-2.22908100	1.93913200	3.12400100
C	-2.76038800	0.92650400	0.95770900
C	-0.59874400	2.12301700	5.48527200
H	0.10074900	0.19588900	4.75740800
C	-2.27760300	3.19131200	3.98311700
C	-2.79688500	2.00002700	1.84909300
C	-1.88371000	2.94874200	5.44015000
H	-0.23674400	2.00791900	6.51341800

H	-1.59478900	3.93861100	3.55127900
H	-3.27024800	2.92375000	1.52575700
H	-2.68440700	2.40314900	5.95858400
H	-3.28031900	3.63174200	3.92162600
H	-1.75990200	3.90568700	5.95962600
H	0.18846200	2.65364600	4.93271800
H	-1.42688900	0.15949100	5.60383900
C	-2.21758200	-2.18171000	5.08768200
H	-1.91527600	-1.81097500	6.07741300
H	-2.91941600	-1.45420100	4.67211000
C	-2.90600900	-3.55207700	5.26552600
H	-3.30850300	-3.85418600	4.29280300
H	-3.76204800	-3.44183500	5.94016800
C	-1.93204400	-4.63945100	5.79345700
H	-2.01699300	-5.53811200	5.17358200
H	-2.20141800	-4.93571000	6.81332000
C	-0.45824900	-4.16722900	5.78553300
H	0.21777900	-5.02076300	5.90099500
H	-0.29235500	-3.51776400	6.65736500
C	2.23732500	-3.41412900	1.56759300
C	2.00880000	-3.87322900	0.26734000
C	3.55211600	-3.25721000	2.02835300
C	3.07398800	-4.16264100	-0.59255600
H	0.98847700	-3.99246600	-0.06943700
C	4.64408100	-3.51174900	1.18802400
H	3.70347700	-2.90704700	3.04301100
C	4.37470600	-3.95325900	-0.11583000
H	5.21100400	-4.14982900	-0.77807200
C	-3.20114500	1.06109900	-0.45205400
C	-2.79333500	2.18055000	-1.18597900

C	-3.93142200	0.04874100	-1.08701900
C	-3.08574900	2.30220700	-2.54937600
H	-2.19688300	2.93419500	-0.68625700
C	-4.22560800	0.12520600	-2.44732900
H	-4.23901000	-0.80932500	-0.50728300
C	-3.79758900	1.25971600	-3.15237700
H	-4.01970300	1.32378500	-4.21101600
C	-4.95393000	-1.00322300	-3.19062500
C	-5.39000800	-2.13584600	-2.24634000
H	-5.90767200	-2.91319900	-2.81913700
H	-4.53135400	-2.60252200	-1.75196400
H	-6.07917700	-1.77597500	-1.47414200
C	-3.99526700	-1.60353400	-4.24267600
H	-4.49665700	-2.39808400	-4.80855400
H	-3.65152400	-0.84636800	-4.95492100
H	-3.11534100	-2.03540500	-3.75372400
C	-6.20926800	-0.44378700	-3.89219100
H	-6.90085300	-0.00902000	-3.16187900
H	-5.95778500	0.33460600	-4.61951200
H	-6.73497400	-1.24356400	-4.42735400
C	-2.69595300	3.55201400	-3.35395800
C	-1.49542700	4.28966600	-2.73193400
H	-0.61989200	3.63667200	-2.69368400
H	-1.24229500	5.15999600	-3.34773100
H	-1.71251000	4.66216100	-1.72506400
C	-3.91601100	4.49955200	-3.37167600
H	-4.78506100	4.01227300	-3.82789800
H	-4.19466600	4.79731700	-2.35432800
H	-3.69114600	5.40722100	-3.94539200
C	-2.31358500	3.18796200	-4.80364100

H	-3.16228600	2.79126200	-5.37034600
H	-1.96933700	4.08632500	-5.32898400
H	-1.50668000	2.45063800	-4.81222900
C	6.09985700	-3.31474400	1.63708300
C	6.19857400	-2.78179100	3.07578100
H	5.74866800	-3.47290900	3.79674500
H	7.25114200	-2.65427200	3.35017200
H	5.70838700	-1.80738900	3.18262900
C	6.83822500	-4.66881000	1.56820200
H	6.36364300	-5.40348300	2.22792000
H	6.83428300	-5.07899900	0.55349200
H	7.88261700	-4.55107200	1.88062200
C	6.79578400	-2.30187400	0.70093100
H	6.79723200	-2.64402900	-0.33871900
H	6.29537100	-1.32731100	0.73229600
H	7.83880400	-2.15681800	1.00539500
C	2.84673200	-4.66995000	-2.02558600
C	3.76940900	-5.87390800	-2.31232200
H	3.58839200	-6.68439200	-1.59757000
H	3.57642900	-6.25890300	-3.32008900
H	4.83062800	-5.60983900	-2.26117300
C	1.39313400	-5.12035700	-2.25389500
H	0.67971200	-4.30225000	-2.13025100
H	1.29076800	-5.50856700	-3.27358100
H	1.11292800	-5.92295400	-1.56173400
C	3.16699400	-3.53292900	-3.02005100
H	2.50976600	-2.67186200	-2.86442900
H	4.20685100	-3.19891300	-2.91895800
H	3.02934200	-3.88207800	-4.05049500
O	0.37705500	-1.41255000	0.90776100



O	-2.11531900	-1.36707100	0.58745300
P	-0.74801300	-1.58129200	-0.25580100
O	-0.79616200	-2.83373700	-1.03281400
O	-0.47123000	-0.29329500	-1.13409000
H	3.19629800	0.25876500	-3.72314600
C	2.58926800	0.94576700	-3.12075700
C	2.17215400	1.18610200	-0.52245400
C	2.65333000	0.49102000	0.62331800
C	2.22625000	0.80238700	1.91526200
C	1.27575900	1.80567200	2.05379100
C	0.76861600	2.49451500	0.93405800
C	1.21656100	2.20721800	-0.35274800
C	2.79168300	0.57352800	-1.67416500
C	3.58414400	-0.44098000	-1.19598900
H	2.59784600	0.25424100	2.77620700
H	0.91046100	2.05942900	3.04084300
H	0.01900400	3.26589900	1.08129200
H	0.83925400	2.75002500	-1.21192200
H	-0.11220600	0.48925400	-0.66308900
H	4.19405300	-1.14925600	-1.73531700
N	3.53197900	-0.47663500	0.18238600
H	3.82733500	-1.27433100	0.73137600
C	1.12698100	0.65309700	-3.47698800
O	0.22836800	1.46779100	-3.42522800
O	0.96994400	-0.63593700	-3.81129000
C	-0.37760000	-1.10536100	-4.03709700
H	-0.49871000	-1.28390800	-5.10924900
H	-0.48154000	-2.03329400	-3.47510800
H	-1.09674400	-0.36738700	-3.68669200
C	2.98354300	2.38194000	-3.45931700

C	3.87562900	3.08833100	-2.64749700
C	2.50692600	2.99838400	-4.62362900
C	4.27770000	4.38170300	-2.98406900
H	4.25258500	2.62435800	-1.74251600
C	2.90607500	4.28959100	-4.96165200
H	1.80471200	2.47444700	-5.26375900
C	3.79309800	4.98880300	-4.14133000
H	4.96819700	4.91432900	-2.33571500
H	2.51870900	4.75166400	-5.86561800
H	4.10067000	5.99773800	-4.40200600

**R-TS1**

C	-1.62169300	-0.53121200	1.92321600
C	-2.46525600	0.57117500	1.69997600
H	-0.27356700	-1.95650500	1.03926700
C	-0.93511500	-1.11273500	0.86111500
C	-2.61318000	1.09464500	0.40130100
C	-1.99897000	0.40041800	-0.65813400
C	-1.13206700	-0.67916900	-0.45480600
C	-3.35743700	2.35831500	0.12268000
C	-3.00965900	3.57510300	0.75959600
C	-4.36105300	2.36178800	-0.85481700
C	-1.80324500	3.65906900	1.67768600
C	-3.76655700	4.72562200	0.47851600
C	-5.05033900	3.52551100	-1.23787800
C	-1.29613100	5.09175600	1.86151200
H	-1.00897100	3.01253900	1.28984600
C	-3.48010300	6.06688000	1.13343800
C	-4.76549200	4.67579800	-0.49516400
C	-2.45886100	5.99618000	2.27087000

H	-0.50043800	5.10574900	2.61525600
H	-3.10304600	6.75742600	0.36355100
H	-5.32244900	5.58351500	-0.71169100
H	-2.93084900	5.58376400	3.17334900
H	-4.42185500	6.50498500	1.48757300
H	-2.11274100	7.00459400	2.52525800
H	-0.85449900	5.46045500	0.92462800
H	-2.05353600	3.26392600	2.66907600
C	-3.26791000	1.03241000	2.89242400
H	-2.61211700	1.49864000	3.64186200
H	-4.00799900	1.78250000	2.60337600
C	-3.96195000	-0.18654800	3.53717300
H	-4.70116300	-0.56682000	2.82426000
H	-4.51738100	0.14008900	4.42334900
C	-2.95915400	-1.31254800	3.90660900
H	-3.32559800	-2.26934600	3.52014100
H	-2.88509700	-1.42145600	4.99451500
C	-1.54489600	-1.05473600	3.33405500
H	-0.94179700	-1.96765000	3.37877900
H	-1.03773000	-0.31430900	3.96993400
C	-0.41136400	-1.32213400	-1.58726600
C	-1.10399400	-1.96155700	-2.61517200
C	0.99030000	-1.25614400	-1.63084000
C	-0.42258200	-2.52188800	-3.70648200
H	-2.18577200	-1.99906100	-2.56981700
C	1.70134100	-1.80550700	-2.69893500
H	1.50464500	-0.74889300	-0.82292800
C	0.97133300	-2.42917400	-3.72630100
H	1.51504300	-2.85314500	-4.56184600
C	-5.91095500	3.59158800	-2.44564400

C	-5.89330500	4.76066500	-3.21234000
C	-6.65817000	2.49732200	-2.91055200
C	-6.57849600	4.85960300	-4.42801700
H	-5.29463400	5.59716600	-2.87409000
C	-7.29563300	2.53396700	-4.14752400
H	-6.69548500	1.60232400	-2.31202500
C	-7.25186800	3.72668400	-4.88786200
H	-7.74386900	3.75790000	-5.85217900
C	-7.96638000	1.29004600	-4.74630500
C	-7.96507400	0.09691100	-3.77481200
H	-8.46840800	-0.75577200	-4.24415200
H	-6.94996400	-0.22165300	-3.51512200
H	-8.50171200	0.33016000	-2.84820400
C	-7.17100400	0.87647100	-6.00529000
H	-7.61741200	-0.01252300	-6.46716800
H	-7.16041700	1.67645800	-6.75388500
H	-6.13506300	0.64181000	-5.73866000
C	-9.42625700	1.60492800	-5.13205000
H	-10.00598300	1.89962600	-4.25002200
H	-9.49090800	2.41840200	-5.86210200
H	-9.90255800	0.72173900	-5.57422100
C	-6.56975200	6.19235700	-5.18946200
C	-5.12567800	6.71740800	-5.32912000
H	-4.48828200	5.98061600	-5.82022800
H	-5.11541900	7.63861900	-5.92447100
H	-4.67841900	6.95001900	-4.35764500
C	-7.40876200	7.21492900	-4.39218100
H	-8.44463000	6.87316300	-4.28849900
H	-7.00261700	7.35961900	-3.38520700
H	-7.41656300	8.18779900	-4.89947100

C	-7.17036700	6.06171500	-6.59878700
H	-8.22252900	5.75879600	-6.56637400
H	-7.12192600	7.02880700	-7.11177600
H	-6.61806100	5.33318400	-7.20056900
C	3.23222600	-1.73404100	-2.79864000
C	3.86582100	-1.03898100	-1.58260900
H	3.63652900	-1.56753100	-0.65112400
H	4.95538900	-1.01754200	-1.69471500
H	3.52148800	-0.00377300	-1.48128300
C	3.80840000	-3.16337700	-2.89194300
H	3.53948600	-3.74652000	-2.00455800
H	3.43033800	-3.69707100	-3.76926800
H	4.90226100	-3.13128300	-2.96309300
C	3.62576200	-0.94096200	-4.06435800
H	3.21862000	-1.39851300	-4.97174800
H	3.25378300	0.08929600	-4.00623100
H	4.71647000	-0.89893400	-4.16928700
C	-1.22979300	-3.19242200	-4.82606000
C	-0.32891500	-3.75781100	-5.93545800
H	0.36341100	-4.51785400	-5.55449400
H	-0.94886000	-4.22914800	-6.70549500
H	0.25719500	-2.96968200	-6.42219300
C	-2.05502100	-4.35156700	-4.22623800
H	-2.75753600	-3.99099400	-3.46936900
H	-2.63627400	-4.84653300	-5.01326600
H	-1.40234900	-5.09907200	-3.76024700
C	-2.19041800	-2.15681200	-5.45288400
H	-2.90056200	-1.76637400	-4.71899000
H	-1.63903900	-1.31314900	-5.88077500
H	-2.76641200	-2.62588500	-6.26020300

O	-2.23980200	0.82278100	-1.96576400
O	-4.68329900	1.15030100	-1.44855400
P	-3.73534500	0.49667200	-2.60786500
O	-4.09038600	-0.93483800	-2.74288800
O	-3.73190000	1.38095800	-3.87348700
H	-2.85318400	2.10583500	-4.18087500
C	-1.45405500	3.93766500	-3.75392500
C	-1.93337400	3.01846200	-4.80698800
O	-0.35817900	3.89261100	-3.20291100
S	-0.62248200	1.95868000	-5.38922400
O	-1.08262200	1.06368600	-6.47052500
C	0.76814700	2.95581000	-5.97506100
H	0.40497600	3.50905400	-6.84268100
H	1.06932300	3.62273800	-5.16607000
H	1.56861000	2.27078500	-6.26263900
C	0.06750600	1.04343900	-4.01635200
H	0.78801800	0.34066100	-4.43703500
H	0.51203300	1.75200900	-3.32024700
H	-0.74931600	0.50802800	-3.53589700
C	-2.65821800	3.60057900	-5.99389100
C	-2.16804900	4.74561600	-6.64378900
C	-3.79890400	2.96793100	-6.50276300
C	-2.79492900	5.24059600	-7.78479200
H	-1.30130900	5.26277100	-6.23877600
C	-4.42885700	3.46772600	-7.64219400
H	-4.19113800	2.09335500	-5.99990000
C	-3.92629400	4.59600600	-8.29023400
H	-2.40836100	6.13068300	-8.27283500
H	-5.31452300	2.96786700	-8.02276600
H	-4.41911600	4.98034800	-9.17868500

O	-2.39895500	4.83317900	-3.42999000
C	-2.04882300	5.73886000	-2.37071400
H	-1.17680500	6.33490600	-2.65235700
H	-2.92454200	6.37170500	-2.23568500
H	-1.83846400	5.18467300	-1.45530600

### S-TS1

C	-1.93636300	-1.20772700	1.33741200
C	-2.81615900	-0.12014300	1.20186000
H	-0.38615200	-2.37640300	0.40485600
C	-1.07568300	-1.54436700	0.28391200
C	-2.79532600	0.64090700	0.00746100
C	-2.01032700	0.18478000	-1.05395000
C	-1.11804100	-0.88601000	-0.94260000
C	-3.57382200	1.90955800	-0.13606200
C	-3.38673600	2.99330600	0.74558200
C	-4.49762800	2.05866700	-1.18701000
C	-2.25363100	3.09488000	1.74007000
C	-4.19546500	4.13617100	0.62205200
C	-5.35952300	3.16141500	-1.29043000
C	-2.65573900	3.69793900	3.11009800
H	-1.51827400	3.75994000	1.26979100
C	-3.95235100	5.27238500	1.58344900
C	-5.19094900	4.18571700	-0.34714500
C	-3.81382600	4.71601000	3.01035700
H	-2.93625000	2.89939000	3.80567700
H	-3.02886700	5.80469700	1.30881200
H	-5.83063300	5.06193500	-0.41272800
H	-4.75982500	4.22669700	3.27117200
H	-4.76751400	6.00233900	1.52655600

H	-3.67030200	5.53132000	3.72812300
H	-1.76845600	4.17733900	3.53908900
H	-1.75003700	2.13686700	1.87837500
C	-3.81660900	0.21148900	2.29591700
H	-3.47332200	1.07965500	2.86965500
H	-4.76238200	0.51716000	1.83552000
C	-4.03816200	-0.94657200	3.27228800
H	-4.58921500	-1.75665700	2.77531500
H	-4.65666700	-0.60595000	4.11069700
C	-2.68909200	-1.47534800	3.76103700
H	-2.81704700	-2.22896400	4.54649200
H	-2.11634100	-0.64739900	4.20246900
C	-1.91688200	-2.07521400	2.58411300
H	-2.35498100	-3.05273500	2.33416100
H	-0.87638600	-2.27846700	2.86780400
C	-0.23289600	-1.24584300	-2.08398700
C	-0.76557300	-1.77952700	-3.26107600
C	1.13877800	-0.99820700	-1.99779500
C	0.06163200	-2.09645000	-4.34467600
H	-1.83685000	-1.92635900	-3.32940700
C	1.98961200	-1.25649900	-3.07750000
H	1.53022900	-0.56465500	-1.08300600
C	1.43183000	-1.82692300	-4.22749400
H	2.07979300	-2.05065600	-5.06275800
C	-6.45183200	3.26405100	-2.29446800
C	-6.25772500	2.97745800	-3.65515300
C	-7.71488600	3.68556400	-1.86988600
C	-7.29937100	3.09302800	-4.57334200
H	-5.28132700	2.66669800	-3.98863300
C	-8.78458200	3.82373600	-2.76537300



H	-7.86655700	3.88284600	-0.81342400
C	-8.55372500	3.52025600	-4.10791600
H	-9.36705100	3.60768600	-4.81757700
C	-10.15292900	4.28211900	-2.24099300
C	-10.00690700	5.66972200	-1.57952500
H	-9.64568400	6.40887700	-2.30331900
H	-10.97404100	6.01298100	-1.19311600
H	-9.30125800	5.64702700	-0.74299900
C	-10.66480100	3.26670800	-1.19647900
H	-11.64109600	3.57890500	-0.80648100
H	-10.77568200	2.27301700	-1.64396400
H	-9.97785300	3.17646300	-0.34922200
C	-11.20231000	4.39189700	-3.35913500
H	-10.90374000	5.11522700	-4.12603800
H	-11.37703900	3.42679300	-3.84704400
H	-12.15591200	4.72820000	-2.93774400
C	-7.11707300	2.75270400	-6.05911400
C	-8.06175600	1.58812300	-6.42804900
H	-7.95235400	1.32948600	-7.48809200
H	-7.82790700	0.69941500	-5.83251000
H	-9.11100000	1.84628800	-6.25137400
C	-5.67762100	2.32355900	-6.38926500
H	-4.96080400	3.12196500	-6.16794600
H	-5.36924500	1.43354300	-5.83248600
H	-5.60003500	2.09352600	-7.45764500
C	-7.46312000	3.98838400	-6.91730400
H	-7.34304200	3.75917800	-7.98287600
H	-8.49503700	4.31839500	-6.76041400
H	-6.80316100	4.82876500	-6.67214200
C	3.47394700	-0.87764900	-2.98137900

C	4.23689900	-1.16373200	-4.28524200
H	3.82264500	-0.59408400	-5.12423100
H	5.28618700	-0.87083000	-4.16922600
H	4.21638100	-2.22757500	-4.54610400
C	3.59070400	0.63466000	-2.68607500
H	4.64526200	0.93466500	-2.65228500
H	3.08449400	1.22542400	-3.45535500
H	3.14195400	0.89120000	-1.72185600
C	4.13721000	-1.67894900	-1.84155200
H	3.64979800	-1.48788900	-0.87984500
H	4.07908700	-2.75546500	-2.03770500
H	5.19466400	-1.40476000	-1.74323300
C	-0.55186500	-2.69826600	-5.61833000
C	-1.35810300	-3.96241700	-5.24932300
H	-0.71638900	-4.70904000	-4.76747600
H	-2.18086200	-3.73044500	-4.56726200
H	-1.78984000	-4.41206500	-6.15141800
C	-1.49967900	-1.66657600	-6.26964400
H	-0.94837600	-0.77023100	-6.57705800
H	-1.96246600	-2.09707300	-7.16665300
H	-2.29476100	-1.35423000	-5.58822900
C	0.51673800	-3.09902500	-6.64918300
H	1.08788300	-2.23411300	-7.00620000
H	1.22388500	-3.83045600	-6.24142000
H	0.03217500	-3.55144800	-7.52122000
O	-2.04785000	0.87314800	-2.25665700
O	-4.59373000	1.04303200	-2.13451400
P	-3.37976400	0.82397200	-3.20856400
O	-3.63229600	-0.41946800	-3.96609900
O	-3.12400000	2.15200900	-3.99807300

H	-2.12799300	2.68275100	-3.69101100
C	-0.58252600	3.48043800	-2.02824800
C	-0.90546000	3.50352300	-3.47811600
O	-1.12341300	4.16858500	-1.17260500
S	-1.62116600	5.04177700	-3.95049900
O	-0.83952800	6.30213500	-3.88904000
C	-2.15755000	4.71521100	-5.64196700
H	-2.75786700	3.80371500	-5.65096800
H	-2.72832800	5.58776200	-5.96501800
H	-1.25603400	4.59675400	-6.24366500
C	-3.17288800	5.21240000	-3.05066500
H	-3.62169500	6.14709700	-3.39270000
H	-3.80204200	4.35085900	-3.27048800
H	-2.91510000	5.24111000	-1.99353500
C	0.15753000	3.02785200	-4.43703600
C	0.13494600	1.69954300	-4.88278000
C	1.19887600	3.87085500	-4.85944600
C	1.12640900	1.23164700	-5.74379500
H	-0.63602300	1.02279800	-4.53589400
C	2.17831300	3.40344700	-5.73519100
H	1.23977300	4.89399300	-4.49805800
C	2.14332500	2.08131300	-6.18060400
H	1.10314600	0.19670300	-6.06343300
H	2.97389600	4.06935800	-6.05747000
H	2.90953000	1.71233600	-6.85682000
O	0.37184800	2.57739400	-1.75925500
C	0.68734000	2.38878700	-0.37203300
H	0.86260800	3.34956700	0.11647000
H	-0.12685700	1.86175100	0.12782300
H	1.59018500	1.78014900	-0.36451300

**R-TS2**

C	-0.27534600	-3.55311400	3.84597100
C	-1.19486600	-2.52432800	3.57908600
H	1.62379000	-4.40224500	3.41992500
C	0.93570200	-3.60242500	3.16993100
C	-0.85054900	-1.51903500	2.66302300
C	0.36001600	-1.63694000	1.94977000
C	1.27823200	-2.68846400	2.15452100
C	-1.75791000	-0.36720600	2.37929500
C	-2.17286300	0.52993300	3.39113600
C	-2.19807200	-0.15557500	1.06616400
C	-1.59111200	0.42565300	4.79037600
C	-3.08939000	1.54824500	3.07414700
C	-3.11573700	0.84376200	0.73458600
C	-1.73149000	1.72136100	5.59351600
H	-0.54088900	0.12283200	4.72372100
C	-3.54823900	2.57074800	4.10006800
C	-3.56289200	1.67024500	1.76316900
C	-3.18059300	2.20658200	5.54016100
H	-1.41062500	1.54913200	6.62748600
H	-3.08964900	3.53958100	3.85244900
H	-4.27605400	2.45647900	1.52654600
H	-3.84073900	1.40693200	5.90483600
H	-4.63129500	2.72059700	4.00509000
H	-3.33610800	3.07168900	6.19512000
H	-1.07116400	2.49430700	5.17693400
H	-2.09837200	-0.37360700	5.34551000
C	-2.55263600	-2.67067800	4.21985100
H	-2.48690500	-2.50975900	5.30565800

H	-3.25440600	-1.92931100	3.83051200
C	-3.07928300	-4.09854800	3.96005600
H	-3.25765800	-4.19737000	2.88278600
H	-4.05035000	-4.22472700	4.45171600
C	-2.08423600	-5.19461900	4.42986100
H	-1.93735400	-5.92390300	3.62556700
H	-2.49522500	-5.74765400	5.28184600
C	-0.70741800	-4.61079800	4.82822700
H	0.03944300	-5.40863300	4.89935900
H	-0.78924000	-4.16906000	5.83171100
C	2.47039200	-2.93935700	1.29209600
C	3.06368300	-4.21619200	1.27266700
C	2.98236800	-1.97370800	0.41214900
C	4.10974700	-4.53483700	0.40475000
H	2.67767200	-4.98862300	1.92186700
C	3.95700800	-2.28316800	-0.53864600
H	2.58201500	-0.97778700	0.44433500
C	4.51979000	-3.56257100	-0.51670900
H	5.28662000	-3.81592000	-1.24017600
C	-3.58212900	1.02459600	-0.67074400
C	-2.88658100	1.87595300	-1.53375100
C	-4.72668200	0.35906000	-1.12292500
C	-3.32876000	2.08692100	-2.84528200
H	-1.98308400	2.34458600	-1.16785000
C	-5.19563500	0.53942500	-2.42920100
H	-5.24541200	-0.29693100	-0.43424800
C	-4.48087800	1.40869000	-3.26351300
H	-4.83158400	1.55942200	-4.27814800
C	-6.42780900	-0.19987400	-2.97218300
C	-7.38547500	0.79437600	-3.66226600

H	-8.27452700	0.26813600	-4.02918200
H	-7.71218600	1.57054000	-2.96149200
H	-6.91994800	1.29042500	-4.51905500
C	-7.21380200	-0.91539200	-1.86079900
H	-8.10280300	-1.39286200	-2.28776700
H	-6.61833200	-1.69846800	-1.38382800
H	-7.54685700	-0.21309900	-1.08851300
C	-5.95778600	-1.25603000	-3.99663100
H	-5.40580500	-0.78899700	-4.81916800
H	-5.30193900	-1.99201400	-3.52053100
H	-6.81628300	-1.79048500	-4.42158700
C	-2.62953500	3.07426400	-3.79186200
C	-1.24891700	3.49846400	-3.26047900
H	-0.60569600	2.63509400	-3.06518300
H	-0.75144800	4.13784200	-3.99802100
H	-1.32959600	4.07169800	-2.33104300
C	-3.52183000	4.33031600	-3.91094200
H	-4.50524700	4.08013800	-4.32399100
H	-3.67739700	4.79145500	-2.92934800
H	-3.05426200	5.07281300	-4.56915700
C	-2.43705200	2.46388300	-5.19620600
H	-3.38695100	2.17812100	-5.65830700
H	-1.96242800	3.19946800	-5.85592400
H	-1.79743300	1.57935100	-5.16231000
C	4.30126700	-1.29320500	-1.66128300
C	3.83583300	0.14056900	-1.34504000
H	4.26209400	0.50333000	-0.40261300
H	4.17098500	0.81343600	-2.14289100
H	2.74655000	0.22535300	-1.28566100
C	5.81916600	-1.25810800	-1.92686900

H	6.36759700	-0.94996900	-1.02940100
H	6.20954100	-2.23036400	-2.24390200
H	6.04362700	-0.54173100	-2.72554500
C	3.55914000	-1.77339300	-2.93166300
H	3.88647000	-2.77646000	-3.22761700
H	2.47813900	-1.81048600	-2.76083900
H	3.75434200	-1.09379700	-3.77091500
C	4.81456300	-5.90068900	0.43035400
C	4.80226500	-6.54827500	-0.97112500
H	5.28105300	-5.91244300	-1.72160800
H	5.34252600	-7.50205900	-0.95022200
H	3.77928700	-6.74888400	-1.30640900
C	6.27871000	-5.68109900	0.87188400
H	6.31885200	-5.22836700	1.86867500
H	6.81862500	-6.63533700	0.90468400
H	6.80687900	-5.01547800	0.18161600
C	4.15604300	-6.88430600	1.41180200
H	4.18390900	-6.51153700	2.44141100
H	3.11111200	-7.08415600	1.14704400
H	4.69076400	-7.84009100	1.39095000
O	0.59880100	-0.65886000	0.99554500
O	-1.72979300	-0.98198000	0.05979200
P	-0.15318700	-0.81064900	-0.46570300
O	0.13881300	-2.12638800	-1.12810900
O	0.05682900	0.49229300	-1.18582200
H	-1.03427700	-2.83353100	-2.52784800
C	-1.64813800	-3.49318300	-3.13436300
S	-0.40007300	-5.27339900	-1.63482300
O	-0.63032100	-6.74502500	-1.87557500
C	1.36795200	-4.90016200	-1.66252300

H	1.71230300	-5.06494500	-2.68364000
H	1.48253100	-3.85146100	-1.38481300
H	1.87259000	-5.56179100	-0.95865000
C	-0.78525100	-4.86882900	0.09282000
H	-0.18119900	-5.50267000	0.74639400
H	-0.55757000	-3.81265600	0.23930000
H	-1.84840200	-5.06727200	0.24195700
C	-1.15685900	-1.36644800	-5.60873400
C	-0.21928500	-0.58001900	-4.88343600
C	1.02595100	-0.23456300	-5.40180900
C	1.32762600	-0.68363900	-6.68533400
C	0.40919200	-1.44879600	-7.42938100
C	-0.83132500	-1.79512600	-6.90364700
C	-2.27861500	-1.57513800	-4.73324200
C	-2.00638700	-0.84794300	-3.56282800
H	1.73118800	0.35315400	-4.82343900
H	2.29052700	-0.43632600	-7.12203500
H	0.67624300	-1.76987700	-8.43200900
H	-1.53745400	-2.38322000	-7.48301700
H	-3.21708800	-2.05004600	-4.97334700
H	-2.60610900	-0.72639300	-2.67378100
N	-0.79056300	-0.27010000	-3.65589500
H	-0.32747800	0.16434700	-2.83471300
C	-0.90197800	-4.02971900	-4.30818100
O	0.30041500	-3.89616400	-4.42013200
O	-1.65949900	-4.68599400	-5.20879700
C	-0.91948300	-5.30372500	-6.27989000
H	-1.67332900	-5.72816100	-6.94269600
H	-0.31356300	-4.55861300	-6.79664500
H	-0.27291300	-6.08833100	-5.87904900



C	-2.97714600	-3.82078300	-2.66015900
C	-3.85313600	-4.72934300	-3.29134800
C	-3.38178900	-3.21729600	-1.44668600
C	-5.08978500	-5.01614400	-2.72325700
H	-3.55266300	-5.20498300	-4.21428200
C	-4.61362800	-3.52036900	-0.88301900
H	-2.71792000	-2.51932400	-0.94942800
C	-5.47457800	-4.41944500	-1.51982200
H	-5.75543100	-5.71711900	-3.21785100
H	-4.90171800	-3.05151200	0.05329900
H	-6.44066900	-4.65261100	-1.08164100

**S-TS2**

C	0.01270500	-3.48562600	3.91013700
C	-0.96586800	-2.50096800	3.67791500
H	1.92623700	-4.27321800	3.36876600
C	1.18968700	-3.50023300	3.16834400
C	-0.72226700	-1.49661500	2.72387000
C	0.47147500	-1.55863200	1.98072600
C	1.44227600	-2.56374600	2.15239000
C	-1.69416600	-0.40195000	2.42009600
C	-2.13049800	0.50445300	3.41614500
C	-2.14369100	-0.22753300	1.09917100
C	-1.51619800	0.47161300	4.80552500
C	-3.08731200	1.48133100	3.08935000
C	-3.08115400	0.75165100	0.75712000
C	-1.68232800	1.79270900	5.56099800
H	-0.45800500	0.20084600	4.72663700
C	-3.57915400	2.50684700	4.09732800
C	-3.56097600	1.57069600	1.77694300

C	-3.15183000	2.21411300	5.53725800
H	-1.32172800	1.67514100	6.58954700
H	-3.18782400	3.49258600	3.80567400
H	-4.29044300	2.33751300	1.52641500
H	-3.76408300	1.40144400	5.95307300
H	-4.67160800	2.58832900	4.02924500
H	-3.32523200	3.09614500	6.16451300
H	-1.06854100	2.57404300	5.09222500
H	-1.98454600	-0.31793300	5.40572800
C	-2.26290000	-2.67088200	4.43025900
H	-2.10866700	-2.44201300	5.49458400
H	-3.02236000	-1.97563300	4.06473000
C	-2.77387900	-4.12330500	4.31331200
H	-3.13086900	-4.27760500	3.28952700
H	-3.64567200	-4.24606700	4.96519000
C	-1.68650900	-5.17817400	4.65547600
H	-1.57622900	-5.87887700	3.81935300
H	-1.98993100	-5.77818900	5.52039300
C	-0.31069400	-4.53597800	4.94196800
H	0.46943000	-5.30410400	4.97424900
H	-0.33671900	-4.07560700	5.94028500
C	2.58566900	-2.72474400	1.21467600
C	3.05931000	-4.01171800	0.91039800
C	3.12765900	-1.63582700	0.51737900
C	3.99848400	-4.22675900	-0.10197000
H	2.64317100	-4.85879700	1.44002200
C	4.00989700	-1.81787000	-0.54688100
H	2.80020200	-0.64269500	0.77196500
C	4.43618200	-3.11808100	-0.83593000
H	5.11655700	-3.27569300	-1.66657600

C	-3.51306000	0.96022100	-0.65571300
C	-2.72102600	1.73591400	-1.50786500
C	-4.72212800	0.43202000	-1.11959600
C	-3.12873600	2.01167000	-2.81781200
H	-1.77582700	2.10319500	-1.13278300
C	-5.15480400	0.67417600	-2.42867900
H	-5.31605600	-0.16713300	-0.43934800
C	-4.34567400	1.47036100	-3.24895000
H	-4.67272800	1.67056000	-4.26332300
C	-6.45094500	0.07904100	-2.99680800
C	-7.33247000	1.19823300	-3.59074800
H	-8.26125300	0.77689600	-3.99348200
H	-7.59477500	1.93405900	-2.82266800
H	-6.82864900	1.72852000	-4.40419600
C	-7.27671300	-0.65219100	-1.92592800
H	-8.19557400	-1.04772700	-2.37260600
H	-6.72899200	-1.49586700	-1.49452200
H	-7.56252800	0.02025700	-1.10970000
C	-6.08367000	-0.92939900	-4.10745200
H	-5.51913500	-0.45089600	-4.91362100
H	-5.45951100	-1.73393300	-3.70388800
H	-6.98657500	-1.37722000	-4.54032800
C	-2.32203100	2.92993900	-3.74823000
C	-0.92016200	3.22865200	-3.18750800
H	-0.36000200	2.31383000	-2.97315900
H	-0.35257800	3.81930300	-3.91521800
H	-0.97081300	3.81087300	-2.26113200
C	-3.09253600	4.26231300	-3.88654700
H	-4.08534800	4.10404400	-4.32196700
H	-3.22661200	4.73772900	-2.90850600

H	-2.54384000	4.95729500	-4.53395100
C	-2.15866000	2.29967000	-5.14746900
H	-3.12216800	2.09805300	-5.62579600
H	-1.60764100	2.98703700	-5.79996000
H	-1.60418600	1.36028400	-5.09738400
C	4.41026600	-0.65459600	-1.46447500
C	3.92269200	0.70552400	-0.93512900
H	4.32705500	0.91930400	0.06082300
H	4.26168200	1.50048300	-1.60897700
H	2.83009500	0.75490700	-0.88787900
C	5.94111300	-0.59825500	-1.63554200
H	6.43373500	-0.42976900	-0.67132900
H	6.34348200	-1.52402000	-2.05986400
H	6.21833400	0.22227100	-2.30780100
C	3.73434300	-0.89462700	-2.83469700
H	4.06526700	-1.83600000	-3.28780900
H	2.64683900	-0.93564600	-2.71527200
H	3.97677400	-0.08138800	-3.53038100
C	4.52656600	-5.62237700	-0.46585400
C	4.17651600	-5.93911200	-1.93674500
H	4.64138600	-5.22613300	-2.62478100
H	4.52715200	-6.94234800	-2.20719600
H	3.09510800	-5.89658800	-2.10347600
C	6.06093800	-5.64284400	-0.29176000
H	6.33558100	-5.43172900	0.74756300
H	6.46478100	-6.62640700	-0.56083200
H	6.54796300	-4.89392900	-0.92389800
C	3.93378300	-6.72872800	0.42176300
H	4.15336900	-6.55753400	1.48121900
H	2.84784600	-6.80882300	0.30555600

H	4.36557000	-7.69633400	0.14397400
O	0.63401400	-0.59927200	0.99471700
O	-1.67774900	-1.06159400	0.09708300
P	-0.10474200	-0.91987800	-0.44550100
O	0.20782300	-2.30516600	-0.94142900
O	0.10490900	0.29065000	-1.30949700
H	-1.34475800	-3.01217300	-2.13422500
C	-1.62120300	-3.82980300	-2.78876100
S	-1.35523000	-5.25801400	-0.78073900
O	-2.01512000	-6.60713800	-0.72993900
C	0.43440700	-5.40287900	-0.63119400
H	0.79956000	-5.91927200	-1.52047300
H	0.84034600	-4.39063500	-0.57138100
H	0.65338400	-5.98446900	0.26667900
C	-1.73633700	-4.30795500	0.70849500
H	-1.37148200	-4.85717600	1.57870500
H	-1.25107800	-3.33847100	0.61204200
H	-2.81951200	-4.18997900	0.74074800
C	-1.29326700	-1.83709900	-5.57505900
C	-0.36000000	-1.02725300	-4.86091300
C	0.91096200	-0.73490100	-5.35950100
C	1.26019100	-1.29841000	-6.58157600
C	0.36464500	-2.12470800	-7.29363000
C	-0.90584300	-2.39548800	-6.80571200
C	-2.46778400	-1.91739400	-4.76339700
C	-2.21610100	-1.17133800	-3.61353000
H	1.59966700	-0.10712000	-4.80394900
H	2.24423400	-1.09947900	-6.99646900
H	0.67830100	-2.55185400	-8.24177400
H	-1.59007000	-3.03180300	-7.35959500

H	-3.39068800	-2.42413700	-5.00290900
H	-2.84588400	-0.98054700	-2.75673200
N	-0.96315200	-0.63756600	-3.67845800
H	-0.50895900	-0.15125700	-2.88847800
C	-3.06812300	-4.18335100	-2.85784900
O	-3.60096900	-4.92772600	-3.65414200
O	-3.72950500	-3.58494000	-1.84043200
C	-5.10376500	-3.98176300	-1.69137300
H	-5.46831000	-3.42891300	-0.82632100
H	-5.67784000	-3.72160800	-2.58269600
H	-5.16350100	-5.05959700	-1.52136400
C	-0.60914000	-4.31743400	-3.68090400
C	0.67518200	-3.72693600	-3.58768900
C	-0.82936200	-5.35156400	-4.62250400
C	1.70050300	-4.15079300	-4.42248100
H	0.84236500	-2.96181300	-2.83770100
C	0.20811900	-5.76863800	-5.44256200
H	-1.81174700	-5.79907700	-4.69484800
C	1.47086800	-5.16942200	-5.34851700
H	2.67629800	-3.68218900	-4.35064700
H	0.03715700	-6.56127300	-6.16476100
H	2.27445500	-5.50032600	-6.00053200

### R-TS3

C	0.12507400	-3.19717400	4.71378800
C	-0.80967800	-2.22868200	4.30371900
H	1.91791700	-4.28269500	4.21083700
C	1.18101600	-3.55669800	3.87679800
C	-0.69042400	-1.61966300	3.03952000
C	0.29061100	-2.12831200	2.17018600

C	1.26669900	-3.04678100	2.57877700
C	-1.47149300	-0.41881500	2.61612200
C	-1.44079000	0.76905900	3.38931200
C	-2.12029300	-0.41146200	1.37053000
C	-0.59613000	0.86564000	4.64803900
C	-2.15994000	1.88775100	2.93949200
C	-2.74538500	0.73655100	0.84931400
C	-0.32755400	2.30713800	5.08906000
H	0.34563100	0.32681600	4.49378500
C	-2.21756600	3.18926000	3.72025100
C	-2.79362200	1.84618800	1.69957500
C	-1.64167000	3.08625300	5.13317500
H	0.16466100	2.30389900	6.06870300
H	-1.65637100	3.95318400	3.16232000
H	-3.33053400	2.73051400	1.36942700
H	-2.34855000	2.56073300	5.79013000
H	-3.25498600	3.54563800	3.75270100
H	-1.49884900	4.08795600	5.55490300
H	0.35891000	2.79791400	4.38642500
H	-1.09569900	0.35441600	5.47838500
C	-1.97475100	-2.00525100	5.23648500
H	-1.64206100	-1.51455700	6.16247600
H	-2.72335300	-1.35361300	4.77861100
C	-2.59539000	-3.37055000	5.60252600
H	-3.03368800	-3.79473000	4.69311200
H	-3.41941600	-3.21648600	6.30800700
C	-1.54957300	-4.35535900	6.19224400
H	-1.61913300	-5.31652600	5.67224000
H	-1.76050100	-4.55448200	7.24901700
C	-0.10084600	-3.82624700	6.06451600

H	0.61772400	-4.63282100	6.24446600
H	0.06951400	-3.07583900	6.85062200
C	2.35506600	-3.39028900	1.62294600
C	2.04282200	-4.04626300	0.42642200
C	3.65819500	-2.93514700	1.83975600
C	3.00217600	-4.22093800	-0.57155900
H	1.02120100	-4.36526400	0.27131100
C	4.64585400	-3.06798600	0.84910500
H	3.88722200	-2.43858200	2.77974700
C	4.29165200	-3.70860300	-0.34368000
H	5.03325300	-3.80417700	-1.12463600
C	-3.24014900	0.84764200	-0.54706800
C	-3.19159000	2.09452700	-1.18236900
C	-3.71168000	-0.25365800	-1.27946300
C	-3.60691200	2.26971400	-2.50740200
H	-2.79885900	2.94272000	-0.63558900
C	-4.06085600	-0.13463800	-2.62198800
H	-3.77437600	-1.21093600	-0.79052200
C	-4.01563300	1.13740500	-3.21569700
H	-4.30320900	1.23638700	-4.25555100
C	-4.43292000	-1.36118700	-3.46682200
C	-4.51187600	-2.64886400	-2.62805000
H	-4.79339400	-3.48798700	-3.27404500
H	-3.55264200	-2.89812000	-2.16224800
H	-5.26688600	-2.56995800	-1.83788500
C	-3.33678700	-1.55866000	-4.53754100
H	-3.56025300	-2.43352800	-5.16022700
H	-3.25645900	-0.68840000	-5.19817600
H	-2.36439000	-1.71673700	-4.05913900
C	-5.79716400	-1.14339200	-4.15320400



H	-6.58784600	-0.99931200	-3.40833600
H	-5.79152400	-0.26699800	-4.80953500
H	-6.05903700	-2.01495000	-4.76488000
C	-3.65318800	3.68596700	-3.10208200
C	-2.32115200	4.42814400	-2.86578700
H	-1.48461500	3.89191900	-3.32161000
H	-2.36602900	5.43145400	-3.30631400
H	-2.10803200	4.55047400	-1.79951500
C	-4.79041700	4.46171400	-2.39967200
H	-5.75375200	3.96369100	-2.55509900
H	-4.61713100	4.52359500	-1.32010000
H	-4.86278300	5.48330600	-2.79328700
C	-3.93725400	3.68057200	-4.61340500
H	-4.91336000	3.24022900	-4.84253100
H	-3.94341600	4.70886500	-4.99161400
H	-3.17297100	3.12527400	-5.16634100
C	6.04542300	-2.47940100	1.08173800
C	6.71065900	-3.21007700	2.26688100
H	6.81534400	-4.27953000	2.05376300
H	7.70870800	-2.79907200	2.46032200
H	6.12046700	-3.10847700	3.18364200
C	6.94896700	-2.61700800	-0.15502200
H	7.10927400	-3.66521700	-0.42923000
H	6.52472000	-2.09051200	-1.01750800
H	7.92925000	-2.17606800	0.05571800
C	5.92810200	-0.97245300	1.40318400
H	5.46745300	-0.43004700	0.57047400
H	5.33573600	-0.79441200	2.30792400
H	6.92189600	-0.54378400	1.57729700
C	2.62664700	-4.85652800	-1.91833400

C	3.80471100	-5.65520300	-2.50919100
H	4.14803700	-6.42726000	-1.81151900
H	3.48904700	-6.14947000	-3.43454000
H	4.66008700	-5.01864600	-2.75913800
C	1.41685100	-5.80195400	-1.78036900
H	0.50700600	-5.26424900	-1.50068200
H	1.22957400	-6.29522500	-2.74094900
H	1.60738000	-6.58049100	-1.03276600
C	2.24316300	-3.71896900	-2.89136300
H	1.38232900	-3.16171200	-2.50637400
H	3.08036200	-3.02570600	-3.03939300
H	1.96937300	-4.12671100	-3.87190400
O	0.34548900	-1.66039300	0.87147400
O	-2.15147700	-1.59776600	0.65138500
P	-0.84457700	-2.09819800	-0.20772400
O	-0.97299200	-3.55733800	-0.44555900
O	-0.53948800	-1.14633400	-1.37264400
H	1.76477500	-1.02578900	-3.01354800
C	2.07161200	-0.01256000	-2.73198100
C	1.33988700	1.43405500	-0.56765200
C	1.81977600	1.34268000	0.75556400
C	1.54489600	2.28454200	1.73973900
C	0.75635700	3.37000000	1.36631900
C	0.25225000	3.47794100	0.06141200
C	0.52195400	2.51397200	-0.90957400
C	1.72257600	0.17011000	-1.25251800
C	2.52759000	-0.51761800	-0.29073200
H	1.91884200	2.17421600	2.75260500
H	0.51970700	4.13436400	2.09962300
H	-0.37011300	4.32880300	-0.19820600

H	0.09404200	2.59603100	-1.89982400
H	0.62482900	-0.48334000	-1.19605700
H	3.01918300	-1.47303100	-0.39064200
N	2.55792600	0.15117400	0.85268900
H	2.93774700	-0.23845500	1.70615900
C	3.58500700	-0.00072300	-2.94761600
O	4.42599300	0.18200800	-2.08955100
O	3.88542300	-0.29152900	-4.22399300
C	5.28776700	-0.36105400	-4.53043800
H	5.76936700	-1.14010400	-3.93353400
H	5.34112800	-0.60023600	-5.59209200
H	5.77167700	0.59687000	-4.32445100
C	1.32228500	0.94083900	-3.64568500
C	0.00394300	0.63765500	-4.00270600
C	1.89892700	2.13203900	-4.09539000
C	-0.71610400	1.50394600	-4.82239000
H	-0.46473400	-0.25849100	-3.60965200
C	1.17809100	2.99834900	-4.91662500
H	2.91368600	2.38824700	-3.80239800
C	-0.12912400	2.68125400	-5.28953800
H	-1.73939100	1.25767400	-5.08345300
H	1.63729800	3.91947000	-5.26417200
H	-0.69104500	3.35442900	-5.93080600

### S-TS3

C	0.02321300	-3.38619600	4.52325000
C	-0.88690400	-2.37864900	4.15299200
H	1.80625300	-4.47059000	3.98987600
C	1.09211600	-3.70796300	3.68917400
C	-0.72462700	-1.68872200	2.93735800

C	0.27255300	-2.15059100	2.05608900
C	1.21846000	-3.11631200	2.42855900
C	-1.48414600	-0.45740700	2.56387700
C	-1.45472300	0.70147200	3.38073100
C	-2.09978700	-0.39106800	1.30540700
C	-0.71264100	0.70093200	4.70605300
C	-2.08951500	1.86953700	2.92610600
C	-2.66815200	0.78938700	0.80202700
C	-0.43452700	2.09848700	5.26588200
H	0.22078900	0.13668900	4.59994500
C	-2.11328400	3.14862900	3.74420500
C	-2.67209100	1.89290400	1.65827200
C	-1.70216900	2.95009100	5.20368900
H	-0.06831800	2.01089600	6.29570200
H	-1.43136000	3.87560800	3.27825000
H	-3.14157800	2.81158100	1.31577400
H	-2.50623200	2.43976000	5.75191000
H	-3.11273700	3.59724700	3.68490800
H	-1.55270600	3.92208200	5.68836600
H	0.35855100	2.58694200	4.68689000
H	-1.30117700	0.15875600	5.45436100
C	-2.07772400	-2.20395300	5.06334600
H	-1.76971300	-1.77781300	6.02894300
H	-2.80635200	-1.51676300	4.62531400
C	-2.72195700	-3.58334500	5.31926600
H	-3.13319400	-3.94259400	4.37010400
H	-3.56775600	-3.46673400	6.00592700
C	-1.70529300	-4.61585100	5.87717700
H	-1.77106200	-5.54267300	5.29770600
H	-1.94916900	-4.87583600	6.91347500

C	-0.24738300	-4.09917400	5.82304200
H	0.45637700	-4.92552600	5.96892000
H	-0.09013800	-3.40413600	6.66107100
C	2.32812000	-3.43645800	1.49101800
C	2.04466500	-3.94553900	0.22309300
C	3.65259800	-3.11626400	1.82907900
C	3.05332200	-4.11709900	-0.73317800
H	1.01341900	-4.15927300	-0.02412300
C	4.68604100	-3.25566800	0.89464400
H	3.85285400	-2.73939900	2.82752400
C	4.35982300	-3.75766500	-0.37705900
H	5.15252600	-3.86324300	-1.10827700
C	-3.16525400	0.90746400	-0.59007100
C	-2.88766500	2.07600700	-1.31199200
C	-3.88119000	-0.12300100	-1.21174400
C	-3.32013300	2.23936100	-2.63044200
H	-2.29886600	2.84702700	-0.83204900
C	-4.30097300	-0.01034900	-2.53774300
H	-4.08762600	-1.02018900	-0.64889200
C	-4.02089900	1.18072000	-3.22089400
H	-4.35577000	1.28461400	-4.24814700
C	-5.03277800	-1.15043200	-3.26021800
C	-5.24361700	-2.37434000	-2.35302100
H	-5.75526000	-3.16387800	-2.91478300
H	-4.29248700	-2.78131200	-1.99337000
H	-5.86341300	-2.13100500	-1.48300100
C	-4.18951500	-1.59984900	-4.47352000
H	-4.70197100	-2.40104200	-5.01968700
H	-4.01343300	-0.77575800	-5.17313700
H	-3.21723100	-1.97956400	-4.14244800

C	-6.41192500	-0.65587300	-3.74490700
H	-7.02664600	-0.33139200	-2.89790500
H	-6.32112900	0.18921600	-4.43520000
H	-6.94505100	-1.45966900	-4.26692500
C	-3.08494700	3.53467100	-3.42193900
C	-2.17633100	4.52086200	-2.66898600
H	-1.18951900	4.08469100	-2.48328900
H	-2.03438200	5.42437300	-3.27243000
H	-2.61095800	4.82861900	-1.71138100
C	-4.45133800	4.21280000	-3.66349200
H	-5.12456900	3.56133000	-4.23046800
H	-4.94102600	4.45211900	-2.71271900
H	-4.32429800	5.14408600	-4.22921700
C	-2.41625000	3.22486000	-4.77785800
H	-3.02536200	2.55064400	-5.38875000
H	-2.27807100	4.15126500	-5.34884500
H	-1.43794600	2.76408700	-4.61989700
C	6.13439000	-2.83939900	1.18973100
C	6.30620700	-2.28655100	2.61387400
H	6.03048300	-3.02623200	3.37292800
H	7.35316000	-2.01186400	2.78015000
H	5.70200000	-1.38622800	2.77874800
C	7.06447400	-4.06094700	1.03005900
H	6.78672300	-4.85343800	1.73334200
H	7.01349900	-4.47796100	0.01967900
H	8.10544200	-3.77763100	1.22559300
C	6.55756100	-1.73672600	0.19207400
H	6.50632100	-2.08708700	-0.84366600
H	5.91047700	-0.85561500	0.27942200
H	7.58847900	-1.41884800	0.38677100

C	2.69480300	-4.57506300	-2.15460000
C	3.88345500	-5.27007600	-2.84394700
H	4.24500400	-6.11999400	-2.25400700
H	3.57230800	-5.64588900	-3.82448200
H	4.72505500	-4.58945900	-3.01362300
C	1.49753300	-5.54794700	-2.14088500
H	0.57897600	-5.05985700	-1.80541200
H	1.32201500	-5.92259100	-3.15576900
H	1.69646100	-6.40882000	-1.49224100
C	2.29861800	-3.32330900	-2.97127700
H	1.43786800	-2.81215100	-2.52946800
H	3.13868100	-2.61909200	-3.03126000
H	2.02908700	-3.60300000	-3.99651900
O	0.37152800	-1.59109400	0.79968700
O	-2.12764600	-1.54329600	0.53504100
P	-0.79987100	-1.93015700	-0.35571200
O	-0.88671300	-3.36982400	-0.71466700
O	-0.49236300	-0.86169100	-1.39781100
H	2.63709400	-0.45943400	-2.94944200
C	2.28931800	0.51056800	-2.58884200
C	1.56595700	1.41913700	-0.17884900
C	2.12682000	1.10845000	1.07206300
C	1.96037000	1.89741100	2.20398400
C	1.20049100	3.05508100	2.04656800
C	0.61529500	3.37699100	0.81321500
C	0.78052500	2.56255800	-0.30635000
C	1.89565800	0.29887600	-1.10656100
C	2.74564700	-0.55742600	-0.31327500
H	2.39387800	1.62730900	3.16169900
H	1.05201900	3.71354600	2.89539700

H	0.01453700	4.27767800	0.73057600
H	0.31340400	2.79597600	-1.25385300
H	0.85968600	-0.33213500	-1.15886900
H	3.20432800	-1.49581400	-0.59333800
N	2.84611100	-0.09528100	0.91863600
H	3.23673500	-0.65383000	1.67121900
C	1.02212000	0.82195700	-3.37610700
O	0.42048300	1.87967800	-3.35284500
O	0.61992600	-0.25869100	-4.04411100
C	-0.73596400	-0.22425300	-4.53777700
H	-0.84267800	0.54292500	-5.30761200
H	-0.91080400	-1.21589000	-4.95240400
H	-1.41445700	-0.02853300	-3.70711300
C	3.43031100	1.50552400	-2.70732900
C	4.73517700	1.01414600	-2.57138400
C	3.23839200	2.88173100	-2.86507700
C	5.82974300	1.87607600	-2.58628100
H	4.89496000	-0.05589800	-2.45259700
C	4.33557000	3.74445500	-2.88717100
H	2.23371400	3.26899400	-2.97885400
C	5.63126900	3.24883800	-2.74423200
H	6.83434200	1.47561600	-2.48201700
H	4.17292700	4.81113800	-3.01442000
H	6.48094200	3.92554100	-2.75878800

**R-pdt**

C	1.82802100	-1.53710900	-0.13895100
C	0.73567800	-0.54072200	-0.50620200
O	1.91824000	-2.15420200	0.90135000
C	1.20950300	0.83671700	-0.03120400



C	1.07342800	1.20388300	1.31070300
C	1.81380100	1.72332400	-0.92608600
C	1.52648000	2.44692000	1.74823400
H	0.60228100	0.51213100	2.00201300
C	2.26402200	2.97009500	-0.49019200
H	1.93128300	1.43441500	-1.96746900
C	2.12089800	3.33472300	0.84878300
H	1.41257500	2.72496400	2.79237100
H	2.72405100	3.65542300	-1.19679300
H	2.46813100	4.30604500	1.18971900
O	2.75050000	-1.60349900	-1.12166400
C	3.89269100	-2.42562800	-0.83339900
H	4.53023400	-2.35909500	-1.71503400
H	3.58545000	-3.45948200	-0.65629500
H	4.41632100	-2.05358800	0.05102000
H	0.69584000	-0.50935900	-1.60081300
C	-1.83079200	-0.19794800	-0.31734500
C	-2.90071200	-0.83764800	0.36668900
C	-4.22368900	-0.40276800	0.25184400
C	-4.46877300	0.69682300	-0.56331900
C	-3.42205200	1.34964800	-1.24500400
C	-2.10810900	0.91390800	-1.12837000
C	-0.62125700	-0.90609700	0.02572000
C	-0.98257100	-1.91119400	0.88882300
H	-5.03084900	-0.90273500	0.78044200
H	-5.48616300	1.06119300	-0.67332300
H	-3.64953500	2.21042500	-1.86725100
H	-1.30439100	1.43231300	-1.64306700
H	-0.36342000	-2.64486000	1.37960700
N	-2.35127800	-1.87713600	1.09079500

H -2.86219200 -2.50780500 1.68746000

**S-pdt**

C -1.82818800 -1.53707300 -0.13873700  
C -0.73580700 -0.54078800 -0.50617100  
O -1.91828800 -2.15421600 0.90154200  
C -1.20940500 0.83672200 -0.03125800  
C -1.07251200 1.20425900 1.31049500  
C -1.81432700 1.72306000 -0.92595900  
C -1.52532600 2.44737100 1.74798300  
H -0.60090200 0.51268900 2.00166900  
C -2.26434100 2.96993600 -0.49010100  
H -1.93248900 1.43388400 -1.96719300  
C -2.12036500 3.33492400 0.84866600  
H -1.41078400 2.72571200 2.79196800  
H -2.72485800 3.65503900 -1.19660000  
H -2.46738400 4.30633400 1.18957200  
O -2.75091100 -1.60329700 -1.12123700  
C -3.89317500 -2.42517000 -0.83272800  
H -4.53121700 -2.35803300 -1.71395800  
H -3.58617900 -3.45922700 -0.65632700  
H -4.41618700 -2.05343800 0.05218700  
H -0.69610700 -0.50954700 -1.60080600  
C 1.83073300 -0.19794900 -0.31730800  
C 2.90072100 -0.83802500 0.36624200  
C 4.22367700 -0.40308500 0.25146000  
C 4.46866100 0.69694800 -0.56315100  
C 3.42186900 1.35012100 -1.24437100  
C 2.10793200 0.91430800 -1.12780600  
C 0.62120400 -0.90627200 0.02556000

C	0.98260500	-1.91183500	0.88804400
H	5.03091200	-0.90332400	0.77968400
H	5.48604400	1.06136200	-0.67307200
H	3.64926400	2.21121200	-1.86621200
H	1.30414400	1.43295500	-1.64214100
H	0.36356700	-2.64574200	1.37861000
N	2.35139000	-1.87797000	1.08980100
H	2.86230200	-2.50869200	1.68641200

**S-Me-cat**

C	-2.14847300	-1.44669200	1.21227300
C	-2.94782100	-0.29066300	1.23285000
H	-0.73150100	-2.61590400	0.10034900
C	-1.36193800	-1.73109600	0.10180600
C	-2.95717900	0.57260000	0.12034900
C	-2.23107600	0.18703200	-1.02326400
C	-1.39894200	-0.93845200	-1.05309200
C	-3.70433600	1.86665000	0.11527500
C	-3.45571200	2.90400400	1.03581000
C	-4.63178600	2.11134200	-0.90533700
C	-2.39552400	2.86282800	2.10951400
C	-4.16374300	4.11583700	0.92855700
C	-5.32605400	3.31580700	-1.05458000
C	-2.92148700	3.35585700	3.47836000
H	-1.58057100	3.53039100	1.79291700
C	-3.86146900	5.18497400	1.94839800
C	-5.08909700	4.30528700	-0.09332900
C	-3.86213900	4.58396900	3.36556300
H	-3.45595100	2.53904500	3.97286300
H	-2.87341300	5.62404800	1.74299100

H	-5.62524300	5.24767100	-0.16636100
H	-4.88897300	4.28381600	3.60306900
H	-4.58721000	6.00206300	1.87524200
H	-3.58301600	5.35170700	4.09537200
H	-2.05921800	3.58890000	4.11294000
H	-1.95056700	1.87142400	2.20337200
C	-3.83202500	-0.11937400	2.44592700
H	-4.32483800	0.85457300	2.45167900
H	-4.63910900	-0.86196000	2.36070800
C	-3.09412900	-0.36413600	3.78566100
H	-3.84325600	-0.61969300	4.54344700
H	-2.62549500	0.56616000	4.12024100
C	-2.01489400	-1.47167000	3.70009300
H	-2.04433000	-2.10542100	4.59326400
H	-1.01920800	-1.01393700	3.67185300
C	-2.17115500	-2.33079100	2.43357000
H	-3.12362900	-2.88027400	2.48205600
H	-1.37826200	-3.08422800	2.37562700
C	-0.54354100	-1.29203600	-2.21540100
C	-1.07084200	-1.43548400	-3.50386600
C	0.82256600	-1.52375600	-2.00861900
C	-0.25136000	-1.79216600	-4.57697100
H	-2.12923200	-1.28232900	-3.67751200
C	1.66391400	-1.87803300	-3.06724600
H	1.23763300	-1.40247000	-1.01094100
C	1.11134800	-2.00777100	-4.34479600
H	1.75716400	-2.28169600	-5.17745300
C	-6.17962300	3.57773500	-2.23933800
C	-6.00771600	4.77475700	-2.95443300
C	-7.11899300	2.64658700	-2.69735300

C	-6.75497000	5.04641900	-4.10245700
H	-5.25717400	5.48604600	-2.62051800
C	-7.87723100	2.89190100	-3.84762300
H	-7.25178000	1.71458200	-2.15855300
C	-7.68207700	4.09091700	-4.53812500
H	-8.25977600	4.28432000	-5.43964900
O	-2.28660200	1.00288600	-2.16574600
O	-4.80433900	1.12064200	-1.88050000
P	-3.65588600	1.04785400	-3.02661400
O	-3.94533500	-0.02598800	-3.99469200
O	-3.47700600	2.53600600	-3.60849700
H	-4.24358100	2.79790500	-4.14759100
C	-6.57738300	6.34473300	-4.85210800
H	-5.60204400	6.79621400	-4.64465100
H	-6.66164600	6.19756600	-5.93423200
H	-7.34500200	7.07479400	-4.56399400
C	-8.87735200	1.86819200	-4.32790500
H	-9.34430500	2.17615600	-5.26828300
H	-8.39964200	0.89486100	-4.48932000
H	-9.67547100	1.71758600	-3.59071200
C	-0.84293900	-1.96292600	-5.95575800
H	-1.80387300	-1.44583500	-6.03488400
H	-0.17385500	-1.56986700	-6.72960100
H	-1.01659700	-3.02257800	-6.18558800
C	3.14371900	-2.07689800	-2.84096600
H	3.55883300	-2.81505000	-3.53547000
H	3.69844400	-1.14113100	-2.99107300
H	3.35043000	-2.41683400	-1.82060000

**Me-R-TS2**

C	0.04156400	-2.97797600	4.84293000
C	-0.94511700	-2.00021200	4.62877900
H	1.83481800	-3.89469800	4.08935100
C	1.05763300	-3.15663000	3.90885800
C	-0.91297900	-1.21876500	3.46286400
C	0.05341800	-1.51528200	2.48181100
C	1.08036800	-2.44095700	2.70348300
C	-1.77710800	-0.02065400	3.25763600
C	-1.70099400	1.08324700	4.14099100
C	-2.52401700	0.08296500	2.07351900
C	-0.76248000	1.06765000	5.33316700
C	-2.44504000	2.23755000	3.84782800
C	-3.22831000	1.25326600	1.73573600
C	-0.37052300	2.47321600	5.79366500
H	0.12867500	0.48179700	5.08944800
C	-2.38141900	3.49012600	4.70602800
C	-3.20092500	2.28815900	2.67740800
C	-1.63275500	3.30350200	6.02774700
H	0.23124100	2.40542100	6.70745600
H	-1.87618700	4.27309200	4.12181600
H	-3.76874800	3.19126200	2.47142900
H	-2.27395800	2.78222300	6.75233700
H	-3.39856000	3.86062800	4.88779900
H	-1.39394700	4.28183300	6.46065100
H	0.25666800	2.95176000	5.02948000
H	-1.23926300	0.54951800	6.17555700
C	-2.04192700	-1.92868300	5.66132700
H	-1.64588400	-1.53884100	6.61034200
H	-2.83658600	-1.24809400	5.34449300
C	-2.61064200	-3.34308500	5.90643300

H	-3.14353000	-3.65194800	5.00091500
H	-3.35463600	-3.29846100	6.70971800
C	-1.50535100	-4.38191900	6.24360200
H	-1.59890900	-5.24373300	5.57436300
H	-1.63214100	-4.76230300	7.26353400
C	-0.07948300	-3.80076700	6.09953500
H	0.66380900	-4.60505400	6.11244800
H	0.13215600	-3.16659400	6.97342000
C	2.19351300	-2.63044000	1.73842600
C	1.95790900	-3.00715500	0.40943300
C	3.51133100	-2.45948500	2.17818900
C	3.02190600	-3.21874300	-0.46966700
H	0.93583600	-3.15122800	0.07365100
C	4.59317600	-2.64632300	1.30941000
H	3.69311900	-2.16324900	3.20886100
C	4.33112000	-3.02911000	-0.00784900
H	5.16395100	-3.18857000	-0.69061200
C	-3.89190000	1.46678000	0.42536100
C	-3.89118400	2.75360100	-0.13616800
C	-4.51382900	0.43193200	-0.28805400
C	-4.50640000	3.02160800	-1.36142400
H	-3.38708100	3.56346200	0.38392700
C	-5.10957400	0.66560900	-1.52867800
H	-4.51617100	-0.56983200	0.12308100
C	-5.10108700	1.96357400	-2.05418400
H	-5.57387600	2.15286400	-3.01644300
C	-5.77218800	-0.46708900	-2.27579100
C	-4.53678000	4.43122300	-1.90337300
C	6.00676200	-2.40064400	1.78061700
C	2.77101000	-3.65109100	-1.89424400

O	0.04146200	-0.78780300	1.30347000
O	-2.48363000	-0.99313800	1.20157100
P	-1.18266400	-1.04878100	0.16819300
O	-1.10276600	-2.41179700	-0.42740200
O	-1.14392800	0.20529200	-0.66673300
H	0.35151000	1.19863800	-1.06015300
C	2.41601600	1.93969700	-1.23844400
C	0.97496100	1.88381600	-1.63407900
O	3.26257700	2.68888600	-1.68794900
S	1.46472300	0.04696200	-3.17239500
O	2.84178100	-0.54439100	-3.15948900
C	0.18763300	-1.23146200	-3.09504300
H	0.28533700	-1.77655600	-2.15492400
H	-0.78362700	-0.73432600	-3.09102600
H	0.31845600	-1.89299700	-3.95555300
C	1.13963400	0.74617000	-4.81738700
H	1.31261700	-0.04151800	-5.55459400
H	0.11446200	1.11768100	-4.86159400
H	1.84280900	1.56785800	-4.96290900
C	0.29492400	2.79324600	-2.52535900
C	0.95196100	3.81076800	-3.25000900
C	-1.09056200	2.57639200	-2.72042200
C	0.23568400	4.58153600	-4.15860900
H	2.01060500	3.97020200	-3.08407200
C	-1.78766300	3.34191000	-3.64662000
H	-1.58775600	1.80065300	-2.14316900
C	-1.12734600	4.34296000	-4.36758000
H	0.73959700	5.36727800	-4.71367900
H	-2.84593000	3.15959500	-3.79766800
H	-1.67624000	4.94196600	-5.08887500



O	2.63372500	0.95109300	-0.36940200
C	3.99918200	0.73130500	0.03560400
H	4.40535700	1.64350700	0.47406600
H	3.94508400	-0.07025900	0.76778000
H	4.58297900	0.42561000	-0.83495600
C	2.06029700	3.46874100	1.57974800
C	1.57319200	2.25097300	2.14379800
C	2.31633800	1.49463500	3.05379600
C	3.56092900	1.99097200	3.42315400
C	4.05821400	3.20376200	2.89481500
C	3.32586600	3.94150200	1.97499400
C	1.06663200	3.90947700	0.64767100
C	0.03348400	2.97961500	0.68848000
H	1.94056800	0.55034100	3.43480800
H	4.16803800	1.43120000	4.12884700
H	5.03548400	3.55712800	3.21074600
H	3.72291800	4.86355700	1.56012500
H	1.09472700	4.79875000	0.03411400
H	-0.91037500	2.95439700	0.16626700
N	0.32964700	2.00999900	1.60478600
H	-0.12150400	1.10033800	1.62815800
H	-3.54407600	4.89460500	-1.87626500
H	-5.88916100	-0.23133200	-3.33877900
H	2.98823600	-2.83443200	-2.59193100
H	6.13584300	-2.68849700	2.82968700
H	-6.77227100	-0.67698100	-1.87446300
H	-5.18936300	-1.39040700	-2.19166400
H	-4.89201100	4.45531800	-2.93898800
H	-5.20840500	5.06651500	-1.31217000
H	6.73145800	-2.96226600	1.18216800

H	6.27398900	-1.33772800	1.70243700
H	3.40645800	-4.50148400	-2.16900700
H	1.72760700	-3.95141100	-2.03359600

**Me-S-TS2**

C	0.10756800	-3.12939400	4.47378000
C	-0.82865300	-2.11356000	4.20931200
H	1.84473000	-4.18257800	3.77399300
C	1.11169000	-3.41124300	3.55250800
C	-0.76001600	-1.39668900	3.00467600
C	0.20593600	-1.77913200	2.05369200
C	1.18446900	-2.74778100	2.31905500
C	-1.61525400	-0.20734400	2.71139500
C	-1.54329500	0.97041600	3.49460500
C	-2.36103600	-0.19387600	1.52682400
C	-0.57614100	1.05576600	4.66071600
C	-2.28502100	2.09792200	3.10200800
C	-3.09019300	0.92922300	1.10557000
C	-0.18190600	2.49533300	4.99856000
H	0.31485300	0.46244500	4.43275600
C	-2.18948800	3.42513900	3.83543600
C	-3.05560700	2.05006500	1.93561700
C	-1.44074900	3.34634300	5.16745600
H	0.42541900	2.50421500	5.91098800
H	-1.66145500	4.13343900	3.17968700
H	-3.61299200	2.93563700	1.63744300
H	-2.08389600	2.89095100	5.93370200
H	-3.19627900	3.83798900	3.98028700
H	-1.19658600	4.35667200	5.51587300
H	0.43999800	2.90717700	4.19288800

H	-1.02511200	0.59748000	5.55225700
C	-1.91158300	-1.92447900	5.24133600
H	-1.48432000	-1.49673300	6.16018500
H	-2.67233700	-1.22294600	4.88922500
C	-2.55485000	-3.28707900	5.57894100
H	-3.12775400	-3.61365200	4.70447400
H	-3.27506200	-3.15261200	6.39381600
C	-1.50570600	-4.37128500	5.95090000
H	-1.65241100	-5.25297900	5.31796200
H	-1.64431600	-4.70276600	6.98622500
C	-0.05193100	-3.87703600	5.77254100
H	0.64656900	-4.71897700	5.82598700
H	0.19917500	-3.21005200	6.61080400
C	2.30945900	-2.98822100	1.37943800
C	2.10228200	-3.16397000	0.00584300
C	3.62280600	-2.98880100	1.87459800
C	3.18273300	-3.30882300	-0.86969300
H	1.09405800	-3.17398700	-0.39380700
C	4.71780100	-3.15665400	1.02284000
H	3.79011500	-2.82878000	2.93720600
C	4.48091000	-3.31085200	-0.34838400
H	5.32660900	-3.41784700	-1.02541400
C	-3.74566000	0.95870300	-0.22457200
C	-3.53146700	2.04712800	-1.08071700
C	-4.52373300	-0.11271500	-0.67830400
C	-4.06779600	2.06851200	-2.37057900
H	-2.88815200	2.85858900	-0.75383400
C	-5.07374300	-0.11687300	-1.96226600
H	-4.67994000	-0.96628500	-0.02764100
C	-4.83623300	0.97964100	-2.79756300

H	-5.25465200	0.98383500	-3.80235800
C	-5.90139700	-1.28912700	-2.43095800
C	-3.78227900	3.22022400	-3.30579300
C	6.12447800	-3.17373700	1.57191700
C	2.93190100	-3.39663800	-2.35545300
O	0.26630100	-1.07941200	0.86371700
O	-2.25177600	-1.28663900	0.68143600
P	-0.92897200	-1.20651000	-0.31997300
O	-0.85485400	-2.46442700	-1.11271500
O	-0.84436400	0.15099000	-0.96711800
H	0.13245400	1.65213600	-1.34635200
C	0.86492900	2.13234600	-1.98790300
S	0.36008900	0.75241200	-3.69692500
O	1.48297800	-0.21408700	-3.84344200
C	-1.24603700	-0.09585100	-3.72986200
H	-1.12460400	-0.99688800	-3.12559100
H	-2.00049900	0.54654800	-3.27274700
H	-1.46674200	-0.32609100	-4.77612700
C	0.24876300	1.77638800	-5.18994300
H	0.23632800	1.10441300	-6.05133000
H	-0.66498700	2.37451900	-5.14418500
H	1.12101300	2.43009800	-5.21052300
C	2.58224100	3.07830100	1.57051600
C	2.08475100	1.75654800	1.78292100
C	2.87702300	0.72910000	2.30630500
C	4.19918600	1.03177300	2.59772500
C	4.72056100	2.32767600	2.38497200
C	3.92692400	3.34917200	1.88267800
C	1.49382300	3.84339600	1.03174900
C	0.41450400	2.99065600	0.92893200

H	2.47956800	-0.26908700	2.44824800
H	4.84708300	0.25246300	2.98943600
H	5.76158400	2.52590400	2.62511800
H	4.33791700	4.34318100	1.72649800
H	1.50489400	4.89275800	0.76986400
H	-0.58915600	3.16653900	0.57564300
N	0.76575300	1.74411200	1.38806300
H	0.22513200	0.89899400	1.24091100
C	0.47666900	3.48308600	-2.50752500
O	1.05979900	4.11399100	-3.36939000
O	-0.64903700	3.91780200	-1.91317500
C	-1.05397100	5.25383900	-2.26441600
H	-1.25585600	5.32392600	-3.33532400
H	-1.95849400	5.44084600	-1.68808800
H	-0.26745500	5.96344900	-1.99746400
C	2.24719300	1.79176500	-1.74959300
C	2.49965200	0.58354900	-1.06162300
C	3.33593900	2.60313400	-2.14666700
C	3.80060500	0.20629400	-0.75587300
H	1.66819100	-0.03753400	-0.76036300
C	4.62749000	2.22593800	-1.81924000
H	3.15082800	3.52659700	-2.67973800
C	4.86129600	1.03165600	-1.12257000
H	3.97737400	-0.71459600	-0.21544800
H	5.46151800	2.86291500	-2.09823400
H	5.87752700	0.75004300	-0.86233600
H	-5.35878700	-2.23203200	-2.29784800
H	-2.73141700	3.22329000	-3.62644400
H	2.65614700	-2.41427900	-2.75961400
H	6.20955800	-2.55427600	2.47142300

H	-6.16506400	-1.19556100	-3.48926200
H	-6.83533500	-1.37096000	-1.86107600
H	-4.40401400	3.16891800	-4.20507100
H	-3.96833100	4.18742500	-2.82495700
H	2.10033100	-4.07409200	-2.57621400
H	3.81851000	-3.74742400	-2.89406000
H	6.84595500	-2.80350800	0.83560500
H	6.43433400	-4.19075700	1.84700200

### **S-Cy-cat**

C	-2.27105800	-1.48945000	1.32870400
C	-3.03549600	-0.31332700	1.42078200
H	-0.95205100	-2.66936800	0.11176300
C	-1.55604400	-1.76811300	0.16960600
C	-3.08326000	0.57913200	0.33165500
C	-2.43356100	0.20039300	-0.86062600
C	-1.63770200	-0.94736200	-0.96251600
C	-3.79766200	1.89064000	0.40189000
C	-3.48749200	2.89456100	1.34122000
C	-4.76138400	2.18818600	-0.56931200
C	-2.38037100	2.80213400	2.36319000
C	-4.17442900	4.12310600	1.30094400
C	-5.42260200	3.41825200	-0.66508000
C	-2.83026400	3.26388900	3.76988800
H	-1.56904100	3.46476600	2.02747200
C	-3.81142100	5.15170900	2.34276200
C	-5.12866000	4.36949500	0.31812800
C	-3.76472200	4.50086600	3.73663400
H	-3.34488600	2.43938000	4.27249700
H	-2.82525400	5.58244500	2.11181700

H	-5.63514500	5.33061300	0.28886200
H	-4.78457500	4.19878200	4.00050700
H	-4.52576500	5.98187100	2.32762600
H	-3.45302800	5.23938600	4.48323000
H	-1.93380200	3.47531500	4.36336600
H	-1.94965800	1.80099700	2.40617700
C	-3.84837600	-0.15314700	2.68451700
H	-4.31625900	0.83120500	2.74206300
H	-4.67699900	-0.87417500	2.62448000
C	-3.04609800	-0.45122700	3.97563500
H	-3.76005100	-0.70647800	4.76676100
H	-2.53454700	0.45743700	4.30661400
C	-2.00407100	-1.58416600	3.80417600
H	-2.00308400	-2.24033900	4.68149100
H	-0.99904100	-1.15224400	3.73311600
C	-2.25257300	-2.40443500	2.52705600
H	-3.21625500	-2.92915500	2.61372400
H	-1.48571300	-3.17719500	2.40668700
C	-0.86791000	-1.29563800	-2.18422300
C	-1.48113500	-1.38793800	-3.43786200
C	0.50254700	-1.56776400	-2.07782200
C	-0.74429400	-1.71970400	-4.57678600
H	-2.54456000	-1.20739100	-3.53663000
C	1.26229500	-1.91102800	-3.19937100
H	0.98765600	-1.48837500	-1.10783900
C	0.62404000	-1.97758800	-4.44295100
H	1.20569900	-2.23298200	-5.32493000
C	-6.23734700	3.74202200	-1.86105800
C	-5.98979100	4.94100200	-2.54673200
C	-7.13770300	2.82473900	-2.41799900

C	-6.58835500	5.20950100	-3.78053700
H	-5.26953300	5.64529900	-2.13951500
C	-7.73564200	3.05482900	-3.66026400
H	-7.33965000	1.89382800	-1.90082700
C	-7.44482500	4.24761000	-4.33209200
H	-7.88133600	4.42709900	-5.30985600
O	-2.52590600	1.03904800	-1.98499300
O	-5.00737200	1.22300200	-1.55322000
P	-3.93692400	1.14620700	-2.76952600
O	-4.32624700	0.10323200	-3.73885900
O	-3.73615800	2.63340700	-3.34193100
H	-4.51727700	2.92972000	-3.84227400
C	-6.25035100	6.47868400	-4.53578300
C	-5.41983200	6.17545200	-5.80145600
C	-7.49815600	7.30857900	-4.89790900
H	-5.62475700	7.09937300	-3.87774600
C	-5.04950900	7.45609800	-6.55929300
H	-6.00244300	5.51603500	-6.46030000
H	-4.51666600	5.61879800	-5.52106400
C	-7.12295900	8.59038200	-5.65273300
H	-8.16640600	6.70317900	-5.52579800
H	-8.05873600	7.54620700	-3.98575500
C	-6.29625900	8.27955500	-6.90730100
H	-4.48922900	7.20605000	-7.46855100
H	-4.37852400	8.06313300	-5.93425500
H	-8.02930100	9.14743000	-5.92029700
H	-6.53845500	9.24303800	-4.98788100
H	-6.00976700	9.20873800	-7.41499700
H	-6.91691600	7.71186000	-7.61608300
C	-8.57790800	1.96618700	-4.29308200



C	-9.87395900	2.47376300	-4.95016100
C	-7.73374300	1.16271000	-5.30970500
H	-8.86792100	1.26945400	-3.49317000
C	-10.67994600	1.31791700	-5.55743200
H	-9.62807700	3.18881200	-5.74744600
H	-10.47497200	3.02066100	-4.21325200
C	-8.54004200	0.01701800	-5.93300100
H	-7.39602600	1.84836000	-6.10113600
H	-6.83195900	0.77479200	-4.82102300
C	-9.84158800	0.52356900	-6.56776500
H	-11.58944000	1.70398100	-6.03433500
H	-11.00910000	0.64506000	-4.75218400
H	-7.92893200	-0.50839900	-6.67690200
H	-8.78058700	-0.71785700	-5.15121600
H	-10.42343000	-0.31577500	-6.96846700
H	-9.59776400	1.17340700	-7.42128700
C	-1.43262400	-1.77315700	-5.92532900
C	-0.90523100	-0.67934800	-6.87716800
C	-1.32711800	-3.15975100	-6.59080900
H	-2.49847800	-1.56699200	-5.75575000
C	-1.62673500	-0.71269200	-8.23013900
H	0.17295700	-0.82743800	-7.03440100
H	-1.02052500	0.30203700	-6.40187300
C	-2.04962800	-3.19200100	-7.94363600
H	-0.26719400	-3.41077300	-6.74019100
H	-1.73615600	-3.92217100	-5.91677300
C	-1.52719400	-2.09742400	-8.88344700
H	-1.21447000	0.05503800	-8.89718900
H	-2.68624800	-0.46099300	-8.07753900
H	-1.93793000	-4.17988900	-8.40821500

H	-3.12652100	-3.04179900	-7.77920800
H	-2.07926200	-2.11321300	-9.83163900
H	-0.47491800	-2.30534900	-9.12833500
C	2.74575600	-2.19095500	-3.06726800
C	3.10365800	-3.63446600	-3.47707000
C	3.60084900	-1.18152000	-3.86095000
H	3.01188600	-2.07846300	-2.00563400
C	4.60398500	-3.91364100	-3.32218100
H	2.81094100	-3.79285300	-4.52442600
H	2.51476700	-4.34129000	-2.87996100
C	5.10088300	-1.46188300	-3.70574000
H	3.32864300	-1.23936500	-4.92410000
H	3.36114800	-0.16258200	-3.53399000
C	5.44580800	-2.90121600	-4.10969600
H	4.83268100	-4.93629700	-3.64738500
H	4.87379100	-3.85553900	-2.25736400
H	5.68156200	-0.74758200	-4.30276700
H	5.39124600	-1.30261400	-2.65678600
H	6.51524900	-3.09452600	-3.95901200
H	5.25084600	-3.02990900	-5.18461300

### **Cy-R-TS2**

C	-0.72580000	-3.22361800	4.30056100
C	-1.48565300	-2.08297700	3.98808800
H	1.05586900	-4.33382700	3.93438100
C	0.48158400	-3.45611800	3.65635500
C	-0.98810000	-1.15650000	3.05781700
C	0.21987100	-1.44616000	2.39258800
C	0.97702100	-2.60464400	2.65198800
C	-1.73569200	0.08560600	2.70180700

C	-2.06839400	1.07399600	3.65712000
C	-2.09923200	0.28788100	1.36453200
C	-1.55352900	0.96273700	5.08156000
C	-2.83002600	2.18694900	3.25860000
C	-2.87535700	1.37472400	0.95553200
C	-1.54484400	2.30417400	5.81926000
H	-0.55224000	0.51940600	5.07044400
C	-3.18285000	3.31011400	4.21907700
C	-3.24168500	2.30392900	1.92626100
C	-2.91343600	2.97342800	5.68739900
H	-1.28404700	2.14314900	6.87180900
H	-2.59234000	4.19723000	3.94582700
H	-3.84131700	3.16079200	1.62788800
H	-3.68606400	2.28746400	6.06250600
H	-4.23293400	3.59530100	4.07601200
H	-2.97283400	3.88340800	6.29573800
H	-0.77364100	2.96106600	5.39407400
H	-2.18267600	0.26700700	5.65118100
C	-2.85827000	-2.01532900	4.61147000
H	-2.78050700	-1.81932200	5.69090100
H	-3.44637100	-1.20083500	4.18215500
C	-3.57822500	-3.36410400	4.40158800
H	-3.75008700	-3.48535900	3.32591400
H	-4.56561100	-3.32895000	4.87548100
C	-2.75844600	-4.56729000	4.93984800
H	-2.72661900	-5.35631000	4.18056600
H	-3.24538300	-5.00109500	5.82055300
C	-1.30898200	-4.17476600	5.31367500
H	-0.68484800	-5.06902400	5.41490700
H	-1.32073900	-3.69045200	6.30084900

C	2.19678300	-2.98673300	1.88963900
C	2.56440900	-4.34369600	1.79434300
C	3.00719200	-2.05292900	1.23254600
C	3.69160100	-4.75891000	1.08742300
H	1.94987100	-5.10258200	2.26862600
C	4.11112300	-2.44173800	0.46474800
H	2.76761800	-1.00101100	1.29577100
C	4.45493400	-3.79386300	0.41247100
H	5.31479200	-4.11053900	-0.16885200
C	-3.27660000	1.52262700	-0.47096900
C	-2.58103100	2.38350000	-1.31903600
C	-4.34335400	0.77248100	-0.98546600
C	-2.93762800	2.51669100	-2.66879300
H	-1.71215900	2.90928200	-0.93510600
C	-4.73214400	0.89418900	-2.31997100
H	-4.86903000	0.08118100	-0.33168500
C	-4.02572200	1.78169700	-3.14519400
H	-4.30751100	1.86451500	-4.18933300
O	0.64964500	-0.52467500	1.45135000
O	-1.65889000	-0.61211500	0.40637900
P	-0.05334300	-0.50955800	-0.04074700
O	0.18805800	-1.78906300	-0.79207400
O	0.27798900	0.82300200	-0.64988300
H	-0.48401400	-2.30215000	-2.59369000
C	-1.04897400	-2.87276300	-3.32345300
S	0.35628600	-4.79476900	-2.14017700
O	0.53288200	-6.21067300	-2.63515300
C	1.96165200	-3.99062400	-1.95476300
H	2.36318800	-3.85835400	-2.95934600
H	1.77900300	-3.02544700	-1.48026200

H	2.60530100	-4.61877100	-1.34270900
C	-0.20520800	-4.81799000	-0.41548100
H	0.48493200	-5.43811600	0.16059300
H	-0.20467400	-3.78527300	-0.06043800
H	-1.21049100	-5.24424600	-0.40713800
C	-0.59976200	-0.25683800	-5.39301900
C	0.25403000	0.45797300	-4.50545100
C	1.45198400	1.03124100	-4.92333400
C	1.79460600	0.88537600	-6.26673600
C	0.96224900	0.19091500	-7.16468800
C	-0.23206600	-0.38280200	-6.74049300
C	-1.71011600	-0.72146300	-4.60758000
C	-1.51266700	-0.21575200	-3.31183000
H	2.08934800	1.57002000	-4.22949200
H	2.72155500	1.32022900	-6.62831700
H	1.25868000	0.10707500	-8.20604700
H	-0.87508700	-0.91009500	-7.43972200
H	-2.60590600	-1.20623600	-4.96244200
H	-2.13657600	-0.30824600	-2.43671500
N	-0.34987500	0.46448300	-3.25504200
H	0.04806600	0.77138500	-2.34429300
C	-0.27982200	-3.14474500	-4.56734600
O	0.90691900	-2.89662600	-4.65805300
O	-0.99537400	-3.70091000	-5.56522100
C	-0.22551000	-4.05480300	-6.73055600
H	-0.95084600	-4.43429600	-7.45001700
H	0.29395400	-3.17773700	-7.11914100
H	0.50406400	-4.82670300	-6.47368000
C	-2.37819700	-3.29849800	-2.93885500
C	-3.22357900	-4.10814000	-3.72827700

C	-2.83589600	-2.87129600	-1.66967500
C	-4.48244300	-4.46638300	-3.25995100
H	-2.88323700	-4.44820900	-4.69644300
C	-4.09869100	-3.22834400	-1.21629600
H	-2.18962300	-2.26273000	-1.04888500
C	-4.92739900	-4.02723400	-2.00903300
H	-5.12492500	-5.08908400	-3.87505400
H	-4.43224200	-2.88108800	-0.24310700
H	-5.91562100	-4.30757100	-1.65590100
C	-2.09428000	3.41070400	-3.55855300
C	-2.20742400	3.11246900	-5.06137600
C	-2.36988900	4.90755500	-3.30068800
H	-1.04704700	3.22735600	-3.27447400
C	-1.22896600	3.97533900	-5.86649400
H	-3.23099800	3.32709000	-5.40160100
H	-2.02394500	2.05076500	-5.25297900
C	-1.41370700	5.79465500	-4.10929500
H	-3.41130000	5.12700100	-3.57751200
H	-2.27777600	5.12428500	-2.22975200
C	-1.46680300	5.46927500	-5.60834600
H	-1.32399900	3.75252100	-6.93639700
H	-0.20102000	3.70773800	-5.58365000
H	-1.64687200	6.85349000	-3.94062300
H	-0.38887000	5.63653600	-3.74299900
H	-0.73232300	6.07460100	-6.15429700
H	-2.45642100	5.74638800	-6.00083200
C	-5.86914300	0.05683200	-2.86912500
C	-7.04364900	0.91883900	-3.37401400
C	-5.39427800	-0.90382000	-3.97800500
H	-6.24825800	-0.56616300	-2.04554200

C	-8.19164600	0.05422200	-3.91068500
H	-6.68353100	1.58189200	-4.17313100
H	-7.39574300	1.56984200	-2.56474400
C	-6.54238900	-1.76703300	-4.51143600
H	-4.96683100	-0.31627600	-4.80275500
H	-4.59134700	-1.53737800	-3.58990900
C	-7.70827900	-0.90320100	-5.00809500
H	-8.99935100	0.69287600	-4.28926100
H	-8.61767400	-0.53256100	-3.08352300
H	-6.17843800	-2.42361300	-5.31181500
H	-6.89608800	-2.42668100	-3.70613200
H	-8.53503000	-1.53679700	-5.35280600
H	-7.37725400	-0.31659400	-5.87774800
C	4.82159400	-1.36706900	-0.33970200
C	6.25619300	-1.71142600	-0.76586300
C	3.97911000	-0.99069900	-1.58297100
H	4.87371500	-0.46852900	0.29404800
C	6.89919200	-0.55145400	-1.53824500
H	6.24260700	-2.59828300	-1.41537000
H	6.85937900	-1.97247700	0.11278400
C	4.61612200	0.15352600	-2.37907500
H	3.89445000	-1.87814700	-2.22527300
H	2.96011600	-0.72420000	-1.28194700
C	6.06445400	-0.16933300	-2.76813000
H	7.91981100	-0.81956100	-1.83880000
H	6.98610900	0.32049400	-0.87375300
H	4.01693500	0.35677900	-3.27558200
H	4.59769000	1.06929700	-1.77051400
H	6.52113300	0.68207400	-3.28846800
H	6.06659800	-1.00999000	-3.47752200

C	4.06021500	-6.23061300	1.03560600
C	3.91319700	-6.83634700	-0.37733000
C	5.48037800	-6.48506900	1.58240800
H	3.35900600	-6.76841000	1.69118900
C	4.28821400	-8.32364200	-0.40292500
H	4.56286500	-6.28535500	-1.07252300
H	2.88675700	-6.71076600	-0.74245700
C	5.84481500	-7.97457000	1.55782000
H	6.20519800	-5.92698200	0.97367700
H	5.55610000	-6.08405500	2.60035800
C	5.69945400	-8.56041500	0.14773300
H	4.20288200	-8.71110700	-1.42531300
H	3.56486500	-8.88589900	0.20562200
H	6.86730500	-8.11723100	1.92921200
H	5.18224900	-8.52065100	2.24539200
H	5.93244900	-9.63249700	0.15311000
H	6.43235800	-8.08193700	-0.51856000

### Cy-S-TS2

C	0.39471500	-3.64077800	3.50117000
C	-0.66634600	-2.71688300	3.45657700
H	2.29351000	-4.23035000	2.69248200
C	1.48789200	-3.50204200	2.65027800
C	-0.59429300	-1.61727400	2.57916300
C	0.51773100	-1.52404000	1.72735200
C	1.56587800	-2.45723100	1.71997500
C	-1.65671300	-0.57108100	2.47997800
C	-2.03262400	0.20028200	3.60588600
C	-2.26654600	-0.31543500	1.23822800
C	-1.24575600	0.10237800	4.90163700



C	-3.10123900	1.10523200	3.49338400
C	-3.35229100	0.56650500	1.11534100
C	-1.41740300	1.33360300	5.79545900
H	-0.18837900	-0.06541200	4.67149200
C	-3.53352600	2.00001300	4.64274300
C	-3.75814200	1.24114800	2.26924800
C	-2.90622000	1.62466100	5.98708800
H	-0.92205400	1.16006600	6.75787800
H	-3.25311100	3.03518800	4.39840700
H	-4.58395900	1.94399400	2.19078400
H	-3.39698600	0.72909100	6.39365800
H	-4.62878900	1.99708200	4.71421900
H	-3.06563700	2.43164500	6.71156000
H	-0.92965200	2.20368900	5.33497600
H	-1.57123100	-0.77447100	5.47443900
C	-1.85940800	-3.04506100	4.32149200
H	-1.60966200	-2.88150900	5.37981300
H	-2.70273200	-2.38874500	4.09240400
C	-2.27187300	-4.52186500	4.14467100
H	-2.70677700	-4.63658800	3.14621400
H	-3.07160500	-4.75732400	4.85516200
C	-1.08639100	-5.51002900	4.30962900
H	-1.02782100	-6.16442500	3.43213800
H	-1.24921100	-6.16622300	5.17161900
C	0.26664900	-4.78423800	4.47531100
H	1.09509300	-5.49060200	4.35626700
H	0.33422100	-4.39611800	5.50218900
C	2.63497300	-2.40104100	0.69460900
C	3.07773500	-3.57831300	0.07575800
C	3.17282300	-1.18337800	0.26547700

C	4.02168600	-3.55026300	-0.95357600
H	2.65391200	-4.53268600	0.37916400
C	4.07719000	-1.11653000	-0.79652300
H	2.84886600	-0.26394200	0.73712300
C	4.50137100	-2.30882500	-1.39163700
H	5.21286500	-2.27297800	-2.20800800
C	-4.07788700	0.79496200	-0.16109200
C	-3.40495200	1.08971000	-1.35453000
C	-5.48098700	0.77688200	-0.16511200
C	-4.11282600	1.37903900	-2.52565100
H	-2.32052800	1.11349700	-1.37080100
C	-6.21212900	1.05994800	-1.32270500
H	-6.01085000	0.52760500	0.75117900
C	-5.51169200	1.36802700	-2.49424100
H	-6.06721300	1.59525100	-3.40003900
O	0.51401700	-0.49661600	0.79713500
O	-1.86411300	-1.02178400	0.11808100
P	-0.34683700	-0.83795300	-0.56933300
O	-0.01041300	-2.20626900	-1.09305200
O	-0.26351500	0.36600900	-1.46215700
H	-1.20322000	-2.97066400	-2.36023200
C	-1.67970600	-3.70600700	-3.00421000
S	-2.36409800	-4.87585500	-0.78139400
O	-2.93766000	-6.26684600	-0.82133800
C	-0.81984000	-4.86737800	0.16291000
H	-0.14045100	-5.55238600	-0.34918300
H	-0.41557300	-3.85196200	0.13172800
H	-1.01766100	-5.21223900	1.17988000
C	-3.38579400	-3.80160700	0.26197900
H	-3.44000100	-4.22853900	1.26574000

