

## *Supporting Information*

### **Enantioselective Synthesis of 4-Aryl-3,4-Dihydrocoumarins via N-Heterocyclic Carbene Catalyzed $\beta$ -Arylation/Cyclization of $\alpha$ -Bromoenals**

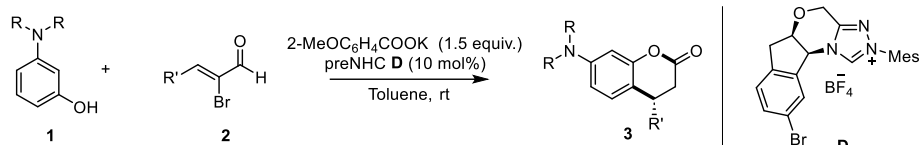
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## 1. General information

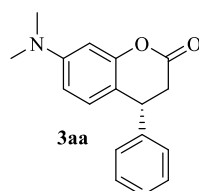
Unless otherwise noted, all starting materials were obtained from commercial supplies and directly used without further purification unless otherwise stated. Unless otherwise indicated, all reactions were carried out under N<sub>2</sub> atmosphere with magnetic stirring. Column chromatography was performed on 300-400 mesh silica gel. Anhydrous toluene and diethyl ether were distilled from sodium and benzophenone.  $\alpha$ -Bromoaldehydes<sup>[1]</sup> and chiral triazolium salts A-D<sup>[2]</sup> were synthesized according to literatures. All <sup>1</sup>H, <sup>13</sup>C, and <sup>19</sup>F NMR spectrometers were recorded on Bruker-400 MHz instruments internally referenced to tetramethylsilane (0.0 ppm) or residue of CDCl<sub>3</sub> (7.26 ppm) signal. <sup>1</sup>H NMR Spectroscopy splitting patterns were designated as singlet (s), doublet (d), triplet (t), quartet (q). Melting points were measured using a XT4A microscopic apparatus. IR spectra were obtained on a Bruker VECTOR22 spectrophotometer in KBr pellets. The substrates 1a-1x<sup>1</sup> were synthesized according to published procedures. Chiral high-performance liquid chromatography (HPLC) analysis was performed using an Agilent 1260 with commercial ChiralPak 4.6 × 250 mm columns.

## 2. General Procedure for the Synthesis of Products 3 and Characterization Data



A mixture of phenol (**1**, 0.2 mmol),  $\alpha$ -bromoaldehydes (**2**, 1.5 equiv.), PreNHC **D** (10 mol%), 2-OMeC<sub>6</sub>H<sub>4</sub>COOK (1.5 equiv.) and toluene (2.0 mL) were added to a 10 mL Schlenk reaction tube under a nitrogen atmosphere. The reaction mixture was stirred at room temperature. After the reaction was complete (monitored by TLC), the mixture was concentrated to dryness. The residue was purified by flash column chromatography to afford the desired product **3** (petroleum ether : ethyl acetate = 20 : 1).

### Characterization data of the products.

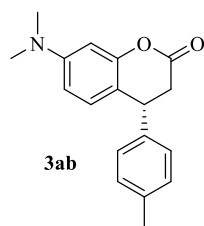


(170, experiment #)

#### (R)-7-(dimethylamino)-4-phenylchroman-2-one

49.7 mg, 93% yield. White solid, m.p. 109-110 °C. R<sub>f</sub> = 0.3 (petroleum ether/ethyl acetate 4:1). [ $\alpha$ ]<sub>D</sub><sup>25</sup> = -28.0 (c = 0.1 in CHCl<sub>3</sub>), 93:7 er, determined by HPLC analysis [Daicel CHIRALPAK IC column, *n*-hexane/*i*-PrOH = 90/10, 1.0 mL/min,  $\lambda$  = 254 nm, t (minor) = 31.1 min, t (major) = 33.0 min]; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.34 – 7.30 (m, 2H), 7.27 – 7.23 (m, 1H), 7.16 – 7.14 (m, 2H), 6.80 (d, *J* = 8.5, 1H), 6.45 (d, *J* = 2.5 Hz, 1H), 6.42 (dd, *J* = 8.5, 2.6 Hz, 1H), 4.29 – 4.18

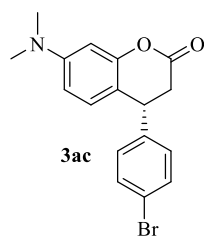
(t,  $J = 6.8$ , 1H), 3.04 (dd,  $J = 15.8$ , 6.0 Hz, 1H), 2.98 – 2.93 (m, 7H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  168.4, 152.7, 151.1, 141.5, 129.1, 128.7, 127.6, 127.4, 112.8, 108.7, 100.5, 40.5, 40.0, 37.8. **IR** (KBr)  $\nu$  3028, 2917, 2849, 1765, 1633, 1133, 803, 703. **HRMS** (ESI) calcd for  $\text{C}_{17}\text{H}_{18}\text{O}_2\text{N}$  ( $[\text{M}+\text{H}]^+$ ) 268.1338 found 268.1339.



(149, experiment #)

**(R)-7-(dimethylamino)-4-(p-tolyl)chroman-2-one**

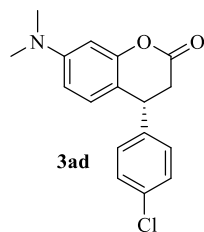
43 mg, 77% yield. White solid, m.p. 83-84 °C.  $R_f = 0.4$  (petroleum ether/ethyl acetate 4:1).  $[\alpha]_D^{25} = -3.1$  ( $c = 0.1$  in  $\text{CHCl}_3$ ), 93:7 er, determined by HPLC analysis [Daicel CHIRALPAK IA column,  $n$ -hexane/ $i$ -PrOH = 90/10, 1.0 mL/min,  $\lambda = 254$  nm,  $t$  (minor) = 13.5 min,  $t$  (major) = 9.4 min];  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.14 (d,  $J = 7.9$  Hz, 2H), 7.05 (d,  $J = 8.1$  Hz, 2H), 6.81 (d,  $J = 8.4$  Hz, 1H), 6.50 – 6.41 (m, 2H), 4.22 (t,  $J = 6.8$  Hz, 1H), 3.03 (dd,  $J = 15.7$ , 6.0 Hz, 1H), 2.97 – 2.92 (m, 7H), 2.33 (s, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  168.5, 152.7, 151.1, 138.5, 137.1, 129.7, 128.7, 127.5, 113.2, 108.7, 100.6, 40.5, 39.7, 37.9, 21.1. **IR** (KBr)  $\nu$  2917, 2851, 2815, 1755, 1130, 823, 797. **HRMS** (ESI) calcd for  $\text{C}_{18}\text{H}_{20}\text{O}_2\text{N}$  ( $[\text{M}+\text{H}]^+$ ) 282.1494 found 282.1492.



(138, experiment #)

**(R)-4-(4-bromophenyl)-7-(dimethylamino)chroman-2-one**

56 mg, 82% yield. White solid, m.p. 86-87 °C.  $R_f = 0.4$  (petroleum ether/ethyl acetate 4:1).  $[\alpha]_D^{25} = -14.2$  ( $c = 0.1$  in  $\text{CHCl}_3$ ), 93:7 er, determined by HPLC analysis [Daicel CHIRALPAK IC column,  $n$ -hexane/ $i$ -PrOH = 90/10, 1.0 mL/min,  $\lambda = 254$  nm,  $t$  (minor) = 33.3 min,  $t$  (major) = 31.6 min];  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.44 (d,  $J = 8.4$  Hz, 2H), 7.03 (d,  $J = 8.4$  Hz, 2H), 6.79 (d,  $J = 8.2$  Hz, 1H), 6.45 – 6.42 (m, 2H), 4.21 (t,  $J = 6.7$  Hz, 1H), 3.03 (dd,  $J = 15.7$ , 6.0 Hz, 1H), 2.95 – 2.88 (m, 7H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  167.9, 152.7, 151.3, 140.7, 132.2, 129.4, 128.6, 121.3, 112.1, 108.8, 100.6, 40.5, 39.6, 37.7. **IR** (KBr)  $\nu$  2922, 2852, 2806, 1749, 1630, 1113, 826, 809. **HRMS** (ESI) calcd for  $\text{C}_{17}\text{H}_{17}\text{O}_2\text{NBr}$  ( $[\text{M}+\text{H}]^+$ ) 346.0443 found 346.0449.

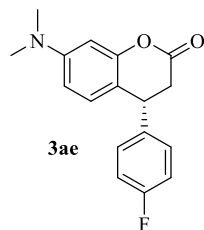


(140, experiment #)

**(R)-4-(4-chlorophenyl)-7-(dimethylamino)chroman-2-one**

54 mg, 87% yield. White solid, m.p. 92-93 °C.  $R_f = 0.3$  (petroleum ether/ethyl acetate 4:1).  $[\alpha]_D^{25} = -31.1$  ( $c = 0.1$  in  $\text{CHCl}_3$ ), 93:7 er, determined by HPLC analysis [Daicel CHIRALPAK IA column,  $n$ -hexane/ $i$ -PrOH = 90/10, 1.0 mL/min,  $\lambda = 254$  nm,  $t$  (minor) = 31.1 min,  $t$  (major) = 29.3 min];

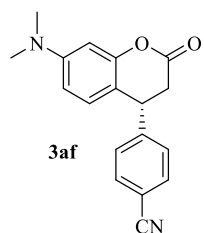
**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.29 (d, *J* = 8.4 Hz, 2H), 7.08 (d, *J* = 8.4 Hz, 2H), 6.79 (d, *J* = 8.1 Hz, 1H), 6.45 – 6.42 (m, 2H), 4.23 (t, *J* = 6.6 Hz, 1H), 3.03 (dd, *J* = 15.7, 6.0 Hz, 1H), 2.95 – 2.89 (m, 7H). **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>) δ 168.0, 152.6, 151.2, 140.1, 133.2, 129.2, 129.0, 128.6, 112.1, 108.7, 100.5, 40.5, 39.5, 37.7. **IR** (KBr)  $\nu$  2986, 2916, 2814, 1766, 1628, 1132, 838, 805. **HRMS** (ESI) calcd for C<sub>17</sub>H<sub>17</sub>O<sub>2</sub>NCl ([M+H]<sup>+</sup>) 302.0948 found 302.0951.



(141, experiment #)

**(R)-7-(dimethylamino)-4-(4-fluorophenyl)chroman-2-one**

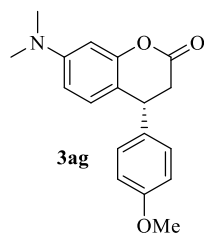
49 mg, 86% yield. White solid, m.p. 88-89 °C. *R<sub>f</sub>* = 0.4 (petroleum ether/ethyl acetate 4:1). [ $\alpha$ ]<sub>D</sub><sup>25</sup> = -20.1 (*c* = 0.1 in CHCl<sub>3</sub>), 87:13 er, determined by HPLC analysis [Daicel CHIRALPAK IC column, *n*-hexane/*i*-PrOH = 90/10, 1.0 mL/min,  $\lambda$  = 254 nm, *t* (minor) = 31.3 min, *t* (major) = 29.2 min]; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.12 (dd, *J* = 8.6, 5.4 Hz, 2H), 7.01 (t, *J* = 8.5 Hz, 2H), 6.80 (d, *J* = 8.2 Hz, 1H), 6.45 – 6.42 (m, 2H), 4.24 (t, *J* = 6.6 Hz, 1H), 3.04 (dd, *J* = 15.7, 6.0 Hz, 1H), 2.95 – 2.91 (m, 7H). **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>) δ 168.1, 162.1 (d, C-F, *J*<sub>C-F</sub> = 245.9 Hz), 152.6, 151.2, 137.3 (d, C-F, *J*<sub>C-F</sub> = 3.9 Hz), 129.2 (d, C-F, *J*<sub>C-F</sub> = 8.1 Hz), 128.6, 115.9 (d, C-F, *J*<sub>C-F</sub> = 21.5 Hz), 112.5, 108.8, 100.5, 40.5, 39.4, 38.0. **<sup>19</sup>F NMR** (376 MHz, CDCl<sub>3</sub>) δ -115.2. **IR** (KBr)  $\nu$  2924, 2848, 2799, 1752, 1629, 1133, 837, 803. **HRMS** (ESI) calcd for C<sub>17</sub>H<sub>17</sub>O<sub>2</sub>NF ([M+H]<sup>+</sup>) 286.1243 found 286.1249.



(165, experiment #)

**(R)-4-(7-(dimethylamino)-2-oxochroman-4-yl)benzotrile**

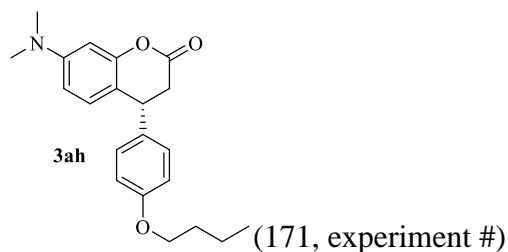
43 mg, 74% yield. White solid, m.p. 87-88 °C. *R<sub>f</sub>* = 0.2 (petroleum ether/ethyl acetate 4:1). [ $\alpha$ ]<sub>D</sub><sup>25</sup> = -38.0 (*c* = 0.1 in CHCl<sub>3</sub>), 88:12 er, determined by HPLC analysis [Daicel CHIRALPAK IA column, *n*-hexane/*i*-PrOH = 90/10, 1.0 mL/min,  $\lambda$  = 254 nm, *t* (minor) = 33.8 min, *t* (major) = 31.0 min]; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.62 – 7.60 (m, 2H), 7.27 – 7.25 (m, 2H), 6.79 (d, *J* = 9.5 Hz, 1H), 6.45 – 6.43 (m, 2H), 4.31 (t, *J* = 6.3 Hz, 1H), 3.08 (dd, *J* = 15.8, 6.2 Hz, 1H), 2.98 – 2.92 (m, 7H). **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>) δ 167.4, 152.7, 151.5, 147.2, 132.9, 128.6, 128.4, 118.7, 111.4, 110.8, 108.9, 100.6, 40.4, 40.2, 37.4. **IR** (KBr)  $\nu$  2921, 2851, 2226, 1765, 1628, 1108, 831, 800. **HRMS** (ESI) calcd for C<sub>18</sub>H<sub>17</sub>O<sub>2</sub>N<sub>2</sub> ([M+H]<sup>+</sup>) 293.1290 found 293.1287.



(139, experiment #)

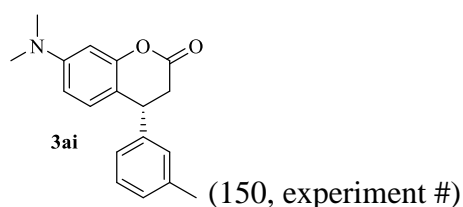
**(R)-7-(dimethylamino)-4-(4-methoxyphenyl)chroman-2-one**

49 mg, 82% yield. White solid, m.p. 92-93 °C.  $R_f = 0.4$  (petroleum ether/ethyl acetate 4:1).  $[\alpha]_D^{25} = -20.8$  ( $c = 0.1$  in  $\text{CHCl}_3$ ), 86:14 er, determined by HPLC analysis [Daicel CHIRALPAK IA column,  $n$ -hexane/ $i$ -PrOH = 80/20, 1.0 mL/min,  $\lambda = 254$  nm,  $t$  (minor) = 11.4 min,  $t$  (major) = 9.1 min];  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.09 – 7.05 (m, 2H), 6.88 – 6.84 (m, 2H), 6.80 (d,  $J = 8.4$  Hz, 1H), 6.46 – 6.41 (m, 2H), 4.21 (dd,  $J = 7.8, 5.8$  Hz, 1H), 3.79 (s, 3H), 3.02 (dd,  $J = 15.7, 5.9$  Hz, 1H), 2.96 – 2.90 (m, 7H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  168.5, 158.9, 152.6, 151.1, 133.5, 128.69, 128.67, 114.4, 113.3, 108.7, 100.6, 55.4, 40.6, 39.3, 38.1. **IR** (KBr)  $\nu$  2918, 2841, 2808, 1748, 1633, 1123, 824, 801. **HRMS** (ESI) calcd for  $\text{C}_{18}\text{H}_{20}\text{O}_3\text{N}$  ( $[\text{M}+\text{H}]^+$ ) 298.1443 found 298.1444.



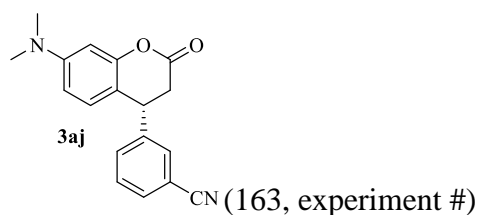
**(R)-4-(4-butoxyphenyl)-7-(dimethylamino)chroman-2-one**

61 mg, 90% yield. Colorless oil.  $R_f = 0.4$  (petroleum ether/ethyl acetate 4:1).  $[\alpha]_D^{25} = -40.7$  ( $c = 0.1$  in  $\text{CHCl}_3$ ), 81:19 er, determined by HPLC analysis [Daicel CHIRALPAK IA column,  $n$ -hexane/ $i$ -PrOH = 90/10, 1.0 mL/min,  $\lambda = 254$  nm,  $t$  (minor) = 14.9 min,  $t$  (major) = 10.7 min];  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.07 – 7.04 (m, 2H), 6.87 – 6.83 (m, 2H), 6.80 (d,  $J = 8.4$  Hz, 1H), 6.45 (d,  $J = 2.5$  Hz, 1H), 6.43 (dd,  $J = 8.4, 2.6$  Hz, 1H), 4.19 (t,  $J = 6.8$  Hz, 1H), 3.94 (t,  $J = 6.5$  Hz, 2H), 3.01 (dd,  $J = 15.7, 5.9$  Hz, 1H), 2.95 (s, 7H), 1.79 – 1.72 (m, 2H), 1.53 – 1.44 (m, 2H), 0.97 (t,  $J = 7.4$  Hz, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  168.5, 158.5, 152.6, 151.1, 133.2, 128.7, 128.6, 115.0, 113.4, 108.7, 100.6, 67.8, 40.5, 39.3, 38.0, 31.4, 19.3, 14.0. **IR** (KBr)  $\nu$  2957, 2929, 2871, 1766, 1109, 831, 801. **HRMS** (ESI) calcd for  $\text{C}_{21}\text{H}_{26}\text{O}_3\text{N}$  ( $[\text{M}+\text{H}]^+$ ) 340.1913 found 340.1909.



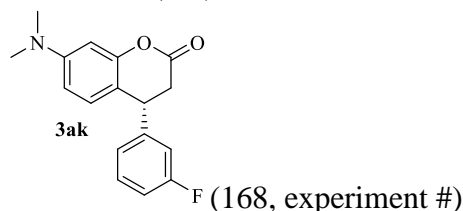
**(R)-7-(dimethylamino)-4-(m-tolyl)chroman-2-one**

40 mg, 71% yield. White solid, m.p. 93-94 °C.  $R_f = 0.4$  (petroleum ether/ethyl acetate 4:1).  $[\alpha]_D^{25} = -18.0$  ( $c = 0.1$  in  $\text{CHCl}_3$ ), 94:6 er, determined by HPLC analysis [Daicel CHIRALPAK IA column,  $n$ -hexane/ $i$ -PrOH = 90/10, 1.0 mL/min,  $\lambda = 254$  nm,  $t$  (minor) = 9.4 min,  $t$  (major) = 8.3 min];  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.22 (t,  $J = 7.5$  Hz, 1H), 7.08 (d,  $J = 7.5$  Hz, 1H), 6.95 (d,  $J = 8.9$  Hz, 2H), 6.81 (d,  $J = 8.4$  Hz, 1H), 6.47 (d,  $J = 2.5$  Hz, 1H), 6.44 (dd,  $J = 8.4, 2.6$  Hz, 1H), 4.21 (t,  $J = 6.8$  Hz, 1H), 3.04 (dd,  $J = 15.7, 6.0$  Hz, 1H), 2.99 – 2.92 (m, 7H), 2.33 (s, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  168.4, 152.7, 151.1, 141.5, 138.7, 129.0, 128.7, 128.3, 128.2, 124.7, 113.0, 108.7, 100.6, 40.5, 40.0, 37.8, 21.6. **IR** (KBr)  $\nu$  2978, 2902, 2808, 1757, 1634, 1131, 800, 788. **HRMS** (ESI) calcd for  $\text{C}_{18}\text{H}_{20}\text{O}_2\text{N}$  ( $[\text{M}+\text{H}]^+$ ) 282.1494 found 282.1488.



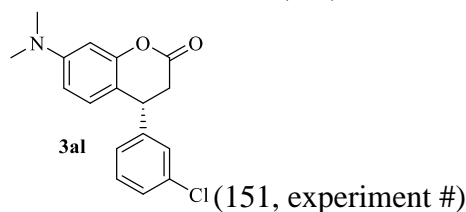
**(R)-3-(7-(dimethylamino)-2-oxochroman-4-yl)benzonitrile**

47 mg, 81% yield. White solid, m.p. 49-50 °C.  $R_f = 0.2$  (petroleum ether/ethyl acetate 4:1).  $[\alpha]_D^{25} = -14.6$  ( $c = 0.1$  in  $\text{CHCl}_3$ ), 85:15 er, determined by HPLC analysis [Daicel CHIRALPAK IA column, *n*-hexane/*i*-PrOH = 90/10, 1.0 mL/min,  $\lambda = 254$  nm,  $t$  (minor) = 22.8 min,  $t$  (major) = 24.0 min];  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.55 (m, 1H), 7.45 – 7.39 (m, 3H), 6.81 – 6.78 (m, 1H), 6.45 (m, 2H), 4.30 (t,  $J = 6.2$  Hz, 1H), 3.07 (dd,  $J = 15.8, 6.1$  Hz, 1H), 2.96 – 2.91 (m, 7H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  167.4, 152.7, 151.5, 143.4, 132.1, 131.19, 131.16, 129.9, 128.6, 118.6, 113.1, 110.7, 108.9, 100.6, 40.4, 39.7, 37.6. **IR** (KBr)  $\nu$  2922, 2852, 2228, 1760, 1627, 1109, 800, 690. **HRMS** (ESI) calcd for  $\text{C}_{18}\text{H}_{17}\text{O}_2\text{N}_2$  ( $[\text{M}+\text{H}]^+$ ) 293.1290 found 293.1288.



**(R)-7-(dimethylamino)-4-(3-fluorophenyl)chroman-2-one**

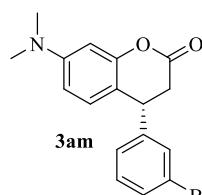
38 mg, 67% yield. White solid, m.p. 65-66 °C.  $R_f = 0.4$  (petroleum ether/ethyl acetate 4:1).  $[\alpha]_D^{25} = -31.2$  ( $c = 0.1$  in  $\text{CHCl}_3$ ), 91:9 er, determined by HPLC analysis [Daicel CHIRALPAK IA column, *n*-hexane/*i*-PrOH = 90/10, 1.0 mL/min,  $\lambda = 254$  nm,  $t$  (minor) = 10.8 min,  $t$  (major) = 10.0 min];  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.26 – 7.20 (m, 1H), 6.92 – 6.87 (m, 2H), 6.80 – 6.76 (m, 2H), 6.40 – 6.37 (m, 2H), 4.19 (t,  $J = 6.5$  Hz, 1H), 3.00 (dd,  $J = 15.8, 6.0$  Hz, 1H), 2.92 – 2.86 (m, 7H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  167.9, 163.3 (d, C-F,  $J_{\text{C-F}} = 246.9$  Hz), 152.7, 151.3, 144.3 (d, C-F,  $J_{\text{C-F}} = 6.7$  Hz), 130.7 (d, C-F,  $J_{\text{C-F}} = 8.5$  Hz), 128.7, 123.3 (d, C-F,  $J_{\text{C-F}} = 2.9$  Hz), 114.7 (q C-F,  $J_{\text{C-F}} = 21.0$  Hz), 114.4 (q, C-F,  $J_{\text{C-F}} = 20.3$  Hz), 111.9, 108.9, 100.6, 40.5, 39.9 (d, C-F,  $J_{\text{C-F}} = 1.5$  Hz), 37.7.  $^{19}\text{F NMR}$  (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -112.13. **IR** (KBr)  $\nu$  2921, 2851, 2805, 1758, 1615, 1118, 817, 798. **HRMS** (ESI) calcd for  $\text{C}_{17}\text{H}_{17}\text{O}_2\text{NF}$  ( $[\text{M}+\text{H}]^+$ ) 286.1243 found 286.1242.



**(R)-4-(3-chlorophenyl)-7-(dimethylamino)chroman-2-one**

44 mg, 73% yield. White solid, m.p. 83-84 °C.  $R_f = 0.5$  (petroleum ether/ethyl acetate 4:1).  $[\alpha]_D^{25} = -16.4$  ( $c = 0.1$  in  $\text{CHCl}_3$ ), 90:10 er, determined by HPLC analysis [Daicel CHIRALPAK IA column, *n*-hexane/*i*-PrOH = 90/10, 1.0 mL/min,  $\lambda = 254$  nm,  $t$  (minor) = 10.6 min,  $t$  (major) = 9.9 min];  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.25 – 7.20 (m, 2H), 7.12 (d,  $J = 1.9$  Hz, 1H), 7.04 – 6.91 (m, 1H), 6.79 (d,  $J = 7.8$  Hz, 1H), 6.43 – 6.41 (m, 2H), 4.21 (t,  $J = 6.6$  Hz, 1H), 3.03 (dd,  $J = 15.8, 6.0$  Hz, 1H), 2.95 – 2.90 (m, 7H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  167.9, 152.7, 151.3, 143.7, 134.9, 130.4, 128.7, 127.9, 127.7, 125.8, 111.8, 108.8, 100.6, 40.5, 39.9, 37.7. **IR** (KBr)  $\nu$  2993, 2923,

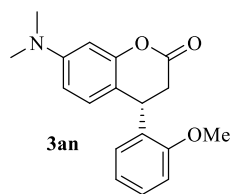
2804, 1756, 1628, 1132, 807, 798. **HRMS** (ESI) calcd for  $C_{17}H_{17}O_2NCl$  ( $[M+H]^+$ ) 302.0948 found 302.0947.



(157, experiment #)

**(R)-4-(3-bromophenyl)-7-(dimethylamino)chroman-2-one**

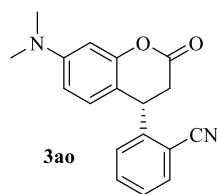
56 mg, 81% yield. White solid, m.p. 87-88 °C.  $R_f = 0.4$  (petroleum ether/ethyl acetate 4:1).  $[\alpha]_D^{25} = -25.3$  ( $c = 0.1$  in  $CHCl_3$ ), 89:11 er, determined by HPLC analysis [Daicel CHIRALPAK IA column, *n*-hexane/*i*-PrOH = 90/10, 1.0 mL/min,  $\lambda = 254$  nm,  $t$  (minor) = 12.1 min,  $t$  (major) = 11.1 min];  **$^1H$  NMR** (400 MHz,  $CDCl_3$ )  $\delta$  7.36 (d,  $J = 6.8$  Hz, 1H), 7.26 – 7.14 (m, 2H), 7.04 (d,  $J = 6.5$  Hz, 1H), 6.76 (d,  $J = 7.7$  Hz, 1H), 6.41 (s, 2H), 4.18 (s, 1H), 3.02 – 2.92 (m, 8H).  **$^{13}C$  NMR** (101 MHz,  $CDCl_3$ )  $\delta$  167.9, 152.7, 151.3, 144.0, 130.8, 130.7, 128.7, 126.3, 123.1, 111.8, 108.8, 100.6, 40.5, 39.8, 37.7. **IR** (KBr)  $\nu$  2920, 2849, 2811, 1754, 1627, 1131, 871, 808. **HRMS** (ESI) calcd for  $C_{17}H_{17}O_2NBr$  ( $[M+H]^+$ ) 346.0443 found 346.0448.



(143, experiment #)

**(R)-7-(dimethylamino)-4-(2-methoxyphenyl)chroman-2-one**

48 mg, 80% yield. White solid, m.p. 111-112 °C.  $R_f = 0.4$  (petroleum ether/ethyl acetate 4:1).  $[\alpha]_D^{25} = -33.6$  ( $c = 0.1$  in  $CHCl_3$ ), 89:11 er, determined by HPLC analysis [Daicel CHIRALPAK IC column, *n*-hexane/*i*-PrOH = 90/10, 1.0 mL/min,  $\lambda = 254$  nm,  $t$  (minor) = 34.7 min,  $t$  (major) = 37.0 min];  **$^1H$  NMR** (400 MHz,  $CDCl_3$ )  $\delta$  7.22 (m, 1H), 6.89 – 6.87 (m, 2H), 6.85 (d,  $J = 4.4$  Hz, 2H), 6.47 – 6.44 (m, 2H), 4.59 (t,  $J = 5.8$  Hz, 1H), 3.84 (s, 3H), 3.06 (dd,  $J = 16.0, 4.9$  Hz, 1H), 3.00 – 2.96 (m, 7H).  **$^{13}C$  NMR** (101 MHz,  $CDCl_3$ )  $\delta$  168.8, 156.9, 153.1, 151.0, 130.0, 128.9, 128.5, 128.3, 120.9, 112.0, 110.6, 108.9, 100.5, 55.2, 40.6, 35.9, 34.7. **IR** (KBr)  $\nu$  2917, 2836, 2801, 1765, 1624, 1130, 811, 765. **HRMS** (ESI) calcd for  $C_{18}H_{20}O_3N$  ( $[M+H]^+$ ) 298.1443 found 298.1445.

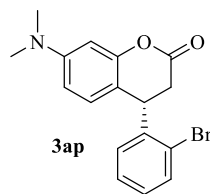


(162, experiment #)

**(R)-2-(7-(dimethylamino)-2-oxochroman-4-yl)benzonitrile**

53 mg, 90% yield. White solid, m.p. 98-99 °C.  $R_f = 0.2$  (petroleum ether/ethyl acetate 4:1).  $[\alpha]_D^{25} = -29.2$  ( $c = 0.1$  in  $CHCl_3$ ), 73:27 er, determined by HPLC analysis [Daicel CHIRALPAK IA column, *n*-hexane/*i*-PrOH = 90/10, 1.0 mL/min,  $\lambda = 254$  nm,  $t$  (minor) = 17.7 min,  $t$  (major) = 15.5 min];  **$^1H$  NMR** (400 MHz,  $CDCl_3$ )  $\delta$  7.70 (d,  $J = 7.2$  Hz, 1H), 7.49 (t,  $J = 7.3$  Hz, 1H), 7.36 (t,  $J = 7.5$  Hz, 1H), 7.05 (d,  $J = 7.9$  Hz, 1H), 6.89 (d,  $J = 8.4$  Hz, 1H), 6.47 – 6.45 (m, 2H), 4.73 (t,  $J = 5.7$  Hz, 1H), 3.16 (dd,  $J = 16.0, 6.5$  Hz, 1H), 3.03 (dd,  $J = 16.0, 5.0$  Hz, 1H), 2.97 (s, 6H).  **$^{13}C$  NMR** (101 MHz,  $CDCl_3$ )  $\delta$  167.3, 153.0, 151.6, 145.8, 133.7, 133.6, 128.8, 128.03, 127.98, 117.7,

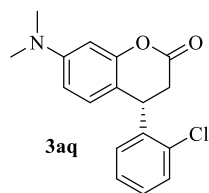
111.9, 110.1, 109.1, 100.5, 40.5, 38.5, 37.1. **IR** (KBr)  $\nu$  2917, 2851, 2810, 2221, 1744, 1628, 1156, 803, 765. **HRMS** (ESI) calcd for C<sub>18</sub>H<sub>17</sub>O<sub>2</sub>N<sub>2</sub> ([M+H]<sup>+</sup>) 293.1290 found 293.1293.



(158, experiment #)

#### (S)-4-(2-bromophenyl)-7-(dimethylamino)chroman-2-one

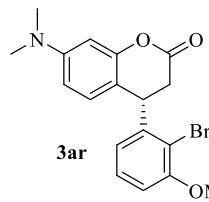
40 mg, 58% yield. White solid, m.p. 116-117 °C.  $R_f$  = 0.4 (petroleum ether/ethyl acetate 4:1).  $[\alpha]_D^{25}$  = -43.6 (c = 0.1 in CHCl<sub>3</sub>), 84:16 er, determined by HPLC analysis [Daicel CHIRALPAK IA column, *n*-hexane/*i*-PrOH = 90/10, 1.0 mL/min,  $\lambda$  = 254 nm, t (minor) = 9.7 min, t (major) = 8.7 min]; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.60 (d,  $J$  = 7.8 Hz, 1H), 7.20 (t,  $J$  = 7.4 Hz, 1H), 7.11 (t,  $J$  = 7.1 Hz, 1H), 6.88 (t,  $J$  = 8.6 Hz, 2H), 6.47 (d,  $J$  = 10.9 Hz, 2H), 4.75 (t,  $J$  = 5.9 Hz, 1H), 3.03 (d,  $J$  = 6.0 Hz, 2H), 2.97 (s, 6H). **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>)  $\delta$  167.9, 153.2, 151.4, 140.6, 133.4, 129.0, 128.9, 128.3, 124.2, 111.3, 109.0, 100.5, 40.5, 39.4, 36.4. **IR** (KBr)  $\nu$  2921, 2850, 2804, 1770, 1625, 1132, 807, 763. **HRMS** (ESI) calcd for C<sub>17</sub>H<sub>17</sub>O<sub>2</sub>NBr ([M+H]<sup>+</sup>) 346.0443 found 346.0445.



