

Supporting Information

**Primary Activation of *para*-Quinone Methides by Chiral Phosphoric Acid for  
Enantioselective Construction of Tetraarylmethanes**

Zhengyu Han,<sup>a</sup> Biao Zhu,<sup>a</sup> Yu Zang,<sup>a</sup> Chaoshen Zhang,<sup>\*,b,c,d</sup> Xiu-Qin Dong,<sup>e</sup>  
Hai Huang<sup>\*,a</sup> and Jianwei Sun<sup>\*,a,c,d</sup>

<sup>a</sup>Jiangsu Key Laboratory of Advanced Catalytic Materials & Technology, School of Petrochemical Engineering, Changzhou University, Changzhou (China)

<sup>b</sup>Shenzhen Bay Laboratory, Shenzhen 518132 (China)

<sup>c</sup>Shenzhen Research Institute, HKUST, No. 9 Yuexing 1st Rd, Shenzhen 518057, China

<sup>d</sup>Department of Chemistry, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong SAR (China)

<sup>e</sup>College of Chemistry and Molecular Sciences, Engineering Research Center of Organosilicon Compounds & Materials, Ministry of Education, Wuhan University, Wuhan, Hubei (China)

**Table of Contents**

I.	General Information .....	S-2
II.	Synthesis of Tertiary Alcohol Substrates .....	S-3
III.	Catalytic Asymmetric Synthesis of Tetraarylmethanes .....	S-11
IV.	Product Derivatizations.....	S-38
V.	Mechanistic Experiments .....	S-41
VI.	DFT Calculations .....	S-42
VII.	Determination of the Absolute Stereochemistry .....	S-54
VIII.	References .....	S-61

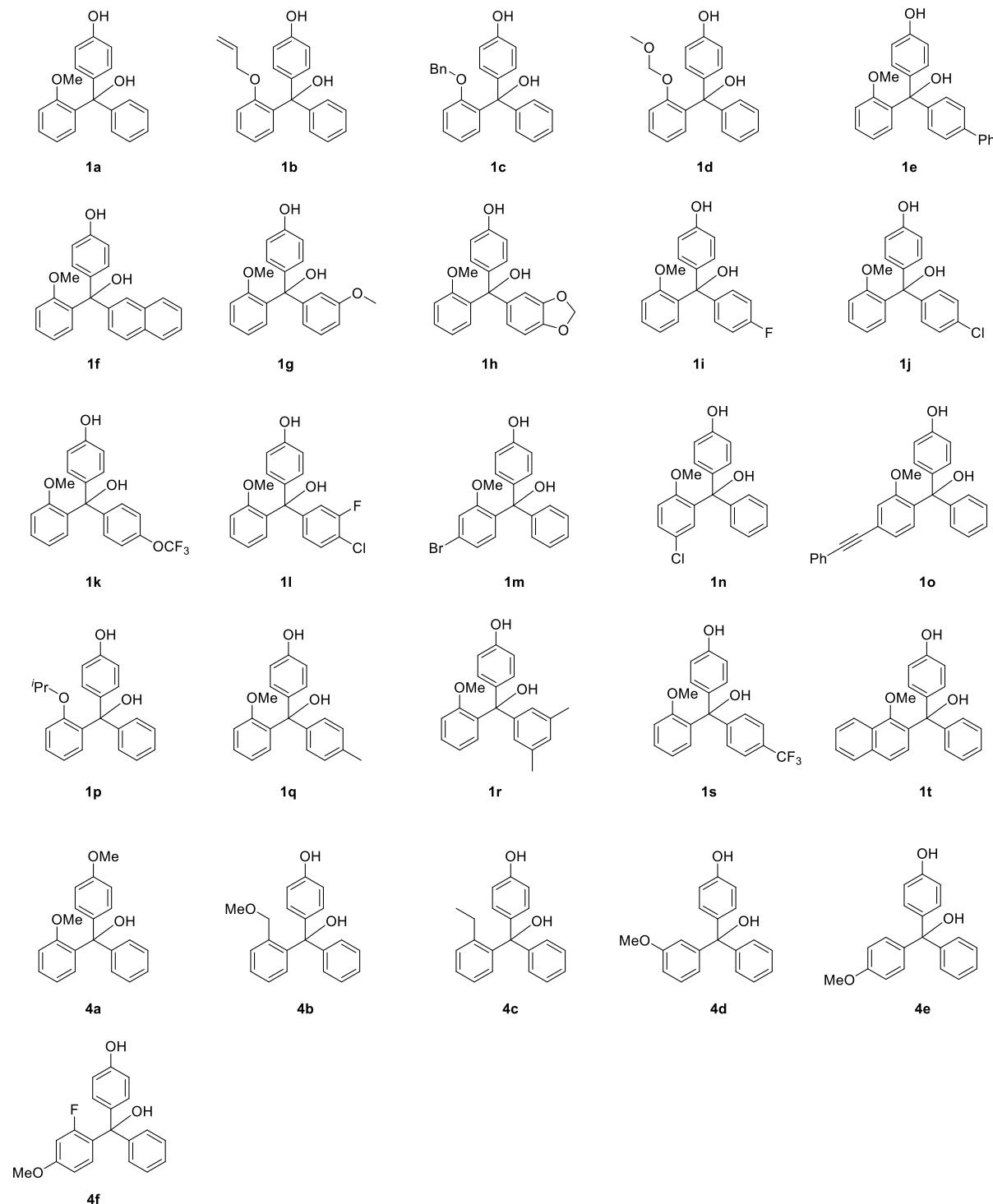
**NMR and HPLC Traces**

## I. General Information

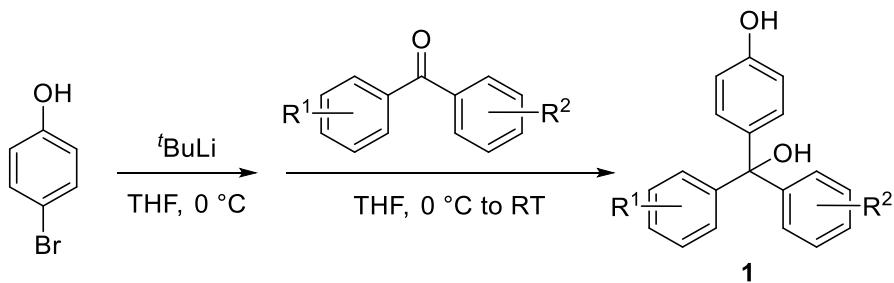
Flash column chromatography was performed over silica gel (200-300 mesh) purchased from Qindao Puke Co., China. All air or moisture sensitive reactions were conducted in oven-dried glassware under nitrogen atmosphere using anhydrous solvents. Anhydrous dichloromethane and tetrahydrofuran were purified by the Innovative® solvent purification system. Anhydrous solvents were purchased from Sigma-Aldrich® and J&K® and used as received. <sup>1</sup>H, <sup>13</sup>C and <sup>19</sup>F spectra were collected on a Bruker AV 400 MHz 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, DMSO-*d*<sub>6</sub> at 2.5 ppm, <sup>13</sup>C NMR: CDCl<sub>3</sub> at 77.0 ppm, DMSO-*d*<sub>6</sub> at 39.5 ppm). Mass spectra were collected on an Agilent GC/MS 5975C system or an API QSTAR XL System. Optical rotations were measured on a RUDOLPH® AUTOPOL I automatic polarimeter with [α]<sub>D</sub> values reported in degrees; concentration (*c*) is in 10 mg/mL. The enantiomeric excesses were determined by chiral HPLC using an Agilent 1260 LC instrument with Daicel Chiralpak AD-H, IC, AS-H or Daicel Chiralcel OD-H column. Unless otherwise noted, the racemic samples in this study were prepared using the racemic phosphoric acid catalyst 1,1'-binaphthyl-2,2'-diyl hydrogenphosphate (10 mol%).

## II. Synthesis of Tertiary Alcohol Substrates

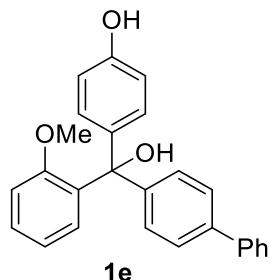
All the substrates were synthesized according to the literature procedures,<sup>1</sup> and the characterization data of **1a – 1d**, **1f – 1i**, **1p**, **1t**, and **4a – 4f** were consistent with those reported in the literature.<sup>1,2</sup>



### General Procedure A: Preparation of Tertiary Alcohol Substrates



Under N<sub>2</sub>, *tert*-butyllithium (1.6 M in pentane, 15.5 mL, 24.8 mmol, 8.2 equiv.) was slowly added to a stirred solution of 4-bromophenol (1.30 g, 7.5 mmol, 2.5 equiv.) in THF (50 mL) at 0 °C. The resulting mixture was stirred at 0 °C for 2 hours. Subsequently, a solution of the corresponding diaryl ketone (3.0 mmol, 1.0 equiv.) in THF (10 mL) was added and the reaction mixture was kept stirring overnight at room temperature. A saturated aqueous solution of NH<sub>4</sub>Cl was added to quench the reaction. The reaction mixture was extracted with EtOAc (3 × 30 mL). The combined organic layers were dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and filtered, then the filtrate was concentrated and the residue was purified by silica gel flash chromatography to afford the desired tertiarymethanol **1**.

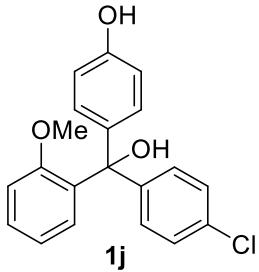


**4-([1,1'-Biphenyl]-4-yl(hydroxy)(2-methoxyphenyl)methyl)phenol (1e)** was prepared according to the General Procedure A as yellow solid (chromatography eluent: hexanes/EtOAc = 15:1 → 10:1) in 63% yield (722 mg).

<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 7.65–7.57 (m, 2H), 7.57–7.49 (m, 2H), 7.49–7.38 (m, 2H), 7.38–7.24 (m, 4H), 7.17–7.10 (m, 2H), 6.97 (dd, *J*<sub>1</sub> = 8.2 Hz, *J*<sub>2</sub> = 1.1 Hz, 1H), 6.89–6.81 (m, 1H), 6.79–6.72 (m, 2H), 6.59 (dd, *J*<sub>1</sub> = 7.7 Hz, *J*<sub>2</sub> = 1.7 Hz, 1H), 5.39 (s, 1H), 3.69 (s, 3H) ppm.

**<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>) δ 157.3, 154.6, 145.9, 140.8, 139.6, 138.8, 135.2, 130.2, 129.2, 129.0, 128.7, 128.2, 127.2, 127.0, 126.3, 120.5, 114.5, 112.0, 81.8, 55.8 ppm.

**HRMS (ES+)** Calcd for C<sub>26</sub>H<sub>22</sub>O<sub>3</sub>Na [M + Na]<sup>+</sup>: 405.1467, Found: 405.1465.

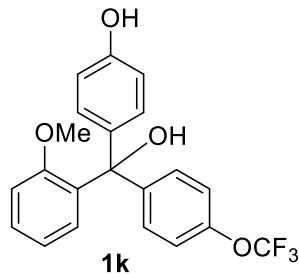


**4-((4-Chlorophenyl)(hydroxy)(2-methoxyphenyl)methyl)phenol (1j)** was prepared according to the General Procedure A as a yellow solid (chromatography eluent: hexanes/EtOAc = 15:1 → 10:1) in 73% yield (746.0 mg).

**<sup>1</sup>H NMR** (400 MHz, DMSO-d<sub>6</sub>) δ 9.34 (s, 1H), 7.31 (d, J = 8.6 Hz, 2H), 7.29–7.26 (m, 1H), 7.15 (d, J = 8.6 Hz, 2H), 7.01 (d, J = 8.0 Hz, 1H), 6.94 (d, J = 8.7 Hz, 2H), 6.91–6.86 (m, 2H), 6.67 (d, J = 8.7 Hz, 2H), 5.68 (s, 1H), 3.49 (s, 3H) ppm.

**<sup>13</sup>C NMR** (101 MHz, DMSO-d<sub>6</sub>) δ 156.7, 156.1, 146.6, 136.5, 134.9, 131.0, 129.3, 128.9, 128.7, 128.4, 127.2, 120.0, 114.2, 112.4, 79.5, 55.3 ppm.

**HRMS (ES+)** Calcd for C<sub>20</sub>H<sub>17</sub>ClO<sub>3</sub> [M + H]<sup>+</sup>: 341.0944, Found: 341.0947.



**4-(Hydroxy(2-methoxyphenyl)(4-(trifluoromethoxy)phenyl)methyl)phenol (1k)** was prepared according to the General Procedure A as a yellow solid (chromatography eluent: hexanes/EtOAc = 15:1 → 10:1) in 66% yield (773.0 mg).

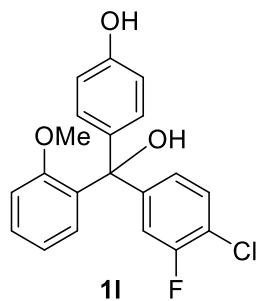
**<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>) δ 7.34–7.22 (m, 3H), 7.15–7.08 (m, 2H), 7.06–6.99 (m, 2H),

6.95 (dd,  $J_1$  = 8.3 Hz,  $J_2$  = 1.1 Hz, 1H), 6.83 (td,  $J_1$  = 7.5 Hz,  $J_2$  = 1.1 Hz, 1H), 6.74–6.67 (m, 2H), 6.50 (dd,  $J_1$  = 7.7 Hz,  $J_2$  = 1.7 Hz, 1H), 3.66 (s, 3H) ppm.

**$^{13}\text{C}$  NMR** (75 MHz,  $\text{CDCl}_3$ )  $\delta$  157.1, 154.9, 148.2, 145.4, 137.9, 134.7, 130.1, 129.2 (2C), 129.1, 120.6, 120.5 (q,  $J$  = 255.7 Hz), 119.9, 114.7, 112.0, 81.7, 55.7 ppm.

**$^{19}\text{F}$  NMR** (282 MHz,  $\text{CDCl}_3$ )  $\delta$  -57.7 ppm.

**HRMS (ES+)** Calcd for  $\text{C}_{21}\text{H}_{17}\text{F}_3\text{O}_4\text{Na} [\text{M} + \text{Na}]^+$ : 413.0977, Found: 413.0973.



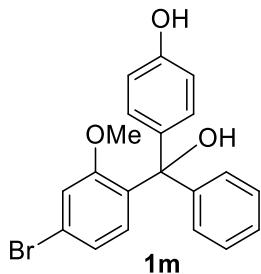
**4-((4-Chloro-3-fluorophenyl)(hydroxy)(2-methoxyphenyl)methyl)phenol (11)** was prepared according to the General Procedure A as a yellow solid (chromatography eluent: hexanes/EtOAc = 15:1 → 10:1) in 51% yield ( 550.0 mg).

**$^1\text{H}$  NMR** (400 MHz,  $\text{DMSO}-d_6$ )  $\delta$  9.38 (s, 1H), 7.46 (t,  $J$  = 8.2 Hz, 1H), 7.32–7.28 (m, 1H), 7.11 (dd,  $J_1$  = 1.9 Hz,  $J_2$  = 11.2 Hz, 1H), 7.02–6.93 (m, 5H), 6.90 (t,  $J$  = 7.5 Hz, 1H), 6.68 (d,  $J$  = 8.6 Hz, 2H), 5.85 (s, 1H), 3.49 (s, 3H) ppm.

**$^{13}\text{C}$  NMR** (101 MHz,  $\text{DMSO}-d_6$ )  $\delta$  156.6, 156.5 (d,  $J$  = 243.0 Hz), 156.2, 149.8 (d,  $J$  = 6.0 Hz), 135.9, 134.4, 129.3, 129.1, 128.7, 128.3, 124.7 (d,  $J$  = 3.0 Hz), 120.1, 117.1 (d,  $J$  = 17.0 Hz), 115.5 (d,  $J$  = 21.0 Hz), 114.3, 112.4, 79.2, 55.3 ppm.

**$^{19}\text{F}$  NMR** (282 MHz,  $\text{DMSO}-d_6$ )  $\delta$  -117.4 ppm.

**HRMS (ES+)**: Calcd for  $\text{C}_{20}\text{H}_{16}\text{ClFO}_3\text{Na} [\text{M} + \text{Na}]^+$ : 381.0670, Found: 381.0666.



**4-((4-Bromo-2-methoxyphenyl)(hydroxy)(phenyl)methyl)phenol (1m)** was prepared according to the General Procedure A as a yellow solid (chromatography eluent: hexanes/EtOAc = 15:1 → 10:1) in 60% yield ( 693.0 mg).

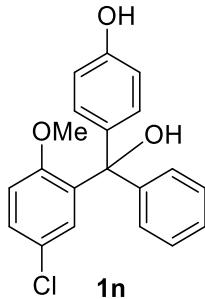
**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.33–7.17 (m, 6H), 7.03 (d, *J* = 8.7 Hz, 2H), 6.86 (d, *J* = 8.7

Hz, 1H), 6.71 (d, *J* = 8.7 Hz, 2H), 6.50 (d, *J* = 2.6 Hz, 1H), 5.23 (s, 1H), 3.62 (s, 3H) ppm.

**<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>) δ 155.9, 154.9, 146.0, 137.7, 137.2, 130.1, 129.1, 128.6, 127.8,

127.5, 127.2, 125.7, 114.7, 113.3, 81.7, 56.1 ppm.

**HRMS (ES+)** Calcd for C<sub>20</sub>H<sub>18</sub>BrO<sub>3</sub> [M + H]<sup>+</sup>: 385.0439, Found: 385.0436.



**4-((5-Chloro-2-methoxyphenyl)(hydroxy)(phenyl)methyl)phenol (1n)** was prepared according to the General Procedure A as a yellow solid (chromatography eluent: hexanes/EtOAc = 15:1 → 10:1) in 47% yield ( 481.0 mg).

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.33–7.16 (m, 5H), 7.06 (d, *J* = 1.9 Hz, 1H), 7.02–6.98 (m,

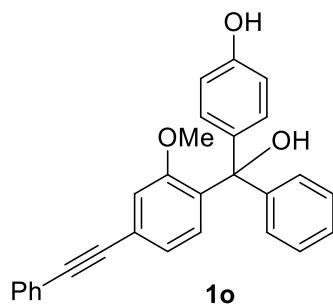
2H), 6.95 (dd, *J*<sub>1</sub> = 8.3 Hz, *J*<sub>2</sub> = 1.9 Hz, 1H), 6.74–6.65 (m, 2H), 6.38 (d, *J* = 8.3 Hz, 1H),

5.12 (s, 2H), 3.64 (s, 3H) ppm.

**<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>) δ 157.8, 154.9, 146.1, 137.8, 134.5, 131.4, 129.1, 127.7, 127.5,

127.2, 123.4, 122.1, 115.5, 114.6, 81.7, 56.1 ppm.

**HRMS (ES+)** Calcd for C<sub>20</sub>H<sub>17</sub>ClO<sub>3</sub> [M + H]<sup>+</sup>: 341.0944, Found: 341.0947.

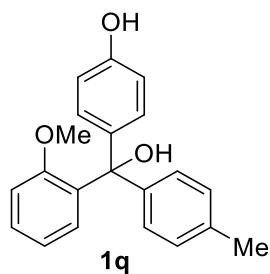


**4-(Hydroxy(2-methoxyphenyl)(4-(phenylethyynyl)phenyl)methyl)phenol (1o)** was prepared according to the General Procedure A as a yellow solid (chromatography eluent: hexanes/EtOAc = 15:1 → 10:1) in 58% yield (573.0 mg).

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.54–7.51 (m, 2H), 7.38–7.19 (m, 8H), 7.10 (d, *J* = 1.5 Hz, 1H), 7.08–7.03 (m, 2H), 7.00 (dd, *J*<sub>1</sub> = 8.0 Hz, *J*<sub>2</sub> = 1.5 Hz, 1H), 6.72 (d, *J* = 8.7 Hz, 2H), 6.51 (d, *J* = 7.9 Hz, 1H), 5.26 (s, 1H), 3.68 (s, 3H) ppm.

**<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>) δ 157.0, 154.8, 146.4, 138.2, 135.8, 131.6, 130.2, 129.2, 128.4, 128.4, 127.7, 127.6, 127.1, 123.9, 123.7, 122.9, 114.9, 114.6, 89.8, 88.8, 81.9, 55.9 ppm.

**HRMS (ES+)** Calcd for C<sub>28</sub>H<sub>22</sub>O<sub>3</sub>Na [M + Na]<sup>+</sup>: 429.1467, Found: 429.1472.



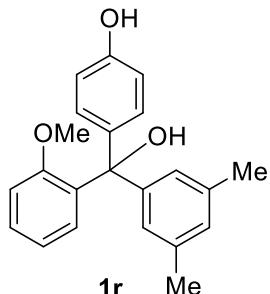
**4-(Hydroxy(2-methoxyphenyl)(p-tolyl)methyl)phenol (1q)** was prepared according to the General Procedure A as a yellow solid (chromatography eluent: hexanes/EtOAc = 15:1 → 10:1) in 54% yield (519.0 mg).

**<sup>1</sup>H NMR** (400 MHz, DMSO-*d*<sub>6</sub>) δ 9.30 (s, 1H), 7.26 (td, *J*<sub>1</sub> = 1.8 Hz, *J*<sub>2</sub> = 7.7 Hz, 1H), 7.07–7.00 (m, 5H), 6.93 (d, *J* = 8.7 Hz, 2H), 6.84 (td, *J*<sub>1</sub> = 0.8 Hz, *J*<sub>2</sub> = 7.5 Hz, 1H), 6.77 (dd, *J*<sub>1</sub> = 1.8 Hz, *J*<sub>2</sub> = 7.7 Hz, 1H), 6.66 (d, *J* = 8.7 Hz, 2H), 5.46 (s, 1H), 3.52 (s, 3H), 2.27 (s, 3H) ppm.

**<sup>13</sup>C NMR** (101 MHz, DMSO-*d*<sub>6</sub>) δ 156.9, 155.9, 144.5, 137.3, 135.5, 135.4, 128.7, 128.7 (2

C), 127.9, 127.4, 119.9, 114.1, 112.3, 80.1, 55.5, 20.6 ppm.

**HRMS** (Cl+) Calcd for C<sub>21</sub>H<sub>20</sub>O<sub>3</sub> [M]<sup>+</sup>: 320.1412, Found: 320.1400.

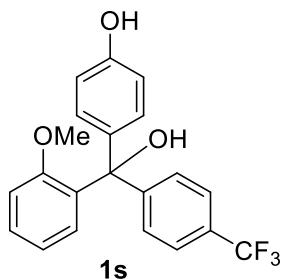


**4-((3,5-Dimethylphenyl)(hydroxy)(2-methoxyphenyl)methyl)phenol (1r)** was prepared according to the General Procedure A as a yellow solid (chromatography eluent: hexanes/EtOAc = 15:1 → 10:1) in 70% yield (702.0 mg).

**<sup>1</sup>H NMR** (300 MHz, DMSO-*d*<sub>6</sub>) δ 9.29 (s, 1H), 7.26 (td, *J*<sub>1</sub> = 7.7 Hz, *J*<sub>2</sub> = 1.8 Hz, 1H), 7.01 (d, *J* = 7.2 Hz, 1H), 6.94 (d, *J* = 8.7 Hz, 2H), 6.88–6.80 (m, 2H), 6.79–6.70 (m, 3H), 6.66 (d, *J* = 8.7 Hz, 2H), 5.44 (s, 1H), 3.53 (s, 3H), 2.18 (s, 6H) ppm.

**<sup>13</sup>C NMR** (75 MHz, DMSO-*d*<sub>6</sub>) δ 157.0, 155.9, 147.4, 137.3, 136.0, 135.5, 128.8, 128.7, 128.7, 127.9, 125.3, 120.0, 114.1, 112.4, 80.2, 55.5, 21.2 ppm.

**HRMS** (ES+) Calcd for C<sub>22</sub>H<sub>23</sub>O<sub>3</sub> [M + H]<sup>+</sup>: 334.1647, Found: 335.1645.



**4-(Hydroxy(2-methoxyphenyl)(4-(trifluoromethyl)phenyl)methyl)phenol (1s)** was prepared according to the General Procedure A as a yellow solid (chromatography eluent: hexanes/EtOAc = 15:1 → 10:1) in 47% yield (528.0 mg).

**<sup>1</sup>H NMR** (400 MHz, DMSO-*d*<sub>6</sub>) δ 9.37 (s, 1H), 7.63 (d, *J* = 8.3 Hz, 2H), 7.38 (d, *J* = 8.2 Hz, 2H), 7.30 (td, *J*<sub>1</sub> = 1.4 Hz, *J*<sub>2</sub> = 7.6 Hz, 1H), 7.01–6.94 (m, 4H), 6.90 (t, *J* = 7.5 Hz, 1H), 6.68

(d,  $J$  = 8.6 Hz, 2H), 5.83 (s, 1H), 3.46 (s, 3H) ppm.

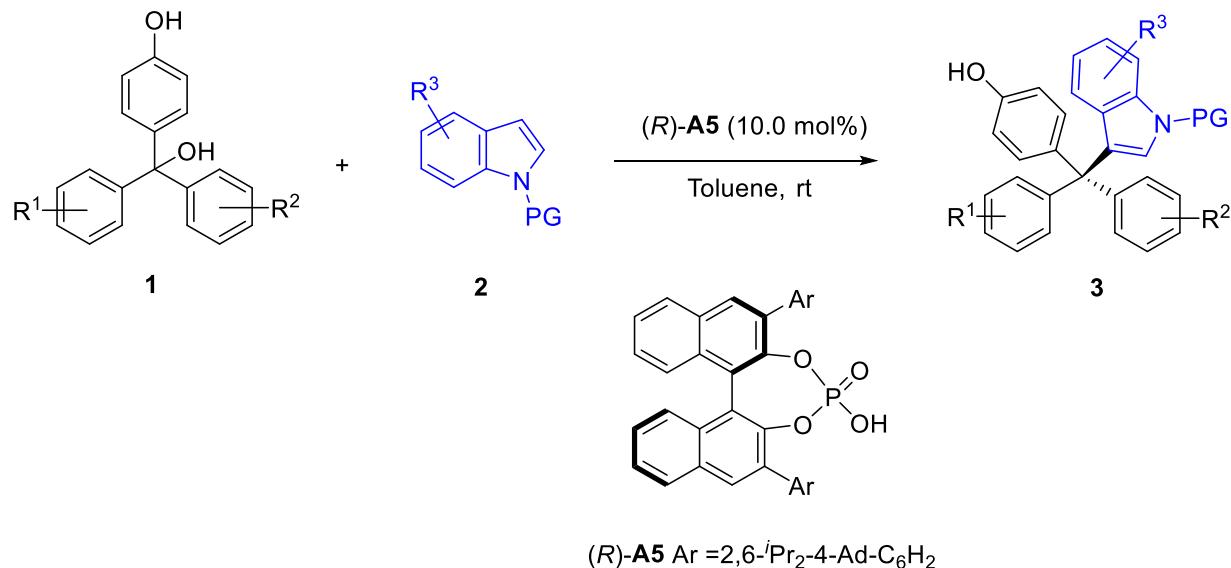
**$^{13}\text{C}$  NMR** (75 MHz, DMSO- $d_6$ )  $\delta$  156.6, 156.2, 152.3, 136.1, 134.7, 129.1, 128.8, 128.4, 128.1, 126.9 (q,  $J$  = 31.7 Hz), 124.5 (q,  $J$  = 272.0 Hz), 124.2 (q,  $J$  = 3.4 Hz), 120.1, 114.3, 112.4, 79.5, 55.3 ppm.

**$^{19}\text{F}$  NMR** (282 MHz, DMSO- $d_6$ )  $\delta$  -60.7 ppm.

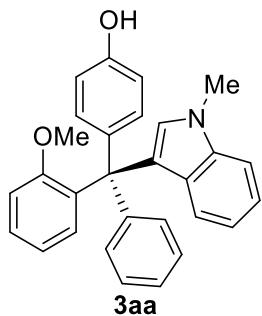
**HRMS** (ES+) Calcd for  $\text{C}_{21}\text{H}_{17}\text{F}_3\text{O}_3\text{Na} [\text{M} + \text{Na}]^+$ : 397.1027, Found: 397.1018.

### III. Catalytic Asymmetric Synthesis of Triarylmethanes

#### General Procedure B.



At room temperature, to an oven-dried 10-mL vial charged with a solution of the tertiary alcohol **1** (0.3 mmol, 1.0 equiv) and **CPA (R)-A5** (28 mg, 0.03 mmol, 10.0 mol%) in toluene (1.5 mL), *N*-protected-indole **2** (0.45 mmol, 1.5 equiv) was added in one portion. The reaction mixture was stirred at room temperature for 1 - 7 days. Upon reaction completing, Et<sub>3</sub>N (0.2 mL) was added and the mixture was stirred for 10 min, then concentrated under reduced pressure and further purified by silica gel flash chromatography to afford the desired product **3**.



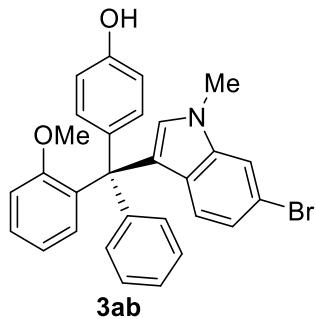
**(S)-4-((2-Methoxyphenyl)(1-methyl-1*H*-indol-3-yl)(phenyl)methyl)phenol (3aa)** was prepared according to the General Procedure B as off-white solid (chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 98% yield (123.0 mg, 92% ee). The reaction time was 3 days.

$[\alpha]_D^{25}$ : +2.50 ( $c = 1.0$ ,  $\text{CHCl}_3$ ). HPLC analysis of the product: Daicel CHIRALPAK IC column; 2% *i*-PrOH in hexanes, 0.4 mL/min; retention times: 39.2 min (major), 43.6 min (minor).

**$^1\text{H NMR}$**  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.32–7.06 (m, 11H), 6.92–6.81 (m, 2H), 6.76 (t,  $J = 1.2$  Hz, 1H), 6.68–6.59 (m, 4H), 4.84 (s, 1H), 3.69 (s, 3H), 3.14 (s, 3H) ppm.

**$^{13}\text{C NMR}$**  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  158.3, 153.0, 146.1, 137.8, 137.5, 136.2, 131.5, 130.7, 130.0, 129.9, 128.2, 128.1, 126.9, 125.3, 122.4, 122.1, 120.9, 120.2, 118.5, 113.7, 113.4, 108.8, 57.3, 55.3, 32.7 ppm.

**HRMS (ES+)** Calcd for  $\text{C}_{29}\text{H}_{25}\text{NO}_2\text{Na} [\text{M} + \text{Na}]^+$ : 442.1792, Found: 442.1783.



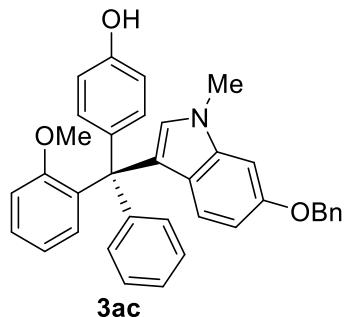
**(S)-4-((6-Bromo-1-methyl-1*H*-indol-3-yl)(2-methoxyphenyl)(phenyl)methyl)phenol (3ab)** was prepared according to the General Procedure B as yellow solid (chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 99% yield (149.0 mg, 94% ee). The reaction time was 7 days.

$[\alpha]_D^{25}$ : +1.98 ( $c = 1.0$ ,  $\text{CHCl}_3$ ). HPLC analysis of the product: Daicel CHIRALPAK IC column; 2% *i*-PrOH in hexanes, 0.4 mL/min; retention times: 37.2 min (major), 41.4 min (minor).

**$^1\text{H NMR}$**  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  7.34 (d,  $J = 1.8$  Hz, 1H), 7.28–7.07 (m, 8H), 7.02 (d,  $J = 8.6$  Hz, 2H), 6.89–6.73 (m, 3H), 6.65–6.52 (m, 3H), 6.46 (d,  $J = 8.5$  Hz, 1H), 5.23 (s, 1H), 3.56 (s, 3H), 3.08 (s, 3H) ppm.

**$^{13}\text{C NMR}$**  (75 MHz,  $\text{CDCl}_3$ )  $\delta$  158.2, 153.1, 145.8, 138.3, 137.5, 135.8, 131.4, 130.5, 130.4, 129.9, 128.3, 127.0, 125.4, 123.6, 122.3, 121.7, 120.3, 114.7, 113.8, 113.5, 111.9, 77.2, 57.1, 55.3, 32.7 ppm.

**HRMS** (ES+) Calcd for C<sub>29</sub>H<sub>24</sub>BrNO<sub>2</sub>Na [M + Na]<sup>+</sup>: 520.0888, Found: 520.0887.



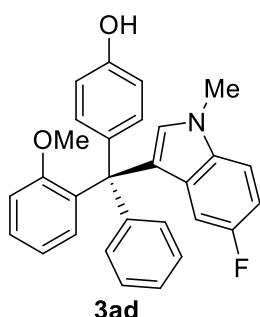
**(S)-4-((6-(BenzylOxy)-1-methyl-1H-indol-3-yl)(2-methoxyphenyl)(phenyl)methyl)phenol (3ac)** was prepared according to the General Procedure B as brown solid (chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 99% yield (156.0 mg, 80% ee). The reaction time was 24 h.

[ $\alpha$ ]<sub>D</sub><sup>25</sup>: +3.24 ( $c$  = 1.0, CHCl<sub>3</sub>). HPLC analysis of the product: Daicel CHIRALPAK IC column; 5% *i*-PrOH in hexanes, 1.0 mL/min; retention times: 10.9 min (major), 12.5 min (minor).

**<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>)  $\delta$  7.46–7.25 (m, 6H), 7.24–7.11 (m, 6H), 7.06 (d,  $J$  = 8.7 Hz, 2H), 6.88–6.74 (m, 3H), 6.64 (d,  $J$  = 8.8 Hz, 2H), 6.53–6.42 (m, 3H), 5.04 (s, 2H), 3.61 (s, 3H), 3.12 (s, 3H) ppm.

**<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>)  $\delta$  158.3, 154.9, 153.1, 146.2, 138.2, 137.8, 137.4, 136.2, 131.5, 130.7, 129.9, 129.1, 128.5, 128.2, 127.8, 127.6, 126.9, 125.3, 123.1, 122.9, 122.3, 120.3, 113.7, 113.4, 108.7, 93.6, 70.4, 57.3, 55.3, 32.7 ppm.

**HRMS** (ES+) Calcd for C<sub>36</sub>H<sub>31</sub>NO<sub>3</sub>Na [M + Na]<sup>+</sup>: 548.2202, Found: 548.2210.



**(S)-4-((5-Fluoro-1-methyl-1*H*-indol-3-yl)(2-methoxyphenyl)(phenyl)methyl)phenol (3ad)** was prepared according to the General Procedure B as brown solid (chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 99% yield (130.0 mg, 93% ee). The reaction time was 3 days.

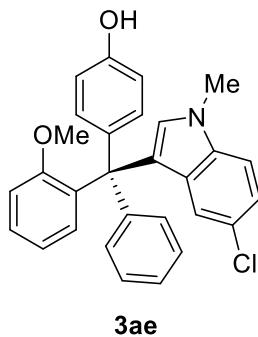
$[\alpha]_D^{25}$ : +1.76 ( $c = 0.5$ , CHCl<sub>3</sub>). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 5% *i*-PrOH in hexanes, 1.0 mL/min; retention times: 14.5 min (minor), 15.4 min (major).

**<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>)  $\delta$  7.33–7.27 (m, 1H), 7.23–7.09 (m, 7H), 7.05 (d,  $J$  = 8.7 Hz, 2H), 6.91–6.77 (m, 3H), 6.70–6.61 (m, 3H), 6.26 (dd,  $J_1$  = 2.5,  $J_2$  = 10.6 Hz, 1H), 3.69 (s, 3H), 3.13 (s, 3H) ppm.

**<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>)  $\delta$  158.3, 156.9 (d,  $J$  = 231.8 Hz), 153.2, 145.8, 137.5, 135.8, 134.2, 131.5, 130.5, 129.9, 128.5 (d,  $J$  = 9.8 Hz), 128.3, 127.0, 125.4, 122.1 (d,  $J$  = 5.3 Hz), 120.3, 113.8, 113.4, 109.5 (d,  $J$  = 9.8 Hz), 109.3 (d,  $J$  = 7.5 Hz), 107.3, 106.9, 57.2, 55.3, 33.0 ppm.

**<sup>19</sup>F NMR** (282 MHz, CDCl<sub>3</sub>)  $\delta$  -125.1 ppm.

**HRMS (ES+)** Calcd for C<sub>29</sub>H<sub>24</sub>FNO<sub>2</sub>Na [M + Na]<sup>+</sup>: 460.1689, Found: 460.1682.



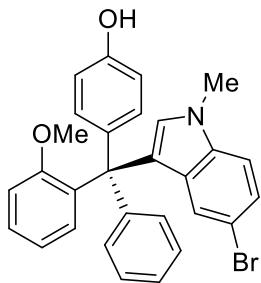
**(S)-4-((5-Chloro-1-methyl-1*H*-indol-3-yl)(2-methoxyphenyl)(phenyl)methyl)phenol (3ae)** was prepared according to the General Procedure B as orange solid (chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 99% yield (136.0 mg, 90% ee). The reaction time was 7 days.

$[\alpha]_D^{25}$ : +3.10 ( $c = 1.0$ ,  $\text{CHCl}_3$ ). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 5% *i*-PrOH in hexanes, 1.0 mL/min; retention times: 15.3 min (minor), 16.1 min (major).

**$^1\text{H NMR}$**  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  7.32–7.25 (m, 1H), 7.21–6.98 (m, 10H), 6.89–6.79 (m, 2H), 6.64 (d,  $J = 8.8$  Hz, 2H), 6.62 (s, 1H), 6.55 (d,  $J = 2.0$  Hz, 1H), 4.88 (s, 1H), 3.65 (s, 3H), 3.12 (s, 3H) ppm.

**$^{13}\text{C NMR}$**  (75 MHz,  $\text{CDCl}_3$ )  $\delta$  158.2, 153.2, 145.8, 137.4, 135.9, 135.8, 131.5, 131.2, 130.5, 129.9, 129.1, 128.3, 127.0, 125.5, 124.3, 121.8, 121.5, 121.3, 120.4, 113.8, 113.5, 109.9, 57.2, 55.3, 32.9 ppm.

**HRMS (ES+)** Calcd for  $\text{C}_{29}\text{H}_{24}\text{ClNO}_2\text{Na} [\text{M} + \text{Na}]^+$ : 476.1393, Found: 476.1390.



**3af**

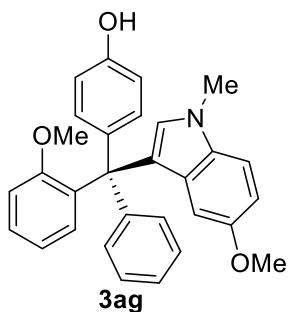
**(S)-4-((5-Bromo-1-methyl-1*H*-indol-3-yl)(2-methoxyphenyl)(phenyl)methyl)phenol (3af)** was prepared according to the General Procedure B as yellow solid (chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 99% yield (149.0 mg, 88% ee). The reaction time was 7 days.

$[\alpha]_D^{25}$ : +10.5 ( $c = 0.5$ ,  $\text{CHCl}_3$ ). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 5% *i*-PrOH in hexanes, 1.0 mL/min; retention times: 15.7 min (minor), 16.6 min (major).

**$^1\text{H NMR}$**  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  7.33–7.27 (m, 1H), 7.23–6.98 (m, 10H), 6.90–6.81 (m, 2H), 6.70–6.64 (m, 2H), 6.63 (s, 1H), 6.58–6.54 (m, 1H), 4.74 (s, 1H), 3.68 (s, 3H), 3.13 (s, 3H) ppm.

**<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>) δ 158.3, 153.2, 145.8, 137.5, 135.9, 135.8, 131.5, 131.2, 130.5, 129.9, 129.1, 128.3, 127.0, 125.5, 124.3, 121.9, 121.6, 121.4, 120.4, 113.8, 113.4, 109.9, 57.2, 55.3, 32.9 ppm.

**HRMS** (ES+) Calcd for C<sub>29</sub>H<sub>24</sub>BrNO<sub>2</sub>Na [M + Na]<sup>+</sup>: 520.0888, Found: 520.0884.



**(S)-4-((5-Methoxy-1-methyl-1H-indol-3-yl)(2-methoxyphenyl)phenol (3ag)** was prepared according to the General Procedure B as yellow solid (chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 99% yield (133.0 mg, 89% ee).

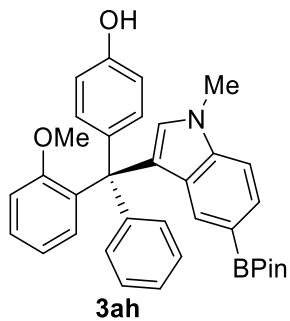
The reaction time was 12 h.

[α]<sub>D</sub><sup>25</sup>: +2.00 (*c* = 0.5, CHCl<sub>3</sub>). HPLC analysis of the product: Daicel CHIRALPAK IC column; 5% *i*-PrOH in hexanes, 1.0 mL/min; retention times: 9.4 min (major), 10.5 min (minor).

**<sup>1</sup>H NMR** (300 MHz, DMSO-*d*<sub>6</sub>) δ 9.18 (s, 1H), 7.30–7.16 (m, 4H), 7.16–7.08 (m, 3H), 7.05 (dd, *J*<sub>1</sub> = 1.7, *J*<sub>2</sub> = 7.8 Hz, 1H), 6.96 (d, *J* = 8.1 Hz, 1H), 6.88 (d, *J* = 8.7 Hz, 2H), 6.82 (t, *J* = 7.5 Hz, 1H), 6.70–6.56 (m, 4H), 5.88 (d, *J* = 2.4 Hz, 1H), 3.66 (s, 3H), 3.36 (s, 3H), 3.09 (s, 3H) ppm.

**<sup>13</sup>C NMR** (75 MHz, DMSO-*d*<sub>6</sub>) δ 158.0, 154.8, 152.3, 145.8, 135.5, 135.3, 132.6, 130.9, 130.2, 129.8, 129.6, 128.3, 127.9, 126.8, 125.2, 120.8, 119.9, 113.7 (2C), 110.15, 110.12, 103.6, 56.8, 55.1, 54.8, 32.4 ppm.

**HRMS** (CI+) Calcd for C<sub>30</sub>H<sub>27</sub>NO<sub>3</sub> [M]<sup>+</sup>: 449.1991, Found: 449.1990.



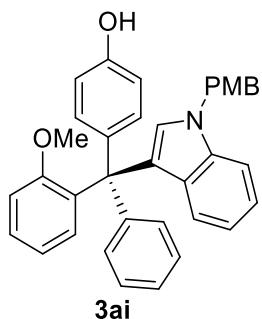
**(S)-4-((2-Methoxyphenyl)(1-methyl-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1*H*-indol-3-yl)(phenyl)methyl)phenol (3ah)** was prepared according to the General Procedure B as yellow solid (chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 43% yield (70.2 mg, 87% ee). The reaction time was 7 days.

$[\alpha]_D^{25}$ : +4.32 ( $c = 0.5$ , CHCl<sub>3</sub>). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 5% *i*-PrOH in hexanes, 1.0 mL/min; retention times: 10.6 min (minor), 13.1 min (major).

**<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>) δ 7.51 (d,  $J = 8.3$  Hz, 1H), 7.31–7.10 (m, 8H), 7.09–7.01 (m, 3H), 6.83 (d,  $J = 7.7$  Hz, 2H) 6.60–6.57 (m, 3H), 3.64 (s, 3H), 3.08 (s, 3H), 1.21 (s, 12H) ppm.

**<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>) δ 158.3, 153.2, 146.2, 139.5, 137.6, 136.5, 131.5, 130.8, 130.4, 130.1, 130.0, 128.0, 127.9, 127.1, 126.9, 125.2, 122.9, 120.4, 113.8, 113.3, 108.2, 83.1, 57.4, 55.3, 32.6, 24.67, 24.65 ppm.

**HRMS (ES+)** Calcd for C<sub>35</sub>H<sub>36</sub>BNO<sub>4</sub>Na [M + Na]<sup>+</sup>: 568.2645, Found: 568.2645.



**(S)-4-((1-(4-Methoxybenzyl)-1*H*-indol-3-yl)(2-methoxyphenyl)(phenyl)methyl)phenol (3ai)** was prepared according to the General Procedure B as yellow solid

(chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 38% yield (60.0 mg, 88% ee).

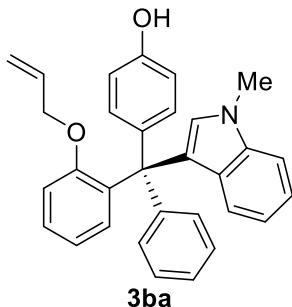
The reaction time was 3 days.

$[\alpha]_D^{25}$ : +0.72 ( $c$  = 0.5, CHCl<sub>3</sub>). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 5% *i*-PrOH in hexanes, 1.0 mL/min; retention times: 21.3 min (major), 24.9 min (minor).

**<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>) δ 7.30–7.12 (m, 8H), 7.08 (d,  $J$  = 8.7 Hz, 2H), 7.04–6.92 (m, 3H), 6.88–6.60 (m, 9H), 5.18 (s, 1H), 4.76 (s, 1H), 3.75 (s, 3H), 3.13 (s, 3H) ppm.

**<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>) δ 158.8, 158.3, 153.1, 146.1, 137.9, 137.0, 135.9, 131.6, 130.7, 130.1, 130.0, 129.6, 128.5, 128.2, 127.5, 126.9, 125.3, 122.6, 122.5, 121.1, 120.2, 118.7, 114.0, 113.8, 113.1, 109.5, 57.4, 55.3, 55.1, 49.4 ppm.

**HRMS** (ES+) Calcd for C<sub>36</sub>H<sub>32</sub>NO<sub>3</sub> [M + H]<sup>+</sup>: 526.2382, Found: 526.2373.



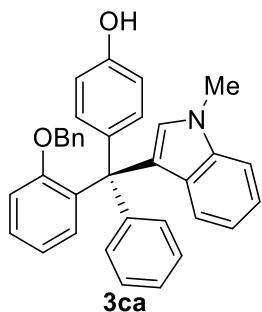
**(S)-4-((2-(Allyloxy)phenyl)(1-methyl-1*H*-indol-3-yl)(phenyl)methyl)phenol** (3ba) was prepared according to the General Procedure B as refous solid (chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 99% yield (94.8 mg, 90% ee). The reaction time was 7 days.

$[\alpha]_D^{25}$ : +2.34 ( $c$  = 1.0, CHCl<sub>3</sub>). HPLC analysis of the product: Daicel CHIRALCEL OD-H column; 2% *i*-PrOH in hexanes, 1.0 mL/min; retention times: 26.2 min (major), 29.7 min (minor).

**<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>) δ 7.24–7.05 (m, 11H), 6.83–6.58 (m, 7H), 5.37–5.25 (m, 1H), 4.87–4.72 (m, 3H), 3.92–3.83 (m, 2H), 3.63 (s, 3H) ppm.

**<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>) δ 157.2, 153.0, 146.1, 137.8, 137.5, 135.9, 133.5, 131.7, 130.9, 130.13, 130.10, 128.2, 128.1, 126.9, 125.3, 122.5, 122.0, 120.9, 120.2, 118.5, 115.9, 113.68, 113.66, 108.8, 68.9, 57.4, 32.6 ppm.

**HRMS** (ES+) Calcd for C<sub>31</sub>H<sub>27</sub>NO<sub>2</sub>Na [M + Na]<sup>+</sup>: 468.1939, Found: 468.1948.



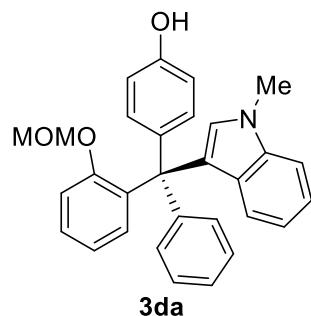
**(S)-4-((2-(Benzyl)phenyl)(1-methyl-1*H*-indol-3-yl)(phenyl)methyl)phenol (3ca)** was prepared according to the General Procedure B as brown solid (chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 68% yield (97.0 mg, 83% ee). The reaction time was 7 days.

[α]<sub>D</sub><sup>25</sup>: -0.64 (*c* = 1.0, CHCl<sub>3</sub>). HPLC analysis of the product: Daicel CHIRALCEL OD-H column; 5% *i*-PrOH in hexanes, 1.0 mL/min; retention times: 14.3 min (major), 17.0 min (minor).

**<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>) δ 7.29–7.27 (m, 2H), 7.23–7.04 (m, 12H), 6.88–6.79 (m, 2H), 6.78–6.65 (m, 4H), 6.54–6.52 (m, 3H), 4.90 (s, 1H), 4.50 (d, *J* = 3.7 Hz, 2H), 3.52 (s, 3H) ppm.

**<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>) δ 157.0, 153.0, 145.9, 137.7, 137.4, 137.2, 135.3, 131.6, 130.9, 130.2, 130.1, 128.1, 128.0, 127.8, 127.0, 126.9, 126.6, 125.2, 122.3, 121.5, 120.8, 120.1, 118.4, 113.7, 113.1, 108.8, 69.5, 57.4, 32.4 ppm.

**HRMS** (ES+) Calcd for C<sub>35</sub>H<sub>29</sub>NO<sub>2</sub>Na [M + Na]<sup>+</sup>: 518.2096, Found: 518.2095.



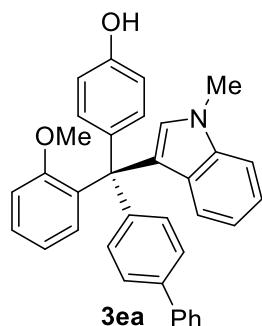
**(S)-4-((2-(Methoxymethoxy)phenyl)(1-methyl-1*H*-indol-3-yl)(phenyl)methyl)phenol (3da)** was prepared according to the General Procedure B as grey solid (chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 42% yield (57.0 mg, 90% ee). The reaction time was 7 days.

$[\alpha]_D^{25}$ : +3.30 ( $c = 1.0$ , CHCl<sub>3</sub>). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 2% *i*-PrOH in hexanes, 1.0 mL/min; retention times: 33.3 min (major), 35.7 min (minor).

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.25–7.07 (m, 12H), 6.87 (t,  $J = 7.4$ , 1H), 6.74 (t,  $J = 7.5$  Hz, 1H),  $\delta$  6.67–6.59 (m, 4H), 4.69 (s, 1H), 4.40 (s, 2H), 3.70 (s, 3H), 2.97 (s, 3H) ppm.

**<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>)  $\delta$  156.2, 153.1, 146.1, 137.5, 135.9, 131.6, 130.8, 130.03, 129.98, 128.3, 128.1, 127.0, 125.4, 122.4, 122.2, 121.2, 121.0, 118.6, 115.2, 113.7, 108.8, 94.1, 57.4, 55.3, 32.7, 29.7 ppm.

**HRMS (ES+)** Calcd for C<sub>30</sub>H<sub>27</sub>NO<sub>3</sub>Na [M + Na]<sup>+</sup>: 472.1889, Found: 472.1887.



**(S)-4-([1,1'-Biphenyl]-4-yl(2-methoxyphenyl)(1-methyl-1*H*-indol-3-yl)methyl)phenol (3ea)** was prepared according to the General Procedure B as yellow solid

(chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 90% yield (134.0 mg, 82% ee).

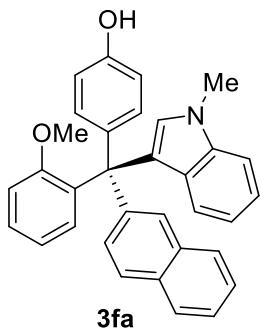
The reaction time was 5 days.

$[\alpha]_D^{25}$ : +10.08 ( $c$  = 0.5, CHCl<sub>3</sub>). HPLC analysis of the product: Daicel CHIRALPAK IC column; 2% *i*-PrOH in hexanes, 1.0 mL/min; retention times: 19.2 min (major), 21.5 min (minor).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.61 – 7.59 (m, 2H), 7.46 (d,  $J$  = 8.3 Hz, 2H), 7.41 (t,  $J$  = 7.7 Hz, 2H), 7.34–7.27 (m, 5H), 7.24 (d,  $J$  = 1.6 Hz, 1H), 7.15–7.06 (m, 3H), 6.89 (dd,  $J_1$  = 8.2 Hz,  $J_2$  = 1.2 Hz, 1H), 6.85 (td,  $J$  = 7.6, 1.2 Hz, 1H), 6.76 (t,  $J$  = 7.5 Hz, 1H), 6.66 (dd,  $J_1$  = 8.5 Hz,  $J_2$  = 3.5 Hz, 3H), 6.63 (s, 1H), 4.69 (s, 1H), 3.70 (s, 3H), 3.15 (s, 3H) ppm.

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 158.3, 153.1, 145.4, 140.8, 137.72, 137.66, 137.5, 136.1, 131.5, 130.7, 130.4, 130.0, 128.6, 128.2, 128.1, 126.8, 126.9, 125.4, 122.5, 122.0, 120.9, 120.3, 118.5, 113.8, 113.4, 108.8, 57.1, 55.3, 32.7 ppm.

HRMS (ES+) Calcd for C<sub>35</sub>H<sub>29</sub>NO<sub>2</sub>Na [M + Na]<sup>+</sup>: 518.2096, Found: 518.2106.



**(S)-4-((2-Methoxyphenyl)(1-methyl-1*H*-indol-3-yl)(naphthalen-2-yl)methyl)phenol (3fa)** was prepared according to the General Procedure B as light yellow solid (chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 99% yield (139.0 mg, 82% ee).

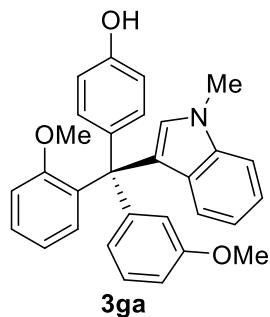
The reaction time was 7 days.

$[\alpha]_D^{25}$ : +5.9 ( $c$  = 1.0, CHCl<sub>3</sub>). HPLC analysis of the product: Daicel CHIRALPAK IC column; 2% *i*-PrOH in hexanes, 0.4 mL/min; retention times: 55.3 min (major), 62.4 min (minor).

**<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>) δ 7.73–7.66 (m, 3H), 7.62 (d, *J* = 8.7 Hz, 1H), 7.40–7.34 (m, 2H), 7.30–7.25 (m, 2H), 7.20–7.18 (m, 2H), 7.11–7.09 (m, 2H), 7.06–7.02 (m, 1H), 6.85–6.81 (m, 2H), 6.71–6.59 (m, 5H), 4.74 (s, 1H), 3.70 (s, 3H), 3.09 (s, 3H) ppm.

**<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>) δ 158.4, 153.1, 143.6, 137.8, 137.5, 135.8, 132.9, 131.7 (2C), 130.8, 130.0, 129.5, 128.4, 128.3, 128.1, 127.7, 127.2, 125.9, 125.31, 125.27, 122.4, 121.8, 120.9, 120.3, 118.6, 113.8, 113.4, 108.8, 57.5, 55.3, 32.7 ppm.

**HRMS** (ES+) Calcd for C<sub>33</sub>H<sub>27</sub>NO<sub>2</sub>Na [M + Na]<sup>+</sup>: 492.1939, Found: 492.1944.



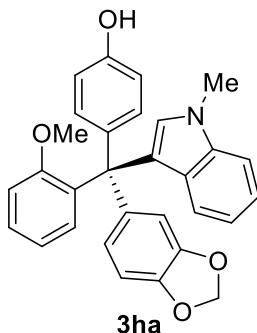
**(R)-4-((2-Methoxyphenyl)(3-methoxyphenyl)(1-methyl-1*H*-indol-3-yl)methyl)phenol (3ga)** was prepared according to the General Procedure B as grey solid (chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 60% yield (81.0 mg, 87% ee). The reaction time was 7 days.

[α]<sub>D</sub><sup>25</sup>: +9.6 (*c* = 0.5, CHCl<sub>3</sub>). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 5% *i*-PrOH in hexanes, 1.0 mL/min; retention times: 15.2 min (major), 17.6 min (minor).

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.24–7.18 (m, 3H), 7.11–7.04 (m, 4H), 6.86–6.78 (m, 4H), 6.75–6.68 (m, 2H), 6.64–6.59 (m, 4H), 4.87 (s, 1H), 3.66 (s, 3H), 3.65 (s, 3H), 3.13 (s, 3H) ppm.

**<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>) δ 158.6, 158.4, 153.1, 148.1, 137.6, 137.5, 136.1, 131.5, 130.7, 130.0, 128.2, 127.6, 123.0, 122.5, 121.9, 120.9, 120.3, 118.5, 116.6, 113.7 (2C), 113.4, 110.0, 108.8, 57.4, 55.3, 55.1, 32.7 ppm.

**HRMS** (CI+) Calcd for C<sub>30</sub>H<sub>27</sub>NO<sub>3</sub> [M]<sup>+</sup>: 449.1991, Found: 449.1990.



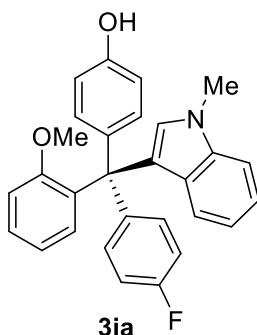
**(R)-4-(Benzo[d][1,3]dioxol-5-yl(2-methoxyphenyl)(1-methyl-1*H*-indol-3-yl)methyl phenol (3ha)** was prepared according to the General Procedure B as grey solid (chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 99% yield (137.0 mg, 76% ee). The reaction time was 7 days.

$[\alpha]_D^{25}$ : +4.5 ( $c = 0.5$ , CHCl<sub>3</sub>). HPLC analysis of the product: Daicel CHIRALPAK IC column; 5% *i*-PrOH in hexanes, 1.0 mL/min; retention times: 10.5 min (major), 12.3 min (minor).

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.25–7.18 (m, 3H), 7.08–7.04 (m, 3H), 6.86–6.59 (m, 10H), 5.87 (dd,  $J_1$  = 7.4 Hz,  $J_2$  = 1.4 Hz, 2H), 4.87 (s, 1H), 3.67 (s, 3H), 3.17 (s, 3H) ppm.

**<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>)  $\delta$  158.3, 153.1, 146.5, 144.9, 140.2, 138.1, 137.5, 136.1, 131.3, 130.6, 129.9, 128.2, 128.1, 123.2, 122.5, 122.1, 120.9, 120.2, 118.5, 113.7, 113.4, 111.1, 108.8, 106.6, 100.6, 57.1, 55.4, 32.7 ppm.

**HRMS (ES+)** Calcd for C<sub>30</sub>H<sub>26</sub>NO<sub>4</sub> [M + H]<sup>+</sup>: 463.1784, Found: 463.1782.



**(R)-4-((4-Fluorophenyl)(2-methoxyphenyl)(1-methyl-1*H*-indol-3-yl)methyl phenol (3ia)** was prepared according to the General Procedure B as brown solid

(chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 99% yield (131.0 mg, 93% ee).

The reaction time was 2 days.

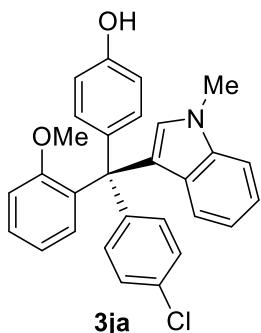
$[\alpha]_D^{25}$ : +6.27 ( $c = 0.5$ , CHCl<sub>3</sub>). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 2% *i*-PrOH in hexanes, 1.0 mL/min; retention times: 40.3 min (minor), 46.5 min (major).

<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 7.30 – 7.20 (m, 2H), 7.18–7.11 (m, 2H), 7.11–6.98 (m, 3H), 6.91–6.68 (m, 5H), 6.65–6.54 (m, 4H), 5.03 (s, 1H), 3.64 (s, 3H), 3.13 (s, 3H) ppm.

<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) δ 160.7 (d,  $J = 242.3$  Hz), 158.1, 153.1, 141.7 (d,  $J = 3.3$  Hz), 137.7, 137.5, 135.9, 131.4 (d,  $J = 7.5$  Hz), 131.3, 130.5, 129.9, 128.3, 128.0, 122.3, 122.0, 121.0, 120.3, 118.6, 113.8, 113.5 (d,  $J = 20.3$  Hz), 113.3, 108.9, 56.8, 55.2, 32.6 ppm.

<sup>19</sup>F NMR (282 MHz, CDCl<sub>3</sub>) δ -118.4 ppm.

HRMS (ES+) Calcd for C<sub>29</sub>H<sub>24</sub>FNO<sub>2</sub>Na [M + Na]<sup>+</sup>: 460.1689, Found: 460.1682.



**(R)-4-((4-Chlorophenyl)(2-methoxyphenyl)(1-methyl-1*H*-indol-3-yl)methyl)phenol (3ja)** was prepared according to the General Procedure B as grey solid (chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 61% yield (84.0 mg, 90% ee).

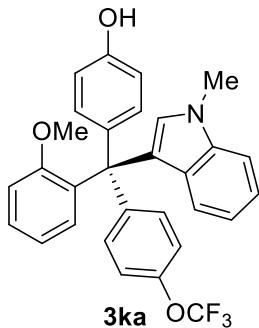
The reaction time was 5 days.

$[\alpha]_D^{25}$ : +4.5 ( $c = 0.5$ , CHCl<sub>3</sub>). HPLC analysis of the product: Daicel CHIRALPAK IC column; 1.5% *i*-PrOH in hexanes, 0.5 mL/min; retention times: 29.7 min (major), 33.9 min (minor).

**<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>) δ 7.29 (dd, *J*<sub>1</sub> = 1.3, *J*<sub>2</sub> = 7.7 Hz, 1H), 7.22–7.17 (m, 2H), 7.15 (s, 4H), 7.09 (t, *J* = 7.6 Hz, 1H), 7.03 (d, *J* = 8.7 Hz, 2H), 6.88–6.79 (m, 2H), 6.79–6.71 (m, 1H), 6.68–6.62 (m, 3H), 6.57 (s, 1H), 4.85 (s, 1H), 3.70 (s, 3H), 3.19 (s, 3H) ppm.

**<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>) δ 158.1, 153.2, 144.7, 137.6, 137.4, 135.5, 131.37, 131.35, 130.9, 130.6, 129.9, 128.4, 127.9, 127.0, 122.3, 121.8, 121.1, 120.3, 118.7, 113.8, 113.2, 108.9, 56.9, 55.2, 32.7 ppm.

**HRMS** (ES+) Calcd for C<sub>29</sub>H<sub>24</sub>ClNO<sub>2</sub>Na [M + Na]<sup>+</sup>: 476.1393, Found: 476.1387.



**(R)-4-((2-Methoxyphenyl)(1-methyl-1*H*-indol-3-yl)(4-(trifluoromethoxy)phenyl)methyl)phenol (3ka)** was prepared according to the General Procedure B as yellow solid (chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 99% yield (151.0 mg, 94% ee). The reaction time was 2 days.

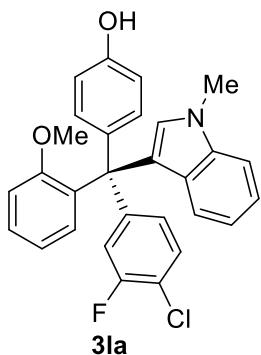
[α]<sub>D</sub><sup>25</sup>: +6.36 (*c* = 1.0, CHCl<sub>3</sub>). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 2% *i*-PrOH in hexanes, 1.0 mL/min; retention times: 24.0 min (major), 26.2 min (minor).

**<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>) δ 7.27–7.15 (m, 6H), 7.13–6.97 (m, 5H), 6.89–6.70 (m, 3H), 6.67–6.56 (m, 3H), 6.55 (s, 1H), 4.87 (s, 1H), 3.68 (s, 3H), 3.14 (s, 3H) ppm.

**<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>) δ 158.0, 153.2, 146.8 (q, *J* = 1.5 Hz), 145.0, 137.6, 137.3, 135.7, 131.4, 131.1, 130.6, 129.9, 128.4, 127.9, 122.3, 121.7, 121.1, 120.5 (q, *J* = 255.0 Hz), 120.3, 119.2, 118.7, 113.9, 113.3, 108.9, 56.9, 55.1, 32.7 ppm.

**<sup>19</sup>F NMR** (282 MHz, CDCl<sub>3</sub>) δ -57.7 ppm.

**HRMS** (ES+) Calcd for C<sub>30</sub>H<sub>25</sub>F<sub>3</sub>NO<sub>3</sub> [M + H]<sup>+</sup>: 504.1787, Found: 504.1784.



**(R)-4-((4-Chloro-3-fluorophenyl)(2-methoxyphenyl)(1-methyl-1*H*-indol-3-yl)methyl)phenol (3la)** was prepared according to the General Procedure B as brown solid (chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 99% yield (141.0 mg, 89% ee). The reaction time was 5 days.

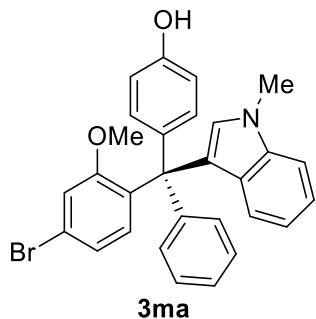
$[\alpha]_D^{25}$ : +6.38 ( $c = 1.0$ , CHCl<sub>3</sub>). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 5% *i*-PrOH in hexanes, 1.0 mL/min; retention times: 11.2 min (minor), 12.4 min (major).

**<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>)  $\delta$  7.34–7.27 (m, 1H), 7.25–7.00 (m, 7H), 6.96 (dd,  $J_1 = 1.8$ ,  $J_2 = 8.7$  Hz, 1H), 6.91–6.74 (m, 3H), 6.65 (t,  $J = 8.3$  Hz, 3H), 6.55 (s, 1H), 4.87 (s, 1H), 3.71 (s, 3H), 3.23 (s, 3H) ppm.

**<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>)  $\delta$  157.9, 157.2 (d,  $J = 243.8$  Hz), 153.3, 147.6 (d,  $J = 6.0$  Hz), 137.6, 136.8, 134.8, 131.3, 130.6, 129.8, 128.6 (d,  $J = 2.3$  Hz), 127.8, 126.5 (d,  $J = 3.8$  Hz), 122.2, 121.3, 121.2, 120.3, 118.8, 118.3, 118.0, 117.4 (d,  $J = 18.0$  Hz), 113.9, 113.0, 109.0, 57.0, 55.1, 32.7 ppm.

**<sup>19</sup>F NMR** (282 MHz, CDCl<sub>3</sub>)  $\delta$  -117.2 ppm.

**HRMS (ES+)** Calcd for C<sub>29</sub>H<sub>24</sub>ClFNO<sub>2</sub> [M + H]<sup>+</sup>: 472.1480, Found: 472.1474.



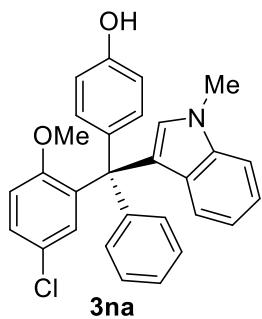
**(S)-4-((4-Bromo-2-methoxyphenyl)(1-methyl-1H-indol-3-yl)(phenyl)methyl)phenol (3ma)** was prepared according to the General Procedure B as brown solid (chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 99% yield (148.0 mg, 91% ee). The reaction time was 5 days.

$[\alpha]_D^{25}$ : -2.60 ( $c = 0.5$ , CHCl<sub>3</sub>). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 5% *i*-PrOH in hexanes, 1.0 mL/min; retention times: 11.9 min (major), 12.7 min (minor).

**<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>) δ 7.24–7.14 (m, 8H), 7.13–7.02 (m, 3H), 6.82–6.73 (m, 2H), 6.68–6.59 (m, 3H), 6.56 (s, 1H), 4.79 (s, 1H), 3.68 (s, 3H), 3.09 (s, 3H) ppm.

**<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>) δ 157.0, 153.2, 145.5, 138.2, 137.5, 137.2, 131.4, 130.6, 130.0, 129.9, 127.9, 127.8, 127.0, 125.5, 125.4, 122.1, 121.2, 121.1, 118.7, 114.6, 113.9, 108.9, 57.3, 55.6, 32.7 ppm.

**HRMS (ES+)** Calcd for C<sub>29</sub>H<sub>25</sub>BrNO<sub>2</sub> [M + H]<sup>+</sup>: 498.1069, Found: 498.1063.



**(S)-4-((5-Chloro-2-methoxyphenyl)(1-methyl-1H-indol-3-yl)(phenyl)methyl)phenol (3na)** was prepared according to the General Procedure B as white solid

(chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 60% yield (81.0 mg, 86% ee).

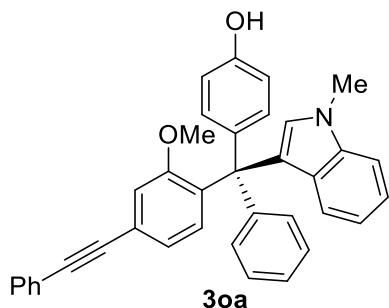
The reaction time was 5 days.

$[\alpha]_D^{25}$ : +2.84 ( $c = 1.0$ , CHCl<sub>3</sub>). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 5% *i*-PrOH in hexanes, 1.0 mL/min; retention times: 14.5 min (major), 16.4 min (minor).

<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 7.22–6.93 (m, 12H), 6.77 (t,  $J = 9.0$  Hz, 1H), 6.69–6.55 (m, 4H), 4.89 (s, 1H), 3.66 (s, 3H), 3.13 (s, 3H) ppm.

<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) δ 158.9, 153.1, 145.5, 137.5, 137.2, 135.2, 132.0, 131.4, 129.9, 129.8, 127.9, 127.0, 125.5, 123.2, 122.2, 121.7, 121.3, 121.1, 118.7, 116.5, 113.8, 108.9, 57.1, 55.5, 32.7 ppm.

HRMS (ES+) Calcd for C<sub>29</sub>H<sub>24</sub>ClNO<sub>2</sub>Na [M + Na]<sup>+</sup>: 476.1393, Found: 476.1385.



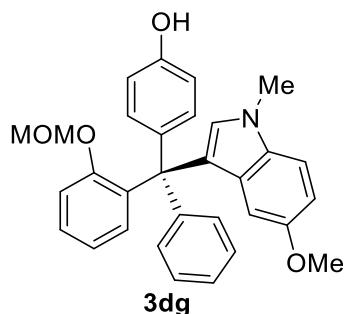
**(S)-4-((2-Methoxy-4-(phenylethynyl)phenyl)(1-methyl-1*H*-indol-3-yl)(phenyl)methyl)phenol (3oa)** was prepared according to the General Procedure B as yellow solid (chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 99% yield (156.0 mg, 90% ee). The reaction time was 5 days.

$[\alpha]_D^{25}$ : +3.30 ( $c = 1.0$ , CHCl<sub>3</sub>). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 3% *i*-PrOH in hexanes, 1.0 mL/min; retention times: 44.3 min (minor), 49.1 min (major).

<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 7.53–7.50 (m, 2H), 7.39–7.31 (m, 3H), 7.25–6.99 (m, 12H), 6.77 (t,  $J = 7.5$  Hz, 1H), 6.70–6.61 (m, 3H), 6.58 (s, 1H), 4.77 (s, 1H), 3.68 (s, 3H), 3.16 (s, 3H) ppm.

**<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>) δ 158.0, 153.2, 145.7, 137.5, 137.4, 136.9, 131.6, 131.5, 130.8, 130.0, 129.9, 128.3, 128.2, 128.0, 127.0, 125.4, 123.8, 123.2, 122.8, 122.3, 121.8, 121.0, 118.6, 116.1, 113.8, 108.9, 89.30, 89.27, 57.4, 55.4, 32.7 ppm.

**HRMS** (ES+) Calcd for C<sub>37</sub>H<sub>29</sub>NO<sub>2</sub>Na [M + Na]<sup>+</sup>: 542.2096, Found: 542.2100.



**(S)-4-((5-Methoxy-1-methyl-1H-indol-3-yl)(2-(methoxymethoxy)phenyl)(phenyl)methyl)phenol (3dg)** was prepared according to the General Procedure B as pink solid (chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 90% yield (129.0 mg, 92% ee).

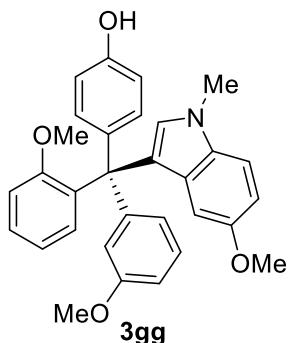
The reaction time was 3 days.

[α]<sub>D</sub><sup>25</sup>: +6.44 (*c* = 1.0, CHCl<sub>3</sub>). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 5% *i*-PrOH in hexanes, 1.0 mL/min; retention times: 13.8 min (major), 17.2 min (minor).

**<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>) δ 7.29–7.06 (m, 11H), 6.93–6.84 (m, 1H), 6.74 (dd, *J*<sub>1</sub> = 2.5, *J*<sub>2</sub> = 8.8 Hz, 1H), 6.65 (d, *J* = 8.8 Hz, 2H), 6.58 (s, 1H), 6.03 (d, *J* = 2.4 Hz, 1H), 4.40 (s, 2H), 3.66 (s, 3H), 3.40 (s, 3H), 2.97 (s, 3H) ppm.

**<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>) δ 156.2, 153.2, 152.8, 146.1, 137.6, 135.8, 132.9, 131.6, 130.8, 130.4, 130.1, 128.5, 128.3, 127.0, 125.4, 121.7, 121.2, 115.2, 113.7, 111.4, 109.5, 103.9, 94.1, 57.4, 55.5, 55.3, 32.8 ppm.

**HRMS** (ES+) Calcd for C<sub>31</sub>H<sub>29</sub>NO<sub>4</sub>Na [M + Na]<sup>+</sup>: 502.1994, Found: 502.1997.



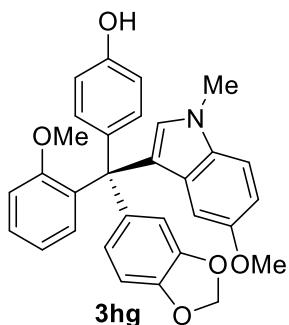
**(R)-4-((5-Methoxy-1-methyl-1*H*-indol-3-yl)(2-methoxyphenyl)(3-methoxyphenyl)methyl)phenol (3gg)** was prepared according to the General Procedure B as orange solid (chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 79% yield (113.0 mg, 83% ee). The reaction time was 7 days.

$[\alpha]_D^{25}$ : +15.2 ( $c = 1.0$ , CHCl<sub>3</sub>). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 5% *i*-PrOH in hexanes, 1.0 mL/min; retention times: 21.0 min (major), 26.4 min (minor).

**<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>) δ 7.27–7.02 (m, 6H), 6.85 (m, 4H), 6.77–6.69 (m, 2H), 6.65–6.57 (m, 3H), 6.04 (d,  $J = 2.5$  Hz, 1H), 3.65 (s, 3H), 3.63 (s, 3H), 3.39 (s, 3H), 3.12 (s, 3H) ppm.

**<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>) δ 158.6, 158.4, 153.2, 152.8, 148.2, 137.5, 136.0, 132.9, 131.6, 130.7, 130.4, 128.5, 128.2, 127.6, 122.9, 121.5, 120.3, 116.6, 113.7, 113.4, 111.2, 110.0, 109.4, 104.0, 57.3, 55.5, 55.4, 55.1, 32.8 ppm.

**HRMS (ES+)** Calcd for C<sub>31</sub>H<sub>29</sub>NO<sub>4</sub>Na [M + Na]<sup>+</sup>: 502.1994, Found: 502.1997.



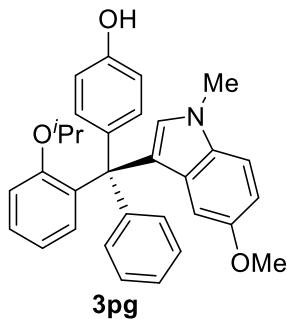
**(R)-4-(Benzo[*d*][1,3]dioxol-5-yl(5-methoxy-1-methyl-1*H*-indol-3-yl)(2-methoxyphenyl)methylphenol (3hg)** was prepared according to the General Procedure B as brown solid (chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 93% yield (137.0 mg, 77% ee). The reaction time was 7 days.

$[\alpha]_D^{25}$ : +4.2 ( $c = 1.0$ , CHCl<sub>3</sub>). HPLC analysis of the product: Daicel CHIRALPAK IC column; 5% *i*-PrOH in hexanes, 1.0 mL/min; retention times: 16.4 min (major), 22.8 min (minor).

**<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>) δ 7.28–7.16 (m, 2H), 7.13–6.99 (m, 3H), 6.90–6.56 (m, 9H), 6.05 (d,  $J = 2.4$  Hz, 1H), 5.88 (q,  $J = 3.0$  Hz, 2H), 3.65 (s, 3H), 3.42 (s, 3H), 3.17 (s, 3H) ppm.

**<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>) δ 158.3, 153.2, 152.8, 146.5, 144.9, 140.3, 138.0, 136.1, 132.9, 131.4, 130.6, 130.3, 128.5, 128.2, 123.2, 121.7, 120.3, 113.7, 113.4, 111.2, 111.2, 109.5, 106.6, 104.0, 100.6, 57.1, 55.5, 55.4, 32.9 ppm.

**HRMS (ES+)** Calcd for C<sub>31</sub>H<sub>28</sub>NO<sub>5</sub> [M + H]<sup>+</sup>: 494.1967, Found: 494.1964.



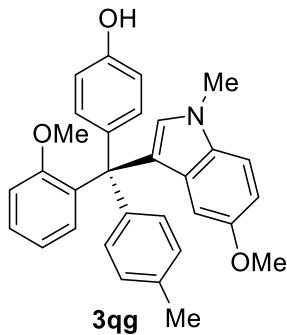
**(S)-4-((2-Isopropoxypyhenyl)(5-methoxy-1-methyl-1*H*-indol-3-yl)(phenyl)methylphenol (3pg)** was prepared according to the General Procedure B as rufous solid (chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 99% yield (143.0 mg, 84% ee). The reaction time was 24 h.

$[\alpha]_D^{25}$ : +5.82 ( $c = 1.0$ , CHCl<sub>3</sub>). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 5% *i*-PrOH in hexanes, 1.0 mL/min; retention times: 11.6 min (major), 13.5 min (minor).

**<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>) δ 7.24–7.05 (m, 10H), 6.82–6.70 (m, 3H), 6.64 (d, *J* = 8.8 Hz, 2H), 6.55 (s, 1H), 6.02 (d, *J* = 2.5 Hz, 1H), 4.90 (s, 1H), 4.28 (p, *J* = 6.0 Hz, 1H), 3.64 (s, 3H), 3.38 (s, 3H), 0.69 (dd, *J*<sub>1</sub> = 6.0, *J*<sub>2</sub> = 20.1 Hz, 6H) ppm.

**<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>) δ 155.5, 153.1, 152.7, 146.1, 137.7, 134.9, 132.8, 131.9, 131.2, 130.7, 130.3, 128.7, 127.8, 126.7, 125.1, 121.9, 118.7, 113.5, 111.4, 111.2, 109.3, 104.0, 67.5, 57.4, 55.5, 32.8, 20.9, 20.8 ppm.

**HRMS** (ES+) Calcd for C<sub>32</sub>H<sub>31</sub>NO<sub>3</sub>Na [M + Na]<sup>+</sup>: 500.2202, Found: 500.2201.



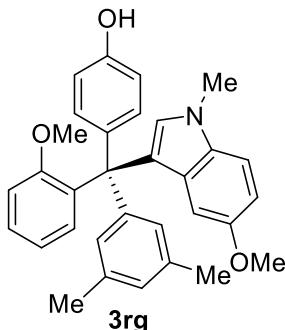
**(S)-4-((5-Methoxy-1-methyl-1*H*-indol-3-yl)(2-methoxyphenyl)(p-tolyl)methyl)phenol (3qg)** was prepared according to the General Procedure B as pink solid (chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 99% yield (139.0 mg, 84% ee). The reaction time was 5 days.

[α]<sub>D</sub><sup>25</sup>: +2.00 (*c* = 1.0, CHCl<sub>3</sub>). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 5% *i*-PrOH in hexanes, 1.0 mL/min; retention times: 14.2 min (minor), 17.4 min (major).

**<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>) δ 7.27–7.15 (m, 2H), 7.13–6.94 (m, 7H), 6.88–6.76 (m, 2H), 6.72 (dd, *J*<sub>1</sub> = 2.5, *J*<sub>2</sub> = 8.8 Hz, 1H), 6.59 (d, *J* = 9.2 Hz, 3H), 6.02 (d, *J* = 2.4 Hz, 1H), 3.62 (s, 3H), 3.38 (s, 3H), 3.10 (s, 3H), 2.28 (s, 3H) ppm.

**<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>) δ 158.4, 153.1, 152.6, 143.0, 138.1, 136.2, 134.6, 132.9, 131.4, 130.6, 130.4, 130.0, 128.5, 128.1, 127.6, 121.8, 120.2, 113.7, 113.5, 111.2, 109.4, 104.0, 56.9, 55.5, 55.4, 32.8, 20.9 ppm.

**HRMS** (ES+) Calcd for C<sub>31</sub>H<sub>29</sub>NO<sub>3</sub>Na [M + Na]<sup>+</sup>: 486.2045, Found: 486.2046.



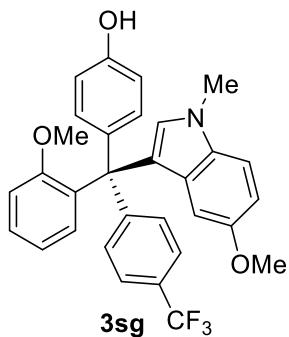
**(R)-4-((3,5-Dimethylphenyl)(5-methoxy-1-methyl-1*H*-indol-3-yl)(2-methoxyphenyl)methyl)phenol (3rg)** was prepared according to the General Procedure B as rufous solid (chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 99% yield (143.0 mg, 82% ee). The reaction time was 5 days.

$[\alpha]_D^{25}$ : +16.95 ( $c = 1.0$ , CHCl<sub>3</sub>). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 5% *i*-PrOH in hexanes, 1.0 mL/min; retention times: 10.5 min (major), 14.3 min (minor).

**<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>) δ 7.30–7.22 (m, 2H), 7.19 (dd,  $J_1 = 1.7$ ,  $J_2 = 7.8$  Hz, 1H), 7.12–7.02 (m, 3H), 6.90–6.78 (m, 5H), 6.73 (dd,  $J_1 = 2.5$ ,  $J_2 = 8.8$  Hz, 1H), 6.67–6.60 (d,  $J = 8.8$ , 2H), 6.58 (s, 1H), 6.03 (d,  $J = 2.4$  Hz, 1H), 3.65 (s, 3H), 3.39 (s, 3H), 3.11 (s, 3H), 2.19 (s, 6H) ppm.

**<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>) δ 158.6, 153.1, 152.7, 146.2, 137.9, 136.3, 136.0, 132.9, 131.7, 130.7, 130.4, 128.6, 128.0, 127.8, 126.9, 121.7, 120.3, 113.6 (2C), 111.2, 109.4, 104.0, 57.2, 55.5, 55.4, 32.8, 21.6 ppm.

**HRMS (ES+)** Calcd for C<sub>32</sub>H<sub>32</sub>NO<sub>3</sub> [M + H]<sup>+</sup>: 478.2382, Found: 478.2372.



**(S)-4-((5-Methoxy-1-methyl-1*H*-indol-3-yl)(2-methoxyphenyl)(4-(trifluoromethyl)phenyl)methyl)phenol (3sg)** was prepared according to the General Procedure B as yellow solid (chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 78% yield (120.0 mg, 91% ee). The reaction time was 7 days.

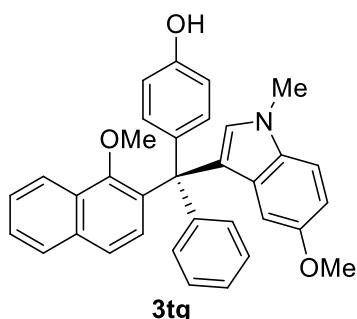
$[\alpha]_D^{25}$ : 2.07 ( $c = 1.0$ , CHCl<sub>3</sub>). HPLC analysis of the product: Daicel CHIRALPAK IC column; 3% *i*-PrOH in hexanes, 1.0 mL/min; retention times: 10.0 min (major), 11.7 min (minor).

**<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>)  $\delta$  7.50–7.33 (m, 4H), 7.33–7.19 (m, 2H), 7.12 (d,  $J$  = 8.8 Hz, 1H), 7.08–6.99 (m, 2H), 6.91–6.81 (m, 2H), 6.76 (dd,  $J_1$  = 8.8 Hz,  $J_2$  = 2.5 Hz, 1H), 6.71–6.63 (m, 2H), 6.52 (s, 1H), 5.98 (d,  $J$  = 2.4 Hz, 1H), 4.90 (s, 1H), 3.66 (s, 3H), 3.39 (s, 3H), 3.14 (s, 3H) ppm.

**<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>)  $\delta$  158.0, 153.4, 153.0, 150.5, 137.0, 135.1, 132.9, 131.5, 130.7, 130.4, 130.1, 128.5, 128.2, 127.4 (q,  $J$  = 32.3 Hz), 124.4 (q,  $J$  = 270.0 Hz), 123.8 (q,  $J$  = 3.8 Hz), 121.0, 120.4, 113.9, 113.1, 111.5, 109.7, 103.7, 57.3, 55.5, 55.1, 32.9 ppm.

**<sup>19</sup>F NMR** (282 MHz, CDCl<sub>3</sub>)  $\delta$  -62.1 ppm.

**HRMS (ES+)** Calcd for C<sub>31</sub>H<sub>26</sub>F<sub>3</sub>NO<sub>3</sub>Na [M + Na]<sup>+</sup>: 540.1762, Found: 540.1765.



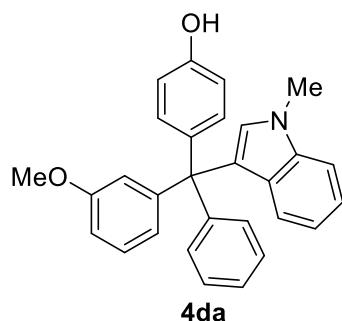
**(S)-4-((5-Methoxy-1-methyl-1*H*-indol-3-yl)(1-methoxynaphthalen-2-yl)(phenyl)methyl)phenol (3tg)** was prepared according to the General Procedure B as yellow solid (chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 88% yield (132.0 mg, 86% ee). The reaction time was 36 h.

$[\alpha]_D^{25}$ : +6.88 ( $c = 1.0$ , CHCl<sub>3</sub>). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 5% *i*-PrOH in hexanes, 1.0 mL/min; retention times: 20.4 min (major), 29.0 min (minor).

**<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>) δ 8.00–7.94 (m, 1H), 7.84–7.76 (m, 1H), 7.48–7.26 (m, 6H), 7.24–7.07 (m, 5H), 7.05 (d,  $J = 8.8$  Hz, 1H), 6.71 (dd,  $J_1 = 2.5$ ,  $J_2 = 8.8$  Hz, 1H), 6.64 (s, 1H), 6.57 (d,  $J = 8.7$  Hz, 2H), 6.00 (d,  $J = 2.5$  Hz, 1H), 3.59 (s, 3H), 3.32 (s, 3H), 2.67 (s, 3H) ppm.

**<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>) δ 154.5, 153.5, 152.7, 146.2, 137.4, 135.4, 134.7, 133.0, 131.8, 130.6, 130.5, 128.7, 128.5, 128.2, 128.0, 127.2, 125.7, 125.6, 125.2, 123.1, 122.5, 121.7, 114.0, 111.4, 109.6, 103.9, 60.0, 57.7, 55.4, 32.8 ppm.

**HRMS** (ES+) Calcd for C<sub>34</sub>H<sub>30</sub>NO<sub>3</sub> [M + H]<sup>+</sup>: 500.2226, Found: 500.2215.

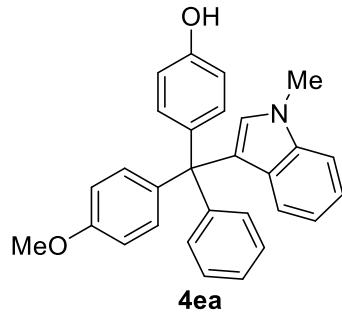


**4-((3-Methoxyphenyl)(1-methyl-1*H*-indol-3-yl)(phenyl)methyl)phenol (4da)** was prepared according to the General Procedure B as grey solid (chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 96% yield (120.8 mg, 0% ee). The reaction time was 3 days.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.26–7.16 (m, 6H), 7.14–7.06 (m, 3H), 6.81–6.65 (m, 8H), 4.94 (d,  $J = 13.9$  Hz, 1H), 3.70 (s, 3H), 3.65 (s, 3H) ppm.

**<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>) δ 158.7, 153.6, 148.7, 146.7, 138.7, 137.6, 131.9, 130.6, 130.0, 128.2, 128.0, 127.3, 125.9, 123.7, 122.9, 122.2, 121.2, 118.6, 117.2, 114.1, 110.5, 108.9, 58.7, 55.1, 32.7 ppm.

**HRMS** (ES+) Calcd for C<sub>29</sub>H<sub>25</sub>NO<sub>2</sub>Na [M + Na]<sup>+</sup>: 442.1792, Found: 442.1783.



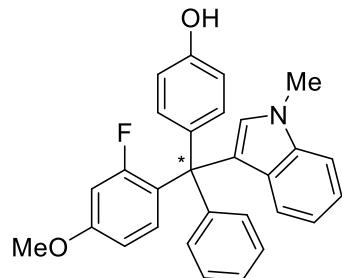
**4-((4-Methoxyphenyl)(1-methyl-1*H*-indol-3-yl)(phenyl)methyl)phenol (4ea)** was prepared according to the General Procedure B as yellow solid (chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 98% yield (123.3 mg, 14% ee). The reaction time was 3 days.

[α]<sub>D</sub><sup>25</sup>: +1.2 (*c* = 1.0, CHCl<sub>3</sub>). HPLC analysis of the product: Daicel CHIRALPAK IC column; 2% *i*-PrOH in hexanes, 0.4 mL/min; retention times: 53.6 min (major), 58.5 min (minor).

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.26–7.10 (m, 9H), 7.06 (d, *J* = 8.7 Hz, 2H), 6.77 (q, *J* = 7.4 Hz, 3H), 6.67–6.62 (m, 4H), 4.97 (s, 1H), 3.77 (s, 3H), 3.69 (s, 3H) ppm.

**<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>) δ 157.4, 153.5, 147.1, 139.2, 139.1, 137.7, 131.8, 131.6, 130.6, 130.0, 128.2, 127.3, 125.8, 122.9, 122.7, 121.1, 118.6, 114.1, 112.5, 108.9, 58.0, 55.1, 32.7 ppm.

**HRMS** (ES+) Calcd for C<sub>29</sub>H<sub>25</sub>NO<sub>2</sub>Na [M + Na]<sup>+</sup>: 442.1792, Found: 442.1783.



**4fa**

**4-((2-Fluoro-4-methoxyphenyl)(1-methyl-1*H*-indol-3-yl)(phenyl)methyl)phenol**

**(4fa):** was prepared according to the General Procedure B as yellow solid (chromatography eluent: hexanes/DCM = 5:2 → 5:4) in 97% yield (131.0 mg, 81% ee).

The reaction time was 2 days.

$[\alpha]_D^{25}$ : -0.92 ( $c = 1.0$ , CHCl<sub>3</sub>). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 10% *i*-PrOH in hexanes, 1.0 mL/min; retention times: 11.3 min (minor), 12.2 min (major).

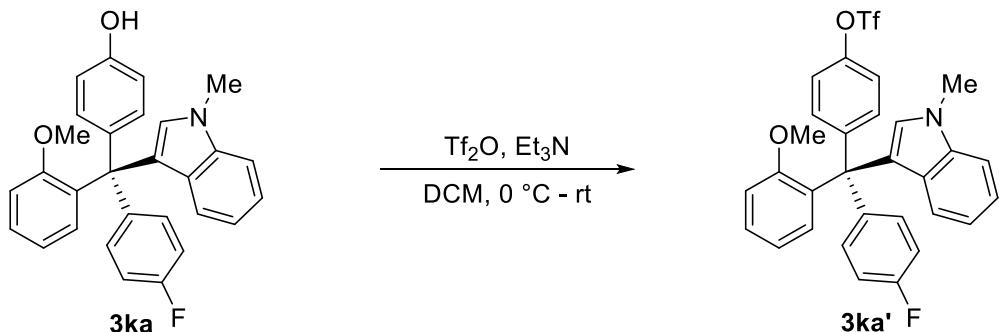
**<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>) δ 7.24–7.05 (m, 10H), 6.75 (t,  $J = 7.8$  Hz, 1H), 6.64–6.51 (m, 6H), 5.00 (s, 1H), 3.73 (s, 3H), 3.65 (s, 3H) ppm.

**<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>) δ 161.5 (d,  $J = 247.9$  Hz), 159.76 (d,  $J = 11.3$  Hz), 153.5, 145.5, 137.6, 137.4, 131.4 (d,  $J = 5.3$  Hz), 131.2, 129.8, 127.8, 127.4, 126.7 (d,  $J = 12.0$  Hz), 125.9, 122.2, 121.1, 121.0, 118.7, 114.2, 109.0, 108.4 (d,  $J = 2.3$  Hz), 102.6 (d,  $J = 26.3$  Hz), 102.4, 56.0, 55.4, 32.7 ppm.

**HRMS (ES+)** Calcd for C<sub>29</sub>H<sub>27</sub>NO<sub>2</sub>FNa [M + Na]<sup>+</sup>: 460.1689, Found: 460.1682.

**<sup>19</sup>F NMR** (282 MHz, CDCl<sub>3</sub>) δ -99.0 ppm.

#### IV. Product Derivatizations



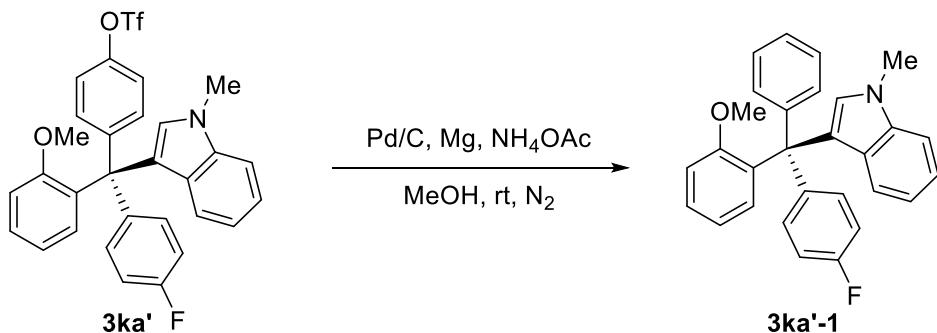
**(R)-4-((4-Fluorophenyl)(2-methoxyphenyl)(1-methyl-1*H*-indol-3-yl)methyl)phenyl trifluoromethanesulfonate (3ka').** At 0 °C, a solution of **3ka** (437.5 mg, 1.0 mmol, 1.0 equiv.) and Et<sub>3</sub>N (121.4 mg, 1.2 mmol, 1.2 equiv.) in DCM (5 mL) was stirred and treated dropwise with Tf<sub>2</sub>O (338.6 mg, 1.2 mmol, 1.2 equiv.), and the mixture was allowed to warm to room temperature and stirred for 1 h. Then the reaction was quenched with water and extracted with DCM, the combined organic layer was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and concentrated under reduced pressure. The residue was further purified by silica gel flash chromatography to afford the desired product **3ka'** as white solid in 73.4% yield (418.2 mg).

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.31–7.09 (m, 10H), 6.91–6.86 (m, 3H), 6.83 (td, *J*<sub>1</sub> = 7.2 Hz, *J*<sub>2</sub> = 1.0 Hz, 1H), 6.76 (td, *J*<sub>1</sub> = 7.6 Hz, *J*<sub>2</sub> = 0.6 Hz, 1H), 6.53 (t, *J* = 8.1 Hz, 2H), 3.71 (s, 3H), 3.16 (s, 3H) ppm.

**<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>) δ 160.9 (d, *J* = 246.4 Hz), 157.7, 147.3, 146.7, 140.2, 137.6, 134.9, 131.6 (d, *J* = 8.1 Hz), 131.5, 130.6, 129.9, 128.8, 127.7, 122.1, 121.4, 121.3, 120.4, 119.7, 118.9, 117.1, 113.9 (d, *J* = 21.2 Hz), 113.1, 109.1, 57.1, 54.9, 32.8 ppm.

**<sup>19</sup>F NMR** (282 MHz, CDCl<sub>3</sub>) δ -72.8, -117.5 ppm.

**HRMS (ES+)** Calcd for C<sub>30</sub>H<sub>24</sub>NO<sub>4</sub>SF<sub>4</sub> [M+H]<sup>+</sup>: 570.1362, Found: 570.1362.



**(R)-3-((4-Fluorophenyl)(2-methoxyphenyl)(phenyl)methyl)-1-methyl-1*H*-indole (3ka'-1).**

Under  $\text{N}_2$ , an oven-dried bottom equipped with magnetic stir bar was charged with triflate **3ka'** (114 mg, 0.2 mmol, 1.0 equiv.), Pd/C (12 mg, 10 wt%), Mg (5.6 mg, 0.24 mmol, 1.2 equiv.),  $\text{NH}_4\text{OAc}$  (18.6 mg, 0.24 mmol, 1.2 equiv.) and MeOH (2 mL). The reaction mixture was stirred at room temperature for 16 h, then the mixture was filtered through a pad of celite and the filtrate was evaporated under reduced pressure, the residue was further purified by silica gel chromatography (eluent: hexanes/EtOAc = 20:1) to afford the desired product **3ka'-1** as light yellow solid (83.5 mg, 99% yield, 93% ee).

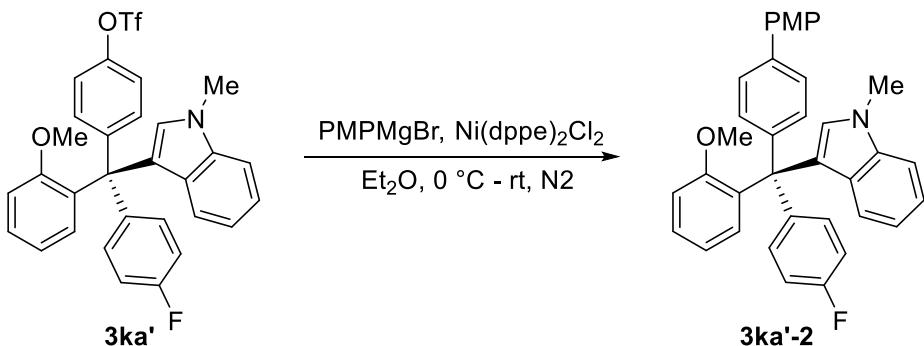
$[\alpha]_D^{25}$ : +6.0 ( $c = 0.5$ ,  $\text{CHCl}_3$ ). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 1% *i*-PrOH in hexanes, 1.0 mL/min; retention times: 6.0 min (major), 6.4 min (minor).

**$^1\text{H NMR}$**  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.32–7.24 (m, 5H), 7.20 (d,  $J = 7.7$  Hz, 1H), 7.15–7.09 (m, 5H), 6.91–6.87 (m, 3H), 6.83 (t,  $J = 7.5$  Hz, 1H), 6.77 (t,  $J = 7.6$  Hz, 1H), 6.53 (t,  $J = 8.1$  Hz, 2H), 3.72 (s, 3H), 3.16 (s, 3H) ppm.

**$^{13}\text{C NMR}$**  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  160.9 (d,  $J = 245.9$  Hz), 157.7, 147.3, 146.7, 137.6, 134.9, 131.6 (d,  $J = 7.7$  Hz), 131.5, 130.6, 129.9, 128.8, 127.7, 122.1, 121.4, 121.3, 120.4, 119.7, 118.9, 114.0, 113.8, 113.1, 109.1, 57.1, 54.9, 32.8 ppm.

**$^{19}\text{F NMR}$**  (282 MHz,  $\text{CDCl}_3$ )  $\delta$  -118.3 ppm.

**HRMS (ES+)** Calcd for  $\text{C}_{29}\text{H}_{24}\text{NOF} [\text{M}+\text{H}]^+$ : 422.1920, Found: 422.1926.



**(R)-3-((4-Fluorophenyl)(4'-methoxy-[1,1'-biphenyl]-4-yl)(2-methoxyphenyl)methyl)-1-methyl-1H-indole (3ka'-2).** Under N<sub>2</sub>, an oven-dried bottom equipped with magnetic stir bar was charged with triflate **3ka'** (114 mg, 0.2 mmol, 1.0 equiv.), Ni(dppe)<sub>2</sub>Cl<sub>2</sub> (5.2 mg, 5 mol%) and Et<sub>2</sub>O (2 mL), then PMPMgBr (0.5 mmol, 5 equiv.) was added dropwise to the mixture at 0 °C. Upon completing, the resulting mixture was allowed to stirred at room temperature for 12 h, then the reaction was quenched with water and extracted with EtOAc, the combined organic layer was dried and evaporated under reduced pressure, further purified by silica gel chromatography (eluent: hexanes/EtOAc = 20:1) to afford the desired product **3ka'-2** as white solid in 70% yield (73.9 mg) and 89% ee.

[ $\alpha$ ]<sub>D</sub><sup>25</sup>: -15.6 ( $c = 1.0$ , CHCl<sub>3</sub>). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 2% *i*-PrOH in hexanes, 1.0 mL/min; retention times: 7.1 min (minor), 7.6 min (major).

<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 7.57–7.54 (m, 2H), 7.45–7.42 (m, 2H), 7.31–7.22 (m, 7H), 7.12 (td,  $J_1 = 10.2$  Hz,  $J_2 = 1.1$  Hz, 1H), 6.99–6.86 (m, 6H), 6.78–6.73 (m, 1H), 6.65–6.61 (m, 2H), 3.82 (s, 3H), 3.70 (s, 3H), 3.16 (s, 3H) ppm.

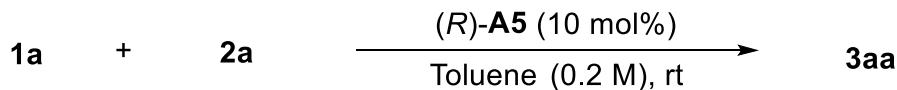
<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) δ 160.8 (d,  $J = 244.2$  Hz), 158.9, 158.2, 144.2, 141.3 (d,  $J = 2.9$  Hz), 137.6, 137.5, 135.7, 133.3, 131.8, 131.7 (d,  $J = 7.5$  Hz), 130.4, 130.3 (d,  $J = 53.2$  Hz), 128.4, 127.8, 127.0, 125.1, 122.4, 121.8, 121.1, 120.3, 118.7, 114.1, 113.6 (d,  $J = 20.7$  Hz), 113.3, 108.9, 57.2, 55.3, 55.2, 32.7 ppm.

<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -118.2 ppm.

HRMS (ES+) Calcd for C<sub>36</sub>H<sub>30</sub>NO<sub>2</sub>Na [M + Na]<sup>+</sup>: 550.2158, Found: 550.2152.

## V. Mechanistic Experiments

### Monitoring the ee values during the reaction process.



At room temperature, to an oven-dried 10-mL vial charged with a solution of the tertiary alcohol **1a** (0.6 mmol) and CPA *(R)*-**A5** (56 mg, 0.06 mmol, 10 mol%) in toluene (3.0 mL), *N*-protected-indole **2a** (0.9 mmol) was added in one portion. The reaction mixture was stirred at the same temperature. Upon the corresponding reaction time, 100  $\mu$ L reaction solution was extracted by syringe and injected to Et<sub>3</sub>N (0.1 mL), then the resulting solution was passed through a short column of silica gel and concentrated under reduced pressure, the crude was analyzed by chiral HPLC for ee values of **1a** and **3aa**.

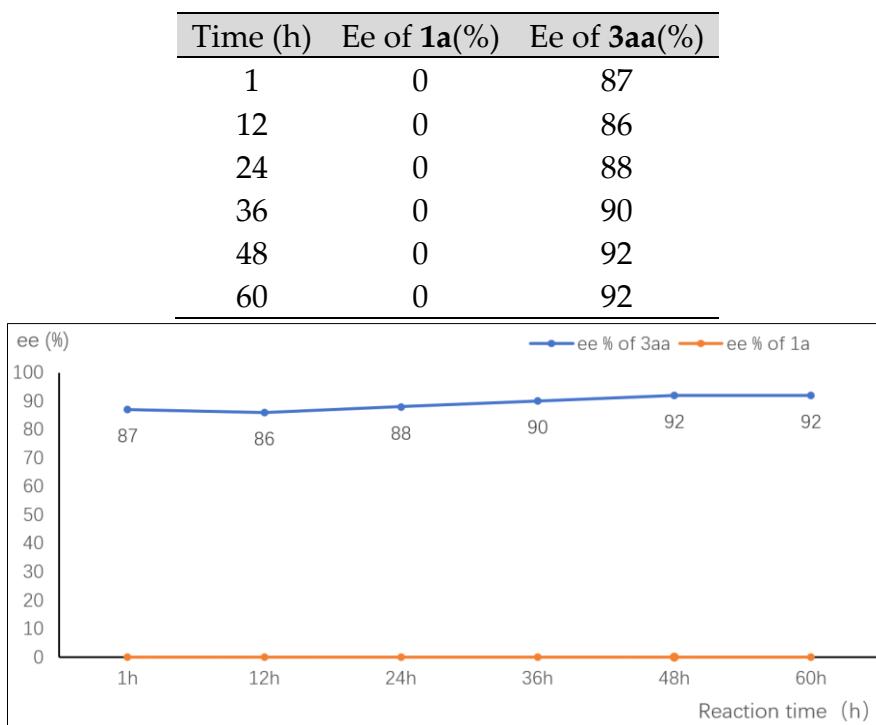


Figure S1. Original data and ee value-time plot of **2a** and **3aa**

## VI. DFT Calculations

### Computational details

All structures were optimized and characterized in toluene with the SMD<sup>3</sup> solvent model (SCRF = SMD) at B3LYP<sup>4</sup>-D3(BJ)<sup>5</sup>/6-31G(d) level. Harmonic frequency analysis calculations at the same level were performed to verify the optimized transition states (TSs, having unique one imaginary frequency). The energies were further improved by M06-2X<sup>6</sup>/6-311+G(d,p) //B3LYP-D3(BJ)/ 6-31G(d) single-point calculations with solvent effects accounted by the SMD solvent model, using the experimental solvent (toluene). All DFT calculations were carried out using Gaussian 09 program.<sup>7</sup> Computed structures are illustrated using the CYLview.<sup>8</sup>

**Cartesian Coordinates in Å, SCF Energies and Free Energies (in a.u.) at 298.15 K  
and 1 atm for the Optimized Structures [BSI= 6-31G(d), BSII=6-311+G(d,p)]**

**TS-S**

B3LYP-D3/BSI SCF energy in toluene: -3907.622981 a.u.

M06-2X/BSII SCF energy in toluene: -3906.886197 a.u.

M06-2X/BSII free energy in toluene: -3905.573469 a.u.