H	-2.92952900	-2.80926000	0.26133400
H	-4.37882800	-3.76861100	-0.18894700
C	0.11508700	-2.51839000	-5.50809400
C	0.99516000	-1.78766800	-4.65521800
C	2.37583300	-1.98211000	-4.67449200
C	2.87674100	-2.91573000	-5.57908600
C	2.02587900	-3.64899300	-6.42853700
C	0.64937000	-3.46173400	-6.39883800
C	-1.21801200	-2.12267500	-5.16168300
C	-1.09609500	-1.16554400	-4.15277500
H	3.03056900	-1.45009300	-3.99363100
H	3.94824200	-3.08621300	-5.62340600
H	2.45525500	-4.37686900	-7.11056900
H	-0.00533900	-4.04294800	-7.04118600
H	-2.13634100	-2.43605500	-5.63595800
H	-1.85485800	-0.64835600	-3.58900900
N	0.21241500	-0.95190000	-3.87155700
H	0.47501500	-0.40628900	-3.04542400
C	-3.11664800	-3.47527900	-3.31673000
O	-3.81114500	-4.10826800	-4.08789100
O	-3.56202700	-2.43660800	-2.58060400
C	-4.96056400	-2.12090500	-2.69783200
H	-5.15087500	-1.37866400	-1.92678500
H	-5.17211200	-1.70353600	-3.68458500
H	-5.56295500	-3.02102000	-2.55065900
C	-0.85722100	-4.75712600	-3.51540400
C	0.50762000	-4.73826300	-3.13372500
C	-1.33838000	-5.80162700	-4.33740600
C	1.36046900	-5.74258000	-3.56833600
H	0.86497700	-3.93069800	-2.50175700

C	-0.47098200	-6.79914800	-4.76080200
H	-2.38305800	-5.80848600	-4.62031700
C	0.87405200	-6.77383900	-4.37641500
H	2.40427000	-5.72295000	-3.28326500
H	-0.84153200	-7.60481800	-5.38737700
H	1.54684600	-7.55848000	-4.71152800
C	-3.35741200	1.73212400	-3.79146800
C	-3.79334800	0.89646400	-5.01158500
C	-3.46206500	3.23575800	-4.12225300
H	-2.29521600	1.52247700	-3.60490400
C	-2.96125700	1.24157700	-6.25222300
H	-4.85426500	1.08815400	-5.22426300
H	-3.71388500	-0.17301200	-4.78312400
C	-2.63884000	3.59344700	-5.36633600
H	-4.51833800	3.49212600	-4.28955700
H	-3.12957400	3.82267100	-3.25803400
C	-3.04392900	2.73935600	-6.57511500
H	-3.29782600	0.64594900	-7.11004400
H	-1.91396700	0.96272600	-6.07001500
H	-2.74980600	4.65997100	-5.59872900
H	-1.57379700	3.42824800	-5.14880300
H	-2.41145700	2.97771600	-7.43918000
H	-4.07632600	2.98839700	-6.86228800
C	-7.72644600	1.00494900	-1.31032900
C	-8.36768100	2.35068900	-1.70546400
C	-8.26560500	-0.12953400	-2.20753700
H	-8.04298800	0.78287500	-0.28044300
C	-9.89965300	2.27948400	-1.67763800
H	-8.03693500	2.62451800	-2.71695100
H	-8.00405800	3.13923700	-1.03572800

C	-9.79769300	-0.19760000	-2.18488500
H	-7.92264100	0.03726200	-3.23845200
H	-7.83496400	-1.08638700	-1.88584600
C	-10.42304400	1.14857900	-2.57245500
H	-10.32670400	3.24116700	-1.98792600
H	-10.23473400	2.10634000	-0.64442400
H	-10.14943600	-0.99090300	-2.85612000
H	-10.13094400	-0.47190300	-1.17329200
H	-11.51700200	1.09101700	-2.51504300
H	-10.17398900	1.37342700	-3.61999300
C	4.49288700	0.25895400	-1.28930500
C	5.72857500	0.27884000	-2.20088400
C	3.30736400	0.95946500	-1.99558600
H	4.73298300	0.86300300	-0.40026000
C	6.09641900	1.71114500	-2.61105900
H	5.52121200	-0.30380700	-3.11045900
H	6.57582600	-0.20819500	-1.70174300
C	3.66432500	2.38896900	-2.41725400
H	3.04340700	0.37662400	-2.88972600
H	2.41932900	0.95426200	-1.35558400
C	4.91956600	2.41629000	-3.29860500
H	6.97288100	1.69963200	-3.27100500
H	6.38568200	2.27928300	-1.71497900
H	2.81630500	2.84594500	-2.94159000
H	3.83985100	2.99559200	-1.51684300
H	5.18978300	3.44935000	-3.55071600
H	4.70231400	1.90688600	-4.24917200
C	4.51917000	-4.86102300	-1.53363600
C	4.92945000	-4.79136800	-3.01375900
C	5.68468800	-5.43345100	-0.69659400

H	3.69166600	-5.58355400	-1.45527200
C	5.35095000	-6.16858200	-3.54108900
H	5.77816600	-4.10302400	-3.12615400
H	4.11154600	-4.37645200	-3.61219800
C	6.13396800	-6.80476300	-1.21765200
H	6.52353400	-4.72387500	-0.73545700
H	5.38231100	-5.50170800	0.35522800
C	6.49898100	-6.75279300	-2.70720400
H	5.64282600	-6.09535200	-4.59613900
H	4.49111100	-6.85463500	-3.50187900
H	6.98425000	-7.17228500	-0.62983500
H	5.31724500	-7.52731500	-1.07260600
H	6.76522200	-7.75334700	-3.06983300
H	7.39080200	-6.12269300	-2.83774900

**S<sup>j</sup>Pr-cat**

C	-2.02160000	-1.12093200	1.37932700
C	-2.87640200	-0.00512700	1.39772500
H	-0.60992400	-2.26777500	0.23741500
C	-1.28302500	-1.41494100	0.23901900
C	-2.98971700	0.80988900	0.25430400
C	-2.30768000	0.40973800	-0.91238700
C	-1.42358800	-0.67556600	-0.94262300
C	-3.80665100	2.06167800	0.24236700
C	-3.57935400	3.14567000	1.11368000
C	-4.79148000	2.21628900	-0.74065200
C	-2.46828600	3.20881000	2.13354700
C	-4.36453300	4.30883200	0.99867900
C	-5.55481100	3.37695100	-0.90813000
C	-2.95394800	3.72259500	3.50991600

H	-1.71306000	3.91147200	1.75154200
C	-4.08568100	5.42895400	1.96957400
C	-5.33886100	4.41078700	0.00998500
C	-3.98454400	4.87621900	3.40248600
H	-3.40093600	2.89345000	4.06665800
H	-3.13823000	5.92253700	1.70483200
H	-5.92643300	5.32111000	-0.07465600
H	-4.97649100	4.51170800	3.69257100
H	-4.86537000	6.19555000	1.90540400
H	-3.73177100	5.68461600	4.09713300
H	-2.07742500	4.04259300	4.08422300
H	-1.95839600	2.25029800	2.23865600
C	-3.70446400	0.17061600	2.64942400
H	-4.24833700	1.11687200	2.64479900
H	-4.47369500	-0.61562700	2.63585200
C	-2.88665200	0.01875400	3.95611900
H	-3.58133200	-0.24338000	4.76200000
H	-2.45117200	0.98442700	4.22954500
C	-1.75639400	-1.03508700	3.85513000
H	-1.70500000	-1.63142900	4.77270800
H	-0.78919700	-0.52908200	3.75412200
C	-1.93430500	-1.95308500	2.63375300
H	-2.85319300	-2.54662300	2.75565900
H	-1.10769300	-2.66810100	2.56186300
C	-0.61785700	-1.03766200	-2.13715400
C	-1.20885300	-1.25399500	-3.38899500
C	0.76500300	-1.20037000	-2.00079300
C	-0.43690200	-1.60758200	-4.49513300
H	-2.28139200	-1.15640700	-3.50647600
C	1.56225800	-1.56209000	-3.09321600

H	1.22264600	-1.02042300	-1.03171500
C	0.94641100	-1.75776800	-4.33074700
H	1.56289800	-2.03221600	-5.18415300
C	-6.41582400	3.55132400	-2.10304200
C	-6.30462600	4.72754300	-2.85665000
C	-7.24989400	2.52634300	-2.57334800
C	-6.98904800	4.88003600	-4.06815000
H	-5.63488100	5.50932200	-2.51108400
C	-7.92531800	2.63971900	-3.78944500
H	-7.34304200	1.61046300	-2.00099700
C	-7.78261500	3.82360300	-4.52524200
H	-8.28967800	3.92841800	-5.48069900
O	-2.46037800	1.16774100	-2.08599000
O	-4.95320800	1.17638400	-1.66410800
P	-3.87311200	1.12050300	-2.87339400
O	-4.17221500	0.00046200	-3.78664300
O	-3.79106200	2.58937200	-3.51907800
H	-4.59667600	2.80212400	-4.02251600
C	-6.83244200	6.14558100	-4.89453900
H	-7.48827900	6.04546000	-5.76947500
C	-8.70070100	1.44715600	-4.32346400
H	-8.93601800	0.80655700	-3.46325100
C	-10.02552800	1.82817700	-4.99763100
H	-9.86058600	2.40191600	-5.91690700
H	-10.58318500	0.92646700	-5.27371500
H	-10.65387900	2.43026900	-4.33242400
C	-7.80349400	0.63255200	-5.27606400
H	-7.53537900	1.23204500	-6.15487700
H	-6.87540800	0.32138200	-4.78429600
H	-8.32495500	-0.26560800	-5.62733200



C	-7.27972500	7.39349700	-4.11607500
H	-7.21508200	8.28686700	-4.74770300
H	-8.31297000	7.29164500	-3.76793300
H	-6.64524900	7.55999800	-3.23784200
C	-5.39023600	6.30036400	-5.40745000
H	-4.68501100	6.40611200	-4.57502600
H	-5.08496100	5.42750100	-5.99503500
H	-5.29600300	7.18921800	-6.04182800
C	-1.10151500	-1.81569200	-5.84565500
H	-2.17576700	-1.64464100	-5.70390000
C	3.06523300	-1.72618700	-2.93998100
H	3.46107800	-2.02211300	-3.92074800
C	3.74031700	-0.40180500	-2.54590600
H	3.39249800	-0.05999800	-1.56411200
H	4.82907800	-0.52046200	-2.49295000
H	3.51360800	0.38585900	-3.27206500
C	3.41438200	-2.84224700	-1.94142900
H	3.05607600	-2.59620300	-0.93495300
H	2.95520600	-3.79175200	-2.23636300
H	4.49964200	-2.98691500	-1.88319000
C	-0.60109000	-0.79107300	-6.87747500
H	-1.12710300	-0.91374500	-7.83165000
H	-0.76518800	0.23191400	-6.52303100
H	0.47191000	-0.91254100	-7.06858300
C	-0.91371000	-3.25341900	-6.35658500
H	-1.44466000	-3.40056200	-7.30449900
H	0.14580700	-3.47744600	-6.52912700
H	-1.29569100	-3.98097300	-5.63252700

C	-0.38157900	-3.40251000	3.94141300
C	-1.24587200	-2.33232100	3.65381600
H	1.47729300	-4.35413000	3.52403200
C	0.82115500	-3.53131500	3.26025500
C	-0.86044200	-1.37145100	2.70562200
C	0.33763100	-1.56780200	1.99166600
C	1.20361500	-2.65269500	2.22991400
C	-1.71611100	-0.19109300	2.38661900
C	-2.08459500	0.75945000	3.36726200
C	-2.15768900	-0.01223100	1.06947100
C	-1.49427400	0.68187400	4.76470000
C	-2.96190300	1.80193400	3.02040100
C	-3.04509600	1.00702100	0.71272400
C	-1.57287600	2.01083000	5.52057300
H	-0.45821200	0.33299500	4.70092700
C	-3.36654600	2.88076800	4.01065000
C	-3.44722200	1.89073700	1.71078400
C	-3.00074700	2.55481400	5.46040800
H	-1.25005800	1.86325500	6.55777200
H	-2.86938800	3.81918300	3.72328500
H	-4.13438500	2.69276000	1.45125400
H	-3.69047500	1.79789600	5.85987500
H	-4.44307500	3.07361800	3.91910400
H	-3.11343100	3.44931900	6.08392900
H	-0.88456200	2.73946600	5.07069600
H	-2.02894500	-0.07472700	5.35301000
C	-2.60285900	-2.38605900	4.31143700
H	-2.51750600	-2.19411000	5.39091100
H	-3.26889800	-1.62184100	3.90411000
C	-3.20592200	-3.79150600	4.10294300

H	-3.38655000	-3.92041000	3.02892200
H	-4.18324100	-3.84794700	4.59520600
C	-2.27179200	-4.92107800	4.61442200
H	-2.18496000	-5.69852900	3.84754200
H	-2.70073400	-5.40256000	5.50041800
C	-0.85530200	-4.40358200	4.96327900
H	-0.15316300	-5.23984300	5.04705700
H	-0.89024400	-3.92579300	5.95295100
C	2.41449900	-2.94471000	1.41382100
C	2.89965300	-4.26325500	1.33474100
C	3.08678700	-1.95895200	0.67594200
C	4.00427100	-4.60091000	0.55114900
H	2.38832800	-5.05198000	1.87440200
C	4.16694300	-2.27329100	-0.15186800
H	2.74518500	-0.93641900	0.72755500
C	4.62321400	-3.59285200	-0.19636300
H	5.46591500	-3.84583100	-0.83728800
C	-3.51539100	1.12785100	-0.69581300
C	-2.80064200	1.91875700	-1.60406200
C	-4.63566800	0.41698500	-1.13002200
C	-3.18870200	1.99916400	-2.94217800
H	-1.90636700	2.41979900	-1.25576600
C	-5.05031100	0.47897300	-2.46701900
H	-5.17161900	-0.20436200	-0.41813400
C	-4.31798400	1.27365200	-3.35041400
H	-4.61500600	1.30603900	-4.39711800
C	-6.26001700	-0.30362000	-2.94948500
C	-7.56105400	0.28651800	-2.37866200
H	-8.43645000	-0.24885300	-2.76525800
H	-7.57458100	0.21009300	-1.28505200

H	-7.66042900	1.34522400	-2.64023800
C	-6.15136600	-1.80199100	-2.62451100
H	-6.99979700	-2.35211700	-3.04788000
H	-5.22989400	-2.23703700	-3.02295800
H	-6.14981300	-1.97740000	-1.54376900
C	-2.41725900	2.81067600	-3.97374900
C	-1.03609300	3.27449600	-3.49726600
H	-0.43925300	2.45226400	-3.09279400
H	-0.48612300	3.72553300	-4.33039900
H	-1.12259400	4.03411300	-2.71117500
C	-3.25168300	4.01636400	-4.44550700
H	-4.22342100	3.70391400	-4.84184800
H	-3.43621400	4.70257400	-3.61049000
H	-2.72442600	4.56969700	-5.23147000
C	4.78969200	-1.19735700	-1.02553200
C	3.78219500	-0.70481300	-2.08244200
H	2.90959300	-0.23203900	-1.61796800
H	4.25175400	0.03113100	-2.74653200
H	3.41818000	-1.53613300	-2.69581500
C	5.33621200	-0.02415800	-0.19632300
H	4.52970500	0.49218200	0.33594900
H	6.06331200	-0.36928400	0.54680800
H	5.82825700	0.70961500	-0.84527200
C	4.53907600	-6.02535300	0.51705600
C	5.27426900	-6.35165600	1.82969100
H	4.58093500	-6.31984400	2.67867900
H	5.71789900	-7.35364900	1.79208000
H	6.07189400	-5.62699600	2.02408600
C	3.45819000	-7.08012700	0.22682100
H	2.70385600	-7.10764200	1.02228500

H	2.93998700	-6.90089500	-0.72111600
H	3.90751000	-8.07841200	0.17533700
O	0.62517600	-0.63908700	1.00087300
O	-1.72948800	-0.89016800	0.08898000
P	-0.14657300	-0.81290200	-0.44648900
O	0.08188500	-2.17338400	-1.04272200
O	0.11337000	0.43829700	-1.23665500
H	-0.85718300	-2.89099100	-2.61832300
C	-1.49882200	-3.53621900	-3.20931800
S	0.30751100	-5.26859200	-2.14537900
O	0.54544600	-6.70572600	-2.55035500
C	1.85713800	-4.33820800	-2.25852100
H	2.09089500	-4.25768400	-3.32084400
H	1.67676400	-3.35243000	-1.82557900
H	2.63472200	-4.87548700	-1.71666100
C	-0.00269700	-5.19163900	-0.35877900
H	0.78618500	-5.74665600	0.15040400
H	-0.00677500	-4.13920600	-0.06991200
H	-0.97569200	-5.65475900	-0.18129500
C	-1.72644800	-1.18191400	-5.59022300
C	-0.71109900	-0.37972300	-4.99479800
C	0.33110200	0.17174100	-5.73509300
C	0.34754700	-0.08864200	-7.10352000
C	-0.64672900	-0.87706700	-7.71513200
C	-1.68350200	-1.42866500	-6.97083500
C	-2.59062700	-1.60287900	-4.52541800
C	-2.10796400	-0.98836400	-3.35721200
H	1.09814100	0.77600500	-5.26164900
H	1.14504300	0.32618000	-7.71270200
H	-0.60130400	-1.05104300	-8.78614300

H	-2.45073400	-2.03354600	-7.44607800
H	-3.51643200	-2.15056000	-4.61121500
H	-2.51260700	-1.00070400	-2.35679100
N	-0.99213800	-0.28540600	-3.63841600
H	-0.41767000	0.13229300	-2.88377900
C	-0.91005100	-3.86460400	-4.53384100
O	0.21260400	-3.51217700	-4.84051800
O	-1.70577400	-4.58816600	-5.34561000
C	-1.09249300	-4.98625600	-6.58738700
H	-1.87104200	-5.51688000	-7.13521300
H	-0.75265700	-4.10735300	-7.13719900
H	-0.24367900	-5.64476600	-6.38784700
C	-2.68730600	-4.04336500	-2.56127000
C	-3.60466300	-4.94242700	-3.14746900
C	-2.92104600	-3.59675100	-1.23813400
C	-4.71480600	-5.37142800	-2.42938800
H	-3.43374000	-5.29491200	-4.15540700
C	-4.03215800	-4.03380700	-0.53056500
H	-2.22040900	-2.90873100	-0.78073600
C	-4.93417300	-4.92197500	-1.12325800
H	-5.41428200	-6.06383200	-2.88830400
H	-4.19545300	-3.67547800	0.48184400
H	-5.80578700	-5.26299300	-0.57191100
H	-2.26544300	2.15236200	-4.84100000
H	-6.29775800	-0.20027200	-4.04242200
H	5.63608600	-1.65529400	-1.55548600
H	5.27508600	-6.07386900	-0.29663800

***i*Pr-S-TS2**

C	-0.09685000	-3.41914300	3.81226600
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C	-1.04697800	-2.40393300	3.60228900
H	1.78466600	-4.24920300	3.25157800
C	1.07023800	-3.45507900	3.05980400
C	-0.77483000	-1.39221000	2.66394400
C	0.40353500	-1.48108900	1.90035000
C	1.34035800	-2.52210200	2.04273300
C	-1.73867000	-0.28282000	2.39745900
C	-2.17014500	0.58486500	3.42875600
C	-2.25021300	-0.10929600	1.10120200
C	-1.47316800	0.57214400	4.77870600
C	-3.21067200	1.49342700	3.17337600
C	-3.30549900	0.77356900	0.83629200
C	-1.68600100	1.86710900	5.56750400
H	-0.40540100	0.37829900	4.63125800
C	-3.70174800	2.47887900	4.21988800
C	-3.78610000	1.53718800	1.90053700
C	-3.17921400	2.19146300	5.62929300
H	-1.26396200	1.75782300	6.57330500
H	-3.38051700	3.48810200	3.92265400
H	-4.60022900	2.23262400	1.71015900
H	-3.71494000	1.33402400	6.06054800
H	-4.79909800	2.50111200	4.21232500
H	-3.37452800	3.05013800	6.28201600
H	-1.15096400	2.69514900	5.08263300
H	-1.84717800	-0.25843900	5.38927400
C	-2.34041500	-2.54884400	4.36632600
H	-2.16209600	-2.35002300	5.43302400
H	-3.08281000	-1.82146200	4.03084000
C	-2.90301500	-3.98118300	4.22831800
H	-3.31193600	-4.09287900	3.21866800

H	-3.74755600	-4.09376100	4.91698000
C	-1.83777100	-5.08108100	4.48982300
H	-1.73870900	-5.71794700	3.60294600
H	-2.15312800	-5.73742400	5.30833400
C	-0.44987100	-4.48704700	4.81535500
H	0.30977100	-5.27595600	4.82862400
H	-0.47403200	-4.05711000	5.82727500
C	2.47616400	-2.74236200	1.10556900
C	2.94878100	-4.04904300	0.89697700
C	3.04803500	-1.71334500	0.33935500
C	3.92274400	-4.34391200	-0.05775400
H	2.52001400	-4.87408100	1.45571000
C	3.98419000	-1.98279800	-0.66007200
H	2.72133100	-0.69861600	0.49998100
C	4.41246800	-3.30183500	-0.84985500
H	5.14484800	-3.51242900	-1.62724700
C	-3.91779400	0.90992300	-0.51259000
C	-3.16049400	1.36974600	-1.60017100
C	-5.28268800	0.66323700	-0.68072100
C	-3.75094000	1.59809600	-2.84823800
H	-2.10819100	1.56523100	-1.44019500
C	-5.89896000	0.85678500	-1.92384900
H	-5.86476600	0.32521400	0.17266200
C	-5.11932400	1.31105400	-2.98907700
H	-5.60700400	1.47037700	-3.94622600
O	0.58492500	-0.49601100	0.94026700
O	-1.76768100	-0.88783100	0.06326200
P	-0.20545400	-0.71751700	-0.48846300
O	0.12067200	-2.05261800	-1.09401100
O	-0.01909700	0.55131900	-1.27824200



H	-0.94392700	-2.79076300	-2.48826200
C	-1.23637600	-3.49246400	-3.26331200
S	-1.59063700	-5.08746100	-0.97750400
O	-2.16497700	-6.48375900	-0.92055900
C	0.12770300	-5.11482600	-0.40302400
H	0.70835700	-5.69919200	-1.11928300
H	0.48187700	-4.08312800	-0.37446800
H	0.15990700	-5.58169100	0.58462600
C	-2.29163400	-4.08996600	0.37016500
H	-2.04408500	-4.55715200	1.32629000
H	-1.88485400	-3.08051600	0.30202400
H	-3.37333900	-4.07074600	0.22327200
C	0.02314200	-1.77734600	-5.60377200
C	0.78360700	-0.92906700	-4.75152100
C	2.15744600	-0.75701500	-4.90086600
C	2.77778800	-1.46818300	-5.92665700
C	2.04759900	-2.32128300	-6.77517000
C	0.67422700	-2.48265600	-6.62535400
C	-1.32041400	-1.76584300	-5.10013800
C	-1.32402700	-0.88417500	-4.00358600
H	2.71867600	-0.10710400	-4.23809300
H	3.84917800	-1.36388400	-6.07109000
H	2.56916700	-2.86570900	-7.55654200
H	0.11862500	-3.15208600	-7.27453300
H	-2.18888300	-2.21540800	-5.55801100
H	-2.13135200	-0.62156600	-3.33476400
N	-0.08600200	-0.38843500	-3.80909200
H	0.15551800	0.09979600	-2.92514500
C	-2.69889600	-3.66486300	-3.45284700
O	-3.26213500	-4.40673100	-4.23347900

O	-3.33747900	-2.81656600	-2.61831200
C	-4.77089200	-2.81220600	-2.67604000
H	-5.07714300	-2.03659900	-1.97654300
H	-5.11056000	-2.57387500	-3.68761400
H	-5.16594700	-3.78945200	-2.38571000
C	-0.18915500	-4.27019900	-3.84388000
C	1.13251300	-3.92761400	-3.46435000
C	-0.39966100	-5.31945600	-4.76766800
C	2.21118400	-4.61122500	-4.00625300
H	1.27885400	-3.13352100	-2.73945900
C	0.68950000	-6.01050100	-5.28070200
H	-1.41353400	-5.57457400	-5.05070400
C	1.99219300	-5.65845200	-4.90532700
H	3.21875400	-4.33444600	-3.71692700
H	0.52924500	-6.82716000	-5.97825400
H	2.83740500	-6.20268200	-5.31748600
C	-7.39511400	0.64515000	-2.09828100
H	-7.63223300	0.85286400	-3.15026600
C	-2.94663900	2.15826500	-4.02481400
H	-2.69227900	1.31434700	-4.68554600
C	-3.76111200	3.15730600	-4.86636400
H	-3.14034300	3.55841200	-5.67502700
H	-4.64288400	2.70275200	-5.32722300
H	-4.09879500	3.99747400	-4.24842200
C	-1.62749500	2.81771600	-3.59641200
H	-1.82174100	3.67925700	-2.94630900
H	-0.96635500	2.13915500	-3.05505900
H	-1.08917700	3.17630800	-4.48044500
C	-8.19246500	1.64104500	-1.23781400
H	-7.90332900	2.67276800	-1.46339300

H	-9.26883900	1.53611100	-1.41748000
H	-8.01212500	1.46943200	-0.17026700
C	-7.82799700	-0.79963400	-1.80231200
H	-7.33644300	-1.50687100	-2.47827800
H	-7.57983400	-1.08631300	-0.77377500
H	-8.91113900	-0.91228900	-1.92696600
C	4.55315700	-0.88301100	-1.54740400
H	4.56485300	-1.28459500	-2.57208600
C	4.43109100	-5.76863600	-0.21044700
H	3.85087700	-6.39422300	0.48112600
C	4.21648800	-6.32692100	-1.62500700
H	4.54118500	-7.37248000	-1.68074900
H	3.16321500	-6.27739600	-1.91713500
H	4.79482500	-5.76149500	-2.36543400
C	6.00954400	-0.57142900	-1.15552600
H	6.63557100	-1.46926600	-1.19306600
H	6.44411900	0.17876300	-1.82692800
H	6.05107700	-0.17810400	-0.13303500
C	3.71581800	0.40191000	-1.56309700
H	2.65698600	0.20862400	-1.75988600
H	3.77394500	0.92924100	-0.60411900
H	4.09491100	1.08744000	-2.33012500
C	5.91018500	-5.86953800	0.20061000
H	6.54162300	-5.26757400	-0.46341300
H	6.05963700	-5.50515900	1.22233300
H	6.26008000	-6.90734000	0.14859400

**S-Me<sub>2</sub>Ph-cat**

C	-2.63317100	-2.19181100	1.69496800
C	-3.19207500	-0.91155400	1.86246400

H	-1.42216800	-3.46726500	0.46422900
C	-1.86915000	-2.48276600	0.57083300
C	-2.96422900	0.08230700	0.89245600
C	-2.23325800	-0.27418300	-0.25623500
C	-1.67212000	-1.54091900	-0.44917200
C	-3.51424200	1.46704200	1.00398500
C	-3.21342800	2.34138400	2.06513000
C	-4.30207900	1.96017000	-0.04578000
C	-2.26326200	2.02162900	3.19354500
C	-3.74427000	3.64559400	2.06525300
C	-4.78813000	3.27213500	-0.10314900
C	-2.82717100	2.41437000	4.58049500
H	-1.34518500	2.60225300	3.02042500
C	-3.41906500	4.52151400	3.24957400
C	-4.52018700	4.09233700	1.00010000
C	-3.63474700	3.73738000	4.55654300
H	-3.46716000	1.60848600	4.95320700
H	-2.37065800	4.85217400	3.19430000
H	-4.90432700	5.10901900	1.00535200
H	-4.70497900	3.51701500	4.64159700
H	-4.03353700	5.42817700	3.23651400
H	-3.37326700	4.36287200	5.41701000
H	-1.98816700	2.49033000	5.28113100
H	-1.95973000	0.97386700	3.18287400
C	-4.09570400	-0.74160400	3.06035800
H	-4.41382100	0.29477400	3.18469900
H	-5.01275000	-1.31396400	2.85693700
C	-3.47221700	-1.28270700	4.37006900
H	-4.28390000	-1.46756500	5.08264200
H	-2.84012000	-0.50990700	4.81868800

C	-2.63305400	-2.56872100	4.16042400
H	-2.83876500	-3.29493700	4.95441600
H	-1.56602600	-2.32642300	4.22466300
C	-2.88723000	-3.20544900	2.78238600
H	-3.92927500	-3.55610700	2.73109700
H	-2.25359300	-4.08721900	2.63963600
C	-0.94280900	-1.91186900	-1.68509600
C	-1.16219100	-3.16384200	-2.25755200
C	-0.01262200	-1.04272300	-2.28255400
C	-0.47456600	-3.57096900	-3.40867400
H	-1.88091400	-3.83756000	-1.80212300
C	0.67229000	-1.41476500	-3.43349800
H	0.16375600	-0.07852400	-1.82738500
C	0.43153300	-2.68541700	-3.98349000
H	0.98884200	-2.97575800	-4.86637700
C	-5.38542900	3.80025600	-1.35357200
C	-4.93358500	5.03386200	-1.84933100
C	-6.28279600	3.04338300	-2.12087100
C	-5.32690900	5.48769100	-3.10949700
H	-4.23348900	5.60674900	-1.25285800
C	-6.66699300	3.45999800	-3.39757300
H	-6.65014100	2.10932900	-1.72089600
C	-6.16058500	4.67037200	-3.87980900
H	-6.46393700	5.01169400	-4.86336300
O	-2.07877100	0.68194200	-1.27562900
O	-4.54949200	1.10827800	-1.12785200
P	-3.36332200	0.94441400	-2.22736800
O	-3.73663500	-0.02914600	-3.26729900
O	-2.94766300	2.42127500	-2.71036900
H	-3.64172000	2.81557600	-3.26792300

C	-4.85657300	6.82004700	-3.71262600
C	-7.55389200	2.59890200	-4.30974000
C	-6.60508700	1.77940900	-5.21309200
H	-5.92834600	1.17742300	-4.59765700
H	-7.16445900	1.09344400	-5.85877000
H	-5.99716100	2.43256600	-5.84819800
C	-8.42578100	1.60612300	-3.50976700
H	-7.81306500	0.85498400	-3.00101900
H	-9.03911900	2.11998700	-2.76295800
H	-9.09779400	1.08013700	-4.19491700
C	-4.22486700	7.75387200	-2.65929500
H	-3.97494600	8.71246200	-3.12444500
H	-4.91086500	7.95118500	-1.83000200
H	-3.30199600	7.32828900	-2.25047400
C	-3.78032300	6.49978700	-4.77116800
H	-2.95578000	5.95634500	-4.29827500
H	-4.17868900	5.87302700	-5.57496700
H	-3.37031900	7.41396400	-5.21439800
C	-0.77241000	-4.96025400	-3.99008100
C	1.65369900	-0.47841200	-4.15266700
C	0.96406400	-0.00126900	-5.44920300
H	0.00978900	0.47151600	-5.19766000
H	1.57761000	0.73456100	-5.98101300
H	0.75540500	-0.83490400	-6.12670400
C	1.99740600	0.77249700	-3.31573100
H	1.11020000	1.39118400	-3.14327700
H	2.42731200	0.50442000	-2.34572700
H	2.73404300	1.37818300	-3.85296300
C	-2.18506500	-4.91524800	-4.61001200
H	-2.43548900	-5.86182600	-5.10193900

H	-2.95114700	-4.69856700	-3.85963400
H	-2.22533400	-4.12209500	-5.36265800
C	0.22179400	-5.35902500	-5.10153400
H	0.00279700	-6.37735200	-5.43776300
H	0.13825400	-4.69259300	-5.96688500
H	1.25681900	-5.33640700	-4.74735600
C	-6.08253000	7.52873400	-4.31141400
C	-7.20619800	7.73985400	-3.49666300
C	-6.14236300	7.96403600	-5.63775500
C	-8.34866000	8.36107500	-3.98986300
H	-7.19002700	7.38628500	-2.46945800
C	-7.29075300	8.58400600	-6.13963900
H	-5.29741100	7.81398700	-6.30046900
C	-8.39785900	8.78439100	-5.32027700
H	-9.20666600	8.50615900	-3.33886500
H	-7.31547800	8.90318400	-7.17799900
H	-9.29254300	9.25971500	-5.71220200
C	-8.48969600	3.51678900	-5.11007200
C	-9.26498800	4.46410800	-4.42237900
C	-8.60632100	3.46008800	-6.50161800
C	-10.11515200	5.33128300	-5.10018800
H	-9.17172700	4.54235200	-3.34294400
C	-9.46256700	4.32706100	-7.18738800
H	-8.02131100	2.74485900	-7.06880900
C	-10.21667500	5.26815600	-6.49179400
H	-10.68747400	6.06809900	-4.54408300
H	-9.52908200	4.26691400	-8.27045100
H	-10.87264700	5.95015300	-7.02537800
C	-0.65382800	-5.99822600	-2.86340300
C	0.50521500	-6.00884700	-2.07089700

C	-1.63861800	-6.95447300	-2.59986900
C	0.67474400	-6.94296000	-1.05351000
H	1.27321500	-5.26100300	-2.24813900
C	-1.47411000	-7.89336400	-1.57692100
H	-2.54972000	-6.97429400	-3.18742100
C	-0.31844700	-7.89292200	-0.80015000
H	1.58085500	-6.92775000	-0.45354900
H	-2.25713800	-8.62344600	-1.38975200
H	-0.19107300	-8.62120700	-0.00401600
C	2.96242200	-1.23546800	-4.42269500
C	3.58322400	-1.91704600	-3.36389100
C	3.58679400	-1.25757000	-5.67314600
C	4.78528400	-2.59371700	-3.54697700
H	3.10299200	-1.92736500	-2.38936700
C	4.79315800	-1.93829600	-5.86308100
H	3.13539900	-0.74662500	-6.51636300
C	5.39800900	-2.60820200	-4.80274900
H	5.24294600	-3.11567200	-2.71073300
H	5.25535700	-1.94394100	-6.84669400
H	6.33398300	-3.13960100	-4.95067300

**Me<sub>2</sub>Ph-R-TS2**

C	-0.29297800	-3.60440500	3.80932500
C	-1.18182900	-2.54546700	3.55761700
H	1.56778200	-4.51426200	3.36292800
C	0.91112400	-3.68560800	3.12483100
C	-0.81181000	-1.54587800	2.64639500
C	0.39279800	-1.69208800	1.92700000
C	1.28213800	-2.77207800	2.11807600
C	-1.69015500	-0.36955600	2.36995100



C	-2.07375000	0.54133500	3.38135000
C	-2.13221100	-0.14864100	1.05946600
C	-1.49308900	0.41920900	4.77938500
C	-2.95697200	1.58908000	3.06434300
C	-3.01787700	0.87781000	0.72739300
C	-1.58917600	1.71931000	5.58195000
H	-0.45357500	0.08179500	4.71092700
C	-3.37832600	2.62819000	4.08967200
C	-3.43071600	1.72393900	1.75466300
C	-3.02112500	2.25321900	5.52965700
H	-1.27342900	1.53699800	6.61573100
H	-2.88668800	3.58015400	3.83998700
H	-4.11823200	2.53299800	1.51871800
H	-3.70762100	1.47689700	5.89601400
H	-4.45569400	2.81536000	3.99643900
H	-3.14634100	3.12382500	6.18376700
H	-0.90348900	2.46925700	5.16433900
H	-2.02568600	-0.36299000	5.33532700
C	-2.53903600	-2.65379300	4.20684300
H	-2.46041400	-2.50183000	5.29310400
H	-3.22011600	-1.88857200	3.82708500
C	-3.11178200	-4.06268800	3.94144500
H	-3.29946600	-4.14855900	2.86467000
H	-4.08338800	-4.16163000	4.43818300
C	-2.14905800	-5.19265600	4.39767700
H	-2.03357800	-5.92282400	3.58910700
H	-2.57033800	-5.73565800	5.25105200
C	-0.75034000	-4.65630400	4.78637300
H	-0.02884400	-5.47821600	4.84427200
H	-0.80810000	-4.22025000	5.79400800

C	2.46875600	-3.05040800	1.25384400
C	3.09727100	-4.31330000	1.29789300
C	2.95779900	-2.12162000	0.32019900
C	4.13109200	-4.64986200	0.42553000
H	2.77118600	-5.05185200	2.01642800
C	3.91965200	-2.46726300	-0.62959700
H	2.56360000	-1.12314800	0.32077600
C	4.48943000	-3.73781200	-0.57163000
H	5.27037000	-4.00329500	-1.27573200
C	-3.48350500	1.06982300	-0.67649600
C	-2.82461800	1.98071300	-1.51132800
C	-4.61107400	0.38505500	-1.14555400
C	-3.29235900	2.22337000	-2.80581200
H	-1.94792900	2.48634500	-1.12780000
C	-5.09240700	0.60274200	-2.44149400
H	-5.11897400	-0.29667700	-0.47326400
C	-4.40905800	1.51118300	-3.25222200
H	-4.80451400	1.72607000	-4.23918700
C	-6.34036200	-0.09363800	-3.00608100
C	-7.21518700	-0.71563300	-1.89702000
H	-8.12558800	-1.13058900	-2.34112300
H	-6.69055200	-1.52842000	-1.38509000
H	-7.51231100	0.03223100	-1.15529400
C	-2.71428900	3.30909900	-3.72816200
C	-1.53861400	4.06300400	-3.07500600
H	-0.71805400	3.37651500	-2.83942000
H	-1.16320200	4.82437500	-3.76607700
H	-1.83576200	4.56939900	-2.15234200
C	4.28712000	-1.51623400	-1.77897500
C	3.99245600	-0.03688000	-1.43930600

H	4.49287500	0.27109700	-0.51550900
H	4.36572000	0.59816800	-2.24960000
H	2.91903800	0.15170600	-1.33467700
C	4.91779900	-5.96928700	0.50939900
C	4.60846800	-6.76464100	1.79443700
H	4.80116100	-6.17377500	2.69471700
H	3.56388800	-7.09579500	1.81554300
H	5.24294300	-7.65559400	1.83503100
O	0.65418100	-0.70785200	0.98508600
O	-1.68254700	-0.98381800	0.05166400
P	-0.10731500	-0.81306300	-0.47670600
O	0.16763200	-2.11584300	-1.17141700
O	0.11550700	0.50587000	-1.16209500
H	-1.00608100	-2.78136900	-2.56972100
C	-1.62080100	-3.42437000	-3.19296100
S	-0.42177100	-5.25033700	-1.70920200
O	-0.68160700	-6.71308700	-1.97204900
C	1.35325100	-4.91309900	-1.70555800
H	1.71043500	-5.07365200	-2.72279900
H	1.48056200	-3.86951300	-1.41663600
H	1.83750700	-5.58892900	-1.00083400
C	-0.82448900	-4.85863000	0.01732700
H	-0.23939700	-5.50849800	0.67235400
H	-0.58268500	-3.80802300	0.17940500
H	-1.89252700	-5.04192200	0.14958800
C	-1.07680200	-1.24972000	-5.62433900
C	-0.14262300	-0.47427500	-4.88356400
C	1.10423300	-0.12017600	-5.39197500
C	1.41309000	-0.55261000	-6.67977600
C	0.49917700	-1.30924000	-7.43757700

C	-0.74428900	-1.66190800	-6.92263200
C	-2.20610700	-1.46485100	-4.75965300
C	-1.93959000	-0.75249700	-3.57897000
H	1.80526700	0.46289800	-4.80379100
H	2.37742400	-0.29763500	-7.10885900
H	0.77132100	-1.61767900	-8.44278100
H	-1.44769700	-2.24162100	-7.51362400
H	-3.14499700	-1.93139600	-5.01370400
H	-2.54421000	-0.64037800	-2.69205200
N	-0.72071000	-0.17913700	-3.65532900
H	-0.26260700	0.24166600	-2.82398300
C	-0.86813000	-3.94832400	-4.36829000
O	0.33743500	-3.83089400	-4.46304800
O	-1.62454700	-4.57427800	-5.29130400
C	-0.88099900	-5.18039400	-6.36668600
H	-1.63303300	-5.57917300	-7.04722600
H	-0.25781700	-4.43377100	-6.86022600
H	-0.25100700	-5.98302300	-5.97524900
C	-2.95909300	-3.74327600	-2.73890000
C	-3.83706300	-4.63432500	-3.39195200
C	-3.37122000	-3.15330500	-1.52113500
C	-5.08230200	-4.91747400	-2.84093100
H	-3.53111600	-5.09993800	-4.31824600
C	-4.61219700	-3.45235500	-0.97491300
H	-2.70602700	-2.46889700	-1.00700500
C	-5.47459200	-4.33425100	-1.63325700
H	-5.74903400	-5.60514100	-3.35241200
H	-4.90608100	-2.99443100	-0.03498900
H	-6.44738000	-4.56457300	-1.20864600
C	-7.19453800	0.94638400	-3.75031100

C	-7.73533200	0.71463600	-5.01830600
C	-7.45670100	2.18266600	-3.13869100
C	-8.50474100	1.68878300	-5.66148600
H	-7.55300700	-0.22608000	-5.52605300
C	-8.21600200	3.15753100	-3.77707100
H	-7.02403400	2.39609800	-2.16599900
C	-8.74417300	2.91503200	-5.04705000
H	-8.90655300	1.48596900	-6.65075300
H	-8.37560200	4.11587300	-3.29256700
H	-9.32898500	3.67826900	-5.55268800
C	-3.86203100	4.30113300	-3.99819800
C	-4.32389600	4.60523400	-5.28166600
C	-4.50687500	4.90614000	-2.90736200
C	-5.39421500	5.48422800	-5.47265600
H	-3.86052000	4.15043900	-6.14975900
C	-5.56675300	5.78800400	-3.09223000
H	-4.18559100	4.66046900	-1.89904800
C	-6.01880000	6.08127300	-4.38150100
H	-5.73898000	5.69515600	-6.48135600
H	-6.04700200	6.24162300	-2.22903800
H	-6.85156400	6.76313200	-4.52986300
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C	7.33352200	-6.11707400	-0.39967500
C	6.87894000	-4.68885600	1.47601500
C	8.67638200	-5.72883000	-0.36574200
H	7.01209800	-6.81712700	-1.16259700
C	8.21524600	-4.30535700	1.51873900
H	6.17414900	-4.25338000	2.17873600
C	9.12370900	-4.82372000	0.59218000
H	9.36864300	-6.13462600	-1.09844000

H	8.54731000	-3.59265900	2.26907100
H	10.16612600	-4.51861600	0.61550900
C	5.78524300	-1.64549700	-2.08674600
C	6.28207100	-1.83577600	-3.37941100
C	6.70931400	-1.56832200	-1.03226100
C	7.65565600	-1.95232400	-3.61304500
H	5.59901300	-1.90676100	-4.21862400
C	8.07637200	-1.69111000	-1.25792200
H	6.34432700	-1.44755000	-0.01654600
C	8.55807700	-1.88496800	-2.55467200
H	8.01485500	-2.10621600	-4.62738900
H	8.76494000	-1.65422800	-0.41889300
H	9.62465600	-1.98891900	-2.73402900
C	3.39303000	-1.91118300	-2.97718300
H	2.34021900	-1.86445700	-2.68500000
H	3.53822900	-1.23186800	-3.82456500
H	3.60202900	-2.93093600	-3.31659700
C	4.53747200	-6.85512800	-0.69396200
H	5.08528900	-7.80368700	-0.67888500
H	3.46949500	-7.09129100	-0.65468400
H	4.73516100	-6.35532100	-1.64681500
C	-5.85995500	-1.23033100	-3.93345000
H	-5.30693300	-0.83333600	-4.79043800
H	-5.19790400	-1.89930100	-3.37861300
H	-6.69883500	-1.82814300	-4.30621700
C	-2.18533000	2.65841000	-5.02147400
H	-1.80254300	3.41815300	-5.71130700
H	-1.36538800	1.97955400	-4.78195900
H	-2.95447200	2.07925500	-5.54050500

**Me<sub>2</sub>Ph-S-TS2**

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C	-0.55623500	-2.19536400	3.87238700
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C	1.58947100	-3.16710500	3.27955000
C	-0.42602600	-1.27418600	2.81870100
C	0.70201100	-1.37283300	1.98156500
C	1.72844000	-2.31589400	2.17094300
C	-1.43467400	-0.21245400	2.51837200
C	-1.76779600	0.79283200	3.45827900
C	-1.98963100	-0.14207700	1.23034900
C	-1.05292700	0.86057000	4.79685200
C	-2.71078500	1.77735100	3.11185400
C	-2.89856200	0.85090800	0.86089600
C	-1.11026000	2.25159600	5.43320400
H	-0.01499600	0.53569800	4.66956200
C	-3.09048700	2.90757000	4.05461600
C	-3.26626200	1.78222600	1.82874400
C	-2.56069000	2.73260500	5.47958000
H	-0.67454100	2.21352700	6.43842100
H	-2.69399200	3.84674400	3.64176000
H	-3.96595300	2.56857200	1.55514400
H	-3.16677900	1.98991900	6.01737100
H	-4.18200100	3.02299600	4.06221400
H	-2.65211200	3.67628000	6.02973600
H	-0.50675300	2.95813300	4.84714200
H	-1.50651900	0.15145400	5.50033400
C	-1.76701600	-2.30765900	4.76533300
H	-1.50388600	-1.96404500	5.77590800
H	-2.57478700	-1.66075700	4.41441700

C	-2.26493600	-3.76783500	4.86830400
H	-2.81553300	-4.01310700	3.95406600
H	-2.98991500	-3.82946900	5.68728800
C	-1.11747300	-4.79248700	5.08232500
H	-1.06629500	-5.47678000	4.22681500
H	-1.31542200	-5.41436900	5.96218100
C	0.25798200	-4.10884300	5.23085300
H	1.05682400	-4.85798600	5.25079300
H	0.29465800	-3.58441600	6.19703500
C	2.83516600	-2.49726600	1.19393400
C	3.40950600	-3.76030700	1.00374400
C	3.27737100	-1.44387500	0.37746600
C	4.38677600	-3.98531600	0.02667000
H	3.06454300	-4.60142700	1.59526000
C	4.17458500	-1.65549000	-0.66568200
H	2.87576000	-0.45614500	0.52769300
C	4.73745200	-2.93127900	-0.82007200
H	5.44912500	-3.10366000	-1.61710100
C	-3.35237700	0.97914700	-0.55329500
C	-2.59931400	1.76670300	-1.42009500
C	-4.52436800	0.36576600	-1.01589400
C	-2.99848300	1.97294500	-2.74706700
H	-1.69406200	2.23169800	-1.05098300
C	-4.94149900	0.54045900	-2.33618800
H	-5.10421800	-0.23200300	-0.32190100
C	-4.16208500	1.34255500	-3.18737400
H	-4.50790300	1.49524400	-4.20324000
O	0.74493000	-0.51283700	0.89379400
O	-1.62897000	-1.07867100	0.27324200
P	-0.11742500	-0.99483800	-0.42301900



O	0.18035200	-2.41896900	-0.79916200
O	-0.01542000	0.10274300	-1.44574100
H	-1.25609700	-3.39501100	-1.83236200
C	-1.49697100	-4.23607700	-2.47052300
S	-1.22613200	-5.43444200	-0.09753100
O	-1.71386600	-6.82844600	0.20571800
C	0.49492100	-5.23092200	0.40954300
H	1.09229500	-5.93937200	-0.15852600
H	0.77194100	-4.20134900	0.17641400
H	0.56506800	-5.43459000	1.48081900
C	-1.98884800	-4.26116600	1.05815700
H	-1.68310500	-4.53301300	2.07029100
H	-1.65681400	-3.25359700	0.80452900
H	-3.06959500	-4.34646300	0.94403100
C	-1.44277000	-2.50370100	-5.46046900
C	-0.47745200	-1.62259400	-4.88120300
C	0.72513800	-1.31078400	-5.51732600
C	0.97360600	-1.92288200	-6.74050900
C	0.04491400	-2.81348900	-7.32400800
C	-1.15710900	-3.10686300	-6.69940200
C	-2.53232400	-2.57280900	-4.54357600
C	-2.20462300	-1.74722700	-3.46364600
H	1.43965800	-0.63227300	-5.06313700
H	1.90233500	-1.70909600	-7.26176800
H	0.28039900	-3.27112100	-8.28036700
H	-1.86804700	-3.79100300	-7.15357900
H	-3.45461100	-3.11979900	-4.66921700
H	-2.76889500	-1.50436100	-2.57453600
N	-0.98363900	-1.18868100	-3.67080400
H	-0.51424000	-0.60102800	-2.96219400

C	-2.90474200	-4.71221300	-2.47809900
O	-3.36012300	-5.63999400	-3.11629200
O	-3.64916200	-3.96370700	-1.62934100
C	-5.01497600	-4.38734000	-1.48238800
H	-5.53813800	-4.33205700	-2.43974800
H	-5.05260200	-5.41362700	-1.10882100
H	-5.45468000	-3.69392100	-0.76592500
C	-0.46889500	-4.70086000	-3.33959400
C	0.77333200	-4.01614700	-3.29571300
C	-0.65268000	-5.73844700	-4.29192300
C	1.77522200	-4.33175200	-4.20374800
H	0.91635900	-3.25105700	-2.54003900
C	0.36327300	-6.04758600	-5.17949100
H	-1.59846200	-6.26287700	-4.32010900
C	1.57327200	-5.33712000	-5.14859200
H	2.71089900	-3.78309800	-4.18048300
H	0.21692400	-6.83409600	-5.91360100
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C	-6.21276800	-0.11581400	-2.89974700
C	-2.14083200	2.87478900	-3.65360900
C	-2.93619400	3.39806700	-4.86968200
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H	-3.20665700	2.58105600	-5.54681800
H	-3.85568300	3.90948100	-4.56976000
C	-7.12654300	-0.67972900	-1.79015700
H	-6.63485600	-1.49234700	-1.24382300
H	-7.41415700	0.09249600	-1.07074200
H	-8.04107700	-1.08057500	-2.23850300
C	4.39644600	-0.54846800	-1.71554800
C	5.01776300	-5.38621000	-0.07953400

C	5.70933200	-5.70195500	1.26359100
H	6.19050900	-6.68605000	1.23768000
H	6.48028100	-4.95018300	1.45879600
H	5.01131800	-5.68204900	2.10498300
C	5.82107600	-0.59228300	-2.31159000
H	5.97221800	-1.49815500	-2.90713100
H	5.97548200	0.26736100	-2.97141200
H	6.59409600	-0.57348200	-1.53841200
C	-0.95770900	2.04191400	-4.18612000
H	-0.35047200	1.64700100	-3.36798400
H	-1.33818800	1.19643400	-4.76448400
H	-0.32182400	2.64356200	-4.84564900
C	-5.77833000	-1.29692800	-3.79141500
H	-5.15413300	-0.96813700	-4.62695500
H	-5.18760600	-1.99683900	-3.19387800
H	-6.64317700	-1.83954400	-4.18991800
C	3.40043800	-0.84638800	-2.86478000
H	3.65439400	-1.80681400	-3.32564600
H	2.37197000	-0.91401500	-2.50257800
H	3.45360600	-0.06893900	-3.63650000
C	6.10582900	-5.46341400	-1.17155500
H	5.71238600	-5.24738200	-2.16851100
H	6.91838100	-4.75896600	-0.96354000
H	6.52640700	-6.47366900	-1.19501700
C	-1.66480600	4.08362400	-2.83271900
C	-0.31351600	4.37424200	-2.61967600
C	-2.61930100	4.93221400	-2.25073600
C	0.07441200	5.47765600	-1.85339900
H	0.45596400	3.73528000	-3.03656300
C	-2.23872400	6.03459200	-1.49112500

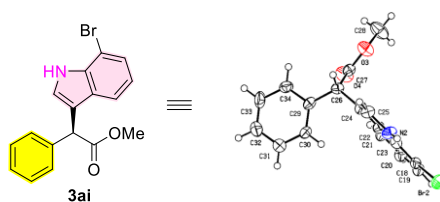
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C	-0.88482200	6.31379300	-1.28781300
H	1.13235100	5.67319500	-1.69951400
H	-2.99935500	6.67370500	-1.05032000
H	-0.58461300	7.17040200	-0.69075100
C	-7.01991000	0.93820400	-3.67255200
C	-7.48437100	0.74032900	-4.97574100
C	-7.32916200	2.15244600	-3.03930000
C	-8.23575000	1.72241900	-5.62852600
H	-7.25978100	-0.18094500	-5.50160700
C	-8.07895900	3.13151000	-3.68333500
H	-6.95631300	2.33454600	-2.03527700
C	-8.53743200	2.92031300	-4.98646200
H	-8.58021900	1.54563600	-6.64393100
H	-8.30128700	4.06392700	-3.17133100
H	-9.11867600	3.68479100	-5.49426800
C	3.91744300	-6.40316600	-0.42702700
C	3.23171200	-6.27446500	-1.64504800
C	3.56144900	-7.46359000	0.41305000
C	2.24125800	-7.17848300	-2.01986000
H	3.45741600	-5.43741300	-2.29713800
C	2.55815000	-8.36728400	0.04891300
H	4.06208500	-7.59576500	1.36566500
C	1.89692900	-8.23327900	-1.16962400
H	1.72302700	-7.04696100	-2.96359500
H	2.29299800	-9.17426800	0.72632900
H	1.10878100	-8.92673900	-1.44681900
C	4.13201400	0.83622500	-1.10198200
C	2.90166900	1.48981200	-1.25204600
C	5.11049800	1.45692600	-0.31130400

C	2.65915200	2.72174600	-0.64105700
H	2.09104600	1.02752500	-1.79894900
C	4.87729800	2.69255800	0.29006200
H	6.06499500	0.96656700	-0.14812700
C	3.64824900	3.33398900	0.12570600
H	1.68414500	3.18641200	-0.75715100
H	5.65584900	3.15026600	0.89497700
H	3.46144600	4.29273000	0.60222500

### IX. The Stereochemistry of Product

The absolute stereochemistry of the **3ai** and (*R*)-**HA-10** were determined by X-ray crystallography. The suitable crystals were selected and mounted on a suitable support on a Bruker D8 VENTURE diffractometer.

The single crystal of compound **3ai** was obtained by slow evaporation of its solution in hexanes/DCM/EtOAc (20:1:1) at 0 °C. X-ray crystal structure was determined at 170 K with the ellipsoid contour at 50% probability levels. The X-ray data have been deposited at the Cambridge Crystallographic Data Center (CCDC: 2307251)

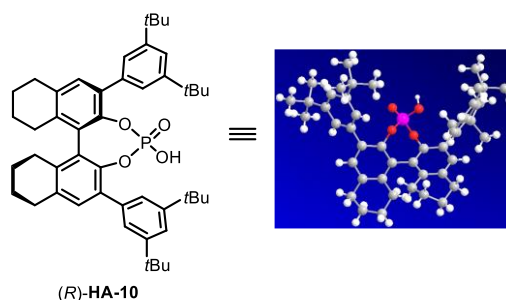


**Table S6 Crystal Data and Structure Refinement for 3ai.**

Identification code	<b>3ai</b>
Empirical formula	C <sub>17</sub> H <sub>14</sub> BrNO <sub>2</sub>
Formula weight	344.20
Temperature/K	170
Crystal system	monoclinic
Space group	P21
a/Å	8.1154(11)

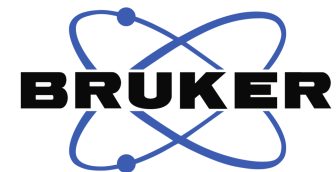
b/Å	10.5749(13)
c/Å	17.941(2)
$\alpha/^\circ$	90
$\beta/^\circ$	92.885(4)
$\gamma/^\circ$	90
Volume/Å <sup>3</sup>	1537.8(3)
Z	4
$\rho_{\text{calc}}/\text{cm}^3$	1.487
$\mu/\text{mm}^{-1}$	2.676
F(000)	696.0
Crystal size/mm <sup>3</sup>	0.15 × 0.08 × 0.05
Radiation	MoK $\alpha$ ( $\lambda = 0.71073$ )
2 $\Theta$ range for data collection/ $^\circ$	4.472 to 52.93
Index ranges	-8 ≤ h ≤ 10, -13 ≤ k ≤ 12, -22 ≤ l ≤ 22
Reflections collected	15202
Independent reflections	5800 [R <sub>int</sub> = 0.0707, R <sub>sigma</sub> = 0.1025]
Data/restraints/parameters	5800/1/381
Goodness-of-fit on F <sup>2</sup>	0.990
Final R indexes [ $I \geq 2\sigma(I)$ ]	R <sub>1</sub> = 0.0479, wR <sub>2</sub> = 0.0874
Final R indexes [all data]	R <sub>1</sub> = 0.0986, wR <sub>2</sub> = 0.1056
Largest diff. peak/hole / e Å <sup>-3</sup>	0.29/-0.57
Flack parameter	0.024(11)

The single crystal of compound (*R*)-**HA-10** was obtained by slow evaporation of its solution in DCM/CH<sub>3</sub>CN (1:3) at 0 °C. X-ray crystal structure was determined at 100 K with the ellipsoid contour at 50% probability levels. The X-ray data have been deposited at the Cambridge Crystallographic Data Center (CCDC: 2330415).



**Table S7 Crystal Data and Structure Refinement for (R)-HA-10.**

Identification code	(R)-HA-10
Empirical formula	C <sub>48</sub> H <sub>61</sub> O <sub>4</sub> P
Formula weight	732.93
Temperature/K	100.00
Crystal system	monoclinic
Space group	C2
a/Å	22.3569(8)
b/Å	15.3432(8)
c/Å	13.0072(5)
α/°	90
β/°	101.568(2)
γ/°	90
Volume/Å <sup>3</sup>	4371.2(3)
Z	4
ρ <sub>calc</sub> /cm <sup>3</sup>	1.114
μ/mm <sup>-1</sup>	0.103
F(000)	1584.0
Crystal size/mm <sup>3</sup>	0.12 × 0.08 × 0.05
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	4.282 to 52.812
Index ranges	-27 ≤ h ≤ 27, -19 ≤ k ≤ 19, -16 ≤ l ≤ 16
Reflections collected	25471
Independent reflections	8593 [R <sub>int</sub> = 0.0712, R <sub>sigma</sub> = 0.0732]
Data/restraints/parameters	8593/1/510
Goodness-of-fit on F <sup>2</sup>	1.035
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0527, wR <sub>2</sub> = 0.1193
Final R indexes [all data]	R <sub>1</sub> = 0.0707, wR <sub>2</sub> = 0.1320
Largest diff. peak/hole / e Å <sup>-3</sup>	0.27/-0.31
Flack parameter	0.09(7)



Current Data Parameters  
NAME HNMR-YX-5-p27  
EXPNO 1055  
PROCNO 1

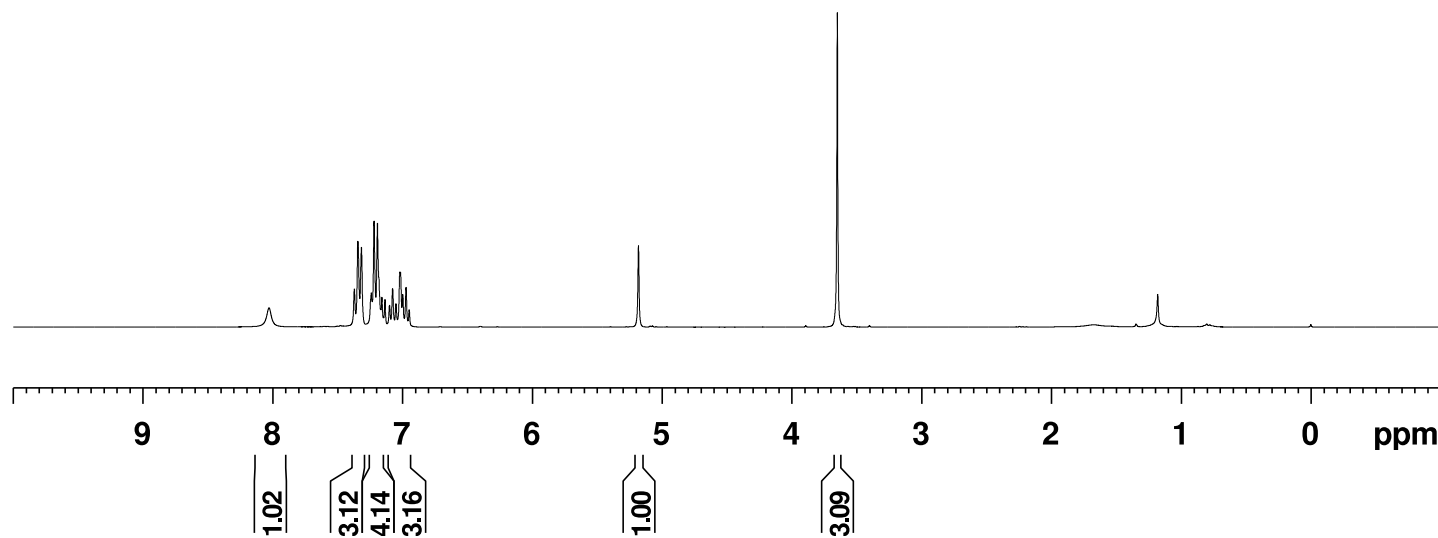
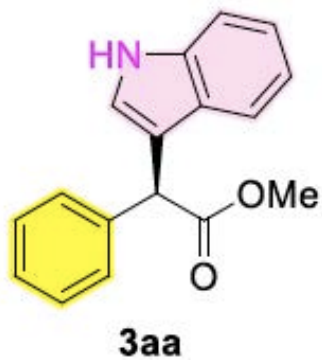
F2 - Acquisition Parameters  
Date\_ 20230711  
Time 20.49  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 128  
DW 83.200 usec  
DE 6.50 usec  
TE 300.1 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 300.1318534 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 14.00000000 W

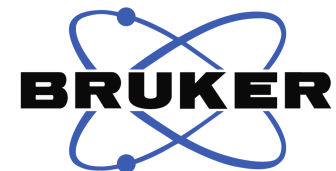
F2 - Processing parameters  
SI 65536  
SF 300.1300436 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

8.028  
7.371  
7.344  
7.316  
7.240  
7.219  
7.193  
7.158  
7.135  
7.100  
7.076  
7.050  
7.020  
7.015  
6.998  
6.972  
6.948  
5.181

— 3.649







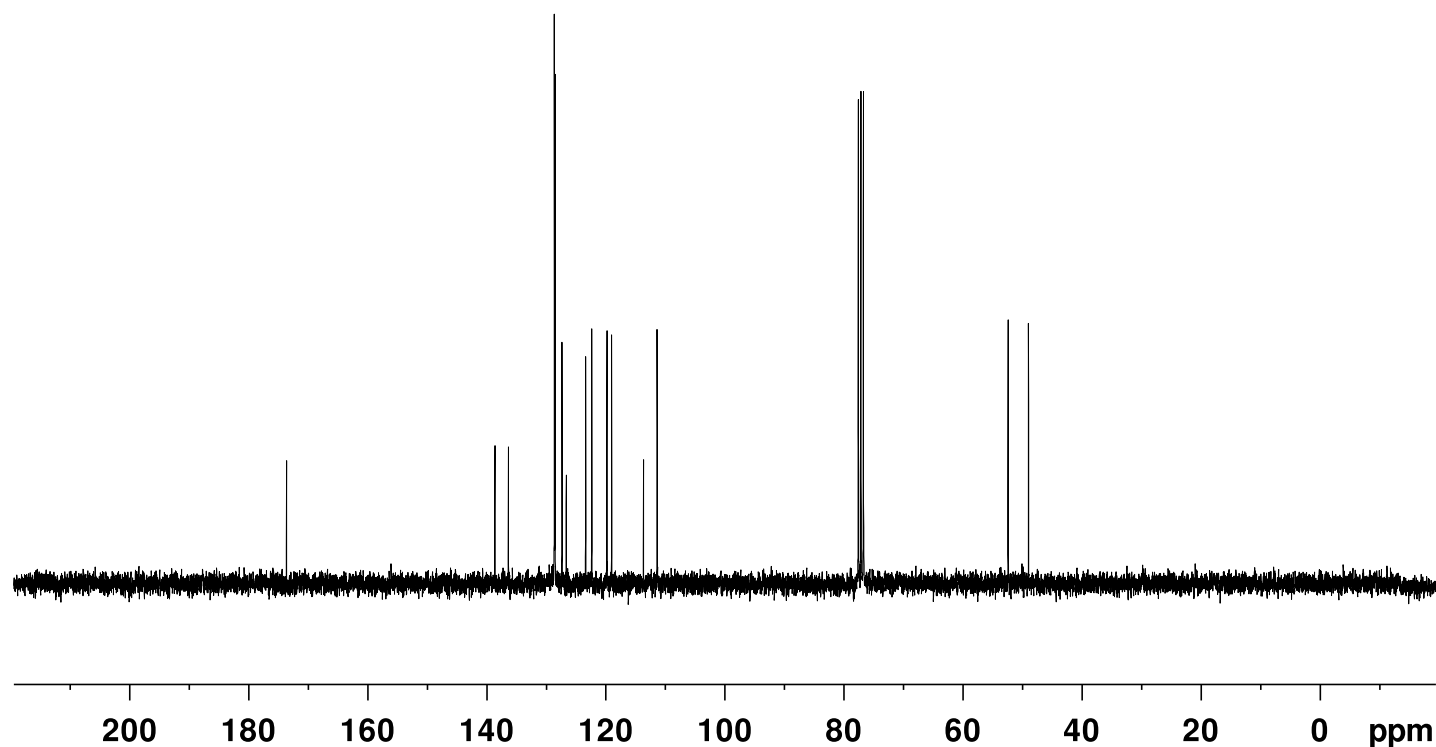
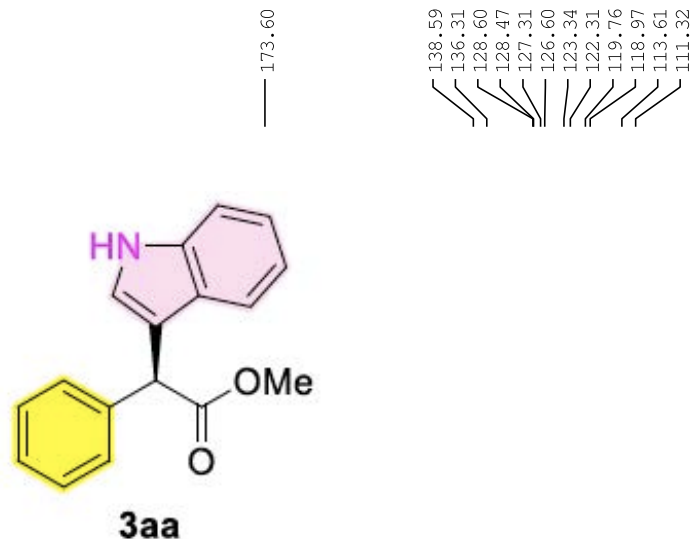
Current Data Parameters  
NAME CNMR-YX-5-p27  
EXPNO 1061  
PROCNO 1

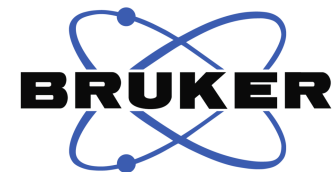
F2 - Acquisition Parameters  
Date\_ 20230712  
Time 1.46  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 100  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE 300.7 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 75.4752949 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 34.20000076 W

==== CHANNEL f2 =====  
SFO2 300.1312005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W  
PLW13 0.14000000 W

F2 - Processing parameters  
SI 32768  
SF 75.4677485 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



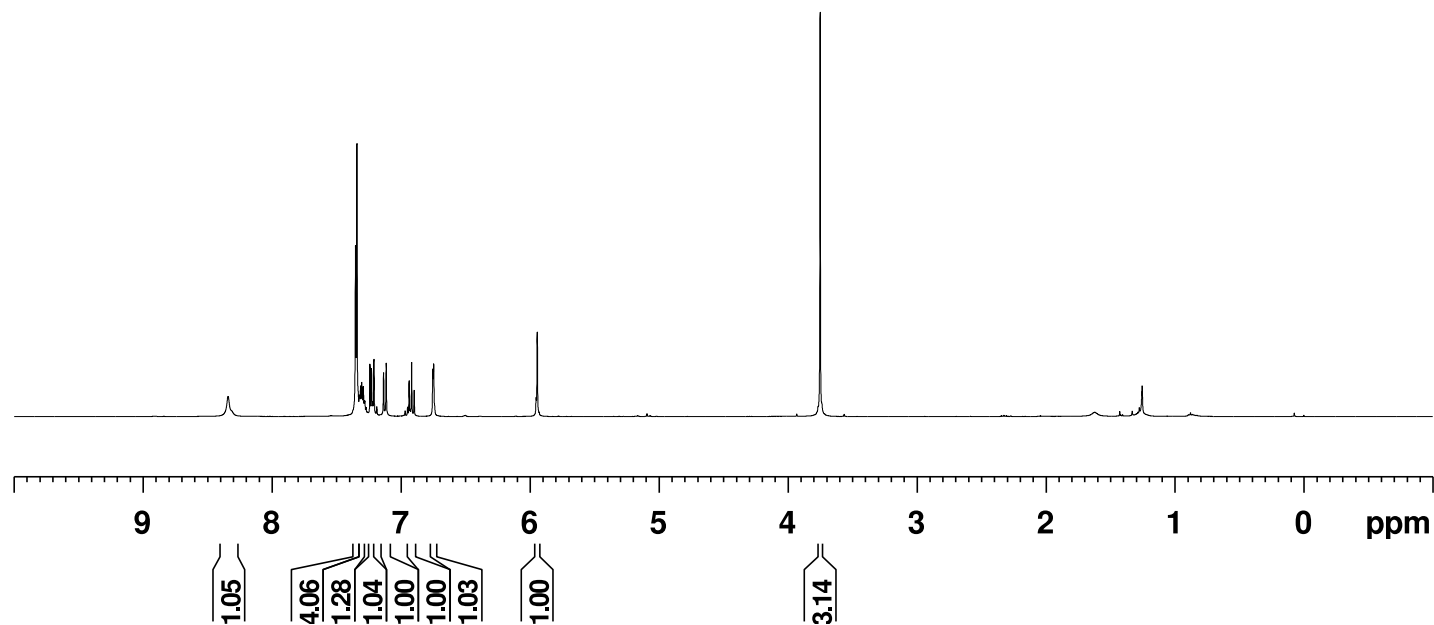
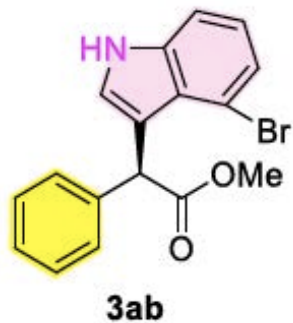


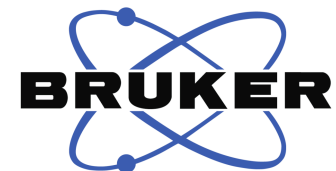
Current Data Parameters  
NAME HNMR-YX-6-p51  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231019  
Time 2.45 h  
INSTRUM Avance  
PROBHD Z116098\_0833 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8196.722 Hz  
FIDRES 0.250144 Hz  
AQ 3.9976959 sec  
RG 101  
DW 61.000 usec  
DE 13.54 usec  
TE 293.6 K  
D1 1.00000000 sec  
TD0 1  
SF01 400.1324708 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 20.73200035 W

F2 - Processing parameters  
SI 65536  
SF 400.1300175 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

7.353  
7.342  
7.323  
7.313  
7.305  
7.292  
7.284  
7.280  
7.241  
7.229  
7.220  
7.210  
7.135  
7.114  
6.948  
6.937  
6.917  
6.898  
6.753  
6.747  
5.943  
— 3.750

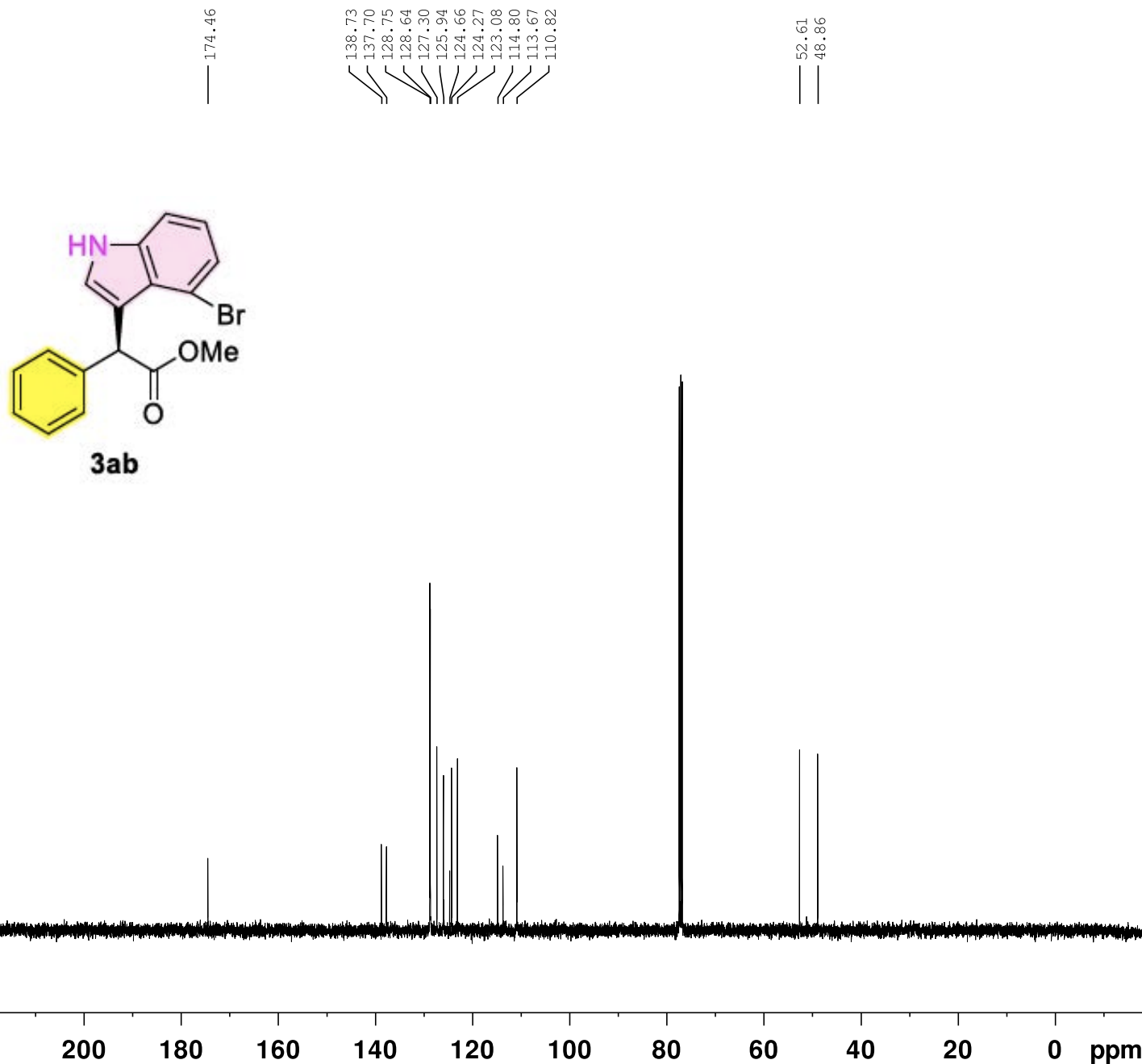


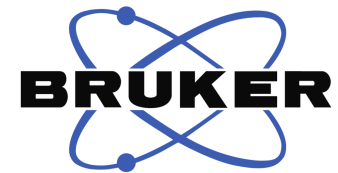


Current Data Parameters  
NAME CNMR-YX-6-p51  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231019  
Time 2.52 h  
INSTRUM Avance  
PROBHD Z116098\_0833 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 100  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 46.0295  
DW 21.000 usec  
DE 6.50 usec  
TE 294.3 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 3.33 usec  
P1 10.00 usec  
PLW1 87.89900208 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 20.73200035 W  
PLW12 0.25595000 W  
PLW13 0.12874000 W

F2 - Processing parameters  
SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



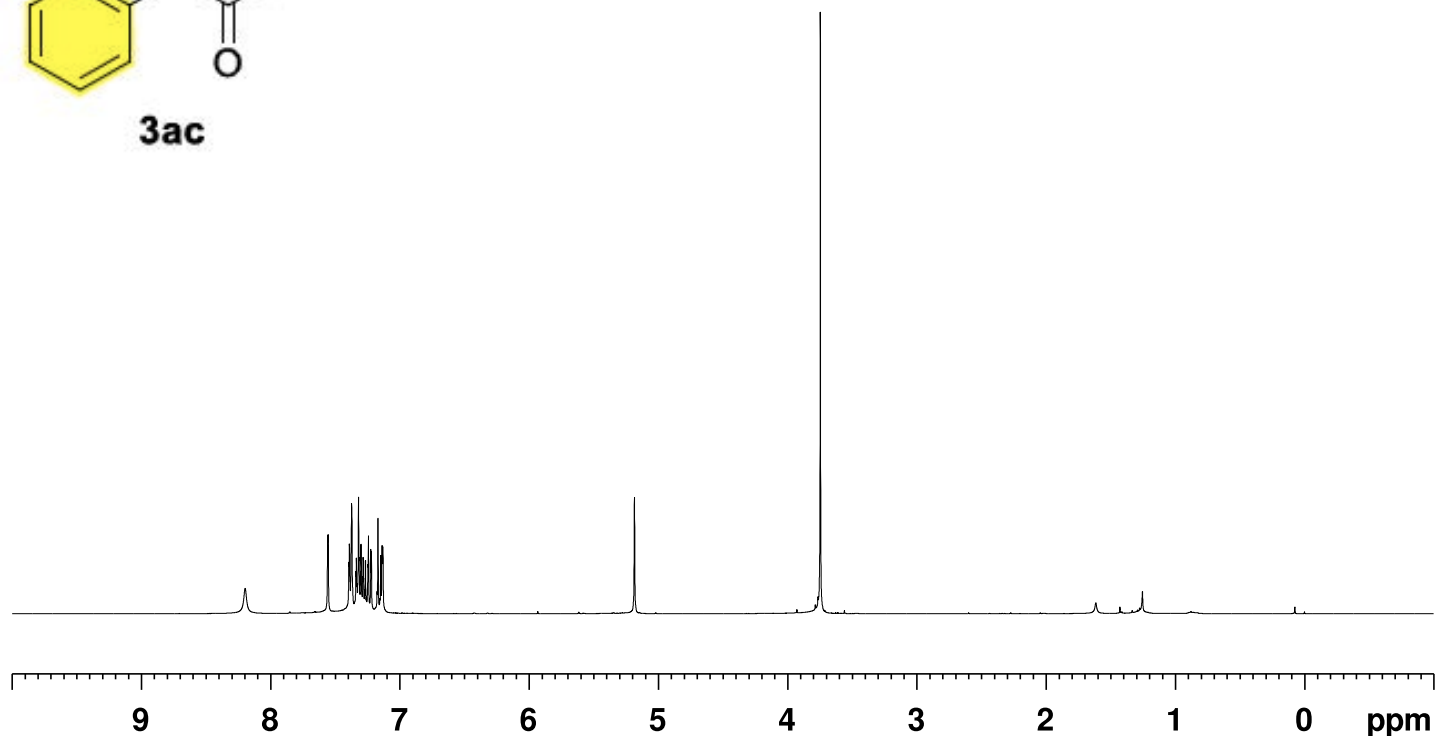


Current Data Parameters  
NAME NMR-YX-6-p52  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231107  
Time 11.21 h  
INSTRUM Avance  
PROBHD z116098\_0833 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8196.722 Hz  
FIDRES 0.250144 Hz  
AQ 3.9976959 sec  
RG 100.806  
DW 61.000 usec  
DE 13.54 usec  
TE 294.0 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1324708 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 20.73200035 W

F2 - Processing parameters  
SI 65536  
SF 400.1300169 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

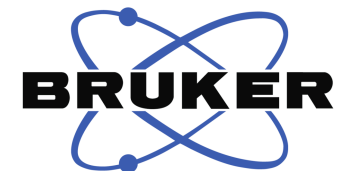
7.390  
7.373  
7.371  
7.340  
7.336  
7.331  
7.319  
7.315  
7.300  
7.287  
7.283  
7.280  
7.272  
7.266  
7.245  
7.242  
7.224  
7.220  
7.175  
7.169  
7.147  
7.137  
7.132  
5.184  
3.746



1.06  
1.04  
2.10  
2.27  
1.09  
1.42  
2.20

1.00

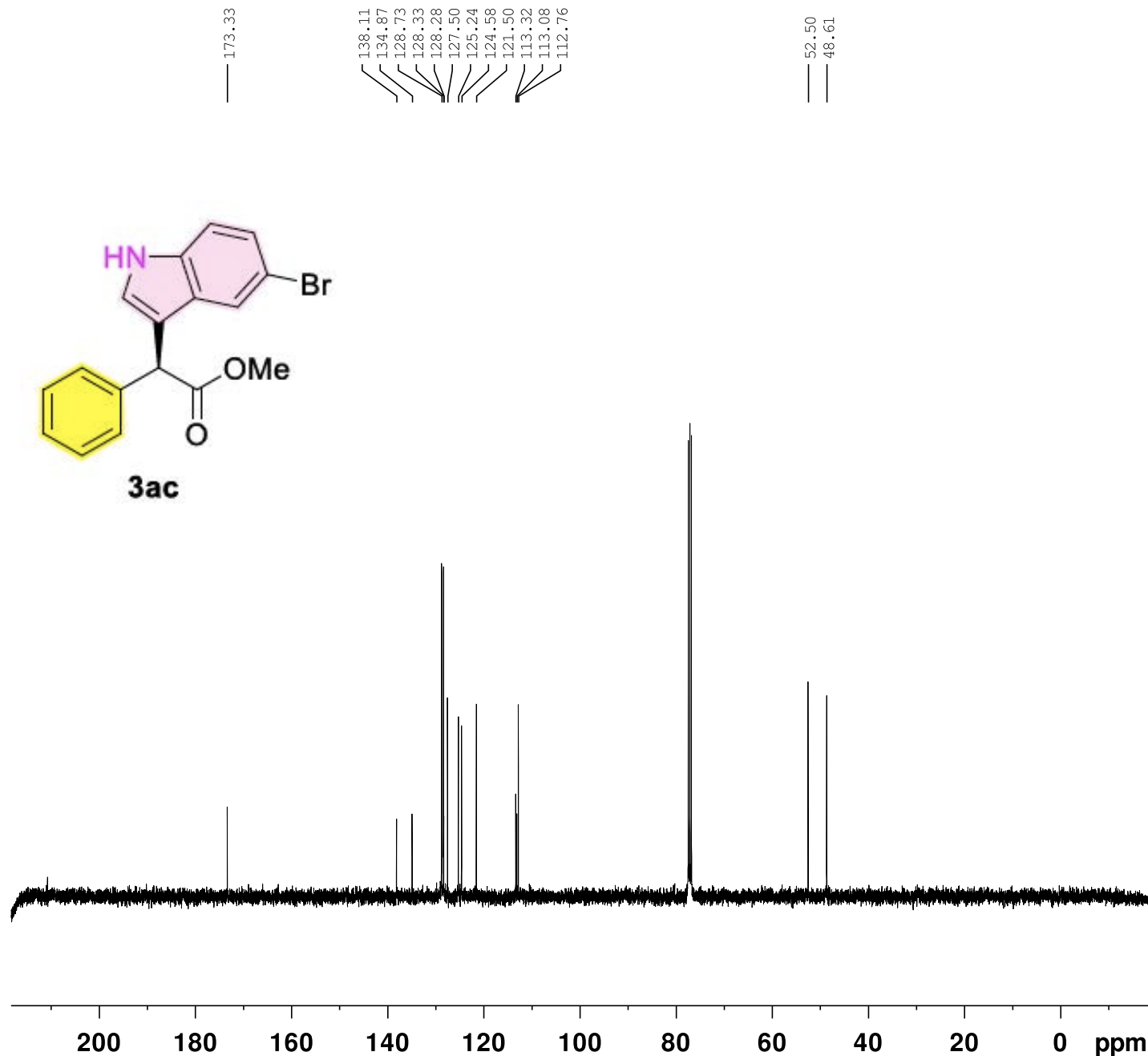
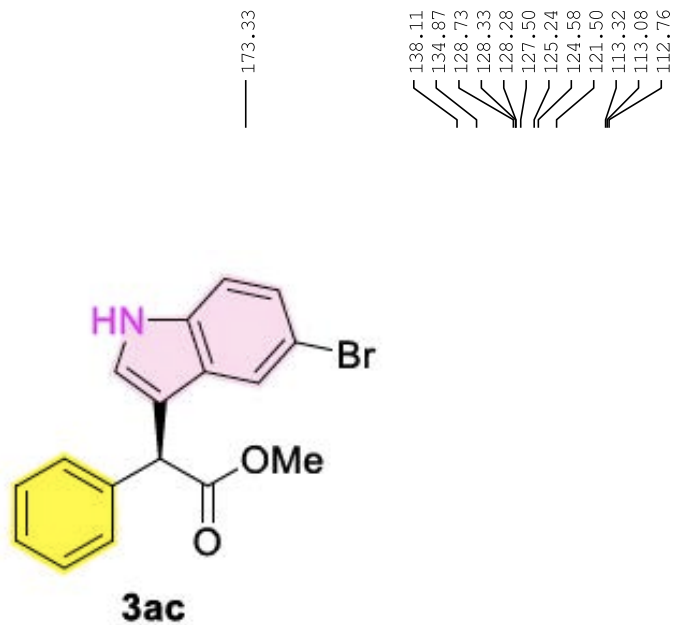
3.04

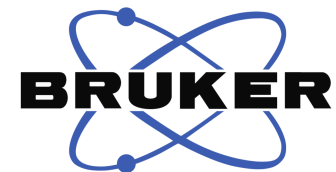


Current Data Parameters  
NAME NMR-YX-6-p52  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231107  
Time 11.28 h  
INSTRUM Avance  
PROBHD z116098\_0833 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 100  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 47.4244  
DW 21.000 usec  
DE 6.50 usec  
TE 294.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 3.33 usec  
P1 10.00 usec  
PLW1 87.8990208 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 20.73200035 W  
PLW12 0.25595000 W  
PLW13 0.12874000 W

F2 - Processing parameters  
SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



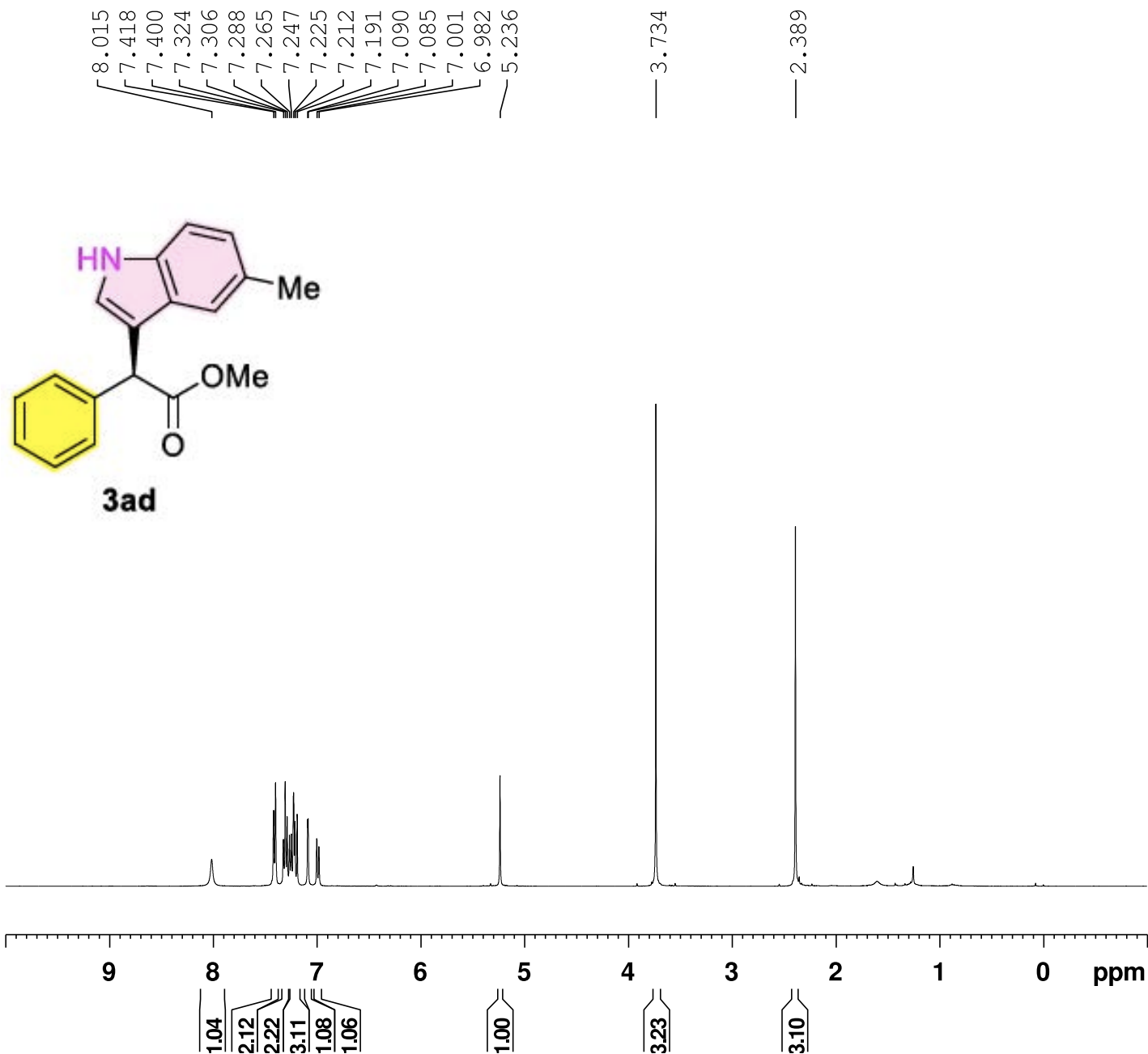


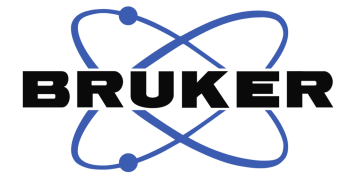
Current Data Parameters  
NAME HNMR-YX-6-p54  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231027  
Time 14.13  
INSTRUM spect  
PROBHD 5 mm PADUL 13C  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 4  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9845889 sec  
RG 90.23  
DW 60.800 usec  
DE 6.50 usec  
TE 291.9 K  
D1 1.00000000 sec  
TD0 1

=====  
CHANNEL f1  
NUC1 1H  
P1 9.90 usec  
PLW1 23.00000000 W  
SFO1 400.1924713 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1900263 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





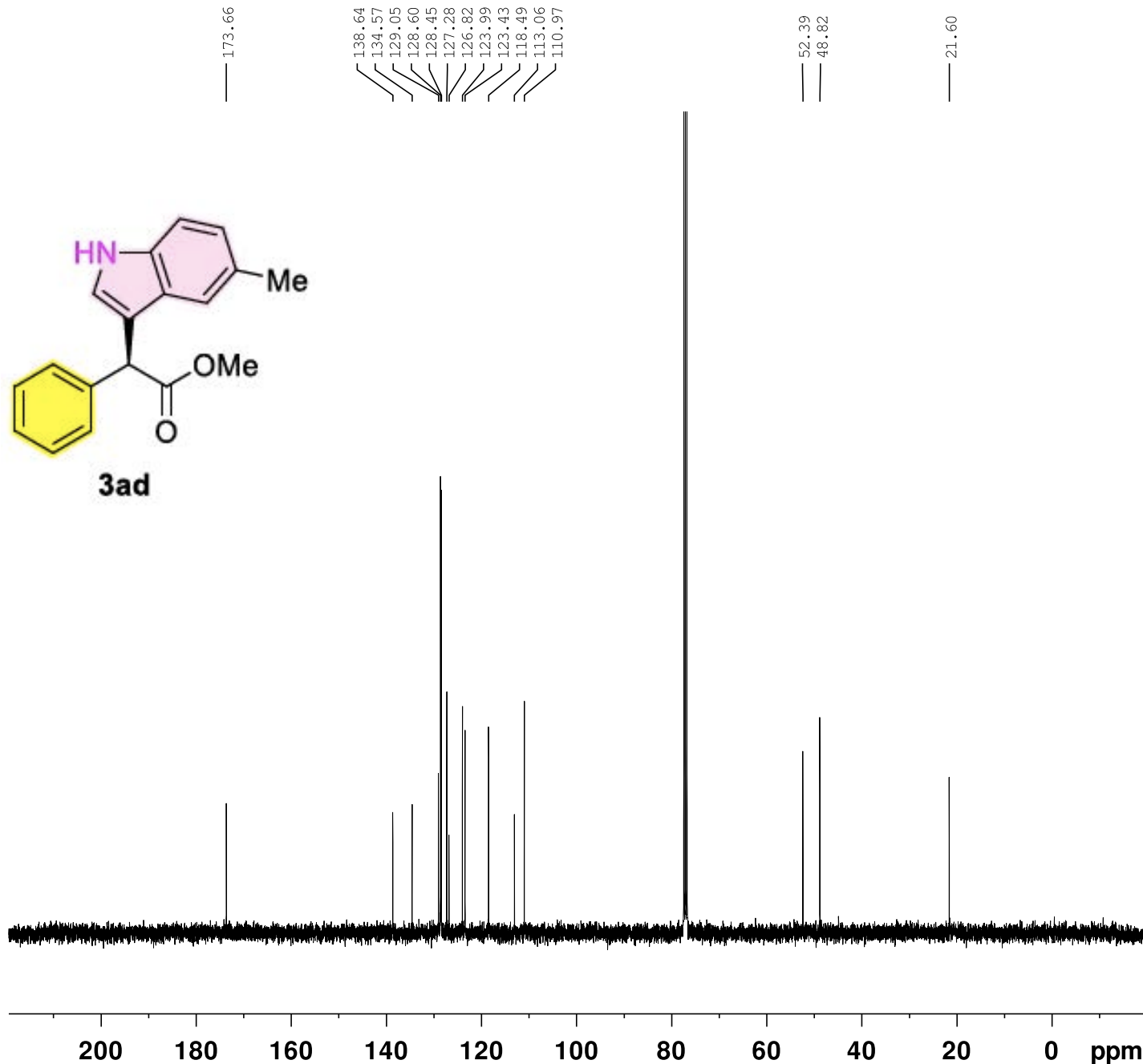
Current Data Parameters  
NAME CNMR-YX-6-p54  
EXPNO 2  
PROCNO 1

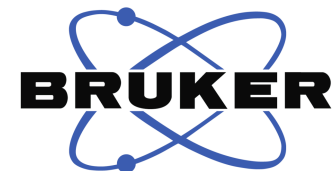
F2 - Acquisition Parameters  
Date\_ 20231027  
Time 14.20  
INSTRUM spect  
PROBHD 5 mm PADUL 13C  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 100  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 35.06  
DW 20.800 usec  
DE 6.50 usec  
TE 292.5 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 9.80 usec  
PLW1 47.40000153 W  
SFO1 100.6379178 MHz

==== CHANNEL f2 =====  
CPDPRG[2] waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 23.00000000 W  
PLW12 0.30712000 W  
PLW13 0.24877000 W  
SFO2 400.1916008 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6278560 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