(152, experiment #)

#### (S)-4-(2-chlorophenyl)-7-(dimethylamino)chroman-2-one

56 mg, 93% yield. White solid, m.p. 110-111 °C.  $R_f$  = 0.5 (petroleum ether/ethyl acetate 4:1).  $[\alpha]_D^{25}$  = -48.4 (c = 0.1 in CHCl<sub>3</sub>), 89:11 er, determined by HPLC analysis [Daicel CHIRALPAK IA column, *n*-hexane/*i*-PrOH = 90/10, 1.0 mL/min,  $\lambda$  = 254 nm, t (minor) = 9.2 min, t (major) = 8.2 min]; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.41 (dd,  $J$  = 7.6, 1.7 Hz, 1H), 7.21 – 7.10 (m, 2H), 6.95 – 6.70 (m, 2H), 6.59 – 6.41 (m, 2H), 4.76 (t,  $J$  = 5.9 Hz, 1H), 3.04 (d,  $J$  = 6.1 Hz, 2H), 2.97 (s, 6H). **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>)  $\delta$  168.0, 153.3, 151.4, 139.0, 133.6, 130.1, 128.9, 128.80, 128.75, 127.6, 111.2, 109.0, 100.5, 40.5, 36.9, 36.2. **IR** (KBr)  $\nu$  2921, 2849, 2809, 1773, 1625, 1132, 808, 765. **HRMS** (ESI) calcd for C<sub>17</sub>H<sub>17</sub>O<sub>2</sub>NCl ([M+H]<sup>+</sup>) 302.0948 found 302.0943.



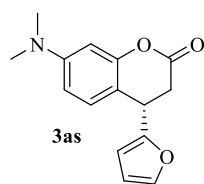
(144, experiment #)

#### (S)-4-(2-bromo-3-methoxyphenyl)-7-(dimethylamino)chroman-2-one

50 mg, 66% yield. White solid, m.p. 105-106 °C.  $R_f$  = 0.3 (petroleum ether/ethyl acetate 4:1).  $[\alpha]_D^{25}$  = -21.1 (c = 0.1 in CHCl<sub>3</sub>), 92:8 er, determined by HPLC analysis [Daicel CHIRALPAK IC column, *n*-hexane/*i*-PrOH = 90/10, 1.0 mL/min,  $\lambda$  = 254 nm, t (minor) = 30.2 min, t (major) = 24.4 min]; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.48 (d,  $J$  = 8.8 Hz, 1H), 6.87 (d,  $J$  = 8.0 Hz, 1H), 6.67 (dd,  $J$  = 8.8, 3.0 Hz, 1H), 6.54 – 6.38 (m, 3H), 4.68 (t,  $J$  = 6.0 Hz, 1H), 3.66 (s, 3H), 3.02 – 3.00 (m, 2H), 2.96 (s, 6H). **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>)  $\delta$  167.9, 159.5, 153.1, 151.4, 141.6, 133.9, 128.9, 115.2, 114.4, 114.1, 111.0, 109.0, 100.5, 55.5, 40.5, 39.5, 36.3. **IR** (KBr)  $\nu$  2919, 2841,



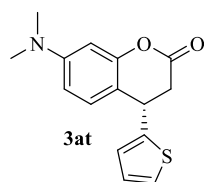
2812, 1761, 1633, 1141, 808, 795. **HRMS** (ESI) calcd for C<sub>18</sub>H<sub>19</sub>O<sub>3</sub>Br ([M+H]<sup>+</sup>) 376.0548 found 376.0550.



(153, experiment #)

**(S)-7-(dimethylamino)-4-(furan-2-yl)chroman-2-one**

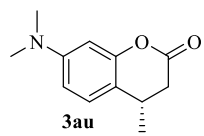
31 mg, 61% yield. White solid, m.p. 93-94 °C.  $R_f = 0.5$  (petroleum ether/ethyl acetate 4:1).  $[\alpha]_D^{25} = -20.0$  (c = 0.1 in CHCl<sub>3</sub>), 87:13 er, determined by HPLC analysis [Daicel CHIRALPAK IA column, *n*-hexane/*i*-PrOH = 90/10, 1.0 mL/min,  $\lambda = 254$  nm, t (minor) = 11.9 min, t (major) = 9.4 min]; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.34 (dd,  $J = 1.9, 0.8$  Hz, 1H), 6.99 (d,  $J = 8.5$  Hz, 1H), 6.46 (dd,  $J = 8.5, 2.6$  Hz, 1H), 6.41 (d,  $J = 2.6$  Hz, 1H), 6.27 (dd,  $J = 3.3, 1.9$  Hz, 1H), 6.00 (d,  $J = 3.3$  Hz, 1H), 4.29 (t,  $J = 5.8$  Hz, 1H), 3.15 (dd,  $J = 15.9, 5.5$  Hz, 1H), 2.97 – 2.94 (m, 7H). **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>)  $\delta$  168.0, 154.2, 152.4, 151.4, 142.5, 128.5, 110.4, 110.4, 108.7, 106.6, 100.7, 40.5, 34.7, 34.1. **IR** (KBr)  $\nu$  2921, 2359, 2341, 1750, 1635, 1134, 1119, 801, 748. **HRMS** (ESI) calcd for C<sub>15</sub>H<sub>16</sub>O<sub>3</sub>N ([M+H]<sup>+</sup>) 258.1130 found 258.1129.



(155, experiment #)

**(S)-7-(dimethylamino)-4-(thiophen-2-yl)chroman-2-one**

35 mg, 64% yield. White solid, m.p. 86-87 °C.  $R_f = 0.4$  (petroleum ether/ethyl acetate 4:1).  $[\alpha]_D^{25} = -25.1$  (c = 0.1 in CHCl<sub>3</sub>), 88:12 er, determined by HPLC analysis [Daicel CHIRALPAK IA column, *n*-hexane/*i*-PrOH = 90/10, 1.0 mL/min,  $\lambda = 254$  nm, t (minor) = 15.0 min, t (major) = 10.8 min]; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.20 (dd,  $J = 5.1, 1.2$  Hz, 1H), 6.99 (d,  $J = 8.5$  Hz, 1H), 6.93 (dd,  $J = 5.1, 3.5$  Hz, 1H), 6.81 – 6.80 (m, 1H), 6.47 (dd,  $J = 8.4, 2.6$  Hz, 1H), 6.43 (d,  $J = 2.5$  Hz, 1H), 4.51 (t,  $J = 6.0$  Hz, 1H), 3.09 (d,  $J = 6.0$  Hz, 2H), 2.96 (s, 6H). **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>)  $\delta$  167.8, 152.3, 151.4, 145.3, 128.5, 127.2, 125.0, 124.9, 112.6, 108.7, 100.6, 40.5, 38.3, 35.6. **IR** (KBr)  $\nu$  3087, 2904, 2808, 1751, 1635, 1119, 824, 707. **HRMS** (ESI) calcd for C<sub>15</sub>H<sub>16</sub>O<sub>2</sub>NS ([M+H]<sup>+</sup>) 274.0902 found 274.0899.

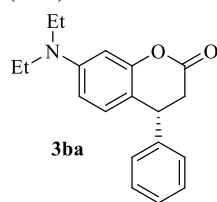


(169, experiment #)

**(S)-7-(dimethylamino)-4-methylchroman-2-one**

26 mg, 64% yield. Colorless oil.  $R_f = 0.5$  (petroleum ether/ethyl acetate 4:1).  $[\alpha]_D^{25} = -12.6$  (c = 0.1 in CHCl<sub>3</sub>), 90:10 er, determined by HPLC analysis [Daicel CHIRALPAK IA column, *n*-hexane/*i*-PrOH = 99/1, 0.8 mL/min,  $\lambda = 254$  nm, t (minor) = 17.3 min, t (major) = 16.4 min]; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.7 – 7.05 (m, 1H), 6.48 (dd,  $J = 8.5, 2.6$  Hz, 1H), 6.40 (d,  $J = 2.6$  Hz, 1H), 3.13 – 3.04 (m, 1H), 2.93 (s, 6H), 2.80 (dd,  $J = 15.7, 5.4$  Hz, 1H), 2.51 (dd,  $J = 15.7, 7.6$  Hz, 1H), 1.30 – 1.28 (m, 3H). **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>)  $\delta$  169.1, 152.2, 150.9, 126.8, 115.3, 108.7,

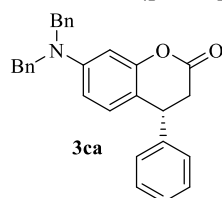
100.9, 40.6, 37.6, 28.7, 20.3. **IR** (KBr)  $\nu$  2958, 2922, 2805, 1769, 1629, 1121, 827, 799. **HRMS** (ESI) calcd for  $C_{12}H_{16}O_2N([M+H]^+)$  206.1181 found 206.1180.



(167, experiment #)

**(R)-7-(diethylamino)-4-phenylchroman-2-one**

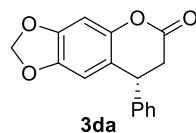
44 mg, 74% yield. Colorless oil.  $R_f = 0.6$  (petroleum ether/ethyl acetate 4:1).  $[\alpha]_D^{25} = -29.3$  ( $c = 0.1$  in  $CHCl_3$ ), 86:14 er, determined by HPLC analysis [Daicel CHIRALPAK IA column, *n*-hexane/*i*-PrOH = 90/10, 1.0 mL/min,  $\lambda = 254$  nm,  $t$  (minor) = 7.7 min,  $t$  (major) = 7.2 min];  **$^1H$  NMR** (400 MHz,  $CDCl_3$ )  $\delta$  7.33 – 7.28 (m, 2H), 7.27 – 7.22 (m, 1H), 7.17 – 7.15 (m, 2H), 6.75 (d,  $J = 8.5$  Hz, 1H), 6.40 (d,  $J = 2.6$  Hz, 1H), 6.36 (dd,  $J = 8.5, 2.6$  Hz, 1H), 4.22 (t,  $J = 6.8$  Hz, 1H), 3.32 (q,  $J = 7.1$  Hz, 4H), 3.06 – 2.91 (m, 2H), 1.15 (t,  $J = 7.1$  Hz, 6H).  **$^{13}C$  NMR** (101 MHz,  $CDCl_3$ )  $\delta$  168.5, 153.0, 148.4, 141.7, 129.0, 128.9, 127.7, 127.4, 111.7, 108.0, 99.7, 44.6, 40.1, 37.9, 12.6. **IR** (KBr)  $\nu$  3027, 2970, 2927, 1765, 1627, 1114, 801, 699. **HRMS** (ESI) calcd for  $C_{19}H_{22}O_2N([M+H]^+)$  296.1651 found 296.1650.



(166, experiment #)

**(R)-7-(dibenzylamino)-4-phenylchroman-2-one**

36 mg, 43% yield. White solid, m.p. 51-52 °C.  $R_f = 0.5$  (petroleum ether/ethyl acetate 4:1).  $[\alpha]_D^{25} = -24.7$  ( $c = 0.1$  in  $CHCl_3$ ), 90:10 er, determined by HPLC analysis [Daicel CHIRALPAK IA column, *n*-hexane/*i*-PrOH = 90/10, 1.0 mL/min,  $\lambda = 254$  nm,  $t$  (minor) = 13.9 min,  $t$  (major) = 12.0 min];  **$^1H$  NMR** (400 MHz,  $CDCl_3$ )  $\delta$  7.39 – 7.34 (m, 6H), 7.32 – 7.26 (m, 7H), 7.21 – 7.18 (m, 2H), 6.73 (d,  $J = 8.6$  Hz, 1H), 6.52 (d,  $J = 2.6$  Hz, 1H), 6.47 (dd,  $J = 8.5, 2.7$  Hz, 1H), 4.69 (s, 4H), 4.26 – 4.23 (m, 1H), 3.02 (qd,  $J = 15.8, 7.0$  Hz, 2H).  **$^{13}C$  NMR** (101 MHz,  $CDCl_3$ )  $\delta$  168.3, 152.7, 149.8, 141.3, 138.0, 129.1, 128.9, 128.8, 127.7, 127.5, 127.2, 126.6, 113.5, 108.8, 100.8, 54.6, 40.1, 37.6. **IR** (KBr)  $\nu$  3026, 2918, 2849, 1763, 1626, 1116, 801, 695. **HRMS** (ESI) calcd for  $C_{29}H_{26}O_2N([M+H]^+)$  420.1964 found 420.1963.

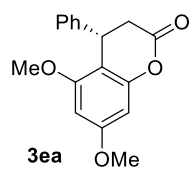


(806, experiment #)

**(R)-9-phenyl-8,9-dihydro-7H-[1,3]dioxolo[4,5-f]chromen-7-one**

29.1 mg, 54% yield. White solid, m.p. 81-82 °C.  $R_f = 0.4$  (petroleum ether/ethyl acetate 4:1).  $[\alpha]_D^{25} = -14.0$  ( $c = 0.1$  in  $CHCl_3$ ), 91:9 er, determined by HPLC analysis [Daicel CHIRALPAK IC column, *n*-hexane/*i*-PrOH = 70/30, 1.0 mL/min,  $\lambda = 277$  nm,  $t$  (minor) = 13.9 min,  $t$  (major) = 15.2 min];  **$^1H$  NMR** (400 MHz,  $CDCl_3$ )  $\delta$  7.37 – 7.33 (m, 2H), 7.31 – 7.29 (m, 1H), 7.14 (d,  $J = 7.2$  Hz, 2H), 6.66 (s, 1H), 6.39 (s, 1H), 5.95 (d,  $J = 1.9$  Hz, 2H), 4.22 (t,  $J = 6.7$  Hz, 1H), 3.07 – 2.93 (m, 2H).  **$^{13}C$  NMR** (101 MHz,  $CDCl_3$ )  $\delta$  167.75, 147.67, 146.36, 144.57, 140.58, 129.30,

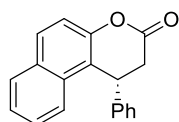
127.85, 127.62, 118.07, 107.44, 101.86, 99.29, 40.79, 37.15. **IR** (KBr)  $\nu$  3395, 2923, 2851, 1760, 1647, 1149, 802, 703. **HRMS** (ESI) calcd for C<sub>16</sub>H<sub>13</sub>O<sub>4</sub> ([M+H]<sup>+</sup>) 269.0814 found 269.0804.



(804, experiment #)

### (S)-5,7-dimethoxy-4-phenylchroman-2-one<sup>3</sup>

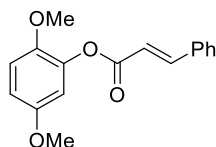
22.3 mg, 39% yield. White solid, m.p. 117-118 °C.  $R_f$  = 0.5 (petroleum ether/ethyl acetate 4:1).  $[\alpha]_D^{25}$  = -21.0 (c = 0.1 in CHCl<sub>3</sub>), 82:18 er, determined by HPLC analysis [Daicel CHIRALPAK OD-H column, *n*-hexane/*i*-PrOH = 90/10, 1.0 mL/min,  $\lambda$  = 254 nm, t (minor) = 10.4 min, t (major) = 23.3 min]; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.28 – 7.27 (m, 1H), 7.25 – 7.24 (m, 1H), 7.22 – 7.20 (m, 1H), 7.12 – 7.10 (m, 2H), 6.32 (dd,  $J$  = 21.0, 2.3 Hz, 2H), 4.55 (t,  $J$  = 4.4 Hz, 1H), 3.82 (s, 3H), 3.74 (s, 3H), 3.01 (d,  $J$  = 4.5 Hz, 2H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  167.80, 160.81, 157.57, 153.25, 141.68, 128.97, 127.24, 126.88, 106.16, 95.25, 94.06, 55.94, 55.71, 37.22, 34.63. **IR** (KBr)  $\nu$  3031, 2923, 2851, 1773, 1623, 1130, 810, 706. **HRMS** (ESI) calcd for C<sub>17</sub>H<sub>17</sub>O<sub>4</sub> ([M+H]<sup>+</sup>) 285.1127 found 285.1131.



(805, experiment #)

### (R)-1-phenyl-1,2-dihydro-3H-benzo[f]chromen-3-one

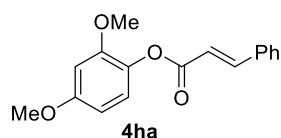
44.8 mg, 82% yield. White solid, m.p. 115-116 °C.  $R_f$  = 0.4 (petroleum ether/ethyl acetate 4:1).  $[\alpha]_D^{25}$  = -38.0 (c = 0.1 in CHCl<sub>3</sub>), 86:14 er, determined by HPLC analysis [Daicel CHIRALPAK IC column, *n*-hexane/*i*-PrOH = 70/30, 1.0 mL/min,  $\lambda$  = 277 nm, t (minor) = 10.3 min, t (major) = 9.2 min]; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.89 – 7.86 (m, 2H), 7.79 (d,  $J$  = 8.1 Hz, 1H), 7.50 – 7.42 (m, 2H), 7.35 (d,  $J$  = 8.9 Hz, 1H), 7.29 – 7.27 (m, 1H), 7.26 – 7.25 (m, 1H), 7.23 – 7.19 (m, 1H), 7.14 – 7.12 (m, 2H), 4.95 (dd,  $J$  = 6.7, 2.3 Hz, 1H), 3.26 – 3.14 (m, 2H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  167.25, 149.91, 140.64, 131.21, 131.11, 130.05, 129.35, 128.87, 127.71, 127.58, 127.05, 125.38, 123.17, 117.71, 117.67, 37.76, 37.59. **IR** (KBr)  $\nu$  3026, 2924, 2851, 1761, 1625, 1136, 814, 702. **HRMS** (ESI) calcd for C<sub>19</sub>H<sub>14</sub>O<sub>2</sub>Na ([M+Na]<sup>+</sup>) 297.0891 found 297.0892.



(802, experiment #)

### 2,5-dimethoxyphenyl cinnamate

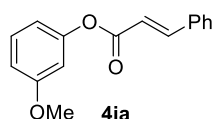
15.4 mg, 48% yield. White solid,  $R_f$  = 0.4 (petroleum ether/ethyl acetate 4:1). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.89 (d,  $J$  = 16.0 Hz, 1H), 7.60 – 7.58 (m, 2H), 7.43 – 7.41 (m, 3H), 6.94 (d,  $J$  = 8.9 Hz, 1H), 6.78 – 6.73 (m, 2H), 6.67 (d,  $J$  = 16.0 Hz, 1H), 3.79 (d,  $J$  = 10.4 Hz, 6H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  165.02, 153.90, 146.80, 145.61, 140.41, 134.37, 130.78, 129.10, 128.45, 117.05, 113.57, 111.62, 109.66, 56.73, 55.94.



(803, experiment #)

### 2,4-dimethoxyphenyl cinnamate

50.0 mg, 88% yield. White solid, m.p.  $R_f = 0.3$  (petroleum ether/ethyl acetate 4:1).  $^1\text{H NMR}$  (400 MHz, Chloroform-*d*)  $\delta$  7.88 (d,  $J = 16.0$  Hz, 1H), 7.60 – 7.58 (m, 2H), 7.42 – 7.41 (m, 3H), 7.03 (d,  $J = 8.7$  Hz, 1H), 6.67 (d,  $J = 16.0$  Hz, 1H), 6.58 (d,  $J = 2.6$  Hz, 1H), 6.48 (dd,  $J = 8.7, 2.7$  Hz, 1H), 3.82 (d,  $J = 2.3$  Hz, 6H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  165.50, 158.51, 151.97, 146.48, 134.39, 133.66, 130.66, 129.04, 128.38, 122.99, 117.19, 104.02, 100.34, 55.98, 55.71.

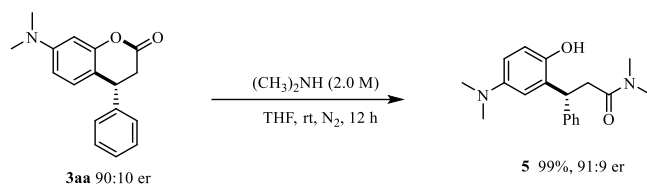


(808, experiment #)

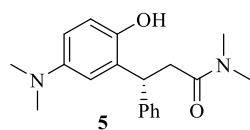
### 3-methoxyphenyl cinnamate

21.5 mg, 42% yield. White solid,  $R_f = 0.6$  (petroleum ether/ethyl acetate 4:1).  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.88 (d,  $J = 16.1$  Hz, 1H), 7.61 – 7.58 (m, 2H), 7.44 – 7.42 (m, 3H), 7.31 (t,  $J = 8.2$  Hz, 1H), 6.82 – 6.79 (m, 2H), 6.74 (t,  $J = 2.3$  Hz, 1H), 6.63 (d,  $J = 16.0$  Hz, 1H), 3.82 (s, 3H).  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  187.16, 165.43, 160.67, 151.93, 149.15, 146.75, 134.33, 131.70, 131.08, 130.85, 129.96, 129.14, 128.90, 128.44, 117.44, 113.99, 111.87, 107.77, 55.57.

## 3. Product Transformation



To a 10 mL Schlenk tube,  $(\text{CH}_3)_2\text{NH}$  (2.0 M, 10.0 equiv.) was added to a mixture of **3aa** (0.2 mmol) in THF (4.0 mL) under a nitrogen atmosphere. After the reaction mixture was stirred at room temperature for 12 h, the reaction was complete (monitored by TLC), the mixture was concentrated to dryness. The residue was purified by flash column chromatography to afford the desired product **5** (petroleum ether : ethyl acetate = 6 : 1).



(174, experiment #)

### (*R*)-3-(5-(dimethylamino)-2-hydroxyphenyl)-*N,N*-dimethyl-3-phenylpropanamide

62 mg, 99% yield. White solid, m.p. 151-152 °C.  $R_f = 0.1$  (petroleum ether/ethyl acetate 2:1).  $[\alpha]_D^{25} = -38.0$  ( $c = 0.1$  in  $\text{CHCl}_3$ ), 91:9 er, determined by HPLC analysis [Daicel CHIRALPAK IA column, *n*-hexane/*i*-PrOH = 90/10, 1.0 mL/min,  $\lambda = 254$  nm,  $t$  (minor) = 30.2 min,  $t$  (major) = 27.1 min];  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.30 – 7.29 (m, 4H), 7.21 – 7.17 (m, 1H), 6.68 (d,  $J =$

8.6 Hz, 1H), 6.36 (d,  $J = 2.7$  Hz, 1H), 6.18 (dd,  $J = 8.6, 2.7$  Hz, 1H), 4.89 (dd,  $J = 8.1, 5.3$  Hz, 1H), 3.12 – 3.10 (m, 2H), 3.01 (s, 3H), 2.94 (s, 3H), 2.86 (s, 6H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  173.1, 155.3, 150.4, 145.1, 129.4, 128.5, 128.1, 126.2, 120.8, 105.8, 102.3, 40.6, 40.1, 37.7, 37.3, 36.1.

#### 4. X-Ray Crystal Structure of Enantiopure **3ac**

The crystal of **3ac** (CCDC 2342120) suitable for X-ray analysis was prepared by slow evaporation of the solvent of the solution of **3ac** in *n*-hexane/acetone at room temperature (Figure S1).

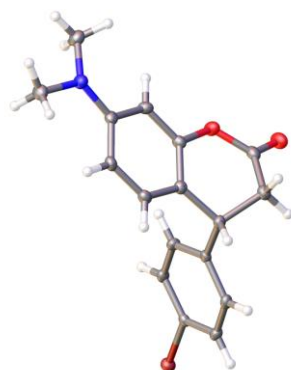


Figure S1. X-ray crystal structure of **3ac**

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

Identification code	MX10532
Empirical formula	$\text{C}_{17}\text{H}_{16}\text{BrNO}_2$
Formula weight	346.22
Temperature/K	170.00(10)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
$a/\text{\AA}$	5.7063(4)
$b/\text{\AA}$	7.9223(4)
$c/\text{\AA}$	32.7085(16)
$\alpha/^\circ$	90
$\beta/^\circ$	90
$\gamma/^\circ$	90
Volume/ $\text{\AA}^3$	1478.65(15)
Z	4
$\rho_{\text{calc}}/\text{cm}^3$	1.555
$\mu/\text{mm}^{-1}$	2.784
F(000)	704.0
Crystal size/ $\text{mm}^3$	$0.28 \times 0.04 \times 0.03$
Radiation	Mo $K\alpha$ ( $\lambda = 0.71073$ )
$2\theta$ range for data collection/ $^\circ$	4.982 to 61.38

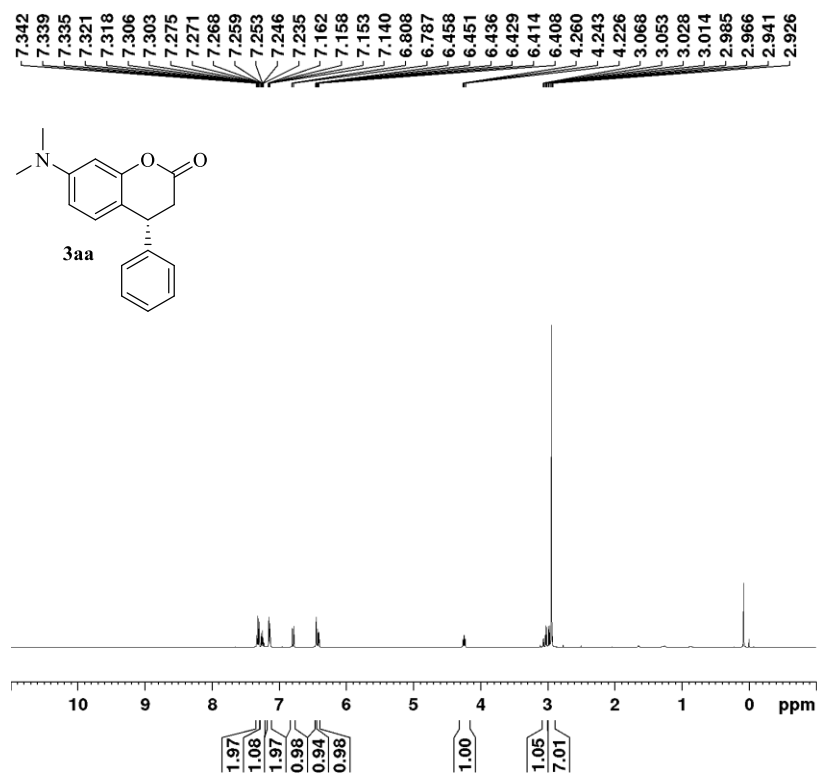
Index ranges	-7 ≤ h ≤ 8, -11 ≤ k ≤ 10, -44 ≤ l ≤ 43
Reflections collected	16468
Independent reflections	4006 [R <sub>int</sub> = 0.0444, R <sub>sigma</sub> = 0.0457]
Data/restraints/parameters	4006/0/192
Goodness-of-fit on F <sup>2</sup>	1.040
Final R indexes [I ≥ 2σ(I)]	R <sub>1</sub> = 0.0406, wR <sub>2</sub> = 0.0789
Final R indexes [all data]	R <sub>1</sub> = 0.0540, wR <sub>2</sub> = 0.0825
Largest diff. peak/hole / e Å <sup>-3</sup>	0.97/-0.55
Flack parameter	-0.004(6)

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## 5. Reference

- [1] (a) H. Byeon, S. Ryu, E. J. Yoob and J. W. Yang., *Adv. Synth. Catal.*, **2021**, 363, 5085. (b) L.-L. Shang, Y. F. X. -L. Gao, Z.-R. Chen, Y. Xia, W.-W. Jin and C. -J. Liu., *Chin. J. Chem.*, **2020**, 38, 1595.
- [2] (a) C.-G. Zhao, F.-Y. Li and J. W., *Angew. Chem. Int. Ed.*, **2016**, 128, 1852. (b) S. Kobayashi, T. Kinoshita, H. Uehara, T. Sudo and I. Ryu., *Org. Lett.*, **2009**, 11, 3934. (c) C. D. Campbell, C. Concellon and A. D. Smith, *Tetrahedron. Asymmetry*, **2011**, 22, 797.
- [3] G.-T. Li, Z.-K. Li, Q. Gu and S.-L. You, *Org. Lett.*, **2017**, 19, 1318.