P	1.49769800	0.22710400	-0.91362600
O	2.73025800	1.33428700	-1.00499200
O	2.15883000	-0.79517100	0.22055100
O	1.47904000	-0.41438500	-2.27747000
O	0.27475000	0.79909300	-0.26447500
C	-4.20590400	-0.91476600	0.57743300
C	-3.63686000	-1.29748200	1.93951300
C	-4.04231100	-2.53545000	2.46996400
C	-2.69870100	-0.54867700	2.66082100
C	-3.53985100	-2.99578200	3.68721300
C	-2.21153600	-0.99867100	3.88856800
C	-2.63011900	-2.22271000	4.41043300
C	-3.36731300	-1.29561900	-0.58585000
C	-3.75845600	-0.99559200	-1.91232300
C	-2.05462700	-1.77263400	-0.39133700
C	-2.85159800	-1.05060100	-2.96149000
C	-1.14637700	-1.83583700	-1.43215900
C	-1.50687500	-1.37246400	-2.71106500
C	-5.68396300	-1.17651300	0.51438100
C	-6.22585700	-2.06965400	-0.42526700
C	-6.56595300	-0.66849400	1.50852000
C	-7.57404200	-2.42667600	-0.41904900
C	-7.91881500	-1.02167400	1.51551500
C	-8.42083800	-1.89553100	0.54991400
O	-0.59815600	-1.18594200	-3.68398200
C	-4.07234800	1.18285900	0.53240100
C	-5.00660000	1.71257900	-0.46979500

C	-4.24347100	2.09328100	-1.59198400
C	-1.78103200	2.16781100	-2.19225600
H	-3.86756100	-3.95904700	4.06933700
H	-5.56734000	-2.53135300	-1.14975200
H	-7.94861200	-3.12822900	-1.15810800
H	-8.58332800	-0.62150300	2.27178600
H	-9.47348400	-2.16400900	0.57024700
H	0.26608400	-0.94631400	-3.22785000
H	-1.86066300	3.19649400	-2.54973300
H	-0.84097900	2.01140700	-1.66630200
H	-1.84903800	1.47262800	-3.03321700
H	-4.76055100	-0.63364300	-2.11153900
H	-3.14158300	-0.74760100	-3.96324800
H	-1.72317900	-2.06846900	0.59579600
H	-4.25455500	1.30353400	1.58976600
C	3.43224000	-1.28068700	0.02466900
C	4.52700000	-0.44370900	0.21677900
C	5.83517800	-0.96238700	-0.07774100
C	5.97958000	-2.35743000	-0.37342900
C	4.82645600	-3.18216900	-0.42771400
C	3.55528900	-2.66762700	-0.28511300
H	6.90349500	0.91887900	0.06095600
C	7.00010600	-0.14628900	-0.11668600
C	7.27405500	-2.88608500	-0.62990400
H	4.95230600	-4.24259700	-0.62433100
C	8.38409800	-2.07183800	-0.63354800
C	8.23898400	-0.68528500	-0.38816700
H	7.36716800	-3.94872400	-0.84217900
H	9.36747500	-2.48579300	-0.84000400
H	9.11160100	-0.03825700	-0.42041100
C	4.31202000	0.93789300	0.73752200
C	4.99156700	1.42580100	1.91022200
C	3.36970600	1.76231900	0.13497200

C	5.84664800	0.61901700	2.71277200
C	4.78048200	2.78465100	2.31988400
C	3.06474600	3.07339100	0.60400900
C	6.49805800	1.13830200	3.81081500
H	5.98104700	-0.42528500	2.45986000
C	5.48164900	3.29542700	3.44633200
C	3.81951600	3.57701800	1.64161400
C	6.33142000	2.49533100	4.17558400
H	7.14195900	0.49568300	4.40551800
H	5.31669400	4.33222000	3.73113900
H	3.62428000	4.58492600	1.99956200
H	6.85774300	2.89505900	5.03830700
C	1.88471000	3.81804900	0.06508100
C	1.85717200	4.28474200	-1.26975500
C	0.76395800	4.02617700	0.90497800
C	0.71828300	4.95161800	-1.72963500
C	-0.35017200	4.70690400	0.39485600
C	-0.39750400	5.17794300	-0.91730800
H	0.69803900	5.31579700	-2.75479100
H	-1.20439300	4.86077400	1.04679100
C	2.33632800	-3.52356200	-0.43984000
C	1.48798900	-3.76412600	0.66923100
C	2.02791200	-4.10186100	-1.69489500
C	0.35883800	-4.57081400	0.50116300
C	0.89235700	-4.91704200	-1.80234700
C	0.04278600	-5.16447400	-0.72417600
H	-0.28832900	-4.74621700	1.35620800
H	0.65614500	-5.36592700	-2.76375600
C	0.69348800	3.52670600	2.34952400
H	1.62902400	3.01779300	2.58731100
C	3.04466300	4.12288600	-2.21420800
H	3.81021100	3.53379900	-1.70341500
C	-1.58387100	5.95823500	-1.47218300

H	-1.67781000	5.68814900	-2.53467800
C	1.77452600	-3.20582400	2.06146600
H	2.67380800	-2.58729400	2.01246700
C	2.88905800	-3.88080400	-2.93819900
H	3.57567900	-3.05563300	-2.73311700
C	-1.18644400	-6.04919400	-0.87886900
H	-1.18864300	-6.42845400	-1.90977400
H	-0.13721600	-2.18470600	-1.25476900
H	-4.75218400	-3.14564600	1.92138700
H	-1.48873400	-0.39163800	4.42591900
H	-2.24313800	-2.57521600	5.36248600
H	-2.33132500	0.39542400	2.28408600
O	-6.02531900	0.18640100	2.41747500
C	-6.78599500	0.57195400	3.55930900
H	-7.12732400	-0.30495300	4.12253500
H	-6.10492400	1.15753400	4.17982700
H	-7.64683700	1.19454700	3.28388200
C	2.66641600	3.36233900	-3.49690700
H	3.55563400	3.20702700	-4.12044500
H	2.24518800	2.38114800	-3.26129400
H	1.93725600	3.91972200	-4.09831800
C	3.67184900	5.49119500	-2.54155800
H	2.96695900	6.13857300	-3.07804000
H	3.97749400	6.01542500	-1.62814900
H	4.55904900	5.36597900	-3.17481200
C	-1.29995900	7.47223100	-1.40912900
H	-0.37605900	7.72521300	-1.94129700
H	-2.12109800	8.04649800	-1.85665400
H	-1.18449500	7.79809500	-0.36779600
C	-2.92230400	5.63604600	-0.79167700
H	-3.11424100	4.55894100	-0.75629300
H	-2.95167000	6.01368900	0.23736600
H	-3.74938800	6.10812800	-1.33457000

C	0.62733100	-2.31218600	2.56089800
H	0.88384400	-1.86950600	3.53170600
H	0.43198000	-1.49828200	1.85807000
H	-0.29694500	-2.88380800	2.69801600
C	2.06739500	-4.33969500	3.06239100
H	2.32384500	-3.92600700	4.04606600
H	1.19845100	-4.99634300	3.19301900
H	2.90712400	-4.95975300	2.72655800
C	-2.49029900	-5.25550300	-0.67561100
H	-3.36392400	-5.90548500	-0.81500400
H	-2.54481900	-4.83348500	0.33525000
H	-2.56250200	-4.42421800	-1.38327000
C	-1.13340600	-7.26465600	0.06447000
H	-1.16131100	-6.95305200	1.11584700
H	-1.99008800	-7.92792600	-0.10903400
H	-0.21617300	-7.84556300	-0.08611300
C	2.06274600	-3.47671900	-4.17055600
H	1.41830800	-2.62409700	-3.95165100
H	2.73196500	-3.19881800	-4.99417700
H	1.42805900	-4.29623200	-4.52935400
C	3.728444000	-5.13410700	-3.25278100
H	3.07937500	-5.98946700	-3.47991600
H	4.37253300	-4.95980600	-4.12377900
H	4.36811600	-5.42159900	-2.41123100
C	0.54826700	4.69390700	3.34200200
H	0.56447800	4.32435200	4.37504300
H	1.36463700	5.41752800	3.22948400
H	-0.39522100	5.23470700	3.19775800
C	-0.42380100	2.48495500	2.54070600
H	-0.44631200	2.14093300	3.58302000
H	-1.41284000	2.90066300	2.30726800
H	-0.23946000	1.62571200	1.89066100
C	-2.77004000	1.43896400	-0.03263300

H	-1.78308200	1.20778300	0.34643900
N	-2.88037300	1.90052200	-1.26880500
C	-4.79409300	2.58637600	-2.76798700
C	-6.18578300	2.70953600	-2.80555500
C	-6.97046300	2.35835900	-1.69648700
C	-6.39418200	1.86120900	-0.52387600
H	-4.17552700	2.86215000	-3.61560700
H	-6.66341200	3.08986800	-3.70360100
H	-8.04905500	2.47591400	-1.74972500
H	-7.01505600	1.60012300	0.32426700

### TS-*R*

B3LYP-D3/BSI SCF energy in toluene: -3907.620941 a.u.

M06-2X/BSII SCF energy in toluene: -3906.885508 a.u.

M06-2X/BSII free energy in toluene: -3905.572188 a.u.

P	1.29770500	0.17357000	-0.94295600
O	2.83602800	0.78171000	-0.80482300
O	1.44871800	-1.18321100	0.02571600
O	1.17603000	-0.21982700	-2.39155200
O	0.29637800	1.05101900	-0.24946200
C	-4.38992000	-0.32818800	0.88983100
C	-3.88389800	-1.04380200	2.14690700
C	-4.68759600	-2.08685000	2.64806500
C	-2.65904600	-0.80491700	2.82752700
C	-4.35183500	-2.82418000	3.78122800
C	-2.35013100	-1.50352000	4.00357600
C	-3.18857600	-2.50895600	4.47781100
C	-3.70506300	-0.64761500	-0.38927700
C	-4.11577400	-0.06211500	-1.60958200
C	-2.48186300	-1.34199500	-0.38746400
C	-3.29249300	-0.07047100	-2.72760400
C	-1.64576000	-1.34023000	-1.48940200
C	-2.00251000	-0.62201100	-2.64502800
C	-5.89863500	-0.26908300	0.90248700

C	-6.67765200	-0.87106400	-0.09811200
C	-6.56603300	0.25994500	2.02430300
C	-8.07148000	-0.90825900	0.00283000
C	-7.95223300	0.22445000	2.12696300
C	-8.71549500	-0.35598000	1.10841700
O	-1.14041400	-0.41518100	-3.65659300
C	-3.89201000	1.69443800	1.13183300
C	-4.82385700	2.61865200	0.45104400
C	-4.16614100	3.10770800	-0.69773000
C	-1.85472000	2.86474100	-1.72589900
H	-5.00504800	-3.62368800	4.11743200
H	-6.19778700	-1.35197400	-0.94176500
H	-8.64865600	-1.38640300	-0.78385800
H	-8.43780900	0.64456100	3.00366000
H	-9.79880200	-0.38764800	1.18581300
H	-0.21570800	-0.40272100	-3.26535300
H	-0.93661400	2.33020500	-1.47807100
H	-2.23702100	2.52490100	-2.69142700
H	-1.66787900	3.94193400	-1.75717700
H	-5.04921700	0.48770700	-1.65790200
H	-3.58988000	0.43433200	-3.64199000
H	-2.15471000	-1.85679000	0.50482000
H	-3.82749800	1.65292500	2.21185900
C	2.60072300	-1.94367200	-0.00270300
C	3.76458000	-1.44847500	0.57664700
C	4.95932900	-2.24833800	0.51941500
C	4.87727200	-3.58361800	0.00772500
C	3.63811600	-4.05952600	-0.48953000
C	2.51741900	-3.25958700	-0.54948100
H	6.33491500	-0.74824800	1.27233200
C	6.23677000	-1.77094000	0.92851000
C	6.04071300	-4.40008700	-0.01537300
H	3.57666600	-5.08461100	-0.84372300

C	7.25383300	-3.91564200	0.41785900
C	7.35038200	-2.58117300	0.87958600
H	5.95404900	-5.41480800	-0.39719400
H	8.13869400	-4.54581900	0.39043700
H	8.31410000	-2.18861400	1.19317300
C	3.77348200	-0.09458800	1.20000400
C	4.21744400	0.12990100	2.54825700
C	3.34041700	0.99585400	0.45834600
C	4.50179500	-0.92699900	3.45733200
C	4.35478600	1.47830600	3.01559400
C	3.45306300	2.34344800	0.91084200
C	4.93085900	-0.66583800	4.74069900
H	4.36906500	-1.95249900	3.13170400
C	4.81599100	1.71357300	4.33978700
C	3.99946100	2.55305600	2.16050800
C	5.10329100	0.66684900	5.18651000
H	5.13577900	-1.49101300	5.41769200
H	4.92533500	2.74248800	4.67514700
H	4.12311500	3.57019900	2.52223700
H	5.44933200	0.85930100	6.19854900
C	2.96576400	3.47679900	0.06588300
C	3.55485600	3.74101100	-1.19307200
C	1.89989200	4.29138500	0.52496100
C	3.05870700	4.79696800	-1.96638600
C	1.44887600	5.33824200	-0.28545900
C	2.00505900	5.60465100	-1.53871500
H	3.50923900	4.99749200	-2.93560700
H	0.62818500	5.95708900	0.06771200
C	1.22839400	-3.78834200	-1.10102100
C	0.27038200	-4.32547100	-0.21335100
C	0.97479800	-3.76273900	-2.49247400
C	-0.94631100	-4.78793900	-0.72513800
C	-0.25105100	-4.25826000	-2.95510300

C	-1.23055200	-4.75726400	-2.09236600
H	-1.69375600	-5.17211800	-0.03620500
H	-0.46687800	-4.23083800	-4.01904600
C	1.18899800	4.06463500	1.85893100
H	1.57079900	3.14097100	2.29926000
C	4.74299200	2.94853700	-1.73447400
H	4.97671100	2.14544600	-1.03165600
C	1.46724200	6.72452100	-2.41740600
H	2.08395100	6.75561300	-3.32566500
C	0.52344900	-4.39892300	1.28956200
H	1.55887900	-4.09847300	1.47430100
C	2.01085700	-3.22306500	-3.47781900
H	2.56060800	-2.42760400	-2.96500300
C	-2.57565600	-5.22935400	-2.62722300
H	-2.53668800	-5.15681300	-3.72255800
H	-0.69389100	-1.85126500	-1.44814300
H	-5.60343100	-2.33480300	2.12611900
H	-1.43553500	-1.27662500	4.53702600
H	-2.91972400	-3.04800200	5.38210600
C	4.42797600	2.29042700	-3.08970000
H	5.26699200	1.65841400	-3.40693100
H	3.53589000	1.66219600	-3.02133000
H	4.26582800	3.04002700	-3.87437300
C	5.99749800	3.83806900	-1.82616000
H	5.85323400	4.66553200	-2.53156700
H	6.24968800	4.27108900	-0.85065900
H	6.85944500	3.25285900	-2.17067700
C	1.57667700	8.09810800	-1.73236000
H	2.61196700	8.31818500	-1.44788200
H	1.23033900	8.89541100	-2.40173800
H	0.96564500	8.13992500	-0.82237400
C	0.01662700	6.44282900	-2.85173600
H	-0.05914700	5.48031700	-3.37091700

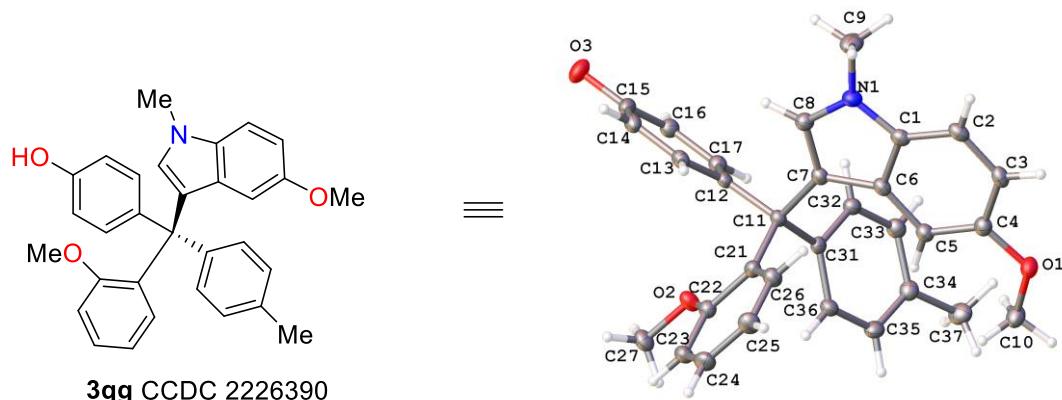
H	-0.65529300	6.41423300	-1.98435000
H	-0.34823400	7.22517300	-3.52922100
C	-0.37708700	-3.41298200	2.04968800
H	-0.13591300	-3.41106600	3.11958600
H	-0.24042800	-2.39942500	1.66257800
H	-1.43625600	-3.67828000	1.95300100
C	0.36545100	-5.82931000	1.83386200
H	0.62379000	-5.86347600	2.89975900
H	-0.66480900	-6.19120700	1.73313100
H	1.01956800	-6.53148900	1.30378500
C	-3.72271400	-4.32150500	-2.14365200
H	-4.68283300	-4.66117300	-2.55344700
H	-3.80209700	-4.33314600	-1.04970900
H	-3.56382100	-3.28350100	-2.45237800
C	-2.85055600	-6.70050400	-2.26795400
H	-2.93260500	-6.83746400	-1.18266200
H	-3.79203300	-7.04096900	-2.71692600
H	-2.04659700	-7.35408500	-2.62604400
C	1.39707700	-2.60288900	-4.74312400
H	0.57637800	-1.92385300	-4.50834600
H	2.16272700	-2.03690100	-5.28614900
H	1.01577600	-3.37077400	-5.42863500
C	3.00913000	-4.32329200	-3.89071600
H	2.48611000	-5.15075800	-4.38767300
H	3.75096800	-3.92314400	-4.59360700
H	3.54922700	-4.73407700	-3.03408800
C	1.47037900	5.20398400	2.85362900
H	0.97965800	5.00880100	3.81585200
H	2.54461500	5.32075700	3.03907200
H	1.09535000	6.16326000	2.47572800
C	-0.32109300	3.86032200	1.65585800
H	-0.80472700	3.56858000	2.59687700
H	-0.81962700	4.76894200	1.29686000

H	-0.47352800	3.06771500	0.92364900
C	-2.66861600	1.82949400	0.36975500
H	-1.72809300	1.31582100	0.49493000
N	-2.85132200	2.58624600	-0.69458400
C	-4.74254800	3.97632800	-1.61358600
C	-6.05166900	4.39093400	-1.35015300
C	-6.72142700	3.95349500	-0.19992100
C	-6.11813600	3.07651100	0.70816000
H	-4.19999500	4.32524700	-2.48610100
H	-6.54663800	5.06914600	-2.03879300
H	-7.73128600	4.30336300	-0.00584100
H	-6.65626300	2.76167700	1.59257600
H	-5.98228400	0.69759800	2.82857700
O	-1.81516100	0.11474800	2.29943500
C	-0.51542200	0.32462400	2.86367700
H	0.02386800	-0.61858000	2.98845300
H	0.02059000	0.93286400	2.13608500
H	-0.58845400	0.84172200	3.82863300

## VII. Determination of the Absolute Stereochemistry

The absolute stereochemistry of product **3qg** was unambiguously determined by X-ray diffraction. The X-ray data have been deposited at the Cambridge Crystallographic Data Center (CCDC 2226390). The stereochemistry of other products was assumed by analogy.

The X-ray data were collected by SuperNova, Dual, Cu at zero, Atlas diffractometer. A suitable crystal of **3qg** was obtained from petroleum ether and dichloromethane by vapor deposition. The crystal was kept at 100.01(10) K during data collection. Using Olex2,1 the structure was solved with the SHELXT2 structure solution program using Intrinsic Phasing and refined with the SHELXL refinement package using Least Squares minimization.



**Table S1. Crystal data and structure refinement for 3qg.**

Identification code	<b>3qg</b>
Empirical formula	C <sub>32</sub> H <sub>33</sub> NO <sub>4</sub>
Formula weight	495.59
Temperature/K	100.01(10)
Crystal system	monoclinic
Space group	P2 <sub>1</sub>
a/Å	13.02736(13)
b/Å	7.62610(7)
c/Å	13.31312(13)
α/°	90

$\beta/\circ$	97.9813(9)
$\gamma/\circ$	90
Volume/ $\text{\AA}^3$	1309.82(2)
Z	2
$\rho_{\text{calc}} \text{g/cm}^3$	1.257
$\mu/\text{mm}^{-1}$	0.655
F(000)	528.0
Crystal size/mm <sup>3</sup>	0.2 $\times$ 0.18 $\times$ 0.18
Radiation	CuK $\alpha$ ( $\lambda = 1.54184$ )
2 $\Theta$ range for data collection/ $\circ$	6.704 to 153.748
Index ranges	-14 $\leq$ h $\leq$ 16, -9 $\leq$ k $\leq$ 9, -16 $\leq$ l $\leq$ 13
Reflections collected	8645
Independent reflections	5291 [ $R_{\text{int}} = 0.0181$ , $R_{\text{sigma}} = 0.0226$ ]
Data/restraints/parameters	5291/1/342
Goodness-of-fit on F <sup>2</sup>	1.032
Final R indexes [ $I >= 2\sigma(I)$ ]	$R_1 = 0.0247$ , $wR_2 = 0.0647$
Final R indexes [all data]	$R_1 = 0.0256$ , $wR_2 = 0.0652$
Largest diff. peak/hole / e $\text{\AA}^{-3}$	0.18/-0.12
Flack parameter	0.01(6)

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

Atom x	y	z	U(eq)
O(1) 3162.7 (8)	972.6 (16)	2076.8 (9)	22.3 (2)
O(2) 8585.2 (9)	4059.0 (15)	4674.8 (8)	21.5 (2)
O(3) 11191.1 (9)	6004.7 (18)	1769.9 (10)	29.0 (3)
N(1) 6773.2 (11)	430.7 (19)	412.6 (10)	19.8 (3)
C(1) 5823.3 (12)	389 (2)	749.6 (11)	17.6 (3)
C(2) 4896.6 (12)	-372 (2)	300.8 (11)	20.1 (3)
C(3) 4030.4 (12)	-145 (2)	773.4 (12)	20.1 (3)
C(4) 4093.6 (12)	808 (2)	1687.9 (12)	18.9 (3)
C(5) 5011.1 (12)	1537 (2)	2150.6 (11)	17.8 (3)
C(6) 5904.3 (12)	1342 (2)	1668.8 (11)	16.6 (3)
C(7) 6959.9 (12)	1968 (2)	1881.6 (11)	16.4 (3)
C(8) 7442.4 (12)	1376 (2)	1090.7 (12)	19.0 (3)
C(9) 7023.8 (14)	-465 (3)	-485.8 (13)	29.7 (4)
C(10) 3161.8 (13)	2023 (2)	2967.5 (13)	24.7 (3)
C(11) 7453.5 (11)	2991 (2)	2821.3 (11)	15.7 (3)
C(12) 8449.5 (12)	3896 (2)	2565.7 (11)	16.5 (3)
C(13) 9312.1 (12)	2855 (2)	2452.0 (11)	19.5 (3)

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

Atom x	y	z	$U(\text{eq})$
C(14) 10214.1 (12)	3571 (2)	2183.1 (12)	21.3 (3)
C(15) 10285.5 (12)	5373 (2)	2032.7 (11)	21.1 (3)
C(16) 9447.1 (12)	6436 (2)	2165.8 (12)	20.7 (3)
C(17) 8544.9 (12)	5703 (2)	2428.6 (11)	18.7 (3)
C(21) 7756.3 (11)	1716 (2)	3716.6 (11)	17.2 (3)
C(22) 8337.3 (12)	2317 (2)	4629.8 (12)	18.4 (3)
C(23) 8620.4 (12)	1172 (2)	5432.8 (12)	21.2 (3)
C(24) 8324.2 (13)	-582 (2)	5350.5 (13)	24.5 (3)
C(25) 7749.0 (14)	-1201 (2)	4470.4 (13)	24.4 (3)
C(26) 7473.0 (12)	-45 (2)	3663.6 (12)	20.8 (3)
C(27) 9178.8 (13)	4692 (2)	5583.2 (12)	24.4 (3)
C(31) 6622.5 (11)	4303 (2)	3070.0 (11)	15.9 (3)
C(32) 6149.7 (12)	5418 (2)	2308.4 (11)	17.7 (3)
C(33) 5285.6 (12)	6407 (2)	2440.7 (12)	20.5 (3)
C(34) 4846.9 (12)	6311 (2)	3338.1 (12)	20.6 (3)
C(35) 5335.8 (13)	5252 (2)	4111.0 (12)	21.1 (3)
C(36) 6213.5 (12)	4275 (2)	3984.2 (11)	18.6 (3)
C(37) 3860.3 (14)	7281 (2)	3451.2 (14)	27.7 (4)
O(1S) 1244.8 (9)	-501.3 (19)	1447.0 (9)	29.1 (3)
C(1S) 859.2 (16)	17 (3)	433.7 (15)	36.8 (4)

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

Atom	$U_{11}$	$U_{22}$	$U_{33}$	$U_{23}$	$U_{13}$	$U_{12}$
O(1)	16.1 (5)	26.4 (6)	24.3 (6)	-5.5 (5)	1.9 (4)	-2.5 (4)
O(2)	25.0 (6)	20.5 (6)	17.4 (5)	0.0 (4)	-3.4 (4)	-3.4 (4)
O(3)	19.3 (6)	34.1 (7)	35.6 (7)	-2.6 (6)	10.5 (5)	-5.4 (5)
N(1)	22.4 (7)	21.9 (6)	15.3 (6)	-2.1 (5)	3.3 (5)	-1.4 (5)
C(1)	21.5 (7)	16.5 (7)	14.6 (6)	1.5 (6)	1.4 (5)	0.5 (6)
C(2)	26.2 (8)	18.2 (7)	14.6 (7)	-0.2 (6)	-1.7 (6)	-0.6 (6)
C(3)	19.2 (7)	19.0 (7)	20.2 (7)	-0.3 (6)	-3.7 (6)	-2.2 (6)
C(4)	18.1 (7)	18.4 (7)	19.7 (7)	1.4 (6)	1.2 (6)	0.6 (6)
C(5)	18.9 (7)	17.7 (7)	16.3 (7)	-0.5 (6)	0.3 (5)	-0.6 (6)
C(6)	18.8 (7)	15.1 (7)	14.8 (6)	0.6 (6)	-1.2 (5)	-0.1 (6)
C(7)	17.2 (7)	16.1 (7)	15.3 (7)	1.2 (5)	0.1 (5)	-0.3 (5)
C(8)	19.5 (7)	19.9 (7)	17.8 (7)	-0.3 (6)	2.8 (5)	-1.6 (6)
C(9)	29.5 (8)	37.9 (10)	23.0 (8)	-12.4 (8)	8.8 (7)	-5.4 (8)
C(10)	19.0 (7)	28.1 (8)	27.4 (8)	-6.7 (7)	5.0 (6)	-0.8 (6)
C(11)	15.8 (6)	17.0 (7)	13.7 (7)	0.0 (6)	0.0 (5)	-0.7 (6)

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

<b>Atom</b>	<b><math>\mathbf{U}_{11}</math></b>	<b><math>\mathbf{U}_{22}</math></b>	<b><math>\mathbf{U}_{33}</math></b>	<b><math>\mathbf{U}_{23}</math></b>	<b><math>\mathbf{U}_{13}</math></b>	<b><math>\mathbf{U}_{12}</math></b>
C(12)	15.5 (7)	21.5 (7)	11.8 (6)	-0.3 (5)	-0.5 (5)	-1.4 (6)
C(13)	19.2 (7)	21.6 (7)	16.6 (7)	0.2 (6)	-1.3 (6)	0.9 (6)
C(14)	16.8 (7)	28.3 (8)	18.4 (7)	-3.5 (6)	0.5 (6)	2.9 (6)
C(15)	16.7 (7)	30.3 (8)	16.3 (7)	-3.0 (6)	2.7 (6)	-4.3 (6)
C(16)	21.2 (7)	21.8 (8)	18.9 (7)	-1.2 (6)	2.3 (6)	-3.7 (6)
C(17)	18.6 (7)	20.7 (8)	16.6 (7)	-2.2 (6)	1.8 (6)	-0.6 (6)
C(21)	15.1 (6)	20.0 (7)	16.3 (7)	2.2 (6)	1.7 (5)	0.6 (5)
C(22)	16.7 (7)	20.7 (7)	17.6 (7)	0.1 (6)	1.8 (5)	-0.2 (6)
C(23)	20.6 (7)	27.5 (8)	15.0 (7)	1.3 (6)	0.2 (6)	-0.6 (6)
C(24)	26.0 (8)	27.4 (8)	19.7 (8)	8.6 (6)	1.9 (6)	1.4 (7)
C(25)	28.1 (8)	20.2 (8)	24.6 (8)	4.5 (6)	2.1 (7)	-2.7 (6)
C(26)	21.3 (7)	21.3 (8)	19.1 (7)	1.4 (6)	0.7 (6)	-1.2 (6)
C(27)	24.7 (8)	26.4 (8)	20.5 (8)	-3.8 (6)	-3.1 (6)	-2.2 (7)
C(31)	14.3 (6)	16.4 (7)	16.6 (7)	-1.6 (6)	1.0 (5)	-3.5 (5)
C(32)	19.1 (7)	18.5 (7)	15.5 (7)	-0.2 (6)	2.3 (5)	-2.2 (6)
C(33)	21.8 (7)	18.9 (7)	20.3 (7)	1.9 (6)	1.0 (6)	0.1 (6)
C(34)	19.9 (7)	20.0 (7)	22.1 (8)	-4.1 (6)	3.1 (6)	-0.1 (6)
C(35)	22.8 (8)	24.5 (8)	16.4 (7)	-3.4 (6)	4.6 (6)	-2.2 (6)
C(36)	19.8 (7)	21.4 (7)	14.2 (7)	-0.6 (6)	0.5 (5)	-1.1 (6)
C(37)	28.2 (9)	28.7 (9)	27.3 (9)	-1.2 (7)	7.4 (7)	6.6 (7)
O(1S)	22.3 (6)	36.0 (7)	28.0 (6)	0.9 (5)	0.6 (5)	-8.7 (5)
C(1S)	35.8 (10)	45.1 (12)	27.3 (9)	-3.6 (8)	-3.6 (7)	1.2 (9)

**Table S4. Bond Lengths for 3qg.**

<b>Atom</b>	<b>Atom</b>	<b>Length/<math>\text{\AA}</math></b>	<b>Atom</b>	<b>Atom</b>	<b>Length/<math>\text{\AA}</math></b>
O(1)	C(4)	1.3888 (19)	C(12)	C(13)	1.401 (2)
O(1)	C(10)	1.431 (2)	C(12)	C(17)	1.398 (2)
O(2)	C(22)	1.3668 (19)	C(13)	C(14)	1.387 (2)
O(2)	C(27)	1.4262 (18)	C(14)	C(15)	1.394 (2)
O(3)	C(15)	1.3642 (19)	C(15)	C(16)	1.391 (2)
N(1)	C(1)	1.374 (2)	C(16)	C(17)	1.389 (2)
N(1)	C(8)	1.370 (2)	C(21)	C(22)	1.416 (2)
N(1)	C(9)	1.453 (2)	C(21)	C(26)	1.391 (2)
C(1)	C(2)	1.397 (2)	C(22)	C(23)	1.390 (2)
C(1)	C(6)	1.414 (2)	C(23)	C(24)	1.392 (2)
C(2)	C(3)	1.377 (2)	C(24)	C(25)	1.383 (2)
C(3)	C(4)	1.411 (2)	C(25)	C(26)	1.398 (2)
C(4)	C(5)	1.383 (2)	C(31)	C(32)	1.399 (2)
C(5)	C(6)	1.412 (2)	C(31)	C(36)	1.395 (2)
C(6)	C(7)	1.446 (2)	C(32)	C(33)	1.387 (2)

**Table S4. Bond Lengths for 3qg.**

<b>Atom Atom Length/Å</b>	<b>Atom Atom Length/Å</b>
C(7) C(8) 1.375 (2)	C(33) C(34) 1.396 (2)
C(7) C(11) 1.538 (2)	C(34) C(35) 1.391 (2)
C(11) C(12) 1.549 (2)	C(34) C(37) 1.509 (2)
C(11) C(21) 1.546 (2)	C(35) C(36) 1.395 (2)
C(11) C(31) 1.544 (2)	O(1S) C(1S) 1.428 (2)

**Table S5. Bond Angles for 3qg.**

<b>Atom Atom Atom Angle/°</b>	<b>Atom Atom Atom Angle/°</b>
C(4) O(1) C(10) 117.43 (12)	C(17) C(12) C(13) 117.21 (14)
C(22) O(2) C(27) 117.60 (13)	C(14) C(13) C(12) 121.73 (15)
C(1) N(1) C(9) 124.98 (14)	C(13) C(14) C(15) 120.06 (15)
C(8) N(1) C(1) 108.46 (13)	O(3) C(15) C(14) 117.56 (16)
C(8) N(1) C(9) 126.48 (14)	O(3) C(15) C(16) 123.29 (16)
N(1) C(1) C(2) 129.34 (14)	C(16) C(15) C(14) 119.14 (15)
N(1) C(1) C(6) 107.96 (13)	C(17) C(16) C(15) 120.28 (15)
C(2) C(1) C(6) 122.67 (14)	C(16) C(17) C(12) 121.54 (15)
C(3) C(2) C(1) 117.83 (14)	C(22) C(21) C(11) 120.45 (13)
C(2) C(3) C(4) 120.37 (14)	C(26) C(21) C(11) 122.02 (14)
O(1) C(4) C(3) 114.77 (14)	C(26) C(21) C(22) 117.53 (14)
C(5) C(4) O(1) 122.89 (14)	O(2) C(22) C(21) 116.56 (13)
C(5) C(4) C(3) 122.34 (15)	O(2) C(22) C(23) 122.76 (14)
C(4) C(5) C(6) 118.10 (14)	C(23) C(22) C(21) 120.67 (14)
C(1) C(6) C(7) 107.08 (13)	C(22) C(23) C(24) 120.13 (15)
C(5) C(6) C(1) 118.67 (14)	C(25) C(24) C(23) 120.38 (15)
C(5) C(6) C(7) 134.22 (14)	C(24) C(25) C(26) 119.17 (16)
C(6) C(7) C(11) 127.29 (13)	C(21) C(26) C(25) 122.11 (15)
C(8) C(7) C(6) 105.36 (13)	C(32) C(31) C(11) 119.33 (13)
C(8) C(7) C(11) 127.27 (14)	C(36) C(31) C(11) 122.78 (13)
N(1) C(8) C(7) 111.14 (14)	C(36) C(31) C(32) 117.31 (14)
C(7) C(11) C(12) 108.42 (12)	C(33) C(32) C(31) 121.48 (14)
C(7) C(11) C(21) 109.95 (12)	C(32) C(33) C(34) 121.06 (15)
C(7) C(11) C(31) 106.07 (11)	C(33) C(34) C(37) 121.01 (15)
C(21) C(11) C(12) 108.54 (12)	C(35) C(34) C(33) 117.65 (14)
C(31) C(11) C(12) 113.09 (12)	C(35) C(34) C(37) 121.32 (14)
C(31) C(11) C(21) 110.72 (12)	C(34) C(35) C(36) 121.30 (14)
C(13) C(12) C(11) 118.69 (14)	C(35) C(36) C(31) 121.09 (14)
C(17) C(12) C(11) 124.09 (14)	

**Table S6. Torsion Angles for 3qg.**

<b>A</b>	<b>B</b>	<b>C</b>	<b>D</b>	<b>Angle/°</b>	<b>A</b>	<b>B</b>	<b>C</b>	<b>D</b>	<b>Angle/°</b>
O(1)	C(4)	C(5)	C(6)	-177.72 (14)	C(11)	C(12)	C(17)	C(16)	-177.77 (13)
O(2)	C(22)	C(23)	C(24)	178.49 (15)	C(11)	C(21)	C(22)	O(2)	1.4 (2)
O(3)	C(15)	C(16)	C(17)	179.64 (14)	C(11)	C(21)	C(22)	C(23)	-179.34 (14)
N(1)	C(1)	C(2)	C(3)	-176.59 (16)	C(11)	C(21)	C(26)	C(25)	179.76 (15)
N(1)	C(1)	C(6)	C(5)	177.97 (14)	C(11)	C(31)	C(32)	C(33)	169.15 (14)
N(1)	C(1)	C(6)	C(7)	-0.20 (17)	C(11)	C(31)	C(36)	C(35)	-167.94 (14)
C(1)	N(1)	C(8)	C(7)	0.18 (19)	C(12)	C(11)	C(21)	C(22)	53.95 (18)
C(1)	C(2)	C(3)	C(4)	-0.8 (2)	C(12)	C(11)	C(21)	C(26)	-126.20 (15)
C(1)	C(6)	C(7)	C(8)	0.30 (17)	C(12)	C(11)	C(31)	C(32)	66.14 (17)
C(1)	C(6)	C(7)	C(11)	-176.66 (14)	C(12)	C(11)	C(31)	C(36)	-122.84 (15)
C(2)	C(1)	C(6)	C(5)	-0.2 (2)	C(12)	C(13)	C(14)	C(15)	0.9 (2)
C(2)	C(1)	C(6)	C(7)	-178.41 (14)	C(13)	C(12)	C(17)	C(16)	1.5 (2)
C(2)	C(3)	C(4)	O(1)	178.75 (14)	C(13)	C(14)	C(15)	O(3)	179.96 (13)
C(2)	C(3)	C(4)	C(5)	-0.5 (2)	C(13)	C(14)	C(15)	C(16)	0.6 (2)
C(3)	C(4)	C(5)	C(6)	1.5 (2)	C(14)	C(15)	C(16)	C(17)	-1.1 (2)
C(4)	C(5)	C(6)	C(1)	-1.1 (2)	C(15)	C(16)	C(17)	C(12)	0.0 (2)
C(4)	C(5)	C(6)	C(7)	176.49 (16)	C(17)	C(12)	C(13)	C(14)	-2.0 (2)
C(5)	C(6)	C(7)	C(8)	-177.46 (17)	C(21)	C(11)	C(12)	C(13)	48.76 (17)
C(5)	C(6)	C(7)	C(11)	5.6 (3)	C(21)	C(11)	C(12)	C(17)	-131.93 (15)
C(6)	C(1)	C(2)	C(3)	1.2 (2)	C(21)	C(11)	C(31)	C(32)	-171.80 (13)
C(6)	C(7)	C(8)	N(1)	-0.30 (18)	C(21)	C(11)	C(31)	C(36)	-0.79 (19)
C(6)	C(7)	C(11)	C(12)	-161.47 (14)	C(21)	C(22)	C(23)	C(24)	-0.7 (2)
C(6)	C(7)	C(11)	C(21)	80.02 (18)	C(22)	C(21)	C(26)	C(25)	-0.4 (2)
C(6)	C(7)	C(11)	C(31)	-39.73 (19)	C(22)	C(23)	C(24)	C(25)	0.1 (2)
C(7)	C(11)	C(12)	C(13)	-70.63 (16)	C(23)	C(24)	C(25)	C(26)	0.3 (3)
C(7)	C(11)	C(12)	C(17)	108.67 (16)	C(24)	C(25)	C(26)	C(21)	-0.1 (3)
C(7)	C(11)	C(21)	C(22)	172.38 (13)	C(26)	C(21)	C(22)	O(2)	-178.42 (14)
C(7)	C(11)	C(21)	C(26)	-7.8 (2)	C(26)	C(21)	C(22)	C(23)	0.8 (2)
C(7)	C(11)	C(31)	C(32)	-52.56 (17)	C(27)	O(2)	C(22)	C(21)	-179.41 (13)
C(7)	C(11)	C(31)	C(36)	118.46 (15)	C(27)	O(2)	C(22)	C(23)	1.4 (2)
C(8)	N(1)	C(1)	C(2)	178.07 (16)	C(31)	C(11)	C(12)	C(13)	172.04 (13)
C(8)	N(1)	C(1)	C(6)	0.02 (18)	C(31)	C(11)	C(12)	C(17)	-8.7 (2)
C(8)	C(7)	C(11)	C(12)	22.2 (2)	C(31)	C(11)	C(21)	C(22)	-70.74 (17)
C(8)	C(7)	C(11)	C(21)	-96.30 (18)	C(31)	C(11)	C(21)	C(26)	109.11 (16)
C(8)	C(7)	C(11)	C(31)	143.95 (15)	C(31)	C(32)	C(33)	C(34)	-0.8 (2)
C(9)	N(1)	C(1)	C(2)	-4.9 (3)	C(32)	C(31)	C(36)	C(35)	3.2 (2)
C(9)	N(1)	C(1)	C(6)	177.04 (15)	C(32)	C(33)	C(34)	C(35)	3.0 (2)
C(9)	N(1)	C(8)	C(7)	-176.78 (16)	C(32)	C(33)	C(34)	C(37)	-175.30 (16)
C(10)O(1)	C(4)	C(3)	-175.99 (14)	C(33)	C(34)	C(35)	C(36)	-2.1 (2)	
C(10)O(1)	C(4)	C(5)	3.2 (2)	C(34)	C(35)	C(36)	C(31)	-1.1 (2)	
C(11)C(7)	C(8)	N(1)	176.66 (15)	C(36)	C(31)	C(32)	C(33)	-2.4 (2)	
C(11)C(12)	C(13)	C(14)	177.36 (14)	C(37)	C(34)	C(35)	C(36)	176.19 (16)	

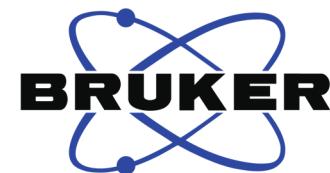
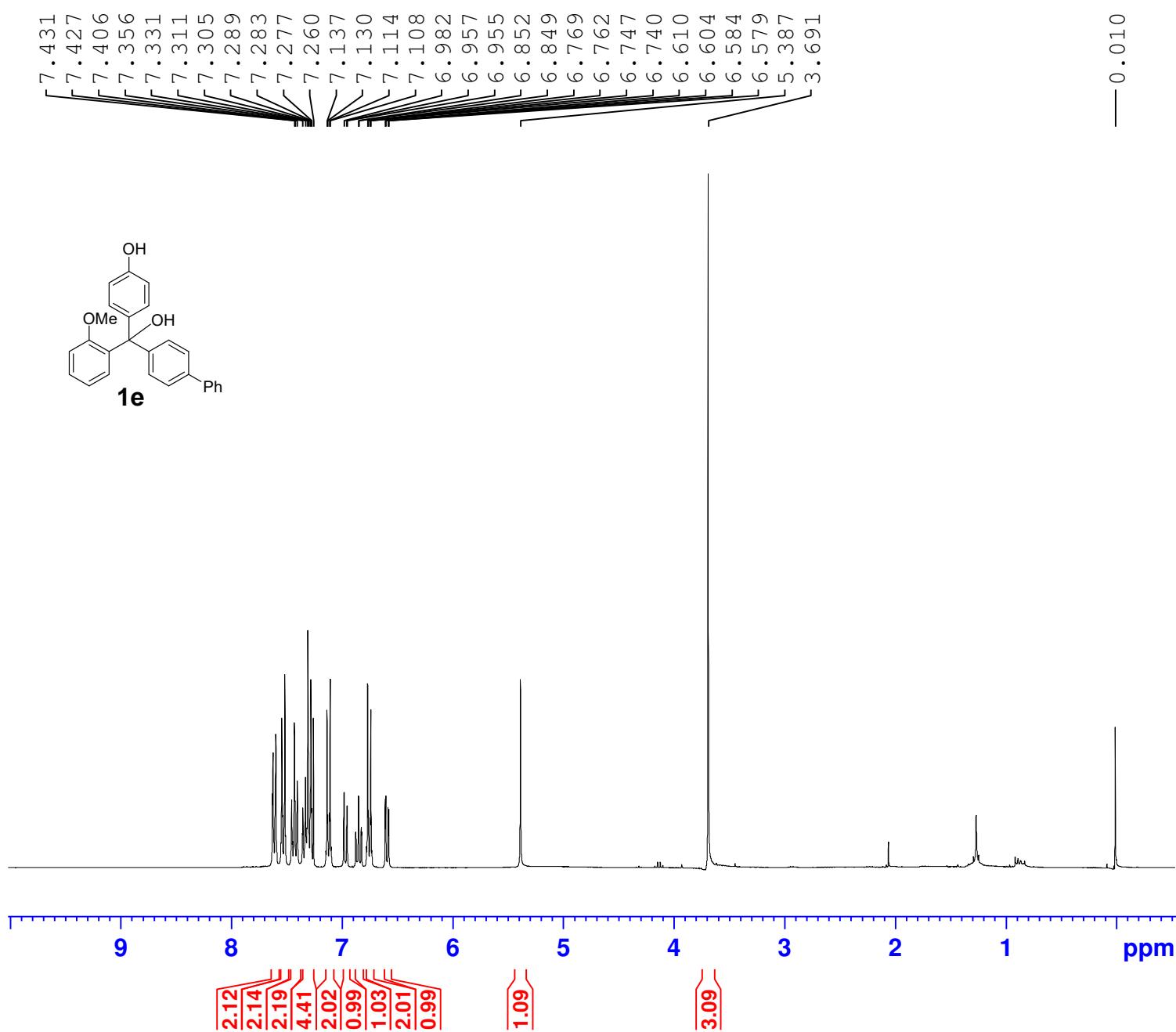
**Table S7. Hydrogen Atom Coordinates ( $\text{\AA} \times 10^4$ ) and Isotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for 3qg.**

Atom	x	y	z	U(eq)
H(3)	11155	7101	1717	44
H(2)	4865	-1024	-311	24
H(3A)	3387	-634	482	24
H(5)	5040	2151	2775	21
H(8)	8148	1593	1024	23
H(9A)	7039	-1734	-367	44
H(9B)	7704	-75	-632	44
H(9C)	6497	-191	-1064	44
H(10A)	3363	3226	2826	37
H(10B)	3656	1537	3519	37
H(10C)	2466	2025	3168	37
H(13)	9278	1627	2562	23
H(14)	10784	2832	2101	26
H(16)	9492	7668	2077	25
H(17)	7980	6447	2517	22
H(23)	9017	1587	6039	25
H(24)	8518	-1359	5902	29
H(25)	7544	-2396	4415	29
H(26)	7079	-474	3060	25
H(27A)	9319	5945	5511	37
H(27B)	9836	4050	5709	37
H(27C)	8789	4517	6154	37
H(32)	6427	5499	1687	21
H(33)	4987	7163	1912	25
H(35)	5067	5194	4738	25
H(36)	6538	3578	4529	22
H(37A)	4030	8464	3711	42
H(37B)	3484	6649	3927	42
H(37C)	3427	7360	2790	42
H(1S)	1856	-142	1598	44
H(1SA)	1315	-441	-31	55
H(1SB)	839	1300	392	55
H(1SC)	159	-452	246	55

### VIII. References

- 1 X. G. Li, M. Duan, Z. Q. Deng, Q. Z. Shao, M. Chen, G. Y. Zhu, K. N. Houk and J. Sun, *Nat. Catal.*, 2020, **3**, 1010-1019.
- 2 Z. Han, Y. Zang, C. Liu, W. Guo, H. Huang and J. Sun, *Chem. Commun.*, 2022, **58**, 7128-7131.
- 3 A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B*. 2009, **113**, 6378-6396.
- 4 (a) L. Noodleman, T. Lovell, W.-G. Han, J. Li, F. Himo, *Chem. Rev.* 2004, **104**, 459-508; (b) L. Noodleman, *J. Chem. Phys.* 1981, **74**, 5737; (c) L. Noodleman, D. A. Case, *Adv. Inorg. Chem.* 1992, **38**, 423-458.
- 5 S. Grimme, J. Antony, Ehrlich, S. H. Krieg, *J. Chem. Phys.* 2010, **132**, 154104.
- 6 (a) Y. Zhao, D. G. Truhlar, *J. Chem. Theory Comput.* 2009, **5**, 324-333; (b) Y. Zhao, D. G. Truhlar, *Theor. Chem. Acc.* 2008, **120**, 215-241; (c) Y. Zhao, D. G. Truhlar, *Acc. Chem. Res.* 2008, **41**, 157-167.
- 7 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, , M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr.; J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian 09, Rev. A.01; Gaussian, Inc.: Wallingford, CT, 2010.
- 8 C. Y. Legault, *CYLView, version 1.0 b*; Université de Sherbrooke: Sherbrooke, Quebec, Canada, 2009. <http://www.cylview.org>.

1e



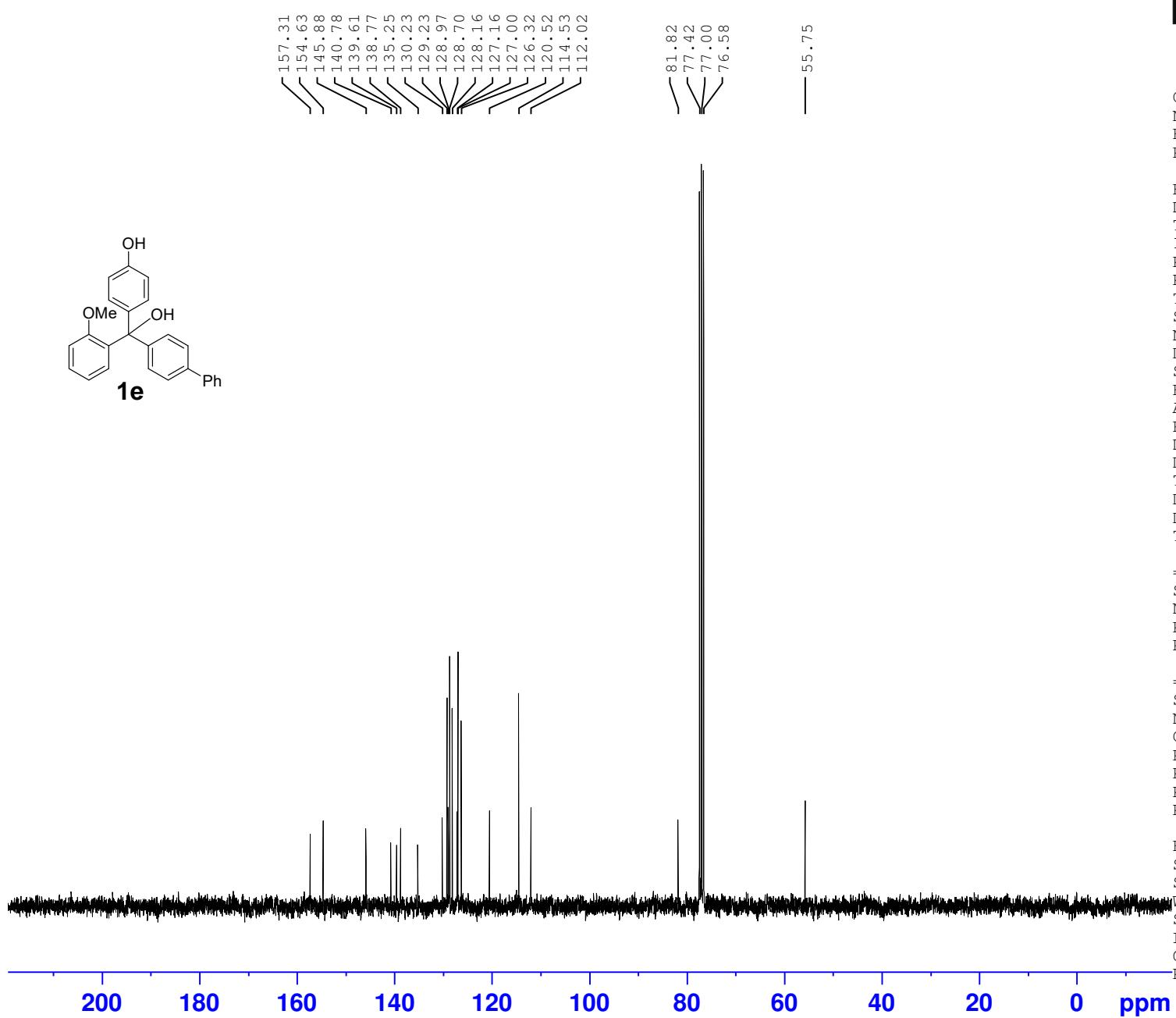
Current Data Parameters  
 NAME 0907sjw  
 EXPNO 5251  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210907  
 Time 13.42  
 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 -59.1 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 300.1300071 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1e



Current Data Parameters  
NAME 1e-ZY-4-71B  
EXPNO 5264  
PROCNO 1

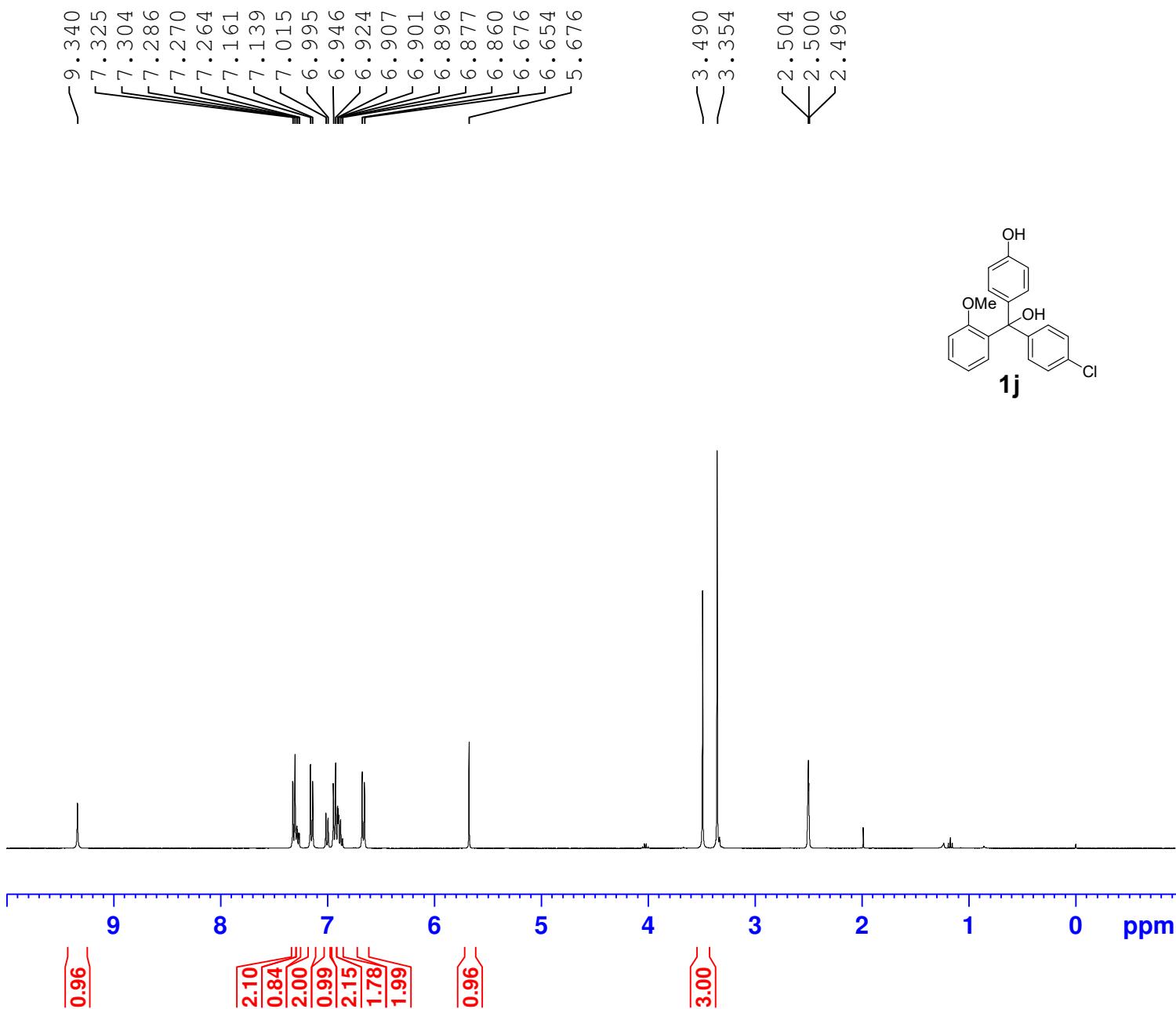
F2 - Acquisition Parameters  
Date\_ 20210908  
Time 11.30  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 350  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE -59.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 ======  
SFO1 75.4752949 MHz  
NUC1 <sup>13</sup>C  
P1 9.50 usec  
PLW1 34.20000076 W

===== CHANNEL f2 ======  
SFO2 300.1312005 MHz  
NUC2 <sup>1</sup>H  
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 75.4677523 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

1j



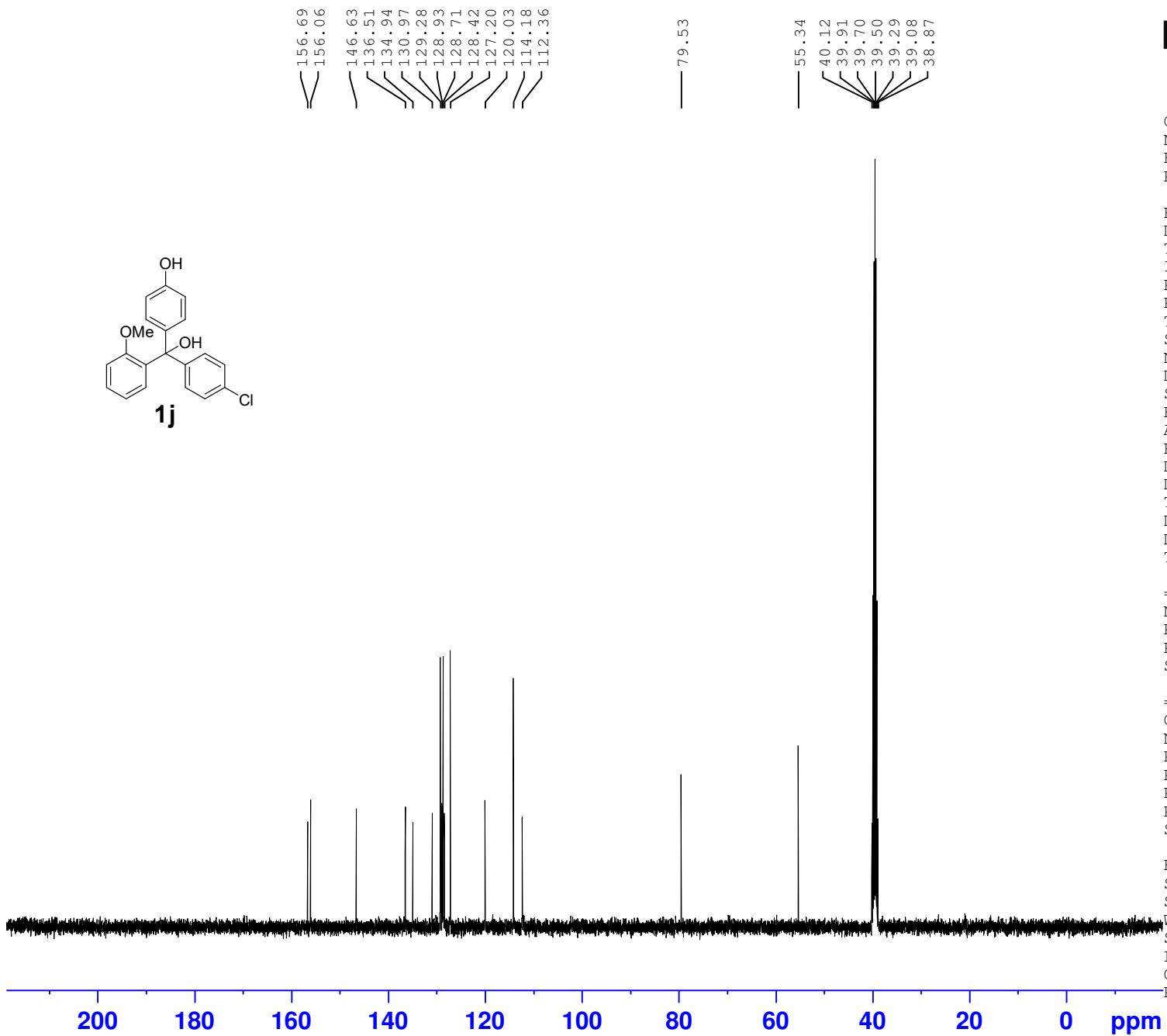
Current Data Parameters  
 NAME 0720-400  
 EXPNO 39  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220720  
 Time 17.01  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 8  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9845889 sec  
 RG 154.68  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 294.4 K  
 D1 1.0000000 sec  
 TD0 1

===== CHANNEL f1 ======  
 NUC1 1H  
 P1 14.68 usec  
 PLW1 14.00000000 W  
 SFO1 400.1924713 MHz

F2 - Processing parameters  
 SI 65536  
 SF 400.1900123 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1j



Current Data Parameters  
 NAME 1j-ZY-4-70A  
 EXPNO 1  
 PROCNO 1

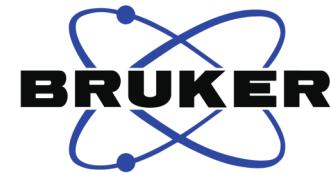
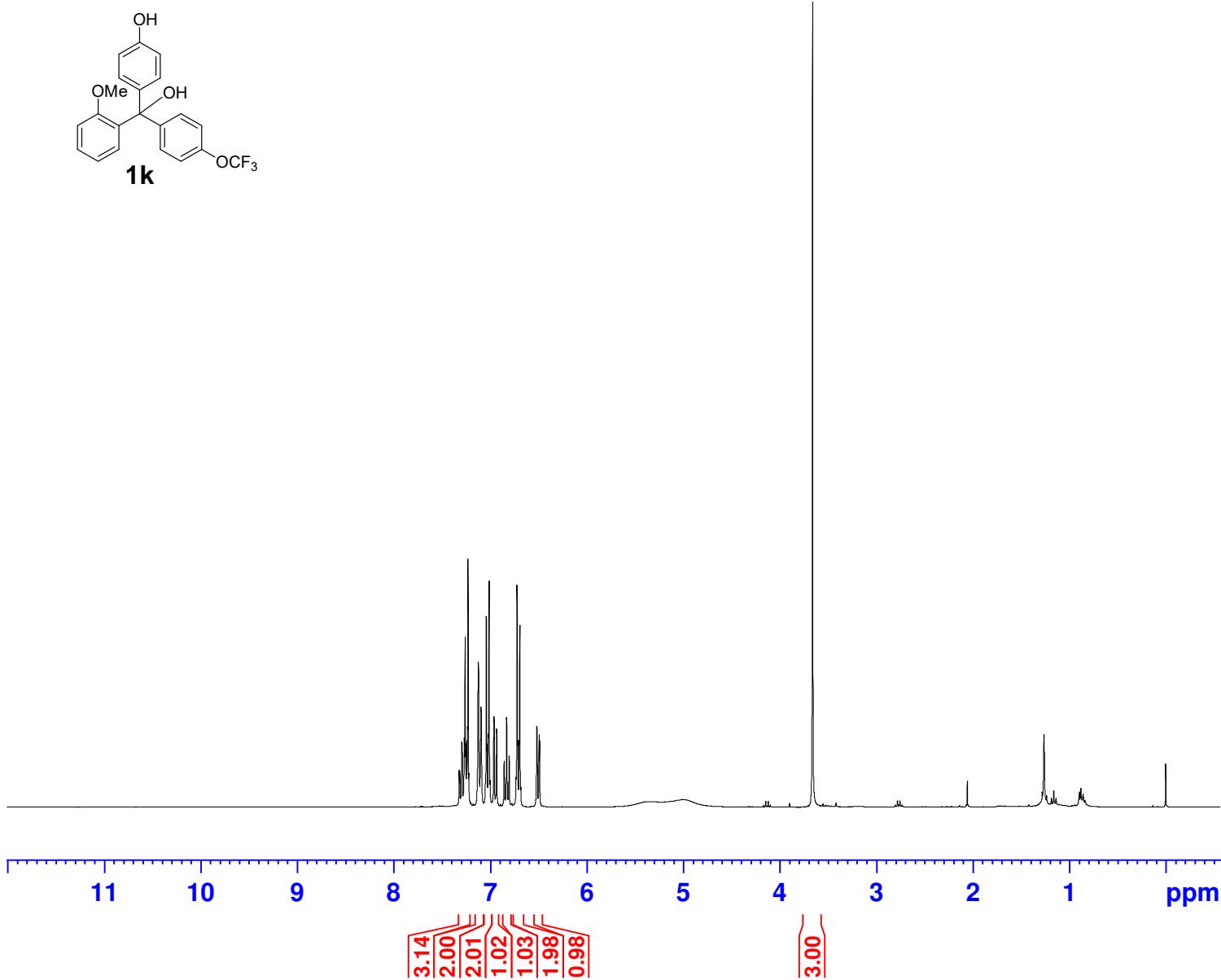
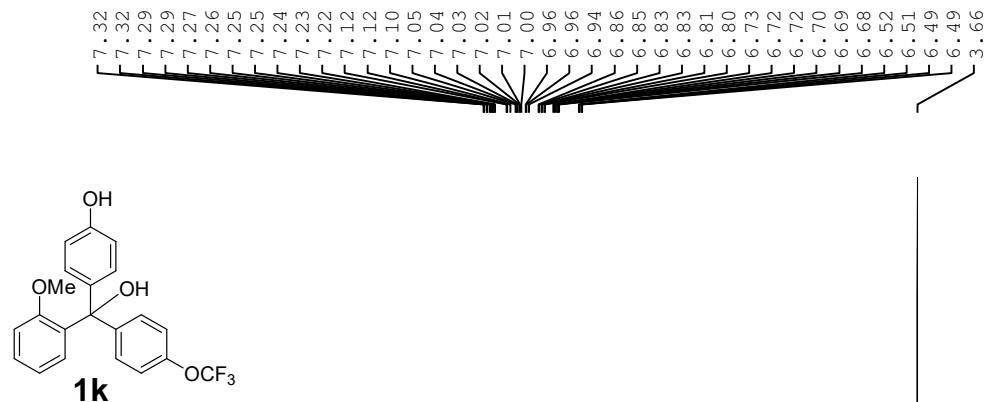
F2 - Acquisition Parameters  
 Date\_ 20220718  
 Time 15.42  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 50  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 193.13  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.1 K  
 D1 2.00000000 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 100.6279052 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

1k



Current Data Parameters  
NAME ZY-4-71A-h-fr  
EXPNO 5248  
PROCNO 1

```

F2 - Acquisition Parameters
Date_          20210907
Time           13.34
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG      zg30
TD             65536
SOLVENT        CDC13
NS              16
DS               2
SWH            6009.615 Hz
FIDRES        0.091699 Hz
AQ             5.4525952 sec
RG              90.5
DW             83.200 used
DE              6.50 used
TE             -59.1 K
D1             1.00000000 sec
TD0                  1

```

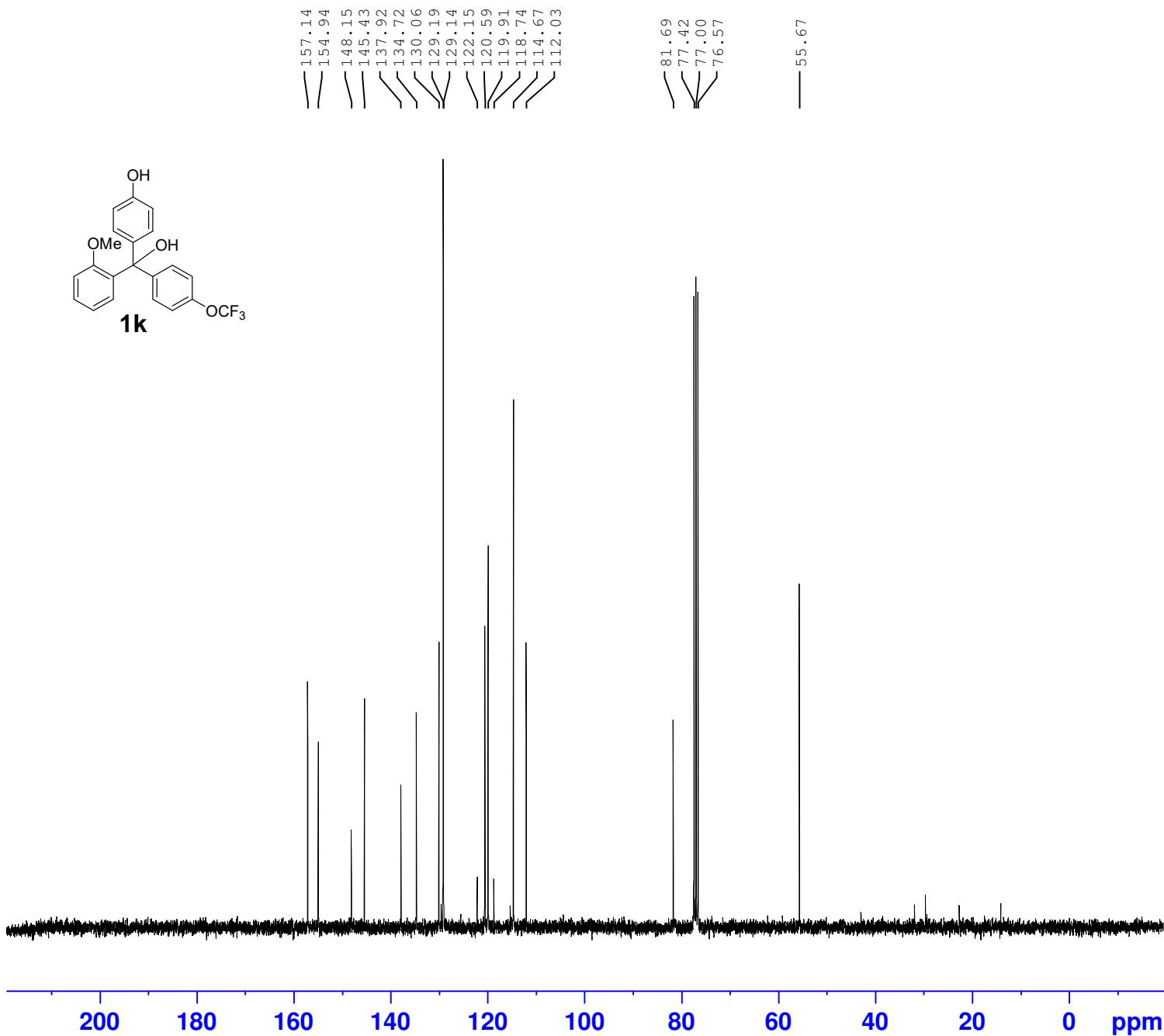
===== CHANNEL f1 =====  
SFO1 300.1318534 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 14.00000000 W

```

F2 - Processing parameters
SI           65536
SF          300.1300115 MHz
WDW          EM
SSB            0
LB           0.30 Hz
GB            0
PC           1.00

```

1k



Current Data Parameters  
 NAME 1k-ZY-4-71A  
 EXPNO 5263  
 PROCNO 1

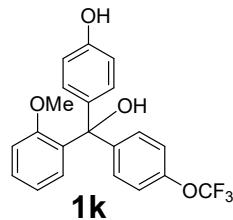
F2 - Acquisition Parameters  
 Date\_ 20210908  
 Time 11.04  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 350  
 DS 4  
 SWH 18028.846 Hz  
 FIDRES 0.275098 Hz  
 AQ 1.8175317 sec  
 RG 203  
 DW 27.733 usec  
 DE 6.50 usec  
 TE -59.1 K  
 D1 2.00000000 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 75.4677535 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

1k



— -57.739

0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm



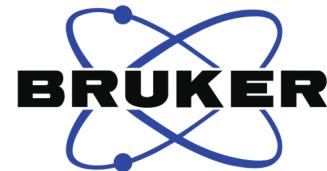
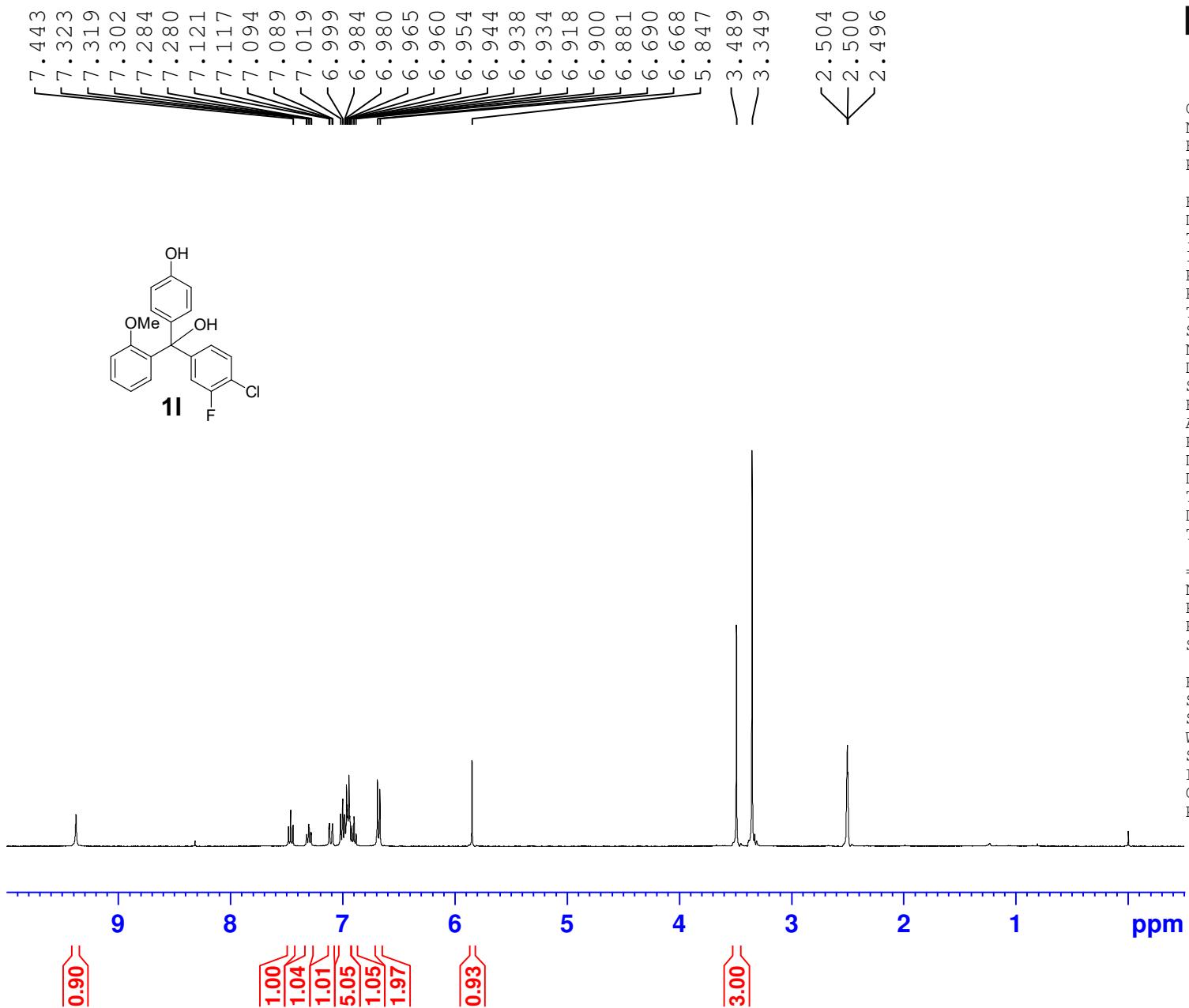
Current Data Parameters  
 NAME 0907sjw  
 EXPNO 5249  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210907  
 Time 13.37  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgfhigqn.2  
 TD 131072  
 SOLVENT CDCl<sub>3</sub>  
 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 -59.1 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

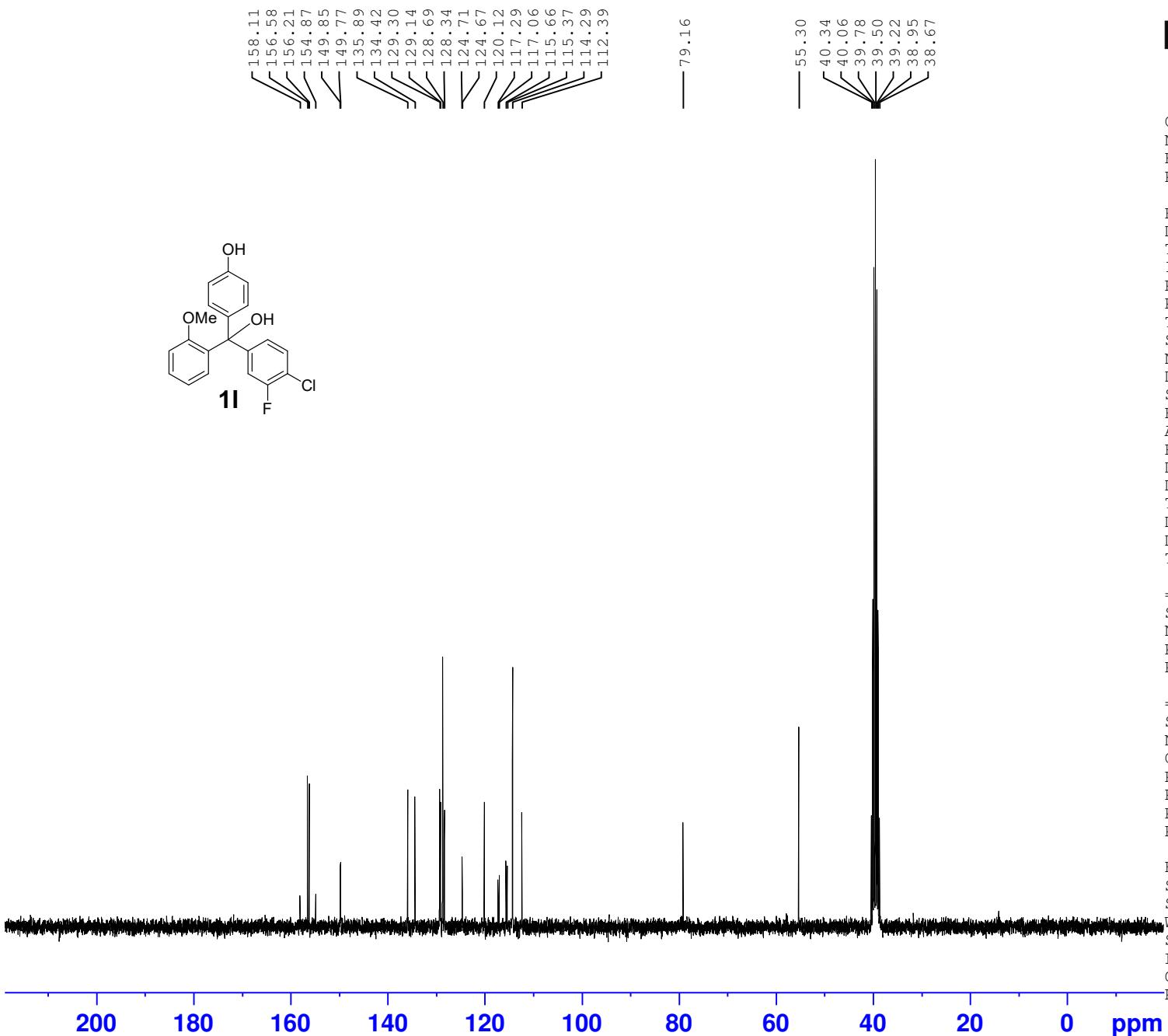


Current Data Parameters  
 NAME 0729-400  
 EXPNO 110  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220729  
 Time 21.44  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 8  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9845889 sec  
 RG 181.41  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 294.7 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 ======  
 NUC1 1H  
 P1 14.68 usec  
 PLW1 14.00000000 W  
 SFO1 400.1924713 MHz

F2 - Processing parameters  
 SI 65536  
 SF 400.1900124 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



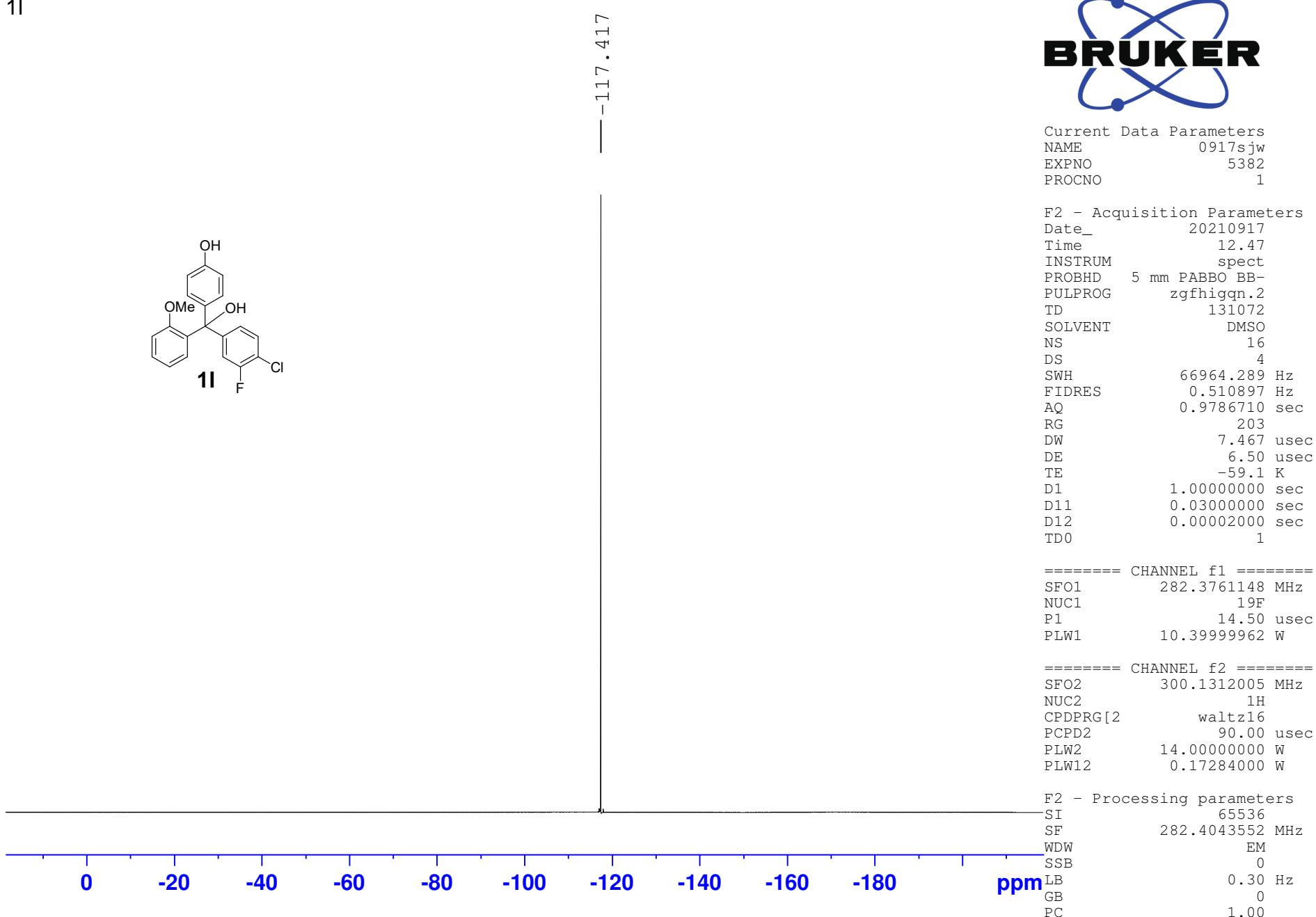
Current Data Parameters  
 NAME 11-ZY-4-78B  
 EXPNO 5462  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210927  
 Time 13.31  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 138  
 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 -59.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

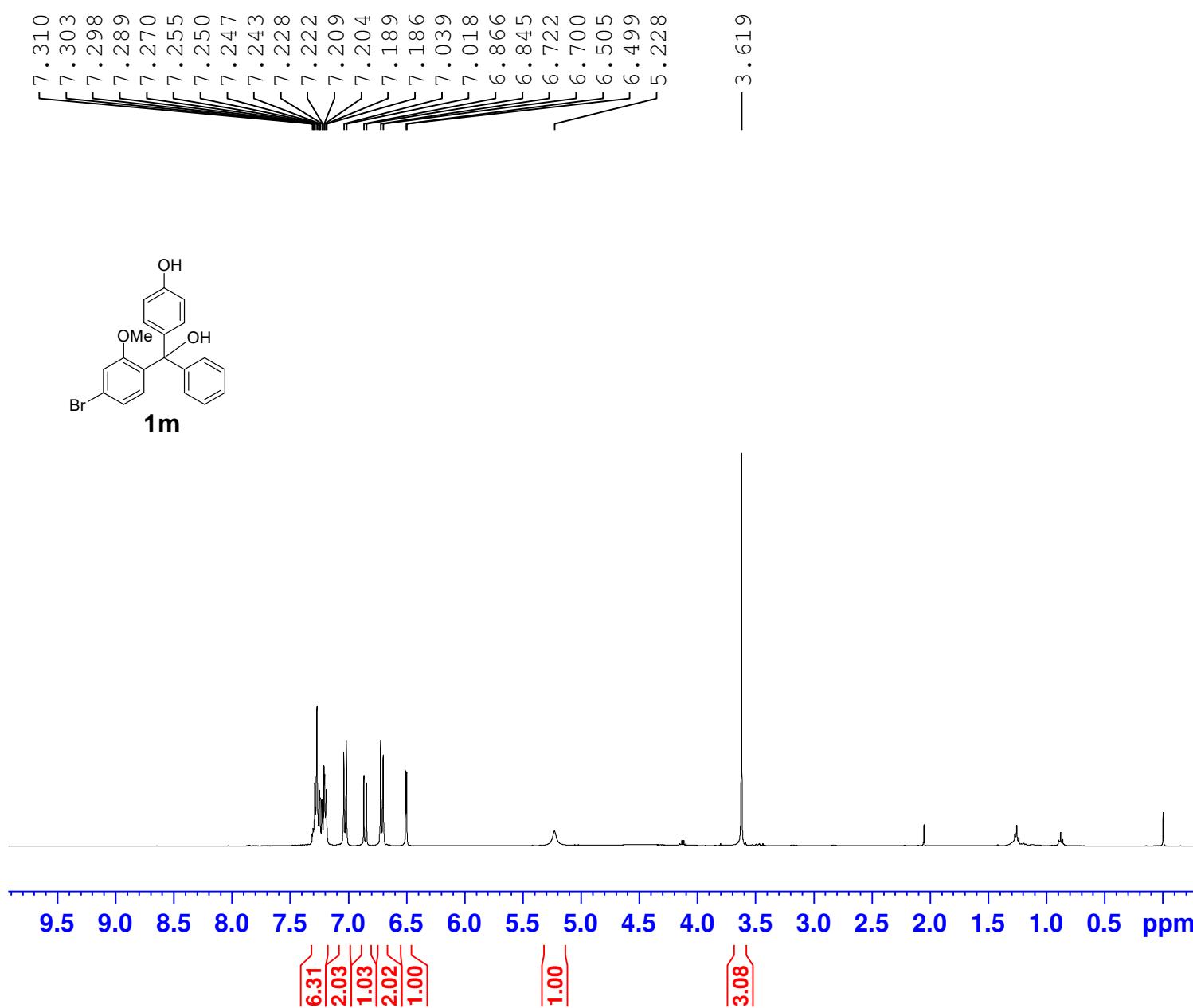
===== CHANNEL f1 ======  
 SFO1 75.4752949 MHz  
 NUC1 <sup>13</sup>C  
 P1 9.50 usec  
 PLW1 34.20000076 W

===== CHANNEL f2 ======  
 SFO2 300.1312005 MHz  
 NUC2 <sup>1</sup>H  
 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 75.4677831 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



1m

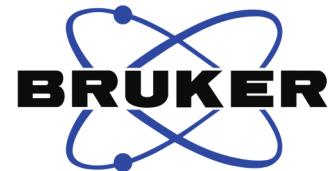
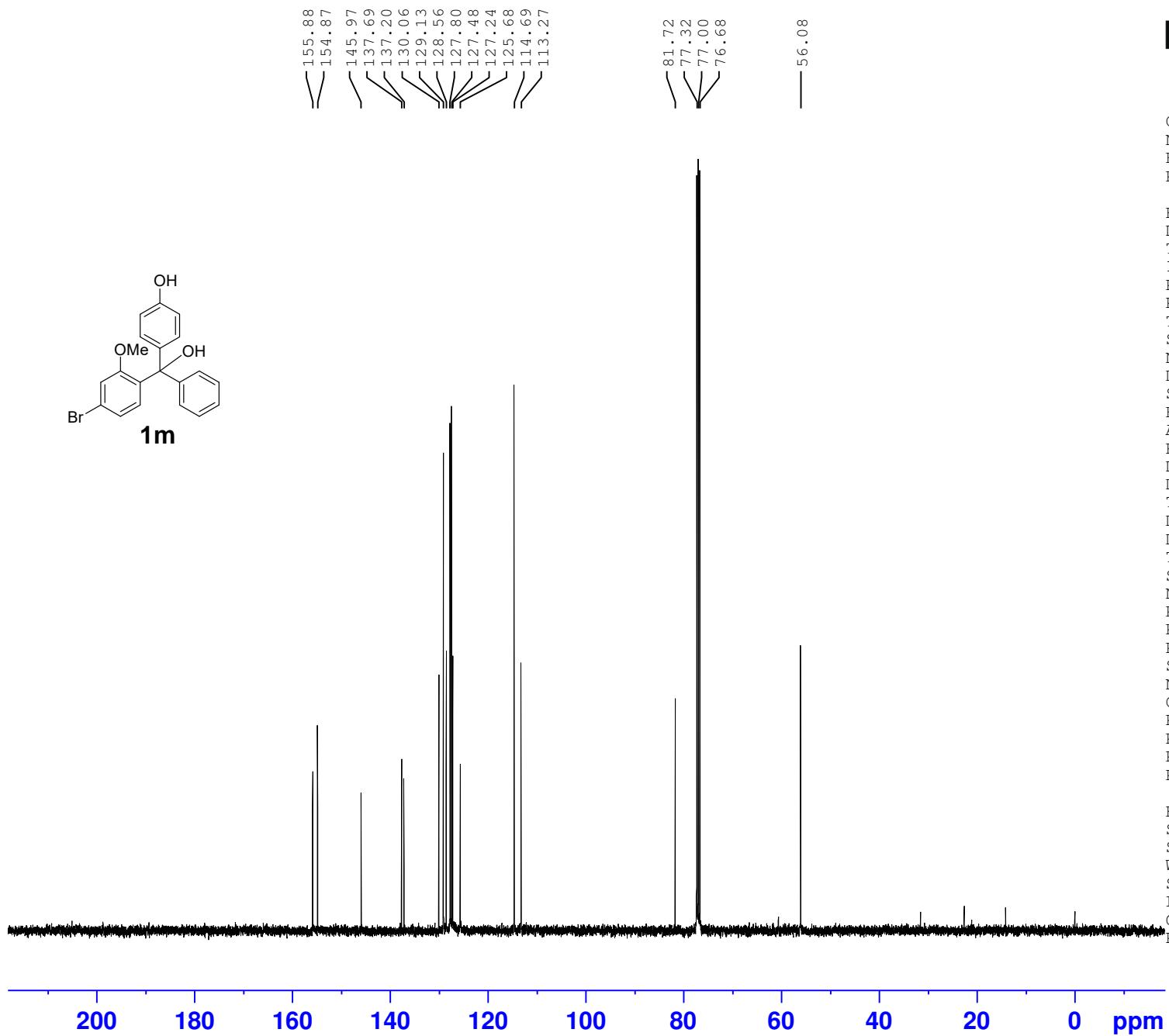
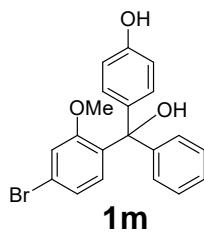


Current Data Parameters  
NAME 0611HH  
EXPNO 16  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220611  
Time 4.44 h  
INSTRUM Avance  
PROBHD Z116098\_0833 (zg30  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
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 292.4 K  
D1 1.0000000 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 400.1300172 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

1m



Current	Data	Parameters
NAME	1m-ZY-4-82	
EXPNO		15
PROCNO		1

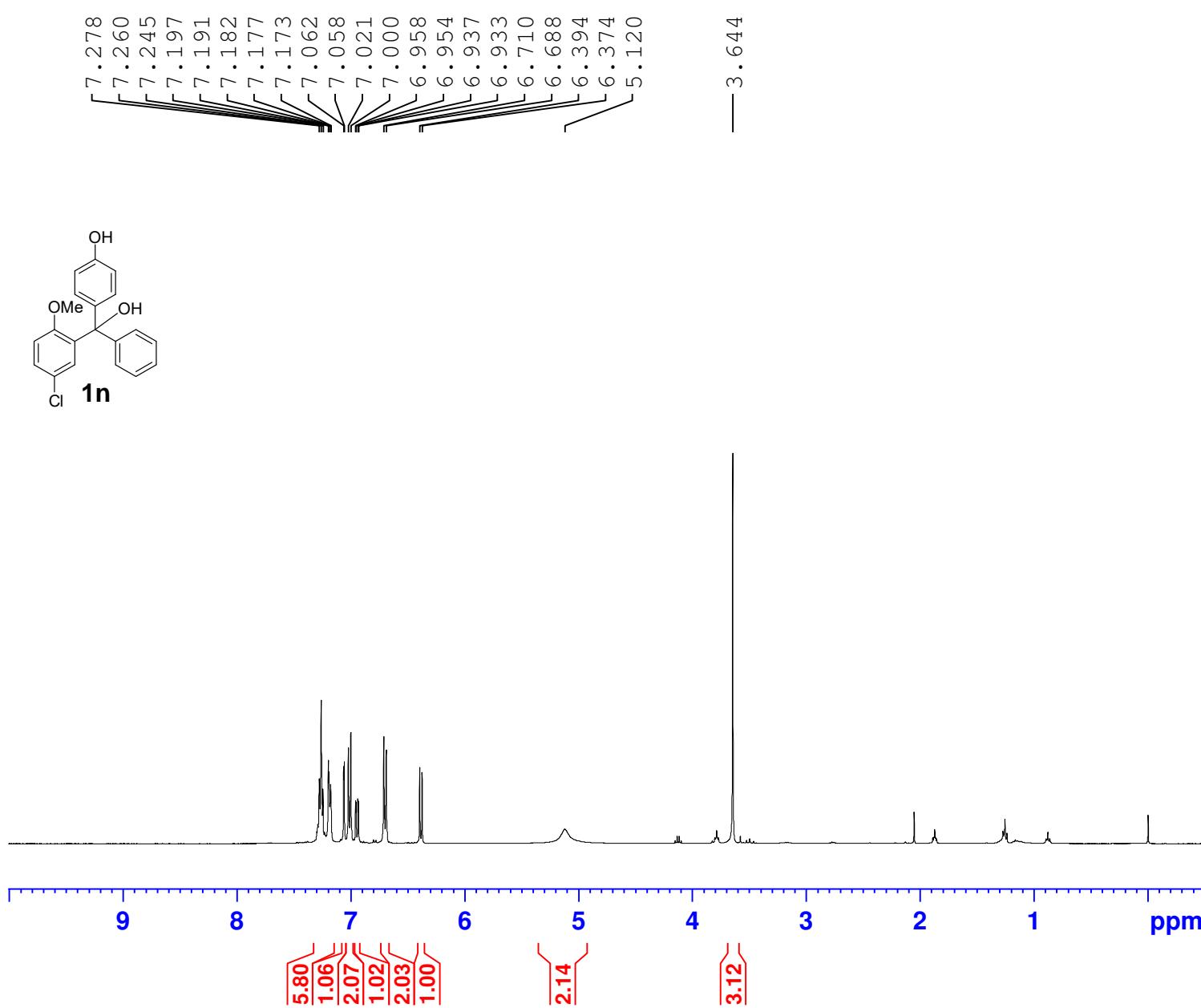
```

F2 - Acquisition Parameters
Date_           20220611
Time            4.42 h
INSTRUM        Avance
PROBHD         Z116098_0833 (
PULPROG        zgpg30
TD              65536
SOLVENT         CDC13
NS              400
DS              4
SWH             23809.523 Hz
FIDRES        0.726609 Hz
AQ              1.3762560 sec
RG              54.9866
DW              21.0000 usec
DE              6.5000 usec
TE              292.8 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0             1
SFO1            100.6228298 MHz
NUC1            13C
P0              3.3300 usec
P1              10.0000 usec
PLW1            87.89900208 W
SFO2            400.1316005 MHz
NUC2            1H
CPDPRG[2       waltz65
PCPD2           90.0000 usec
PLW2            20.73200035 W
PLW12           0.25595000 W
PLW13           0.12874000 W

```

F2 - Processing parameters  
SI 32768  
SF 100.6127766 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

1n

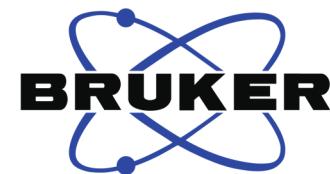
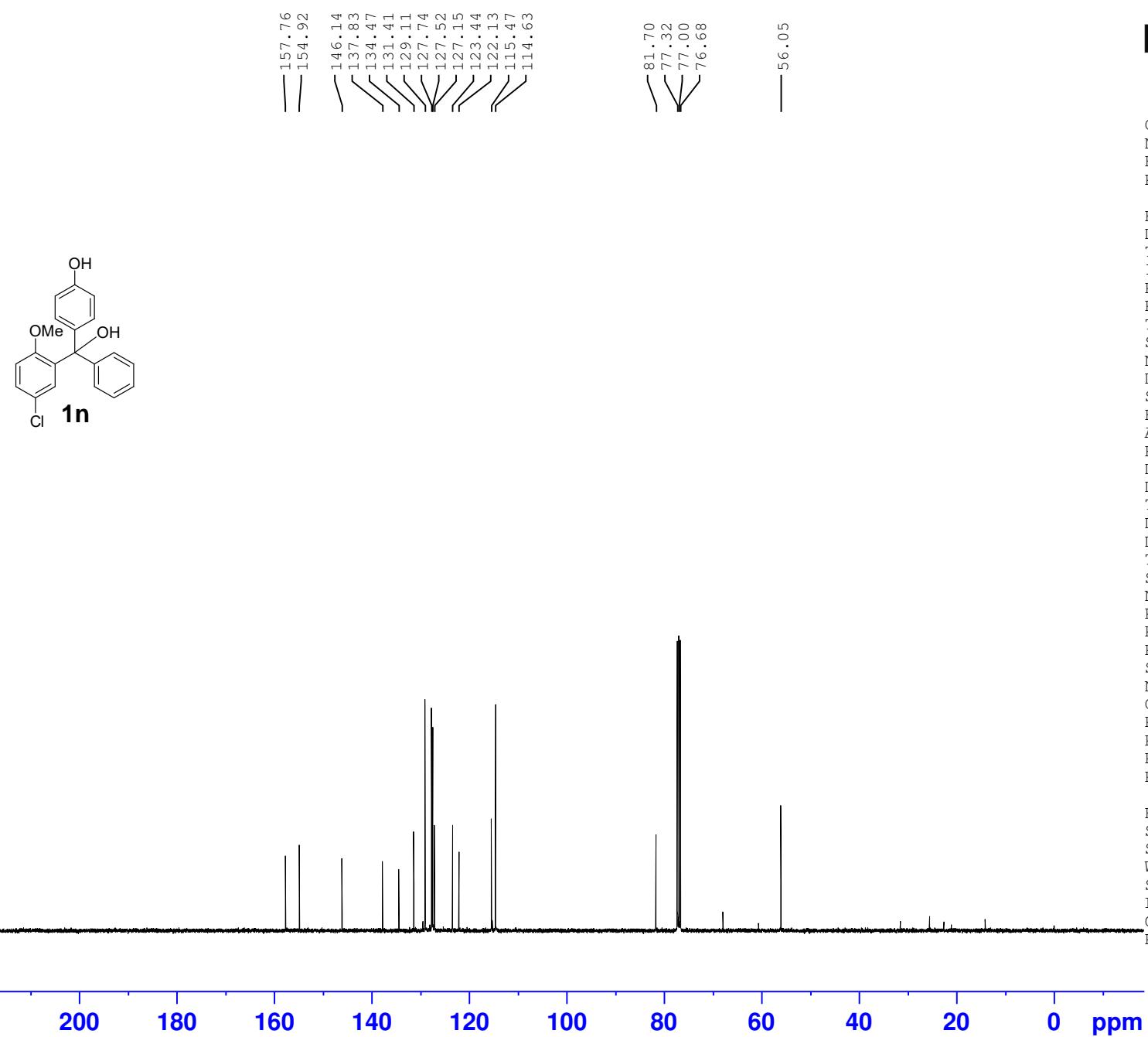


Current Data Parameters  
NAME 0611HH  
EXPNO 14  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220611  
Time 4.14 h  
INSTRUM Avance  
PROBHD Z116098\_0833 (zg30  
PULPROG 65536  
TD 16  
SOLVENT CDCl<sub>3</sub>  
NS 2  
DS 16  
SWH 8196.722 Hz  
FIDRES 0.250144 Hz  
AQ 3.9976959 sec  
RG 82.3452  
DW 61.000 usec  
DE 13.54 usec  
TE 292.2 K  
D1 1.0000000 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 400.1300163 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

1n

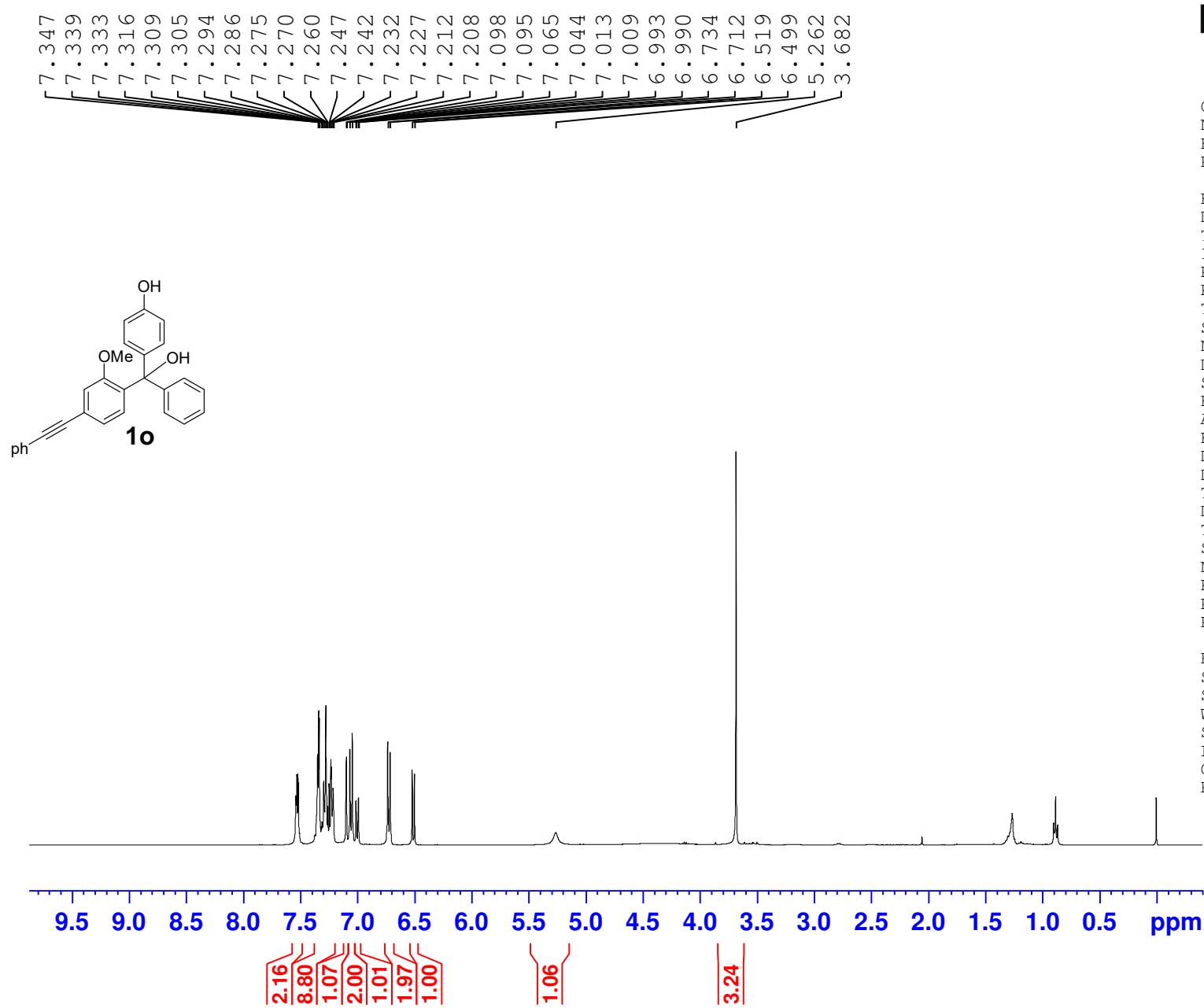


Current Data Parameters  
 NAME 1n-ZY-4-83  
 EXPNO 13  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220611  
 Time 4.12 h  
 INSTRUM Avance  
 PROBHD Z116098\_0833 (zgpg30  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 400  
 DS 4  
 SWH 23809.523 Hz  
 FIDRES 0.726609 Hz  
 AQ 1.3762560 sec  
 RG 54.9866  
 DW 21.000 usec  
 DE 6.50 usec  
 TE 292.7 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 100.6127772 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

1o

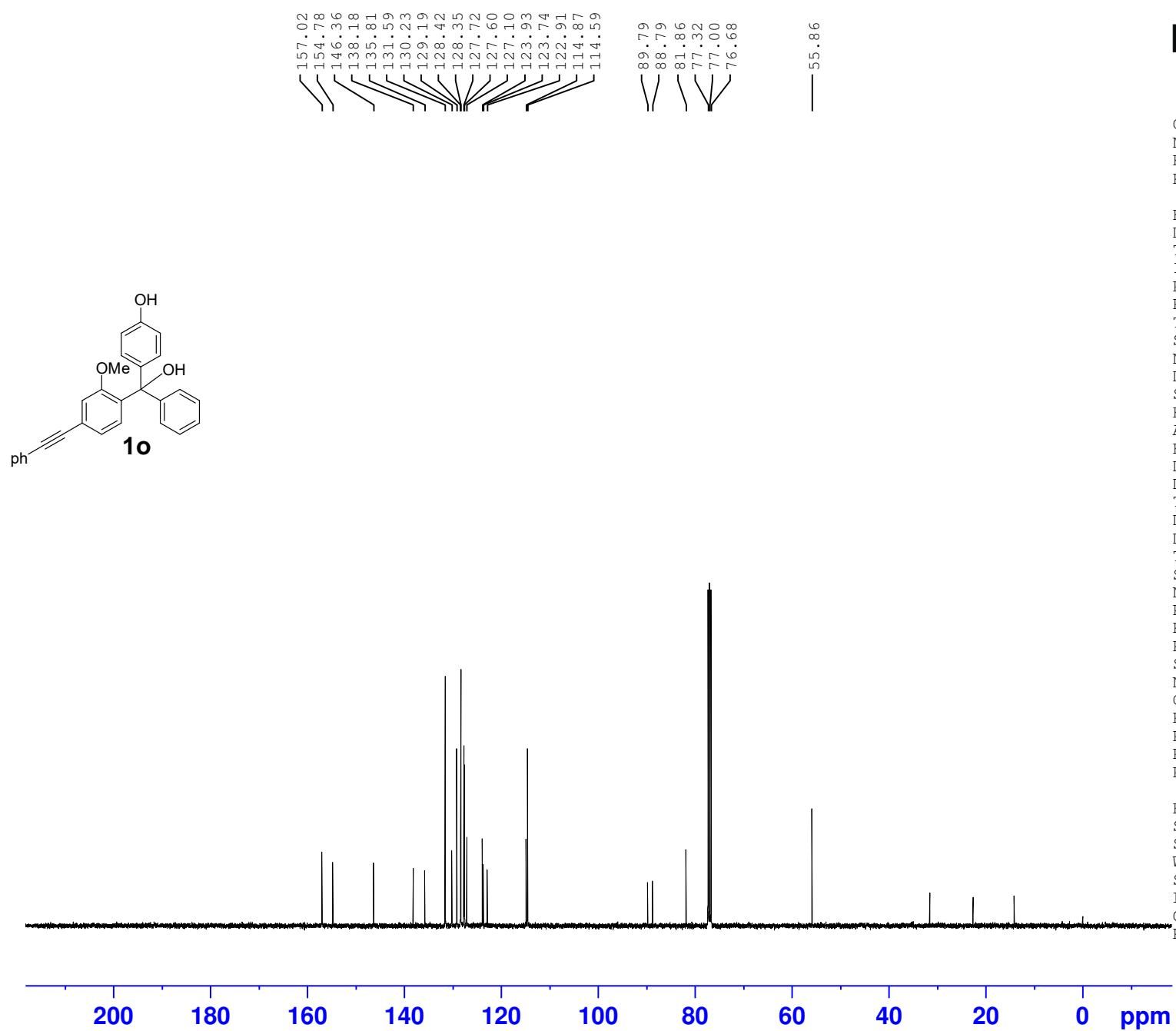


Current Data Parameters  
 NAME 0611HH  
 EXPNO 12  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220611  
 Time 3.45 h  
 INSTRUM Avance  
 PROBHD Z116098\_0833 (zg30  
 PULPROG 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8196.722 Hz  
 FIDRES 0.250144 Hz  
 AQ 3.9976959 sec  
 RG 91.9118  
 DW 61.000 usec  
 DE 13.54 usec  
 TE 292.4 K  
 D1 1.0000000 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 400.1300153 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1o