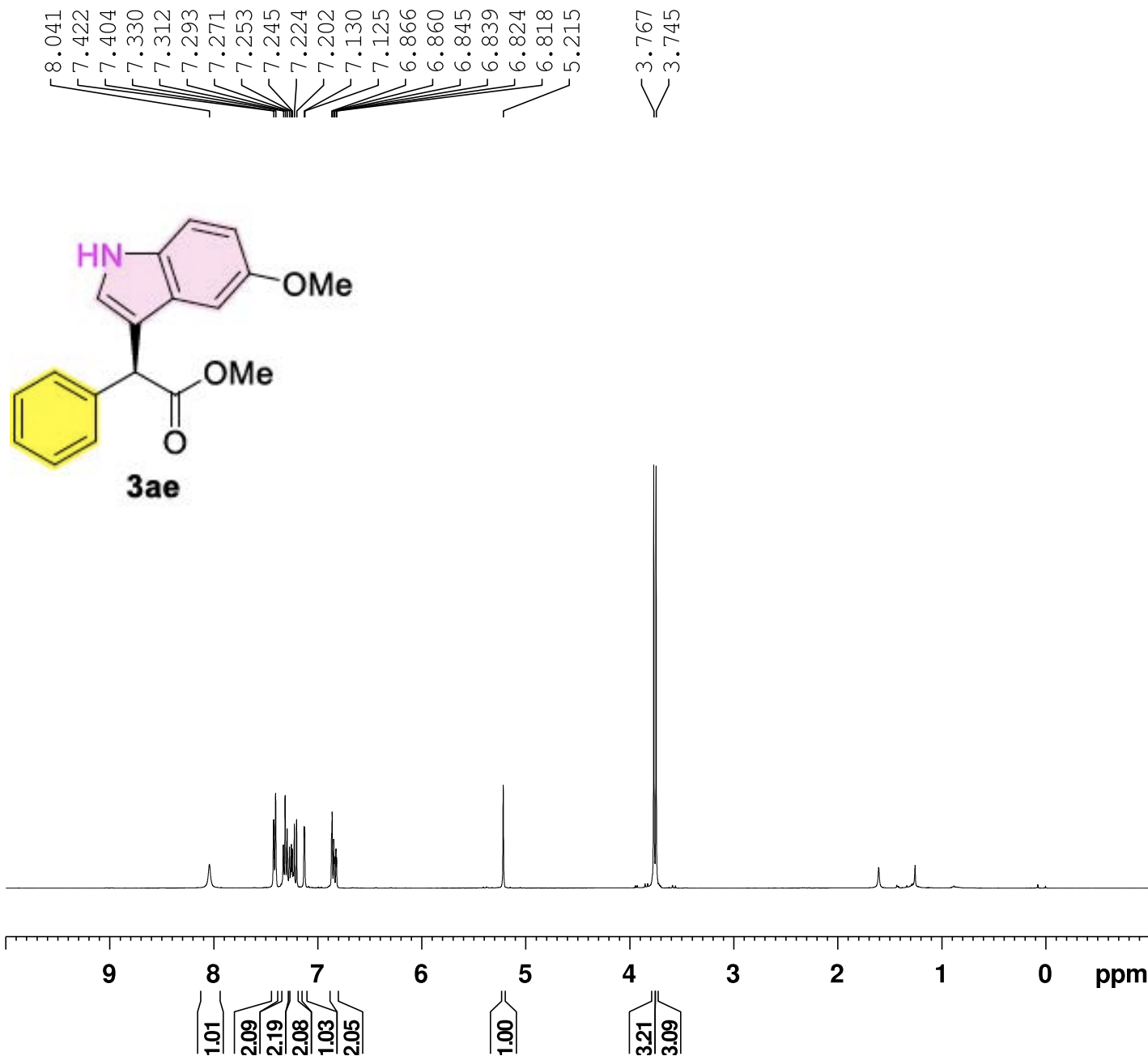




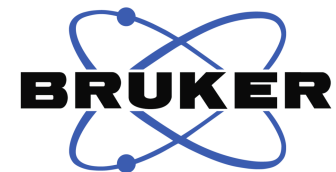
Current Data Parameters  
NAME HNMR-YX-6-p55  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231019  
Time 6.48 h  
INSTRUM Avance  
PROBHD Z116098\_0833 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8196.722 Hz  
FIDRES 0.250144 Hz  
AQ 3.9976959 sec  
RG 101  
DW 61.000 usec  
DE 13.54 usec  
TE 294.0 K  
D1 1.00000000 sec  
TD0 1  
SF01 400.1324708 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 20.73200035 W

F2 - Processing parameters  
SI 65536  
SF 400.1300160 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



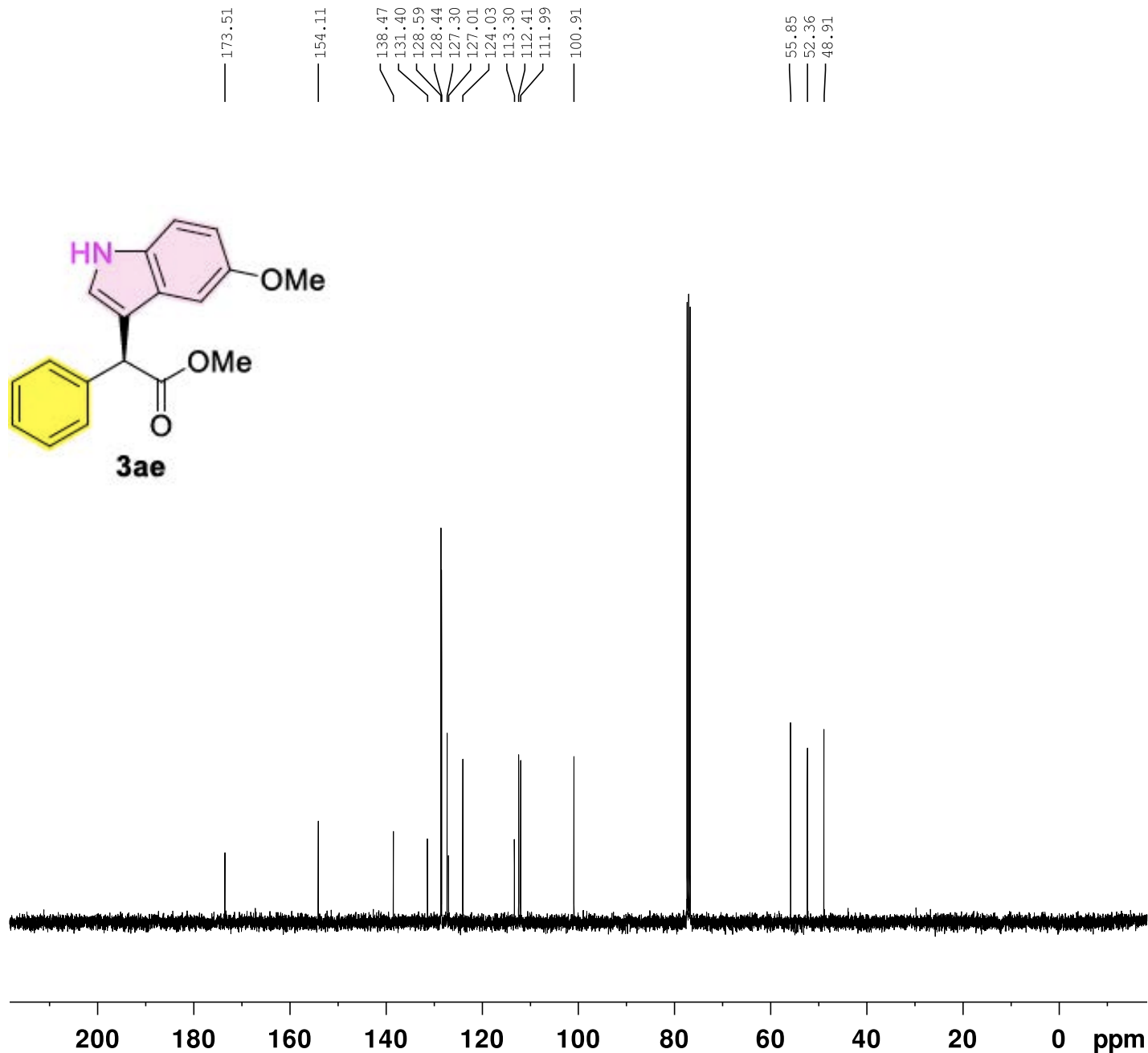


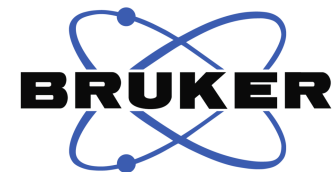


Current Data Parameters  
NAME CNMR-YX-6-p55  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231019  
Time 6.55 h  
INSTRUM Avance  
PROBHD Z116098\_0833 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 100  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 46.0295  
DW 21.000 usec  
DE 6.50 usec  
TE 293.9 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 3.33 usec  
P1 10.00 usec  
PLW1 87.89900208 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 20.73200035 W  
PLW12 0.25595000 W  
PLW13 0.12874000 W

F2 - Processing parameters  
SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



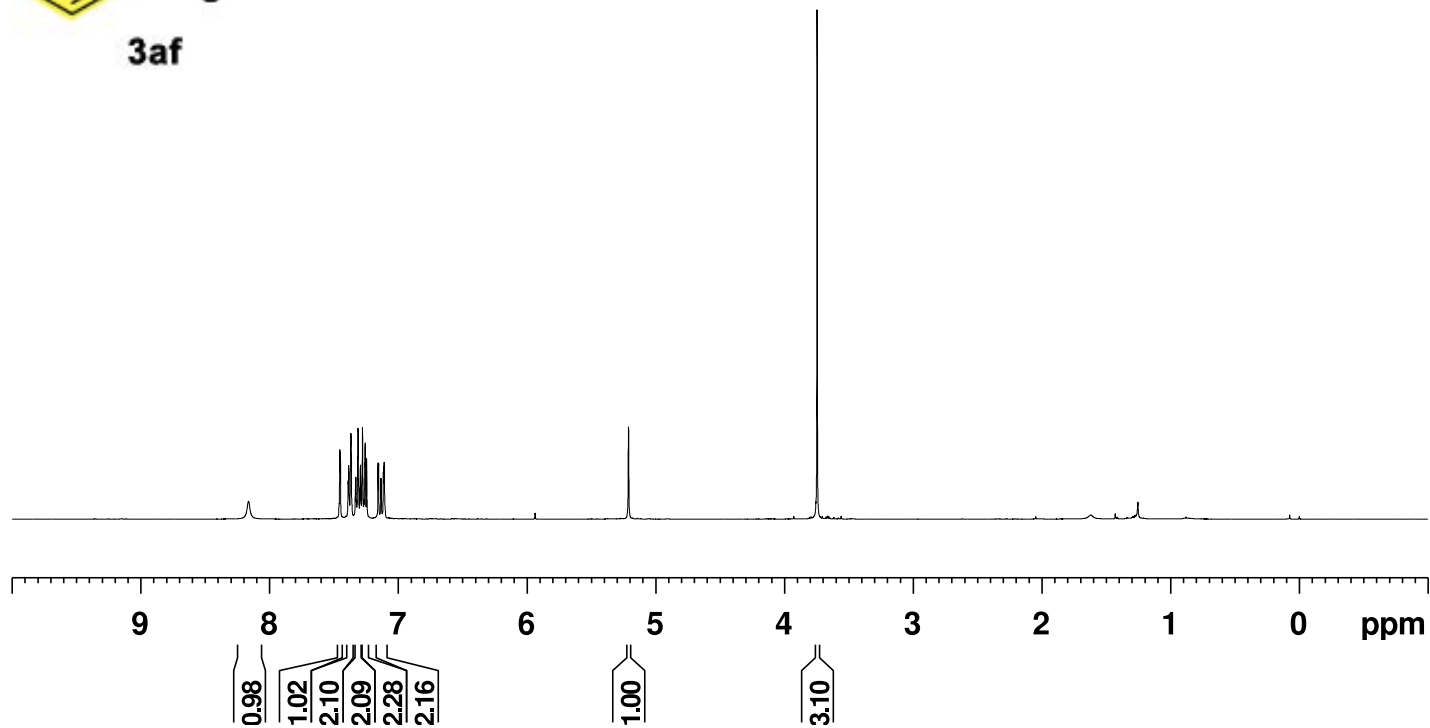
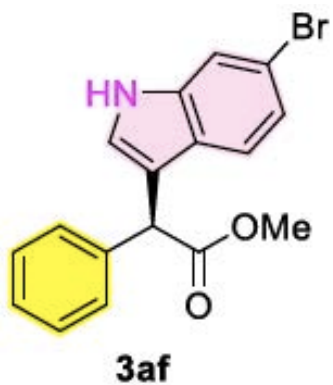


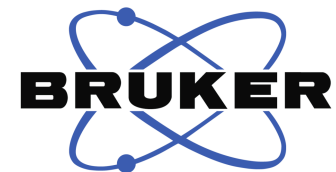
Current Data Parameters  
NAME HNMR-YX-6-p53  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231019  
Time 6.37 h  
INSTRUM Avance  
PROBHD Z116098\_0833 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8196.722 Hz  
FIDRES 0.250144 Hz  
AQ 3.9976959 sec  
RG 101  
DW 61.000 usec  
DE 13.54 usec  
TE 293.4 K  
D1 1.00000000 sec  
TD0 1  
SF01 400.1324708 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 20.73200035 W

F2 - Processing parameters  
SI 65536  
SF 400.1300156 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

7.389  
7.385  
7.367  
7.365  
7.333  
7.329  
7.312  
7.308  
7.297  
7.293  
7.277  
7.259  
7.256  
7.245  
7.157  
7.152  
7.135  
7.131  
7.115  
7.113  
7.109  
7.107  
5.211  
3.745





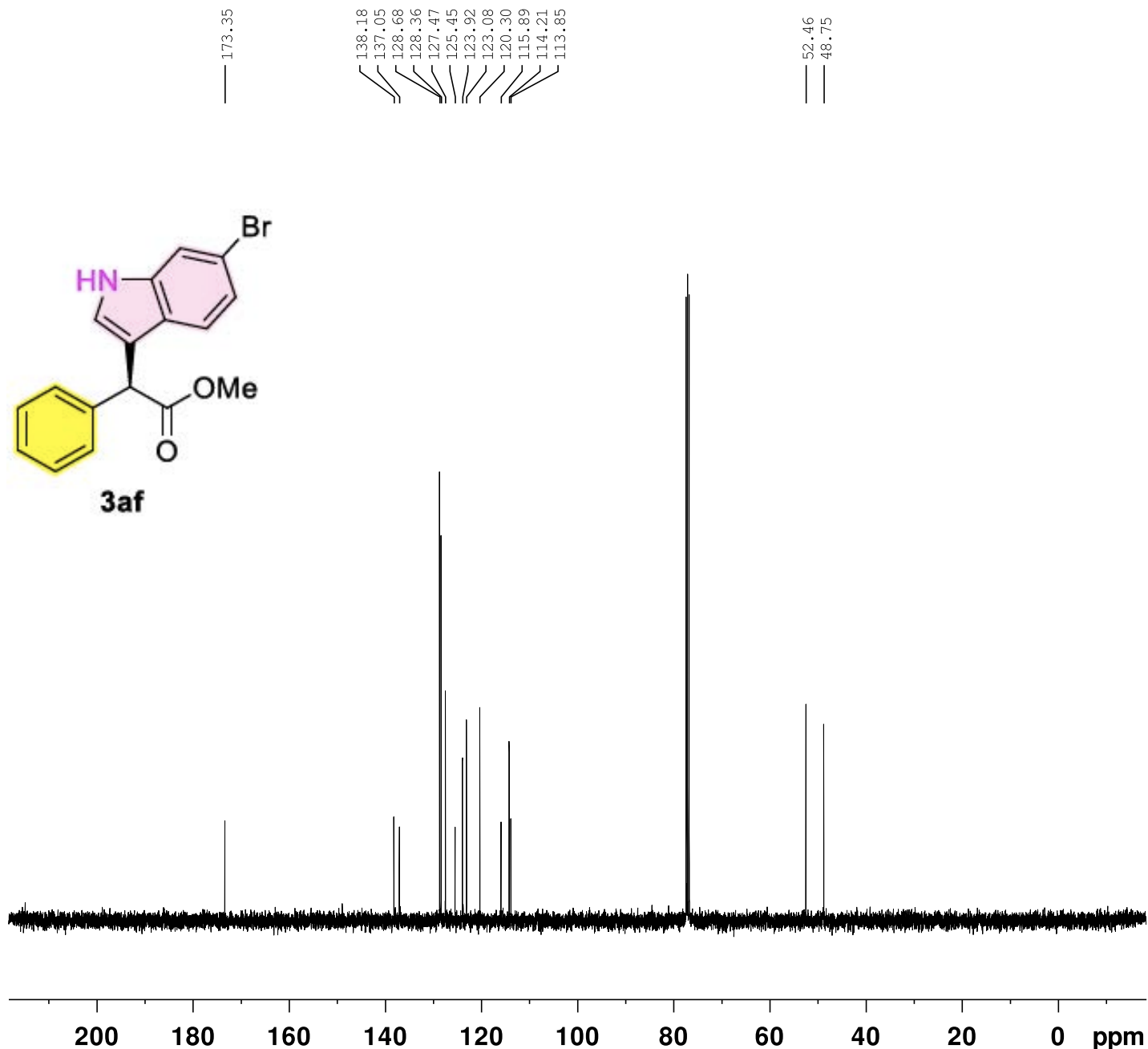
Current Data Parameters  
NAME CNMR-YX-6-p53  
EXPNO 2  
PROCNO 1

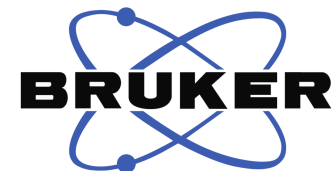
F2 - Acquisition Parameters

Date\_ 20231019  
Time 6.44 h  
INSTRUM Avance  
PROBHD Z116098\_0833 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 100  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 47.2408  
DW 21.000 usec  
DE 6.50 usec  
TE 294.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 3.33 usec  
P1 10.00 usec  
PLW1 87.89900208 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 20.73200035 W  
PLW12 0.25595000 W  
PLW13 0.12874000 W

F2 - Processing parameters

SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



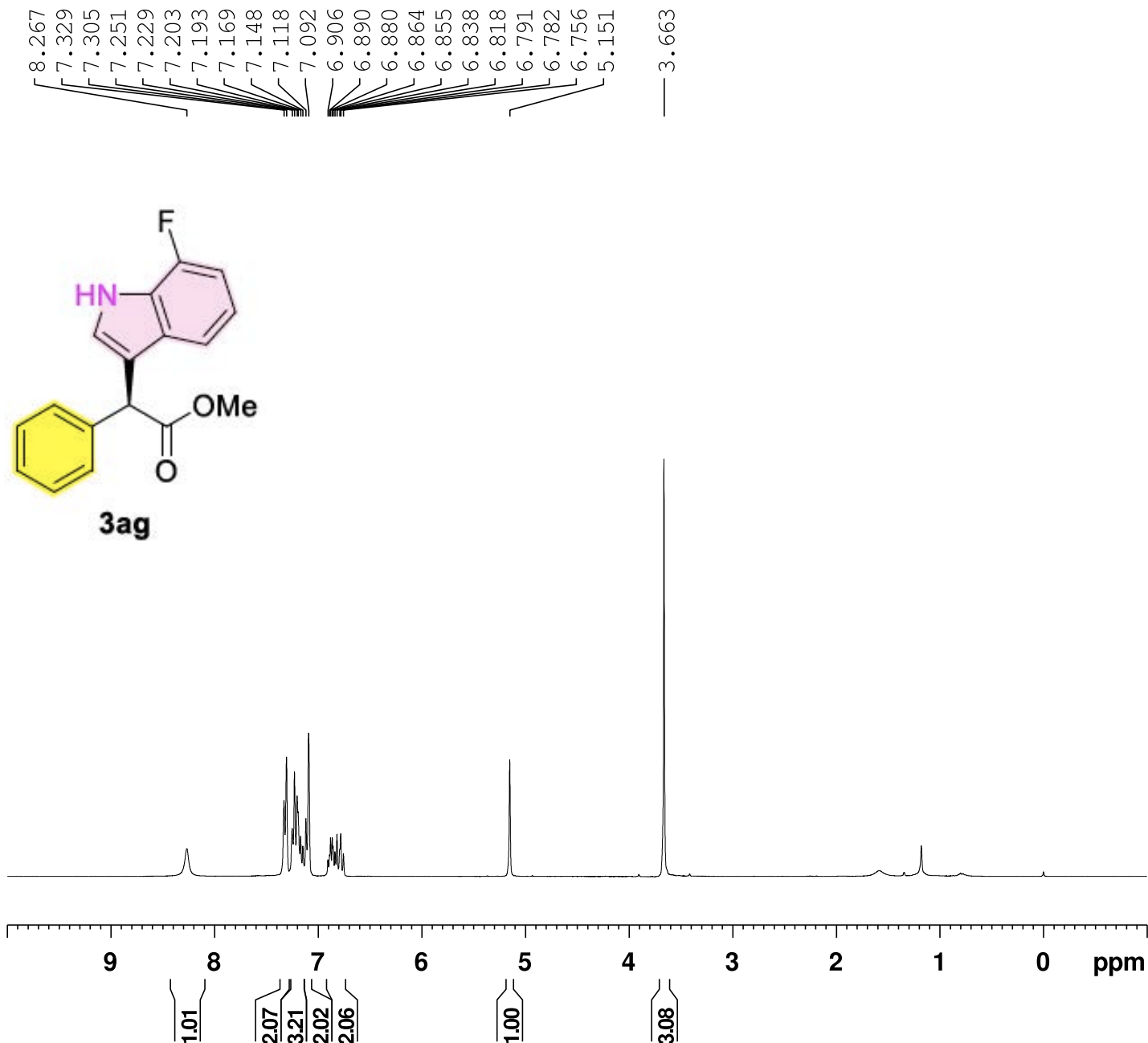


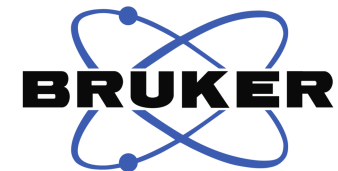
Current Data Parameters  
NAME HNMR-YX-5-p26  
EXPNO 1053  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230711  
Time 20.43  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 144  
DW 83.200 usec  
DE 6.50 usec  
TE 300.1 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 300.1318534 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 14.00000000 W

F2 - Processing parameters  
SI 65536  
SF 300.1300398 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





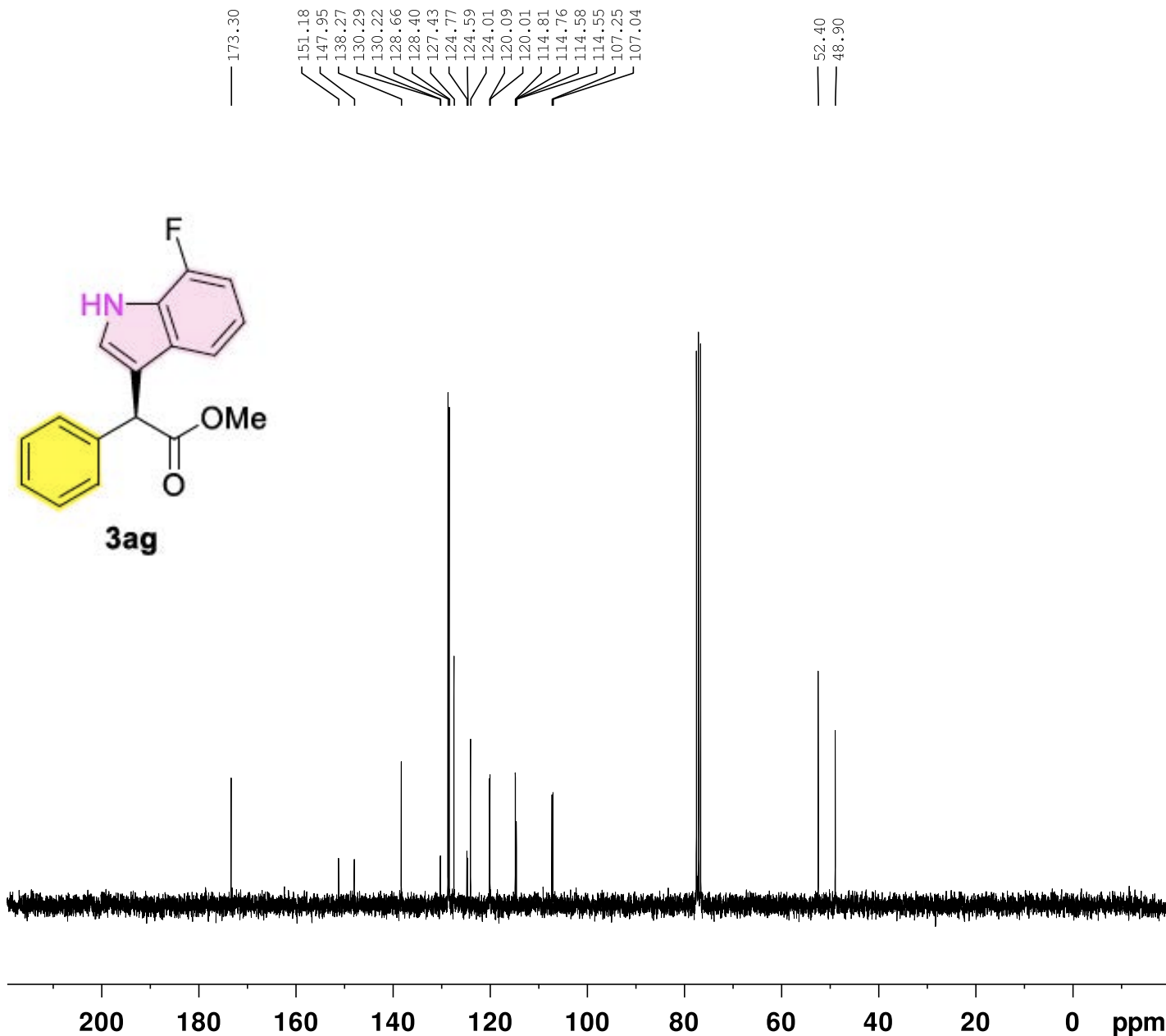
Current Data Parameters  
NAME CNMR-YX-5-p26  
EXPNO 1060  
PROCNO 1

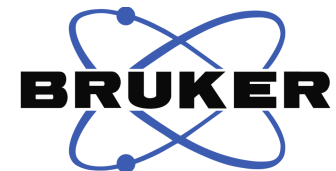
F2 - Acquisition Parameters  
Date\_ 20230712  
Time 1.36  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 100  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE 300.7 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 75.4752949 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 34.20000076 W

==== CHANNEL f2 =====  
SFO2 300.1312005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W  
PLW13 0.14000000 W

F2 - Processing parameters  
SI 32768  
SF 75.4677485 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





Current Data Parameters  
NAME FNMN-YX-5-p26  
EXPNO 1054  
PROCNO 1

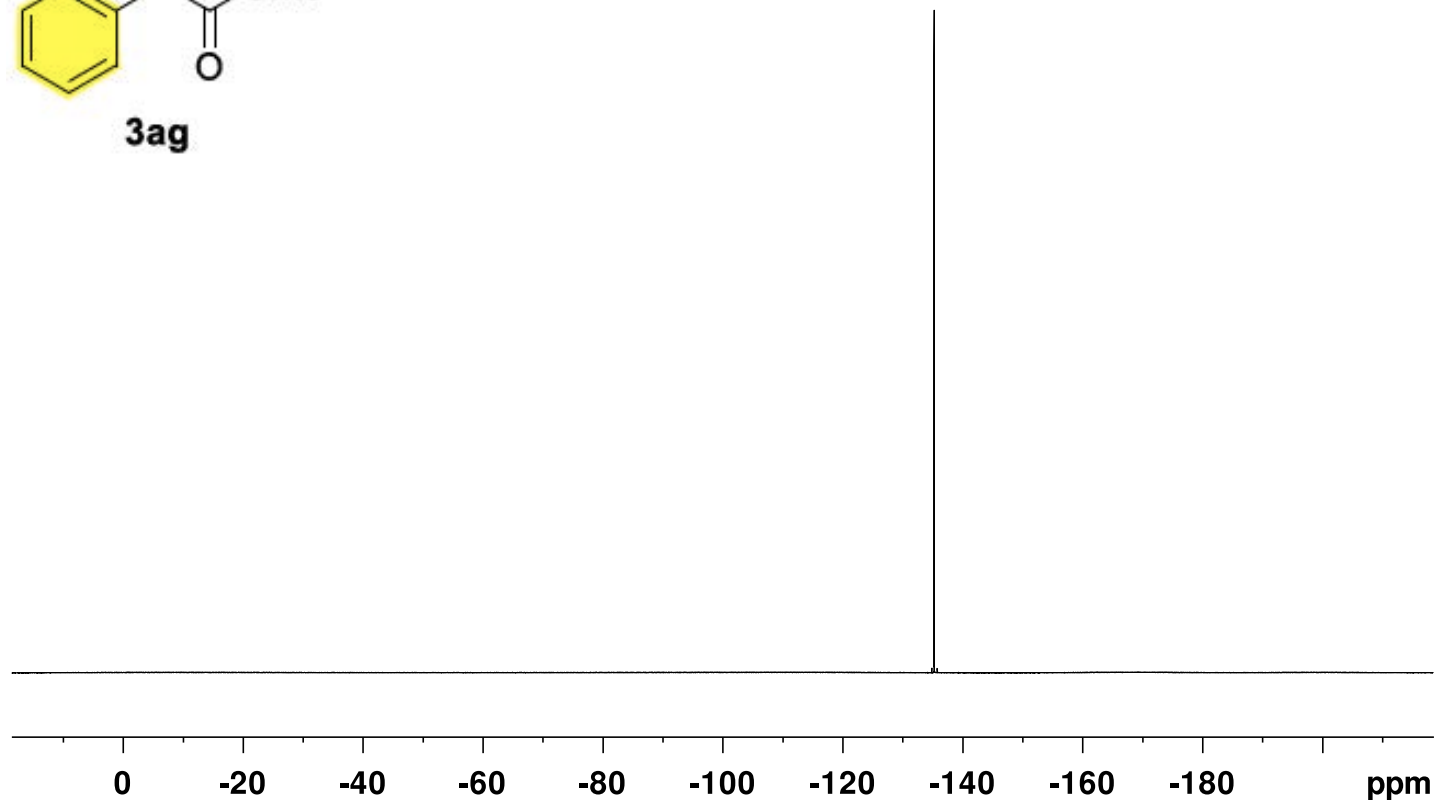
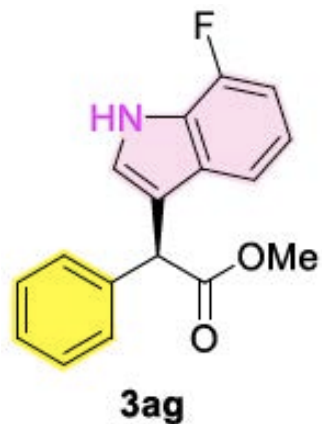
F2 - Acquisition Parameters  
Date\_ 20230711  
Time 20.45  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgfhigqn.2  
TD 131072  
SOLVENT CDCl3  
NS 16  
DS 4  
SWH 66964.289 Hz  
FIDRES 0.510897 Hz  
AQ 0.9786710 sec  
RG 203  
DW 7.467 usec  
DE 6.50 usec  
TE 300.2 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
D12 0.00002000 sec  
TD0 1

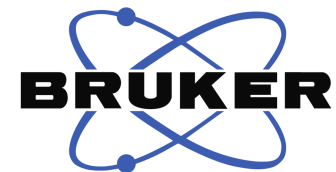
==== CHANNEL f1 =====  
SFO1 282.3761148 MHz  
NUC1 19F  
P1 14.50 usec  
PLW1 10.39999962 W

==== CHANNEL f2 =====  
SFO2 300.1312005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W

F2 - Processing parameters  
SI 65536  
SF 282.4043552 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

-135.27



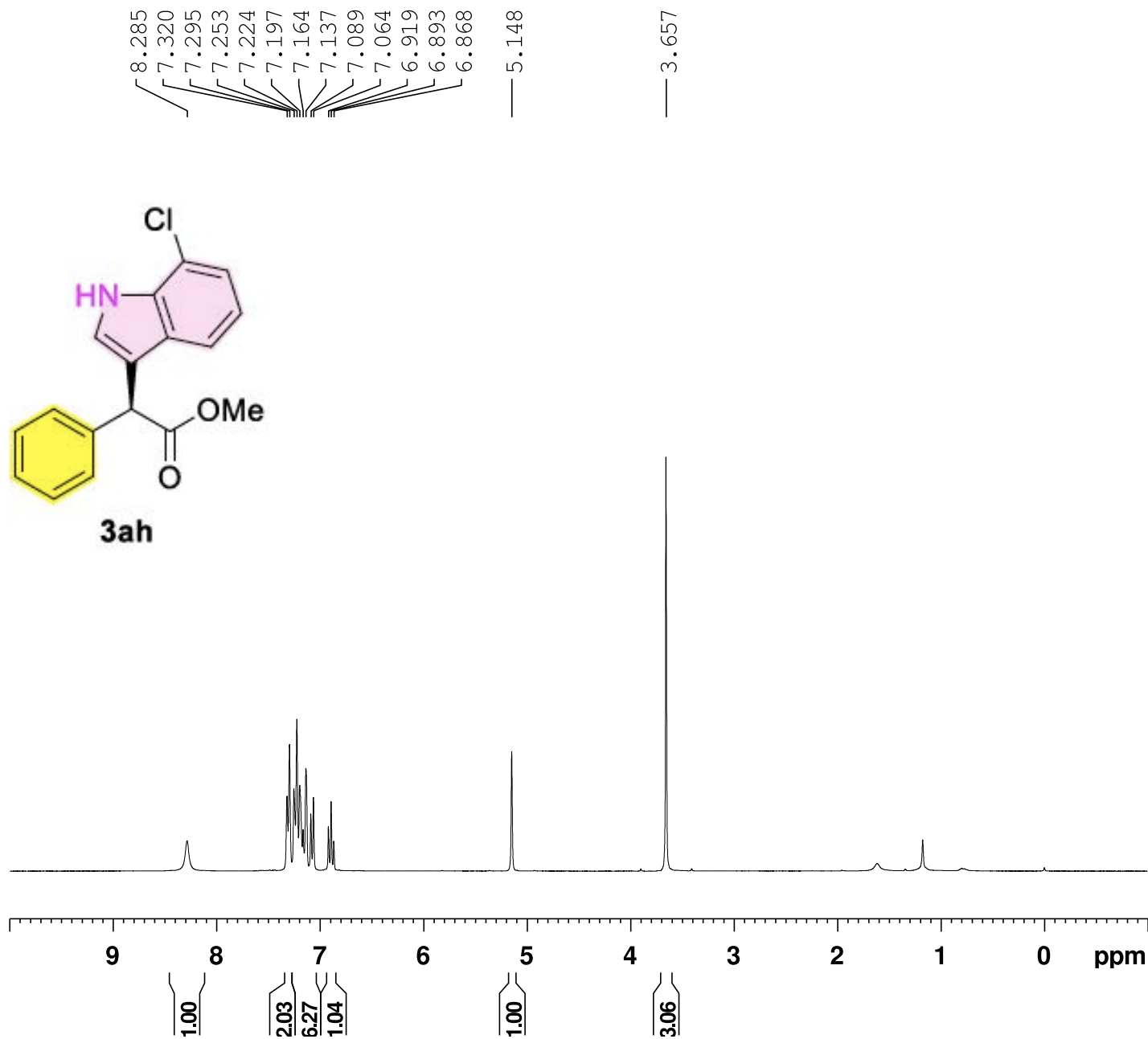


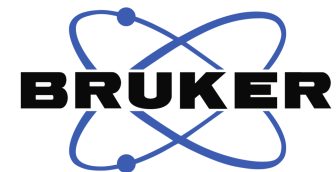
Current Data Parameters  
NAME HNMR-YX-5-p14  
EXPNO 1025  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230705  
Time 21.08  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 128  
DW 83.200 usec  
DE 6.50 usec  
TE 297.6 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 300.1318534 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 14.00000000 W

F2 - Processing parameters  
SI 65536  
SF 300.1300428 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





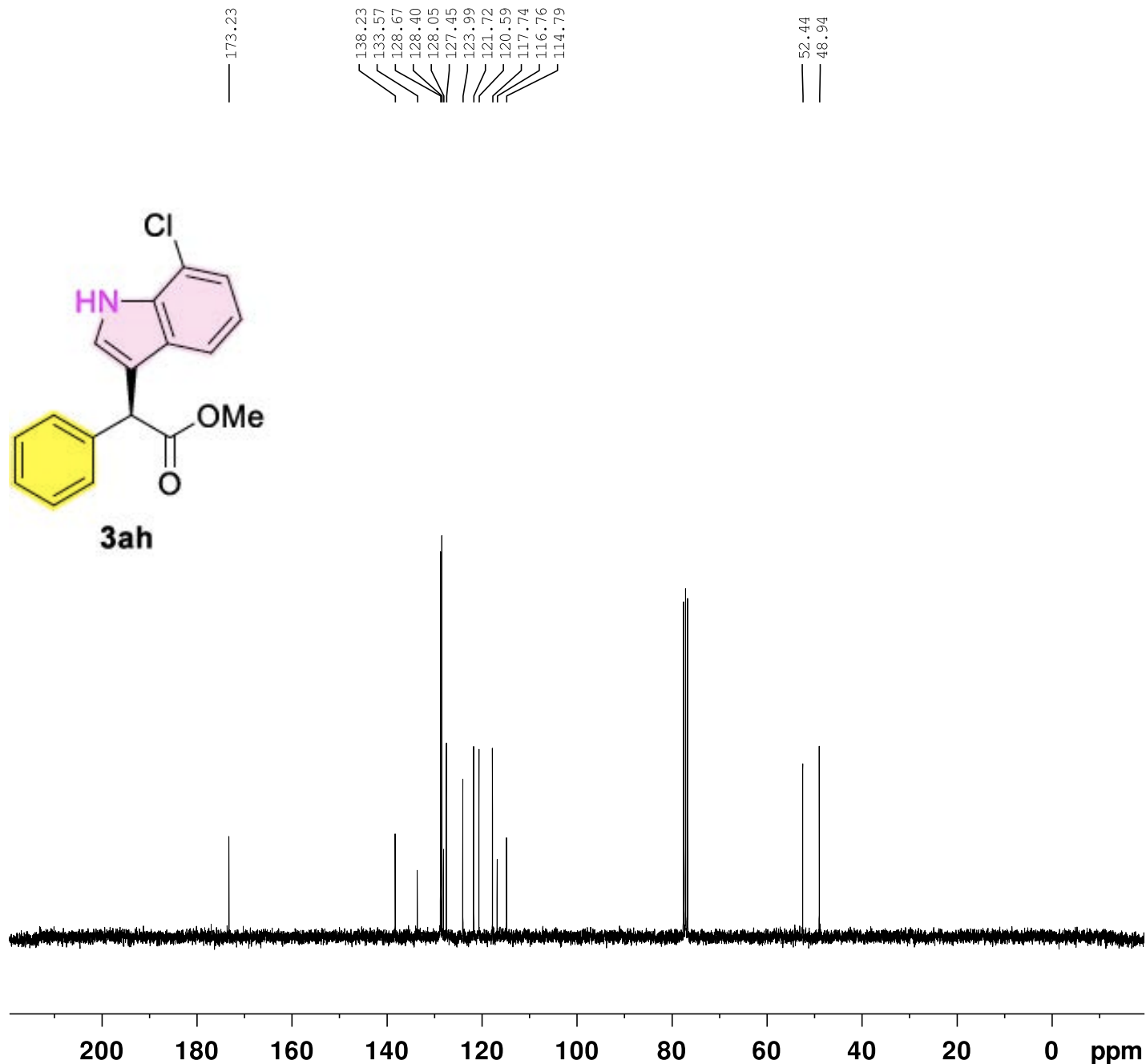
Current Data Parameters  
NAME CNMR-YX-5-p14  
EXPNO 1030  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230706  
Time 1.29  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 100  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE 298.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

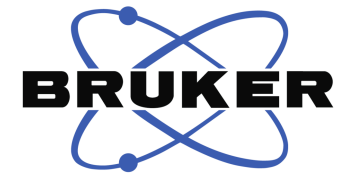
==== CHANNEL f1 =====  
SFO1 75.4752949 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 34.20000076 W

==== CHANNEL f2 =====  
SFO2 300.1312005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W  
PLW13 0.14000000 W

F2 - Processing parameters  
SI 32768  
SF 75.4677485 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





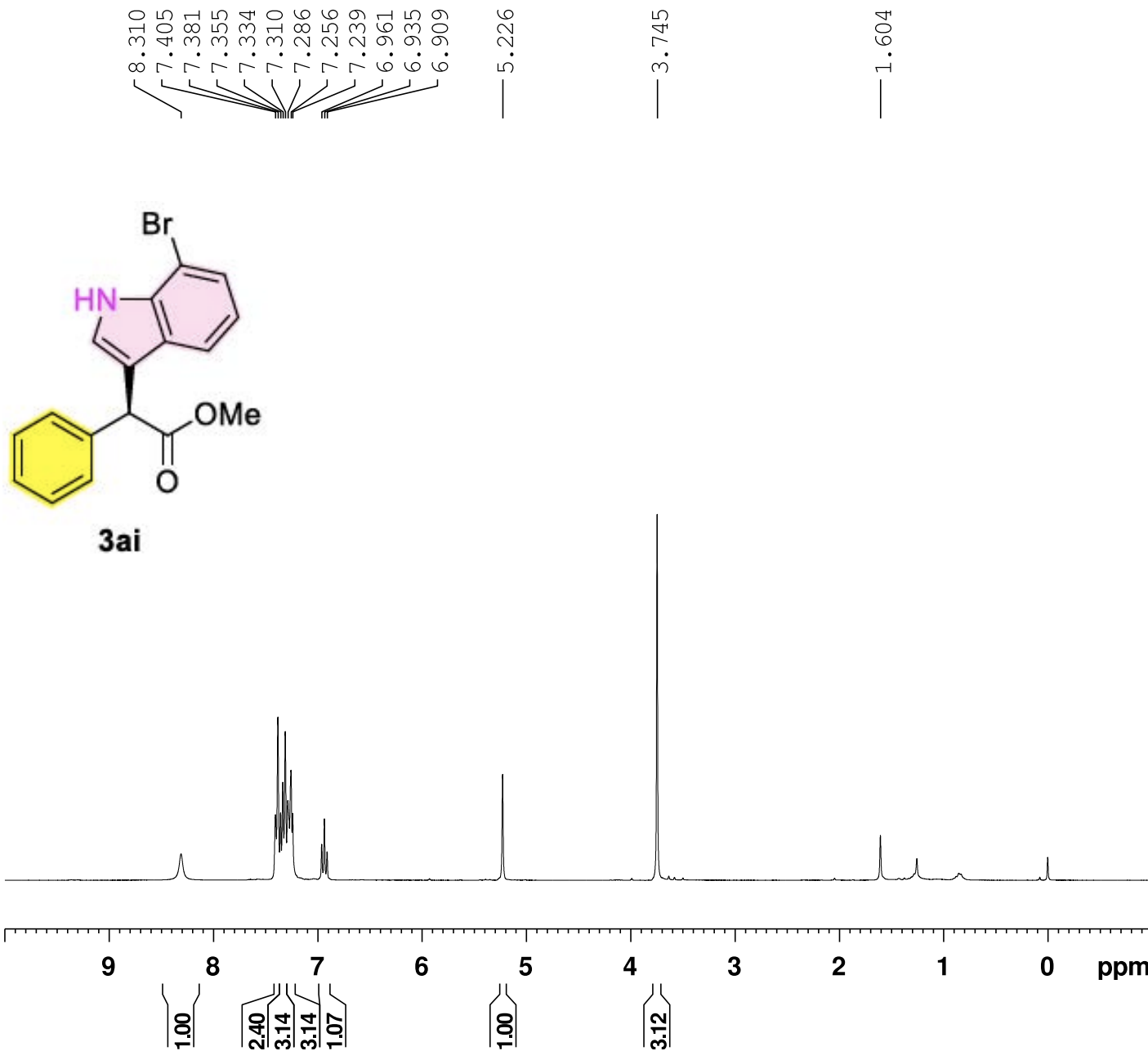


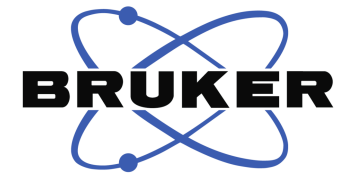
Current Data Parameters  
NAME HNMR-YX-4-p62 (NEW)  
EXPNO 387  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230525  
Time 16.35  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 161  
DW 83.200 usec  
DE 6.50 usec  
TE 293.6 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 300.1318534 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 14.00000000 W

F2 - Processing parameters  
SI 65536  
SF 300.1300127 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





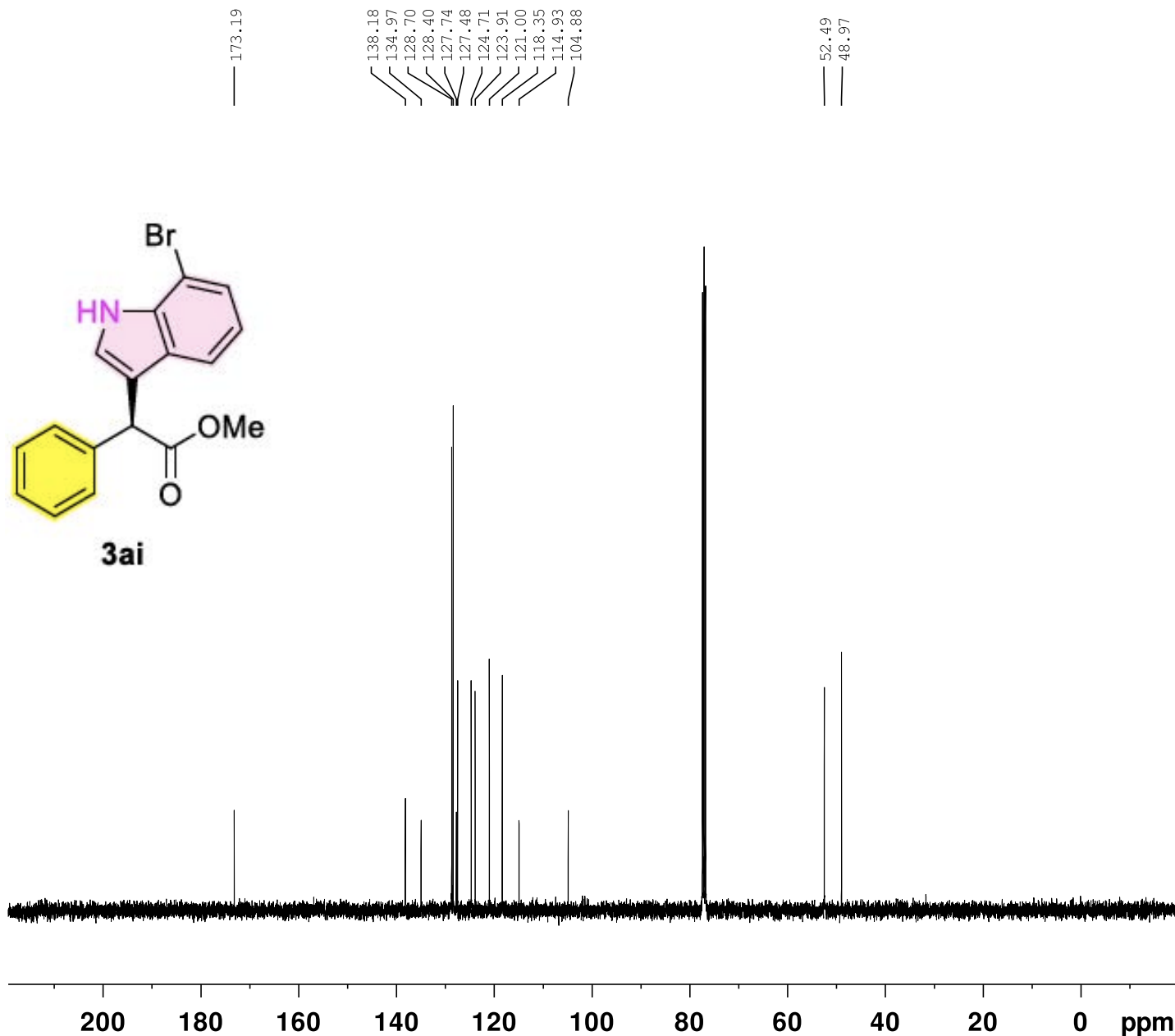
Current Data Parameters  
NAME CNMR-YX-4-p62  
EXPNO 32  
PROCNO 1

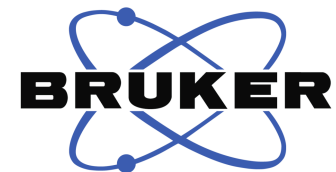
F2 - Acquisition Parameters  
Date\_ 20230525  
Time 21.40  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 100  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 193.13  
DW 20.800 usec  
DE 6.50 usec  
TE 291.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 12.00 usec  
PLW1 53.00000000 W  
SFO1 100.6379178 MHz

==== CHANNEL f2 =====  
CPDPRG[2] waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.37246999 W  
PLW13 0.30170000 W  
SFO2 400.1916008 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6278560 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

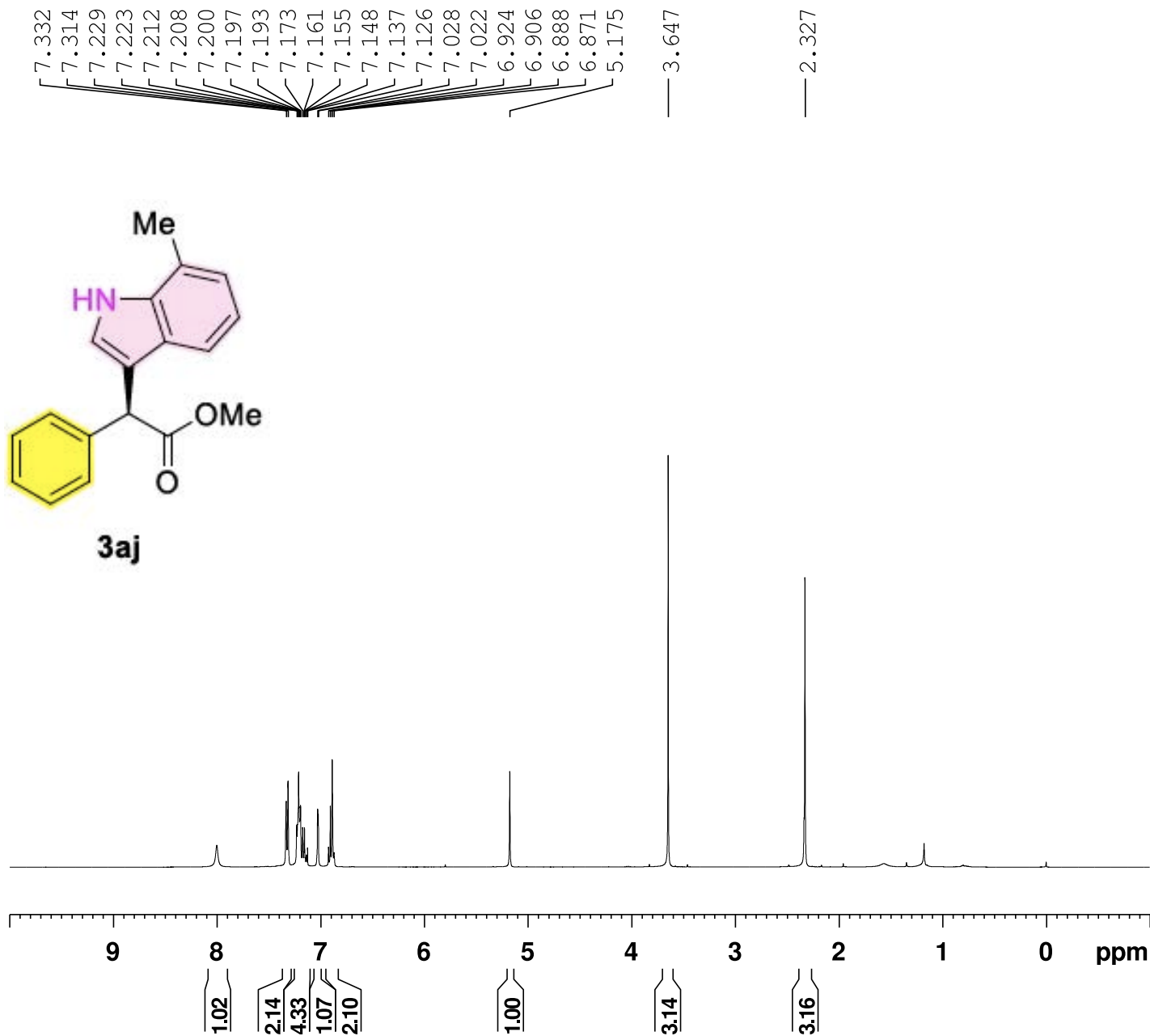


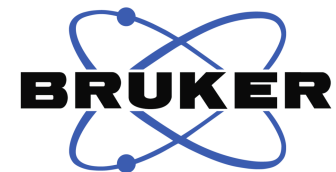


Current Data Parameters  
NAME HNMR-YX-5-p5  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230628  
Time 22.31 h  
INSTRUM Avance  
PROBHD z116098\_0833 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8196.722 Hz  
FIDRES 0.250144 Hz  
AQ 3.9976959 sec  
RG 72.338  
DW 61.000 usec  
DE 13.54 usec  
TE 294.6 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1324708 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 20.73200035 W

F2 - Processing parameters  
SI 65536  
SF 400.1300634 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

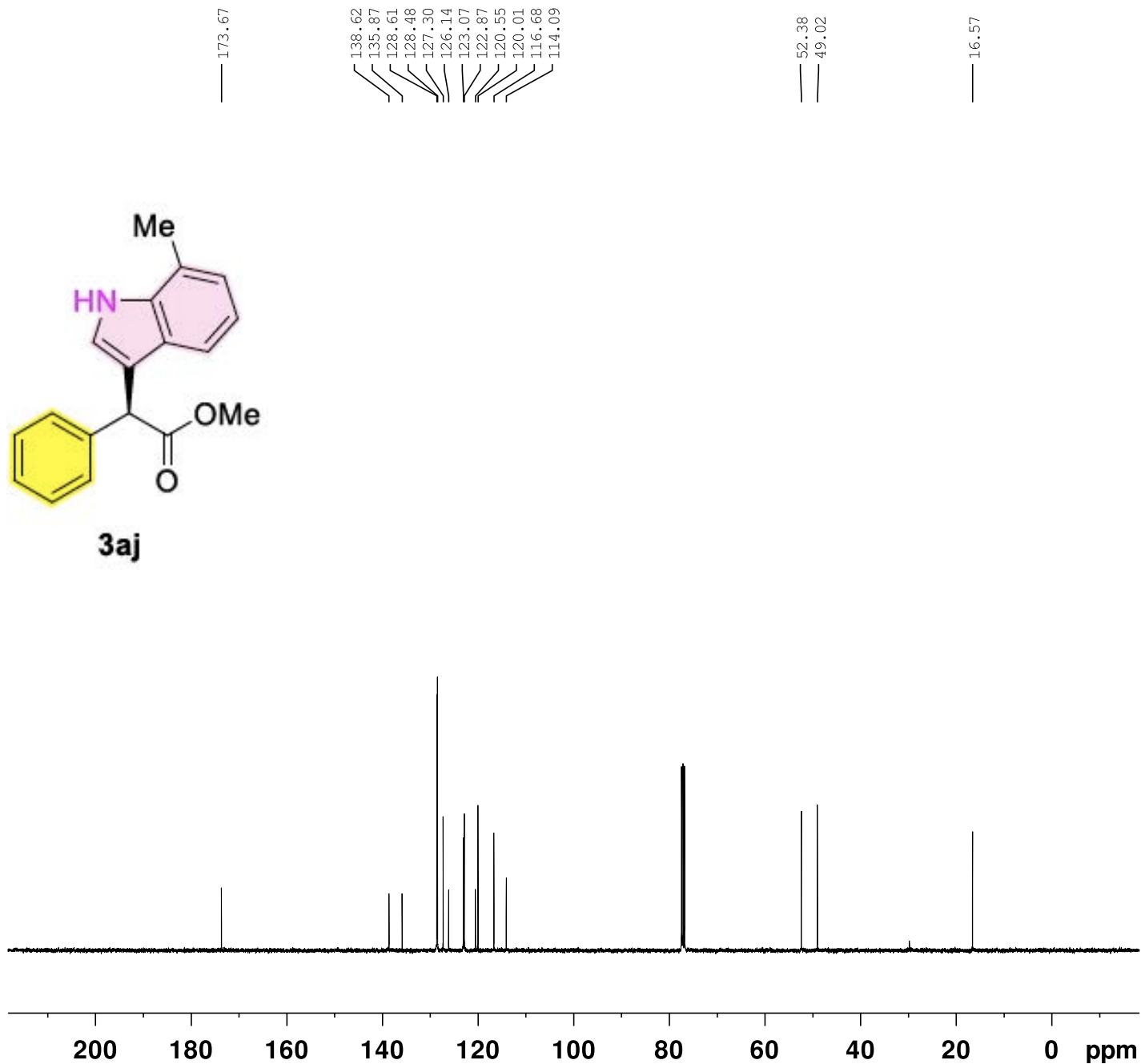


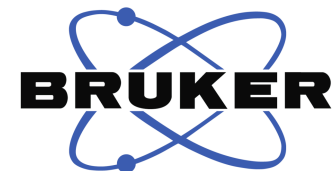


Current Data Parameters  
NAME CNMR-YX-5-p5  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230628  
Time 22.44 h  
INSTRUM Avance  
PROBHD z116098\_0833 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 200  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 51.55  
DW 21.000 usec  
DE 6.50 usec  
TE 295.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 3.33 usec  
P1 10.00 usec  
PLW1 87.89900208 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 20.73200035 W  
PLW12 0.25595000 W  
PLW13 0.12874000 W

F2 - Processing parameters  
SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





Current Data Parameters  
NAME HNMR-YX-4-p84  
EXPNO 423  
PROCNO 1

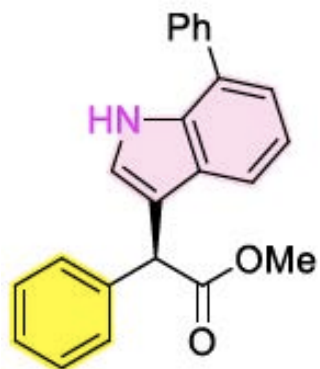
F2 - Acquisition Parameters  
Date\_ 20230606  
Time 15.46  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 161  
DW 83.200 usec  
DE 6.50 usec  
TE 296.0 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 300.1318534 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 14.00000000 W

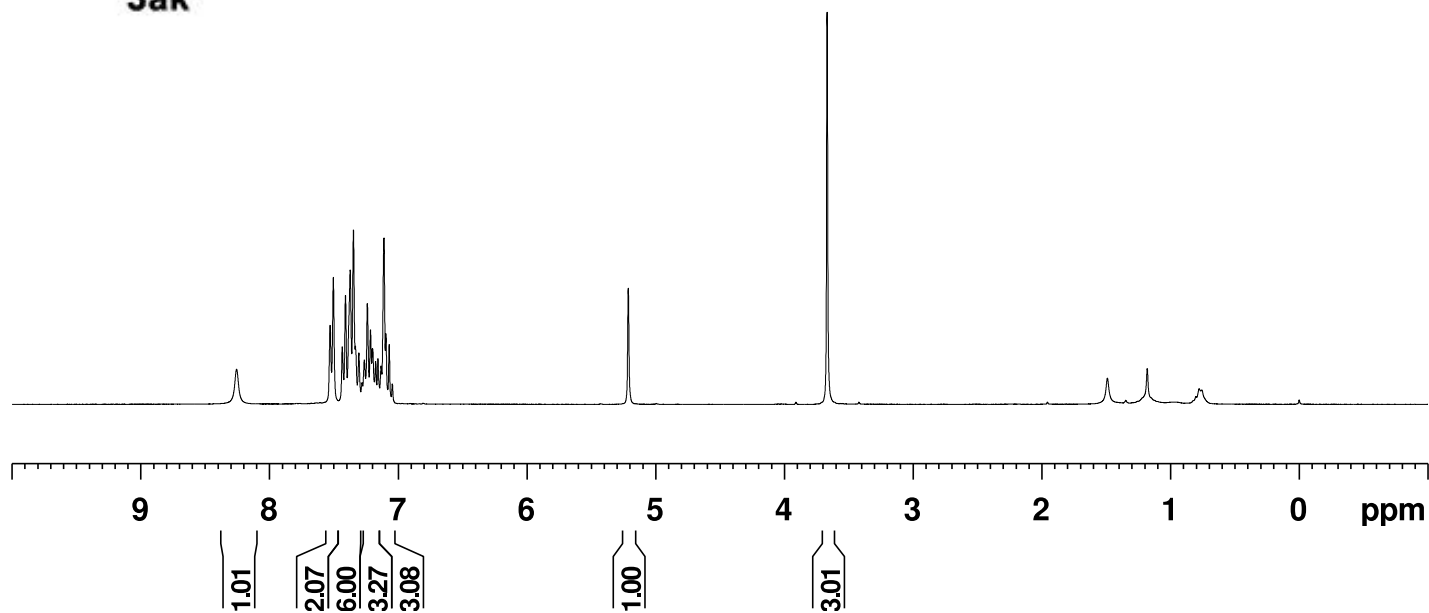
F2 - Processing parameters  
SI 65536  
SF 300.1300376 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

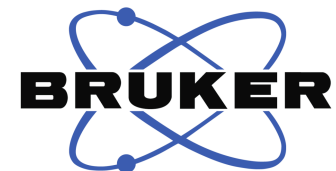
7.529  
7.503  
7.434  
7.409  
7.372  
7.347  
7.331  
7.305  
7.279  
7.263  
7.239  
7.214  
7.199  
7.174  
7.156  
7.133  
7.110  
7.095  
7.069  
7.045  
5.212

3.667



3ak





Current Data Parameters  
NAME CNMR-YX-4-p84  
EXPNO 424  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20230606  
Time 16.01  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 200  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE 296.7 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

==== CHANNEL f1 =====

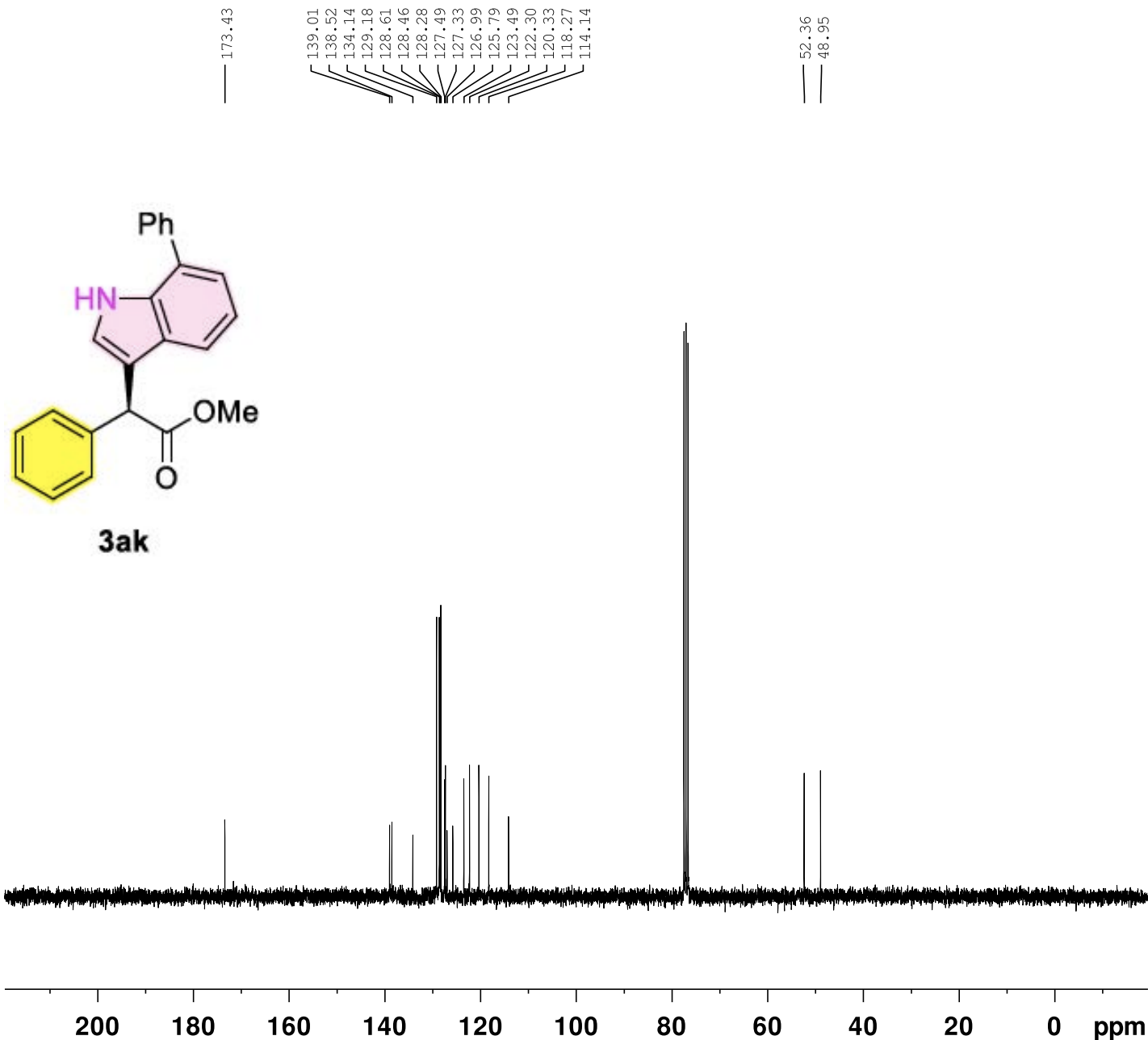
SFO1 75.4752949 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 34.20000076 W

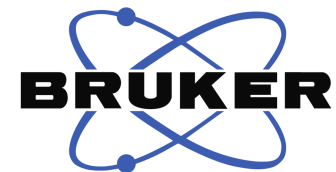
==== CHANNEL f2 =====

SFO2 300.1312005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W  
PLW13 0.14000000 W

F2 - Processing parameters

SI 32768  
SF 75.4677485 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





Current Data Parameters  
NAME HNMR-YX-5-p8  
EXPNO 993  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230703  
Time 15.52  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 114  
DW 83.200 usec  
DE 6.50 usec  
TE 298.8 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 300.1318534 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 14.00000000 W

F2 - Processing parameters  
SI 65536  
SF 300.1300412 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

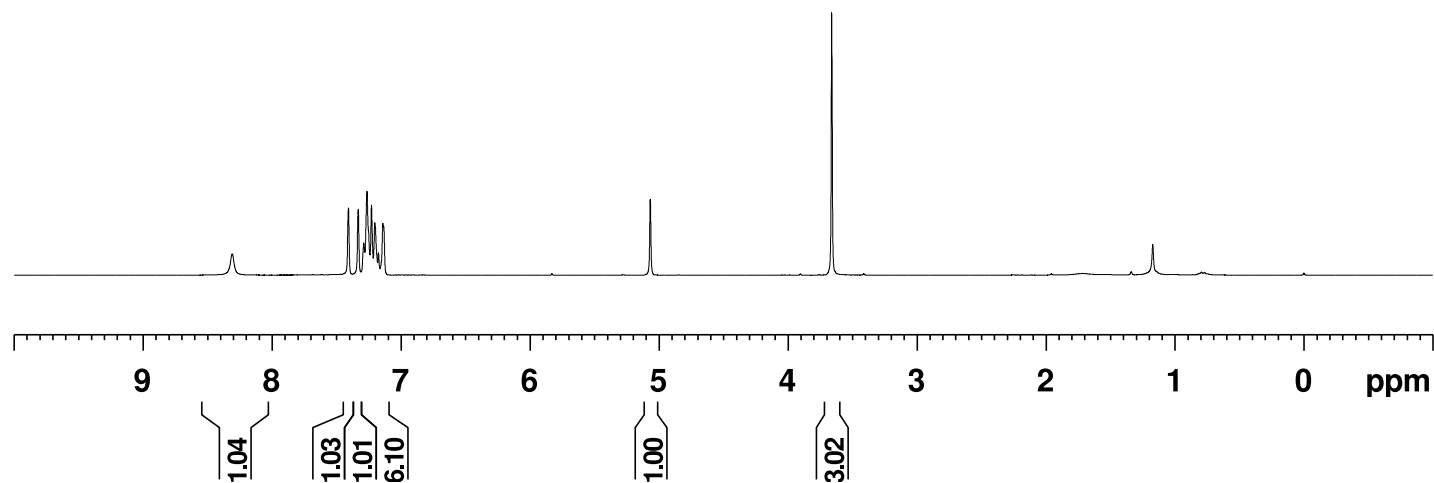
8.309  
7.408  
7.331  
7.289  
7.263  
7.229  
7.203  
7.175  
7.140  
7.134

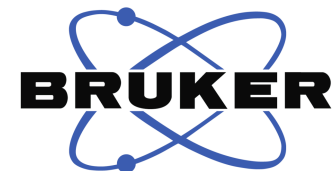
5.067

3.661



3al





Current Data Parameters  
NAME CNMR-YX-5-p8  
EXPNO 997  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20230703  
Time 17.16  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 150  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE 299.3 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

==== CHANNEL f1 =====

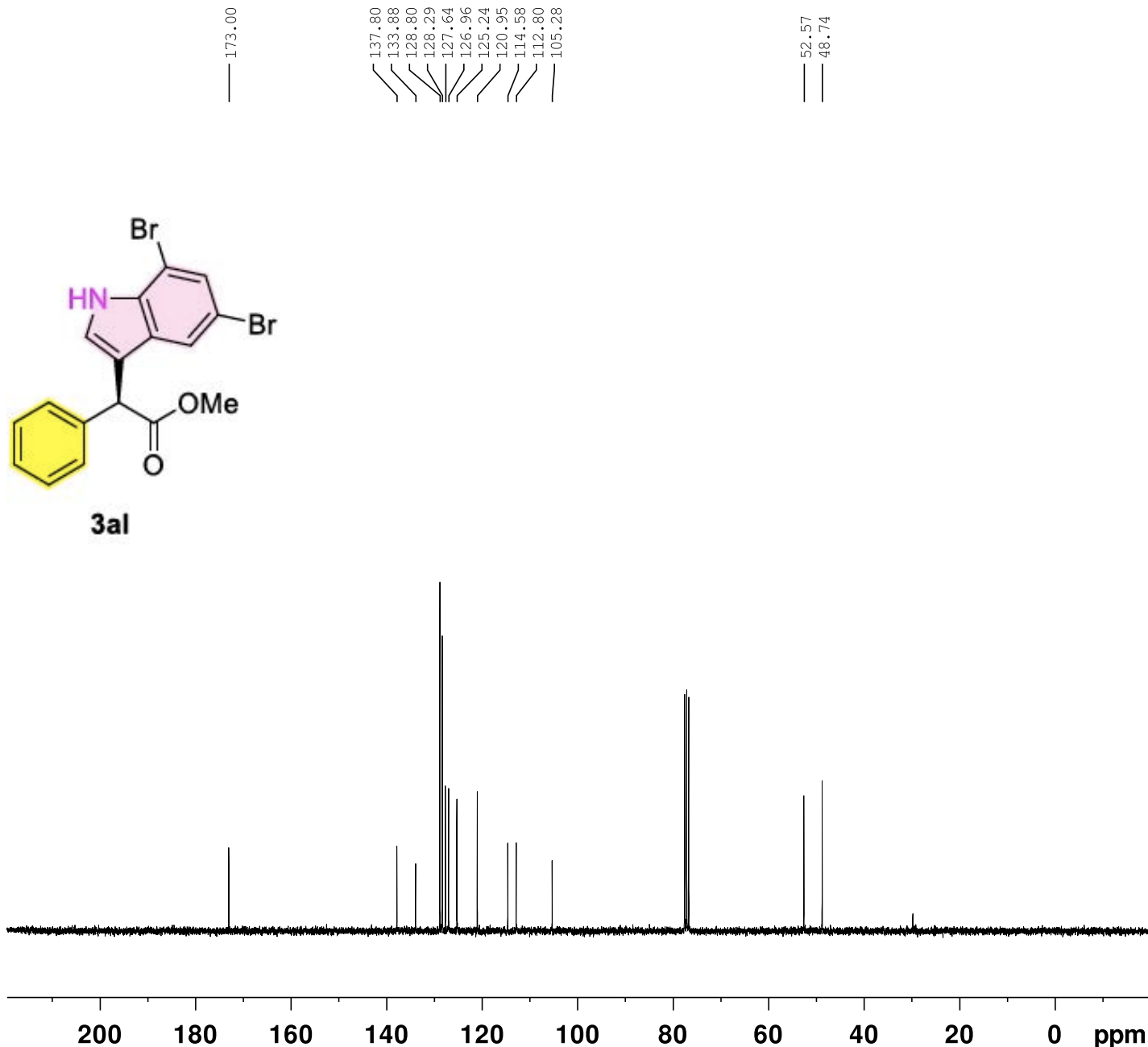
SFO1 75.4752949 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 34.20000076 W

==== CHANNEL f2 =====

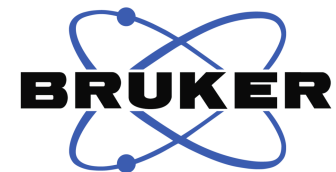
SFO2 300.1312005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W  
PLW13 0.14000000 W

F2 - Processing parameters

SI 32768  
SF 75.4677485 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40







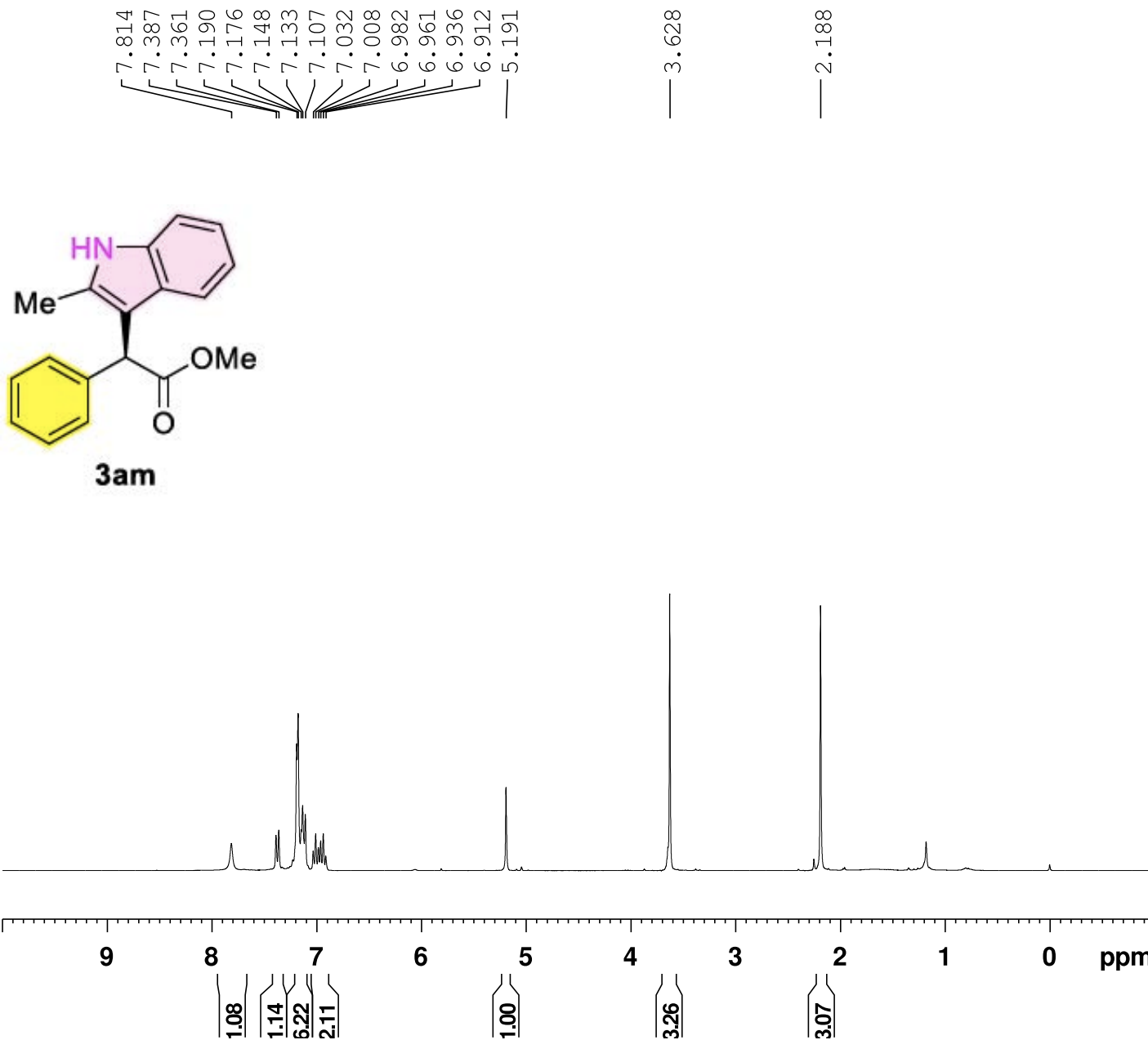
Current Data Parameters  
NAME HNMR-YX-5-p60  
EXPNO 1181  
PROCNO 1

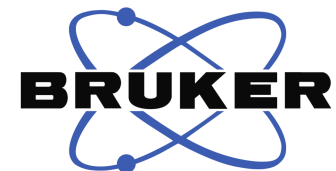
F2 - Acquisition Parameters

Date\_ 20230803  
Time 21.31  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 114  
DW 83.200 usec  
DE 6.50 usec  
TE 298.1 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 300.1318534 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 14.00000000 W

F2 - Processing parameters  
SI 65536  
SF 300.1300456 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





Current Data Parameters  
NAME CNMR-YX-5-p60  
EXPNO 2003  
PROCNO 1

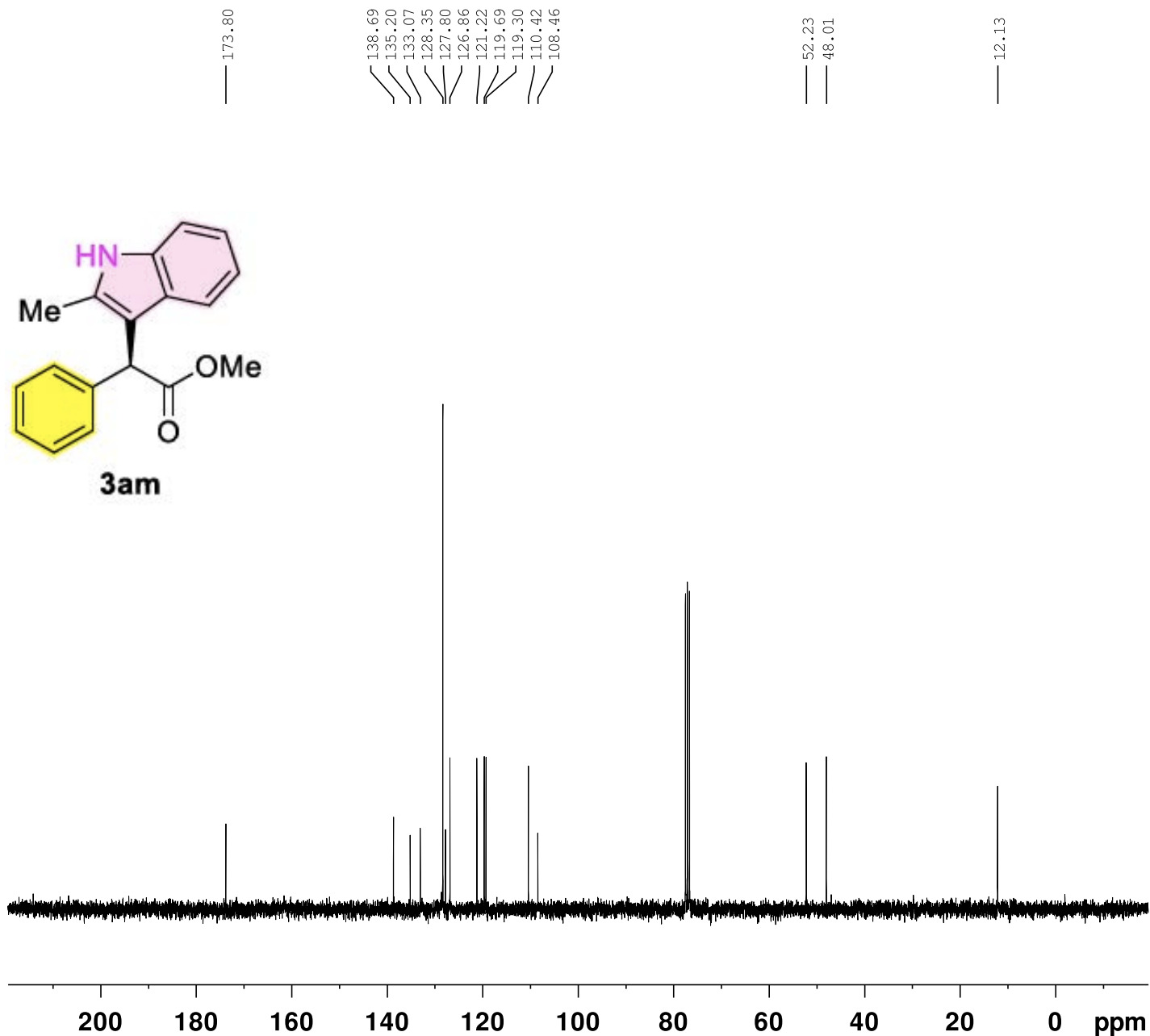
F2 - Acquisition Parameters

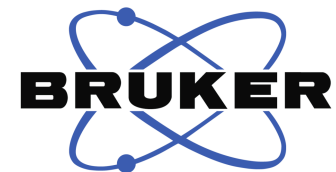
Date\_ 20230804  
Time 16.05  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 50  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE 298.3 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 75.4752949 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 34.20000076 W

==== CHANNEL f2 =====  
SFO2 300.1312005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W  
PLW13 0.14000000 W

F2 - Processing parameters  
SI 32768  
SF 75.4677485 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



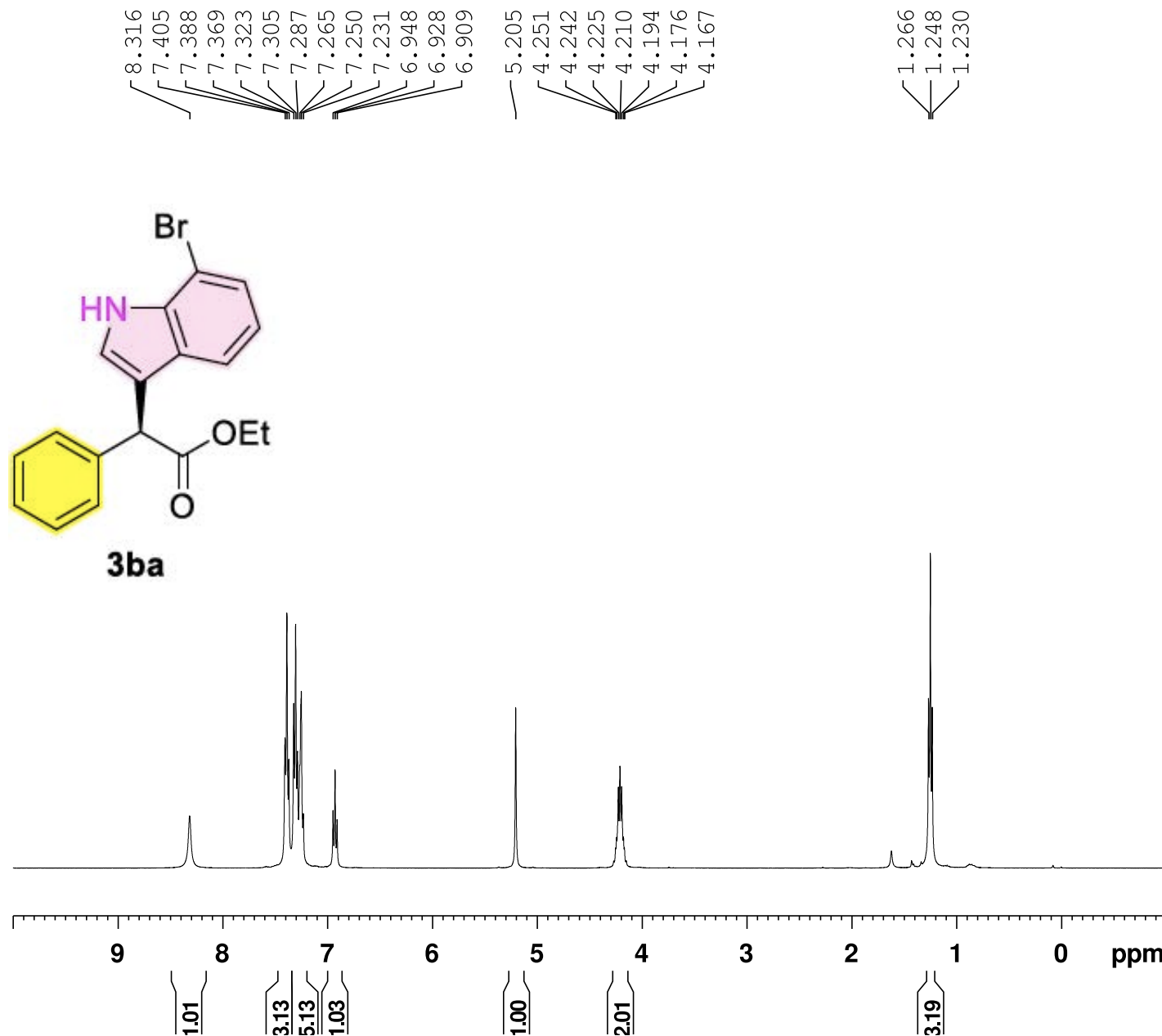


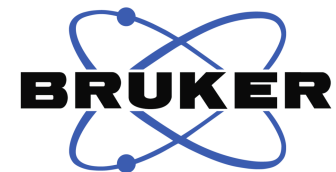
Current Data Parameters  
NAME HNMR-YX-7-p14  
EXPNO 17  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231101  
Time 15.07  
INSTRUM spect  
PROBHD 5 mm PADUL 13C  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 4  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9845889 sec  
RG 75.43  
DW 60.800 usec  
DE 6.50 usec  
TE 291.4 K  
D1 1.00000000 sec  
TD0 1

=====  
CHANNEL f1  
NUC1 1H  
P1 9.90 usec  
PLW1 23.00000000 W  
SFO1 400.1924713 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1900255 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





Current Data Parameters  
NAME CNMR-YX-7-p14  
EXPNO 18  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20231101  
Time 15.14  
INSTRUM spect  
PROBHD 5 mm PADUL 13C  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 100  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 29.75  
DW 20.800 usec  
DE 6.50 usec  
TE 291.9 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

==== CHANNEL f1 =====

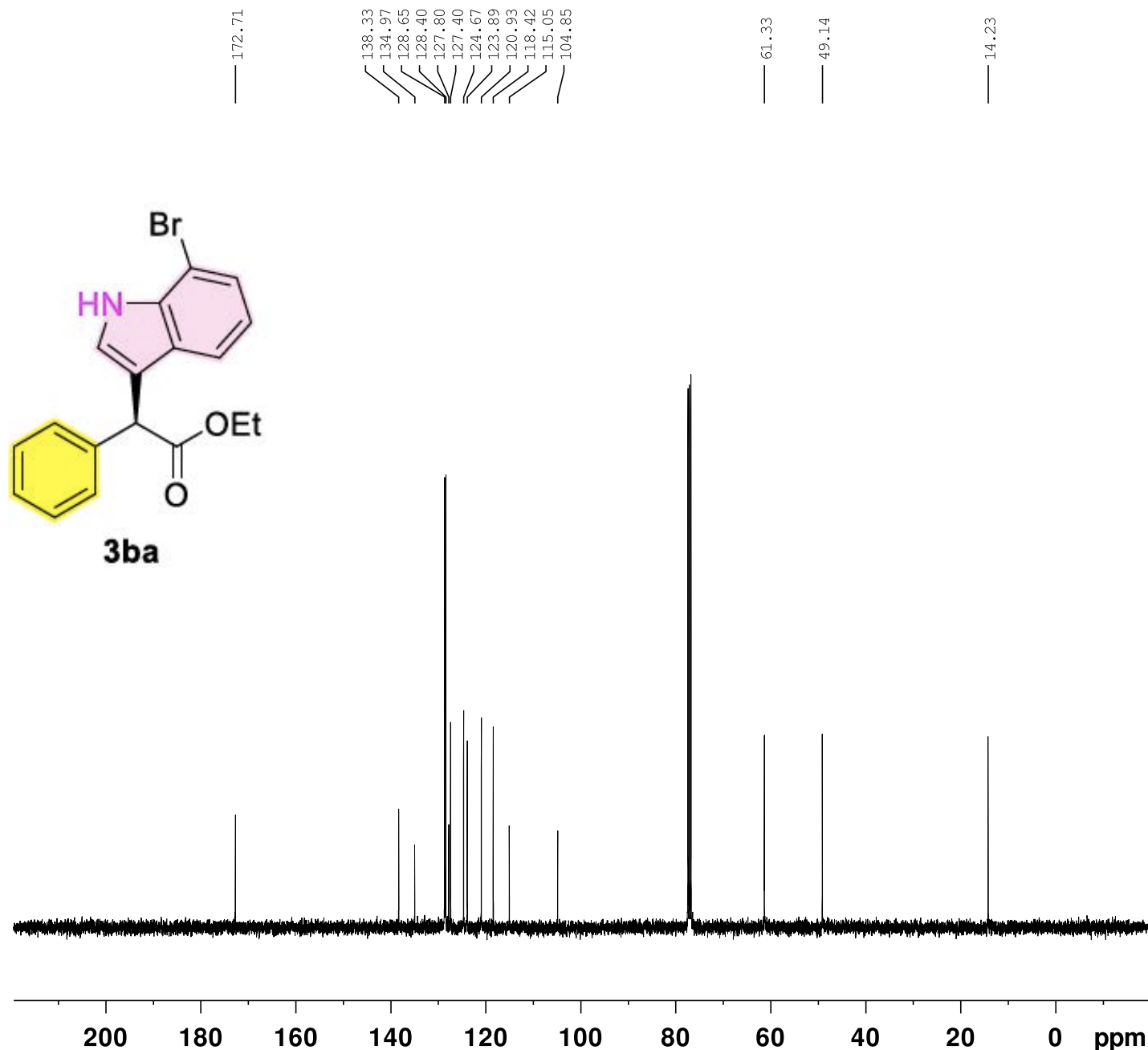
NUC1 13C  
P1 9.80 usec  
PLW1 47.40000153 W  
SFO1 100.6379178 MHz

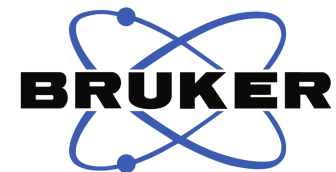
==== CHANNEL f2 =====

CPDPRG[2] waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 23.00000000 W  
PLW12 0.30712000 W  
PLW13 0.24877000 W  
SFO2 400.1916008 MHz

F2 - Processing parameters

SI 32768  
SF 100.6278560 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





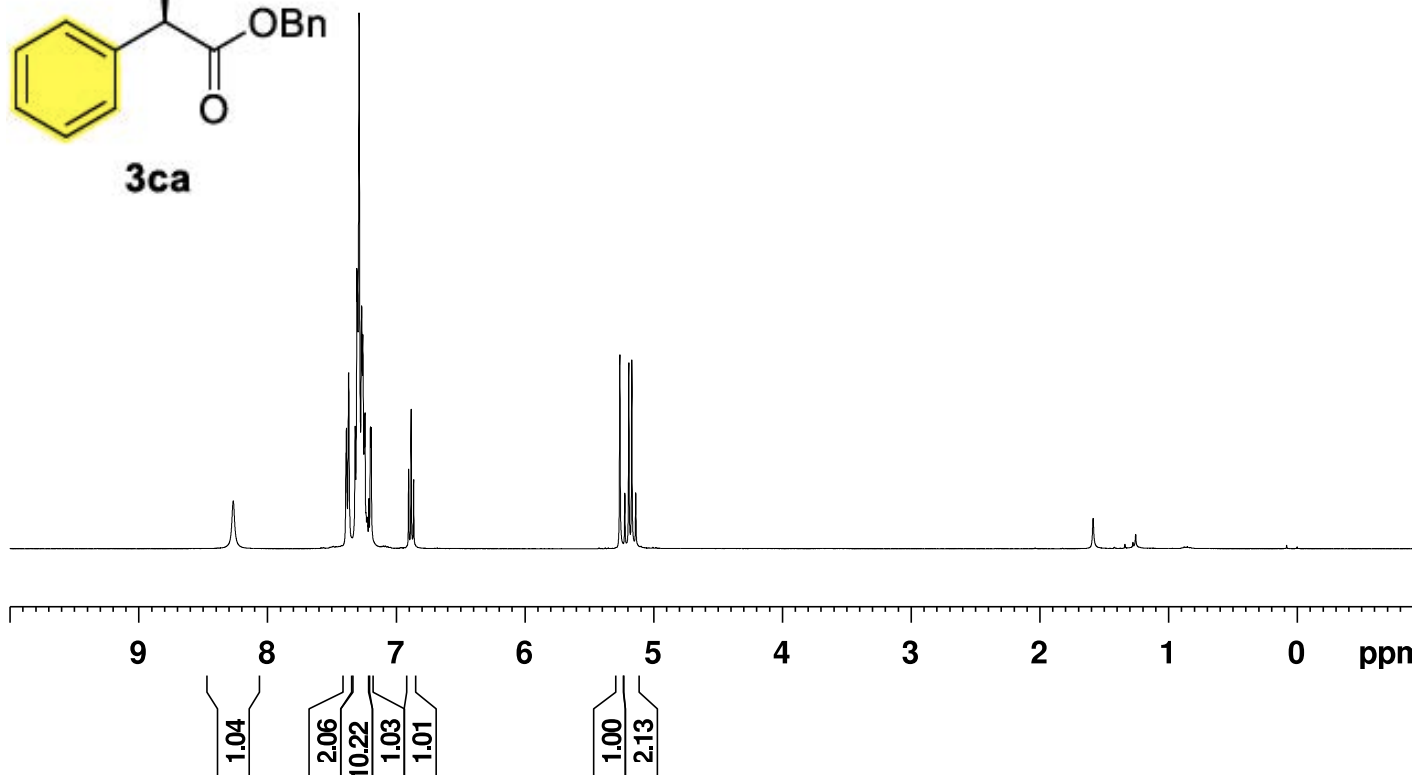
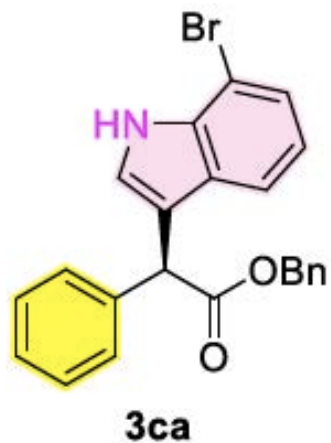
Current Data Parameters  
NAME HNMR-YX-7-p15  
EXPNO 36  
PROCNO 1

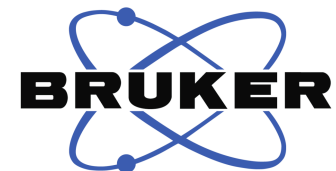
F2 - Acquisition Parameters  
Date\_ 20231109  
Time 15.57  
INSTRUM spect  
PROBHD 5 mm PADUL 13C  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 4  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9845889 sec  
RG 68.24  
DW 60.800 usec  
DE 6.50 usec  
TE 294.0 K  
D1 1.00000000 sec  
TD0 1

=====  
CHANNEL f1  
NUC1 1H  
P1 9.90 usec  
PLW1 23.00000000 W  
SFO1 400.1924713 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1900332 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

8.265  
7.386  
7.368  
7.318  
7.304  
7.300  
7.287  
7.267  
7.258  
7.247  
7.242  
7.212  
7.199  
7.194  
6.902  
6.883  
6.863  
5.261  
5.223  
5.192  
5.169  
5.138