## 6. <sup>1</sup>H, <sup>19</sup>F, <sup>13</sup>C NMR Spectra



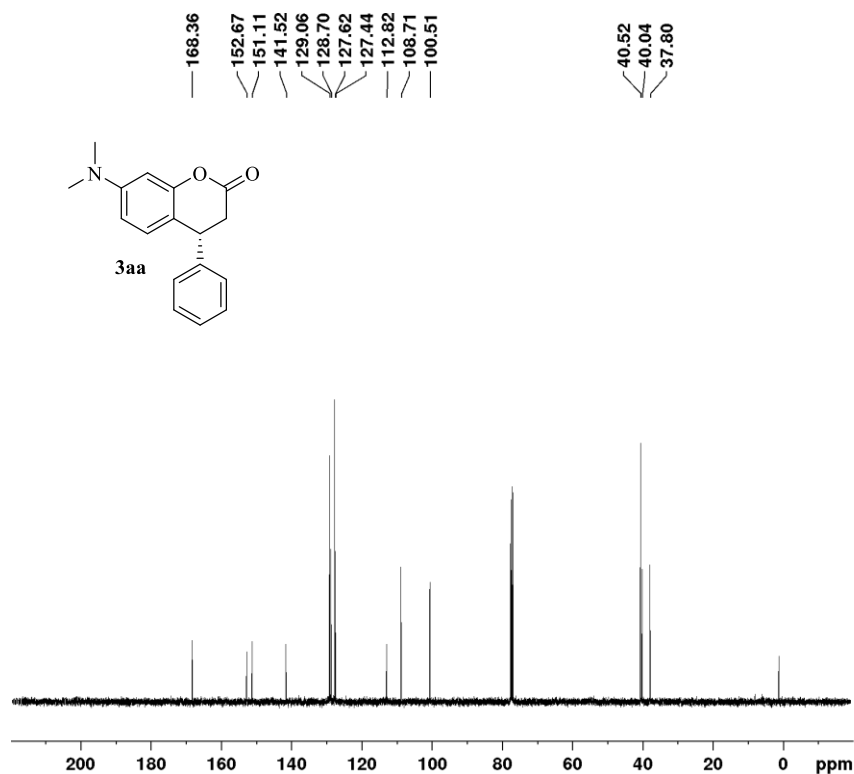
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 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 6  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122265 Hz  
 AQ 4.0894465 sec  
 RG 31.77  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 293.2 K  
 D1 1.00000000 sec  
 D11 0 sec  
 TD0 1

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 SFO1 400.1324710 MHz  
 NUC1 1H  
 P1 9.63 usec  
 PLW1 16.00000000 W

===== CHANNEL f2 =====  
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 NUC2 off  
 CPDPRG[2]  
 PCPD2 0 usec  
 PLW2 0 W  
 PLW12 0 W  
 PLW13 0 W

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 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



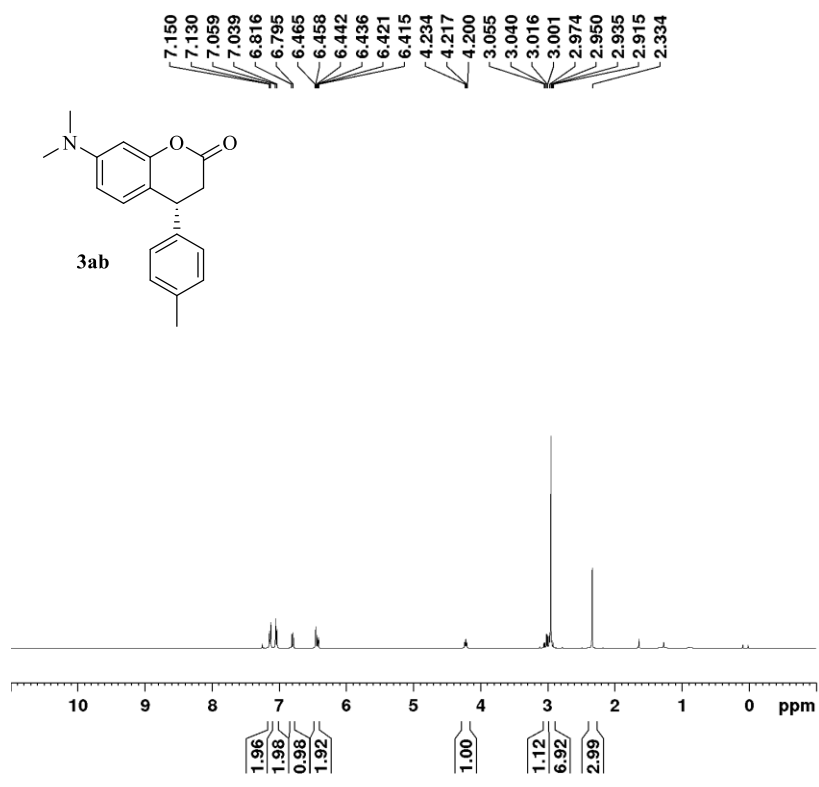
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 NS 36  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 213.76  
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 DE 6.50 usec  
 TE 293.4 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

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 NUC2 1H  
 CPDPRG[2] waitz16  
 PCPD2 80.00 usec  
 PLW2 16.00000000 W  
 PLW12 0.23184000 W  
 PLW13 0.14838000 W

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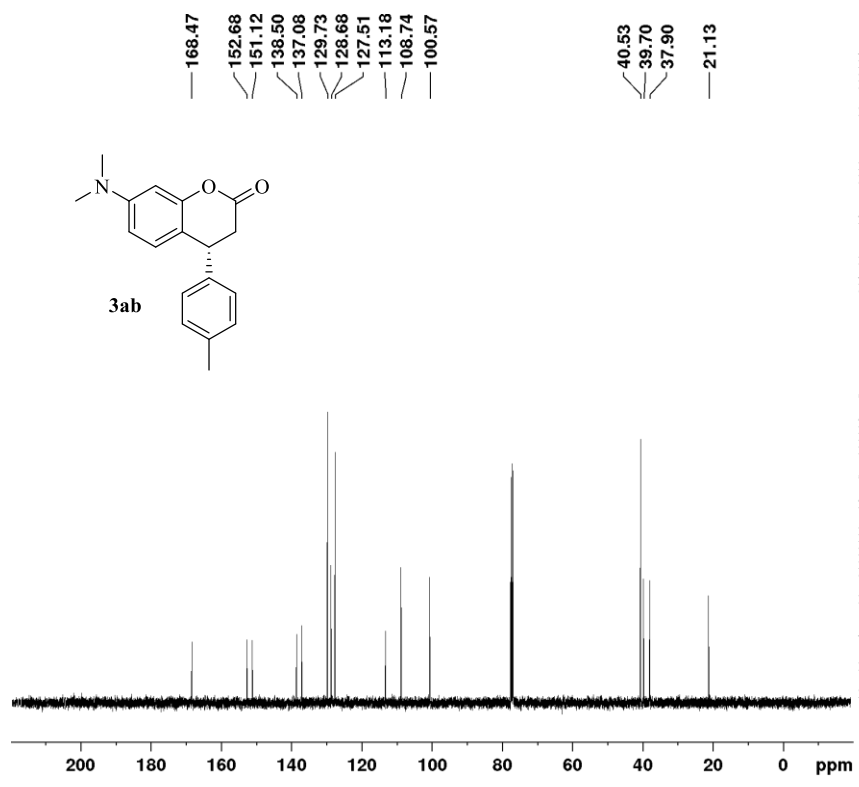
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TD0           1

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NUC1          1H
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PLW1          16.00000000 W

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NUC2          off
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PLW12         0 W
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PROCNO        1

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FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG            213.76
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DE            6.50 usec
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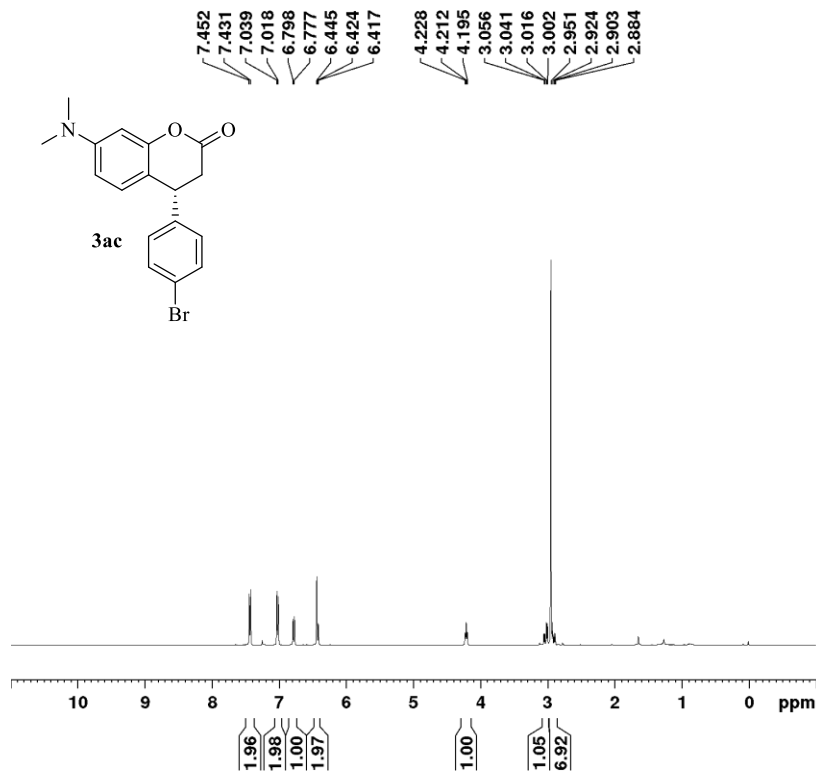
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PC            1.40

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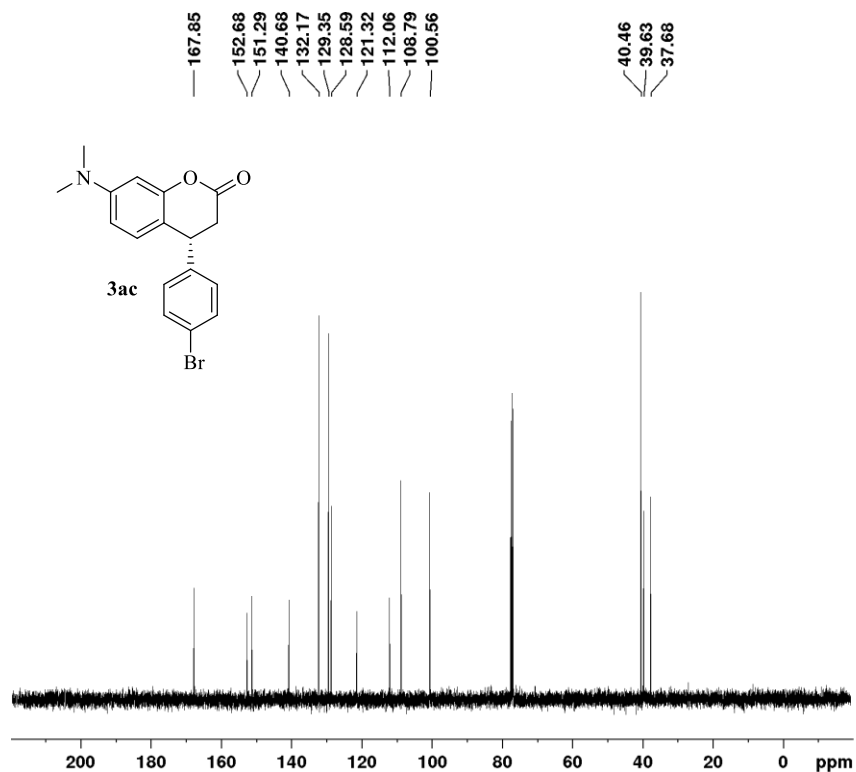
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Current Data Parameters
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PROCNO       1

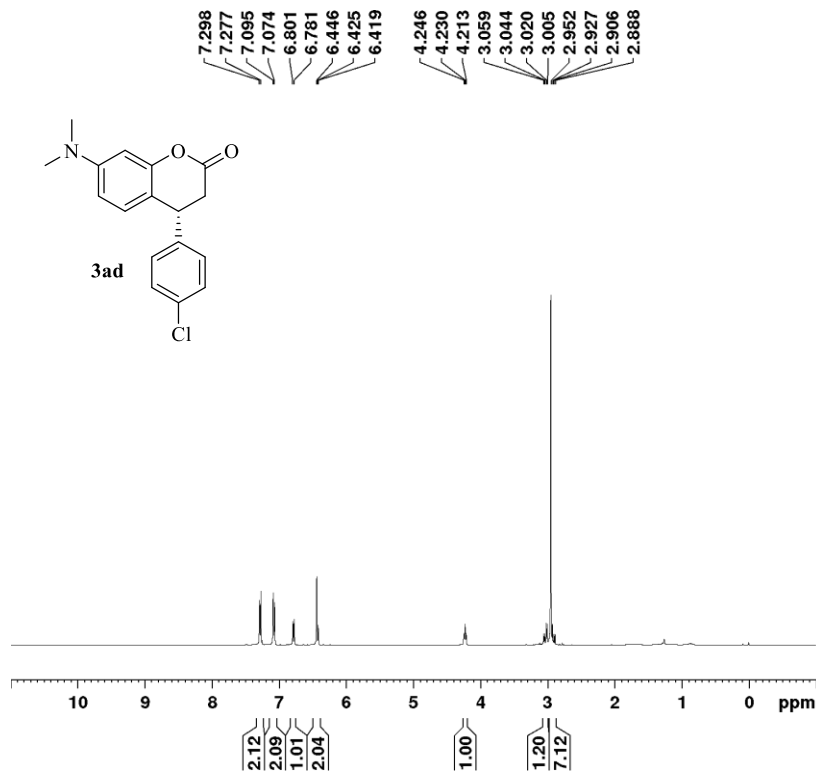
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AQ          1.3631488 sec
RG          213.76
DW          20.800 usec
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TE          303.0 K
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TDO         1

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F1          10.15 usec
PLW1        76.00000000 W

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PLW12       0.23184000 W
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PC          1.40

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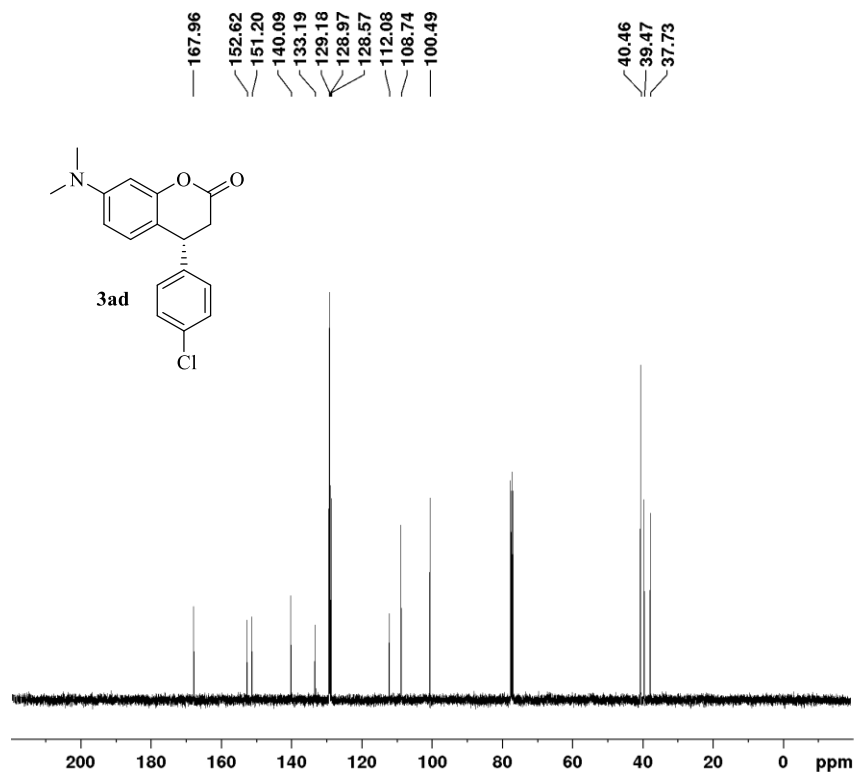


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 SOLVENT CDCl3  
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 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 31.77  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 293.0 K  
 D1 1.00000000 sec  
 TD0 1

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 NUC1 1H  
 F1 9.63 usec  
 PLW1 16.00000000 W

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 SSB 0  
 LB 0.30 Hz  
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 PC 1.00



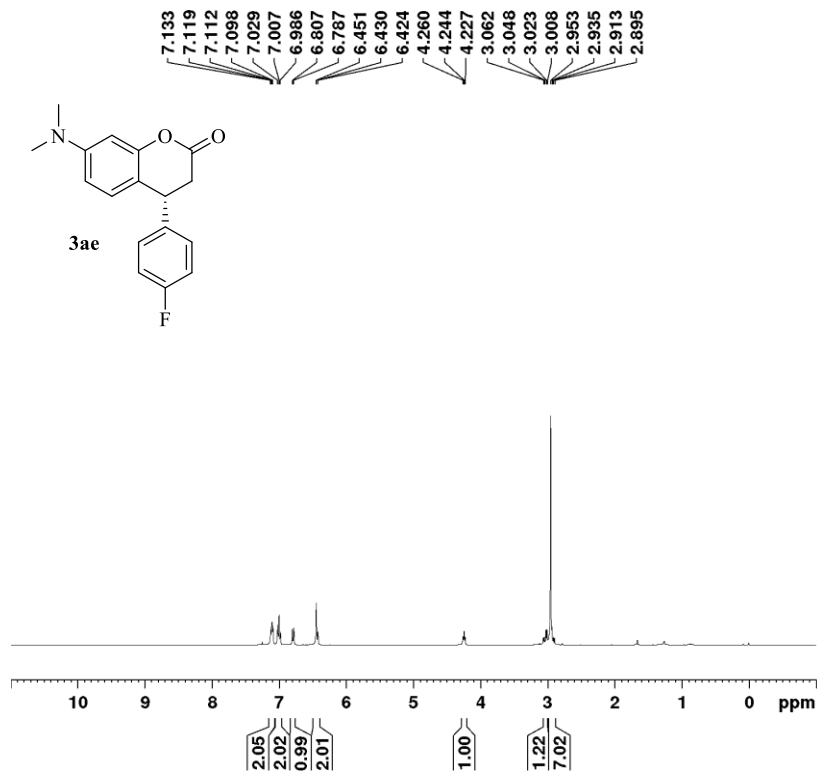
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 DW 20.800 usec  
 DE 6.50 usec  
 TE 293.4 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SF01 100.6228293 MHz  
 NUC1 13C  
 F1 10.15 usec  
 PLW1 76.00000000 W

===== CHANNEL f2 =====  
 SF02 400.1316005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 80.00 usec  
 PLW2 16.00000000 W  
 PLW12 0.23184000 W  
 PLW13 0.14838000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6127648 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

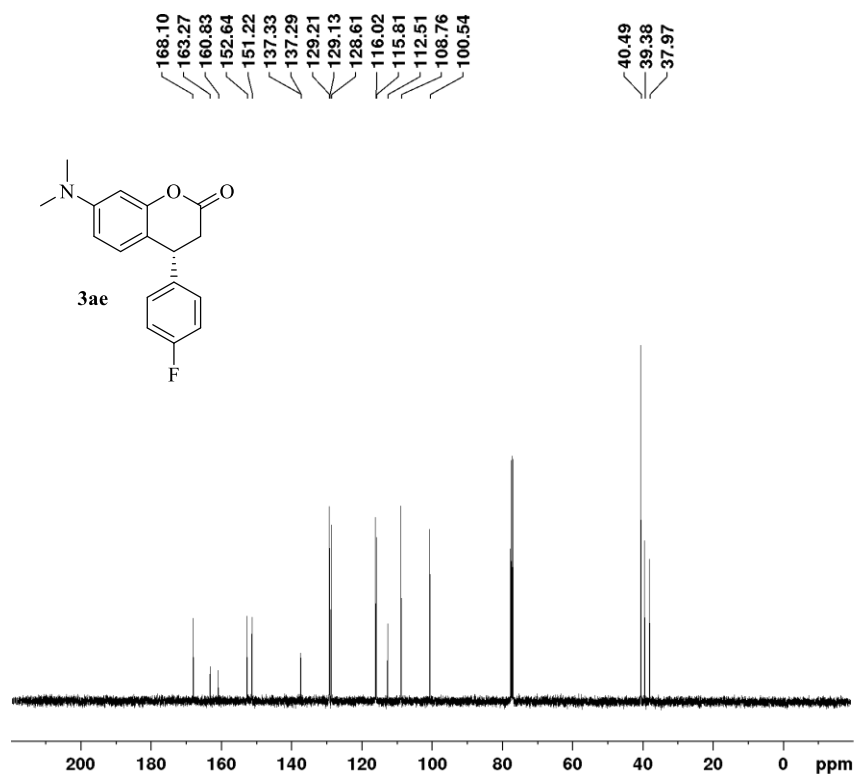


```
Current Data Parameters
NAME          GY
EXPNO         26
PROCNO        1

F2 - Acquisition Parameters
Date_         20220608
Time          15.36
INSTRUM       spect
PROBHD        5 mm PABBO BB/
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            10
DS            2
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894465 sec
RG            31.77
DW            62.400 usec
DE            6.50 usec
TE            295.4 K
D1            1.00000000 sec
TDO           1
```

```
===== CHANNEL f1 =====
SF01         400.1324710 MHz
NUC1          1H
P1            9.63 usec
PLW1         16.00000000 W

F2 - Processing parameters
SI           65536
SF           400.1300099 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00
```



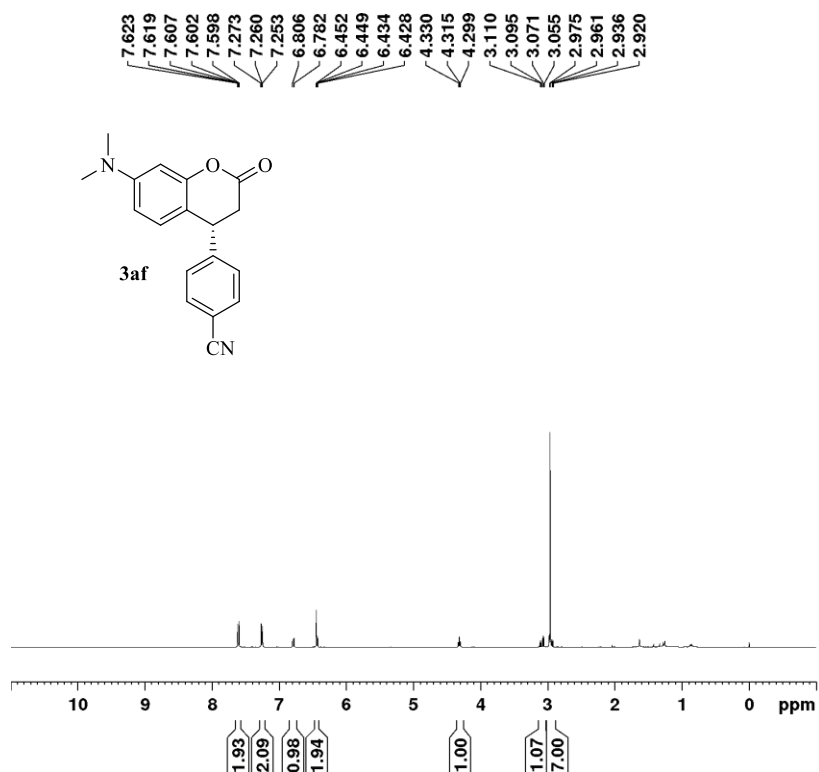
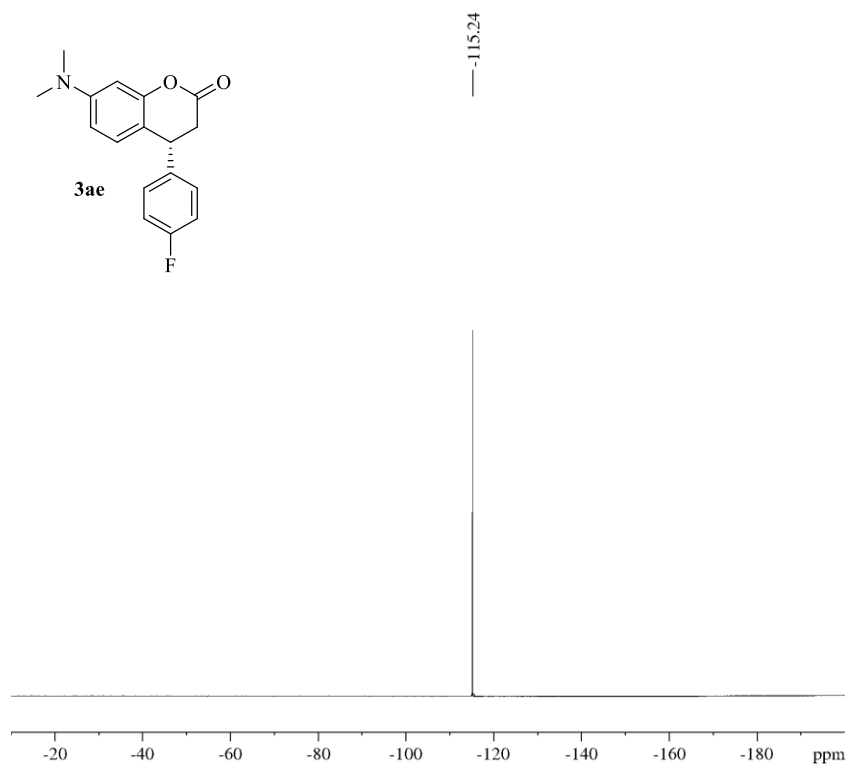
```
Current Data Parameters
NAME          GY
EXPNO         27
PROCNO        1

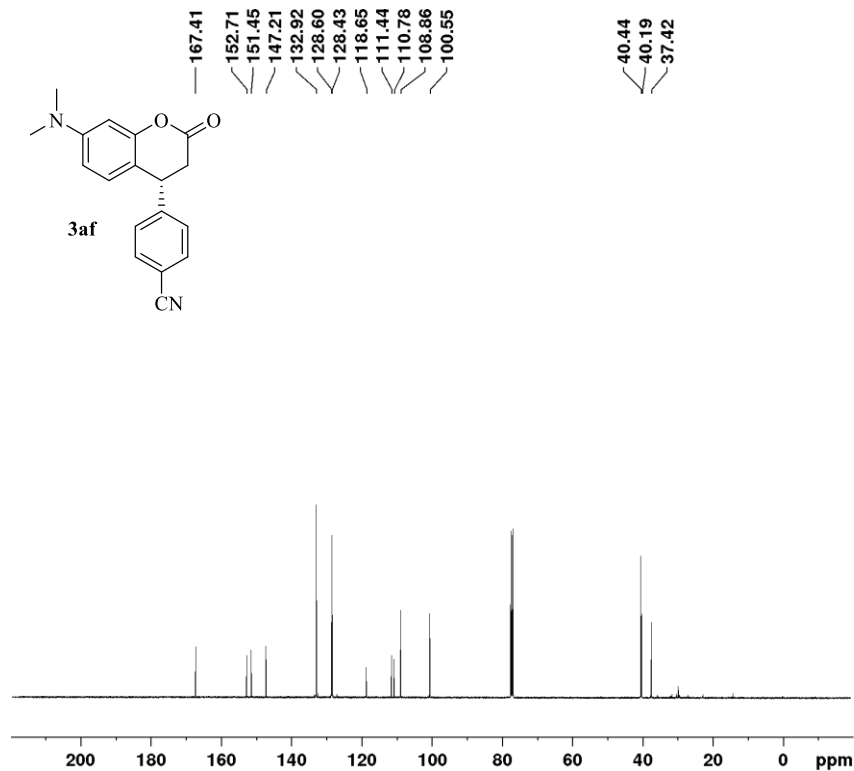
F2 - Acquisition Parameters
Date_         20220608
Time          15.38
INSTRUM       spect
PROBHD        5 mm PABBO BB/
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            64
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG            213.76
DW            20.800 usec
DE            6.50 usec
TE            295.6 K
D1            2.00000000 sec
D11           0.03000000 sec
TDO           1
```

```
===== CHANNEL f1 =====
SF01         100.6228293 MHz
NUC1          13C
P1           10.15 usec
PLW1         76.00000000 W

===== CHANNEL f2 =====
SF02         400.1316005 MHz
NUC2          1H
CPDPRG[2]    waltz16
PCPD2        80.00 usec
PLW2         16.00000000 W
PLW12        0.23184000 W
PLW13        0.14838000 W

F2 - Processing parameters
SI           32768
SF           100.6127615 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
```





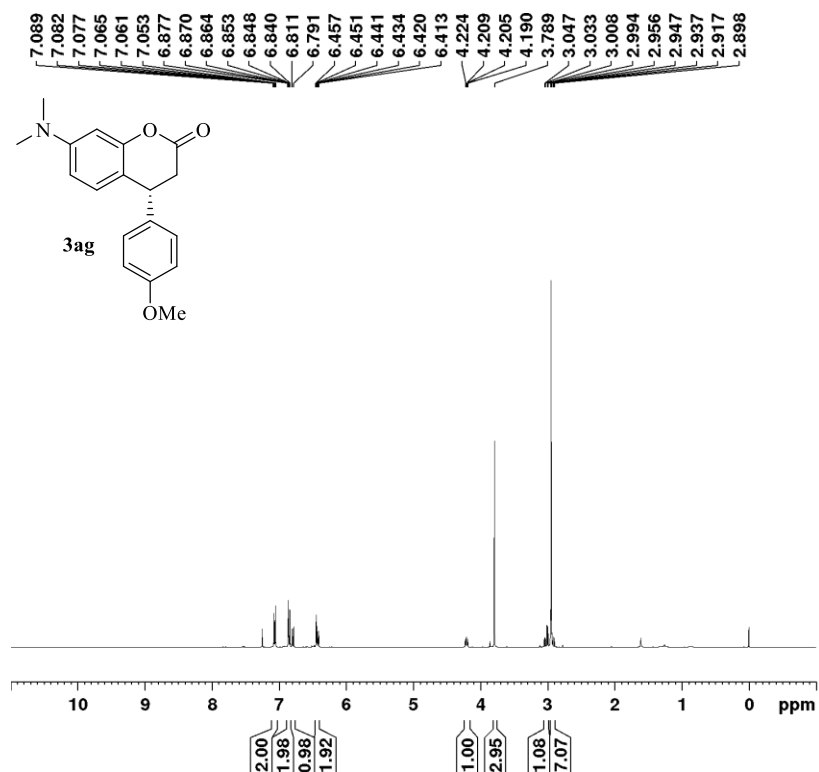
Current Data Parameters  
NAME GY  
EXPNO 128  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220731  
Time 2.54  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631468 sec  
RG 213.76  
DW 20.800 usec  
DE 6.50 usec  
TE 296.1 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1

===== CHANNEL f1 =====  
SFO1 100.6228293 MHz  
NUC1 13C  
P1 10.15 usec  
PLW1 76.00000000 W

===== CHANNEL f2 =====  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 16.00000000 W  
PLW12 0.23184000 W  
PLW13 0.14838000 W

F2 - Processing parameters  
SI 32768  
SF 100.6127607 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

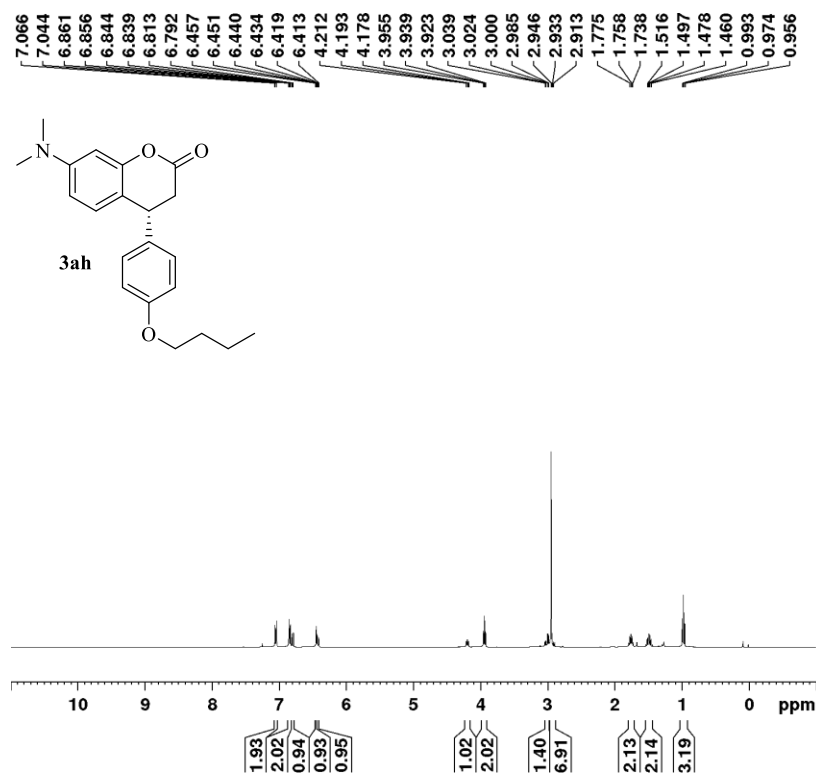
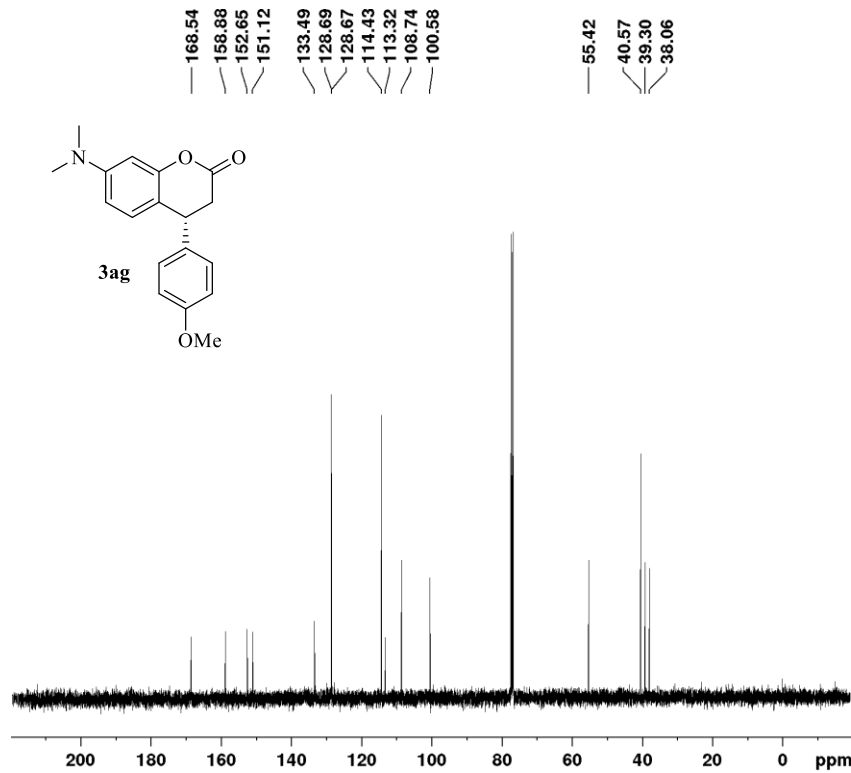


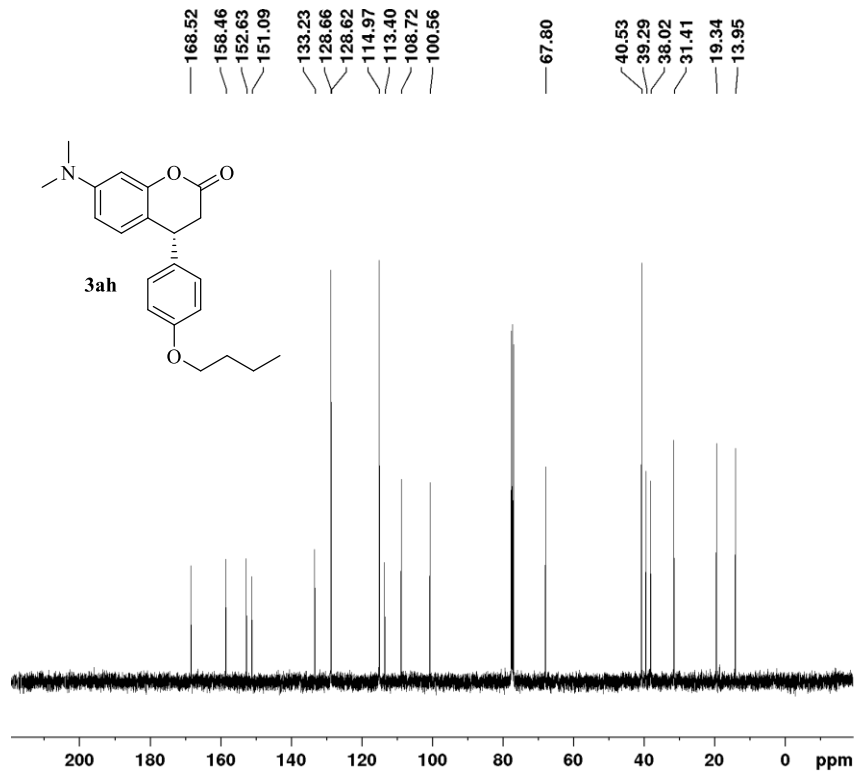
Current Data Parameters  
NAME GY  
EXPNO 24  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220606  
Time 14.56  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 6  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 84.43  
DW 62.400 usec  
DE 6.50 usec  
TE 293.8 K  
D1 1.0000000 sec  
TDO 1