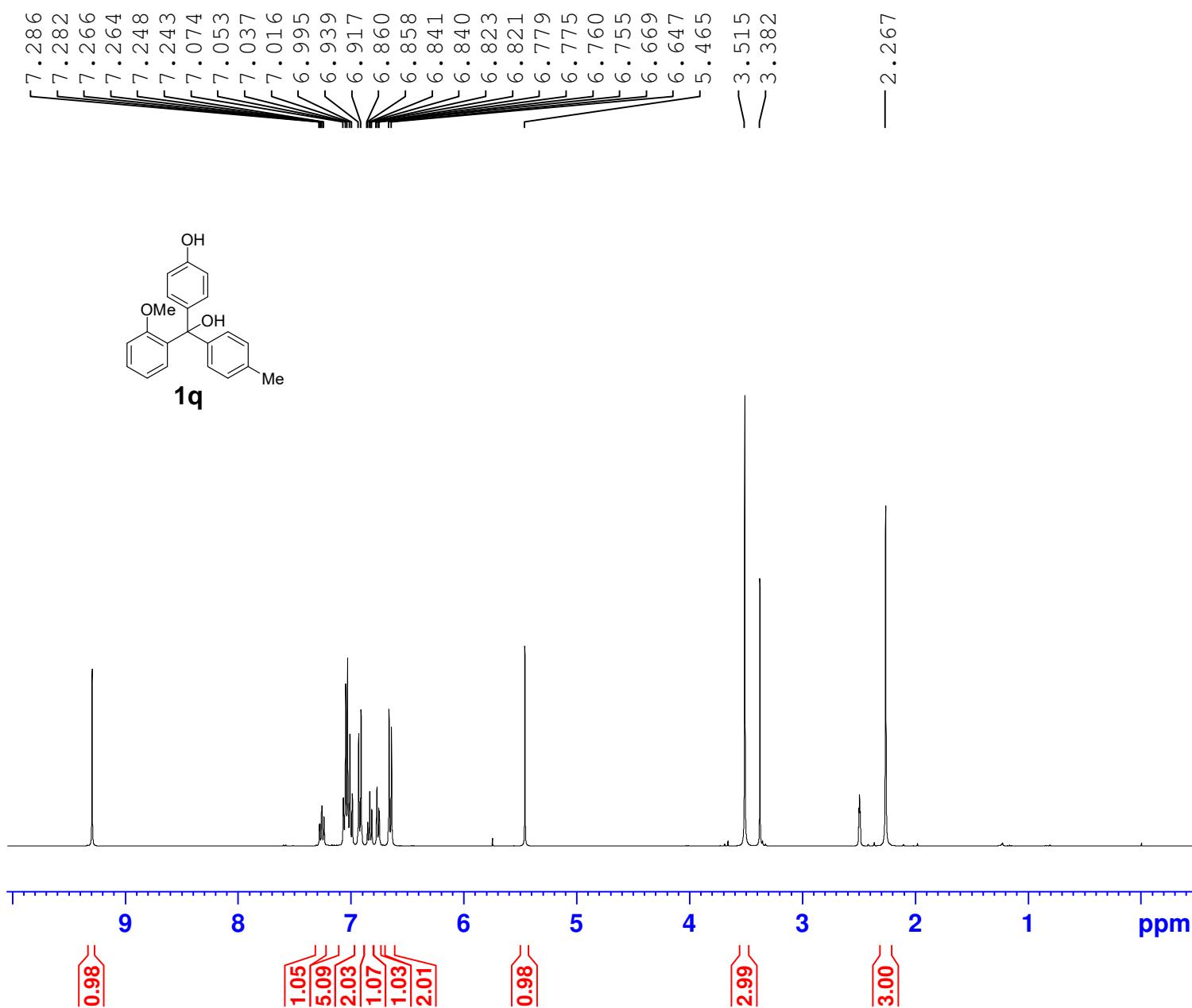


Current Data Parameters  
 NAME 1o-ZY-4-84  
 EXPNO 11  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220611  
 Time 3.43 h  
 INSTRUM Avance  
 PROBHD Z116098\_0833 (zgpg30  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 400  
 DS 4  
 SWH 23809.523 Hz  
 FIDRES 0.726609 Hz  
 AQ 1.3762560 sec  
 RG 53.2129  
 DW 21.000 usec  
 DE 6.50 usec  
 TE 292.9 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 100.6127763 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

1q



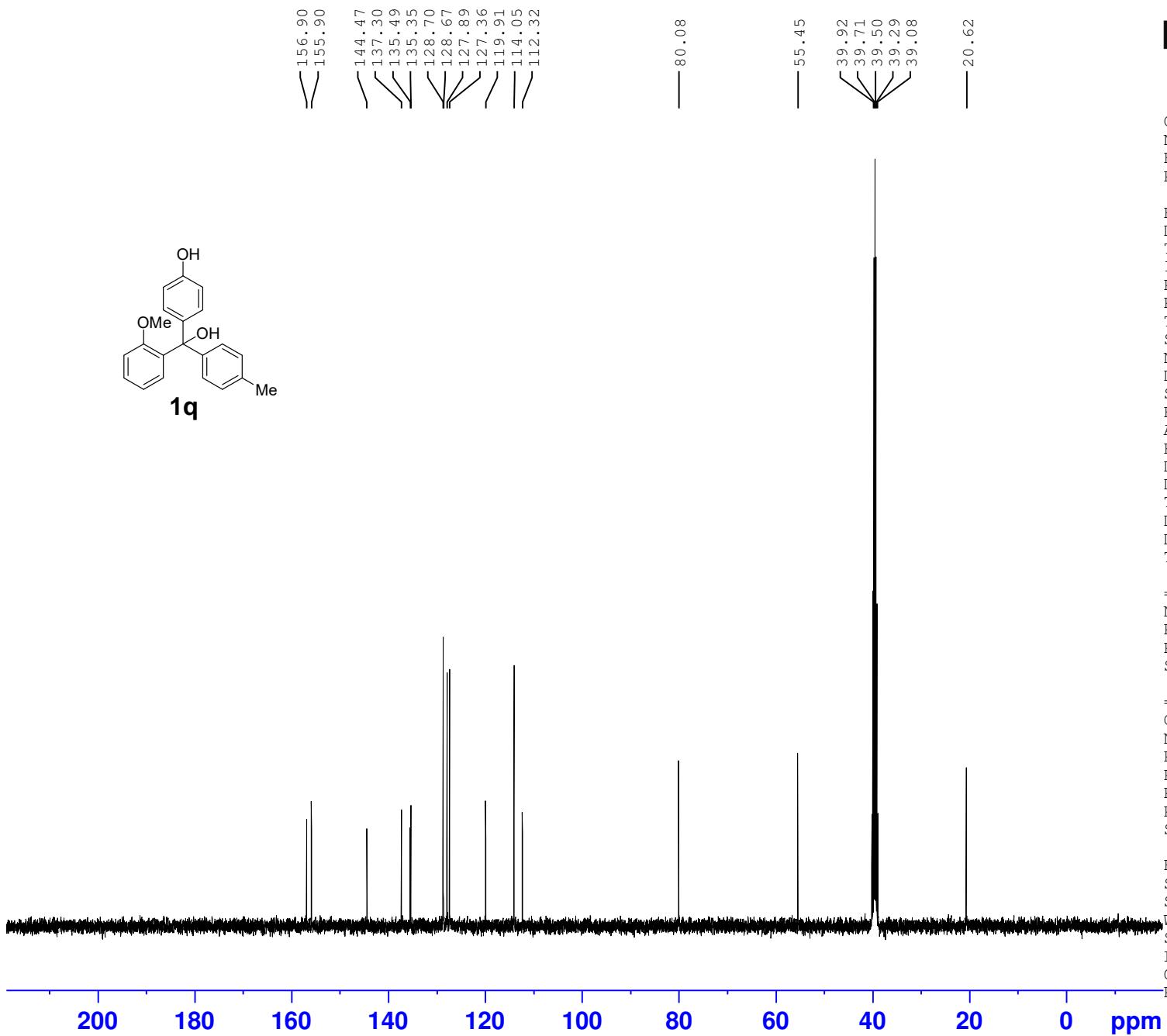
Current Data Parameters  
 NAME 0718-400  
 EXPNO 15  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220718  
 Time 15.33  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 6  
 DS 0  
 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 14.68 usec  
 PLW1 14.00000000 W  
 SFO1 400.1924713 MHz

F2 - Processing parameters  
 SI 65536  
 SF 400.1900135 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1q



Current Data Parameters  
 NAME 1q-ZY-4-69A  
 EXPNO 1  
 PROCNO 1

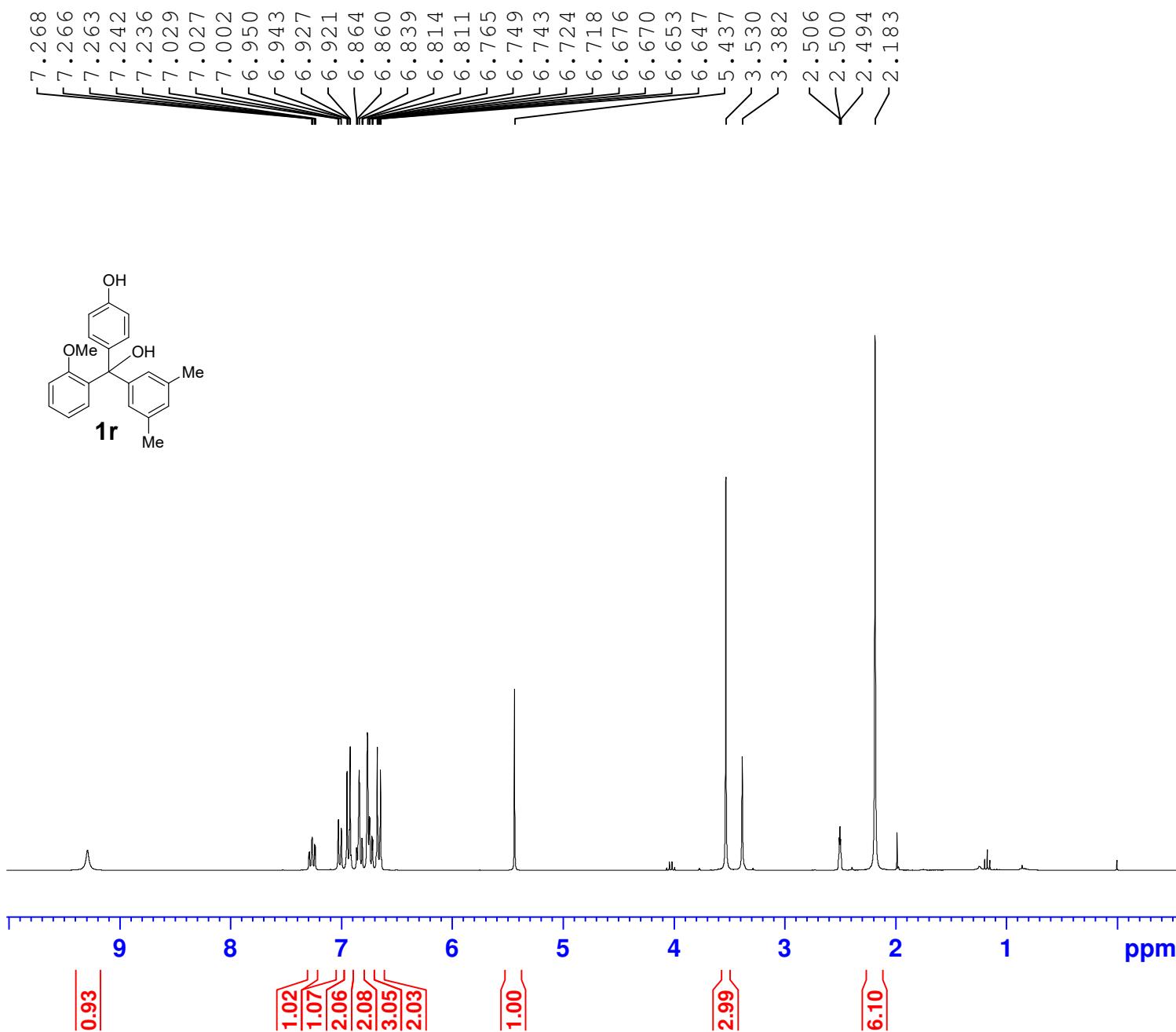
F2 - Acquisition Parameters  
 Date\_ 20220718  
 Time 15.35  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 50  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 193.13  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 294.9 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 <sup>13</sup>C  
 P1 12.00 usec  
 PLW1 53.00000000 W  
 SFO1 100.6379178 MHz

===== CHANNEL f2 =====  
 CPDPRG[2 waltz16  
 NUC2 <sup>1</sup>H  
 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 100.6279048 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

1r



Current Data Parameters  
NAME 0917sjw  
EXPNO 5380  
PROCNO 1

```

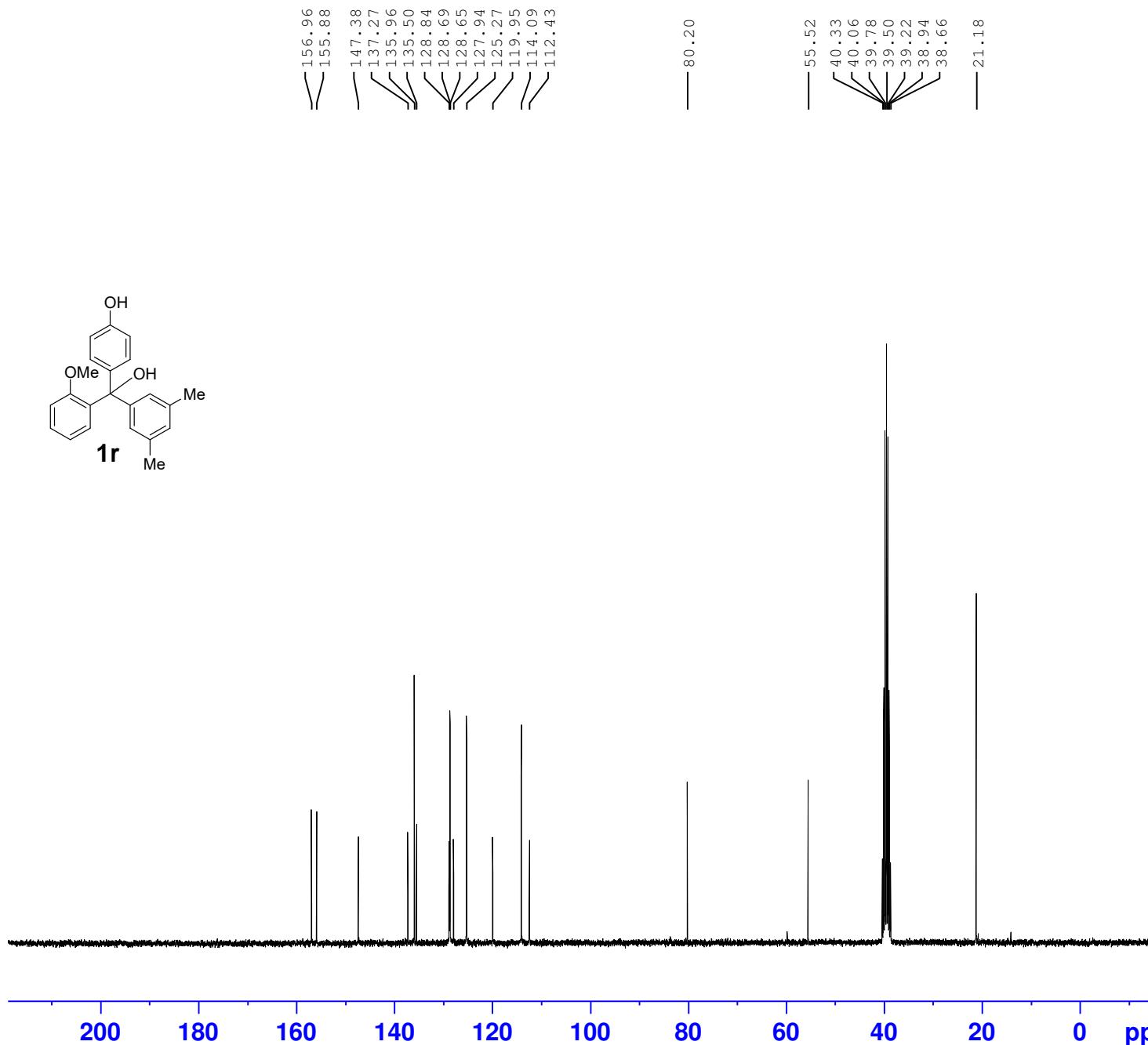
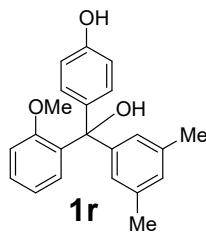
F2 - Acquisition Parameters
Date_          20210917
Time           12.40
INSTRUM       spect
PROBHD        5 mm PABBO BB
PULPROG       zg30
TD             65536
SOLVENT        DMSO
NS              16
DS               2
SWH            6009.615 Hz
FIDRES        0.091699 Hz
AQ             5.4525952 sec
RG              80.6
DW             83.200 used
DE              6.50 used
TE             -59.1 K
D1             1.0000000 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 300.1300023 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

1r



Current Data Parameters  
 NAME 1r-ZY-4-78A  
 EXPNO 5461  
 PROCNO 1

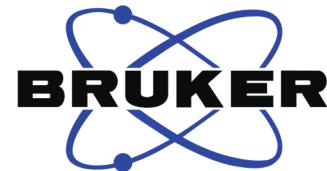
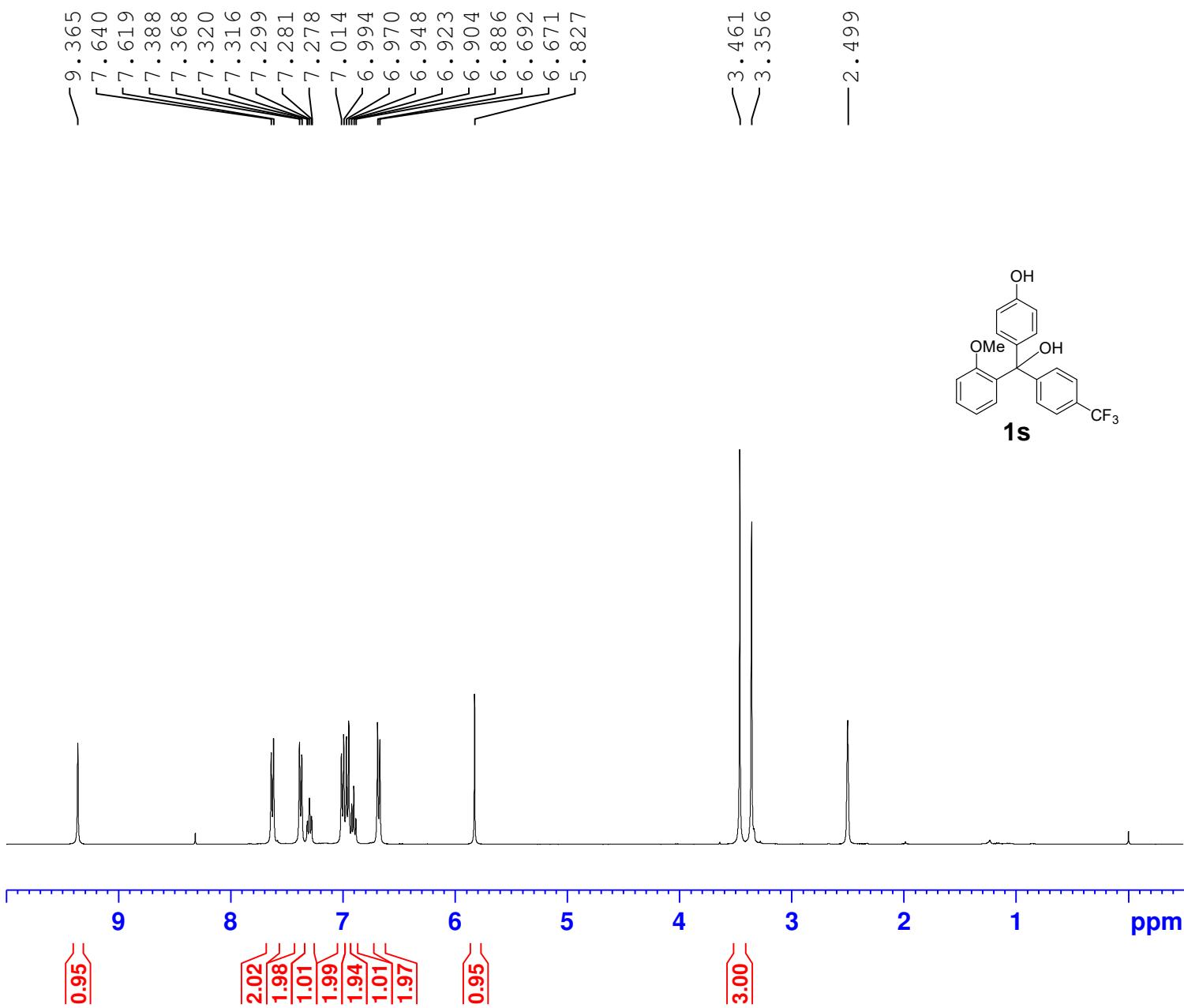
F2 - Acquisition Parameters  
 Date\_ 20210927  
 Time 13.25  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 500  
 DS 4  
 SWH 18028.846 Hz  
 FIDRES 0.275098 Hz  
 AQ 1.8175317 sec  
 RG 203  
 DW 27.733 usec  
 DE 6.50 usec  
 TE -59.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 ======  
 SFO1 75.4752949 MHz  
 NUC1 <sup>13</sup>C  
 P1 9.50 usec  
 PLW1 34.20000076 W

===== CHANNEL f2 ======  
 SFO2 300.1312005 MHz  
 NUC2 <sup>1</sup>H  
 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 75.4677836 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

1s



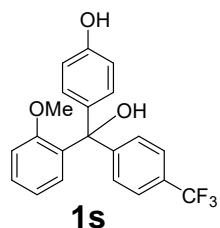
Current Data Parameters  
 NAME 0729-400  
 EXPNO 109  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220729  
 Time 21.40  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 8  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9845889 sec  
 RG 140.02  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 294.7 K  
 D1 1.00000000 sec  
 TD0 1

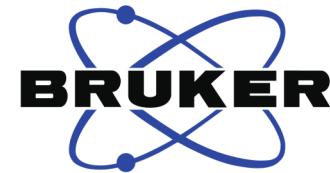
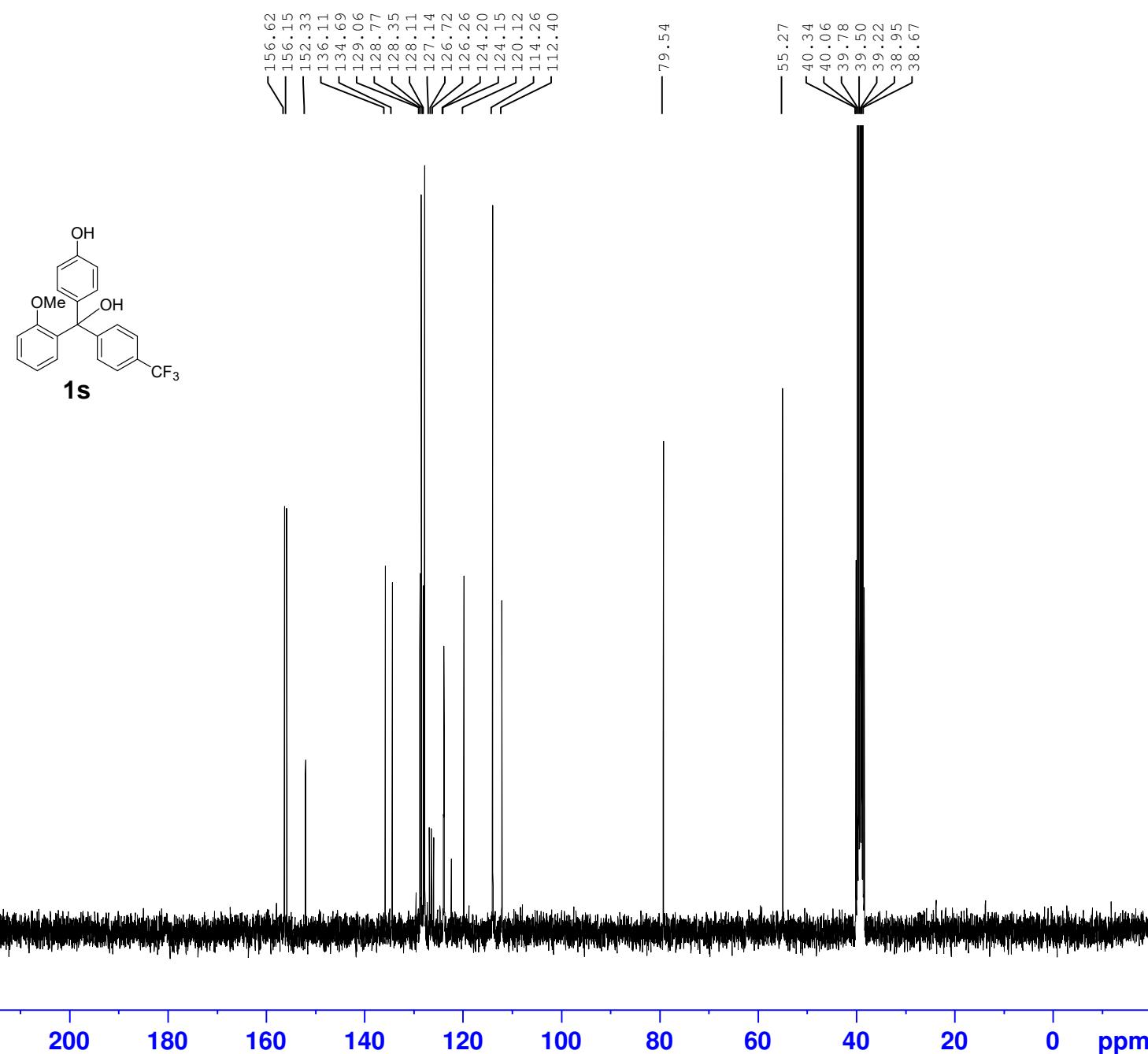
===== CHANNEL f1 ======

NUC1 1H  
 P1 14.68 usec  
 PLW1 14.00000000 W  
 SFO1 400.1924713 MHz

F2 - Processing parameters  
 SI 65536  
 SF 400.1900133 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



1s



Current Data Parameters  
 NAME 1s-ZY-4-70B  
 EXPNO 5299  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210909  
 Time 13.28  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 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 -59.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

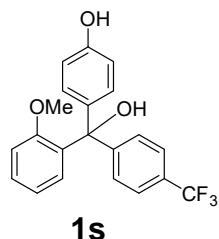
===== CHANNEL f1 ======  
 SFO1 75.4752949 MHz  
 NUC1 13C  
 P1 9.50 usec  
 PLW1 34.20000076 W

===== 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 75.4677830 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

1s

-60.690



Current Data Parameters  
 NAME 0909sjw  
 EXPNO 5300  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210909  
 Time 13.31  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgfhigqn.2  
 TD 131072  
 SOLVENT DMSO  
 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 -59.1 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

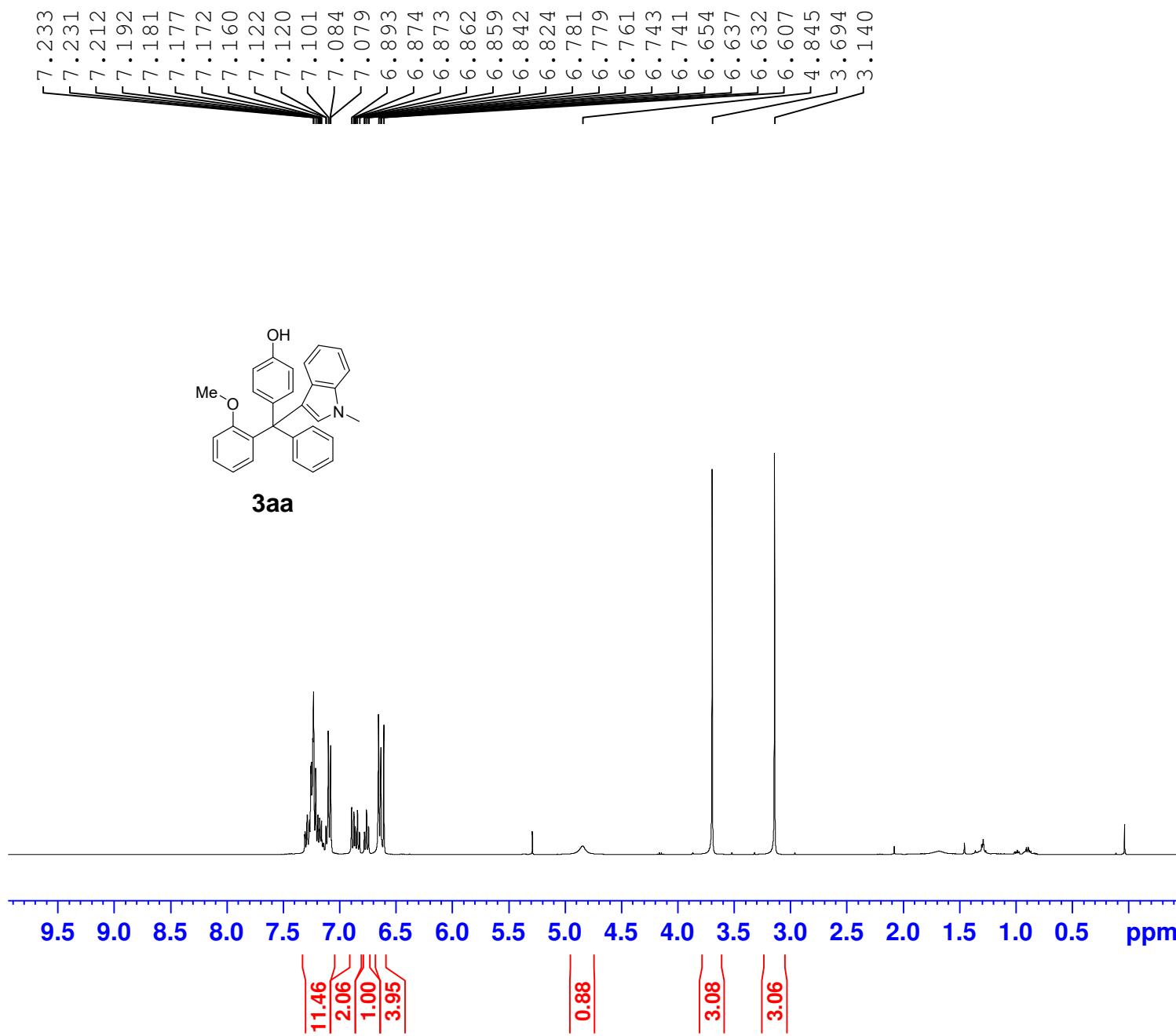
===== CHANNEL f2 ======  
 SFO2 300.1312005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 14.00000000 W  
 PLW12 0.17284000 W

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

0 -20 -40 -60 -80 -100 -120 -140 -160 -180

ppm

3aa

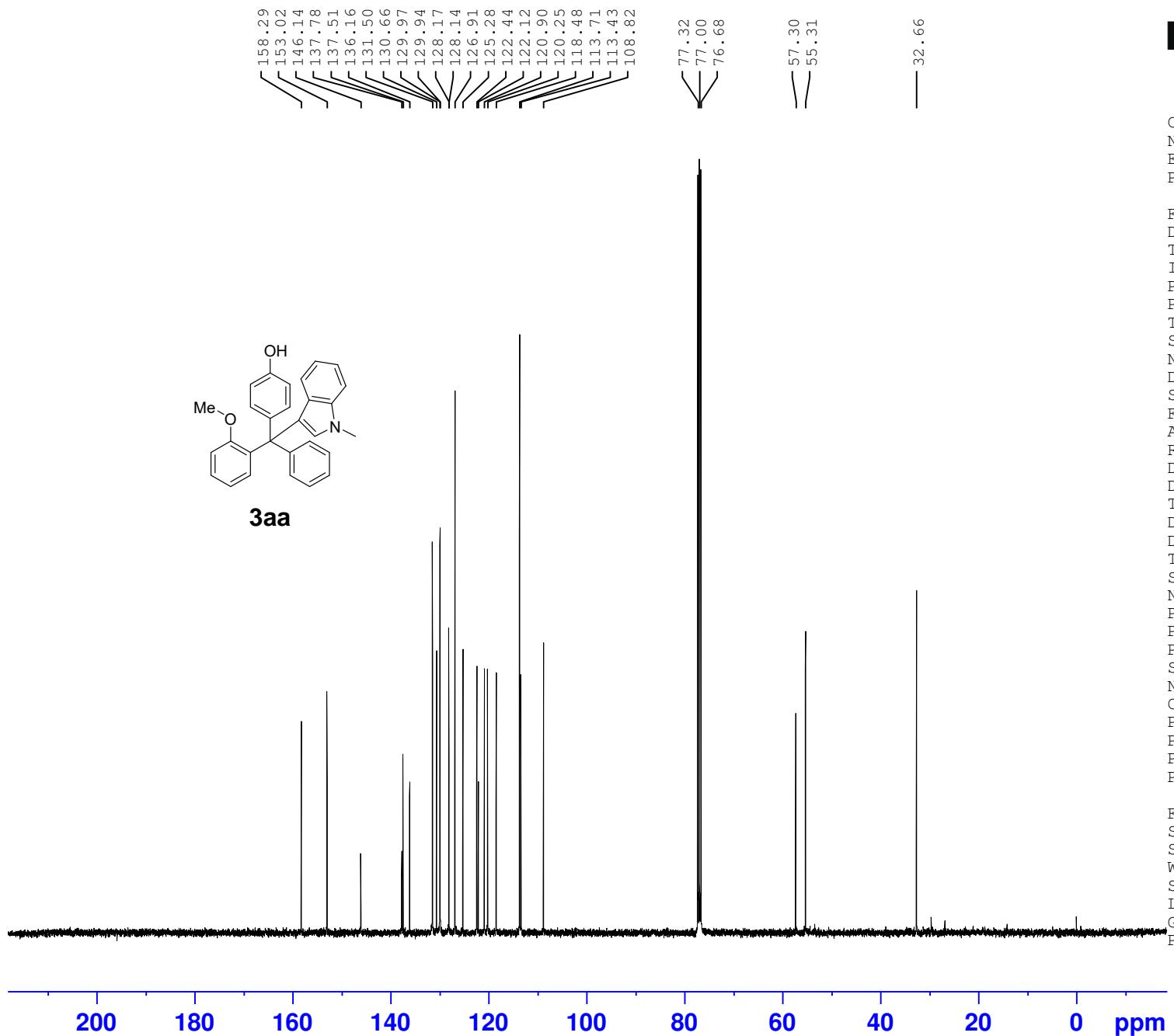


Current Data Parameters  
NAME 0607HH  
EXPNO 4  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220608  
Time 0.46 h  
INSTRUM Avance  
PROBHD Z116098\_0833 (zg30  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 2  
SWH 8196.722 Hz  
FIDRES 0.250144 Hz  
AQ 3.9976959 sec  
RG 60.6061  
DW 61.000 usec  
DE 13.54 usec  
TE 292.0 K  
D1 1.0000000 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 400.1300112 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

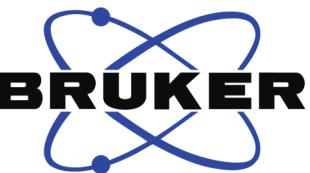
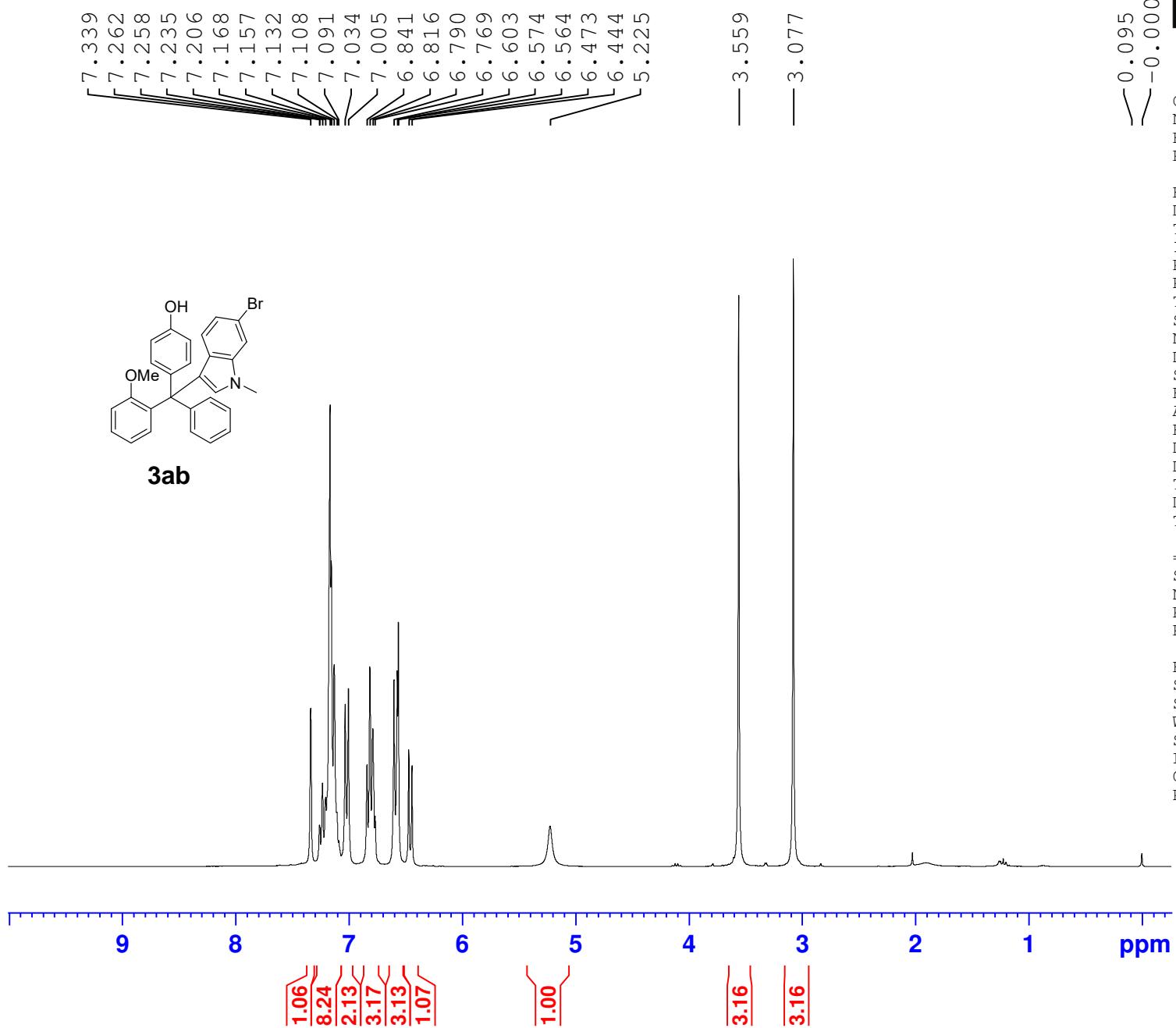
3aa



**BRUKER**

Current Data Parameters  
 NAME 3aa-ZY-4-1  
 EXPNO 5  
 PROCNO 1

3ab



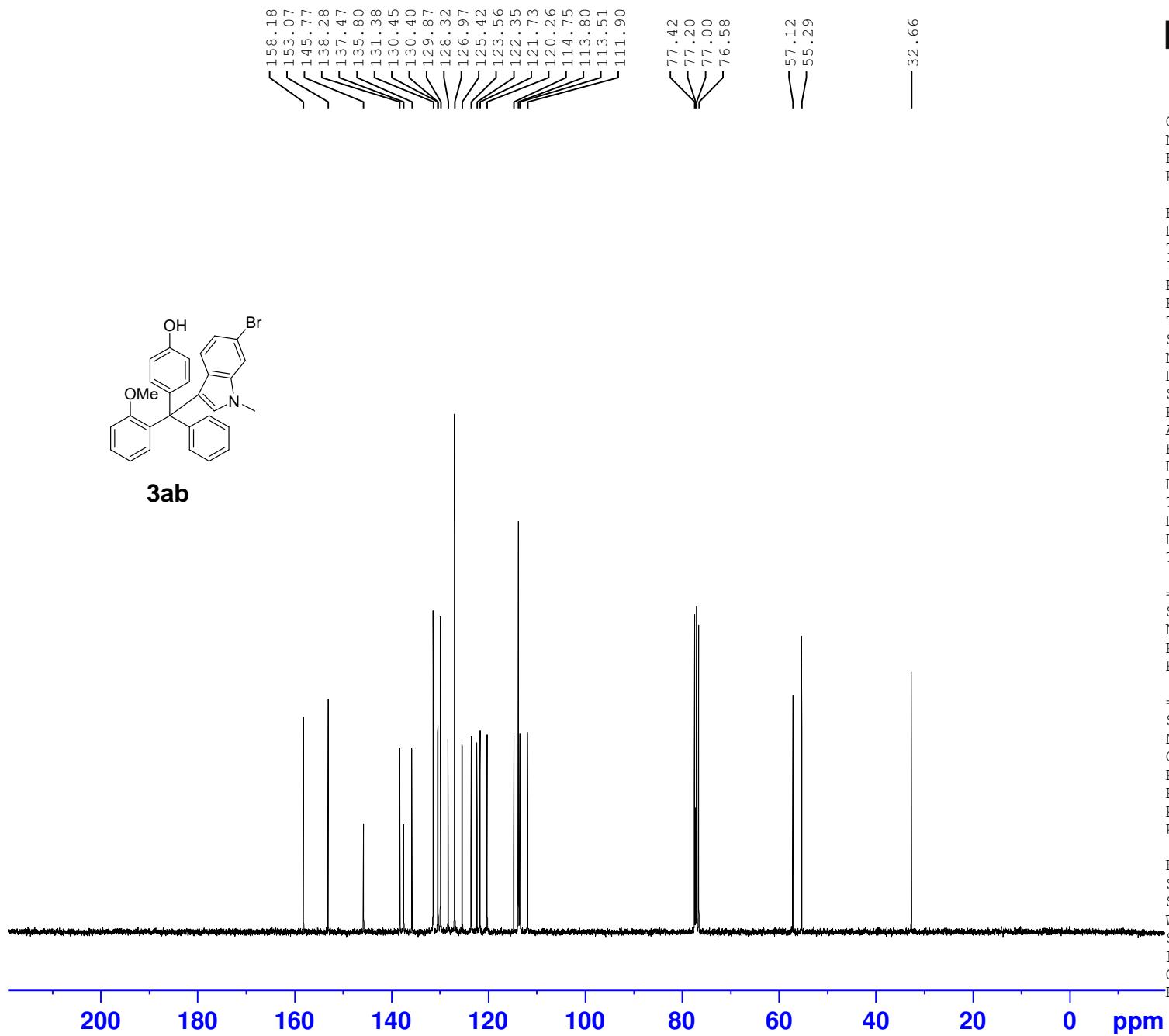
Current Data Parameters  
NAME 0929sjw  
EXPNO 5465  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210929  
Time 10.11  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 32  
DW 83.200 usec  
DE 6.50 usec  
TE -59.1 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 300.1300344 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

3ab



Current Data Parameters  
NAME 3ab-ZY-4-64B  
EXPNO 5496  
PROCNO 1

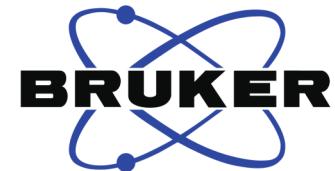
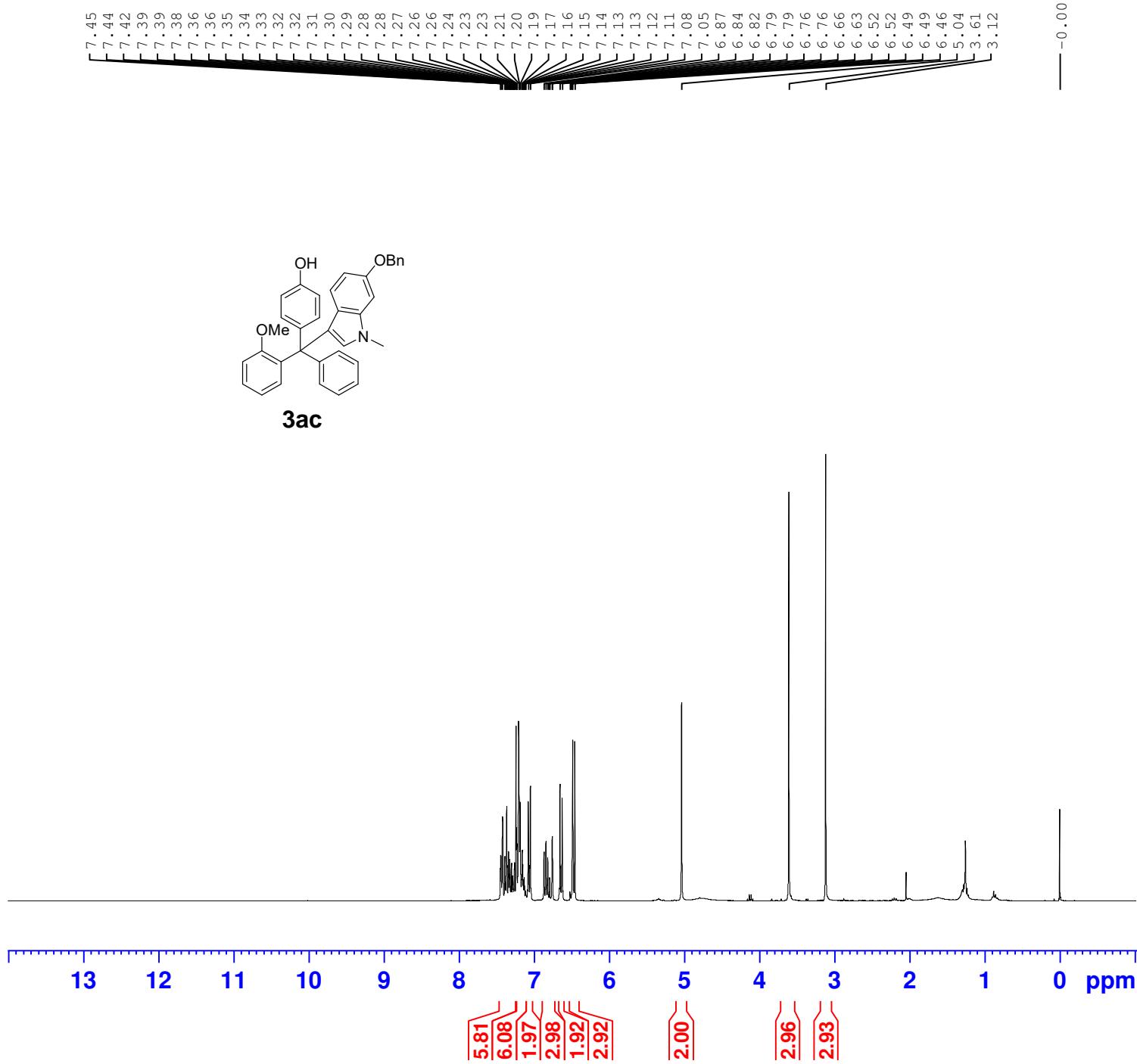
F2 - Acquisition Parameters  
Date\_ 20210930  
Time 12.04  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 500  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE -59.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 ======  
SFO1 75.4752949 MHz  
NUC1 <sup>13</sup>C  
P1 9.50 usec  
PLW1 34.20000076 W

===== CHANNEL f2 ======  
SFO2 300.1312005 MHz  
NUC2 <sup>1</sup>H  
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 75.4677642 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

3ac



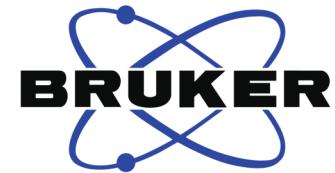
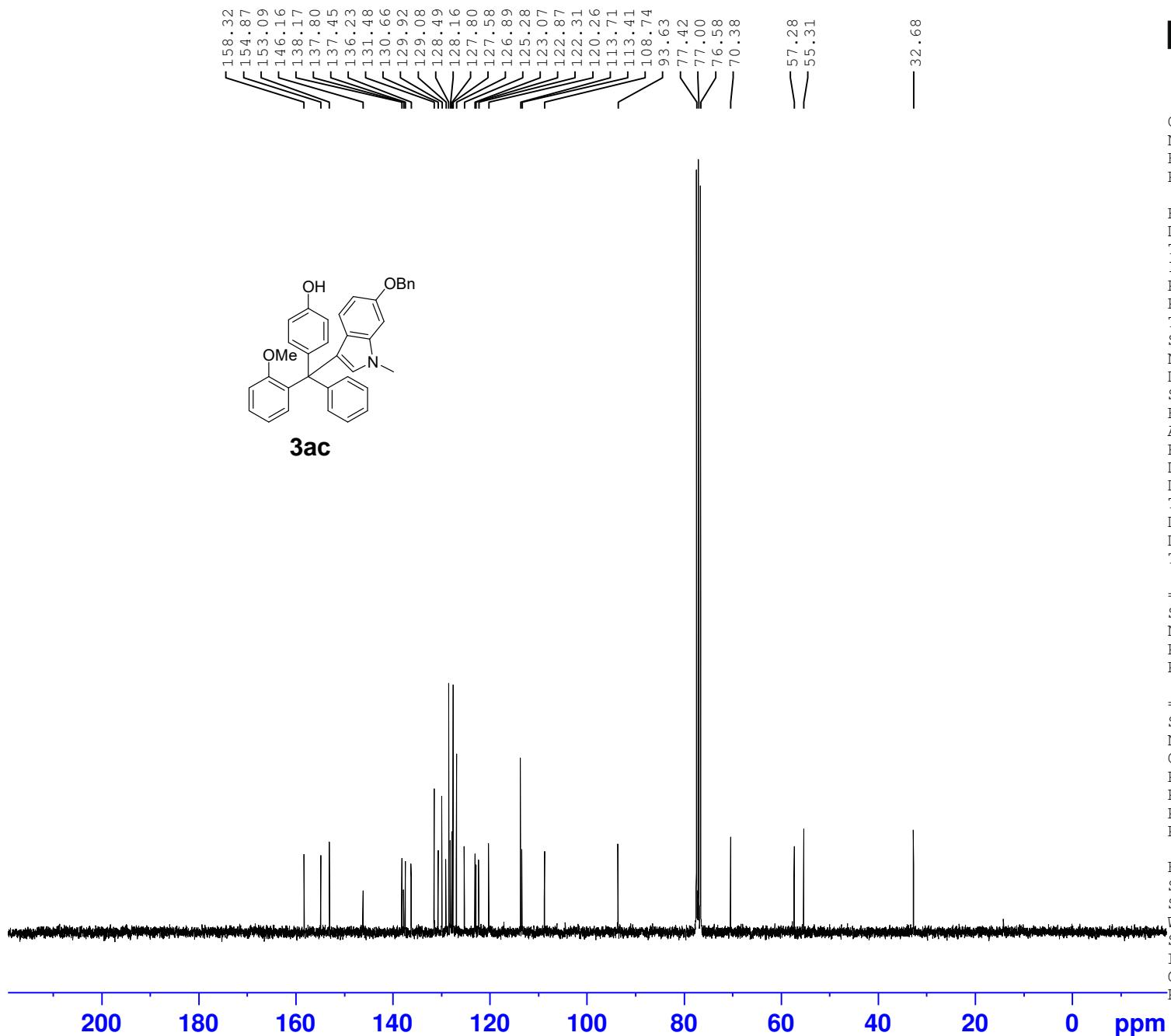
Current Data Parameters  
NAME ZY-4-64G-h-fr  
EXPNO 5413  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210924  
Time 10.18  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
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 -59.1 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 300.1300127 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

3ac



Current Data Parameters  
NAME 3ac-ZY-4-64G  
EXPNO 5338  
PROCNO 1

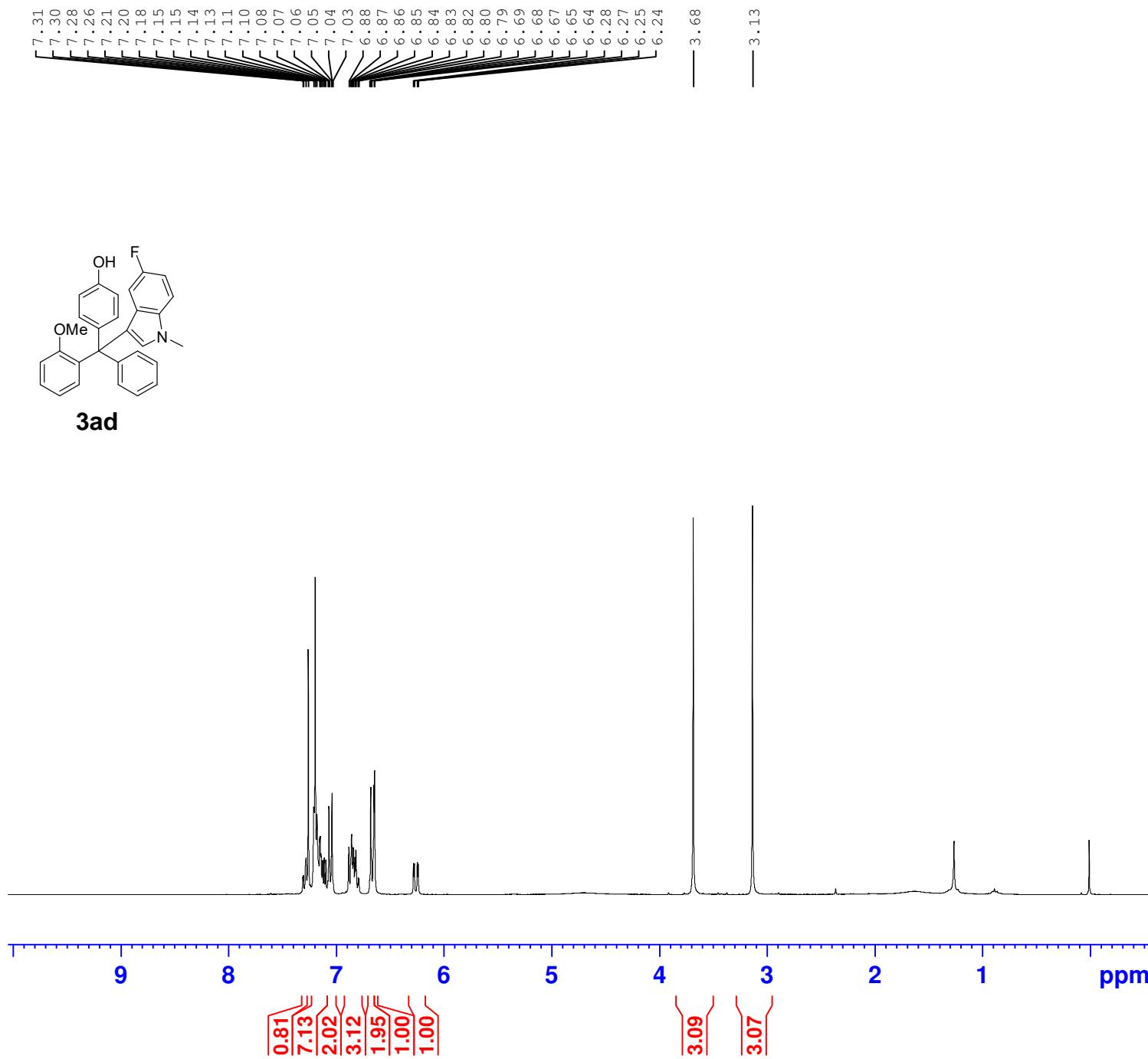
F2 - Acquisition Parameters  
Date\_ 20210915  
Time 11.47  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 800  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE -59.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 75.4752949 MHz  
NUC1 <sup>13</sup>C  
P1 9.50 usec  
PLW1 34.20000076 W

===== CHANNEL f2 =====  
SFO2 300.1312005 MHz  
NUC2 <sup>1</sup>H  
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 75.4677531 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

3ad



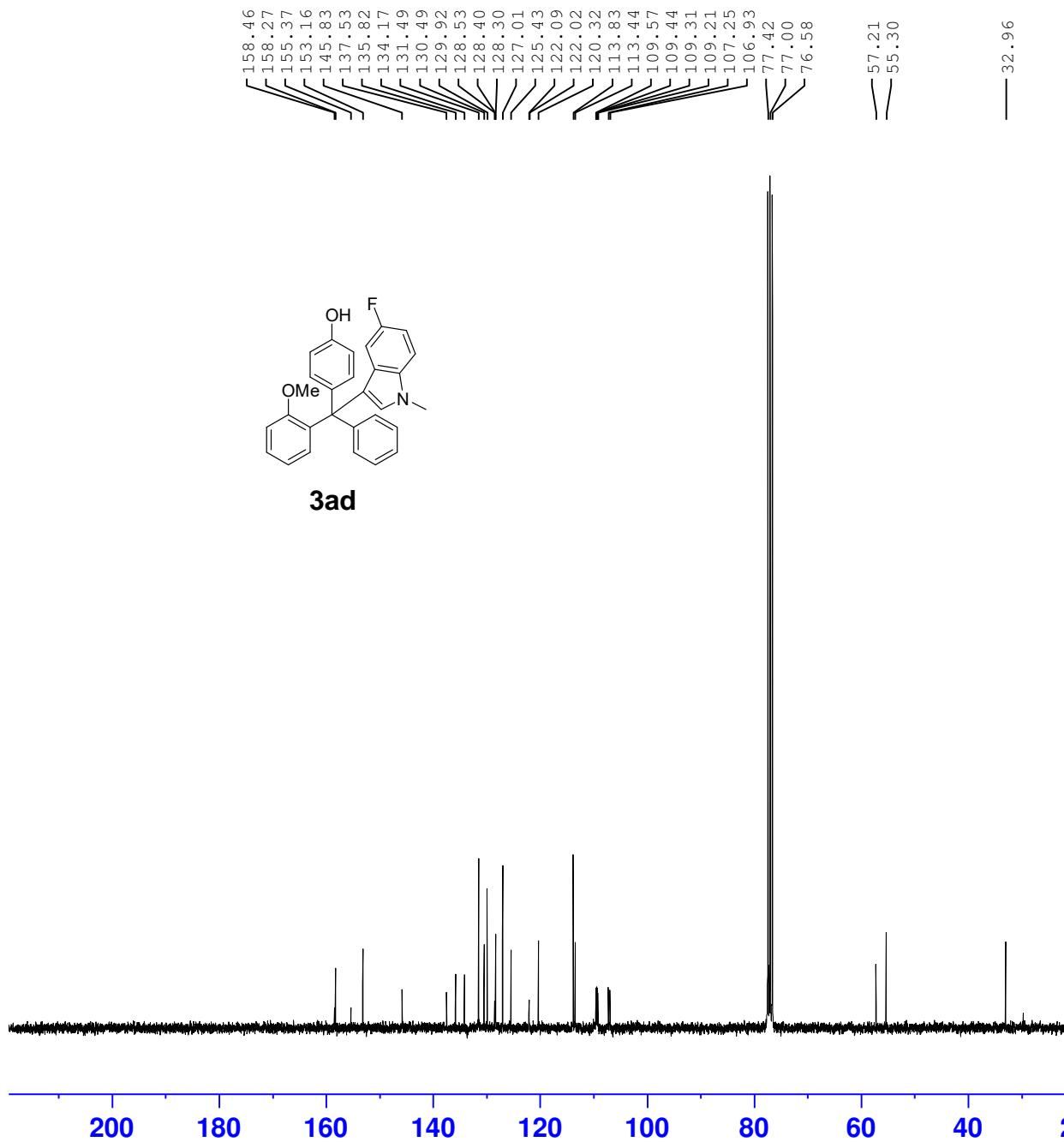
Current Data Parameters  
NAME ZY-4-64C-h-fr  
EXPNO 5542  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211019  
Time 9.45  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 203  
DW 83.200 usec  
DE 6.50 usec  
TE -59.1 K  
D1 1.0000000 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 300.1300072 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

3ad



Current Data Parameters  
NAME 3ad-ZY-4-64C  
EXPNO 5543  
PROCNO 1

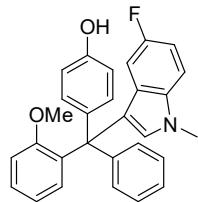
F2 - Acquisition Parameters  
Date\_ 20211019  
Time 10.53  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 1024  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE -59.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 ======  
SFO1 75.4752949 MHz  
NUC1 <sup>13</sup>C  
P1 9.50 usec  
PLW1 34.20000076 W

===== CHANNEL f2 ======  
SFO2 300.1312005 MHz  
NUC2 <sup>1</sup>H  
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 75.4677522 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

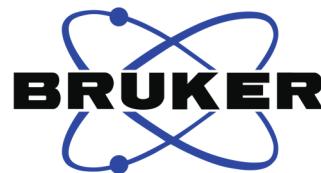
3ad



**3ad**

— -125.149

0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm



Current Data Parameters  
NAME 211010sjw  
EXPNO 5511  
PROCNO 1

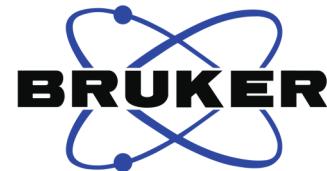
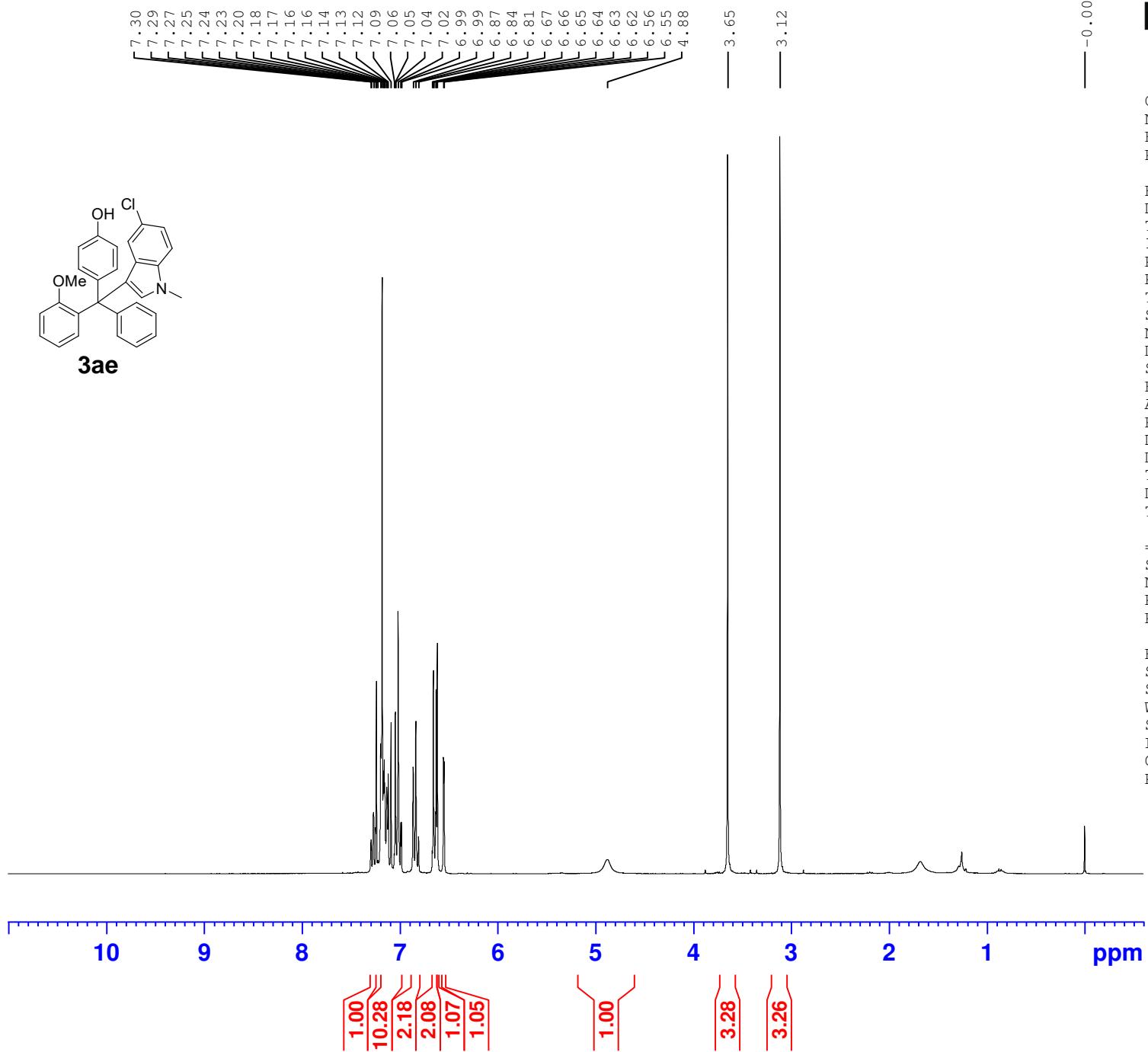
F2 - Acquisition Parameters  
Date\_ 20211010  
Time 9.52  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgfhigqn.2  
TD 131072  
SOLVENT CDCl3  
NS 16  
DS 4  
SWH 66964.289 Hz  
FIDRES 0.510897 Hz  
AQ 0.9786710 sec  
RG 203  
DW 7.467 usec  
DE 6.50 usec  
TE -59.1 K  
D1 1.00000000 sec  
D11 0.03000000 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

3ae



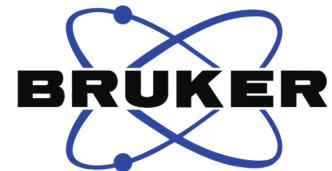
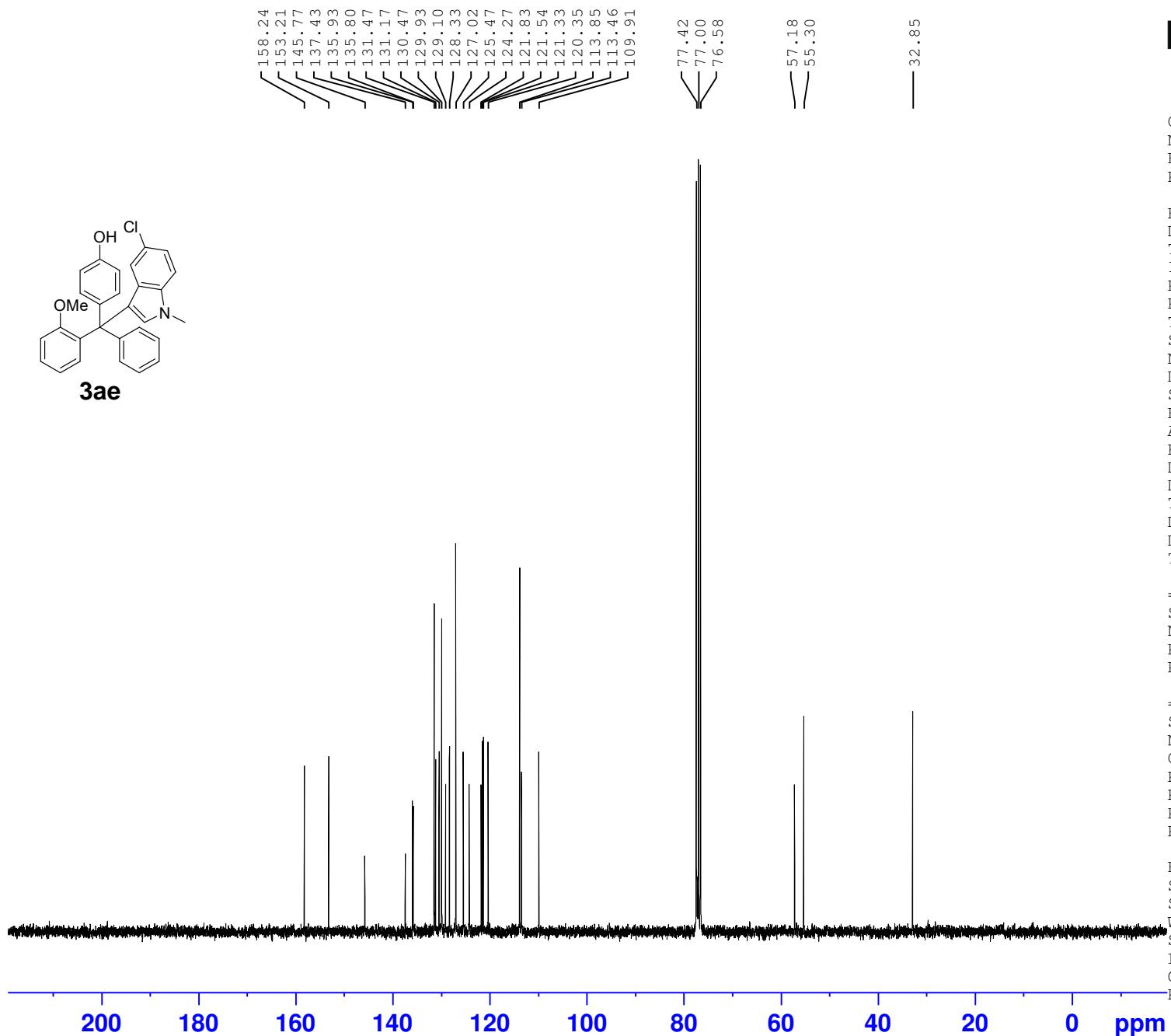
Current Data Parameters  
 NAME ZY-4-64D-h-fr  
 EXPNO 5340  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210914  
 Time 13.44  
 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 -59.1 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 300.1300129 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

3ae



Current Data Parameters  
 NAME 3ae-ZY-4-64D  
 EXPNO 5337  
 PROCNO 1

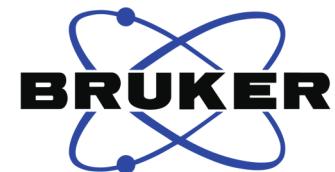
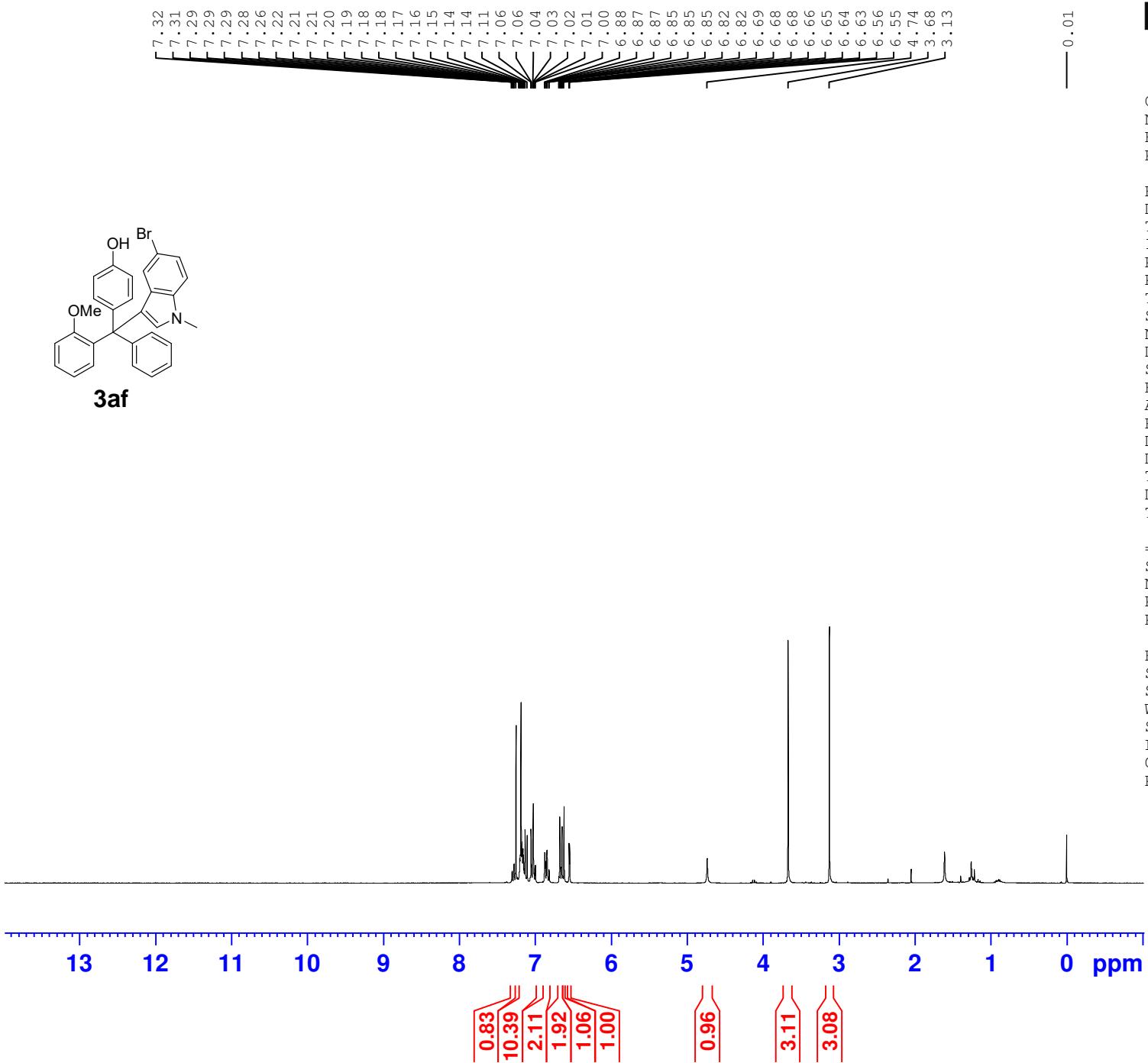
F2 - Acquisition Parameters  
 Date\_ 20210915  
 Time 10.51  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl<sub>3</sub>  
 NS 800  
 DS 4  
 SWH 18028.846 Hz  
 FIDRES 0.275098 Hz  
 AQ 1.8175317 sec  
 RG 203  
 DW 27.733 usec  
 DE 6.50 usec  
 TE -59.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 ======  
 SFO1 75.4752949 MHz  
 NUC1 <sup>13</sup>C  
 P1 9.50 usec  
 PLW1 34.20000076 W

===== CHANNEL f2 ======  
 SFO2 300.1312005 MHz  
 NUC2 <sup>1</sup>H  
 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 75.4677539 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

3af



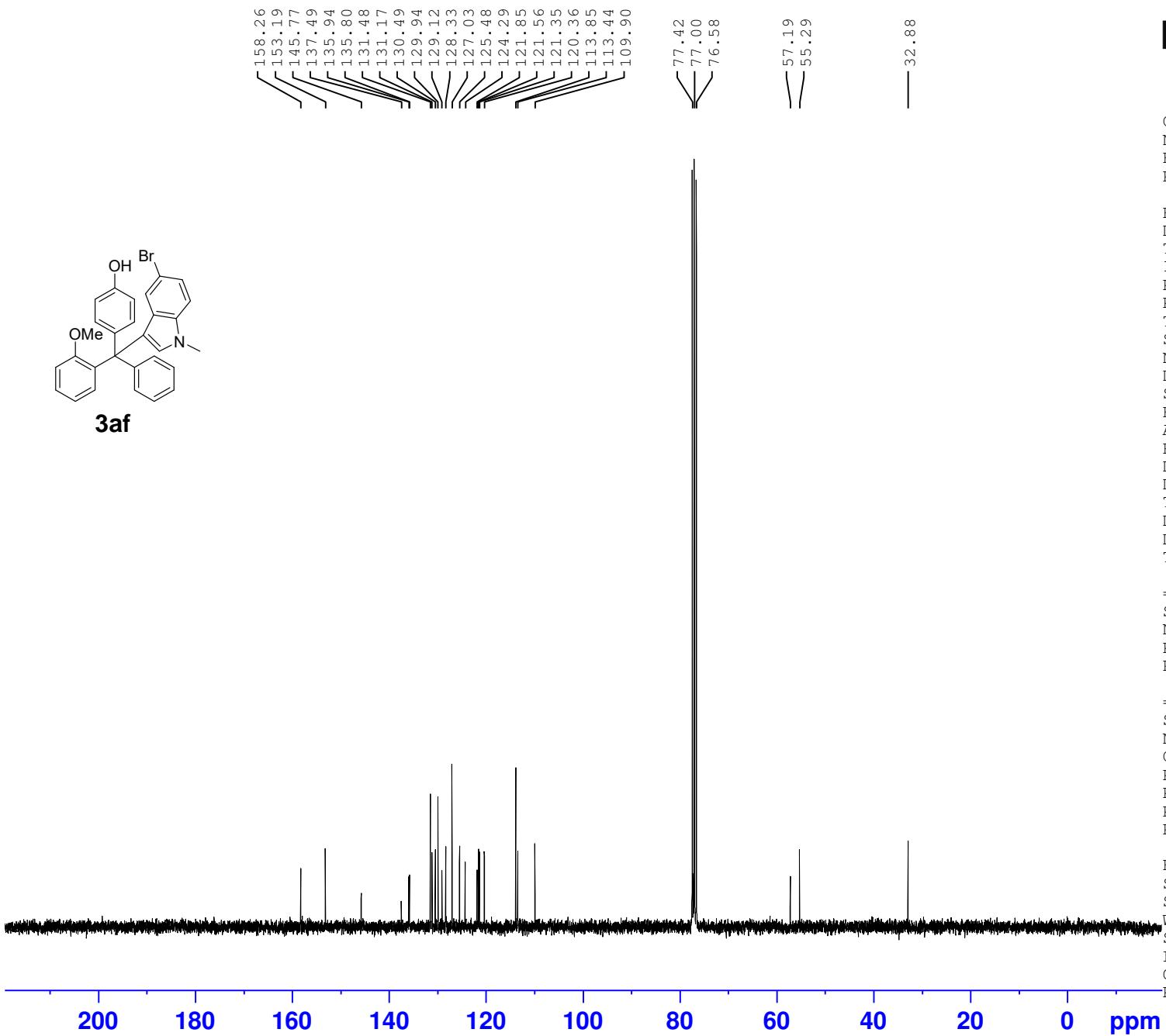
Current Data Parameters  
NAME ZY-4-64E-h-fr  
EXPNO 5617  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211117  
Time 10.35  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
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 -59.1 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 300.1300097 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

3af



Current Data Parameters  
 NAME 3af-ZY-4-64E  
 EXPNO 5618  
 PROCNO 1

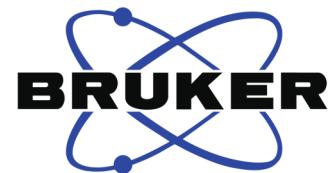
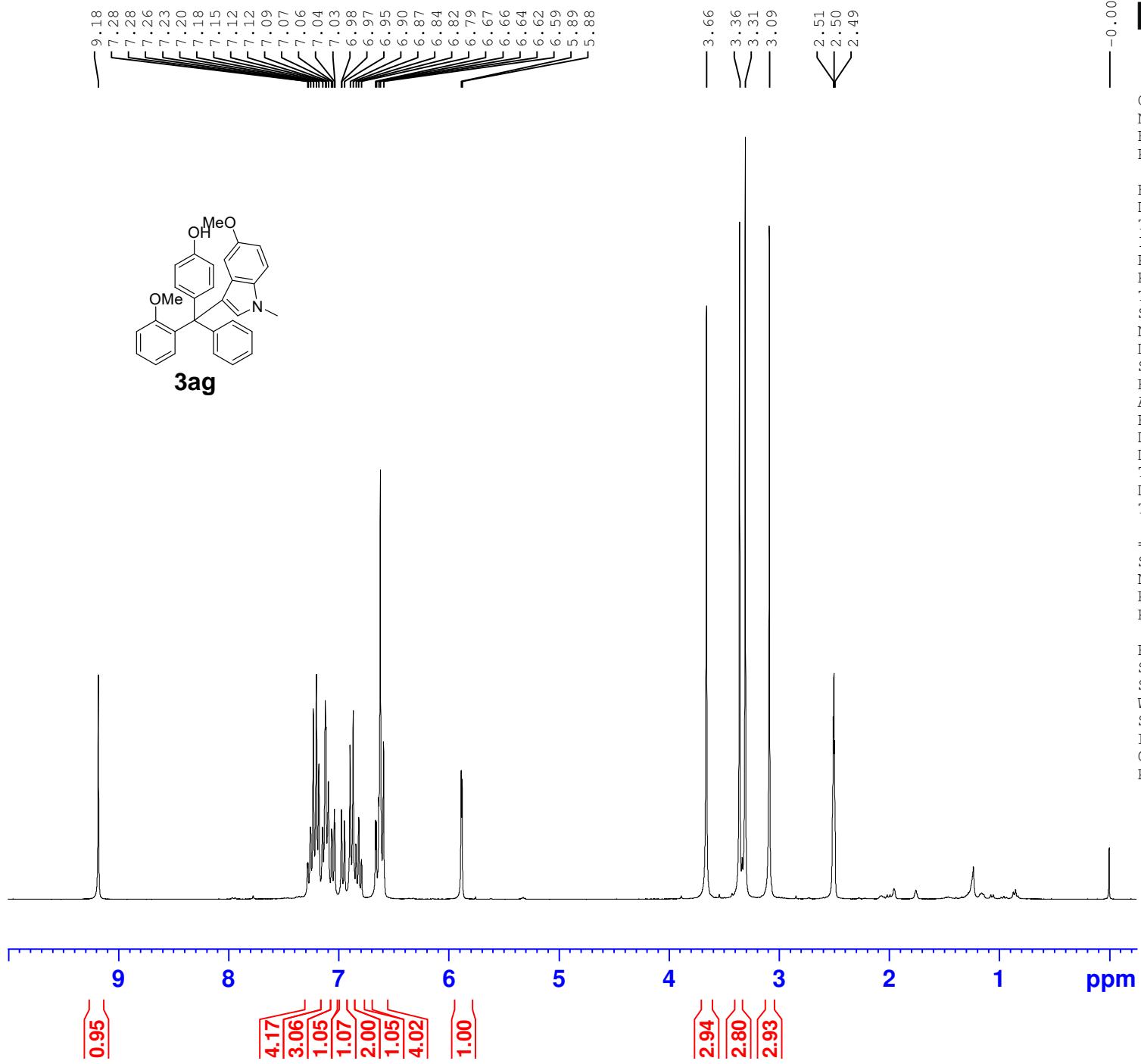
F2 - Acquisition Parameters  
 Date\_ 20211117  
 Time 11.09  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl<sub>3</sub>  
 NS 500  
 DS 4  
 SWH 18028.846 Hz  
 FIDRES 0.275098 Hz  
 AQ 1.8175317 sec  
 RG 203  
 DW 27.733 usec  
 DE 6.50 usec  
 TE -59.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 ======  
 SFO1 75.4752949 MHz  
 NUC1 <sup>13</sup>C  
 P1 9.50 usec  
 PLW1 34.20000076 W

===== CHANNEL f2 ======  
 SFO2 300.1312005 MHz  
 NUC2 <sup>1</sup>H  
 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 75.4677521 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

3ag



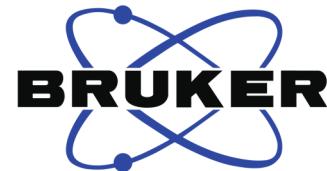
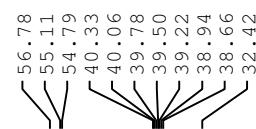
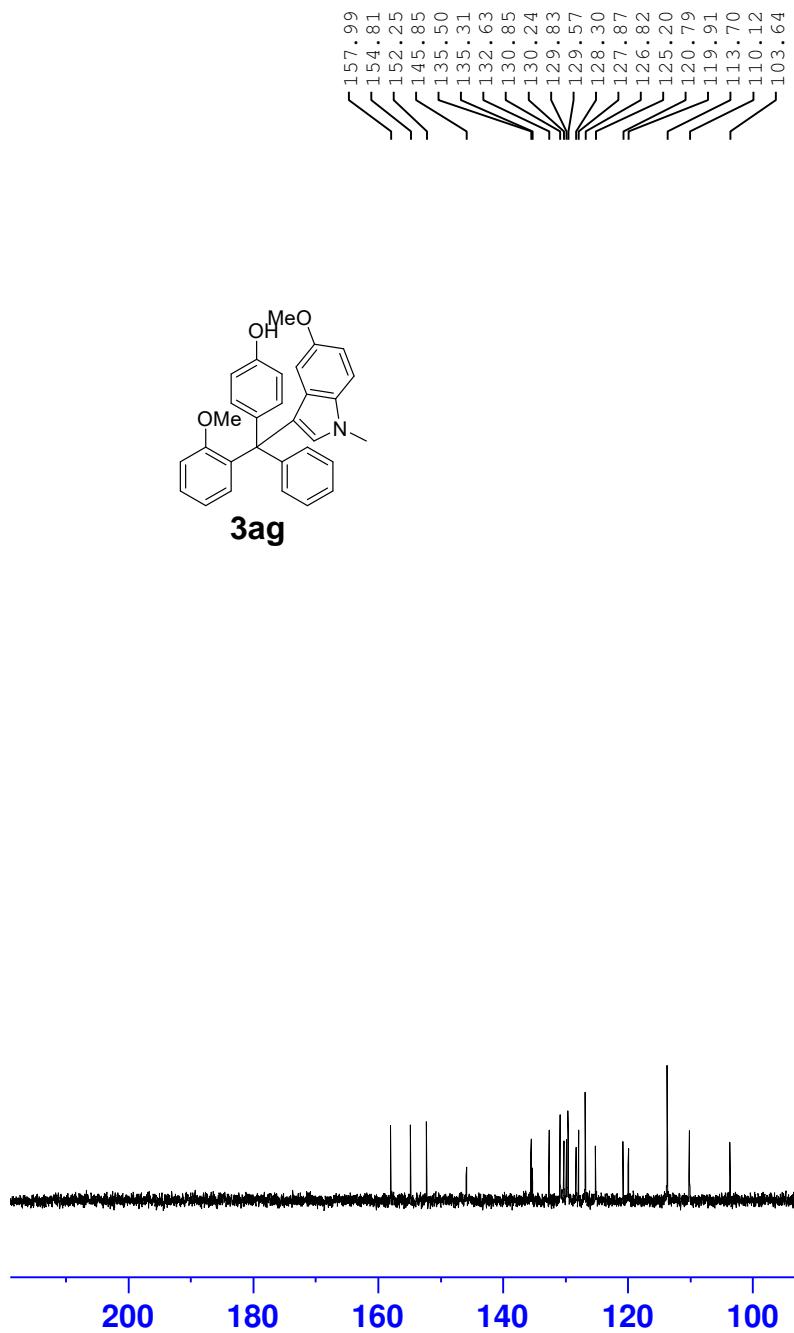
Current Data Parameters  
NAME ZY-4-64H-h-fr  
EXPNO 5301  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210909  
Time 13.35  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
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 -59.1 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 300.1300013 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

3ag



Current Data Parameters  
NAME 3ag-ZY-4-64H  
EXPNO 5311  
PROCNO 1

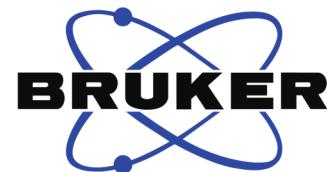
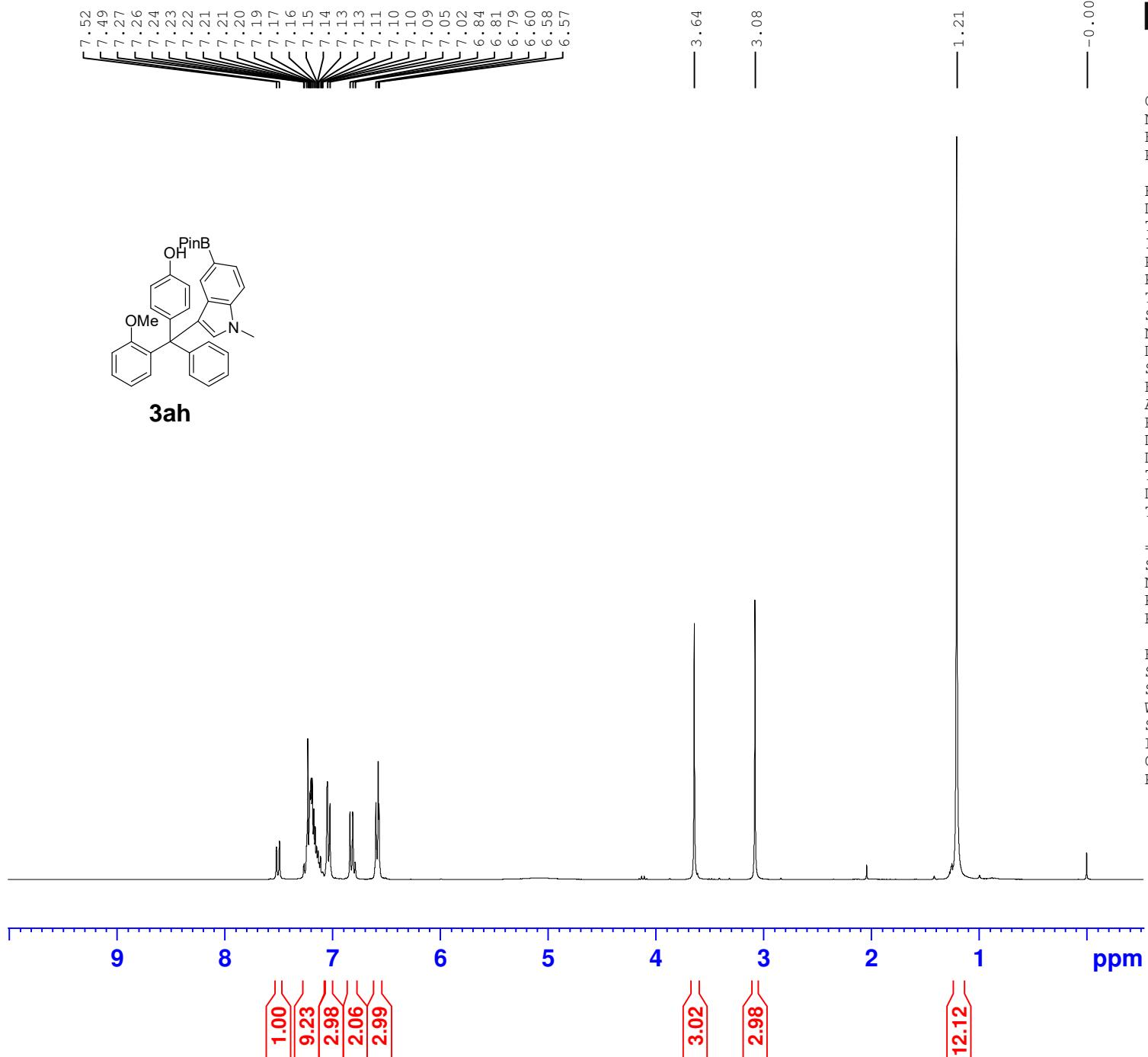
F2 - Acquisition Parameters  
Date\_ 20210910  
Time 13.51  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 473  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE -59.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 ======  
SFO1 75.4752949 MHz  
NUC1 <sup>13</sup>C  
P1 9.50 usec  
PLW1 34.20000076 W

===== CHANNEL f2 ======  
SFO2 300.1312005 MHz  
NUC2 <sup>1</sup>H  
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 75.4677847 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

3ah



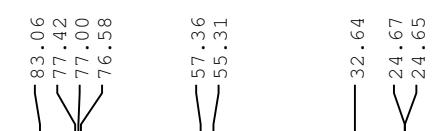
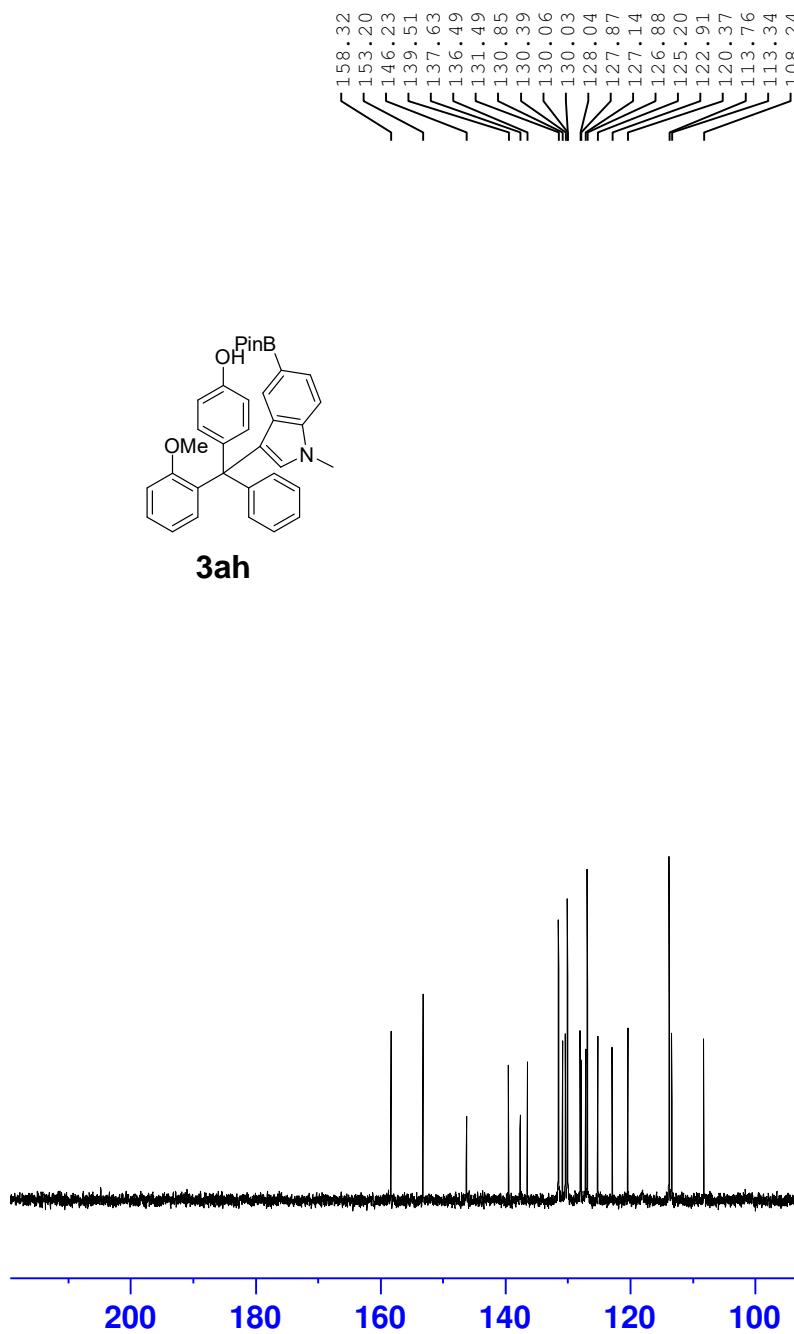
Current Data Parameters  
NAME ZY-4-72-h-fr  
EXPNO 5589  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211029  
Time 23.47  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 80.6  
DW 83.200 usec  
DE 6.50 usec  
TE -59.1 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 300.1300161 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

3ah



Current Data Parameters  
NAME 3ah-ZY-4-72  
EXPNO 5590  
PROCNO 1

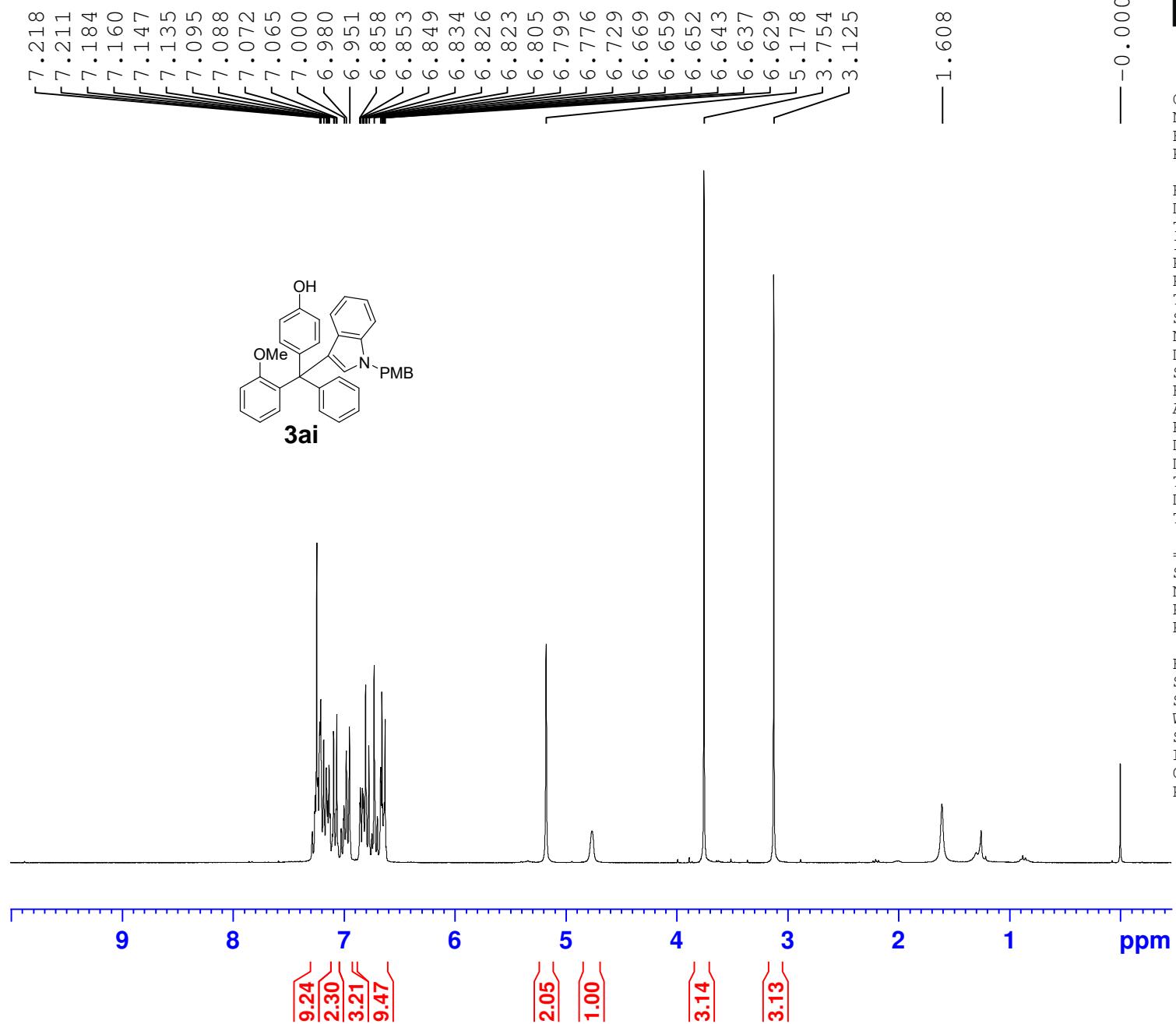
F2 - Acquisition Parameters  
Date\_ 20211030  
Time 0.34  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 700  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE -59.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 ======  
SFO1 75.4752949 MHz  
NUC1 <sup>13</sup>C  
P1 9.50 usec  
PLW1 34.20000076 W

===== CHANNEL f2 ======  
SFO2 300.1312005 MHz  
NUC2 <sup>1</sup>H  
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 75.4677552 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

3ai



Current Data Parameters	
NAME	0914sjw
EXPNO	5338
PROCNO	1

```

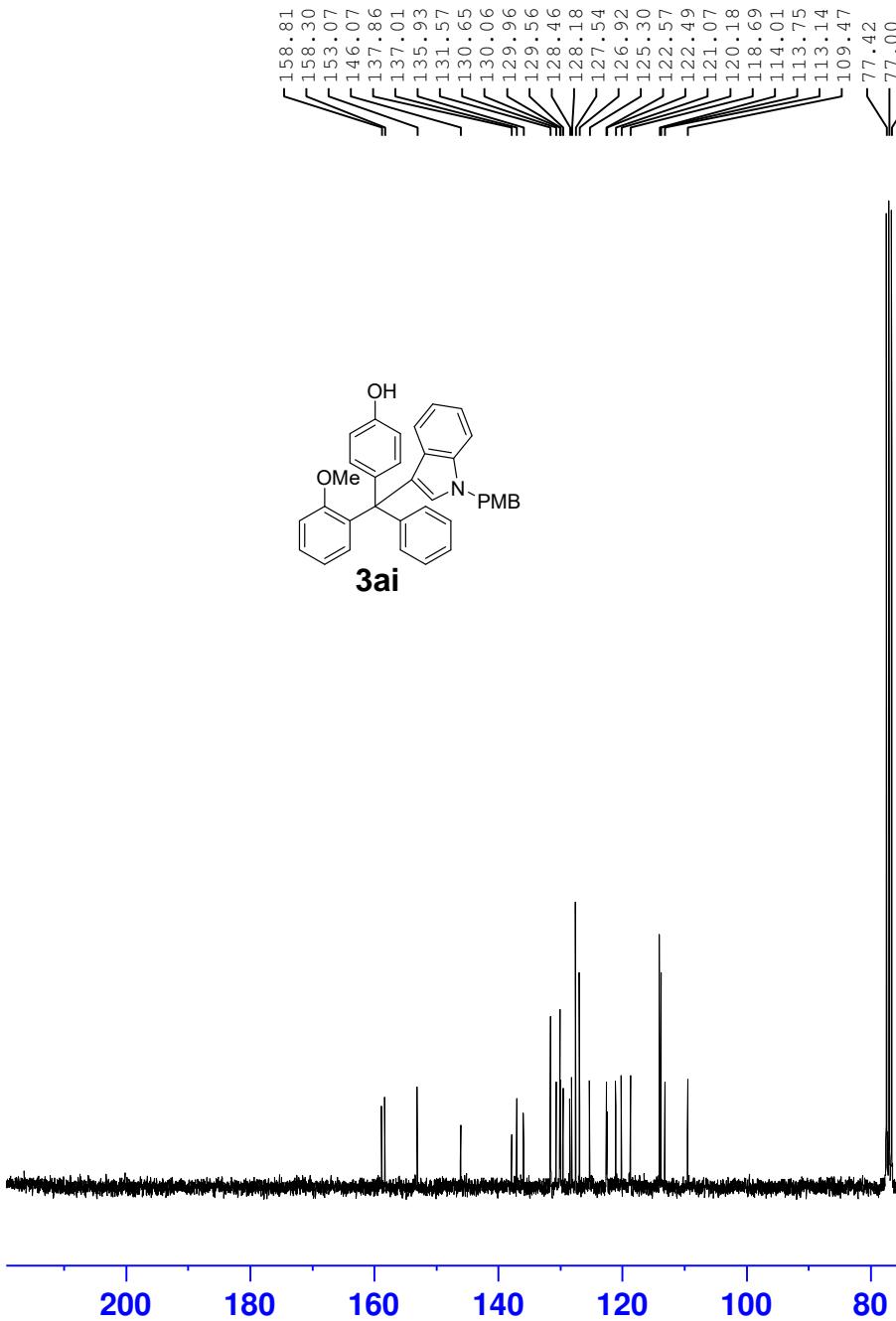
F2 - Acquisition Parameters
Date_           20210914
Time            12.39
INSTRUM        spect
PROBHD         5 mm PABBO BB-
PULPROG        zg30
TD              65536
SOLVENT         CDC13
NS              16
DS              2
SWH             6009.615 Hz
FIDRES         0.091699 Hz
AQ              5.4525952 sec
RG              181
DW              83.200 used
DE              6.50 used
TE              -59.1 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 300.1300113 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

3ai



Current Data Parameters  
 NAME 3ai-ZY-4-64A  
 EXPNO 5339  
 PROCNO 1

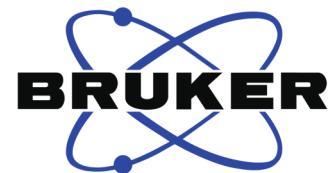
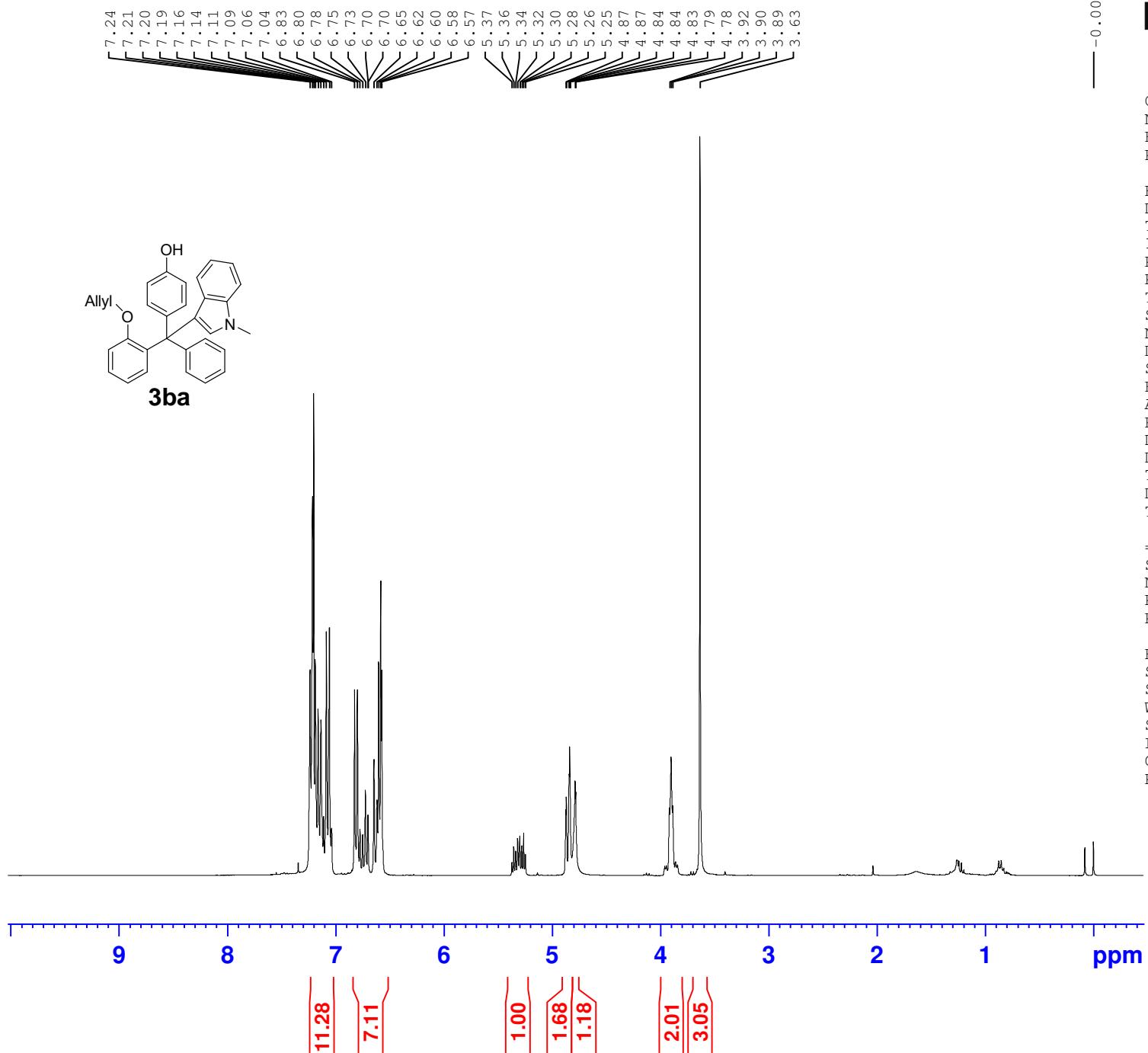
F2 - Acquisition Parameters  
 Date\_ 20210914  
 Time 13.39  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl<sub>3</sub>  
 NS 900  
 DS 4  
 SWH 18028.846 Hz  
 FIDRES 0.275098 Hz  
 AQ 1.8175317 sec  
 RG 203  
 DW 27.733 usec  
 DE 6.50 usec  
 TE -59.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 ======  
 SFO1 75.4752949 MHz  
 NUC1 <sup>13</sup>C  
 P1 9.50 usec  
 PLW1 34.20000076 W