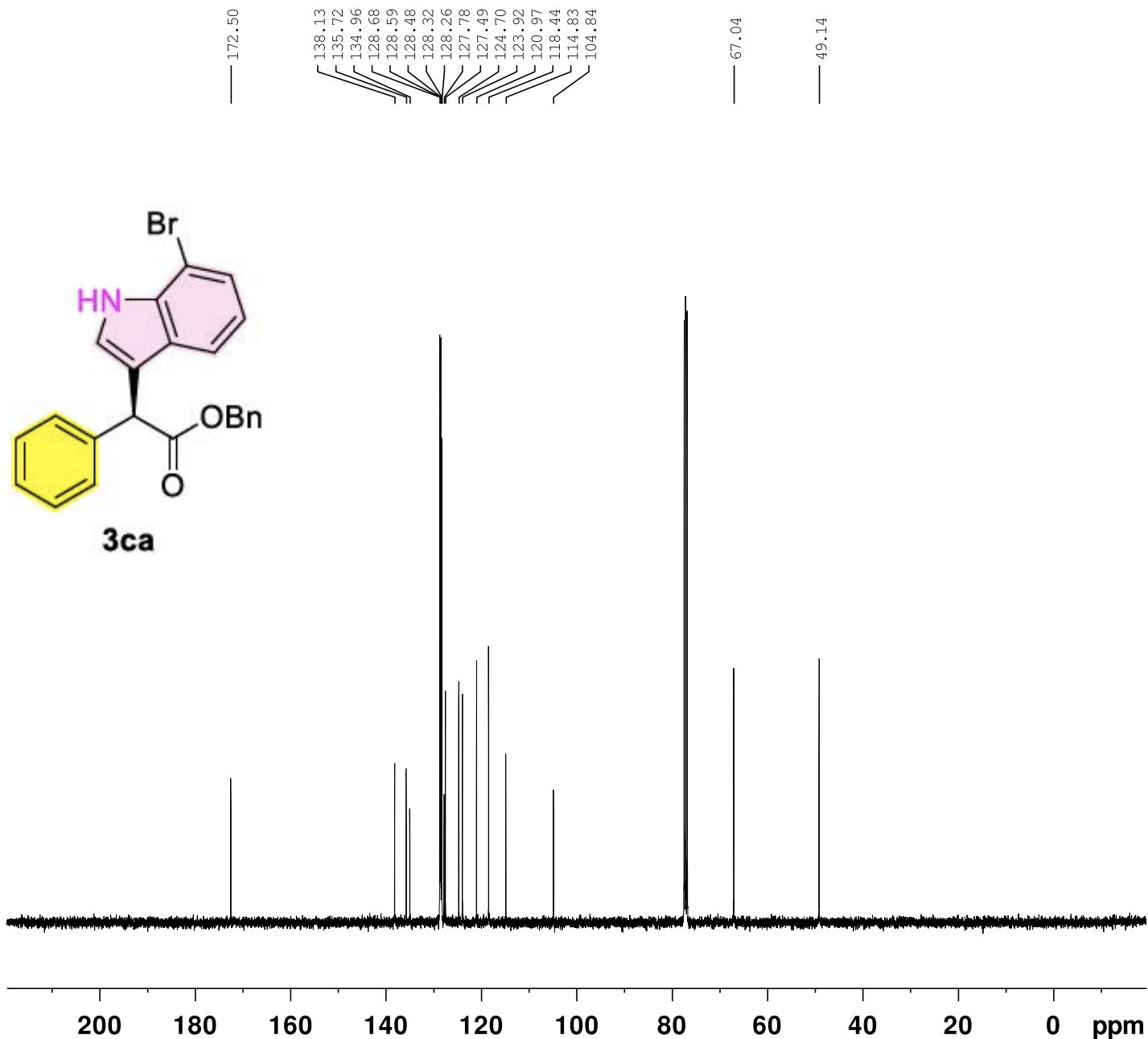
Current Data Parameters  
NAME CNMR-YX-7-p15  
EXPNO 37  
PROCNO 1

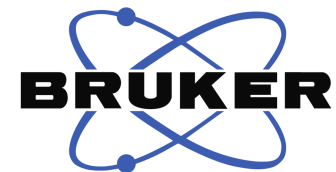
F2 - Acquisition Parameters  
Date\_ 20231109  
Time 16.09  
INSTRUM spect  
PROBHD 5 mm PADUL 13C  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 188  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 37.77  
DW 20.800 usec  
DE 6.50 usec  
TE 294.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 9.80 usec  
PLW1 47.40000153 W  
SFO1 100.6379178 MHz

==== CHANNEL f2 =====  
CPDPRG[2] waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 23.00000000 W  
PLW12 0.30712000 W  
PLW13 0.24877000 W  
SFO2 400.1916008 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6278560 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





Current Data Parameters  
NAME HNMR-YX-5-p25  
EXPNO 1051  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230711  
Time 20.34  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 114  
DW 83.200 usec  
DE 6.50 usec  
TE 300.1 K  
D1 1.00000000 sec  
TD0 1

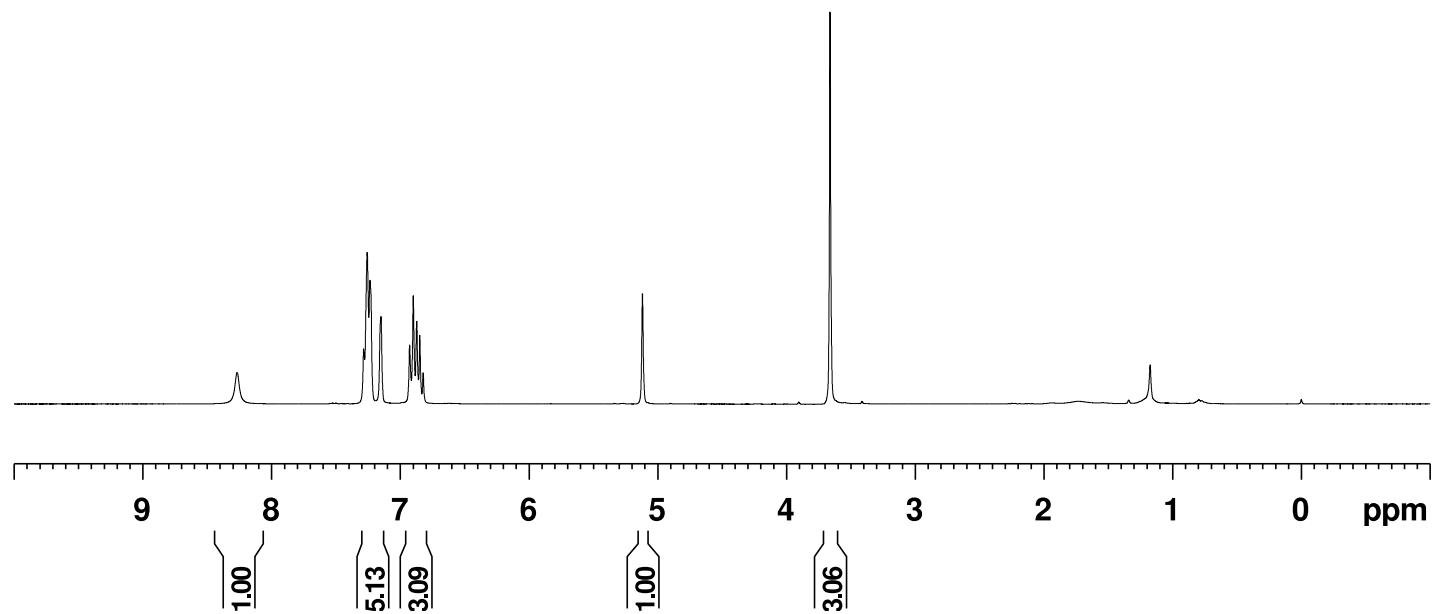
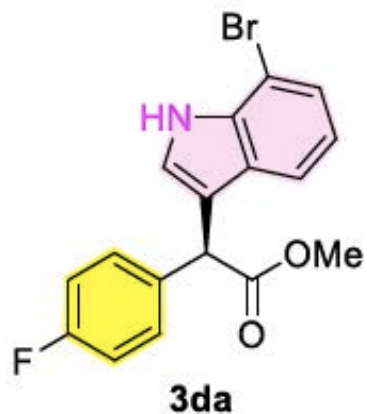
==== CHANNEL f1 =====  
SFO1 300.1318534 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 14.00000000 W

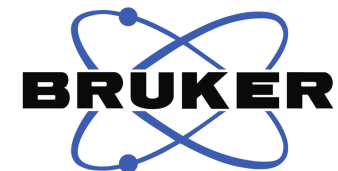
F2 - Processing parameters  
SI 65536  
SF 300.1300408 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

8.267  
7.284  
7.257  
7.234  
7.149  
6.927  
6.899  
6.871  
6.848  
6.822

5.118

3.661





Current Data Parameters  
NAME CNMR-YX-5-p25  
EXPNO 1059  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20230712  
Time 1.26  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 100  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE 300.7 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

==== CHANNEL f1 =====

SFO1 75.4752949 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 34.20000076 W

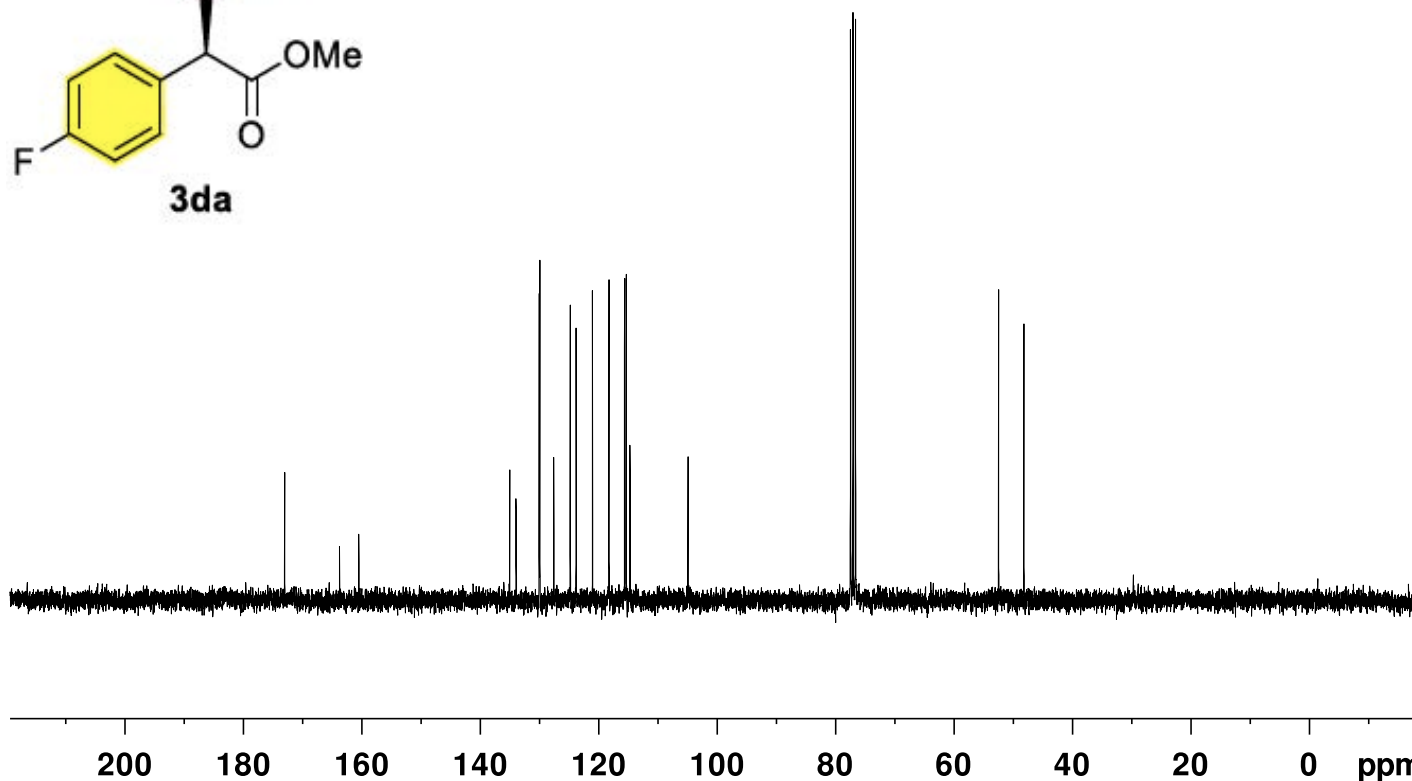
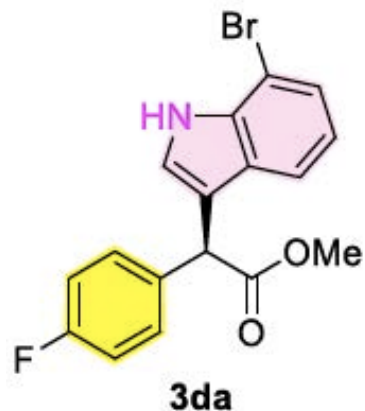
==== CHANNEL f2 =====

SFO2 300.1312005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W  
PLW13 0.14000000 W

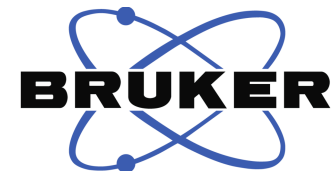
F2 - Processing parameters

SI 32768  
SF 75.4677485 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

173.04  
163.78  
160.52  
135.03  
133.98  
133.94  
130.05  
129.95  
127.60  
124.81  
123.82  
121.06  
118.28  
115.65  
115.36  
114.73  
104.92  
52.49  
48.21







Current Data Parameters  
NAME FNMR-YX-5-p25  
EXPNO 1052  
PROCNO 1

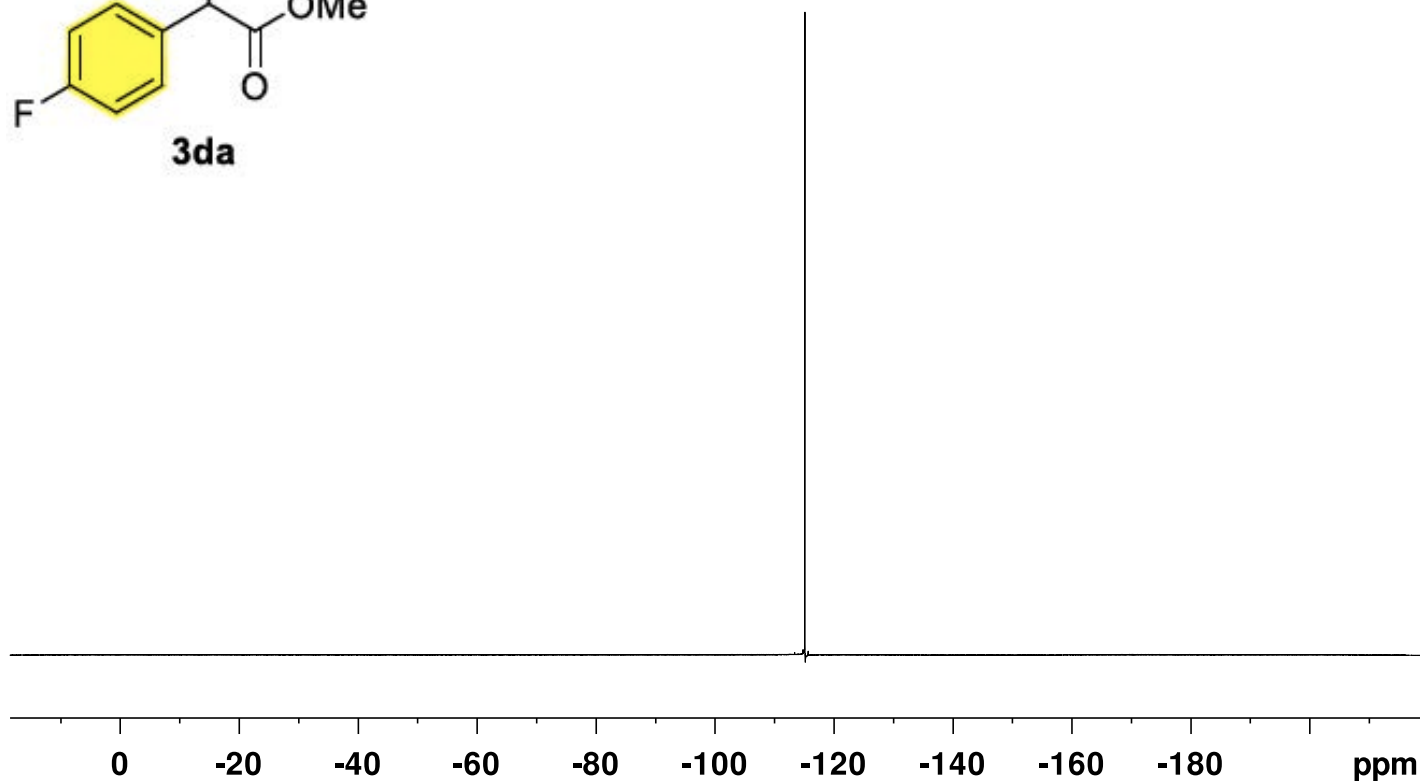
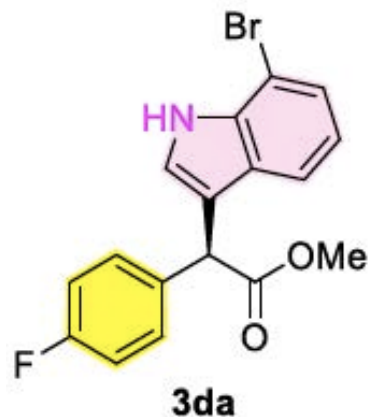
F2 - Acquisition Parameters  
Date\_ 20230711  
Time 20.38  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgfhigqn.2  
TD 131072  
SOLVENT CDCl3  
NS 16  
DS 4  
SWH 66964.289 Hz  
FIDRES 0.510897 Hz  
AQ 0.9786710 sec  
RG 203  
DW 7.467 usec  
DE 6.50 usec  
TE 300.2 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
D12 0.00002000 sec  
TD0 1

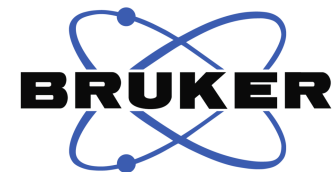
==== CHANNEL f1 =====  
SFO1 282.3761148 MHz  
NUC1 19F  
P1 14.50 usec  
PLW1 10.39999962 W

==== CHANNEL f2 =====  
SFO2 300.1312005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W

F2 - Processing parameters  
SI 65536  
SF 282.4043552 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

-115.14



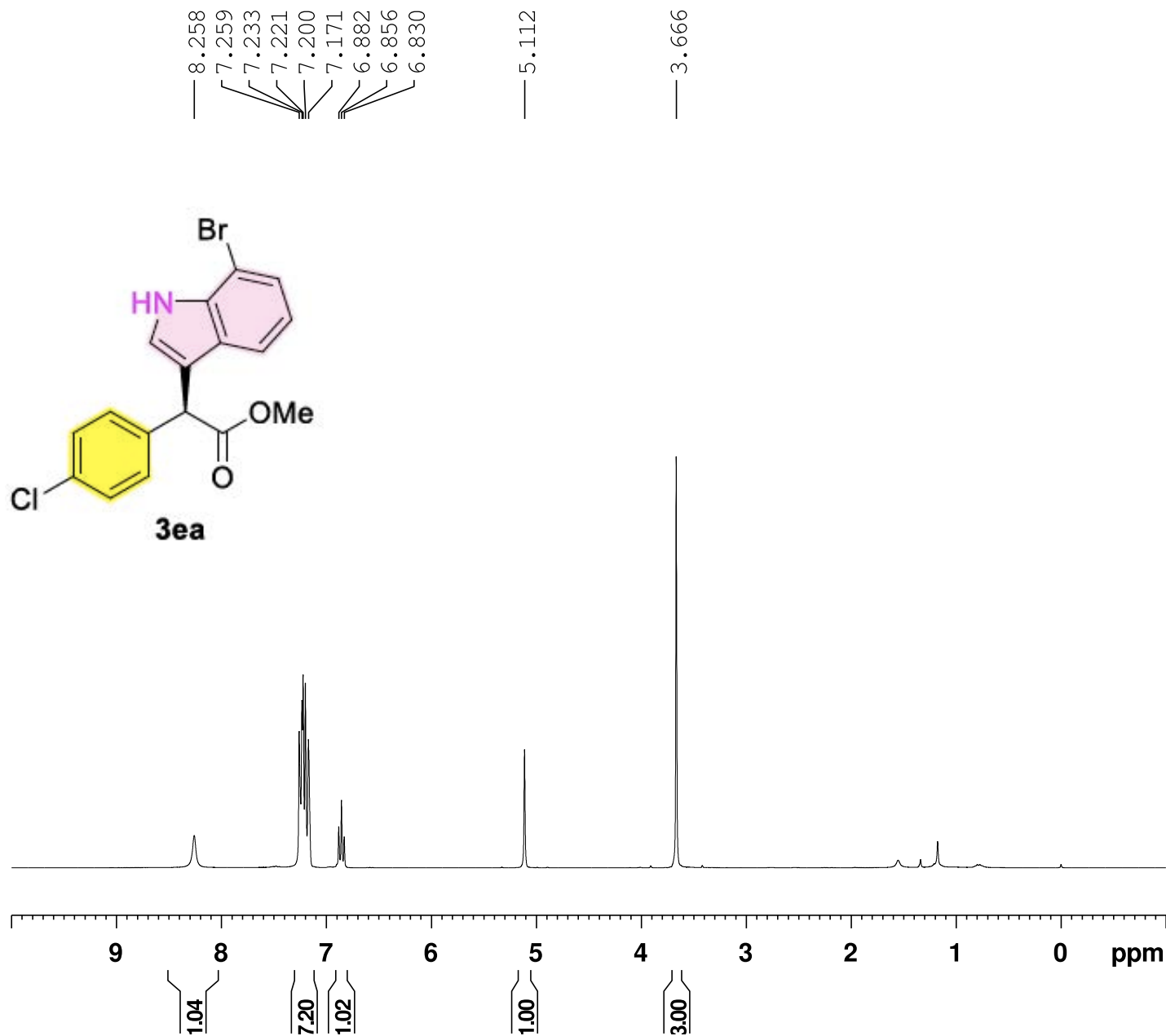


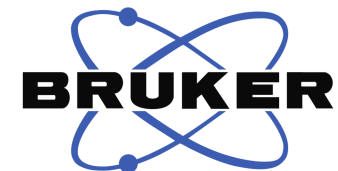
Current Data Parameters  
NAME HNMR-YX-4-p98  
EXPNO 757  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230619  
Time 22.11  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 144  
DW 83.200 usec  
DE 6.50 usec  
TE 296.7 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 300.1318534 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 14.00000000 W

F2 - Processing parameters  
SI 65536  
SF 300.1300381 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





Current Data Parameters  
NAME CNMR-YX-4-p98  
EXPNO 758  
PROCNO 1

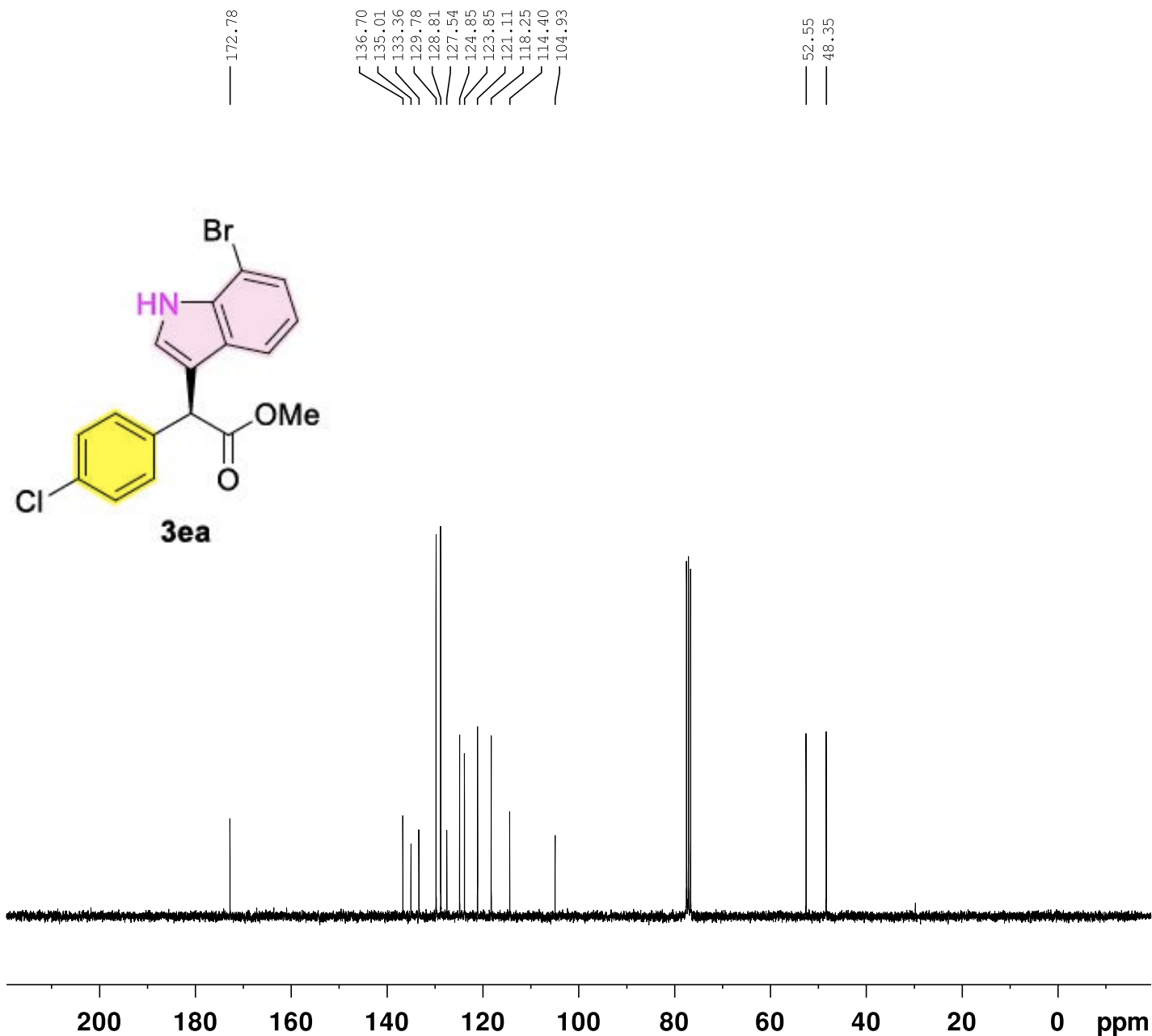
F2 - Acquisition Parameters

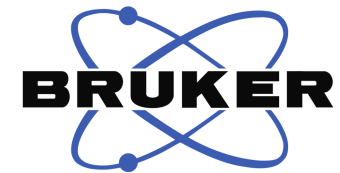
Date\_ 20230619  
Time 22.29  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 250  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE 297.3 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 75.4752949 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 34.20000076 W

==== CHANNEL f2 =====  
SFO2 300.1312005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W  
PLW13 0.14000000 W

F2 - Processing parameters  
SI 32768  
SF 75.4677485 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



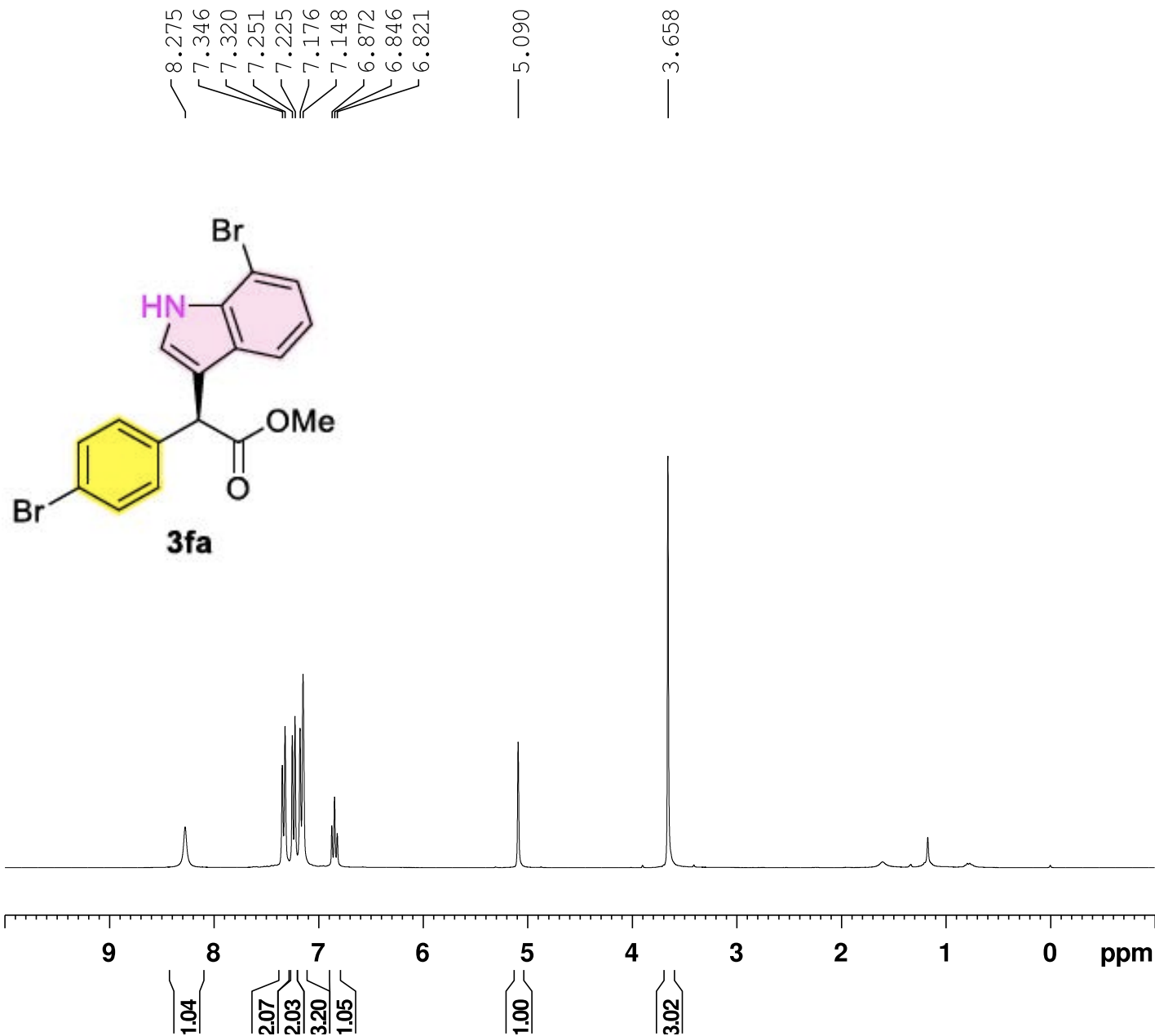


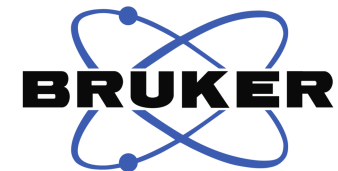
Current Data Parameters  
NAME HNMR-YX-4-p95  
EXPNO 722  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230616  
Time 14.41  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 114  
DW 83.200 usec  
DE 6.50 usec  
TE 296.7 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 300.1318534 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 14.00000000 W

F2 - Processing parameters  
SI 65536  
SF 300.1300417 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





Current Data Parameters  
NAME CNMR-YX-4-p95  
EXPNO 730  
PROCNO 1

F2 - Acquisition Parameters

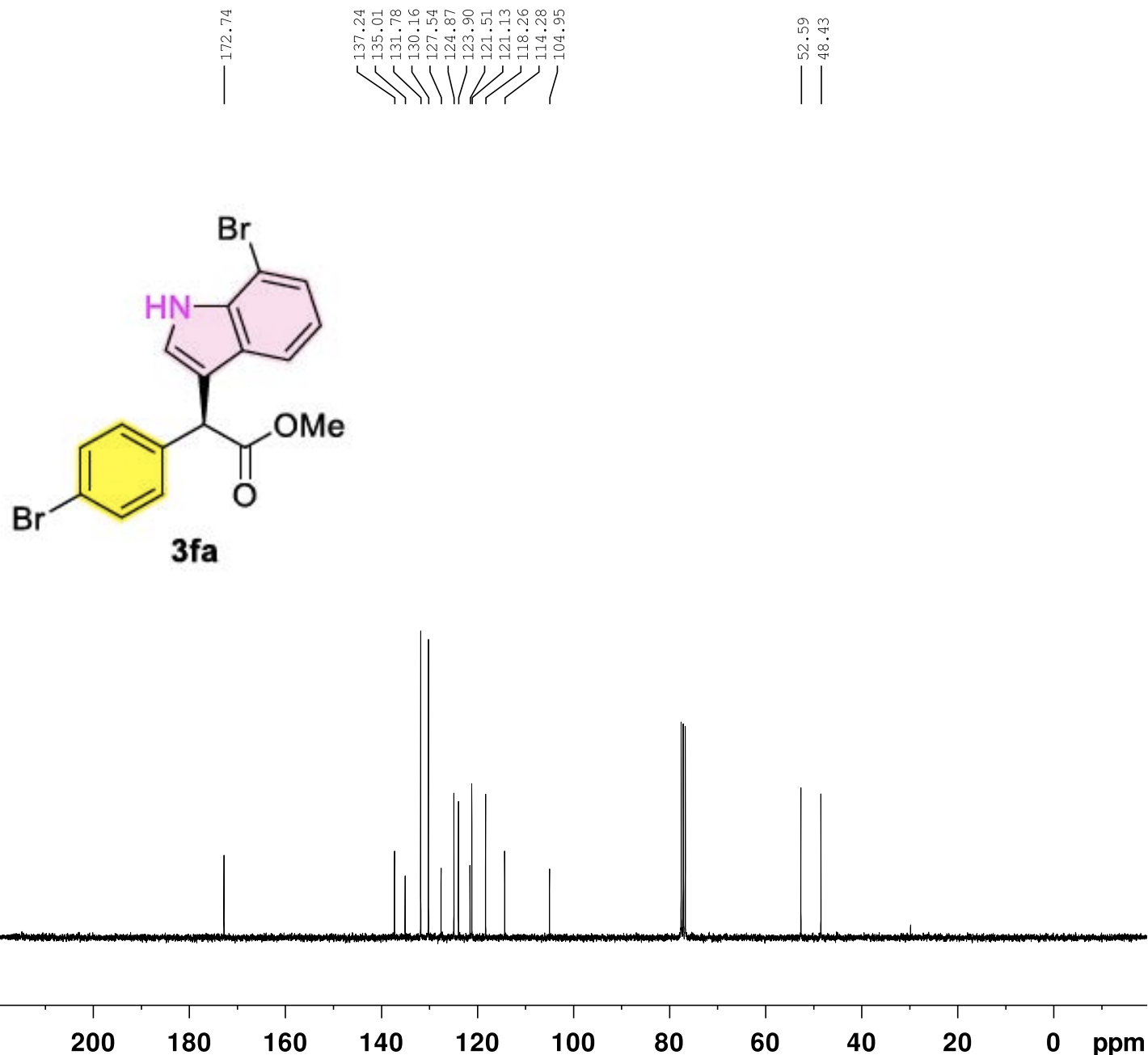
Date\_ 20230616  
Time 16.11  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 200  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE 296.9 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

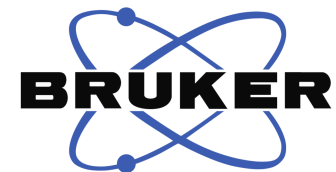
==== CHANNEL f1 =====  
SFO1 75.4752949 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 34.20000076 W

==== CHANNEL f2 =====  
SFO2 300.1312005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W  
PLW13 0.14000000 W

F2 - Processing parameters

SI 32768  
SF 75.4677485 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

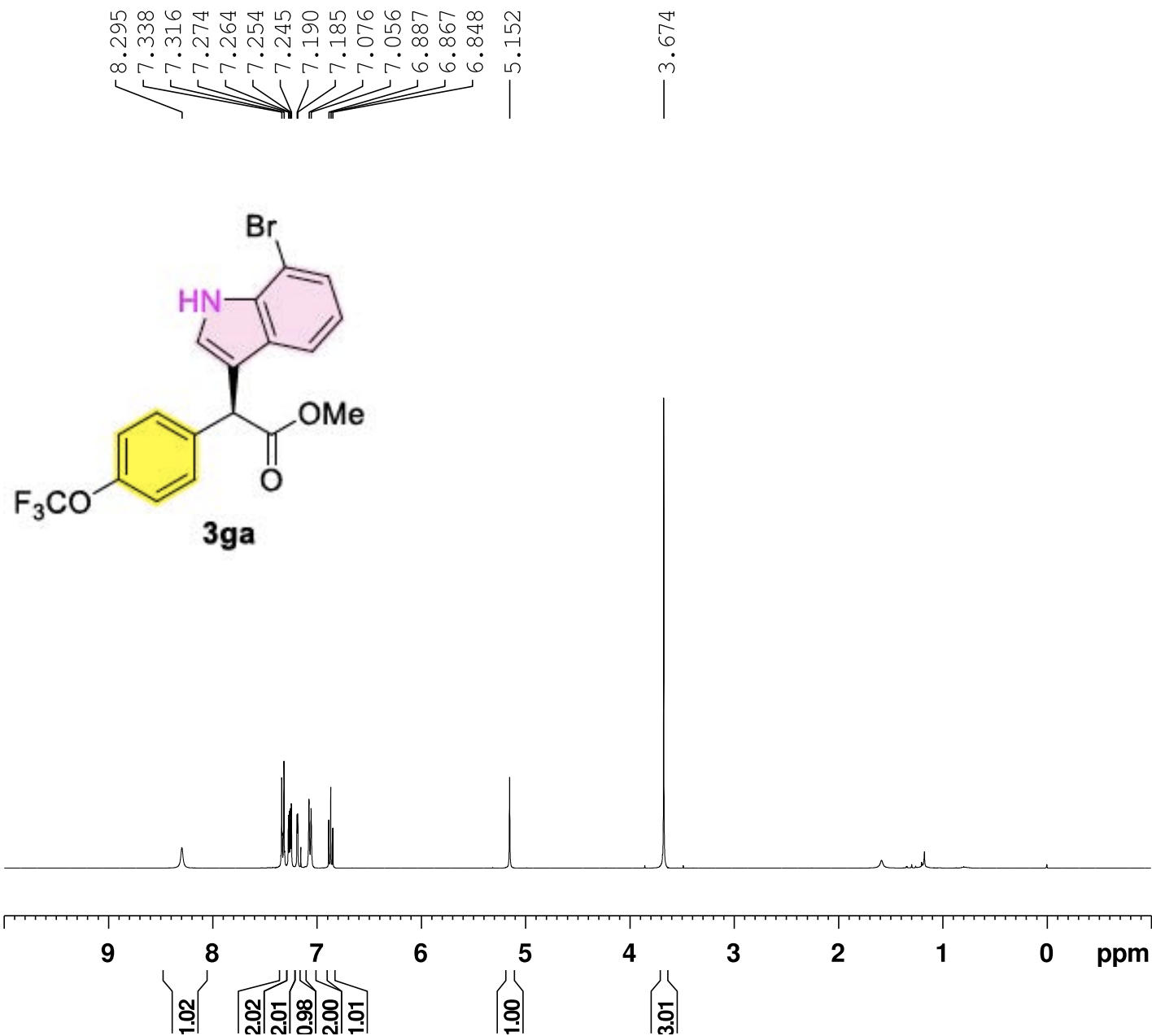


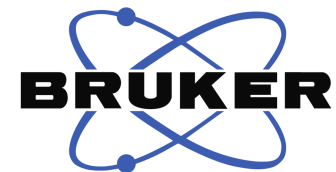


Current Data Parameters  
NAME HNMR-YX-5-p50  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230728  
Time 20.14 h  
INSTRUM Avance  
PROBHD z116098\_0833 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8196.722 Hz  
FIDRES 0.250144 Hz  
AQ 3.9976959 sec  
RG 93.006  
DW 61.000 usec  
DE 13.54 usec  
TE 294.7 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1324708 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 20.73200035 W

F2 - Processing parameters  
SI 65536  
SF 400.1300518 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





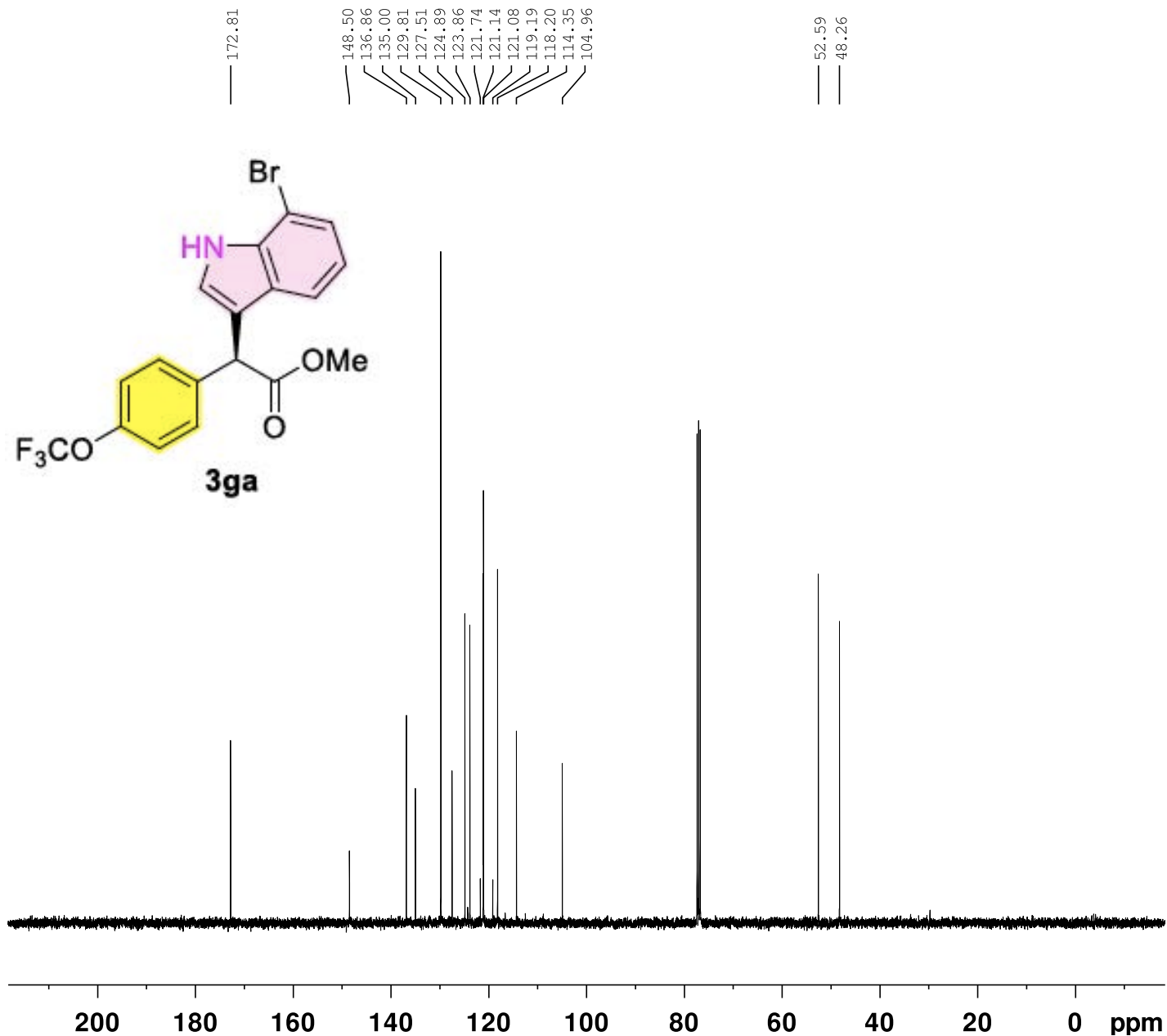
Current Data Parameters  
NAME CNMR-YX-5-p50  
EXPNO 2  
PROCNO 1

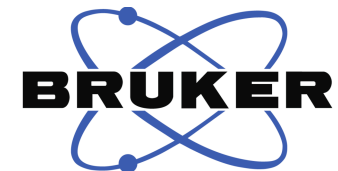
F2 - Acquisition Parameters

Date\_ 20230729  
Time 6.41 h  
INSTRUM Avance  
PROBHD Z116098\_0833 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 200  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 46.0295  
DW 21.000 usec  
DE 6.50 usec  
TE 294.7 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 3.33 usec  
P1 10.00 usec  
PLW1 87.89900208 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 20.73200035 W  
PLW12 0.25595000 W  
PLW13 0.12874000 W

F2 - Processing parameters

SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





Current Data Parameters  
NAME FNMR-YX-5-p50  
EXPNO 3  
PROCNO 1

F2 - Acquisition Parameters

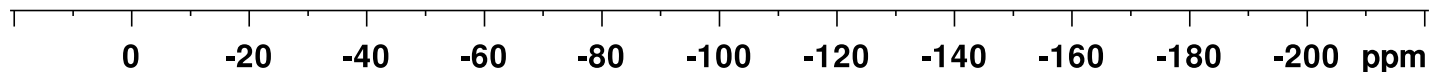
Date\_ 20230729  
Time 7.01 h  
INSTRUM Avance  
PROBHD Z116098\_0833 (  
PULPROG zgig  
TD 131072  
SOLVENT CDCl3  
NS 16  
DS 4  
SWH 90909.094 Hz  
FIDRES 1.387163 Hz  
AQ 0.7208960 sec  
RG 101  
DW 5.500 usec  
DE 6.50 usec  
TE 294.7 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 376.4607164 MHz  
NUC1 19F  
P1 18.00 usec  
PLW1 16.73100090 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 20.73200035 W  
PLW12 0.25595000 W

F2 - Processing parameters

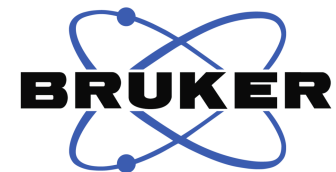
SI 65536  
SF 376.4983662 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



-57.80







Current Data Parameters  
NAME HNMR-YX-4-p93  
EXPNO 532  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230612  
Time 15.59  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 144  
DW 83.200 usec  
DE 6.50 usec  
TE 296.5 K  
D1 1.00000000 sec  
TD0 1

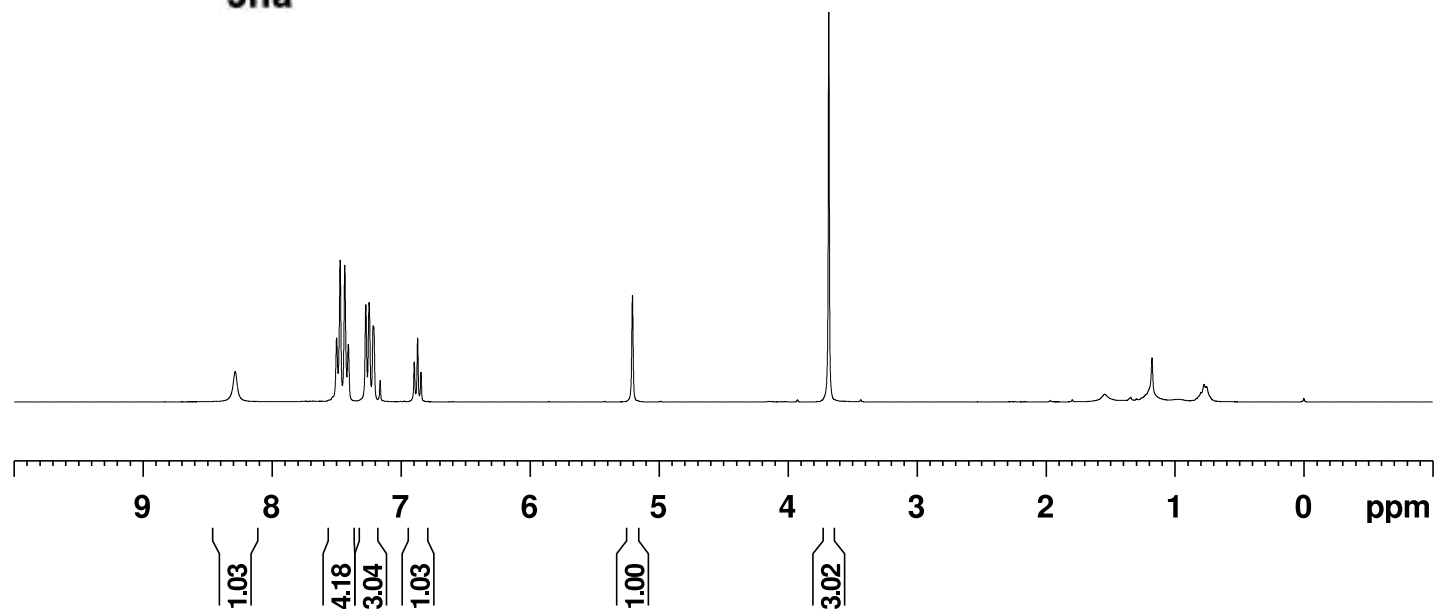
==== CHANNEL f1 =====  
SFO1 300.1318534 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 14.00000000 W

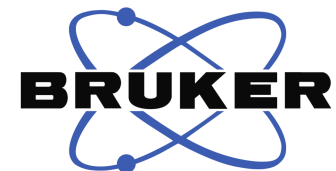
F2 - Processing parameters  
SI 65536  
SF 300.1300359 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

8.285  
7.499  
7.472  
7.436  
7.408  
7.273  
7.247  
7.215  
6.897  
6.871  
6.845

5.205

3.683





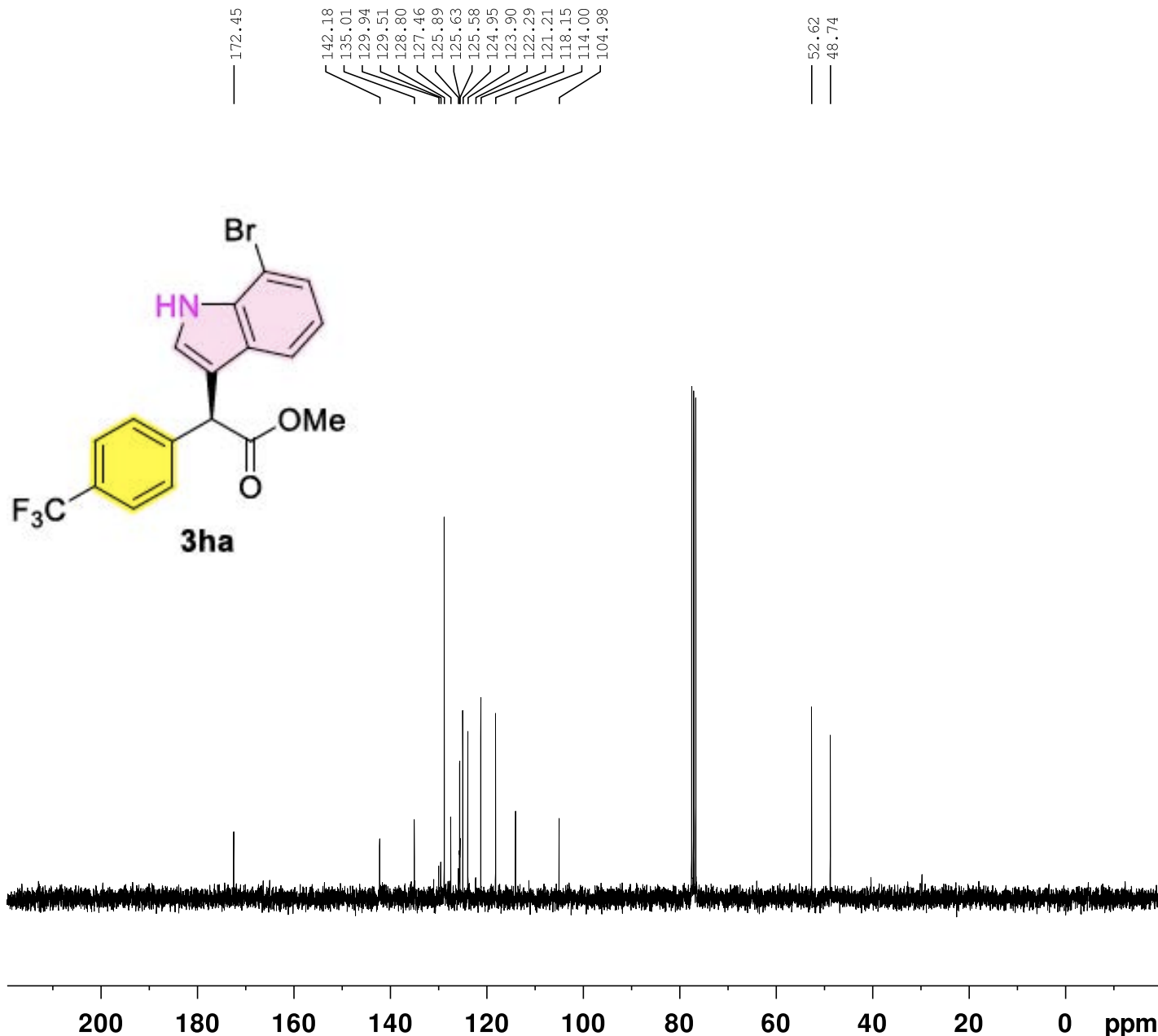
Current Data Parameters  
NAME CNMR-YX-4-p93  
EXPNO 609  
PROCNO 1

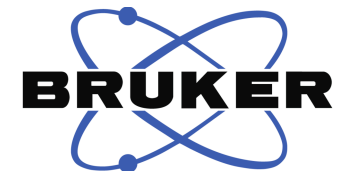
F2 - Acquisition Parameters  
Date\_ 20230614  
Time 15.57  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 81  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE 297.5 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 75.4752949 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 34.20000076 W

==== CHANNEL f2 =====  
SFO2 300.1312005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W  
PLW13 0.14000000 W

F2 - Processing parameters  
SI 32768  
SF 75.4677485 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





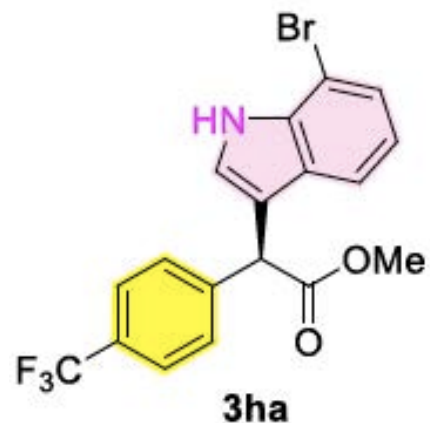
Current Data Parameters  
NAME FNMN-YX-4-p93  
EXPNO 608  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230614  
Time 15.50  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgfhigqn.2  
TD 131072  
SOLVENT CDCl3  
NS 16  
DS 4  
SWH 66964.289 Hz  
FIDRES 0.510897 Hz  
AQ 0.9786710 sec  
RG 203  
DW 7.467 usec  
DE 6.50 usec  
TE 297.1 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
D12 0.00002000 sec  
TD0 1

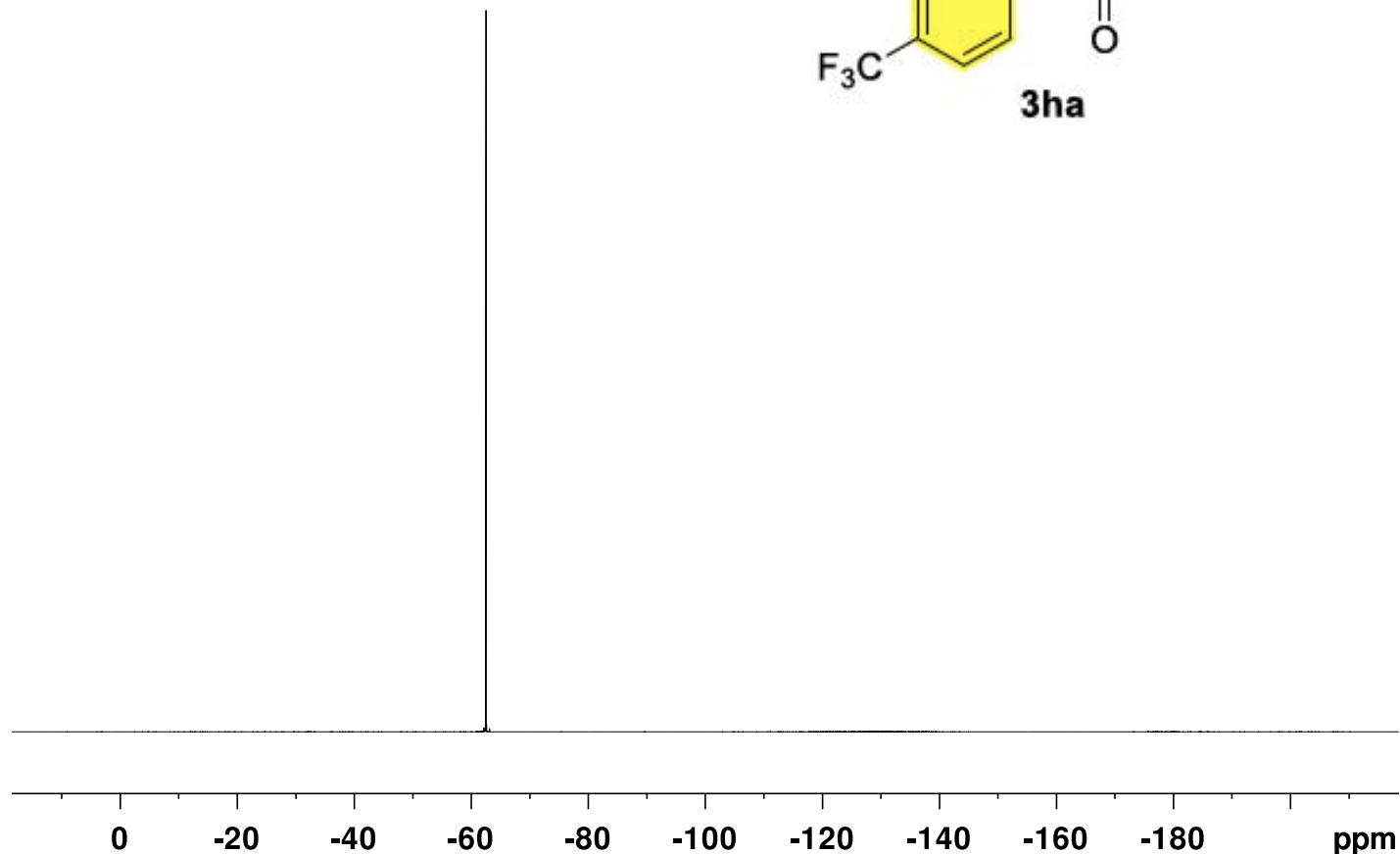
==== CHANNEL f1 =====  
SFO1 282.3761148 MHz  
NUC1 19F  
P1 14.50 usec  
PLW1 10.39999962 W

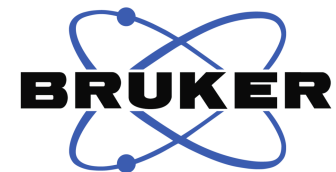
==== CHANNEL f2 =====  
SFO2 300.1312005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W

F2 - Processing parameters  
SI 65536  
SF 282.4043552 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



-62.51



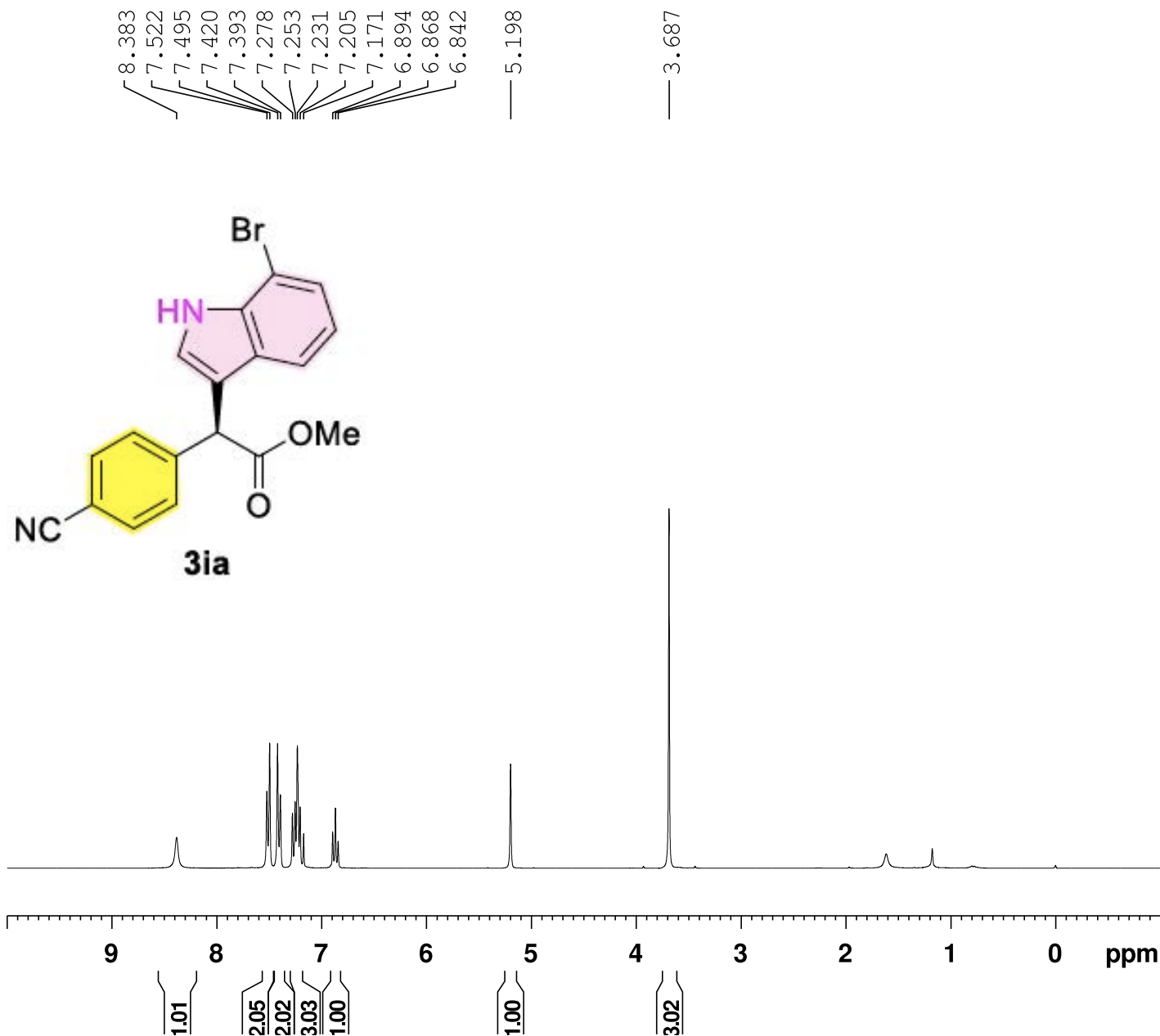


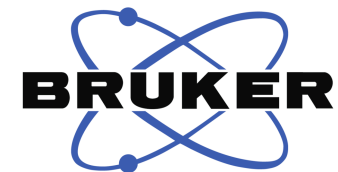
Current Data Parameters  
NAME HNMR-YX-4-p97  
EXPNO 805  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230620  
Time 15.41  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 161  
DW 83.200 usec  
DE 6.50 usec  
TE 296.7 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 300.1318534 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 14.00000000 W

F2 - Processing parameters  
SI 65536  
SF 300.1300332 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





Current Data Parameters  
NAME CNMR-YX-4-p97  
EXPNO 806  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20230620  
Time 16.01  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 300  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE 297.4 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

==== CHANNEL f1 =====

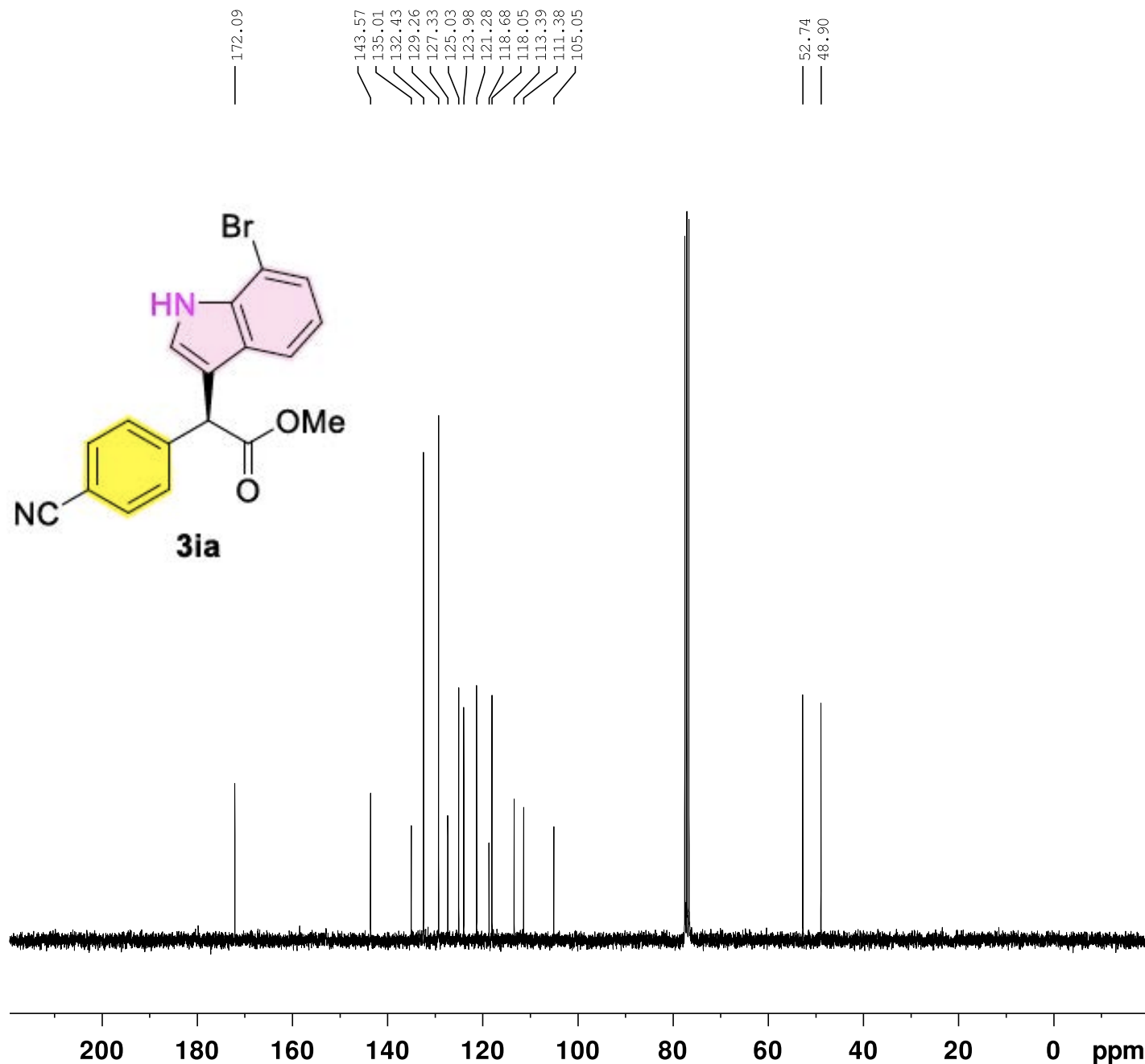
SFO1 75.4752949 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 34.20000076 W

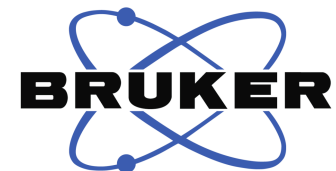
==== CHANNEL f2 =====

SFO2 300.1312005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W  
PLW13 0.14000000 W

F2 - Processing parameters

SI 32768  
SF 75.4677485 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



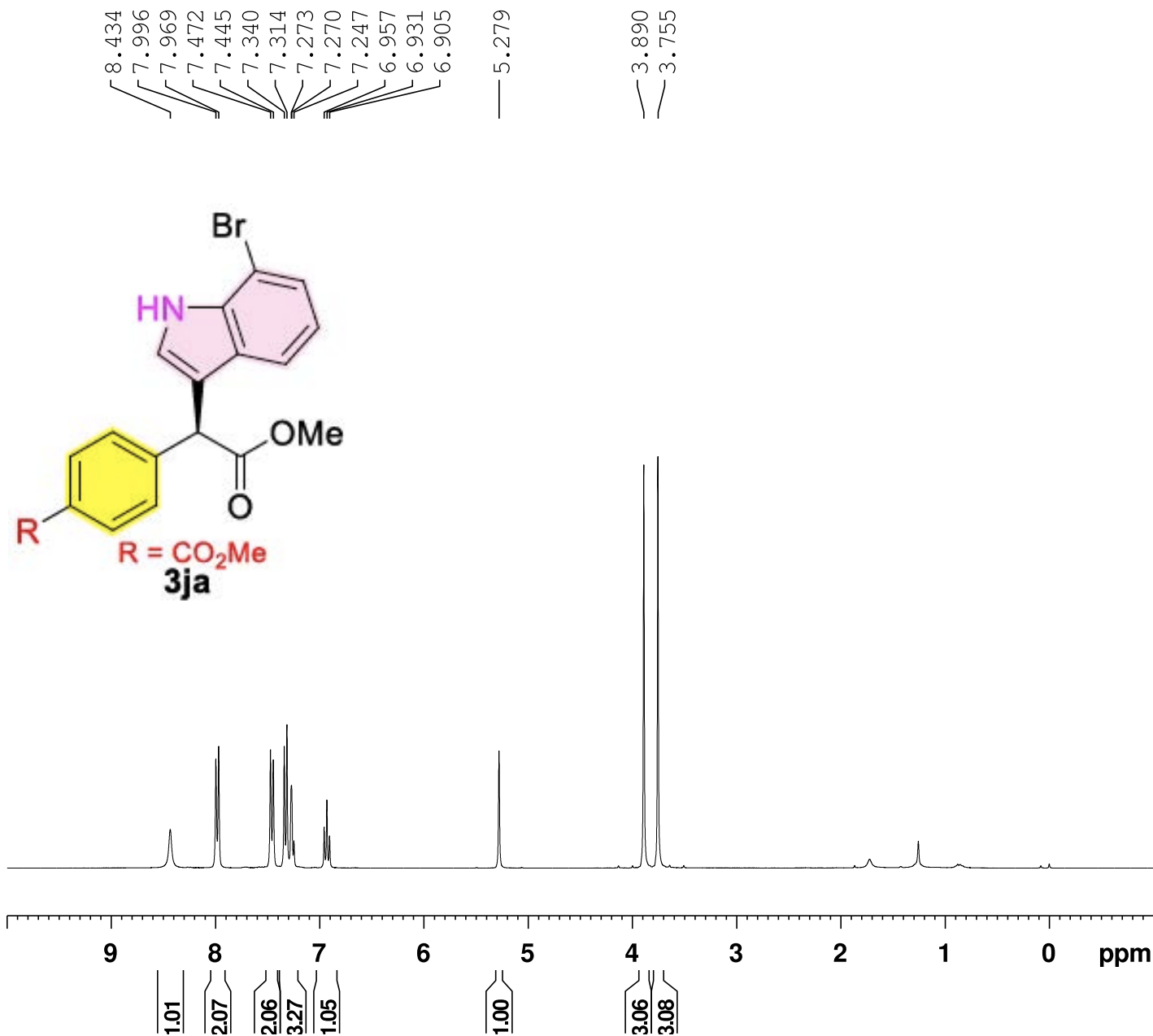


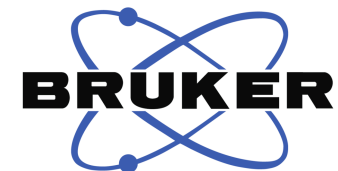
Current Data Parameters  
NAME HNMR-YX-4-p92  
EXPNO 755  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230619  
Time 21.48  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 144  
DW 83.200 usec  
DE 6.50 usec  
TE 296.5 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 300.1318534 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 14.00000000 W

F2 - Processing parameters  
SI 65536  
SF 300.1300107 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





Current Data Parameters  
NAME CNMR-YX-4-p92  
EXPNO 756  
PROCNO 1

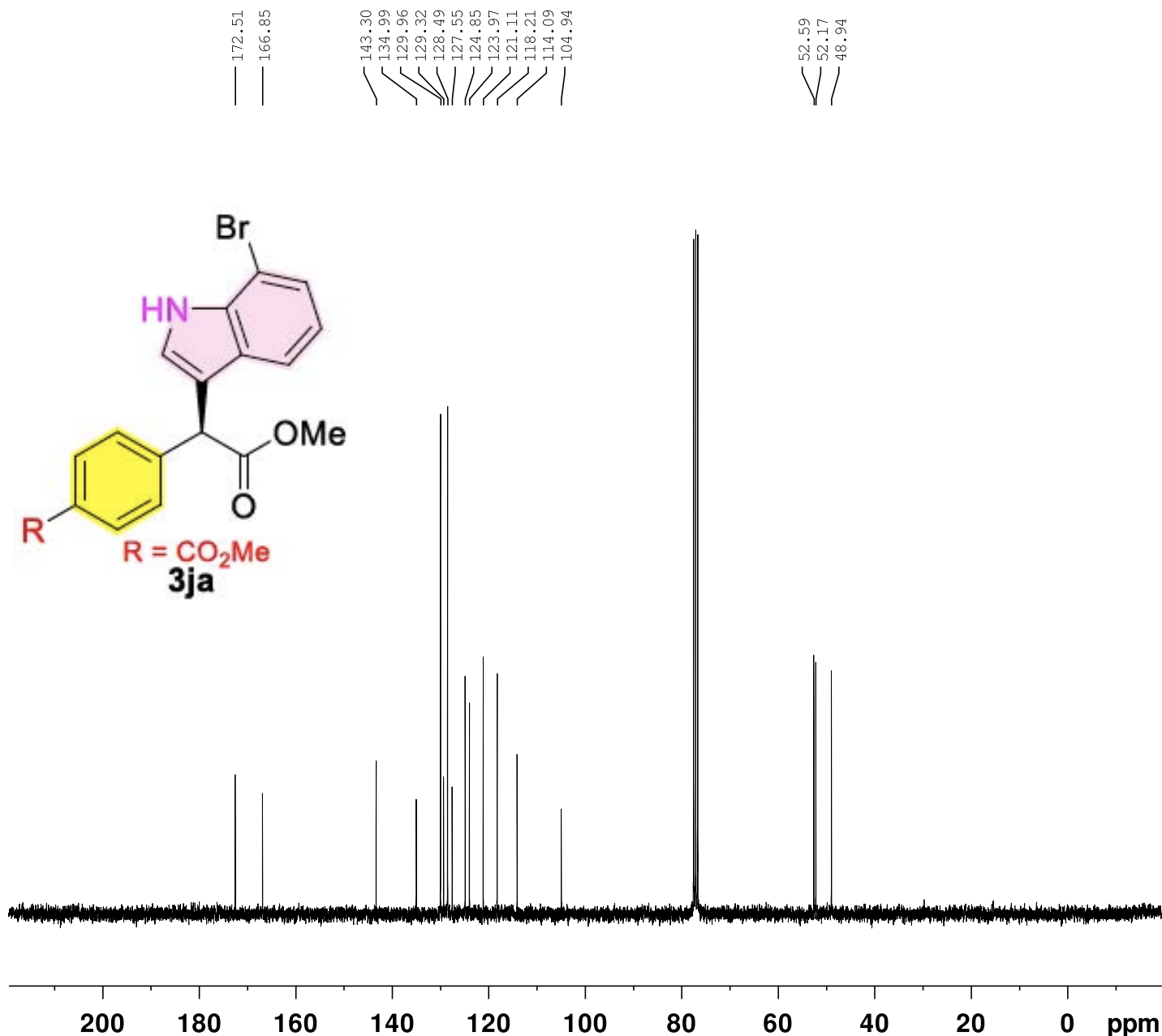
F2 - Acquisition Parameters

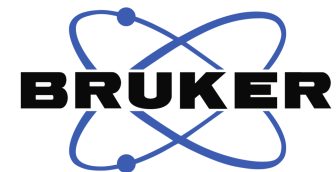
Date\_ 20230619  
Time 22.05  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 250  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE 297.3 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 75.4752949 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 34.20000076 W

==== CHANNEL f2 =====  
SFO2 300.1312005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W  
PLW13 0.14000000 W

F2 - Processing parameters  
SI 32768  
SF 75.4677485 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





Current Data Parameters  
NAME HNMR-YX-4-p99  
EXPNO 725  
PROCNO 1

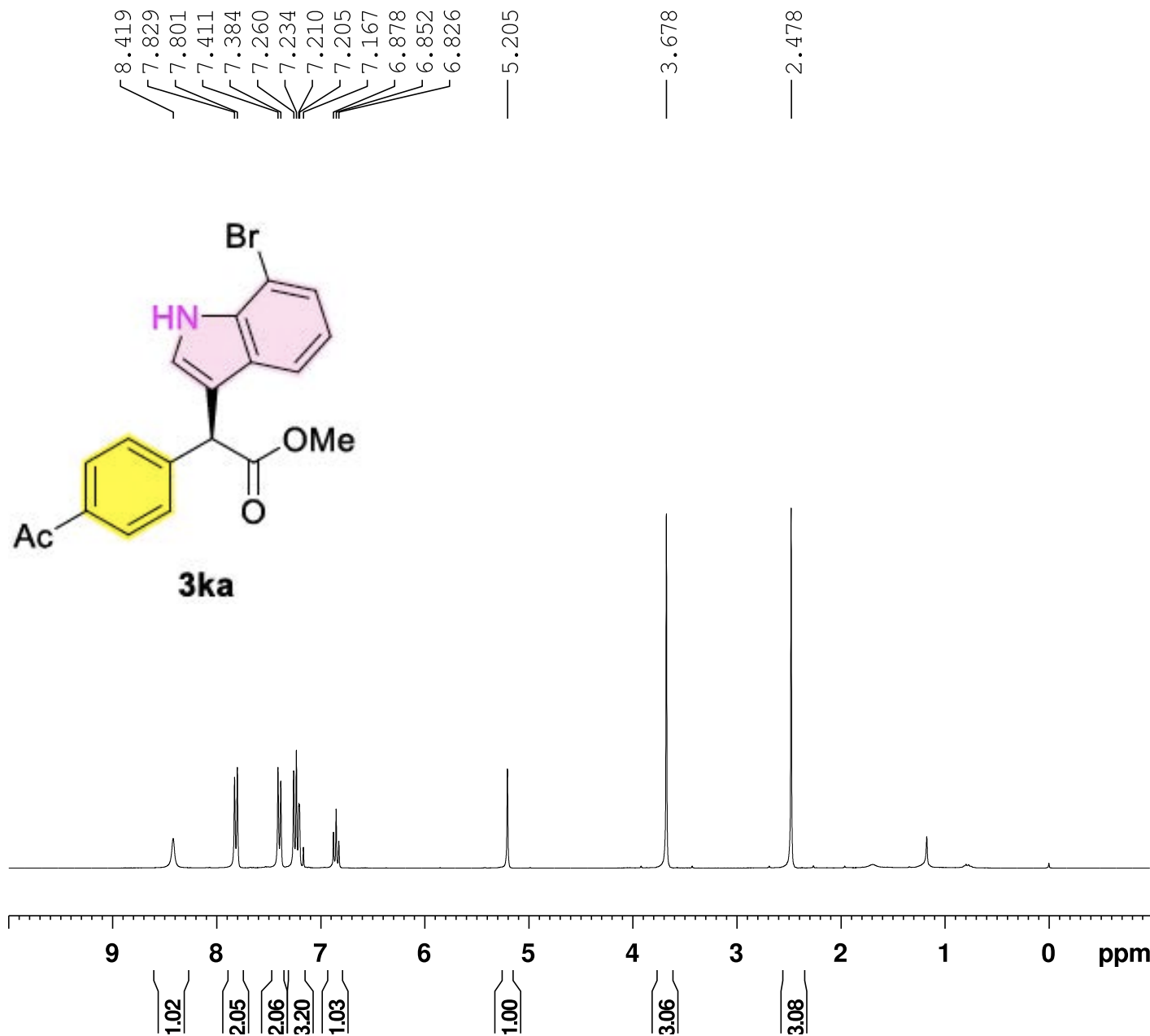
F2 - Acquisition Parameters

Date\_ 20230616  
Time 14.56  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 128  
DW 83.200 usec  
DE 6.50 usec  
TE 296.6 K  
D1 1.00000000 sec  
TD0 1

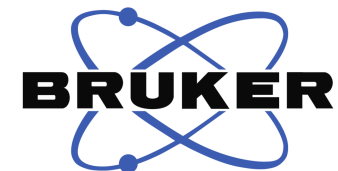
==== CHANNEL f1 =====  
SFO1 300.1318534 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 14.00000000 W

F2 - Processing parameters

SI 65536  
SF 300.1300347 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00







Current Data Parameters  
NAME CNMR-YX-4-p99  
EXPNO 759  
PROCNO 1

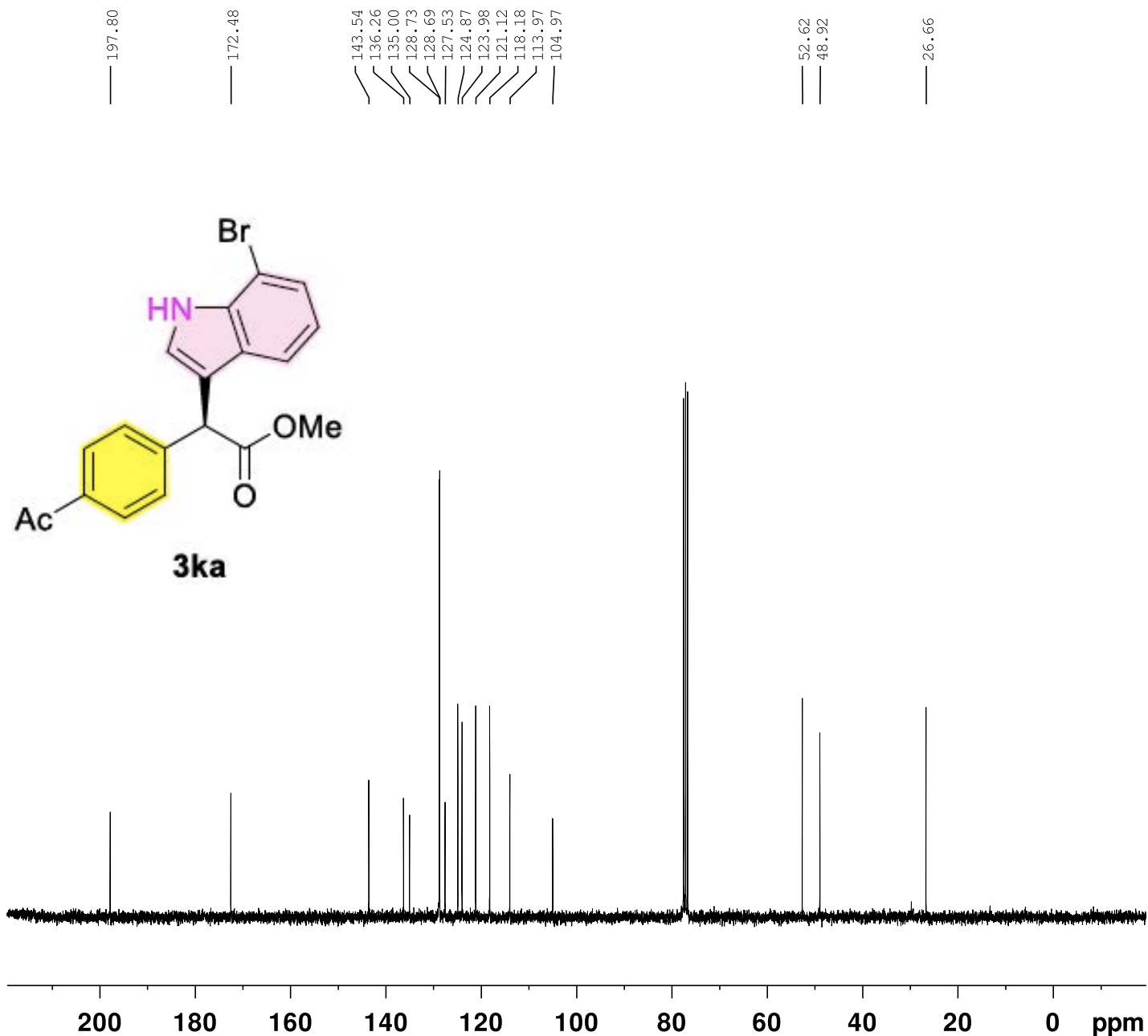
F2 - Acquisition Parameters

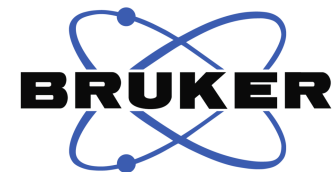
Date\_ 20230619  
Time 22.49  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 250  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE 297.4 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 75.4752949 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 34.20000076 W

==== CHANNEL f2 =====  
SFO2 300.1312005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W  
PLW13 0.14000000 W

F2 - Processing parameters  
SI 32768  
SF 75.4677485 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





Current Data Parameters  
NAME HNMR-YX-4-p100  
EXPNO 701  
PROCNO 1

F2 - Acquisition Parameters

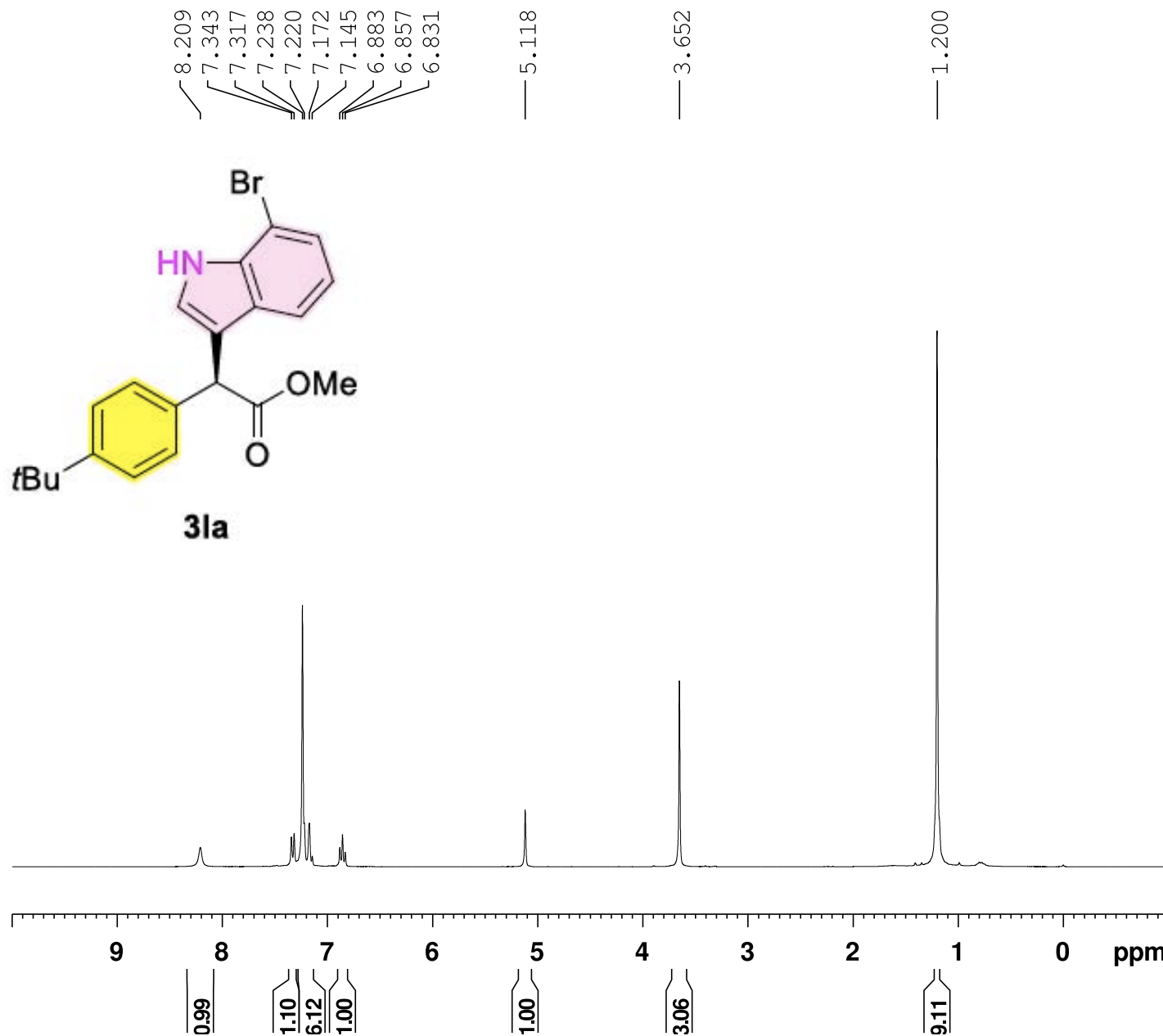
Date\_ 20230615  
Time 14.09  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 90.5  
DW 83.200 usec  
DE 6.50 usec  
TE 296.8 K  
D1 1.00000000 sec  
TD0 1

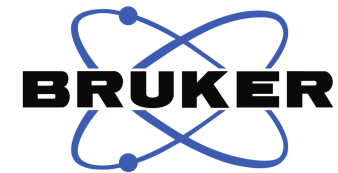
==== CHANNEL f1 =====

SFO1 300.1318534 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 14.00000000 W

F2 - Processing parameters

SI 65536  
SF 300.1300413 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





Current Data Parameters  
NAME CNMR-YX-4-p100  
EXPNO 707  
PROCNO 1

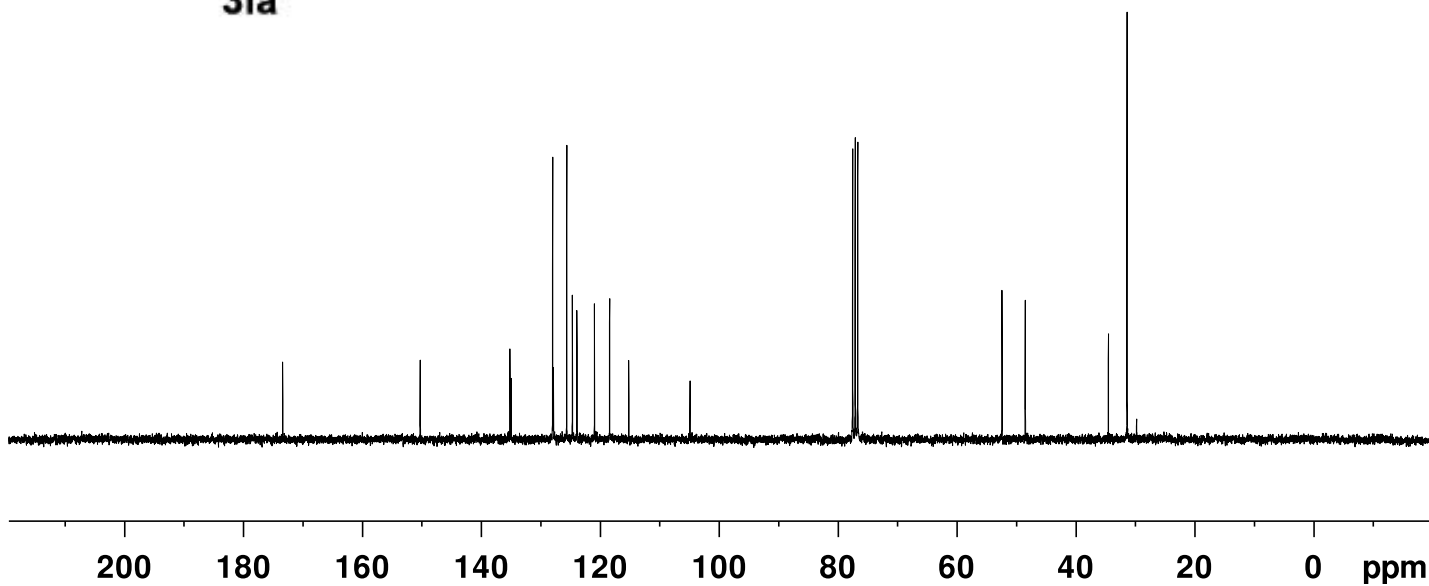
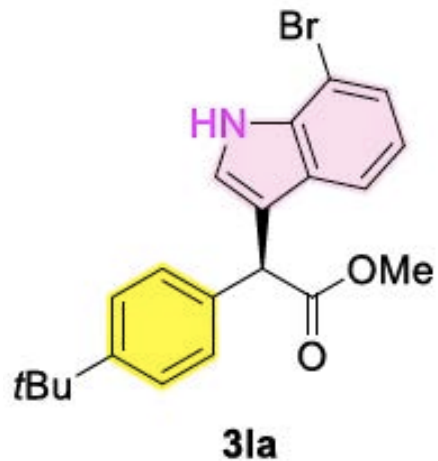
F2 - Acquisition Parameters  
Date\_ 20230615  
Time 15.20  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 200  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE 297.5 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

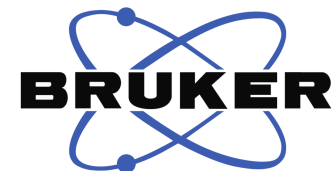
==== CHANNEL f1 =====  
SFO1 75.4752949 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 34.20000076 W  
  
==== CHANNEL f2 =====  
SFO2 300.1312005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W  
PLW13 0.14000000 W

F2 - Processing parameters  
SI 32768  
SF 75.4677485 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

173.36  
150.24  
135.14  
134.95  
127.96  
127.83  
125.60  
124.64  
123.88  
120.93  
118.38  
115.16  
104.85

52.38  
48.48  
34.49  
31.36





Current Data Parameters  
NAME HNMR-YX-4-p96  
EXPNO 723  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230616  
Time 14.45  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 101  
DW 83.200 usec  
DE 6.50 usec  
TE 296.8 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 300.1318534 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 14.00000000 W