===== CHANNEL f1 =====  
SFO1 400.1324710 MHz  
NUC1 1H  
P1 9.63 usec  
PLW1 16.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1300098 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





```

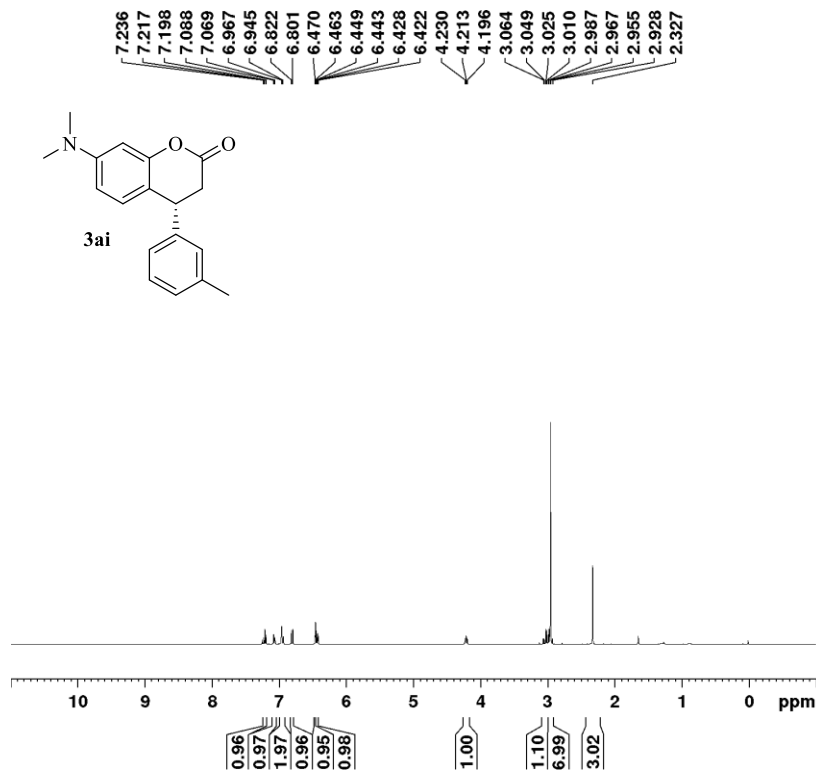
Current Data Parameters
NAME          GYY
EXPNO        208
PROCNO       1

F2 - Acquisition Parameters
Date_        20220927
Time         10.37
INSTRUM     spect
PROBHD      5 mm PABBO BB/
PULPROG     zgpg30
TD           65536
SOLVENT     CDCl3
NS           44
DS           4
SWH          24038.461 Hz
FIDRES      0.366798 Hz
AQ           1.3631468 sec
RG           213.76
DW           20.800 usec
DE           6.50 usec
TE           297.4 K
D1           2.0000000 sec
D11          0.0300000 sec
TDO         1

===== CHANNEL f1 =====
SFO1        100.6228293 MHz
NUC1         13C
P1           10.15 usec
PLW1        76.00000000 W

===== CHANNEL f2 =====
SFO2        400.1316005 MHz
NUC2         1H
CPDPRG[2]   waltz16
PCPD2       80.00 usec
PLW2        16.0000000 W
PLW12       0.23184000 W
PLW13       0.14838000 W

F2 - Processing parameters
SI           32768
SF           100.6127611 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
  
```



```

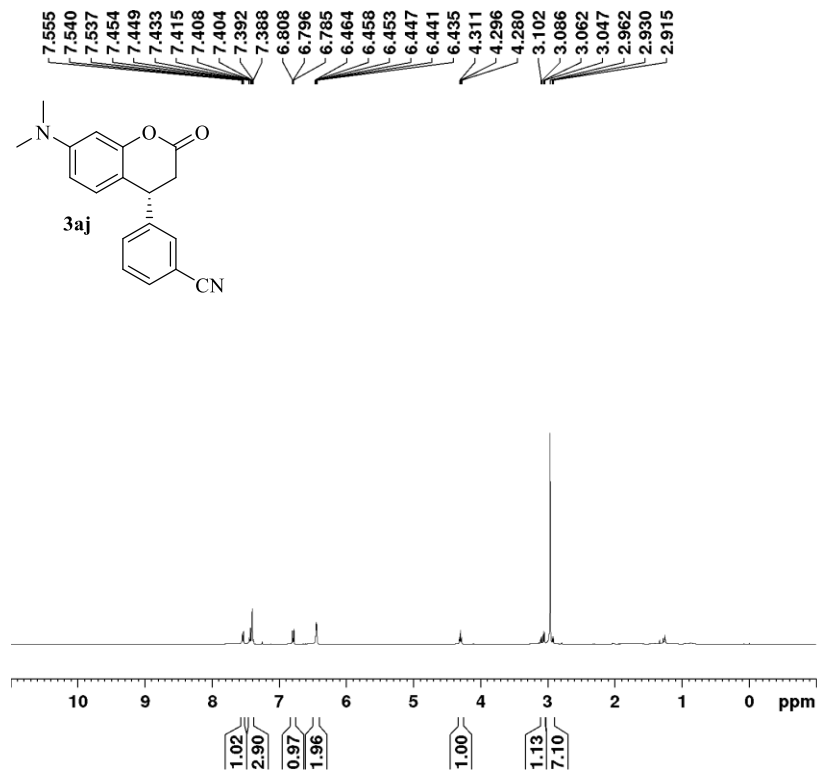
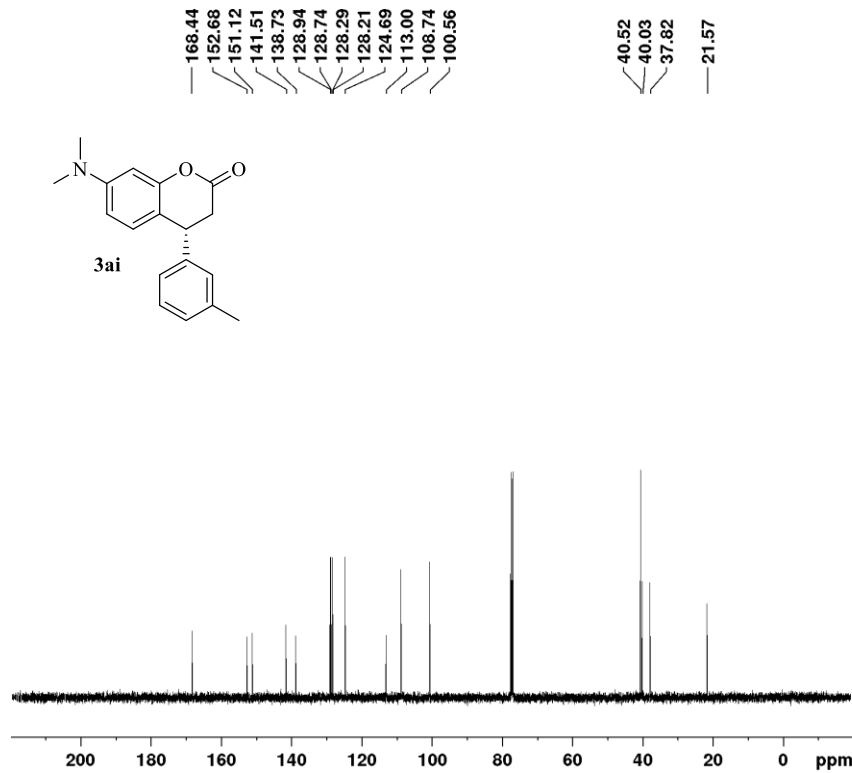
Current Data Parameters
NAME          GYY
EXPNO        53
PROCNO       1

F2 - Acquisition Parameters
Date_        20220622
Time         19.49
INSTRUM     spect
PROBHD      5 mm PABBO BB/
PULPROG     zg30
TD           65536
SOLVENT     CDCl3
NS           4
DS           2
SWH          8012.820 Hz
FIDRES      0.122266 Hz
AQ           4.0894465 sec
RG           58.51
DW           62.400 usec
DE           6.50 usec
TE           298.3 K
D1           1.0000000 sec
D11          0 sec
TDO         1

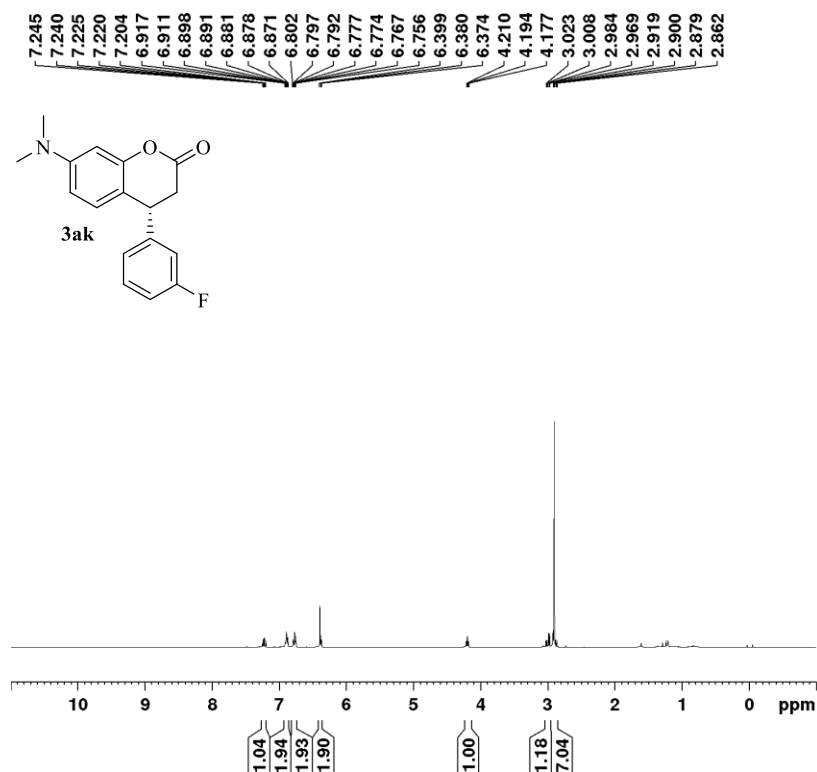
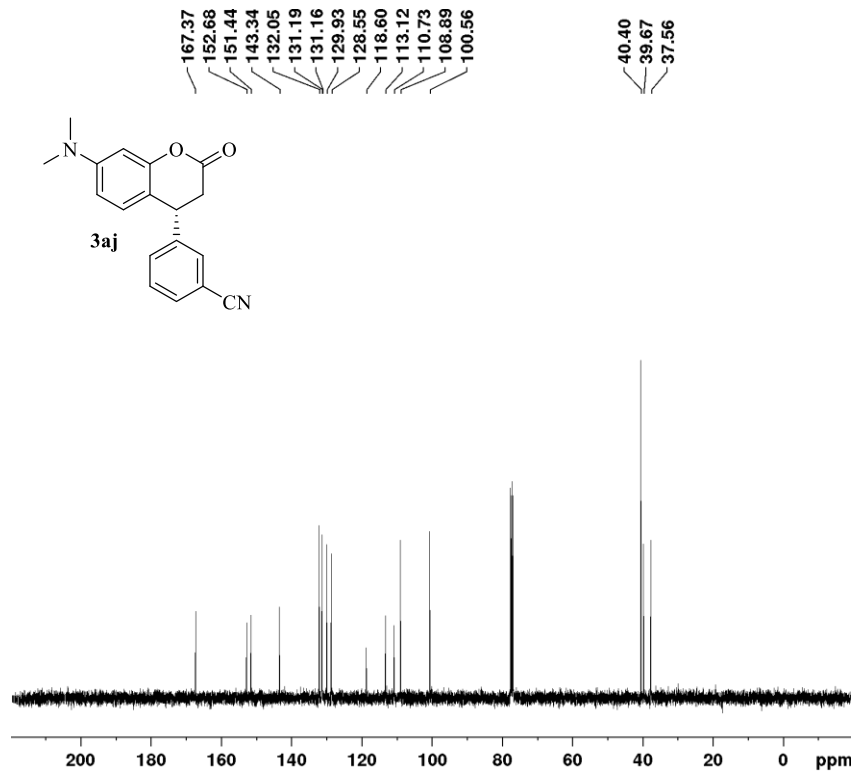
===== CHANNEL f1 =====
SFO1        400.1324710 MHz
NUC1         1H
P1           9.63 usec
PLW1        16.00000000 W

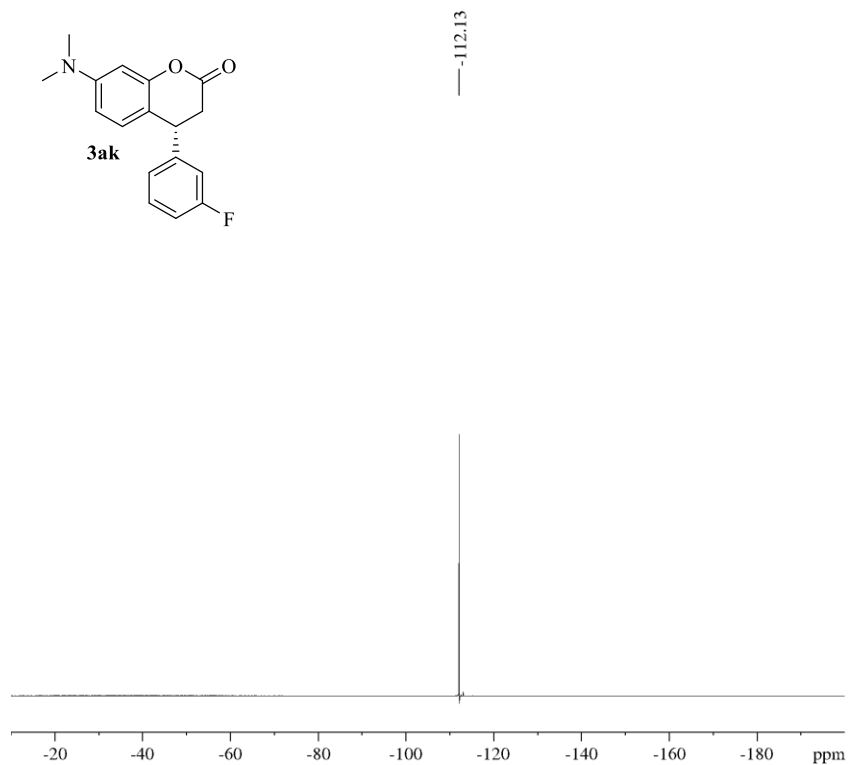
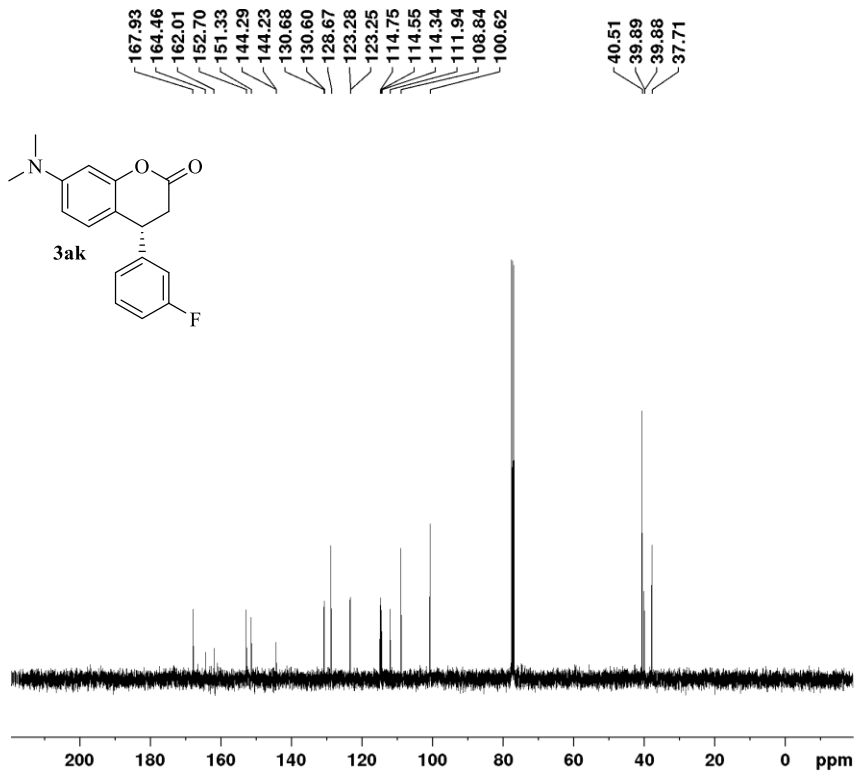
===== CHANNEL f2 =====
SFO2        400.1324710 MHz
NUC2         off
CPDPRG[2]   off
PCPD2       0 usec
PLW2        0 W
PLW12       0 W
PLW13       0 W

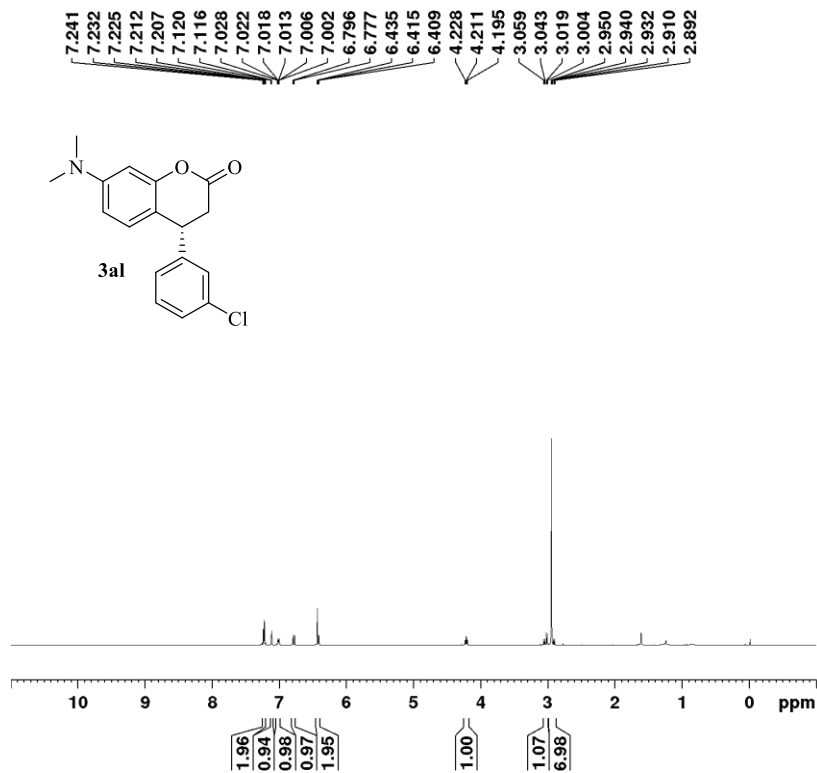
F2 - Processing parameters
SI           65536
SF           400.1300098 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00
  
```











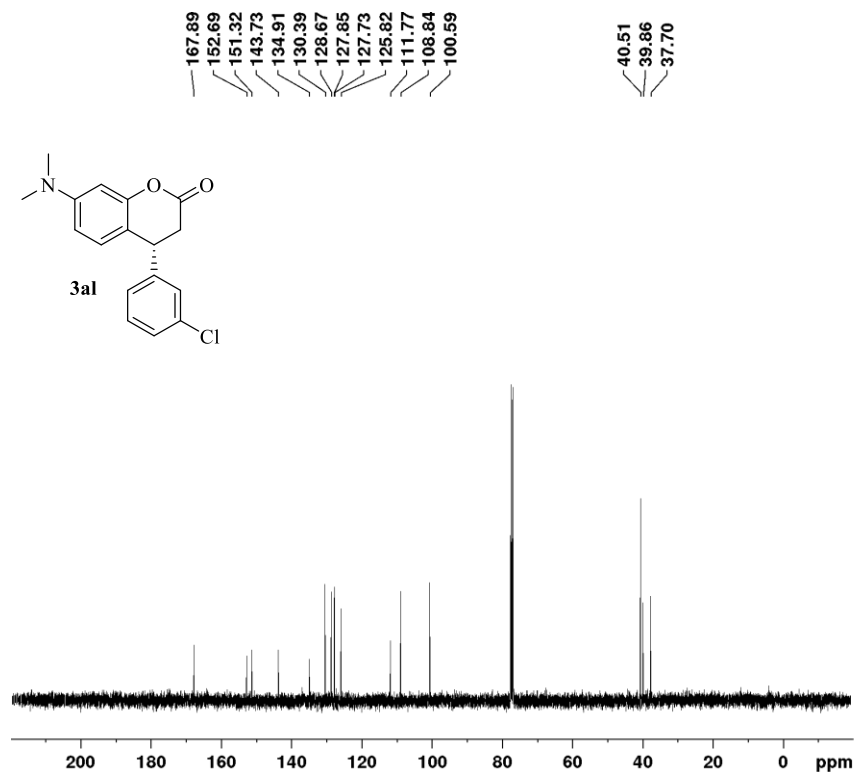
Current Data Parameters  
 NAME GYY  
 EXPNO 57  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220628  
 Time 9.51  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 6  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 84.43  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 295.9 K  
 D1 1.00000000 sec  
 D11 0 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 400.1324710 MHz  
 NUC1 1H  
 P1 9.63 usec  
 PLW1 16.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.1324710 MHz  
 NUC2 off  
 CPDPRG[2]  
 PCPD2 0 usec  
 PLW2 0 W  
 PLW12 0 W  
 PLW13 0 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300172 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



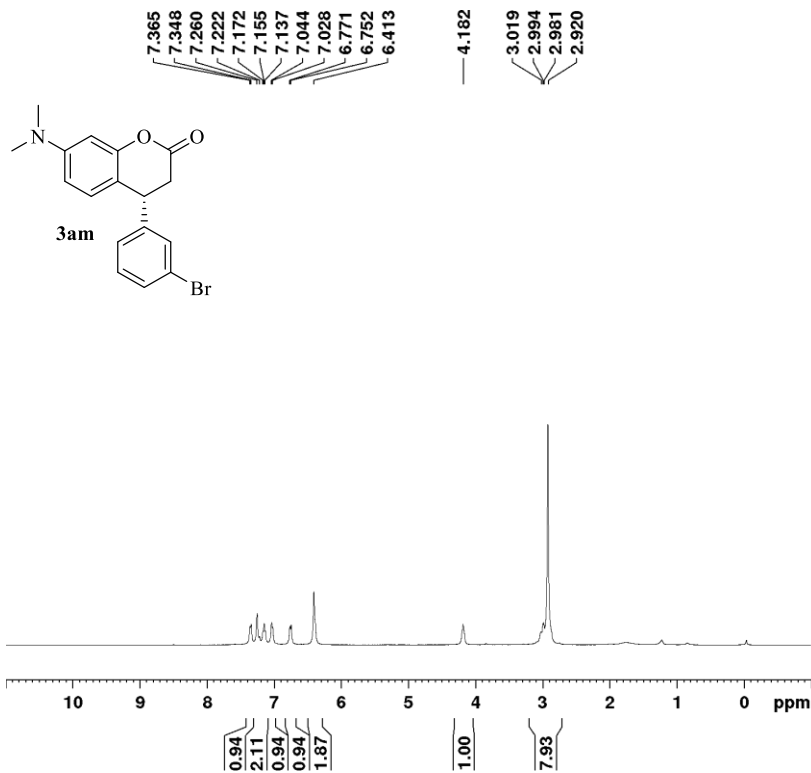
Current Data Parameters  
 NAME GYY  
 EXPNO 58  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220628  
 Time 9.54  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 32  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 213.76  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 100.6228293 MHz  
 NUC1 13C  
 P1 10.15 usec  
 PLW1 76.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.1316005 MHz  
 NUC2 1H  
 CPDPRG[2] waitz16  
 PCPD2 80.00 usec  
 PLW2 16.00000000 W  
 PLW12 0.23184000 W  
 PLW13 0.14838000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6127585 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



```

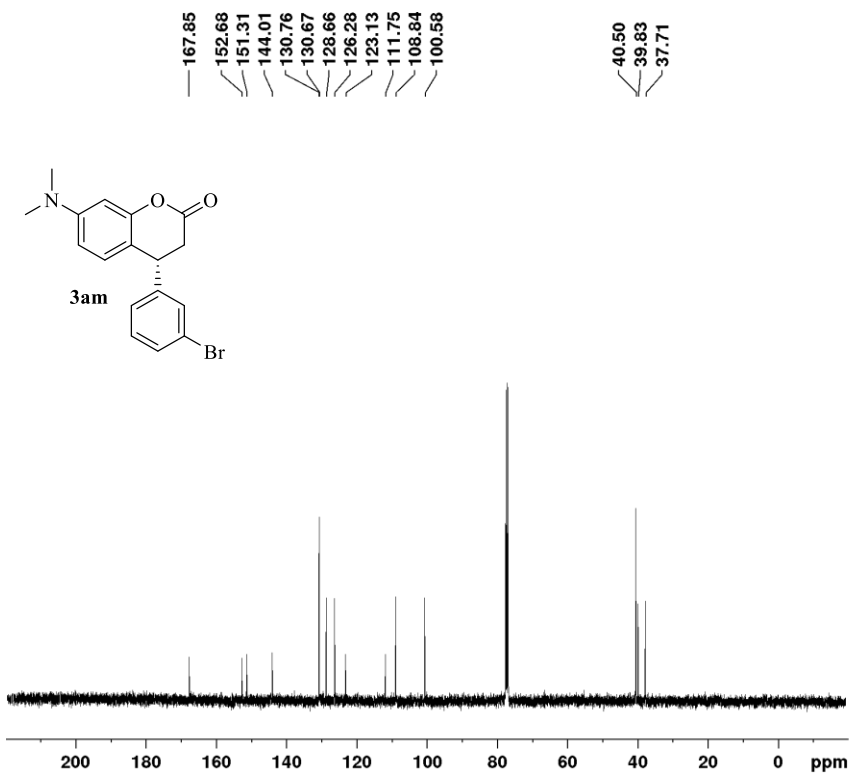
Current Data Parameters
NAME          GYY
EXPNO         101
PROCNO        1

F2 - Acquisition Parameters
Date_         20220721
Time          20.58
INSTRUM       spect
PROBHD        5 mm PABBO BB/
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            5
DS            2
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894465 sec
RG            84.43
DW            62.400 usec
DE            6.50 usec
TE            296.1 K
D1            1.00000000 sec
D11           0 sec
TD0           1

===== CHANNEL f1 =====
SFO1          400.1324710 MHz
NUC1          1H
P1            9.63 usec
PLW1          16.00000000 W

===== CHANNEL f2 =====
SFO2          400.1324710 MHz
NUC2          off
CPDPRG[2]
PCPD2         0 usec
PLW2          0 W
PLW12         0 W
PLW13         0 W

F2 - Processing parameters
SI            65536
SF            400.1300254 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```



```

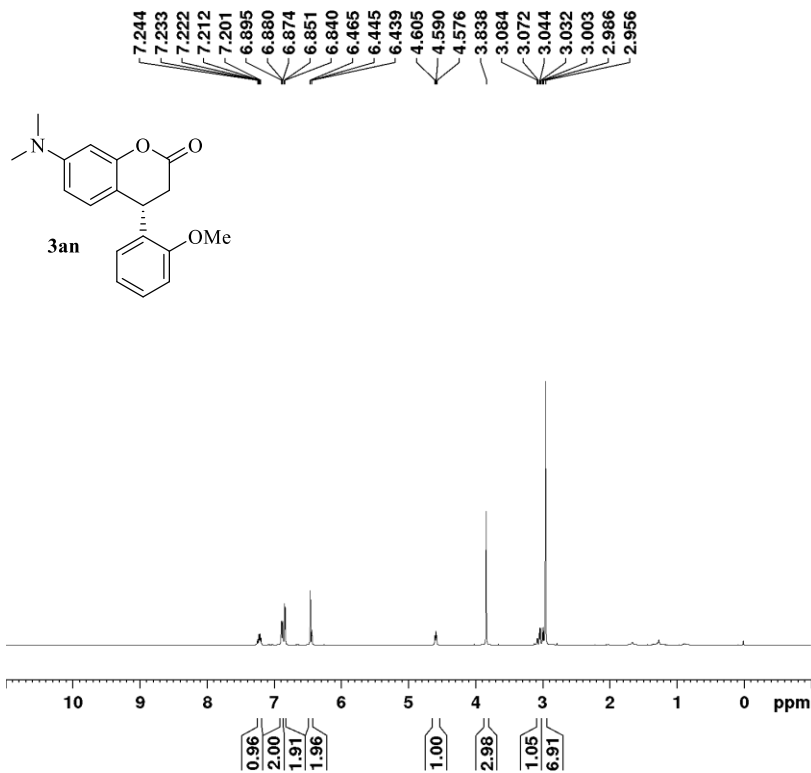
Current Data Parameters
NAME          GYY
EXPNO         102
PROCNO        1

F2 - Acquisition Parameters
Date_         20220721
Time          21.01
INSTRUM       spect
PROBHD        5 mm PABBO BB/
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            154
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG            213.76
DW            20.800 usec
DE            6.50 usec
TE            296.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

===== CHANNEL f1 =====
SFO1          100.6228293 MHz
NUC1          13C
P1            10.15 usec
PLW1          76.00000000 W

===== CHANNEL f2 =====
SFO2          400.1316005 MHz
NUC2          1H
CPDPRG[2]     waltz16
PCPD2         80.00 usec
PLW2          16.00000000 W
PLW12         0.23184000 W
PLW13         0.14838000 W

F2 - Processing parameters
SI            32768
SF            100.6127592 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```

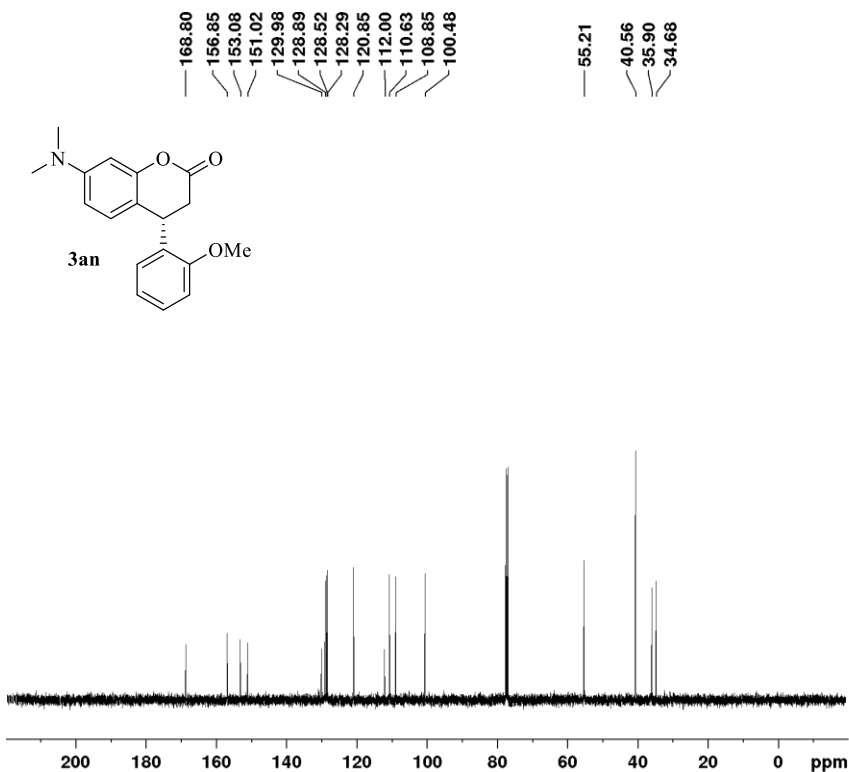


Current Data Parameters  
 NAME GYY  
 EXPNO 42  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220619  
 Time 10.18  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 58.51  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 294.4 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SF01 400.1324710 MHz  
 NUC1 1H  
 F1 9.63 usec  
 PLW1 16.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300098 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