===== CHANNEL f2 ======  
 SFO2 300.1312005 MHz  
 NUC2 <sup>1</sup>H  
 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 75.4677526 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

3ba



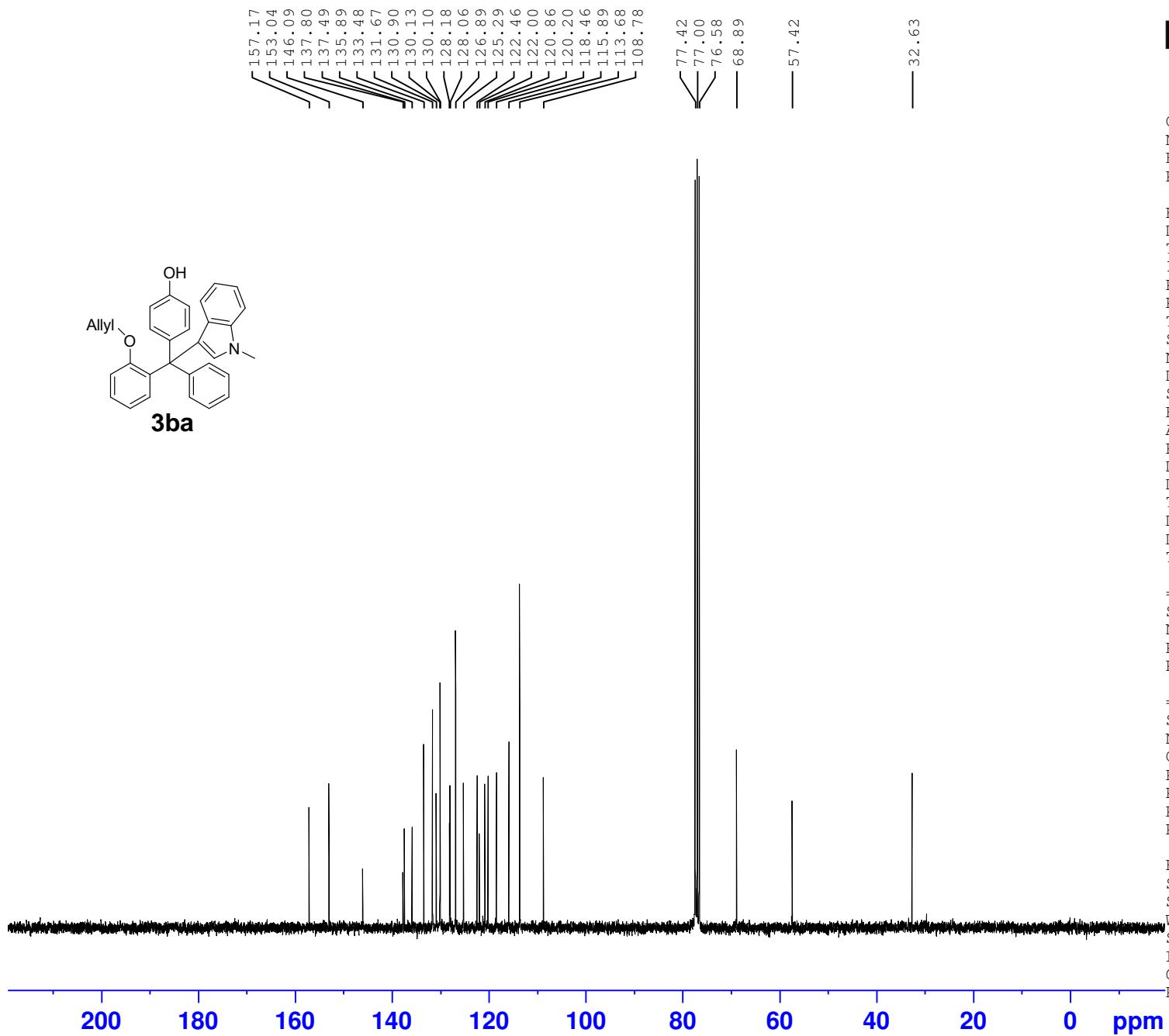
Current Data Parameters  
NAME ZY-4-11D-h-fr  
EXPNO 5723  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211218  
Time 9.11  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 80.6  
DW 83.200 usec  
DE 6.50 usec  
TE -59.1 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 300.1300245 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

3ba



Current Data Parameters  
 NAME 3ca-ZY-4-11D  
 EXPNO 5513  
 PROCNO 1

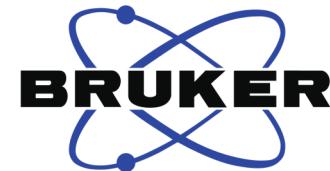
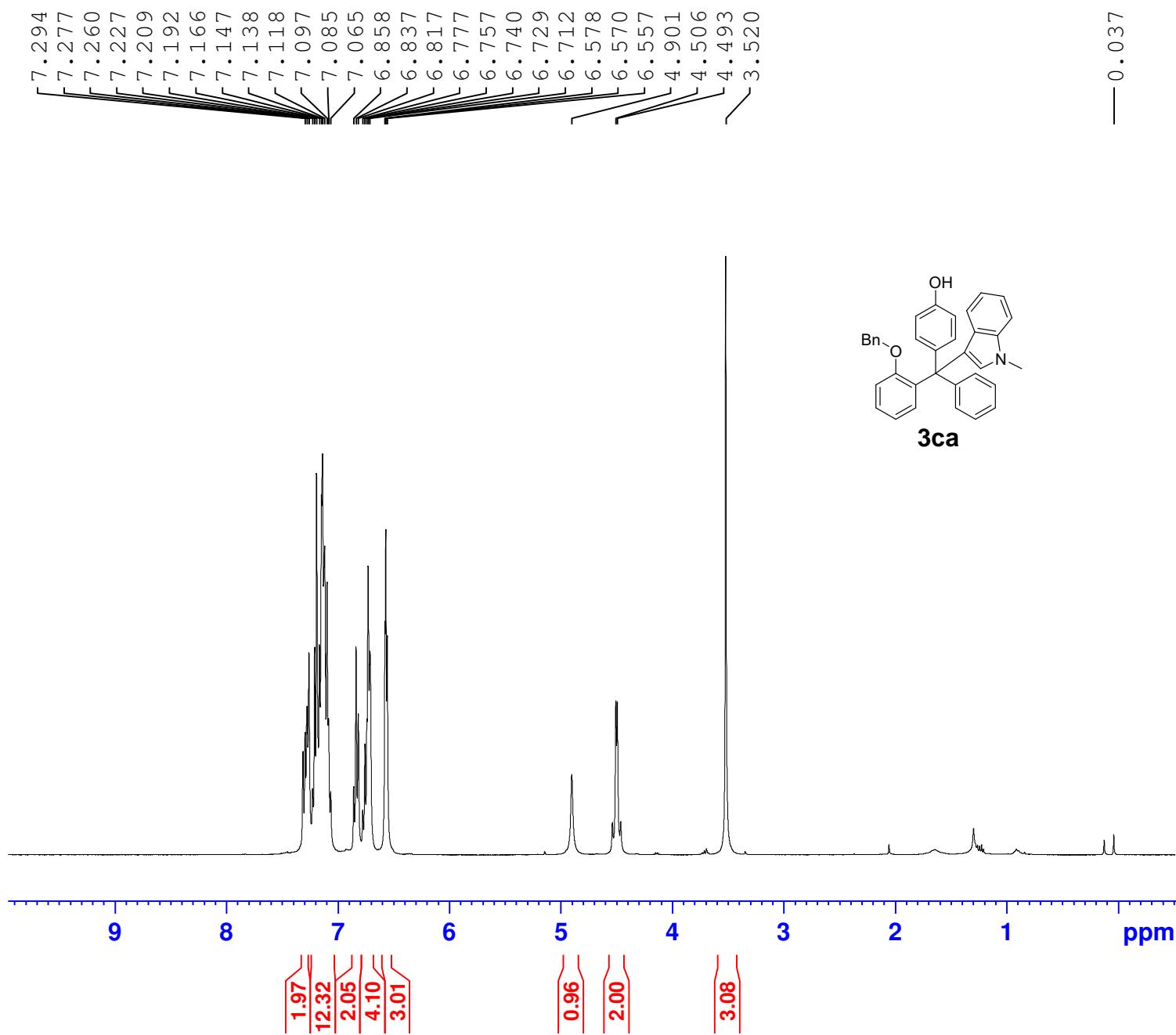
F2 - Acquisition Parameters  
 Date\_ 20211010  
 Time 11.17  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 600  
 DS 4  
 SWH 18028.846 Hz  
 FIDRES 0.275098 Hz  
 AQ 1.8175317 sec  
 RG 203  
 DW 27.733 usec  
 DE 6.50 usec  
 TE -59.1 K  
 D1 2.00000000 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 75.4677539 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

3ca



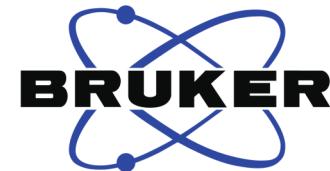
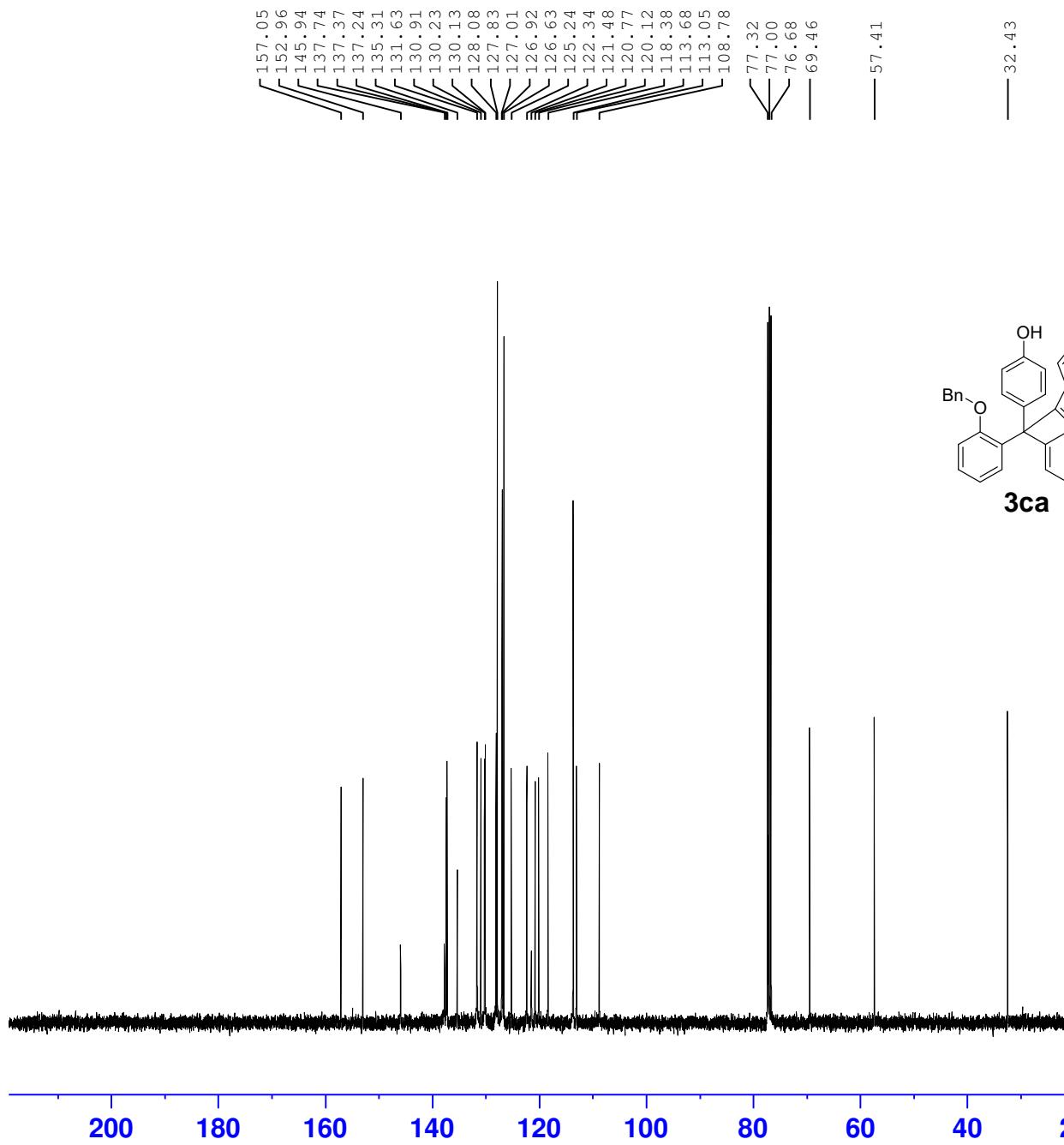
Current Data Parameters  
NAME 211214-400  
EXPNO 230  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211214  
Time 19.41  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 8  
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 292.4 K  
D1 1.0000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 14.40 usec  
PLW1 14.00000000 W  
SFO1 400.1924713 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1900442 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

3ca



Current Data Parameters  
 NAME 3ba-ZY-4-11B  
 EXPNO 234  
 PROCNO 1

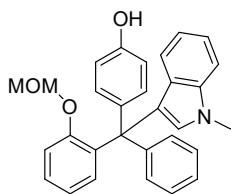
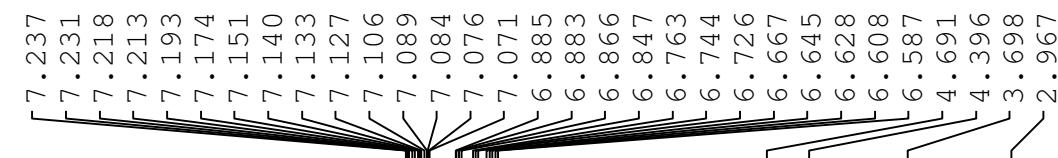
F2 - Acquisition Parameters  
 Date\_ 20211214  
 Time 20.09  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 112  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 193.13  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 293.2 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 ======  
 NUC1 13C  
 P1 9.90 usec  
 PLW1 53.00000000 W  
 SFO1 100.6379178 MHz

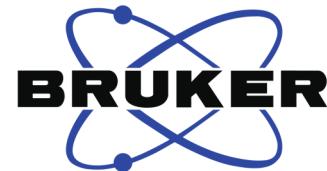
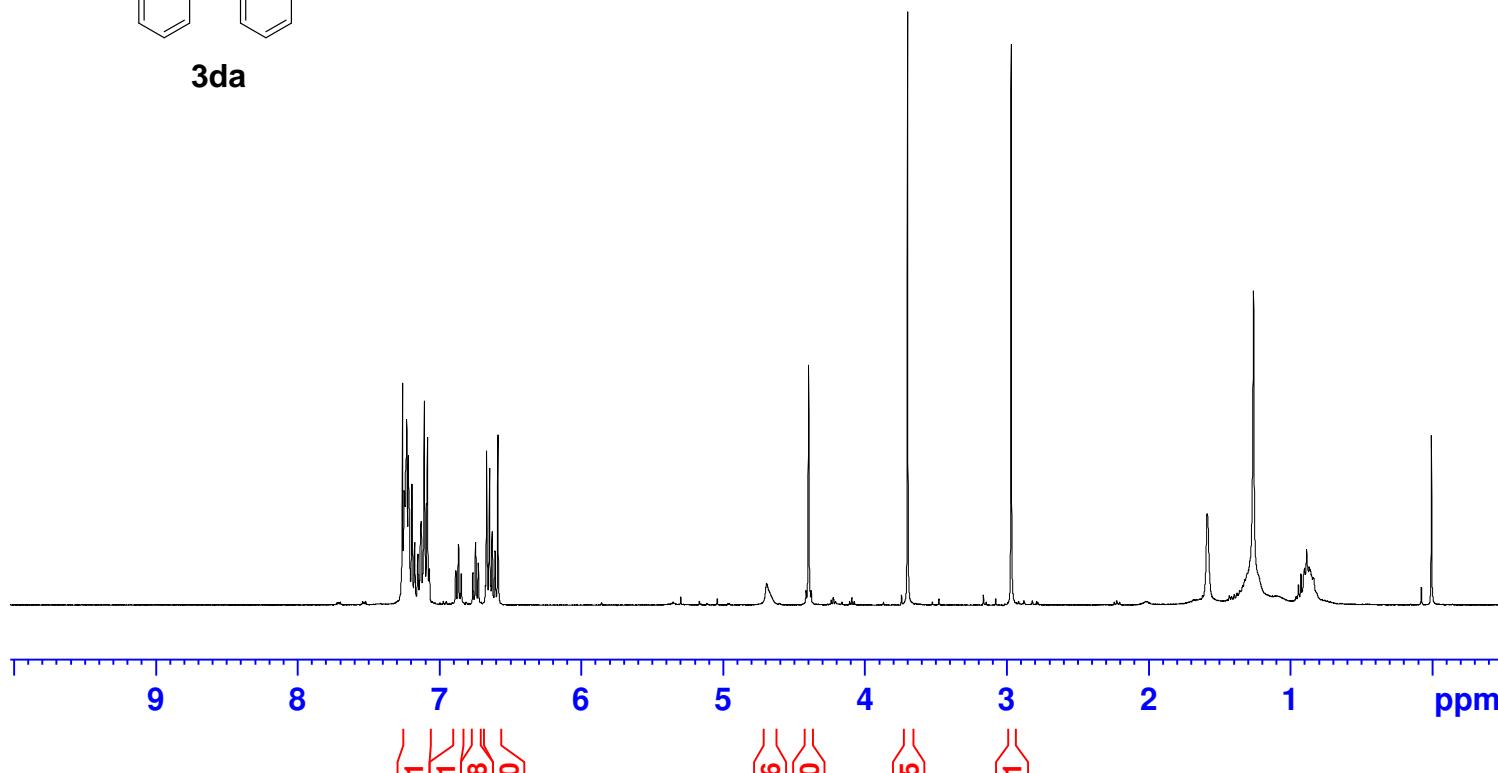
===== CHANNEL f2 ======  
 CPDPRG[2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PLW2 14.00000000 W  
 PLW12 0.35839999 W  
 PLW13 0.29030001 W  
 SFO2 400.1916008 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6278764 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

3da



**3da**



Current Data Parameters  
NAME 0812-400  
EXPNO 58  
PROCNO 1

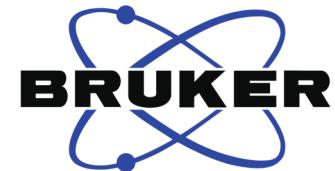
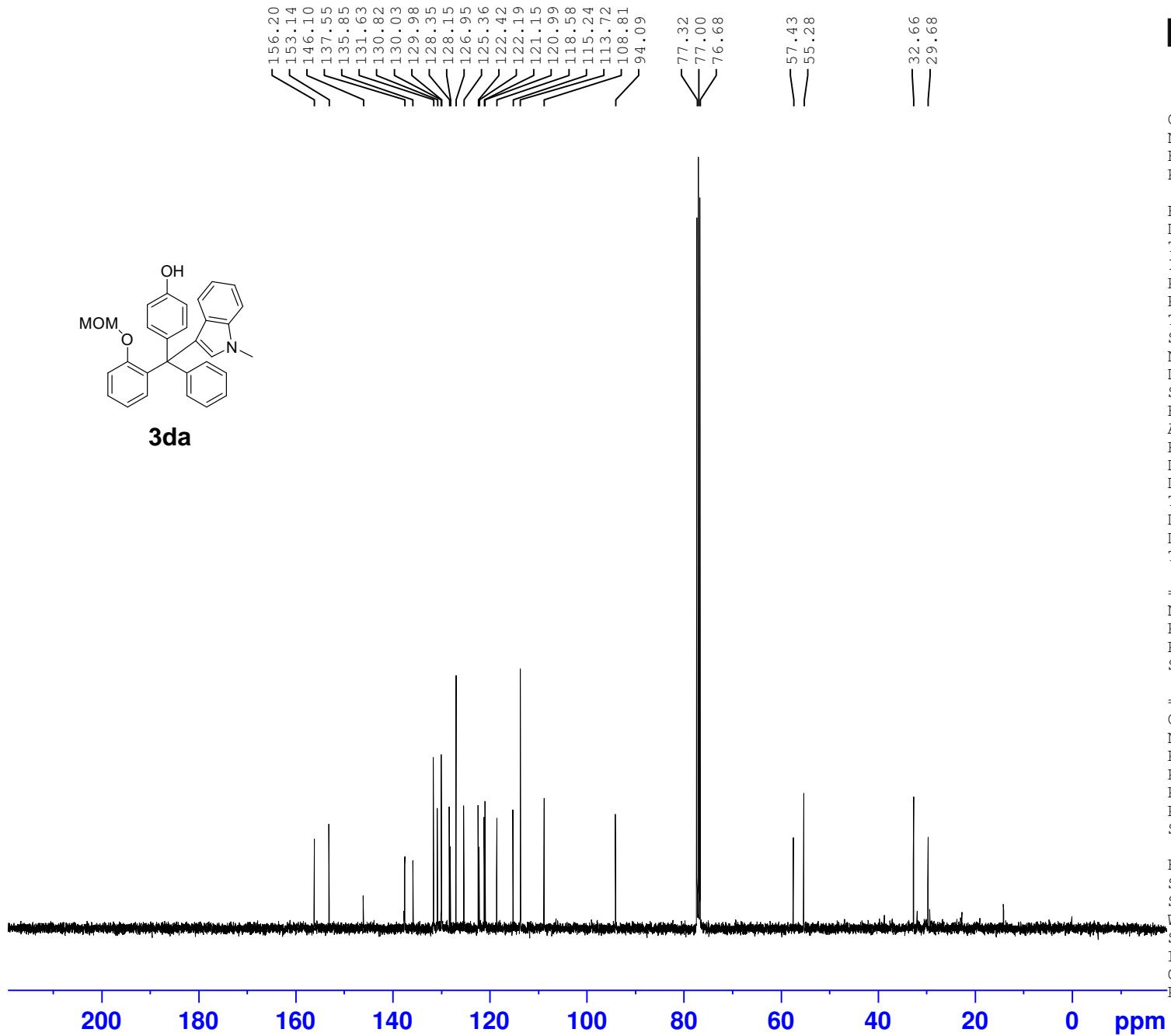
F2 - Acquisition Parameters  
Date\_ 20220812  
Time 22.18  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 8  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9845889 sec  
RG 193.13  
DW 60.800 usec  
DE 6.50 usec  
TE 294.6 K  
D1 1.00000000 sec  
TD0 1

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

NUC1 1H  
P1 14.68 usec  
PLW1 14.00000000 W  
SFO1 400.1924713 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1900165 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

3da



Current Data Parameters  
NAME 3da-ZB-1-50  
EXPNO 1  
PROCNO 1

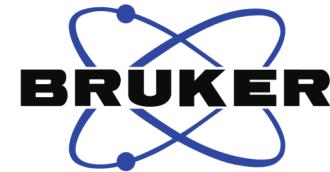
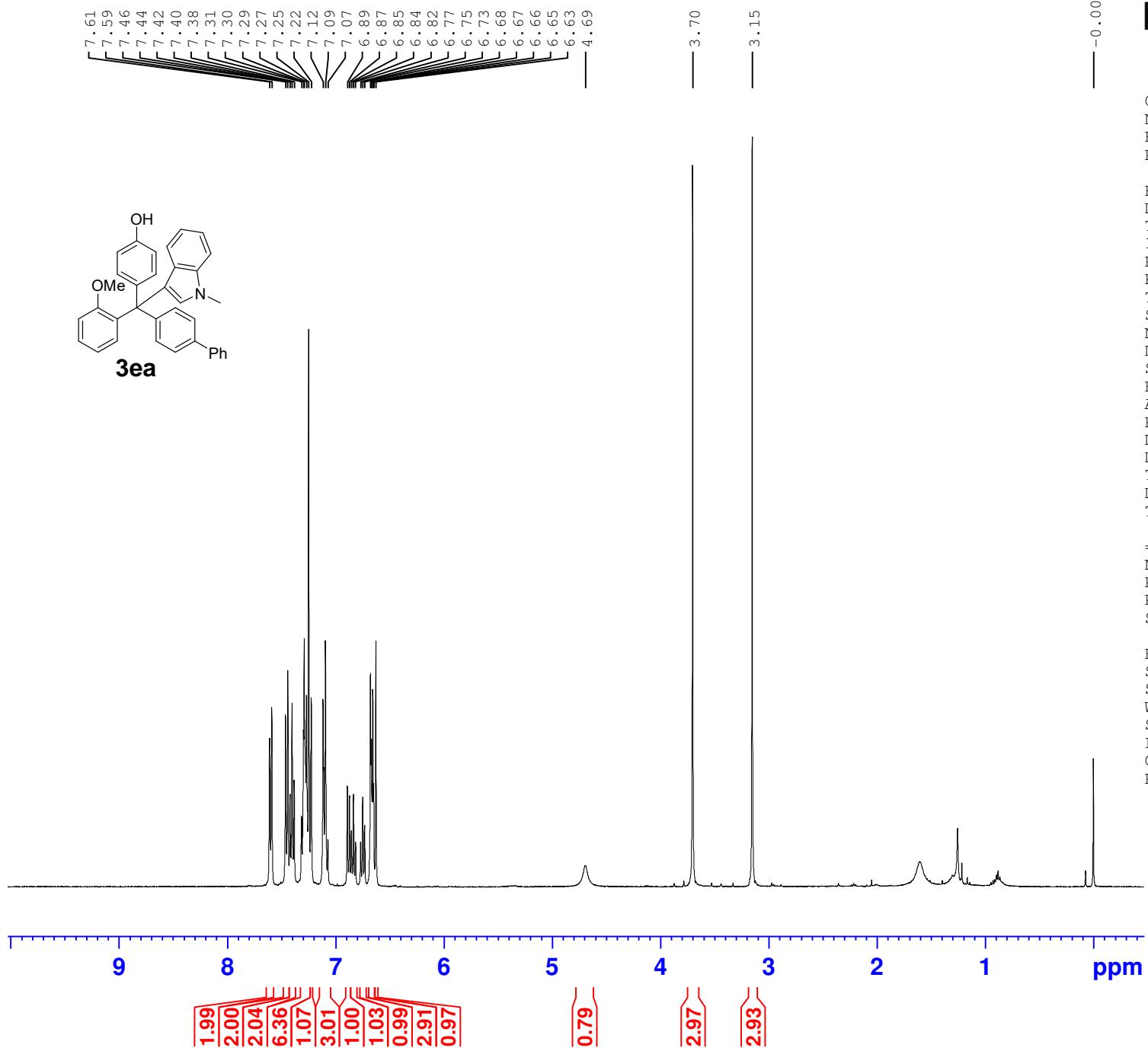
F2 - Acquisition Parameters  
Date\_ 20220808  
Time 22.41  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 400  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 193.13  
DW 20.800 usec  
DE 6.50 usec  
TE 295.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 <sup>13</sup>C  
P1 12.00 usec  
PLW1 53.00000000 W  
SFO1 100.6379178 MHz

===== CHANNEL f2 =====  
CPDPGRG[2 waltz16  
NUC2 <sup>1</sup>H  
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 100.6278628 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

3ea



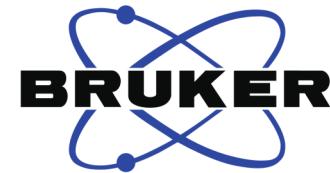
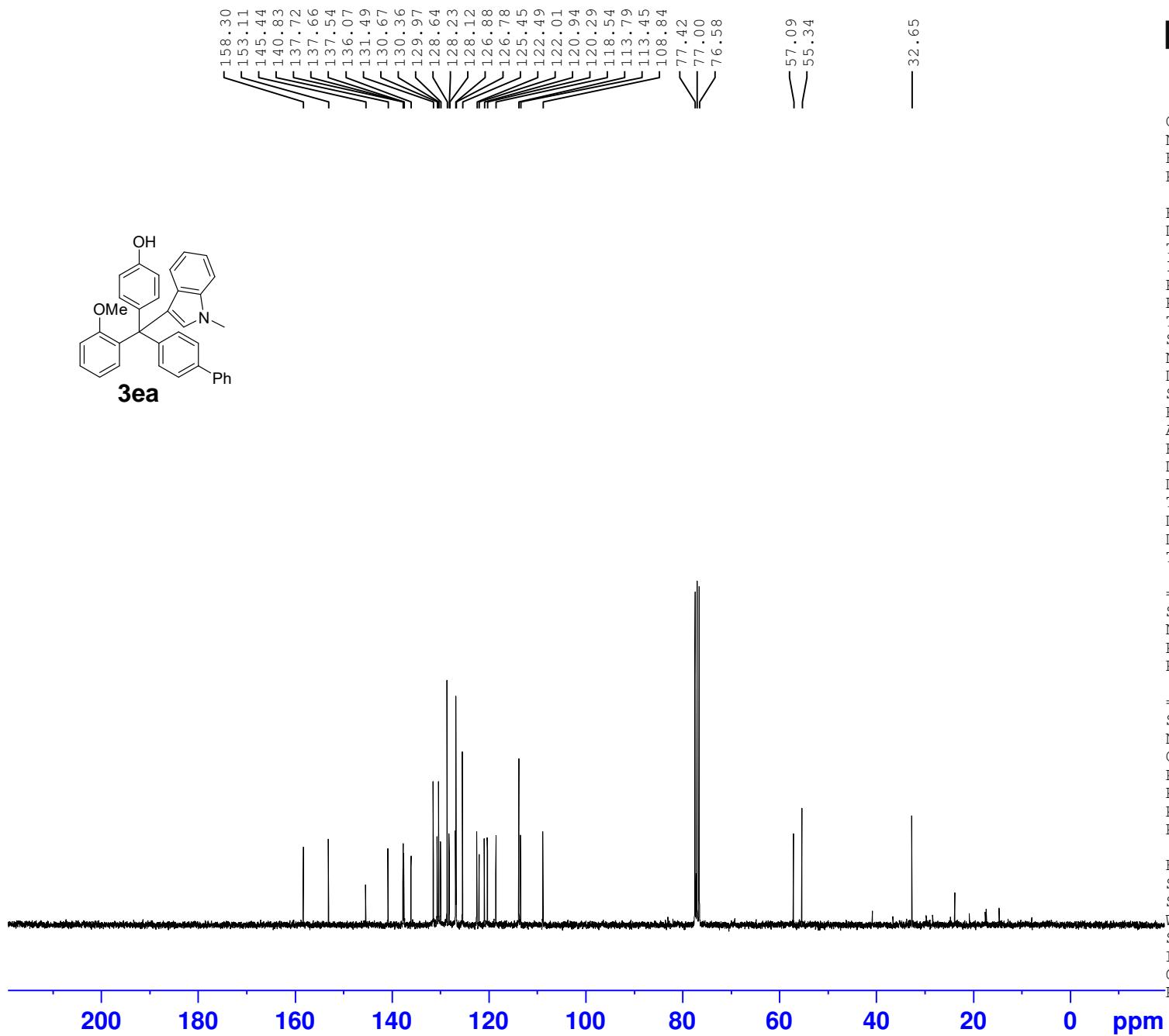
Current Data Parameters  
NAME ZY-4-75F-h-fr  
EXPNO 281  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211223  
Time 19.58  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 8  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9845889 sec  
RG 154.68  
DW 60.800 usec  
DE 6.50 usec  
TE 292.4 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 14.40 usec  
PLW1 14.00000000 W  
SFO1 400.1924713 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1900203 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

3ea



Current Data Parameters  
NAME 3ea-ZY-4-75F  
EXPNO 5617  
PROCNO 1

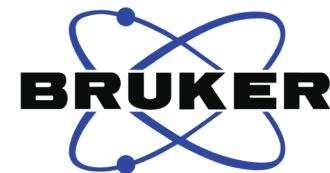
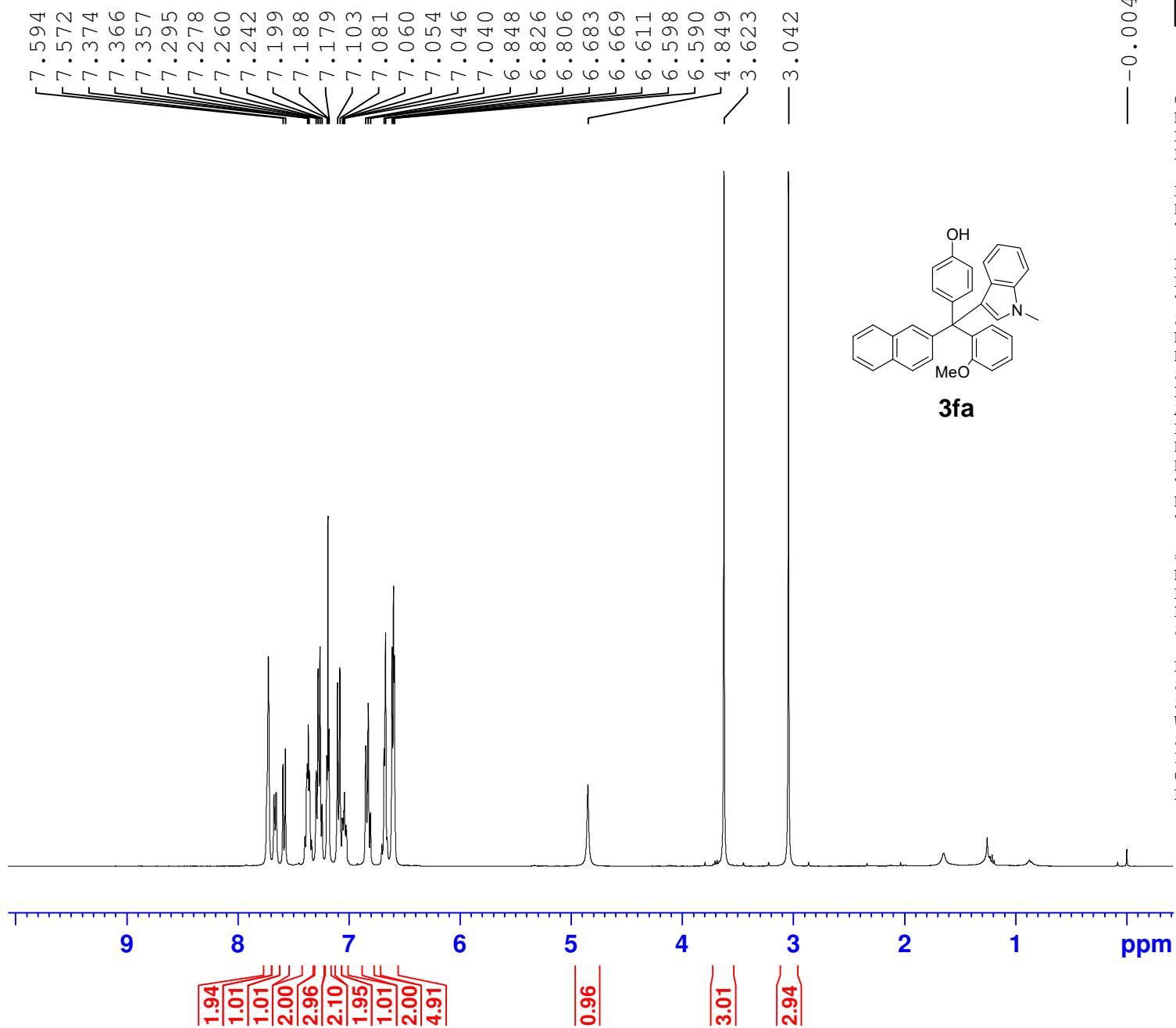
F2 - Acquisition Parameters  
Date\_ 20211118  
Time 10.01  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 500  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE -59.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 ======  
SFO1 75.4752949 MHz  
NUC1 <sup>13</sup>C  
P1 9.50 usec  
PLW1 34.20000076 W

===== CHANNEL f2 ======  
SFO2 300.1312005 MHz  
NUC2 <sup>1</sup>H  
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 75.4677568 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

3fa



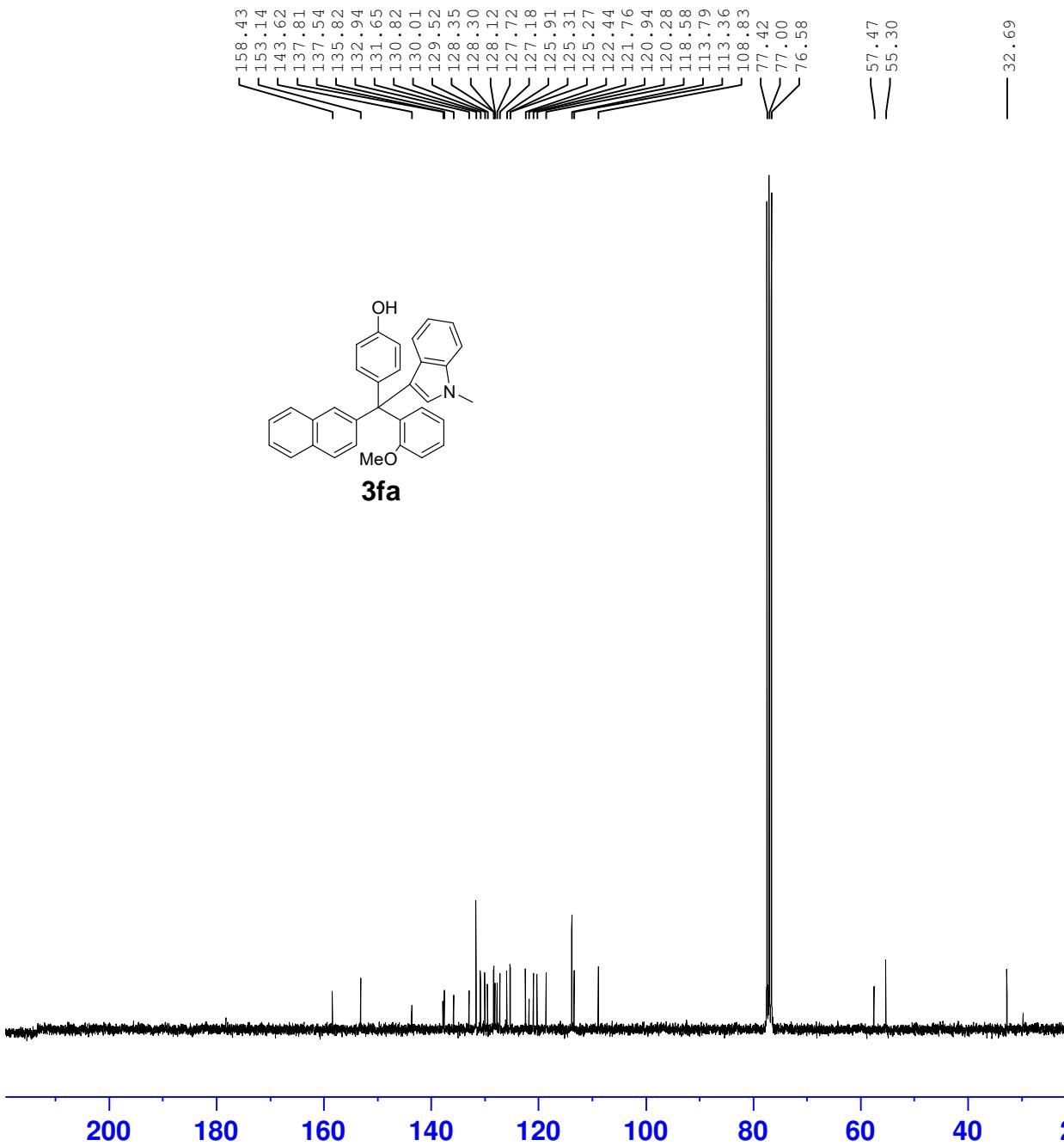
Current Data Parameters  
 NAME 211223-400  
 EXPNO 279  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20211223  
 Time 19.49  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 6  
 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 292.3 K  
 D1 1.0000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.40 usec  
 PLW1 14.00000000 W  
 SFO1 400.1924713 MHz

F2 - Processing parameters  
 SI 65536  
 SF 400.1900447 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

3fa



Current Data Parameters  
 NAME 3fa-ZY-4-11A  
 EXPNO 4252  
 PROCNO 1

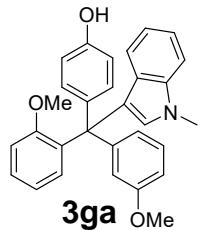
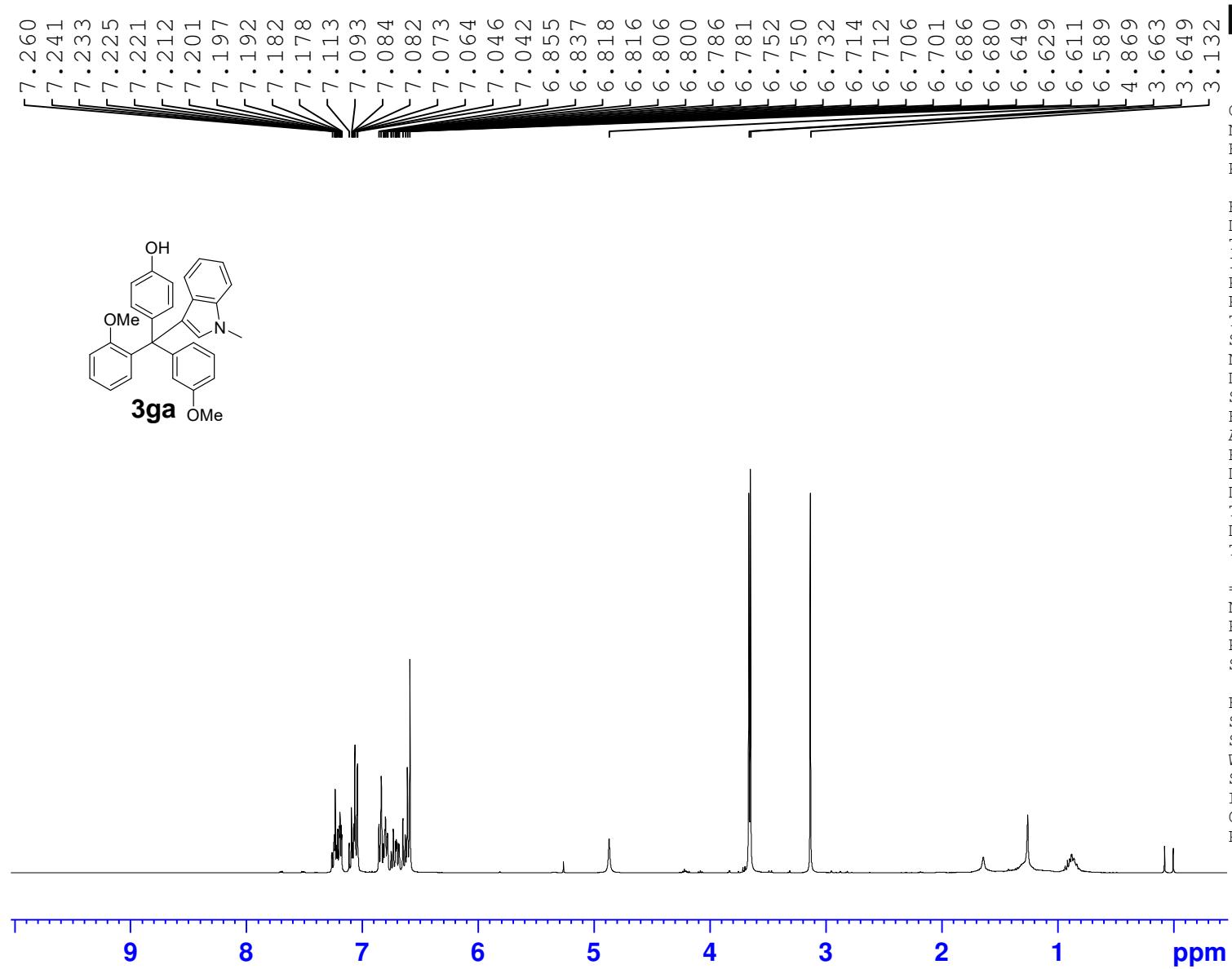
F2 - Acquisition Parameters  
 Date\_ 20210623  
 Time 11.59  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1024  
 DS 4  
 SWH 18028.846 Hz  
 FIDRES 0.275098 Hz  
 AQ 1.8175317 sec  
 RG 203  
 DW 27.733 usec  
 DE 6.50 usec  
 TE 296.2 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 ======  
 SFO1 75.4752949 MHz  
 NUC1 <sup>13</sup>C  
 P1 9.50 usec  
 PLW1 34.20000076 W

===== CHANNEL f2 ======  
 SFO2 300.1312005 MHz  
 NUC2 <sup>1</sup>H  
 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 75.4677518 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

3ga



**BRUKER**

Current Data Parameters  
NAME 0812-400  
EXPNO 69  
PROCNO 1

```

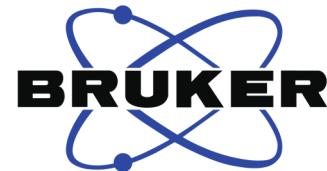
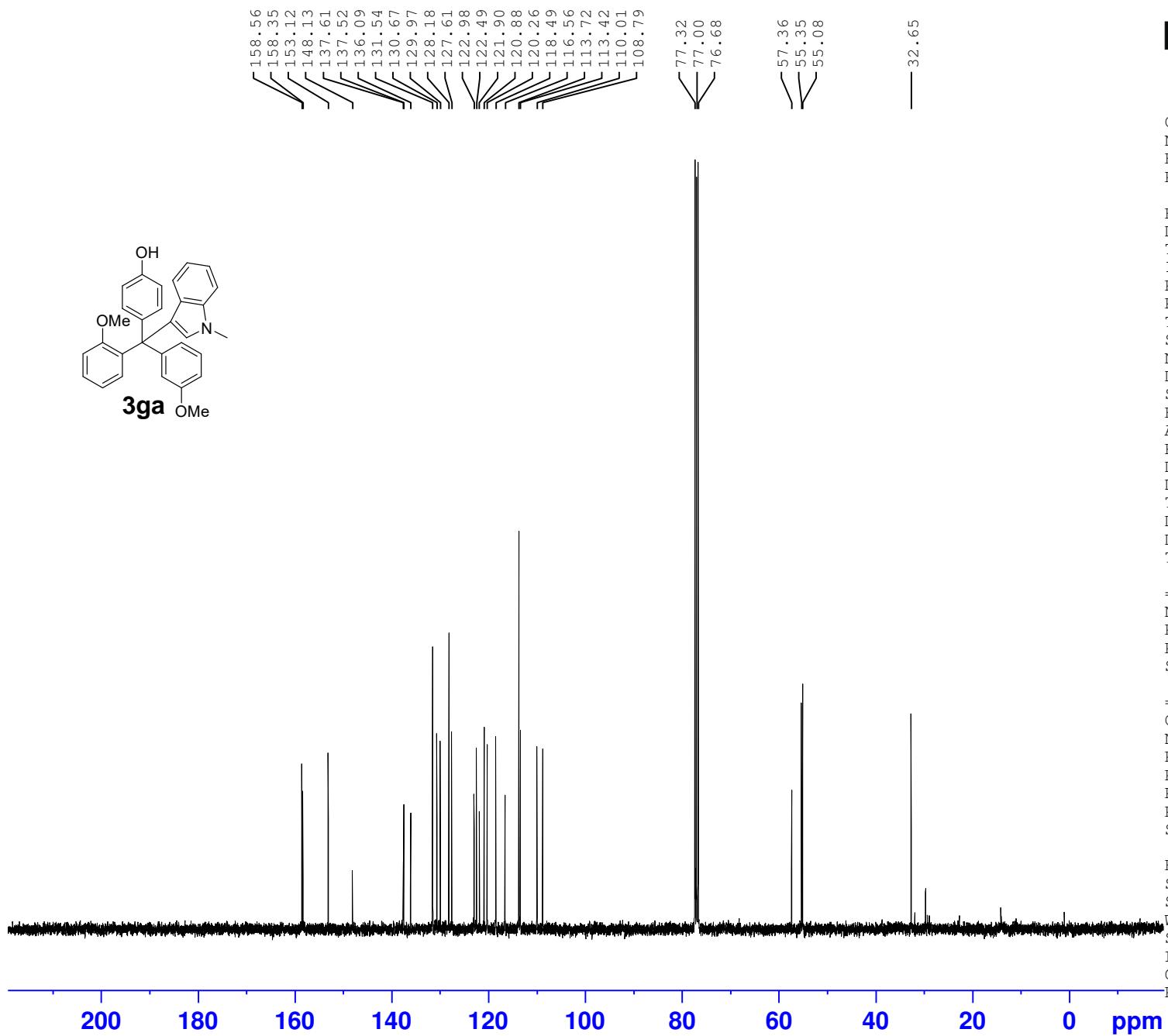
F2 - Acquisition Parameters
Date_           20220812
Time            23.29
INSTRUM         spect
PROBHD         5 mm PABBO BB-
PULPROG        zg30
TD              65536
SOLVENT         CDC13
NS              8
DS              2
SWH             8223.685 Hz
FIDRES         0.125483 Hz
AQ              3.9845889 sec
RG              90.23
DW              60.800 used
DE              6.50 usec
TE              294.7 K
D1              1.00000000 sec
TD0             1

```

```
===== CHANNEL f1 ======  
NUC1          1H  
P1           14.68  usec  
PLW1        14.0000000 W  
SFO1        400.1924713 MHz
```

F2 - Processing parameters  
SI 65536  
SF 400.1900270 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

3ga



Current Data Parameters  
 NAME 3ga-ZB-1-77  
 EXPNO 1  
 PROCNO 1

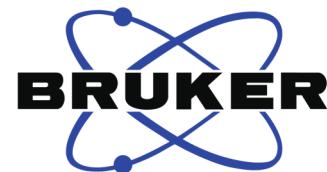
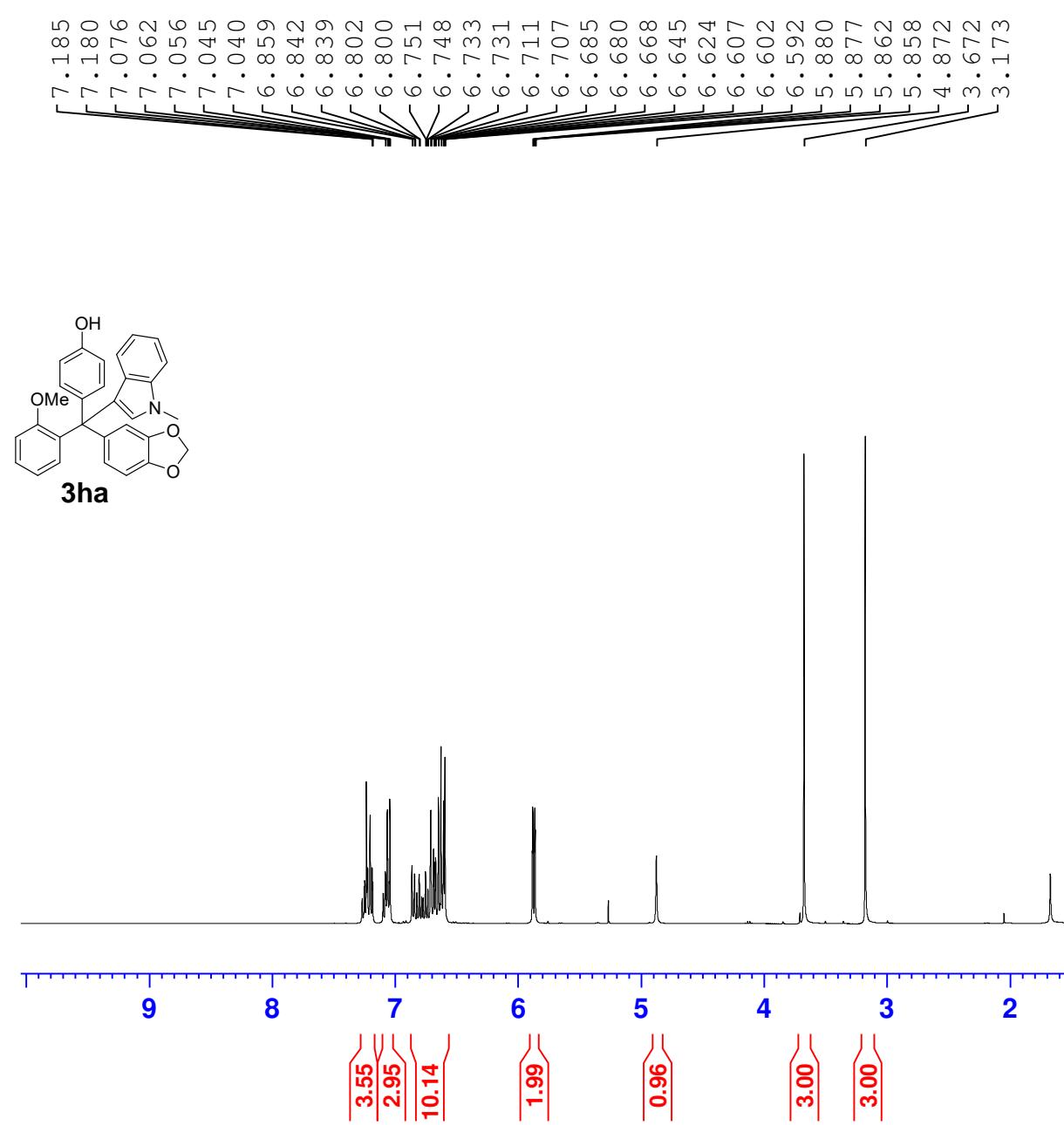
F2 - Acquisition Parameters  
 Date\_ 20220812  
 Time 23.47  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 300  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 193.13  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.4 K  
 D1 2.00000000 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 100.6278644 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

3ha



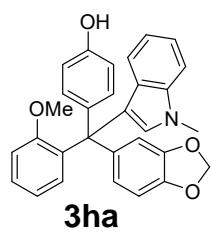
Current Data Parameters  
NAME 0812-400  
EXPNO 61  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220812  
Time 22.31  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 8  
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 294.6 K  
D1 1.0000000 sec  
TD0 1

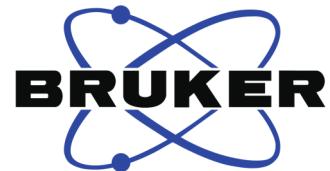
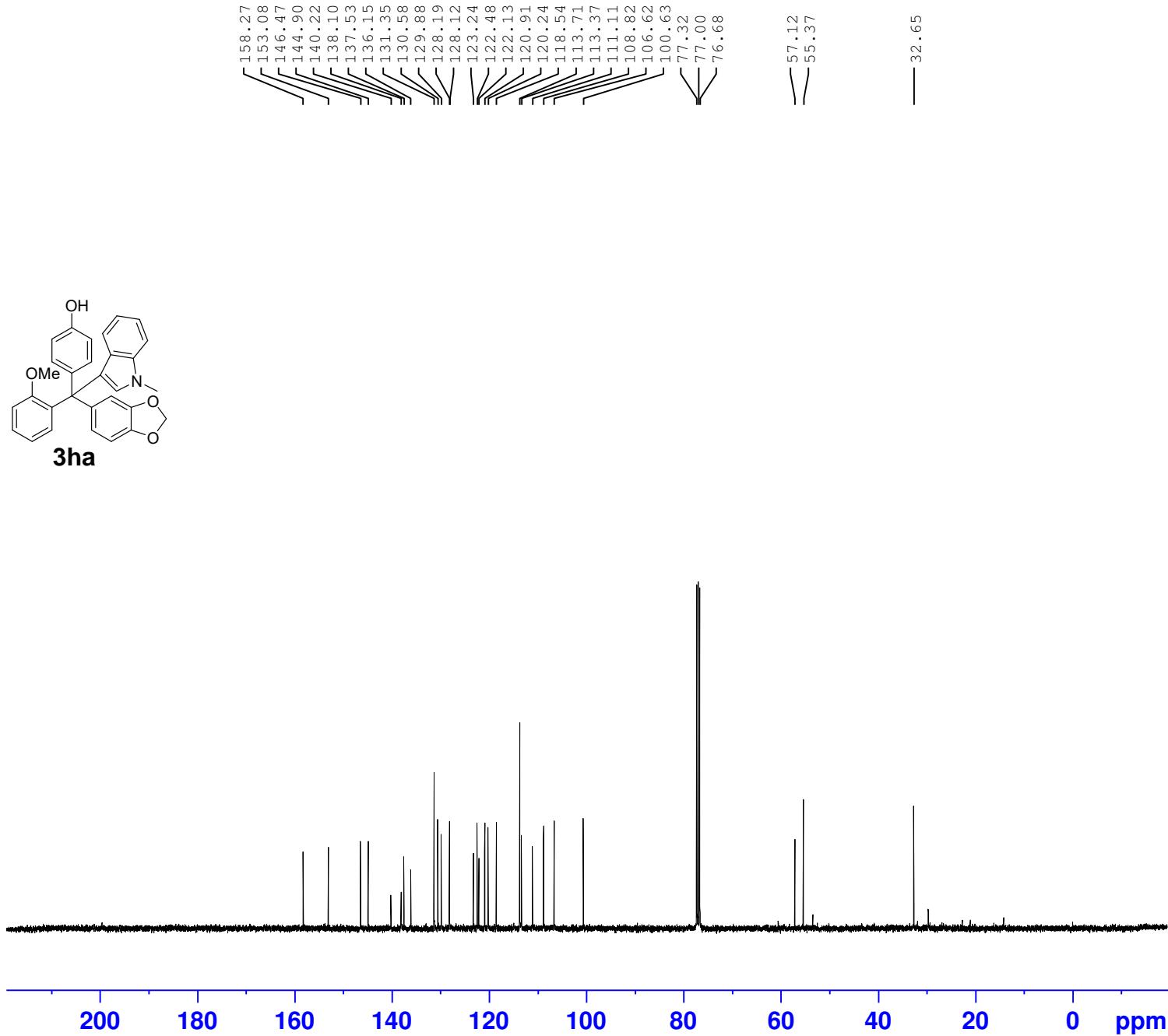
===== CHANNEL f1 ======  
NUC1 1H  
P1 14.68 usec  
PLW1 14.00000000 W  
SFO1 400.1924713 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1900277 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

3ha



**3ha**



Current Data Parameters  
NAME 0811-400-2  
EXPNO 35  
PROCNO 1

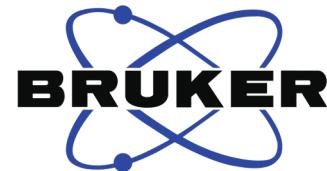
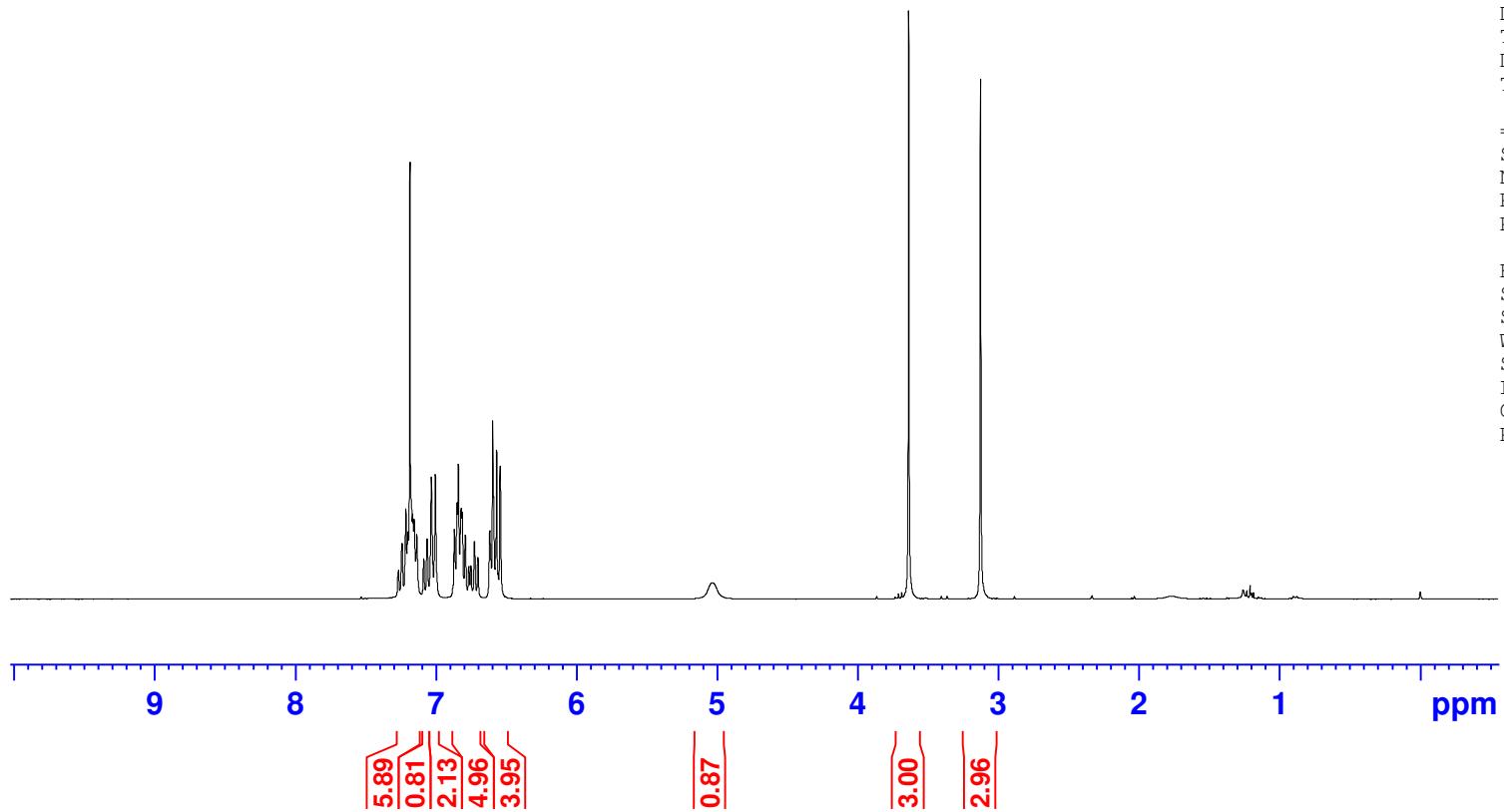
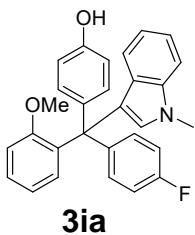
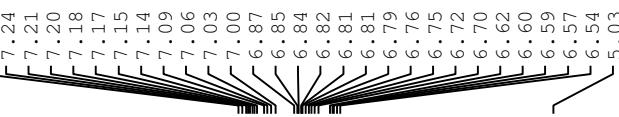
F2 - Acquisition Parameters  
Date\_ 20220812  
Time 0.58  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 300  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 193.13  
DW 20.800 usec  
DE 6.50 usec  
TE 295.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 ======  
NUC1 <sup>13</sup>C  
P1 12.00 usec  
PLW1 53.00000000 W  
SFO1 100.6379178 MHz

===== CHANNEL f2 ======  
CPDPGRG[2 waltz16  
NUC2 <sup>1</sup>H  
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 100.6278652 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

3ia



Current Data Parameters  
NAME ZY-4-75B-h-fr  
EXPNO 5623  
PROCNO 1

```

F2 - Acquisition Parameters
Date_           20211117
Time            12.31
INSTRUM         spect
PROBHD         5 mm PABBO BB-
PULPROG        zg30
TD              65536
SOLVENT         CDC13
NS              16
DS              2
SWH             6009.615 Hz
FIDRES         0.091699 Hz
AQ              5.4525952 sec
RG              57
DW              83.200 used
DE              6.50  usec
TE              -59.1 K
D1              1.00000000 sec
TD0             1

```

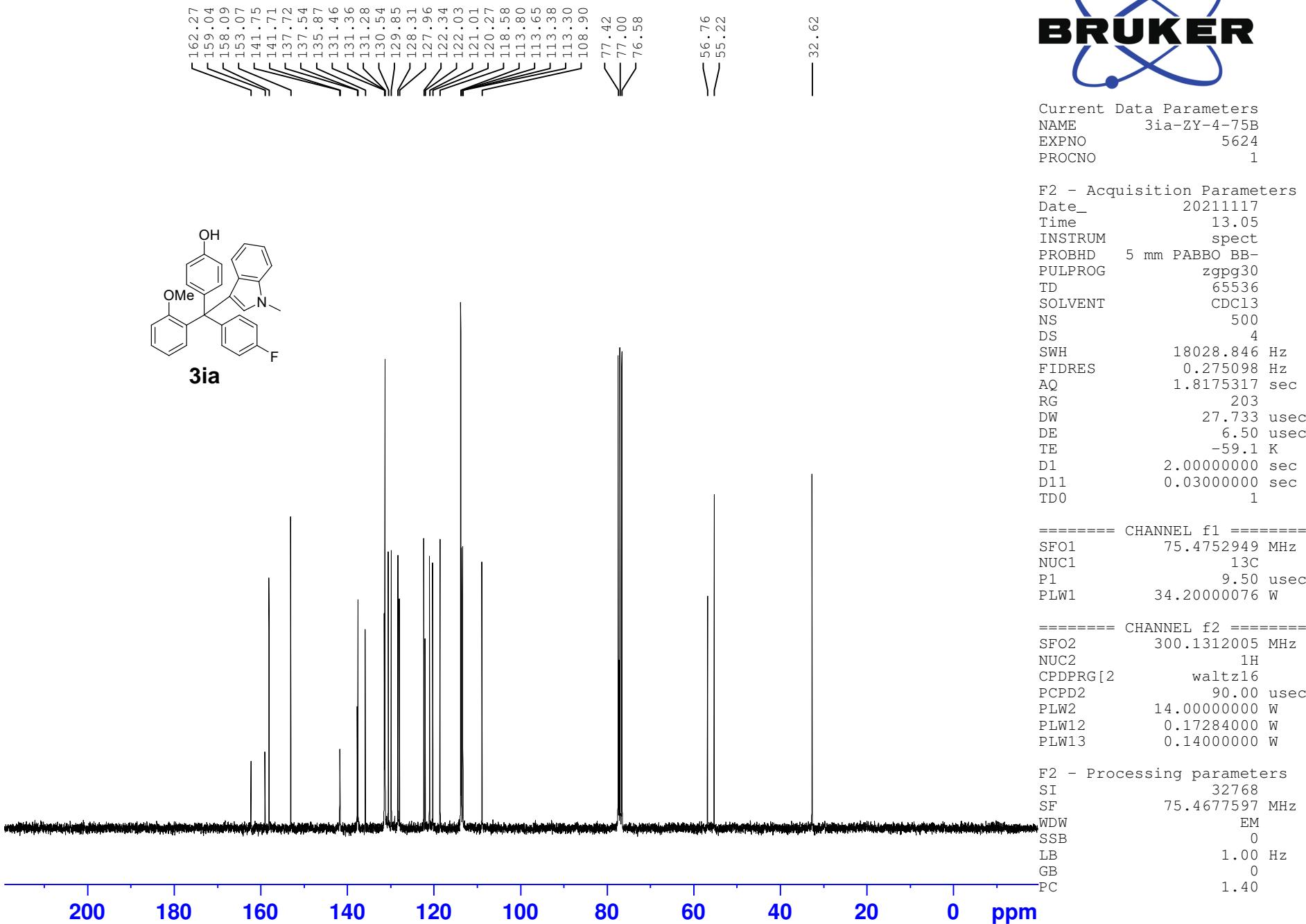
```
===== CHANNEL f1 ======  
SFO1          300.1318534 MHz  
NUC1           1H  
P1             10.00 usec  
PLW1          14.00000000 W
```

```

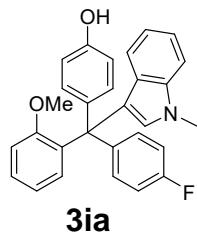
F2 - Processing parameters
SI           65536
SF          300.1300298 MHz
WDW          EM
SSB           0
LB           0.30 Hz
GB           0
PC           1.00

```

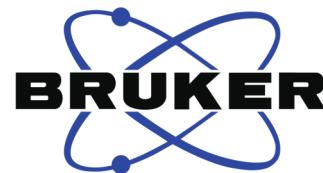
3ia



3ia



— -118.357



Current Data Parameters  
 NAME 0927sjw  
 EXPNO 5451  
 PROCNO 1

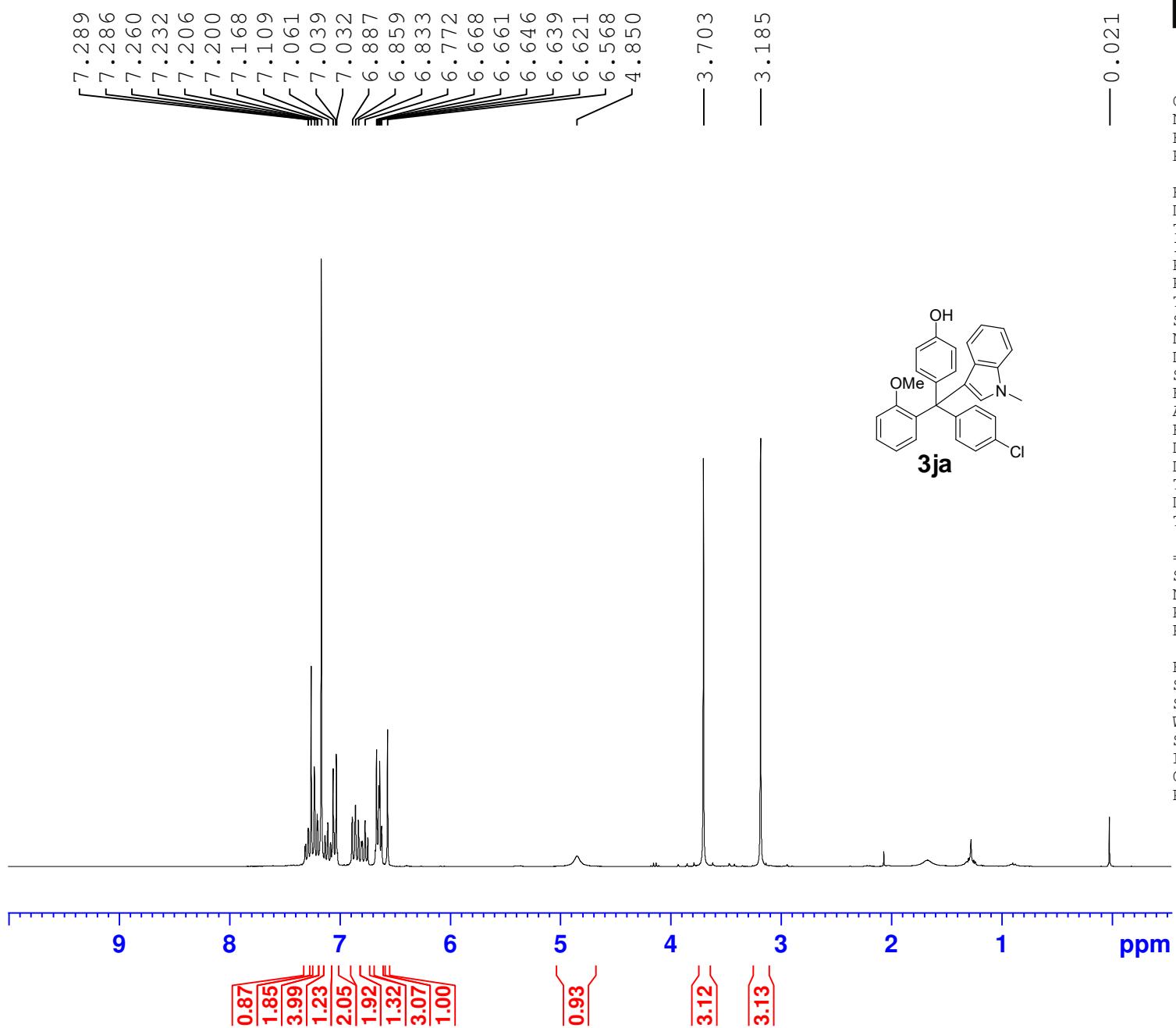
F2 - Acquisition Parameters  
 Date\_ 20210927  
 Time 11.06  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgfhigqn.2  
 TD 131072  
 SOLVENT CDCl3  
 NS 16  
 DS 4  
 SWH 66964.289 Hz  
 FIDRES 0.510897 Hz  
 AQ 0.9786710 sec  
 RG 203  
 DW 7.467 usec  
 DE 6.50 usec  
 TE -59.1 K  
 D1 1.00000000 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

3ja



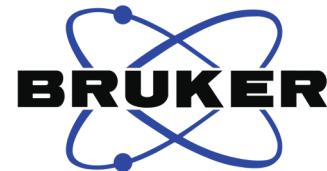
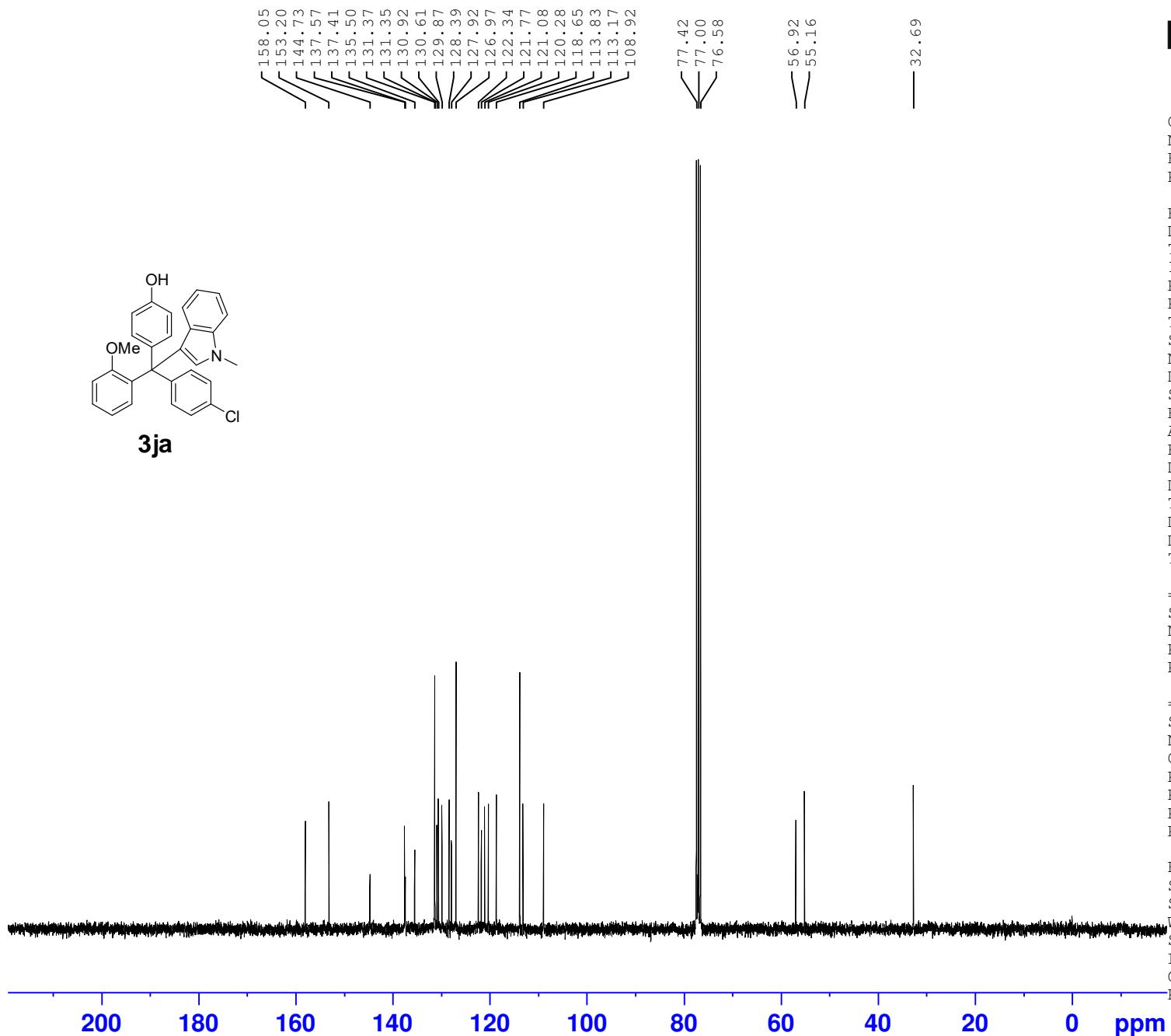
Current Data Parameters  
 NAME 20211030  
 EXPNO 5493  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210930  
 Time 10.19  
 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 -59.1 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 300.1300072 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

3ja



Current Data Parameters  
 NAME 3ja-ZY-4-75C  
 EXPNO 5494  
 PROCNO 1

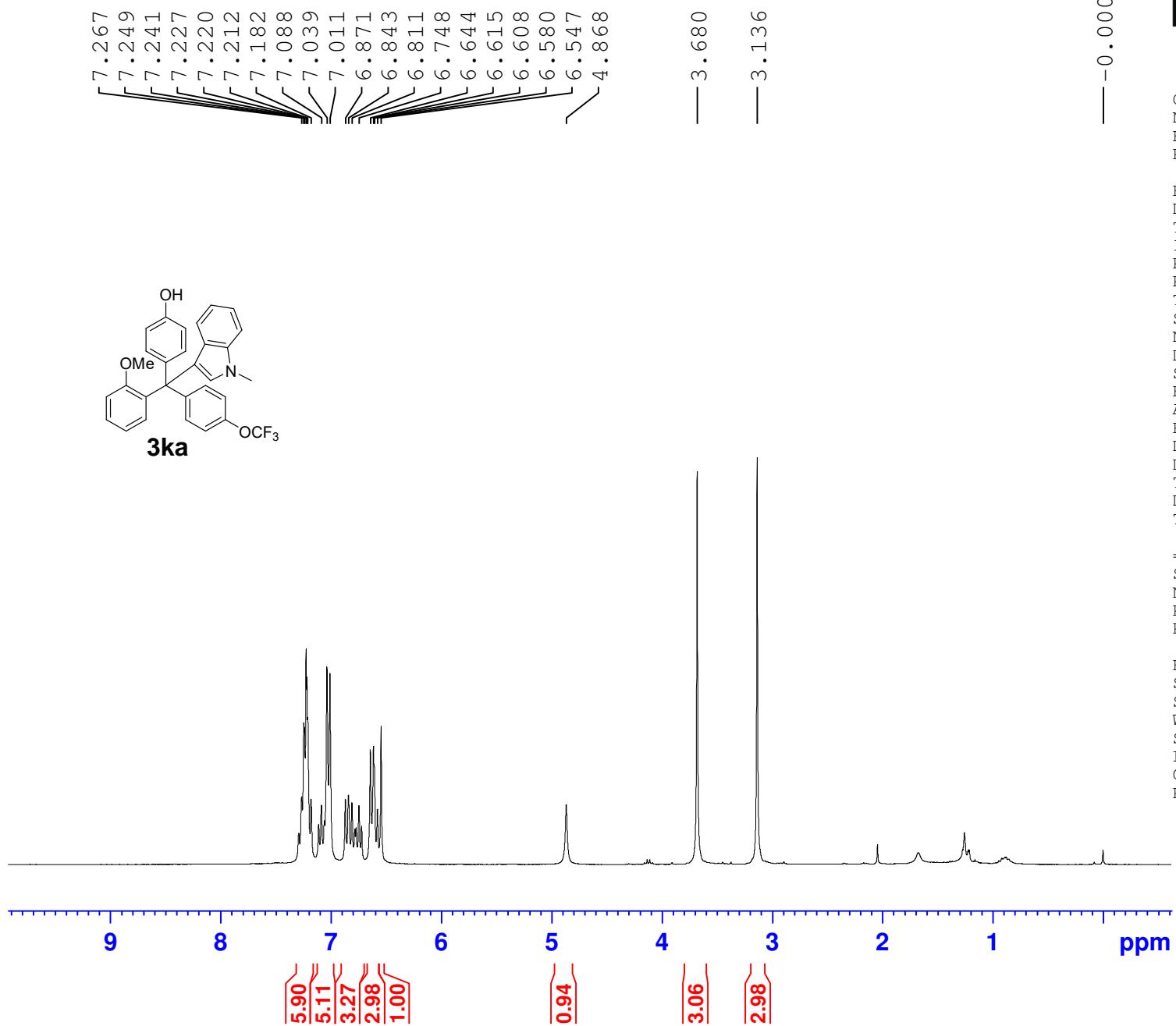
F2 - Acquisition Parameters  
 Date\_ 20210930  
 Time 10.52  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 500  
 DS 4  
 SWH 18028.846 Hz  
 FIDRES 0.275098 Hz  
 AQ 1.8175317 sec  
 RG 203  
 DW 27.733 usec  
 DE 6.50 usec  
 TE -59.1 K  
 D1 2.00000000 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 75.4677536 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

3ka



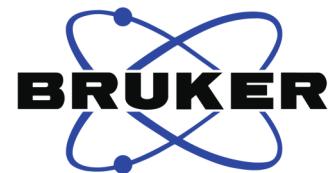
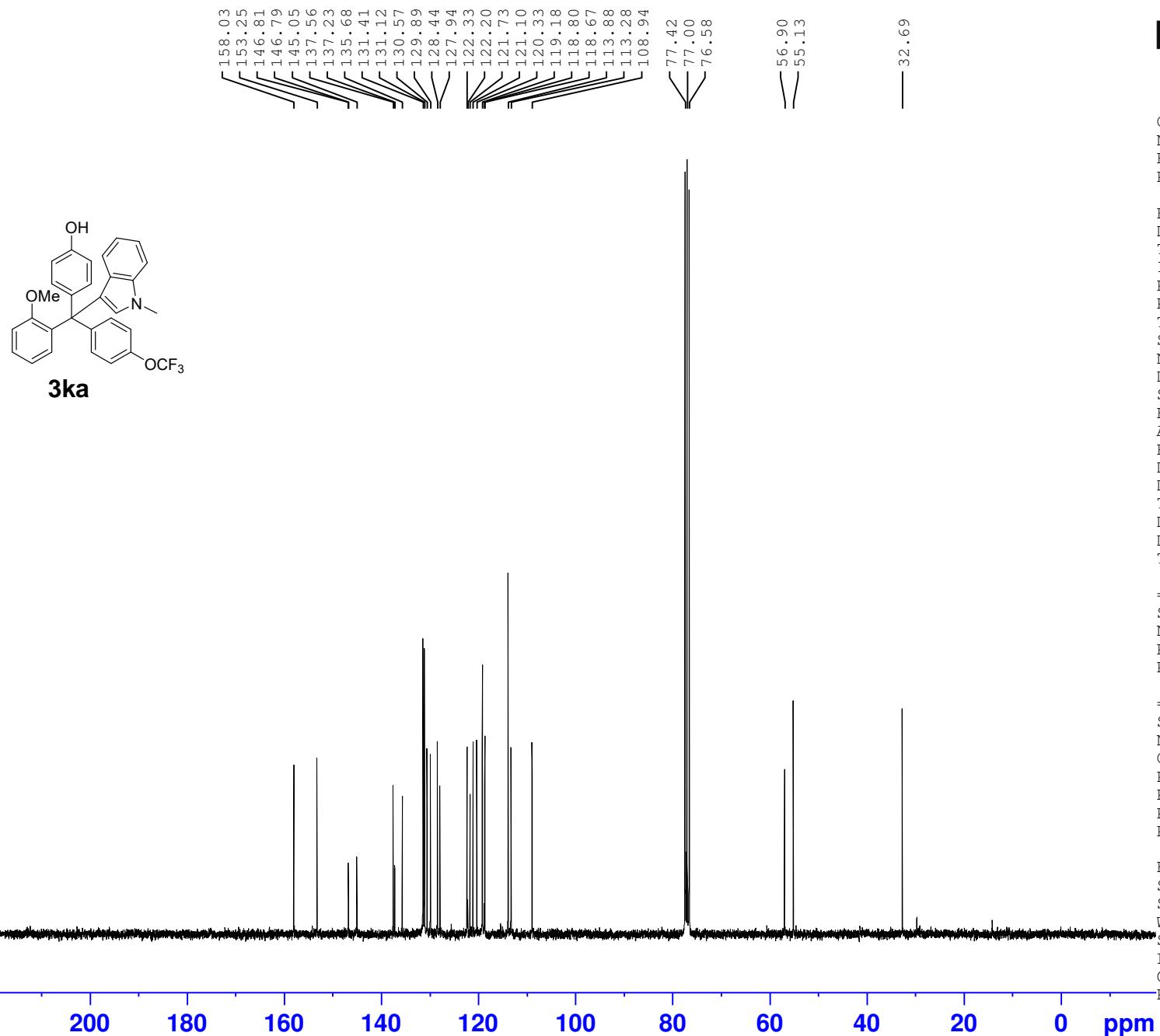
Current Data Parameters  
NAME 211223sjw  
EXPNO 5730  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211223  
Time 9.07  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
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 -59.1 K  
D1 1.0000000 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 300.1300169 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

3ka



Current Data Parameters  
NAME 3ka-ZY-4-75E  
EXPNO 5739  
PROCNO 1

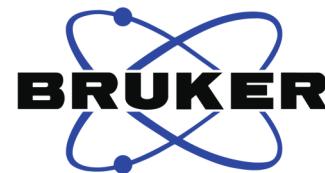
F2 - Acquisition Parameters  
Date\_ 20211224  
Time 10.31  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 1024  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE -59.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 ======  
SFO1 75.4752949 MHz  
NUC1 <sup>13</sup>C  
P1 9.50 usec  
PLW1 34.20000076 W

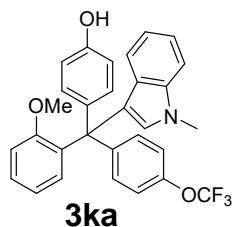
===== CHANNEL f2 ======  
SFO2 300.1312005 MHz  
NUC2 <sup>1</sup>H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W  
PLW13 0.14000000 W

F2 - Processing parameters  
SI 32768  
SF 75.4677548 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

3ka



-57.668



0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm

Current Data Parameters  
NAME 211124sjw (2)  
EXPNO 5628  
PROCNO 1

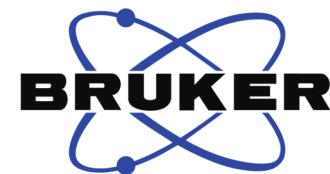
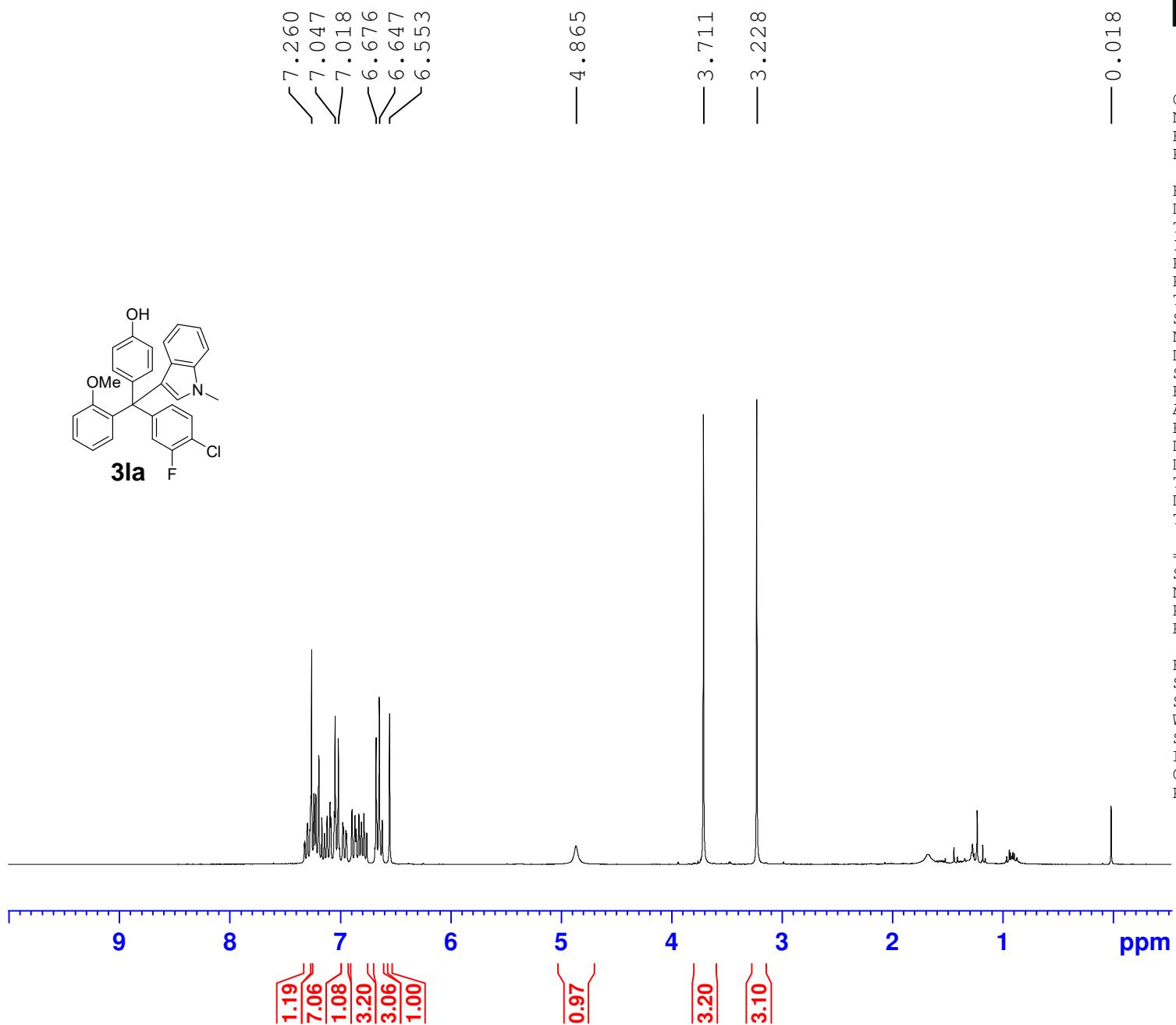
F2 - Acquisition Parameters  
Date\_ 20211124  
Time 9.09  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgfhigqn.2  
TD 131072  
SOLVENT CDCl3  
NS 16  
DS 4  
SWH 66964.289 Hz  
FIDRES 0.510897 Hz  
AQ 0.9786710 sec  
RG 203  
DW 7.467 usec  
DE 6.50 usec  
TE -59.1 K  
D1 1.00000000 sec  
D11 0.03000000 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  
CPDPGRG[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

3la



Current Data Parameters  
 NAME 211015sjw  
 EXPNO 5528  
 PROCNO 1

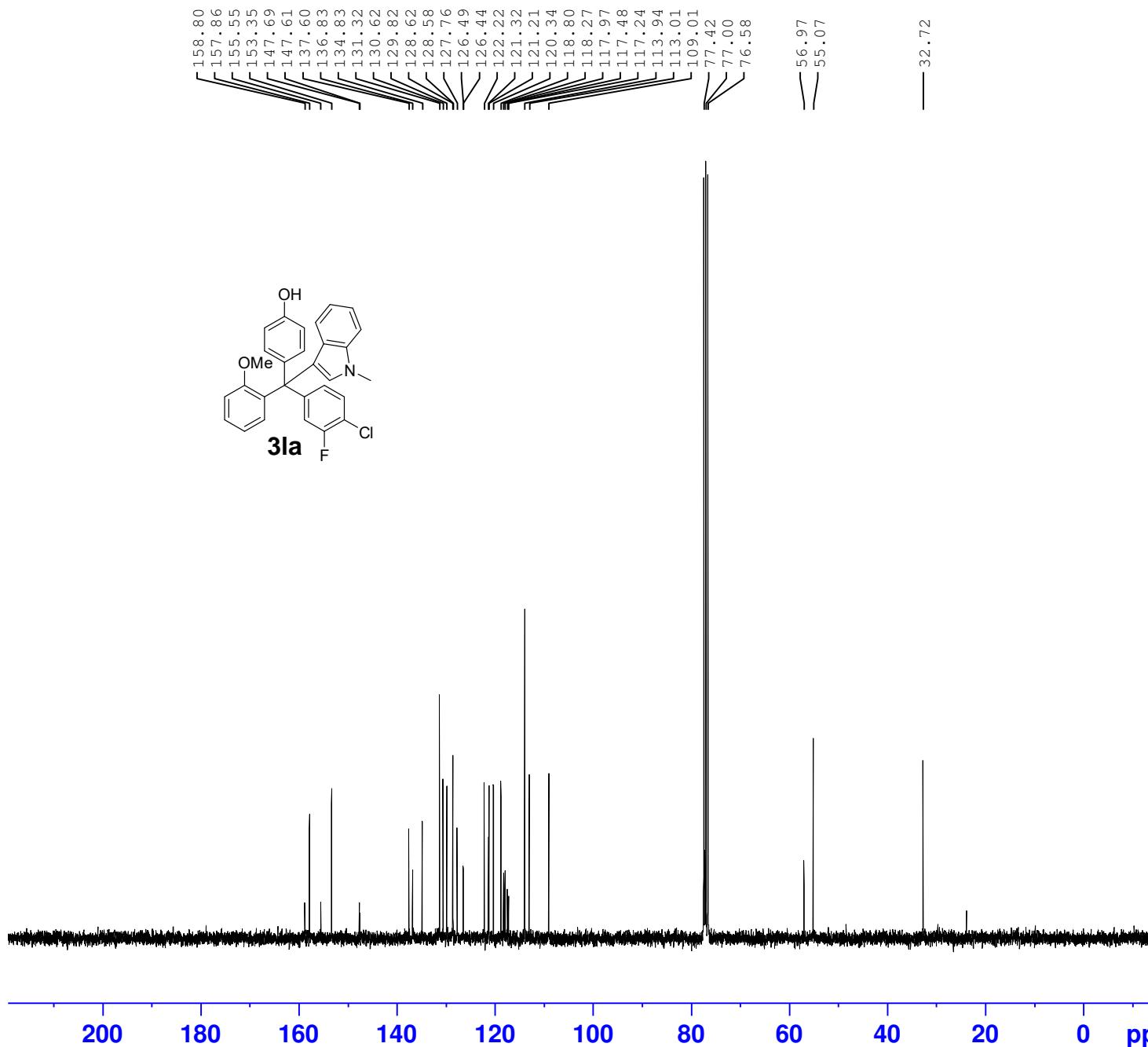
F2 - Acquisition Parameters  
 Date\_ 20211015  
 Time 10.02  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6009.615 Hz  
 FIDRES 0.091699 Hz  
 AQ 5.4525952 sec  
 RG 128  
 DW 83.200 usec  
 DE 6.50 usec  
 TE -59.1 K  
 D1 1.00000000 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 300.1300073 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

3la



Current Data Parameters  
 NAME 3la-ZY-4-93C  
 EXPNO 5537  
 PROCNO 1

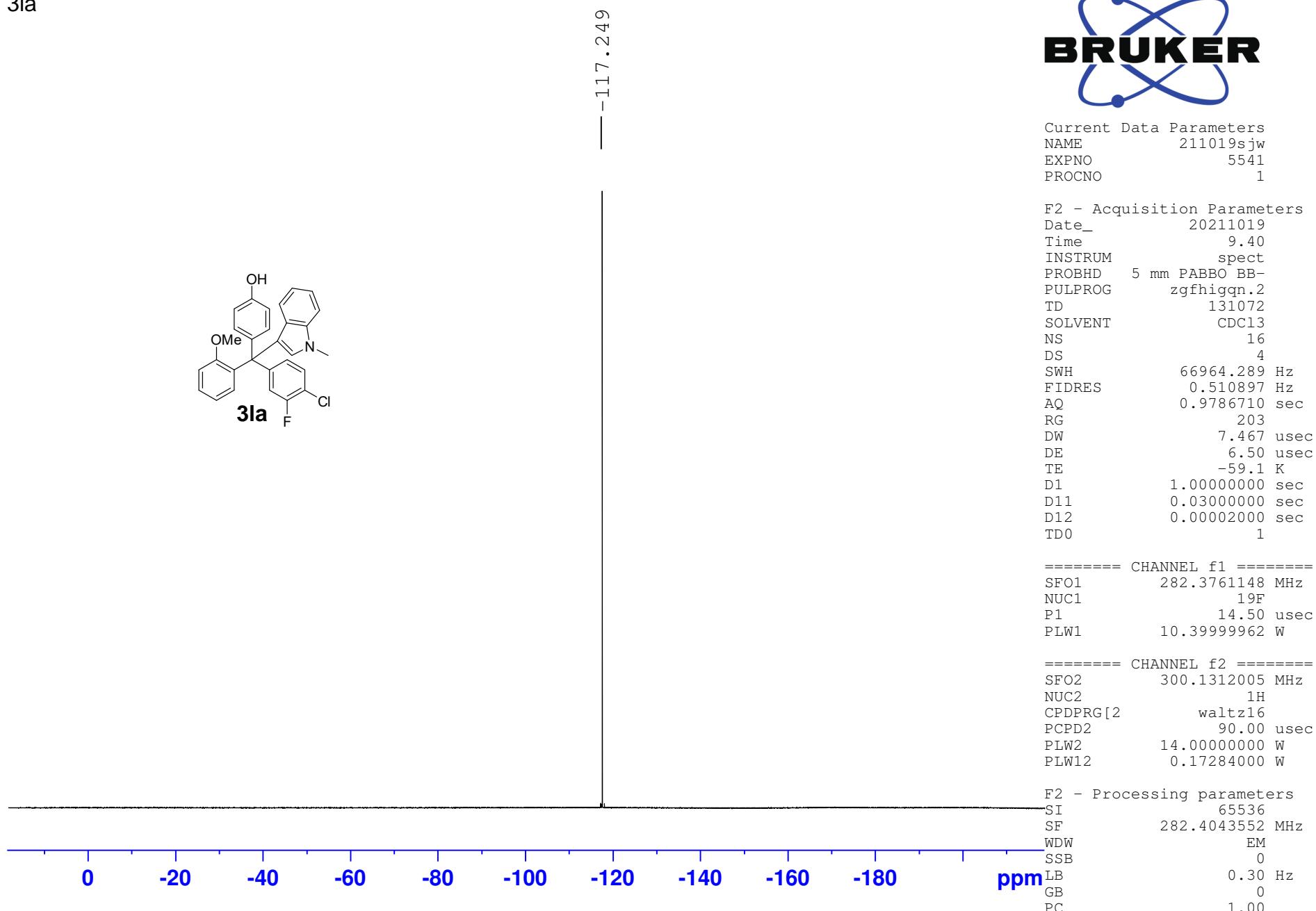
F2 - Acquisition Parameters  
 Date\_ 20211016  
 Time 13.05  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 500  
 DS 4  
 SWH 18028.846 Hz  
 FIDRES 0.275098 Hz  
 AQ 1.8175317 sec  
 RG 203  
 DW 27.733 usec  
 DE 6.50 usec  
 TE -59.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

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

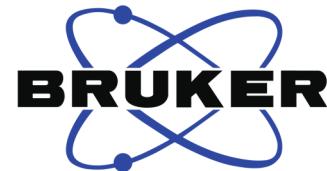
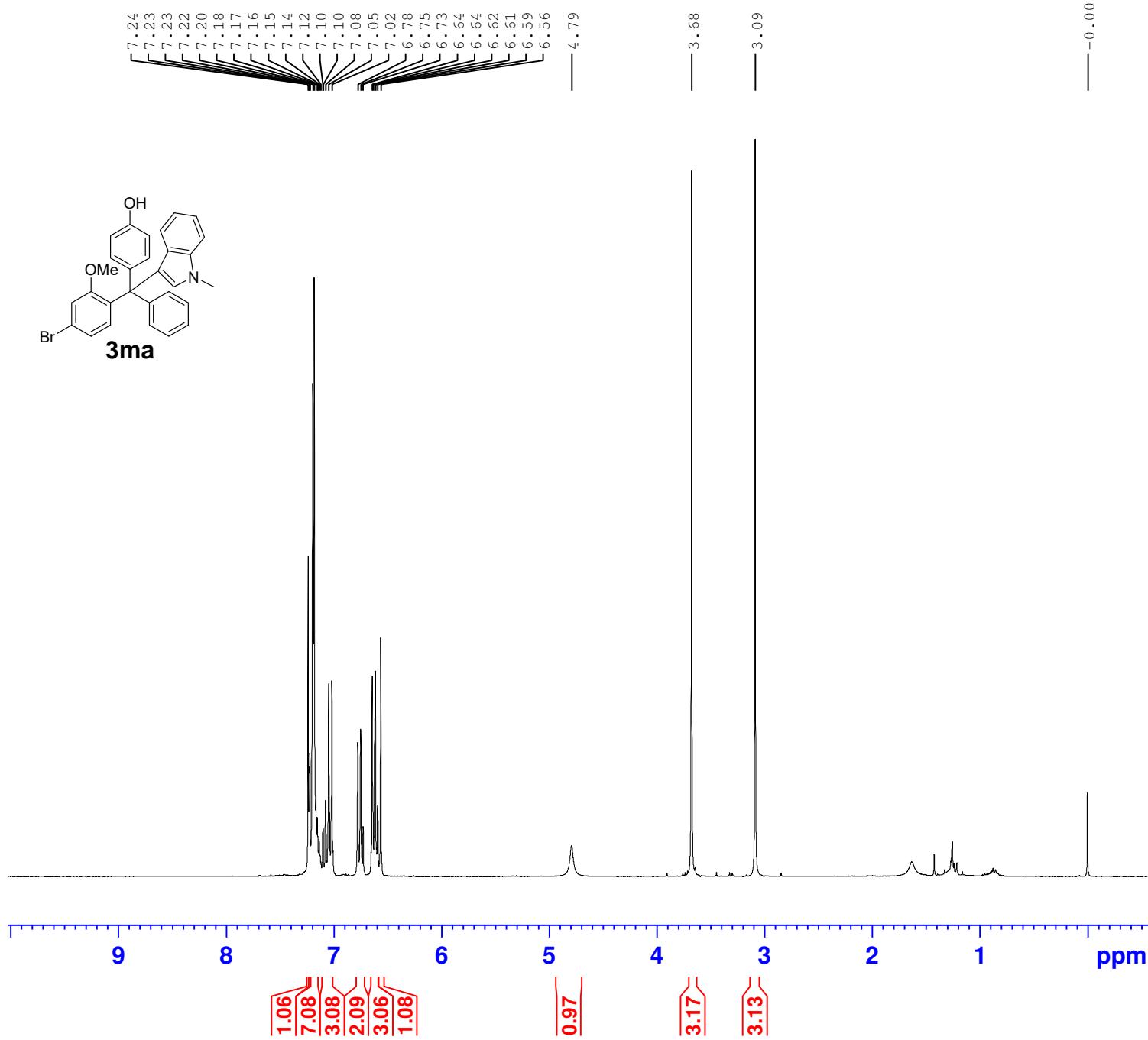
===== CHANNEL f2 ======  
 SFO2 300.1312005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 14.00000000 W  
 PLW12 0.17284000 W  
 PLW13 0.14000000 W

F2 - Processing parameters  
 SI 32768  
 SF 75.4677533 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

3la



3ma



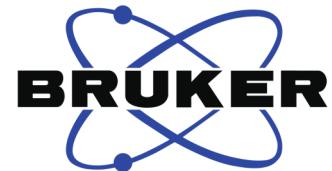
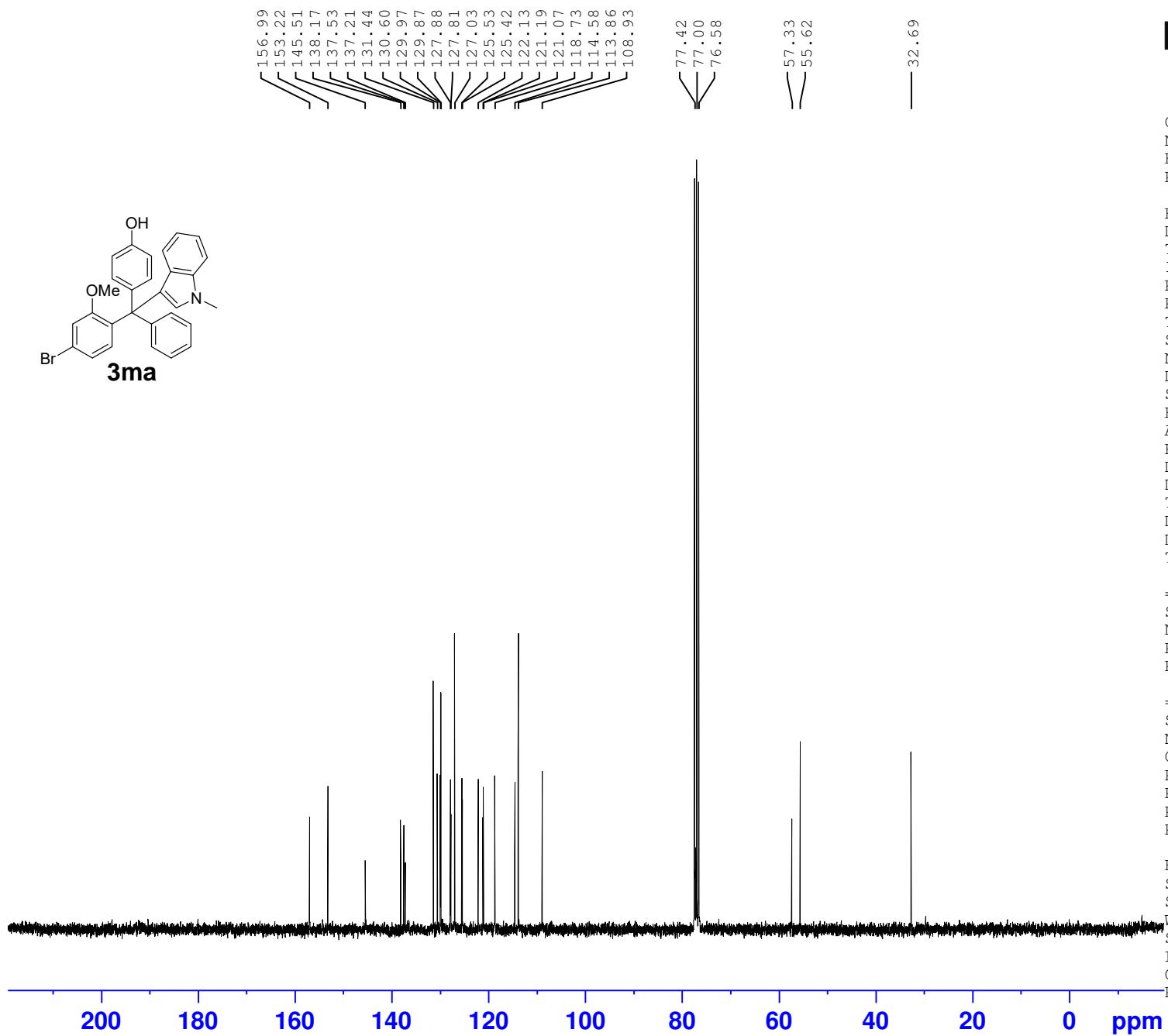
Current Data Parameters  
NAME ZY-4-93D-h-fr  
EXPNO 5529  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211015  
Time 10.06  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
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 -59.1 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 300.1300136 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