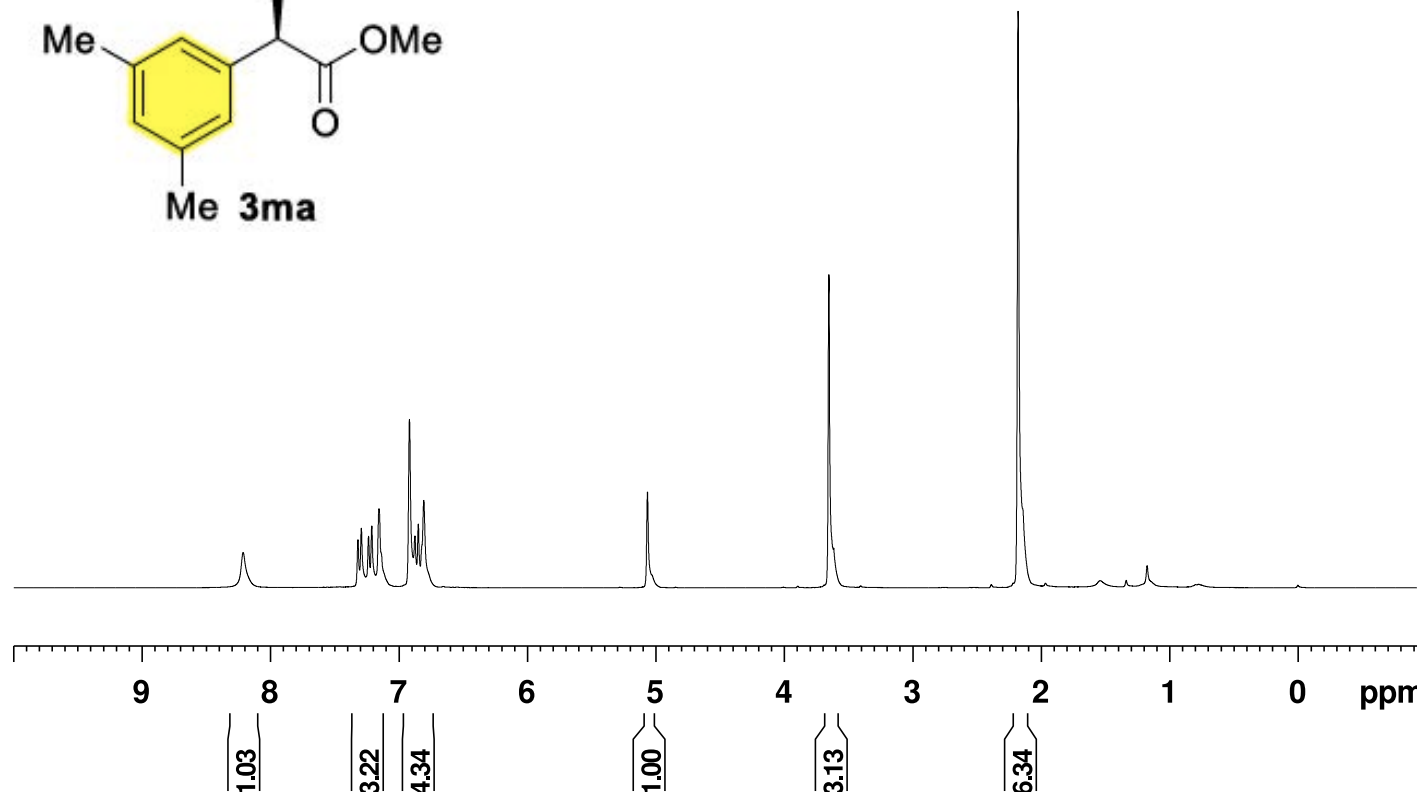
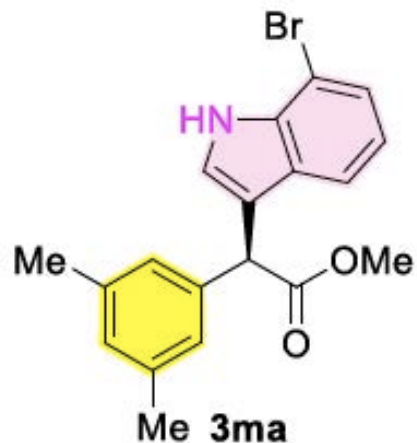
F2 - Processing parameters  
SI 65536  
SF 300.1300439 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

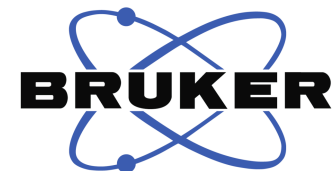
8.213  
7.319  
7.293  
7.237  
7.211  
7.155  
6.918  
6.875  
6.849  
6.806

5.065

3.652

2.179





Current Data Parameters  
NAME CNMR-YX-4-p96  
EXPNO 731  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20230616  
Time 16.28  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 200  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE 297.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

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

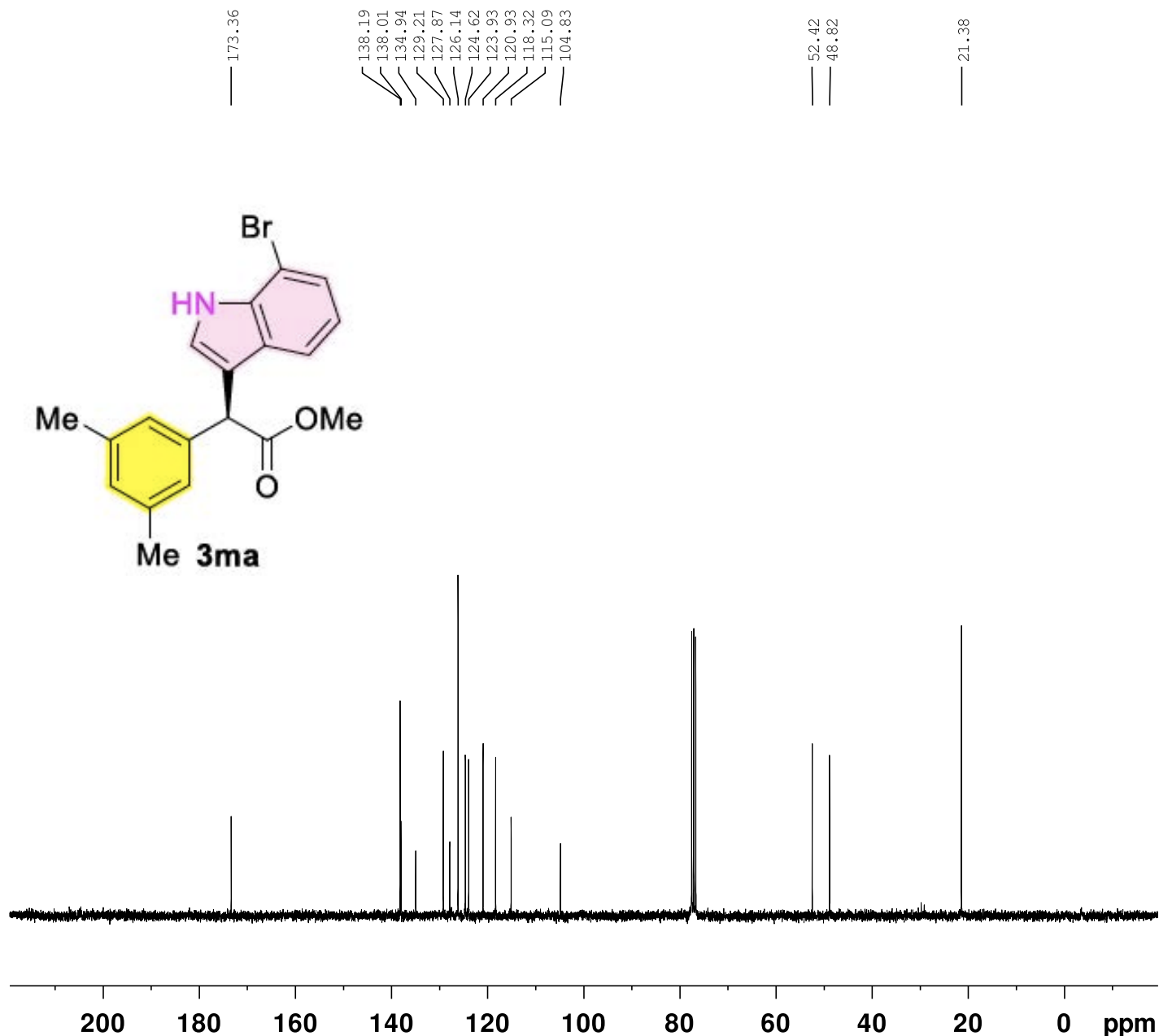
SFO1 75.4752949 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 34.20000076 W

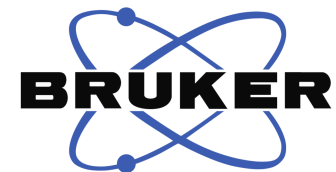
===== CHANNEL f2 =====

SFO2 300.1312005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W  
PLW13 0.14000000 W

F2 - Processing parameters

SI 32768  
SF 75.4677485 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





Current Data Parameters  
NAME HNMR-YX-4-p91  
EXPNO 533  
PROCNO 1

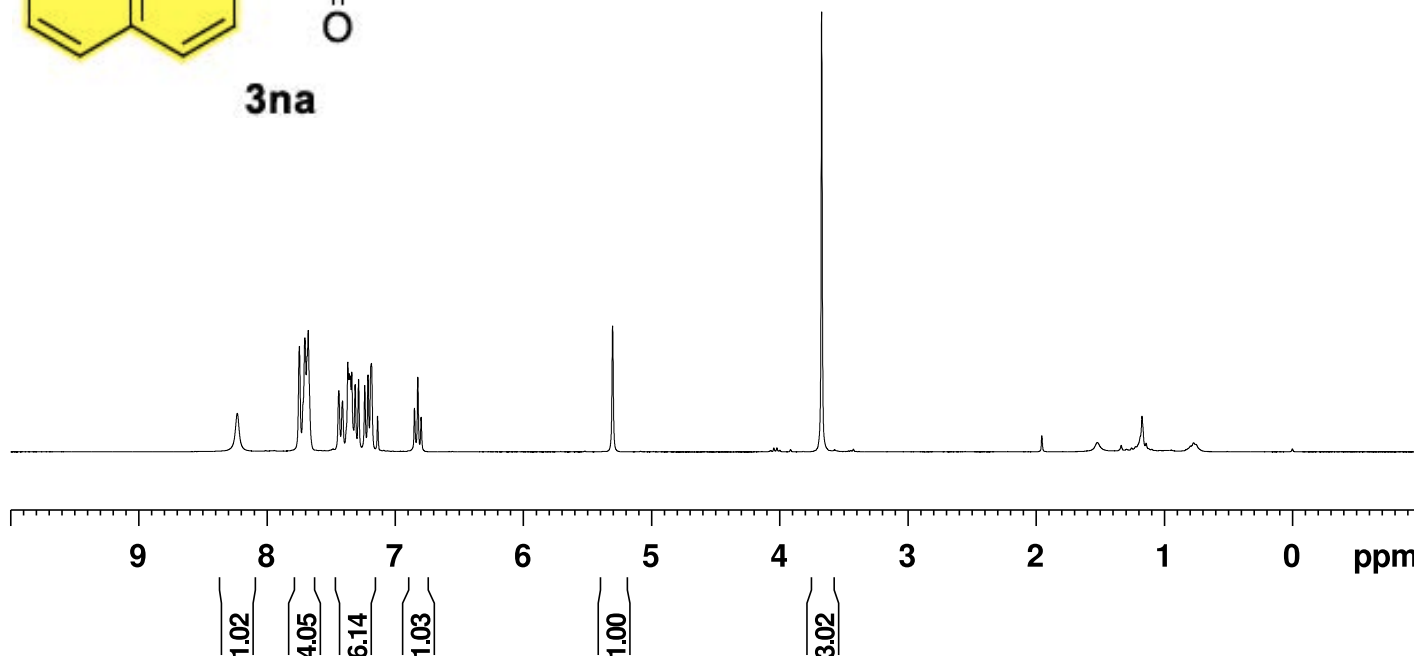
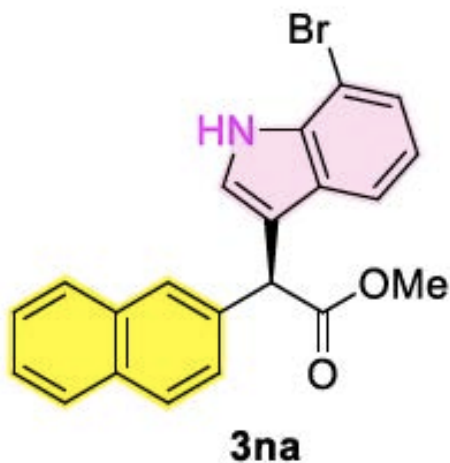
F2 - Acquisition Parameters  
Date\_ 20230612  
Time 16.04  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 128  
DW 83.200 usec  
DE 6.50 usec  
TE 296.5 K  
D1 1.00000000 sec  
TD0 1

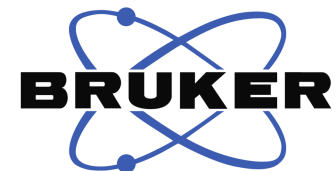
==== CHANNEL f1 =====  
SFO1 300.1318534 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 14.00000000 W

F2 - Processing parameters  
SI 65536  
SF 300.1300434 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

8.232  
7.747  
7.704  
7.678  
7.439  
7.411  
7.369  
7.359  
7.349  
7.339  
7.312  
7.285  
7.237  
7.212  
7.185  
7.137  
6.849  
6.823  
6.797  
5.303

3.673





Current Data Parameters  
NAME CNMR-YX-4-p91  
EXPNO 534  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20230612  
Time 16.11  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 100  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE 297.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

==== CHANNEL f1 =====

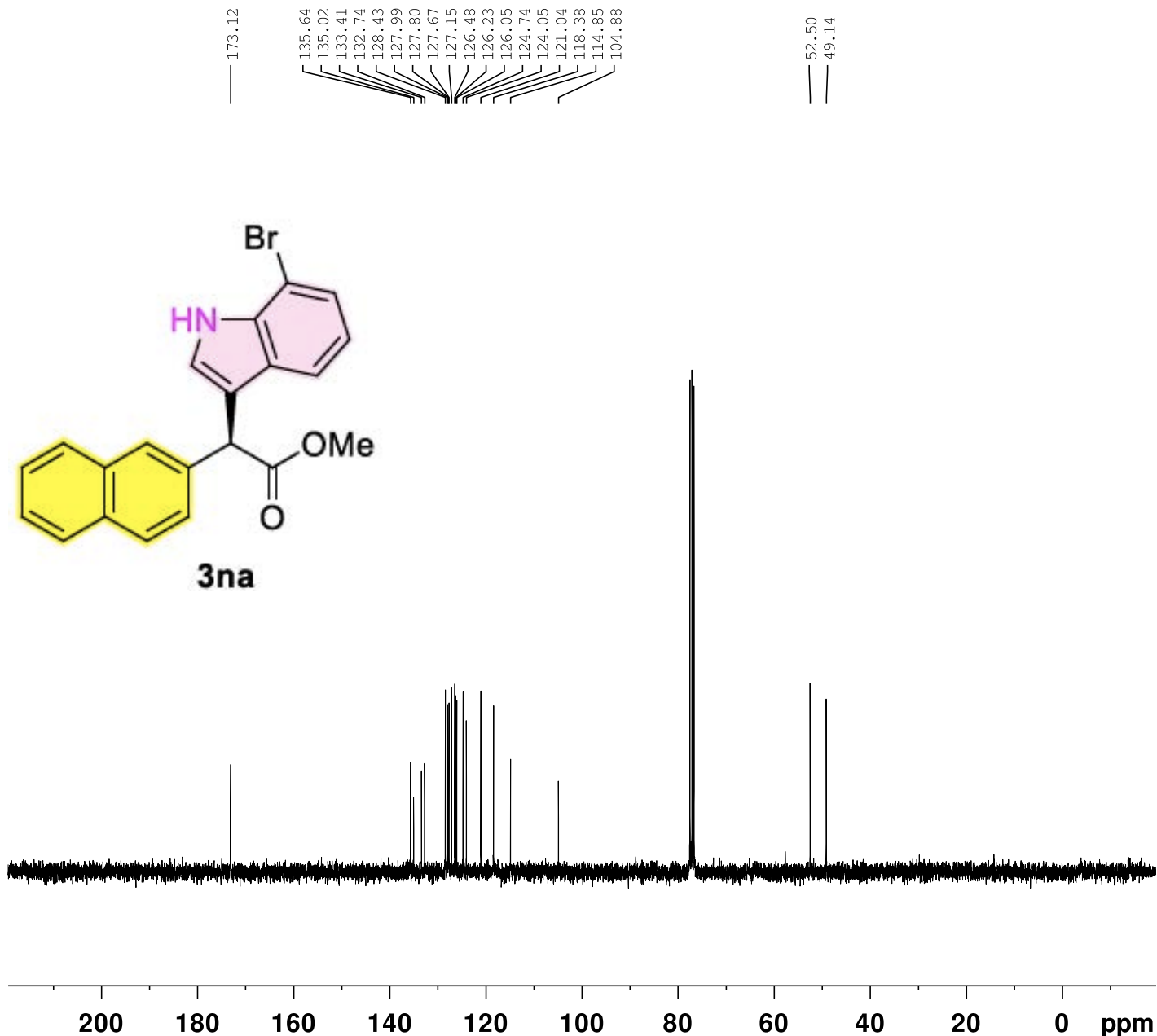
SFO1 75.4752949 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 34.20000076 W

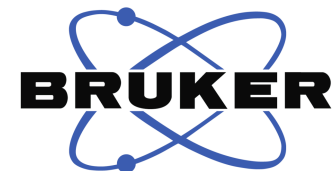
==== CHANNEL f2 =====

SFO2 300.1312005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W  
PLW13 0.14000000 W

F2 - Processing parameters

SI 32768  
SF 75.4677485 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

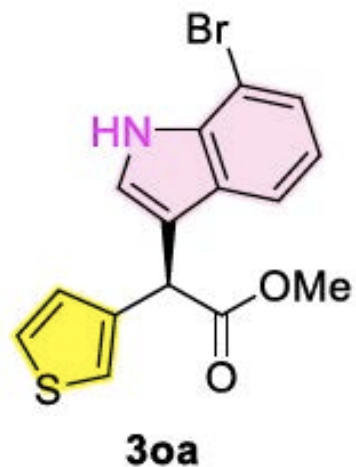
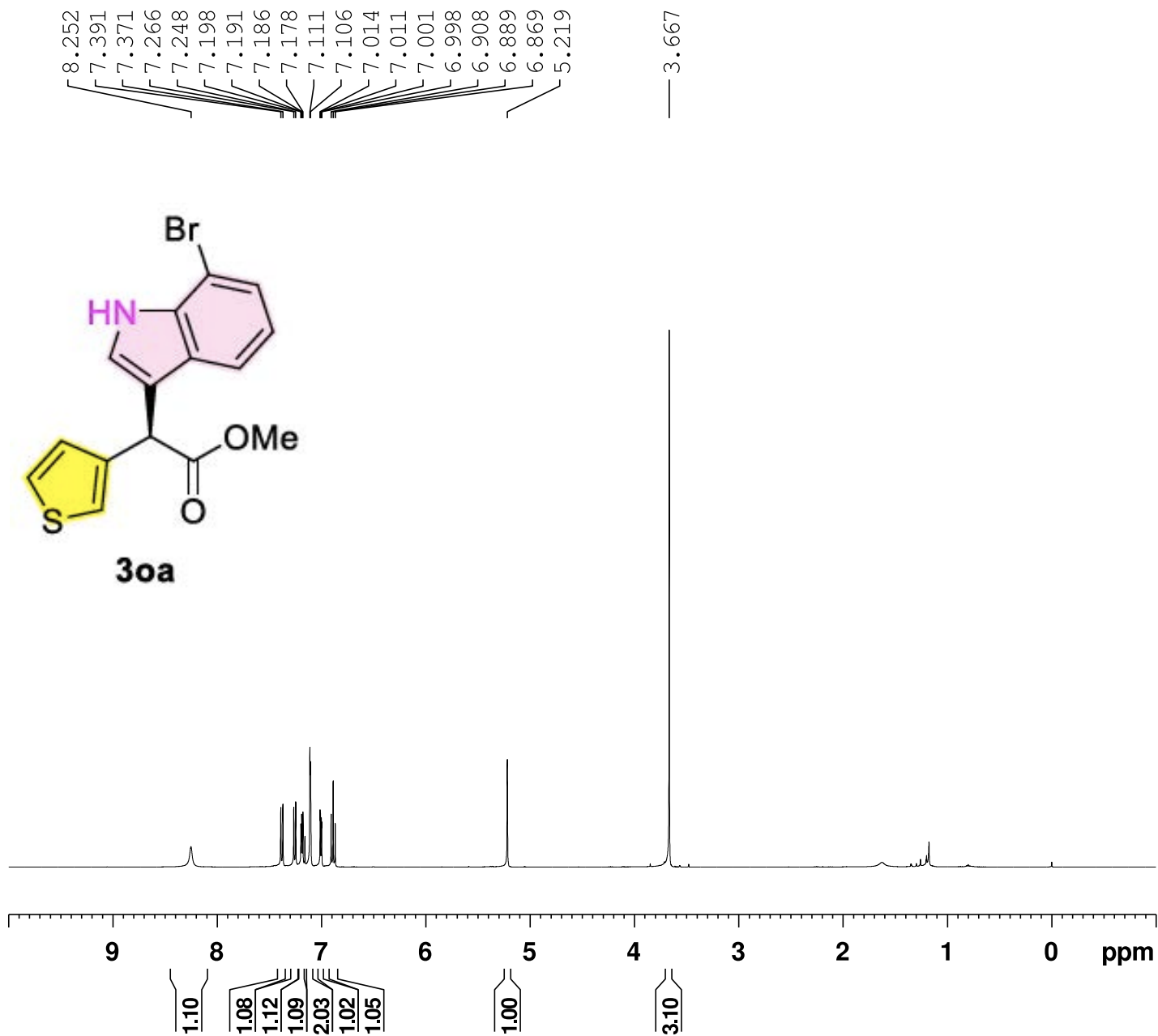




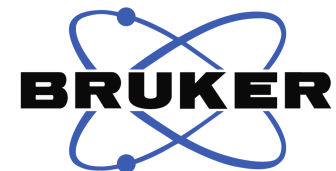
Current Data Parameters  
NAME HNMR-YX-5-p49  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230729  
Time 8.14 h  
INSTRUM Avance  
PROBHD z116098\_0833 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8196.722 Hz  
FIDRES 0.250144 Hz  
AQ 3.9976959 sec  
RG 101  
DW 61.000 usec  
DE 13.54 usec  
TE 294.4 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1324708 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 20.73200035 W

F2 - Processing parameters  
SI 65536  
SF 400.1300498 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



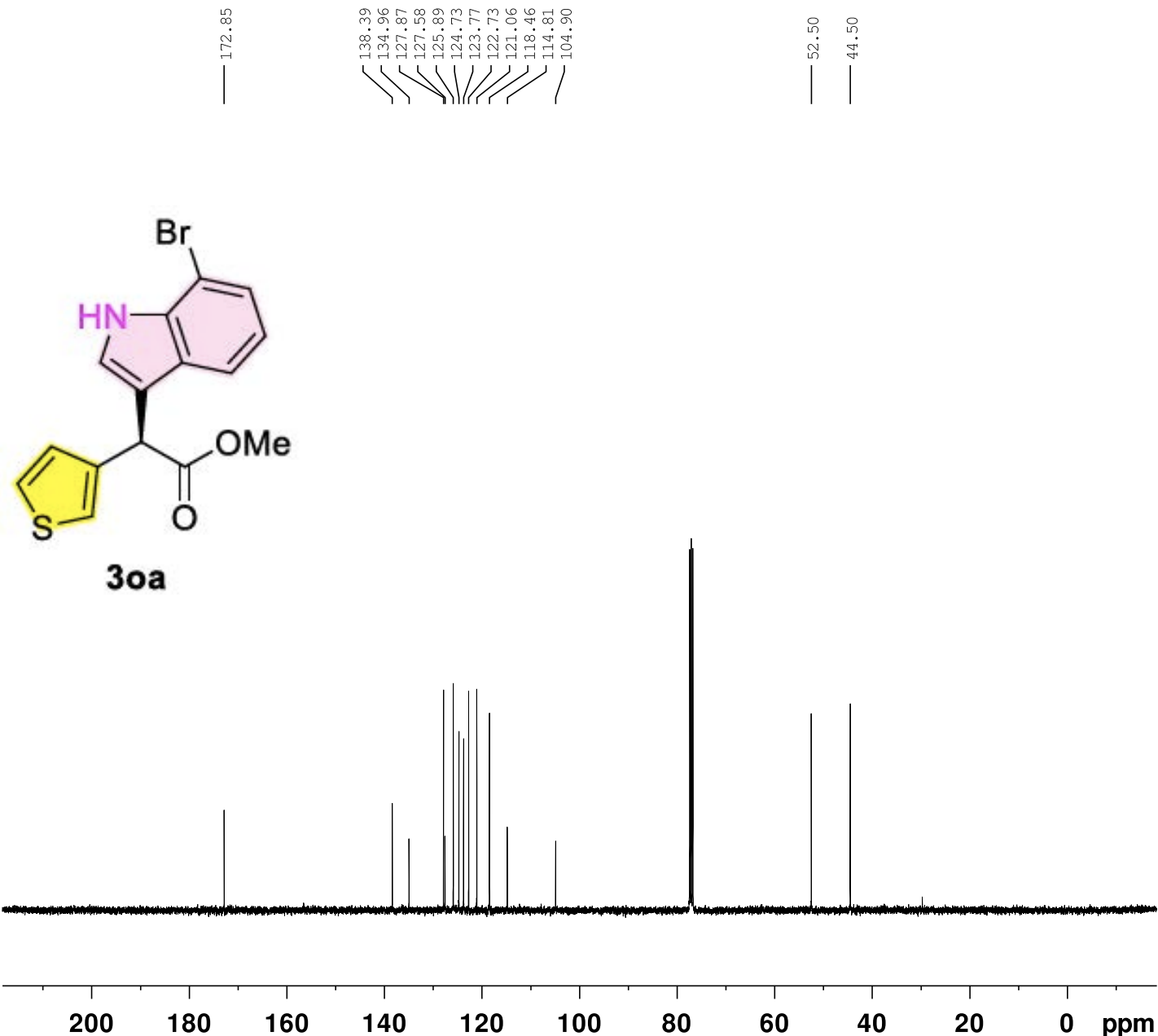




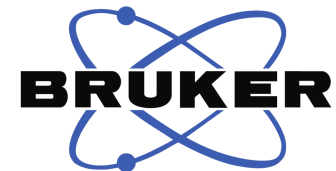
Current Data Parameters  
NAME CNMR-YX-5-p49  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230729  
Time 8.27 h  
INSTRUM Avance  
PROBHD z116098\_0833 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 200  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 44.8788  
DW 21.000 usec  
DE 6.50 usec  
TE 294.7 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 3.33 usec  
P1 10.00 usec  
PLW1 87.89900208 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 20.73200035 W  
PLW12 0.25595000 W  
PLW13 0.12874000 W

F2 - Processing parameters  
SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



7.798  
7.568  
7.566  
7.551  
7.549  
7.531  
7.528  
7.504  
7.502  
7.484  
7.467  
7.450  
7.430  
7.342  
7.331  
7.323  
7.310  
7.039  
7.034  
6.998  
6.980  
6.977  
6.961  
6.955  
6.942  
6.374



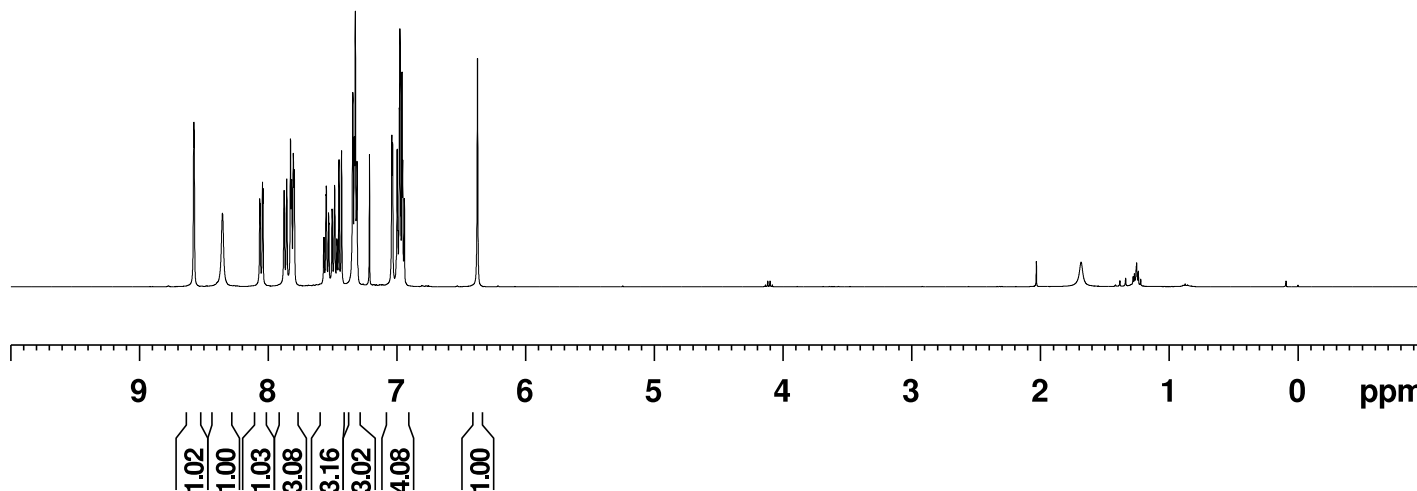
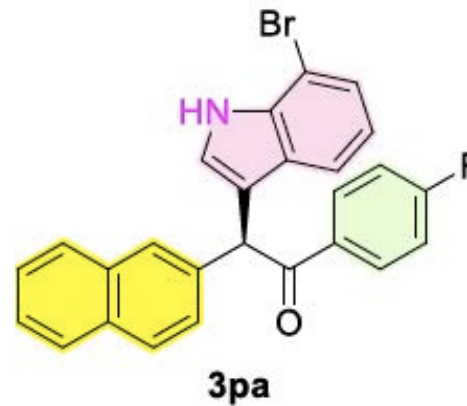
Current Data Parameters  
 NAME NMR-YX-5-p96  
 EXPNO 1  
 PROCNO 1

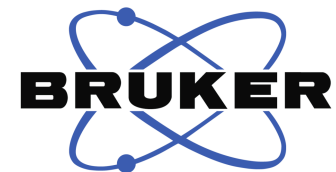
F2 - Acquisition Parameters

Date\_ 20231107  
 Time 10.56 h  
 INSTRUM Avance  
 PROBHD z116098\_0833 (  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8196.722 Hz  
 FIDRES 0.250144 Hz  
 AQ 3.9976959 sec  
 RG 58.8235  
 DW 61.000 usec  
 DE 13.54 usec  
 TE 294.0 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 400.1324708 MHz  
 NUC1 1H  
 P0 3.33 usec  
 P1 10.00 usec  
 PLW1 20.73200035 W

F2 - Processing parameters

SI 65536  
 SF 400.1300283 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





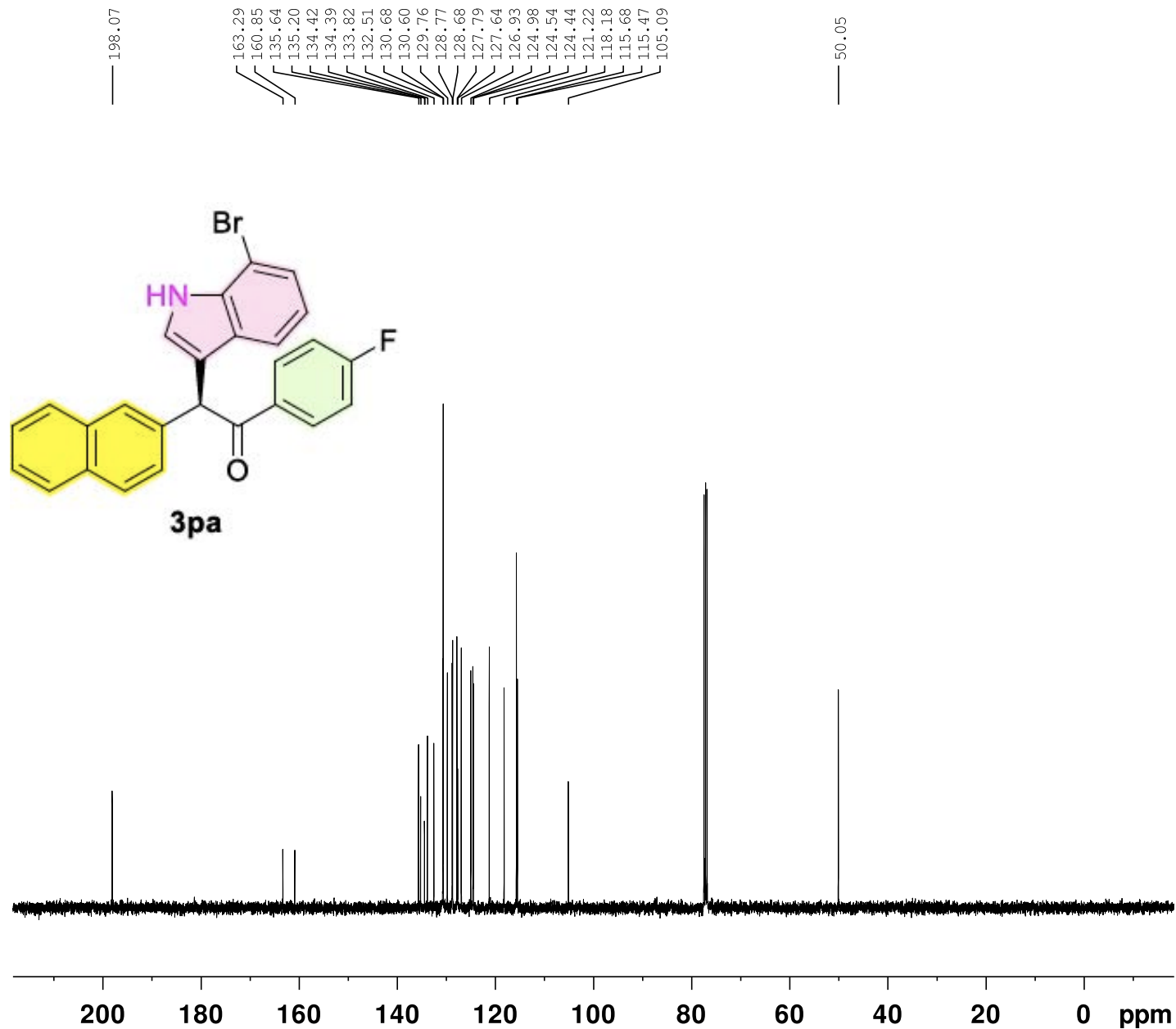
Current Data Parameters  
NAME NMR-YX-5-p96  
EXPNO 2  
PROCNO 1

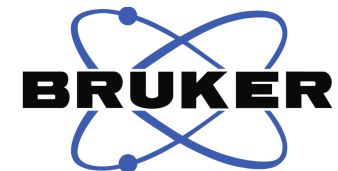
F2 - Acquisition Parameters

Date\_ 20231107  
Time 11.16 h  
INSTRUM Avance  
PROBHD z116098\_0833 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 100  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 46.0295  
DW 21.000 usec  
DE 6.50 usec  
TE 293.9 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 3.33 usec  
P1 10.00 usec  
PLW1 87.89900208 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 20.73200035 W  
PLW12 0.25595000 W  
PLW13 0.12874000 W

F2 - Processing parameters

SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

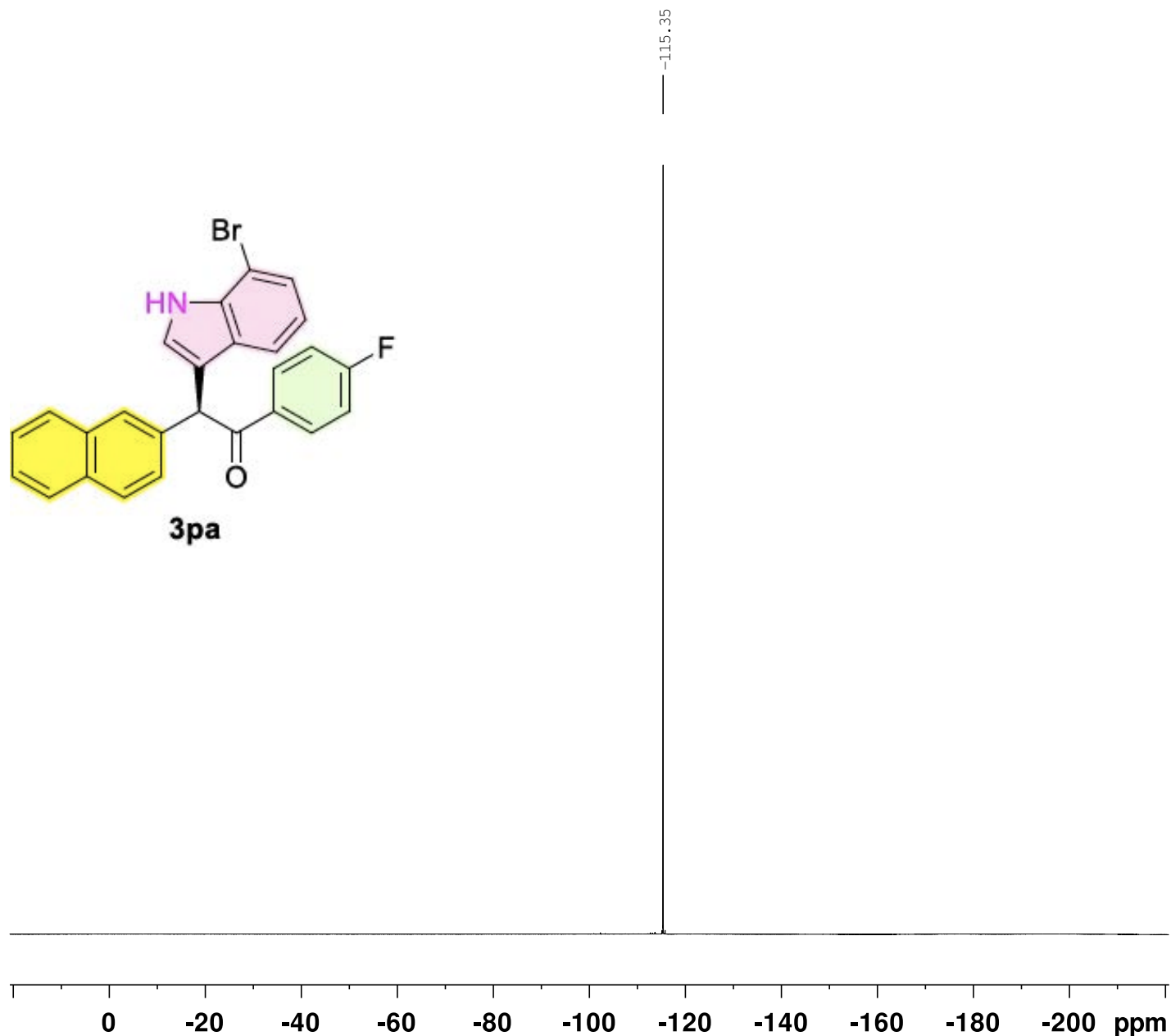


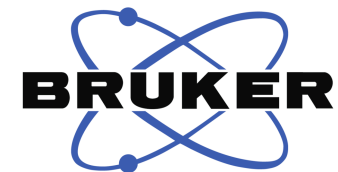


Current Data Parameters  
NAME FNMR-YX-5-p96  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231109  
Time 16.50 h  
INSTRUM Avance  
PROBHD Z116098\_0833 (  
PULPROG zgig  
TD 131072  
SOLVENT CDCl3  
NS 16  
DS 4  
SWH 90909.094 Hz  
FIDRES 1.387163 Hz  
AQ 0.7208960 sec  
RG 101  
DW 5.500 usec  
DE 6.50 usec  
TE 293.5 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 376.4607164 MHz  
NUC1 19F  
P1 18.00 usec  
PLW1 16.73100090 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 20.73200035 W  
PLW12 0.25595000 W

F2 - Processing parameters  
SI 65536  
SF 376.4983662 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



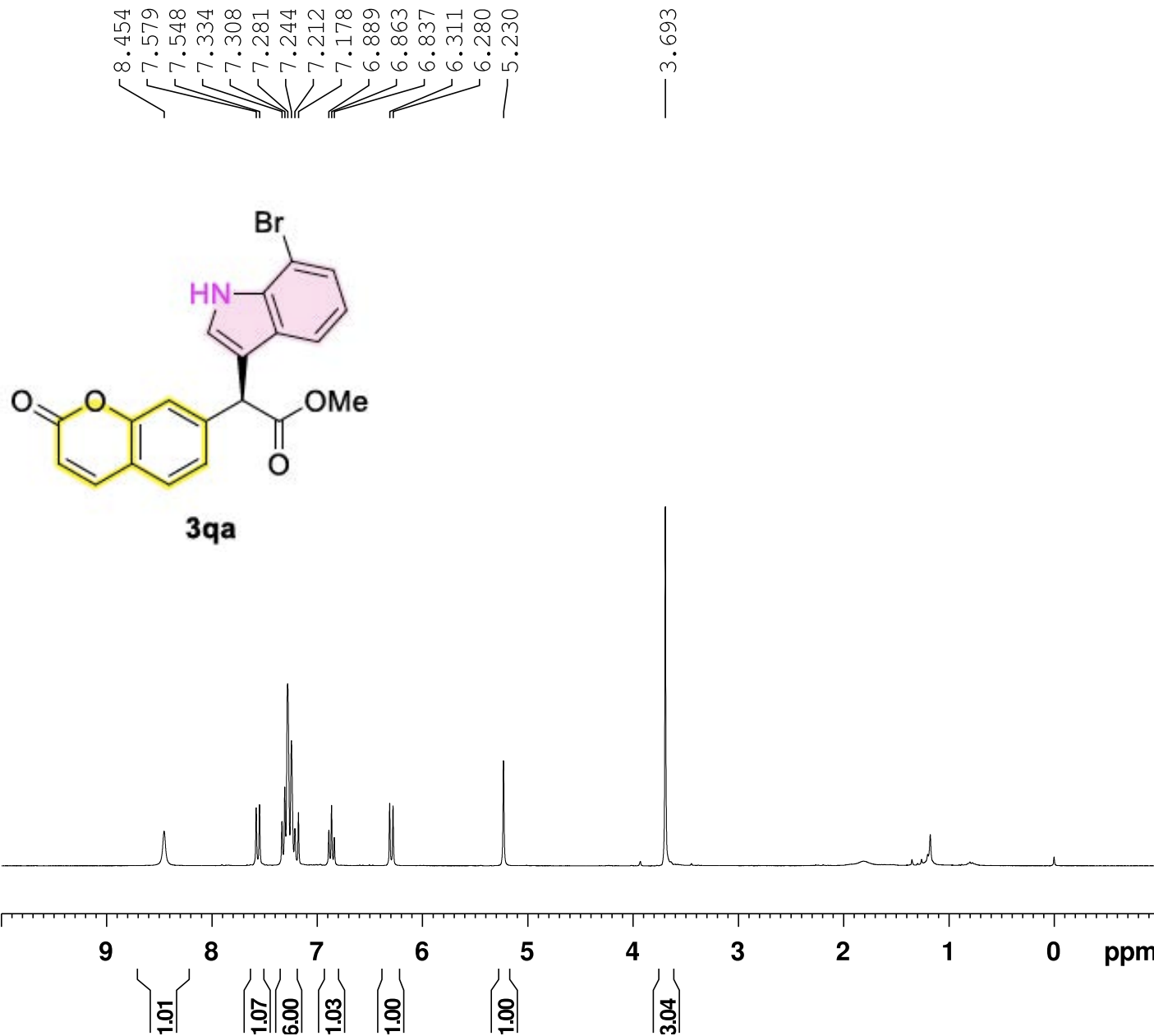


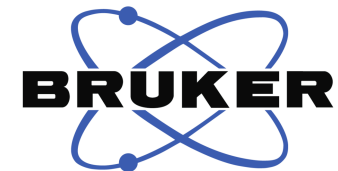
Current Data Parameters  
NAME HNMR-YX-5-p59  
EXPNO 2000  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230804  
Time 15.47  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 181  
DW 83.200 usec  
DE 6.50 usec  
TE 297.6 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 300.1318534 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 14.00000000 W

F2 - Processing parameters  
SI 65536  
SF 300.1300312 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





Current Data Parameters  
NAME CNMR-YX-5-p59  
EXPNO 2007  
PROCNO 1

F2 - Acquisition Parameters

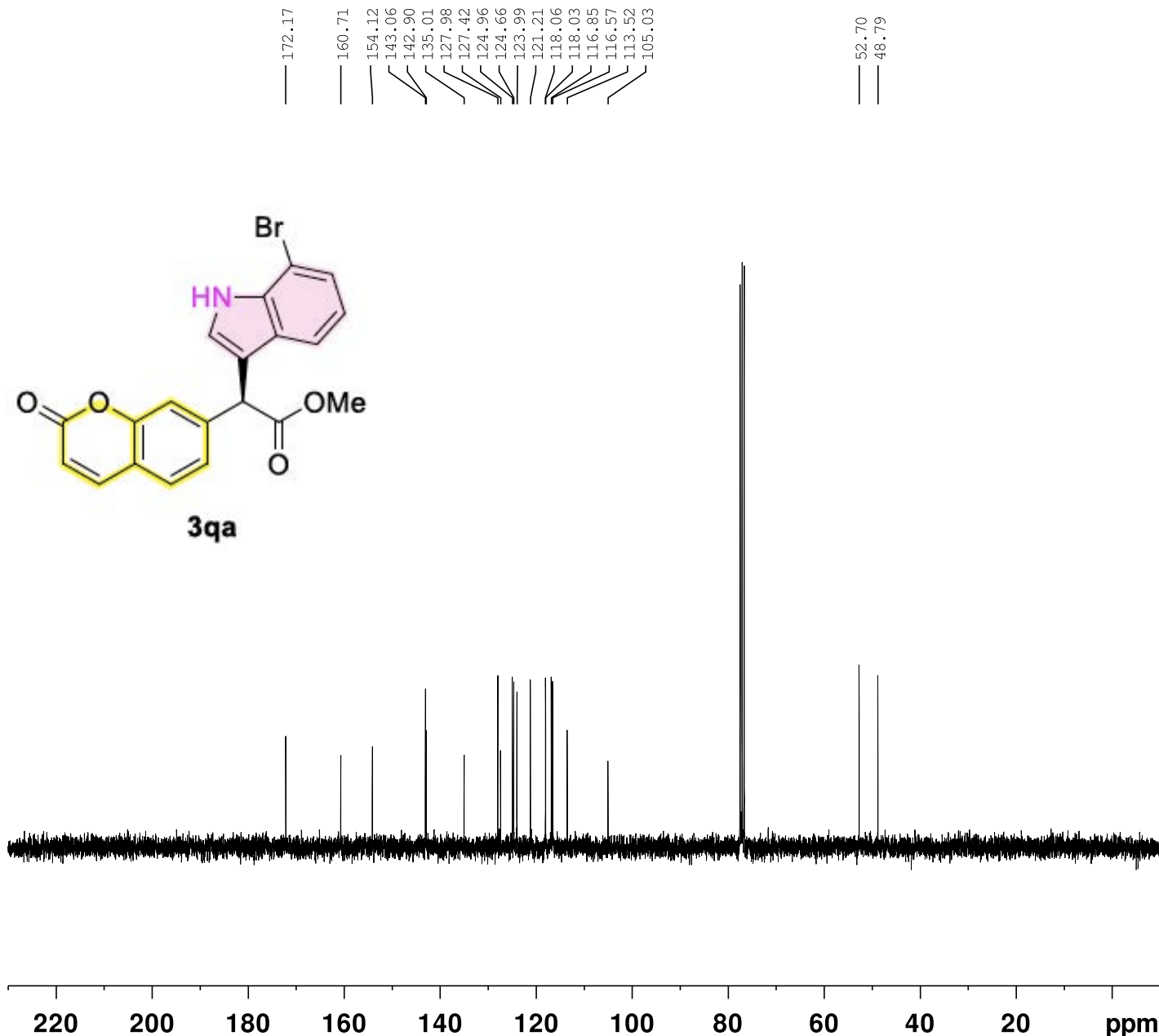
Date\_ 20230804  
Time 16.34  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 100  
DS 4  
SWH 18115.941 Hz  
FIDRES 0.276427 Hz  
AQ 1.8087935 sec  
RG 203  
DW 27.600 usec  
DE 6.50 usec  
TE 298.4 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

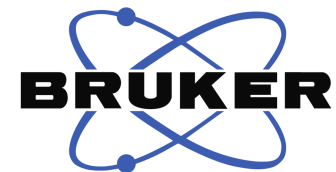
==== CHANNEL f1 =====  
SFO1 75.4760500 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 34.20000076 W

==== CHANNEL f2 =====  
SFO2 300.1312005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W  
PLW13 0.14000000 W

F2 - Processing parameters

SI 32768  
SF 75.4677485 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





Current Data Parameters  
NAME HNMR-YX-6-p18  
EXPNO 149  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20231008  
Time 15.10  
INSTRUM spect  
PROBHD 5 mm PADUL 13C  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 4  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9845889 sec  
RG 61.19  
DW 60.800 usec  
DE 6.50 usec  
TE 294.0 K  
D1 1.00000000 sec  
TD0 1

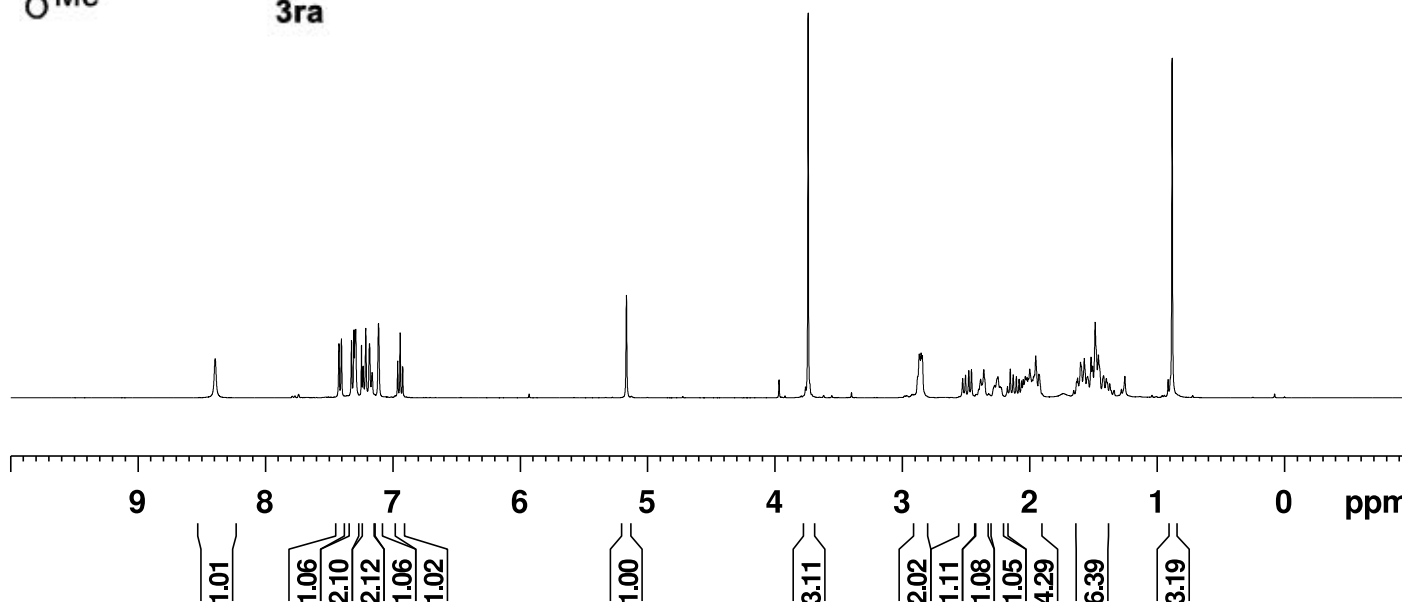
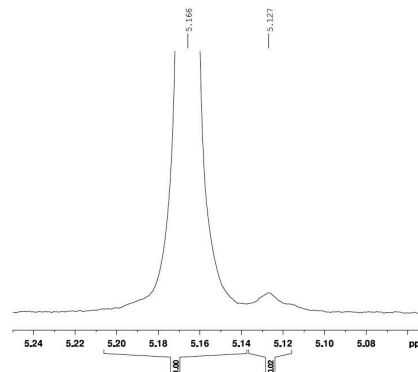
==== CHANNEL f1 =====

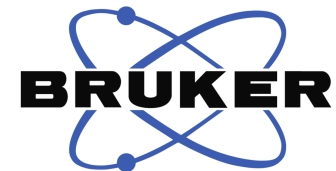
NUC1 1H  
P1 9.90 usec  
PLW1 23.00000000 W  
SFO1 400.1924713 MHz

F2 - Processing parameters

SI 65536  
SF 400.1900197 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

8.394  
7.423  
7.403  
7.324  
7.305  
7.296  
7.291  
7.245  
7.232  
7.212  
7.182  
7.162  
7.112  
6.961  
6.942  
6.923  
5.166  
3.739  
2.867  
2.852  
2.843  
2.504  
2.478  
2.457  
2.360  
2.153  
2.130  
2.035  
2.000  
1.963  
1.953  
1.929  
1.601  
1.572  
1.545  
1.518  
1.505  
1.486  
1.461  
1.420  
0.882





Current Data Parameters  
NAME CNMR-YX-6-p18  
EXPNO 160  
PROCNO 1

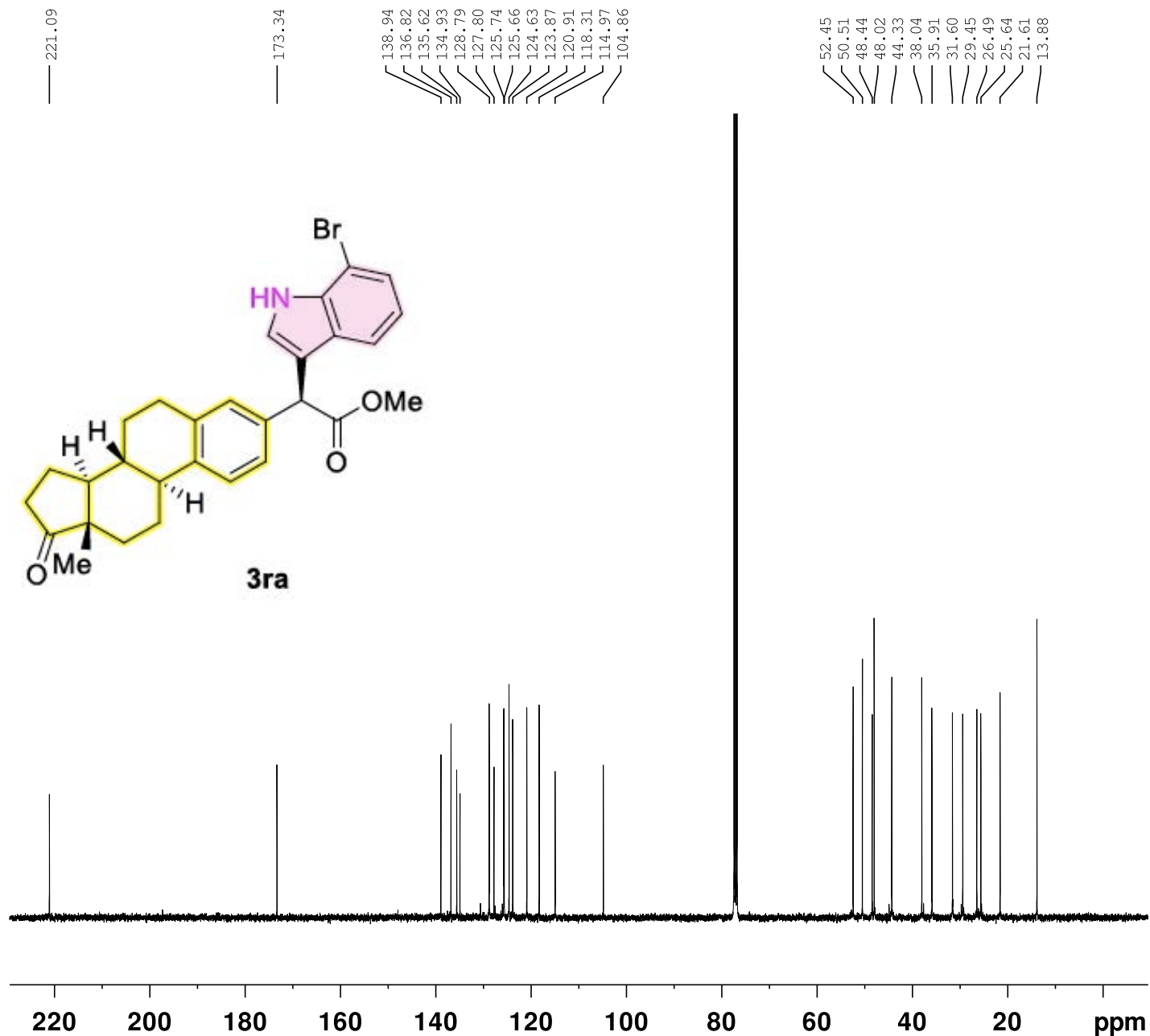
F2 - Acquisition Parameters

Date\_ 20231010  
Time 22.16  
INSTRUM spect  
PROBHD 5 mm PADUL 13C  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 37.77  
DW 20.800 usec  
DE 6.50 usec  
TE 292.5 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

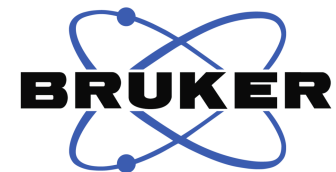
==== CHANNEL f1 =====  
NUC1 13C  
P1 9.80 usec  
PLW1 47.4000153 W  
SFO1 100.6389251 MHz

==== CHANNEL f2 =====  
CPDPRG[2] waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 23.0000000 W  
PLW12 0.30712000 W  
PLW13 0.24877000 W  
SFO2 400.1916008 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6278560 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





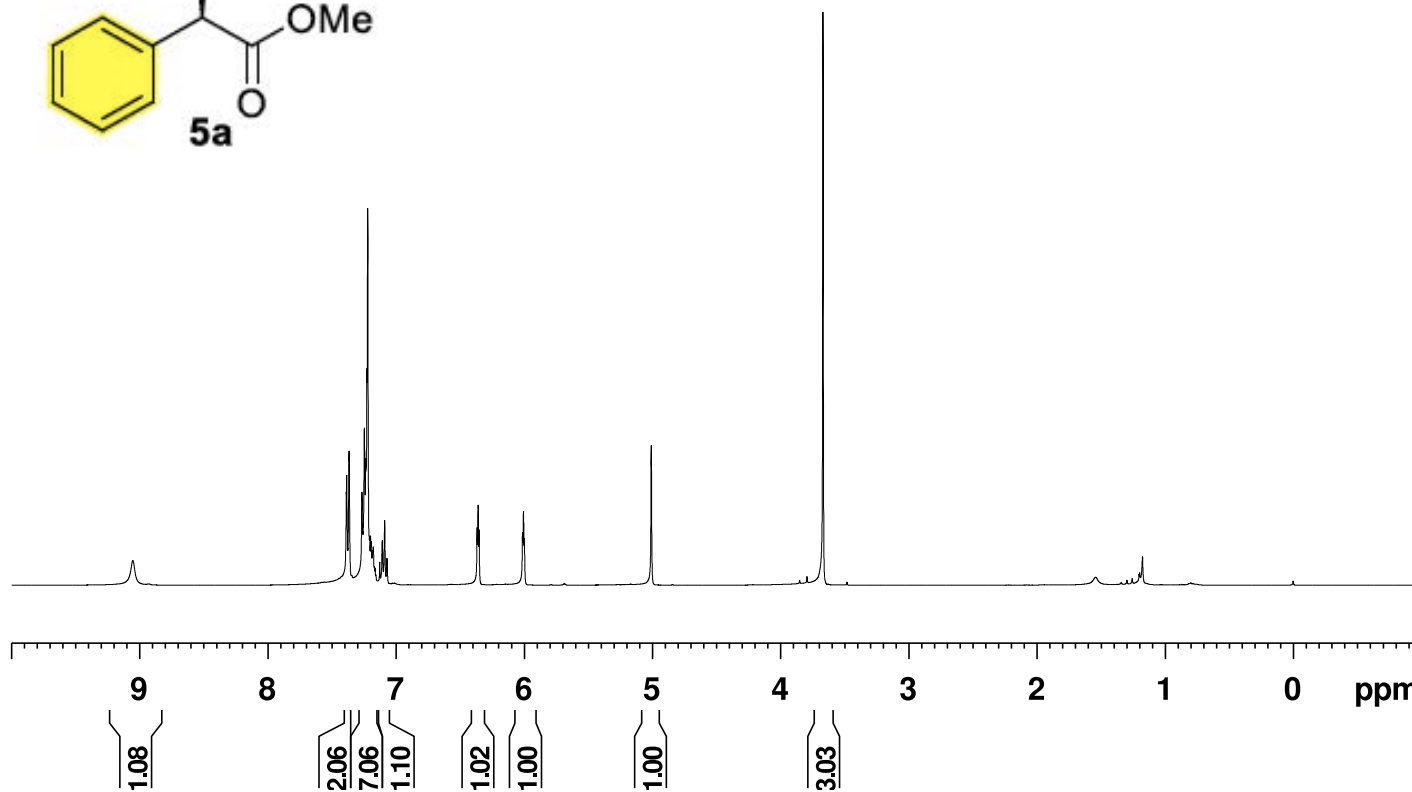
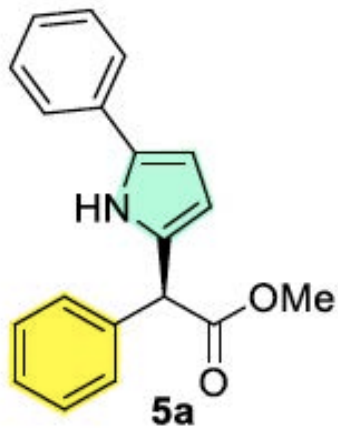


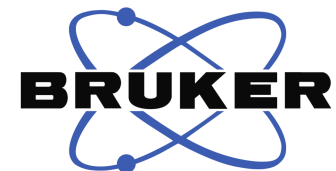
Current Data Parameters  
NAME HNMR-YX-5-p52  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230729  
Time 9.49 h  
INSTRUM Avance  
PROBHD Z116098\_0833 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8196.722 Hz  
FIDRES 0.250144 Hz  
AQ 3.9976959 sec  
RG 54.0541  
DW 61.000 usec  
DE 13.54 usec  
TE 294.6 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1324708 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 20.73200035 W

F2 - Processing parameters  
SI 65536  
SF 400.1300626 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

7.364  
7.266  
7.248  
7.237  
7.234  
7.227  
7.221  
7.206  
7.199  
7.194  
7.191  
7.185  
7.183  
7.178  
7.127  
7.107  
7.089  
7.070  
6.367  
6.360  
6.359  
6.352  
6.012  
6.005  
5.999  
5.009  
3.669

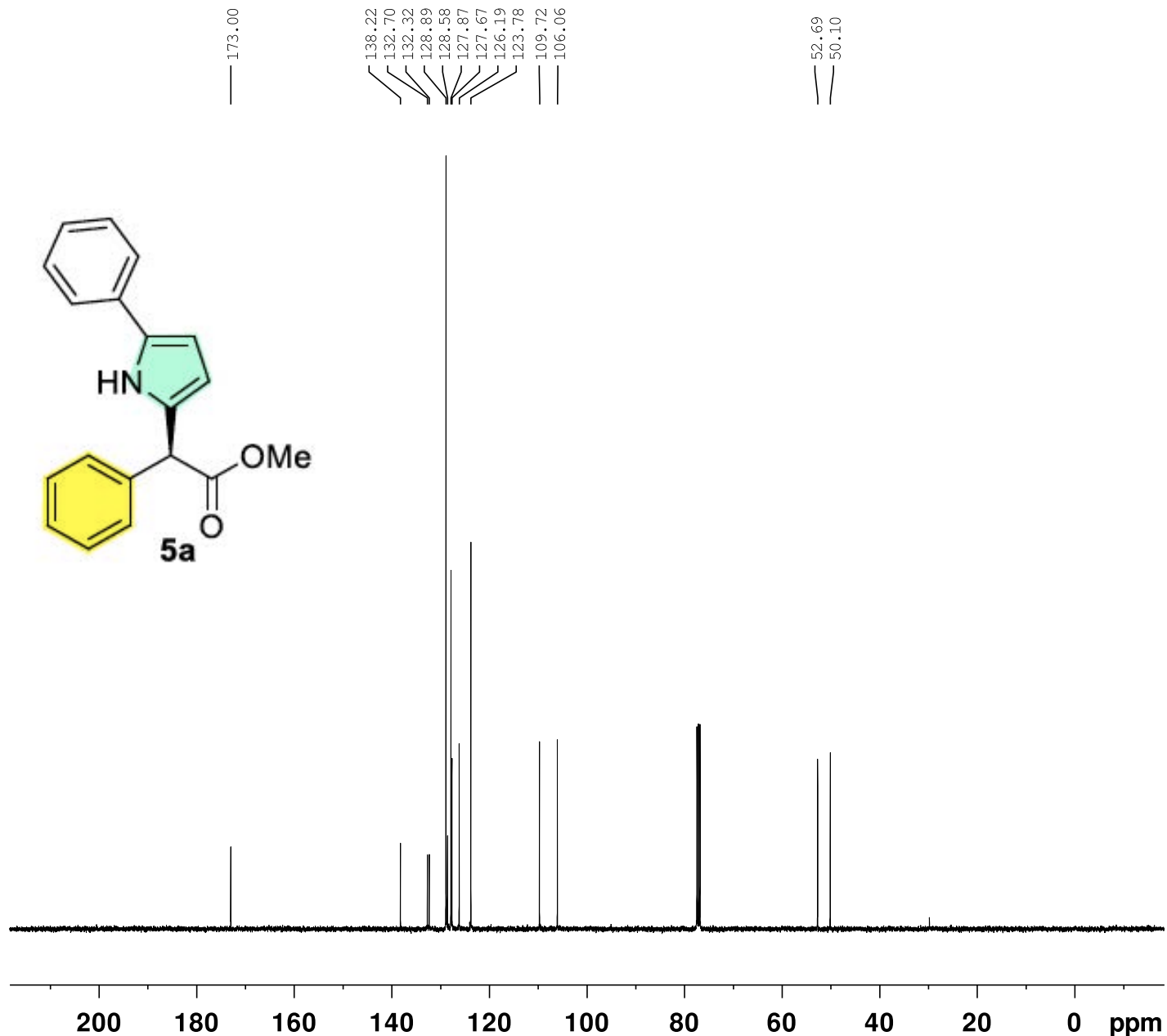


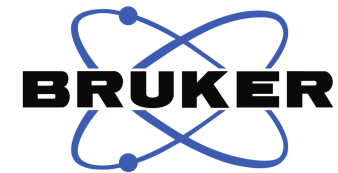


Current Data Parameters  
NAME CNMR-YX-5-p52  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230729  
Time 12.22 h  
INSTRUM Avance  
PROBHD Z116098\_0833 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 200  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 44.7144  
DW 21.000 usec  
DE 6.50 usec  
TE 294.9 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 3.33 usec  
P1 10.00 usec  
PLW1 87.89900208 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 20.73200035 W  
PLW12 0.25595000 W  
PLW13 0.12874000 W

F2 - Processing parameters  
SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



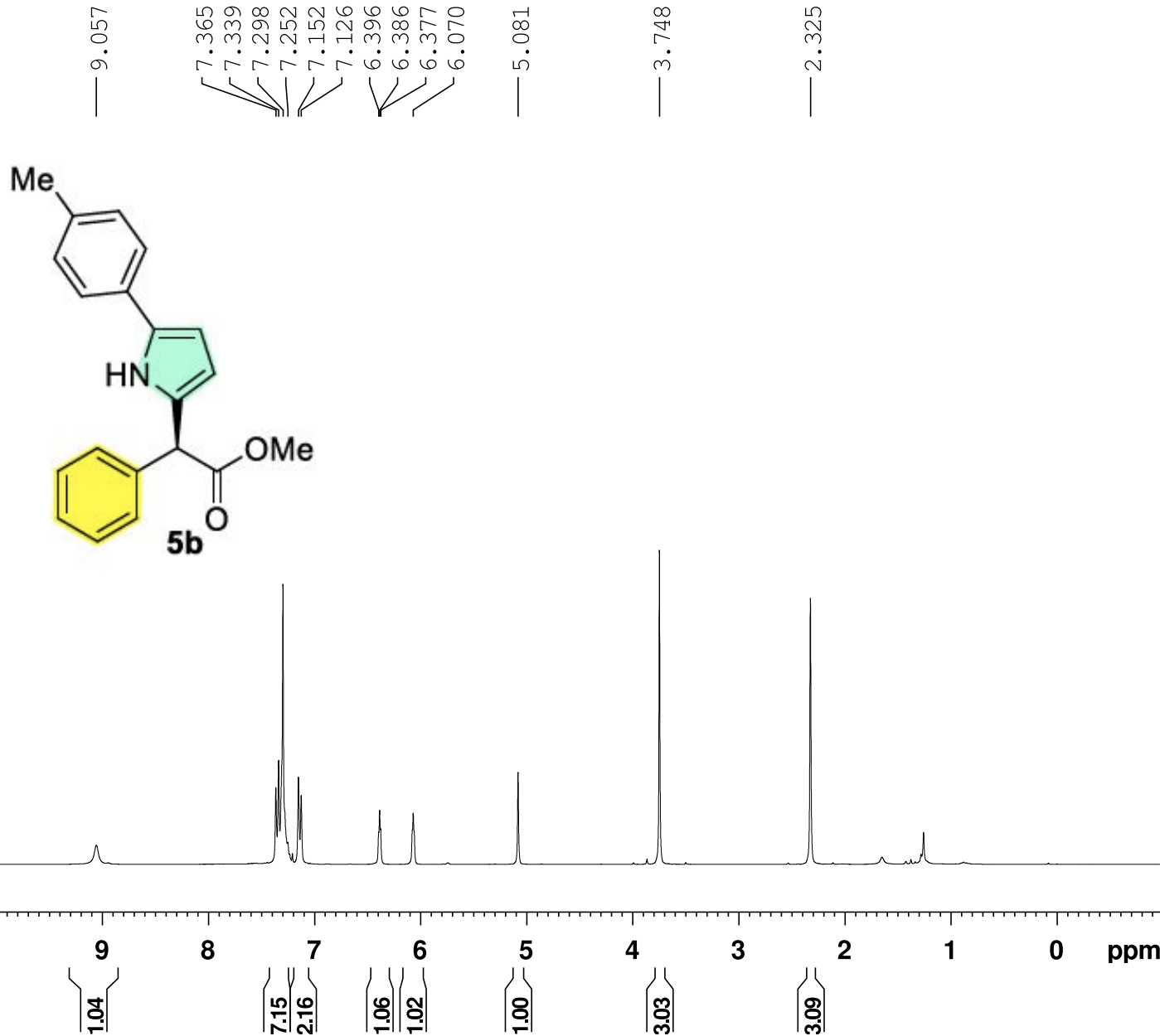


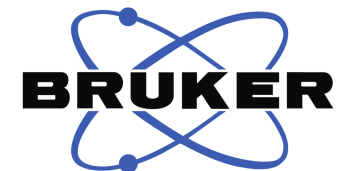
Current Data Parameters  
NAME HNMR-YX-5-p80  
EXPNO 2126  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230908  
Time 14.37  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 101  
DW 83.200 usec  
DE 6.50 usec  
TE 295.9 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 300.1318534 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 14.00000000 W

F2 - Processing parameters  
SI 65536  
SF 300.1300220 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





Current Data Parameters  
NAME CNMR-YX-5-p80  
EXPNO 2130  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20230908  
Time 15.23  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 70  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE 296.5 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

==== CHANNEL f1 =====

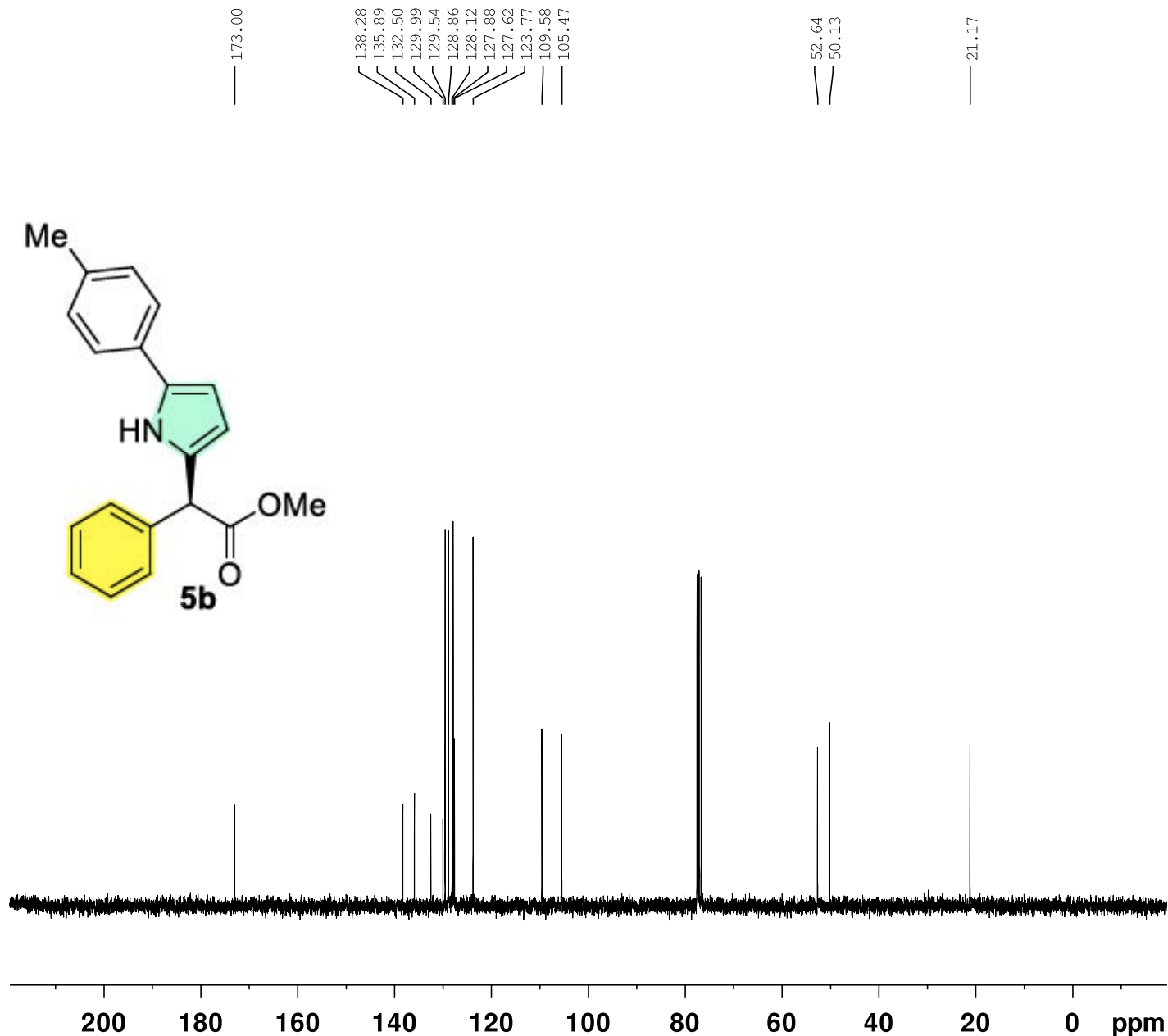
SFO1 75.4752949 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 34.20000076 W

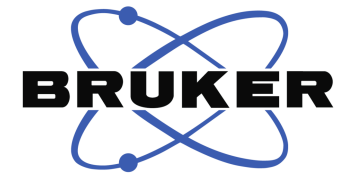
==== CHANNEL f2 =====

SFO2 300.1312005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W  
PLW13 0.14000000 W

F2 - Processing parameters

SI 32768  
SF 75.4677485 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

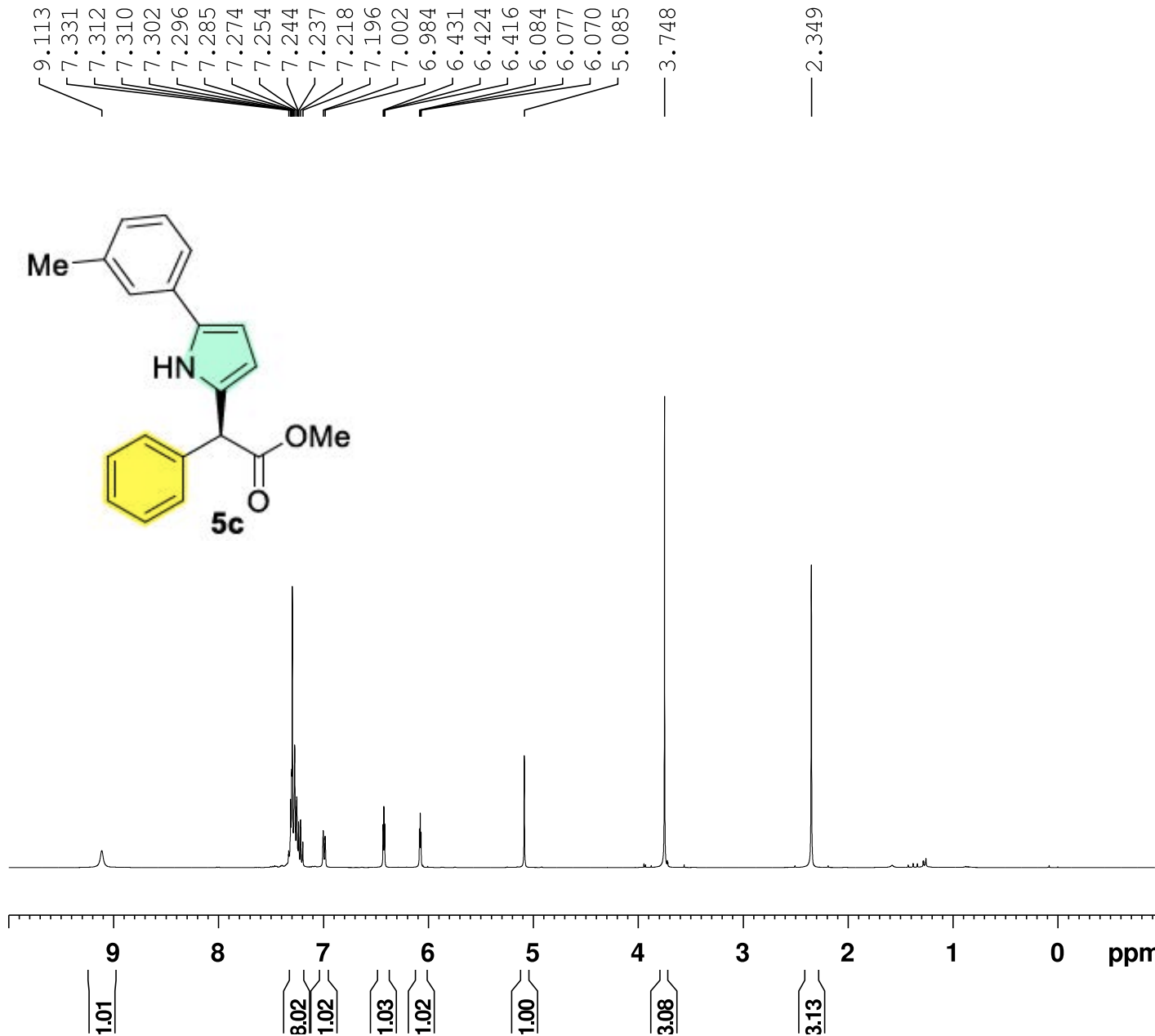


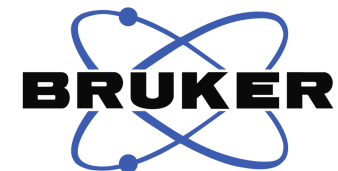


Current Data Parameters  
NAME NMR-YX-6-p31  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231107  
Time 10.44 h  
INSTRUM Avance  
PROBHD Z116098\_0833 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8196.722 Hz  
FIDRES 0.250144 Hz  
AQ 3.9976959 sec  
RG 50  
DW 61.000 usec  
DE 13.54 usec  
TE 294.0 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1324708 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 20.73200035 W

F2 - Processing parameters  
SI 65536  
SF 400.1300352 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





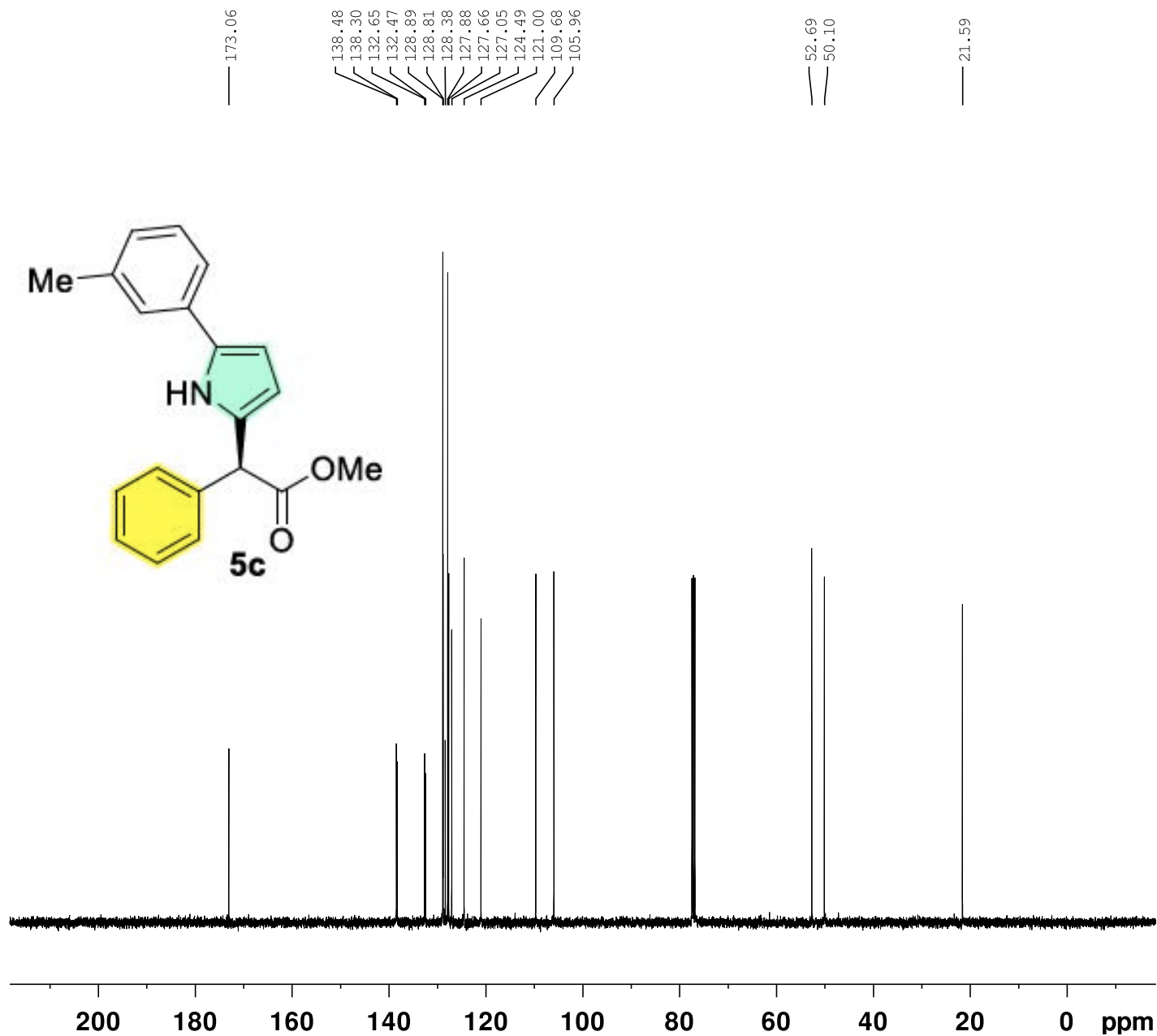
Current Data Parameters  
NAME NMR-YX-6-p31  
EXPNO 2  
PROCNO 1

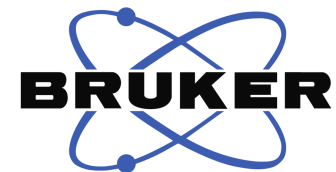
F2 - Acquisition Parameters

Date\_ 20231107  
Time 10.51 h  
INSTRUM Avance  
PROBHD z116098\_0833 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 100  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 43.5965  
DW 21.000 usec  
DE 6.50 usec  
TE 294.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 3.33 usec  
P1 10.00 usec  
PLW1 87.89900208 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 20.73200035 W  
PLW12 0.25595000 W  
PLW13 0.12874000 W

F2 - Processing parameters

SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



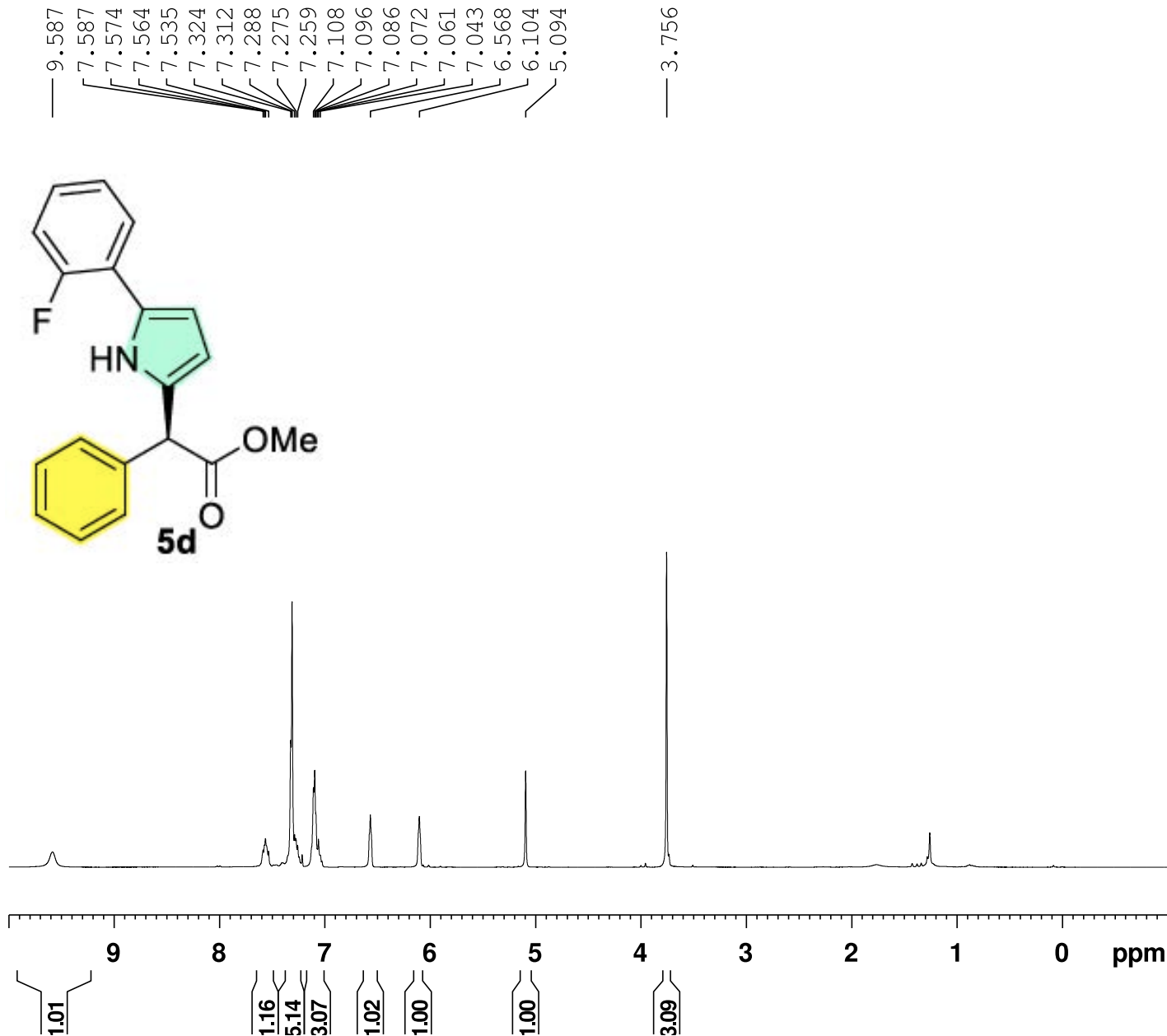


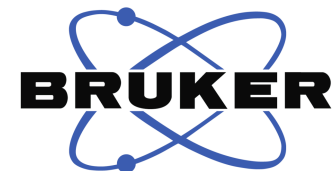
Current Data Parameters  
NAME HNMR-YX-5-p81  
EXPNO 2127  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230908  
Time 14.43  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 101  
DW 83.200 usec  
DE 6.50 usec  
TE 295.8 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 300.1318534 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 14.00000000 W

F2 - Processing parameters  
SI 65536  
SF 300.1300199 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





Current Data Parameters  
NAME CNMR-YX-5-p81  
EXPNO 2132  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230908  
Time 15.34  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 70  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE 296.5 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

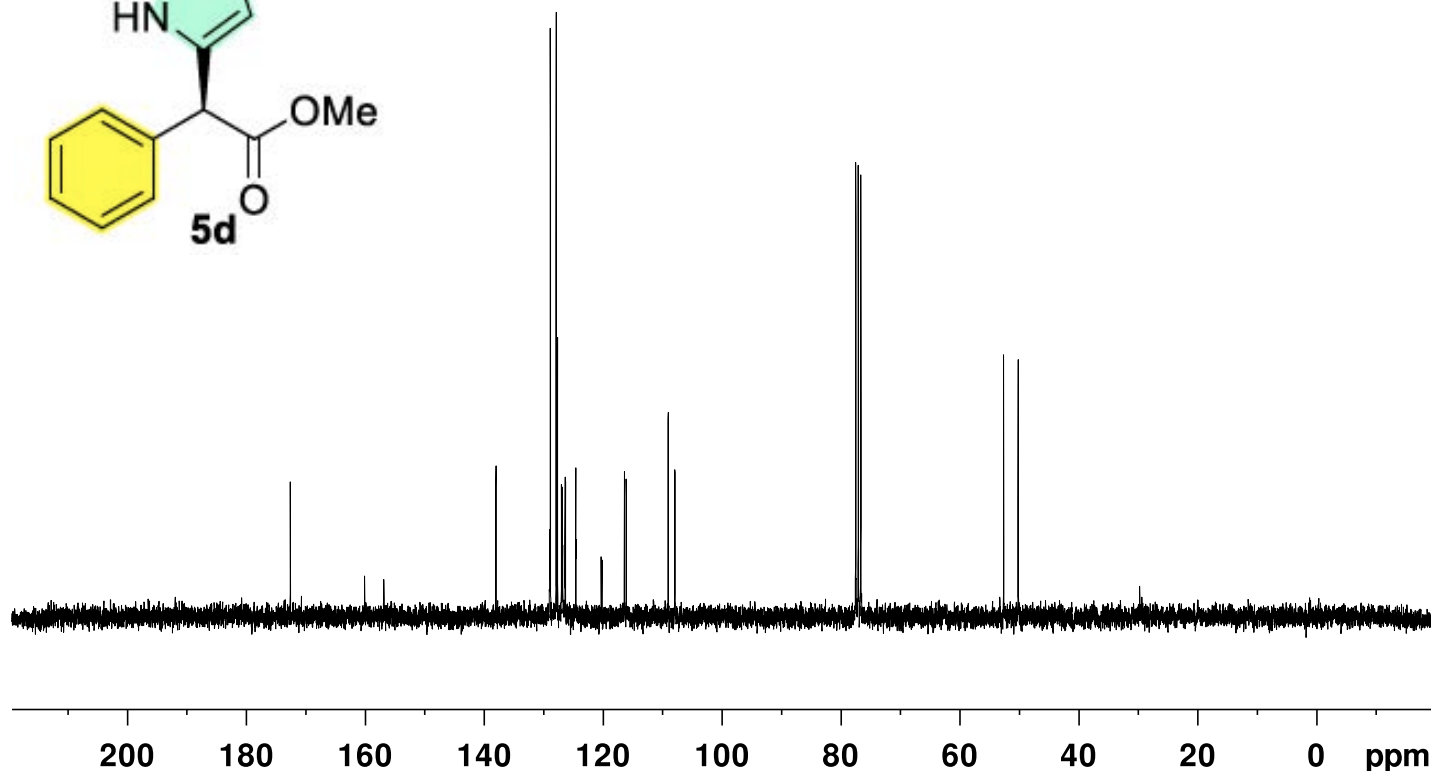
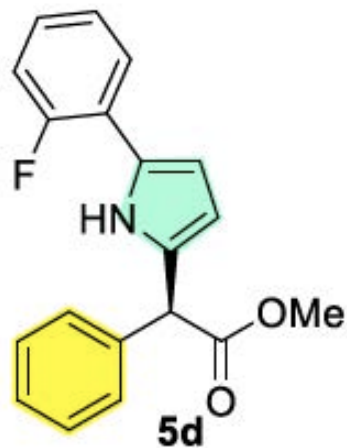
==== CHANNEL f1 =====  
SFO1 75.4752949 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 34.20000076 W

==== CHANNEL f2 =====  
SFO2 300.1312005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W  
PLW13 0.14000000 W

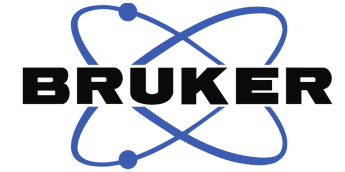
F2 - Processing parameters  
SI 32768  
SF 75.4677485 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

172.62  
160.13  
156.89  
138.04  
129.01  
128.97  
128.88  
127.91  
127.67  
127.02  
126.91  
126.83  
126.80  
126.40  
126.34  
124.62  
124.58  
120.35  
120.19  
116.43  
116.12  
109.06  
107.96

52.66  
50.21







Current Data Parameters  
NAME FNMN-YX-5-p81  
EXPNO 2131  
PROCNO 1

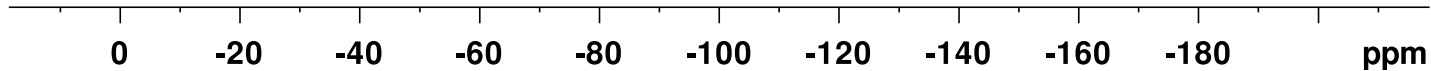
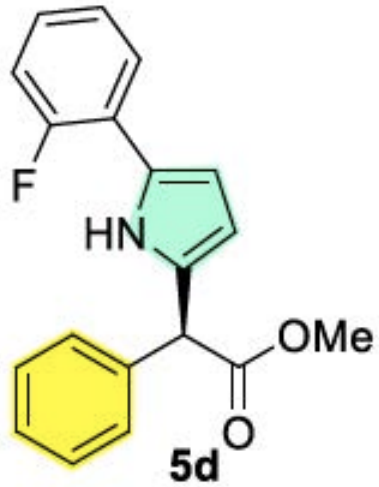
F2 - Acquisition Parameters  
Date\_ 20230908  
Time 15.28  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgfhigqn.2  
TD 131072  
SOLVENT CDCl3  
NS 16  
DS 4  
SWH 66964.289 Hz  
FIDRES 0.510897 Hz  
AQ 0.9786710 sec  
RG 203  
DW 7.467 usec  
DE 6.50 usec  
TE 296.1 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
D12 0.00002000 sec  
TD0 1

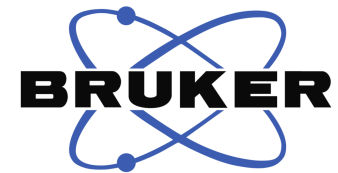
==== CHANNEL f1 =====  
SFO1 282.3761148 MHz  
NUC1 19F  
P1 14.50 usec  
PLW1 10.39999962 W

==== CHANNEL f2 =====  
SFO2 300.1312005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W

F2 - Processing parameters  
SI 65536  
SF 282.4043552 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