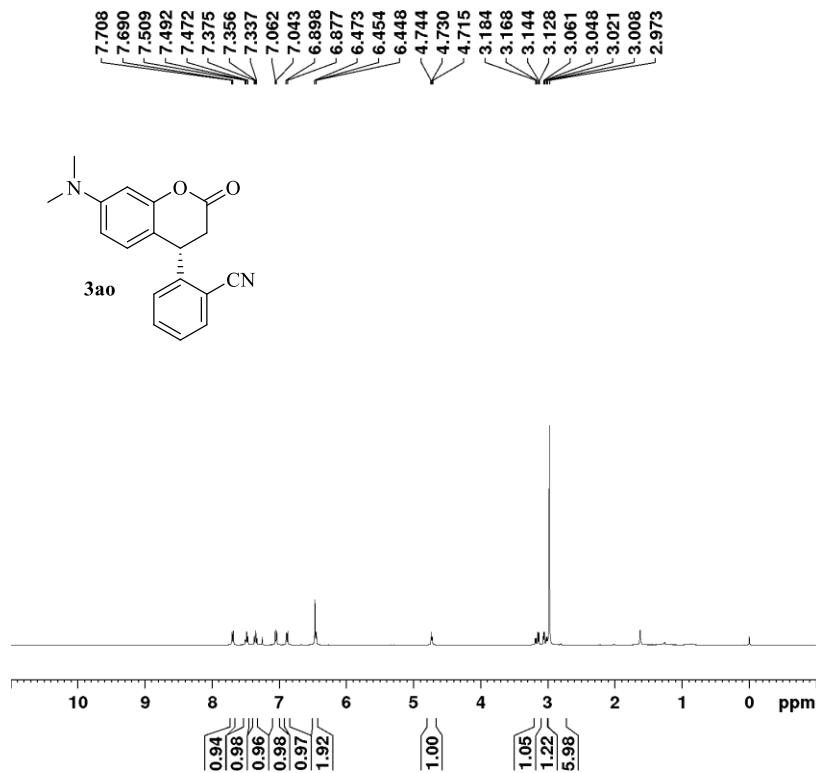
Current Data Parameters  
 NAME GYY  
 EXPNO 43  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220619  
 Time 10.25  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 27  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 213.76  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 294.6 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SF01 100.6228293 MHz  
 NUC1 13C  
 F1 10.15 usec  
 PLW1 76.00000000 W

===== CHANNEL f2 =====  
 SF02 400.1316005 MHz  
 NUC2 1H  
 CPDPRG[2] waitz16  
 PCPD2 80.00 usec  
 PLW2 16.00000000 W  
 PLW12 0.23184000 W  
 PLW13 0.14838000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6127615 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



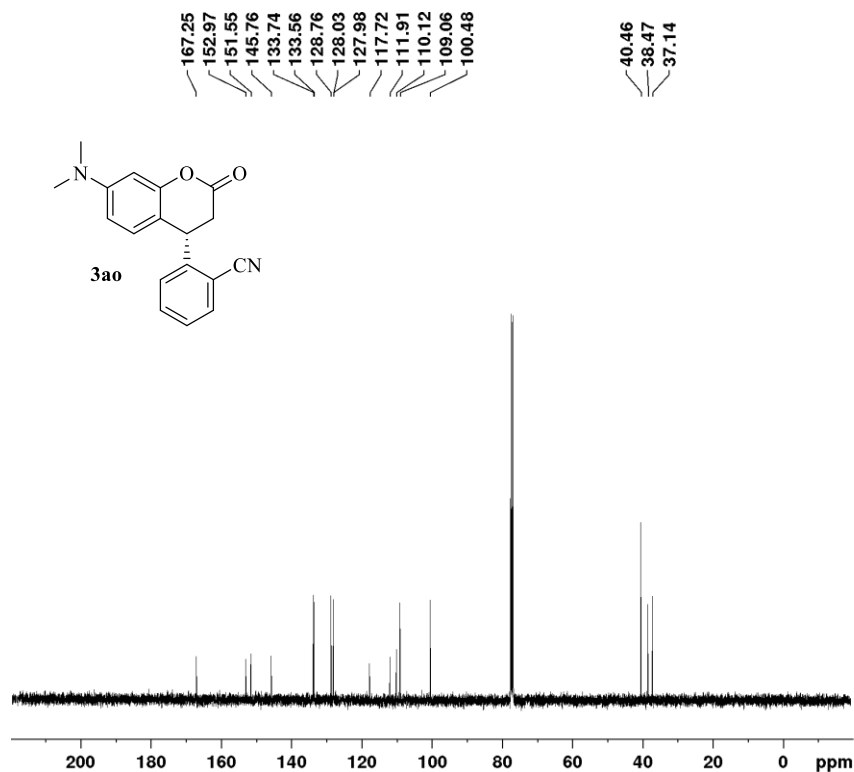
```
Current Data Parameters
NAME          GYY
EXPNO         122
PROCNO        1

F2 - Acquisition Parameters
Date_         20220729
Time          16.47
INSTRUM       spect
PROBHD        5 mm PABBO BB/
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            4
DS            2
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894465 sec
RG            104.2
DW            62.400 usec
DE            6.50 usec
TE            295.3 K
D1            1.00000000 sec
D11           0 sec
TD0           1

===== CHANNEL f1 =====
SFO1          400.1324710 MHz
NUC1          1H
P1            9.63 usec
PLW1          16.00000000 W

===== CHANNEL f2 =====
SFO2          400.1324710 MHz
NUC2          off
CPDPRG[2]
PCPD2         0 usec
PLW2          0 W
PLW12         0 W
PLW13         0 W

F2 - Processing parameters
SI            65536
SF            400.1300099 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
```



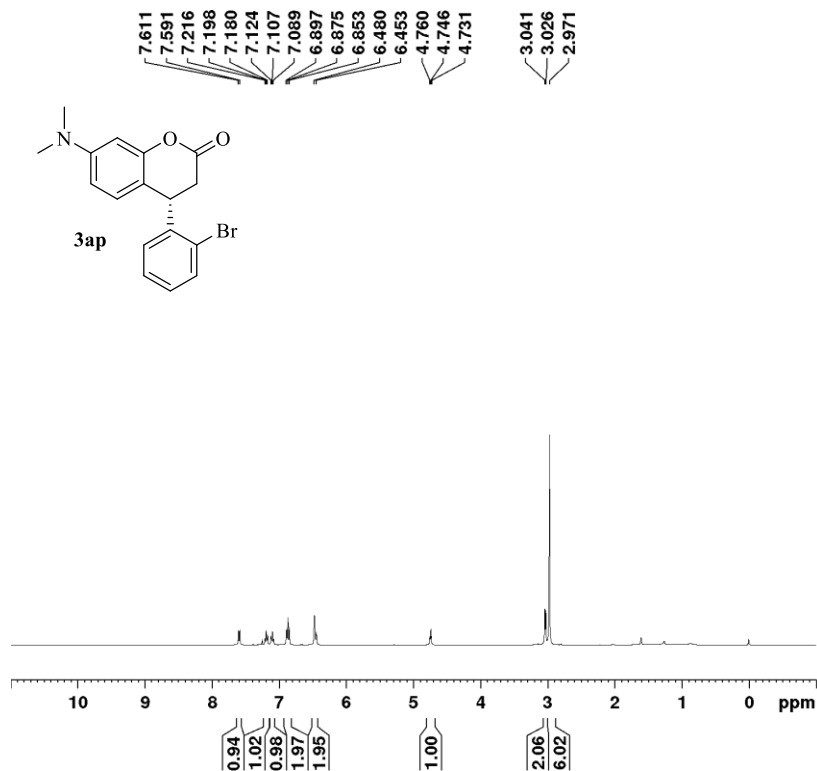
```
Current Data Parameters
NAME          GYY
EXPNO         123
PROCNO        1

F2 - Acquisition Parameters
Date_         20220729
Time          16.49
INSTRUM       spect
PROBHD        5 mm PABBO BB/
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            73
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG            213.76
DW            20.800 usec
DE            6.50 usec
TE            295.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

===== CHANNEL f1 =====
SFO1          100.6228293 MHz
NUC1          13C
P1            10.15 usec
PLW1          76.00000000 W

===== CHANNEL f2 =====
SFO2          400.1316005 MHz
NUC2          1H
CPDPRG[2]     waitz16
PCPD2         80.00 usec
PLW2          16.00000000 W
PLW12         0.23184000 W
PLW13         0.14838000 W

F2 - Processing parameters
SI            32768
SF            100.6127585 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
```



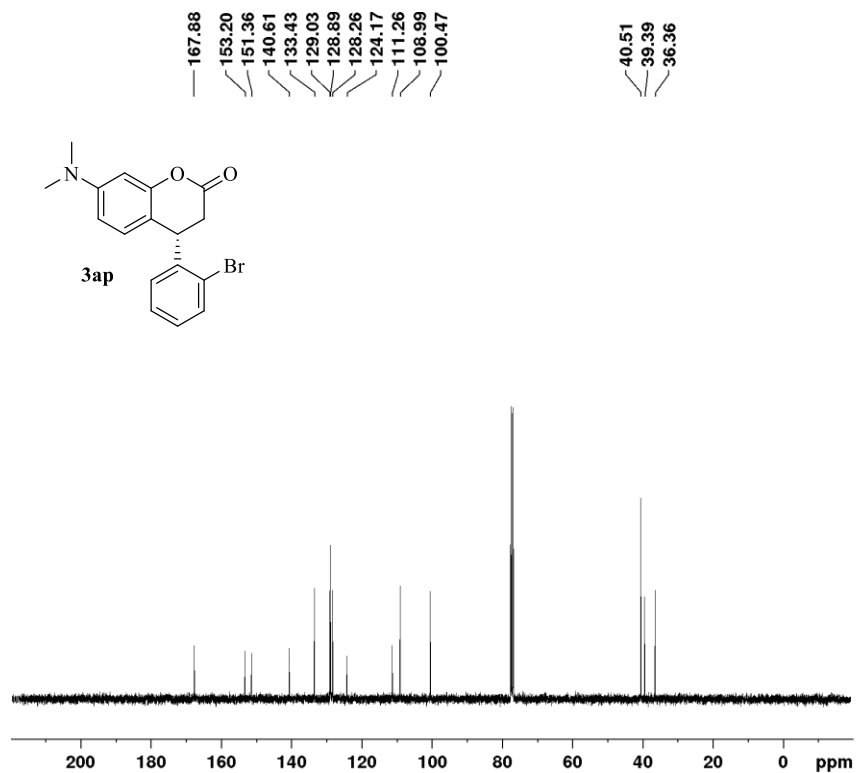
Current Data Parameters  
 NAME GYY  
 EXPNO 88  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220715  
 Time 17.42  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 84.43  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 297.1 K  
 D1 1.00000000 sec  
 D11 0 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 400.1324710 MHz  
 NUC1 1H  
 P1 9.63 usec  
 PLW1 16.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.1324710 MHz  
 NUC2 off  
 CPDPRG[2]  
 PCPD2 0 usec  
 PLW2 0 W  
 PLW12 0 W  
 PLW13 0 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300101 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



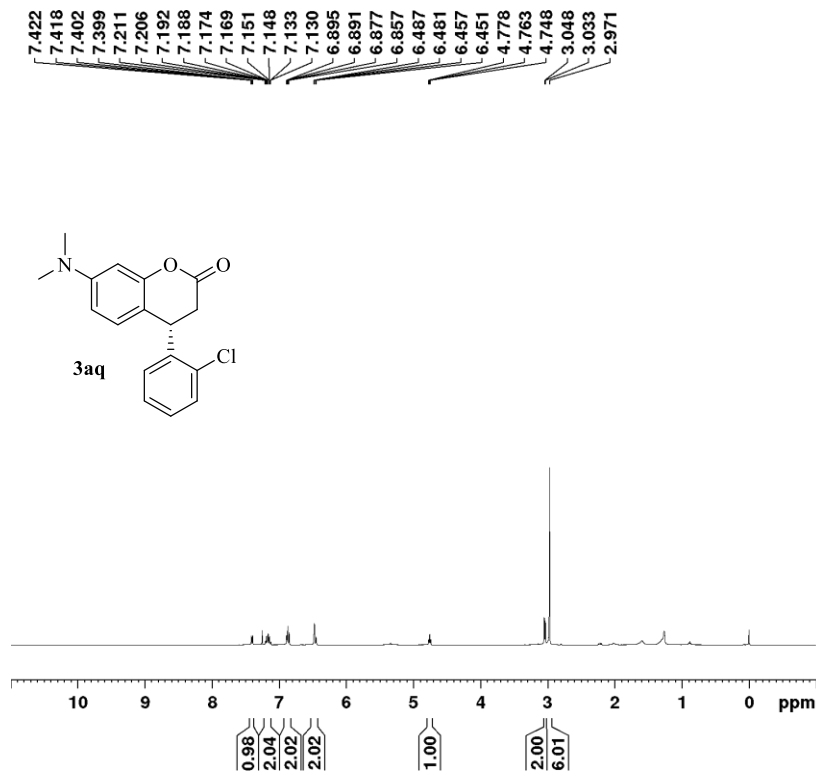
Current Data Parameters  
 NAME GYY  
 EXPNO 89  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220715  
 Time 17.45  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 128  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 213.76  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.3 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 100.6228293 MHz  
 NUC1 13C  
 P1 10.15 usec  
 PLW1 76.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.1316005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 80.00 usec  
 PLW2 16.00000000 W  
 PLW12 0.23184000 W  
 PLW13 0.14838000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6127585 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



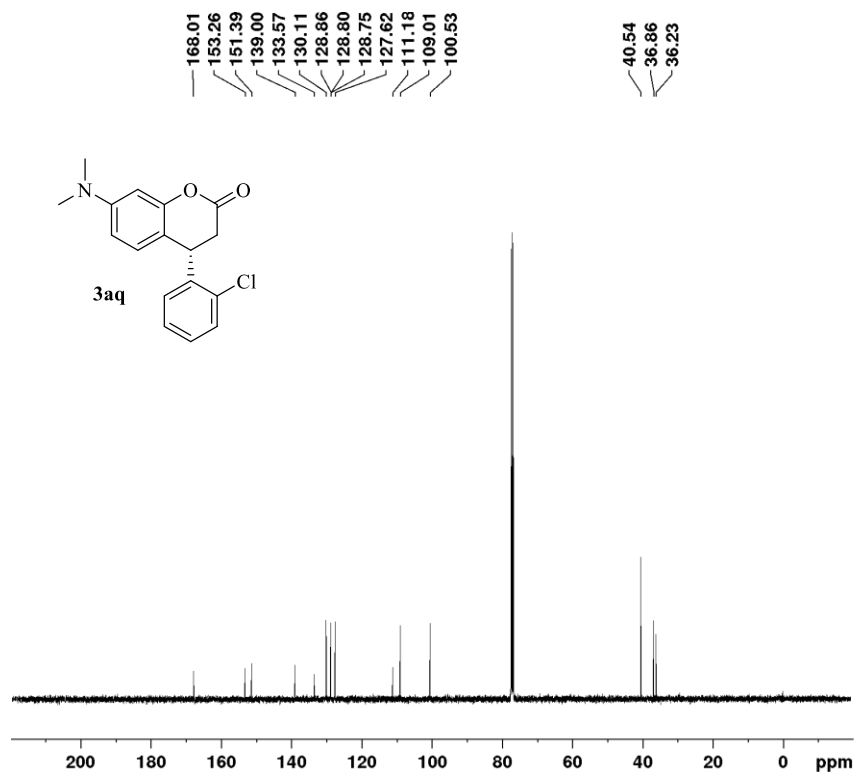
Current Data Parameters  
 NAME GYY  
 EXPNO 166  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220912  
 Time 11.05  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 134.75  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.2 K  
 D1 1.00000000 sec  
 D11 0 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 400.1324710 MHz  
 NUC1 1H  
 P1 9.63 usec  
 PLW1 16.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.1324710 MHz  
 NUC2 off  
 CPDPRG[2]  
 PCPD2 0 usec  
 PLW2 0 W  
 PLW12 0 W  
 PLW13 0 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300103 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



Current Data Parameters  
 NAME GYY  
 EXPNO 148  
 PROCNO 1

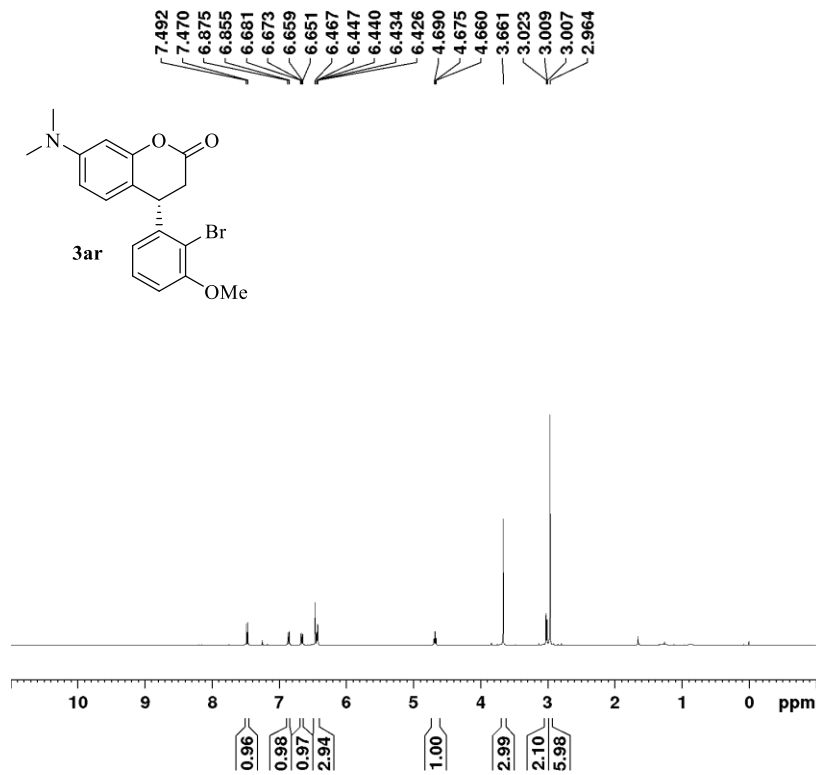
F2 - Acquisition Parameters  
 Date\_ 20220804  
 Time 20.07  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 395  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 213.76  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.7 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 100.6228293 MHz  
 NUC1 13C  
 P1 10.15 usec  
 PLW1 76.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.1316005 MHz  
 NUC2 1H  
 CPDPRG[2] waitz16  
 PCPD2 80.00 usec  
 PLW2 16.00000000 W  
 PLW12 0.23184000 W  
 PLW13 0.14838000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6127556 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40





```

Current Data Parameters
NAME          GYY
EXPNO         45
PROCNO        1

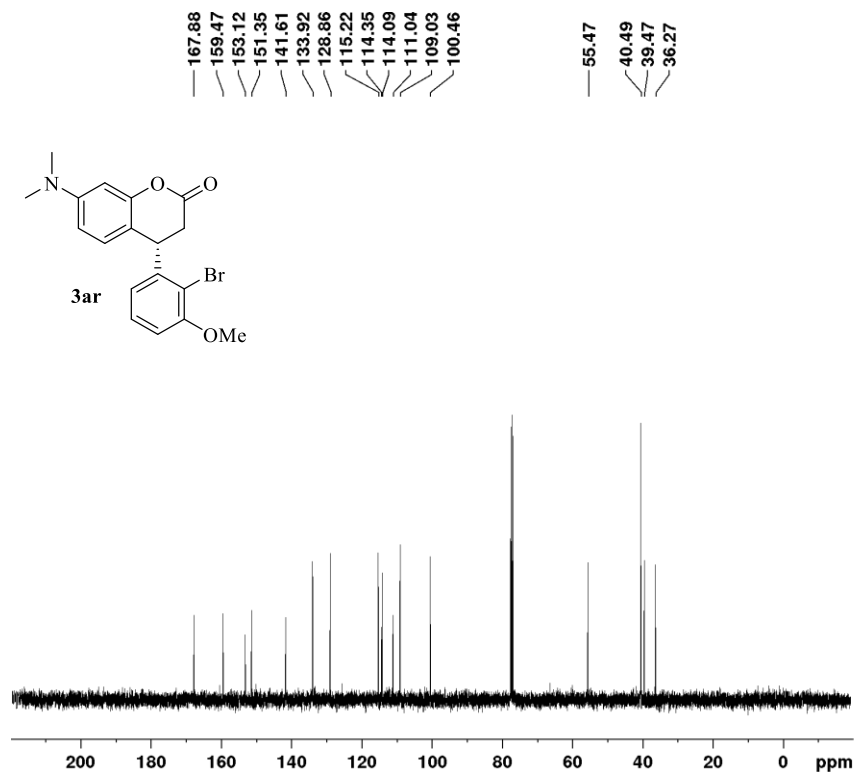
F2 - Acquisition Parameters
Date_         20220621
Time          10.10
INSTRUM       spect
PROBHD        5 mm PABBO BB/
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            8
DS            2
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894465 sec
RG            58.51
DW            62.400 usec
DE            6.50 usec
TE            296.6 K
D1            1.00000000 sec
D11           0 sec
TD0           1

===== CHANNEL f1 =====
SFO1          400.1324710 MHz
NUC1          1H
P1            9.63 usec
PLW1          16.00000000 W

===== CHANNEL f2 =====
SFO2          400.1324710 MHz
NUC2          off
CPDPRG[2]
PCPD2         0 usec
PLW2          0 W
PLW12         0 W
PLW13         0 W

F2 - Processing parameters
SI            65536
SF            400.1300098 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```



```

Current Data Parameters
NAME          GYY
EXPNO         46
PROCNO        1

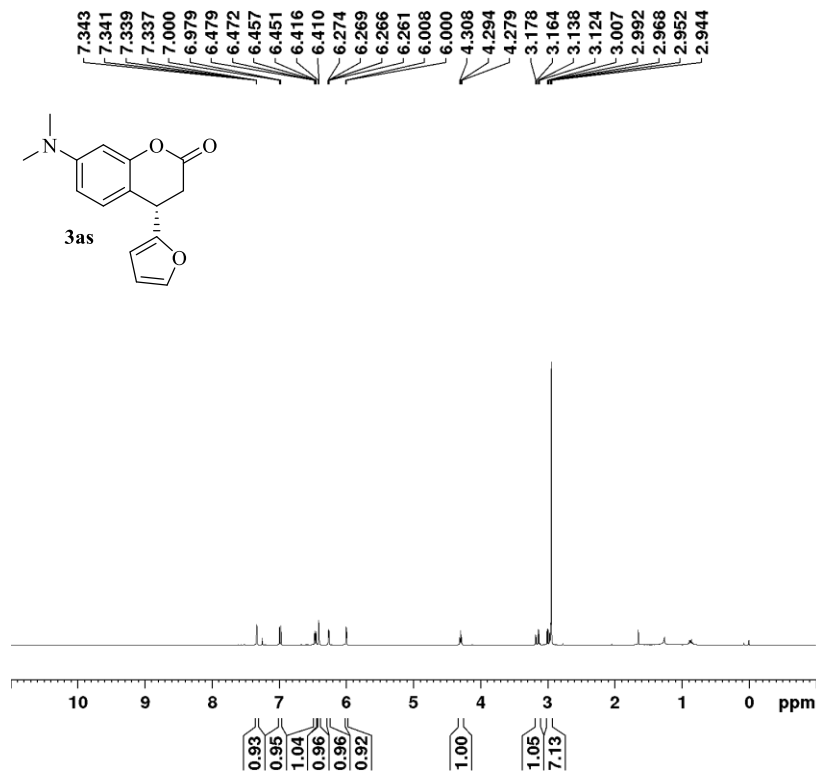
F2 - Acquisition Parameters
Date_         20220621
Time          10.12
INSTRUM       spect
PROBHD        5 mm PABBO BB/
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            12
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG            213.76
DW            20.800 usec
DE            6.50 usec
TE            296.9 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

===== CHANNEL f1 =====
SFO1          100.6228293 MHz
NUC1          13C
P1            10.15 usec
PLW1          76.00000000 W

===== CHANNEL f2 =====
SFO2          400.1316005 MHz
NUC2          1H
CPDPRG[2]     waltz16
PCPD2         80.00 usec
PLW2          16.00000000 W
PLW12         0.23184000 W
PLW13         0.14838000 W

F2 - Processing parameters
SI            32768
SF            100.6127611 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```



```

Current Data Parameters
NAME          GYY
EXPNO         59
PROCNO        1

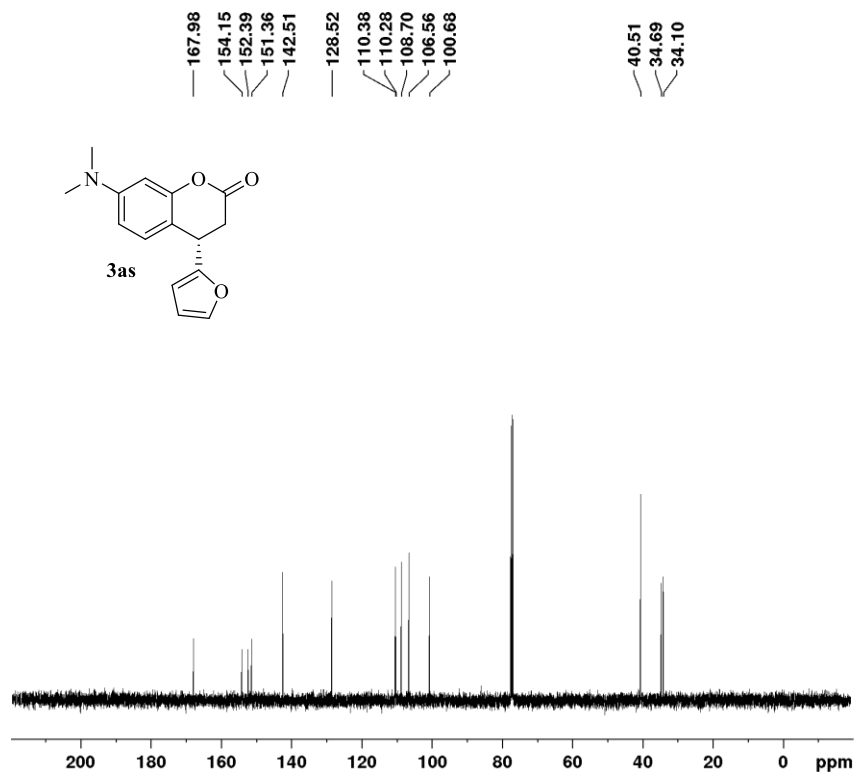
F2 - Acquisition Parameters
Date_         20220628
Time          9.59
INSTRUM       spect
PROBHD        5 mm PABBO BB/
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            5
DS            2
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894465 sec
RG            63.52
DW            62.400 usec
DE            6.50 usec
TE            295.9 K
D1            1.00000000 sec
D11           0 sec
TD0           1

===== CHANNEL f1 =====
SFO1          400.1324710 MHz
NUC1          1H
P1            9.63 usec
PLW1          16.00000000 W

===== CHANNEL f2 =====
SFO2          400.1324710 MHz
NUC2          off
CPDPRG[2]
PCPD2         0 usec
PLW2          0 W
PLW12         0 W
PLW13         0 W

F2 - Processing parameters
SI            65536
SF            400.1300099 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```



```

Current Data Parameters
NAME          GYY
EXPNO         60
PROCNO        1

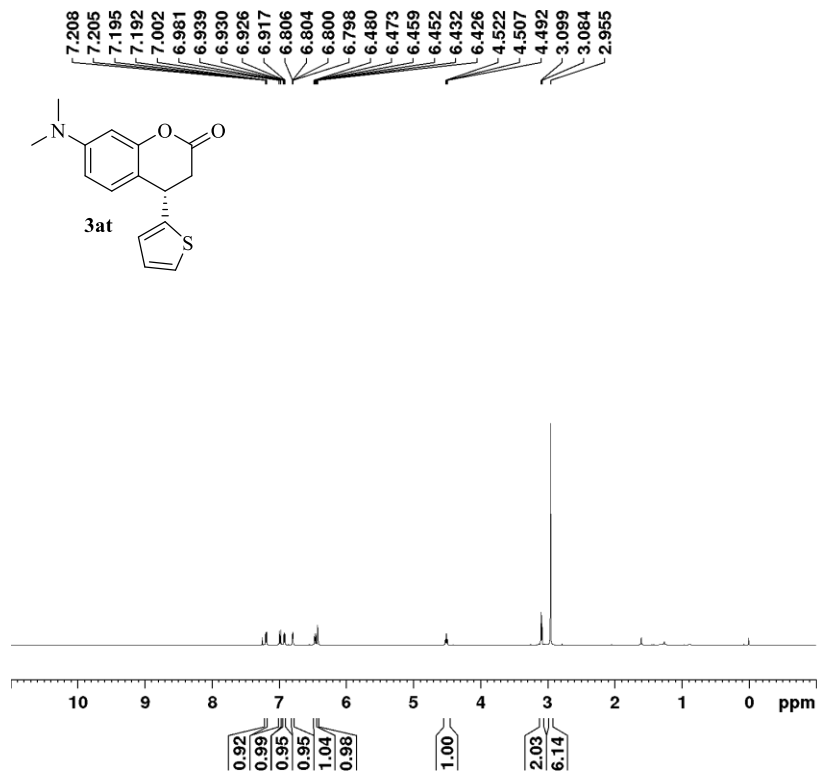
F2 - Acquisition Parameters
Date_         20220628
Time          10.00
INSTRUM       spect
PROBHD        5 mm PABBO BB/
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            21
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG            213.76
DW            20.800 usec
DE            6.50 usec
TE            296.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

===== CHANNEL f1 =====
SFO1          100.6228293 MHz
NUC1          13C
P1            10.15 usec
PLW1          76.00000000 W

===== CHANNEL f2 =====
SFO2          400.1316005 MHz
NUC2          1H
CPDPRG[2]     waitz16
PCPD2         80.00 usec
PLW2          16.00000000 W
PLW12         0.23184000 W
PLW13         0.14838000 W

F2 - Processing parameters
SI            32768
SF            100.6127593 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```

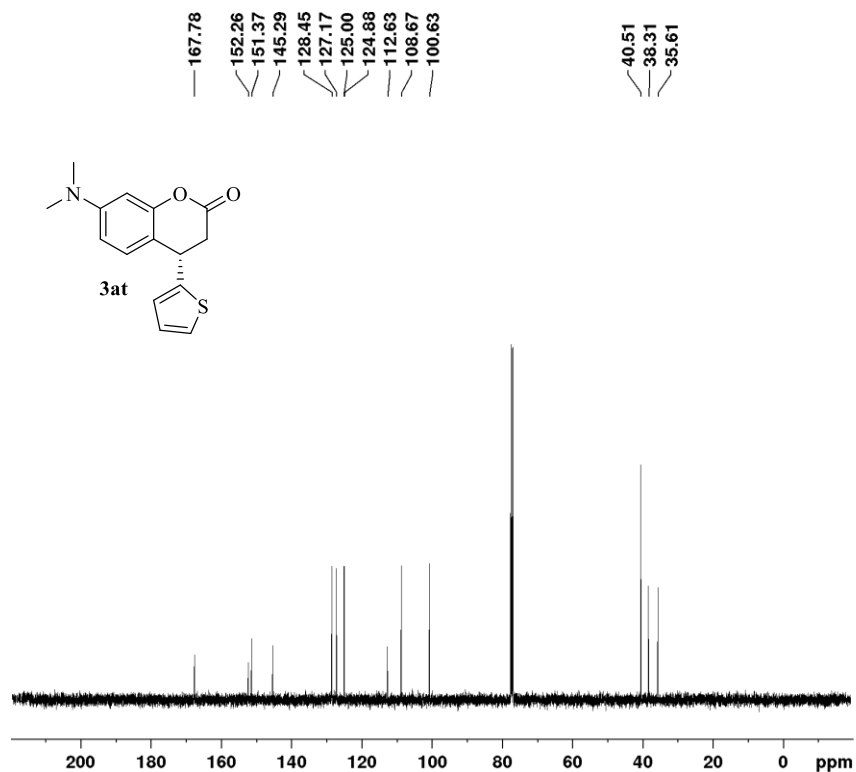


Current Data Parameters  
NAME GY  
EXPNO 222  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221006  
Time 15.18  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 6  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 94.53  
DW 62.400 usec  
DE 6.50 usec  
TE 297.0 K  
D1 1.00000000 sec  
TDO 1

===== CHANNEL f1 =====  
SF01 400.1324710 MHz  
NUC1 1H  
F1 9.63 usec  
PLW1 16.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1300100 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