3ma



Current Data Parameters  
NAME 3ma-ZY-4-93D  
EXPNO 5538  
PROCNO 1

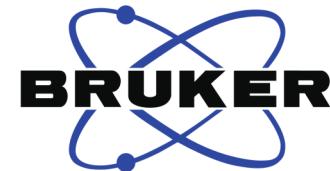
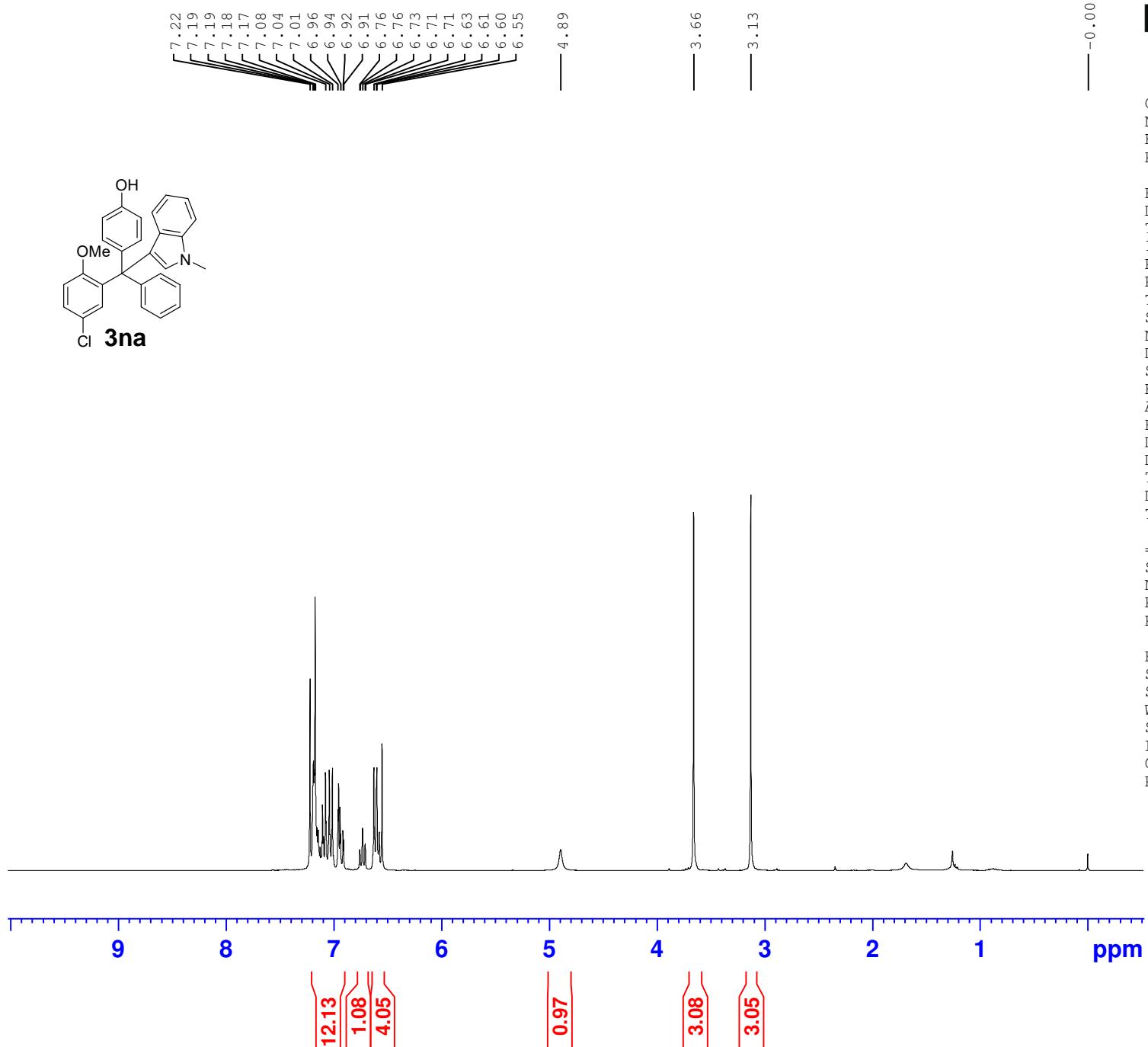
F2 - Acquisition Parameters  
Date\_ 20211016  
Time 13.41  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 500  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE -59.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 ======  
SFO1 75.4752949 MHz  
NUC1 <sup>13</sup>C  
P1 9.50 usec  
PLW1 34.20000076 W

===== CHANNEL f2 ======  
SFO2 300.1312005 MHz  
NUC2 <sup>1</sup>H  
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 75.4677539 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

3na



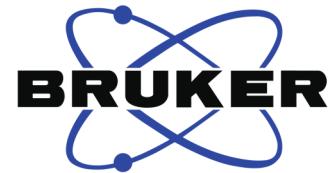
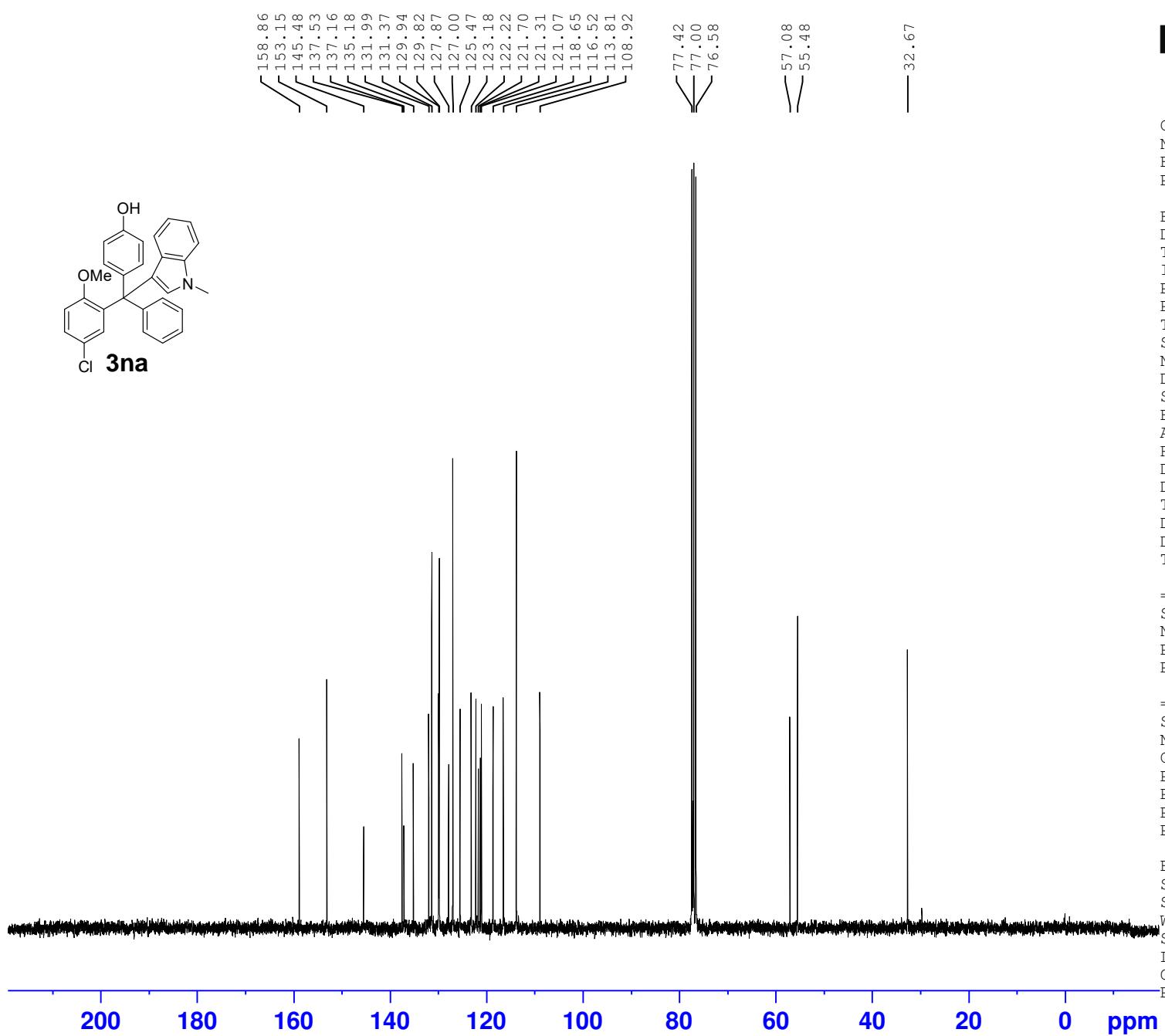
Current Data Parameters  
NAME ZY-4-93E-h-fr  
EXPNO 5618  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211118  
Time 10.06  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
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 -59.1 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 300.1300191 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

3na



Current Data Parameters  
NAME 3na-ZY-4-93E  
EXPNO 5619  
PROCNO 1

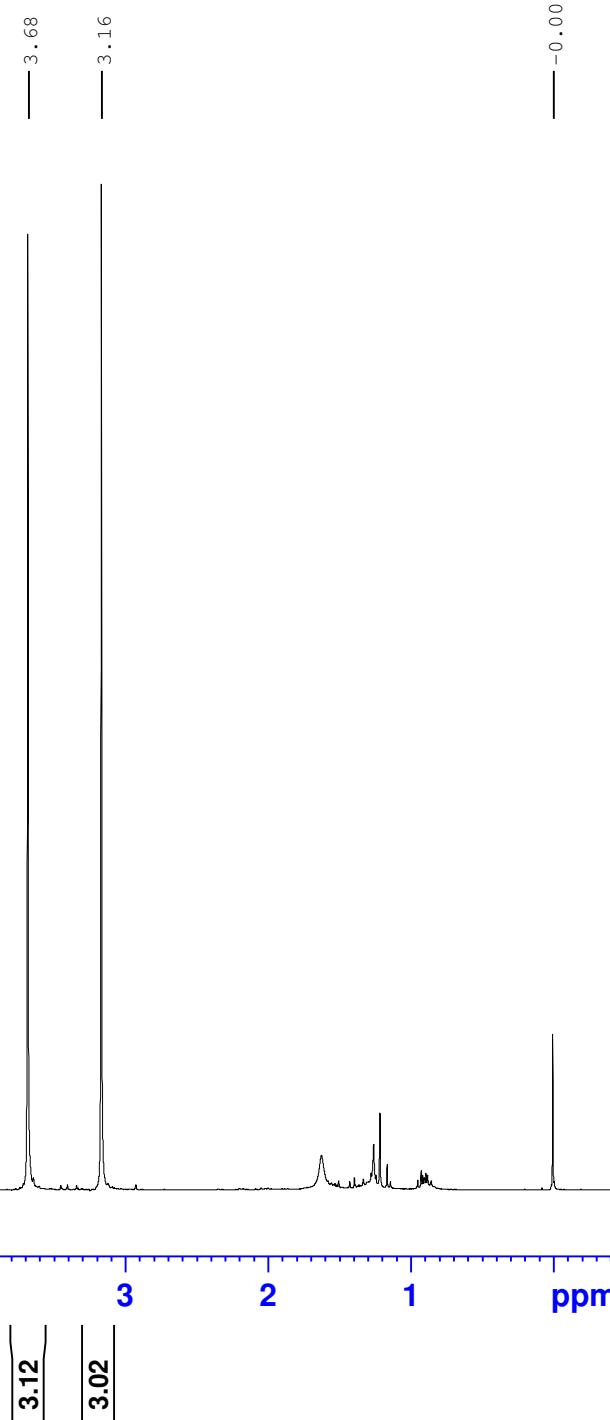
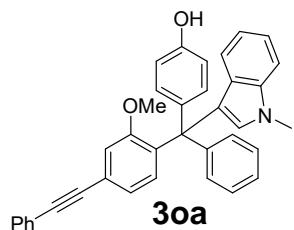
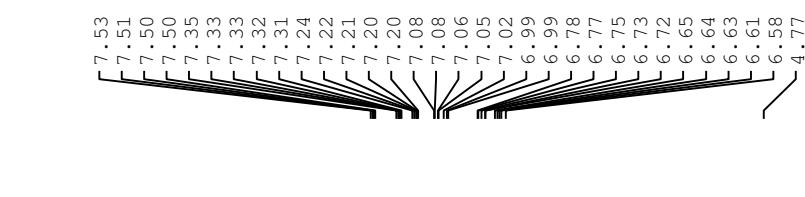
F2 - Acquisition Parameters  
Date\_ 20211118  
Time 10.39  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 500  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE -59.1 K  
D1 2.00000000 sec  
D11 0.03000000 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 75.4677563 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

3oa



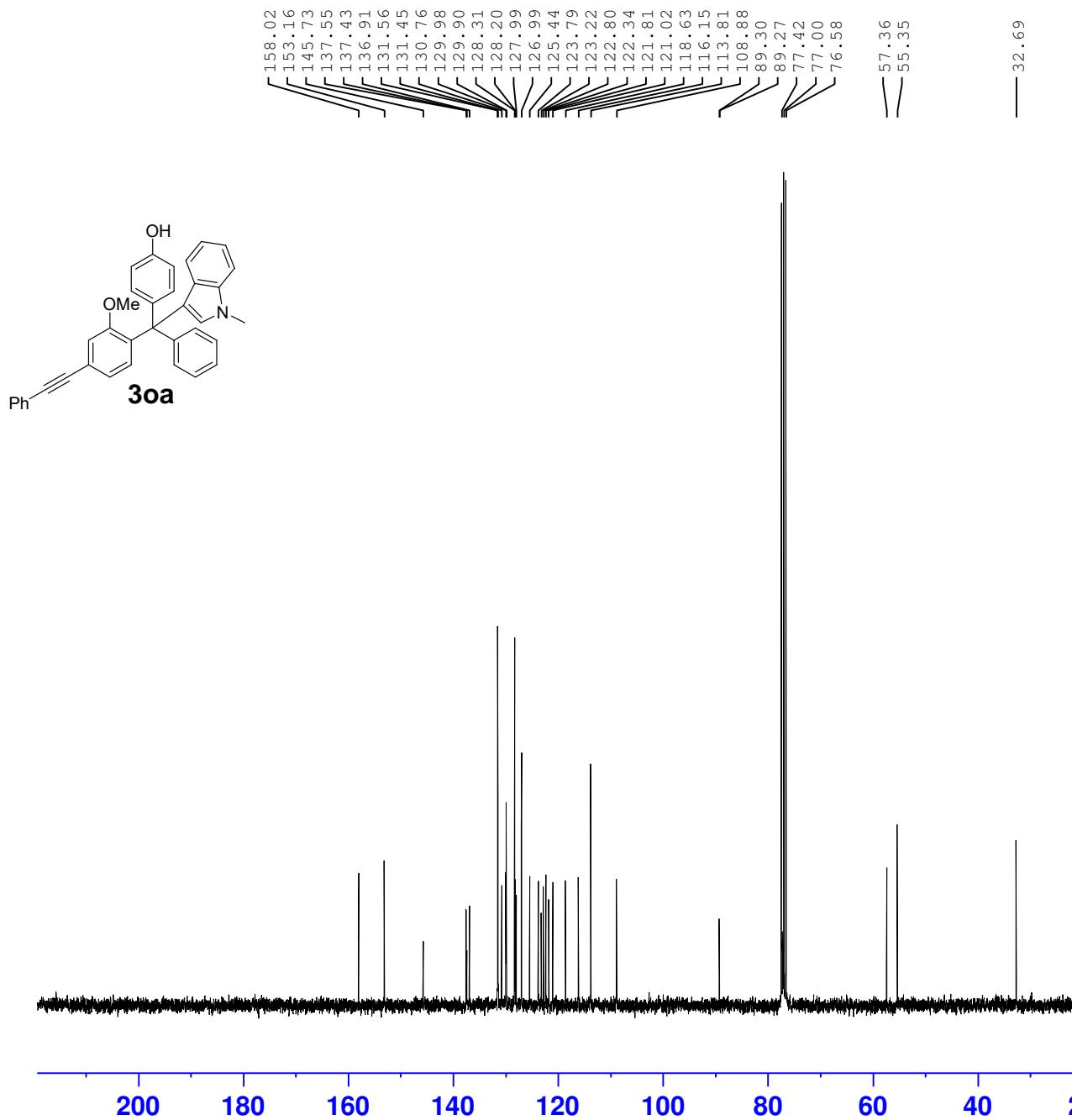
Current Data Parameters  
NAME ZY-4-93F-h-fr  
EXPNO 5531  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211015  
Time 10.16  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
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 -59.1 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 300.1300146 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

3oa



Current Data Parameters  
NAME 3oa-ZY-4-93F  
EXPNO 5539  
PROCNO 1

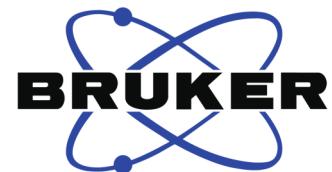
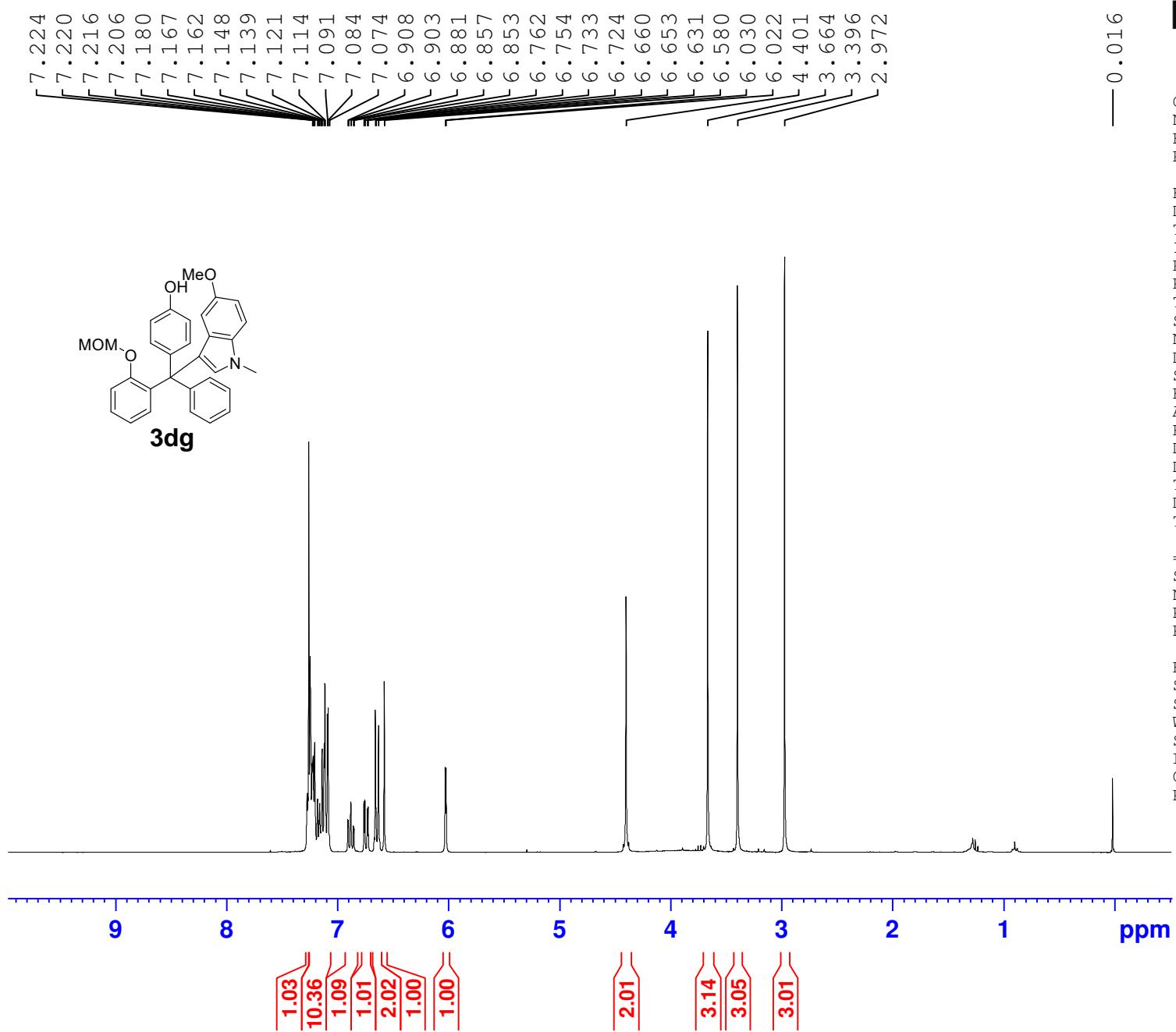
F2 - Acquisition Parameters  
Date\_ 20211016  
Time 14.16  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 500  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE -59.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 ====== SFO1 75.4752949 MHz  
NUC1 <sup>13</sup>C  
P1 9.50 usec  
PLW1 34.20000076 W

===== CHANNEL f2 ====== SFO2 300.1312005 MHz  
NUC2 <sup>1</sup>H  
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 75.4677540 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

3dg



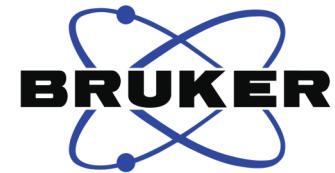
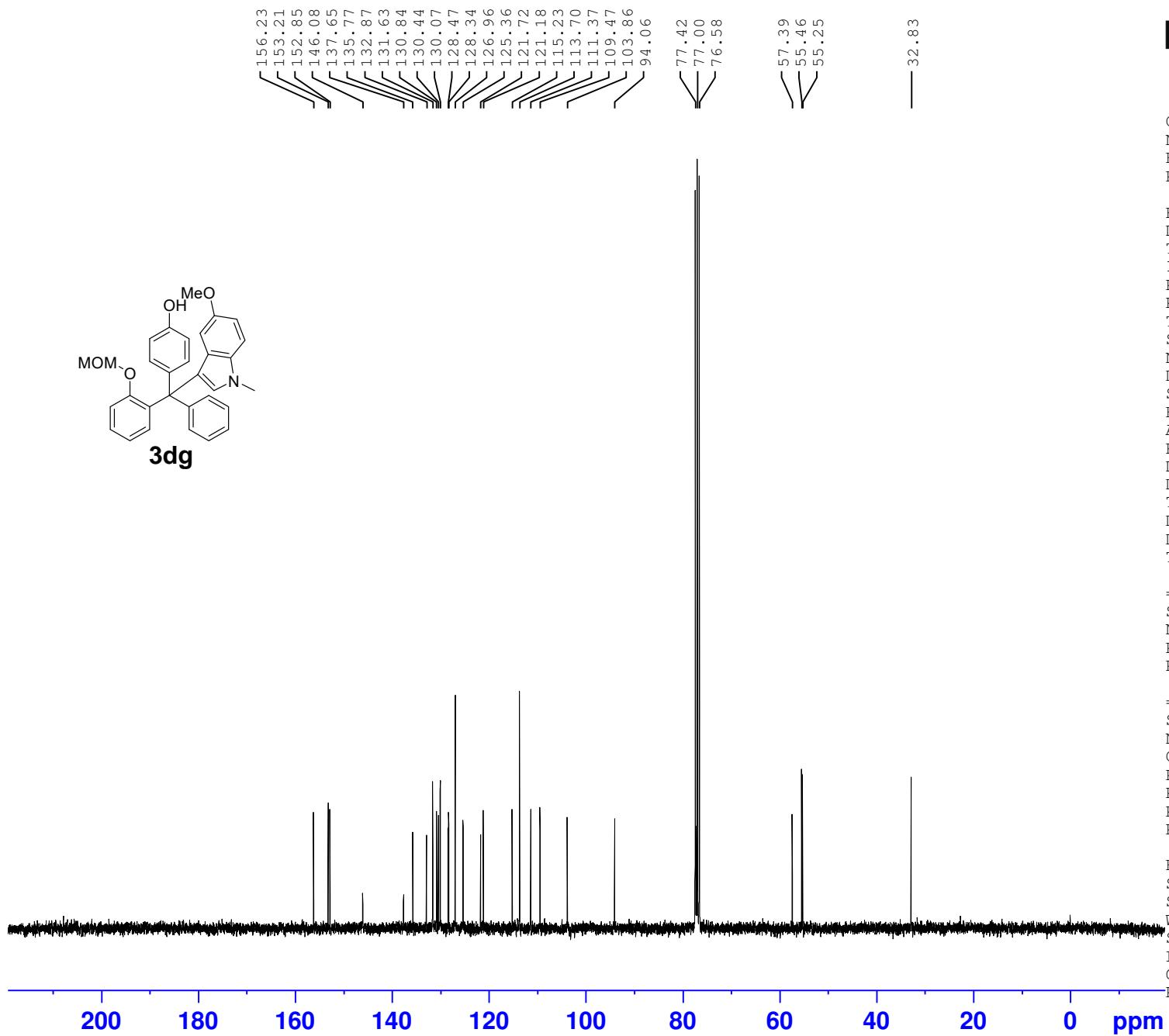
Current Data Parameters  
NAME 211020sjw  
EXPNO 5541  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211020  
Time 9.28  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
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 -59.1 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 300.1300075 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

3dg



Current Data Parameters  
NAME 3dg-ZY-4-86C  
EXPNO 5562  
PROCNO 1

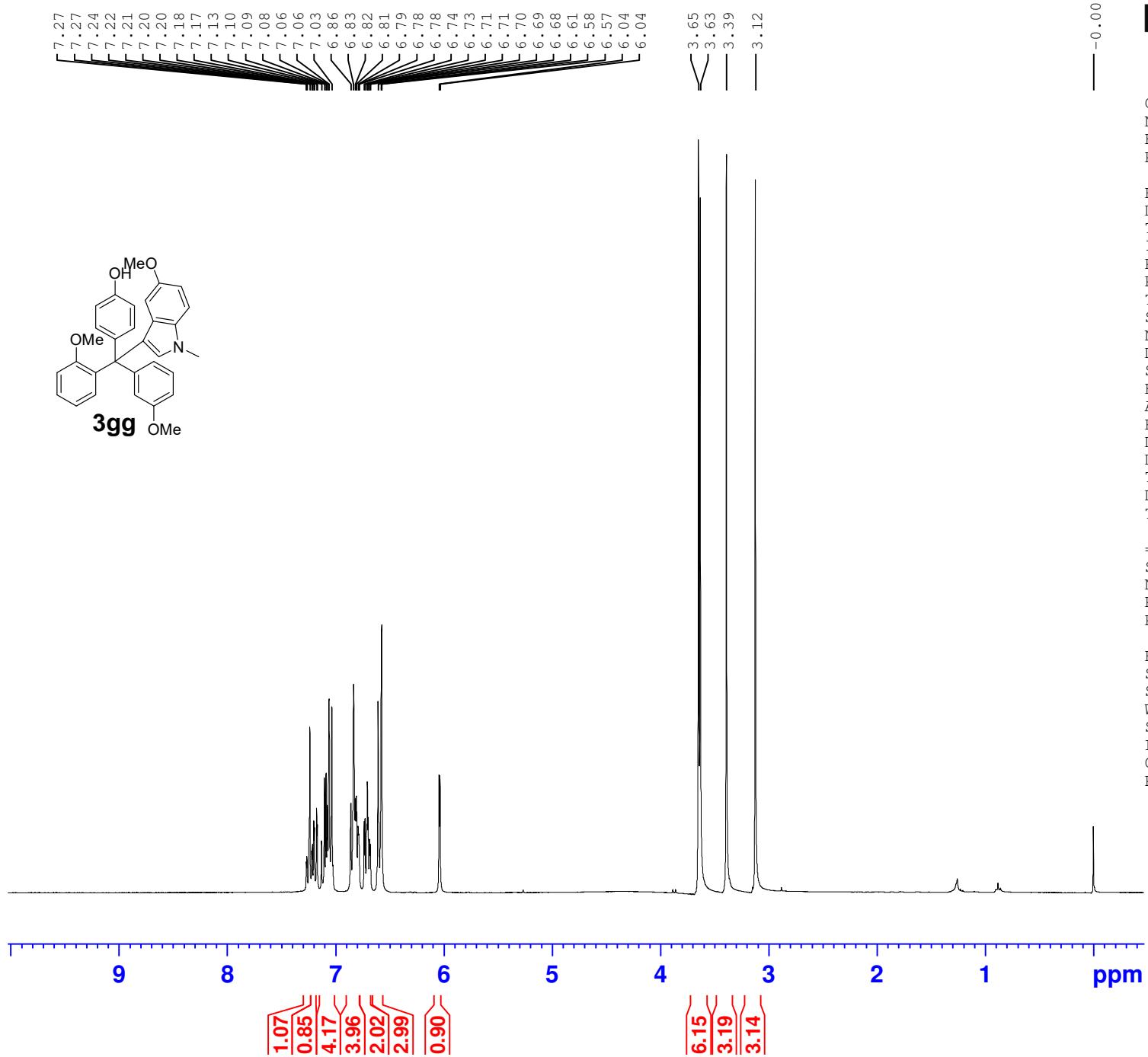
F2 - Acquisition Parameters  
Date\_ 20211022  
Time 12.10  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 500  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE -59.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 ======  
SFO1 75.4752949 MHz  
NUC1 <sup>13</sup>C  
P1 9.50 usec  
PLW1 34.20000076 W

===== CHANNEL f2 ======  
SFO2 300.1312005 MHz  
NUC2 <sup>1</sup>H  
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 75.4677535 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

3gg



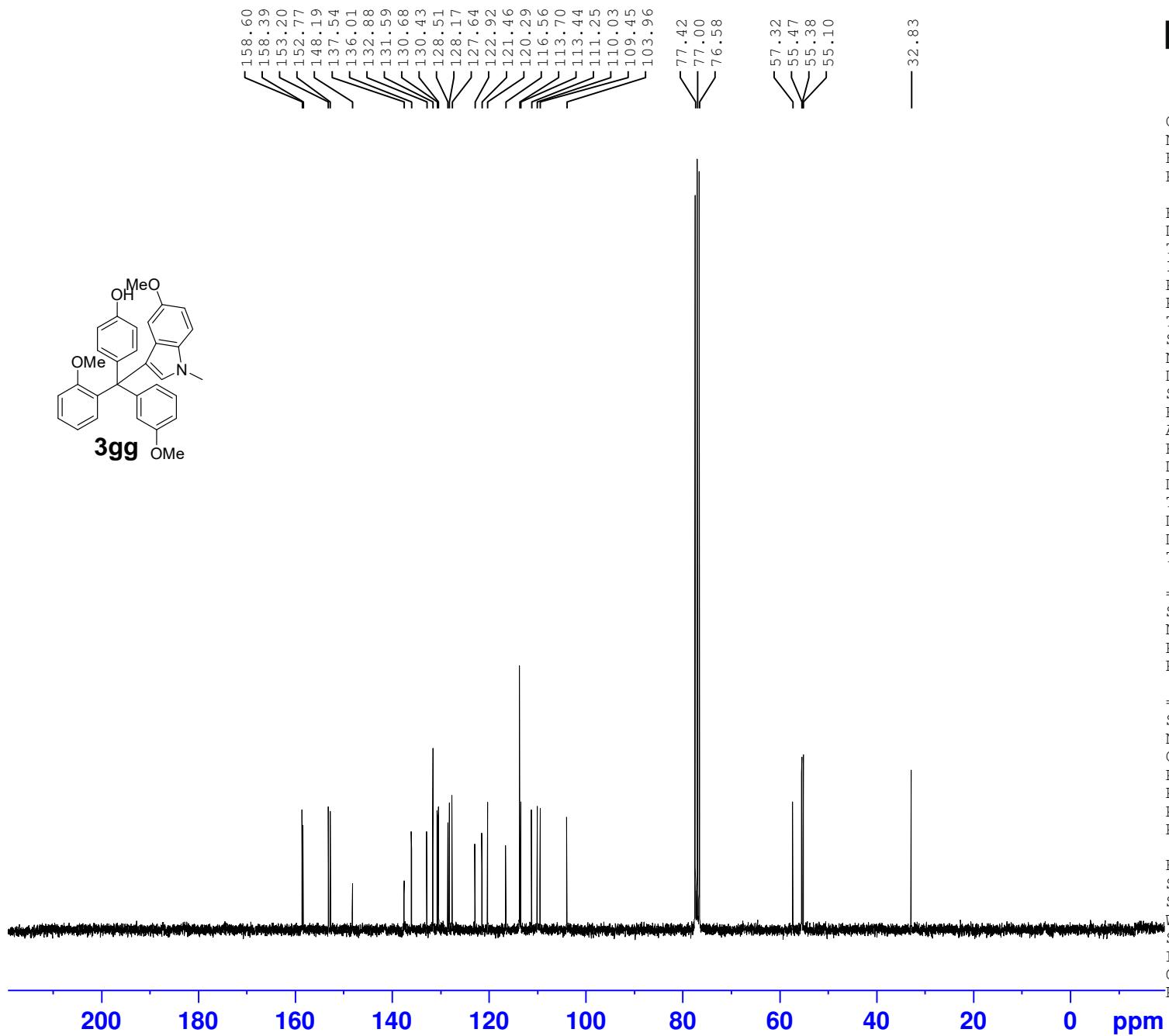
Current Data Parameters  
NAME ZY-4-86E-h-fr  
EXPNO 5543  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211020  
Time 9.37  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
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 -59.1 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 300.1300142 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

3gg



Current Data Parameters  
 NAME 3gg-ZY-4-86E  
 EXPNO 5564  
 PROCNO 1

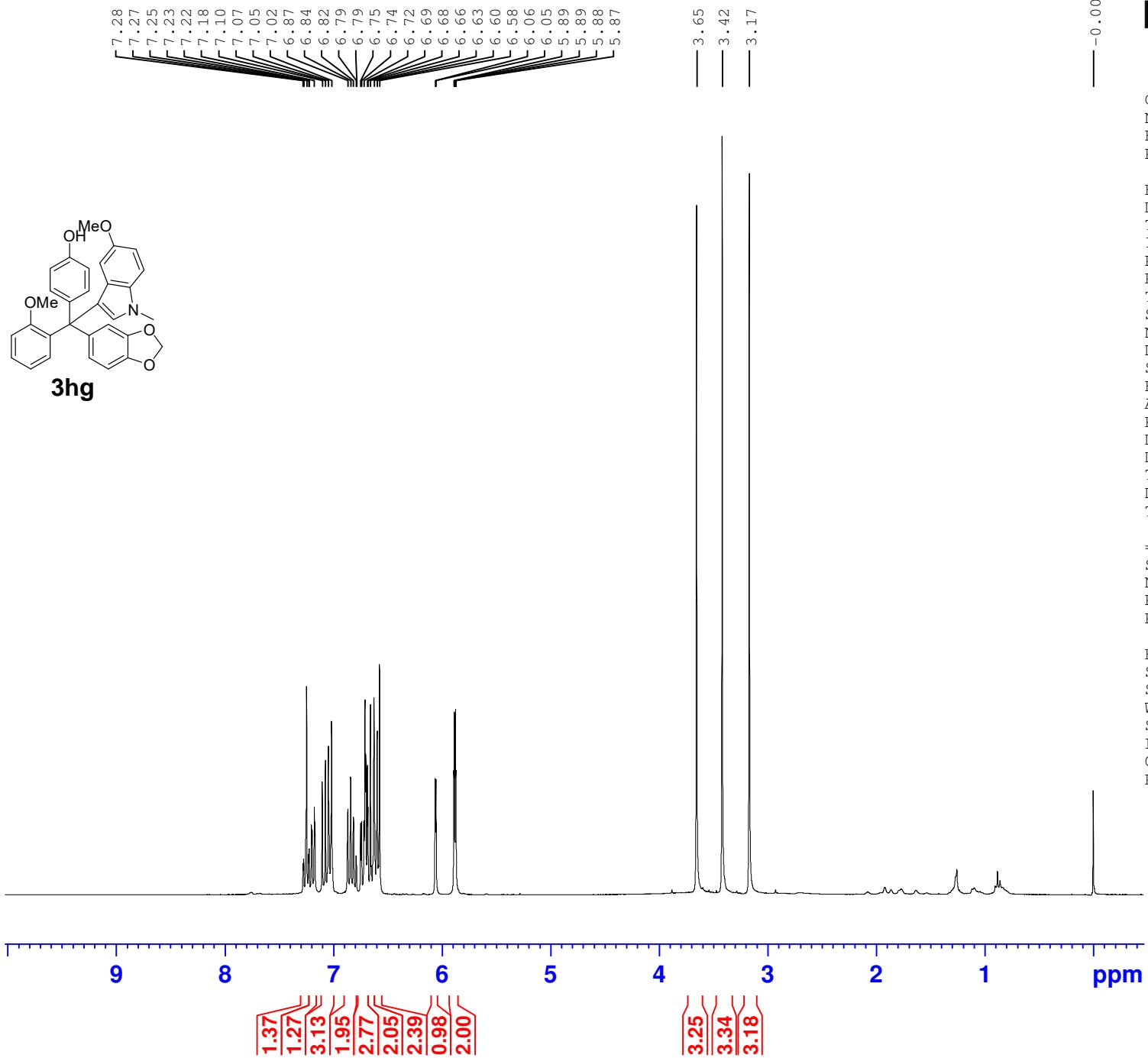
F2 - Acquisition Parameters  
 Date\_ 20211022  
 Time 13.22  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 500  
 DS 4  
 SWH 18028.846 Hz  
 FIDRES 0.275098 Hz  
 AQ 1.8175317 sec  
 RG 203  
 DW 27.733 usec  
 DE 6.50 usec  
 TE -59.1 K  
 D1 2.00000000 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 75.4677539 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

3hg



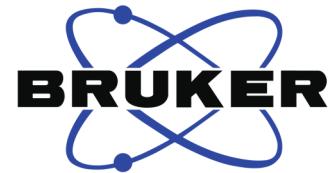
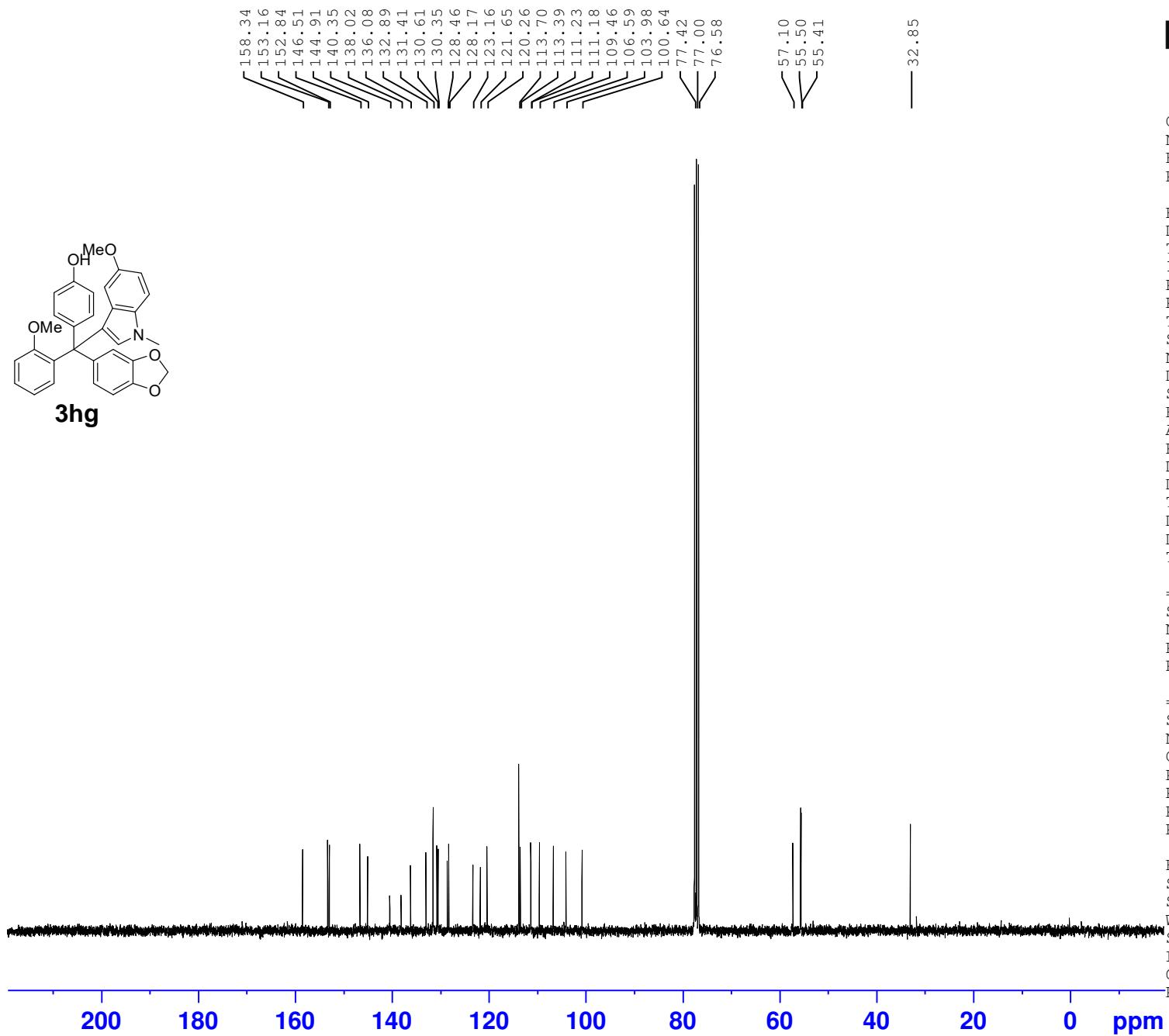
Current Data Parameters  
NAME ZY-4-86F-h-fr  
EXPNO 5544  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211020  
Time 9.42  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
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 -59.1 K  
D1 1.0000000 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 300.1300113 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

3hg



Current Data Parameters  
NAME 3hg-ZY-4-86F  
EXPNO 5555  
PROCNO 1

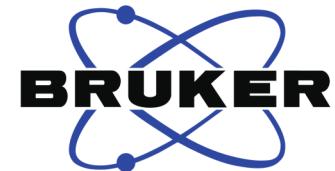
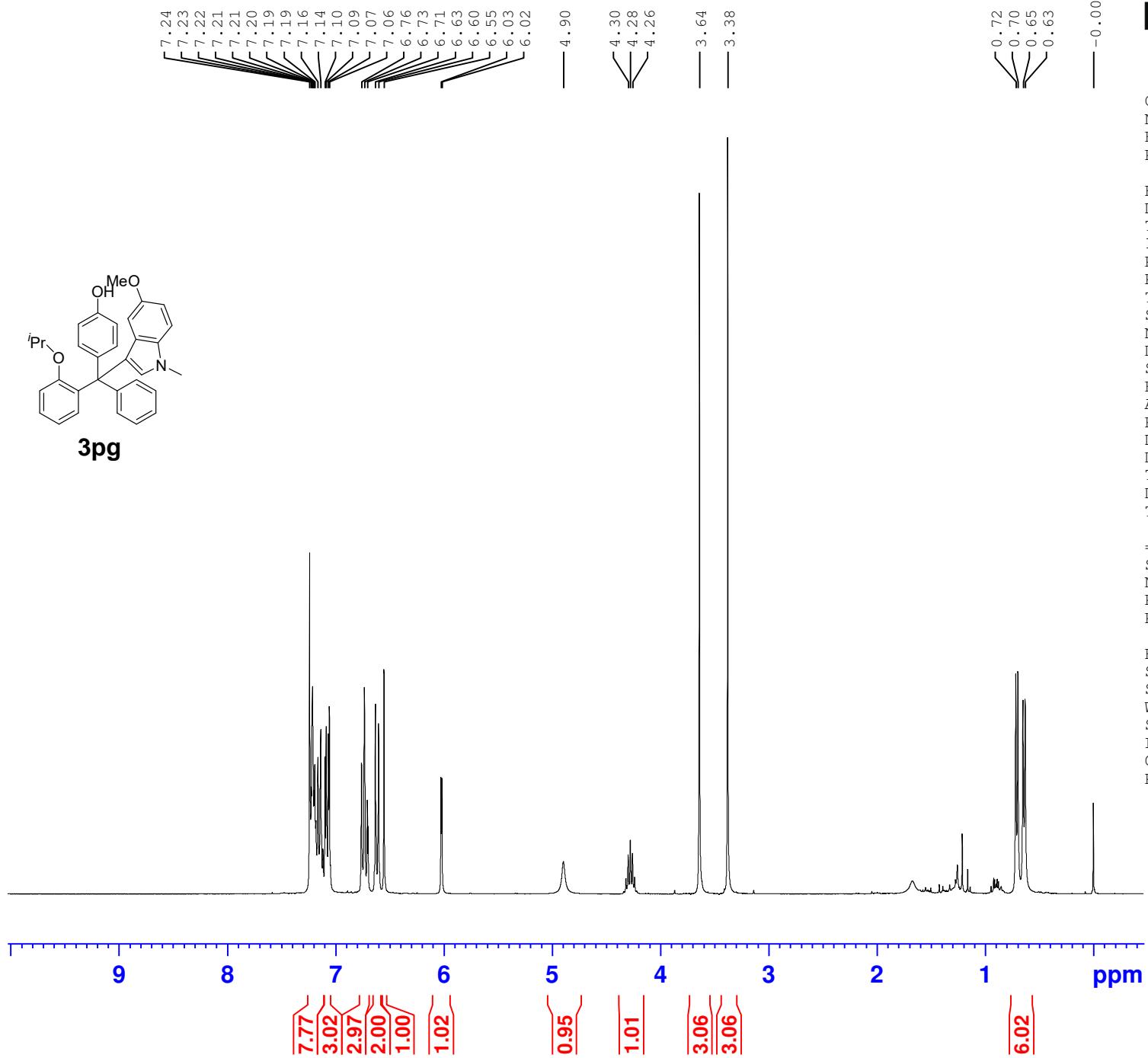
F2 - Acquisition Parameters  
Date\_ 20211023  
Time 10.01  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 700  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE -59.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 ======  
SFO1 75.4752949 MHz  
NUC1 <sup>13</sup>C  
P1 9.50 usec  
PLW1 34.20000076 W

===== CHANNEL f2 ======  
SFO2 300.1312005 MHz  
NUC2 <sup>1</sup>H  
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 75.4677529 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

3pg



Current Data Parameters  
NAME ZY-4-93B-h-fr  
EXPNO 5527  
PROCNO 1

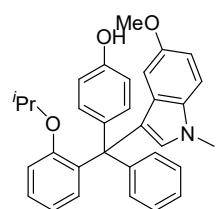
F2 - Acquisition Parameters  
Date\_ 20211015  
Time 9.57  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 101  
DW 83.200 usec  
DE 6.50 usec  
TE -59.1 K  
D1 1.00000000 sec  
TD0 1

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

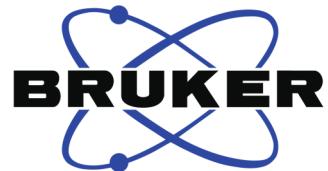
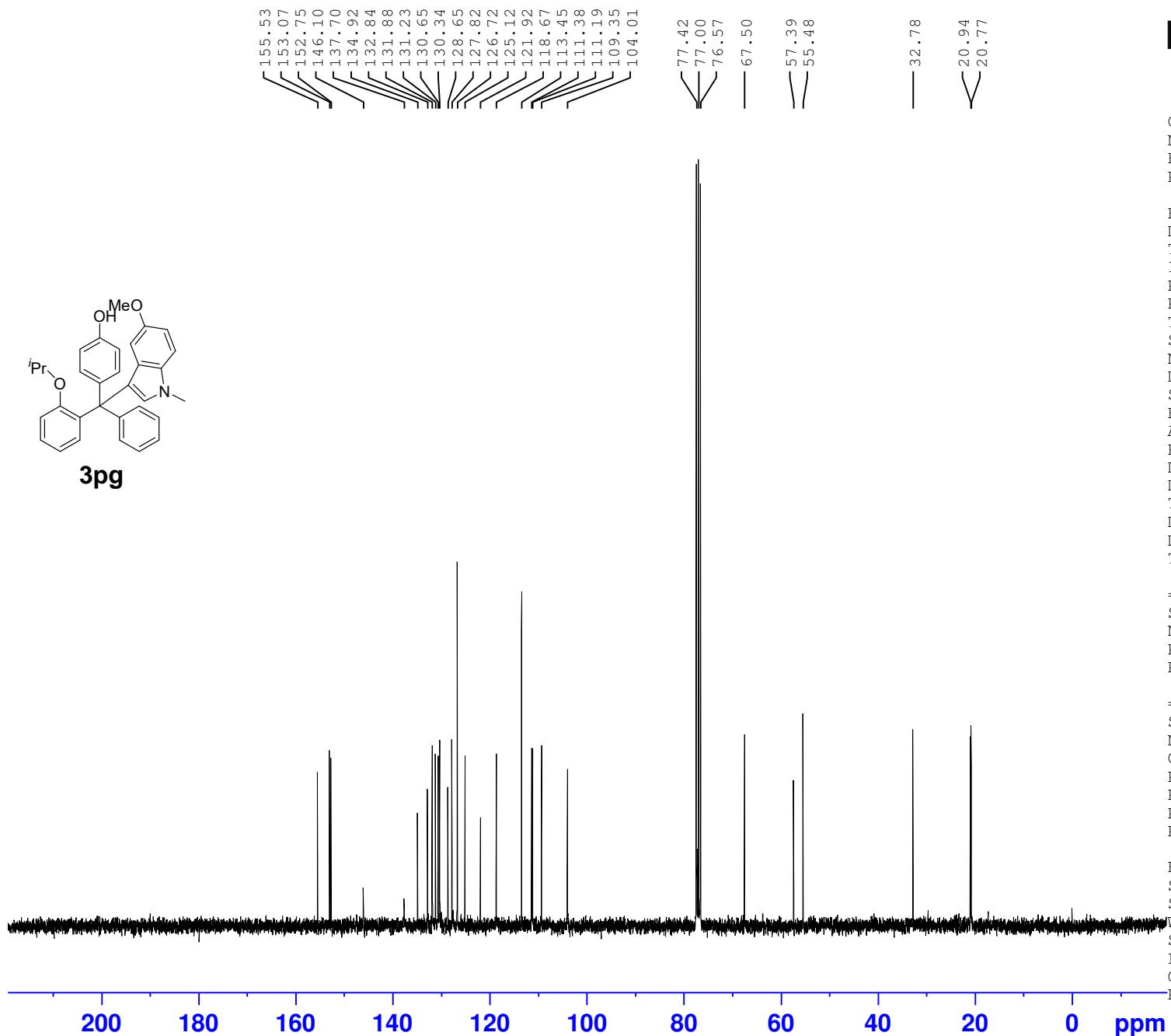
SFO1 300.1318534 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 14.00000000 W

F2 - Processing parameters  
SI 65536  
SF 300.1300132 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

3pg



**3pg**



Current Data Parameters  
NAME 3qg-ZY-4-93B  
EXPNO 5536  
PROCNO 1

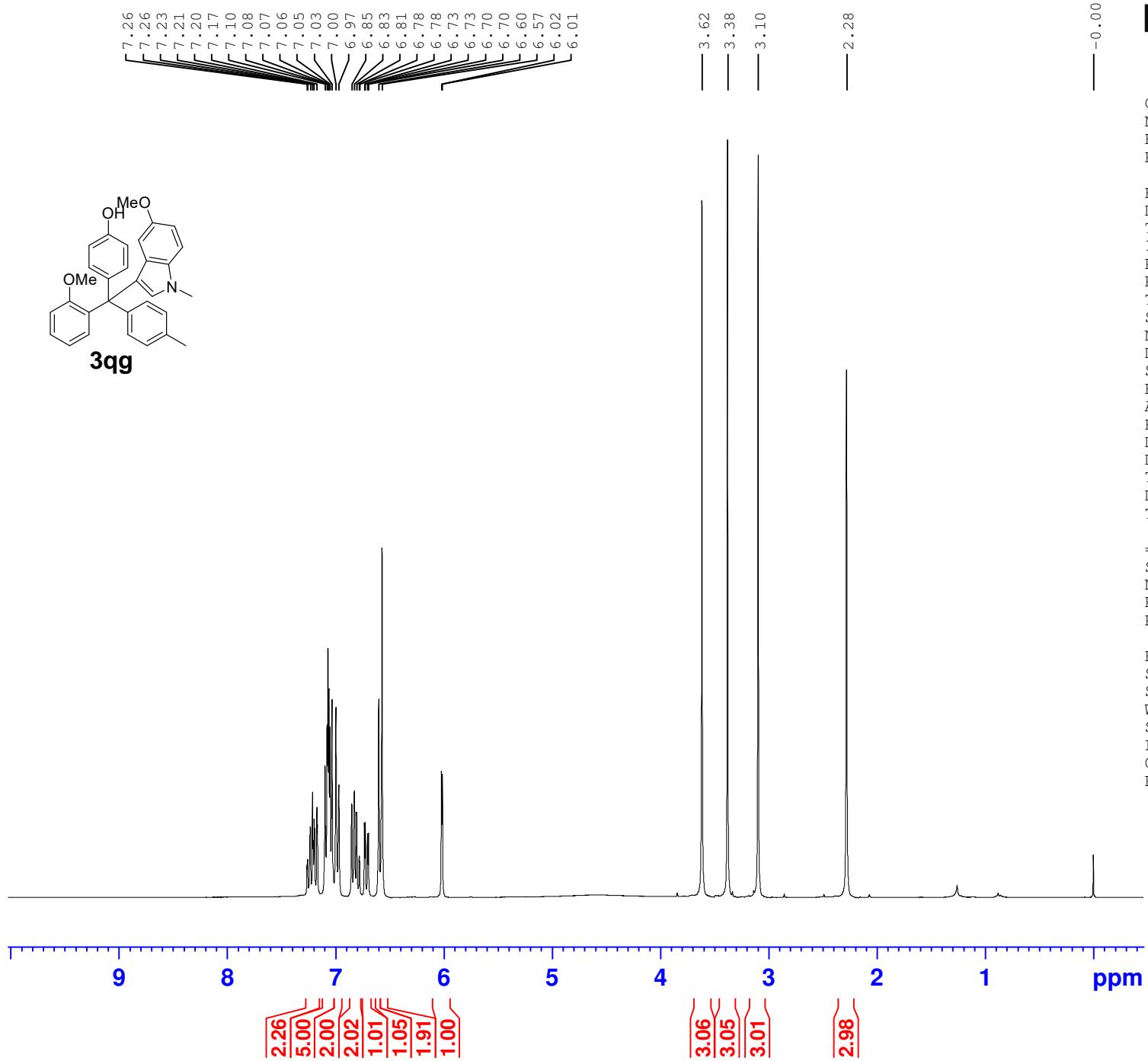
F2 - Acquisition Parameters  
Date\_ 20211016  
Time 12.30  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 500  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE -59.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 ======  
SFO1 75.4752949 MHz  
NUC1 <sup>13</sup>C  
P1 9.50 usec  
PLW1 34.20000076 W

===== CHANNEL f2 ======  
SFO2 300.1312005 MHz  
NUC2 <sup>1</sup>H  
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 75.4677539 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

3qg



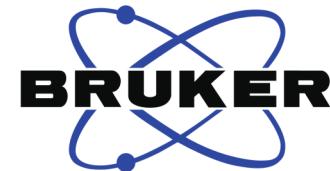
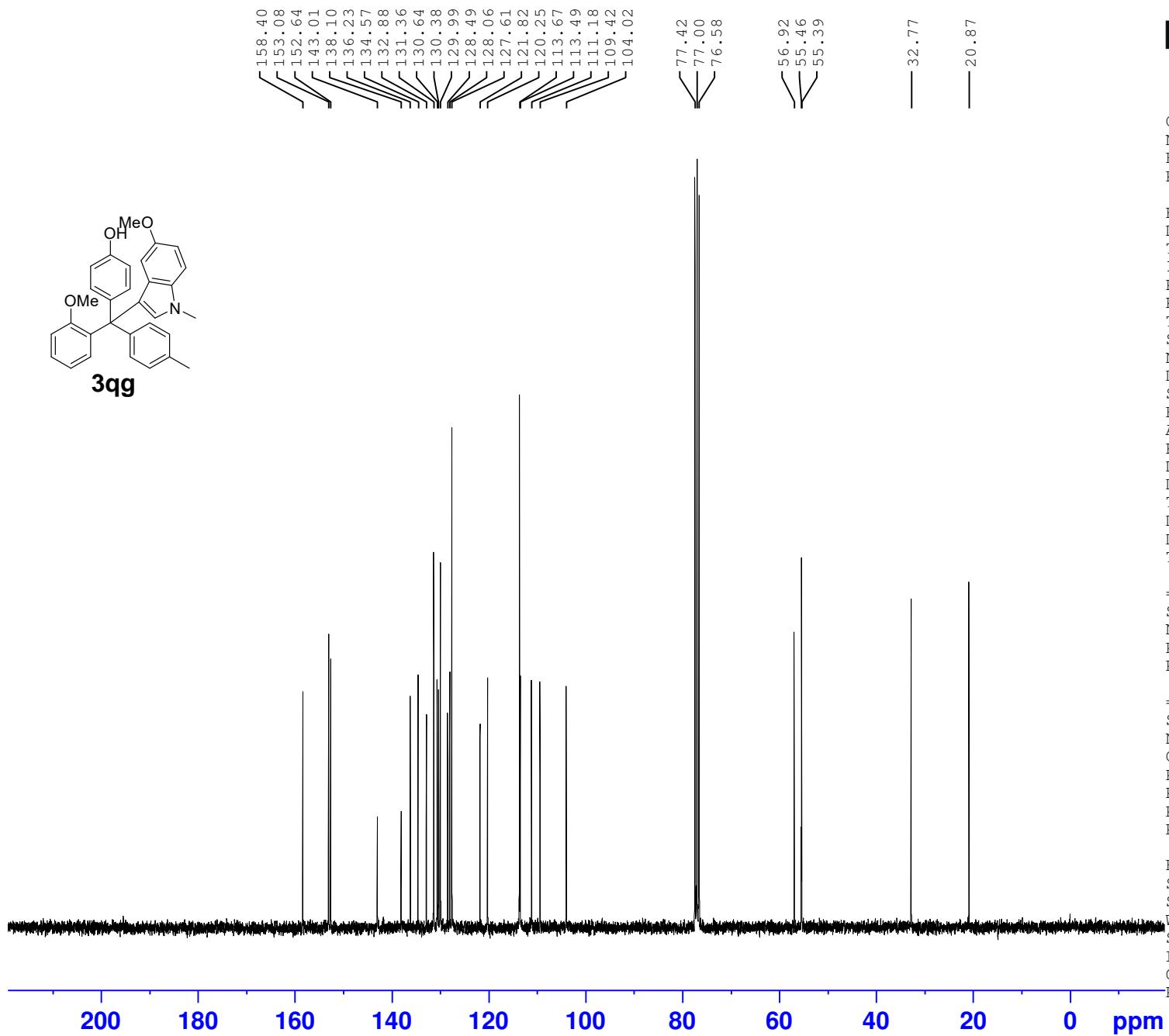
Current Data Parameters  
NAME ZY-4-86A-h-fr  
EXPNO 5540  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211020  
Time 9.22  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 71.8  
DW 83.200 usec  
DE 6.50 usec  
TE -59.1 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 300.1300212 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

3qg



Current Data Parameters  
NAME 3rg-ZY-4-86A  
EXPNO 5561  
PROCNO 1

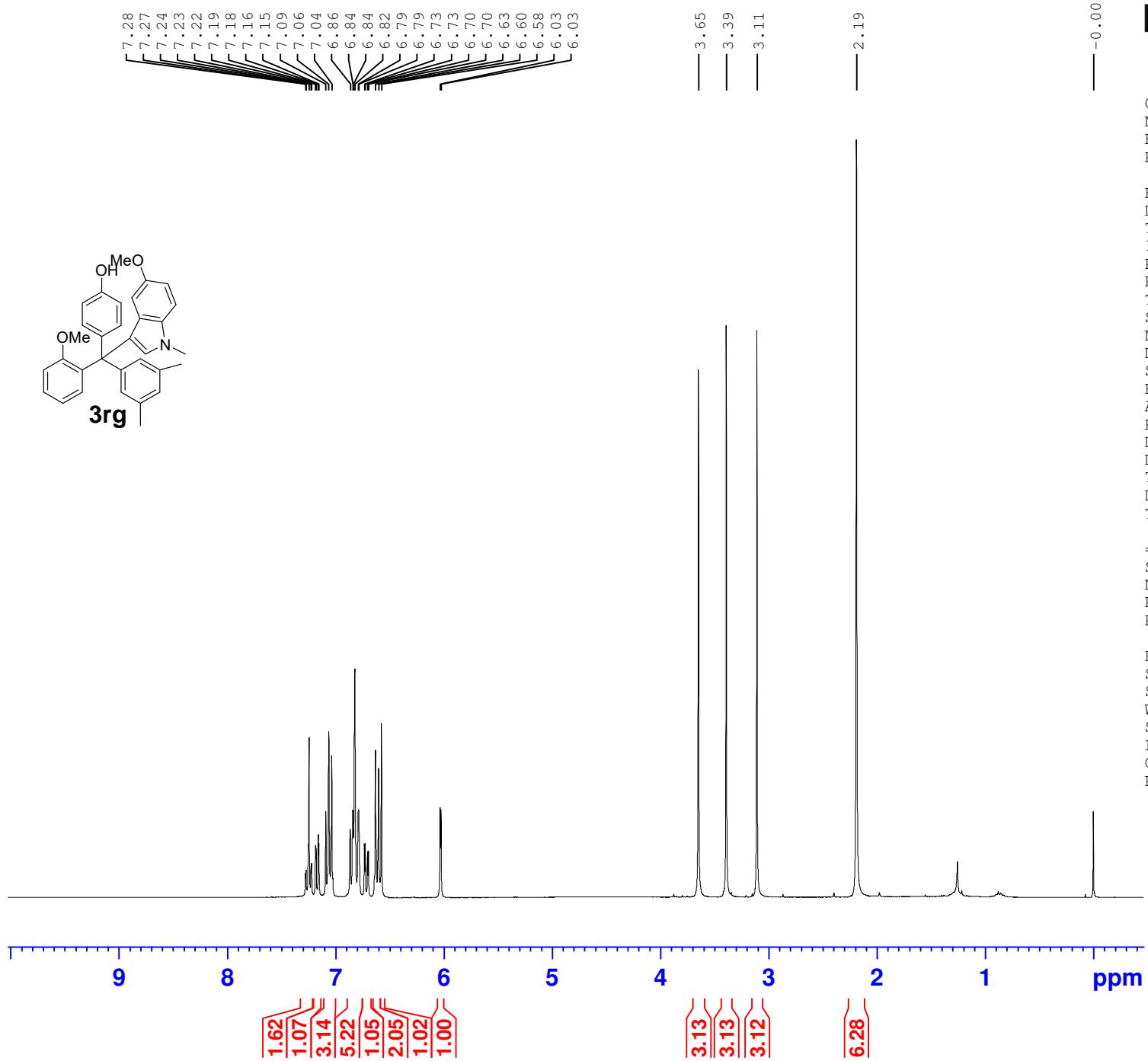
F2 - Acquisition Parameters  
Date\_ 20211022  
Time 11.34  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 500  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE -59.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 ======  
SFO1 75.4752949 MHz  
NUC1 <sup>13</sup>C  
P1 9.50 usec  
PLW1 34.20000076 W

===== CHANNEL f2 ======  
SFO2 300.1312005 MHz  
NUC2 <sup>1</sup>H  
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 75.4677576 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

3rg



Current Data Parameters  
NAME ZY-4-93A-h-fr  
EXPNO 5526  
PROCNO 1

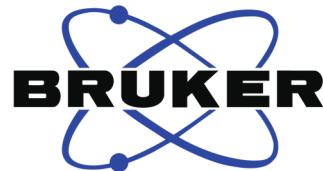
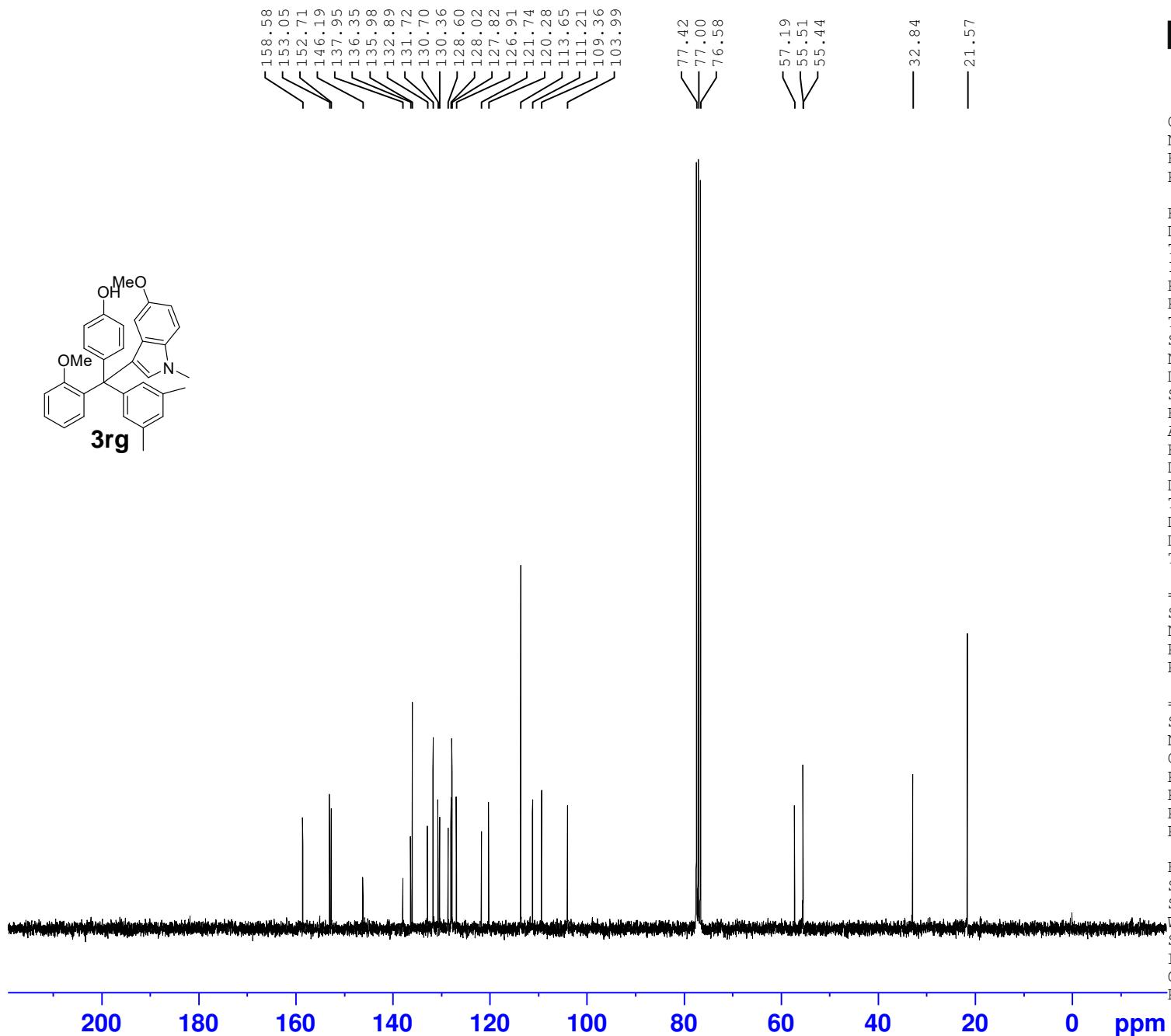
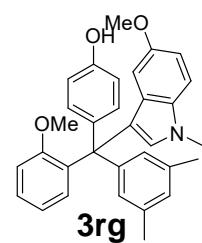
F2 - Acquisition Parameters  
Date\_ 20211015  
Time 9.52  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 128  
DW 83.200 usec  
DE 6.50 usec  
TE -59.1 K  
D1 1.00000000 sec  
TD0 1

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

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

F2 - Processing parameters  
SI 65536  
SF 300.1300119 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

3rg



Current Data Parameters  
NAME 3tg-ZY-4-93A  
EXPNO 5535  
PROCNO 1

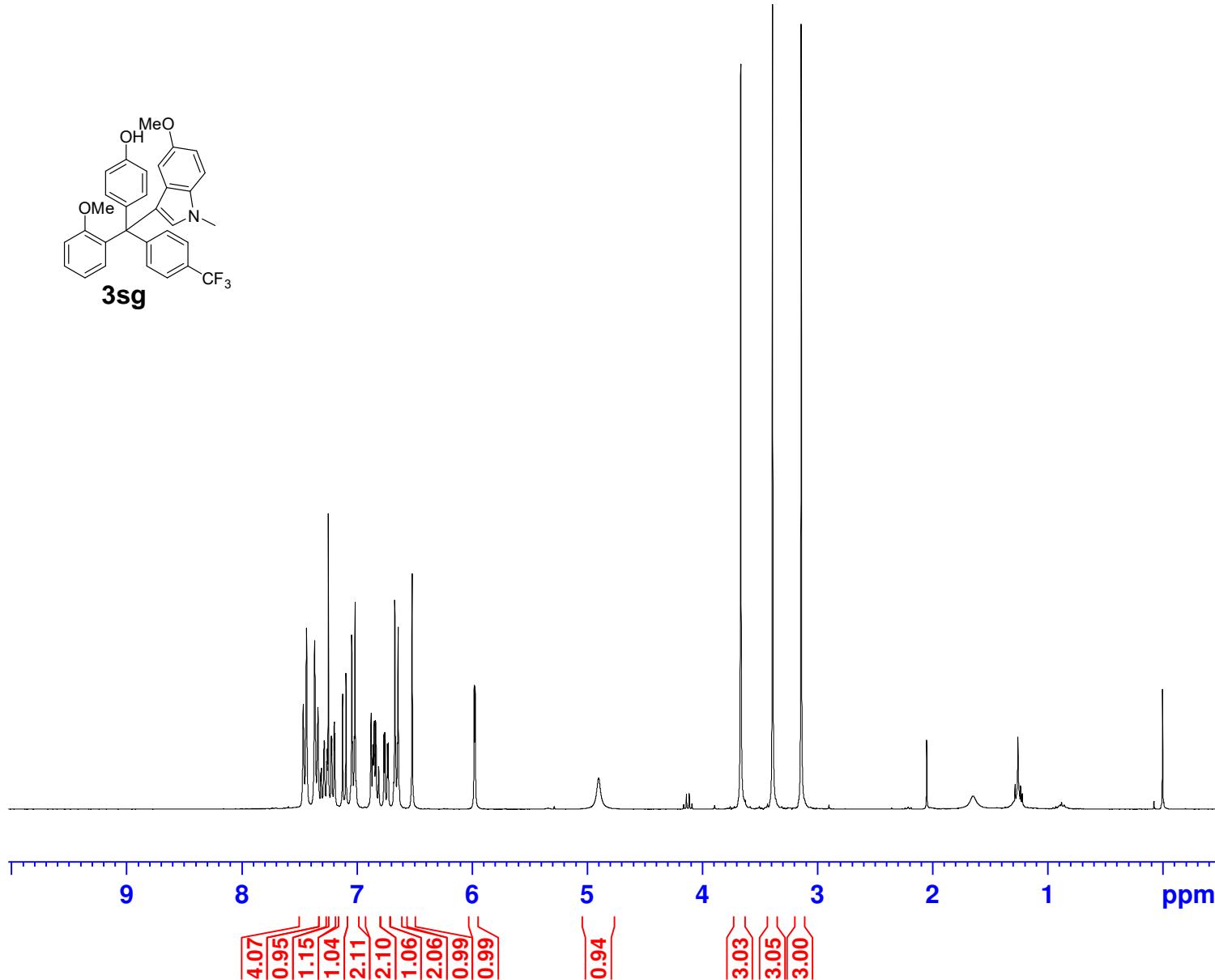
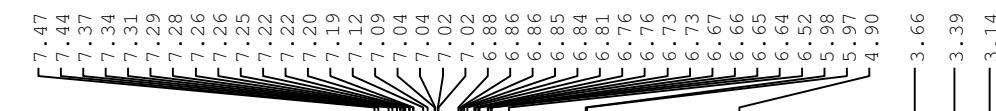
F2 - Acquisition Parameters  
Date\_ 20211016  
Time 11.55  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 500  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE -59.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 ======  
SFO1 75.4752949 MHz  
NUC1 <sup>13</sup>C  
P1 9.50 usec  
PLW1 34.20000076 W

===== CHANNEL f2 ======  
SFO2 300.1312005 MHz  
NUC2 <sup>1</sup>H  
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 75.4677532 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

3sg



Current Data Parameters  
NAME ZY-4-86B-h-fr  
EXPNO 5618  
PROCNO 1

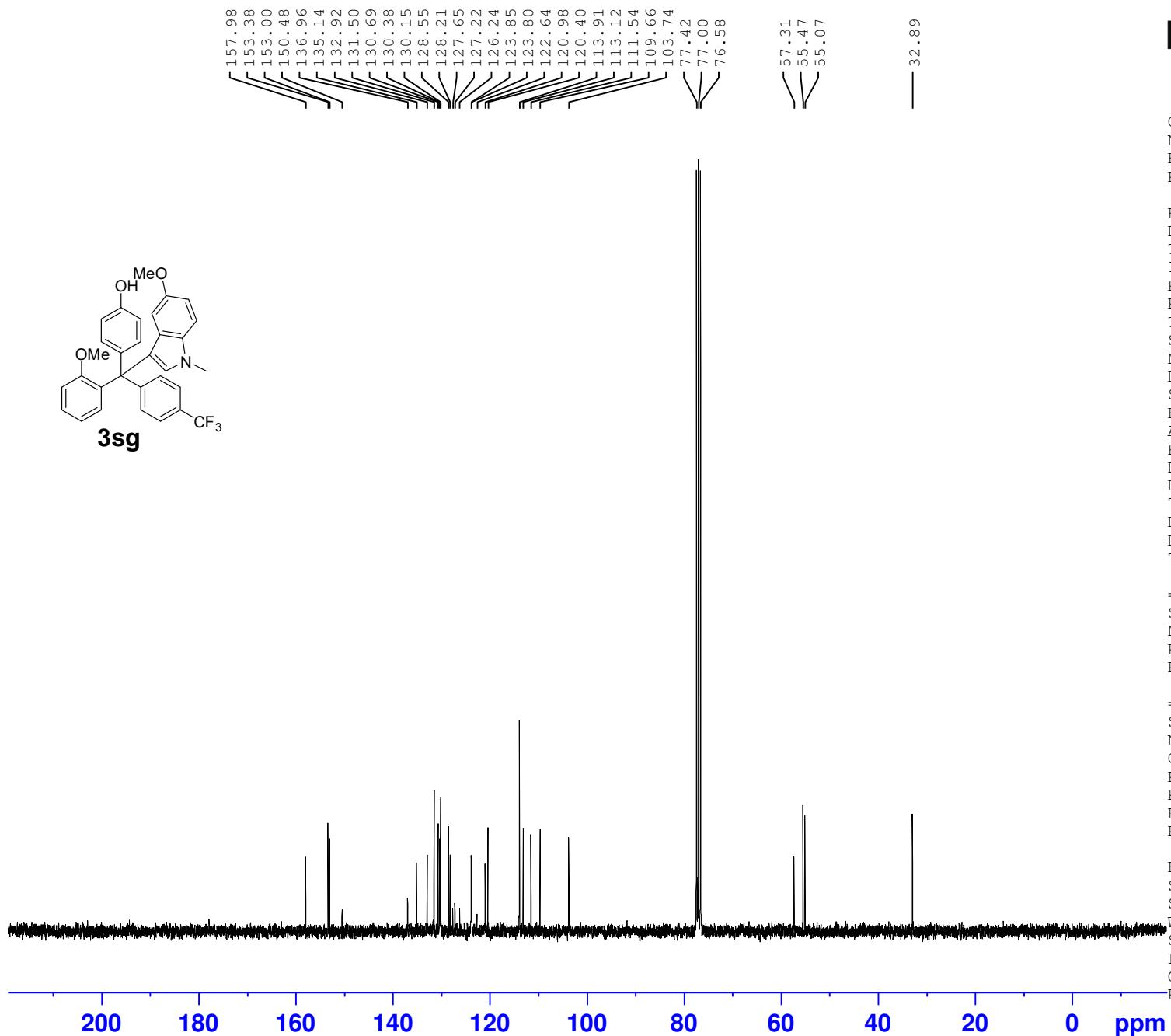
F2 - Acquisition Parameters  
Date\_ 20211116  
Time 10.35  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 161  
DW 83.200 usec  
DE 6.50 usec  
TE -59.1 K  
D1 1.00000000 sec  
TD0 1

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

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

F2 - Processing parameters  
SI 65536  
SF 300.1300108 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

3sg



Current Data Parameters  
NAME 3sg-ZY-4-86B  
EXPNO 5619  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211116  
Time 11.09  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 500  
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 -59.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

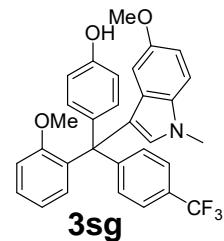
===== CHANNEL f1 ======  
SFO1 75.4752949 MHz  
NUC1 <sup>13</sup>C  
P1 9.50 usec  
PLW1 34.20000076 W

===== CHANNEL f2 ======  
SFO2 300.1312005 MHz  
NUC2 <sup>1</sup>H  
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 75.4677524 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

3sg

-62.094



Current Data Parameters  
 NAME 211029sjw  
 EXPNO 5574  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20211029  
 Time 9.32  
 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 -59.1 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

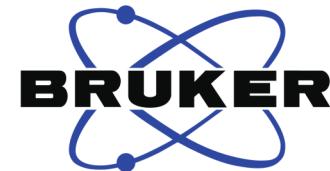
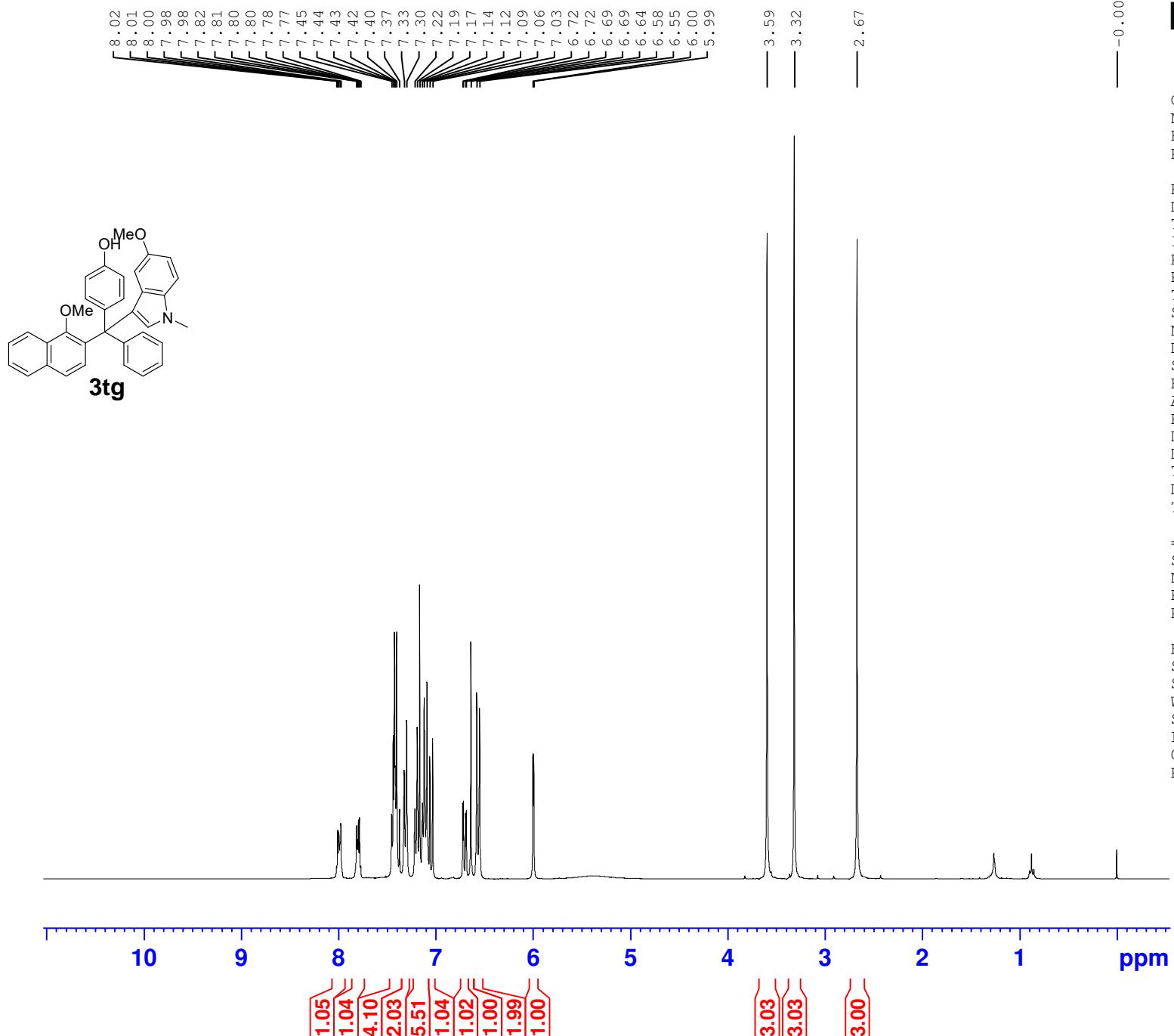
===== CHANNEL f2 ======  
 SFO2 300.1312005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 14.00000000 W  
 PLW12 0.17284000 W

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

0 -20 -40 -60 -80 -100 -120 -140 -160 -180

ppm

3tg



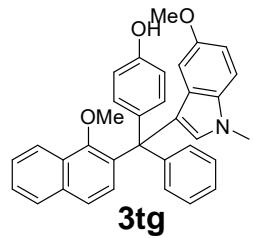
Current Data Parameters  
NAME ZY-4-86D-h-fr  
EXPNO 5542  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211020  
Time 9.33  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 32  
DW 83.200 usec  
DE 6.50 usec  
TE -59.1 K  
D1 1.00000000 sec  
TD0 1

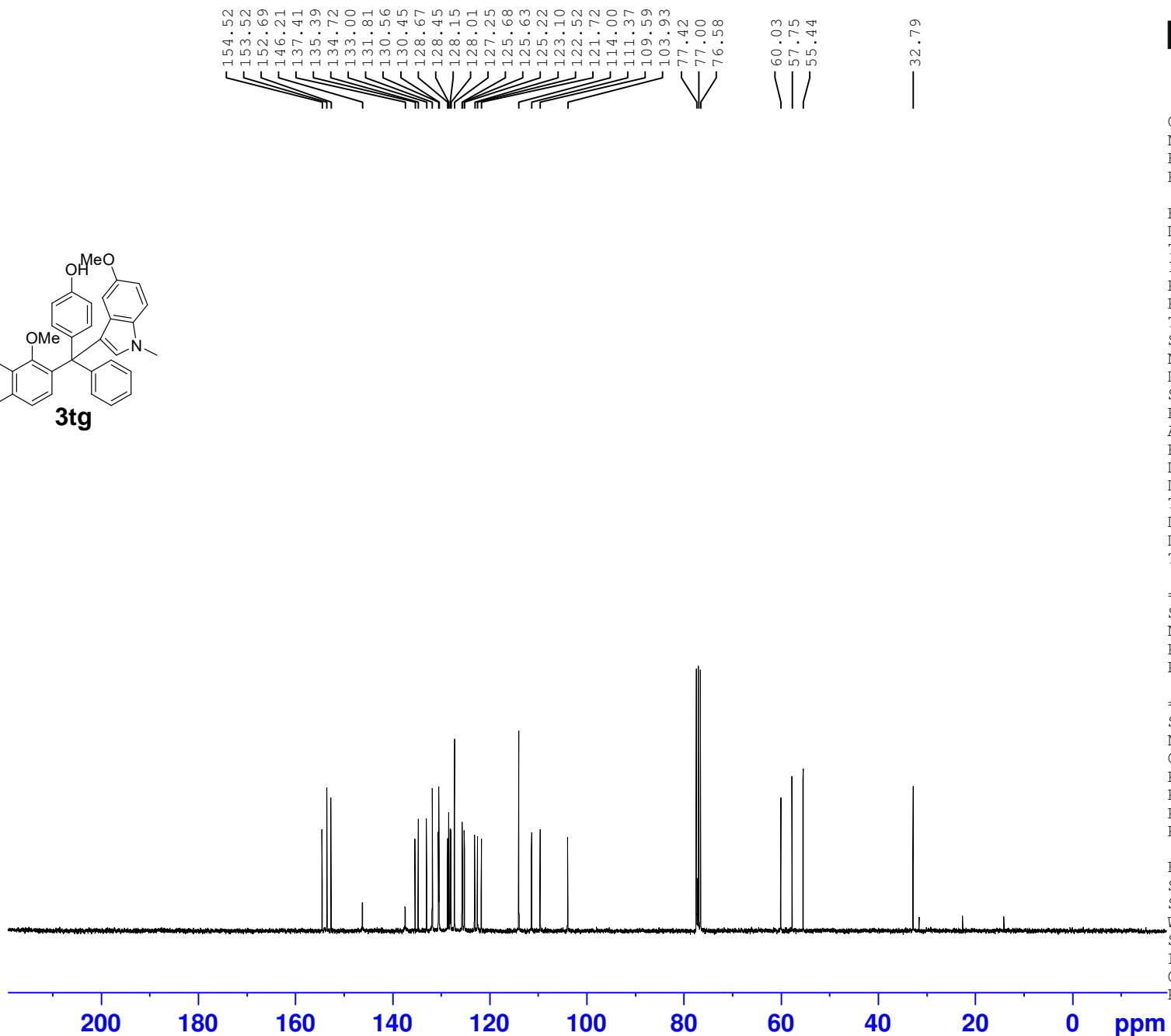
===== CHANNEL f1 =====  
SFO1 300.1318534 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 14.00000000 W

F2 - Processing parameters  
SI 65536  
SF 300.1300352 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

3tg



3tg



Current Data Parameters  
NAME 3pg-ZY-4-86D  
EXPNO 5563  
PROCNO 1

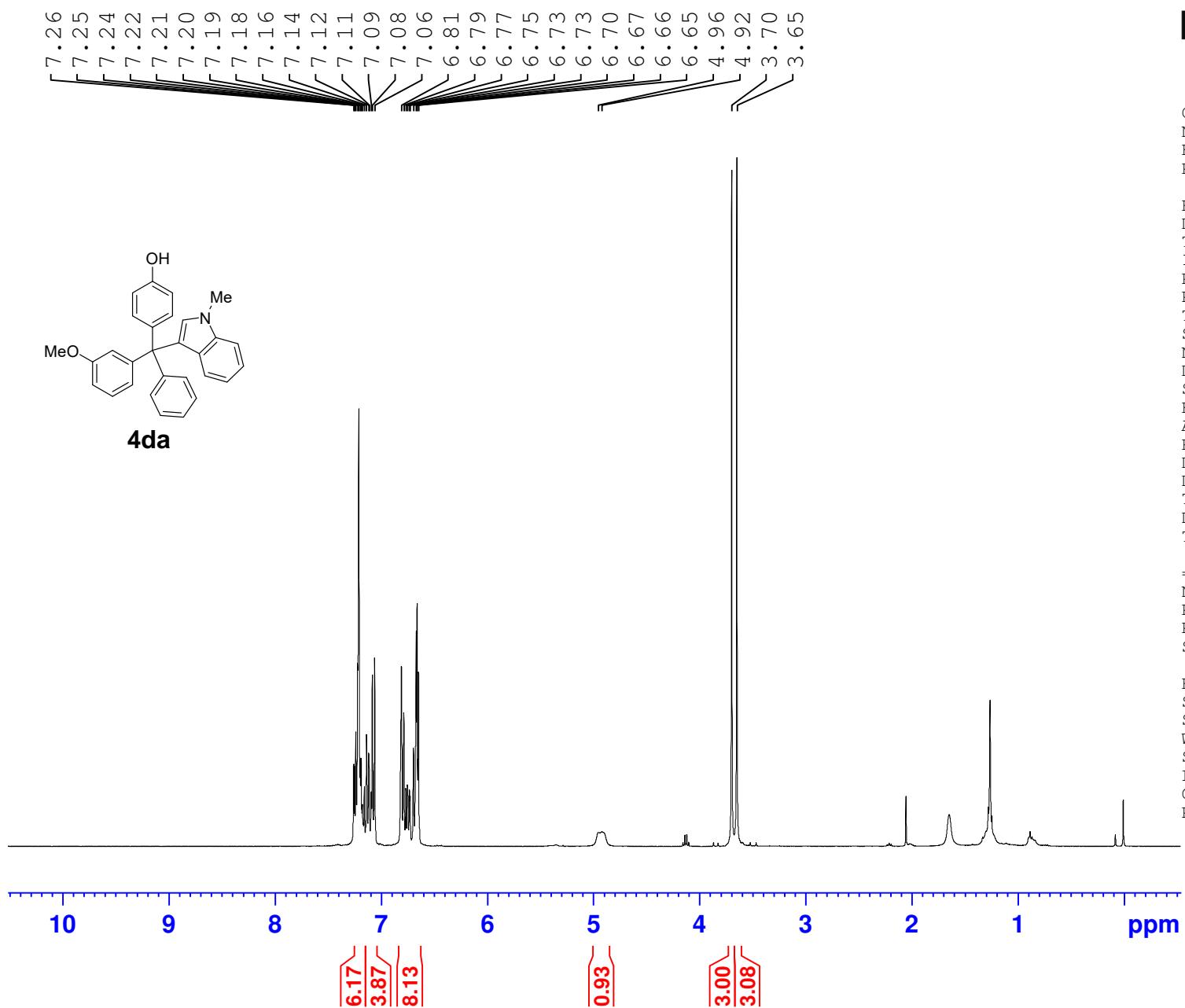
F2 - Acquisition Parameters  
Date\_ 20211022  
Time 12.45  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 500  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE -59.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 ======  
SFO1 75.4752949 MHz  
NUC1 <sup>13</sup>C  
P1 9.50 usec  
PLW1 34.20000076 W

===== CHANNEL f2 ======  
SFO2 300.1312005 MHz  
NUC2 <sup>1</sup>H  
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 75.4677624 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

4da



Current Data Parameters  
NAME 0808-400  
EXPNO 188  
PROCNO 1

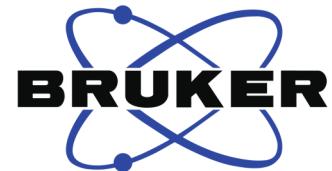
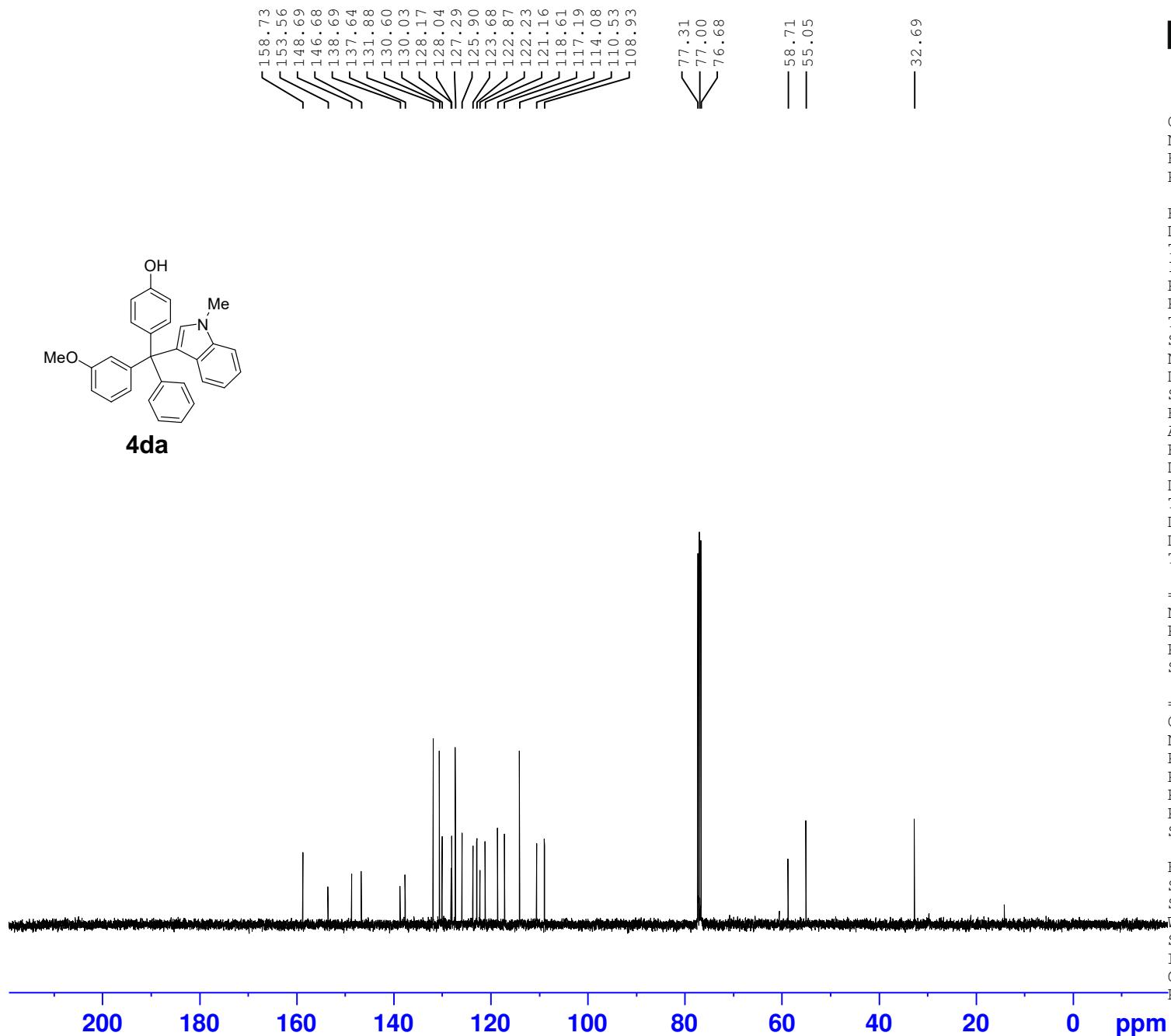
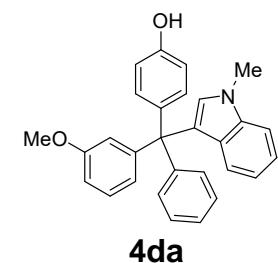
F2 - Acquisition Parameters  
Date\_ 20220808  
Time 21.38  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 8  
DS 0  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9845889 sec  
RG 125.76  
DW 60.800 usec  
DE 6.50 usec  
TE 294.2 K  
D1 1.0000000 sec  
TD0 1

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

NUC1 1H  
P1 14.68 usec  
PLW1 14.00000000 W  
SFO1 400.1924713 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1900204 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

4da



Current Data Parameters  
 NAME 0729-400(2)  
 EXPNO 115  
 PROCNO 1

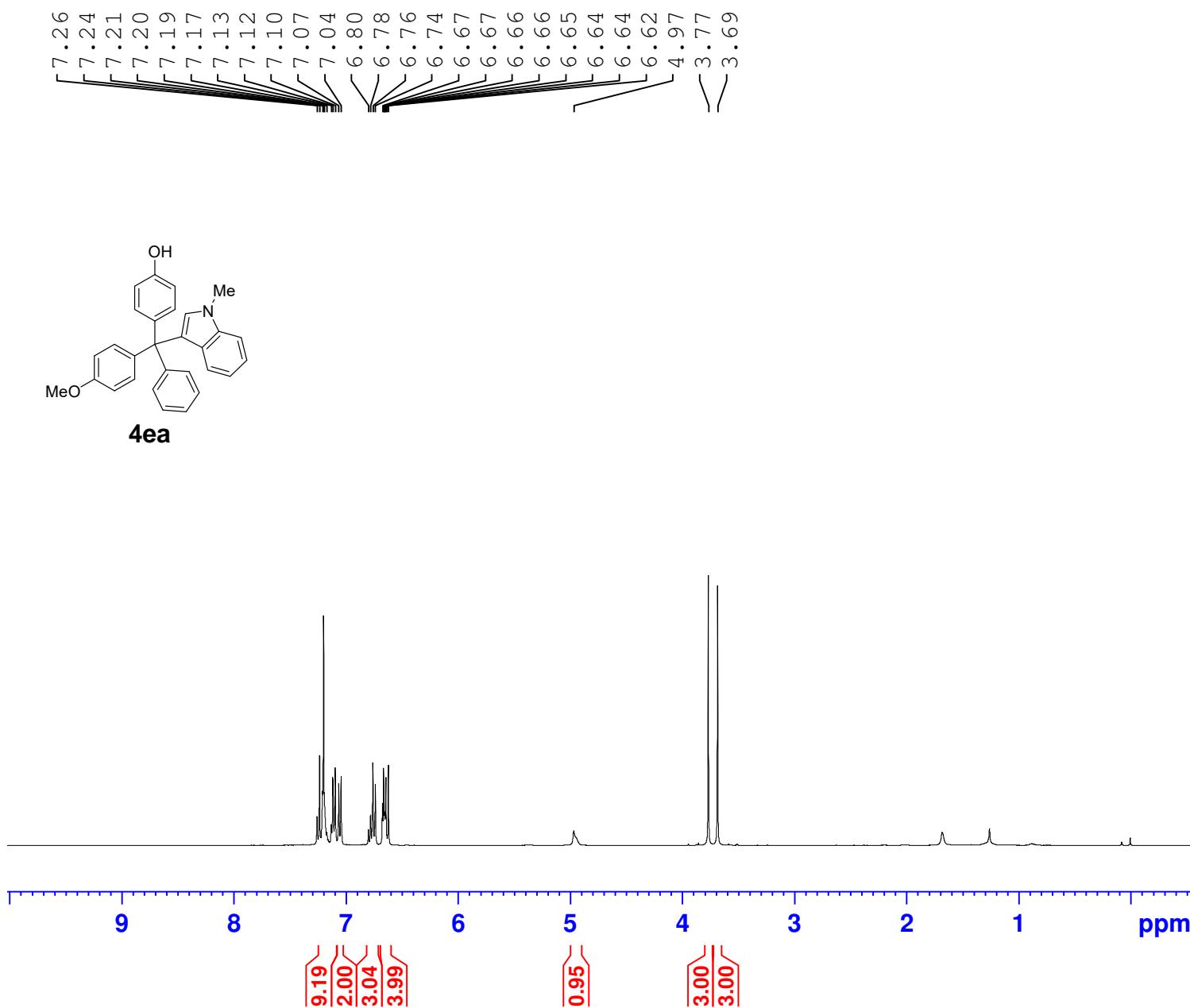
F2 - Acquisition Parameters  
 Date\_ 20220729  
 Time 22.10  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 140  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 193.13  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.4 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 ======  
 NUC1 <sup>13</sup>C  
 P1 12.00 usec  
 PLW1 53.00000000 W  
 SFO1 100.6379178 MHz

===== CHANNEL f2 ======  
 CPDPRG[2 waltz16  
 NUC2 <sup>1</sup>H  
 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 100.6278643 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

4ea



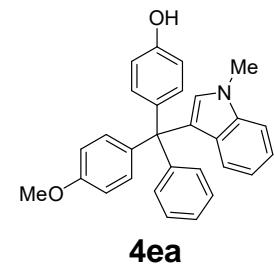
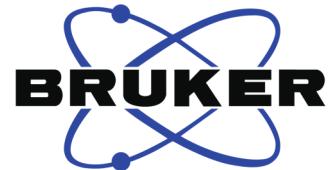
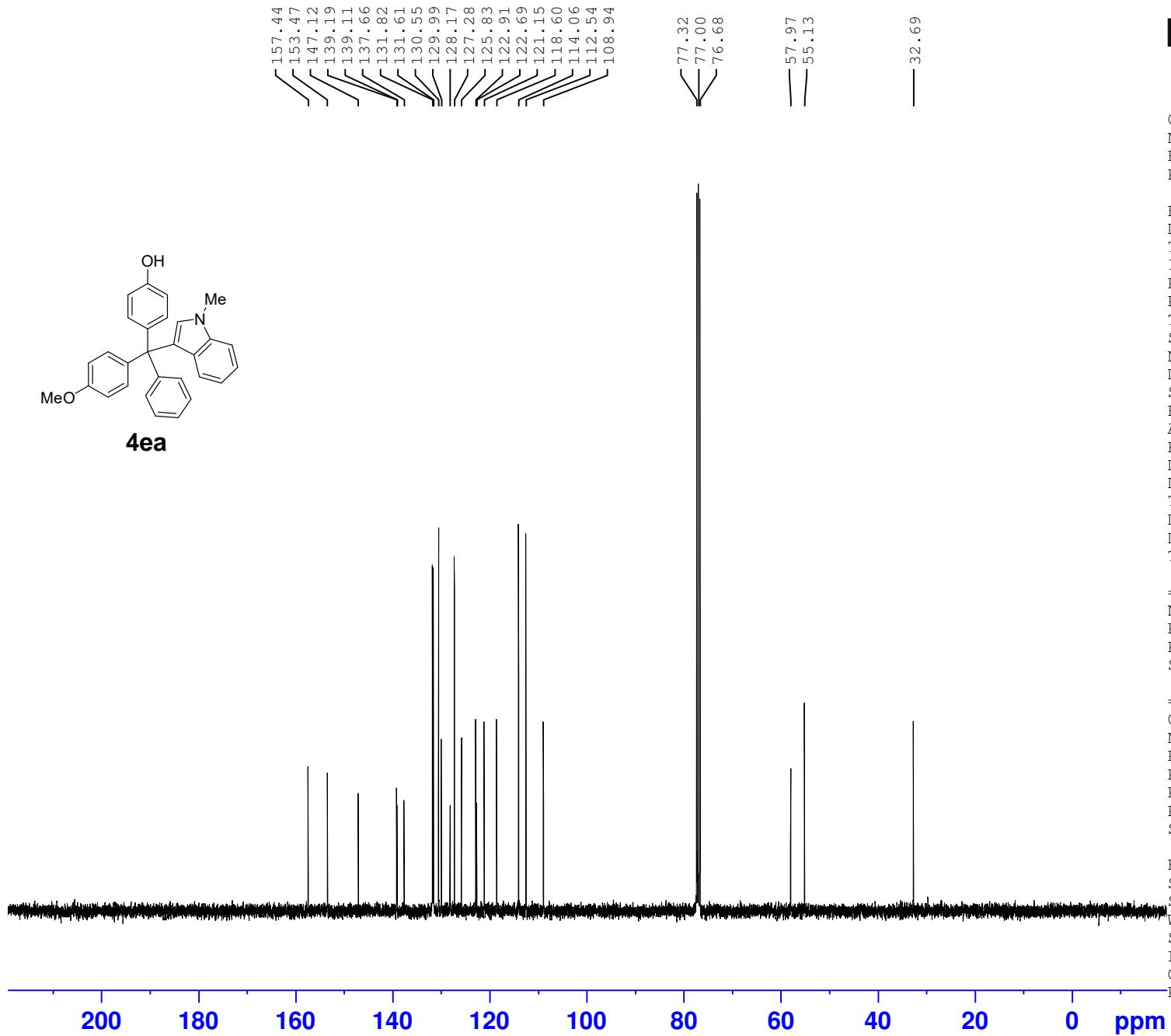
Current Data Parameters  
 NAME 0729-400(2)  
 EXPNO 116  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220729  
 Time 22.19  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl<sub>3</sub>  
 NS 24  
 DS 0  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9845889 sec  
 RG 100.49  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 294.8 K  
 D1 1.0000000 sec  
 TD0 1

===== CHANNEL f1 ======  
 NUC1 1H  
 P1 14.68 usec  
 PLW1 14.00000000 W  
 SFO1 400.1924713 MHz

F2 - Processing parameters  
 SI 65536  
 SF 400.1900260 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

4ea

**4ea**

Current Data Parameters  
 NAME 0729-400(2)  
 EXPNO 117  
 PROCNO 1

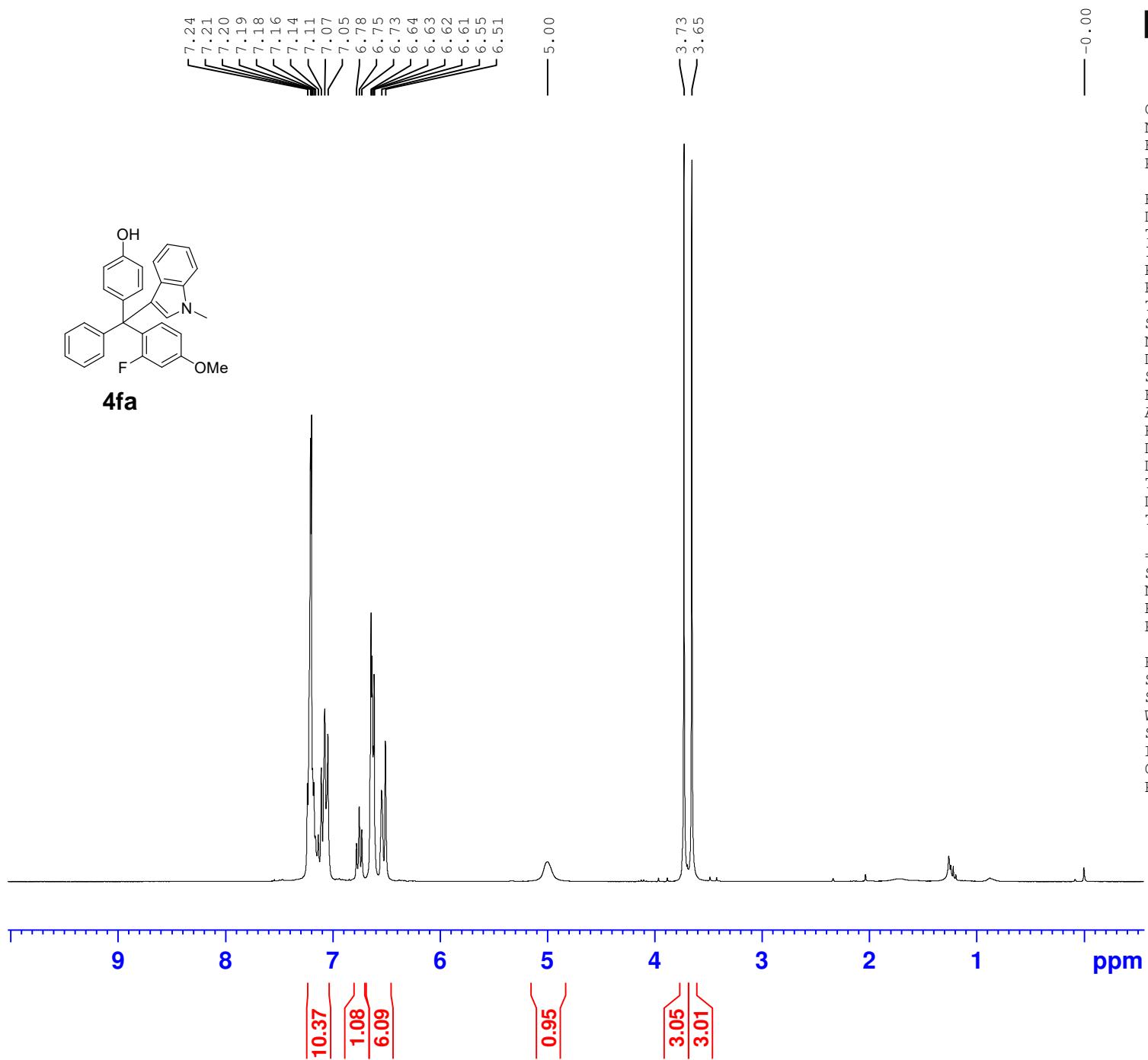
F2 - Acquisition Parameters  
 Date\_ 20220729  
 Time 22.32  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 200  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 193.13  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.5 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 ======  
 NUC1 <sup>13</sup>C  
 P1 12.00 usec  
 PLW1 53.00000000 W  
 SFO1 100.6379178 MHz