-118.61





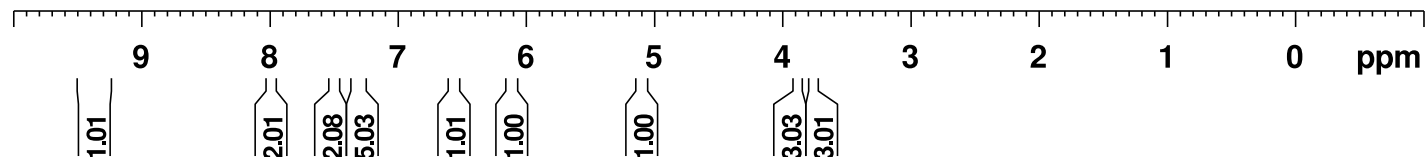
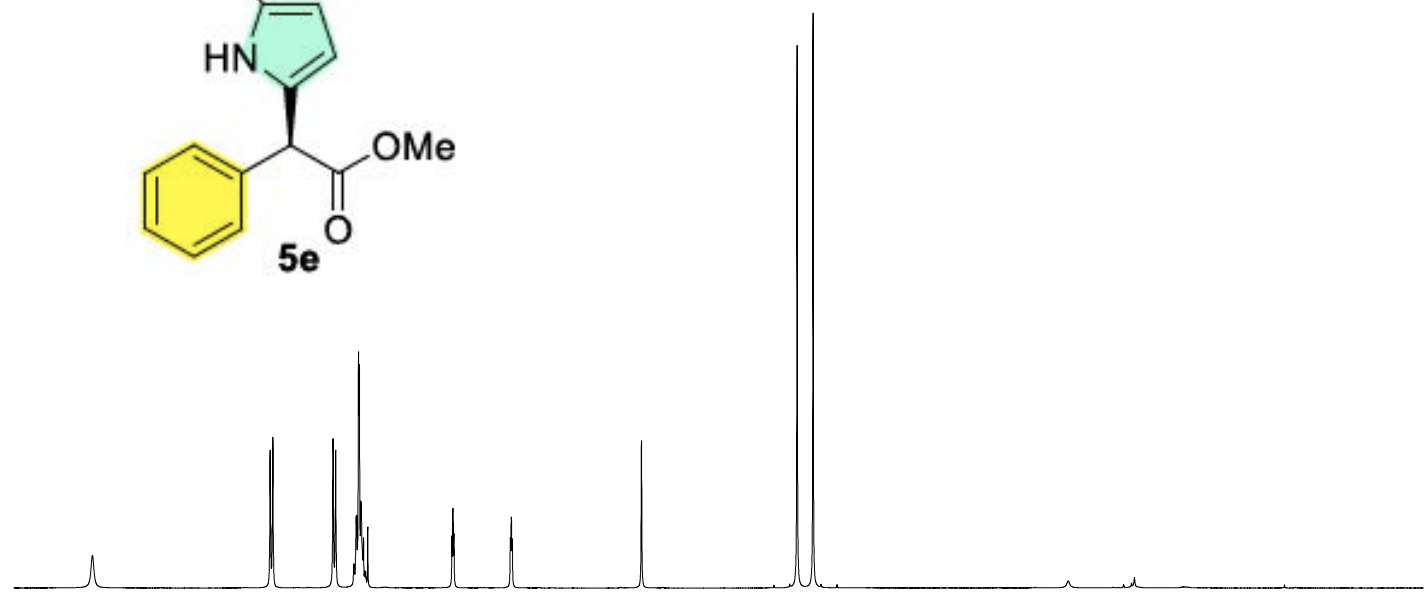
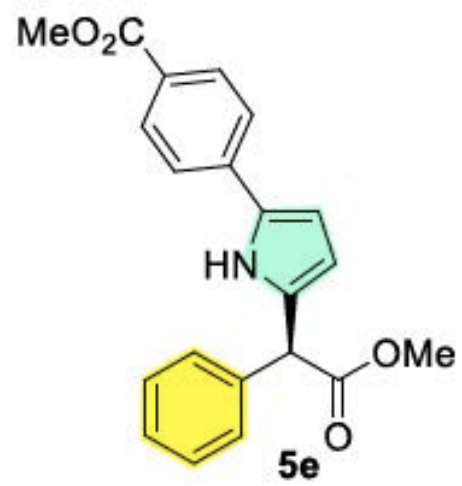
Current Data Parameters  
NAME HNMR-YX-7-p11  
EXPNO 23  
PROCNO 1

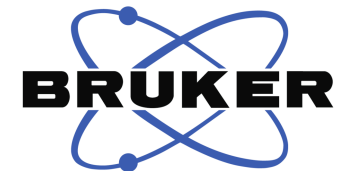
F2 - Acquisition Parameters  
Date\_ 20231103  
Time 9.34  
INSTRUM spect  
PROBHD 5 mm PADUL 13C  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 4  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9845889 sec  
RG 53.3  
DW 60.800 usec  
DE 6.50 usec  
TE 291.9 K  
D1 1.00000000 sec  
TD0 1

=====  
CHANNEL f1  
NUC1 1H  
P1 9.90 usec  
PLW1 23.00000000 W  
SFO1 400.1924713 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1900228 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

7.999  
7.978  
7.508  
7.487  
7.345  
7.341  
7.327  
7.323  
7.309  
7.303  
7.291  
7.287  
7.270  
7.261  
7.254  
6.580  
6.572  
6.565  
6.124  
6.117  
6.110  
5.101  
3.887  
3.763





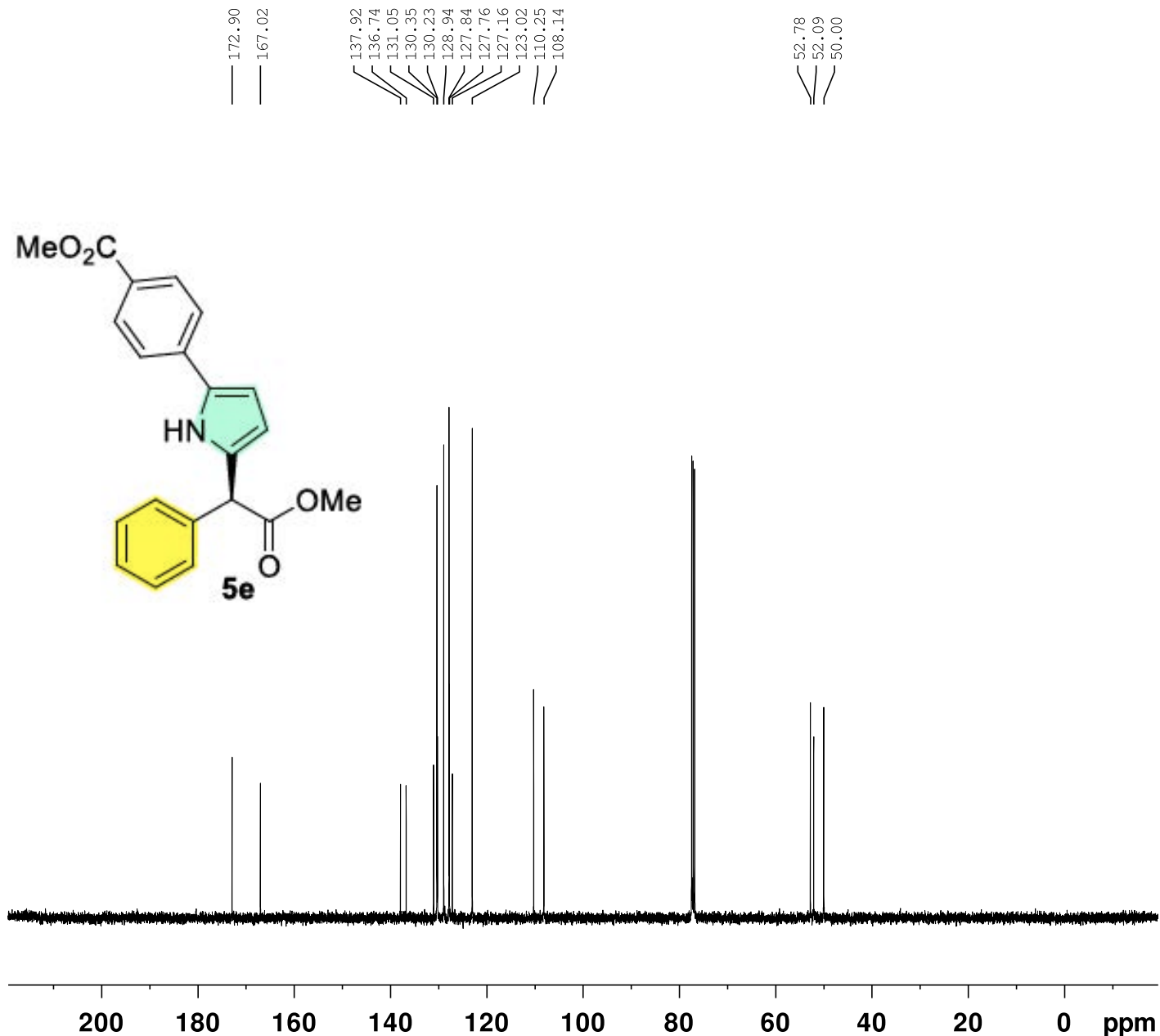
Current Data Parameters  
NAME CNMR-YX-7-p11  
EXPNO 24  
PROCNO 1

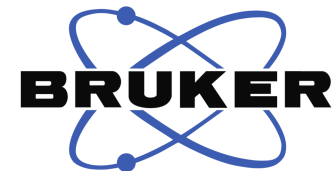
F2 - Acquisition Parameters  
Date\_ 20231103  
Time 9.42  
INSTRUM spect  
PROBHD 5 mm PADUL 13C  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 100  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 37.77  
DW 20.800 usec  
DE 6.50 usec  
TE 292.5 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 9.80 usec  
PLW1 47.4000153 W  
SFO1 100.6379178 MHz

==== CHANNEL f2 =====  
CPDPRG[2] waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 23.00000000 W  
PLW12 0.30712000 W  
PLW13 0.24877000 W  
SFO2 400.1916008 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6278560 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



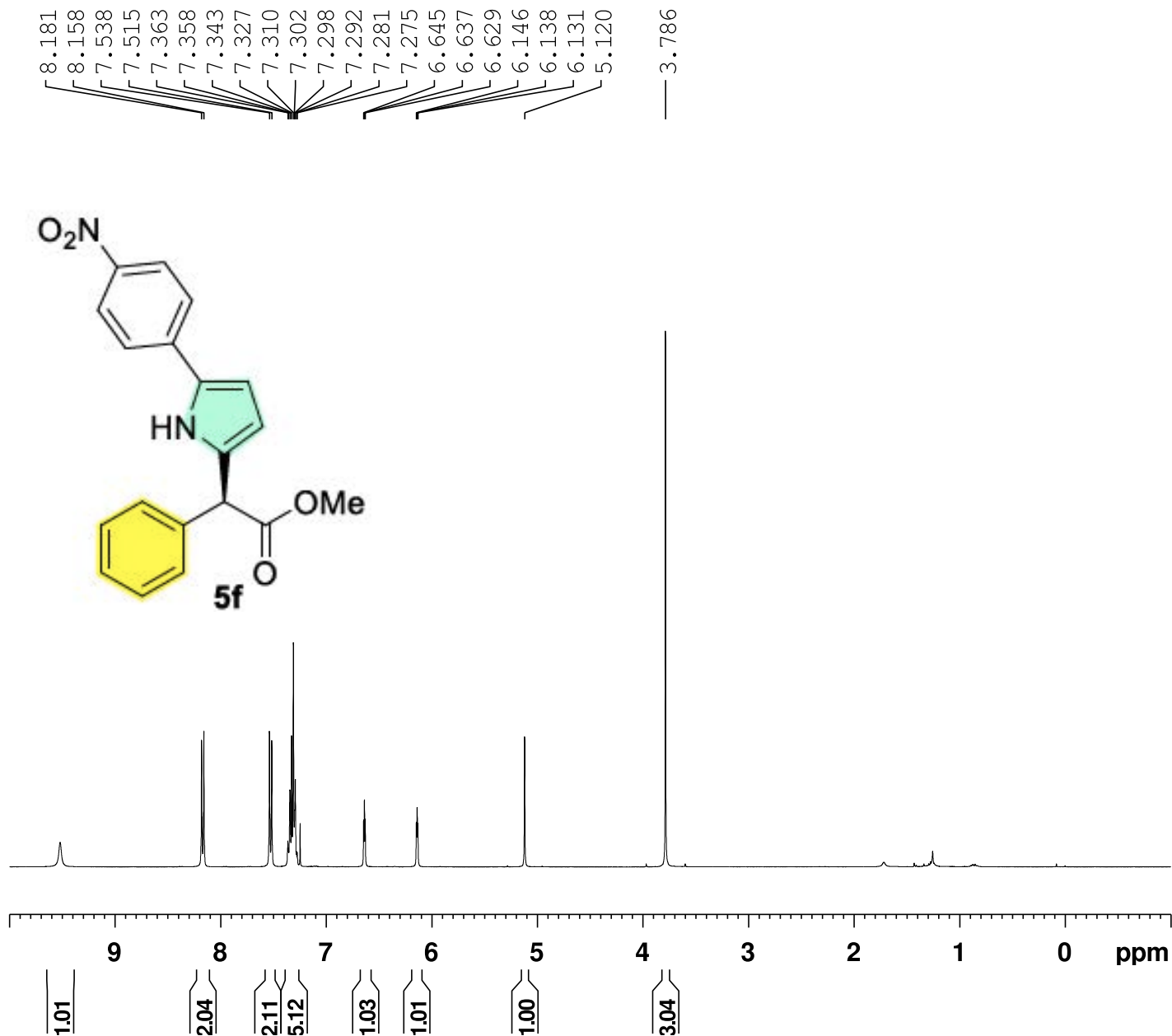


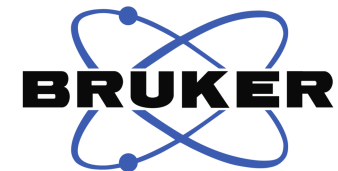
Current Data Parameters  
NAME HNMR-YX-7-p12  
EXPNO 20  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231101  
Time 15.17  
INSTRUM spect  
PROBHD 5 mm PADUL 13C  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 4  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9845889 sec  
RG 75.43  
DW 60.800 usec  
DE 6.50 usec  
TE 291.4 K  
D1 1.00000000 sec  
TD0 1

=====  
CHANNEL f1  
NUC1 1H  
P1 9.90 usec  
PLW1 23.00000000 W  
SFO1 400.1924713 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1900190 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





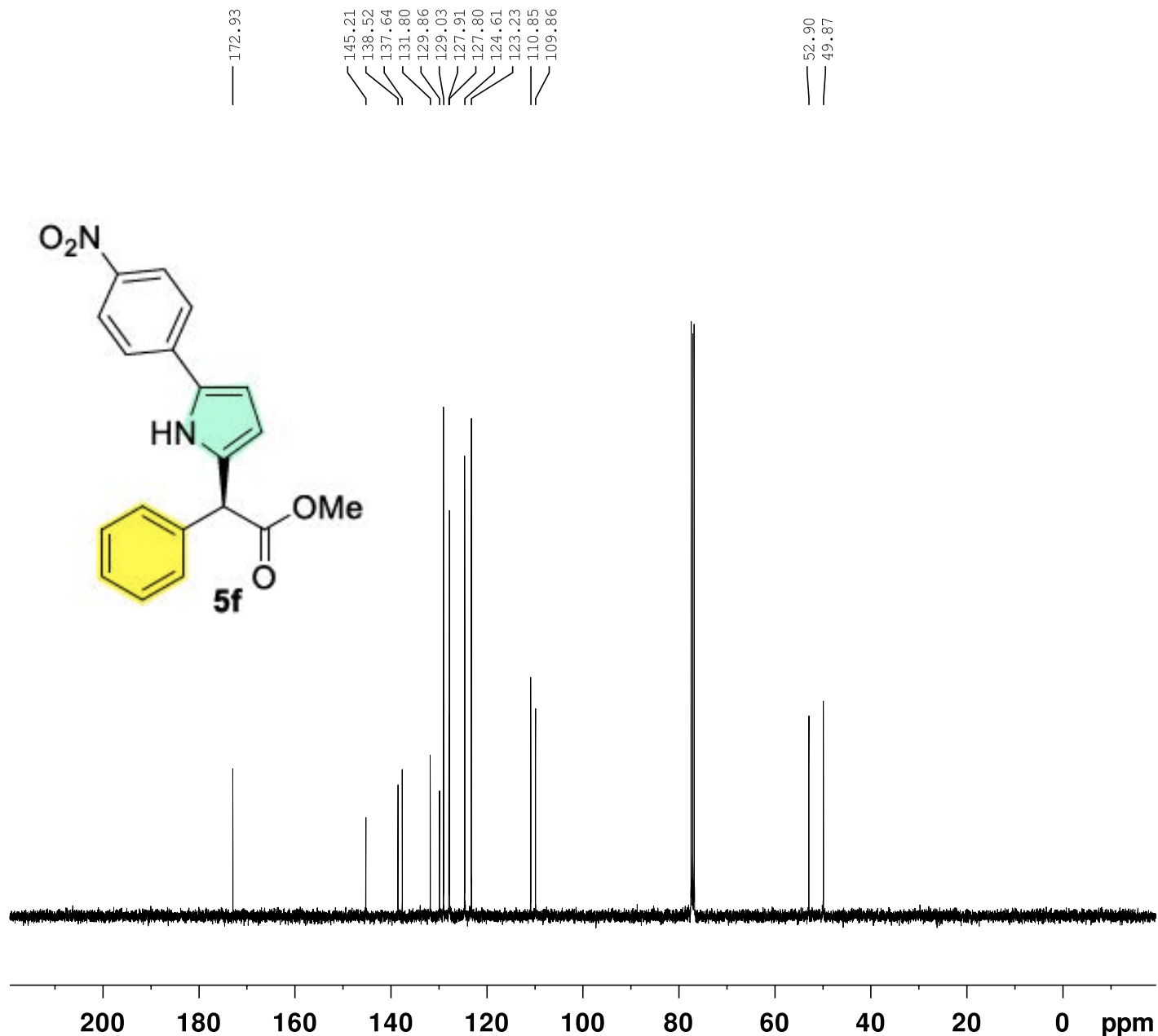
Current Data Parameters  
NAME CNMR-YX-7-p12  
EXPNO 21  
PROCNO 1

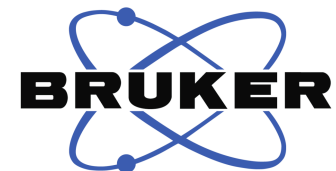
F2 - Acquisition Parameters  
Date\_ 20231101  
Time 15.24  
INSTRUM spect  
PROBHD 5 mm PADUL 13C  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 100  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 50.16  
DW 20.800 usec  
DE 6.50 usec  
TE 292.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 9.80 usec  
PLW1 47.4000153 W  
SFO1 100.6379178 MHz

==== CHANNEL f2 =====  
CPDPRG[2] waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 23.00000000 W  
PLW12 0.30712000 W  
PLW13 0.24877000 W  
SFO2 400.1916008 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6278560 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



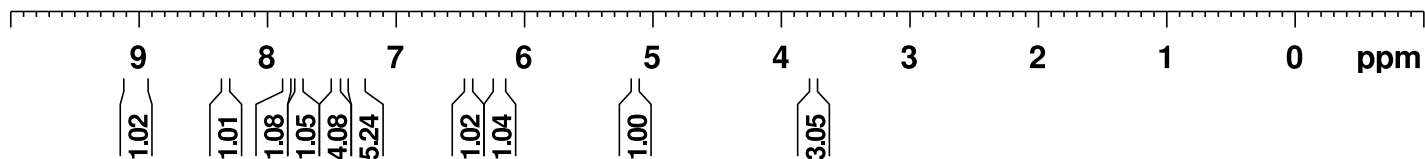
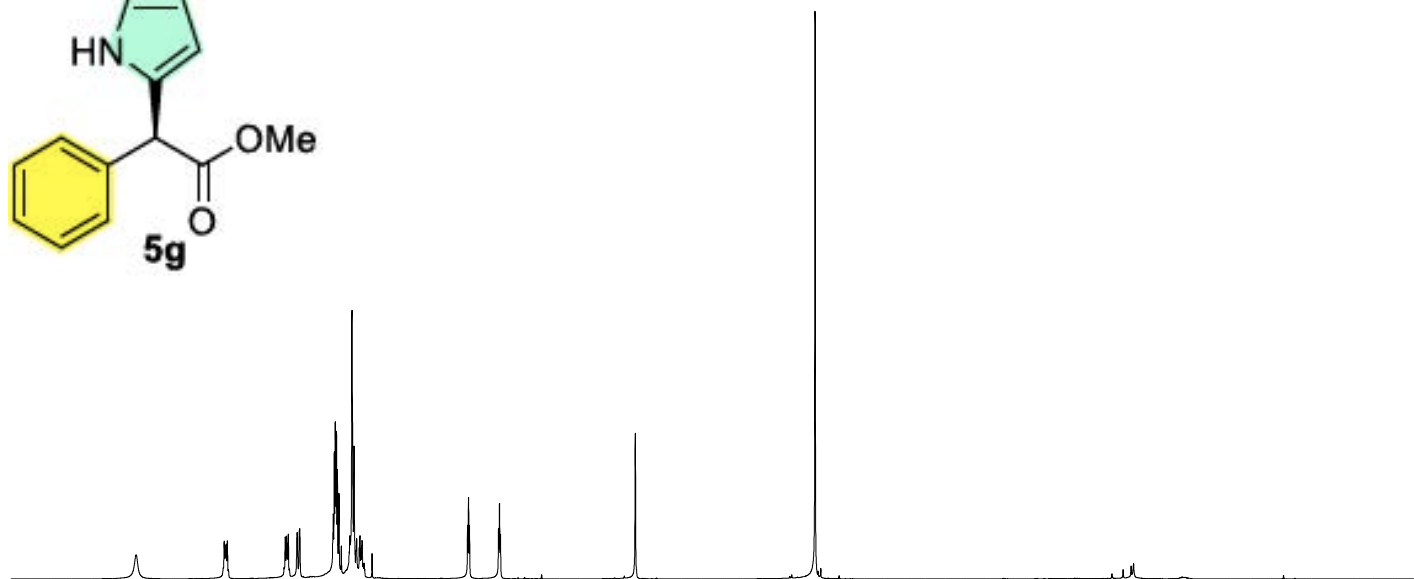
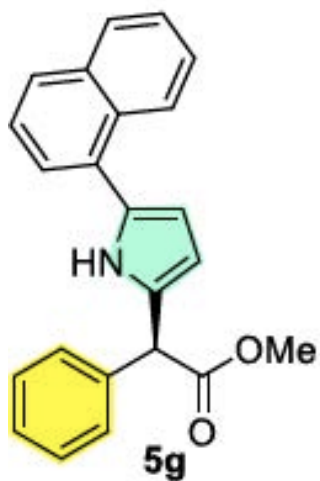


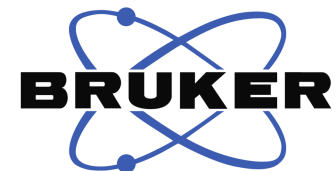
Current Data Parameters  
NAME NMR-YX-6-p33  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231107  
Time 11.52 h  
INSTRUM Avance  
PROBHD Z116098\_0833 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8196.722 Hz  
FIDRES 0.250144 Hz  
AQ 3.9976959 sec  
RG 48.7805  
DW 61.000 usec  
DE 13.54 usec  
TE 294.0 K  
D1 1.00000000 sec  
TD0 1  
SF01 400.1324708 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 20.73200035 W

F2 - Processing parameters  
SI 65536  
SF 400.1300394 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

7.480  
7.472  
7.463  
7.456  
7.443  
7.425  
7.364  
7.358  
7.342  
7.338  
7.326  
7.310  
7.306  
7.296  
7.285  
7.280  
7.272  
7.264  
7.256  
7.248  
7.243  
6.442  
6.434  
6.427  
6.201  
6.194  
6.186  
5.136  
3.736

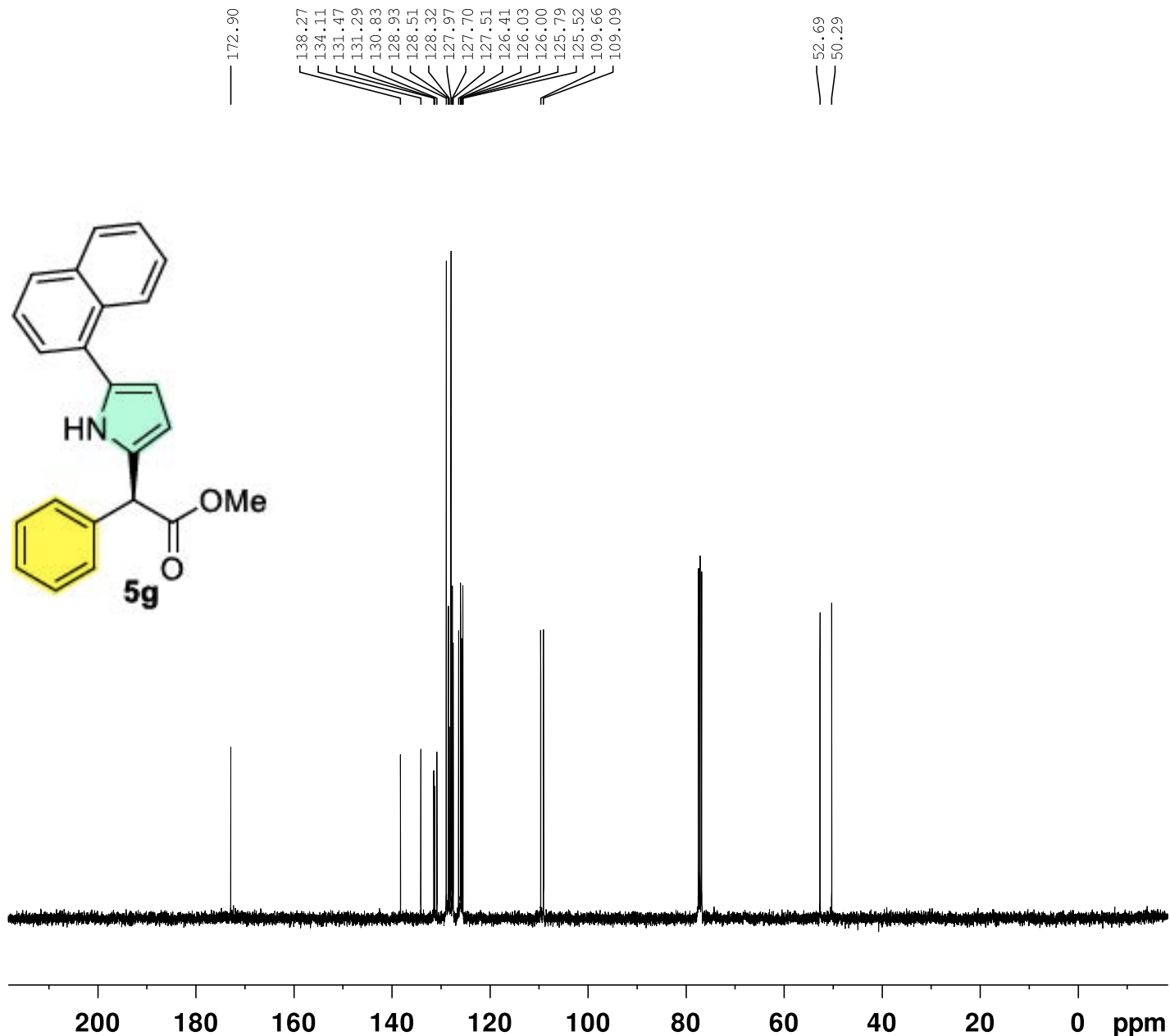


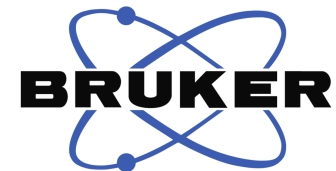


Current Data Parameters  
NAME NMR-YX-6-p33  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231107  
Time 11.59 h  
INSTRUM Avance  
PROBHD Z116098\_0833 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 100  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 44.8788  
DW 21.000 usec  
DE 6.50 usec  
TE 294.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 3.33 usec  
P1 10.00 usec  
PLW1 87.89900208 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 20.73200035 W  
PLW12 0.25595000 W  
PLW13 0.12874000 W

F2 - Processing parameters  
SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



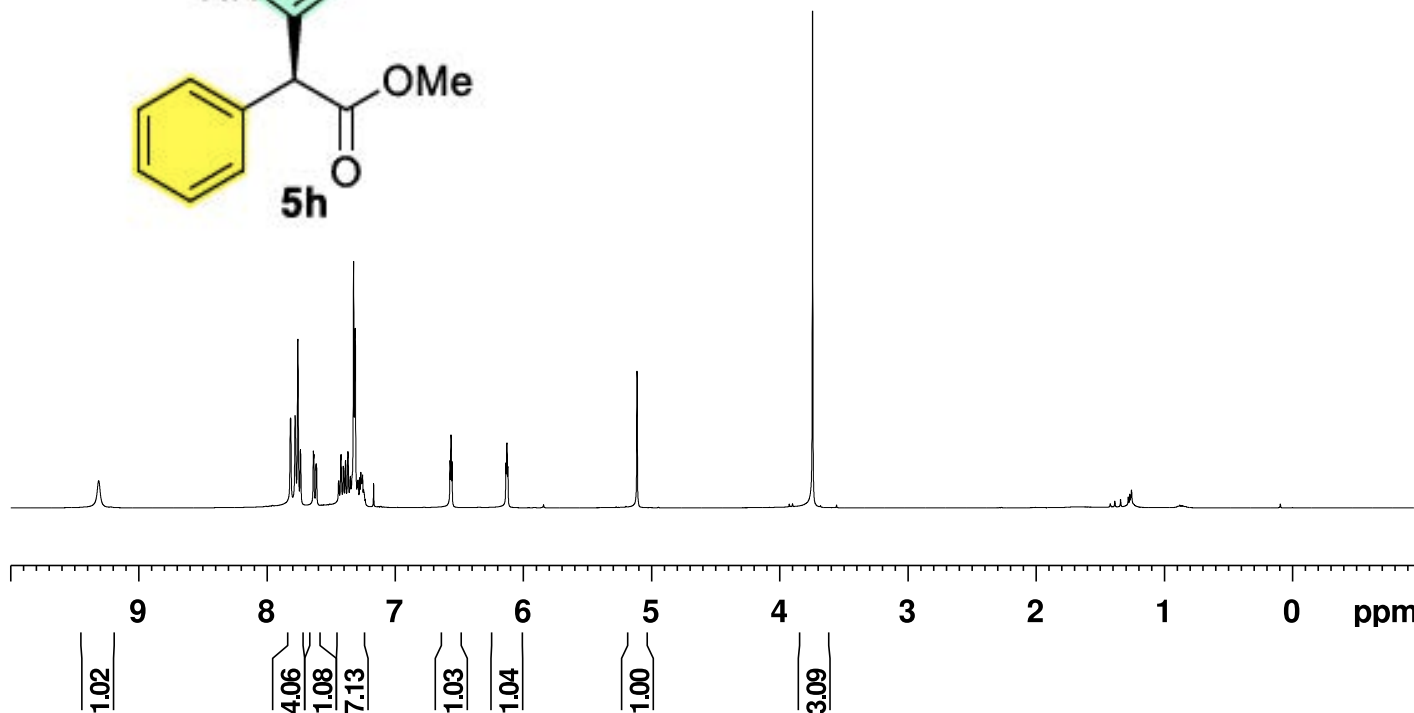
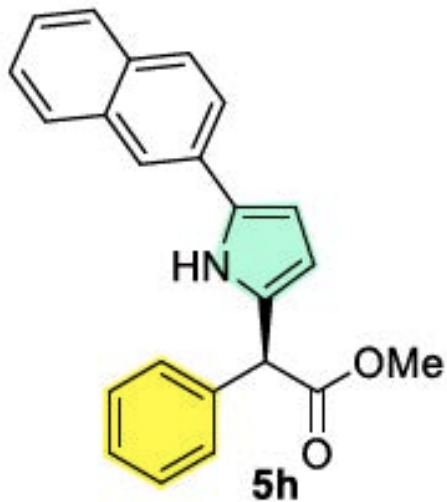


Current Data Parameters  
NAME NMR-YX-6-p32  
EXPNO 1  
PROCNO 1

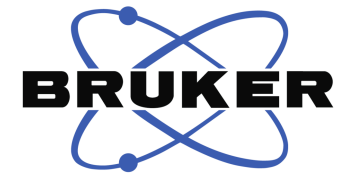
F2 - Acquisition Parameters  
Date\_ 20231107  
Time 11.40 h  
INSTRUM Avance  
PROBHD Z116098\_0833 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8196.722 Hz  
FIDRES 0.250144 Hz  
AQ 3.9976959 sec  
RG 44.4444  
DW 61.000 usec  
DE 13.54 usec  
TE 294.0 K  
D1 1.00000000 sec  
TD0 1  
SF01 400.1324708 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 20.73200035 W

F2 - Processing parameters  
SI 65536  
SF 400.1300464 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

7.613  
7.439  
7.422  
7.405  
7.402  
7.388  
7.386  
7.368  
7.349  
7.324  
7.315  
7.312  
7.297  
7.290  
7.275  
7.268  
7.259  
7.254  
7.247  
6.572  
6.564  
6.556  
6.135  
6.128  
6.121  
5.112  
3.743



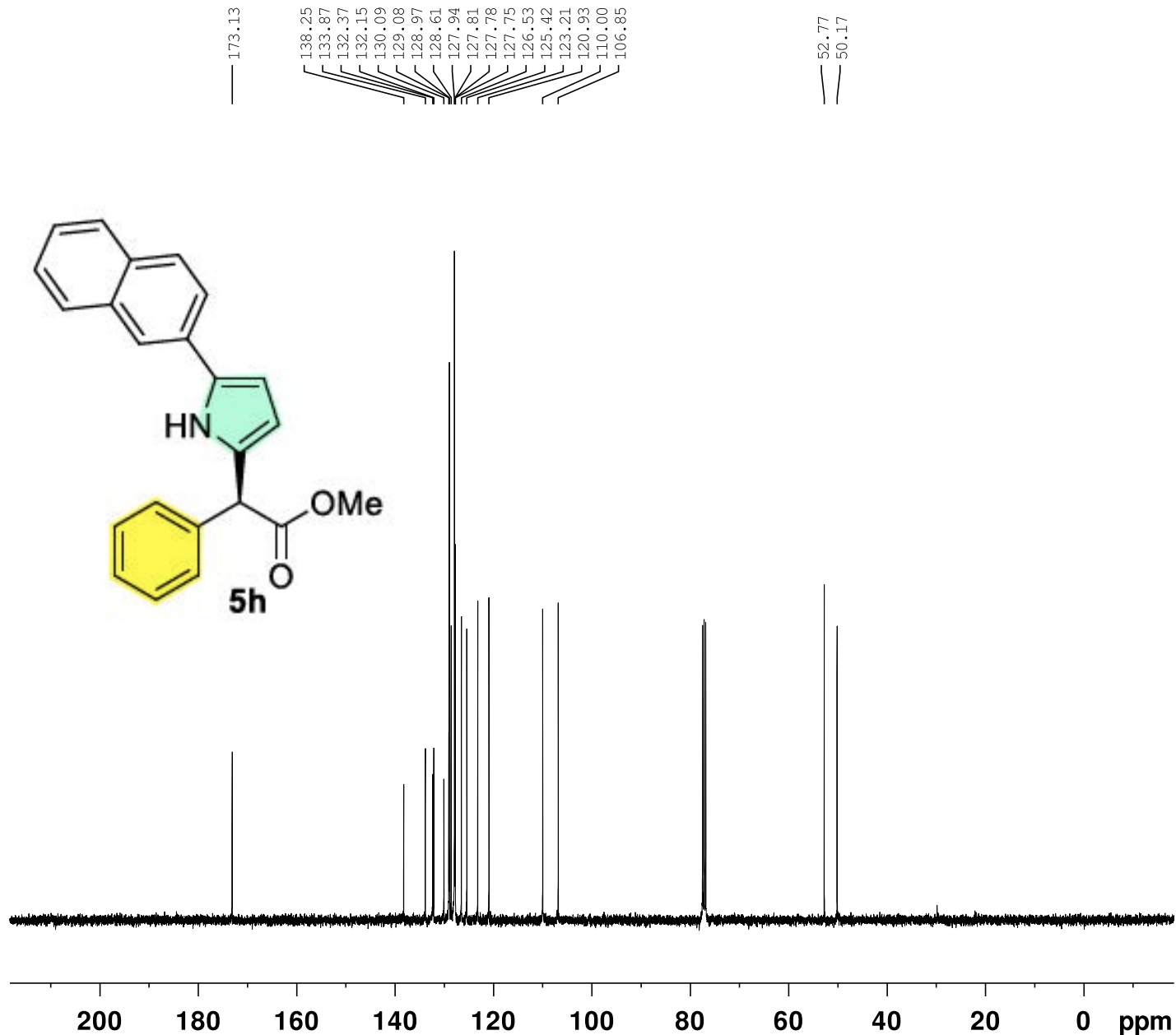


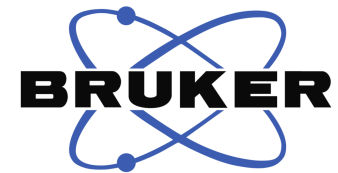


Current Data Parameters  
NAME NMR-YX-6-p32  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231107  
Time 11.47 h  
INSTRUM Avance  
PROBHD Z116098\_0833 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 100  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 47.4244  
DW 21.000 usec  
DE 6.50 usec  
TE 294.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 3.33 usec  
P1 10.00 usec  
PLW1 87.89900208 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 20.73200035 W  
PLW12 0.25595000 W  
PLW13 0.12874000 W

F2 - Processing parameters  
SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



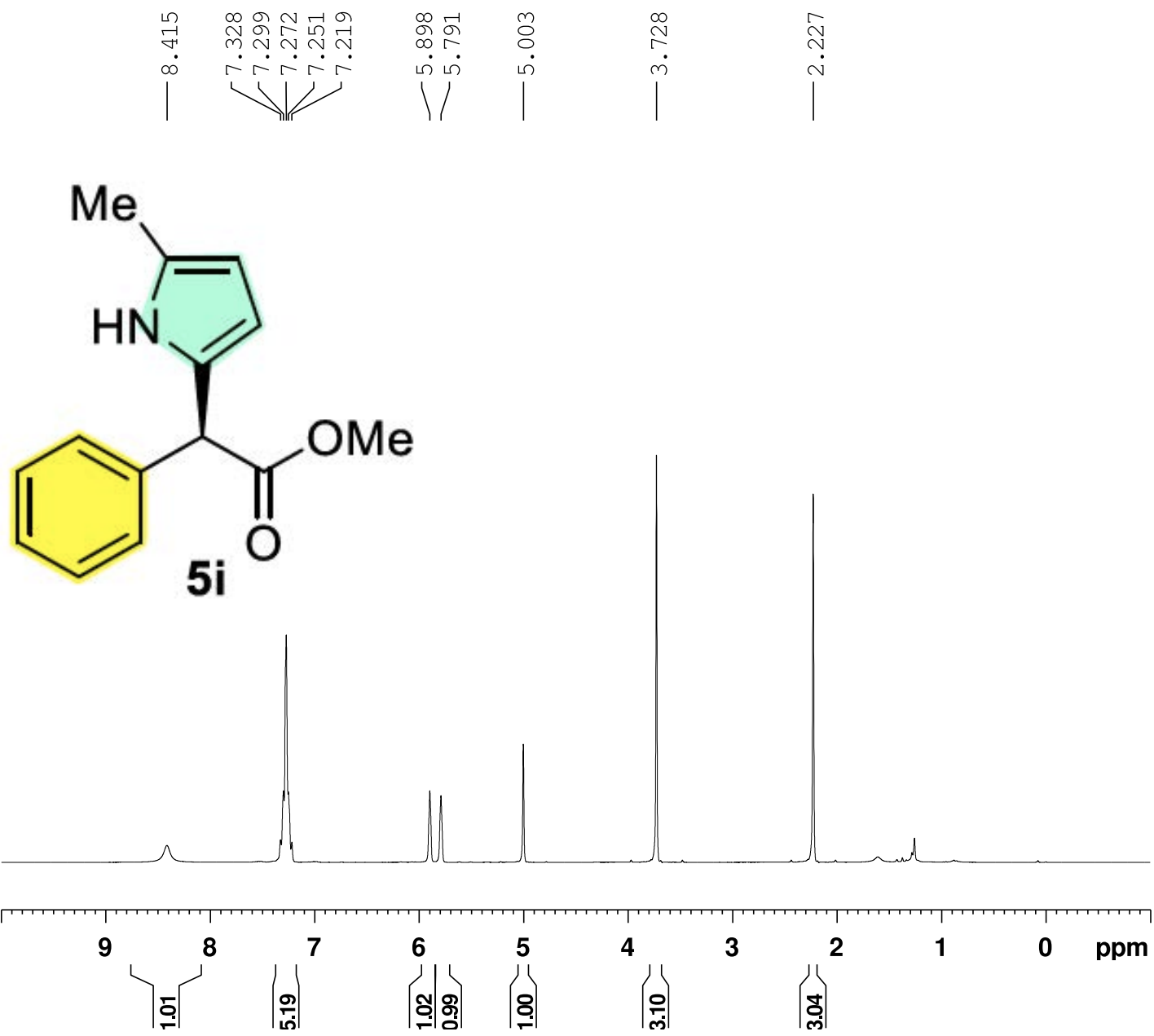


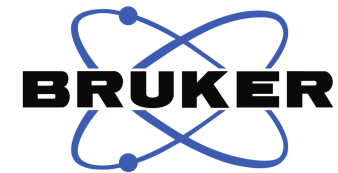
Current Data Parameters  
NAME HNMR-YX-5-p70  
EXPNO 2060  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230809  
Time 20.29  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 101  
DW 83.200 usec  
DE 6.50 usec  
TE 297.9 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 300.1318534 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 14.00000000 W

F2 - Processing parameters  
SI 65536  
SF 300.1300192 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



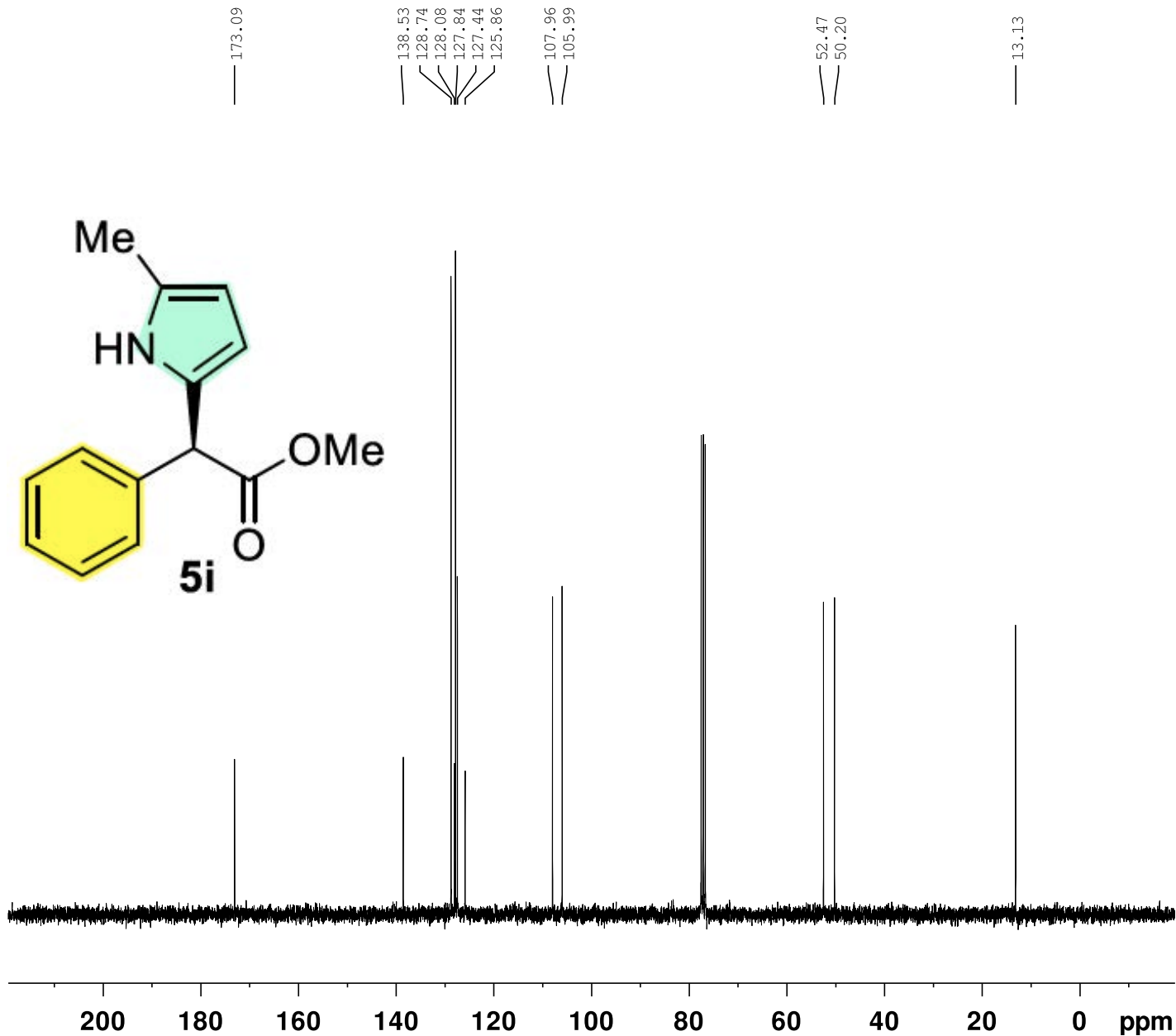


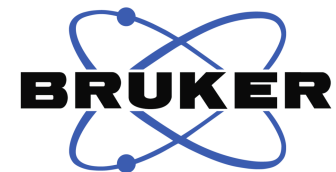
Current Data Parameters  
NAME CNMR-YX-5-p70  
EXPNO 2073  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230810  
Time 2.36  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 150  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE 298.7 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 75.4752949 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 34.20000076 W  
  
==== CHANNEL f2 =====  
SFO2 300.1312005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W  
PLW13 0.14000000 W

F2 - Processing parameters  
SI 32768  
SF 75.4677485 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





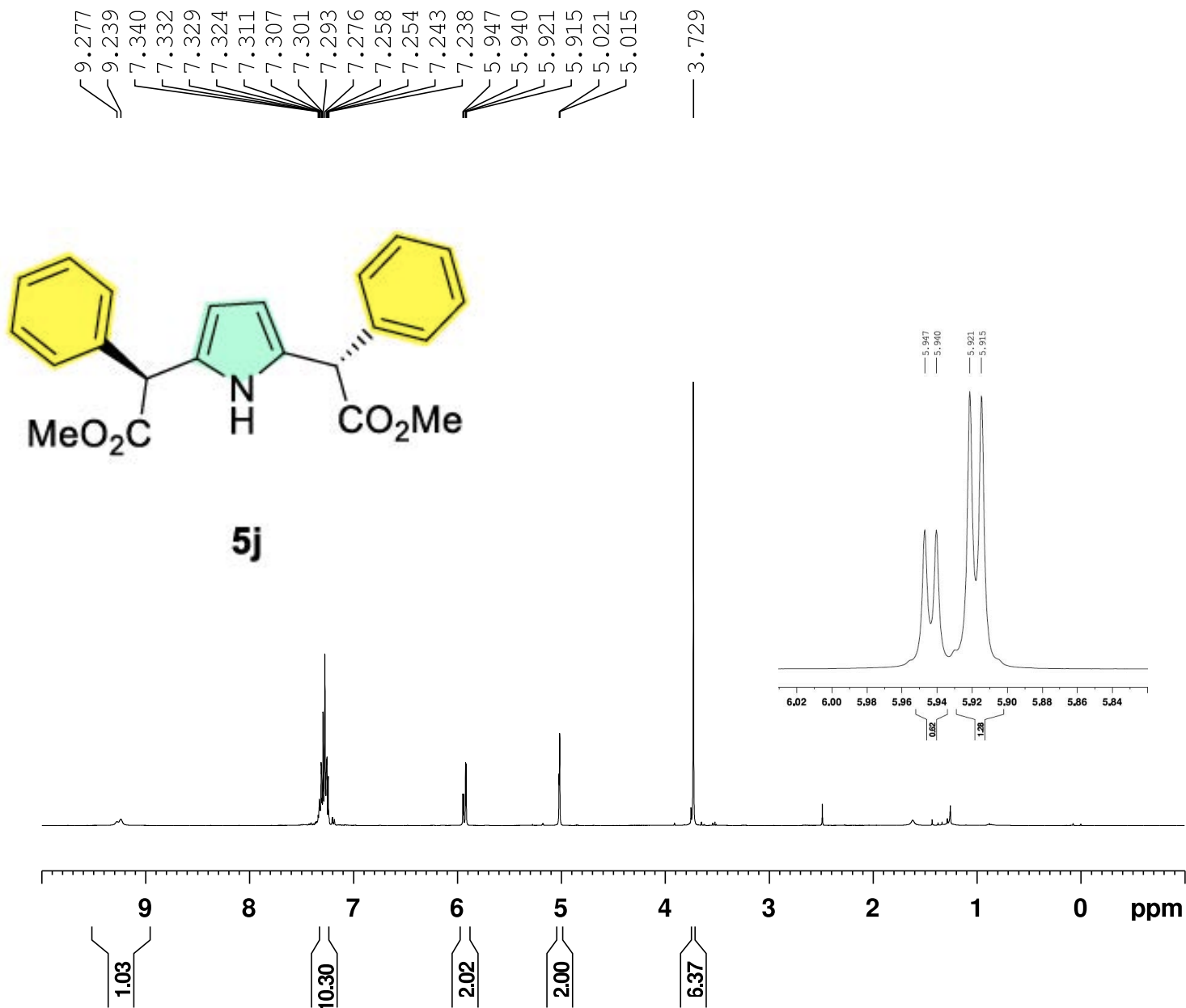
Current Data Parameters  
NAME HNMR-YX-5-p82  
EXPNO 1  
PROCNO 1

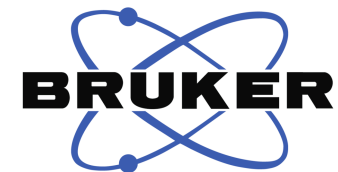
F2 - Acquisition Parameters

Date\_ 20231019  
Time 7.00 h  
INSTRUM Avance  
PROBHD z116098\_0833 (  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 8196.722 Hz  
FIDRES 0.250144 Hz  
AQ 3.9976959 sec  
RG 100.806  
DW 61.000 usec  
DE 13.54 usec  
TE 293.6 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1324708 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 20.73200035 W

F2 - Processing parameters

SI 65536  
SF 400.1300165 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





Current Data Parameters  
NAME CNMR-YX-5-p82  
EXPNO 2135  
PROCNO 1

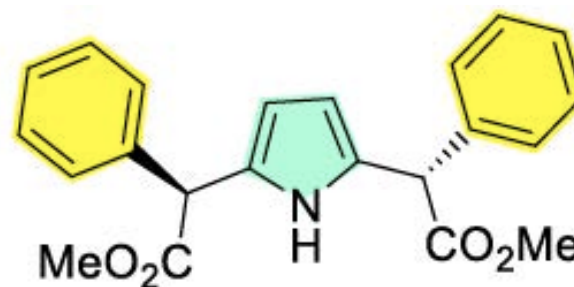
F2 - Acquisition Parameters

Date\_ 20230911  
Time 16.52  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 100  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE 296.8 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

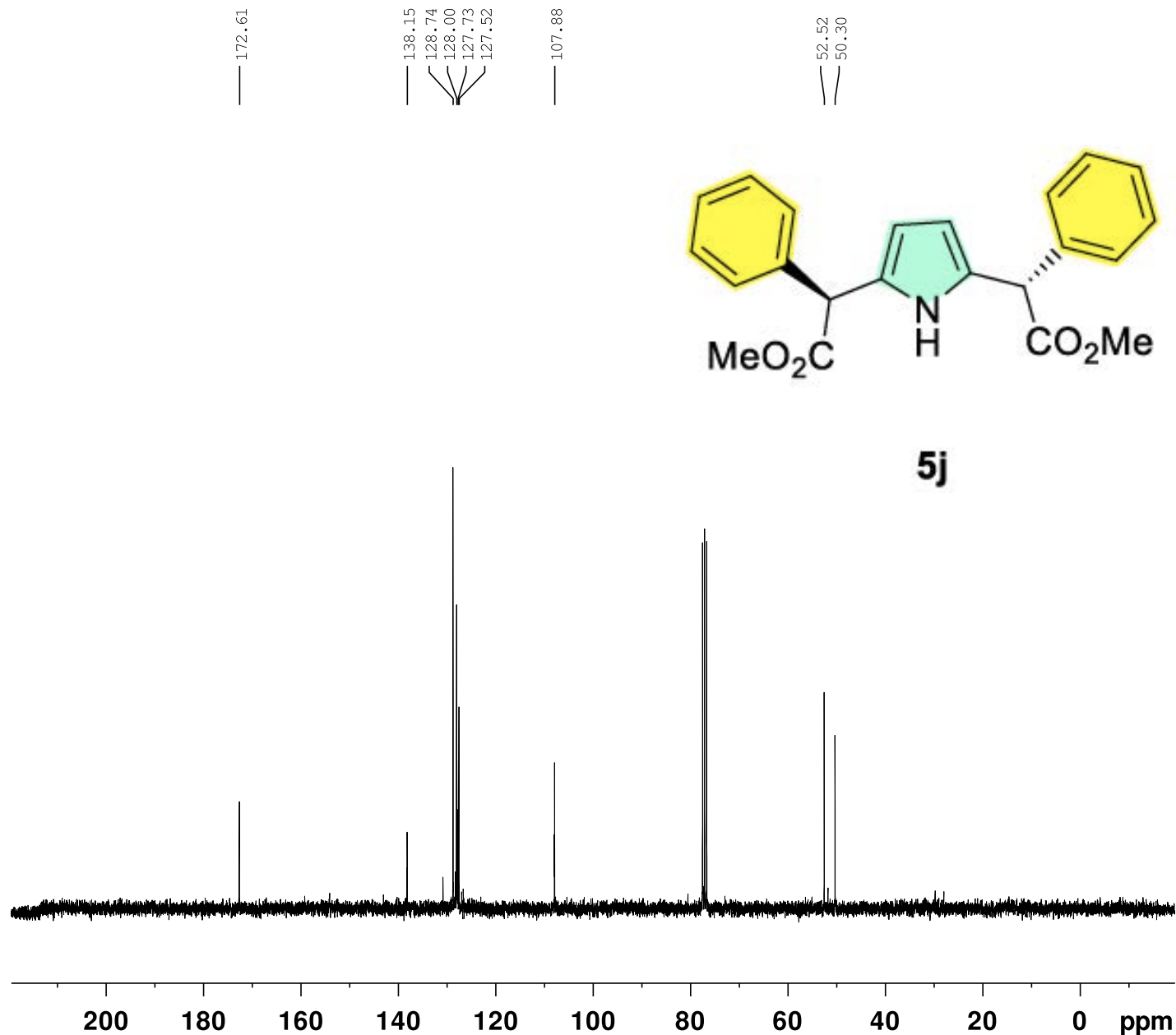
==== CHANNEL f1 =====  
SFO1 75.4752949 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 34.20000076 W

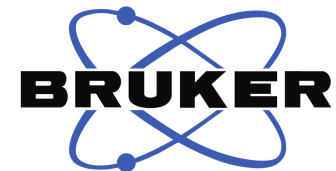
==== CHANNEL f2 =====  
SFO2 300.1312005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W  
PLW13 0.14000000 W

F2 - Processing parameters  
SI 32768  
SF 75.4677485 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



5j



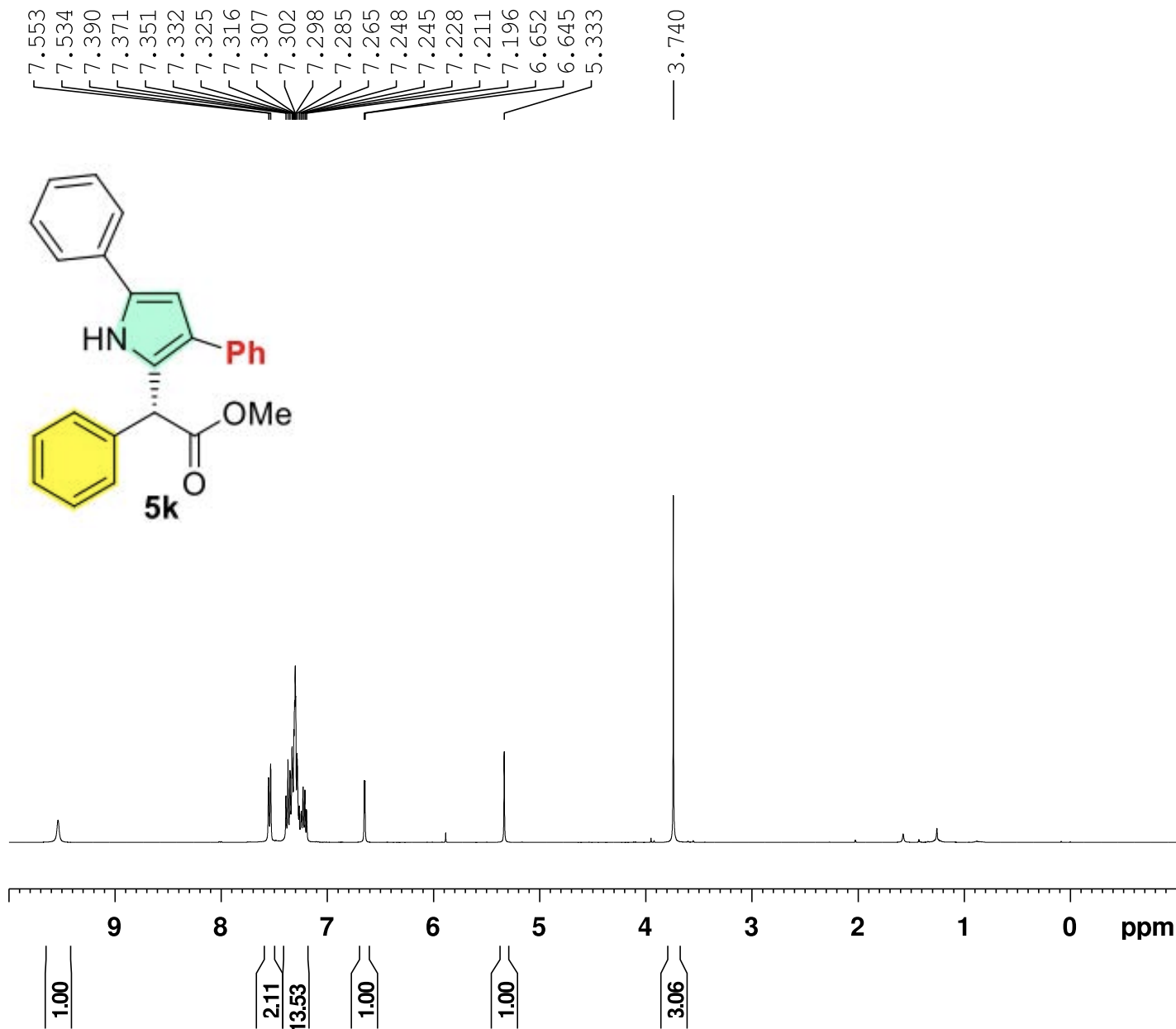


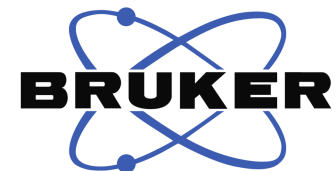
Current Data Parameters  
NAME HNMR-YX-7-p26  
EXPNO 44  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231110  
Time 16.06  
INSTRUM spect  
PROBHD 5 mm PADUL 13C  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 4  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9845889 sec  
RG 53.3  
DW 60.800 usec  
DE 6.50 usec  
TE 292.0 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 9.90 usec  
PLW1 23.00000000 W  
SFO1 400.1924713 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1900391 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





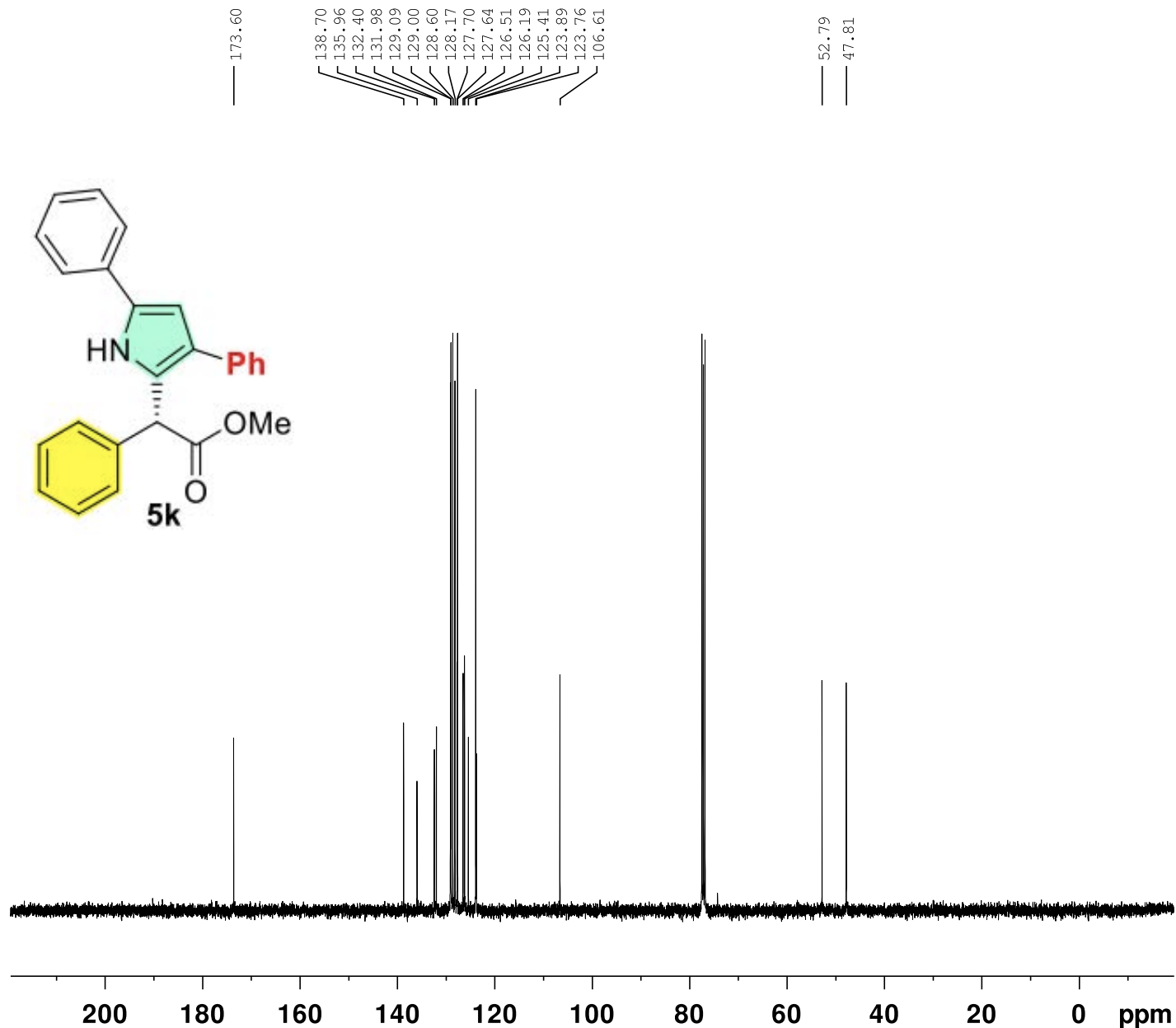
Current Data Parameters  
NAME CNMR-YX-7-p26  
EXPNO 45  
PROCNO 1

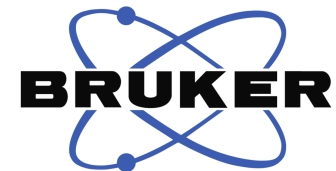
F2 - Acquisition Parameters  
Date\_ 20231110  
Time 16.14  
INSTRUM spect  
PROBHD 5 mm PADUL 13C  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 100  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 35.06  
DW 20.800 usec  
DE 6.50 usec  
TE 292.6 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 9.80 usec  
PLW1 47.4000153 W  
SFO1 100.6379178 MHz

==== CHANNEL f2 =====  
CPDPRG[2] waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 23.00000000 W  
PLW12 0.30712000 W  
PLW13 0.24877000 W  
SFO2 400.1916008 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6278560 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

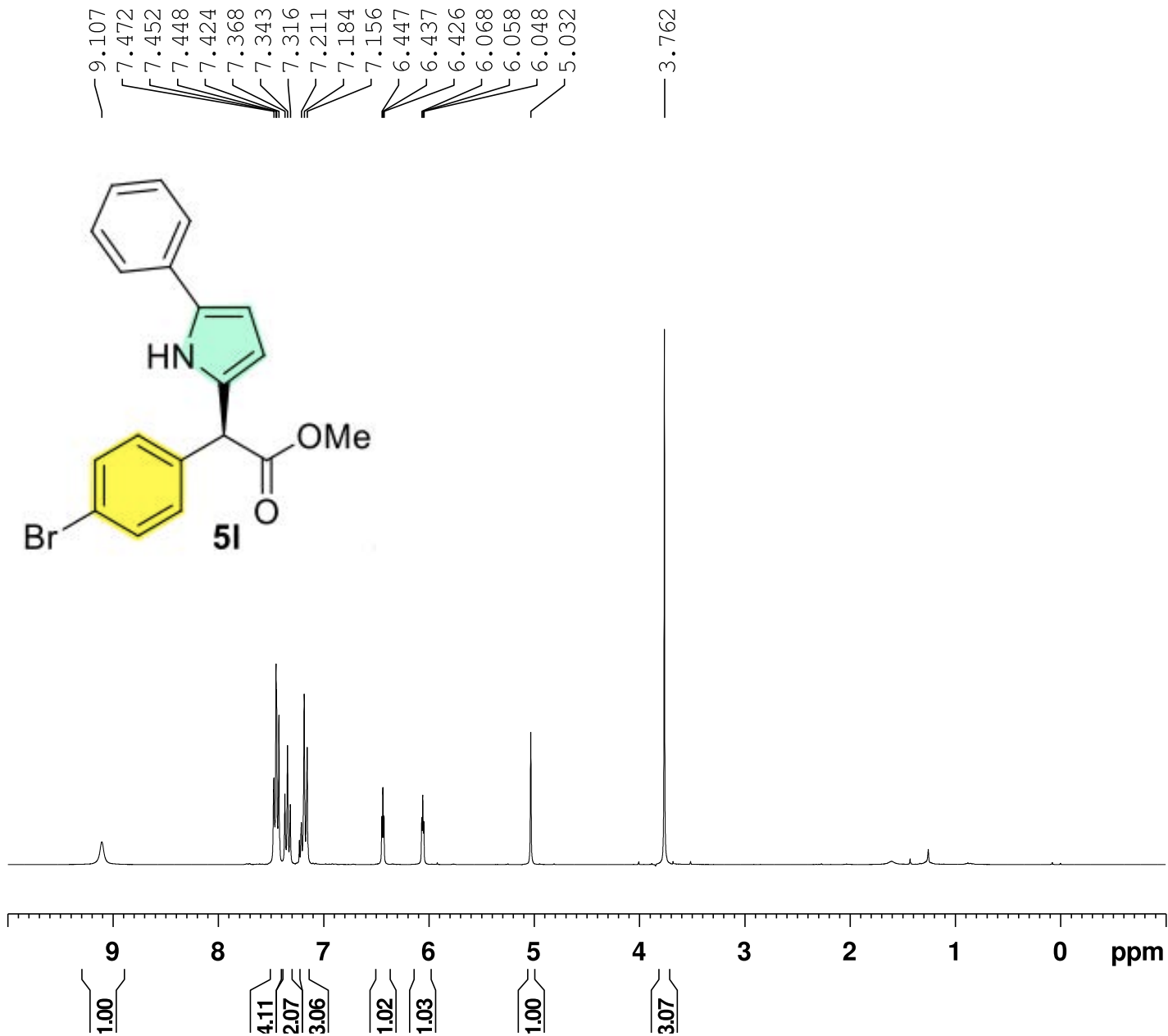




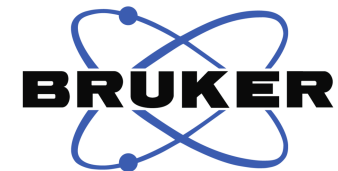
Current Data Parameters  
NAME NMR-YX-7-p67  
EXPNO 2236  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231227  
Time 16.42 h  
INSTRUM spect  
PROBHD Z104275\_0225 (   
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.183399 Hz  
AQ 5.4525952 sec  
RG 114  
DW 83.200 usec  
DE 6.50 usec  
TE 294.4 K  
D1 1.00000000 sec  
TD0 1  
SF01 300.1318533 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 14.00000000 W

F2 - Processing parameters  
SI 65536  
SF 300.1300162 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00







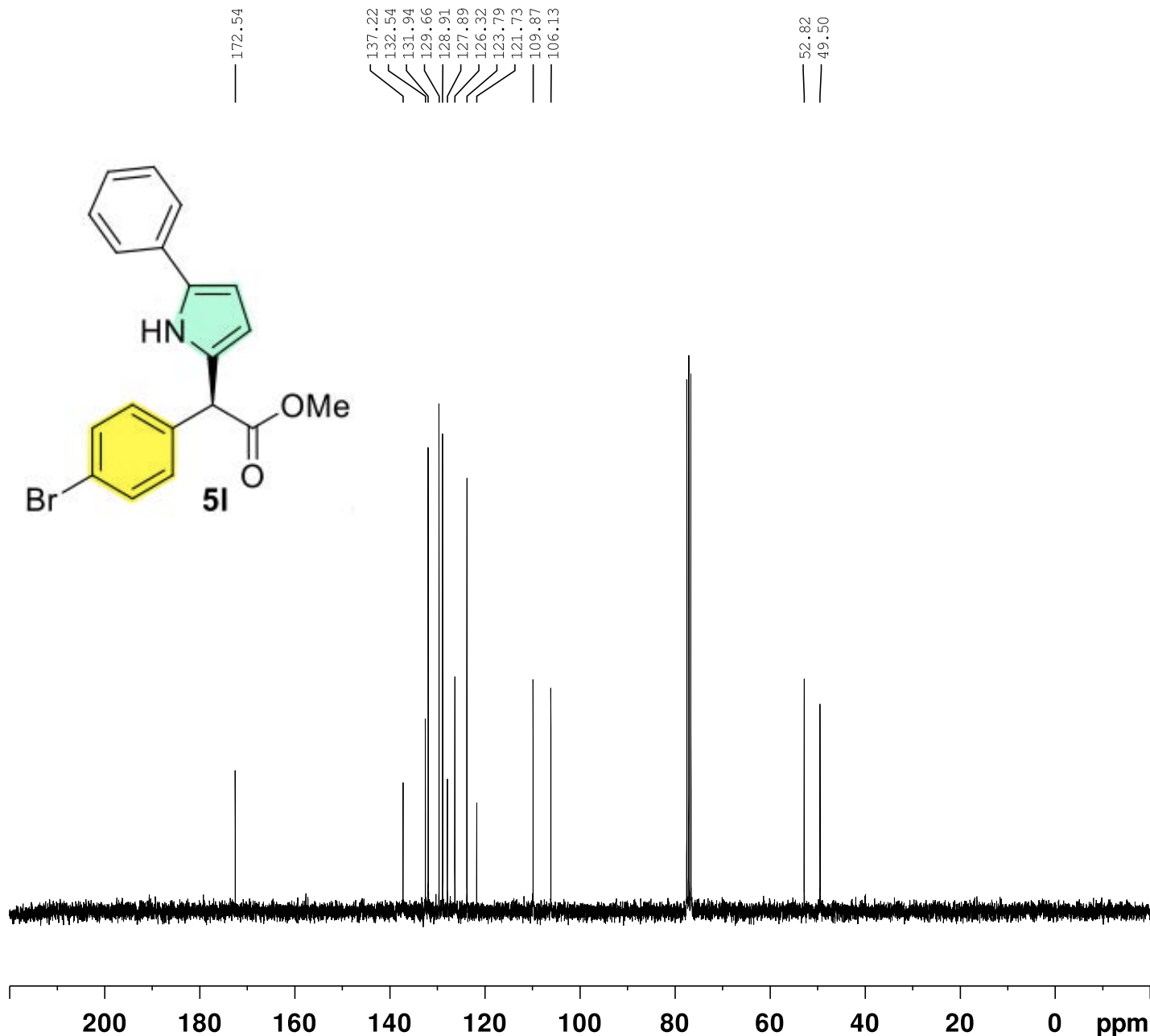
Current Data Parameters  
NAME NMR-YX-7-p67  
EXPNO 2237  
PROCNO 1

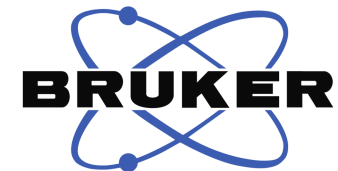
F2 - Acquisition Parameters

Date\_ 20231227  
Time 16.50 h  
INSTRUM spect  
PROBHD z104275\_0225 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 100  
DS 4  
SWH 18115.941 Hz  
FIDRES 0.552855 Hz  
AQ 1.8087935 sec  
RG 203  
DW 27.600 usec  
DE 6.50 usec  
TE 294.9 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 75.4752953 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 34.20000076 W  
SFO2 300.1312005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W  
PLW13 0.08693700 W

F2 - Processing parameters

SI 32768  
SF 75.4677485 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

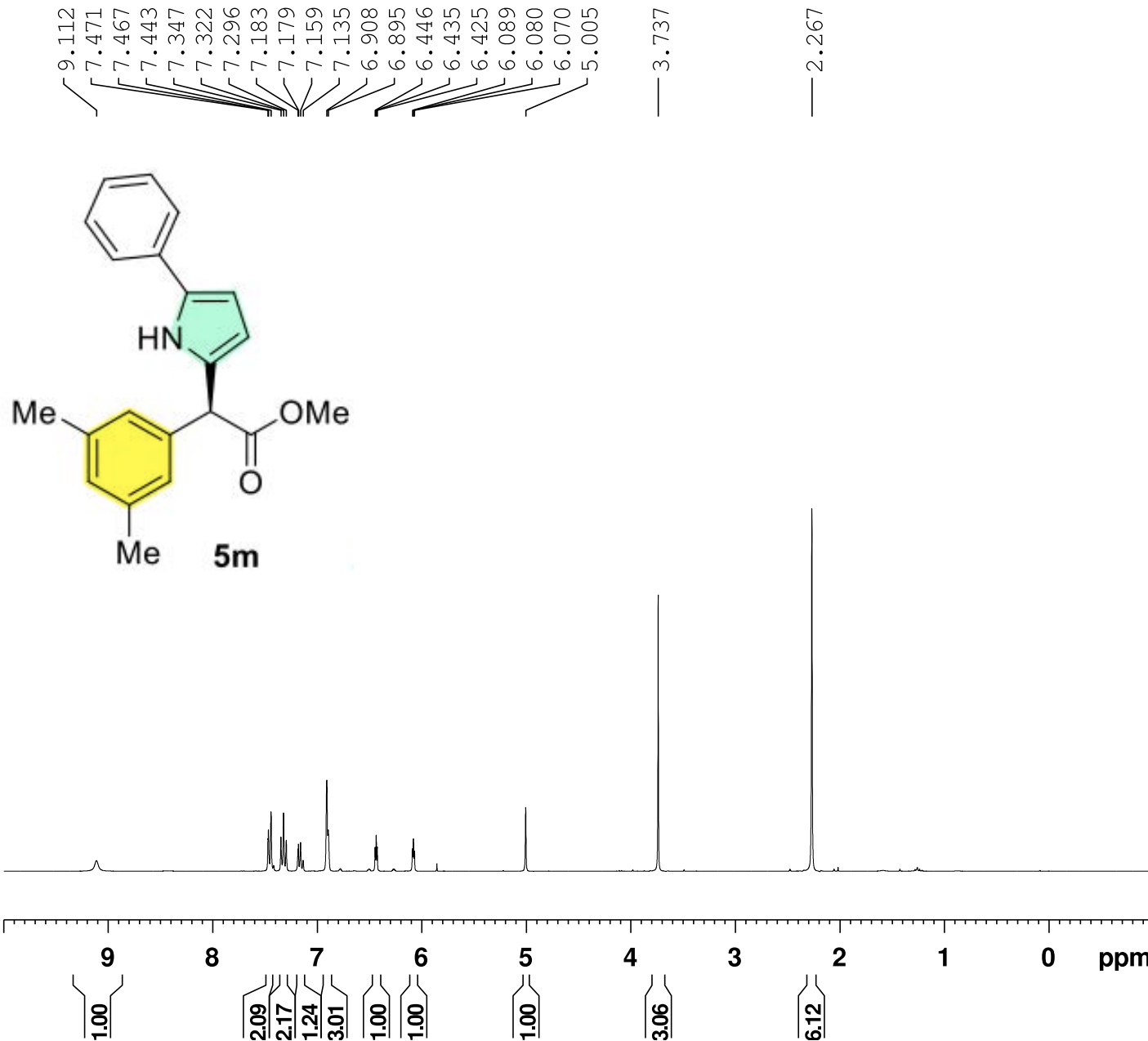


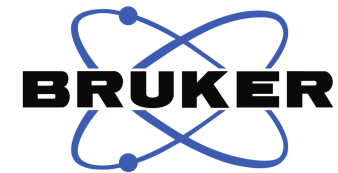


Current Data Parameters  
NAME NMR-YX-7-p68  
EXPNO 2230  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231227  
Time 16.03 h  
INSTRUM spect  
PROBHD Z104275\_0225 (   
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.183399 Hz  
AQ 5.4525952 sec  
RG 57  
DW 83.200 usec  
DE 6.50 usec  
TE 294.4 K  
D1 1.00000000 sec  
TD0 1  
SF01 300.1318533 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 14.00000000 W

F2 - Processing parameters  
SI 65536  
SF 300.1300310 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

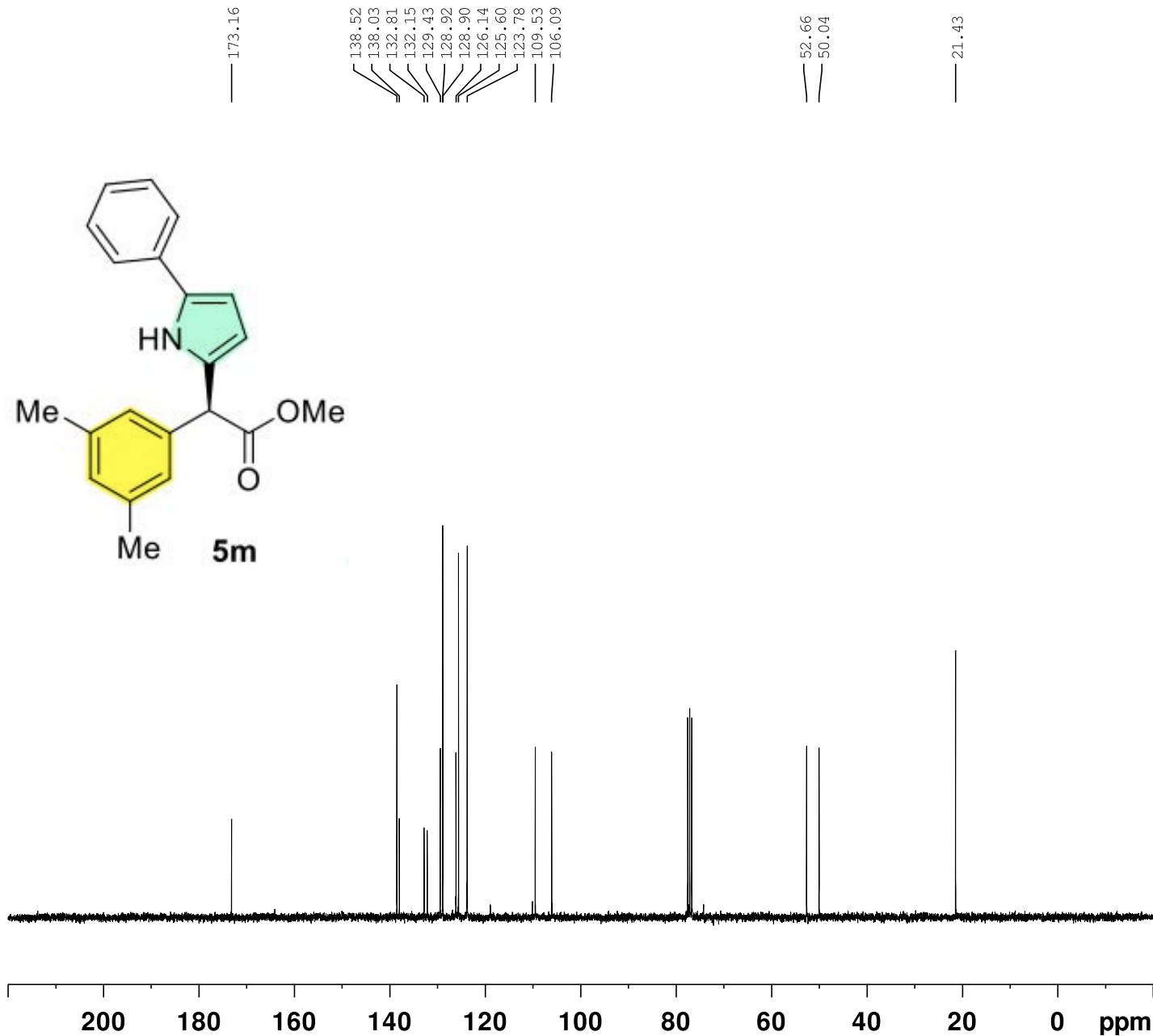


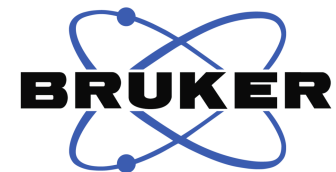


Current Data Parameters  
NAME NMR-YX-7-p68  
EXPNO 2231  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231227  
Time 16.11 h  
INSTRUM spect  
PROBHD z104275\_0225 (   
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 100  
DS 4  
SWH 18115.941 Hz  
FIDRES 0.552855 Hz  
AQ 1.8087935 sec  
RG 203  
DW 27.600 usec  
DE 6.50 usec  
TE 294.9 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 75.4752953 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 34.20000076 W  
SFO2 300.1312005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W  
PLW13 0.08693700 W

F2 - Processing parameters  
SI 32768  
SF 75.4677485 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





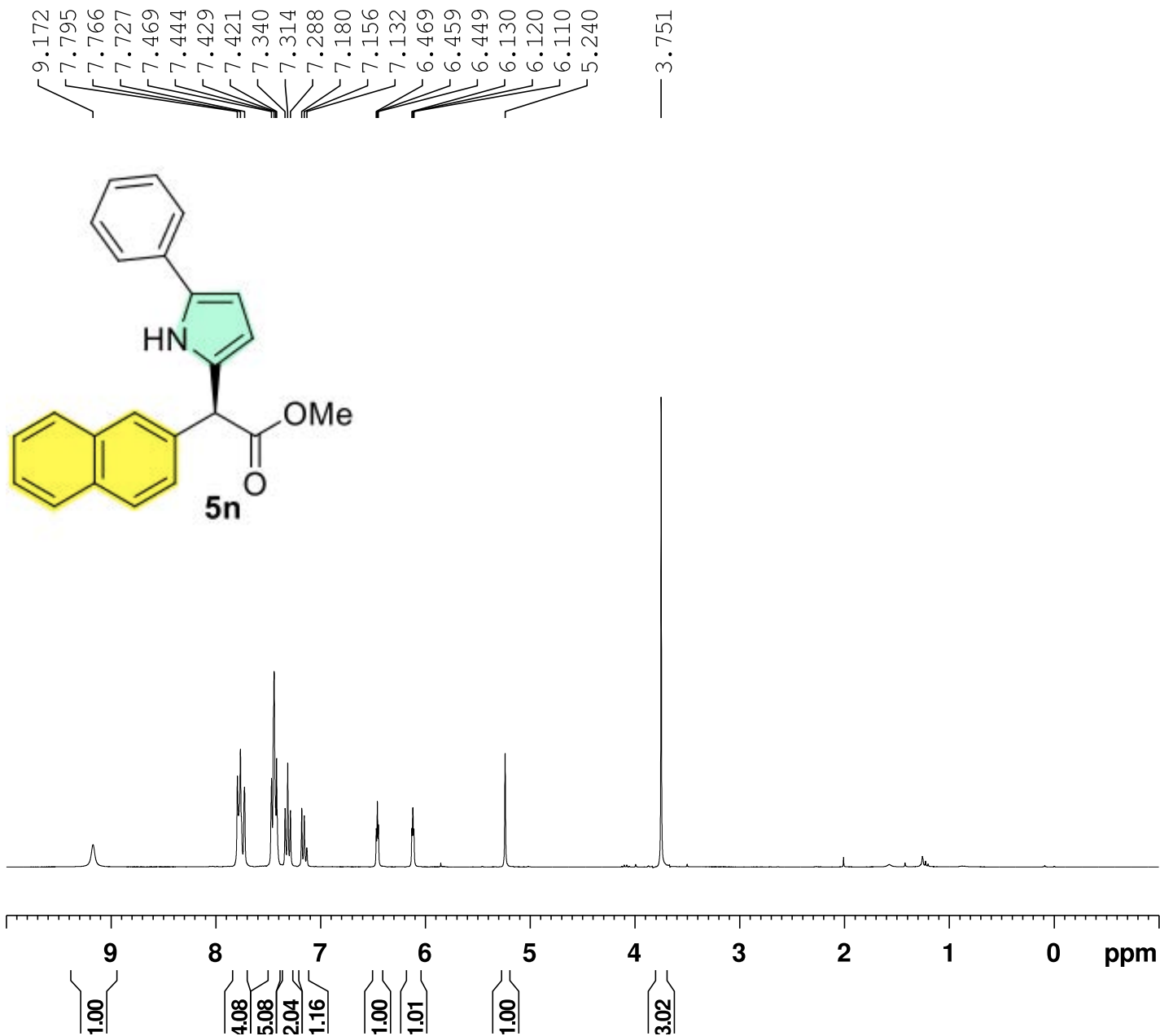
Current Data Parameters  
NAME NMR-YX-7-p66  
EXPNO 2234  
PROCNO 1

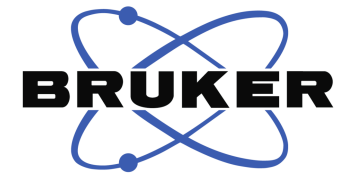
F2 - Acquisition Parameters

Date\_ 20231227  
Time 16.30 h  
INSTRUM spect  
PROBHD Z104275\_0225 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.183399 Hz  
AQ 5.4525952 sec  
RG 71.8  
DW 83.200 usec  
DE 6.50 usec  
TE 294.4 K  
D1 1.00000000 sec  
TD0 1  
SF01 300.1318533 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 14.00000000 W

F2 - Processing parameters

SI 65536  
SF 300.1300309 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

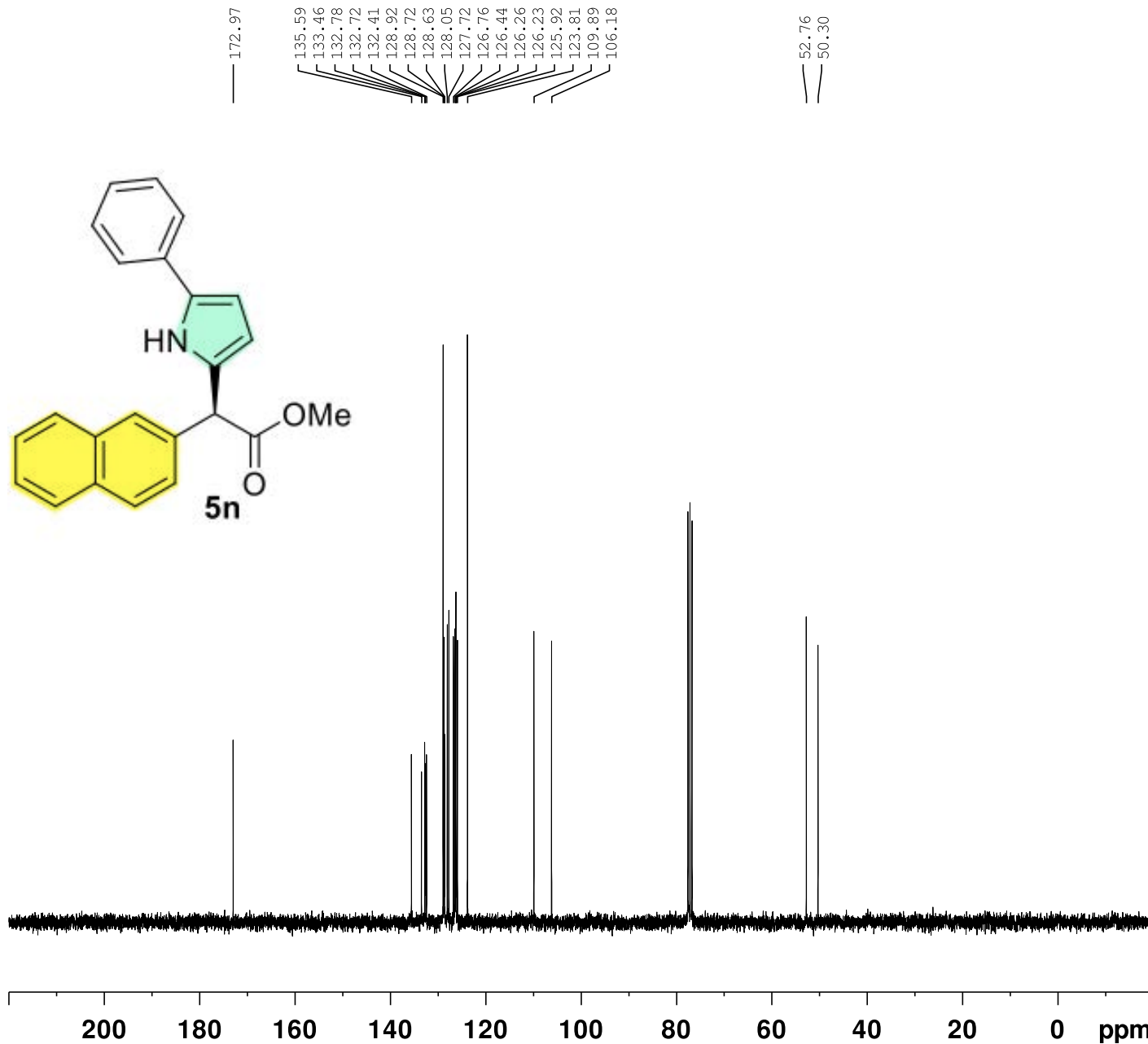


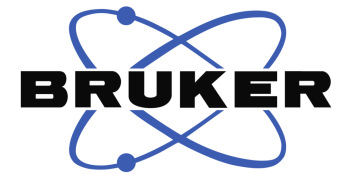


Current Data Parameters  
NAME NMR-YX-7-p66  
EXPNO 2235  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231227  
Time 16.38 h  
INSTRUM spect  
PROBHD z104275\_0225 (zpgg30)  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 100  
DS 4  
SWH 18115.941 Hz  
FIDRES 0.552855 Hz  
AQ 1.8087935 sec  
RG 203  
DW 27.600 usec  
DE 6.50 usec  
TE 294.9 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 75.4752953 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 34.20000076 W  
SFO2 300.1312005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W  
PLW13 0.08693700 W

F2 - Processing parameters  
SI 32768  
SF 75.4677485 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

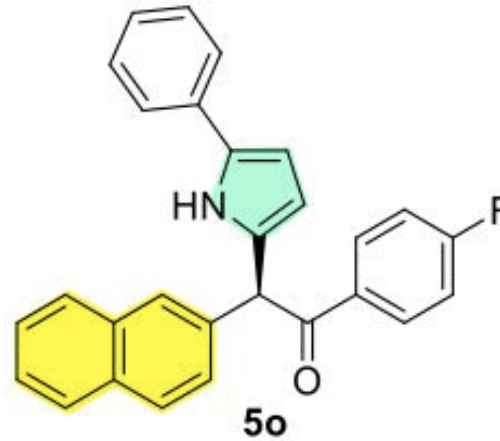




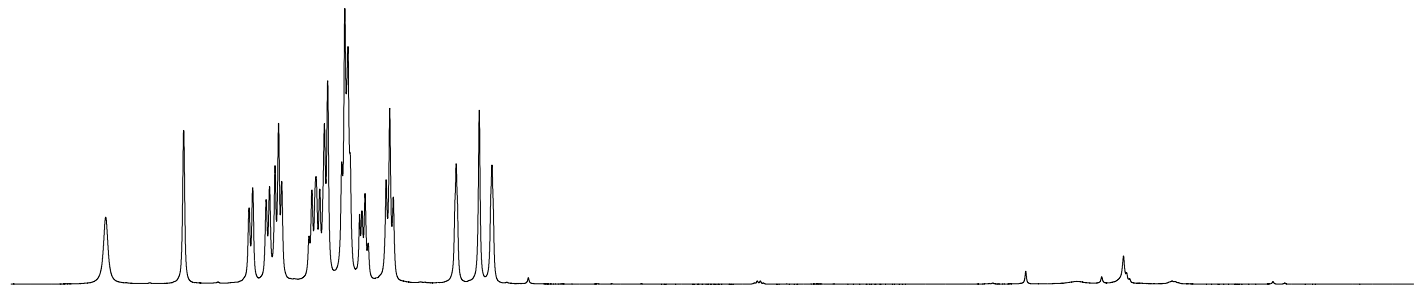
Current Data Parameters  
NAME NMR-YX-7-p62  
EXPNO 2232  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231227  
Time 16.16 h  
INSTRUM spect  
PROBHD Z104275\_0225 (   
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.183399 Hz  
AQ 5.4525952 sec  
RG 90.5  
DW 83.200 usec  
DE 6.50 usec  
TE 294.4 K  
D1 1.00000000 sec  
TD0 1  
SF01 300.1318533 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 14.00000000 W

F2 - Processing parameters  
SI 65536  
SF 300.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

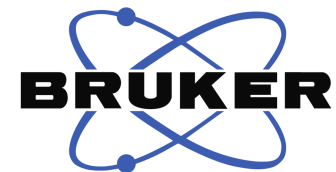


7.941  
7.914  
7.890  
7.676  
7.654  
7.623  
7.593  
7.557  
7.531  
7.422  
7.398  
7.373  
7.358  
7.283  
7.265  
7.240  
7.217  
7.077  
7.048  
7.020  
6.531  
6.351  
6.252