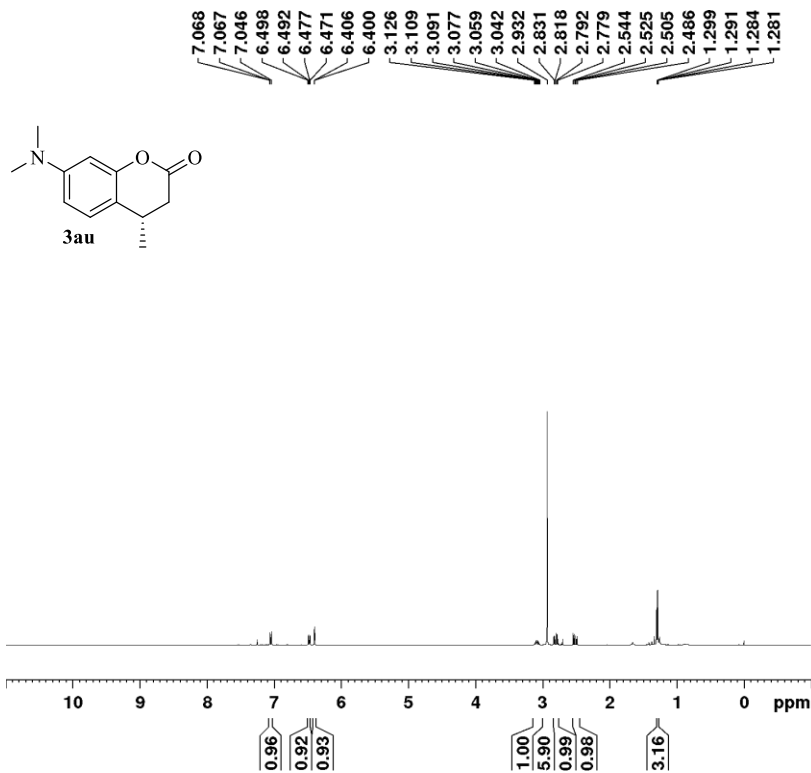
Current Data Parameters  
NAME GY  
EXPNO 223  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221006  
Time 15.22  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 47  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 213.76  
DW 20.800 usec  
DE 6.50 usec  
TE 297.6 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

===== CHANNEL f1 =====  
SF01 100.6228293 MHz  
NUC1 13C  
F1 10.15 usec  
PLW1 76.00000000 W

===== CHANNEL f2 =====  
SF02 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 16.00000000 W  
PLW12 0.23184000 W  
PLW13 0.14838000 W

F2 - Processing parameters  
SI 32768  
SF 100.6127585 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



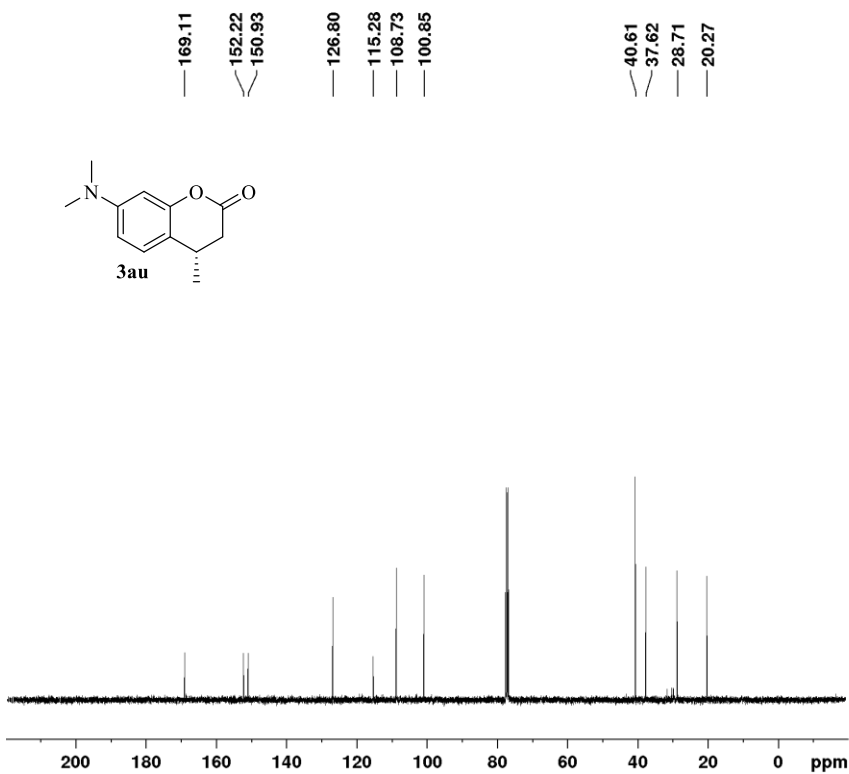
Current Data Parameters  
NAME GYY  
EXPNO 171  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220916  
Time 16.40  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 63.52  
DW 62.400 usec  
DE 6.50 usec  
TE 298.9 K  
D1 1.0000000 sec  
D11 0 sec  
TDO 1

===== CHANNEL f1 =====  
SFO1 400.1324710 MHz  
NUC1 1H  
P1 9.63 usec  
PLW1 16.0000000 W

===== CHANNEL f2 =====  
SFO2 400.1324710 MHz  
NUC2 off  
CPDPRG[2]  
PCPD2 0 usec  
PLW2 0 W  
PLW12 0 W  
PLW13 0 W

F2 - Processing parameters  
SI 65536  
SF 400.1300100 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



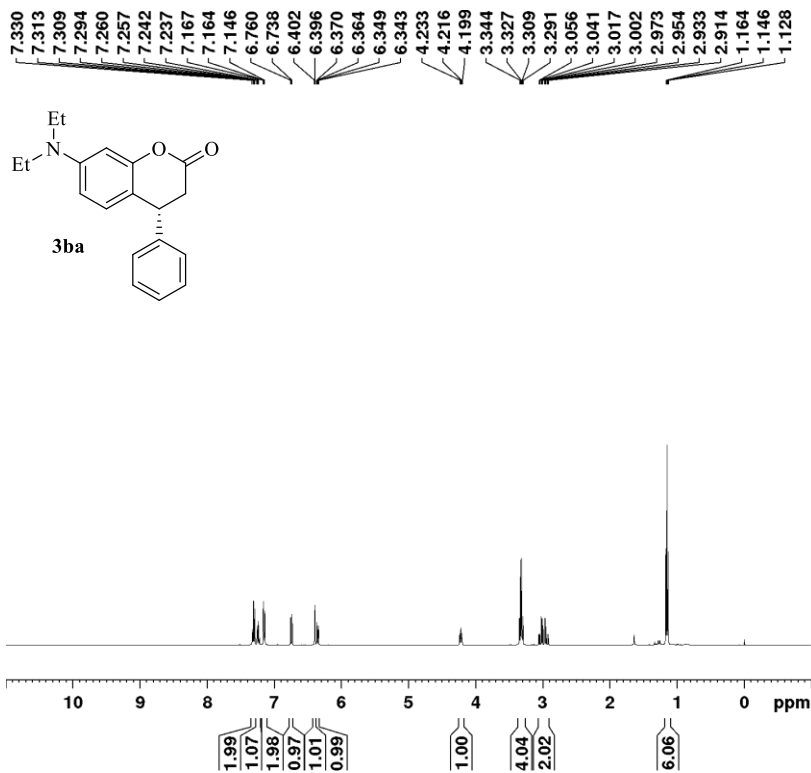
Current Data Parameters  
NAME GYY  
EXPNO 172  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220916  
Time 16.45  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 67  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 213.76  
DW 20.800 usec  
DE 6.50 usec  
TE 299.2 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1

===== CHANNEL f1 =====  
SFO1 100.6228293 MHz  
NUC1 13C  
P1 10.15 usec  
PLW1 76.0000000 W

===== CHANNEL f2 =====  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waitz16  
PCPD2 80.00 usec  
PLW2 16.0000000 W  
PLW12 0.23184000 W  
PLW13 0.14838000 W

F2 - Processing parameters  
SI 32768  
SF 100.6127585 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



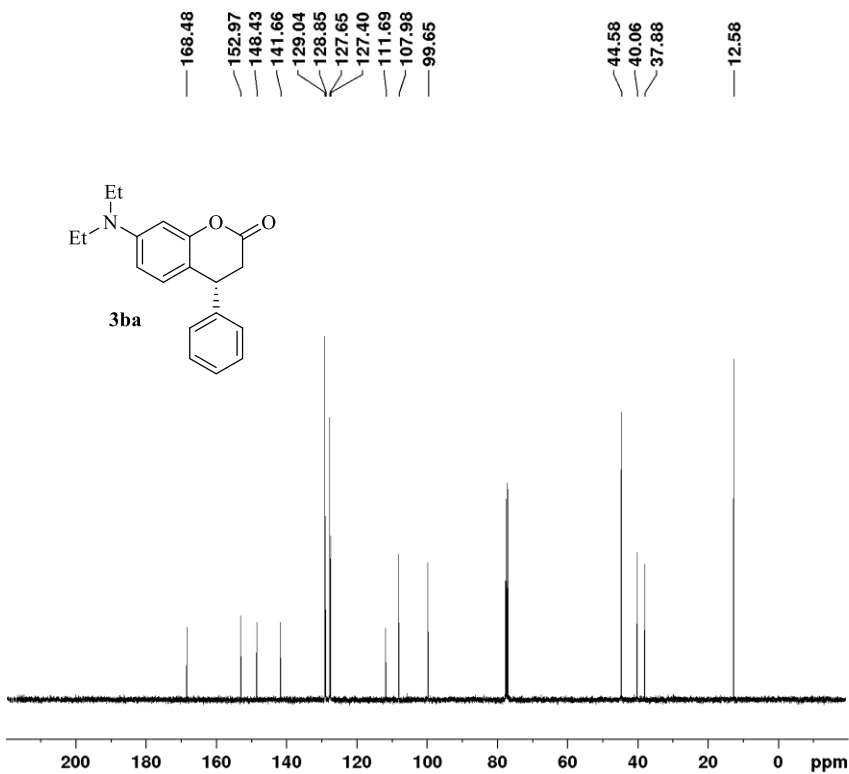
Current Data Parameters  
 NAME GYY  
 EXPNO 147  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220804  
 Time 17.45  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 31.77  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 297.5 K  
 D1 1.00000000 sec  
 D11 0 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 400.1324710 MHz  
 NUC1 1H  
 P1 9.63 usec  
 PLW1 16.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.1324710 MHz  
 NUC2 off  
 CPDPRG[2]  
 PCPD2 0 usec  
 PLW2 0 W  
 PLW12 0 W  
 PLW13 0 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300189 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



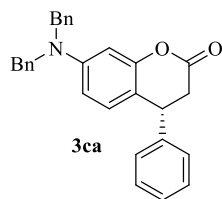
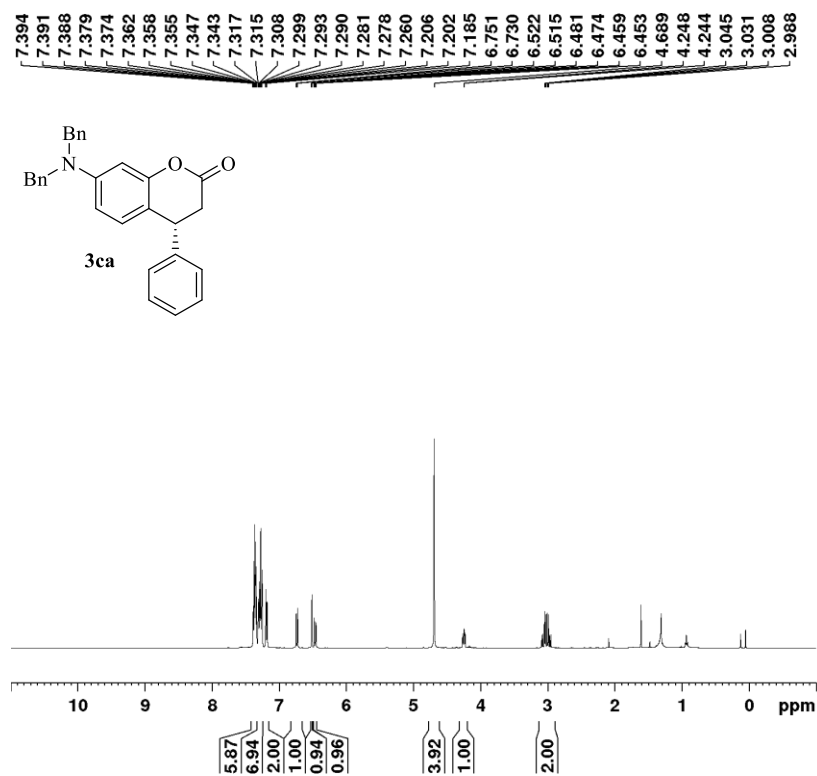
Current Data Parameters  
 NAME GYY  
 EXPNO 149  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220804  
 Time 20.37  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 88  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 213.76  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.8 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 100.6228293 MHz  
 NUC1 13C  
 P1 10.15 usec  
 PLW1 76.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.1316005 MHz  
 NUC2 1H  
 CPDPRG[2] waitz16  
 PCPD2 80.00 usec  
 PLW2 16.00000000 W  
 PLW12 0.23184000 W  
 PLW13 0.14838000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6127615 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



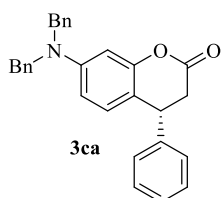
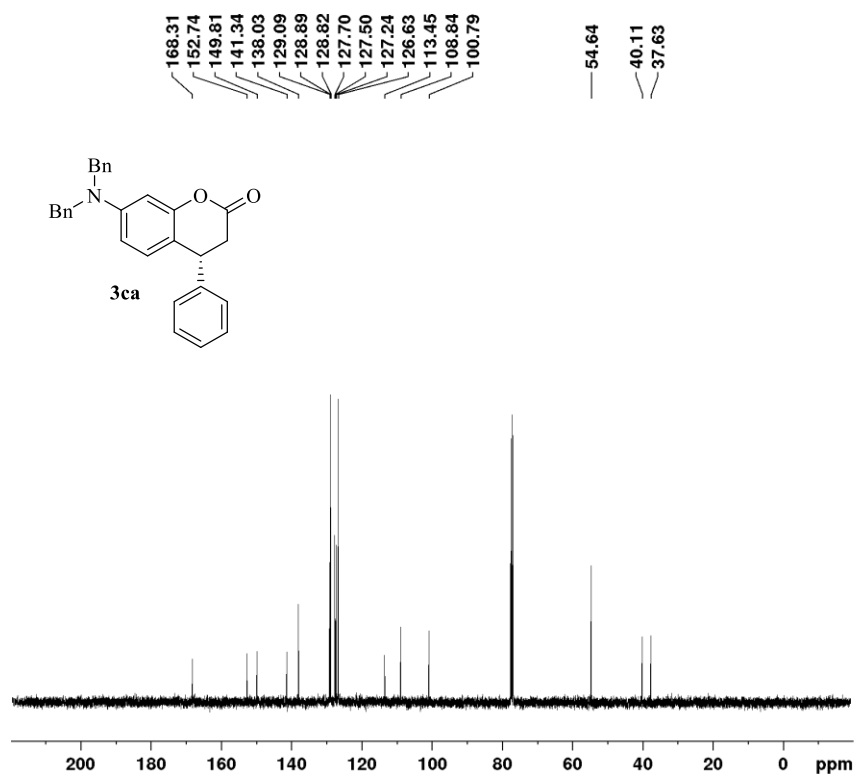
Current Data Parameters  
NAME gyy-sq  
EXPNO 213  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220928  
Time 17.38  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 12  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 71.56  
DW 62.400 usec  
DE 6.50 usec  
TE 298.1 K  
D1 1.00000000 sec  
D11 0 sec  
TDO 1

===== CHANNEL f1 =====  
SFO1 400.1324710 MHz  
NUC1 1H  
P1 9.63 usec  
PLW1 16.00000000 W

===== CHANNEL f2 =====  
SFO2 400.1324710 MHz  
NUC2 off  
CPDPRG2  
PCPD2 0 usec  
PLW2 0 W  
PLW12 0 W  
PLW13 0 W

F2 - Processing parameters  
SI 6536  
SF 400.1299981 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



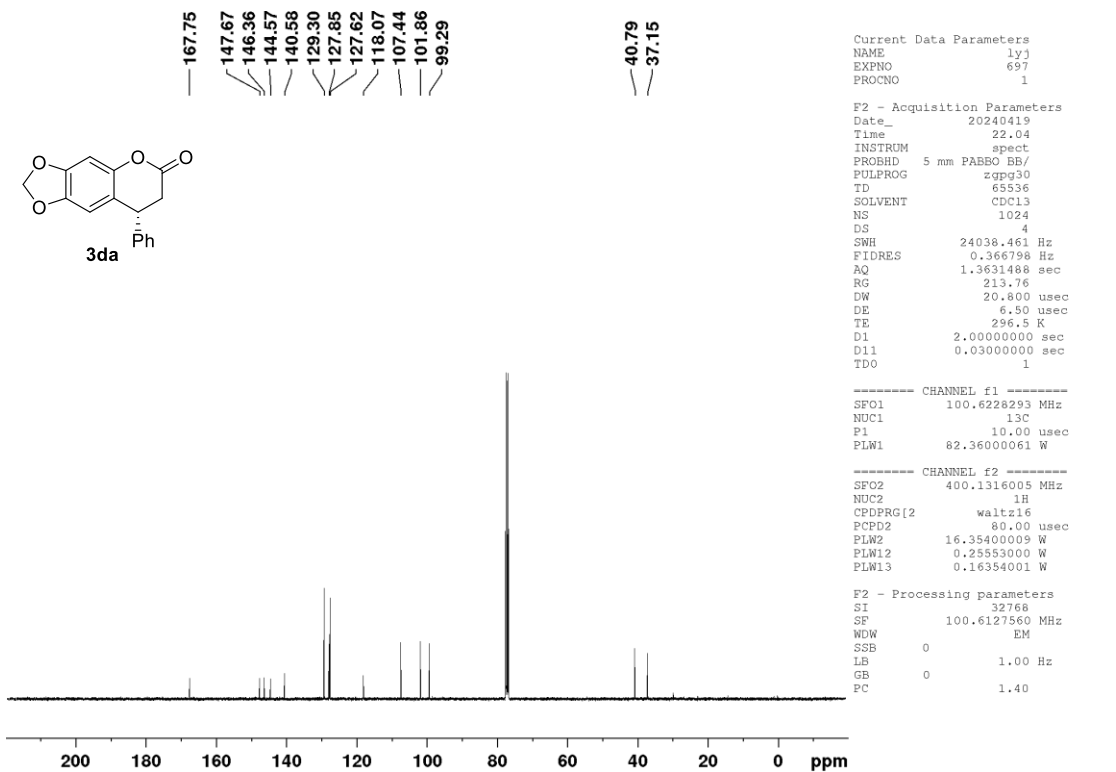
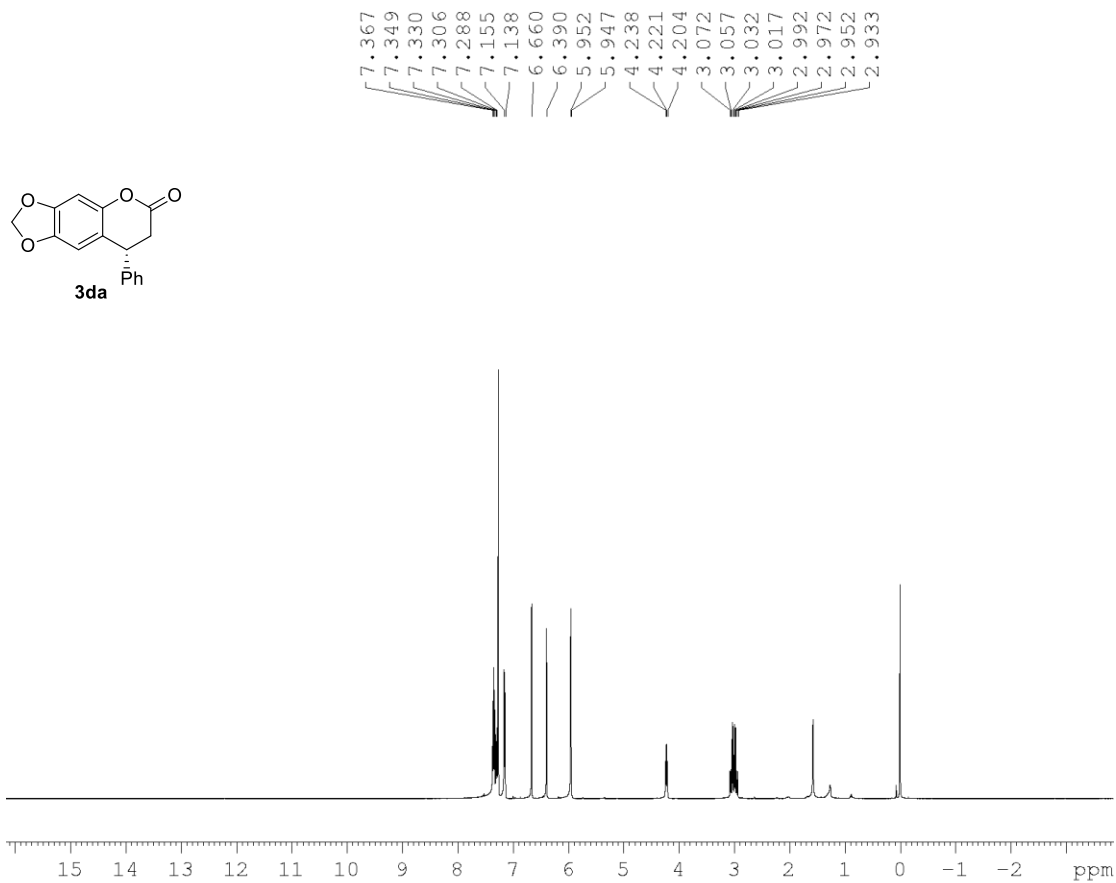
Current Data Parameters  
NAME GYY  
EXPNO 214  
PROCNO 1

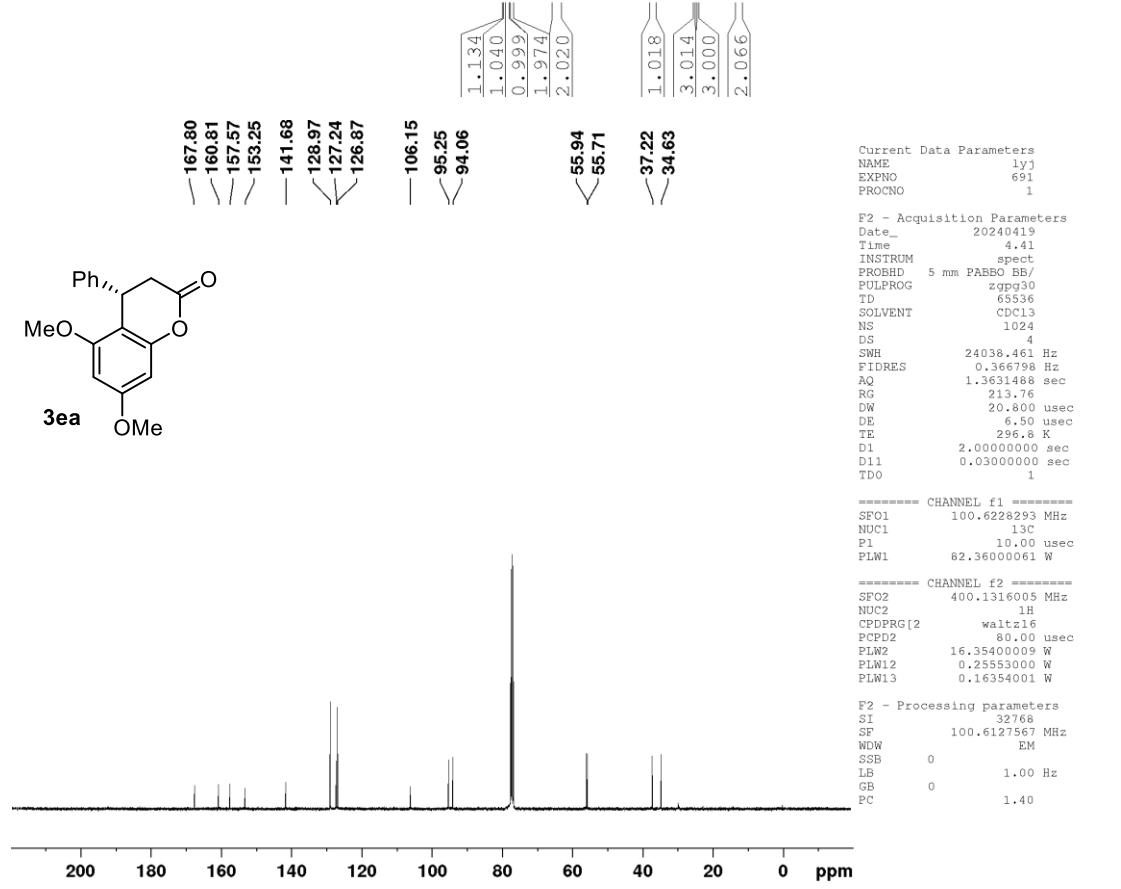
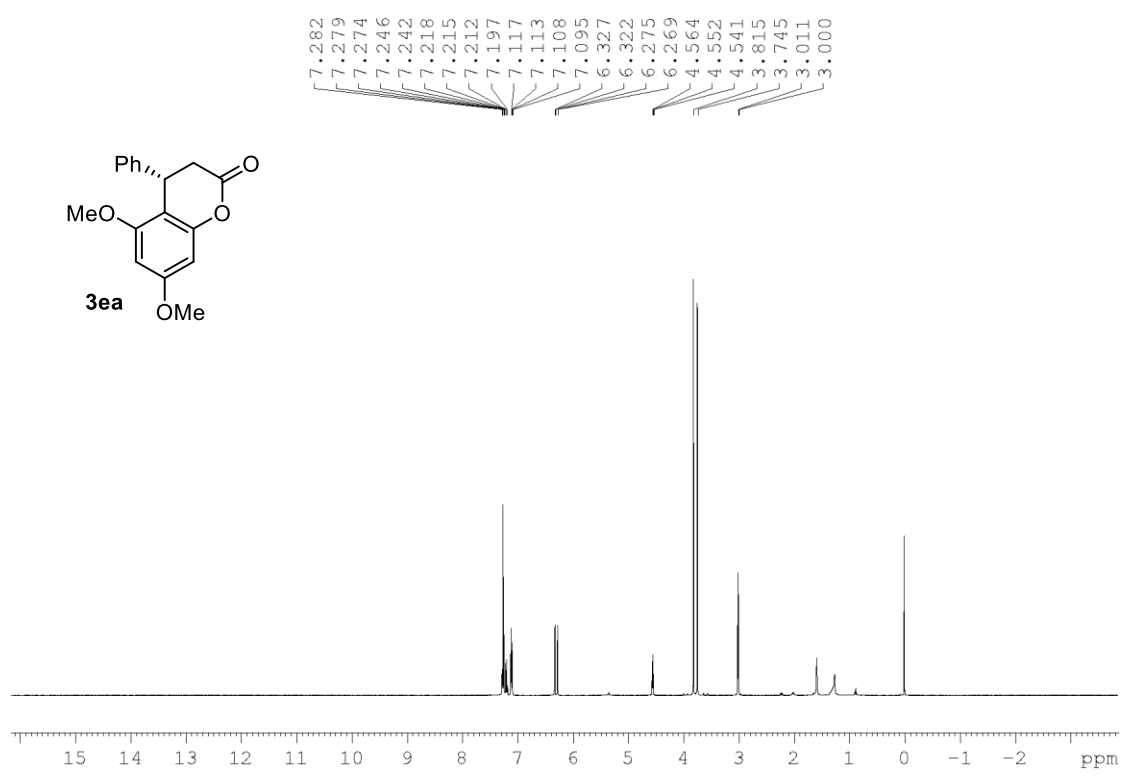
F2 - Acquisition Parameters  
Date\_ 20220928  
Time 17.40  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 47  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 213.76  
DW 20.800 usec  
DE 6.50 usec  
TE 298.5 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

===== CHANNEL f1 =====  
SFO1 100.6228293 MHz  
NUC1 13C  
P1 10.15 usec  
PLW1 76.00000000 W

===== CHANNEL f2 =====  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG2 waitz16  
PCPD2 80.00 usec  
PLW2 16.00000000 W  
PLW12 0.23184000 W  
PLW13 0.14838000 W

F2 - Processing parameters  
SI 32768  
SF 100.6127589 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





Current Data Parameters  
 NAME lyj  
 EXPNO 691  
 PROCNO 1

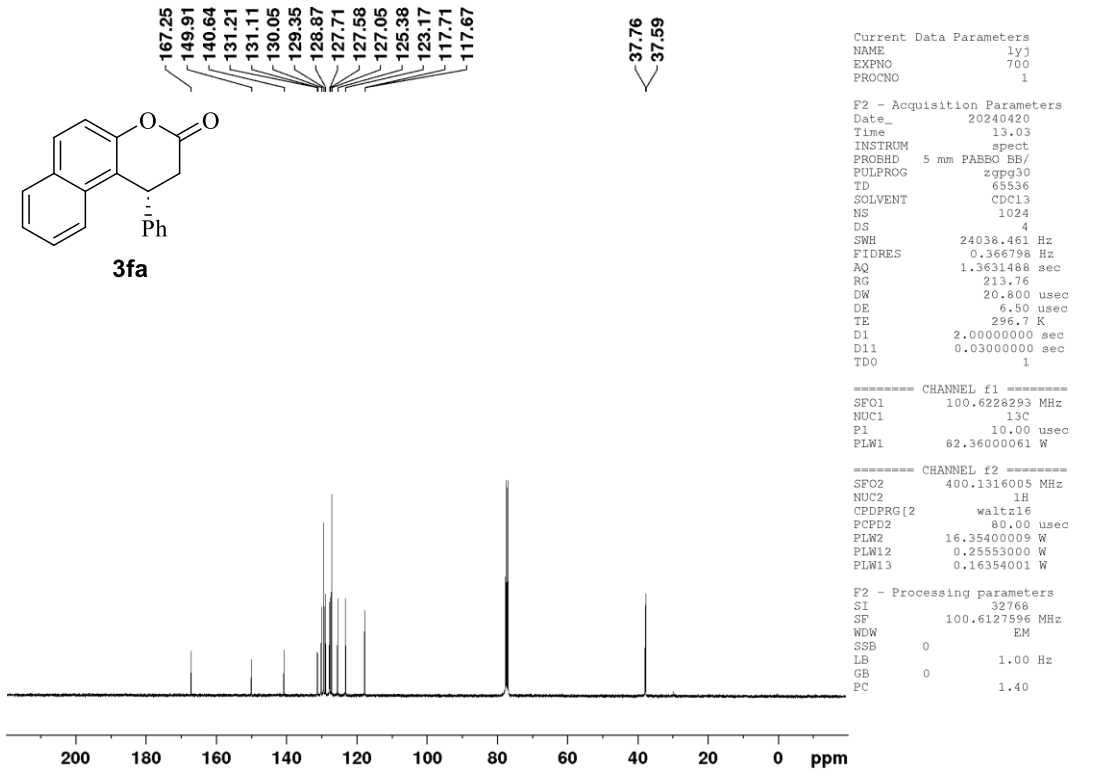
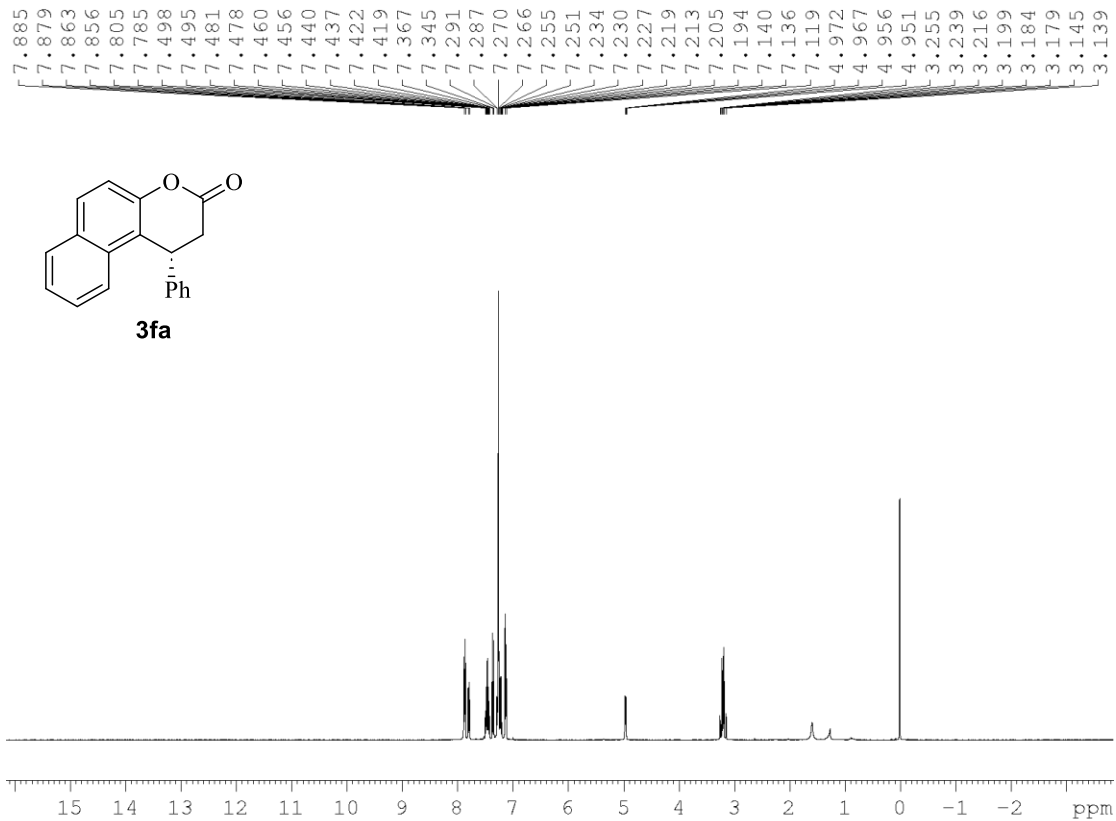
F2 - Acquisition Parameters  
 Date\_ 20240419  
 Time 4.41  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1024  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 213.76  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.8 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 100.6228293 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 62.3600061 W