===== CHANNEL f2 ======  
 CPDPRG[2 waltz16  
 NUC2 <sup>1</sup>H  
 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 100.6278644 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

4fa



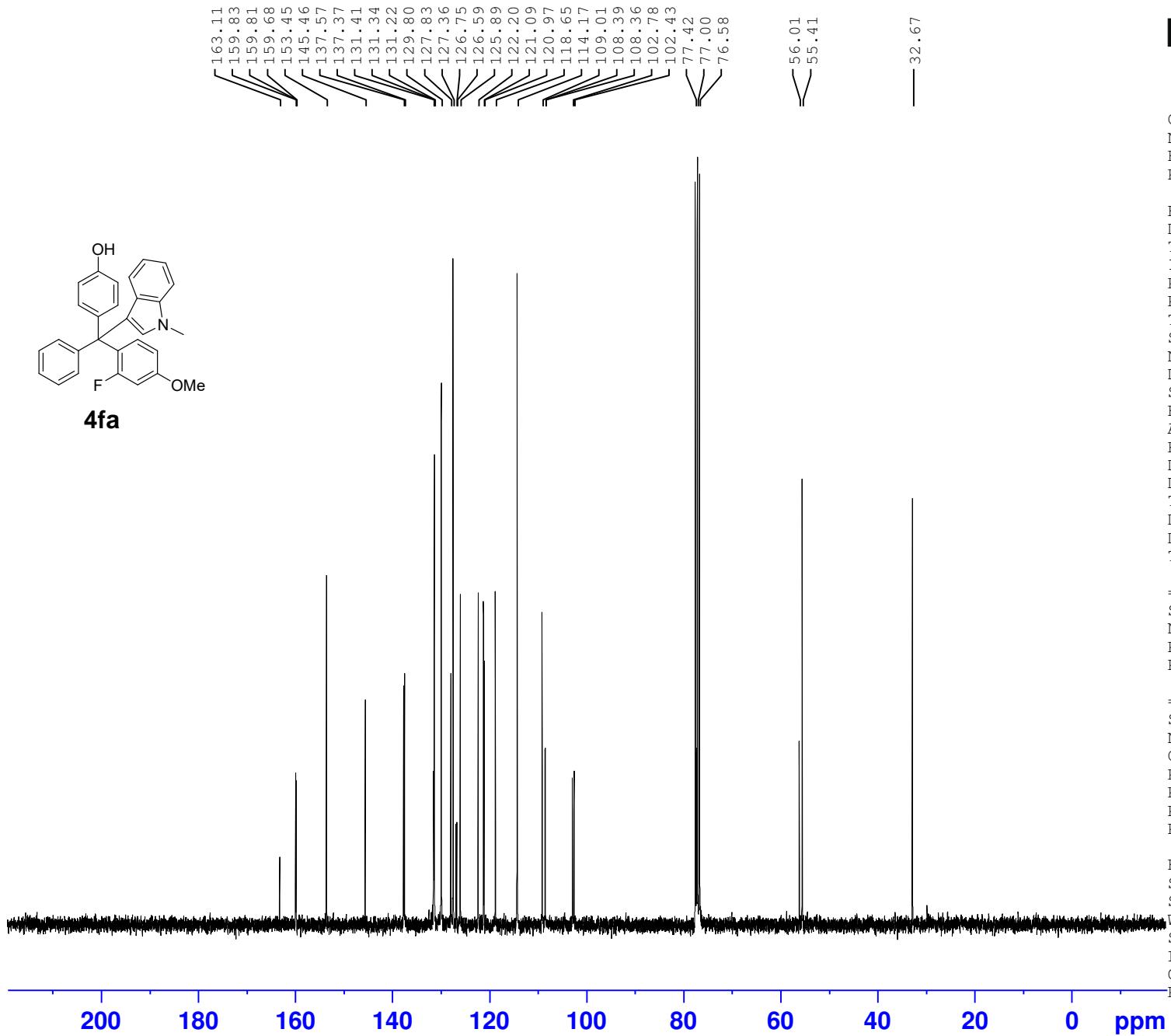
Current Data Parameters  
NAME ZY-4-56B-h-fr  
EXPNO 5620  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211116  
Time 11.14  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 71.8  
DW 83.200 usec  
DE 6.50 usec  
TE -59.1 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 300.1300257 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

4fa



Current Data Parameters  
 NAME ZY-4-56B-c-fr  
 EXPNO 5622  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20211116  
 Time 11.50  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 500  
 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 -59.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

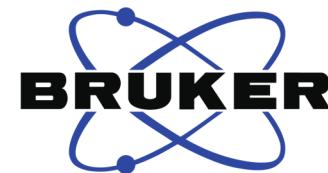
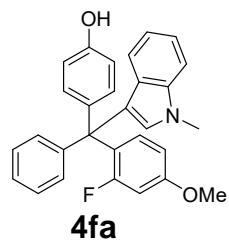
===== CHANNEL f1 ======  
 SFO1 75.4752949 MHz  
 NUC1 13C  
 P1 9.50 usec  
 PLW1 34.20000076 W

===== 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 75.4677583 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

4fa

-99.036



Current Data Parameters  
 NAME 211116sjw  
 EXPNO 5621  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20211116  
 Time 11.16  
 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 -59.1 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

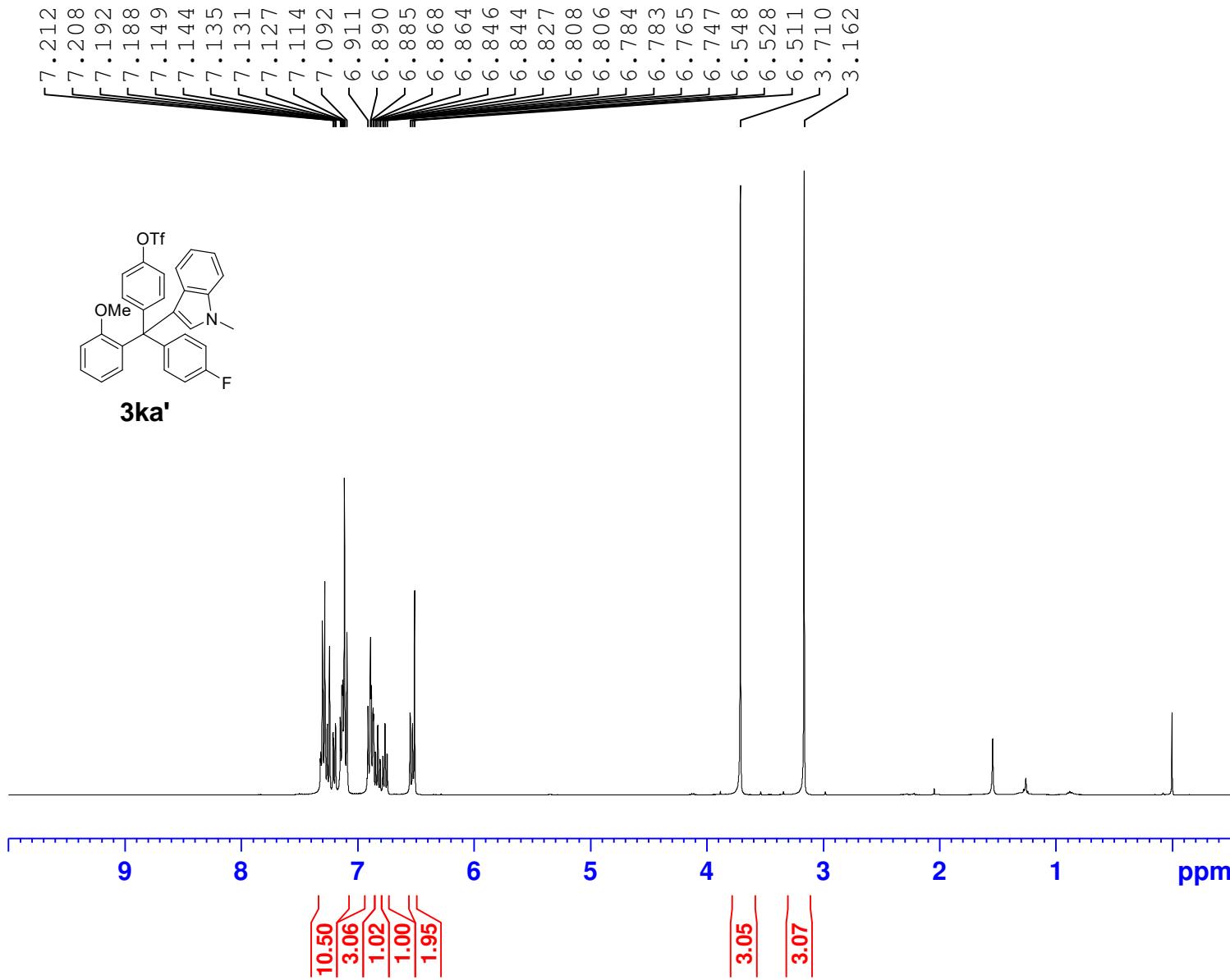
===== CHANNEL f2 ======  
 SFO2 300.1312005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 14.00000000 W  
 PLW12 0.17284000 W

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

0 -20 -40 -60 -80 -100 -120 -140 -160 -180

ppm

3ka'

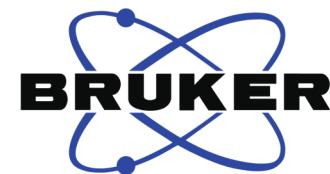
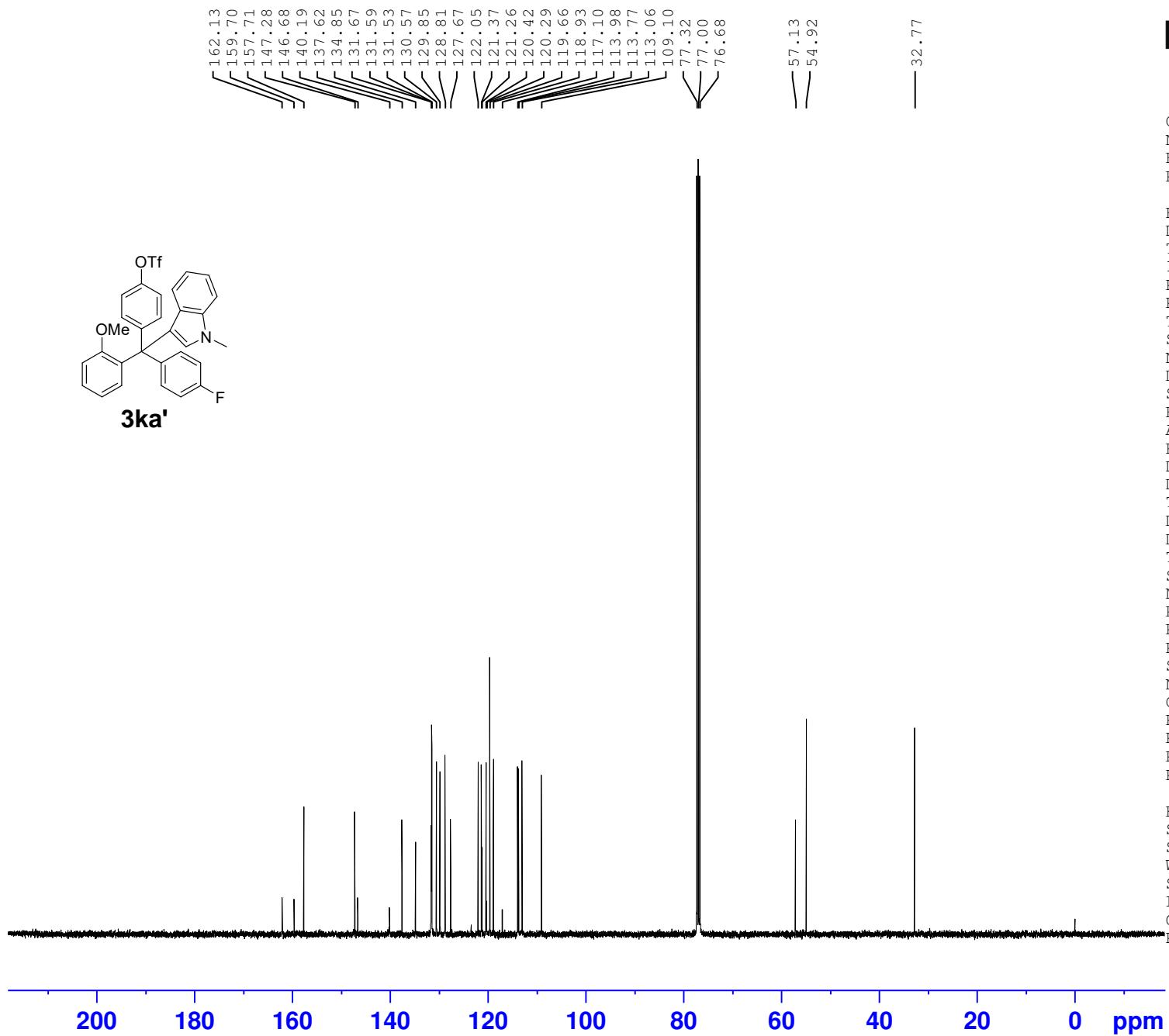


Current Data Parameters  
NAME ZY-5-41-h-fr  
EXPNO 6  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220608  
Time 1.51 h  
INSTRUM Avance  
PROBHD Z116098\_0833 (zg30  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
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 292.1 K  
D1 1.0000000 sec  
TD0 1  
SFO1 400.1324708 MHz  
NUC1 <sup>1</sup>H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 20.73200035 W

F2 - Processing parameters  
SI 65536  
SF 400.1300170 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

3ka'

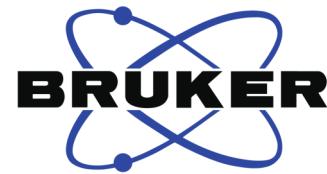
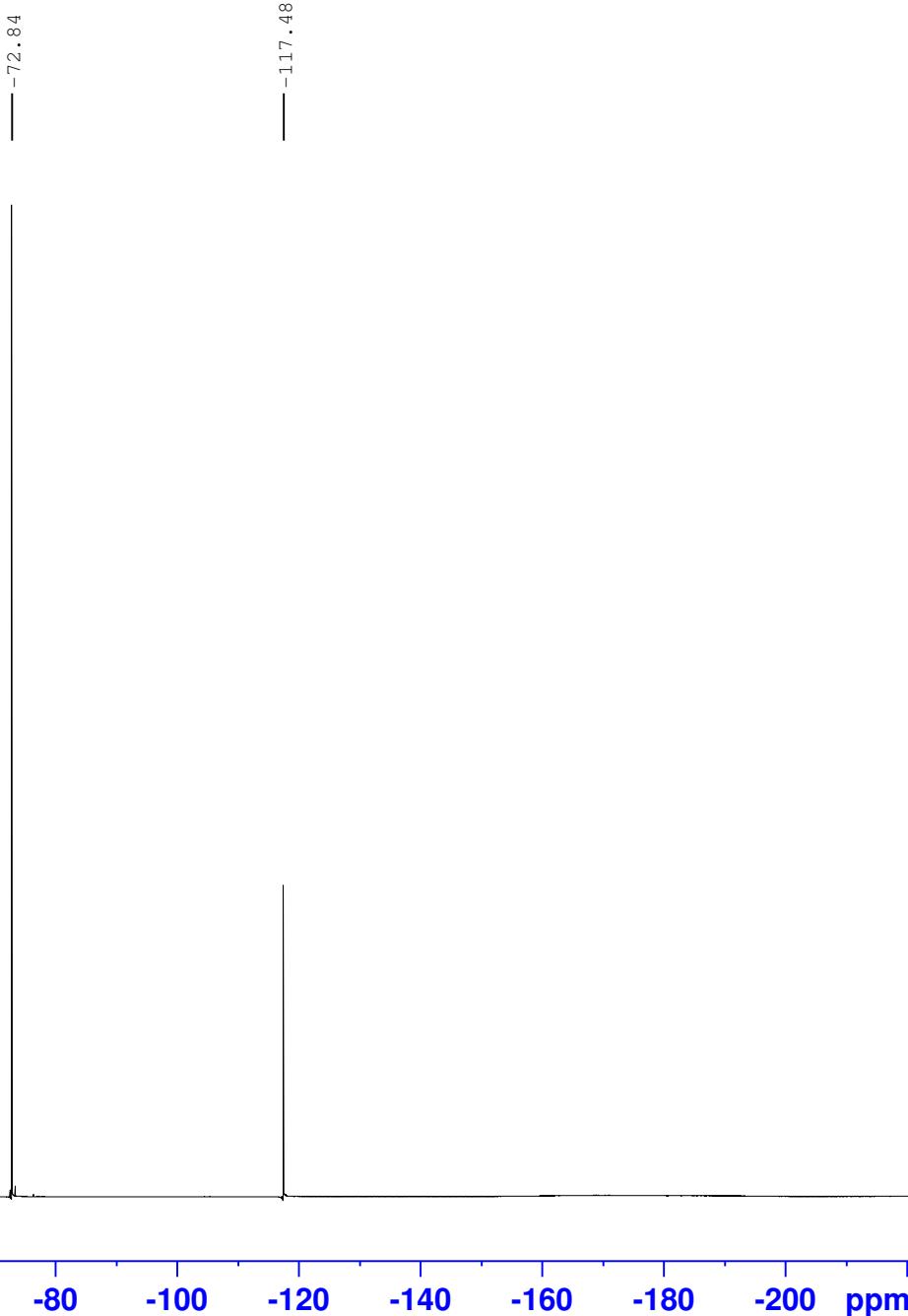
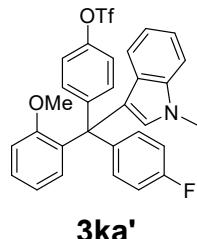


Current Data Parameters  
NAME 3ka'-ZY-5-41OTf  
EXPNO 7  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220608  
Time 2.51 h  
INSTRUM Avance  
PROBHD Z116098\_0833 (   
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 52.9819  
DW 21.000 usec  
DE 6.50 usec  
TE 292.7 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 100.6127748 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

3ka'

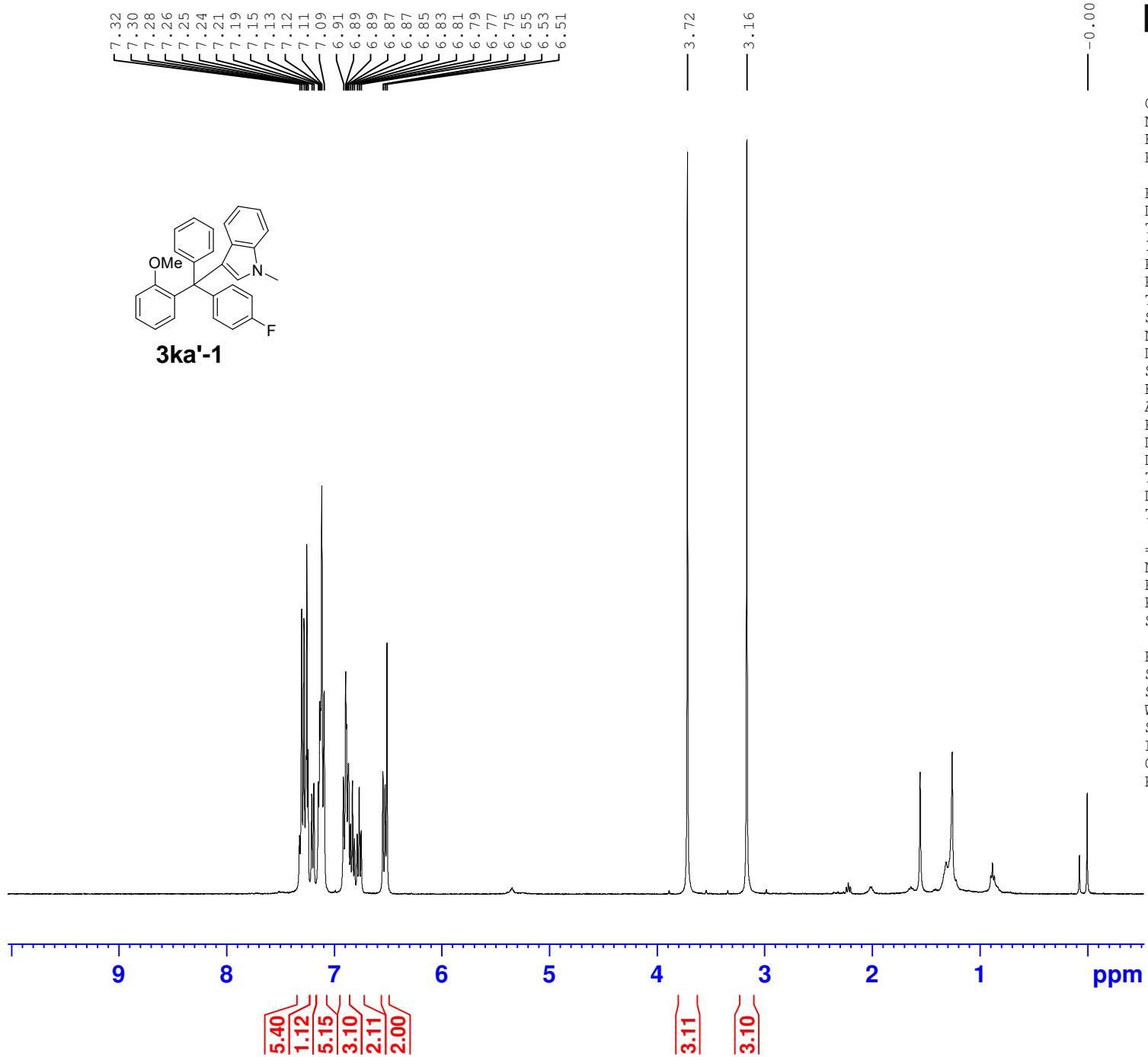


Current Data Parameters  
NAME ZY-5-41-f-fr  
EXPNO 8  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220608  
Time 2.53 h  
INSTRUM Avance  
PROBHD Z116098\_0833 (   
PULPROG zgig  
TD 131072  
SOLVENT CDCl<sub>3</sub>  
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 292.3 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 376.4607164 MHz  
NUC1 <sup>19</sup>F  
P1 18.00 usec  
PLW1 16.73100090 W  
SFO2 400.1316005 MHz  
NUC2 <sup>1</sup>H  
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

3ka'-1



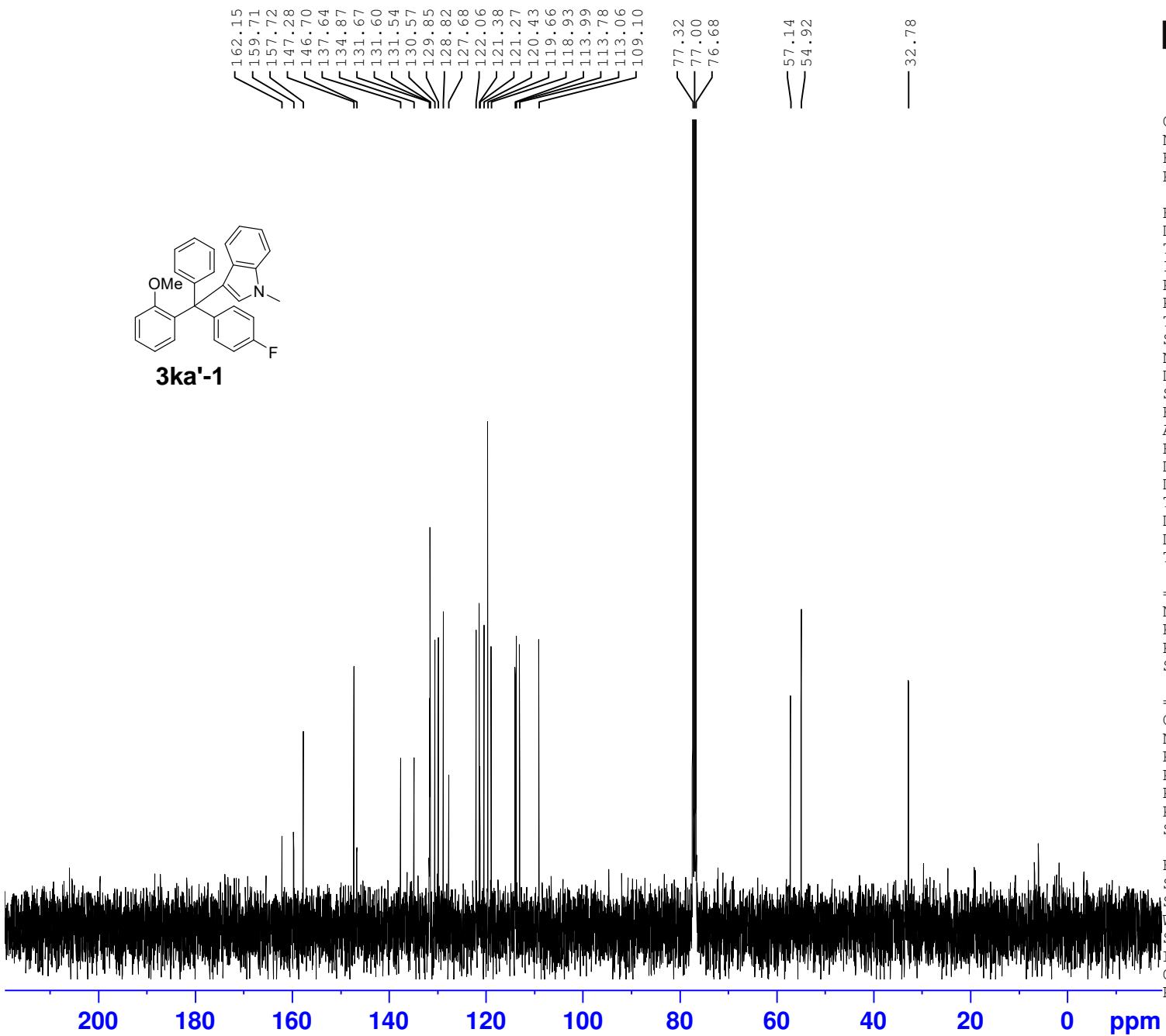
Current Data Parameters  
NAME ZY-5-46-h-fr  
EXPNO 416  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220113  
Time 21.10  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 6  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9845889 sec  
RG 181.41  
DW 60.800 usec  
DE 6.50 usec  
TE 292.6 K  
D1 1.0000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 14.40 usec  
PLW1 14.00000000 W  
SFO1 400.1924713 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1900180 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

3ka'-1



Current Data Parameters  
NAME 3ka'-1-ZY-5-46-OTf  
EXPNO 417  
PROCNO 1

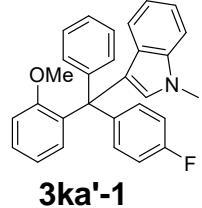
F2 - Acquisition Parameters  
Date\_ 20220113  
Time 21.12  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 190  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 193.13  
DW 20.800 usec  
DE 6.50 usec  
TE 292.9 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 ======  
NUC1 13C  
P1 9.90 usec  
PLW1 53.00000000 W  
SFO1 100.6379178 MHz

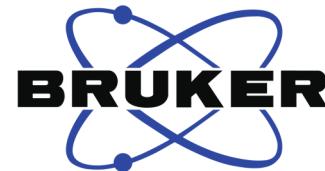
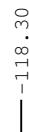
===== CHANNEL f2 ======  
CPDPGRG[2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.35839999 W  
PLW13 0.29030001 W  
SFO2 400.1916008 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6278614 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

3ka'-1



$$3ka' - 1$$



Current	Data	Parameters
NAME	211129sjw	
EXPNO	5668	
PROCNO		1

```

F2 - Acquisition Parameters
Date_           20211129
Time            8.58
INSTRUM         spect
PROBHD         5 mm PABBO BB-
PULPROG        zgfhigqn.2
TD              131072
SOLVENT         CDCI3
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              -59.1 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
PCPDP2     90.00 usec
PLW2      14.00000000 W
PLW12     0.17284000 W

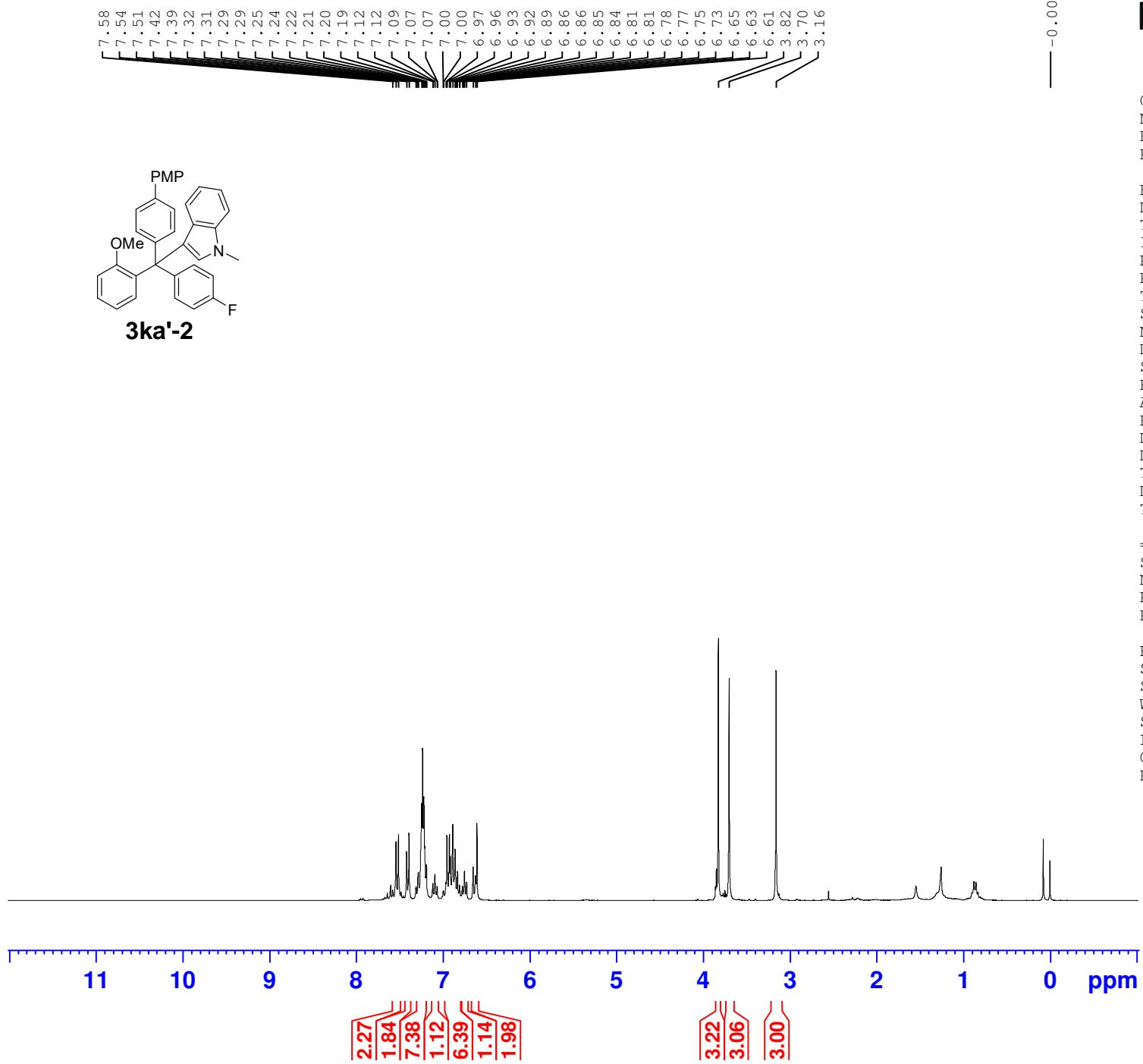
```

```

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

```

3ka'-2



Current Data Parameters  
NAME ZY-5-42-h-fr  
EXPNO 5690  
PROCNO 1

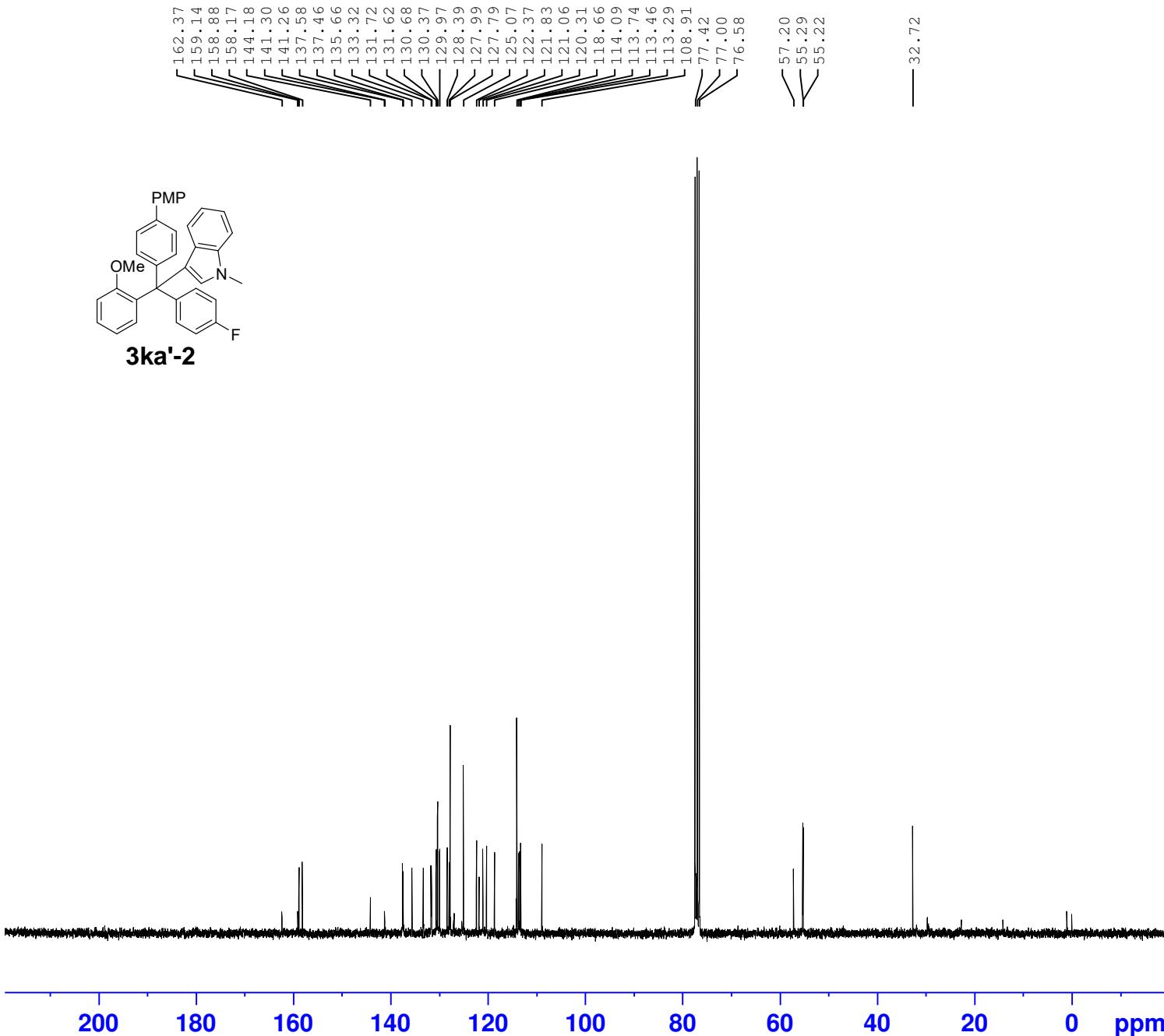
F2 - Acquisition Parameters  
Date\_ 20211207  
Time 9.05  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.091699 Hz  
AQ 5.4525952 sec  
RG 128  
DW 83.200 usec  
DE 6.50 usec  
TE -59.1 K  
D1 1.00000000 sec  
TD0 1

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

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

F2 - Processing parameters  
SI 65536  
SF 300.1300145 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

3ka'-2



Current Data Parameters  
NAME 3ka'-2-ZY-5-42-Kumada  
EXPNO 5691  
PROCNO 1

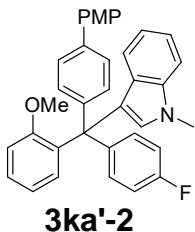
F2 - Acquisition Parameters  
Date\_ 20211207  
Time 10.15  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 4  
SWH 18028.846 Hz  
FIDRES 0.275098 Hz  
AQ 1.8175317 sec  
RG 203  
DW 27.733 usec  
DE 6.50 usec  
TE -59.1 K  
D1 2.0000000 sec  
D11 0.03000000 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 14.0000000 W  
PLW12 0.17284000 W  
PLW13 0.14000000 W

F2 - Processing parameters  
SI 32768  
SF 75.4677538 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

3ka'-2



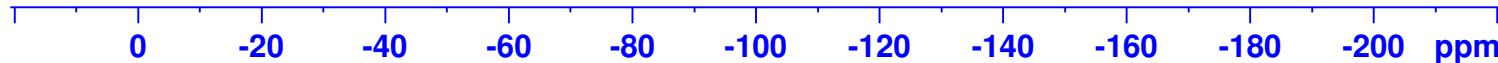
-118.21



Current Data Parameters  
NAME 0607HH  
EXPNO 1  
PROCNO 1

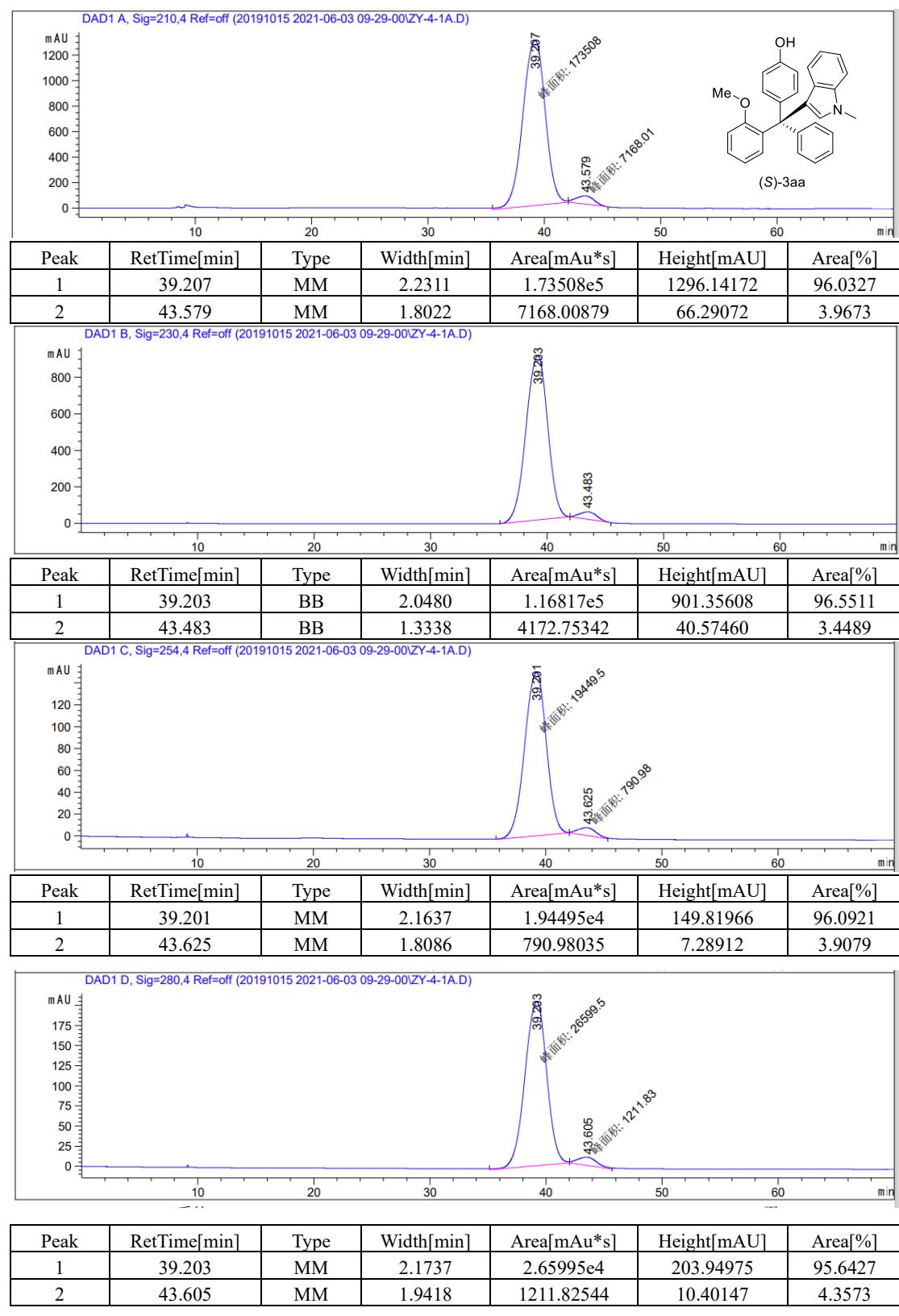
F2 - Acquisition Parameters  
Date\_ 20220607  
Time 21.19 h  
INSTRUM Avance  
PROBHD Z116098\_0833 (   
PULPROG zgig  
TD 131072  
SOLVENT CDCl3  
NS 16  
DS 4  
SWH 90909.094 Hz  
FIDRES 1.387163 Hz  
AQ 0.7208960 sec  
RG 101  
DW 5.500 usec  
DE 6.50 usec  
TE 291.8 K  
D1 1.00000000 sec  
D11 0.03000000 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



Sample Name: ZY-4-1-OP

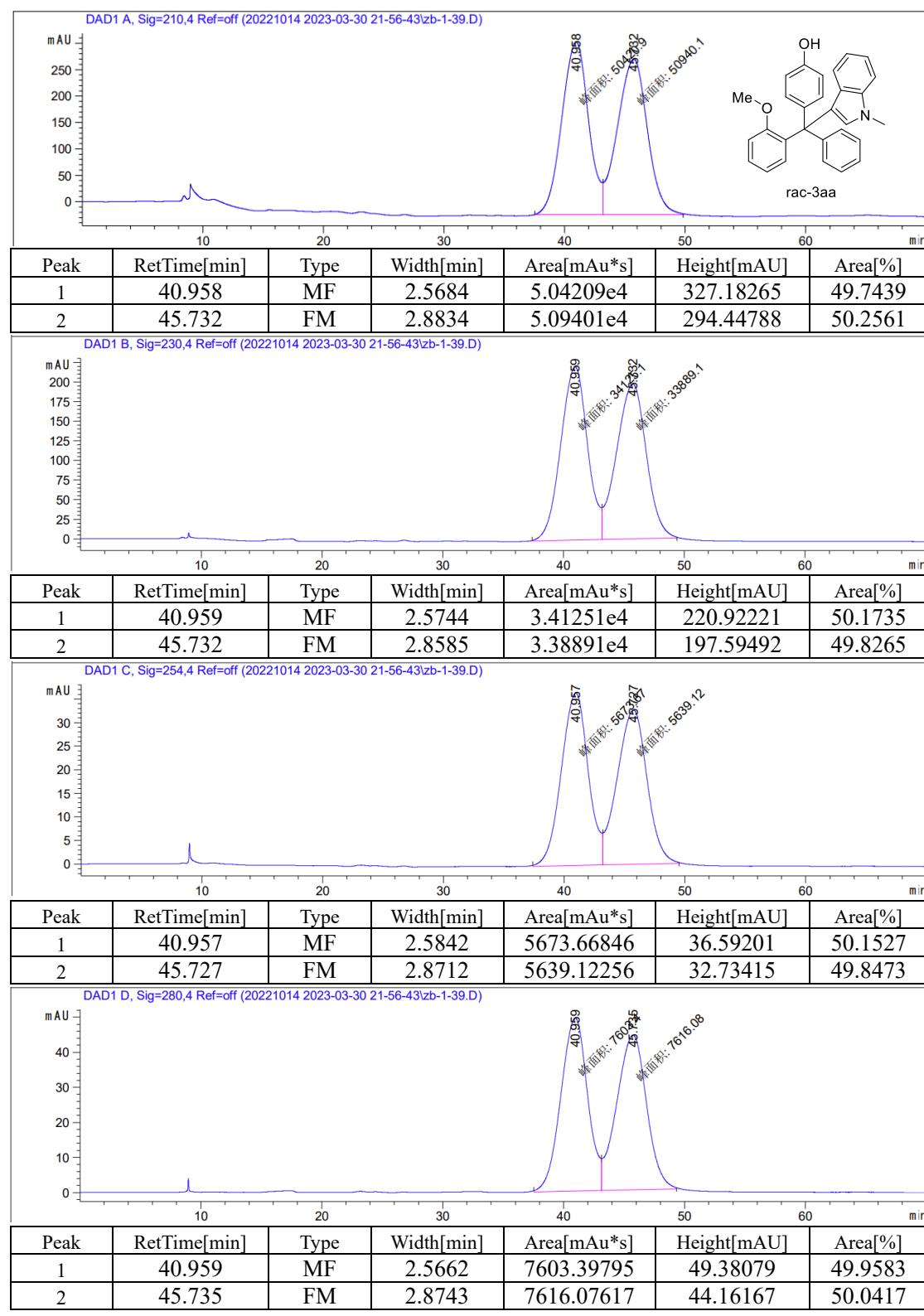
HPLC Condition: IC, *n*-Hexane/iPrOH = 98:2, 0.4 mL/min



End of Report

Sample Name: ZY-4-1-Rac

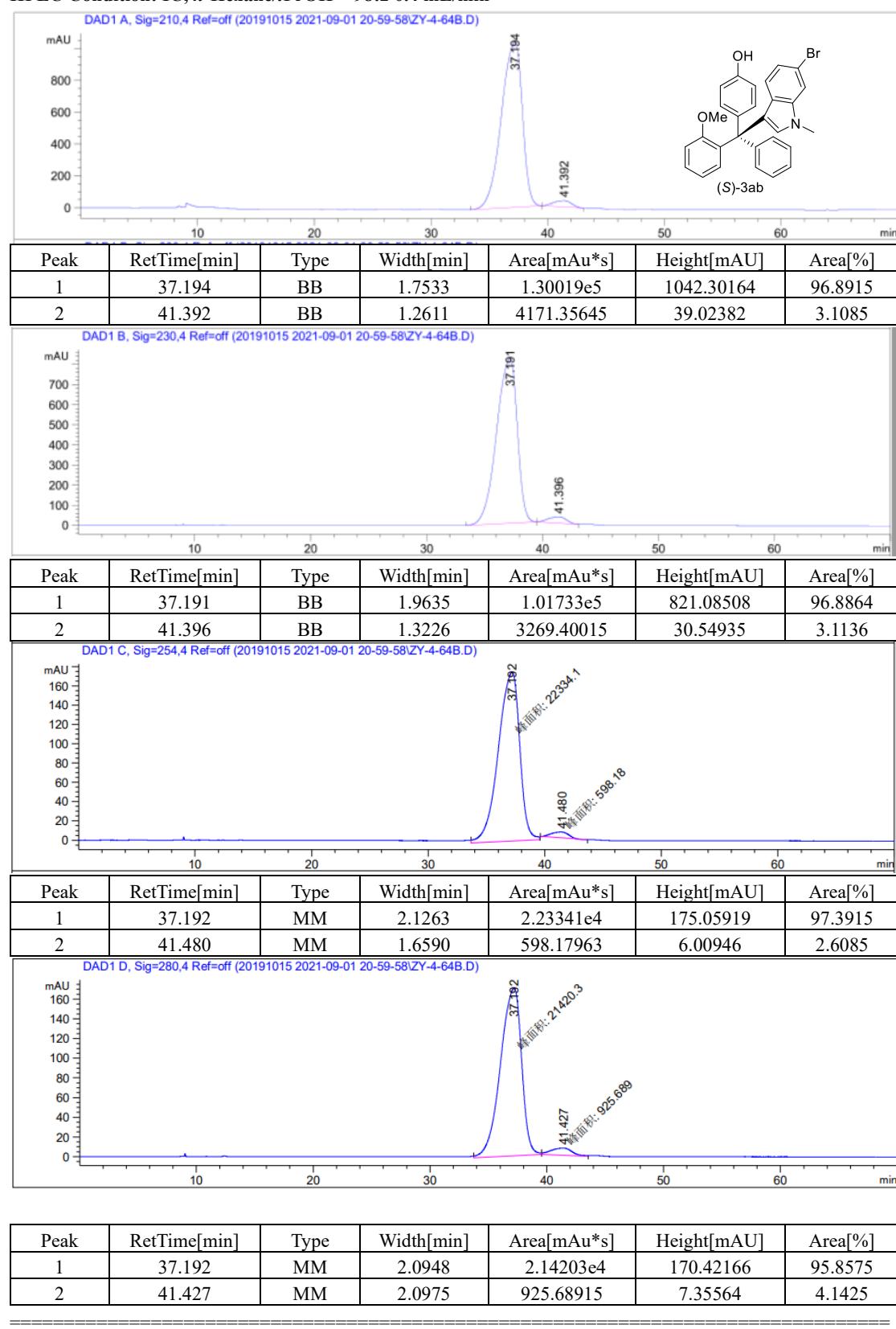
HPLC Condition: IC, n-Hexane/iPrOH = 98:2, 0.4 mL/min



End of Report

Sample Name: ZY-4-64B-OP

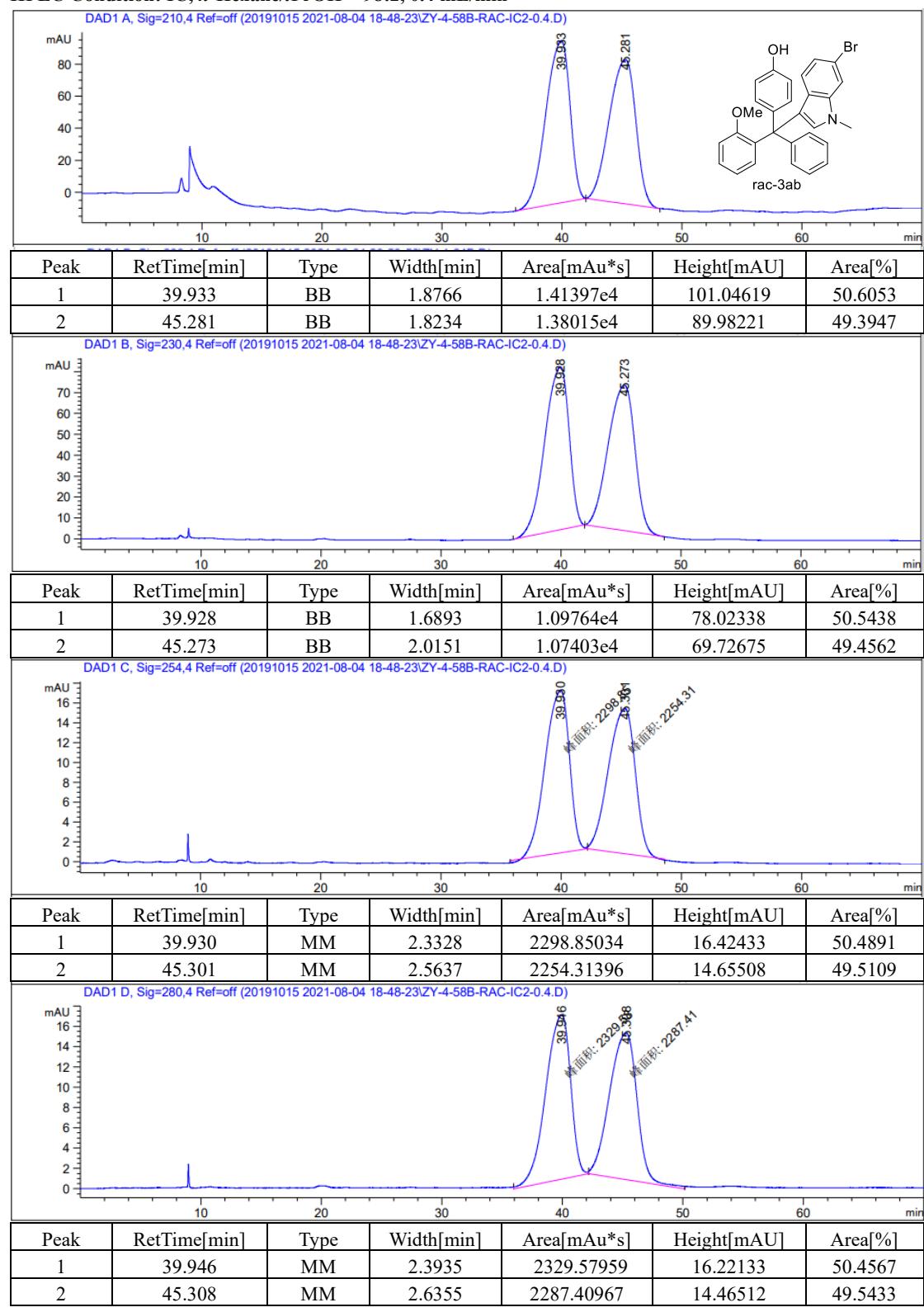
HPLC Condition: IC, *n*-Hexane/iPrOH = 98:2 0.4 mL/min



End of Report

Sample Name: ZY-4-58B-Rac

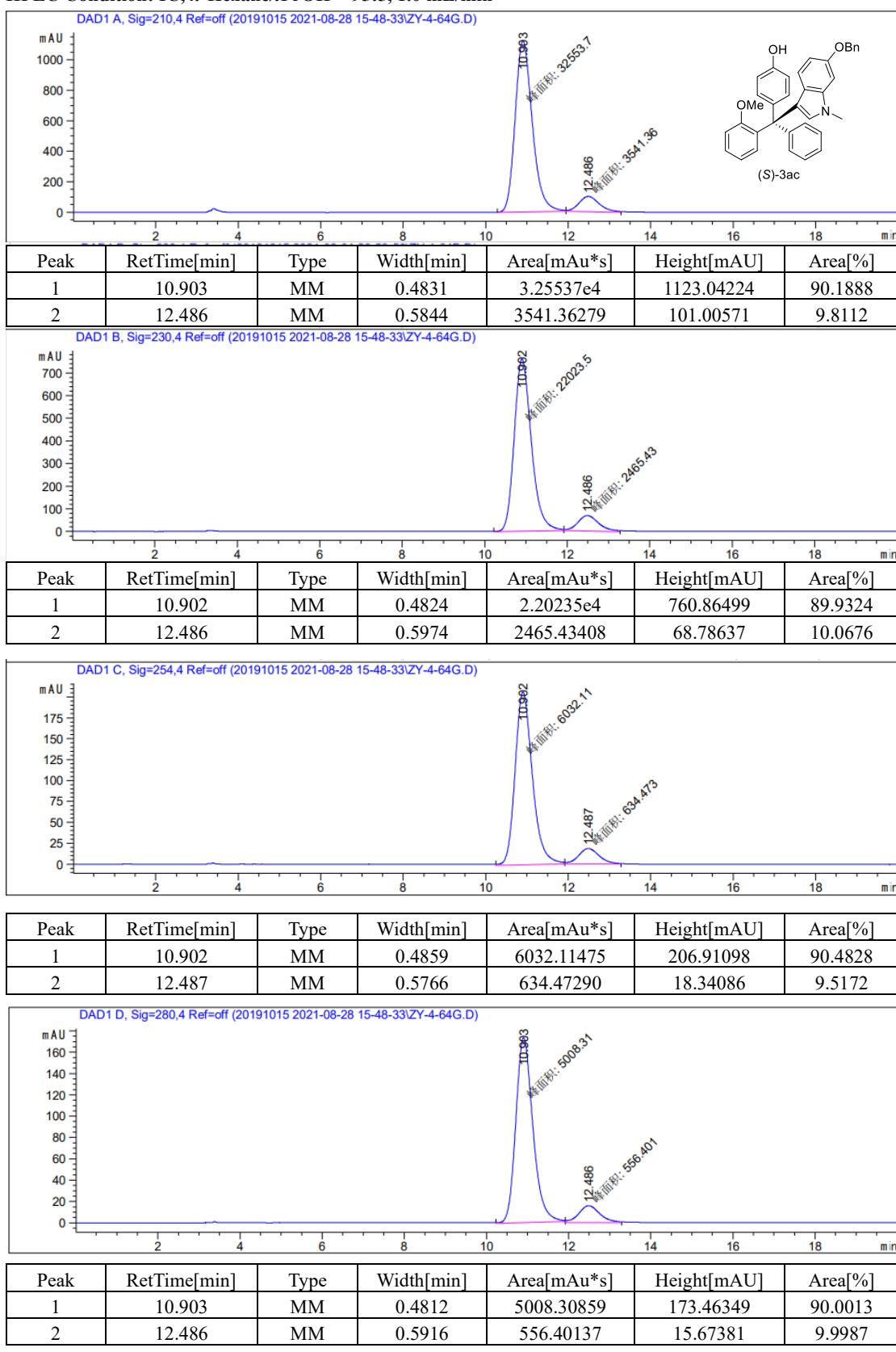
HPLC Condition: IC, *n*-Hexane/iPrOH = 98:2, 0.4 mL/min



End of Report

Sample Name: ZY-4-64G-OP

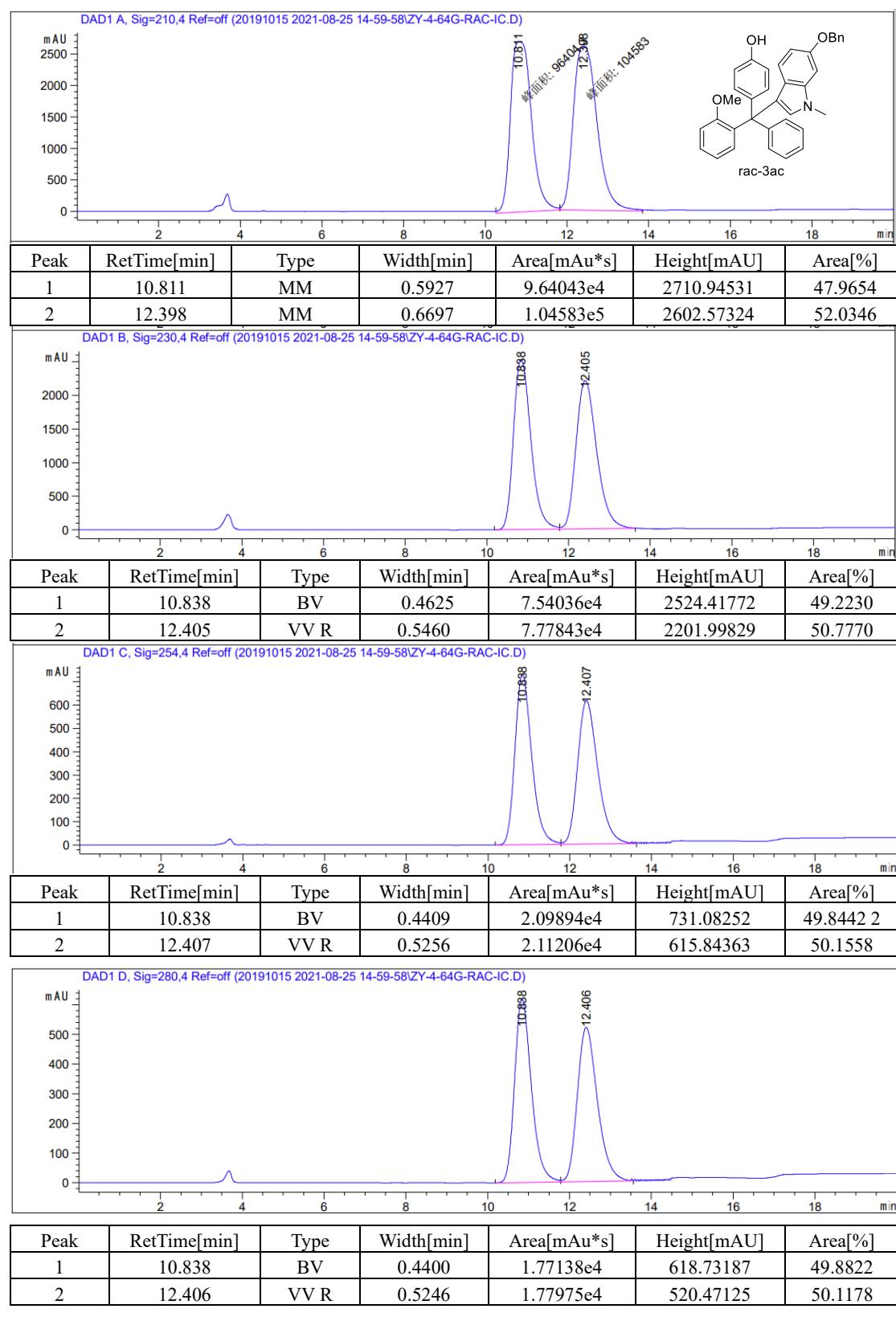
HPLC Condition: IC, *n*-Hexane/iPrOH = 95:5, 1.0 mL/min



End of Report

Sample Name: ZY-4-64G-Rac

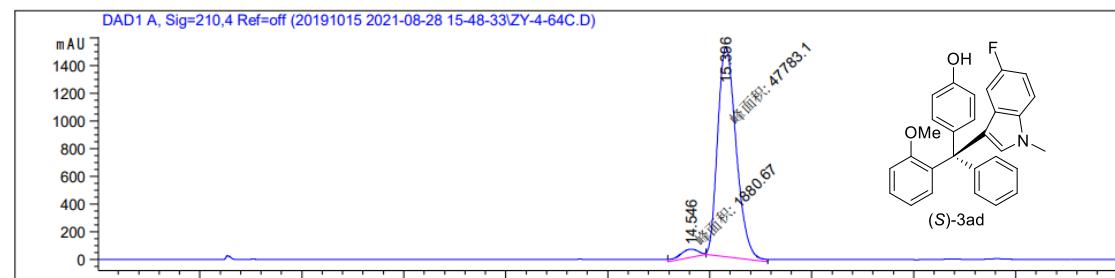
HPLC Condition: IC, n-Hexane/iPrOH = 95:5, 1.0 mL/min



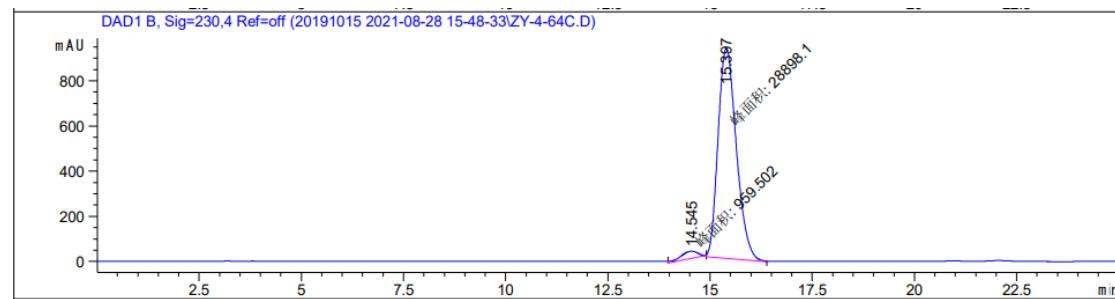
End of Report

Sample Name: ZY-4-64C-OP

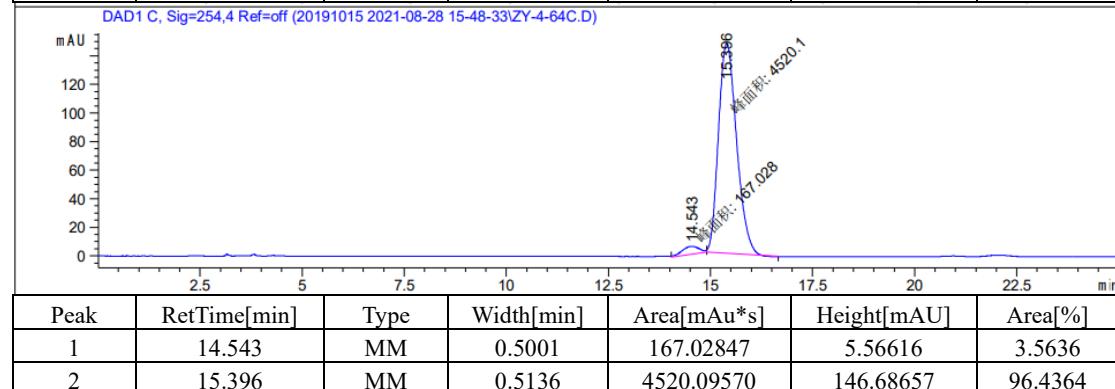
HPLC Condition: AD-H, *n*-Hexane/iPrOH = 95:5, 1.0 mL/min



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	14.546	MM	0.5313	1880.67407	59.00087	3.7868
2	15.396	MM	0.5268	4.77831e4	1511.83679	96.2132



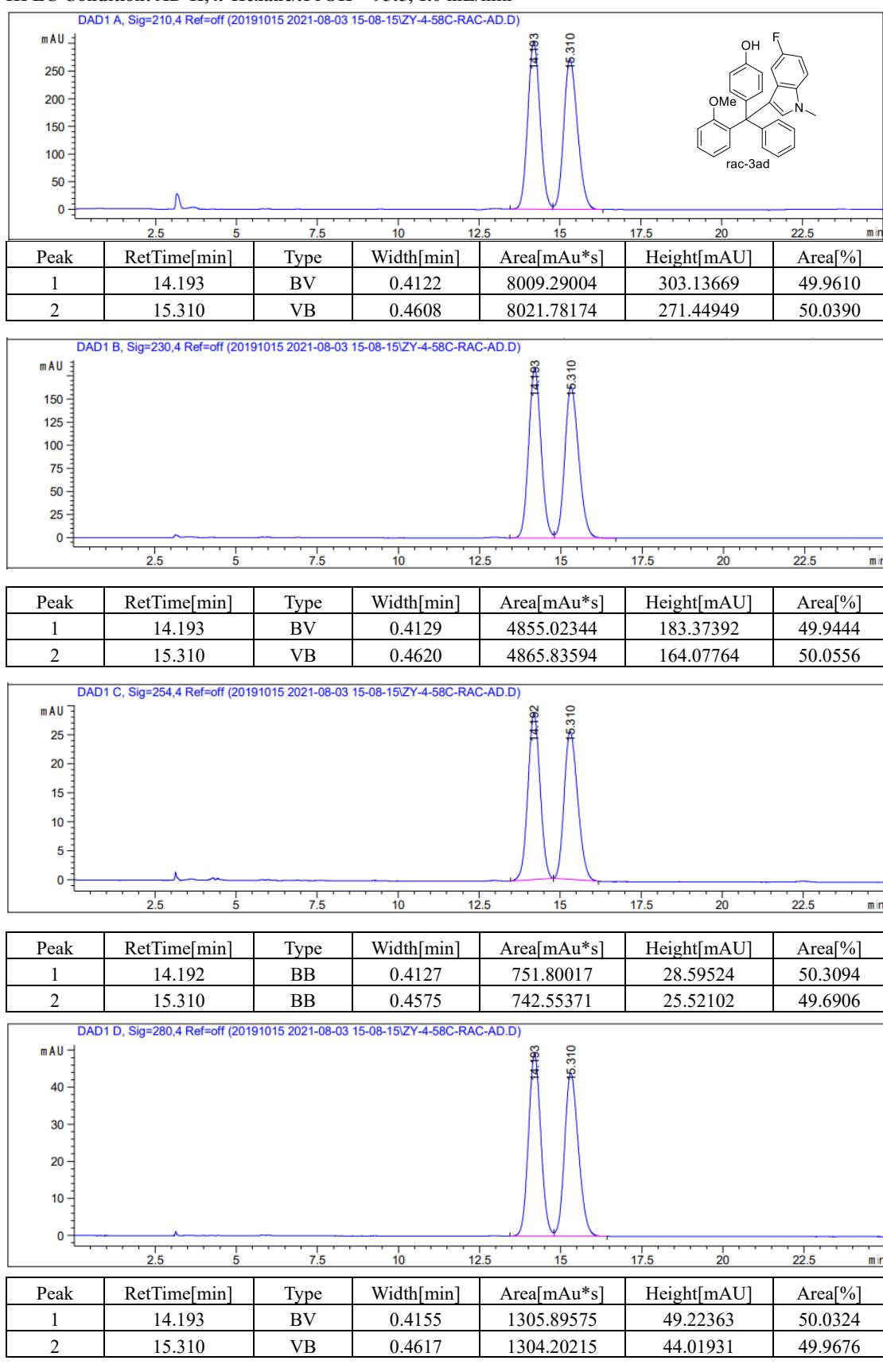
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	14.545	MM	0.4988	959.50208	32.05903	3.2136
2	15.397	MM	0.5182	2.88981e4	929.38043	96.7864



End of Report

Sample Name: ZY-4-58C-Rac

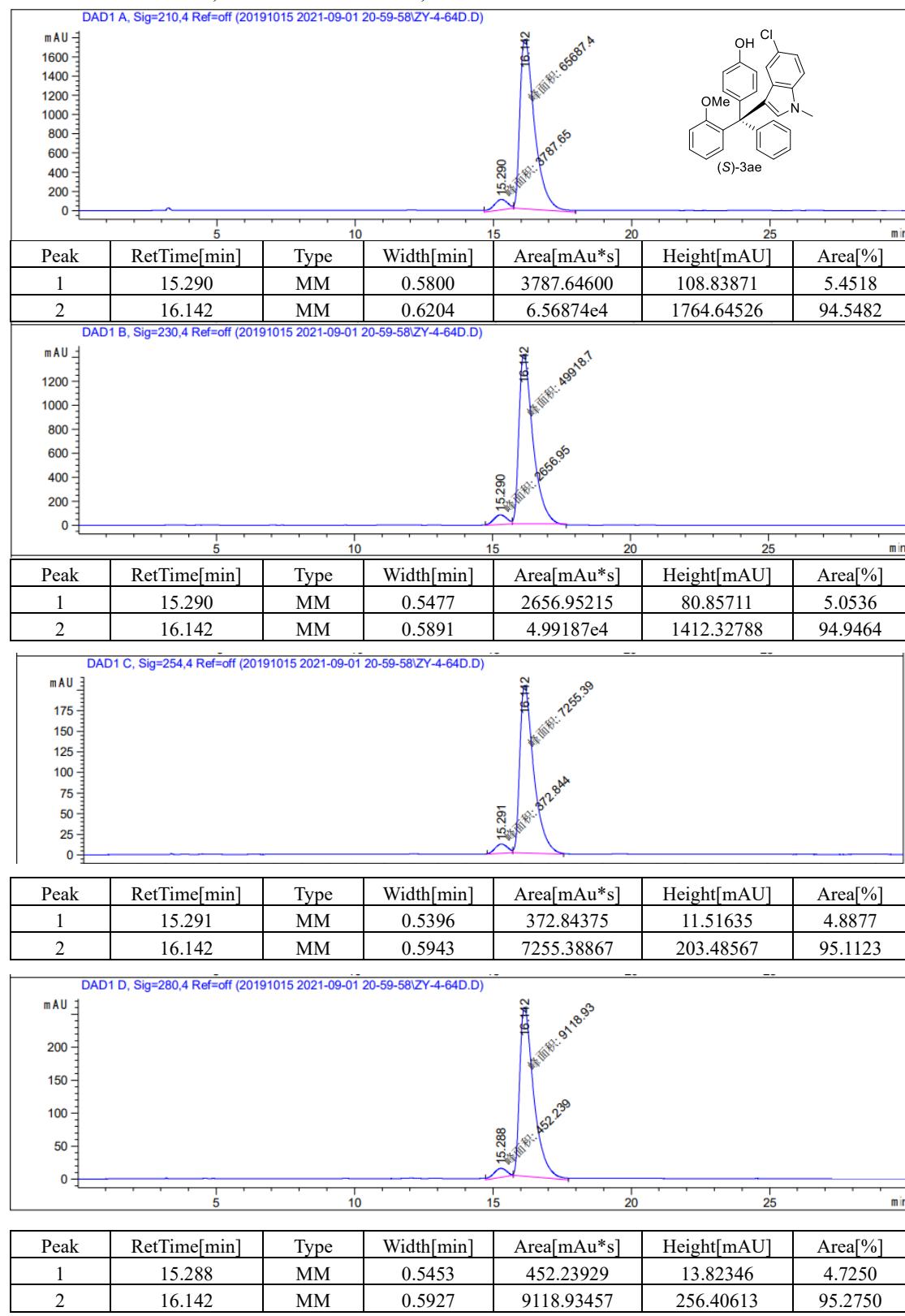
HPLC Condition: AD-H, *n*-Hexane/*i*PrOH = 95:5, 1.0 mL/min



End of Report

Sample Name: ZY-4-64D-OP

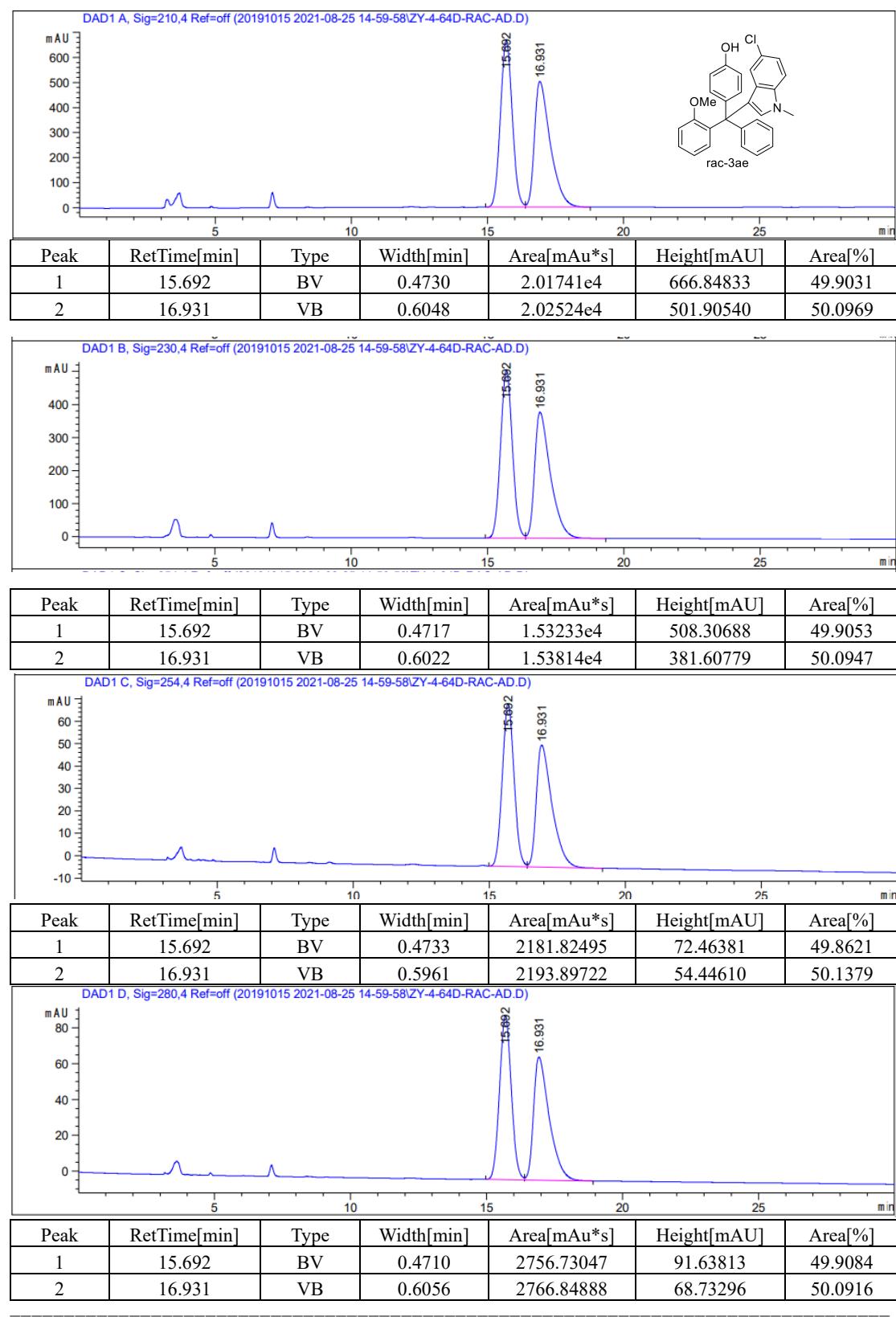
HPLC Condition: AD-H, *n*-Hexane/iPrOH = 95:5, 1.0 mL/min



End of Report

Sample Name: ZY-4-64D-Rac

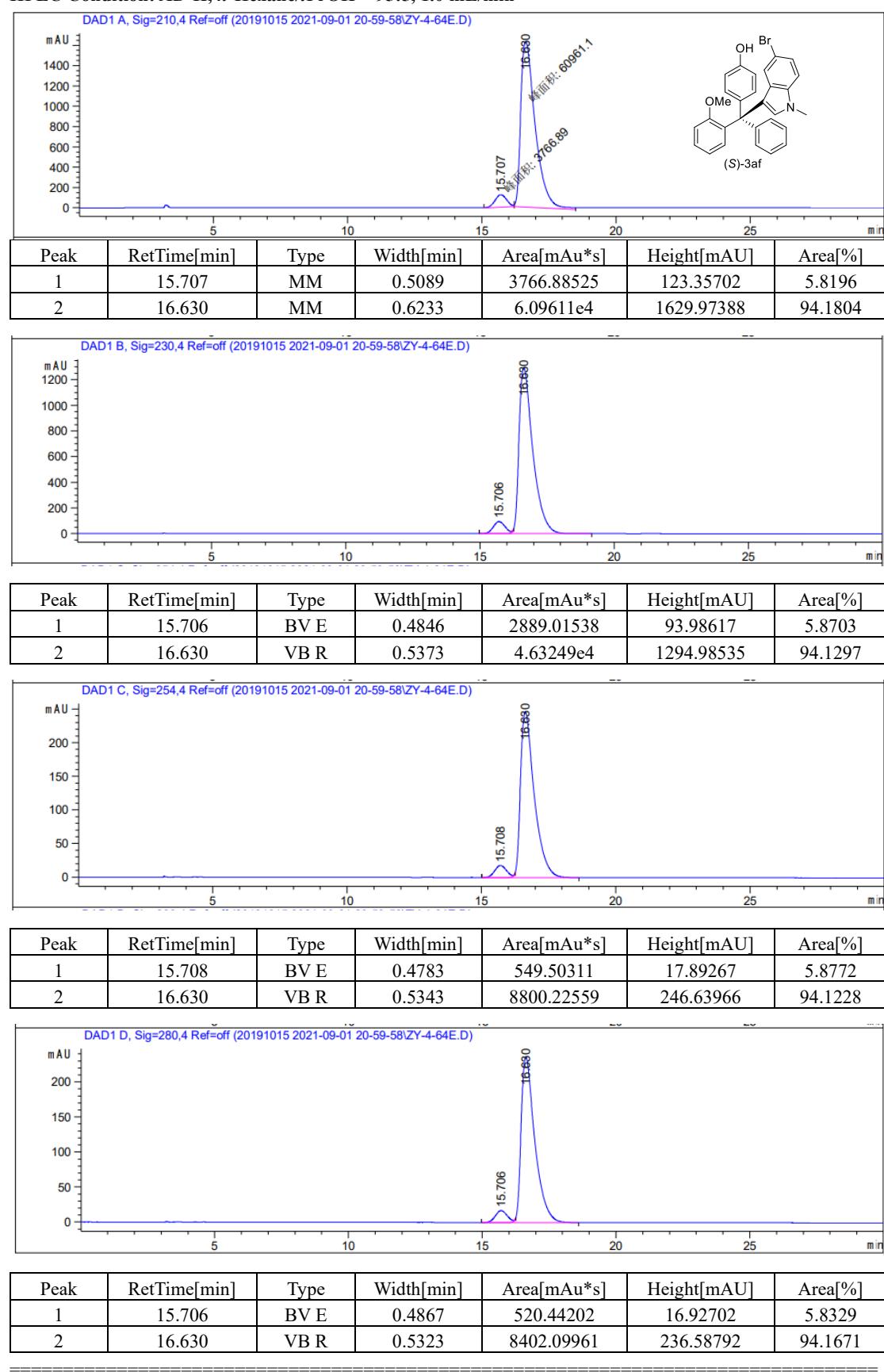
HPLC Condition: AD-H, *n*-Hexane/*i*PrOH = 95:5, 1.0 mL/min



End of Report

Sample Name: ZY-4-64E-OP

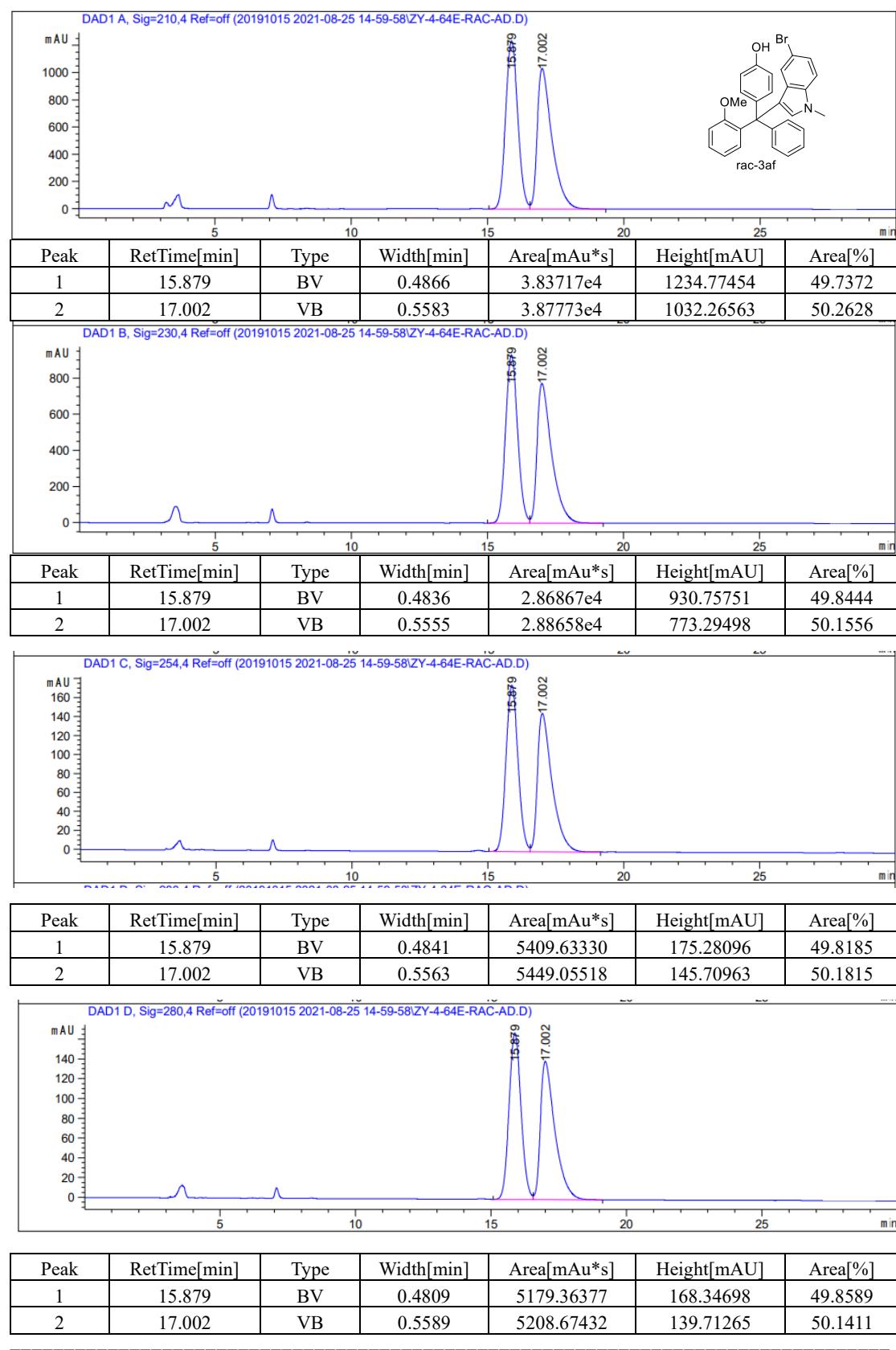
HPLC Condition: AD-H, *n*-Hexane/iPrOH = 95:5, 1.0 mL/min



End of Report

Sample Name: ZY-4-64E-Rac

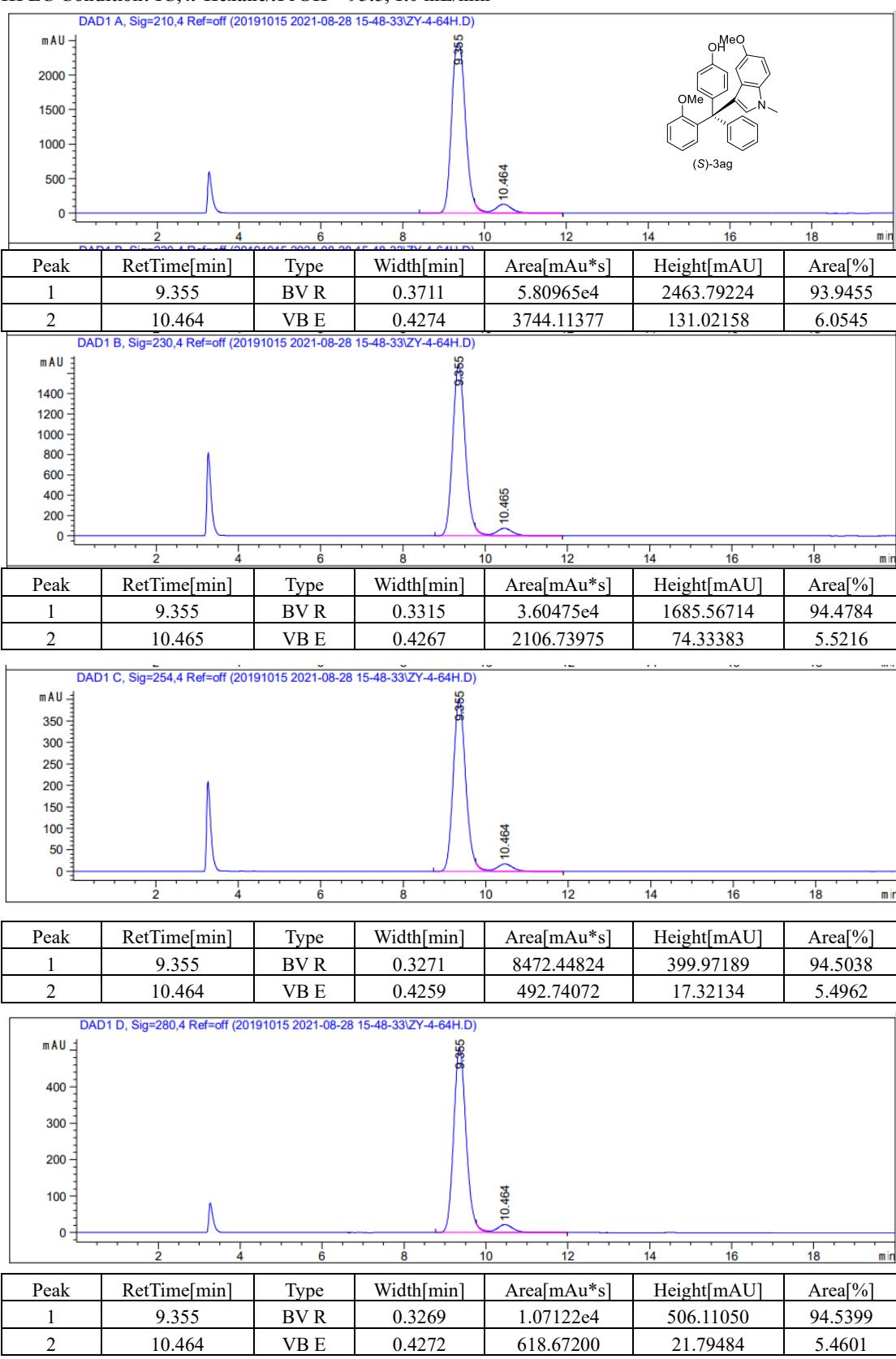
HPLC Condition: AD-H, *n*-Hexane/iPrOH = 95:5, 1.0 mL/min



End of Report

Sample Name: ZY-4-64H-OP

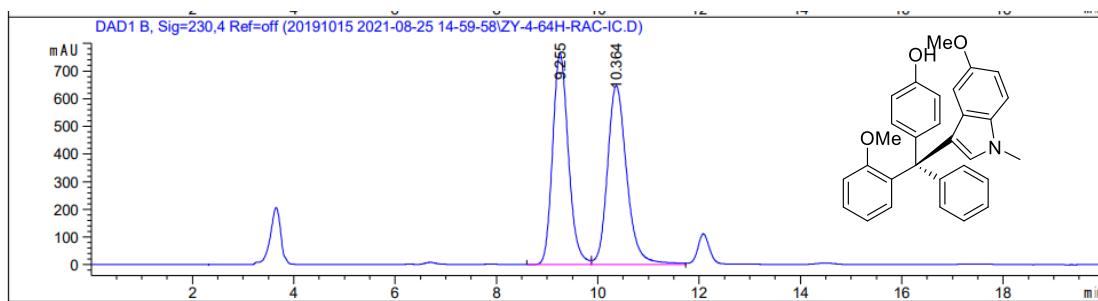
HPLC Condition: IC, *n*-Hexane/iPrOH = 95:5, 1.0 mL/min



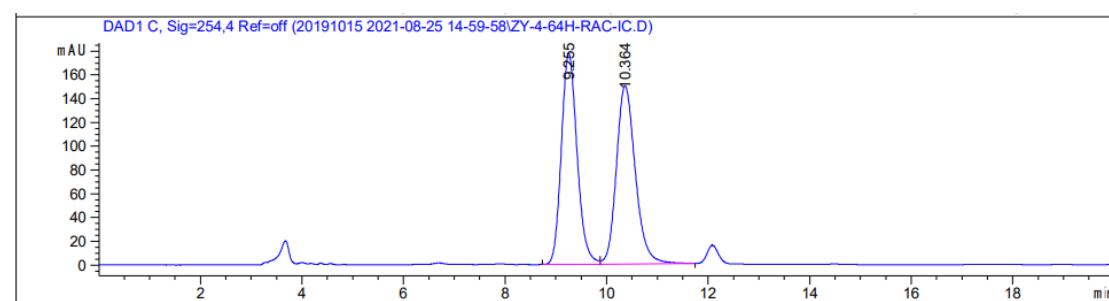
End of Report

Sample Name: ZY-4-64H-Rac

HPLC Condition: IC, n-Hexane/iPrOH = 95:5, 1.0 mL/min



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.255	BV	0.3347	1.65158e4	762.58624	49.0686
2	10.364	VV	0.4071	1.71428e4	647.05078	50.9314



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.255	BV	00.3335	3827.76367	177.55972	49.5941
2	10.364	VB	0.3984	3890.42017	150.07072	50.4059

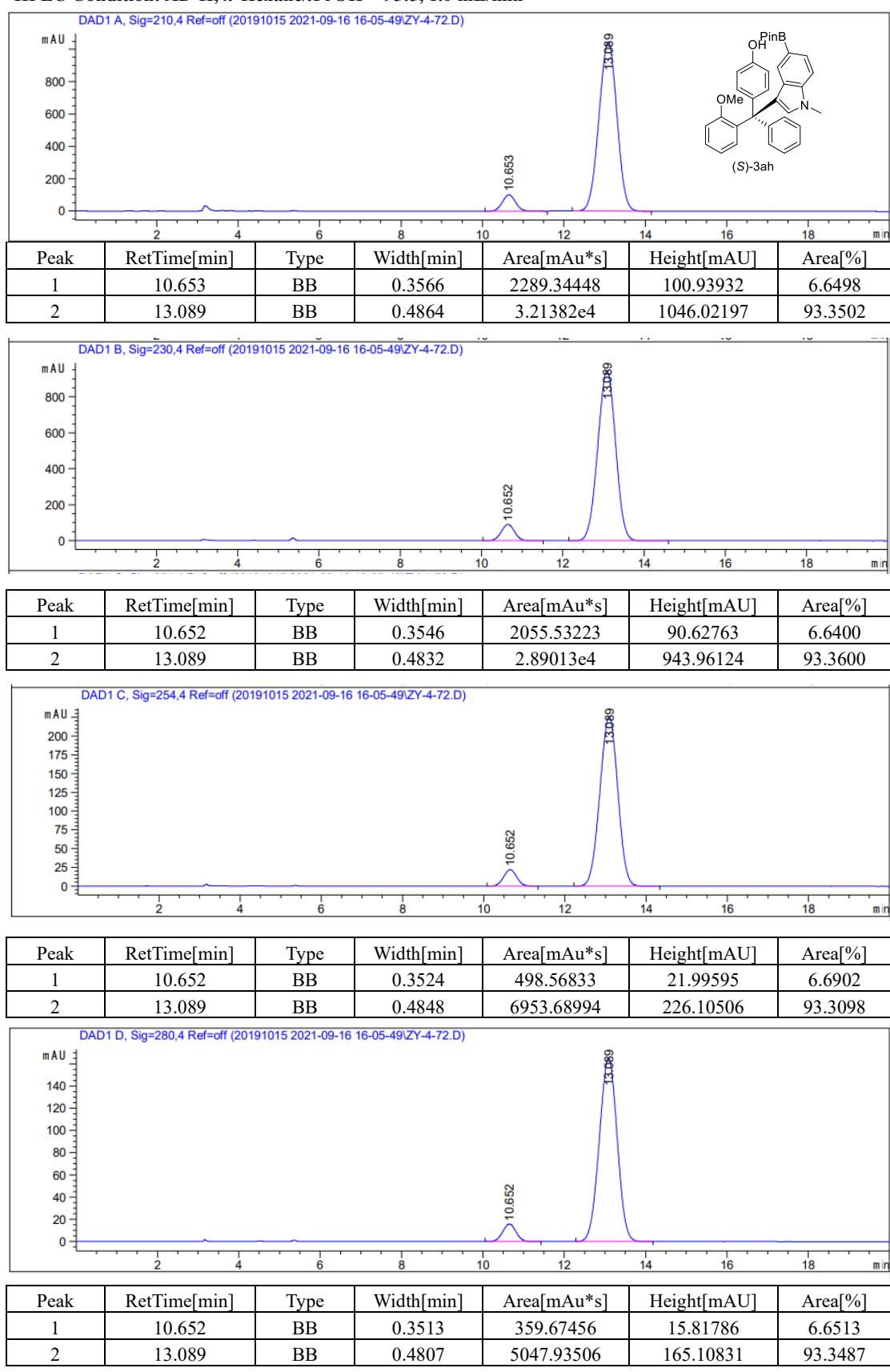
---

---

End of Report

Sample Name: ZY-4-72-OP

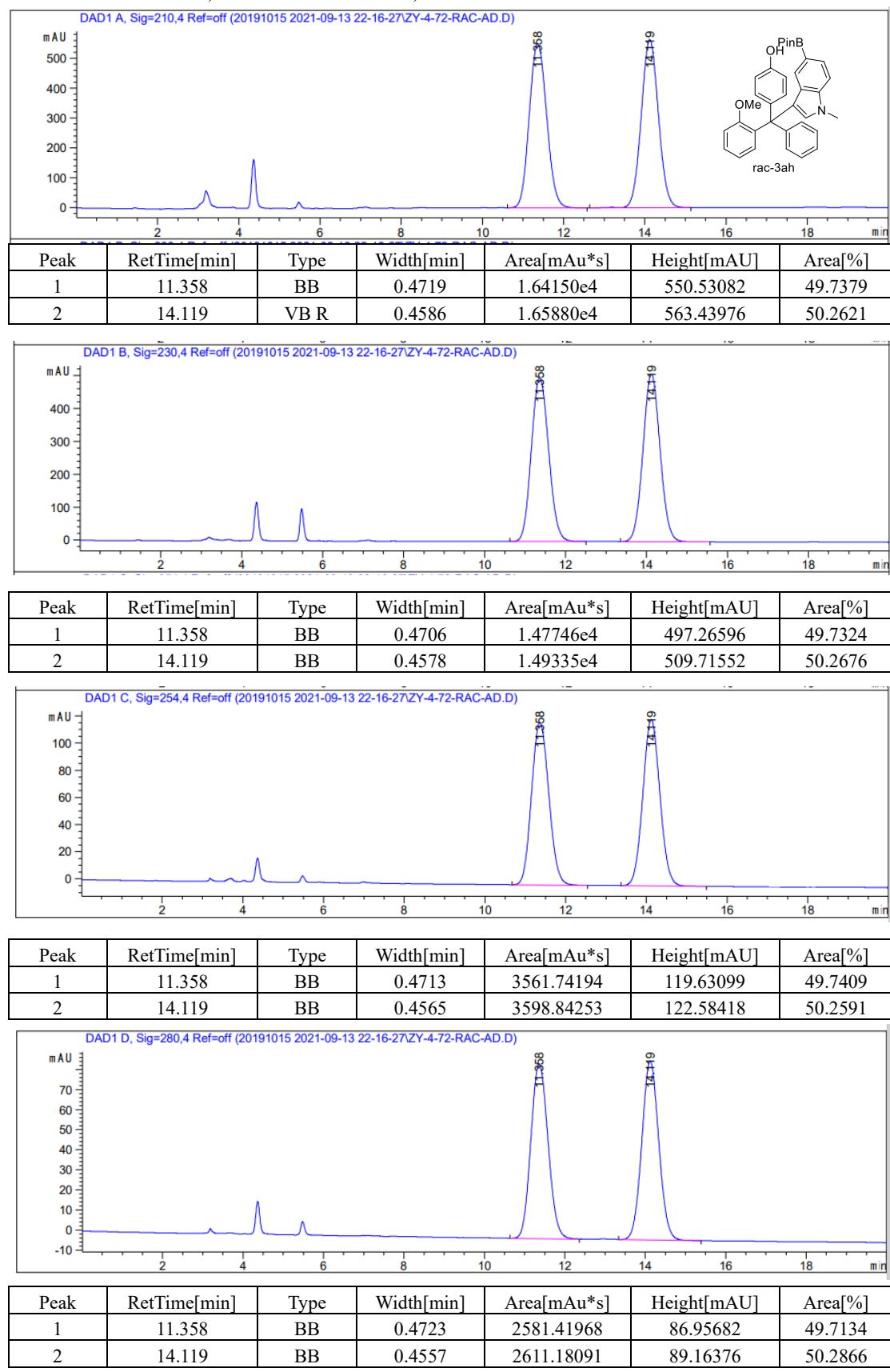
HPLC Condition: AD-H, *n*-Hexane/*i*PrOH = 95:5, 1.0 mL/min



End of Report

Sample Name: ZY-4-72-Rac

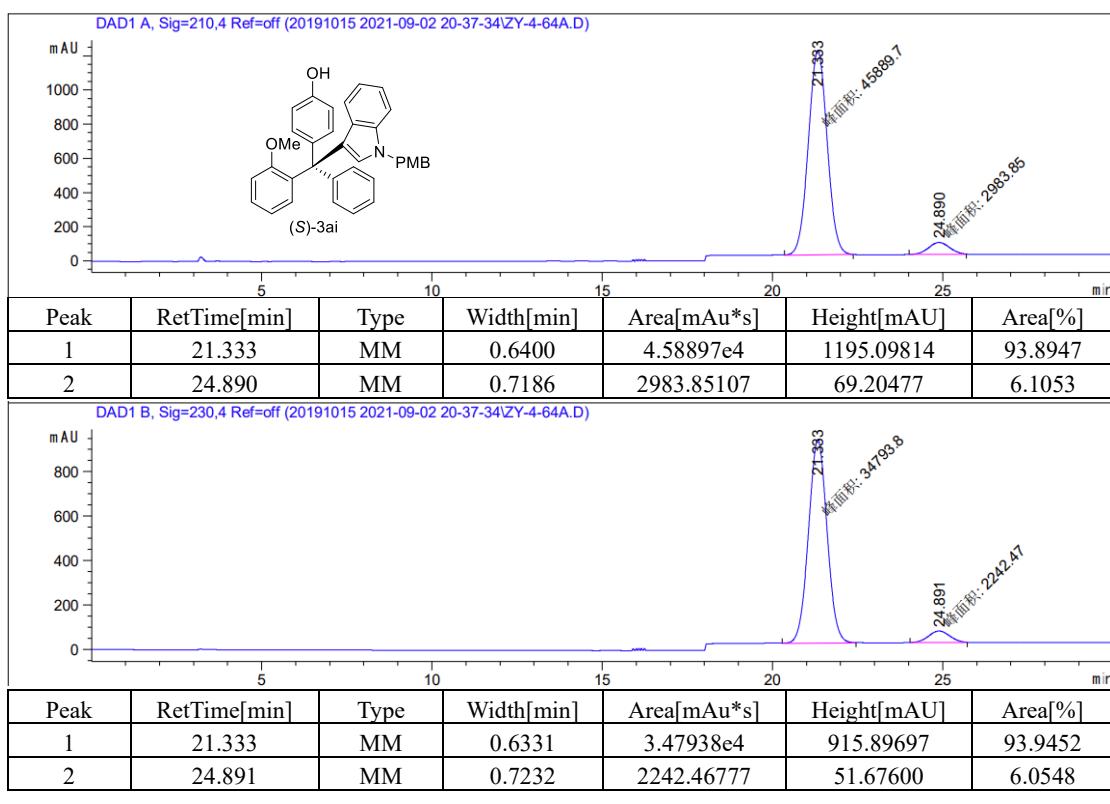
HPLC Condition: AD-H, n-Hexane/iPrOH = 95:5, 1.0 mL/min



End of Report

Sample Name: ZY-4-64A-OP

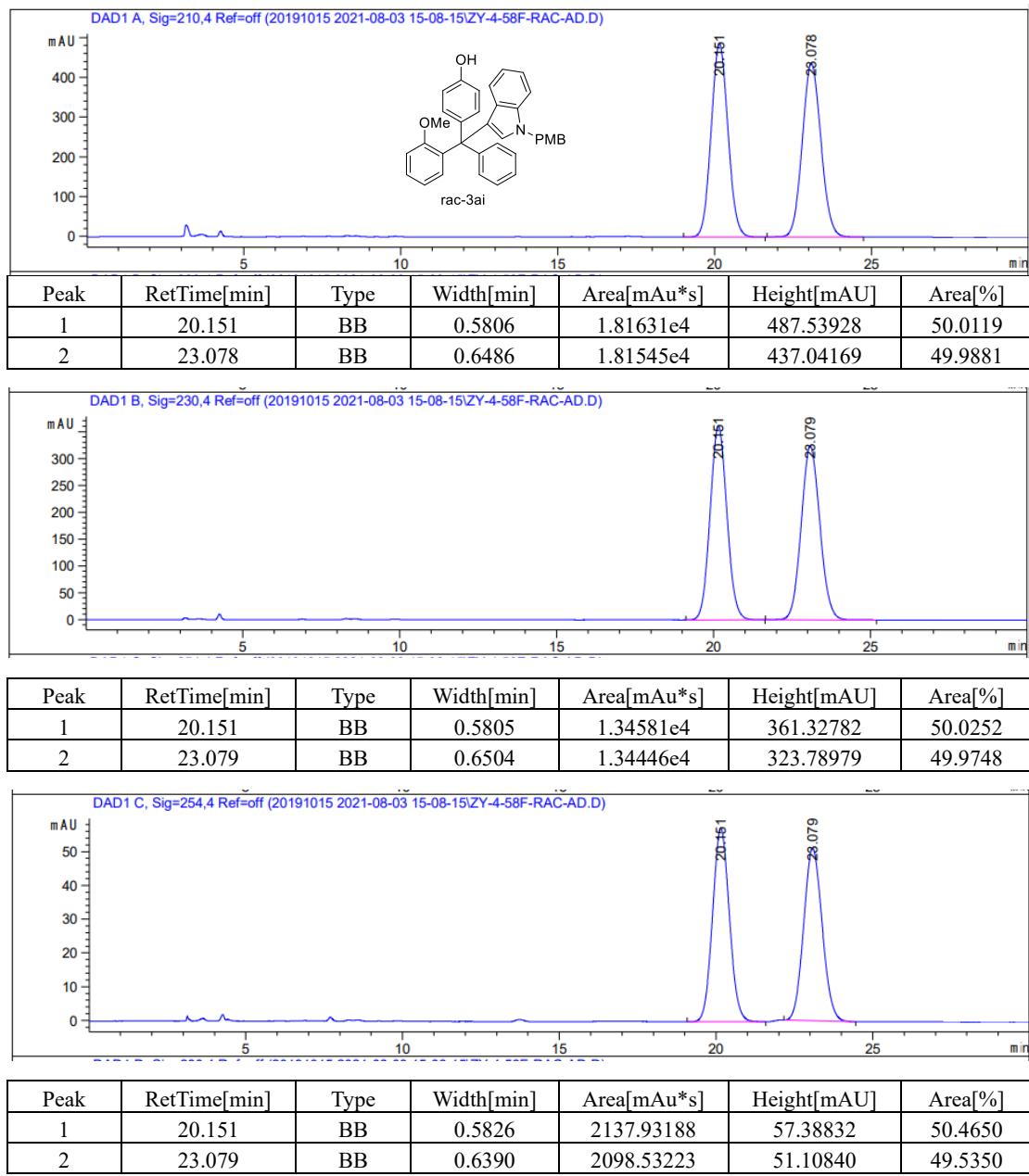
HPLC Condition: AD-H, *n*-Hexane/*i*PrOH = 95:5, 1.0 mL/min