9 8 7 6 5 4 3 2 1 0 ppm

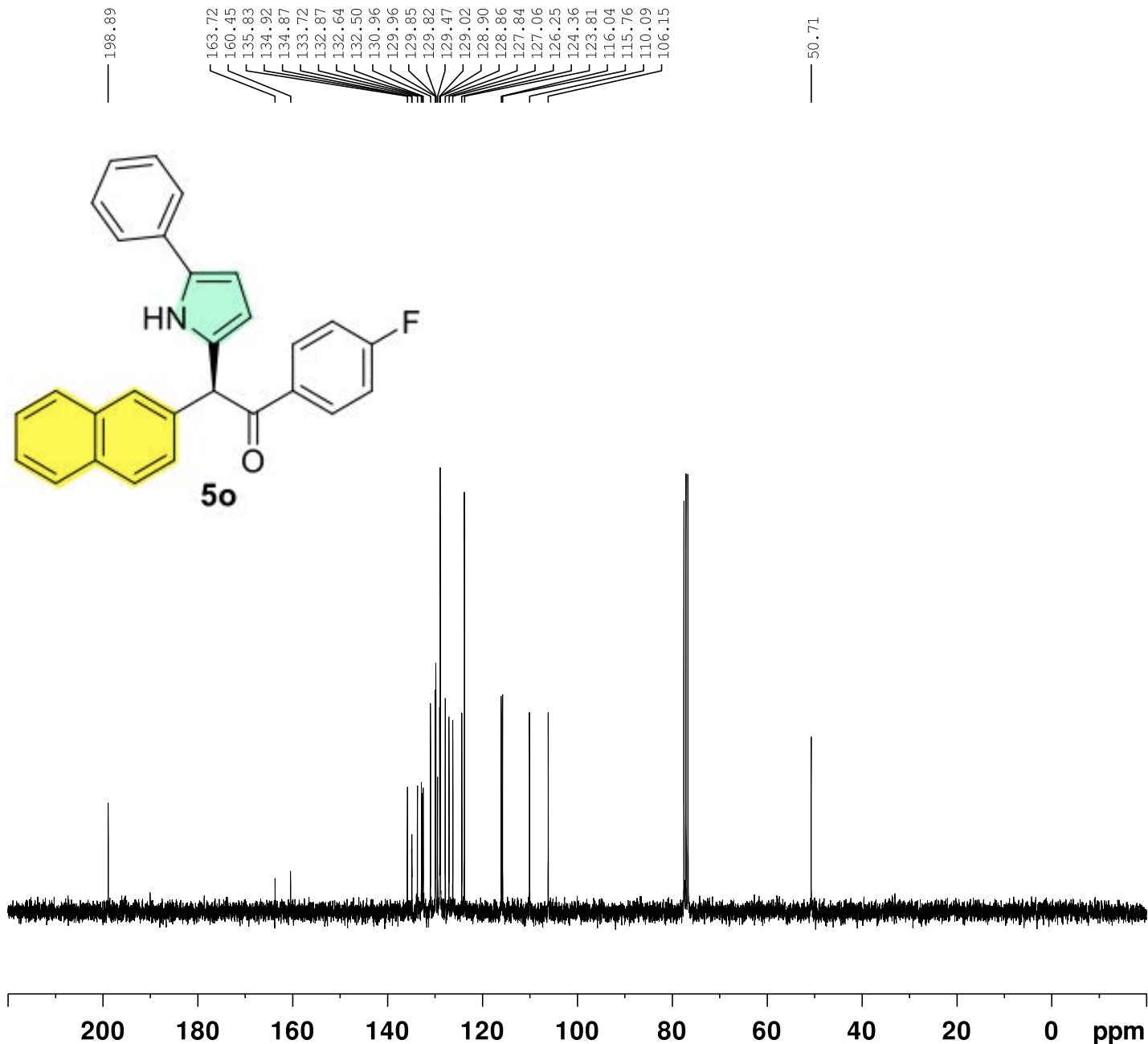
1.03  
1.02  
1.06  
3.14  
4.05  
4.09  
1.11  
2.13  
1.03  
1.03  
1.00

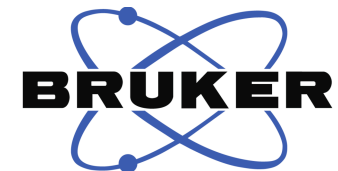


Current Data Parameters  
NAME NMR-YX-7-p62  
EXPNO 2233  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231227  
Time 16.24 h  
INSTRUM spect  
PROBHD z104275\_0225 (zgpg30)  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 100  
DS 4  
SWH 18115.941 Hz  
FIDRES 0.552855 Hz  
AQ 1.8087935 sec  
RG 203  
DW 27.600 usec  
DE 6.50 usec  
TE 294.9 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 75.4752953 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 34.20000076 W  
SFO2 300.1312005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W  
PLW13 0.08693700 W

F2 - Processing parameters  
SI 32768  
SF 75.4677485 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

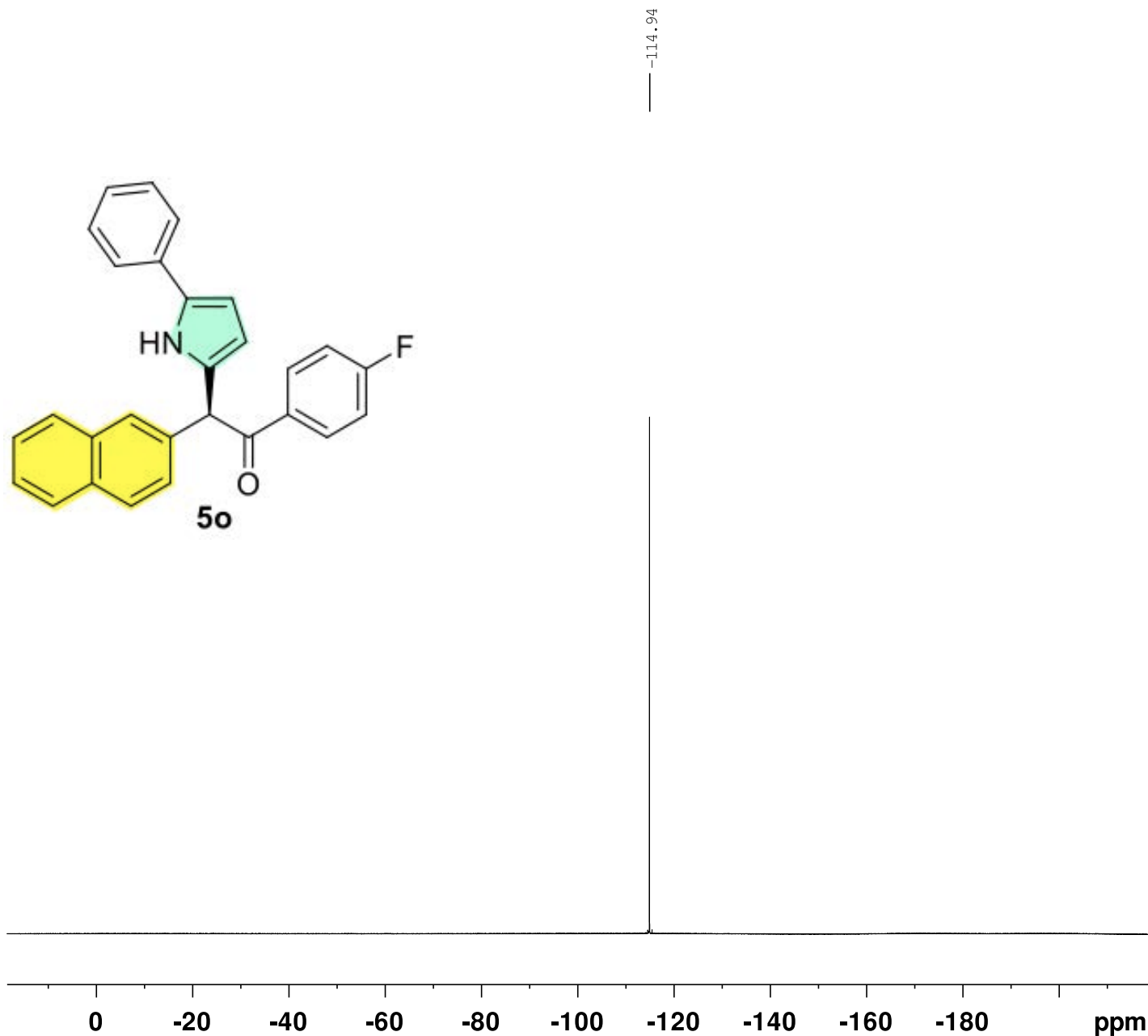




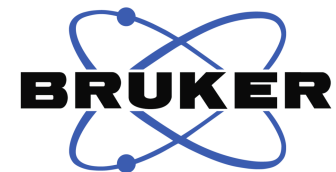
Current Data Parameters  
NAME NMR-YX-7-p62  
EXPNO 2239  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231227  
Time 20.22 h  
INSTRUM spect  
PROBHD z104275\_0225 (  
PULPROG zgfhigqn.2  
TD 131072  
SOLVENT CDCl3  
NS 16  
DS 4  
SWH 66964.289 Hz  
FIDRES 1.021794 Hz  
AQ 0.9786710 sec  
RG 203  
DW 7.467 usec  
DE 6.50 usec  
TE 293.7 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
D12 0.00002000 sec  
TD0 1  
SFO1 282.3761148 MHz  
NUC1 19F  
P1 14.50 usec  
PLW1 10.39999962 W  
SFO2 300.1312005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W

F2 - Processing parameters  
SI 65536  
SF 282.4043552 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





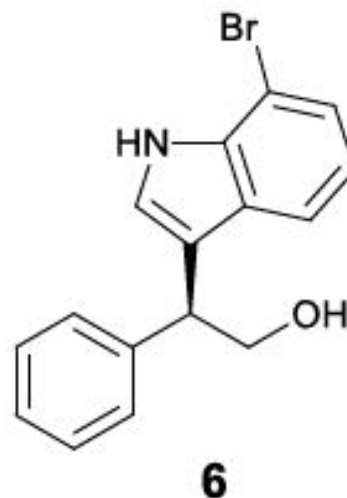


Current Data Parameters  
NAME HNMR-YX-5-p87  
EXPNO 150  
PROCNO 1

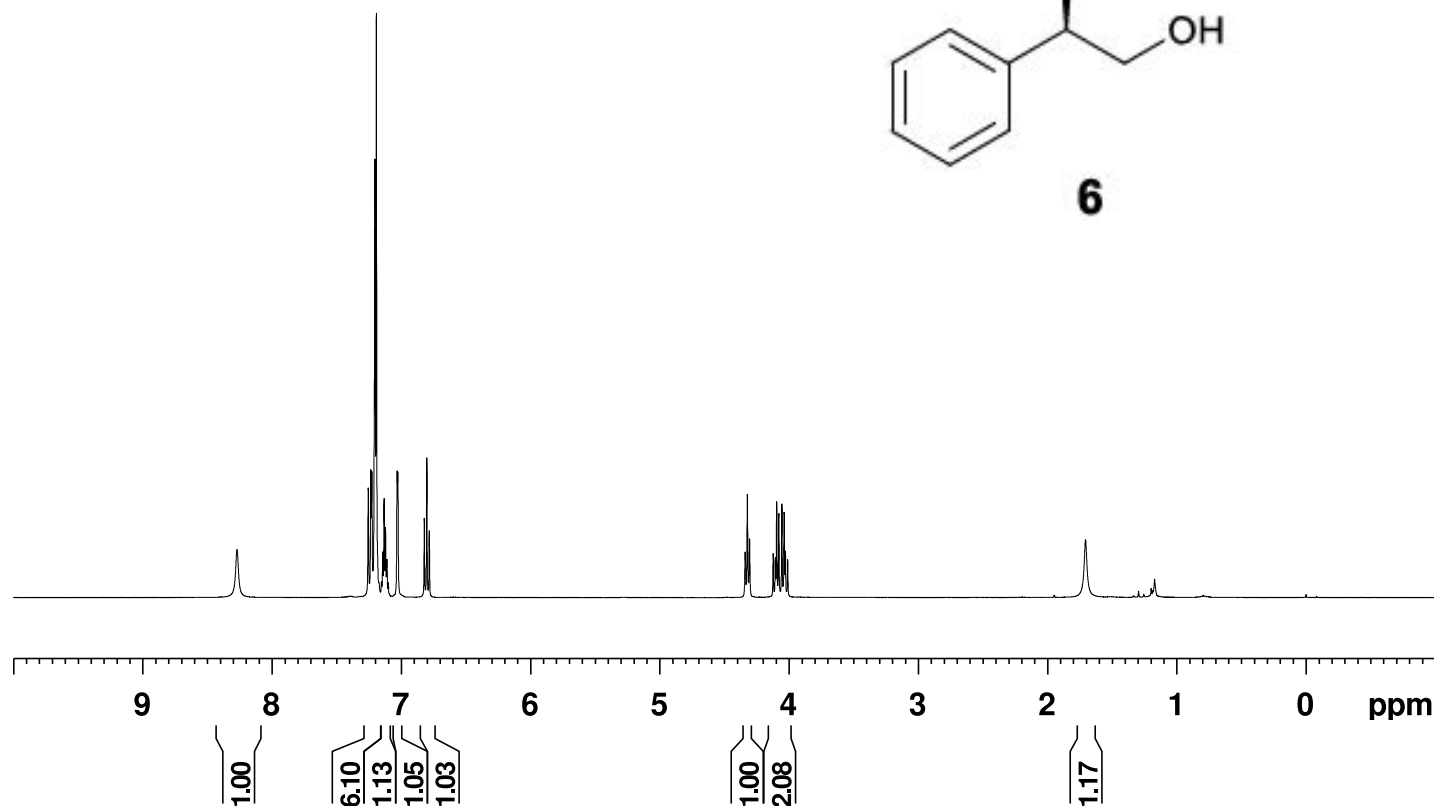
F2 - Acquisition Parameters  
Date\_ 20231008  
Time 15.14  
INSTRUM spect  
PROBHD 5 mm PADUL 13C  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 4  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9845889 sec  
RG 61.19  
DW 60.800 usec  
DE 6.50 usec  
TE 293.9 K  
D1 1.00000000 sec  
TD0 1

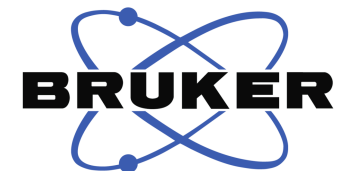
=====  
CHANNEL f1  
NUC1 1H  
P1 9.90 usec  
PLW1 23.00000000 W  
SFO1 400.1924713 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1900647 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



8.271  
7.256  
7.236  
7.228  
7.205  
7.194  
7.144  
7.133  
7.123  
7.111  
7.033  
7.028  
6.823  
6.803  
6.784  
4.340  
4.323  
4.306  
4.123  
4.107  
4.096  
4.080  
4.056  
4.038  
4.029  
4.011  
— 1.706





Current Data Parameters  
NAME CNMR-YX-5-p87  
EXPNO 151  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231008  
Time 15.21  
INSTRUM spect  
PROBHD 5 mm PADUL 13C  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 100  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 29.75  
DW 20.800 usec  
DE 6.50 usec  
TE 294.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 9.80 usec  
PLW1 47.4000153 W  
SFO1 100.6379178 MHz

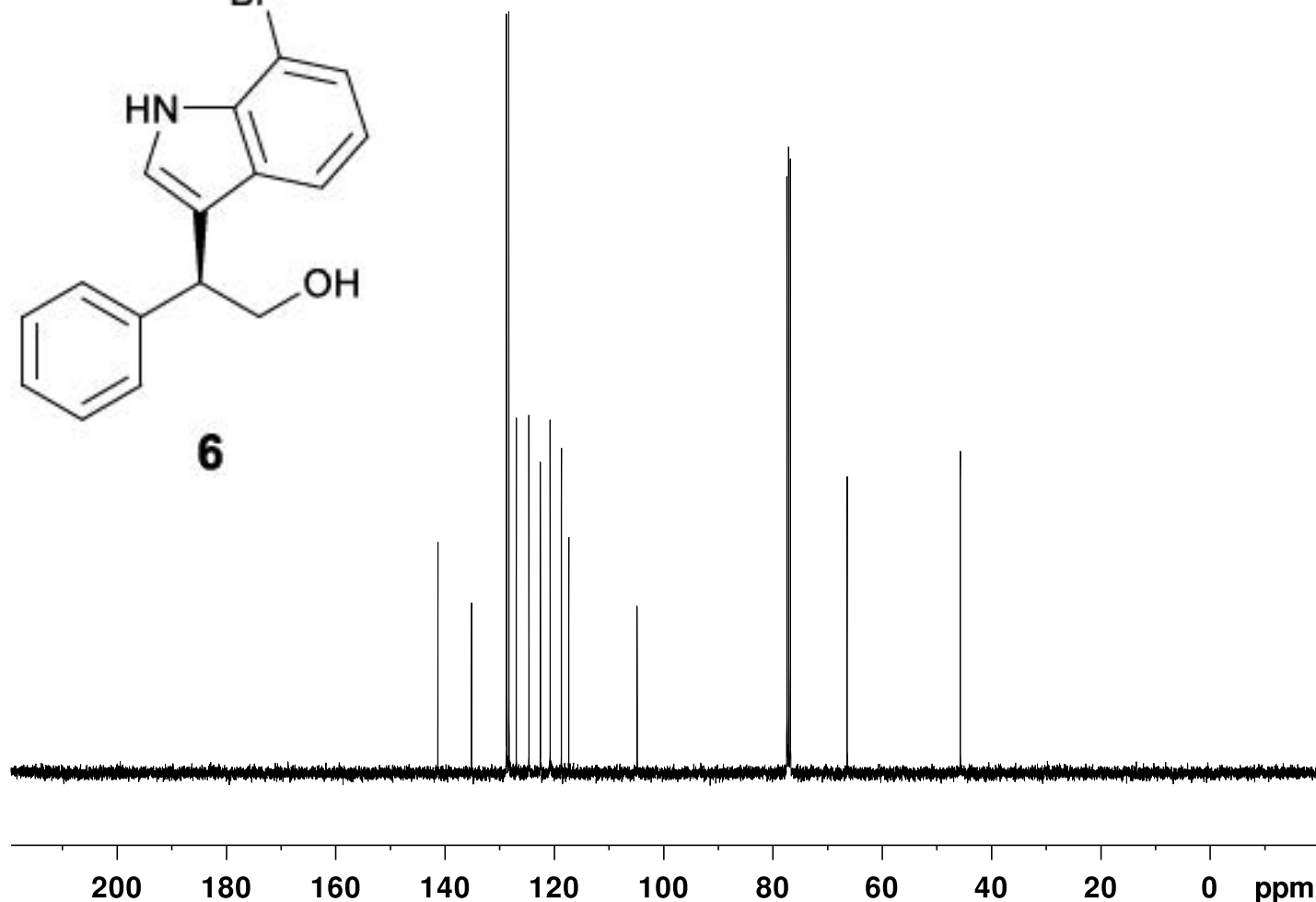
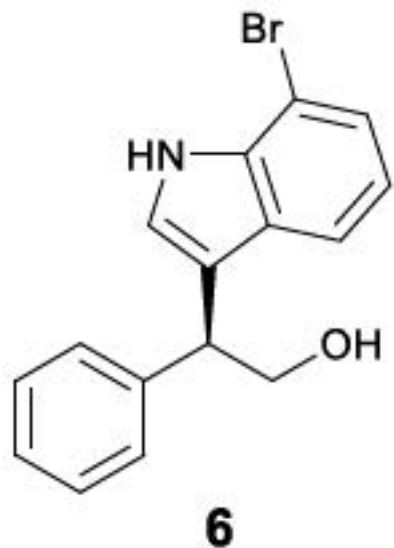
==== CHANNEL f2 =====  
CPDPRG[2] waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 23.0000000 W  
PLW12 0.30712000 W  
PLW13 0.24877000 W  
SFO2 400.1916008 MHz

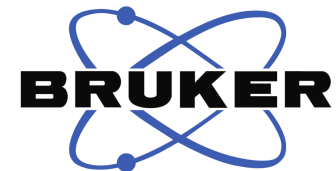
F2 - Processing parameters  
SI 32768  
SF 100.6278560 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

141.31  
135.15  
128.75  
128.34  
128.28  
126.96  
124.66  
122.55  
120.77  
118.71  
117.36  
104.85

66.42

45.71





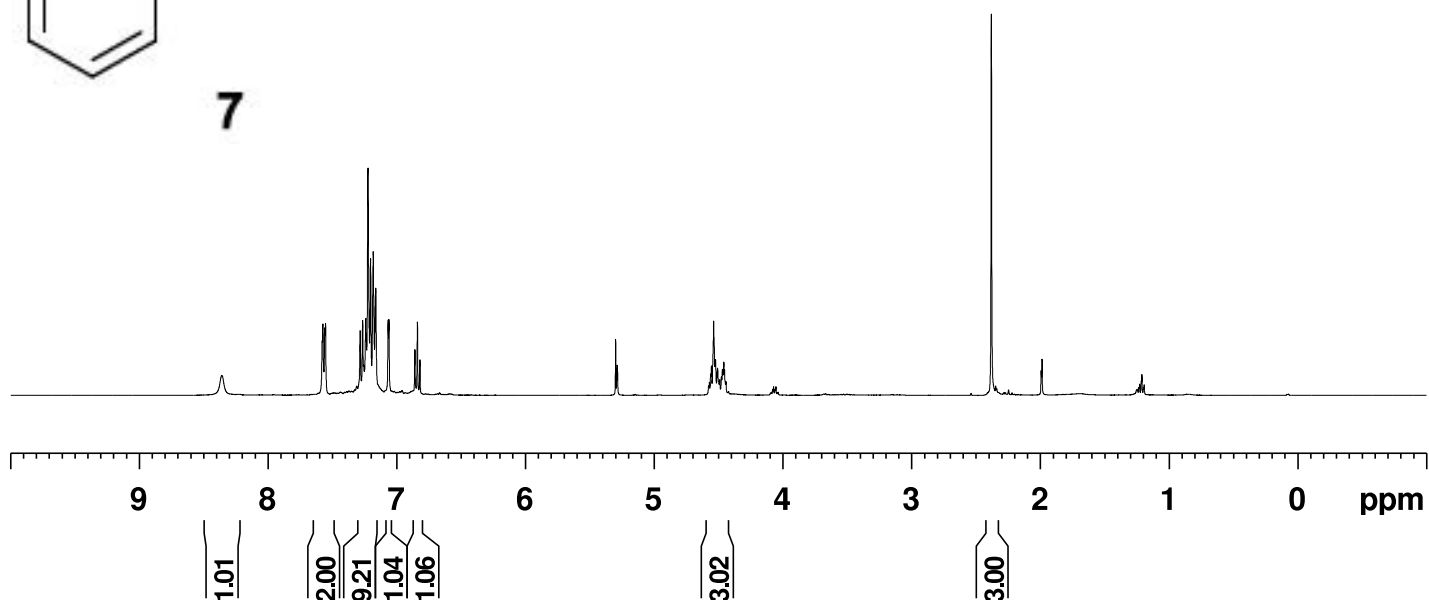
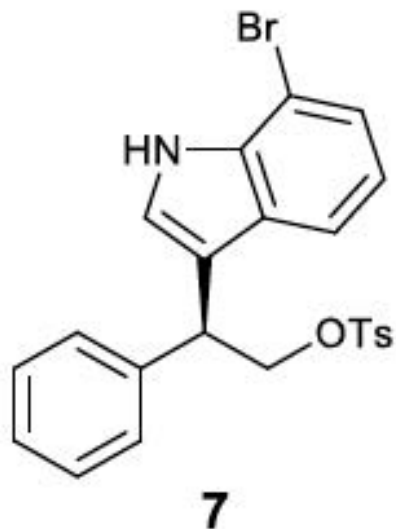
Current Data Parameters  
NAME HNMR-YX-7-p42  
EXPNO 51  
PROCNO 1

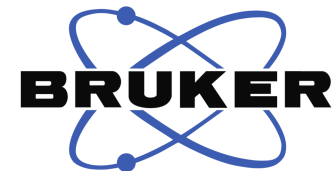
F2 - Acquisition Parameters  
Date\_ 20231114  
Time 16.00  
INSTRUM spect  
PROBHD 5 mm PADUL 13C  
PULPROG zg30  
TD 65536  
SOLVENT CD2Cl2  
NS 4  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9845889 sec  
RG 75.43  
DW 60.800 usec  
DE 6.50 usec  
TE 293.2 K  
D1 1.00000000 sec  
TD0 1

=====  
CHANNEL f1  
NUC1 1H  
P1 9.90 usec  
PLW1 23.00000000 W  
SFO1 400.1924713 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1900326 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

7.574  
7.558  
7.553  
7.285  
7.265  
7.242  
7.224  
7.204  
7.183  
7.163  
7.067  
7.061  
6.859  
6.840  
6.820  
5.300  
4.578  
4.571  
4.562  
4.555  
4.539  
4.524  
4.508  
4.500  
4.491  
4.478  
4.470  
4.466  
4.459  
4.454  
4.443  
2.381





Current Data Parameters  
NAME CNMR-YX-7-p42  
EXPNO 52  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20231114  
Time 16.06  
INSTRUM spect  
PROBHD 5 mm PADUL 13C  
PULPROG zgpg30  
TD 65536  
SOLVENT CD2Cl2  
NS 83  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 29.75  
DW 20.800 usec  
DE 6.50 usec  
TE 293.6 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

==== CHANNEL f1 =====

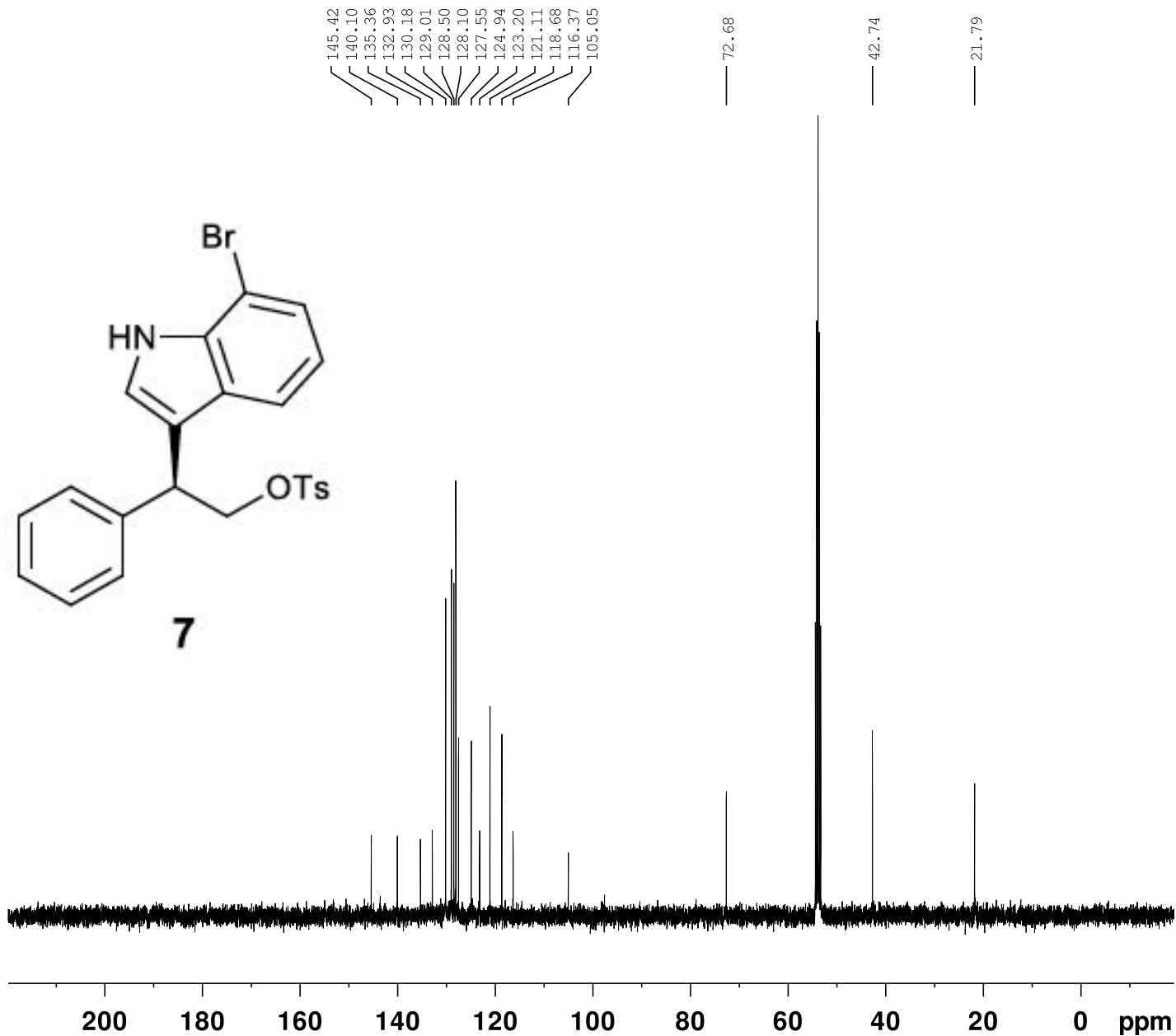
NUC1 13C  
P1 9.80 usec  
PLW1 47.4000153 W  
SFO1 100.6379178 MHz

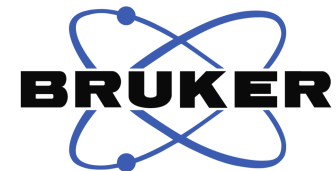
==== CHANNEL f2 =====

CPDPRG[2] waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 23.0000000 W  
PLW12 0.30712000 W  
PLW13 0.24877000 W  
SFO2 400.1916008 MHz

F2 - Processing parameters

SI 32768  
SF 100.6278157 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





Current Data Parameters  
NAME HNMR-YX-7-p52A  
EXPNO 63  
PROCNO 1

F2 - Acquisition Parameters

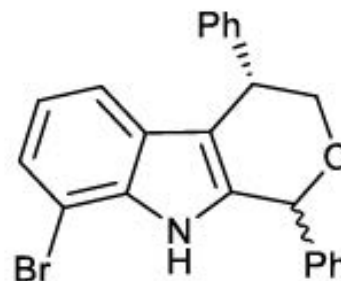
Date\_ 20231125  
Time 10.54  
INSTRUM spect  
PROBHD 5 mm PADUL 13C  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 4  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9845889 sec  
RG 75.43  
DW 60.800 usec  
DE 6.50 usec  
TE 294.6 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====

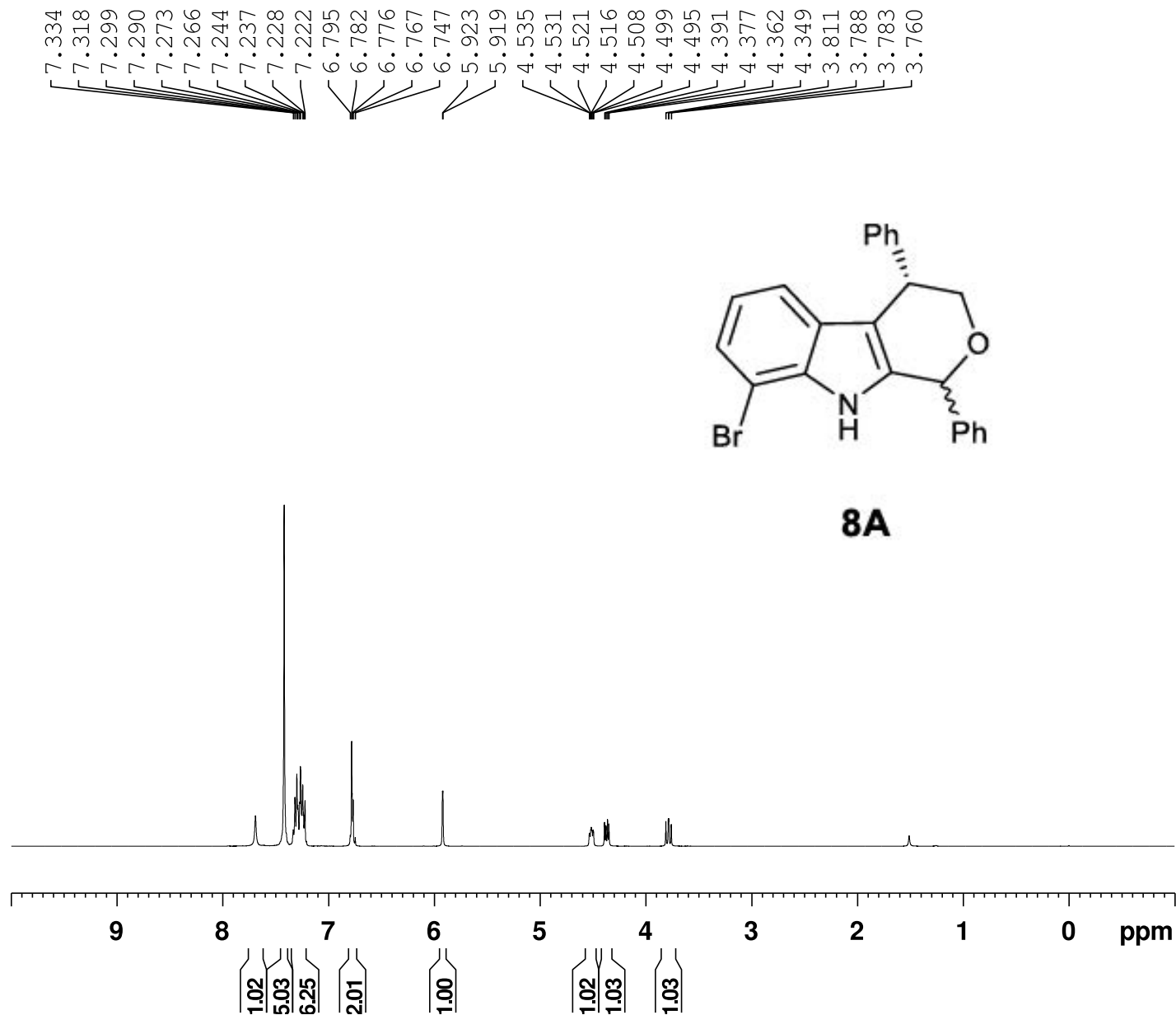
NUC1 1H  
P1 9.90 usec  
PLW1 23.00000000 W  
SFO1 400.1924713 MHz

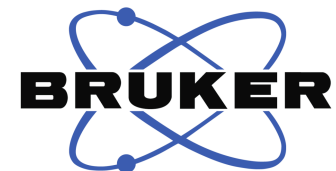
F2 - Processing parameters

SI 65536  
SF 400.1900290 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



8A





Current Data Parameters  
NAME CNMR-YX-7-p52A  
EXPNO 64  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231125  
Time 10.58  
INSTRUM spect  
PROBHD 5 mm PADUL 13C  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 50  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 35.06  
DW 20.800 usec  
DE 6.50 usec  
TE 295.1 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 9.80 usec  
PLW1 47.4000153 W  
SFO1 100.6379178 MHz

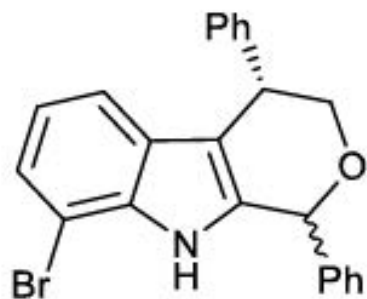
==== CHANNEL f2 =====  
CPDPRG[2] waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 23.0000000 W  
PLW12 0.30712000 W  
PLW13 0.24877000 W  
SFO2 400.1916008 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6278560 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

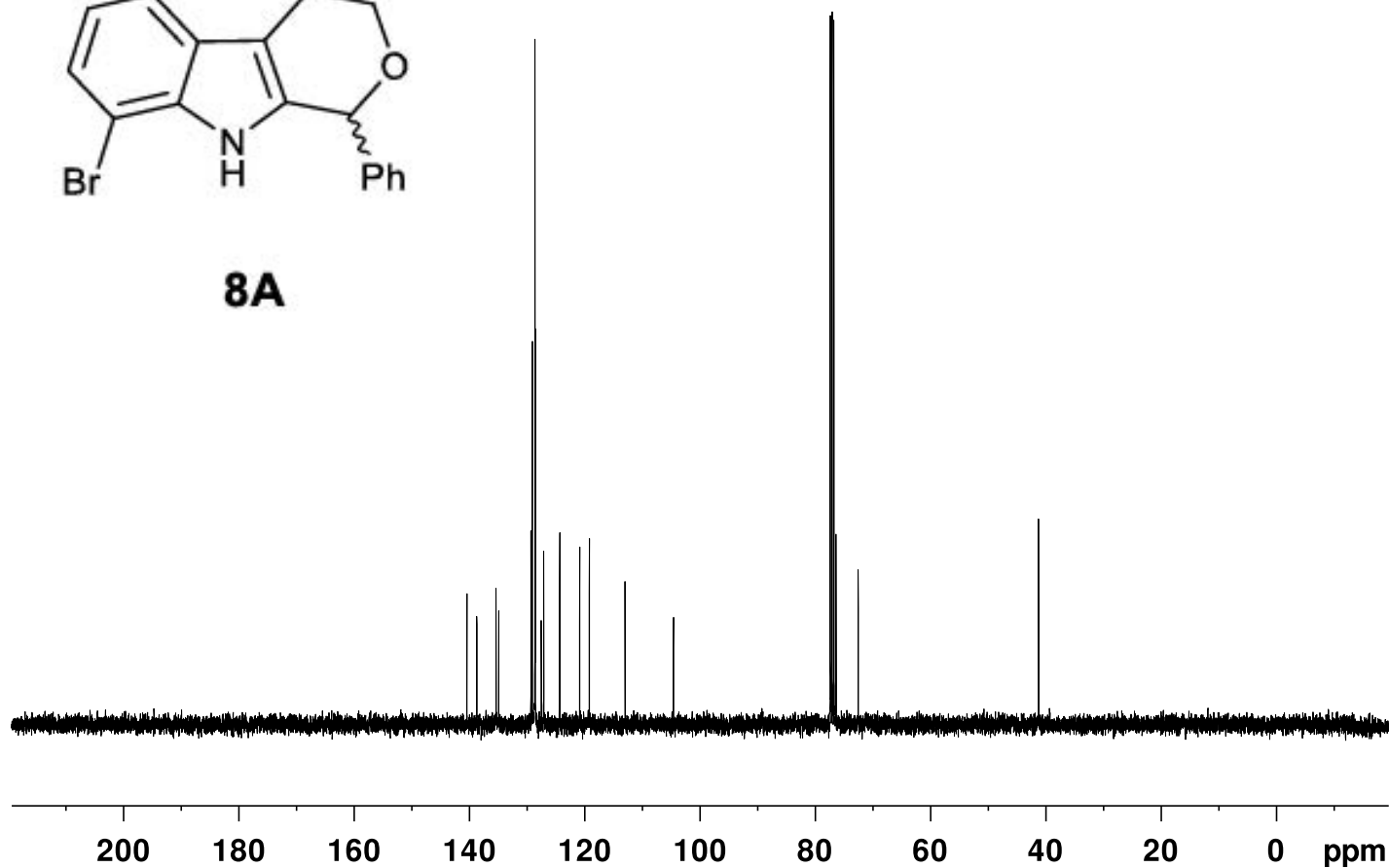
140.43  
138.72  
135.38  
134.91  
129.34  
129.10  
128.63  
128.55  
127.54  
127.12  
124.34  
120.88  
119.21  
113.01  
104.61

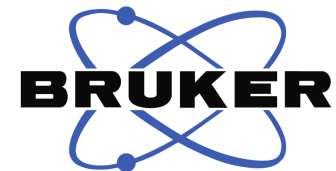
76.41  
72.56

41.27



8A



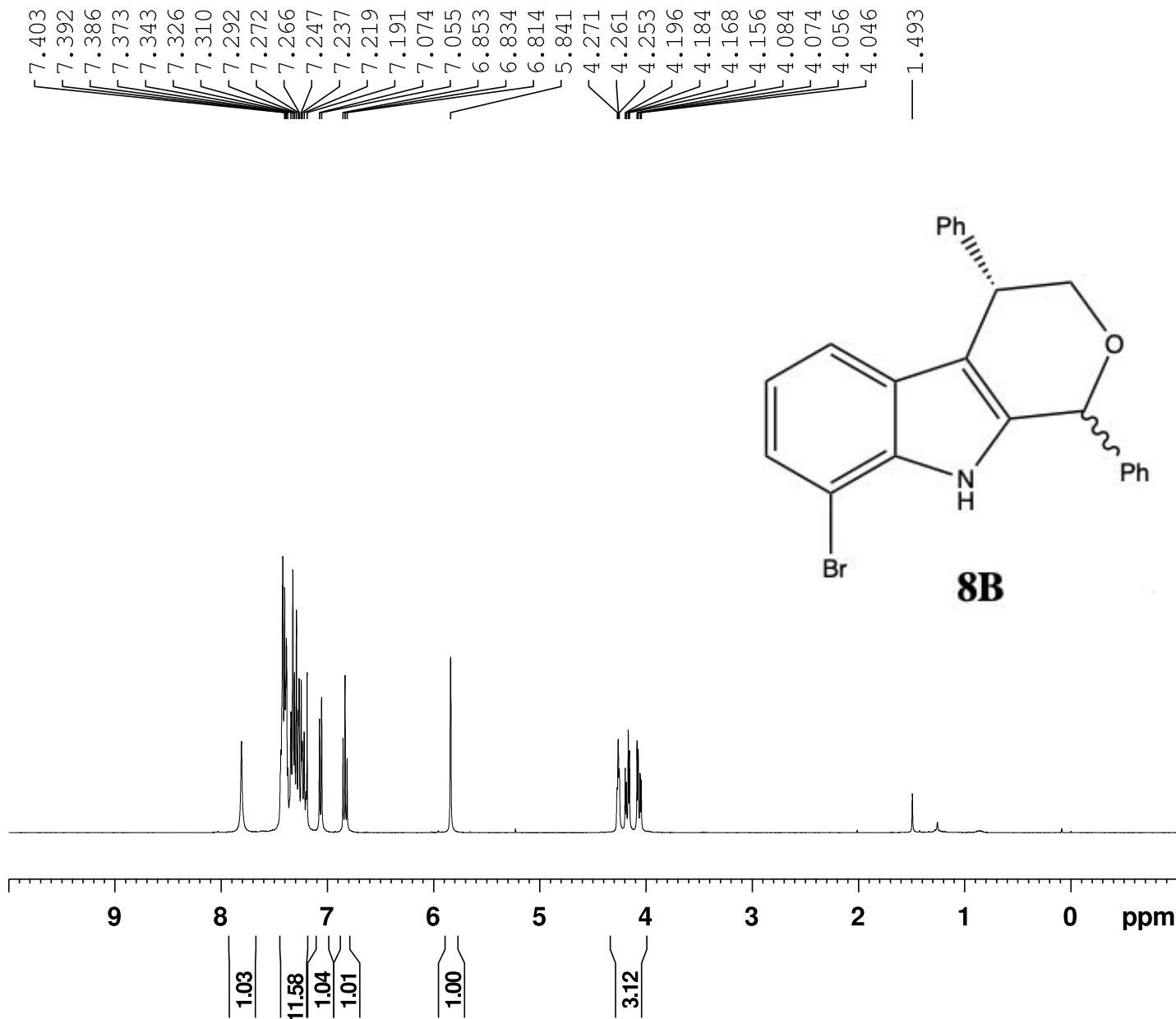
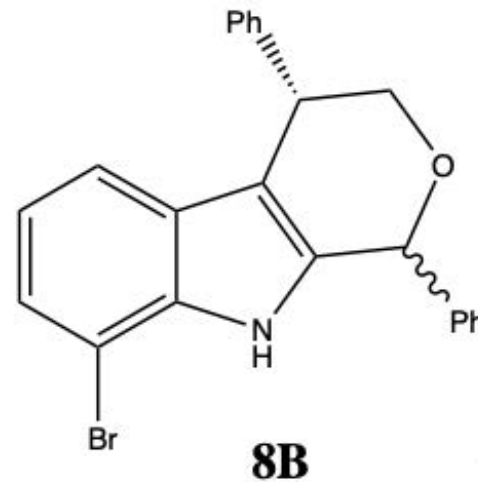


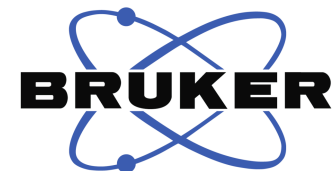
Current Data Parameters  
NAME HNMR-YX-7-p52B  
EXPNO 60  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231125  
Time 10.43  
INSTRUM spect  
PROBHD 5 mm PADUL 13C  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 4  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9845889 sec  
RG 50.16  
DW 60.800 usec  
DE 6.50 usec  
TE 294.5 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 9.90 usec  
PLW1 23.00000000 W  
SFO1 400.1924713 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1900414 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





Current Data Parameters  
NAME CNMR-YX-7-p52B  
EXPNO 61  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231125  
Time 10.47  
INSTRUM spect  
PROBHD 5 mm PADUL 13C  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 50  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 37.77  
DW 20.800 usec  
DE 6.50 usec  
TE 295.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 9.80 usec  
PLW1 47.4000153 W  
SFO1 100.6379178 MHz

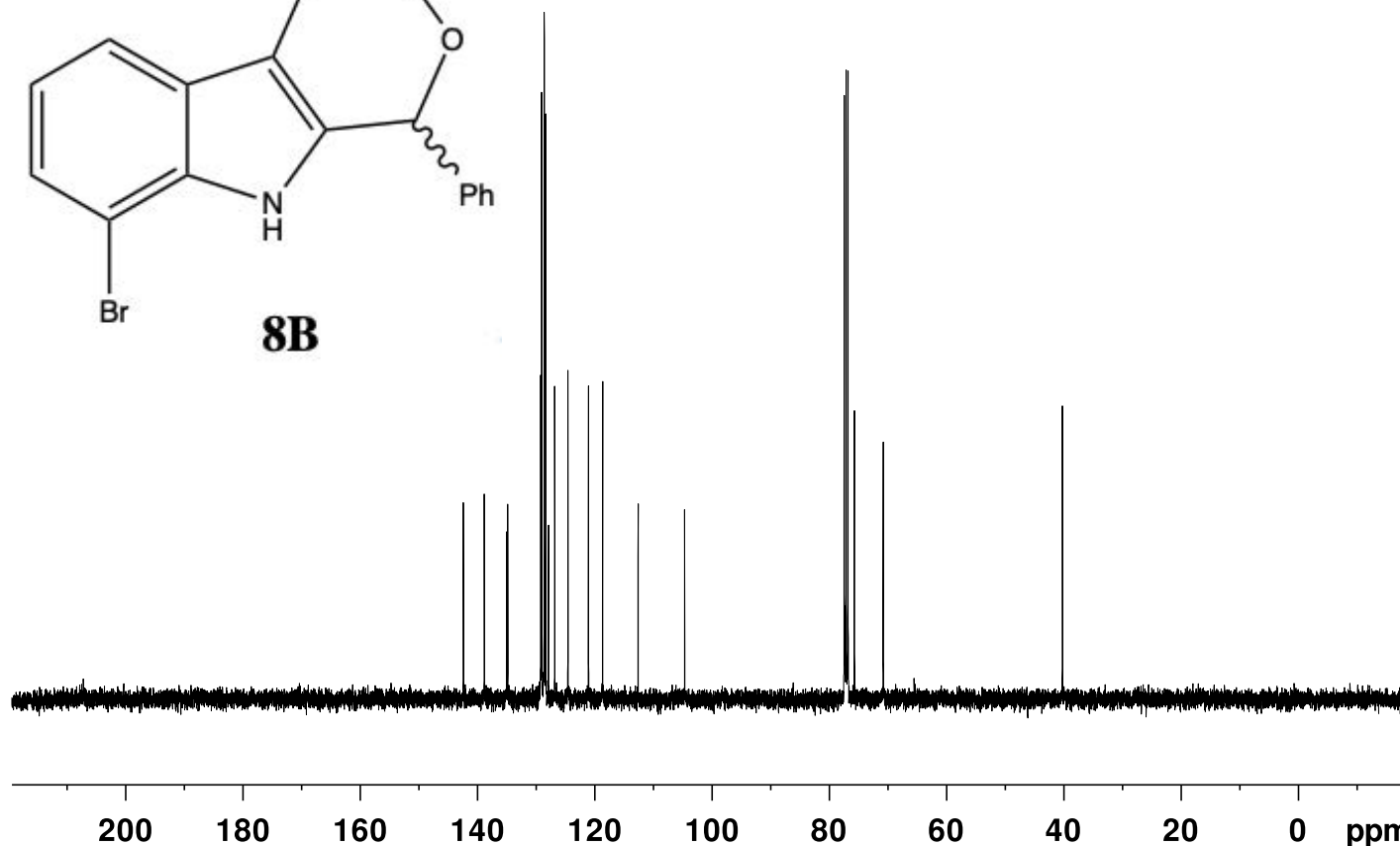
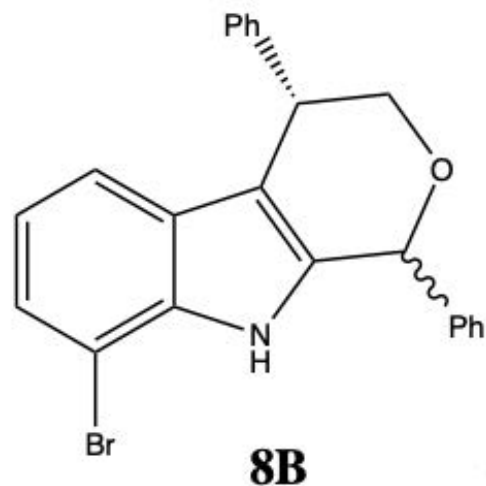
==== CHANNEL f2 =====  
CPDPRG[2] waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 23.0000000 W  
PLW12 0.30712000 W  
PLW13 0.24877000 W  
SFO2 400.1916008 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6278560 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

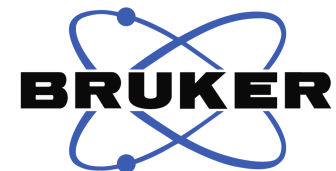
142.42  
138.85  
135.04  
134.85  
129.23  
129.07  
128.63  
128.58  
128.37  
127.90  
126.84  
124.58  
121.08  
118.66  
112.61  
104.67

75.72  
70.80

40.25





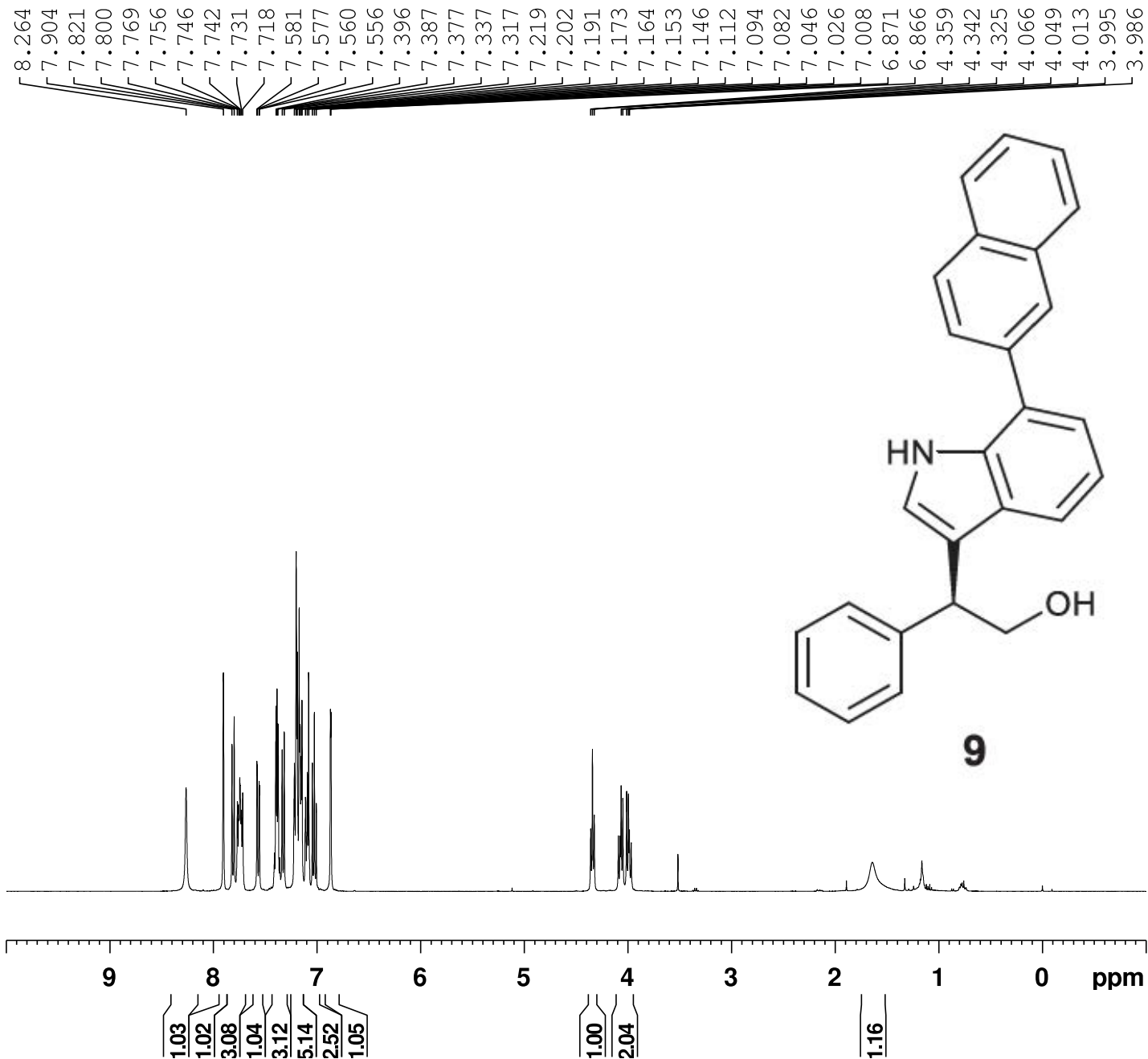
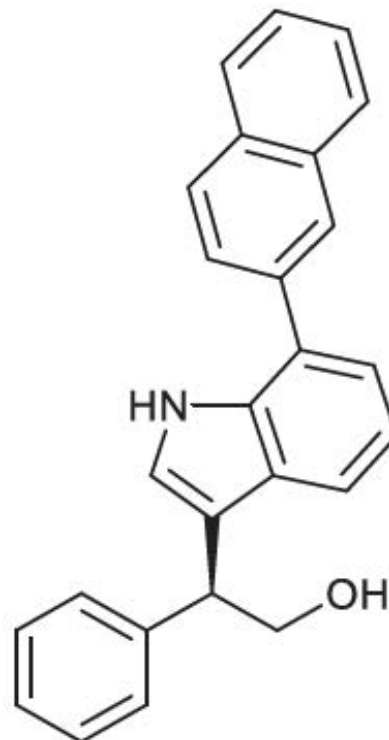


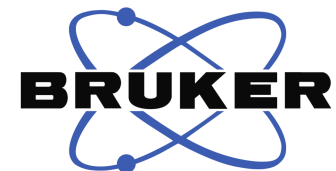
Current Data Parameters  
NAME HNMR-YX-7-p31  
EXPNO 38  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231109  
Time 16.13  
INSTRUM spect  
PROBHD 5 mm PADUL 13C  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 4  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9845889 sec  
RG 29.75  
DW 60.800 usec  
DE 6.50 usec  
TE 293.5 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 9.90 usec  
PLW1 23.00000000 W  
SFO1 400.1924713 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1900851 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





Current Data Parameters  
NAME CNMR-YX-7-p31  
EXPNO 39  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231109  
Time 16.16  
INSTRUM spect  
PROBHD 5 mm PADUL 13C  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 41  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 37.77  
DW 20.800 usec  
DE 6.50 usec  
TE 293.8 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 9.80 usec  
PLW1 47.4000153 W  
SFO1 100.6379178 MHz

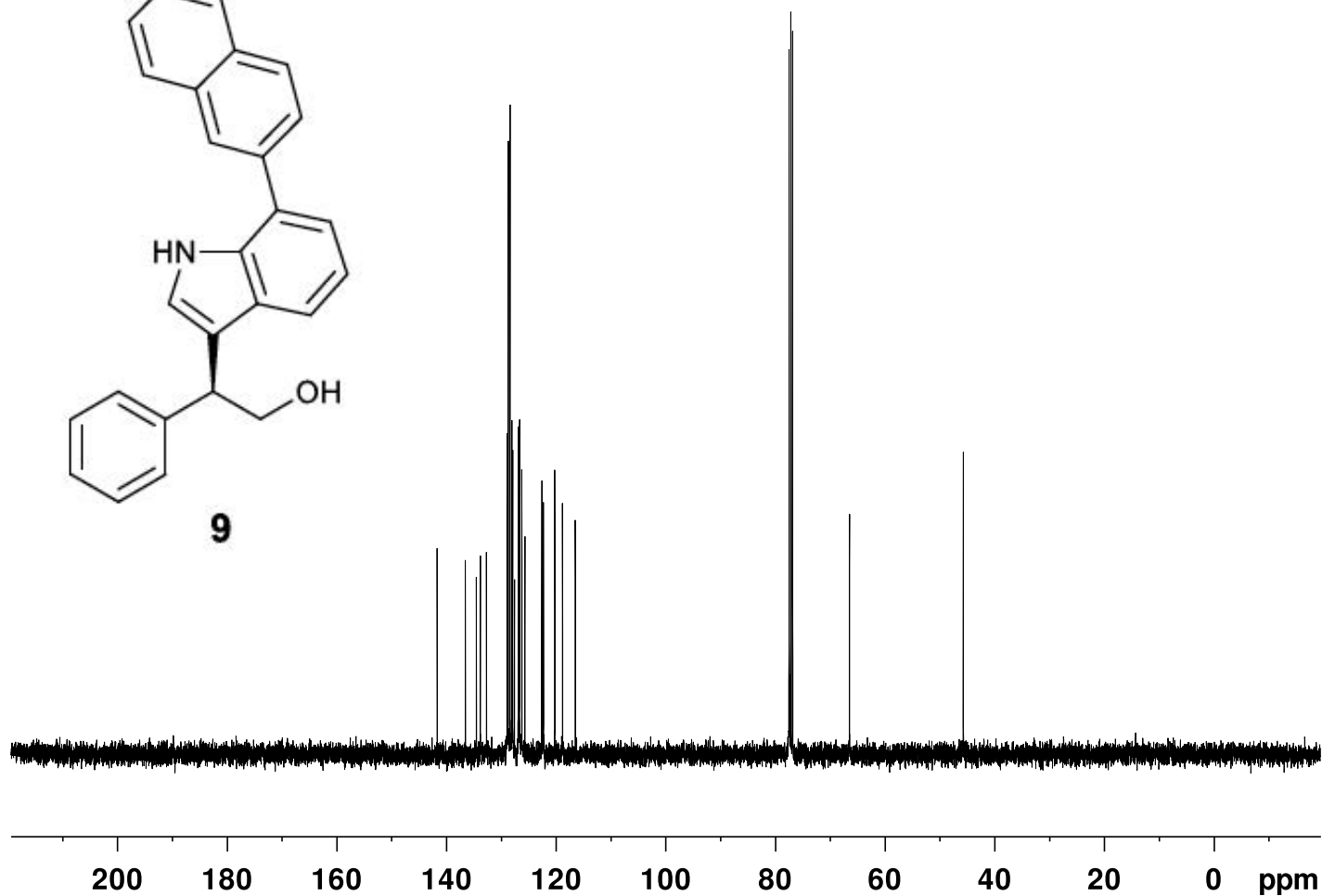
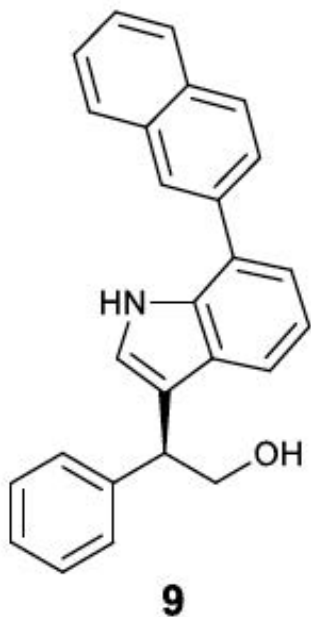
==== CHANNEL f2 =====  
CPDPRG[2] waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 23.0000000 W  
PLW12 0.30712000 W  
PLW13 0.24877000 W  
SFO2 400.1916008 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6278560 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

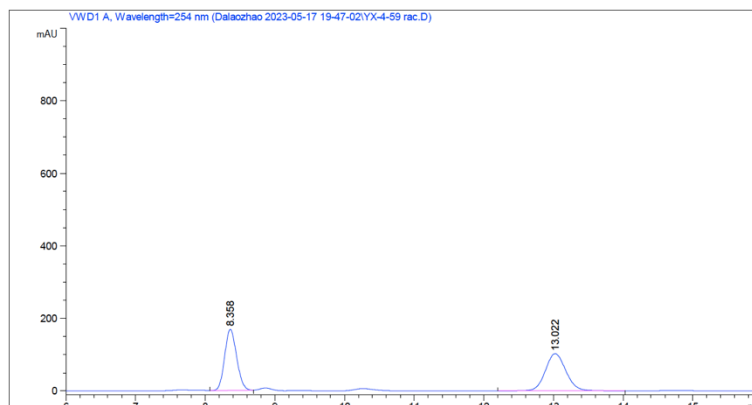
141.70  
136.56  
134.55  
133.80  
132.71  
128.94  
128.73  
128.40  
128.08  
127.91  
127.59  
126.91  
126.86  
126.70  
126.65  
126.25  
125.70  
122.60  
122.31  
120.23  
118.83  
116.49

66.47

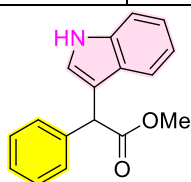
45.70



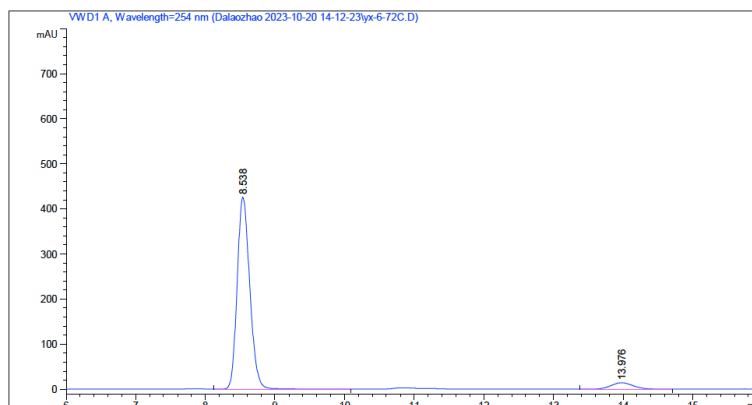
**3aa**, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



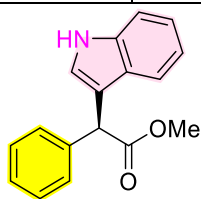
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	8.358	MM	0.1995	2015.11023	168.30583	48.9157
2	13.022	BB	0.3181	2104.45068	102.54544	51.0843



**3aa**  
racemic

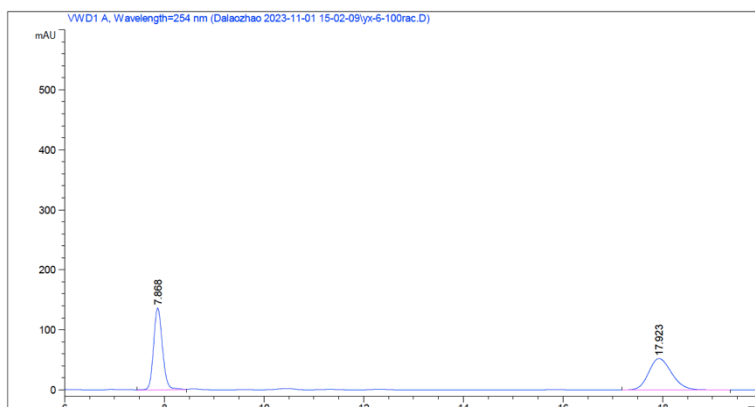


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	8.538	BV R	0.1945	5344.85010	425.78812	94.4476
2	13.976	BB	0.3453	314.21317	14.13033	5.5524

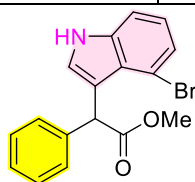


**3aa**  
enantioenriched

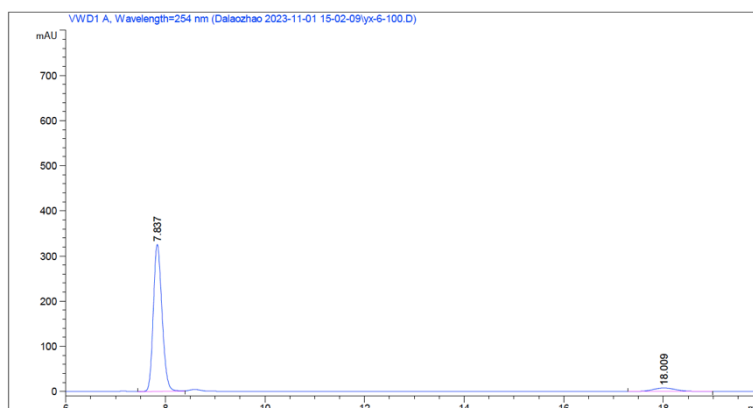
**3ab**, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



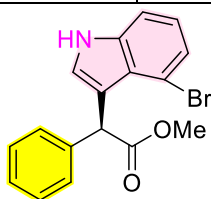
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	7.868	MM	0.2066	1690.90027	136.41212	50.4413
2	17.923	BB	0.4955	1661.31531	52.13615	49.5587



**3ab**  
racemic

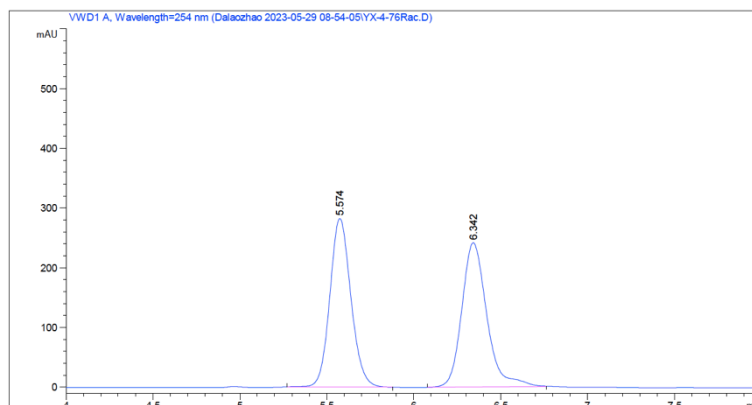


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	7.837	MM	0.2028	3966.52734	325.90671	94.1410
2	18.009	BB	0.4892	246.86372	7.75749	5.8590

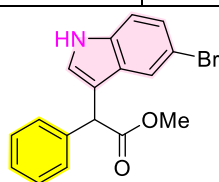


**3ab**  
enantioenriched

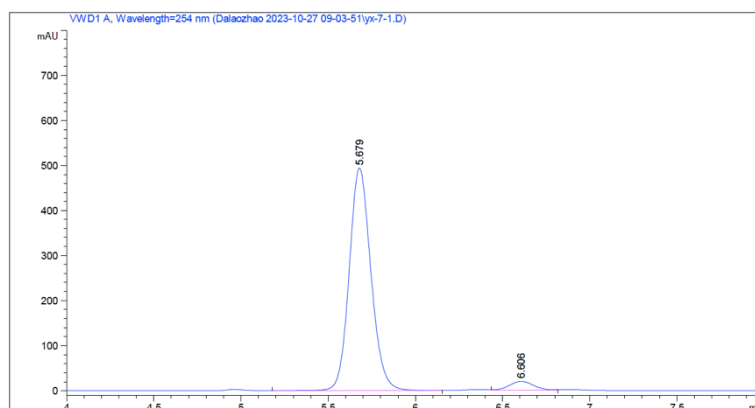
**3ac**, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



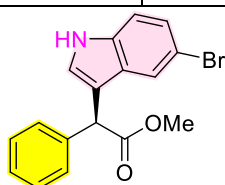
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	5.574	MM	0.1405	2380.12329	282.38724	49.6616
2	6.342	MM	0.1665	2412.56396	241.47307	50.3384



**3ac**  
racemic

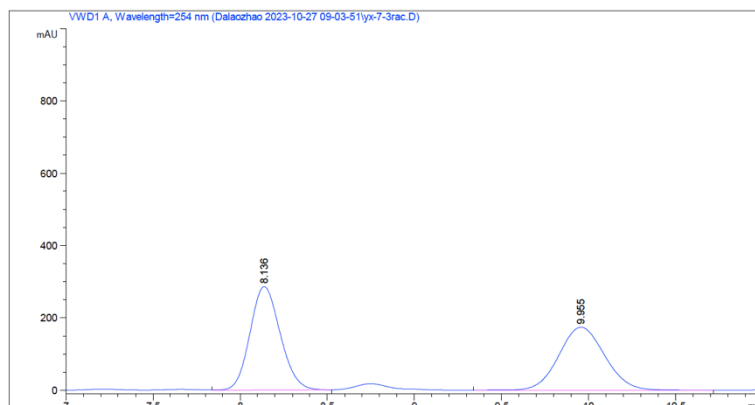


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	5.679	BB	0.1345	4277.72852	494.04504	95.9251
2	6.606	MM	0.1567	181.71617	181.71617	4.0749

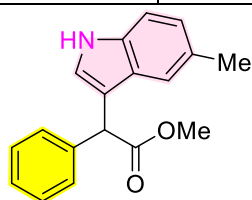


**3ac**  
enantioenriched

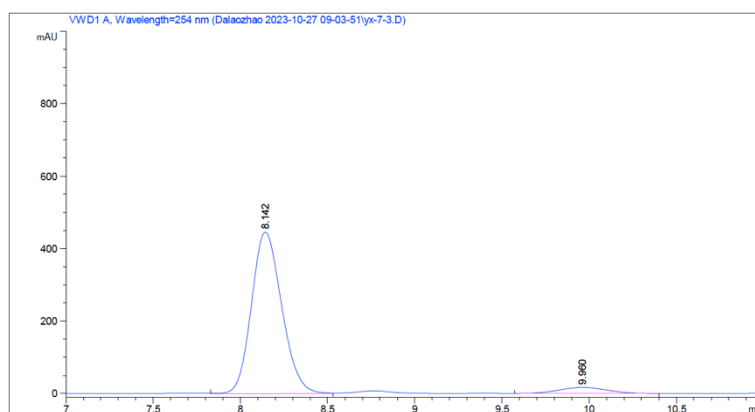
**3ad**, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



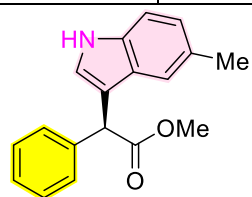
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	8.136	MM	0.2013	3455.89429	286.08041	52.0110
2	9.955	BB	0.2852	3188.65625	173.98116	47.9890



**3ad**  
racemic

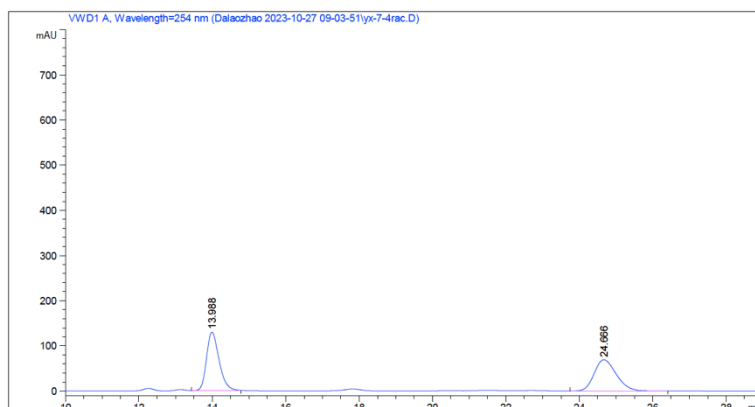


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	8.142	MM	0.2016	5397.20410	446.26401	94.2079
2	9.960	MM	0.3286	331.83267	16.82945	5.7921

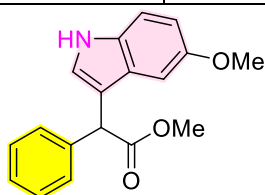


**3ad**  
enantioenriched

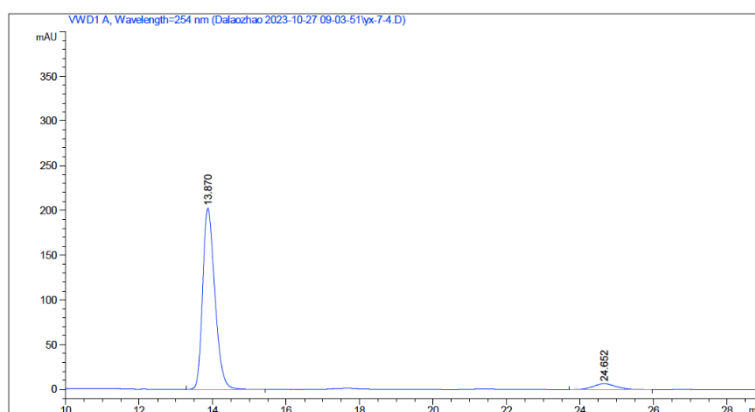
**3ae**, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



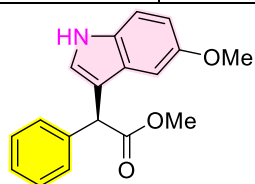
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	13.988	MM	0.3965	3084.40088	129.65916	51.7206
2	24.666	BB	0.6432	2879.17822	69.11674	48.2794



**3ae**  
racemic

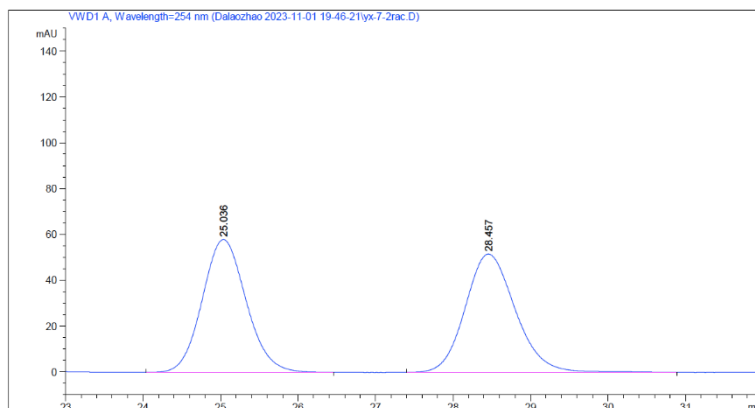


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	13.870	BB	0.3561	4663.82080	202.43958	94.6770
2	24.652	BB	0.6285	262.21152	6.29726	5.3230

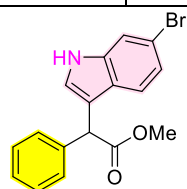


**3ae**  
enantioenriched

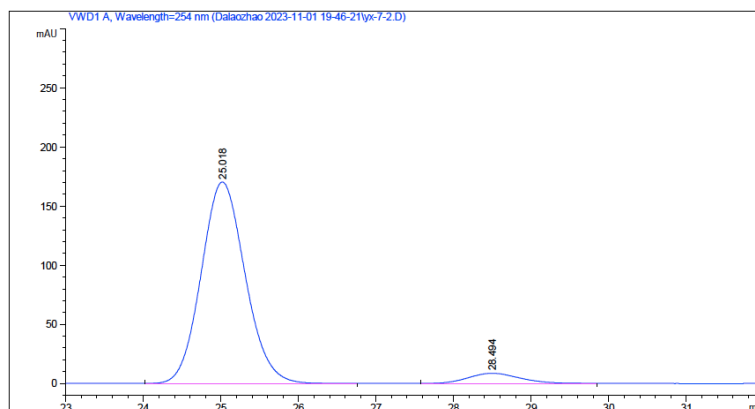
**3af**, HPLC conditions: Daicel CHIRALPAK® AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



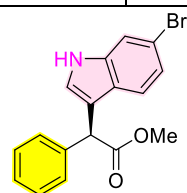
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	25.036	BB	0.6115	2276.97852	57.92403	49.5498
2	28.457	BB	0.6860	2318.35132	51.58177	50.4502



**3af**  
racemic



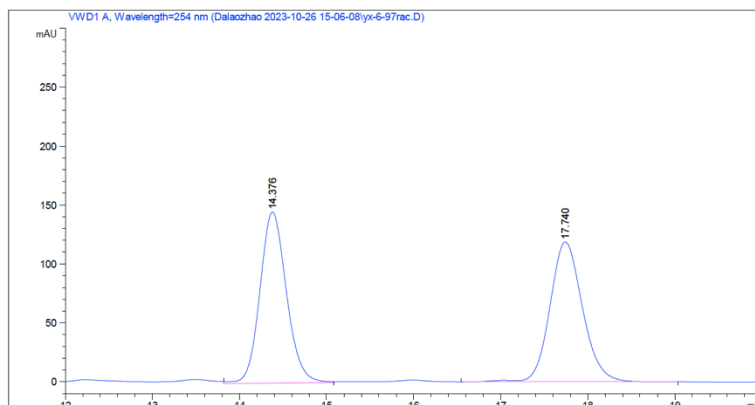
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	25.018	BB	0.6115	6696.18604	170.33723	94.4089
2	28.494	BB	0.6744	396.56339	8.60688	5.5911



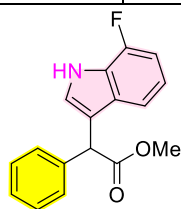
**3af**  
enantioenriched



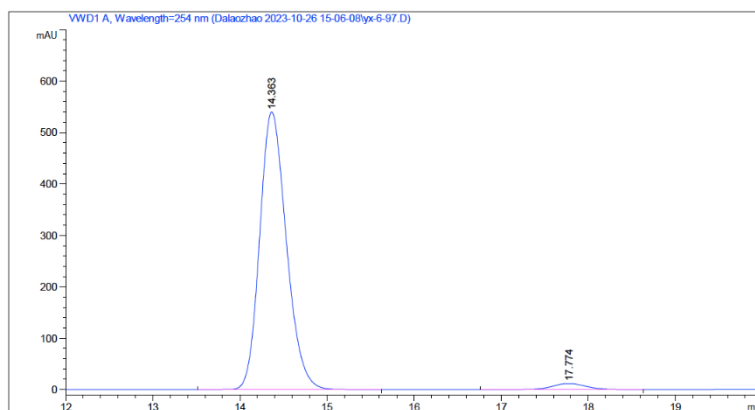
**3ag**, HPLC conditions: Daicel CHIRALPAK® AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



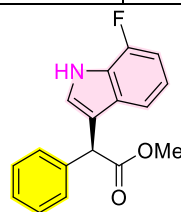
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	14.376	MM	0.3534	3078.99561	145.21498	49.8657
2	17.740	VB R	0.3987	3095.57861	118.76035	50.1343



**3ag**  
racemic

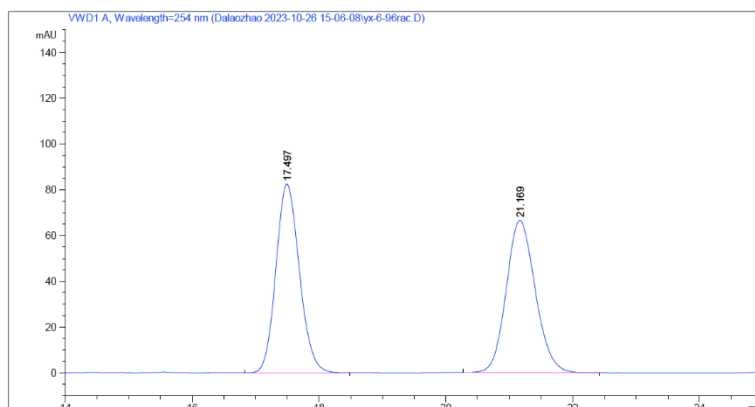


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	14.363	BB	0.3297	1.14879e4	540.09894	97.2197
2	17.774	BB	0.4137	328.53394	12.01425	2.7803

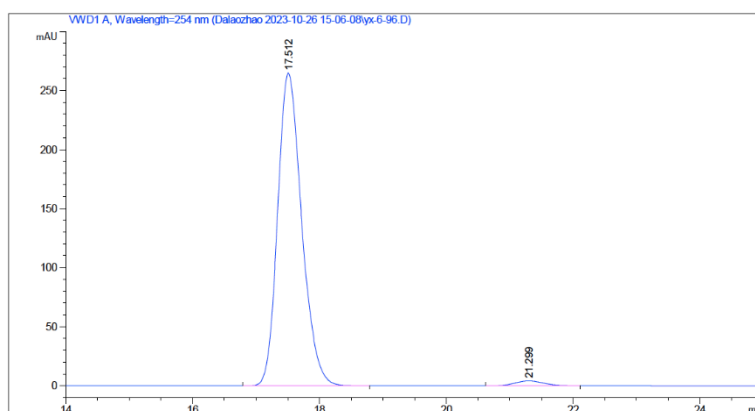
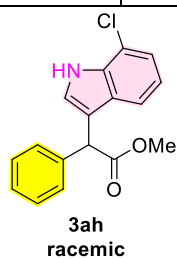


**3ag**  
enantioenriched

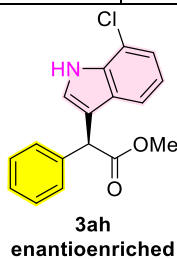
**3ah**, HPLC conditions: Daicel CHIRALPAK® AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



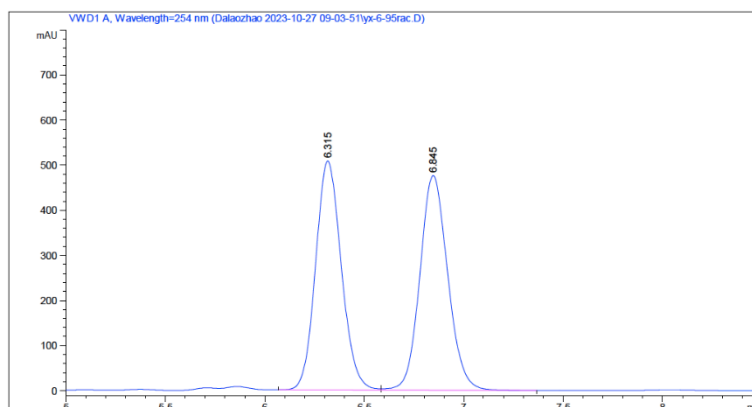
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	17.497	BB	0.4004	2121.39917	82.52696	49.9876
2	21.169	BB	0.4959	2122.45435	66.53132	50.0124



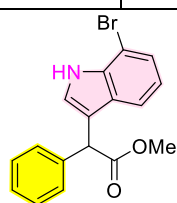
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	17.512	BB	0.4073	6964.32666	264.82855	98.2100
2	21.299	BB	0.4704	126.93218	4.06736	1.7900



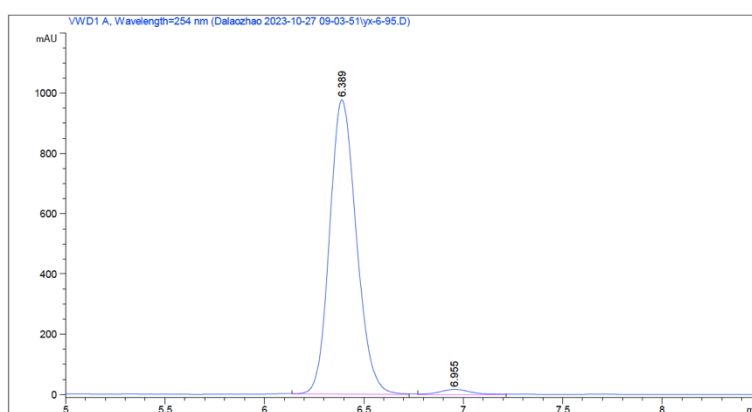
**3ai**, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



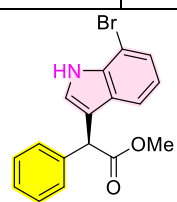
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	6.315	BV	0.1399	4565.25244	507.57706	49.6279
2	6.845	VB	0.1515	4633.71777	475.90207	50.3721



**3ai**  
racemic

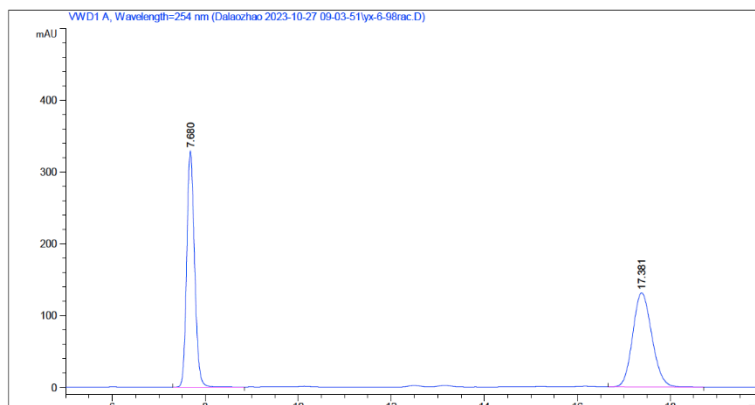


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	6.389	MM	0.1557	9134.68457	977.93396	98.0929
2	6.955	MM	0.1783	177.59837	16.60449	1.9071

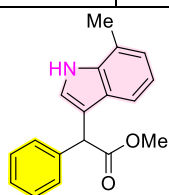


**3ai**  
enantioenriched

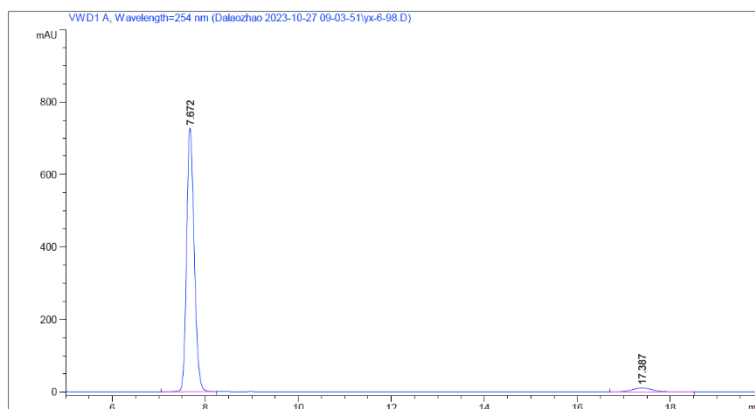
**3aj**, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



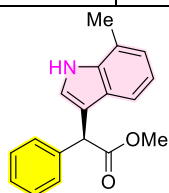
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	7.680	BB	0.1798	3839.78809	329.11990	50.6146
2	17.381	BB	0.4427	3746.53955	131.05153	49.3854



**3aj**  
racemic

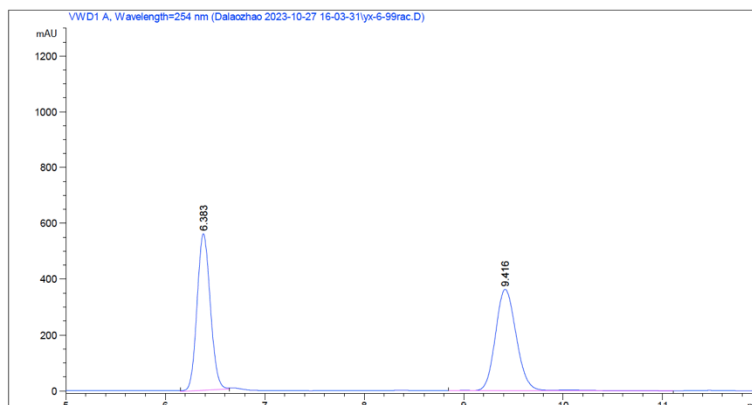


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	7.672	BB	0.1743	8234.94531	727.53772	96.3361
2	17.387	BB	0.4477	313.19550	10.88716	3.6639

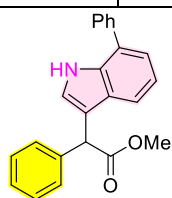


**3aj**  
enantioenriched

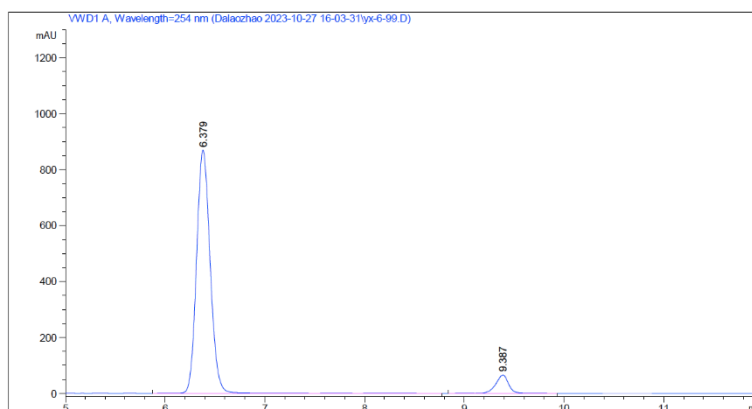
**3ak**, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



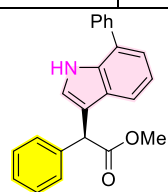
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	6.383	MM	0.1542	5197.50049	561.69751	49.3516
2	9.416	VV R	0.2258	5334.07568	363.45309	50.6484



**3ak**  
racemic

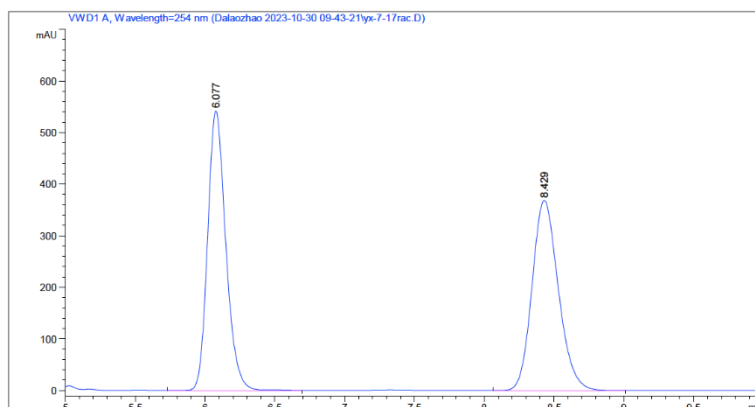


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	6.379	BV R	0.1483	8237.36230	869.79108	93.3530
2	9.387	VB R	0.1334	586.52661	65.64225	6.6470

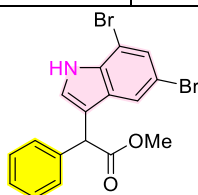


**3ak**  
enantioenriched

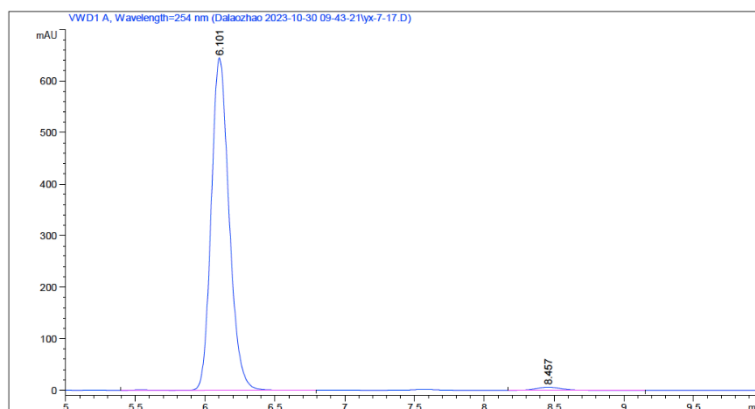
**3a1**, HPLC conditions: Daicel CHIRALPAK® AD-H column; 15% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



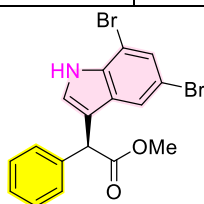
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	6.077	BV R	0.1391	4903.29199	541.56464	50.4061
2	8.429	BB	0.2022	4824.28320	368.59659	49.5939



**3a1**  
racemic

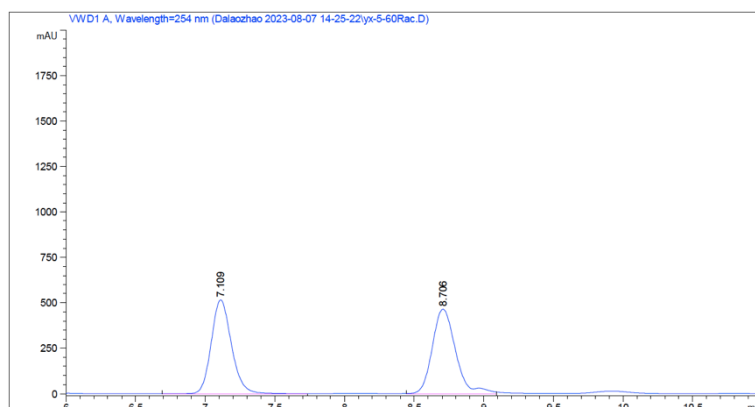


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	6.101	VB R	0.1375	5752.96143	645.16888	98.6777
2	8.457	BB	0.1981	77.09069	5.99429	1.3223

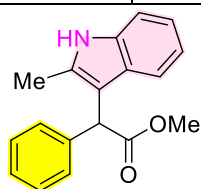


**3a1**  
enantioenriched

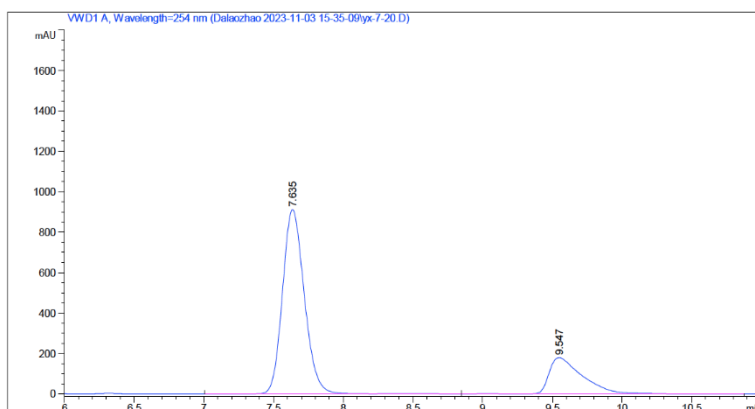
**3am**, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



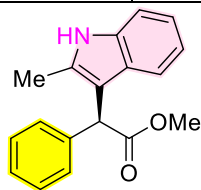
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	7.109	BB	0.1556	5207.08936	515.92908	49.0863
2	8.706	MM	0.1935	5400.93262	465.08133	50.9137



**3am**  
racemic

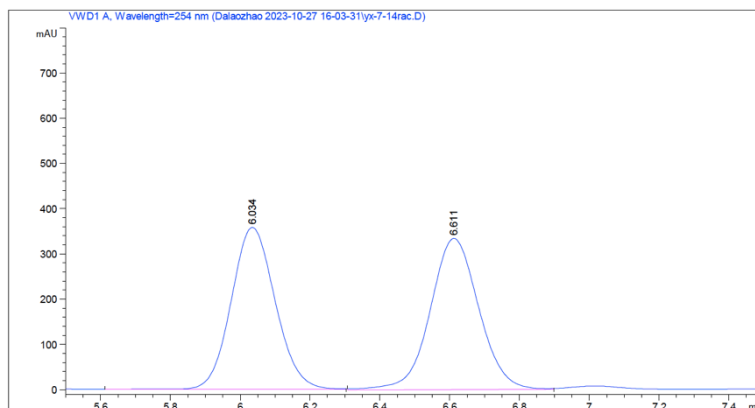


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	7.635	BV R	0.1695	9943.59375	911.83105	76.8718
2	9.547	VB R	0.2382	2991.70679	179.76665	23.1282

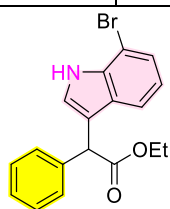


**3am**  
enantioenriched

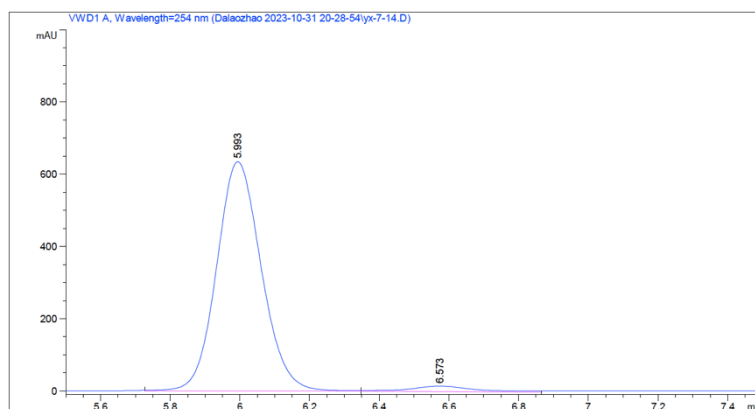
**3ba**, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