===== CHANNEL f2 =====  
 SFO2 400.1316005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 80.00 usec  
 PLW2 16.35400009 W  
 PLW12 0.25553000 W  
 PLW13 0.16354001 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6127567 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40





Current Data Parameters

NAME lyj  
 EXPNO 700  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20240420  
 Time 13.03  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1024  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 213.76  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.7 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TDO 1

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

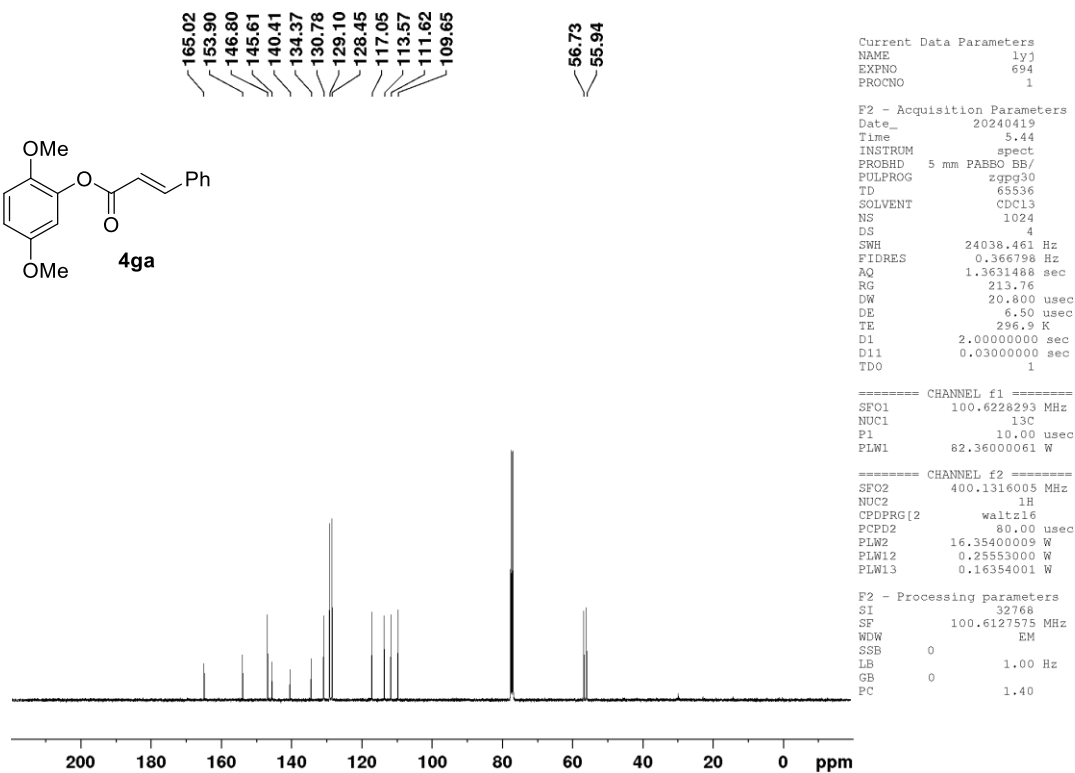
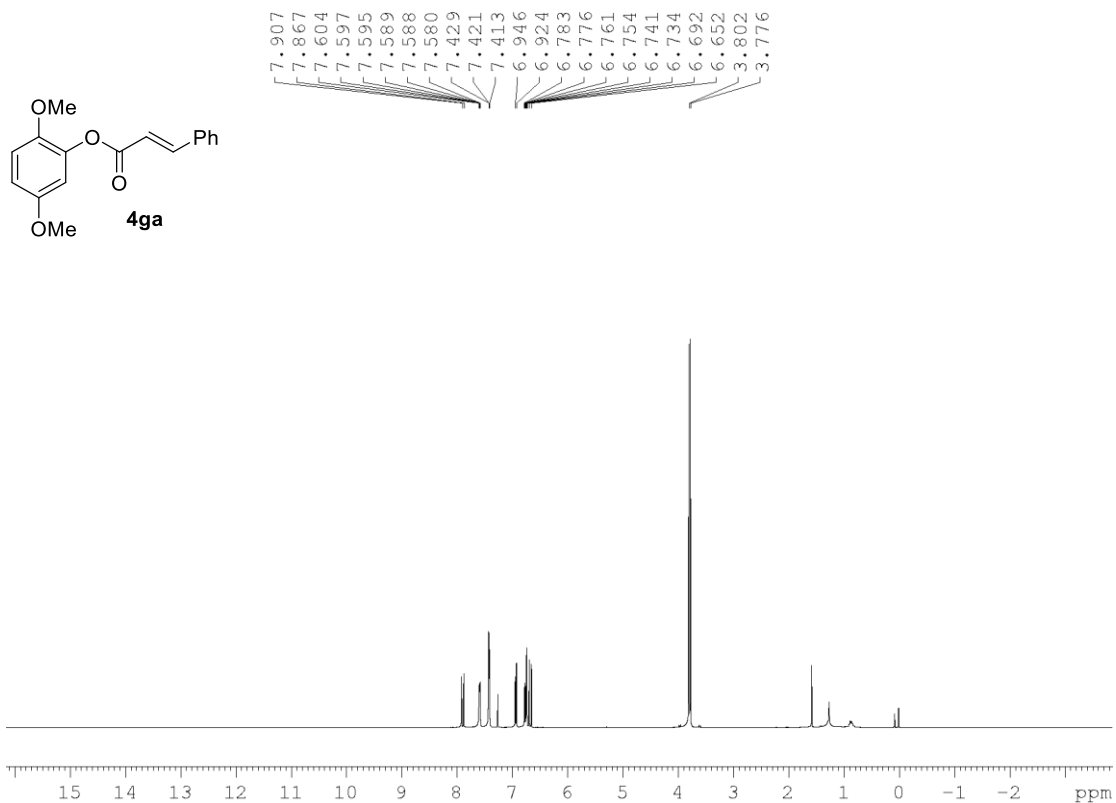
SFO1 100.6228293 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 62.3600061 W

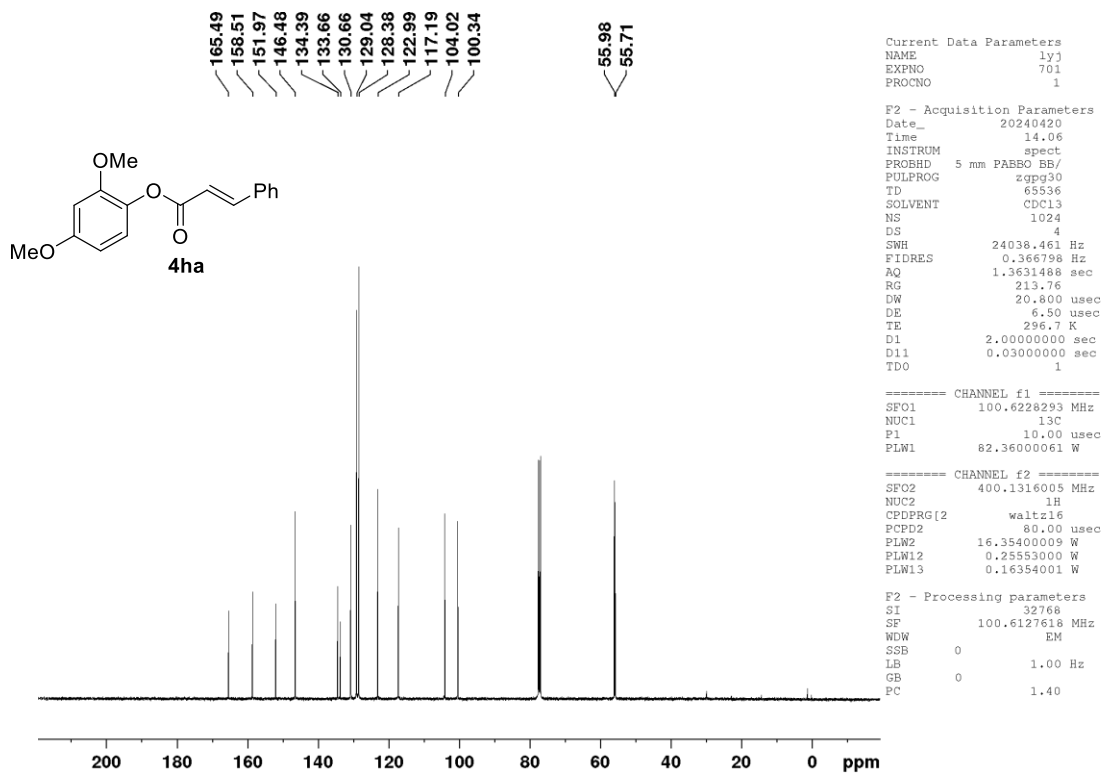
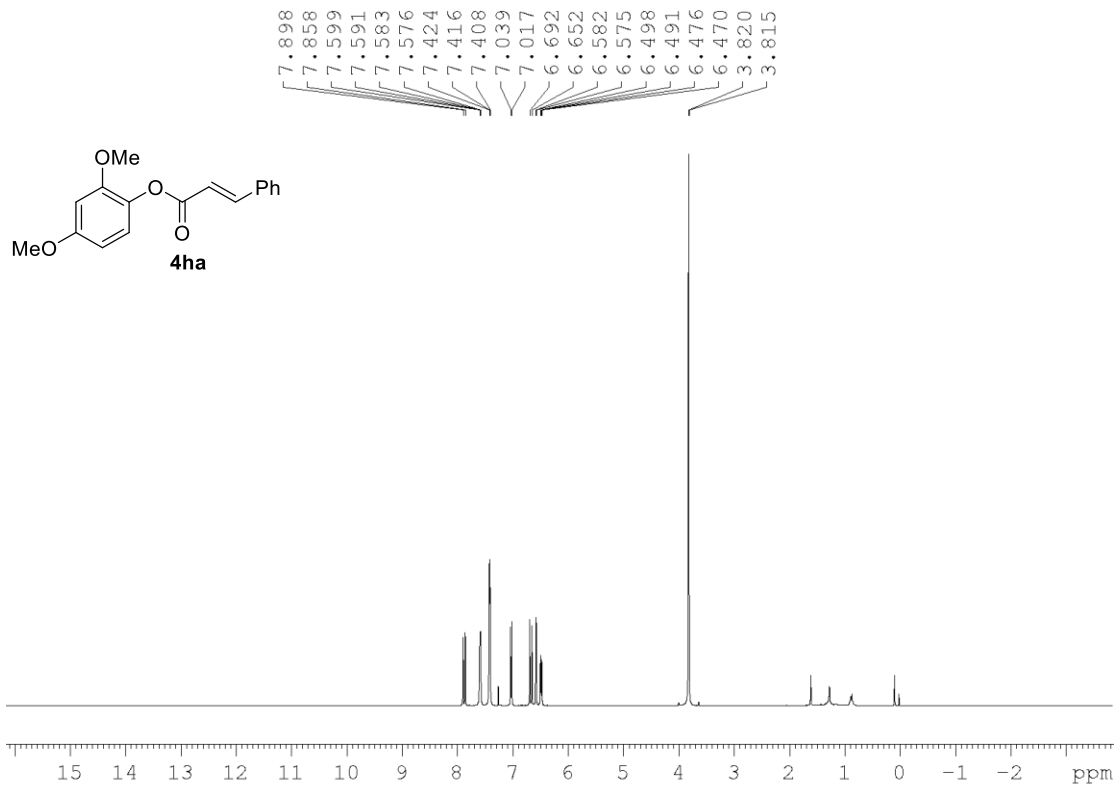
===== CHANNEL f2 =====

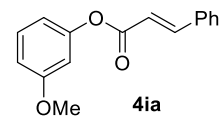
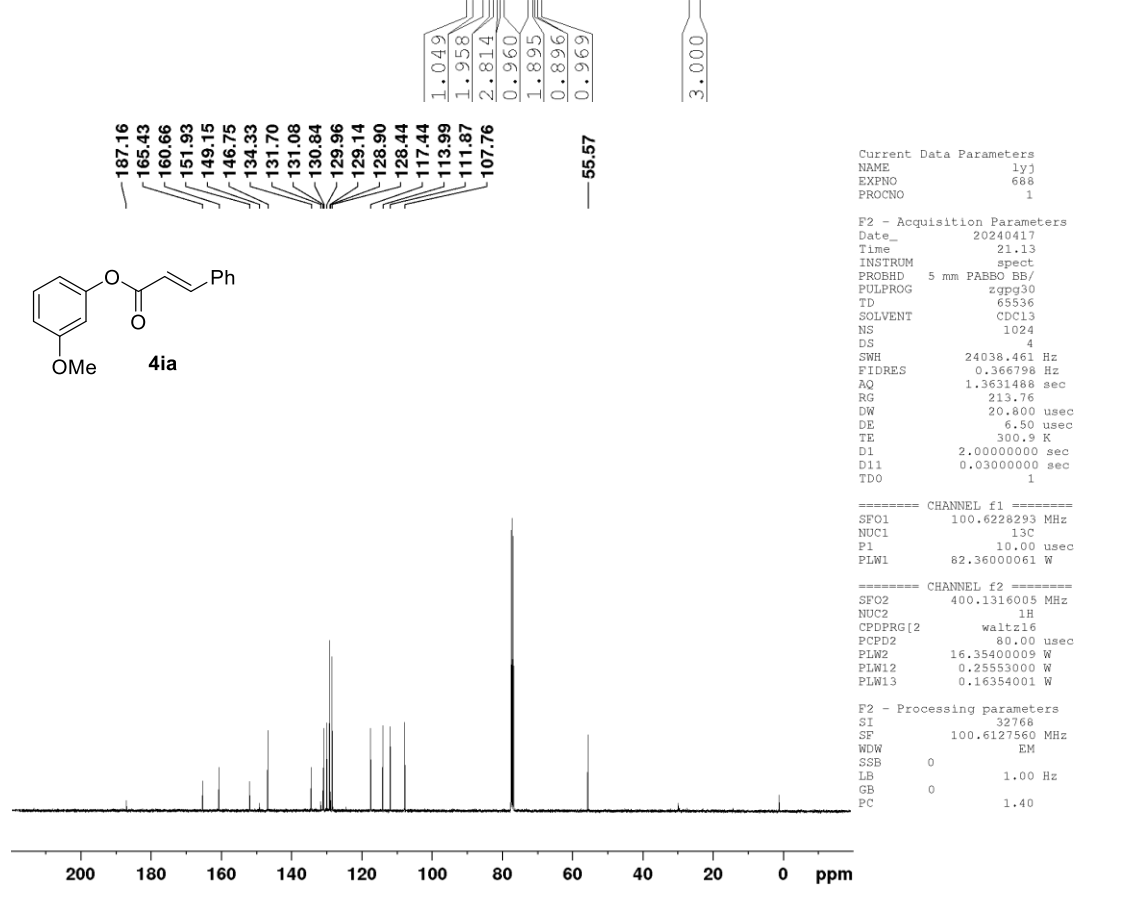
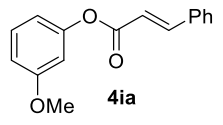
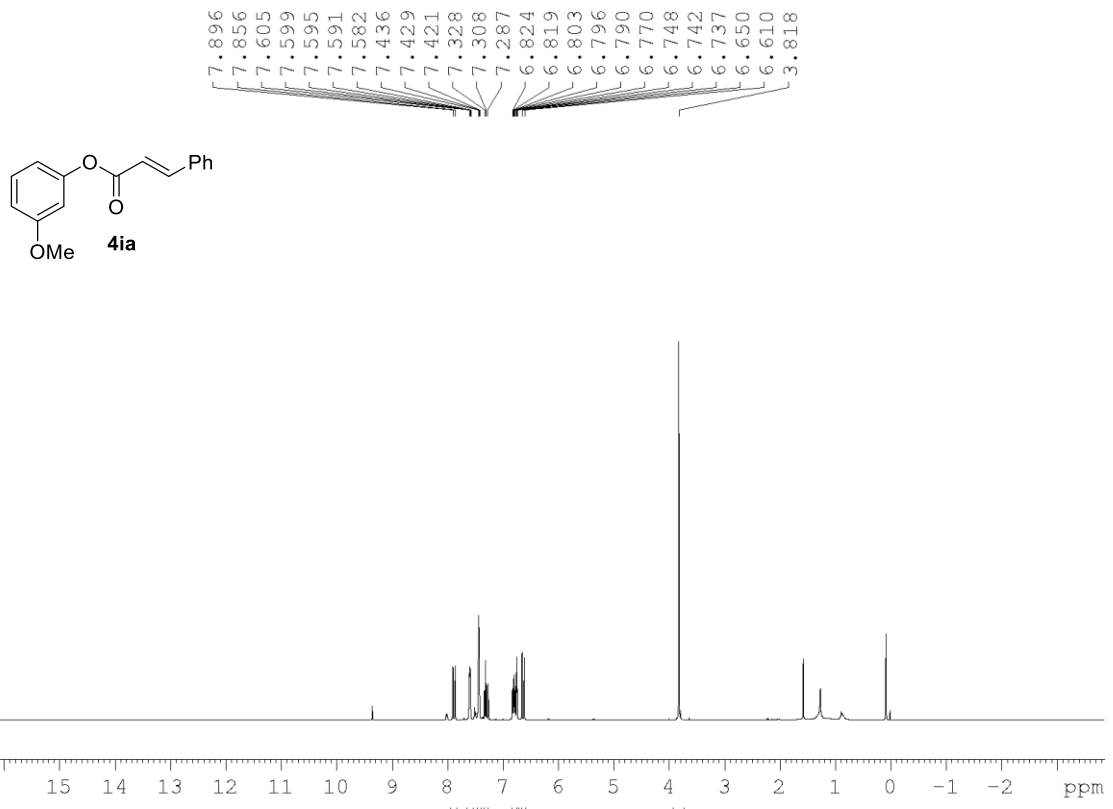
SFO2 400.1316005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 80.00 usec  
 PLW2 16.35400009 W  
 PLW12 0.25553000 W  
 PLW13 0.16354001 W

F2 - Processing parameters

SI 32768  
 SF 100.6127596 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40







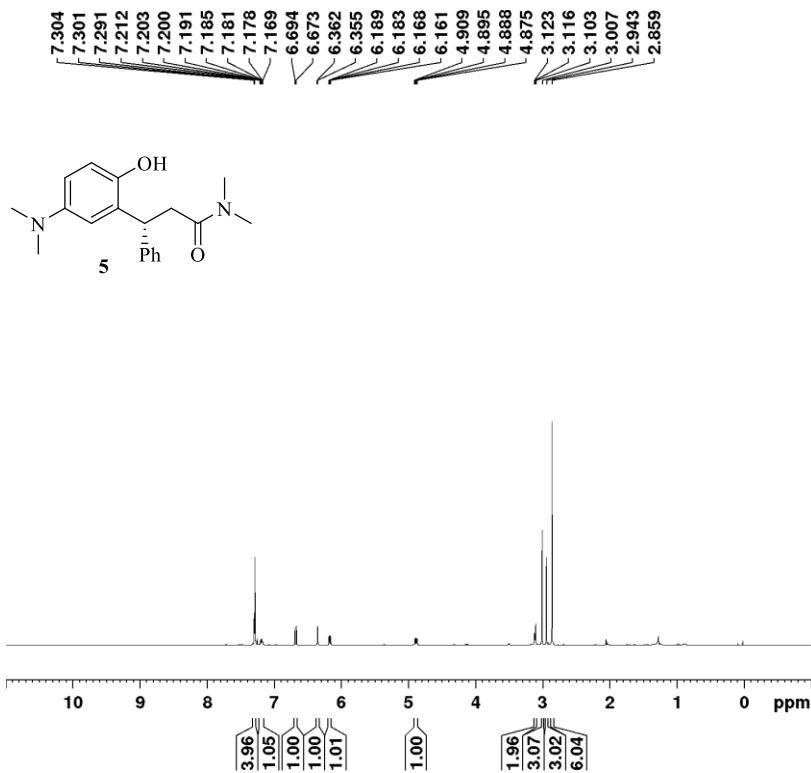
Current Data Parameters  
 NAME lyj  
 EXPNO 688  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20240417  
 Time 21.13  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1024  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 213.76  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 300.9 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 SFO1 100.6228293 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 82.36000061 W

==== CHANNEL f2 =====  
 SFO2 400.1316005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPDZ 80.00 usec  
 PLW2 16.35400009 W  
 PLW12 0.25553000 W  
 PLW13 0.16354001 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6127560 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



```

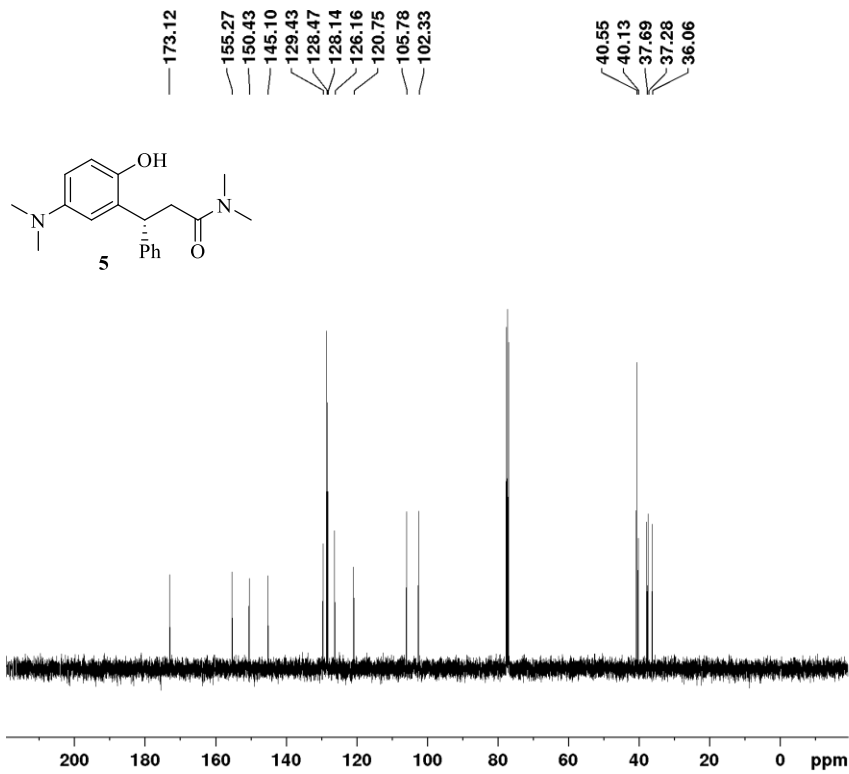
Current Data Parameters
NAME          GYY
EXPNO         215
PROCNO        1

F2 - Acquisition Parameters
Date_         20220928
Time          19.50
INSTRUM       spect
PROBHD        5 mm PABBO BB/
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            11
DS            2
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894465 sec
RG            31.77
DW            62.400 usec
DE            6.50 usec
TE            297.5 K
D1            1.00000000 sec
D11           0 sec
TD0           1

===== CHANNEL f1 =====
SFO1          400.1324710 MHz
NUC1          1H
P1            9.63 usec
PLW1          16.00000000 W

===== CHANNEL f2 =====
SFO2          400.1324710 MHz
NUC2          off
CPDPRG[2]
PCPD2         0 usec
PLW2          0 W
PLW12         0 W
PLW13         0 W

F2 - Processing parameters
SI            65536
SF            400.1300099 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```



```

Current Data Parameters
NAME          GYY
EXPNO         216
PROCNO        1

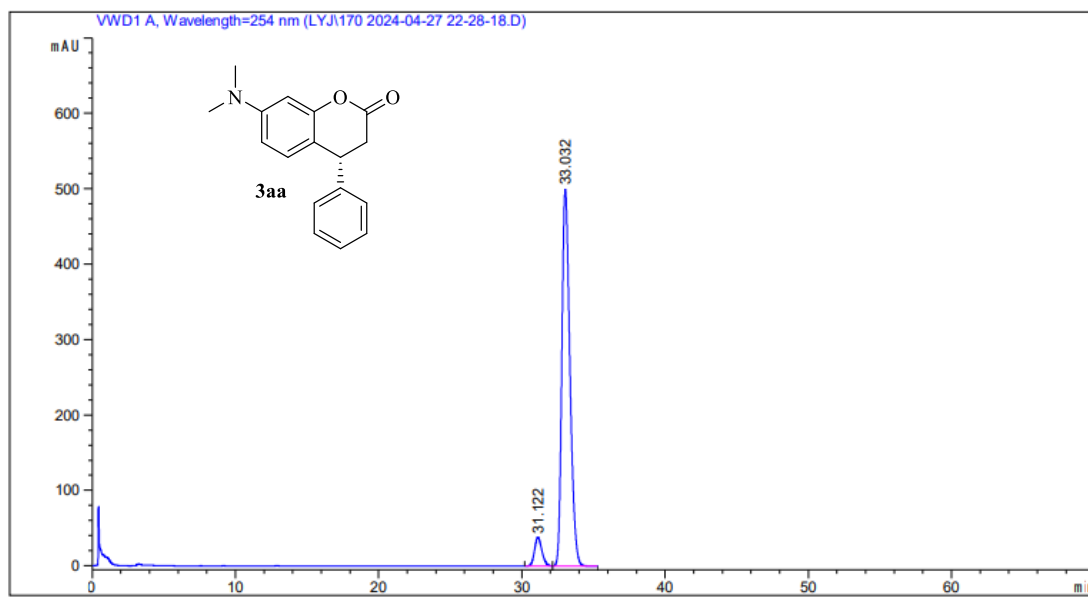
F2 - Acquisition Parameters
Date_         20220928
Time          20.03
INSTRUM       spect
PROBHD        5 mm PABBO BB/
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            18
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG            213.76
DW            20.800 usec
DE            6.50 usec
TE            297.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

===== CHANNEL f1 =====
SFO1          100.6228293 MHz
NUC1          13C
P1            10.15 usec
PLW1          76.00000000 W

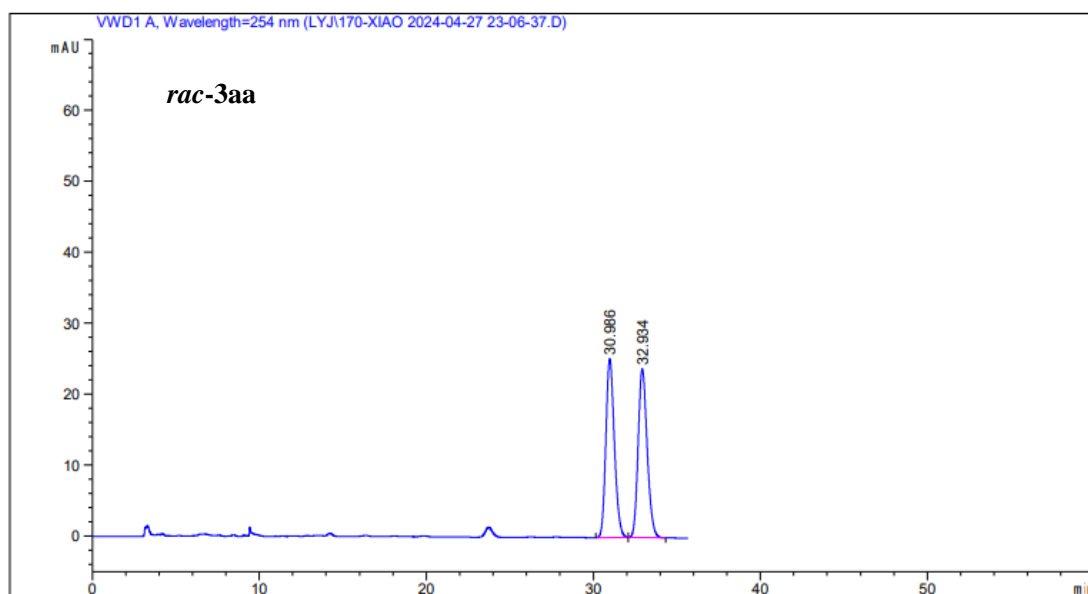
===== CHANNEL f2 =====
SFO2          400.1316005 MHz
NUC2          1H
CPDPRG[2]     waltz16
PCPD2         80.00 usec
PLW2          16.00000000 W
PLW12         0.23184000 W
PLW13         0.14838000 W

F2 - Processing parameters
SI            32768
SF            100.6127626 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```

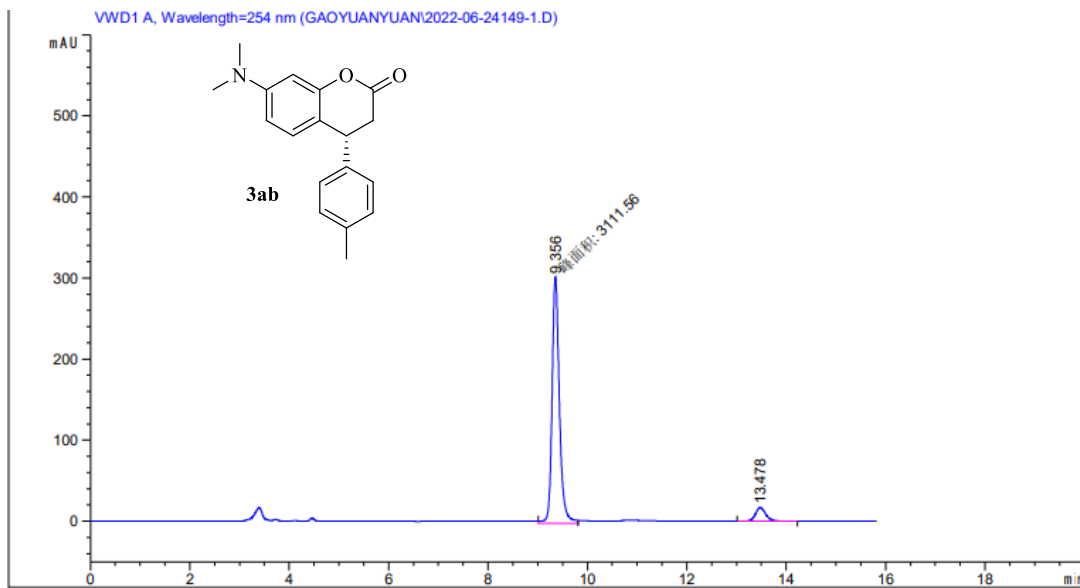
## 6. HPLC Charts of Chiral Products



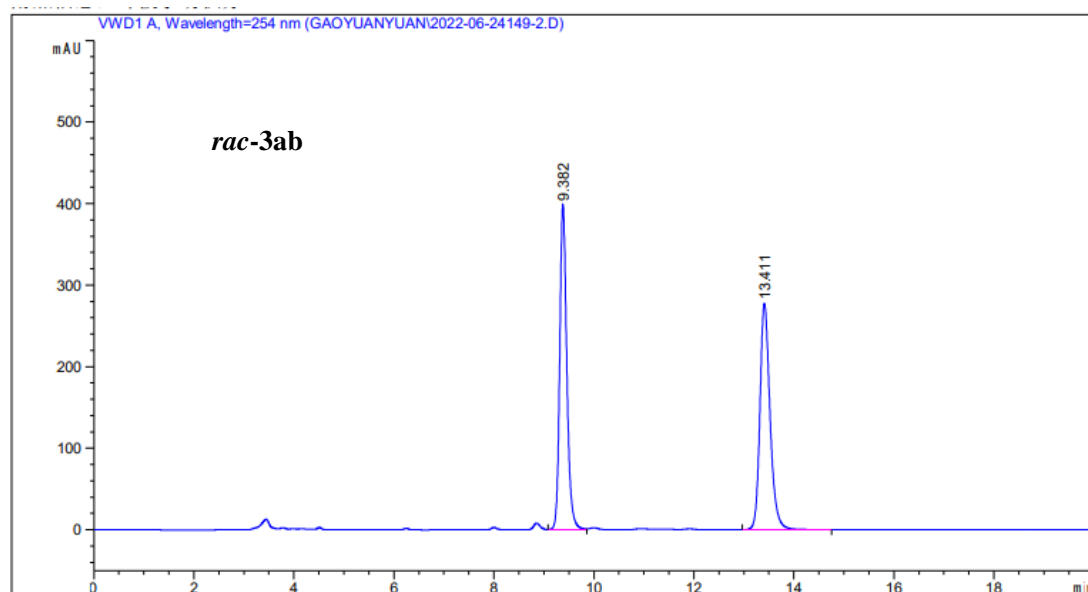
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	31.122	BB	0.5465	1357.86938	38.22024	6.5112
2	33.032	BB	0.6004	1.94966e4	499.52481	93.4888