End of Report

Sample Name: ZY-4-58F-Rac

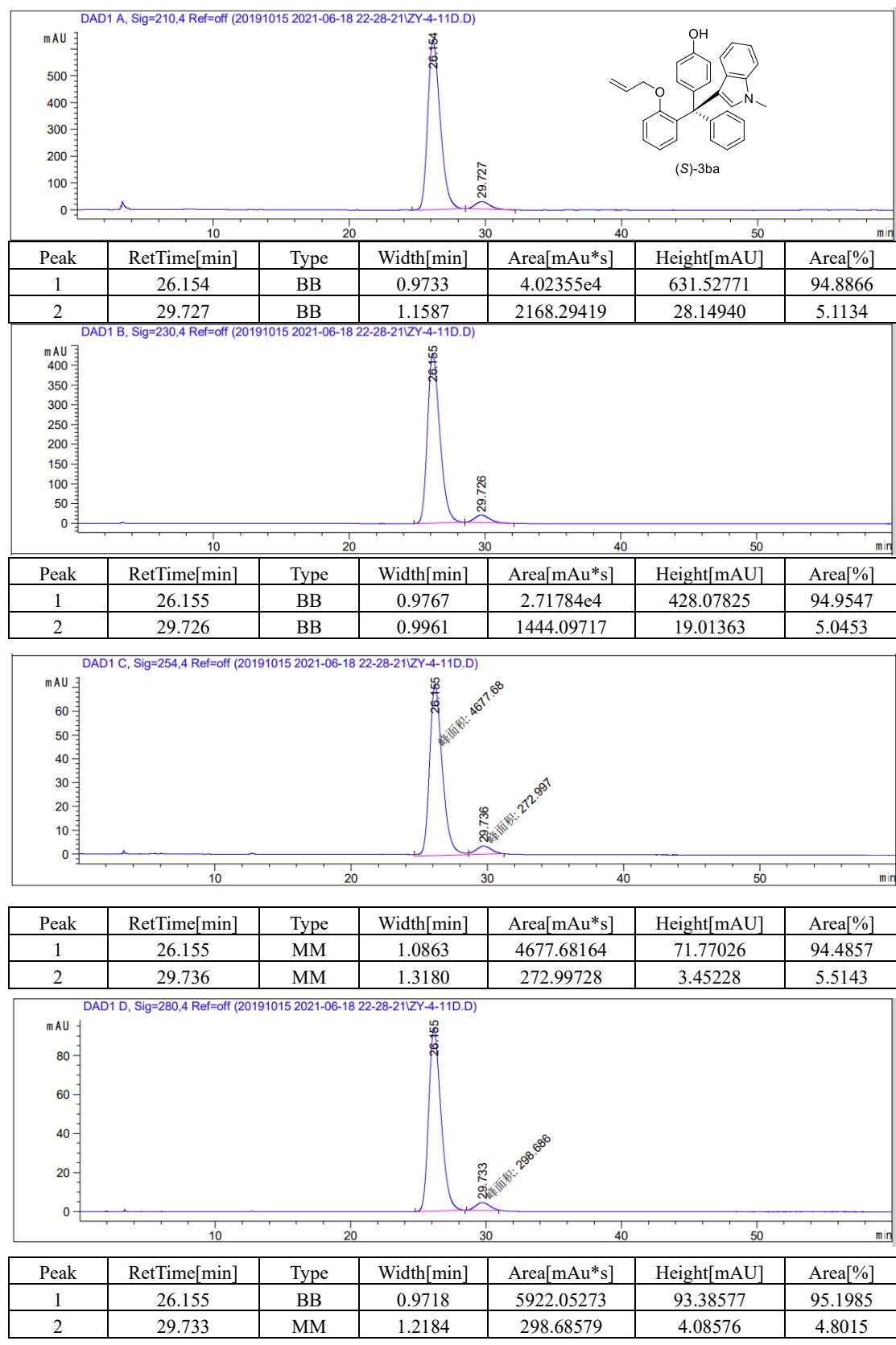
HPLC Condition: AD-H, *n*-Hexane/iPrOH = 95:5, 1.0 mL/min



End of Report

Sample Name: ZY-4-11D-OP

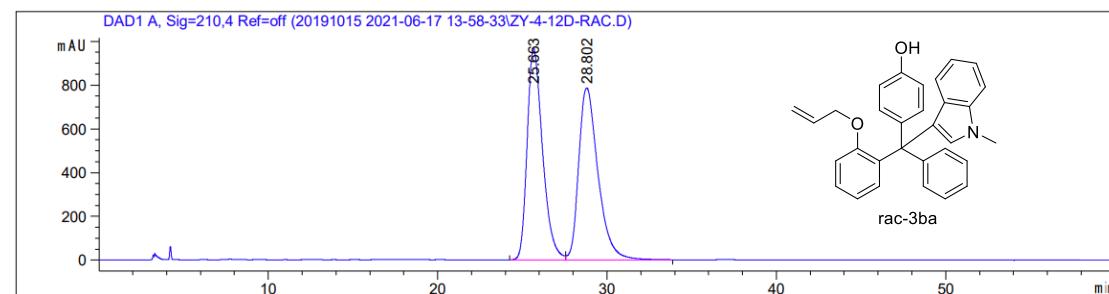
HPLC Condition: OD-H, *n*-Hexane/iPrOH = 98:2, 1.0 mL/min



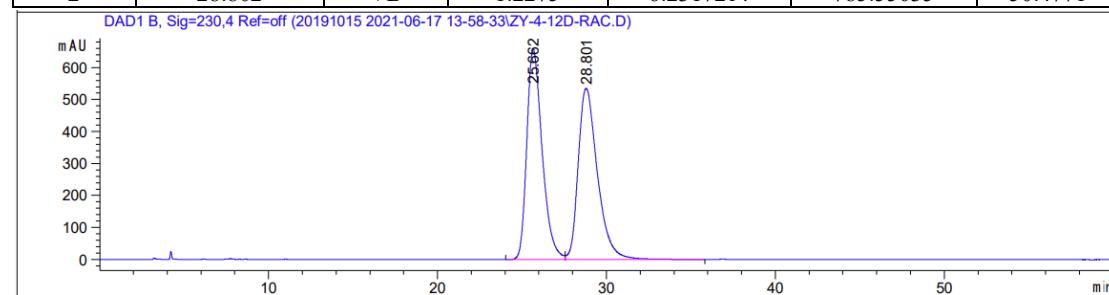
End of Report

**Sample Name: ZY-4-12D-Rac**

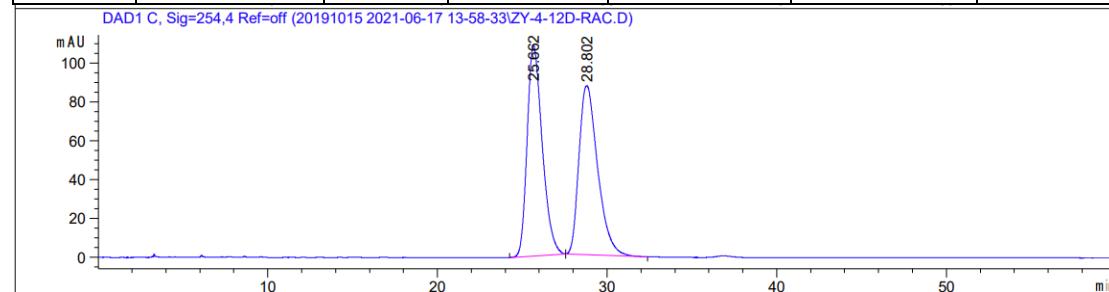
**HPLC Condition: OD-H, n-Hexane/iPrOH = 98:2, 1.0 mL/min**



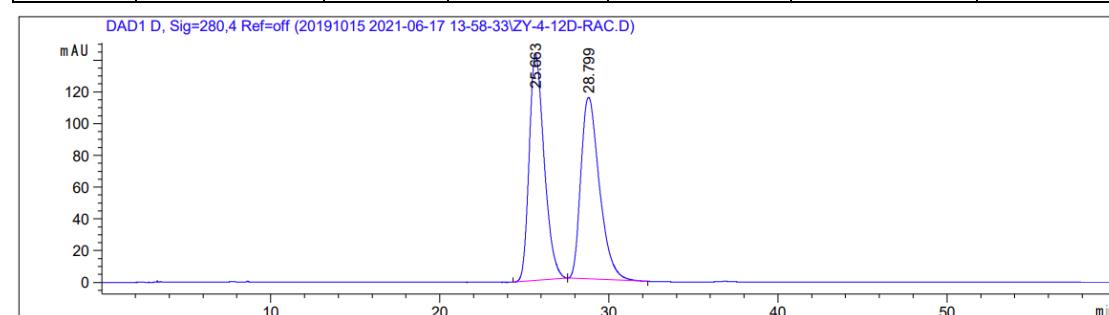
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	25.663	BV	0.9612	6.11391e4	967.52429	49.5229
2	28.802	VB	1.2275	6.23172e4	785.55035	50.4771



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	25.662	BV	0.9602	4.16072e4	659.31635	49.5015
2	28.801	VB	1.2283	4.24452e4	534.60468	50.4985



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	25.662	BB	0.9485	6697.65918	108.44944	50.1161
2	28.802	BB	1.1537	6666.63281	87.02443	49.8839

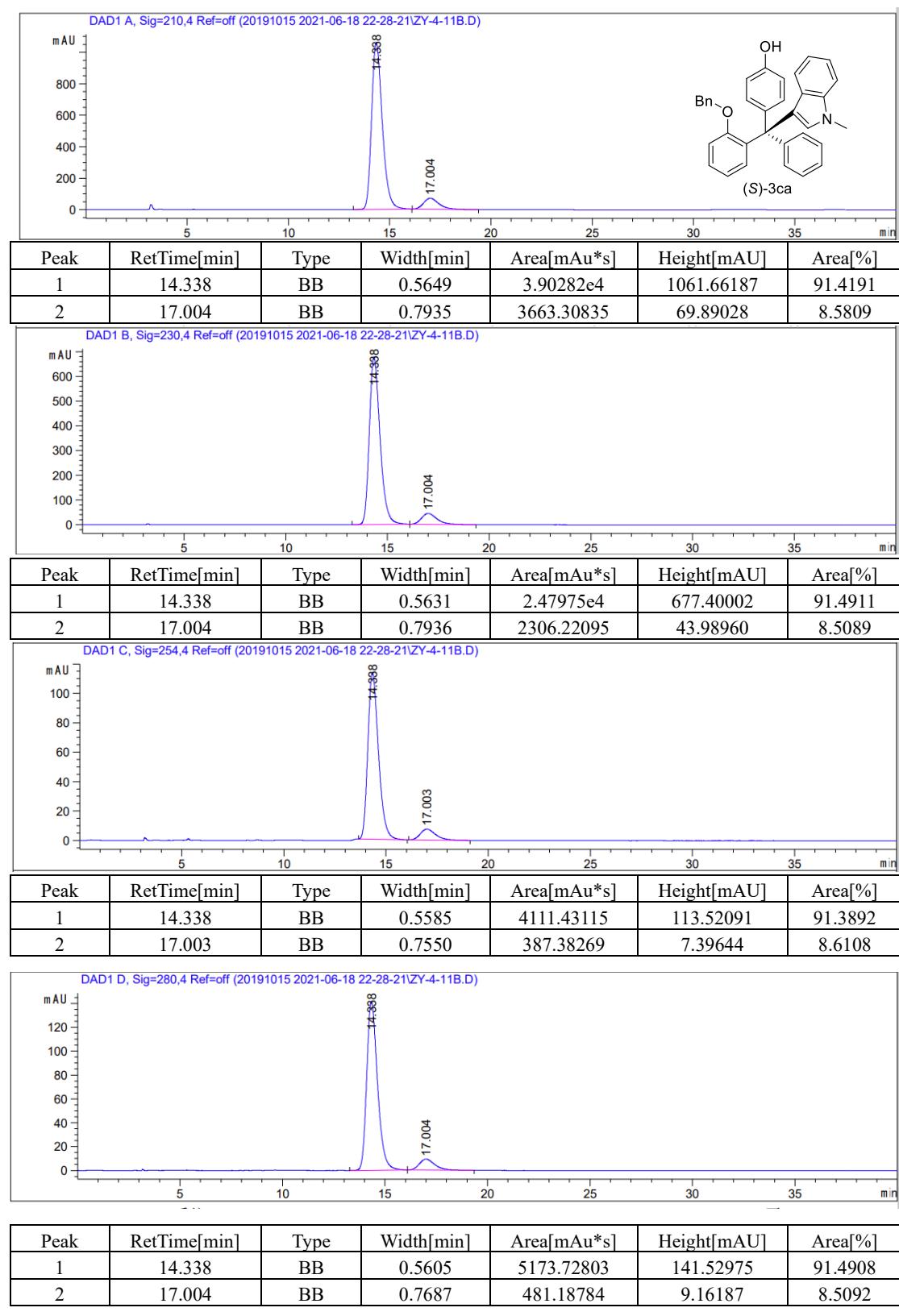


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	25.663	BB	0.9399	8805.01660	142.69490	50.1301
2	28.799	BB	1.1490	8759.31543	114.43378	49.8699

End of Report

Sample Name: ZY-4-11B-OP

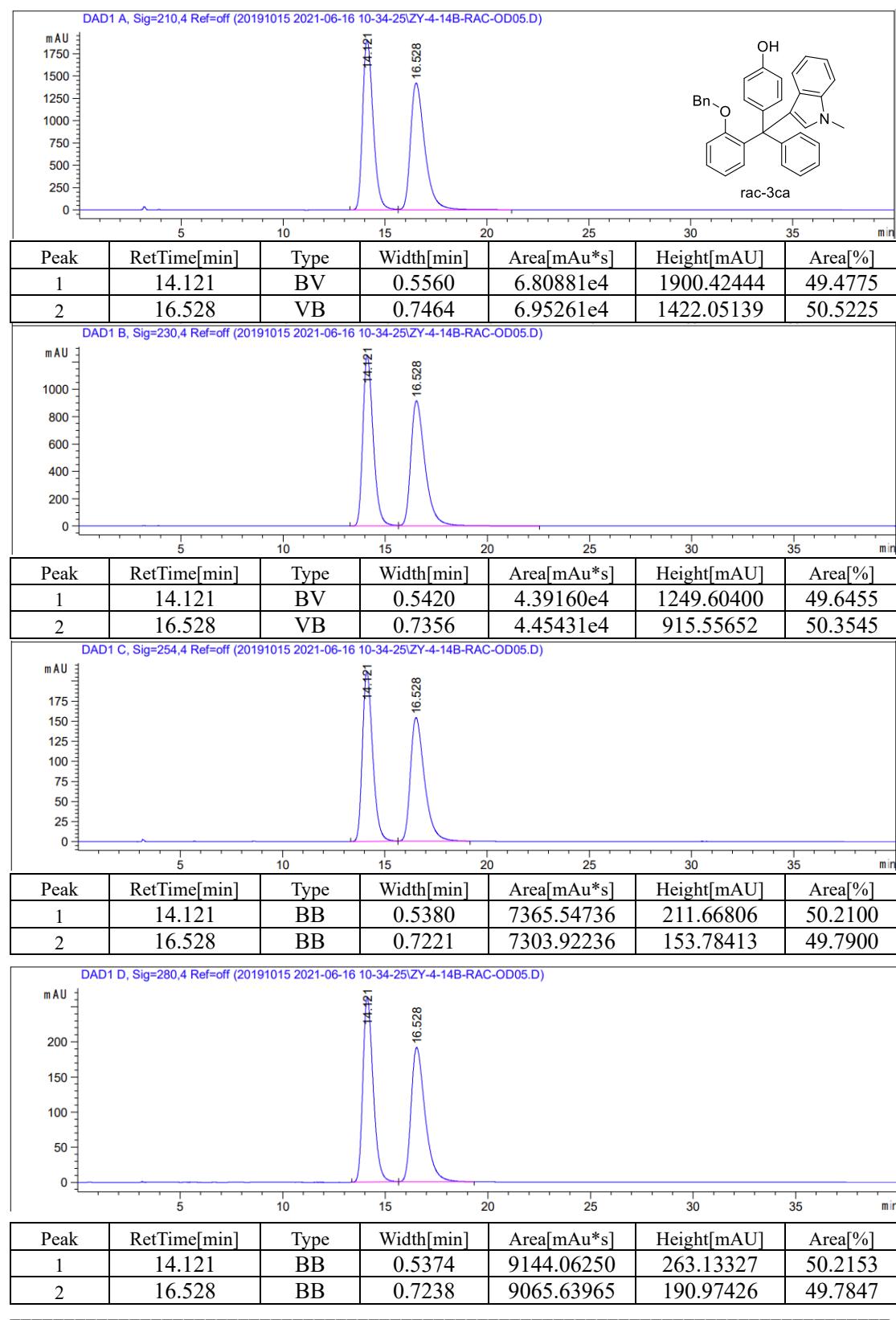
HPLC Condition: OD-H, *n*-Hexane/iPrOH = 95:5, 1.0 mL/min



End of Report

Sample Name: ZY-4-12B-Rac

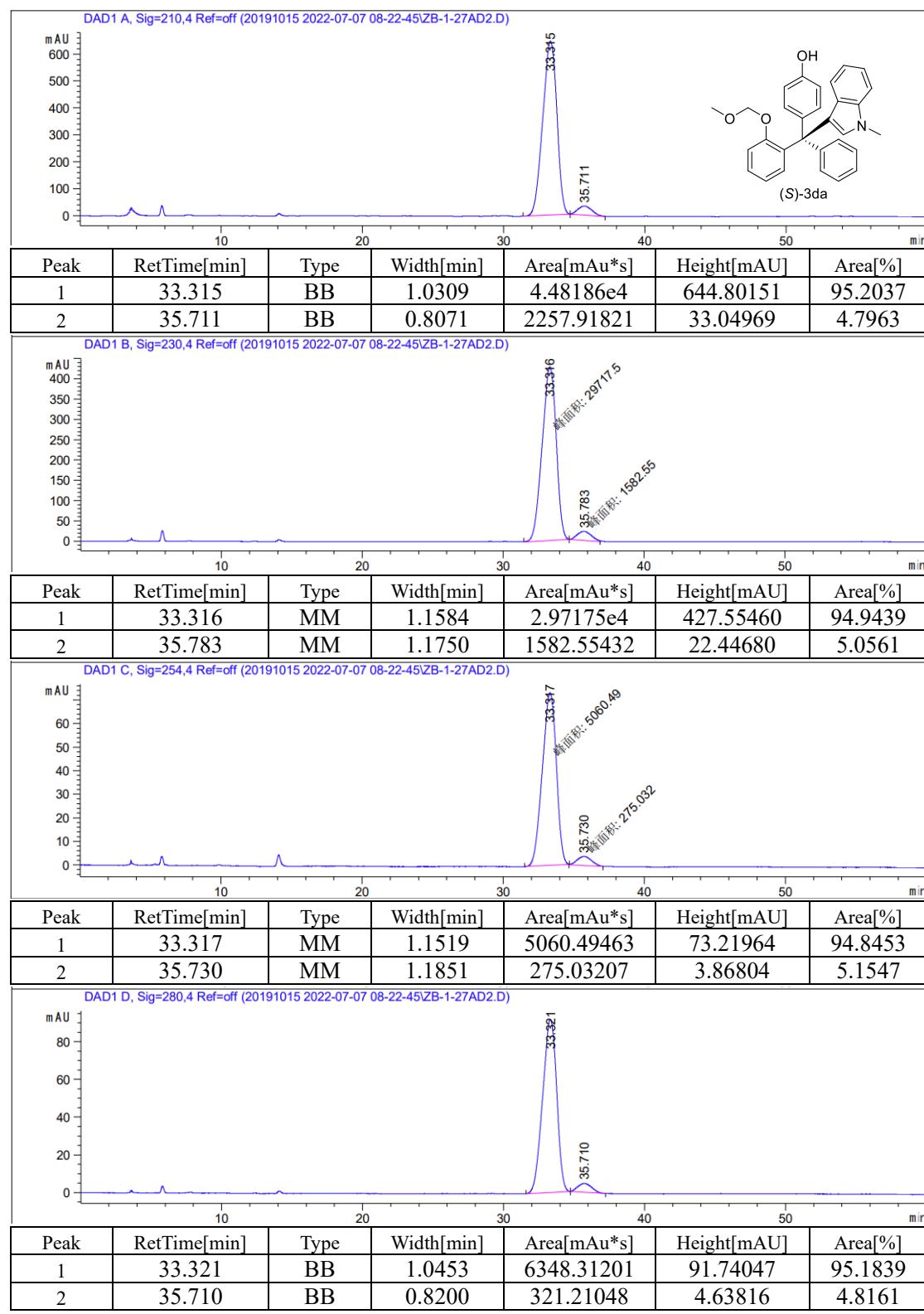
HPLC Condition: OD-H, *n*-Hexane/iPrOH = 95:5, 1.0 mL/min



End of Report

Sample Name: ZY-4-56D-OP

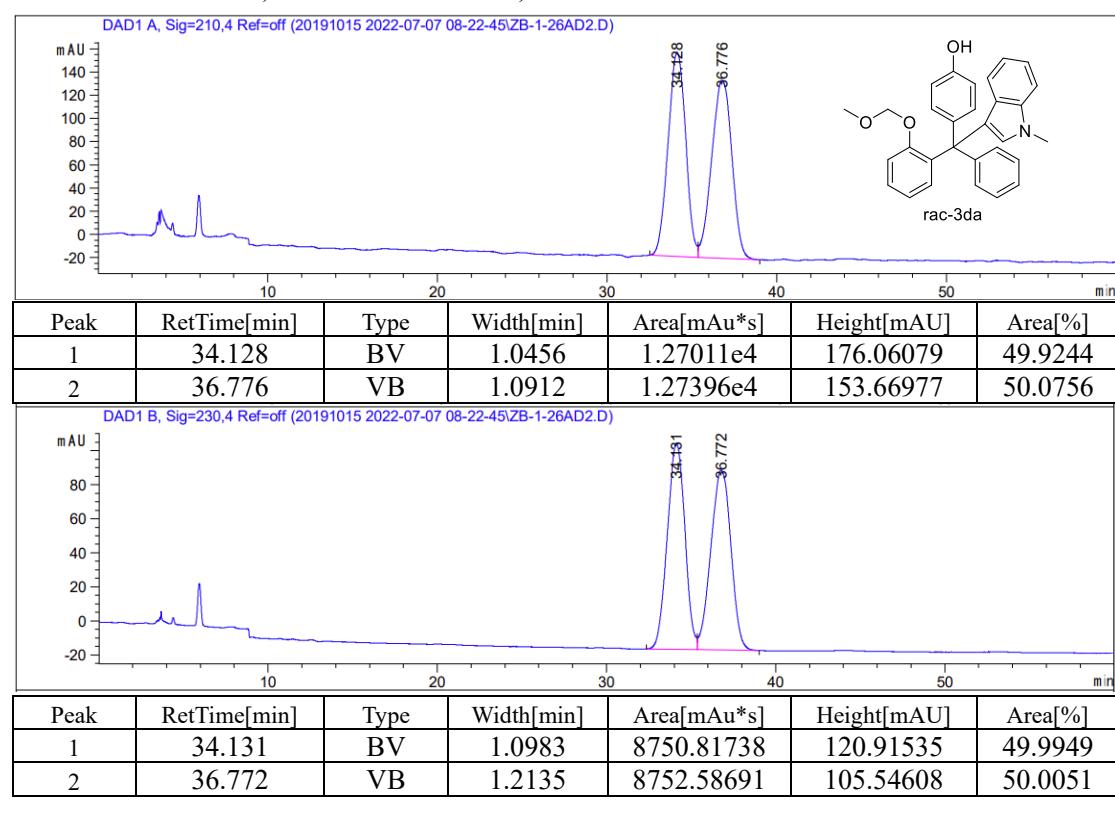
HPLC Condition: AD-H, *n*-Hexane/*i*PrOH = 98:2, 1.0 mL/min



End of Report

**Sample Name: ZY-4-56D-Rac**

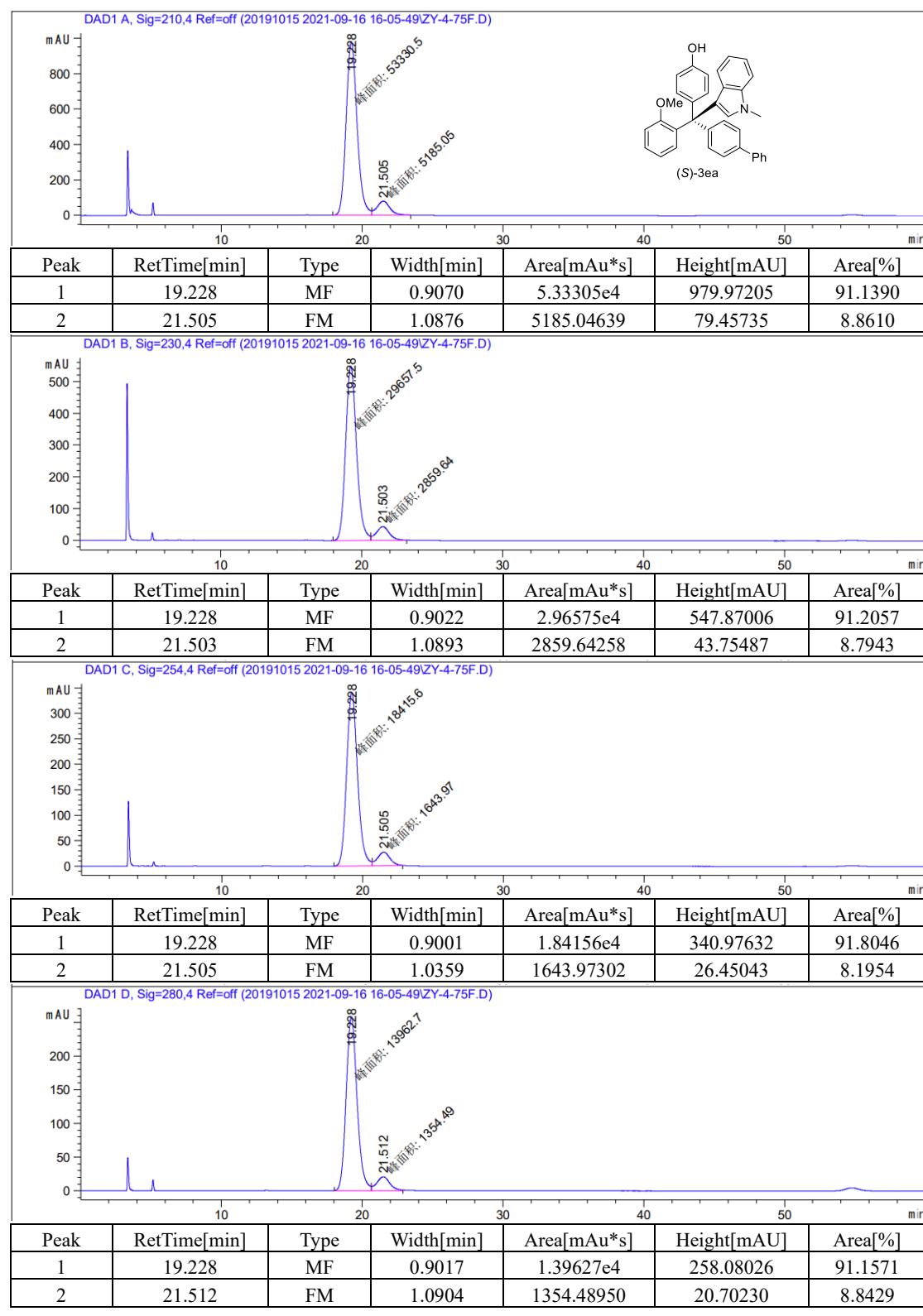
**HPLC Condition: AD-H, *n*-Hexane/iPrOH = 98:2, 1.0 mL/min**



=====  
End of Report

Sample Name: ZY-4-75F-OP

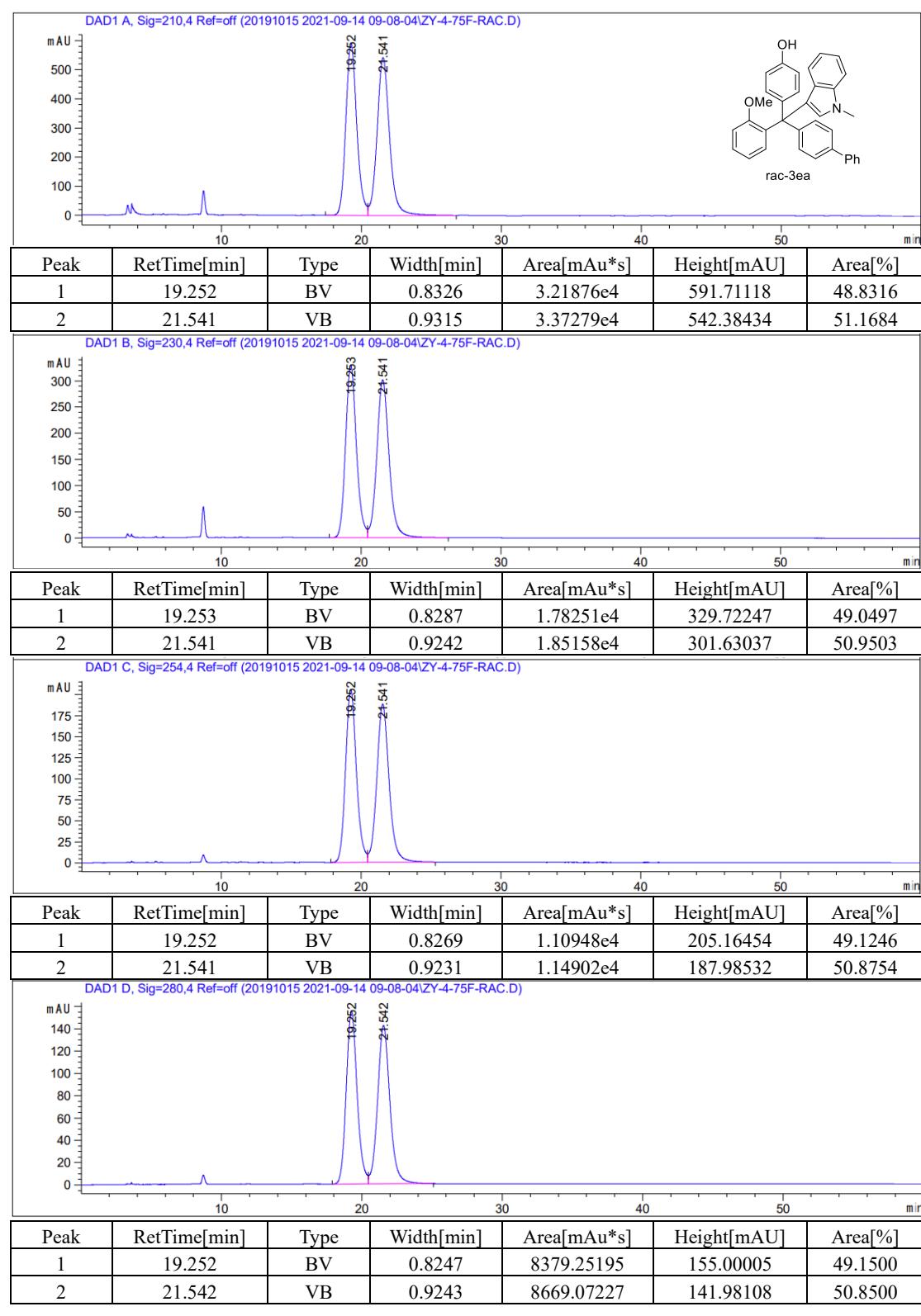
HPLC Condition: IC, *n*-Hexane/iPrOH = 98:2, 1.0 mL/min



End of Report

Sample Name: ZY-4-75F-Rac

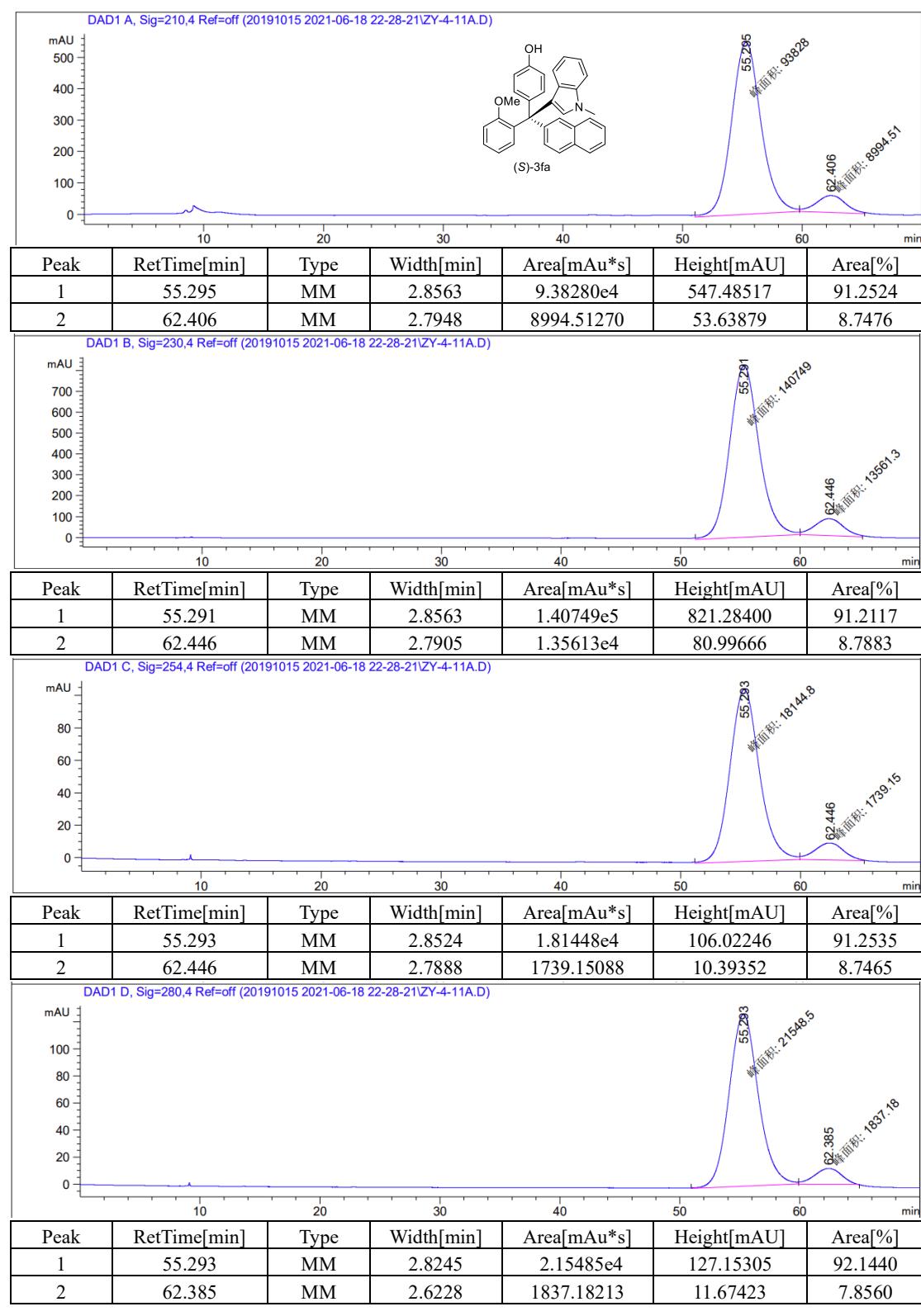
HPLC Condition: IC, *n*-Hexane/iPrOH = 98:2, 1.0 mL/min



End of Report

Sample Name: ZY-4-11A-OP

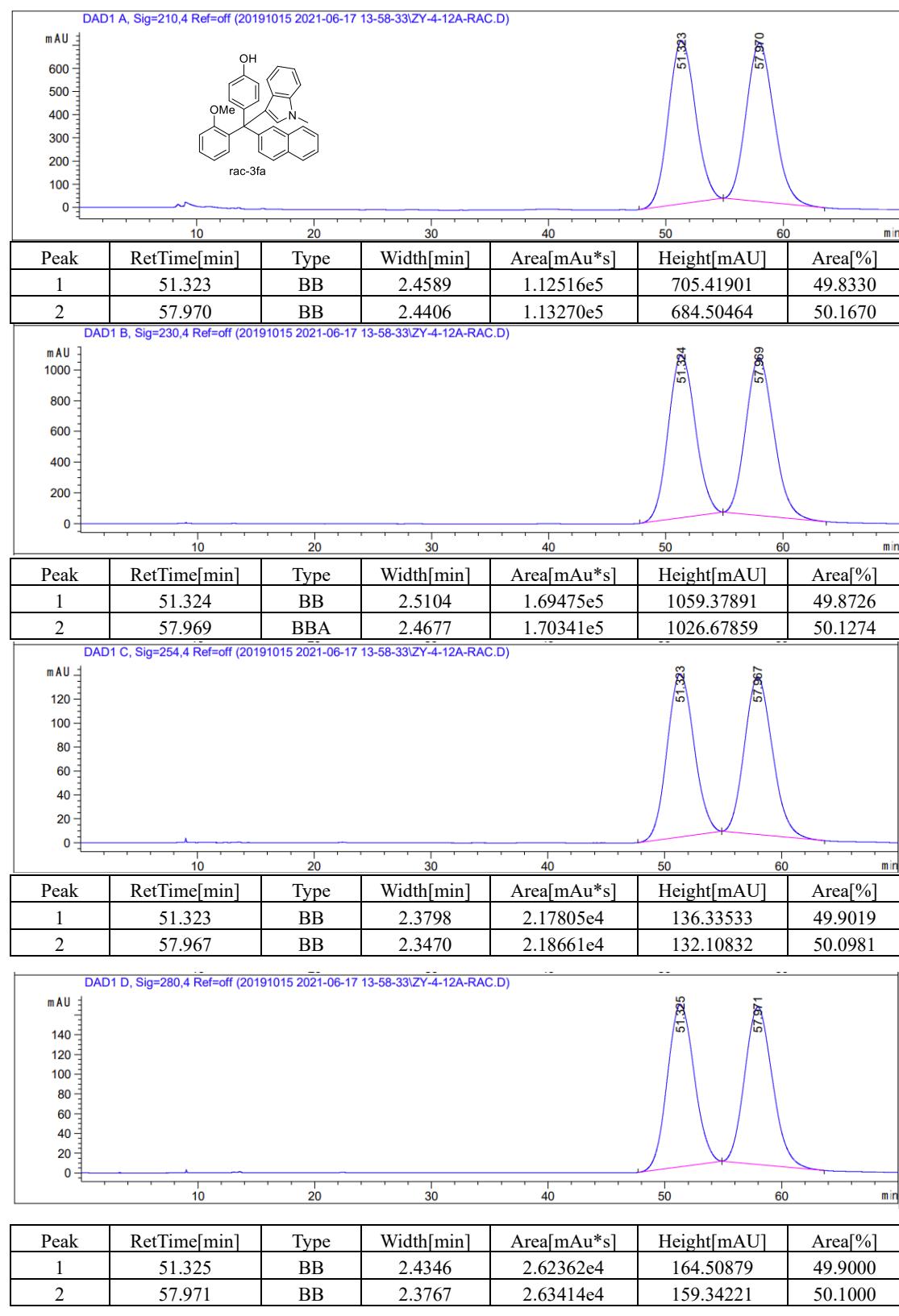
HPLC Condition: IC, *n*-Hexane/iPrOH = 98:2, 0.4 mL/min



End of Report

Sample Name: ZY-4-11A-Rac

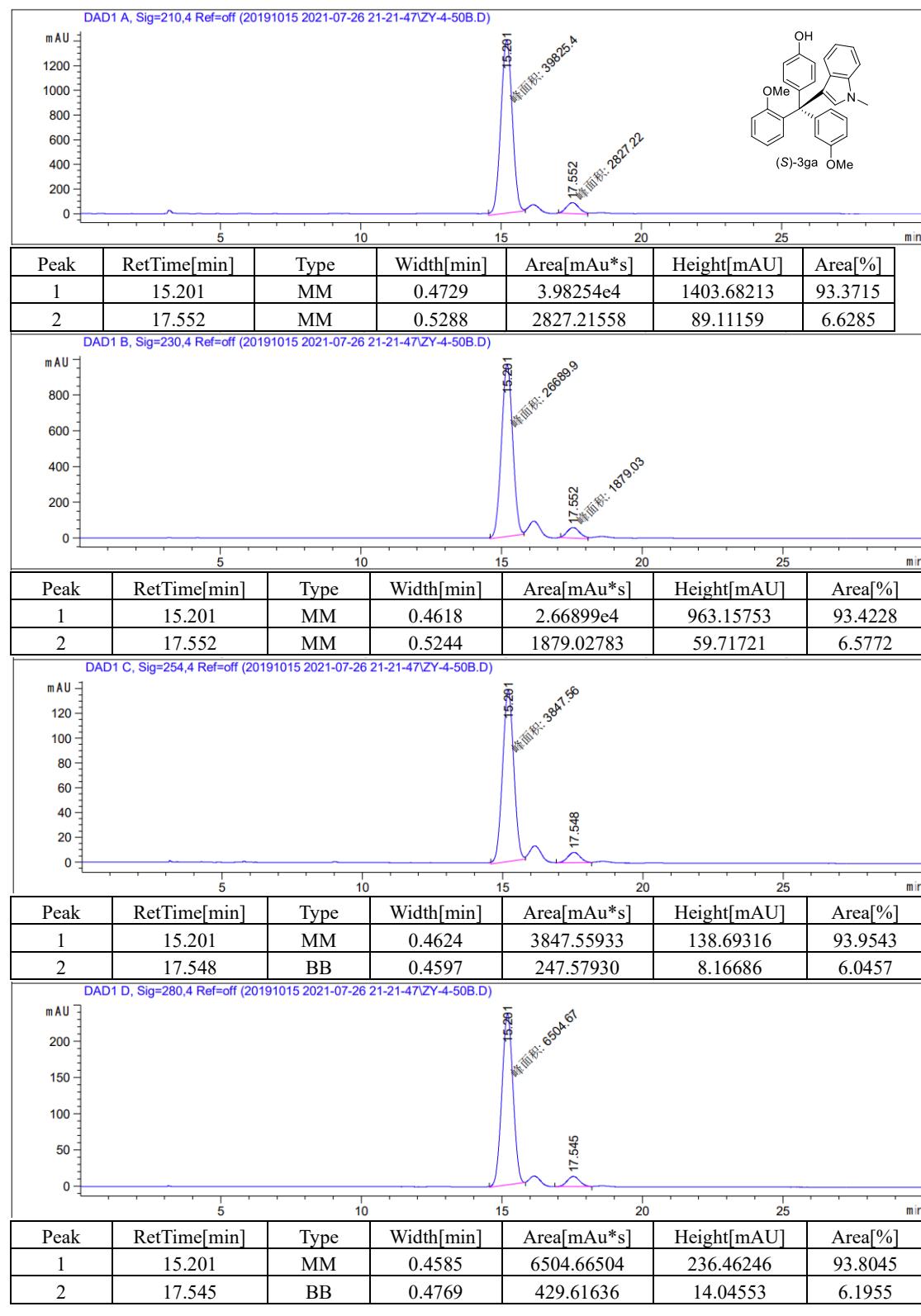
HPLC Condition: IC, *n*-Hexane/iPrOH = 98:2, 0.4 mL/min



End of Report

Sample Name: ZY-4-50B-OP

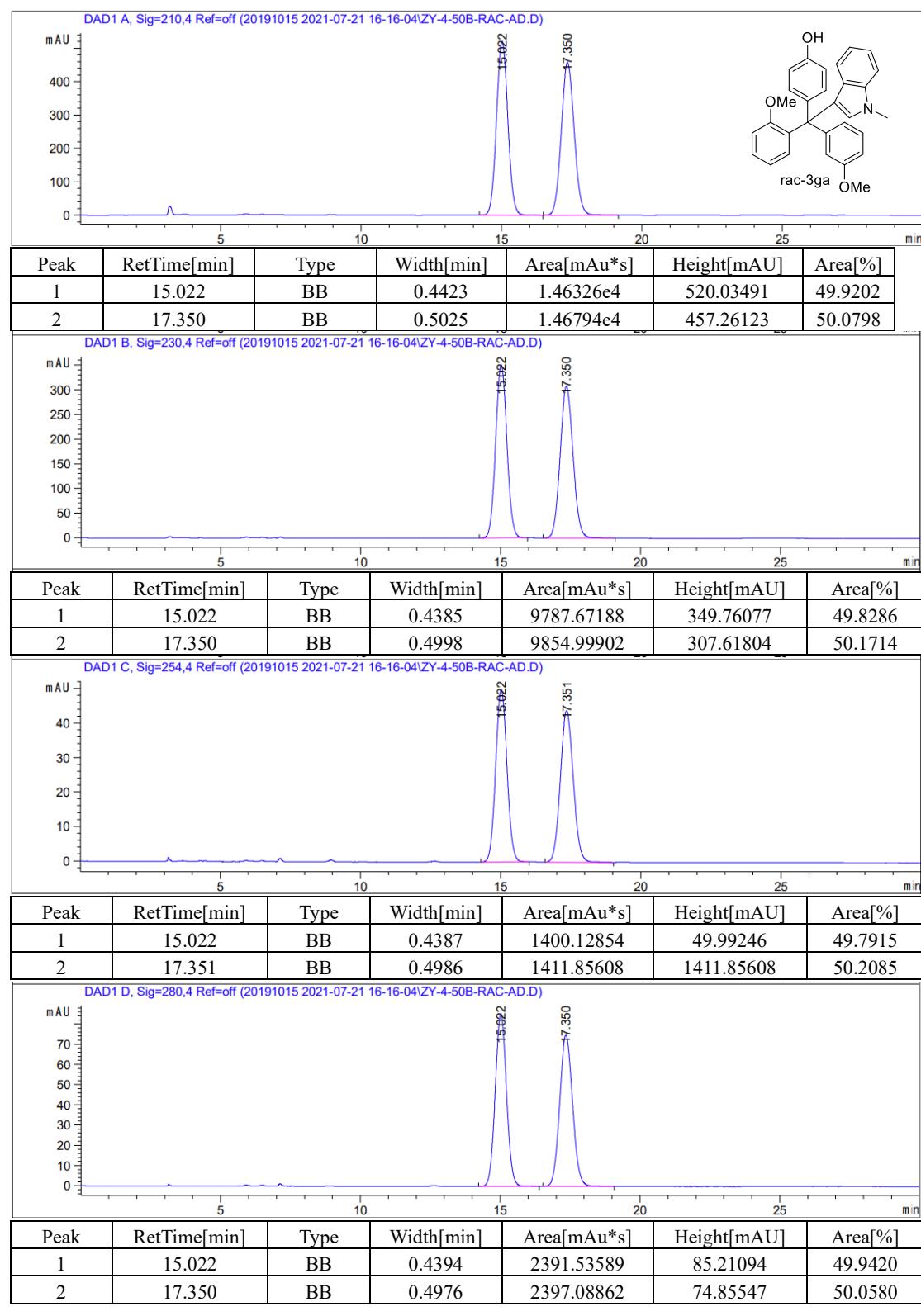
HPLC Condition: AD-H, n-Hexane/iPrOH = 95:5, 1.0 mL/min



End of Report

Sample Name: ZY-4-50B-rac

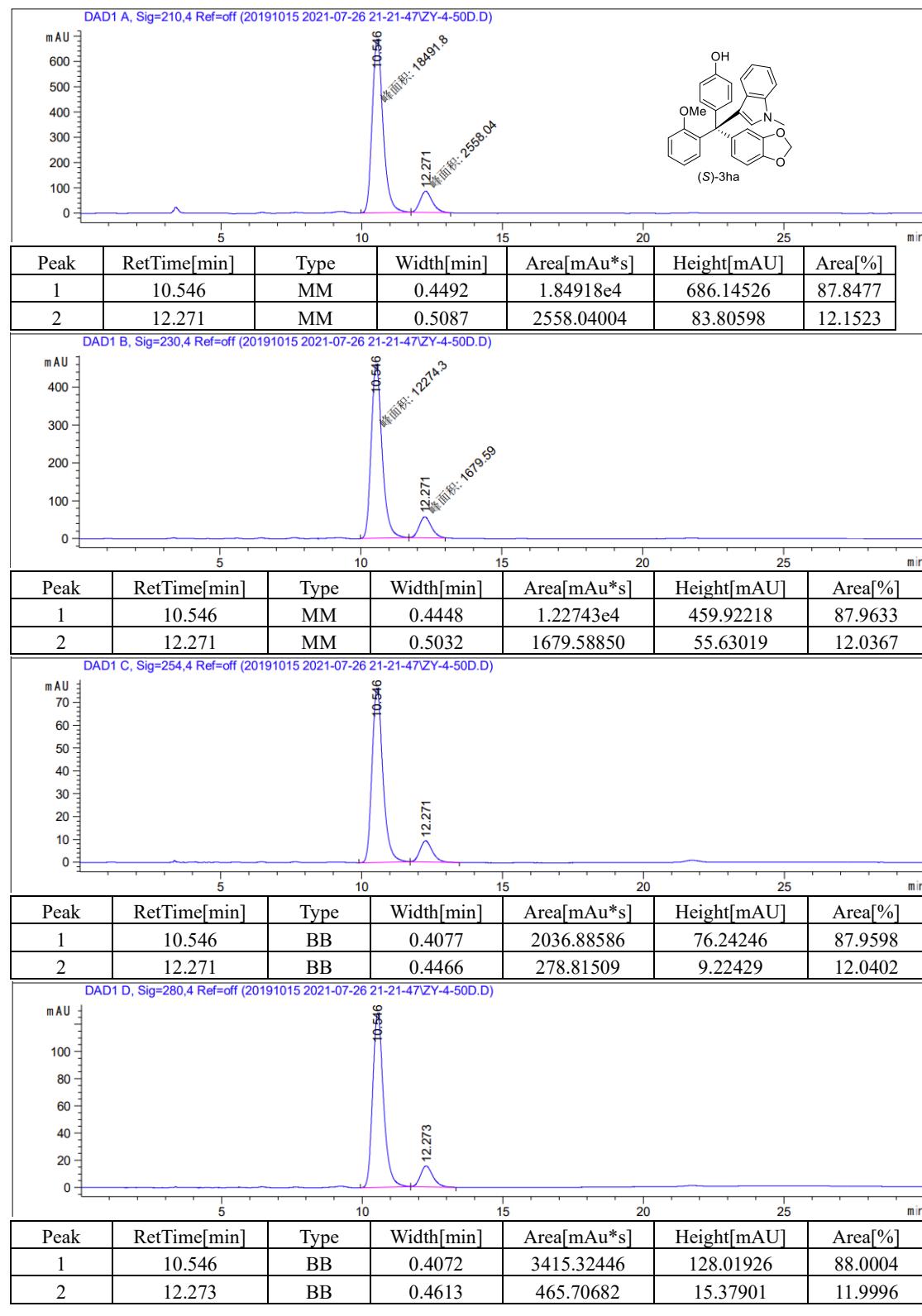
HPLC Condition: AD-H, n-Hexane/iPrOH = 95:5, 1.0 mL/min



End of Report

Sample Name: ZY-4-50D-OP

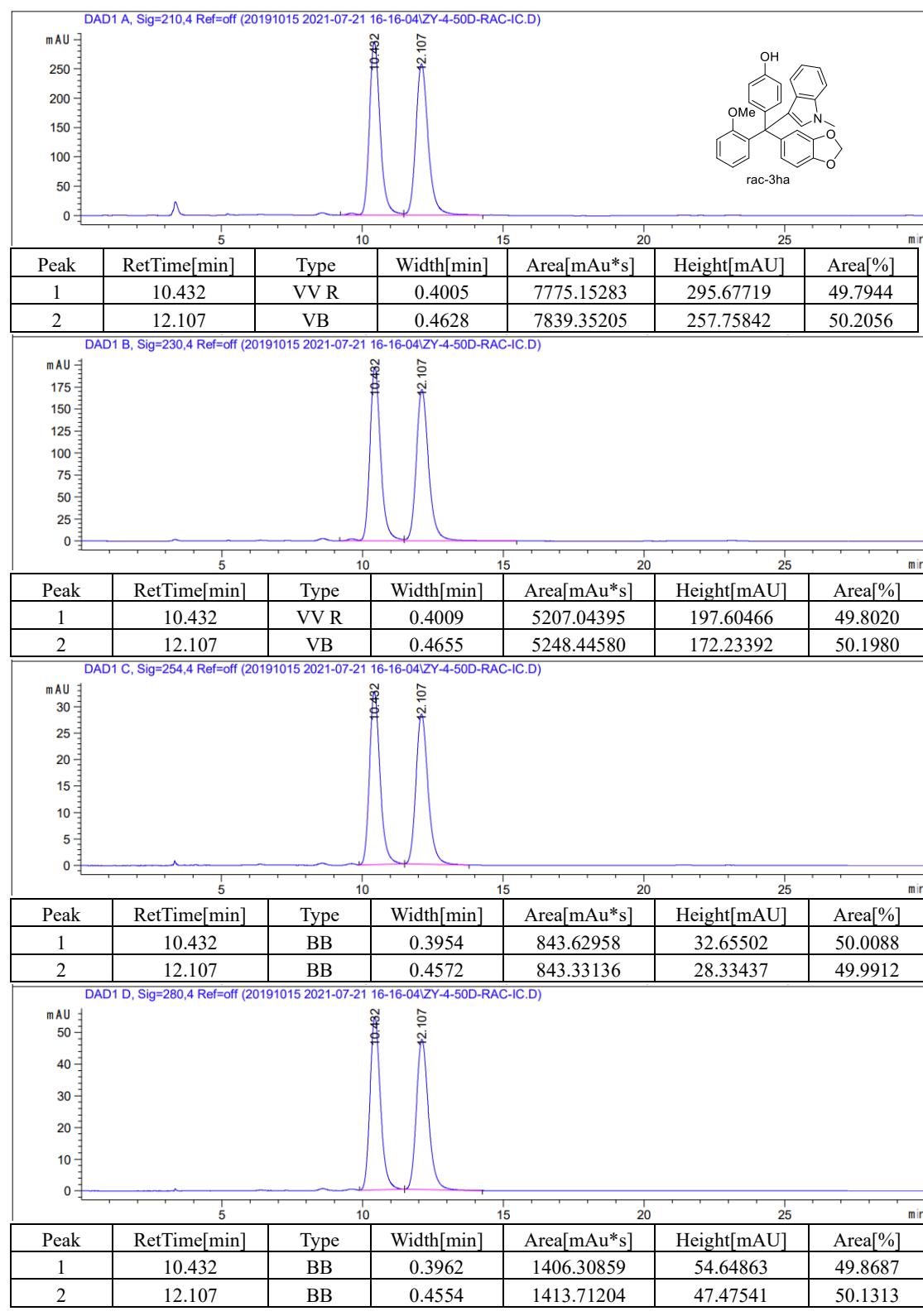
HPLC Condition: IC, *n*-Hexane/iPrOH = 95:5, 1.0 mL/min



End of Report

Sample Name: ZY-4-50D-rac

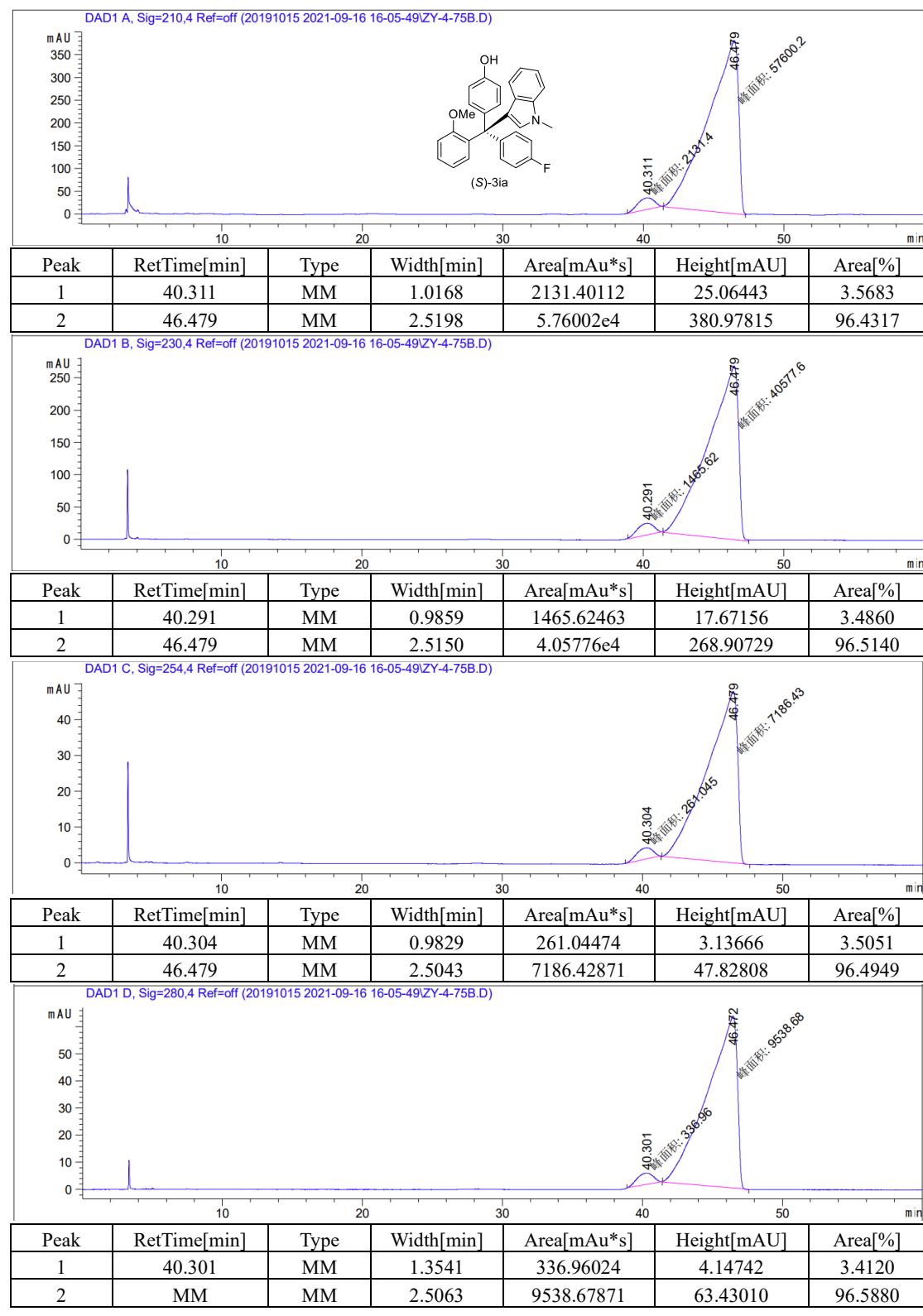
HPLC Condition: IC, *n*-Hexane/iPrOH = 95:5, 1.0 mL/min



End of Report

Sample Name: ZY-4-75B-OP

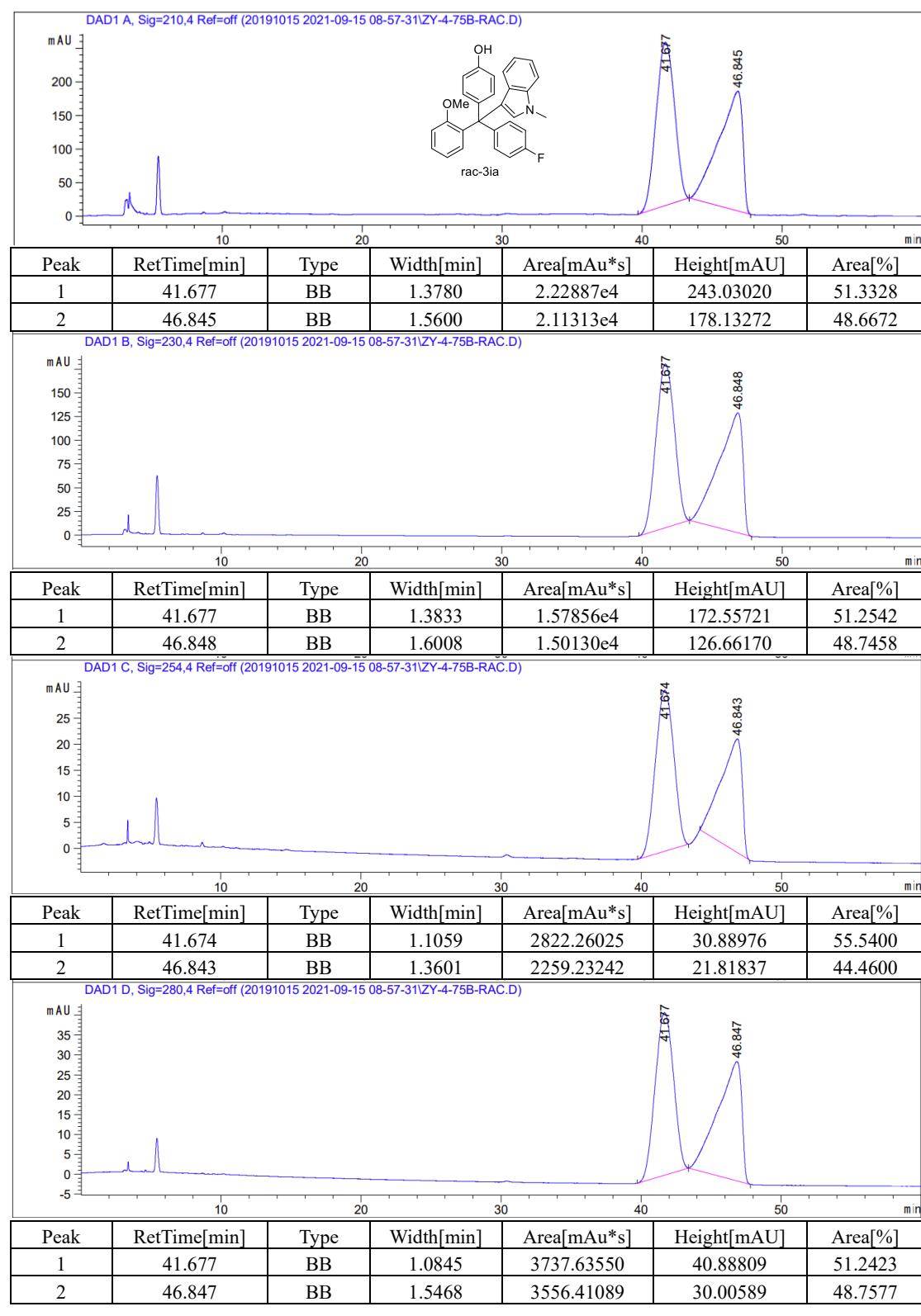
HPLC Condition: AD-H, *n*-Hexane/*i*PrOH = 98:2, 1.0 mL/min



End of Report

Sample Name: ZY-4-75B-Rac

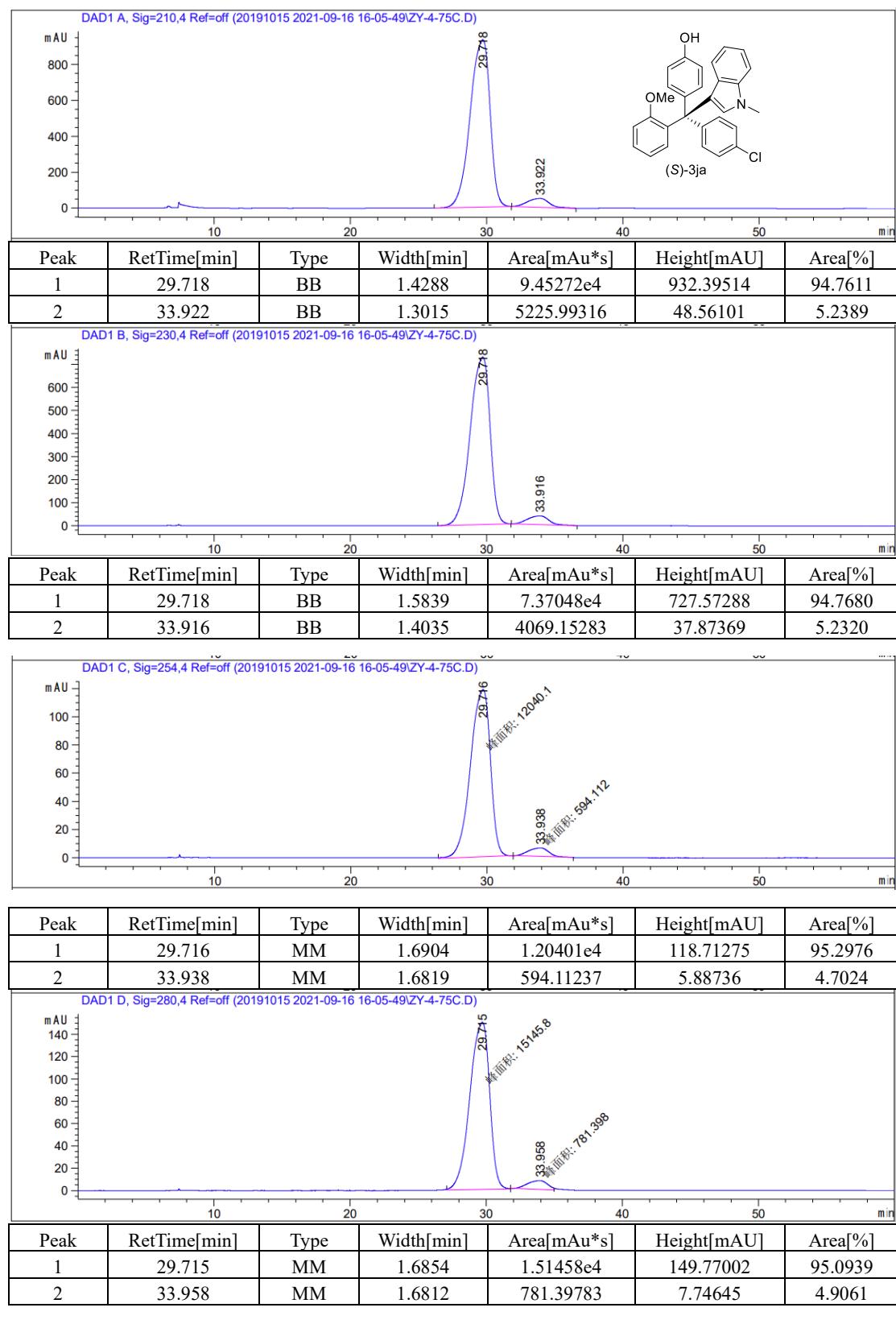
HPLC Condition: AD-H, *n*-Hexane/iPrOH = 98:2, 1.0 mL/min



End of Report

Sample Name: ZY-4-75C-OP

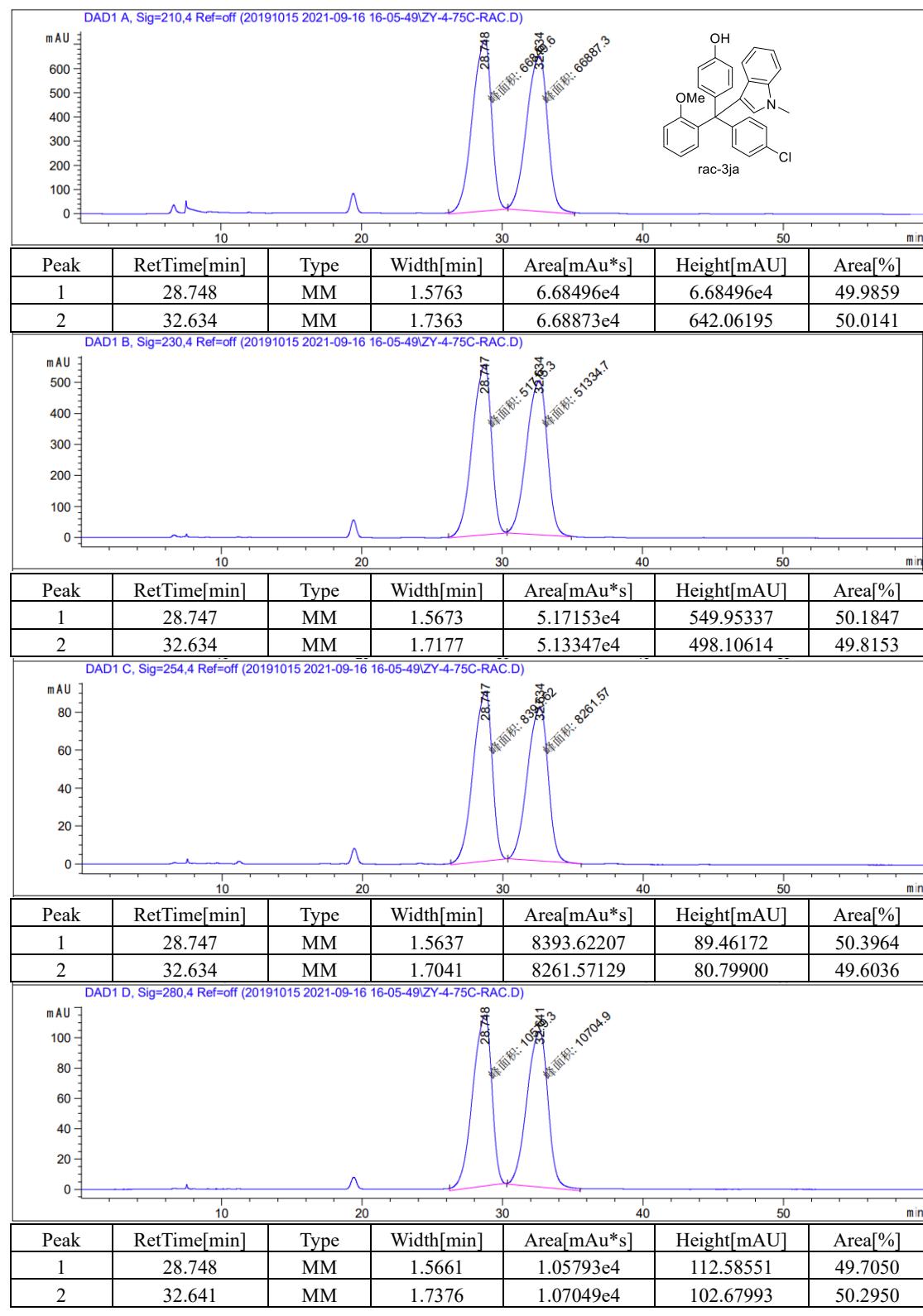
HPLC Condition: IC, *n*-Hexane/iPrOH = 98.5:1.5, 0.5 mL/min



End of Report

Sample Name: ZY-4-75C-Rac

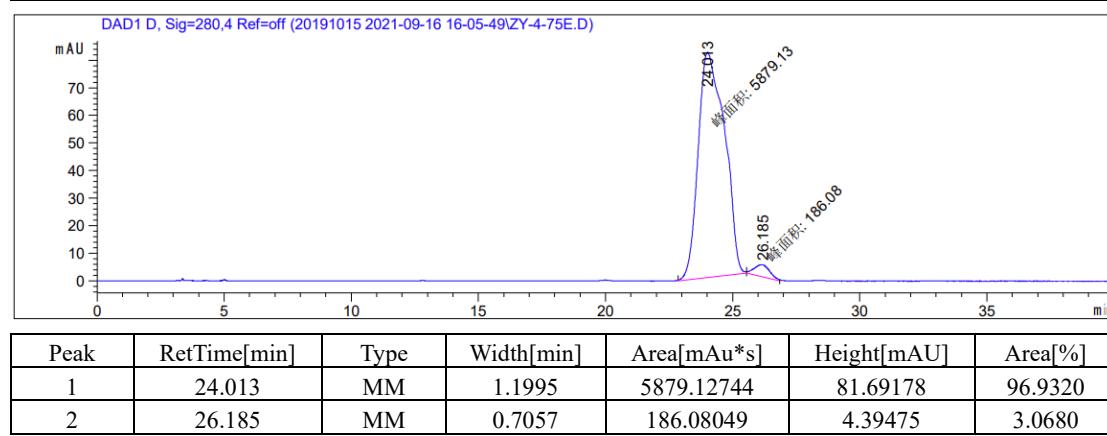
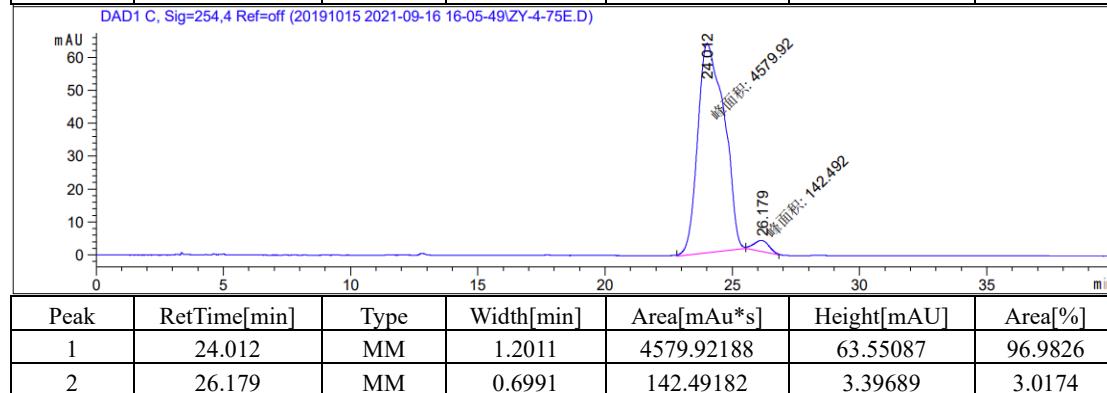
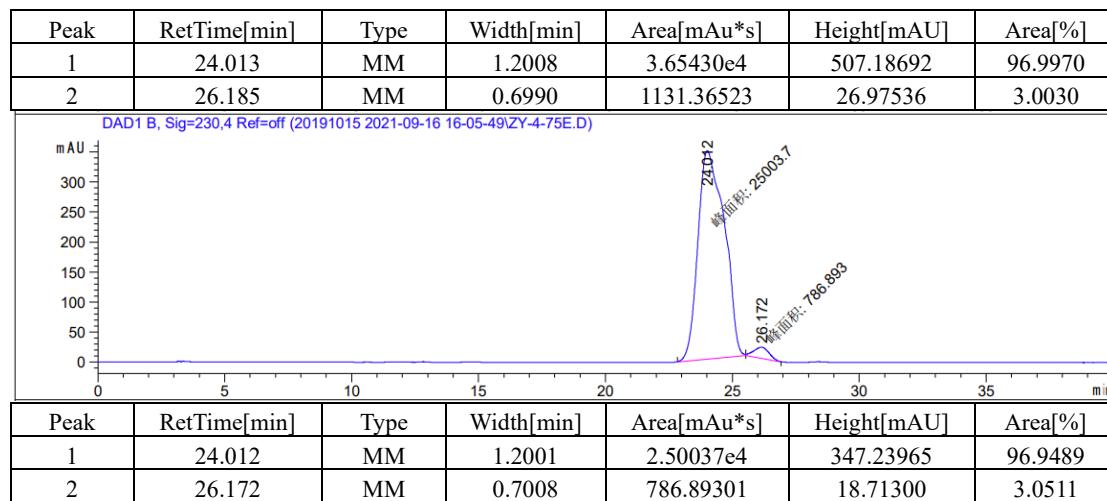
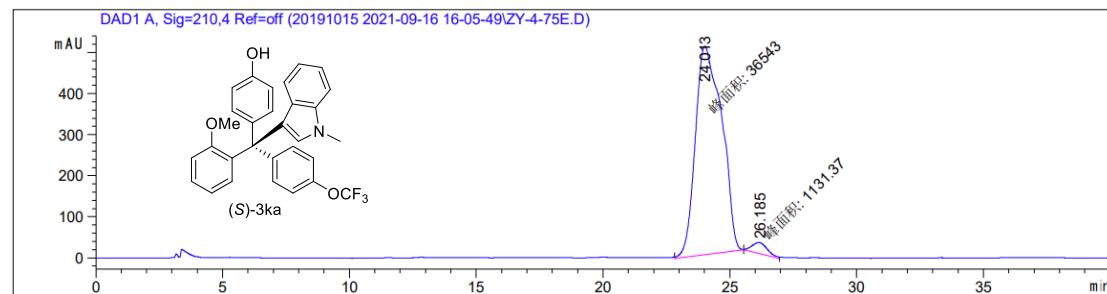
HPLC Condition: IC, n-Hexane/iPrOH = 98.5:1.5, 0.5 mL/min



End of Report

Sample Name: ZY-4-75E-OP

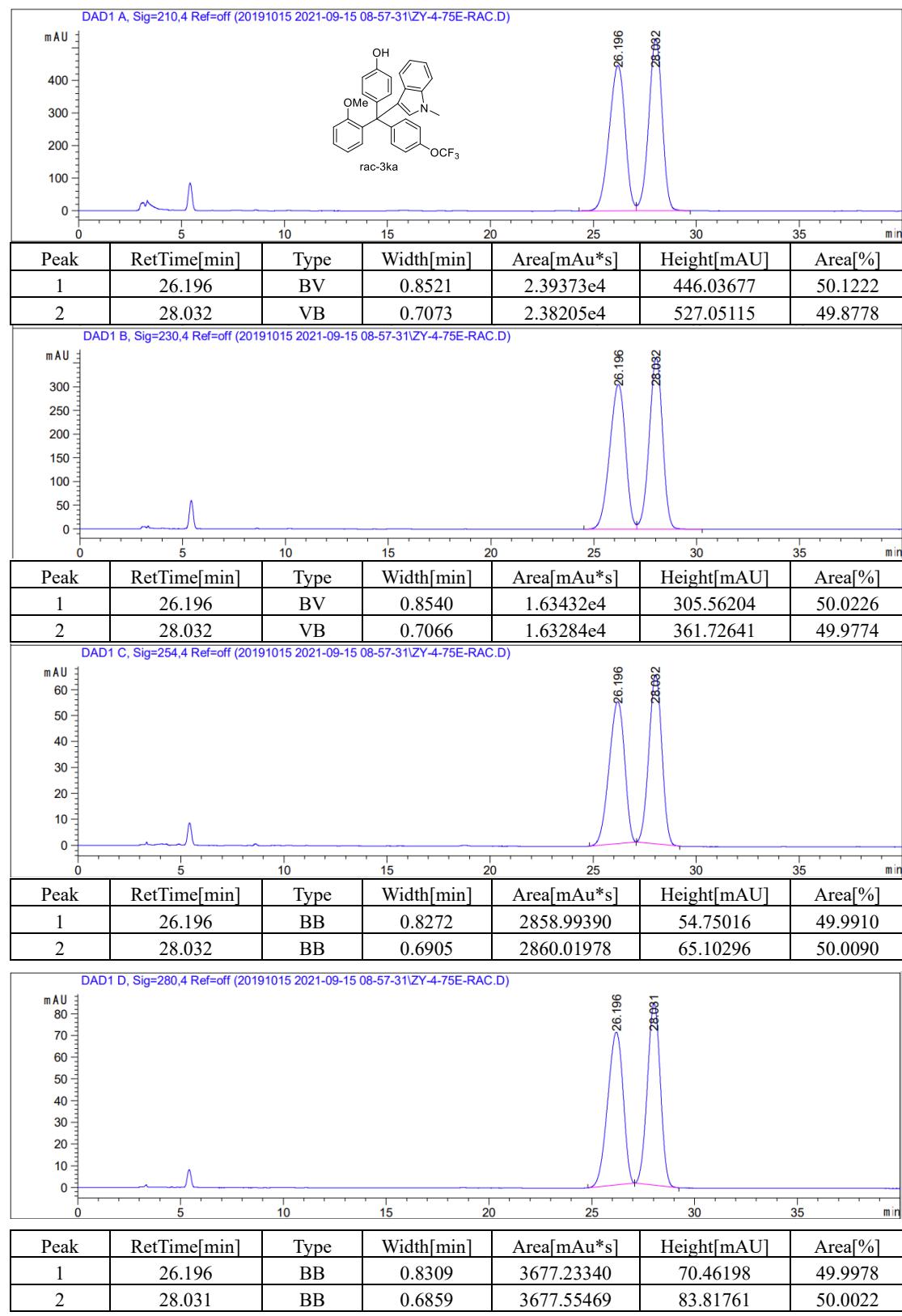
HPLC Condition: AD-H, *n*-Hexane/*i*PrOH = 98:2, 1.0 mL/min



End of Report

Sample Name: ZY-4-75E-Rac

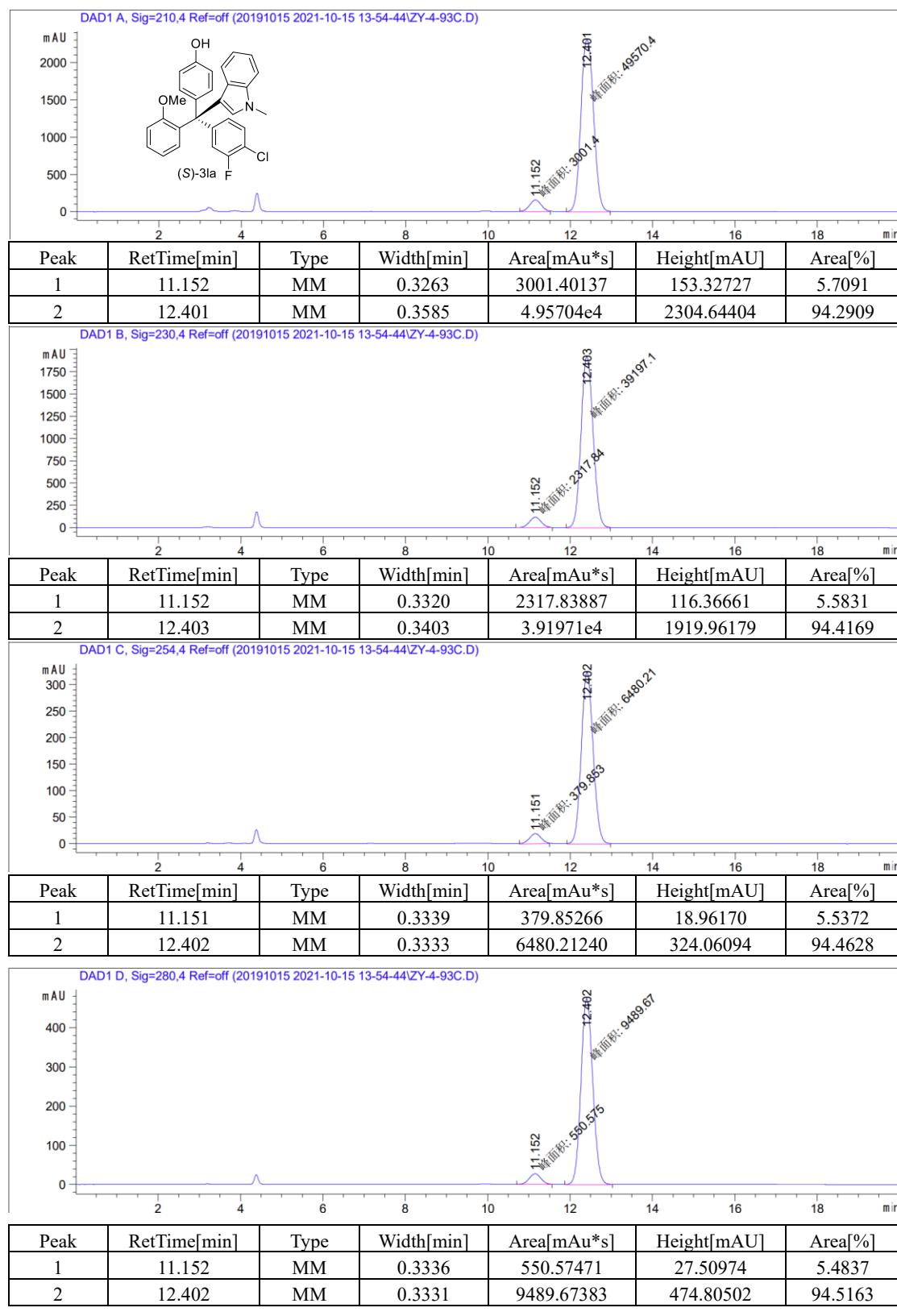
HPLC Condition: AD-H, *n*-Hexane/iPrOH = 98:2, 1.0 mL/min



End of Report

Sample Name: ZY-4-93C-OP

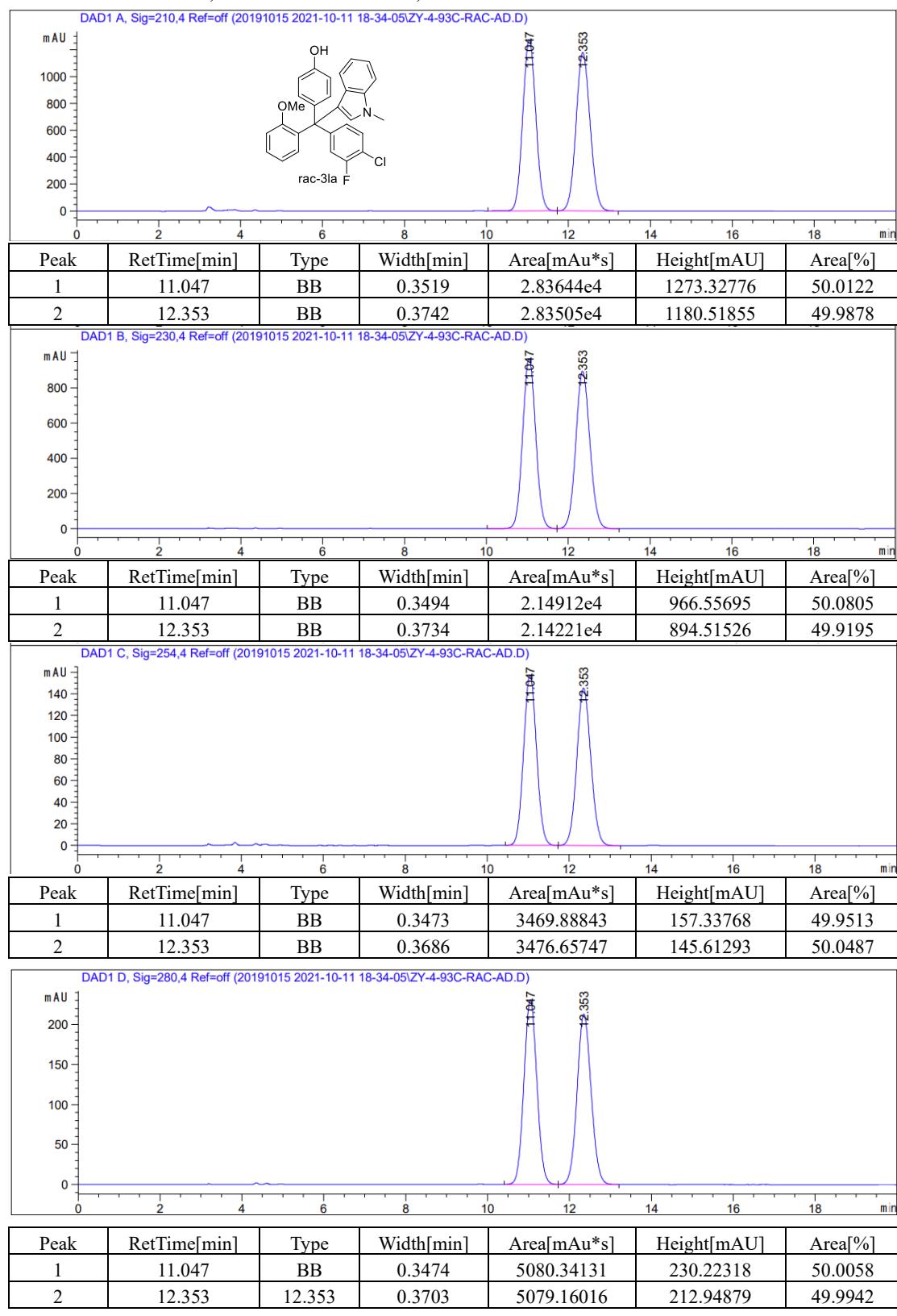
HPLC Condition: AD-H, *n*-Hexane/*i*PrOH = 95:5, 1.0 mL/min



End of Report

Sample Name: ZY-4-93C-Rac

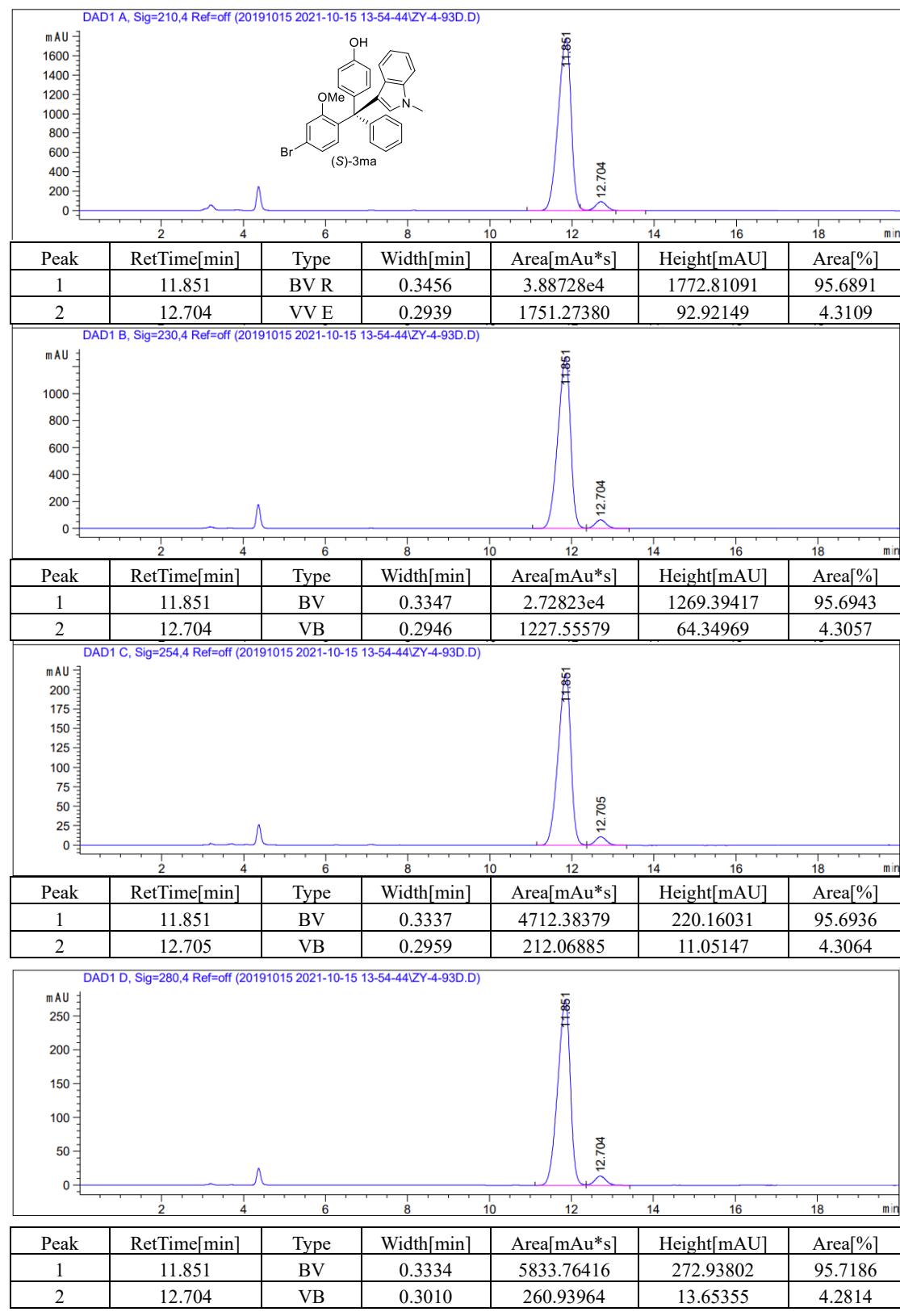
HPLC Condition: AD-H, *n*-Hexane/*i*PrOH = 95:5, 1.0 mL/min



End of Report

Sample Name: ZY-4-93D-OP

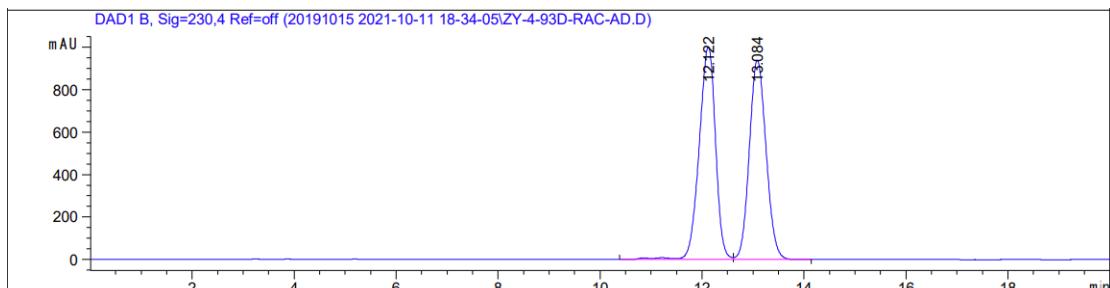
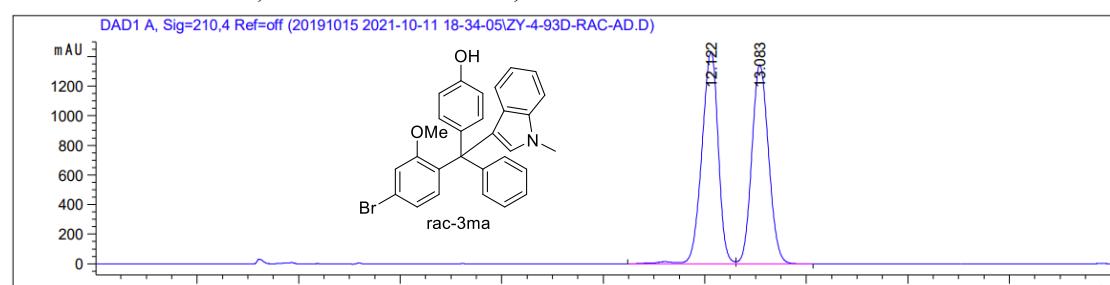
HPLC Condition: AD-H, *n*-Hexane/iPrOH = 95:5, 1.0 mL/min



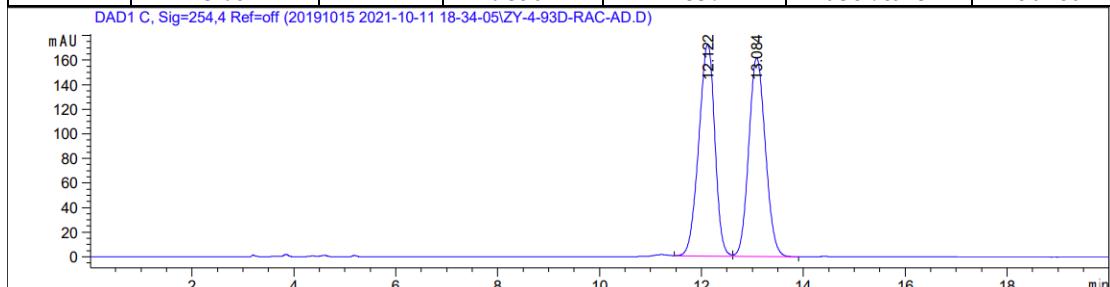
End of Report

Sample Name: ZY-4-93D-Rac

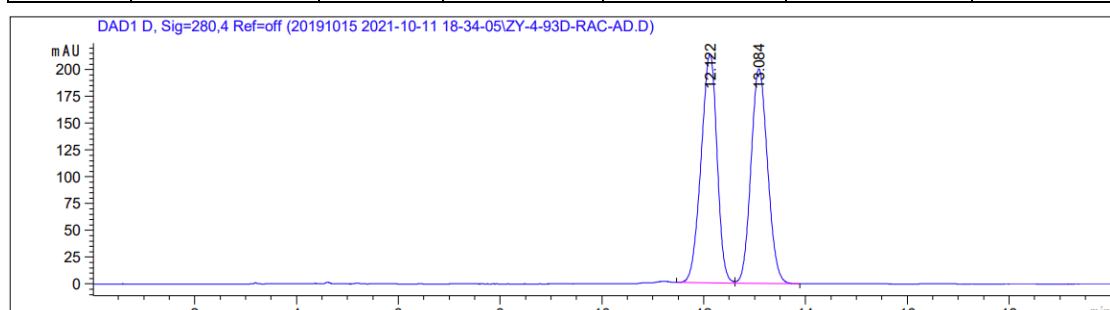
HPLC Condition: AD-H, *n*-Hexane/*i*PrOH = 95:5, 1.0 mL/min



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.122	VV R	0.3412	2.23813e4	1001.10120	51.0814
2	13.084	VB	0.3564	2.14337e4	938.78943	48.9186



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.122	BV	0.3391	3764.80347	172.16327	50.6216
2	13.084	VB	0.3550	3672.34351	161.67903	49.3784

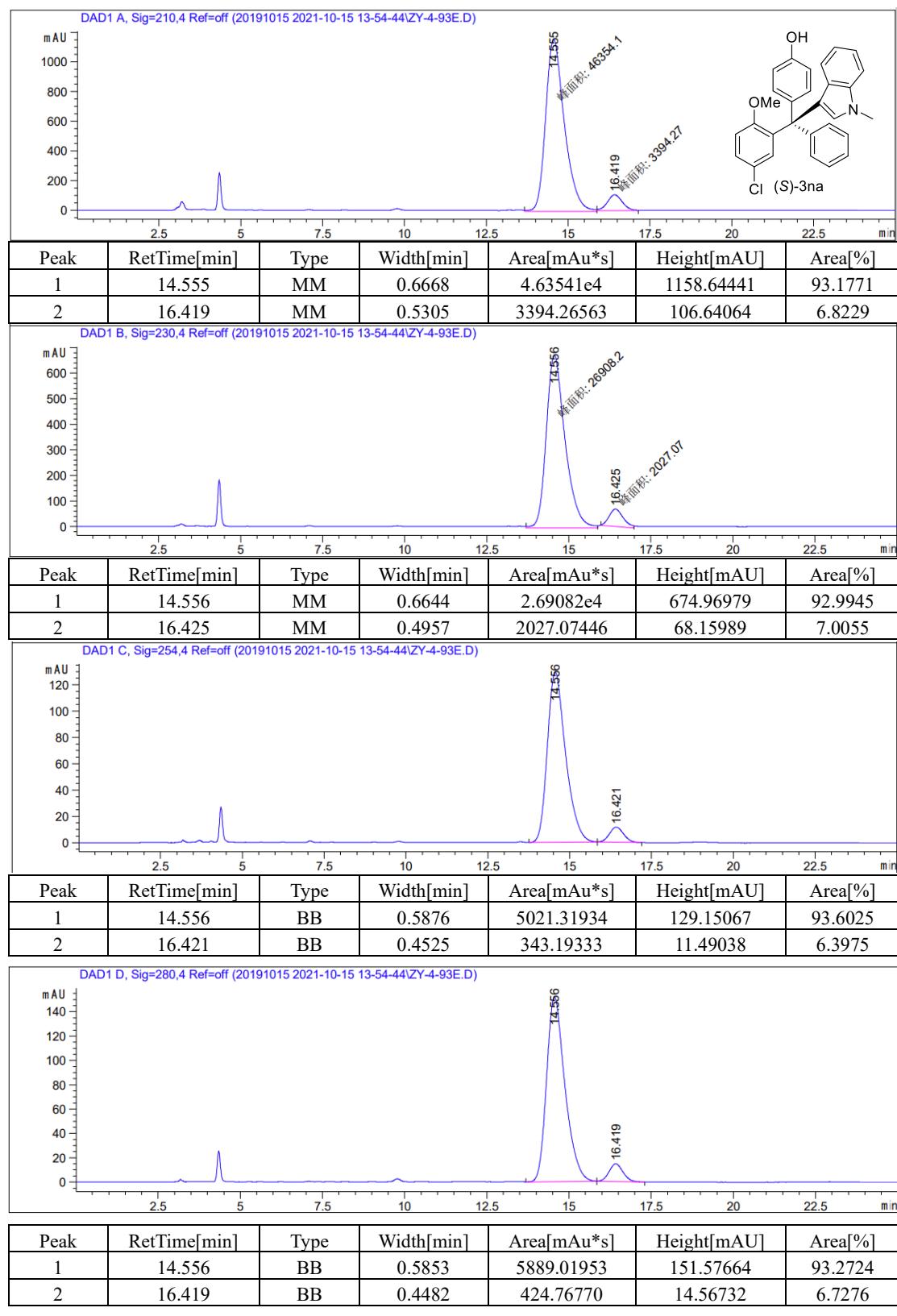


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.122	BV	0.3388	4657.31689	213.27629	50.6255
2	13.084	VB	0.3546	4542.23242	200.25867	49.3745

End of Report

Sample Name: ZY-4-93E-OP

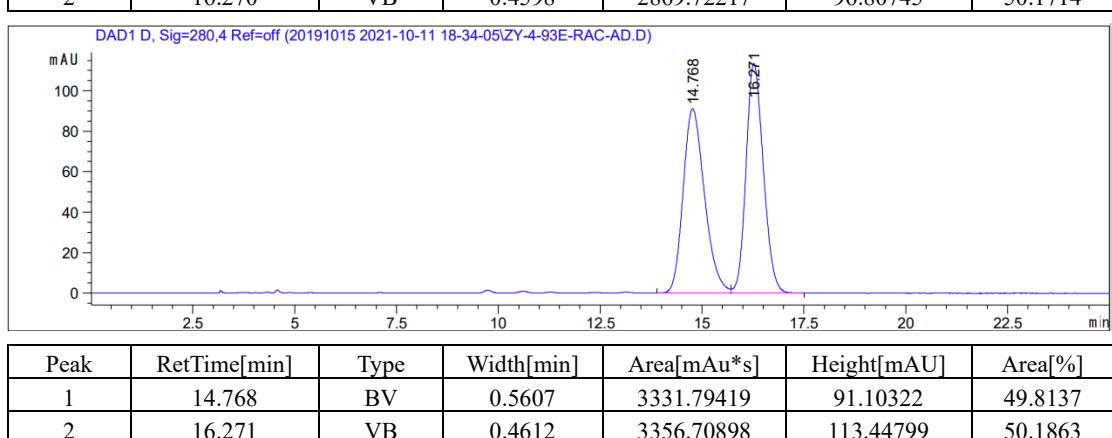
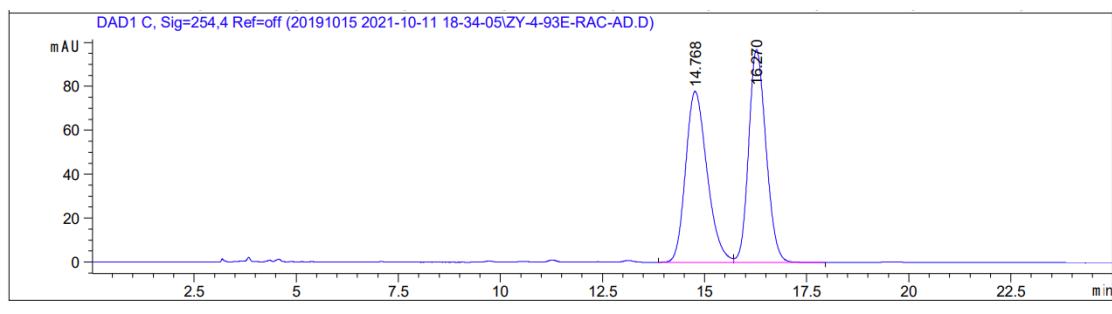
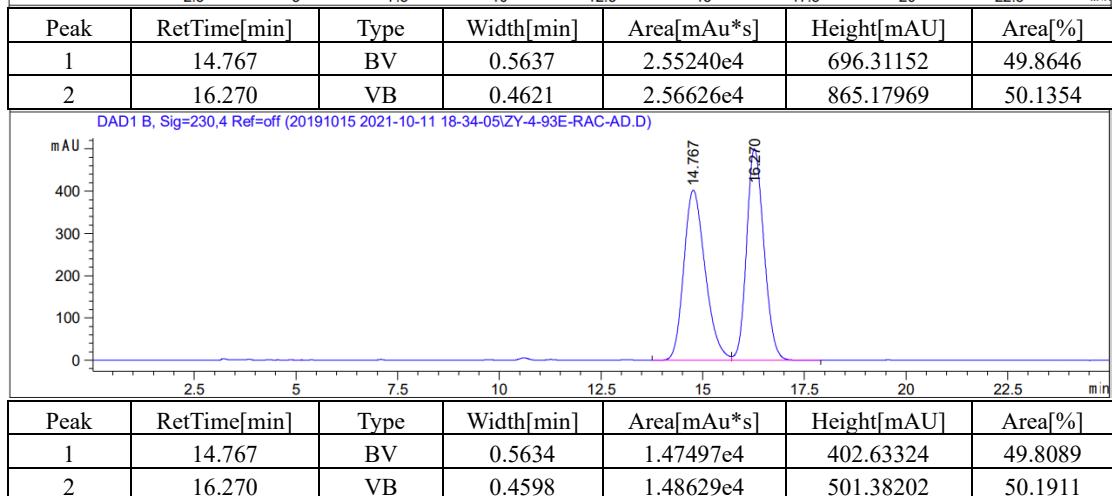
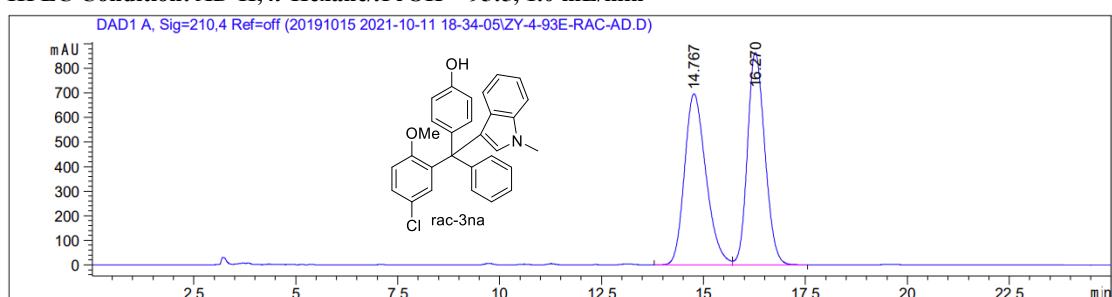
HPLC Condition: AD-H, n-Hexane/iPrOH = 95:5, 1.0 mL/min



End of Report

**Sample Name: ZY-4-93E-Rac**

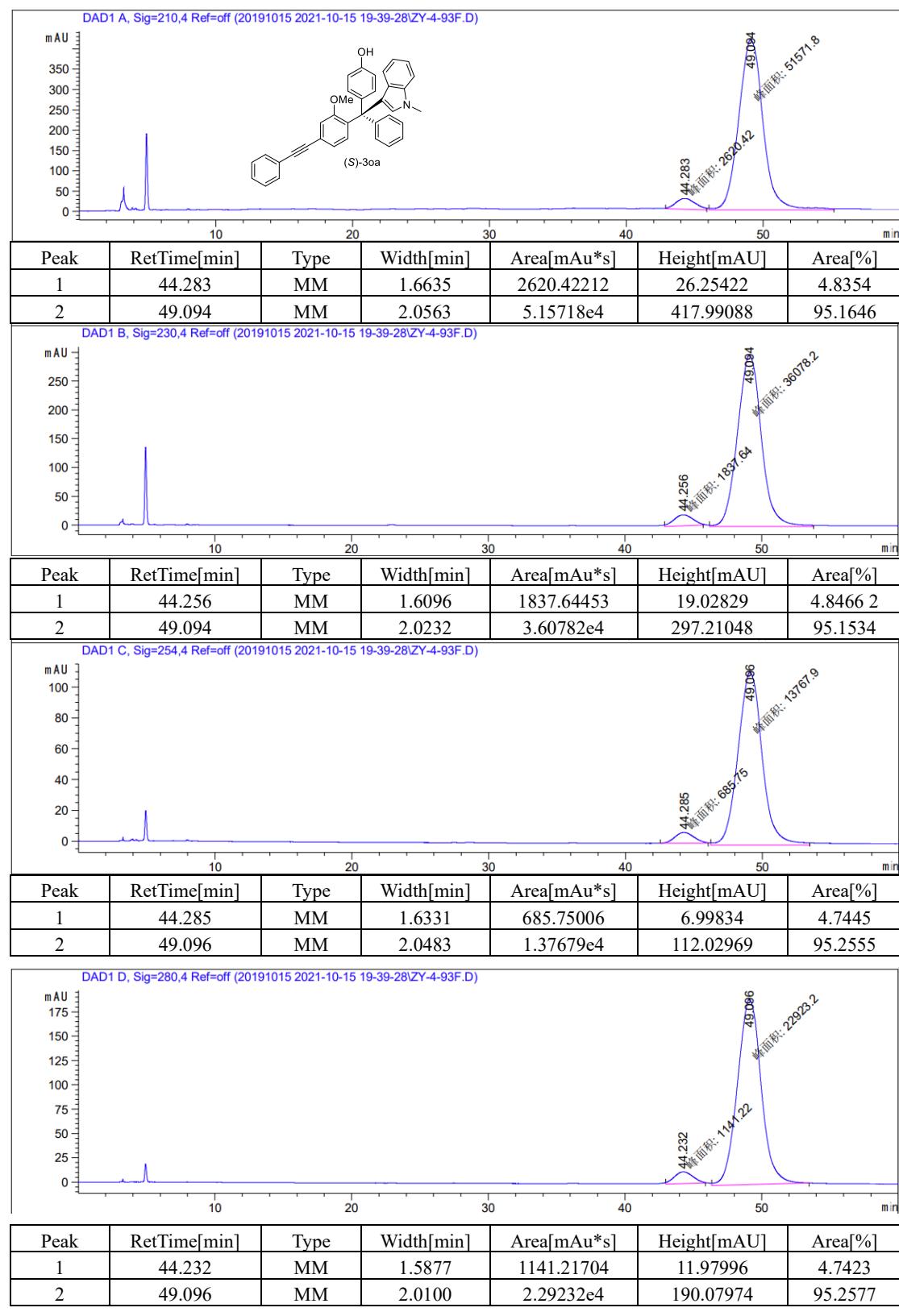
**HPLC Condition: AD-H, n-Hexane/iPrOH = 95:5, 1.0 mL/min**