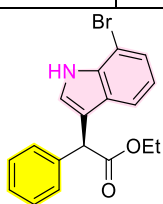
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	6.034	VV R	0.1359	3143.28076	358.17963	49.2399
2	6.611	MM	0.1614	3240.32935	334.52686	50.7601



**3ba**  
racemic



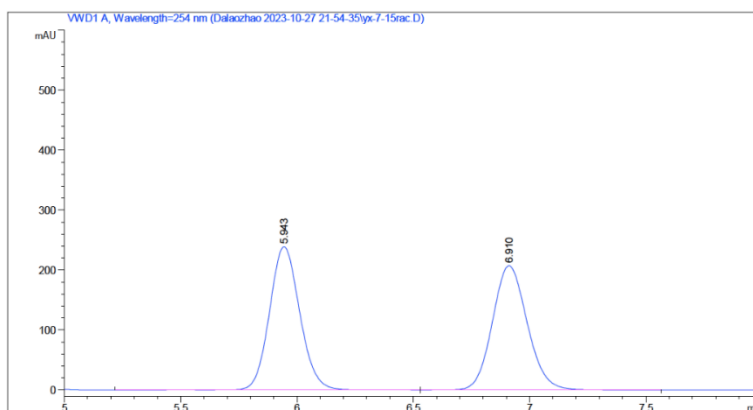
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	5.993	MM	0.1488	5681.47314	636.52856	96.5610
2	6.573	MM	0.2213	202.34578	15.23856	3.4390



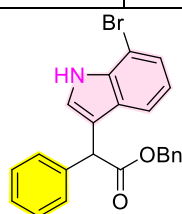
**3ba**  
enantioenriched



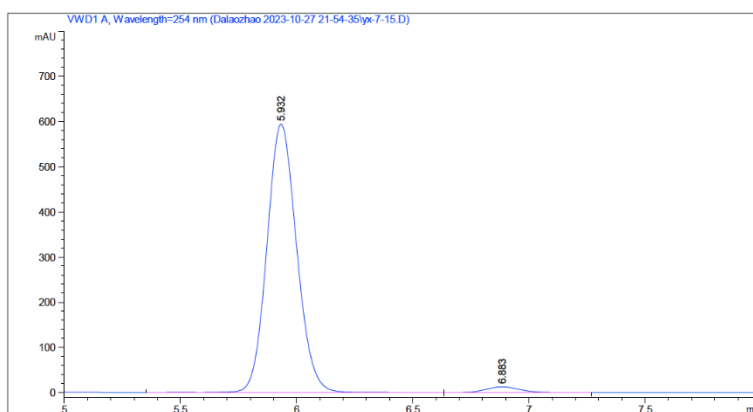
**3ca**, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



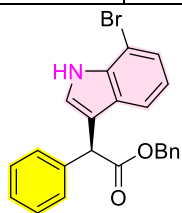
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	5.943	VV R	0.1412	2174.64136	238.87578	50.1834
2	6.910	VB	0.1610	2158.74292	207.04608	49.8166



**3ca**  
racemic

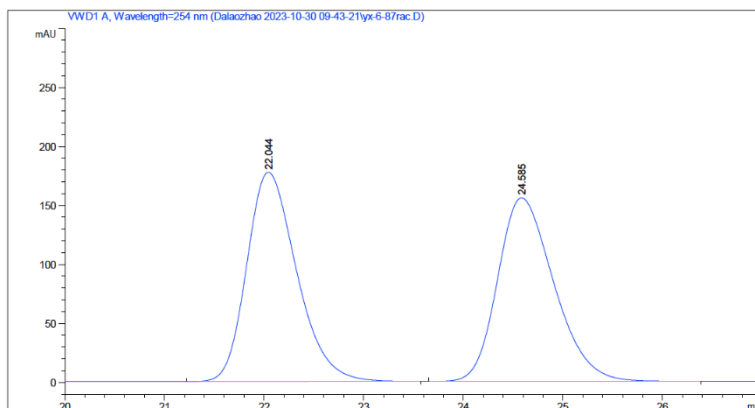


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	5.932	VV R	0.1389	5292.96875	594.27356	97.5667
2	6.883	VB	0.1608	132.00677	12.67865	2.4333

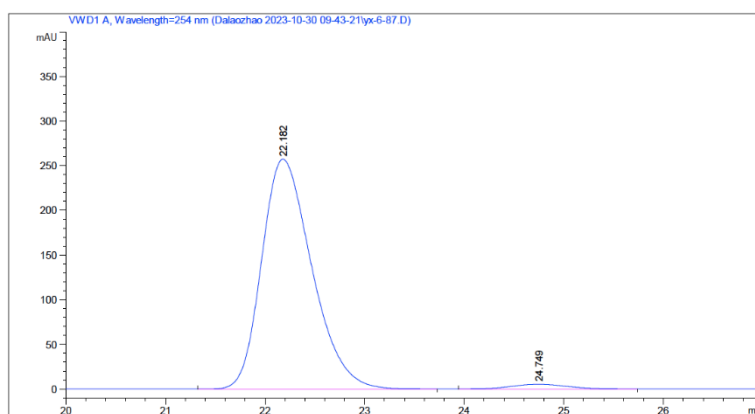
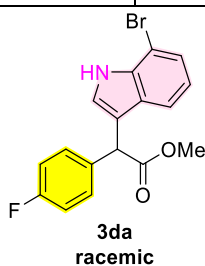


**3ca**  
enantioenriched

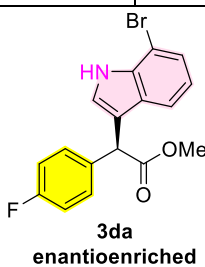
**3da**, HPLC conditions: Daicel CHIRALPAK® AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



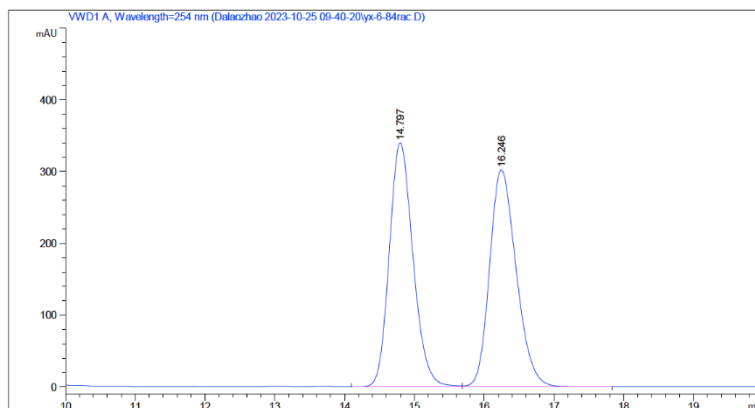
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	22.044	BB	0.5360	6152.14941	177.21953	50.2729
2	24.585	BB	0.6026	6085.36816	155.35538	49.7271



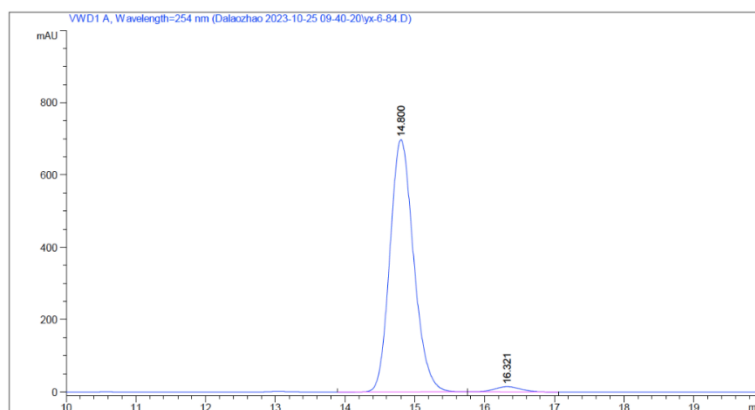
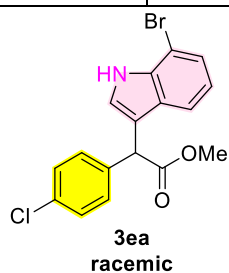
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	22.182	BB	0.5382	8975.84863	257.17630	97.8707
2	24.749	BB	0.5475	195.27715	5.18126	2.1293



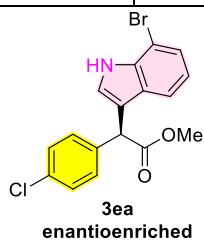
**3ea**, HPLC conditions: Daicel CHIRALPAK® AD-H column; 15% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



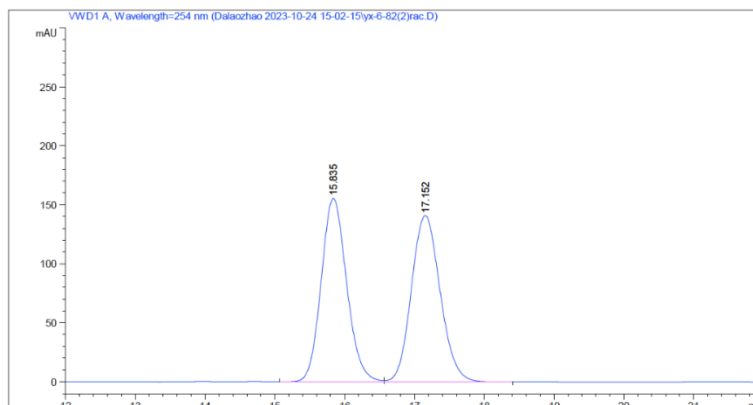
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	14.797	BV	0.3657	8027.72852	340.08710	50.0432
2	16.246	VB	0.4111	8013.86133	302.35474	49.9568



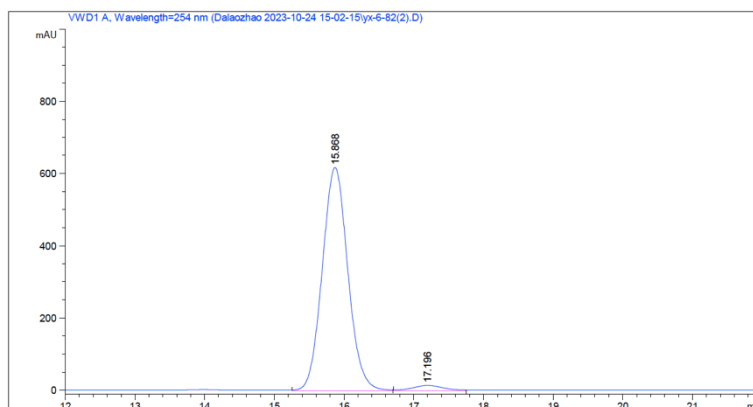
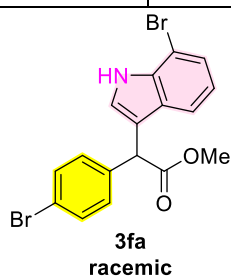
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	14.800	BB	0.3655	1.64477e4	697.21027	97.8224
2	16.321	BB	0.4000	366.13092	14.25980	2.1776



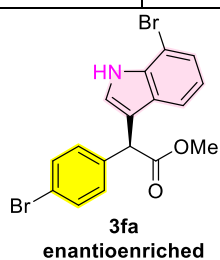
**3fa**, HPLC conditions: Daicel CHIRALPAK® AD-H column; 15% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



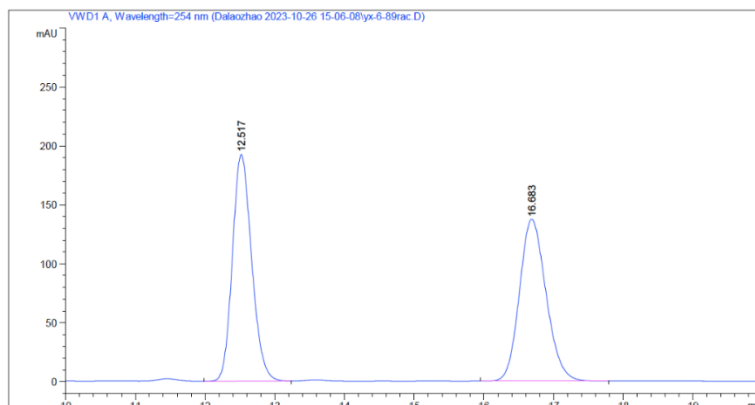
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	15.835	BV	0.3921	3945.65674	155.49304	49.4305
2	17.152	VB	0.4462	4036.58228	140.96289	50.5695



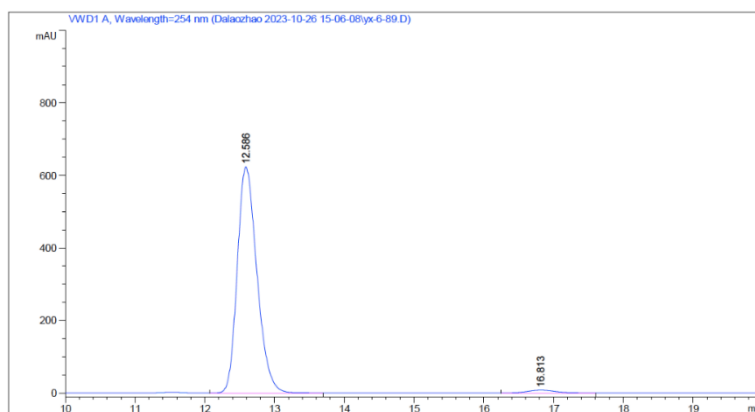
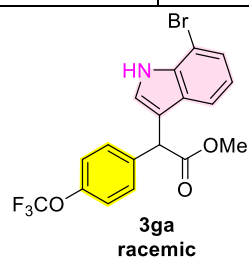
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	15.868	MM	0.4260	1.58054e4	618.36914	97.1078
2	17.196	MM	0.5332	470.73950	14.71398	2.8922



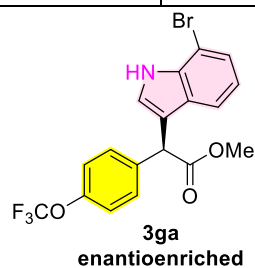
**3ga**, HPLC conditions: Daicel CHIRALPAK® AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



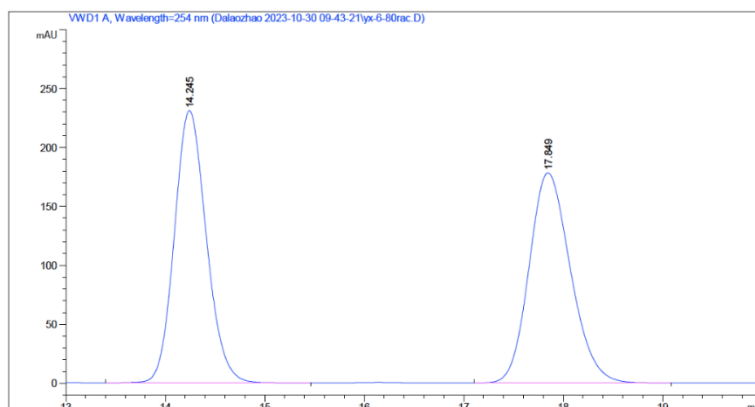
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.517	BB	0.2972	3699.44434	192.33884	50.3786
2	16.683	BB	0.4118	3643.84033	137.20120	49.6214



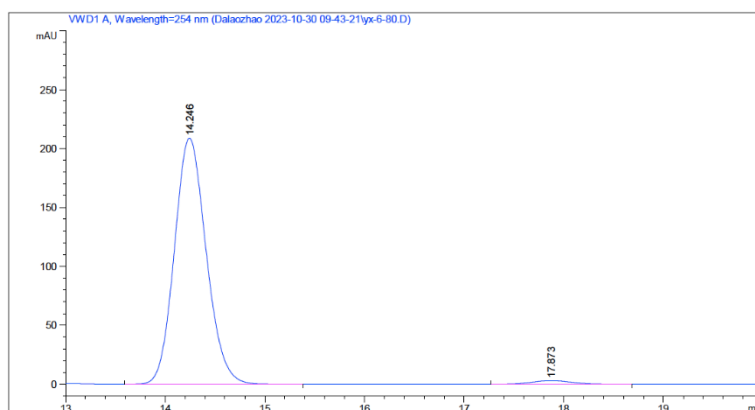
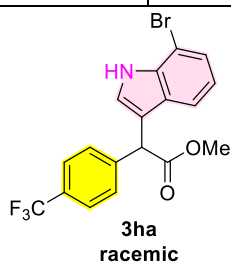
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.586	BB	0.3006	1.21640e4	623.08673	98.4027
2	16.813	BB	0.4083	197.44684	7.48400	1.5973



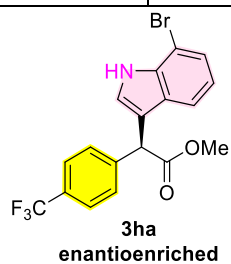
**3ha**, HPLC conditions: Daicel CHIRALPAK® AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



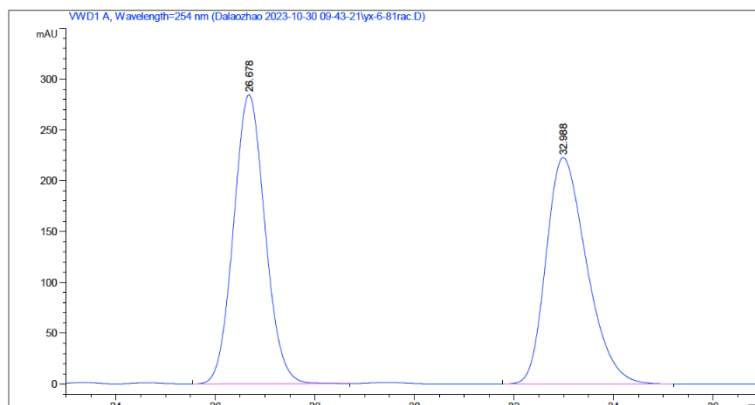
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	14.245	BB	0.3451	5161.00146	231.00645	50.0633
2	17.849	BB	0.4463	5147.94727	178.15005	49.9367



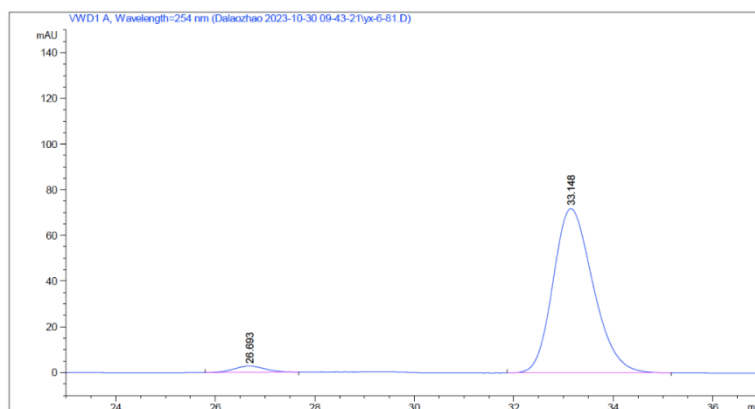
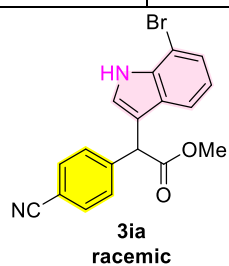
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	14.246	BB	0.3429	4623.15381	208.71748	98.1626
2	17.873	BB	0.4212	86.53774	3.02434	1.8374



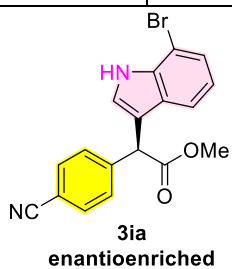
**3ia**, HPLC conditions: Daicel CHIRALPAK® AD-H column; 15% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



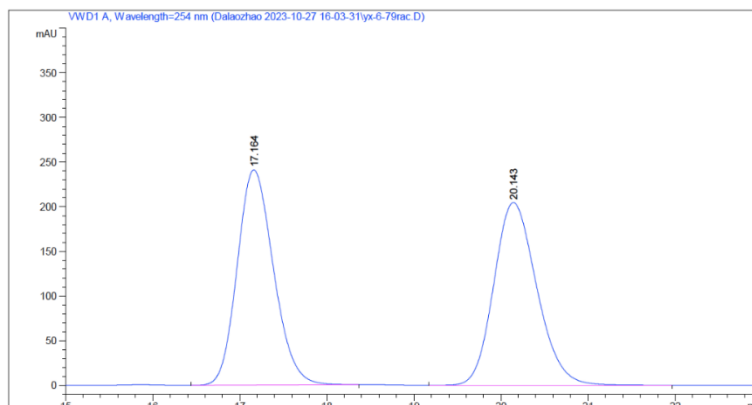
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	26.678	BB	0.6795	1.24803e4	284.33755	49.8446
2	32.988	BB	0.8740	1.25581e4	222.49393	50.1554



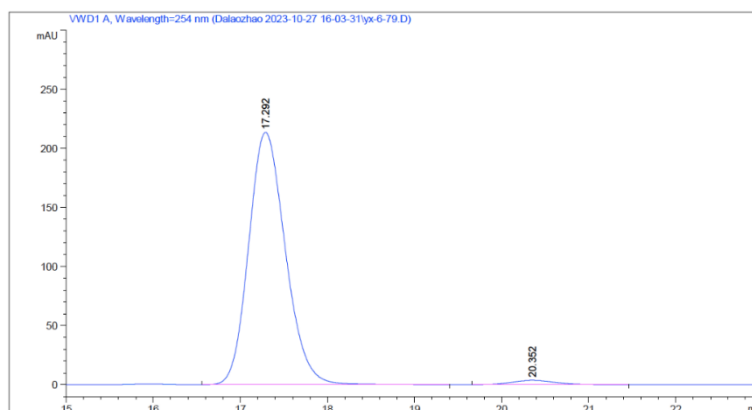
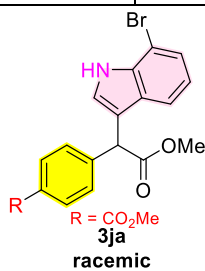
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	26.693	BB	0.5945	116.59806	2.73736	2.8293
2	33.148	BB	0.8642	4004.48364	71.86063	97.1707



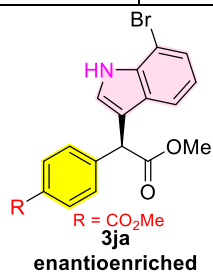
**3ja**, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	17.164	BB	0.4494	6968.07715	241.00447	49.8481
2	20.143	BB	0.5308	7010.54980	204.59828	50.1519

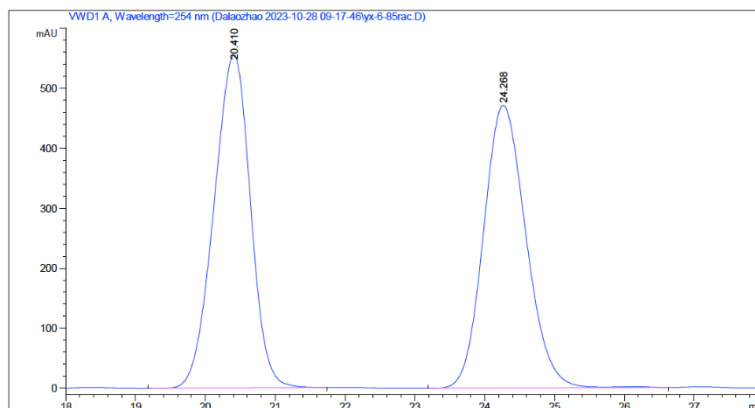


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	17.292	BB	0.4538	6254.04980	213.52275	98.0062
2	20.352	BB	0.5011	127.23135	3.62556	1.9938

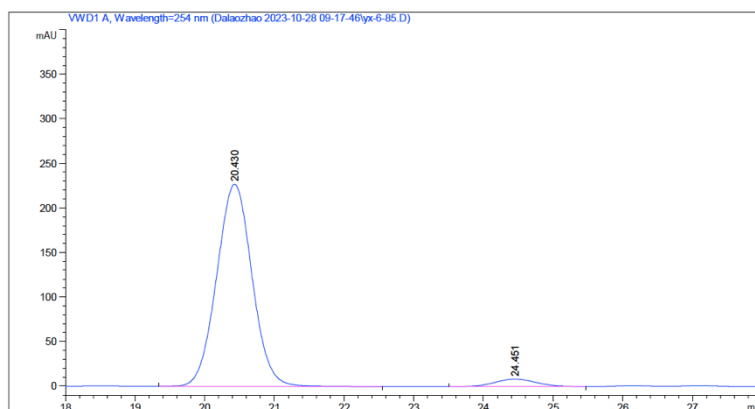
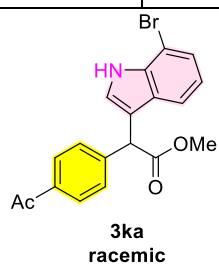




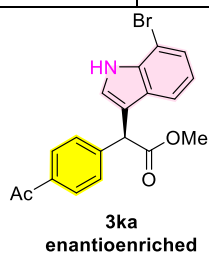
**3ka**, HPLC conditions: Daicel CHIRALPAK® IC column; 15% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



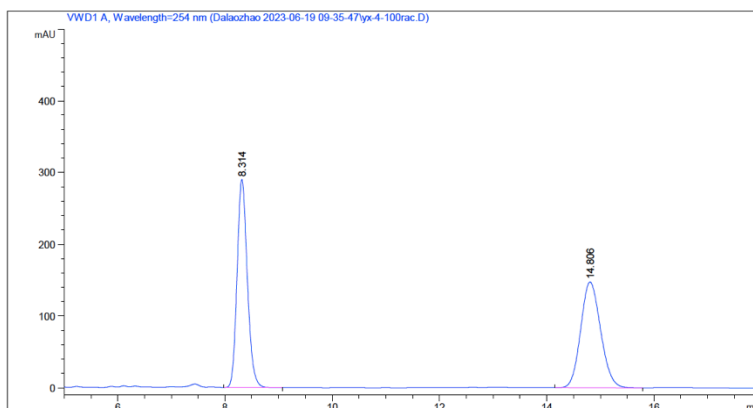
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	20.410	BB	0.5690	2.01584e4	555.48694	50.3390
2	24.268	BV R	0.6524	1.98869e4	471.16019	49.6610



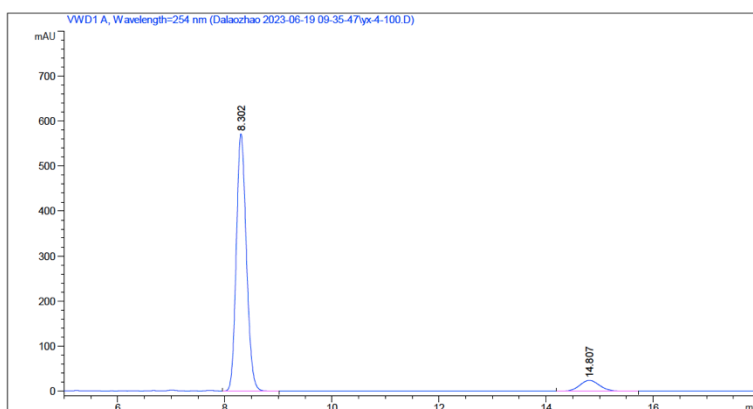
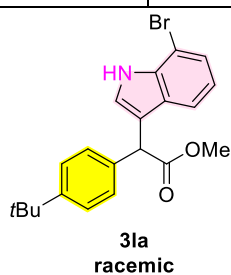
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	20.430	BB	0.5484	8004.04199	226.88336	95.7702
2	24.451	BB	0.6337	353.50439	8.45010	4.2298



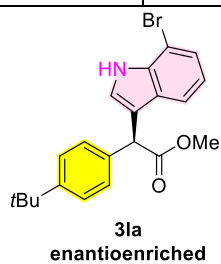
**3la**, HPLC conditions: Daicel CHIRALPAK® AD-H column; 15% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



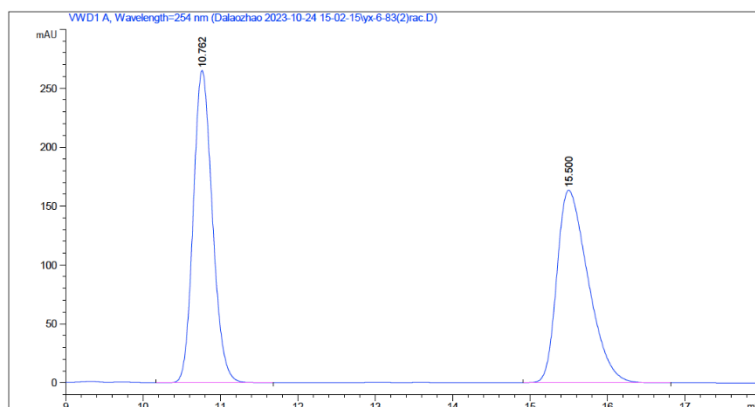
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	8.314	BB	0.2058	3851.20508	290.11786	50.3092
2	14.806	BB	0.4029	3803.87231	147.42479	49.6908



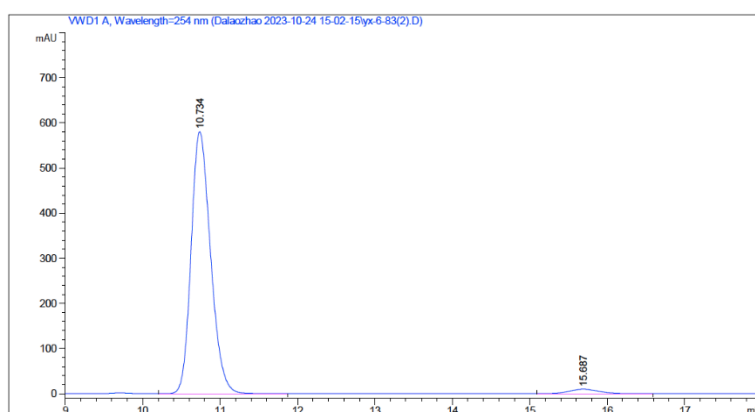
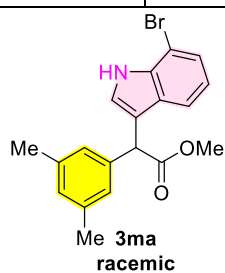
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	8.302	BB	0.2016	7450.64990	571.51685	92.4288
2	14.807	BB	0.3942	610.31415	24.00618	7.5712



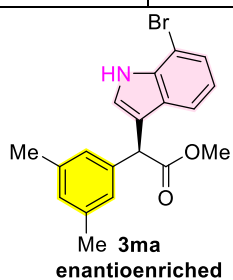
**3ma**, HPLC conditions: Daicel CHIRALPAK® AD-H column; 15% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



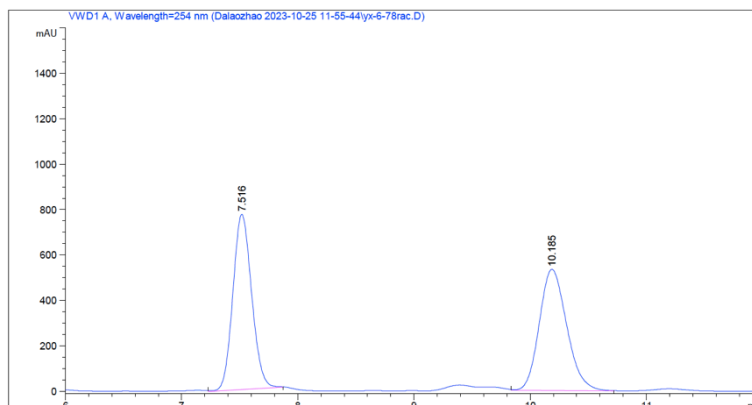
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.762	BB	0.2657	4549.20996	265.13211	49.8721
2	15.500	BB	0.4315	4572.53613	163.31413	50.1279



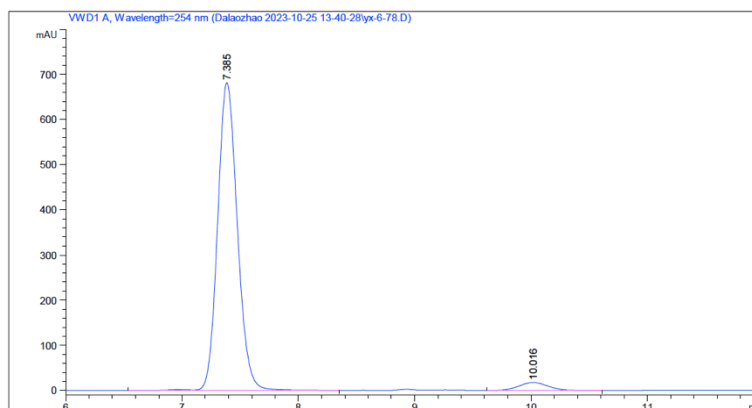
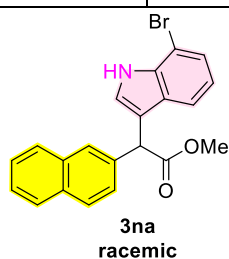
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.734	BB	0.2704	1.01147e4	580.19495	97.5473
2	15.687	BB	0.3998	254.31642	9.72160	2.4527



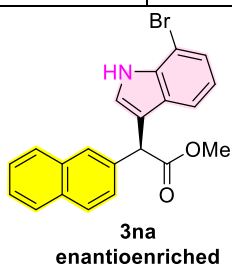
**3na**, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



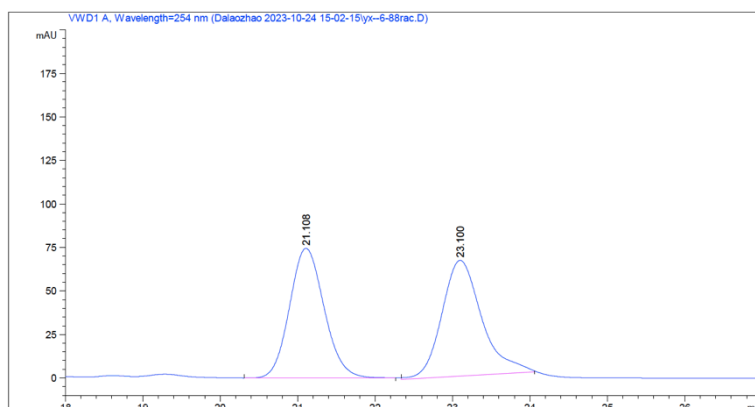
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	7.516	MM	0.1871	8659.59082	771.22919	49.7404
2	10.185	MM	0.2732	8749.97754	533.81573	50.2596



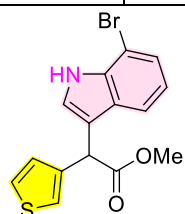
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	7.385	VB R	0.1819	8014.49219	681.64905	96.2623
2	10.016	BB	0.2740	311.18854	17.65883	3.7377



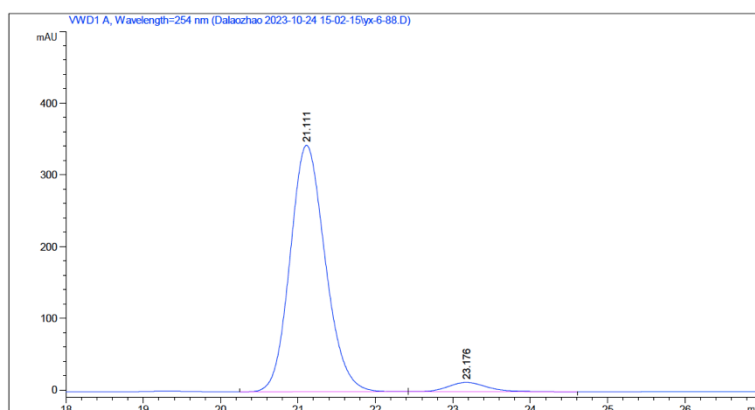
**3oa**, HPLC conditions: Daicel CHIRALPAK® AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



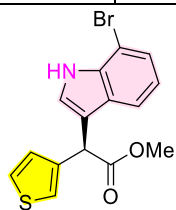
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	21.108	BB	0.4807	2307.20679	74.49439	49.2538
2	23.100	MM	0.5963	2377.11621	66.43819	50.7462



**3oa**  
racemic

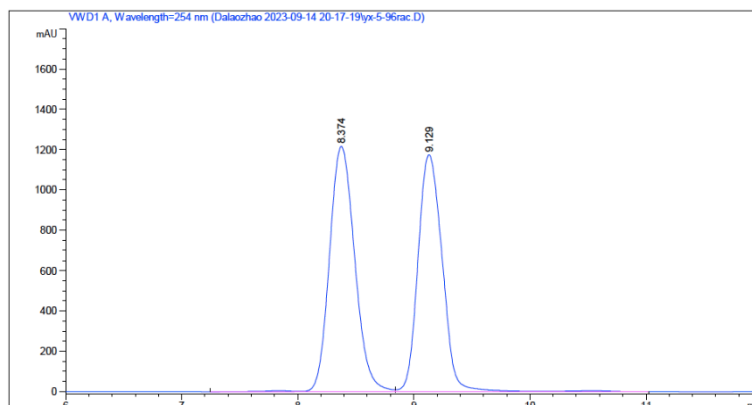


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	21.111	BB	0.4882	1.08321e4	344.01672	95.9764
2	23.176	BB	0.5365	454.10968	12.92601	4.0236

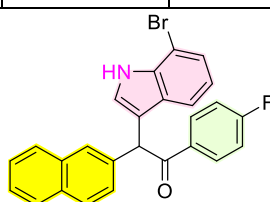


**3oa**  
enantioenriched

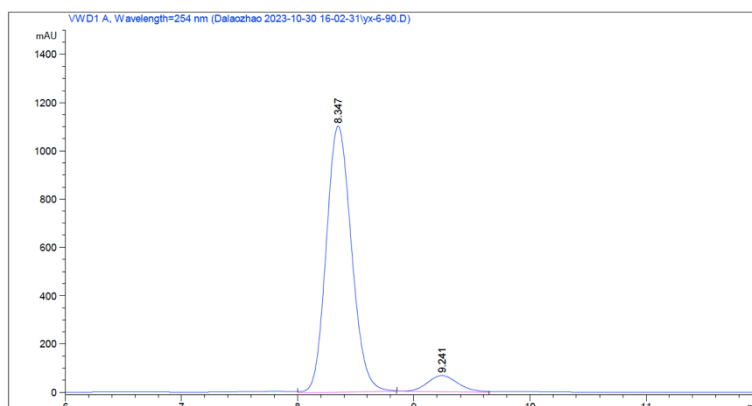
**3pa** HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



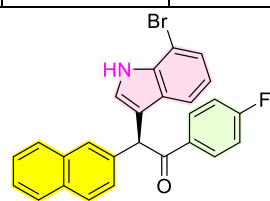
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	8.374	VV R	0.2371	1.84538e4	1216.35229	51.8708
2	9.129	VV R	0.2401	1.71227e4	1174.82178	48.1292



**3pa**  
racemic

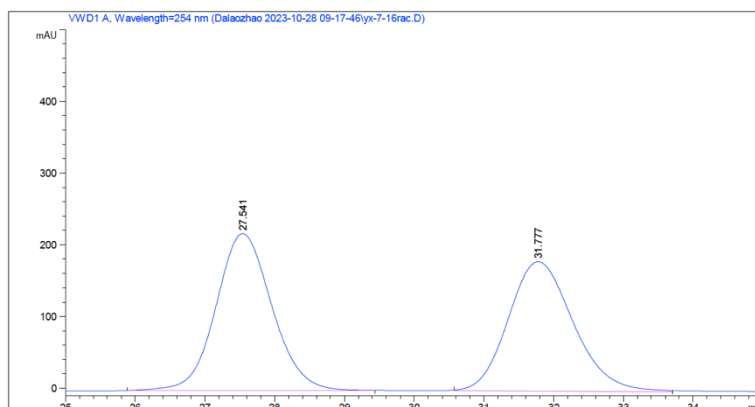


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	8.347	MM	0.2514	1.66403e4	1103.18835	93.1647
2	9.241	MM	0.3053	1220.86670	66.65044	6.8353

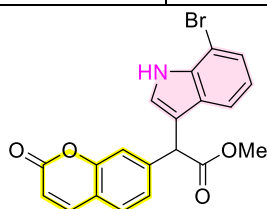


**3pa**  
enantioenriched

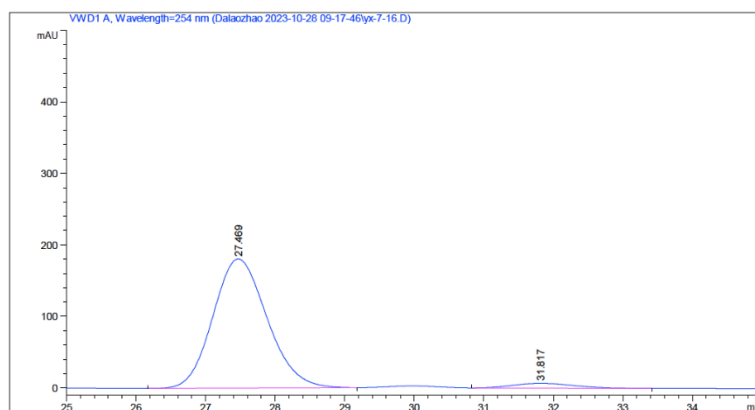
**3qa**, HPLC conditions: Daicel CHIRALPAK® IC column; 25% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



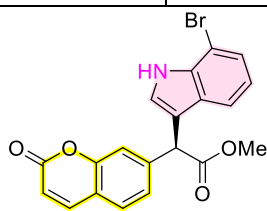
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	27.541	MM	0.9287	1.21949e4	218.84351	51.1606
2	31.777	MM	1.0766	1.16416e4	180.21367	48.8394



**3qa**  
racemic

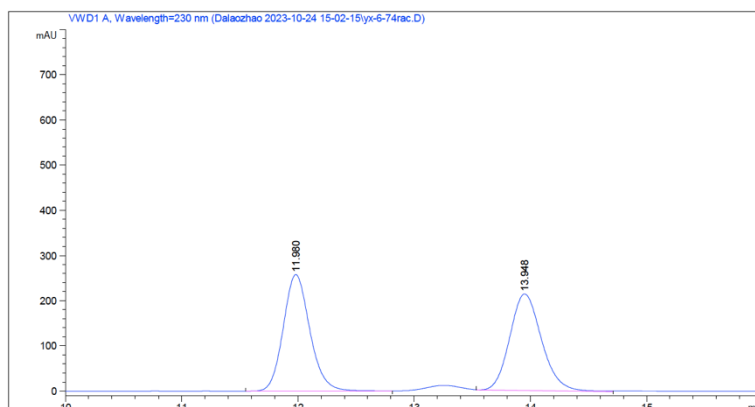


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	27.469	BB	0.8427	9770.35059	180.47118	96.0186
2	31.817	BB	0.8251	405.12115	6.65651	3.9814

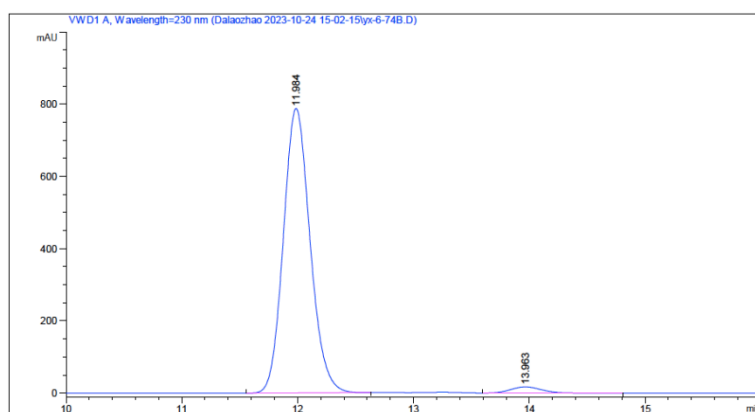
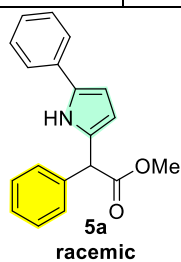


**3qa**  
enantioenriched

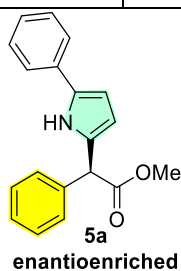
**5a**, HPLC conditions: Daicel CHIRALPAK® AD-H column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 230$  nm.



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	11.980	BV	0.2453	4101.82715	257.90054	50.3258
2	13.948	MM	0.3158	4048.71338	213.66832	49.6742

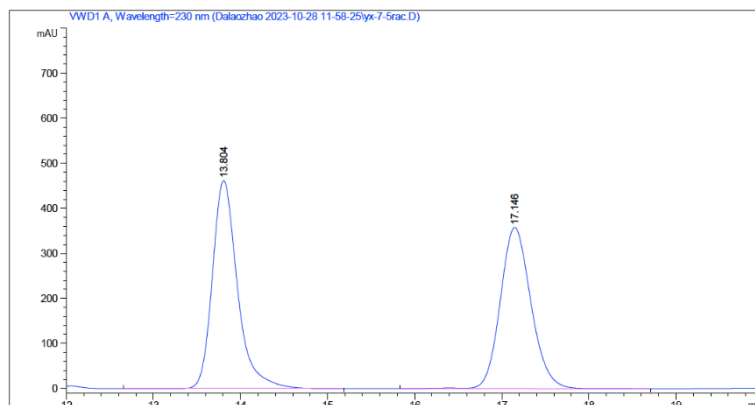


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	11.984	BB	0.2464	1.26049e4	787.72449	97.5269
2	13.963	BB	0.2877	319.64203	17.11760	2.4731

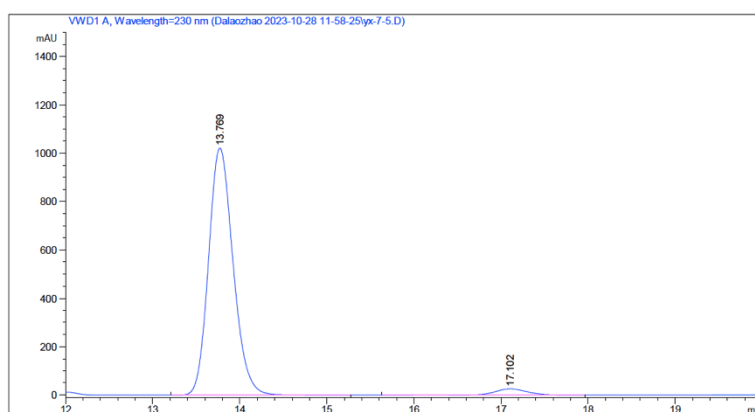
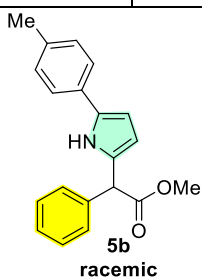




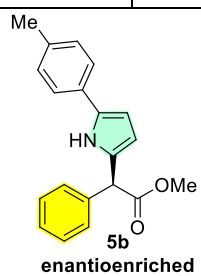
**5b**, HPLC conditions: Daicel CHIRALPAK® AD-H column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 230$  nm.



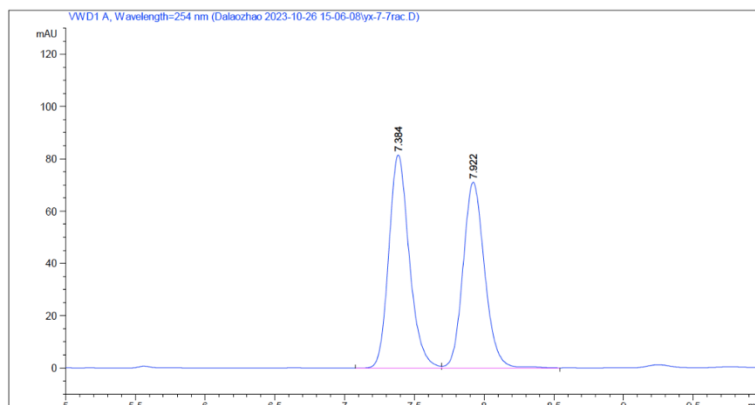
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	13.804	VB R	0.3045	9224.24707	461.63501	51.3050
2	17.146	VB R	0.3774	8754.99219	357.60785	48.6950



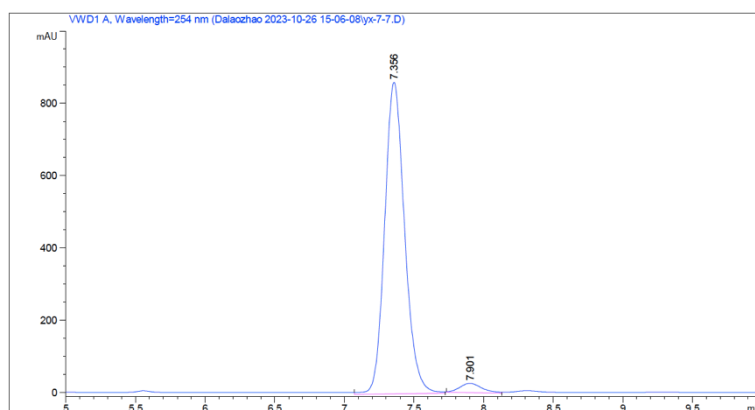
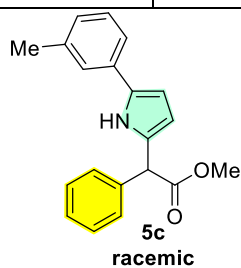
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	13.769	BB	0.3023	1.99722e4	1021.66229	96.6235
2	17.102	VB R	0.4044	697.91931	25.92346	3.3765



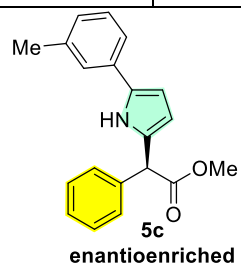
**5c**, HPLC conditions: Daicel CHIRALPAK® AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



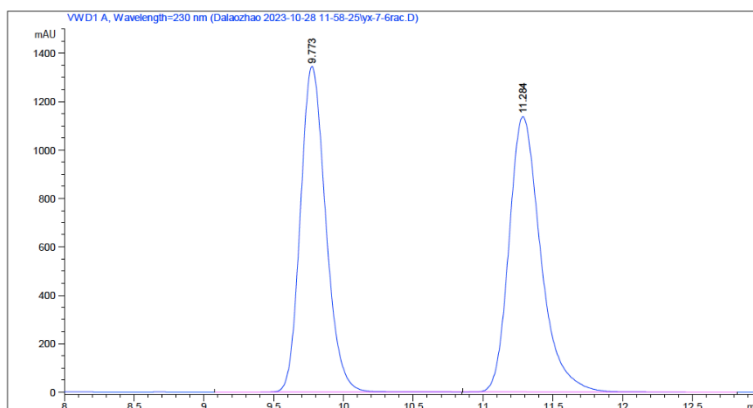
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	7.384	BV	0.1554	831.73621	81.55822	52.1129
2	7.922	VV R	0.1648	764.29108	71.05061	47.8871



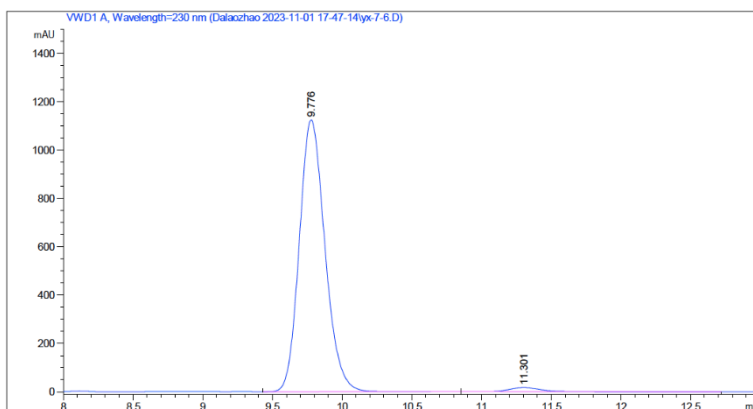
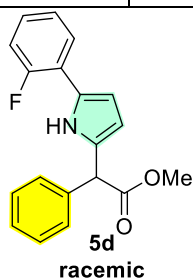
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	7.356	MM	0.1666	8616.14941	861.86407	96.7164
2	7.901	MM	0.1885	292.52292	25.86859	3.2836



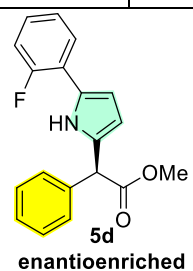
**5d**, HPLC conditions: Daicel CHIRALPAK® AD-H column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 230$  nm.



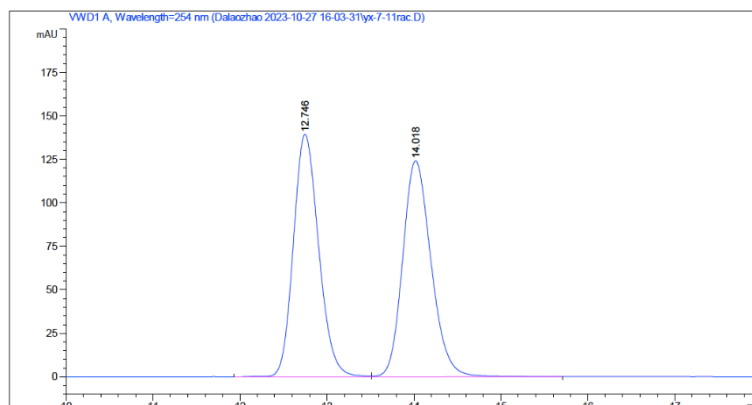
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.773	VB R	0.1948	1.69238e4	1345.37915	48.5949
2	11.284	BB	0.2403	1.79024e4	1137.91150	51.4051



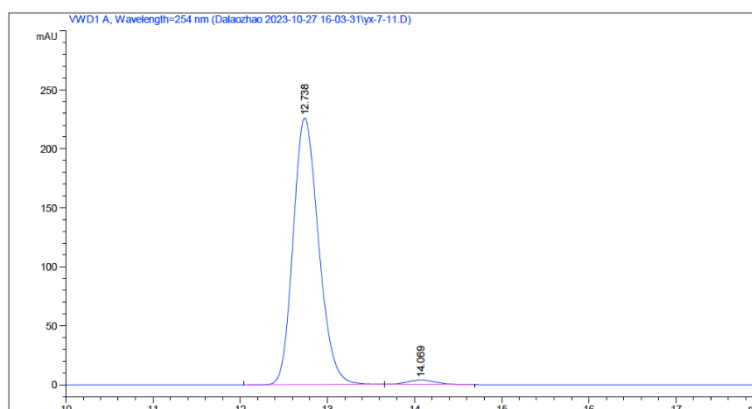
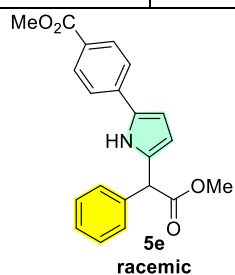
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.776	BB	0.1971	1.43685e4	1124.67297	98.0484
2	11.301	BB	0.2466	285.99020	17.44712	1.9516



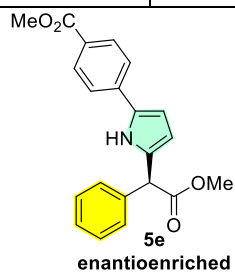
**5e**, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



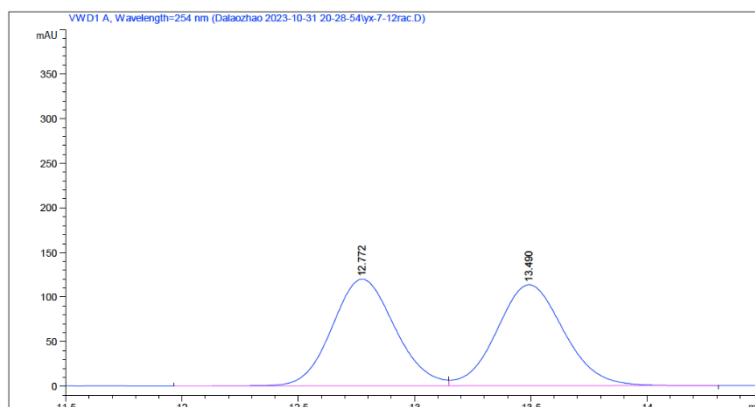
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.746	BV	0.3144	2817.26099	139.42563	50.0241
2	14.018	VB	0.3491	2814.54272	124.06582	49.9759



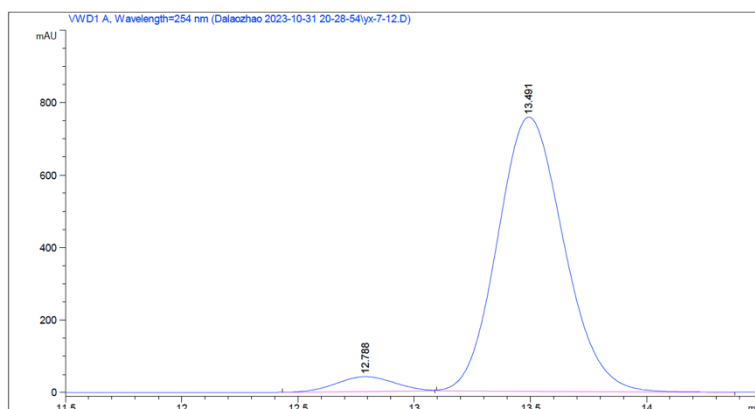
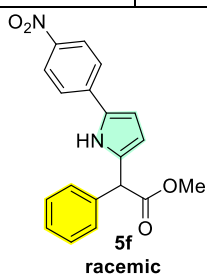
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.738	BB	0.3133	4571.39844	225.89697	98.2464
2	14.069	BB	0.3423	81.59534	3.69189	1.7536



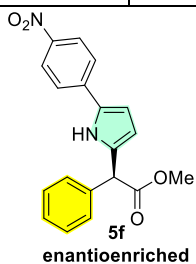
**5f**, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



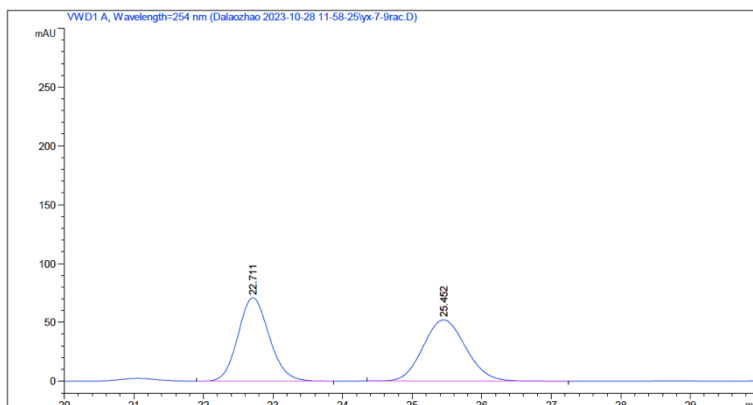
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.772	BV	0.2924	2253.58765	119.71539	49.8494
2	13.490	VB	0.3107	2267.20776	113.24815	50.1506



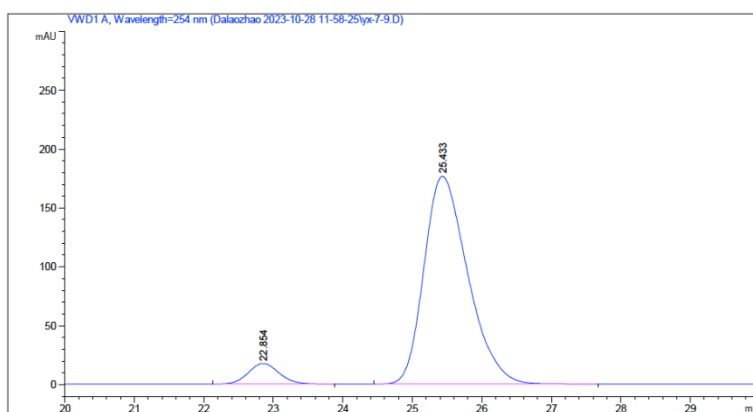
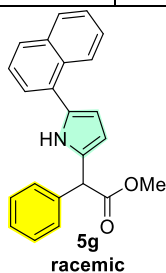
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.788	MM	0.2938	724.97583	41.13110	4.6153
2	13.491	MM	0.3297	1.49830e4	757.39014	95.3847



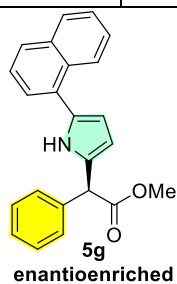
**5g**, HPLC conditions: Daicel CHIRALPAK® AD-H column; 1% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



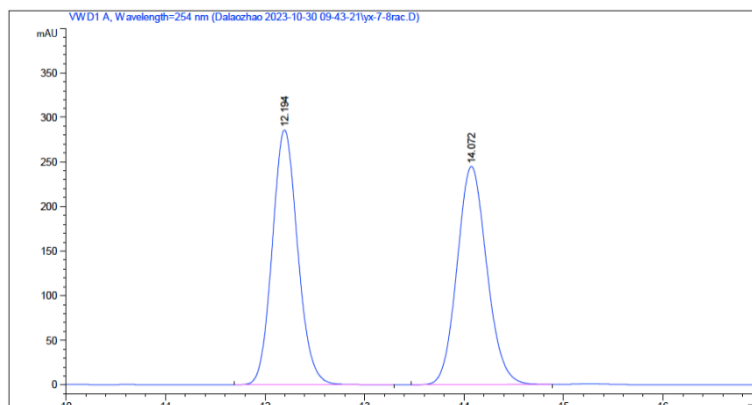
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	22.711	BB	0.4796	2205.57910	70.85541	49.9728
2	25.452	BB	0.6662	2207.97998	51.95373	50.0272



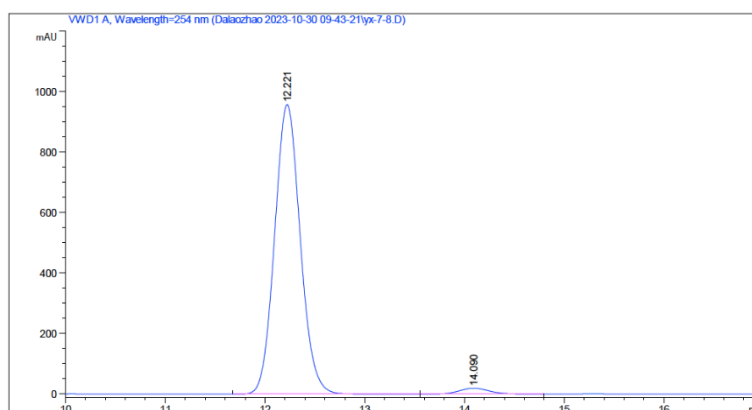
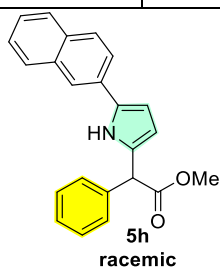
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	22.854	BB	0.4709	536.26276	17.50987	6.5103
2	25.433	BB	0.6726	7700.87598	176.32184	93.4897



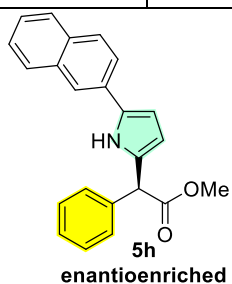
**5h**, HPLC conditions: Daicel CHIRALPAK® AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



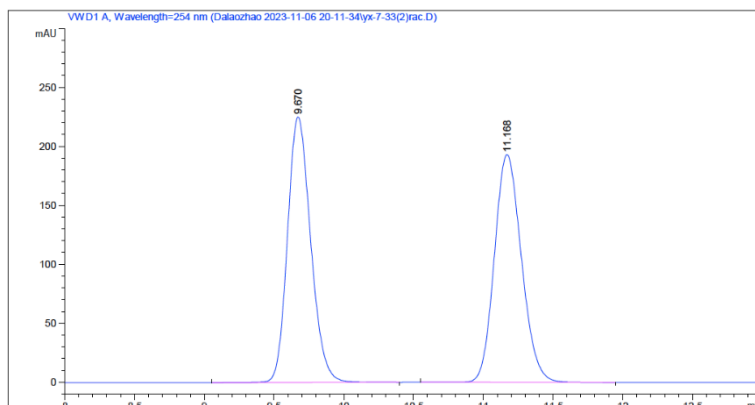
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.194	BB	0.2725	5069.54541	285.70529	49.9270
2	14.072	BB	0.3224	5084.36816	244.74724	50.0730



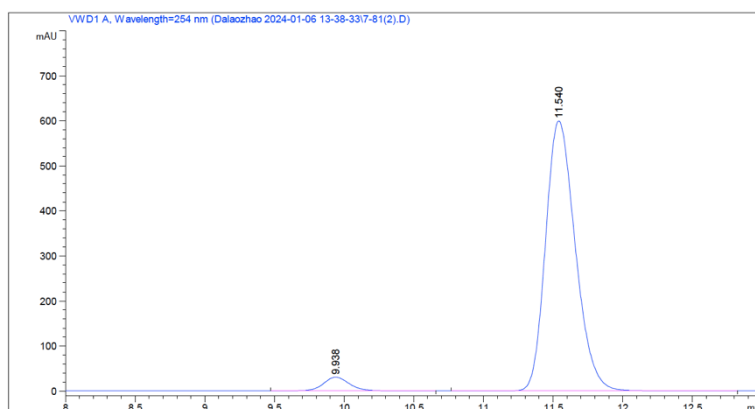
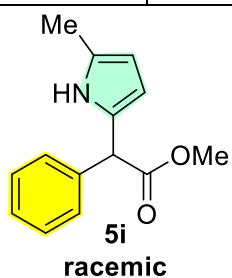
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.221	BB	0.2763	1.70521e4	957.08875	97.7194
2	14.090	BB	0.3185	397.96979	19.24032	2.2806



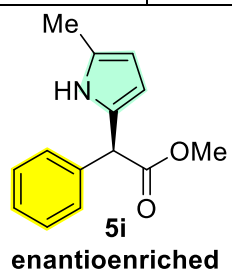
**5i**, HPLC conditions: Daicel CHIRALPAK® IC column; 1% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.670	BB	0.1787	2604.34277	225.04472	49.9632
2	11.168	BB	0.2099	2608.18164	193.17096	50.0368

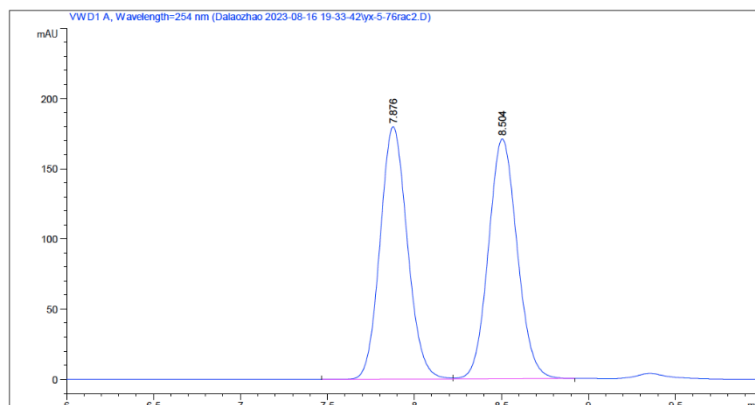


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.938	BB	0.1971	389.88803	30.21919	4.2129
2	11.540	BB	0.2294	8864.76855	599.09741	95.7871

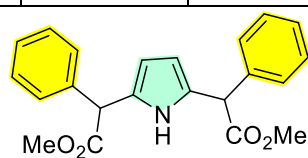




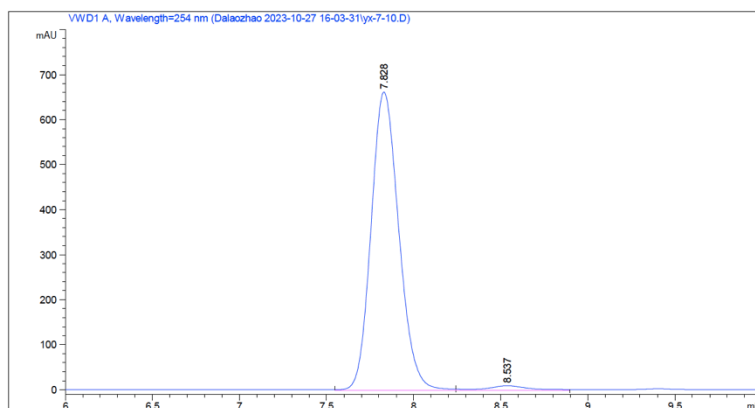
**5j**, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



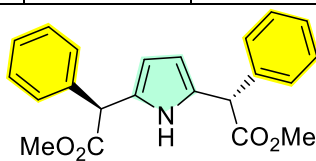
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	7.876	BV	0.1694	1961.60168	179.88727	49.9559
2	8.504	VB	0.1792	1965.06750	170.99181	50.0441



**5j**  
racemic

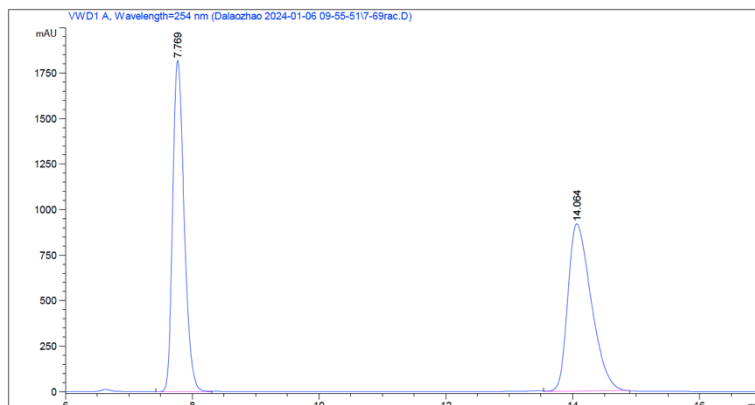


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	7.828	MM	0.1844	7334.12744	662.76801	97.7959
2	8.537	MM	0.2830	165.29617	9.73454	2.2041

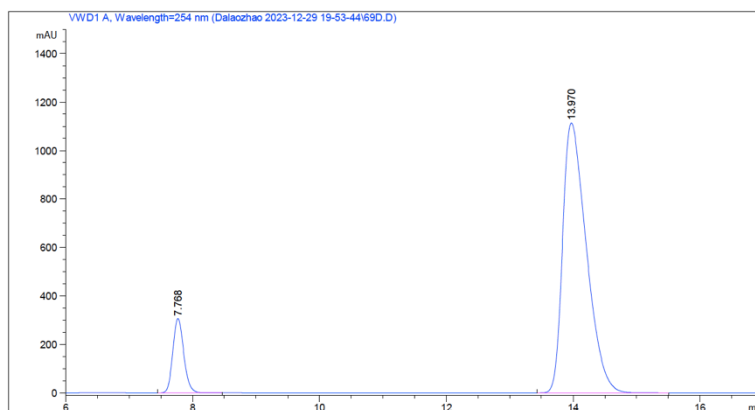
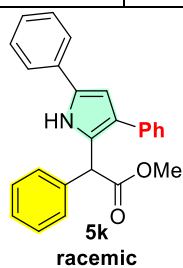


**5j**  
enantioenriched

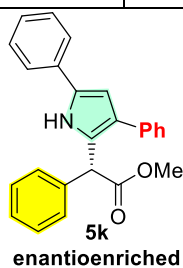
**5k**, HPLC conditions: Daicel CHIRALPAK® AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



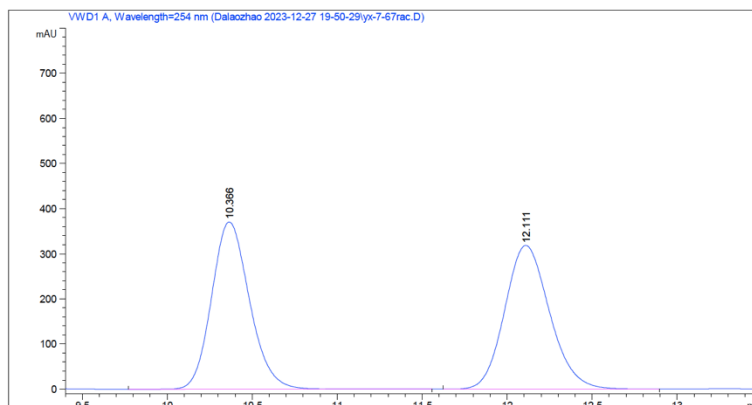
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	7.769	MM	0.2087	2.28026e4	1820.85608	49.2046
2	14.064	MM	0.4268	2.35398e4	919.19678	50.7954



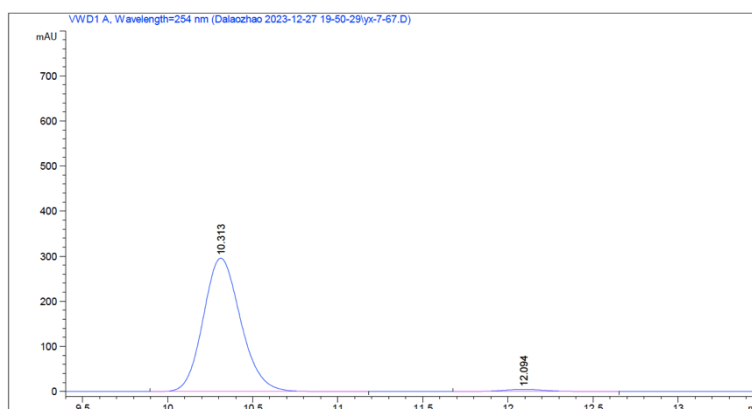
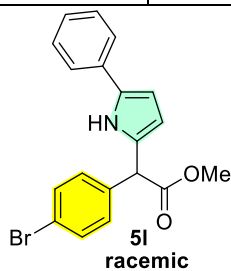
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	7.768	BB	0.1845	3659.41284	306.42999	11.2436
2	13.970	BB	0.3989	2.88873e4	1113.13196	88.7564



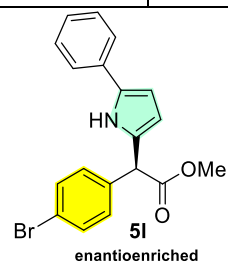
**51**, HPLC conditions: Daicel CHIRALPAK® AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



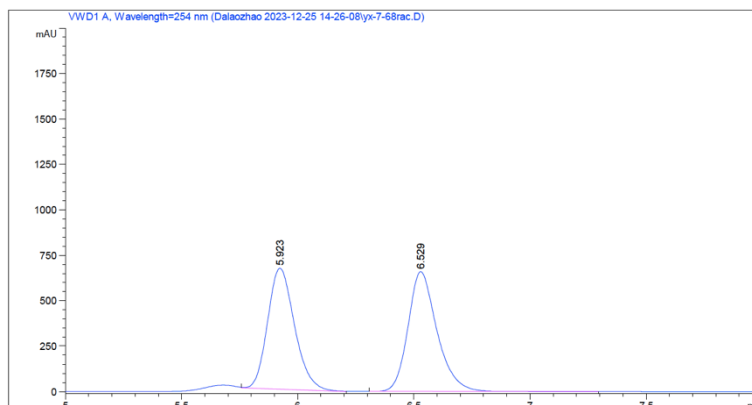
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.366	BB	0.2390	5743.78174	370.79562	49.6202
2	12.111	BB	0.2836	5831.70020	318.36789	50.3798



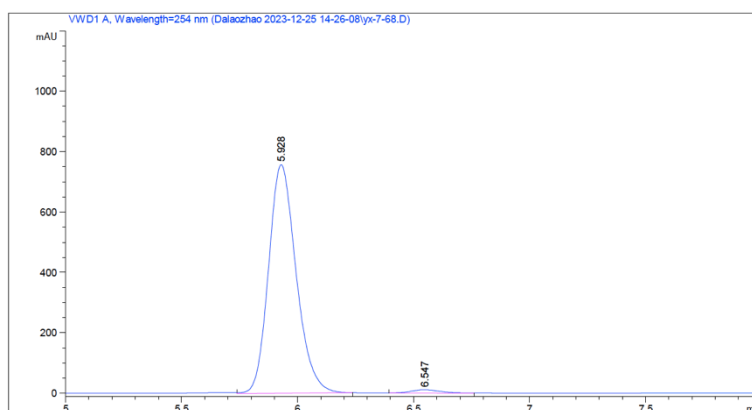
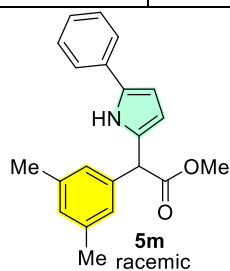
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.313	BB	0.2366	4524.41455	296.02994	98.1893
2	12.094	BB	0.2731	83.43538	4.62413	1.8107



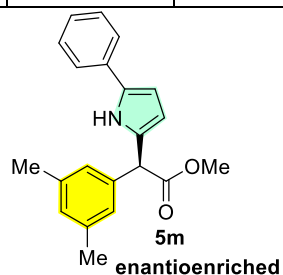
**5m**, HPLC conditions: Daicel CHIRALPAK® AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



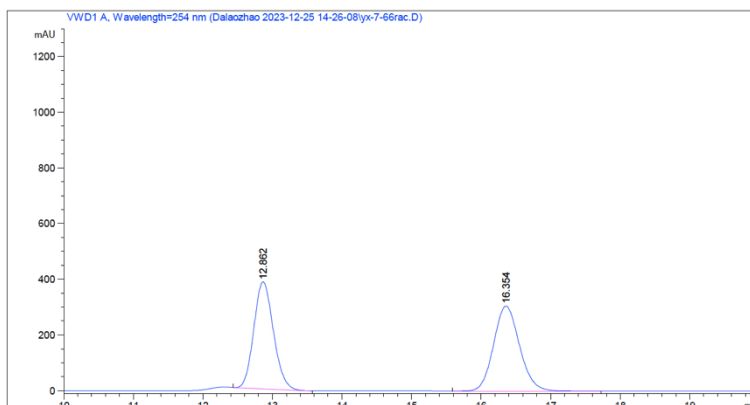
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	5.923	MM	0.1339	5349.33936	665.79333	48.3855
2	6.529	BB	0.1300	5706.31934	659.67432	51.6145



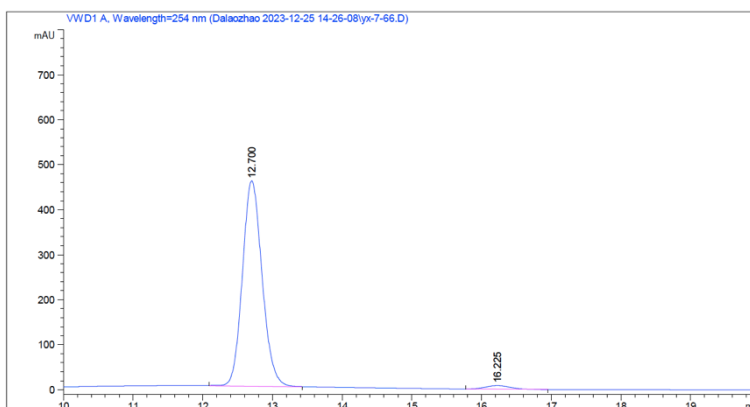
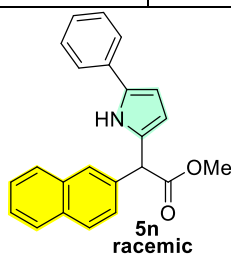
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	5.928	MM	0.1376	6253.89258	757.50269	98.4057
2	6.547	MM	0.1517	101.32139	11.13322	1.5943



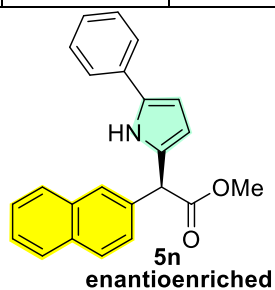
**5n**, HPLC conditions: Daicel CHIRALPAK® AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



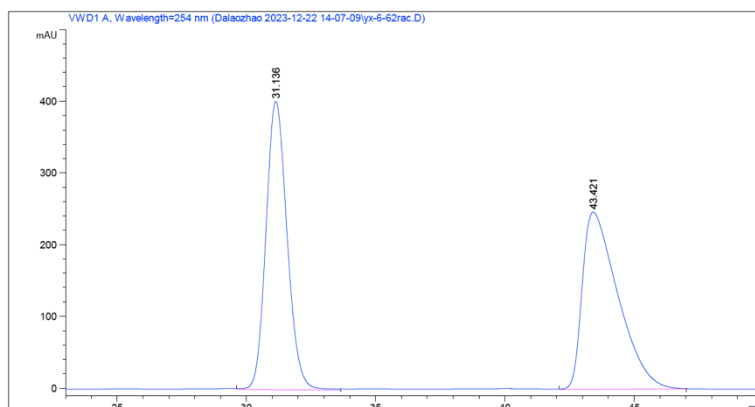
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.862	MM	0.3272	7546.04785	384.33258	48.9830
2	16.354	BB	0.4002	7859.39697	304.46539	51.0170



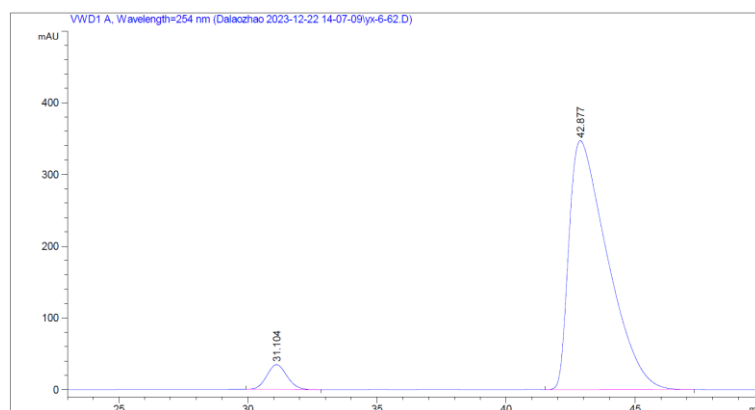
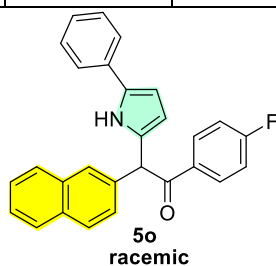
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.700	MM	0.3268	8954.52148	456.68158	97.8199
2	16.225	MM	0.4168	199.56705	7.98092	2.1801



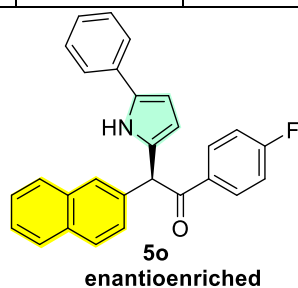
**5o**, HPLC conditions: Daicel CHIRALPAK® AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



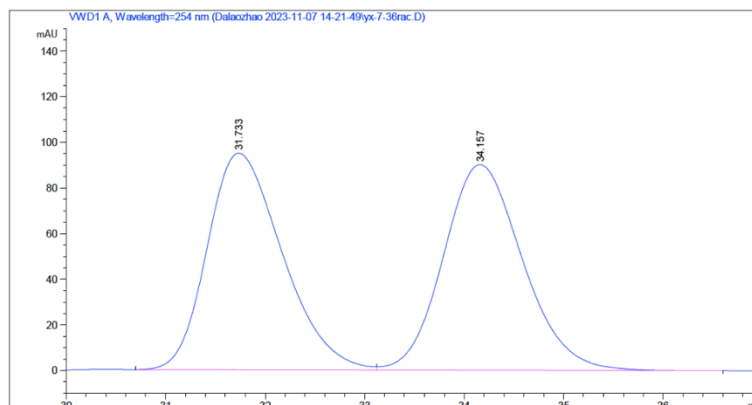
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	31.136	MM	0.9462	2.28110e4	401.79007	49.0546
2	43.421	MM	1.5990	2.36902e4	246.92311	50.9454



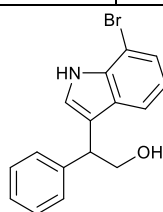
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	31.104	BB	0.8326	1863.81421	34.42153	4.9332
2	42.877	BB	1.5297	3.59170e4	346.89438	95.0668



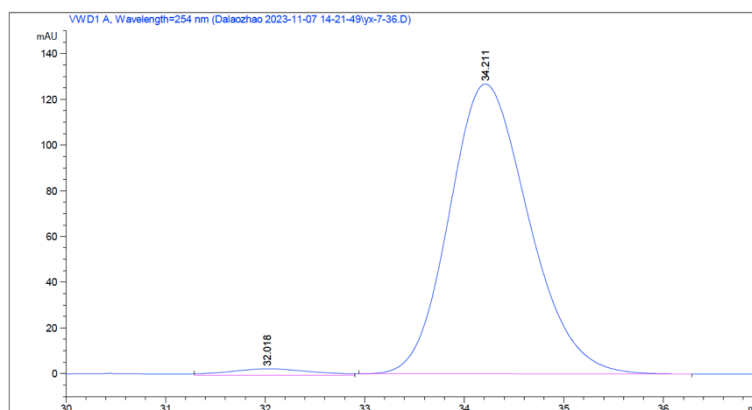
6, HPLC conditions: Daicel CHIRALPAK® AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



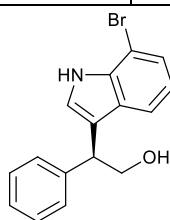
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	31.733	BV	0.8039	4974.74268	94.88175	49.9589
2	34.157	VB	0.8460	4982.93604	90.12096	50.0411



**6**  
racemic

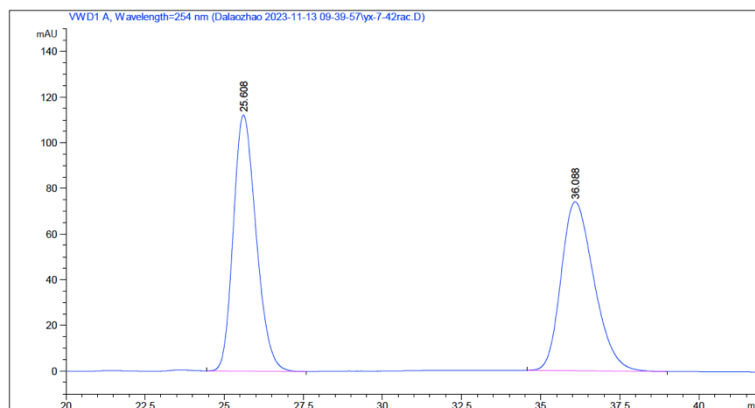


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	32.018	MM	0.9106	142.02074	2.59949	1.9868
2	34.211	BB	0.8561	7006.22852	126.73658	98.0132

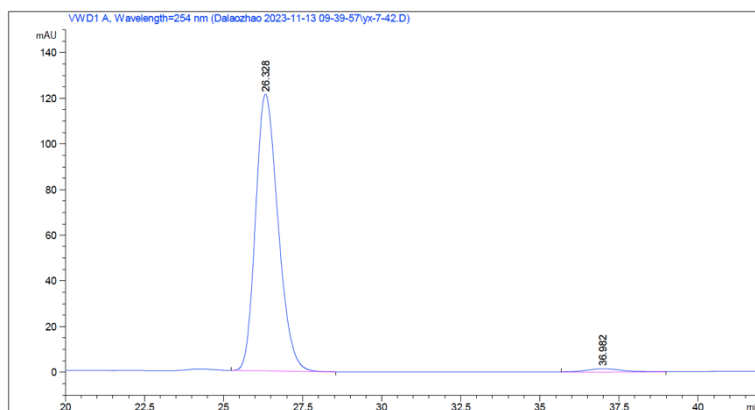
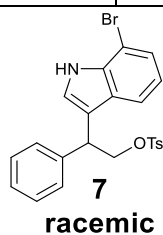


**6**  
enantioenriched

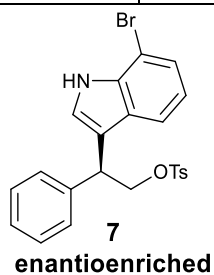
7, HPLC conditions: Daicel CHIRALPAK® AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	25.608	BB	0.7810	5619.25879	112.16592	51.2889
2	36.088	BB	1.1112	5336.83984	73.96053	48.7111

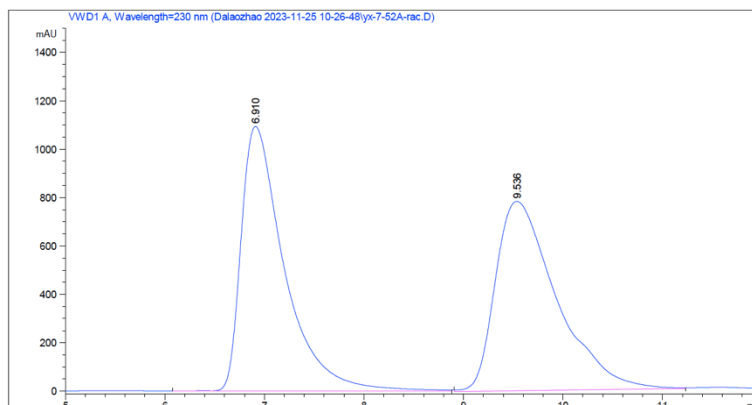


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	26.328	BB	0.7686	5984.24268	121.11806	97.8025
2	36.982	MM	1.4557	134.45738	1.53943	2.1975

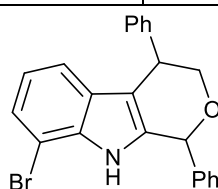




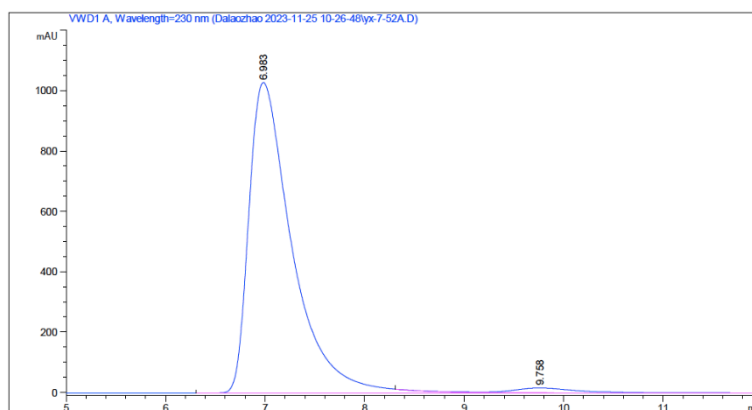
**8A**, HPLC conditions: Daicel CHIRALPAK® AS-H column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 230$  nm.



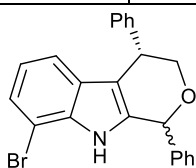
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	6.910	VV R	0.4492	3.29429e4	1093.06238	49.6496
2	9.536	MM	0.7109	3.34079e4	783.18402	50.3504



**8A**  
racemic

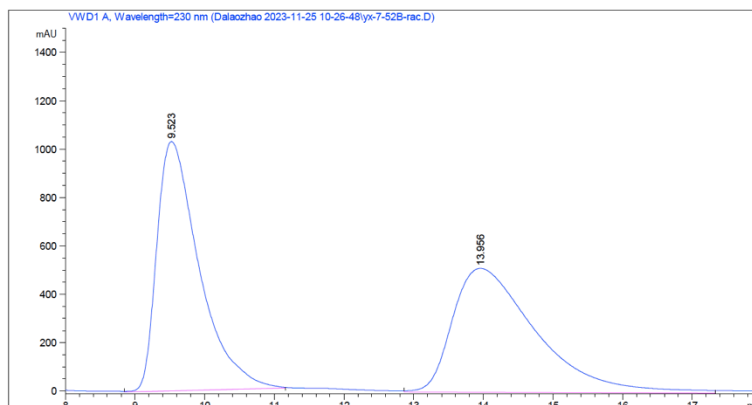


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	6.983	VV R	0.4508	3.11486e4	1028.71729	97.5085
2	9.758	VB E	0.7052	795.88928	16.17228	2.4915

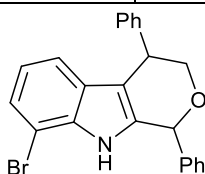


**8A**  
enantiomerically enriched

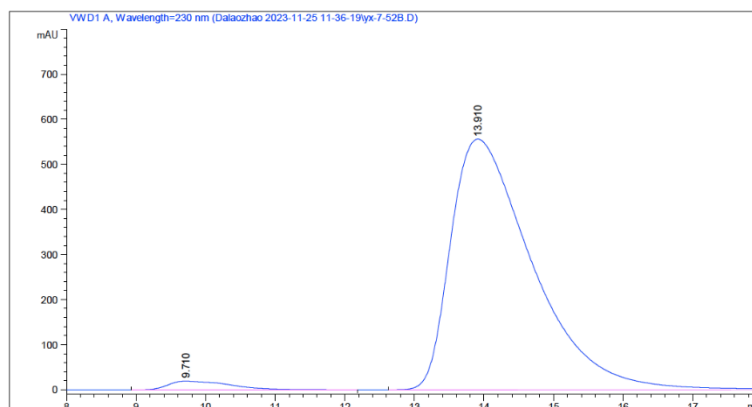
**8B**, HPLC conditions: Daicel CHIRALPAK® AS-H column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 230$  nm.



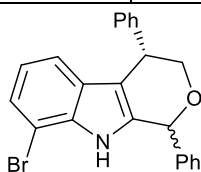
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.523	MM	0.7035	4.35056e4	1030.74377	50.4937
2	13.956	MM	1.3877	4.26548e4	512.29272	49.5063



**8B**  
racemic

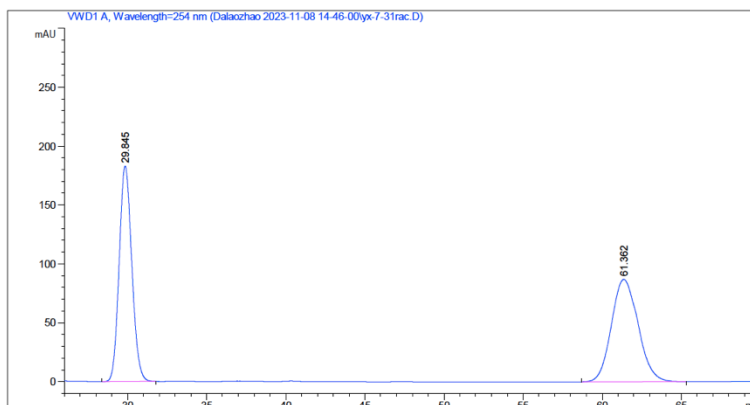


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.710	BB	0.8192	1202.04504	19.55051	2.5799
2	13.910	BB	1.2156	4.53900e4	556.22821	97.4201

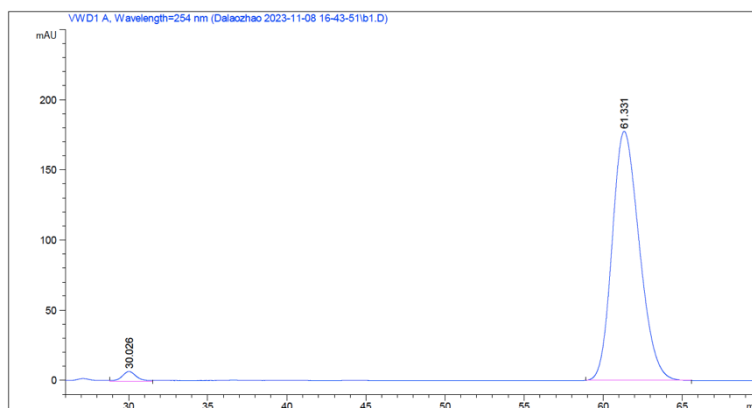
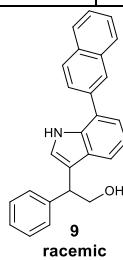


**8B**  
enantioenriched

**9**, HPLC conditions: Daicel CHIRALPAK® AD-H column; 15% *i*-PrOH in *n*-hexane; 1.0 mL/min,  $\lambda = 254$  nm.



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	29.845	BB	0.8633	1.01628e4	183.02049	49.9264
2	61.362	BB	1.6750	1.01927e4	86.84803	50.0736



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	30.026	MM	1.0901	461.42273	7.05464	2.1323
2	61.331	BB	1.7707	2.11778e4	177.48291	97.8677