End of Report

Sample Name: ZY-4-93F-OP

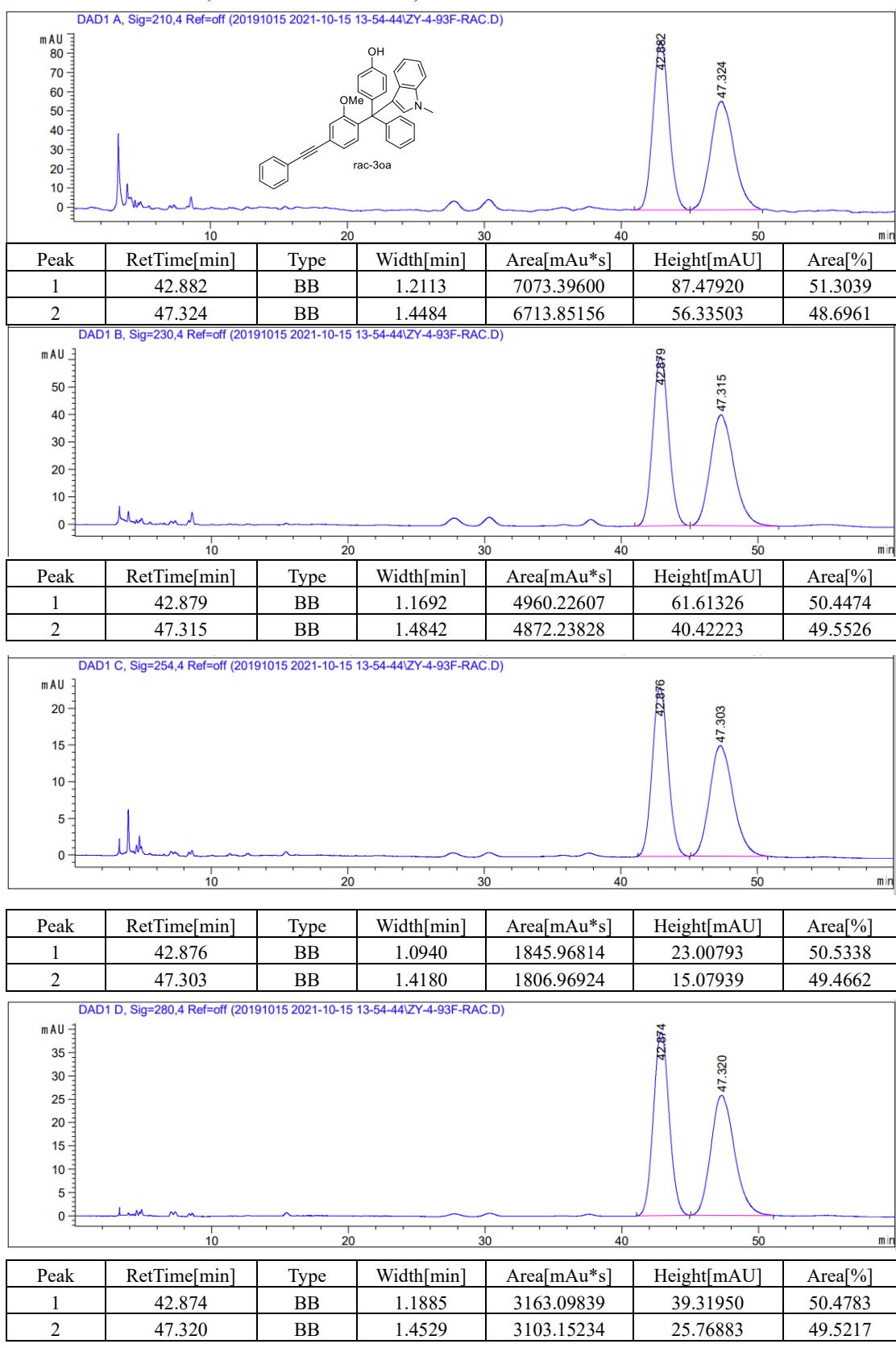
HPLC Condition: AD-H, *n*-Hexane/iPrOH = 97:3, 1.0 mL/min



End of Report

Sample Name: ZY-4-93F-Rac

HPLC Condition: AD-H, *n*-Hexane/iPrOH = 97:3, 1.0 mL/min

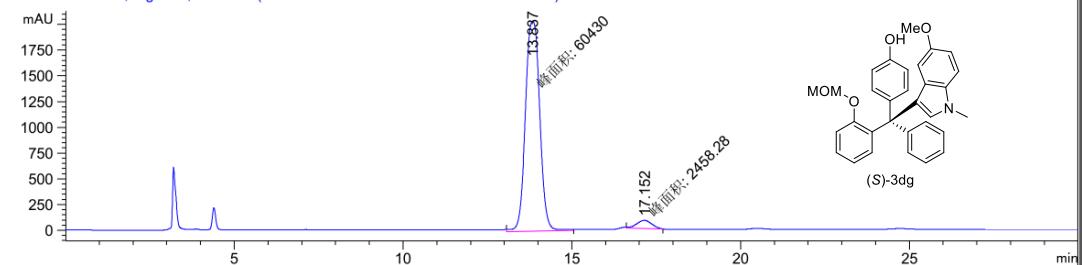


End of Report

Sample Name: ZY-4-86C-OP

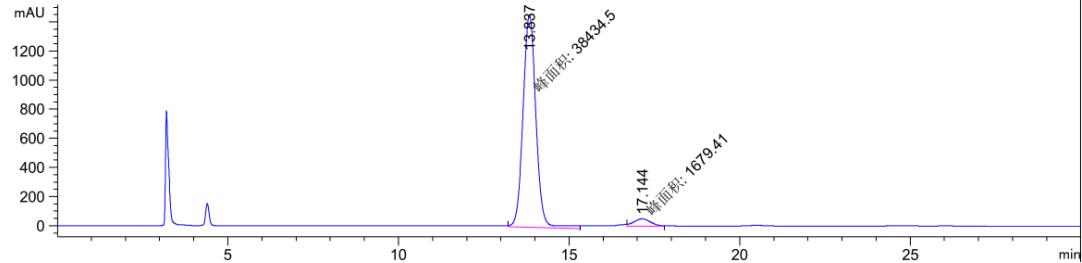
HPLC Condition:AD-H, *n*-Hexane/iPrOH = 95:5, 1.0 mL/min

DAD1 A, Sig=210,4 Ref=off (20191015 2021-09-30 14-39-25|ZY-4-86C.D)



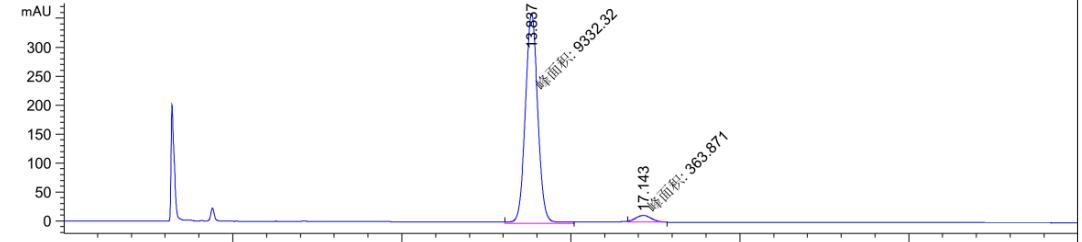
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	13.837	MM	0.4937	6.04300e4	2040.11157	96.0910
2	17.152	MM	0.5195	2458.28223	78.86625	3.9090

DAD1 B, Sig=230,4 Ref=off (20191015 2021-09-30 14-39-25|ZY-4-86C.D)



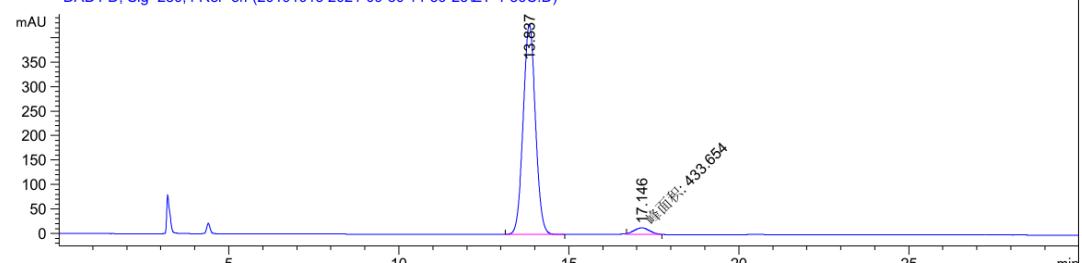
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	13.837	MM	0.4393	3.84345e4	1458.21313	95.8134
2	17.144	MM	0.5659	1679.41260	49.46396	4.1866

DAD1 C, Sig=254,4 Ref=off (20191015 2021-09-30 14-39-25|ZY-4-86C.D)



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	13.837	MM	0.4293	9332.31543	362.34860	96.2473
2	17.143	MM	0.5339	363.87070	11.35797	3.7527

DAD1 D, Sig=280,4 Ref=off (20191015 2021-09-30 14-39-25|ZY-4-86C.D)

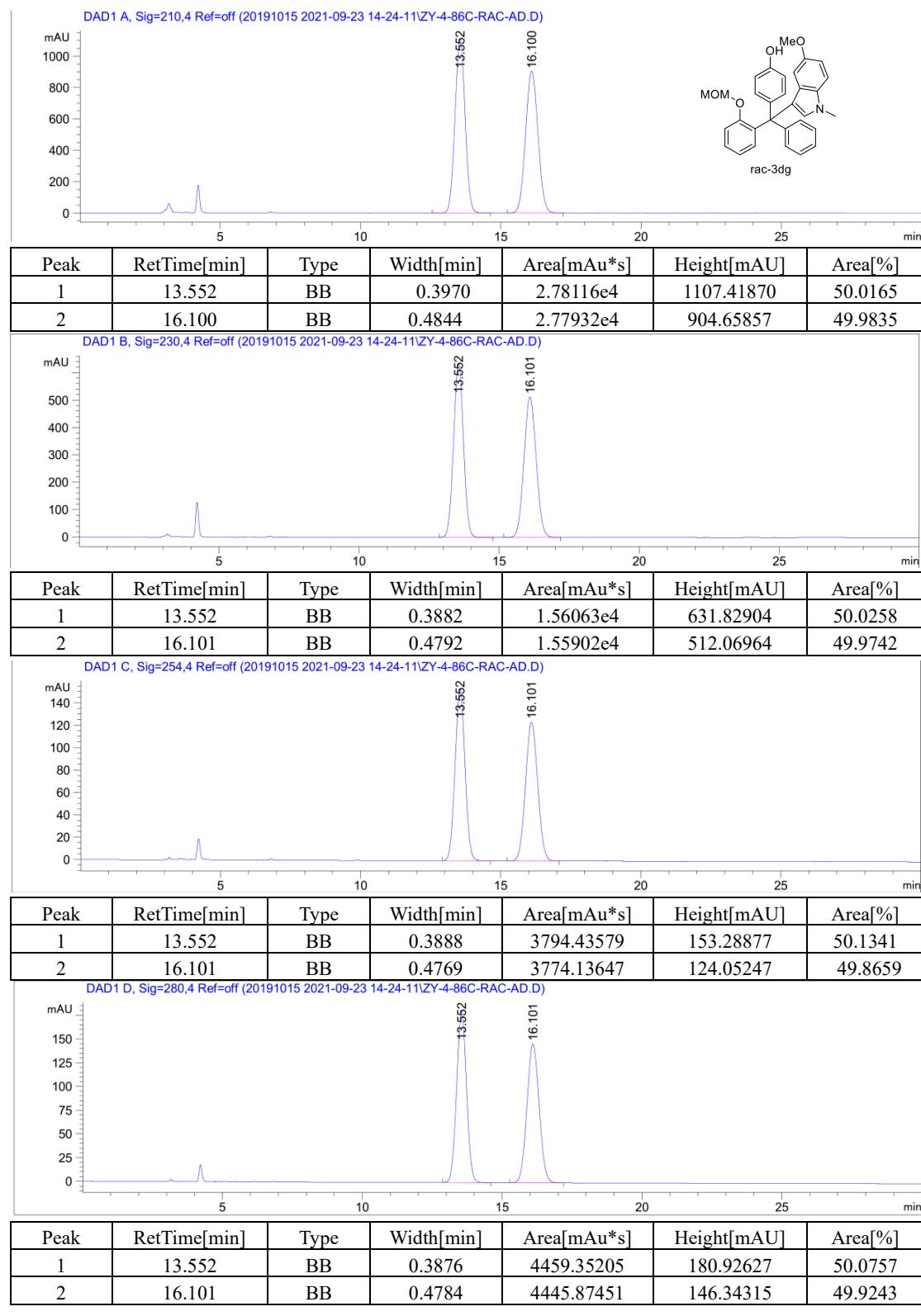


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	13.837	BB	0.3886	1.07547e4	428.76187	96.1241
2	17.146	MM	0.5345	433.65399	13.52119	3.8759

End of Report

**Sample Name: ZY-4-86C-Rac**

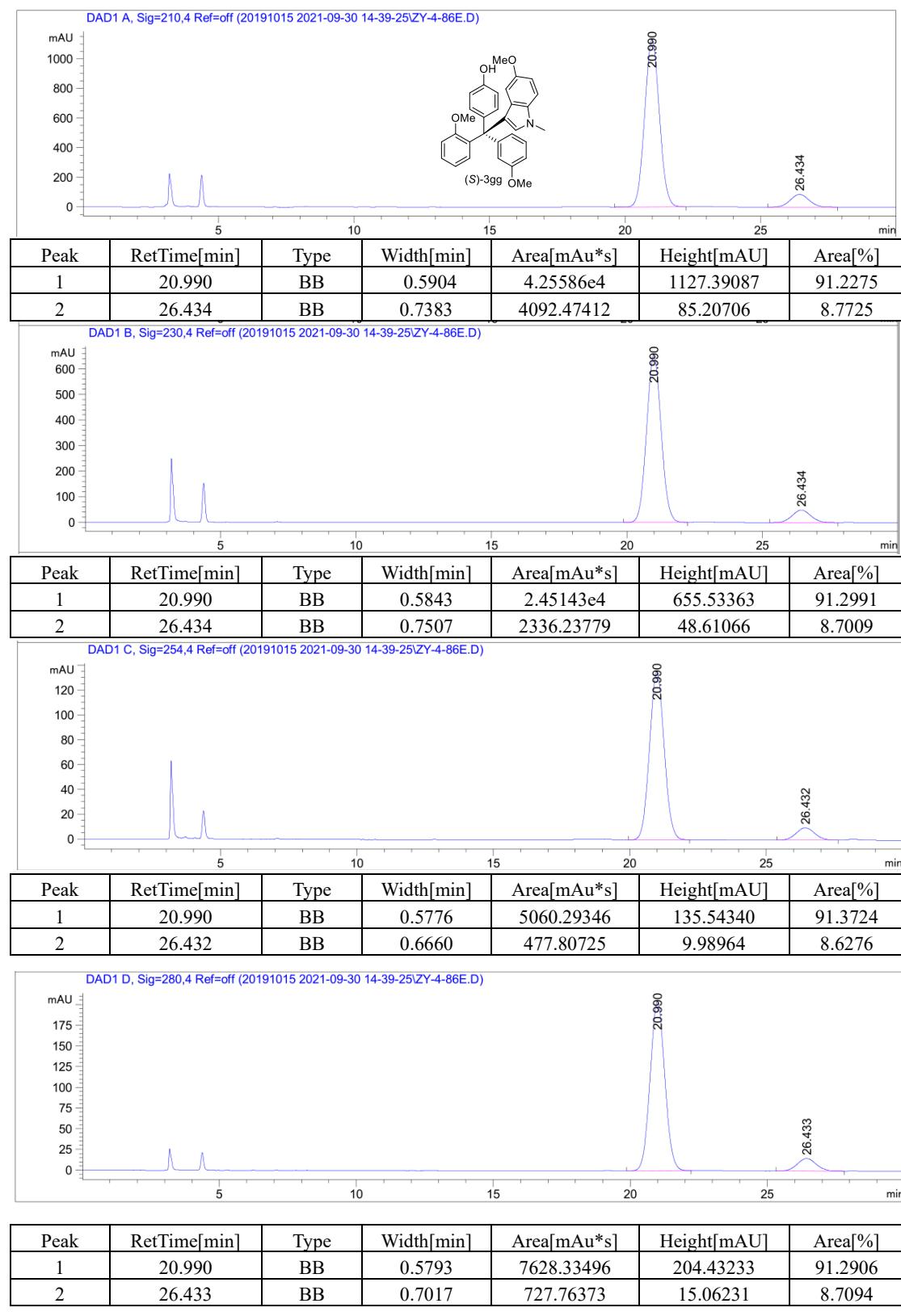
**HPLC Condition:AD-H, n-Hexane/iPrOH = 95:5, 1.0 mL/min**



End of Report

Sample Name: ZY-4-86E-OP

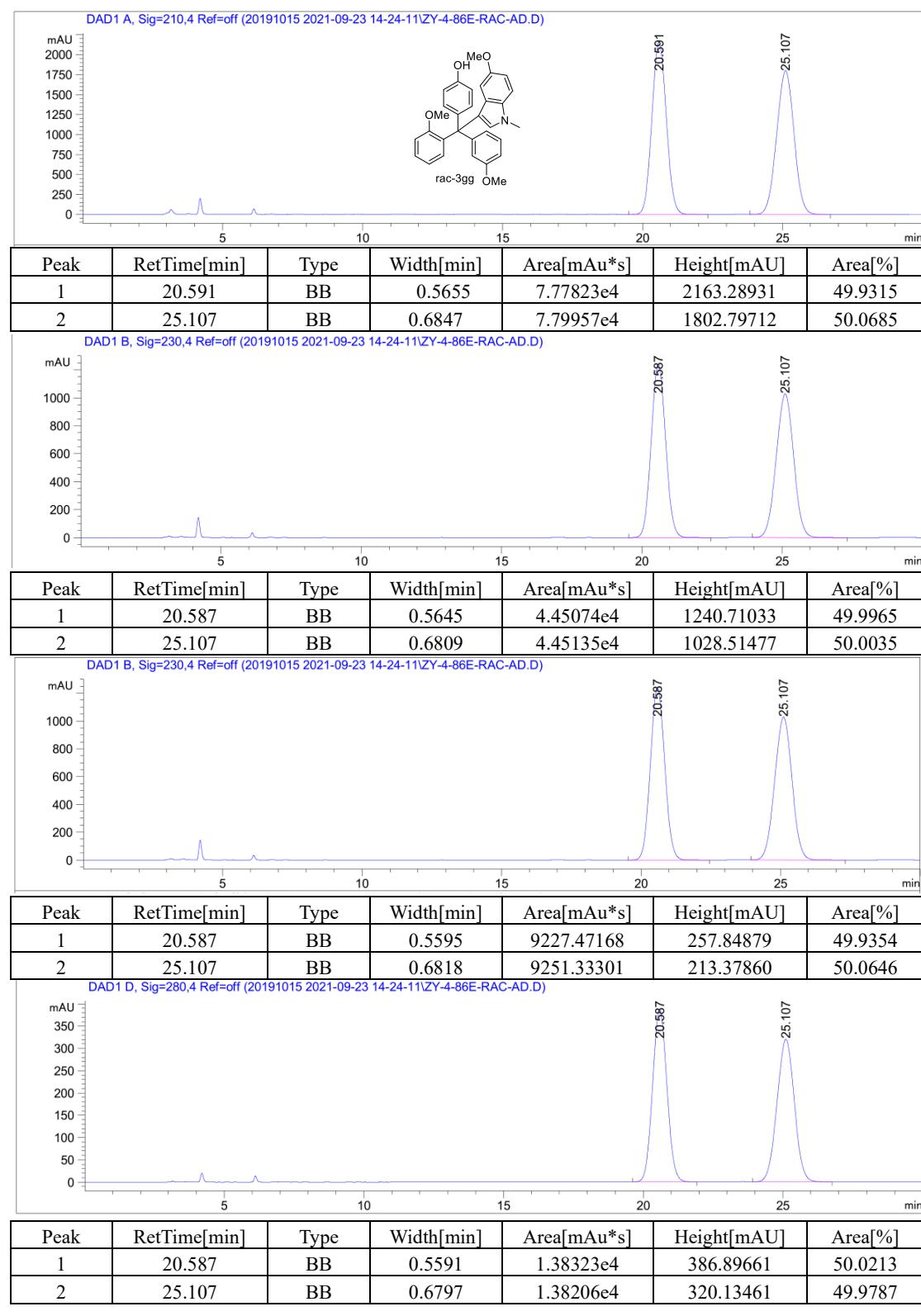
HPLC Condition:AD-H, *n*-Hexane/iPrOH = 95:5, 1.0 mL/min



End of Report

**Sample Name: ZY-4-86E-Rac**

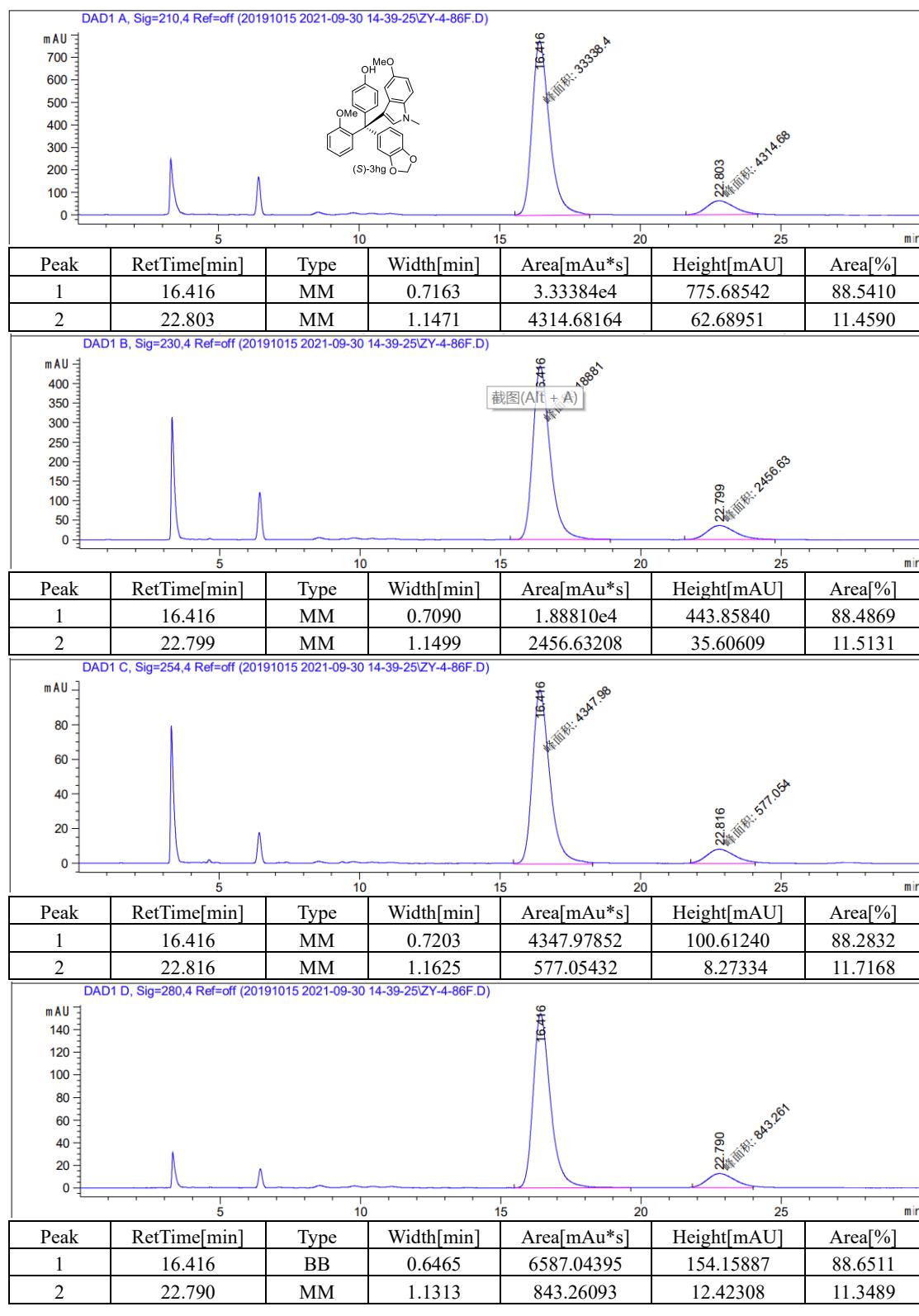
**HPLC Condition:AD-H, n-Hexane/iPrOH = 95:5, 1.0 mL/min**



End of Report

Sample Name: ZY-4-86F-OP

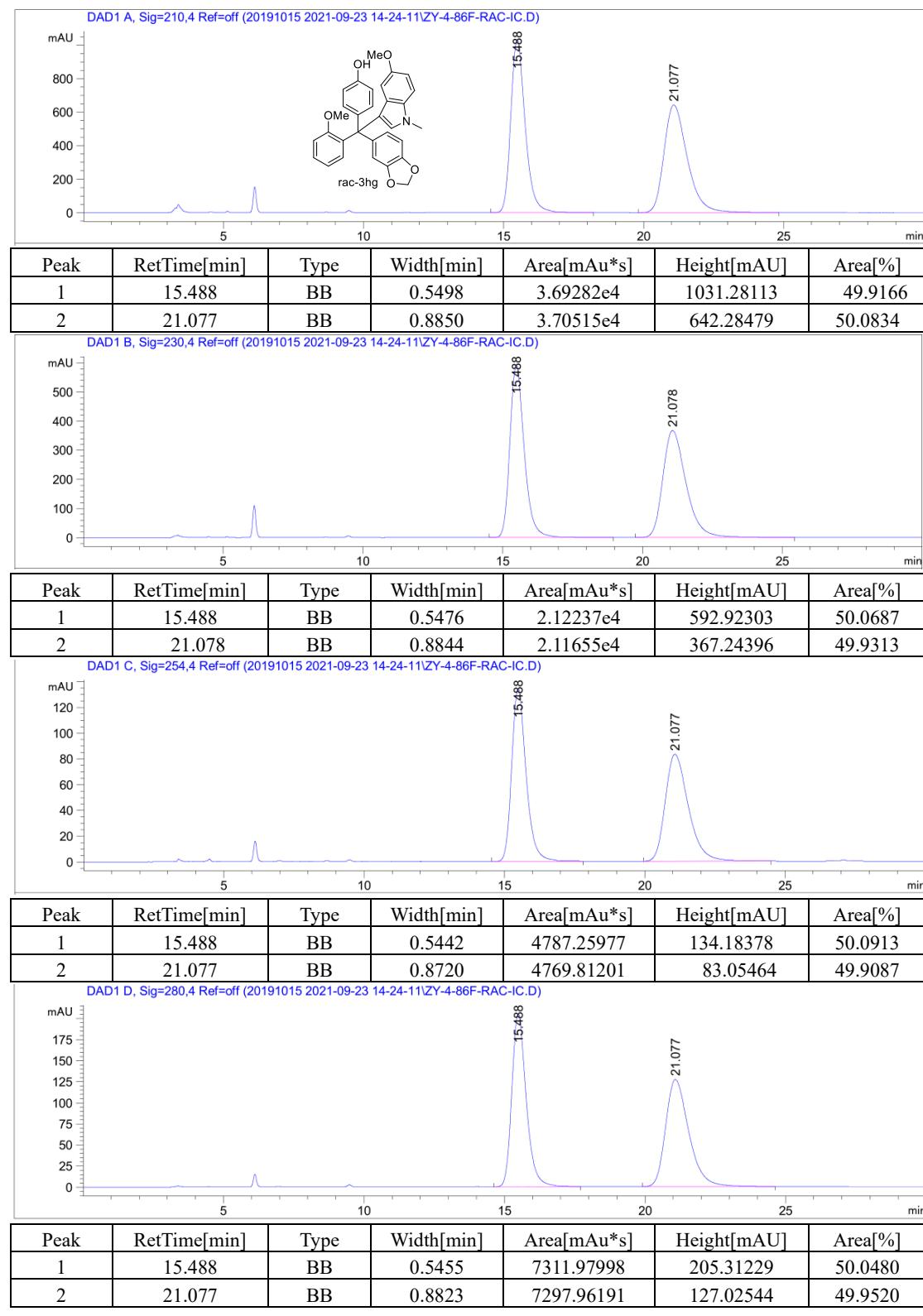
HPLC Condition:IC, *n*-Hexane/*i*PrOH = 95:5, 1.0 mL/min



End of Report

Sample Name: ZY-4-86F-Rac

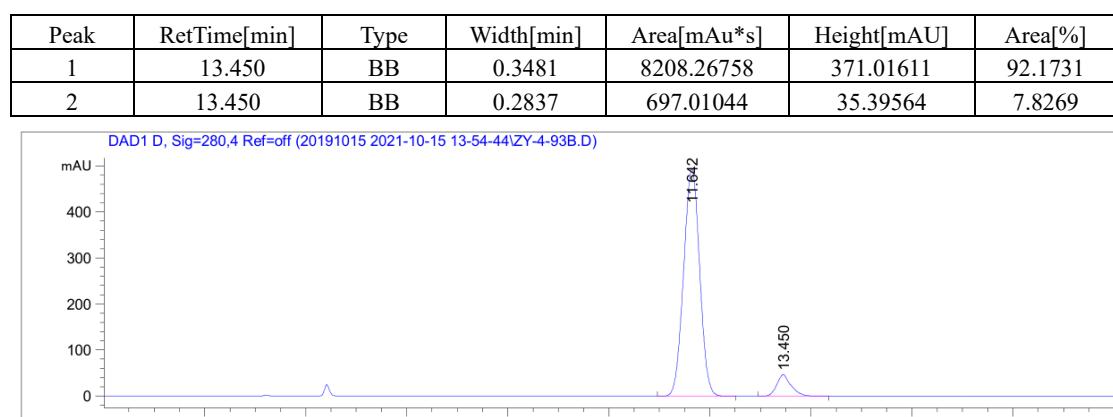
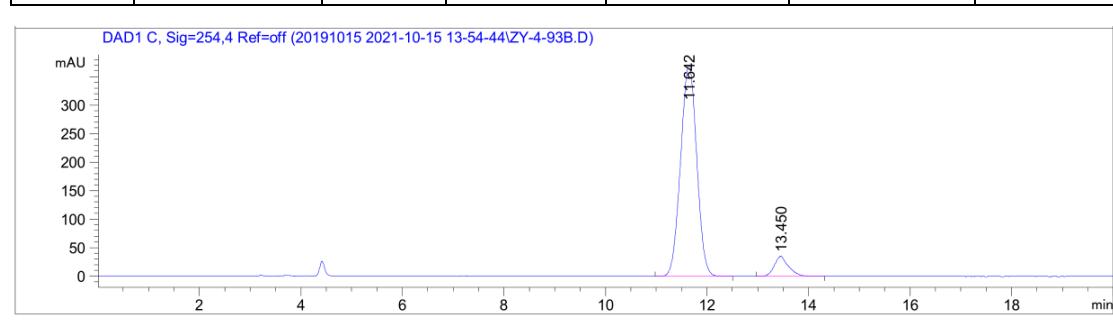
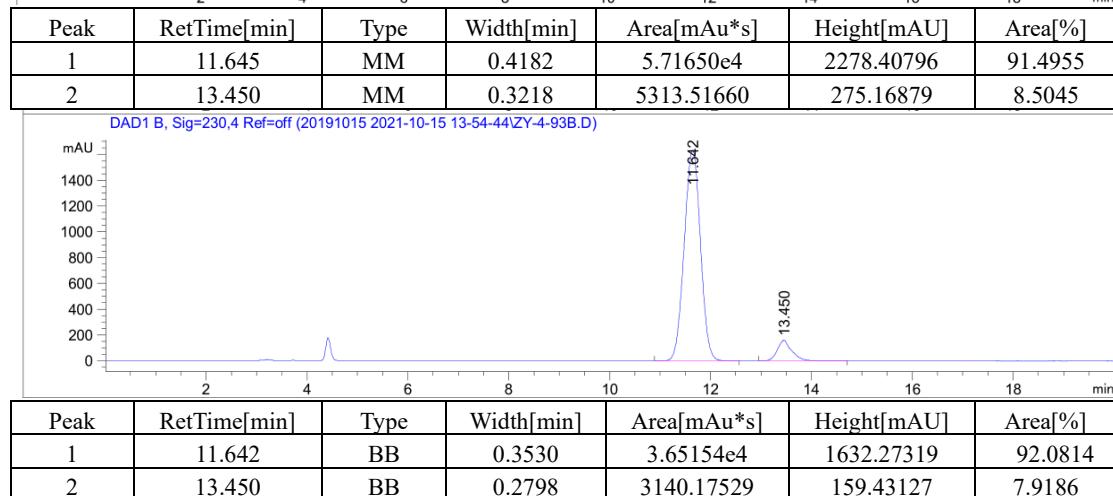
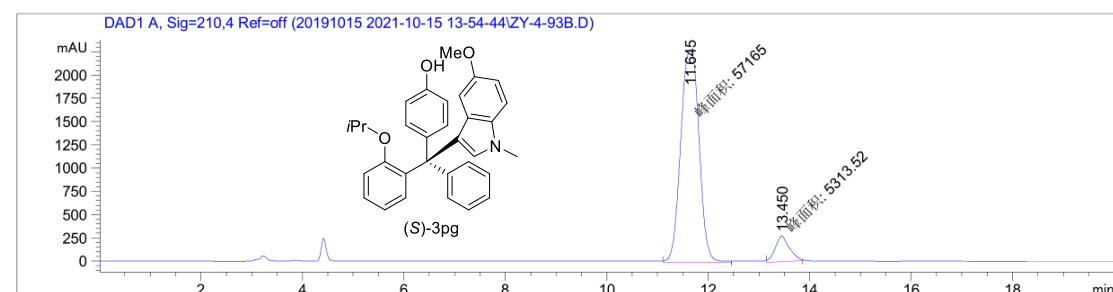
HPLC Condition:IC, *n*-Hexane/iPrOH = 95:5, 1.0 mL/min



End of Report

**Sample Name: ZY-4-93B**

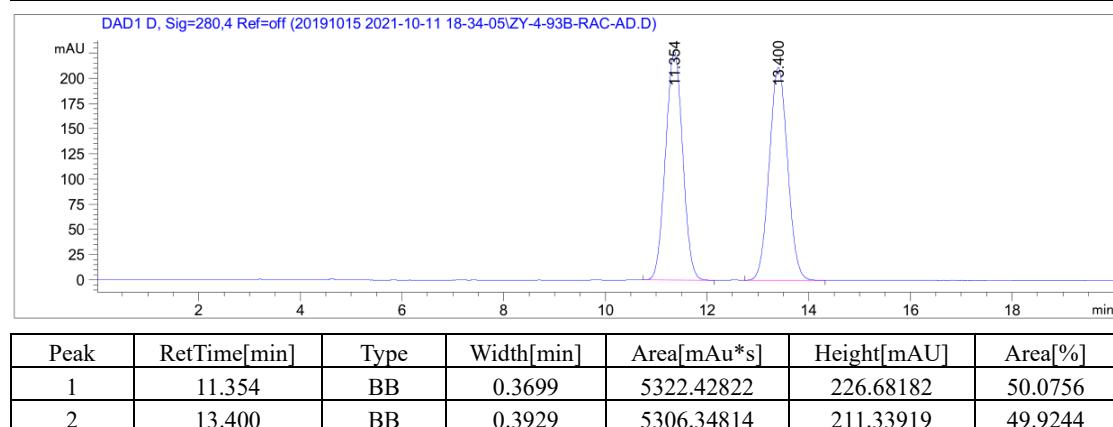
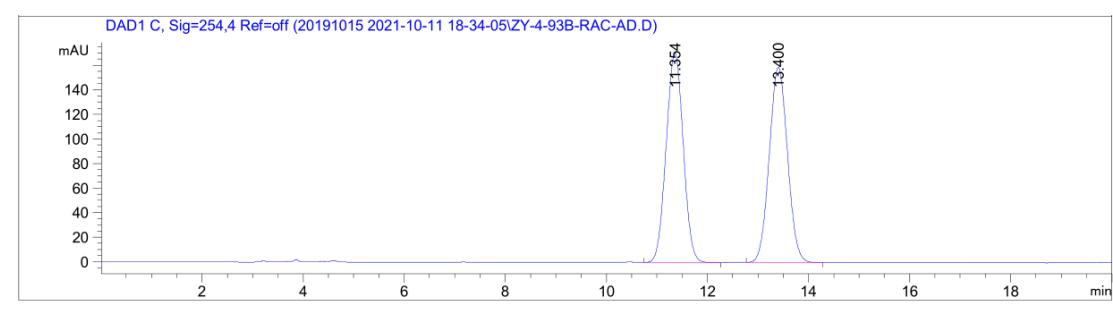
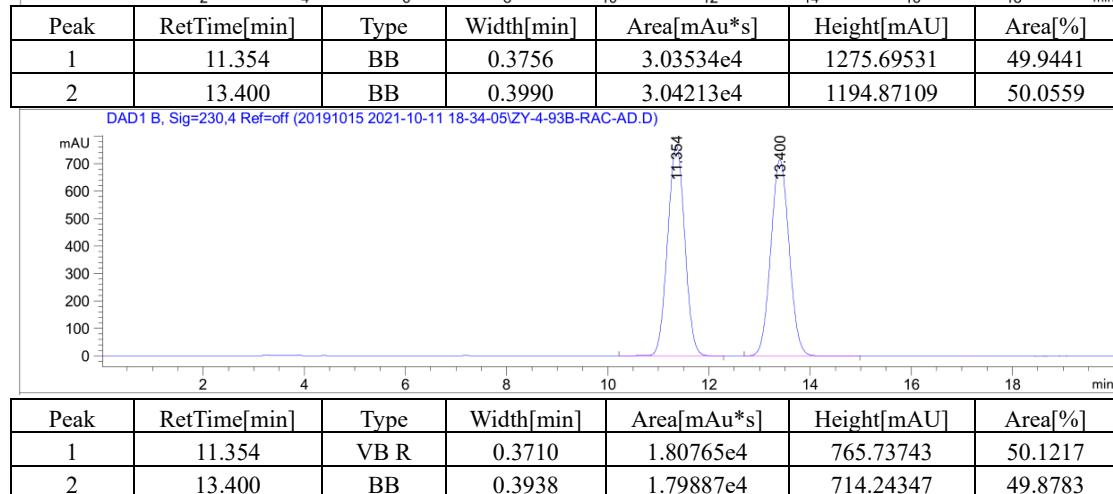
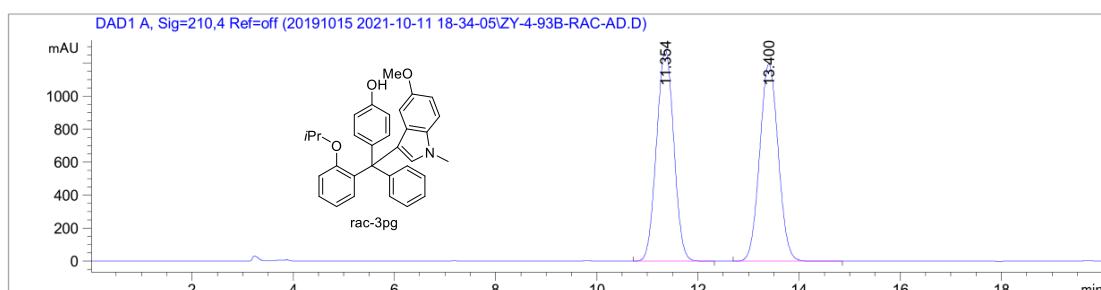
**HPLC Condition:AD-H, n-Hexane/iPrOH = 95:5, 1.0 mL/min**



End of Report

**Sample Name: ZY-4-93B-Rac**

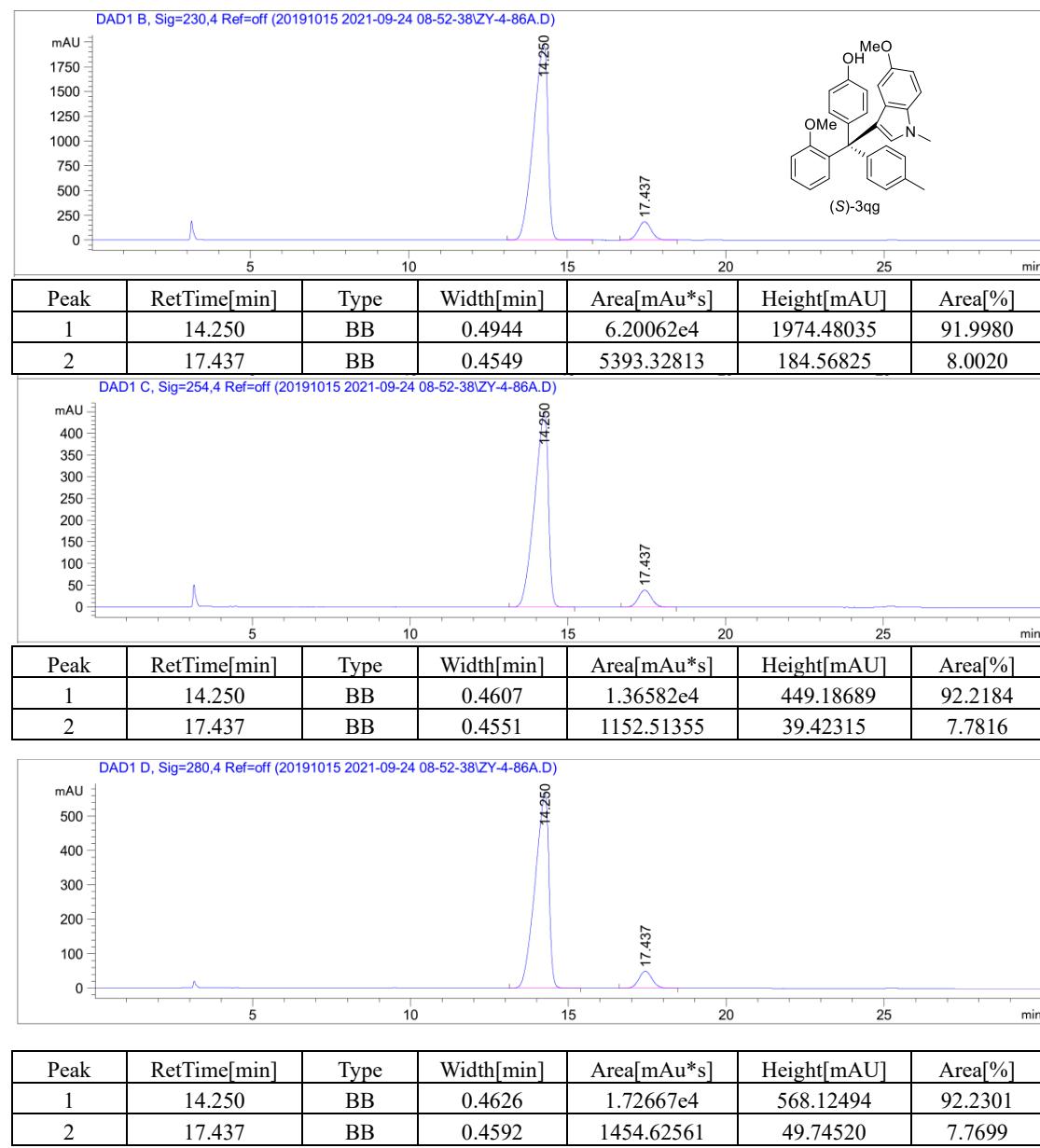
**HPLC Condition:AD-H, n-Hexane/iPrOH = 95:5, 1.0 mL/min**



End of Report

Sample Name: ZY-4-86A-OP

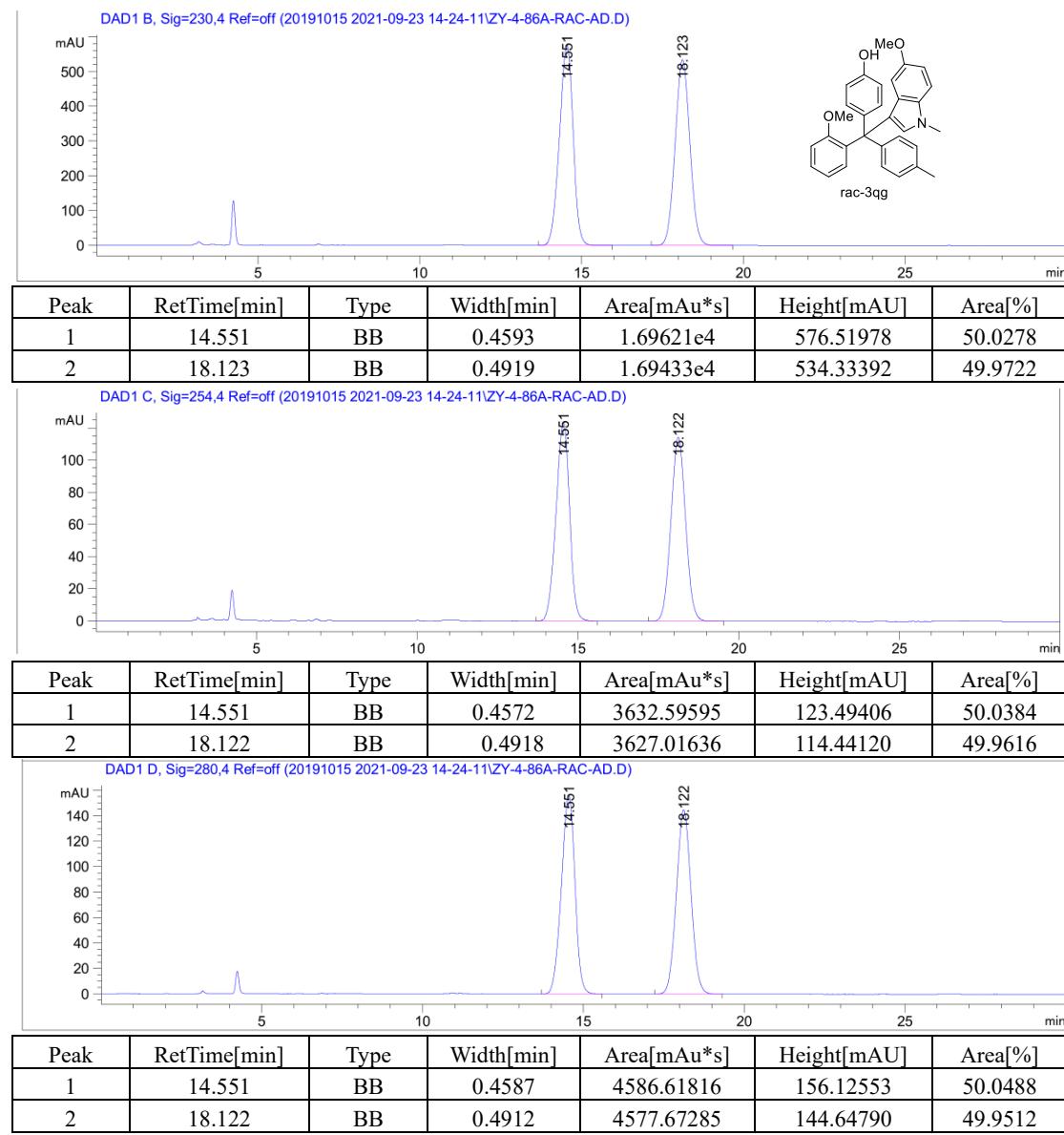
HPLC Condition:AD-H, *n*-Hexane/iPrOH = 95:5, 1.0 mL/min



=====  
End of Report

Sample Name: ZY-4-86A-Rac

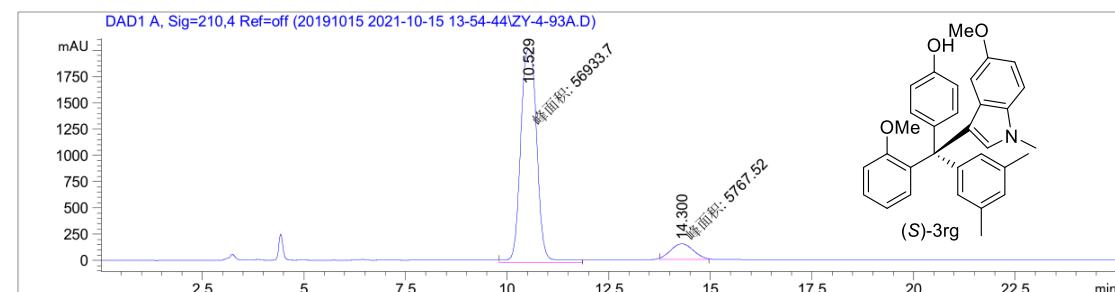
HPLC Condition:AD-H, *n*-Hexane/iPrOH = 95:5, 1.0 mL/min



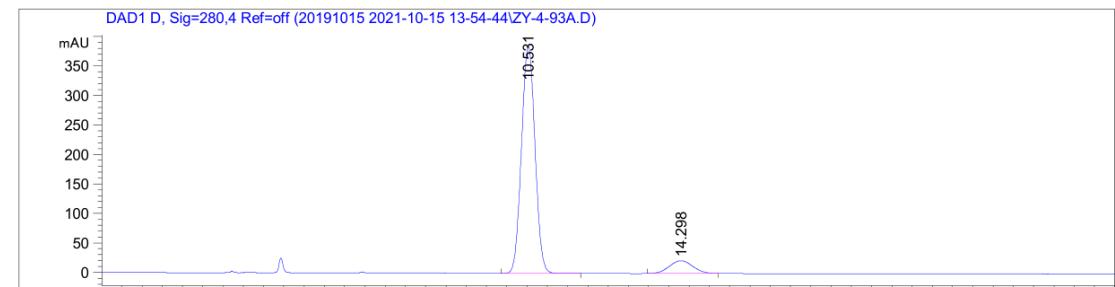
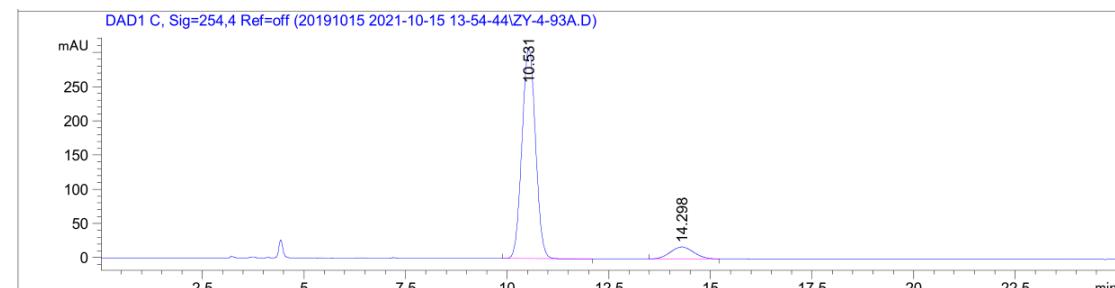
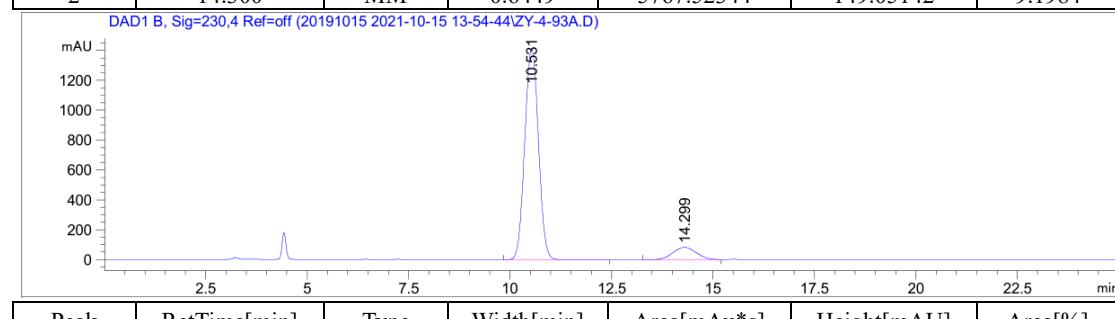
=====  
End of Report

Sample Name: ZY-4-93A-OP

HPLC Condition:AD-H, *n*-Hexane/iPrOH = 95:5, 1.0 mL/min



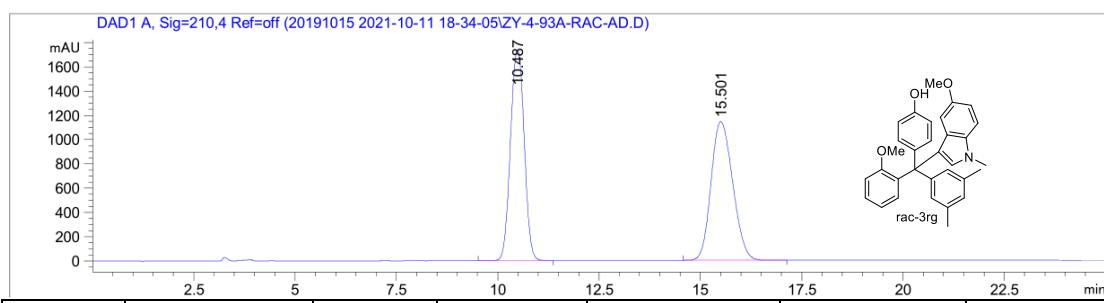
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.529	MM	0.4657	5.69337e4	2037.60828	90.8016
2	14.300	MM	0.6449	5767.52344	149.05142	9.1984



End of Report

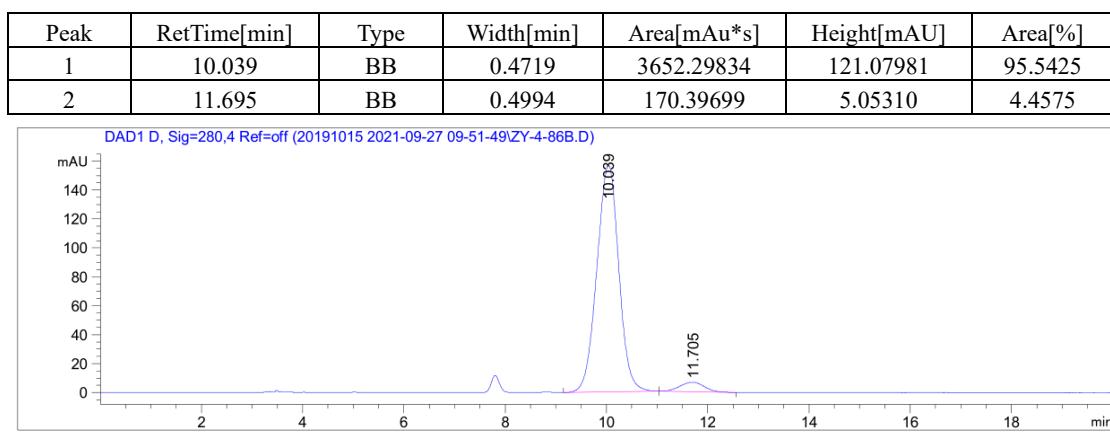
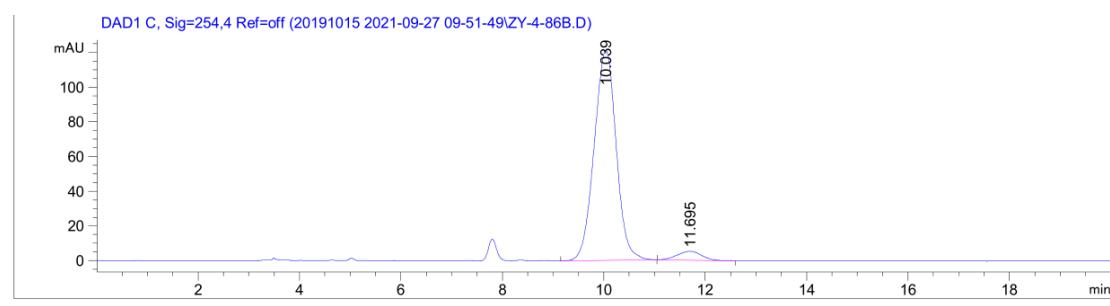
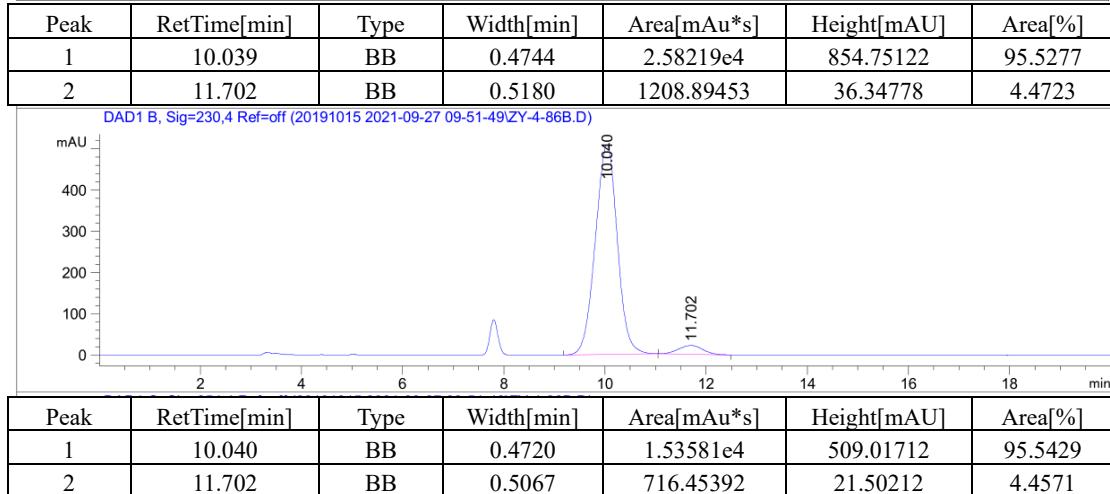
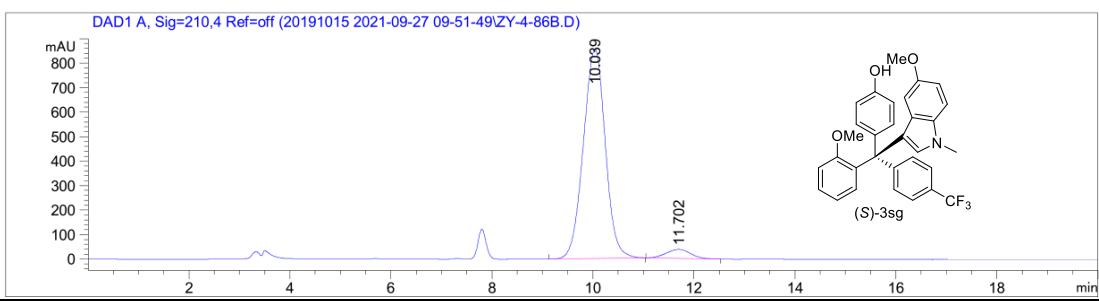
Sample Name: ZY-4-93A-Rac

HPLC Condition:AD-H, *n*-Hexane/iPrOH = 95:5, 1.0 mL/min



Sample Name: ZY-4-86B-OP

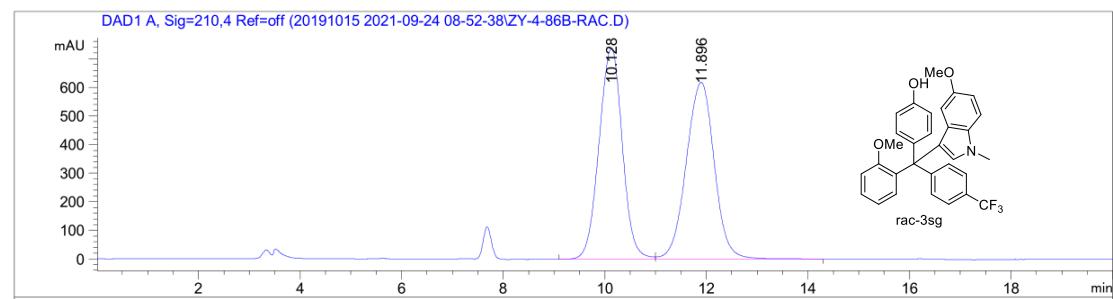
HPLC Condition:IC, *n*-Hexane/iPrOH = 97:3, 1.0 mL/min



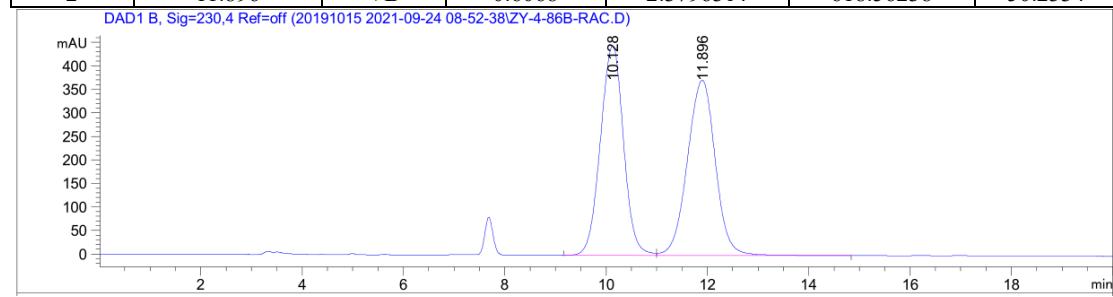
End of Report

Sample Name: ZY-4-86B-Rac

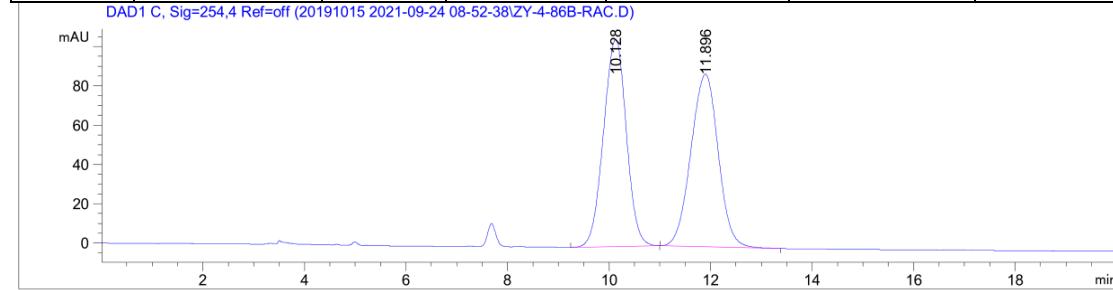
HPLC Condition: IC, n-Hexane/iPrOH = 97:3, 1.0 mL/min



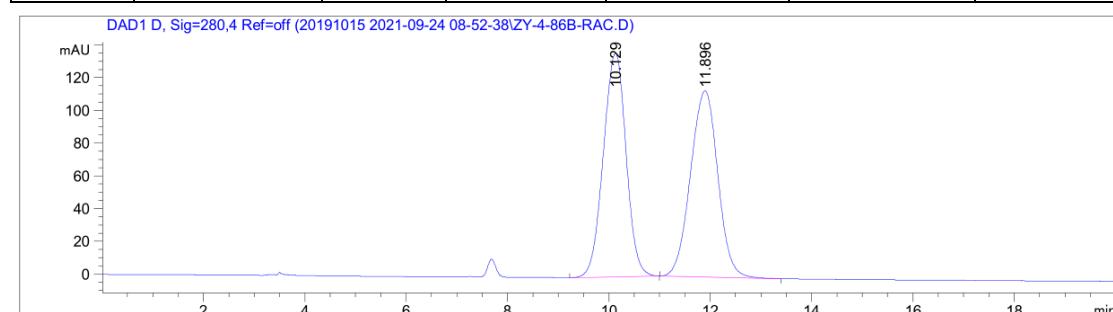
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.128	BV	0.5023	2.35752e4	738.69580	49.7666
2	11.896	VB	0.6068	2.37963e4	618.56238	50.2334



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.128	BV	0.4982	1.41496e4	445.91321	49.7199
2	11.896	VB	0.6037	1.43090e4	372.88580	50.2801



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.128	BB	0.4913	3303.03320	105.50297	50.0900
2	11.896	BB	0.5889	3291.16797	87.88772	49.9100

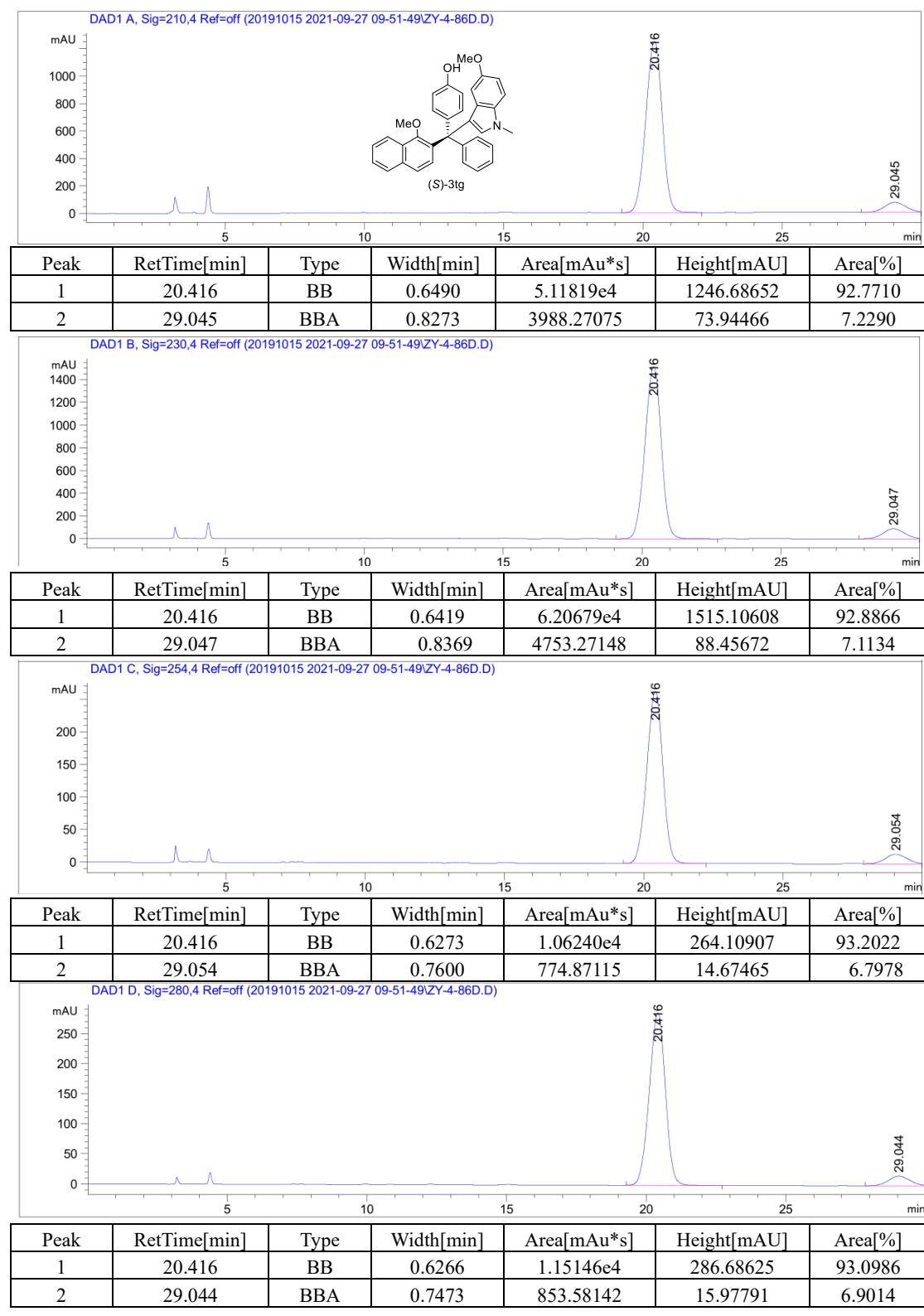


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.129	BB	0.4928	4272.78613	136.63490	50.0372
2	11.896	BB	0.5955	4266.44043	113.76900	49.9628

End of Report

Sample Name: ZY-4-86D-OP

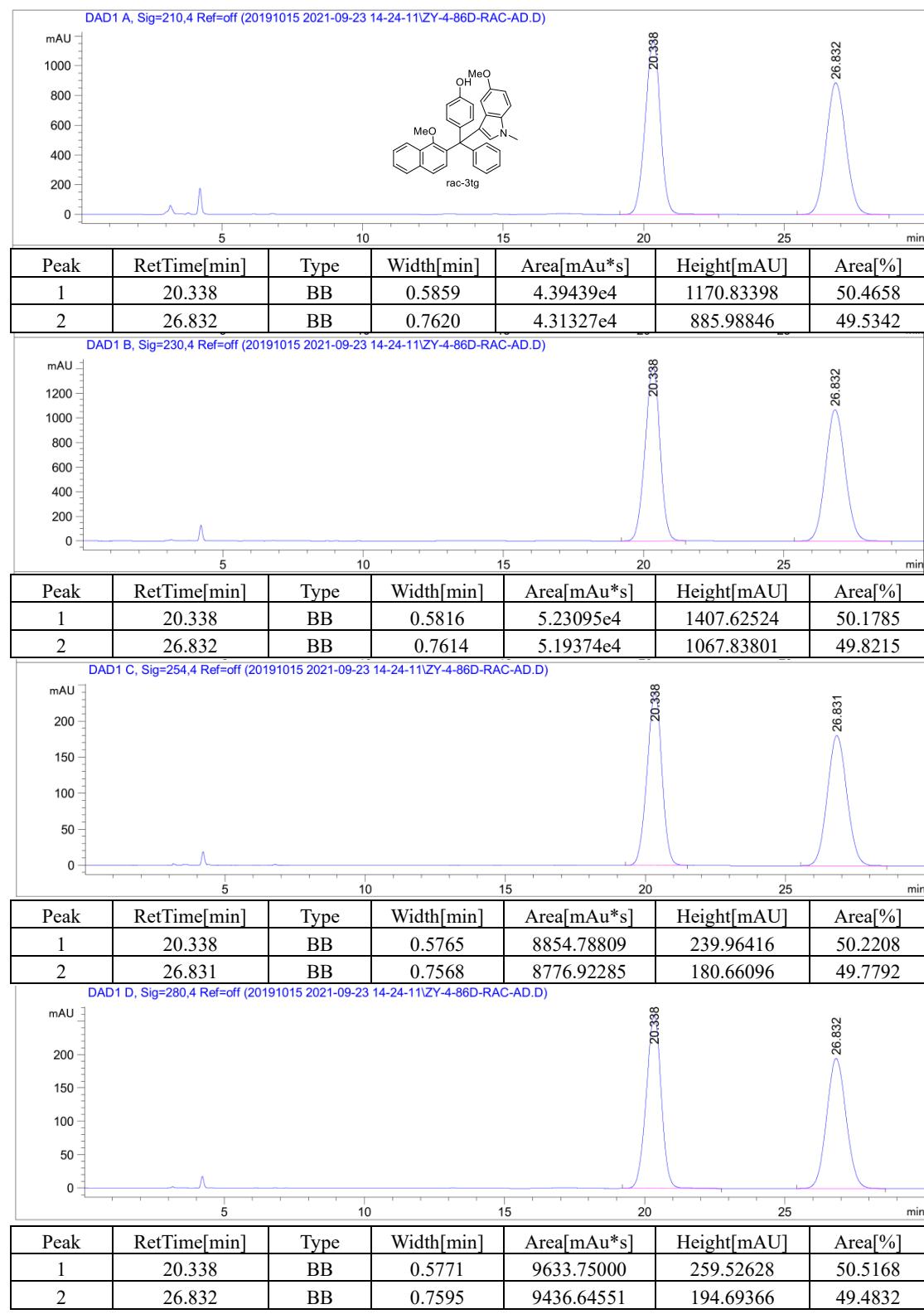
HPLC Condition:AD-H, *n*-Hexane/iPrOH = 95:5, 1.0 mL/min



End of Report

Sample Name: ZY-4-86D-Rac

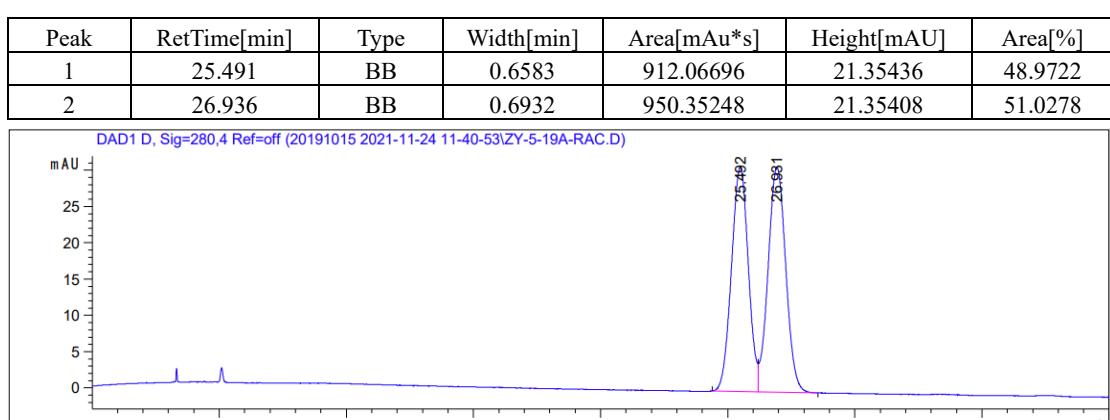
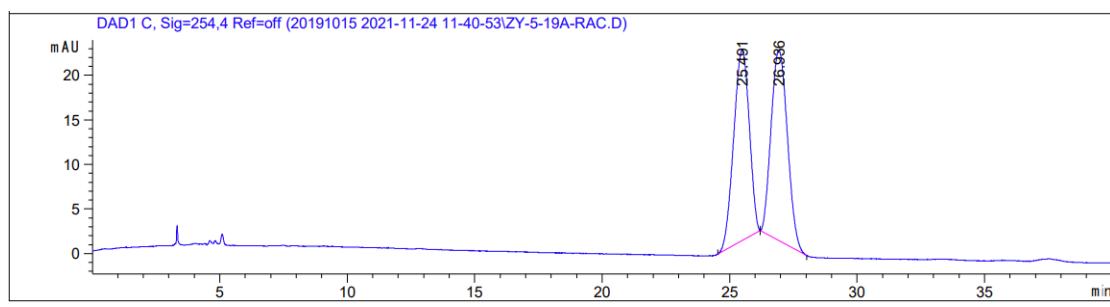
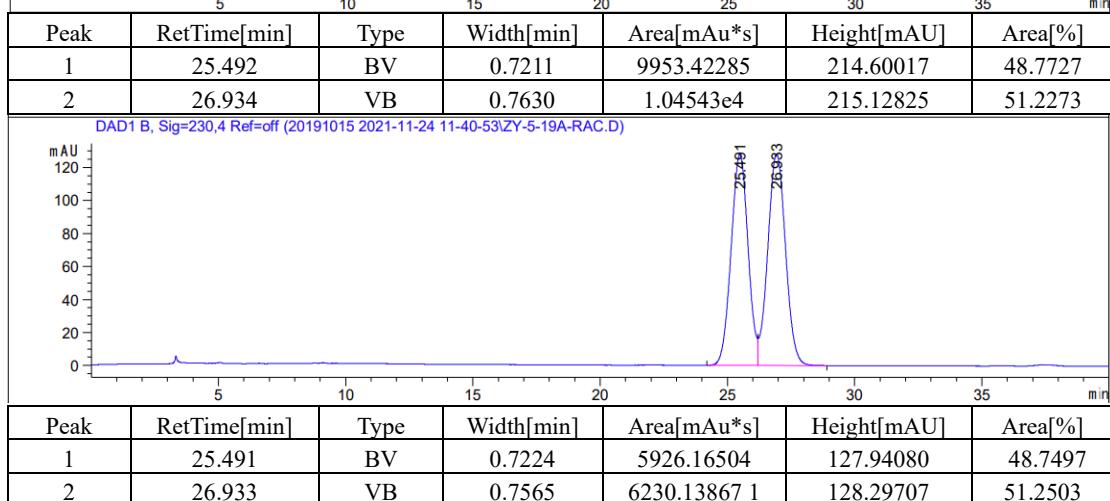
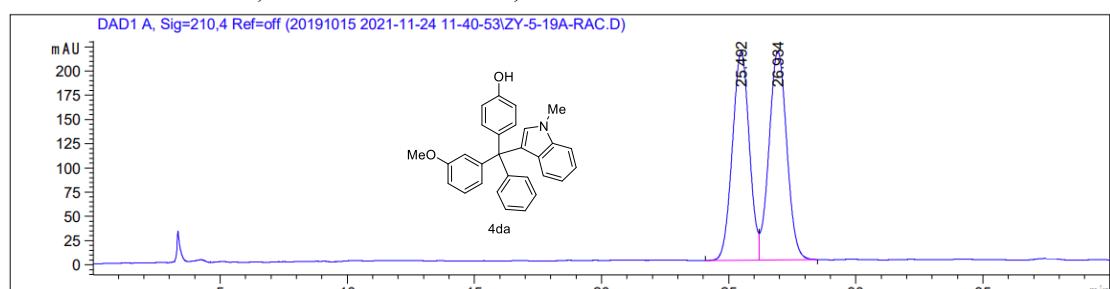
HPLC Condition:AD-H, *n*-Hexane/iPrOH = 95:5, 1.0 mL/min



End of Report

Sample Name: ZY-5-19A

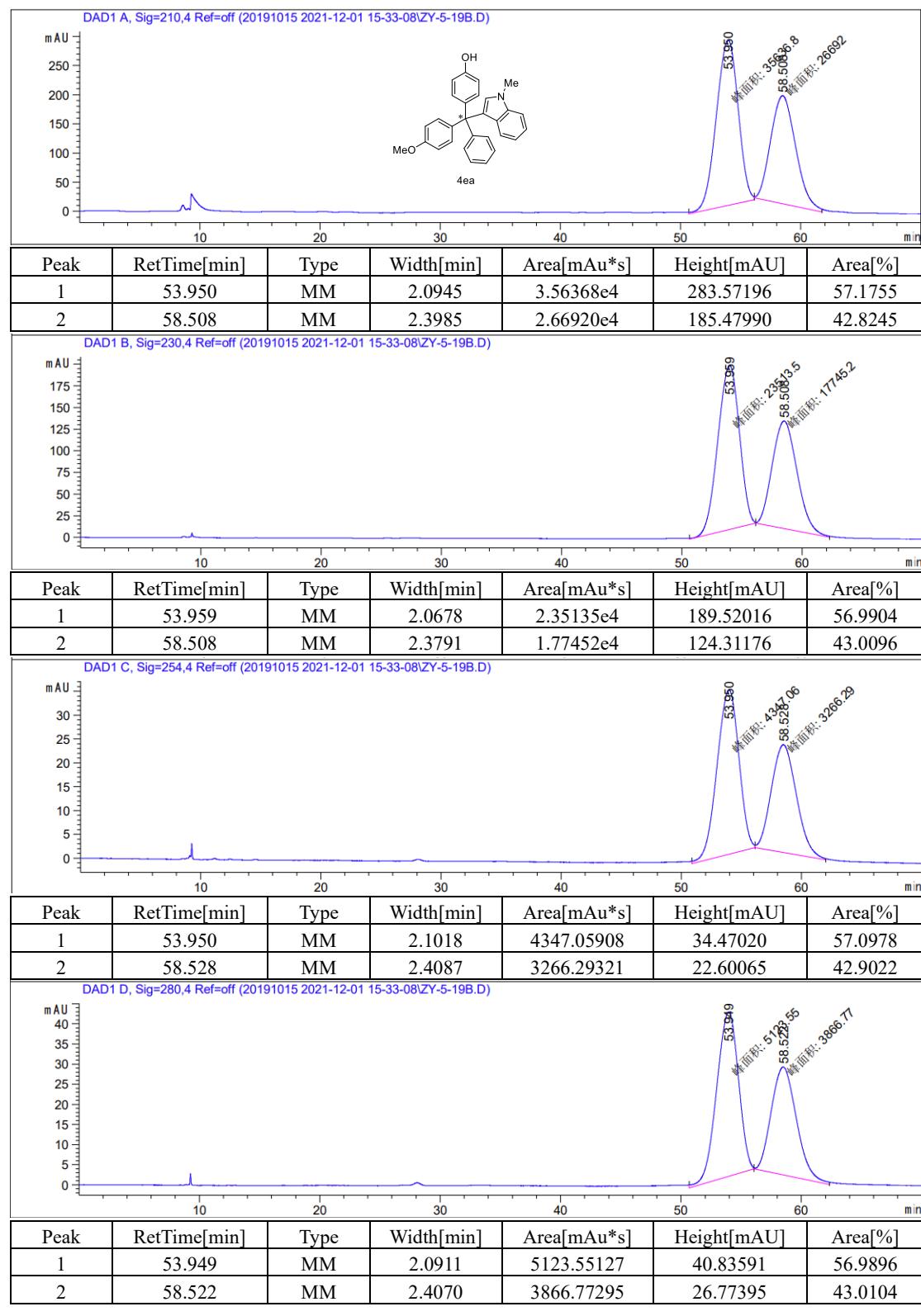
HPLC Condition: AD-H, *n*-Hexane/*i*PrOH = 97:3, 1.0 mL/min



End of Report

Sample Name: ZY-5-19B-OP

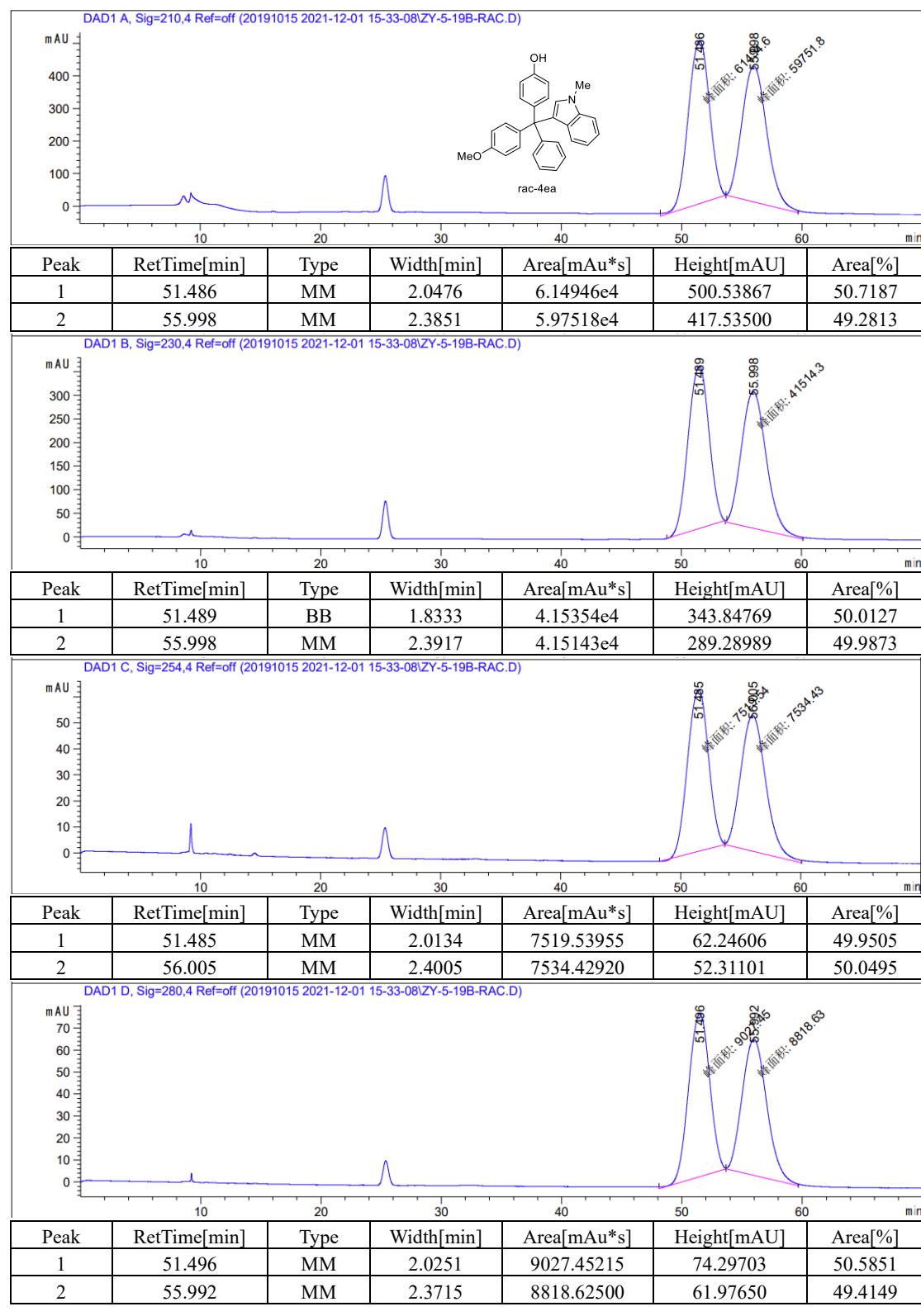
HPLC Condition: IC, *n*-Hexane/iPrOH = 98:2, 0.4 mL/min



End of Report

Sample Name: ZY-5-19B-OP

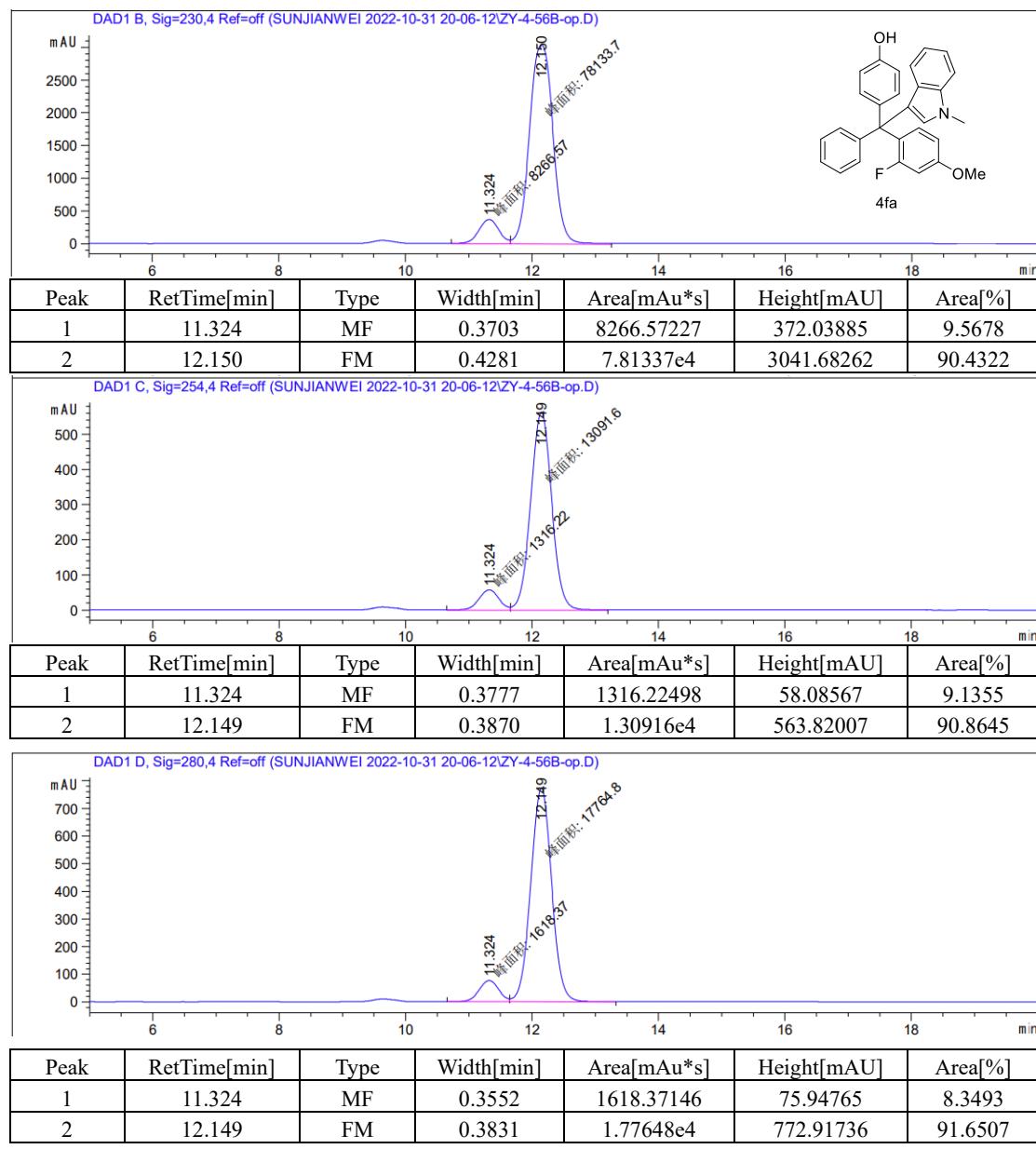
HPLC Condition: IC, *n*-Hexane/iPrOH = 98:2, 0.4 mL/min



End of Report

**Sample Name: ZY-4-56B-OP**

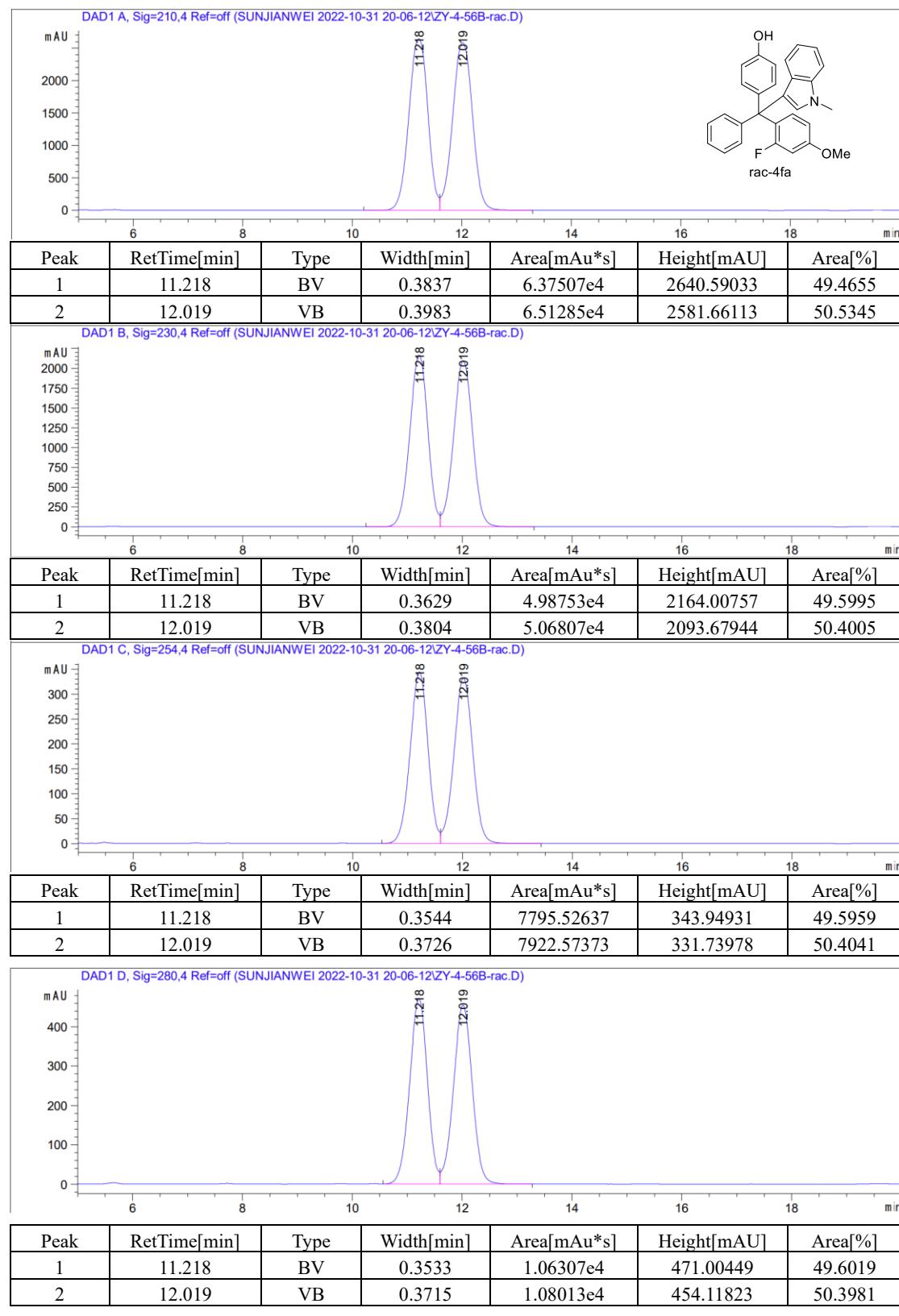
**HPLC Condition: AD-H, *n*-Hexane/*i*PrOH = 90:10, 1.0 mL/min**



End of Report

Sample Name: ZY-4-56B-Rac

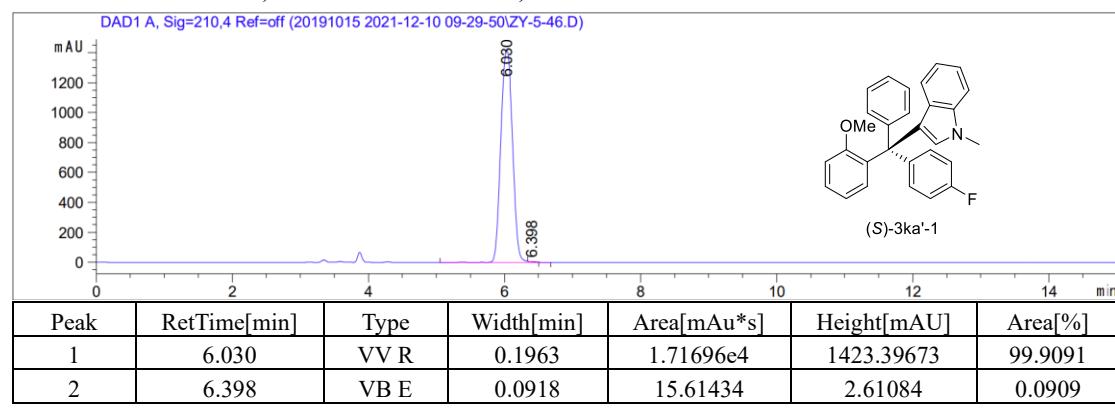
HPLC Condition: AD-H, n-Hexane/iPrOH = 90:10, 1.0 mL/min



End of Report

**Sample Name: ZY-5-46-OP**

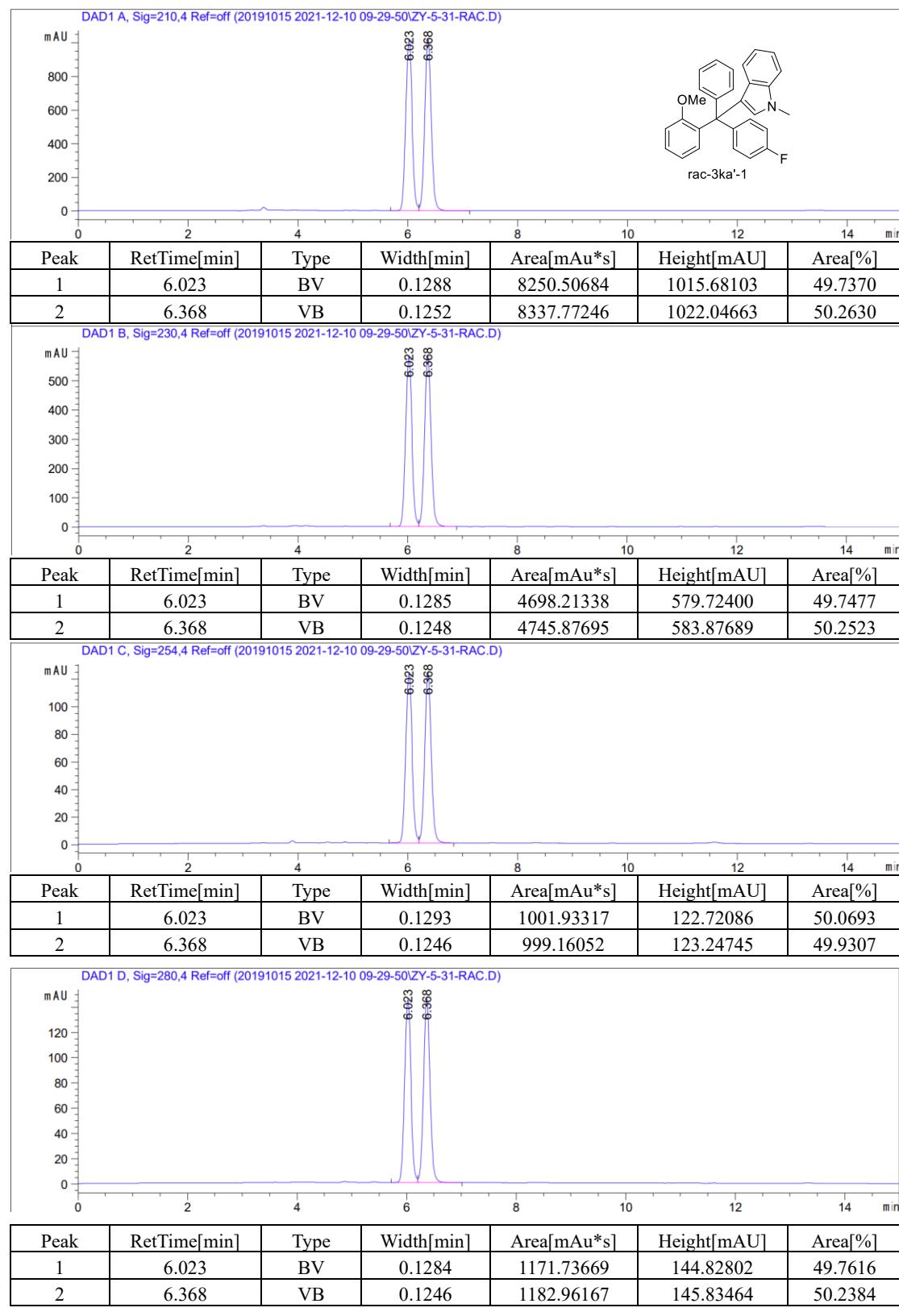
**HPLC Condition: AD-H, *n*-Hexane/*i*PrOH = 99:1, 1.0 mL/min**



End of Report

Sample Name: ZY-5-31-Rac

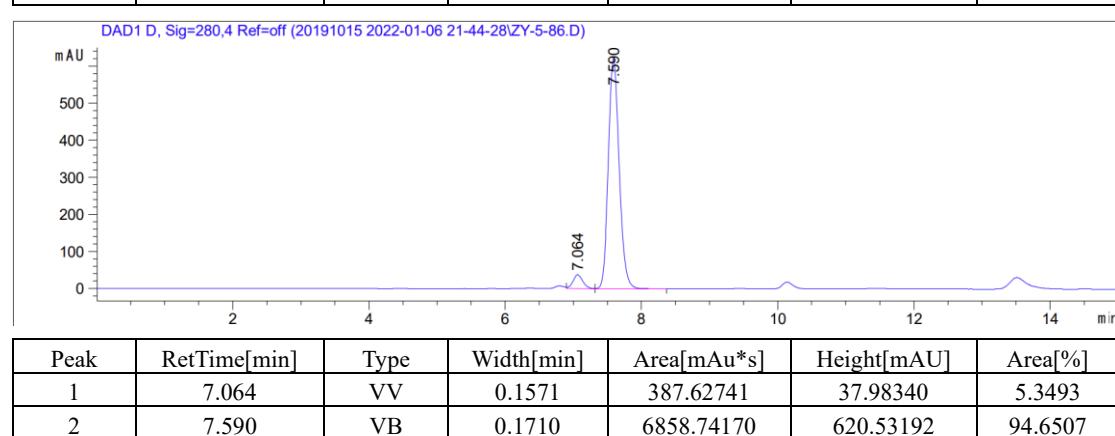
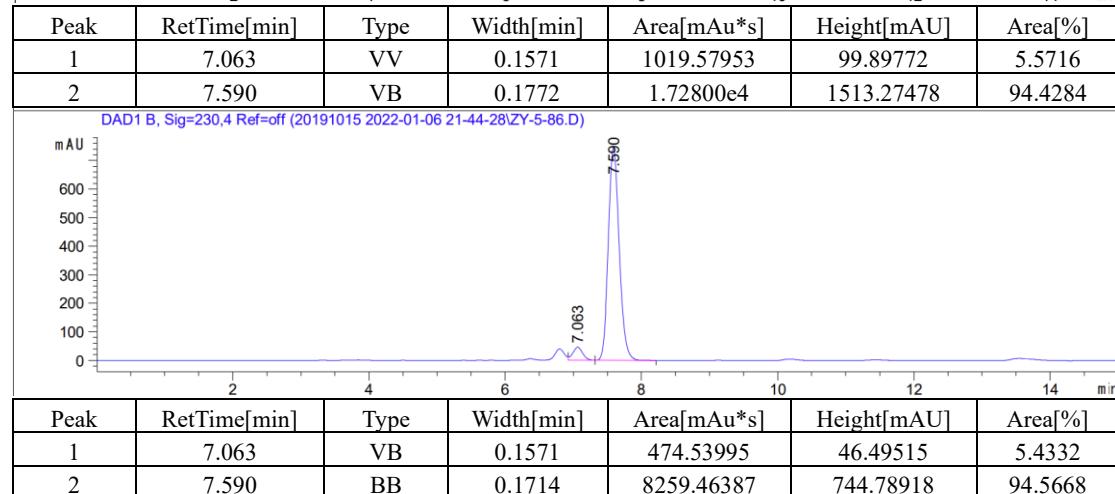
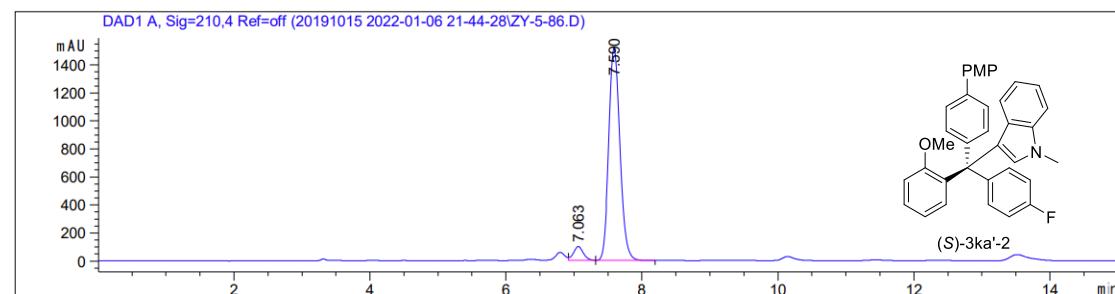
HPLC Condition: AD-H, *n*-Hexane/*i*PrOH = 99:1, 1.0 mL/min



End of Report

Sample Name: ZY-5-86-OP

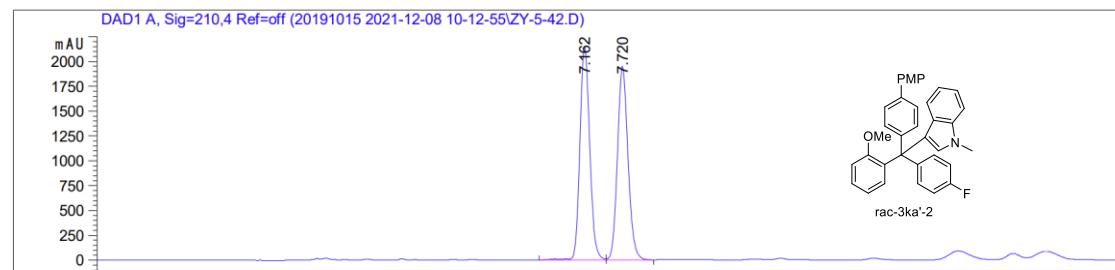
HPLC Condition: AD-H, *n*-Hexane/iPrOH = 98:2, 1.0 mL/min



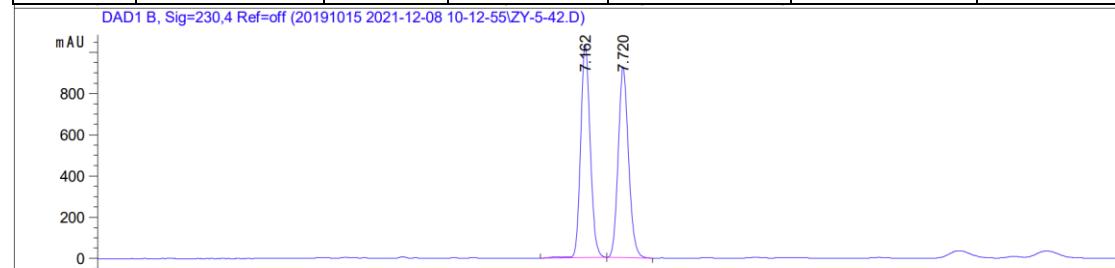
=====  
End of Report

Sample Name: ZY-5-42-Rac

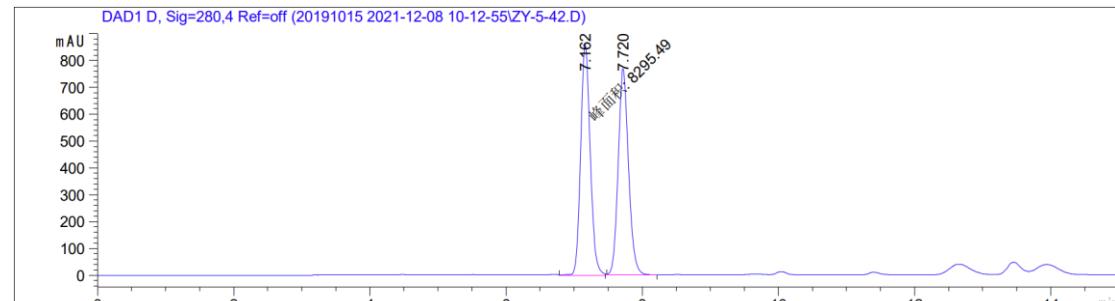
HPLC Condition: AD-H, *n*-Hexane/iPrOH = 98:2, 1.0 mL/min



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	7.162	VV R	0.1533	2.13707e4	2143.65625	49.9968
2	7.720	VB	0.1698	2.13734e4	1951.35425	50.0032



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	7.162	VB R	0.1480	9990.29688	1030.40479	50.1649
2	7.720	BB	0.1652	9924.62891	924.95453	49.8351



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	7.162	MM	0.1610	8295.49121	858.93164	50.0860
2	7.720	VB	0.1655	8267.01855	768.72070	49.9140

=====  
End of Report