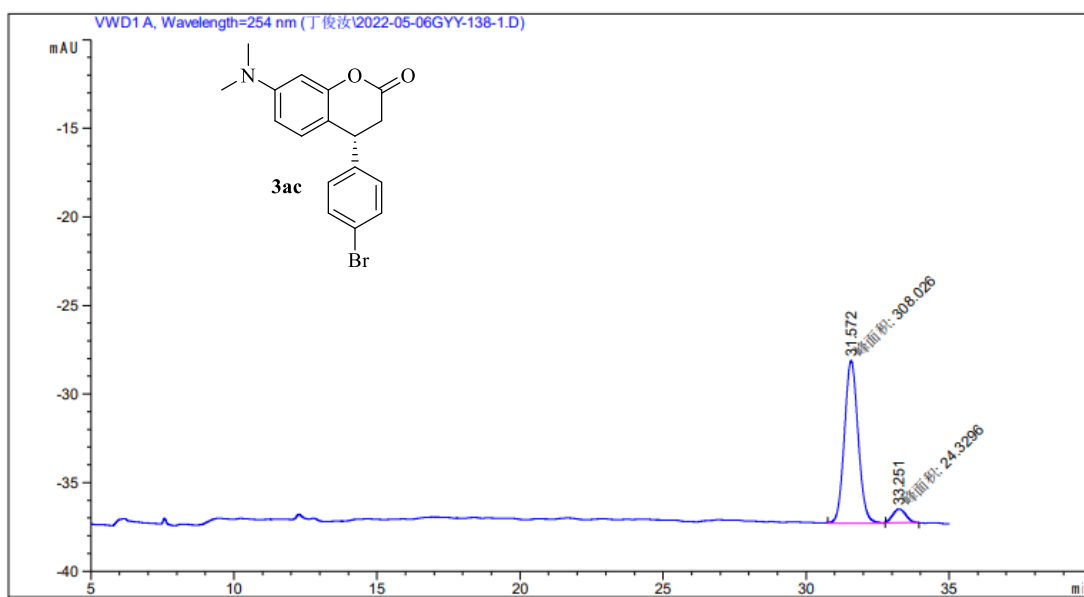
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	30.986	BB	0.5454	892.83173	25.19432	49.9582
2	32.934	BB	0.5776	894.32654	23.78979	50.0418



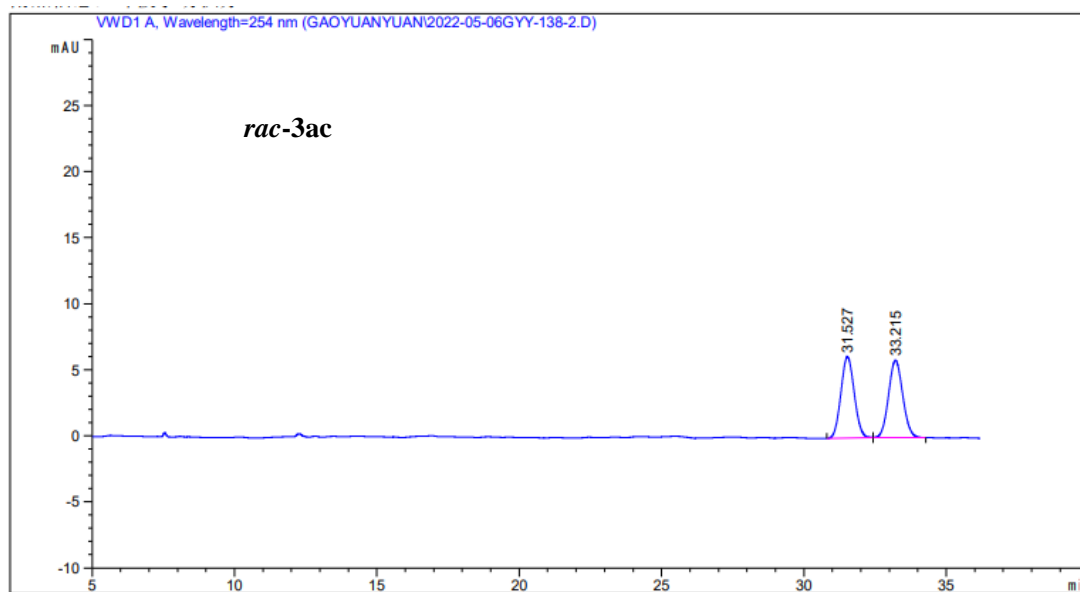
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.356	MM	0.1707	3111.56323	303.85941	92.7665
2	13.478	BB	0.2182	242.62592	16.92815	7.2335



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.382	VV	0.1497	3921.19727	398.75150	50.1569
2	13.411	BB	0.2127	3896.65723	277.64203	49.8431

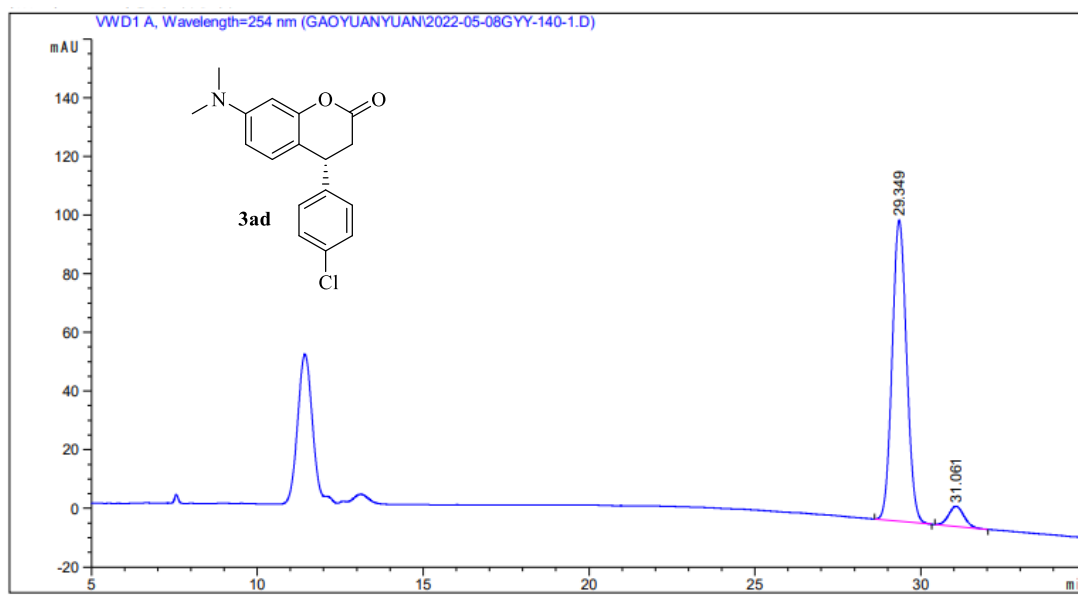


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	31.572	MM	0.5585	308.02609	9.19260	92.6796
2	33.251	MM	0.5256	24.32961	7.71558e-1	7.3204

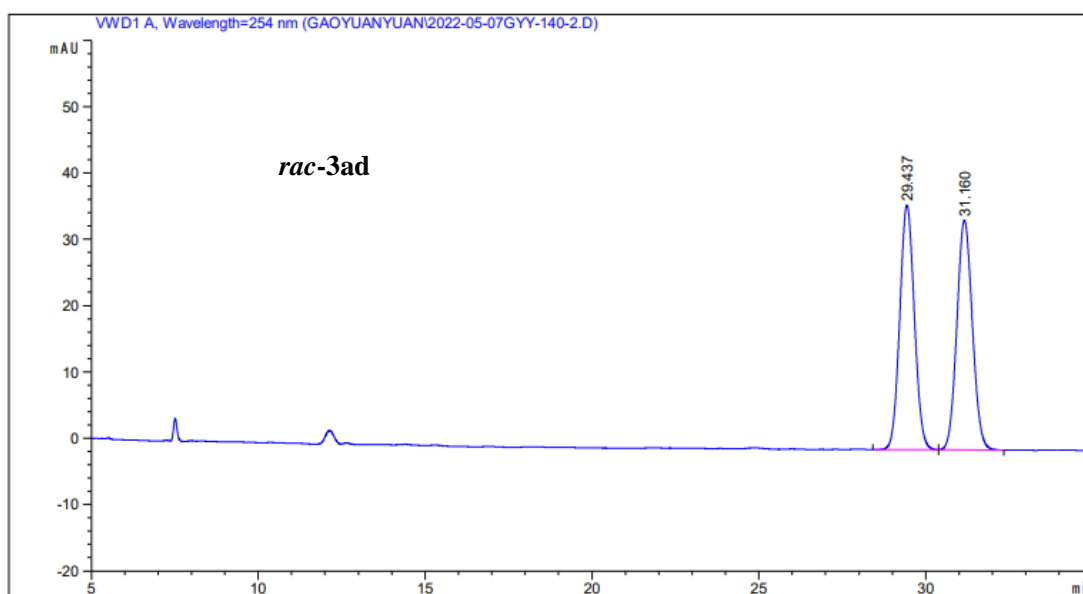


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	31.527	BB	0.5060	200.21280	6.14648	49.8168
2	33.215	BB	0.5330	201.68523	5.83816	50.1832

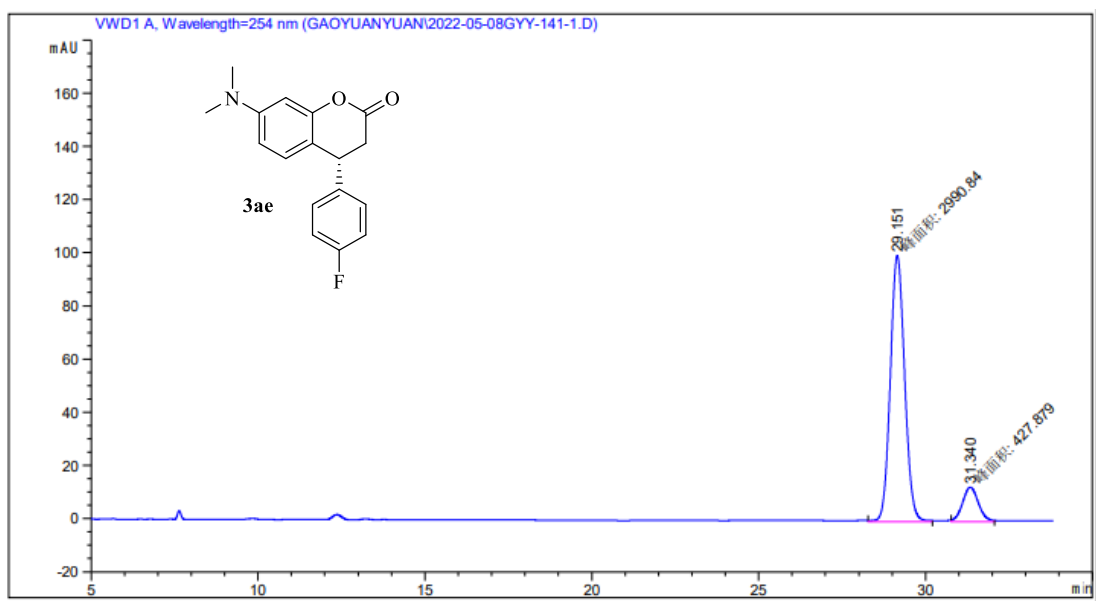




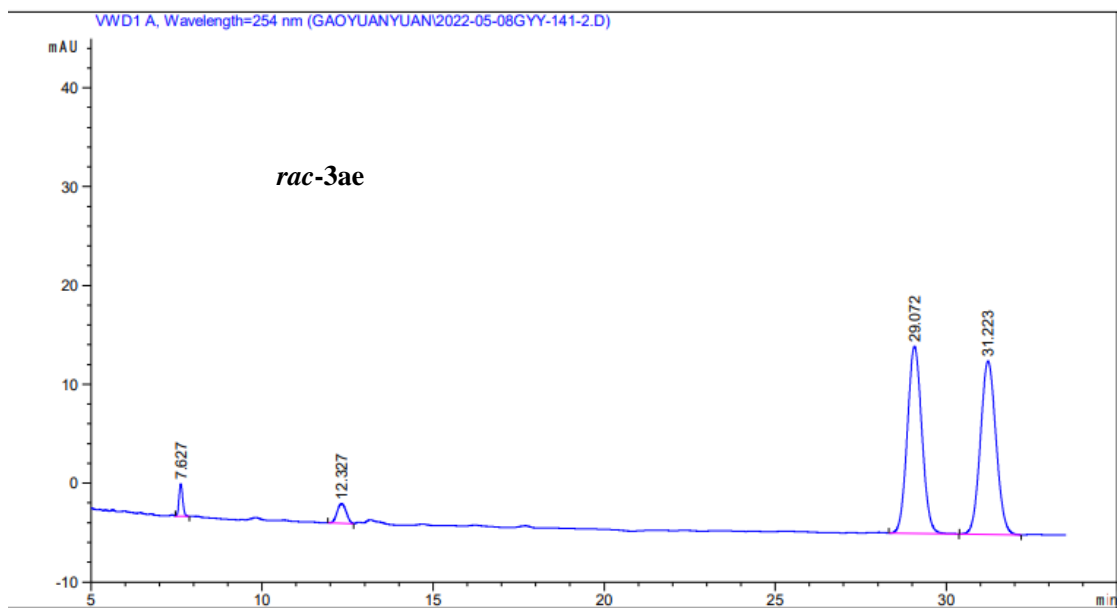
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	29.349	BB	0.4719	3104.30347	102.62521	93.4285
2	31.061	BBA	0.4957	218.34731	6.83510	6.5715



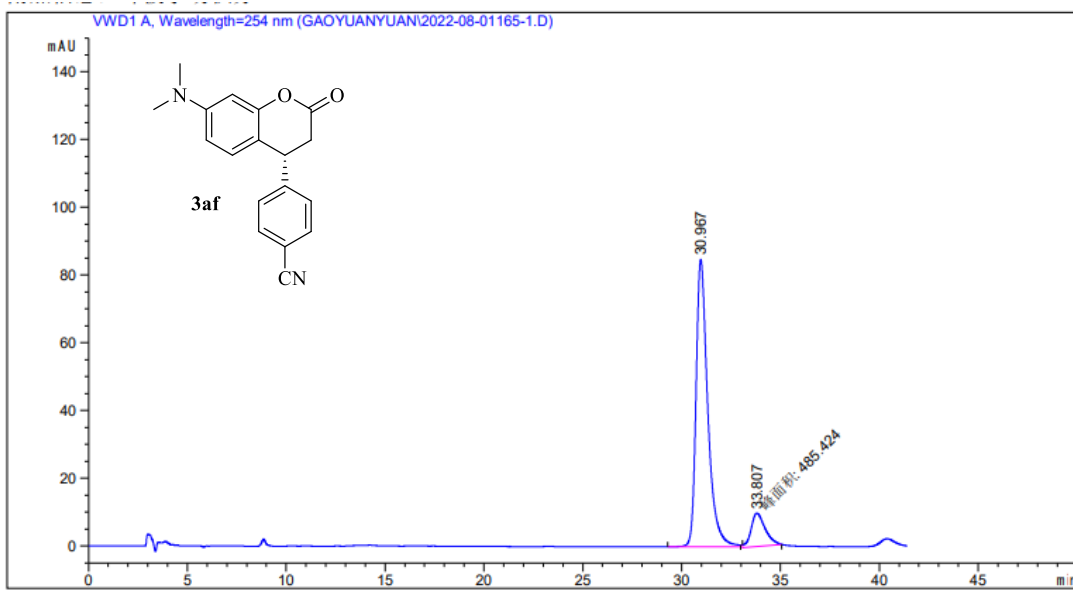
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	29.437	BB	0.4742	1122.75598	36.87444	50.0743
2	31.160	BB	0.5044	1119.42468	34.60501	49.9257



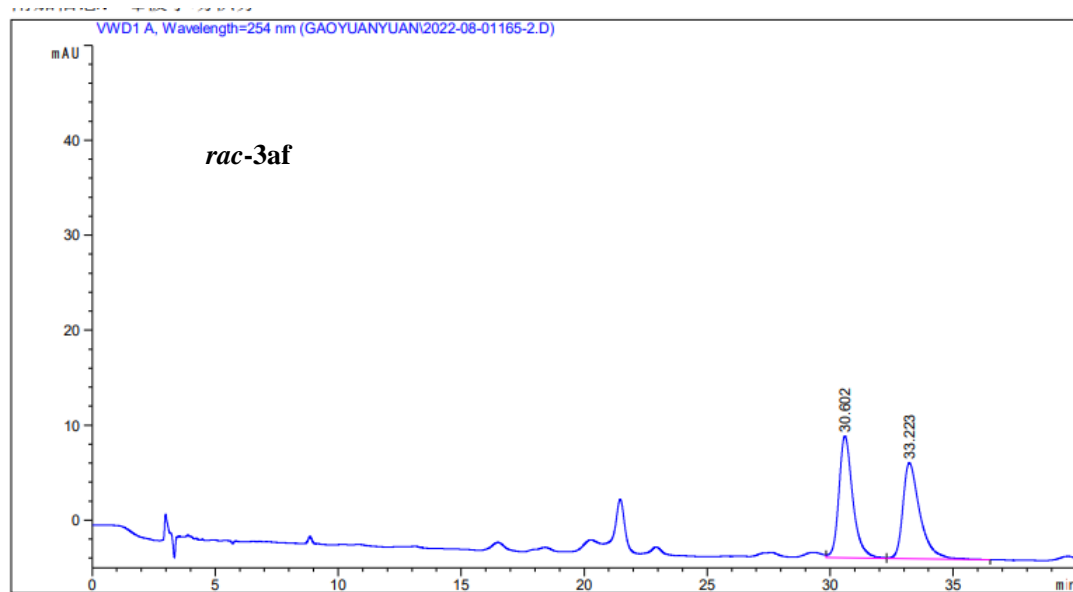
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	29.151	MM	0.4987	2990.83813	99.96323	87.4842
2	31.340	MM	0.5511	427.87927	12.94122	12.5158



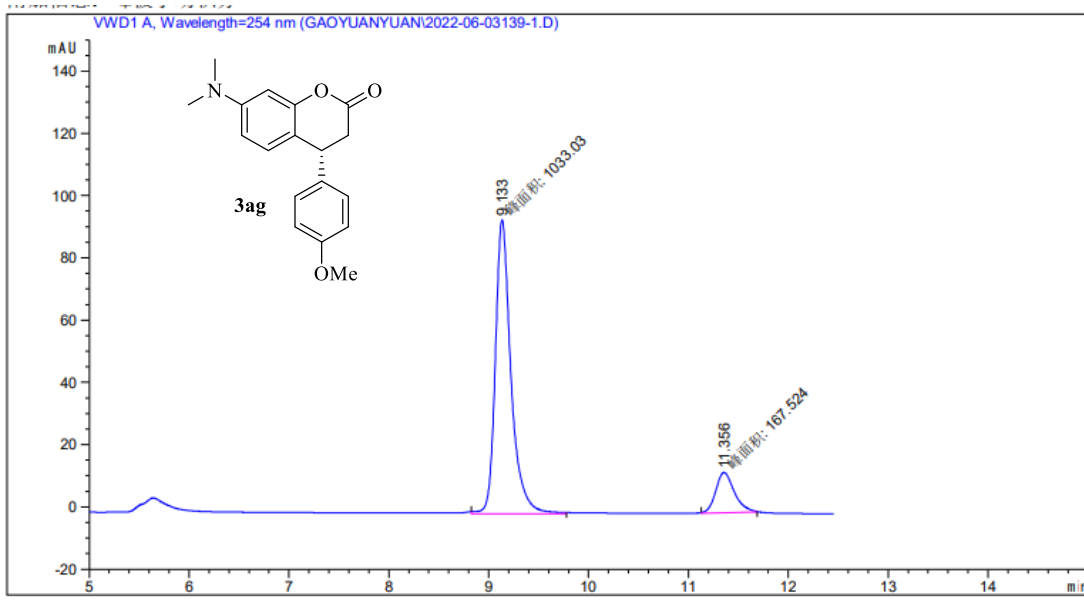
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
3	29.072	BB	0.4604	558.53485	18.92244	47.5208
4	31.223	BB	0.4940	556.06226	17.53439	47.3104



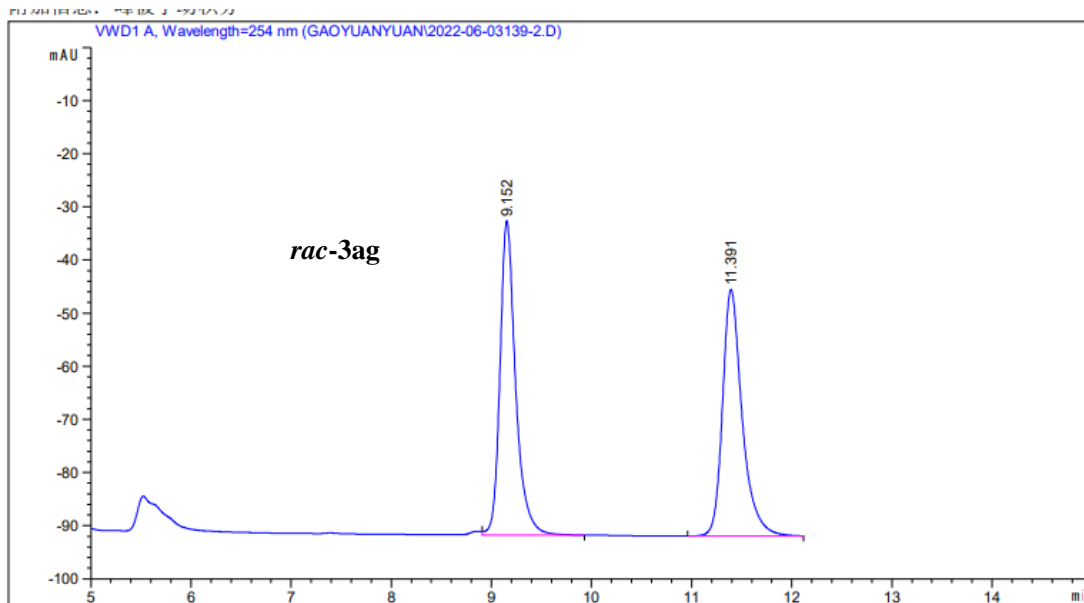
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	30.967	BV	0.6188	3479.00122	84.76335	87.7555
2	33.807	MM	0.8220	485.42407	9.84242	12.2445



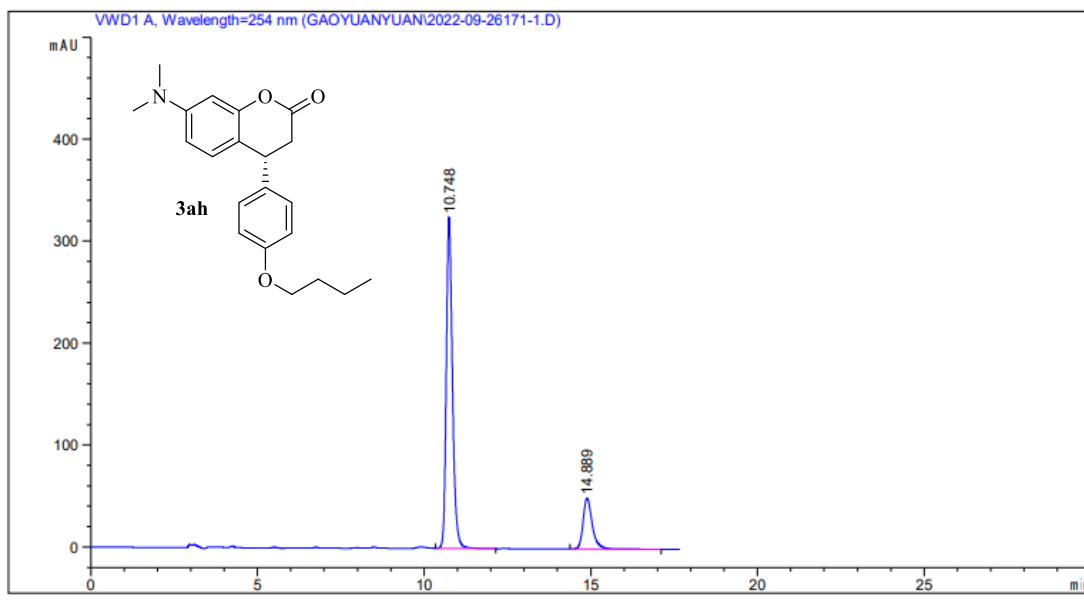
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	30.602	VV	0.5940	503.90137	12.83702	50.7590
2	33.223	VB	0.7165	488.83115	10.10299	49.2410



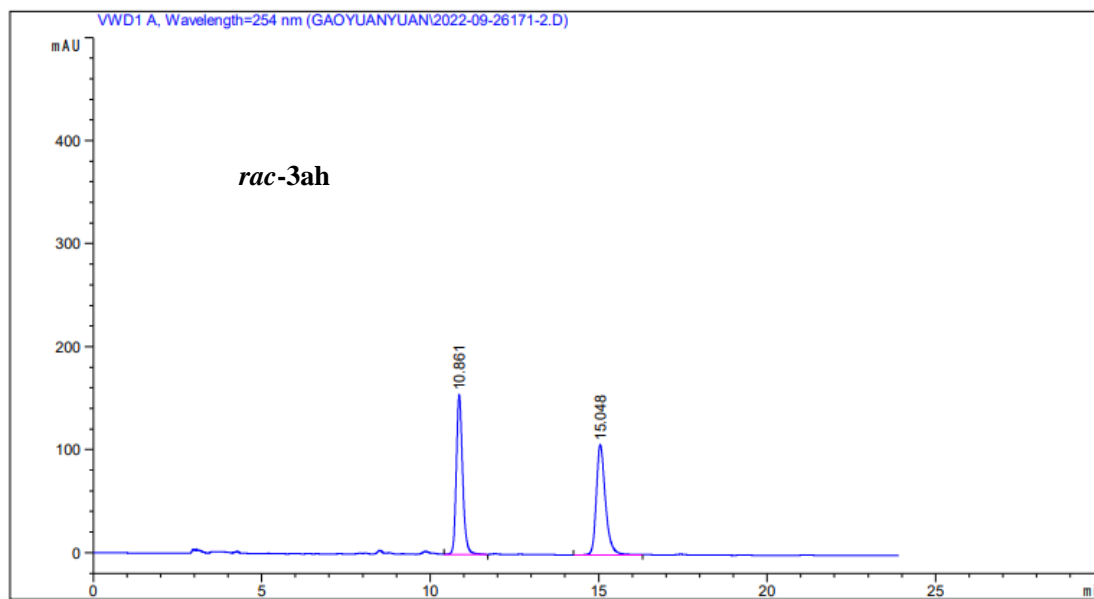
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.133	MM	0.1822	1033.02979	94.48739	86.0461
2	11.356	MM	0.2160	167.52368	12.92853	13.9539



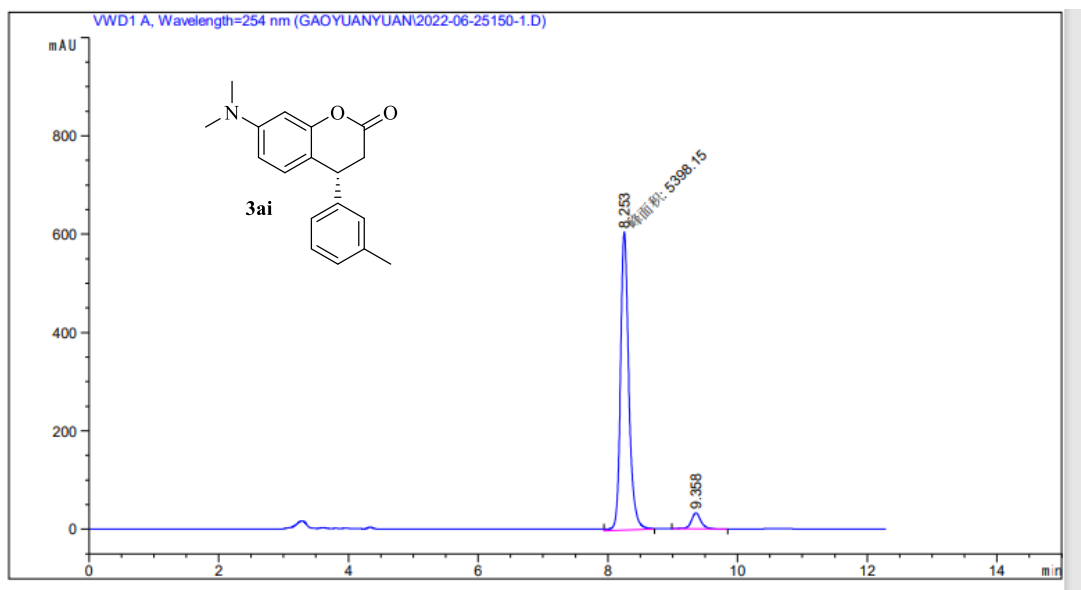
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.152	VB	0.1625	640.45966	59.07540	50.3217
2	11.391	BBA	0.2039	632.27014	46.41124	49.6783



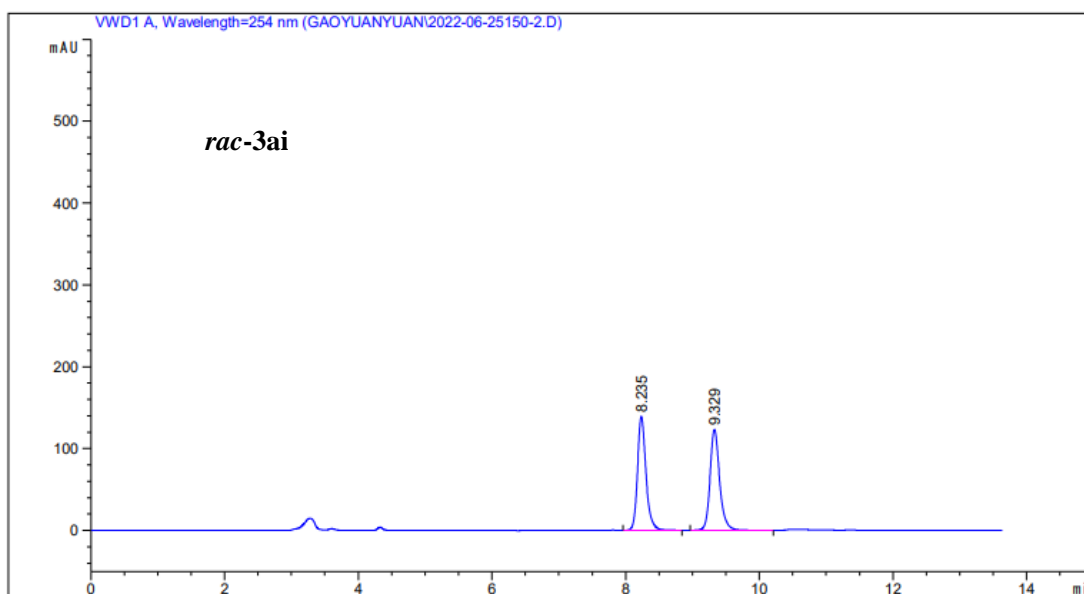
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.748	VB	0.1978	4164.28320	324.37350	81.2929
2	14.889	VB	0.2877	958.28662	49.97046	18.7071



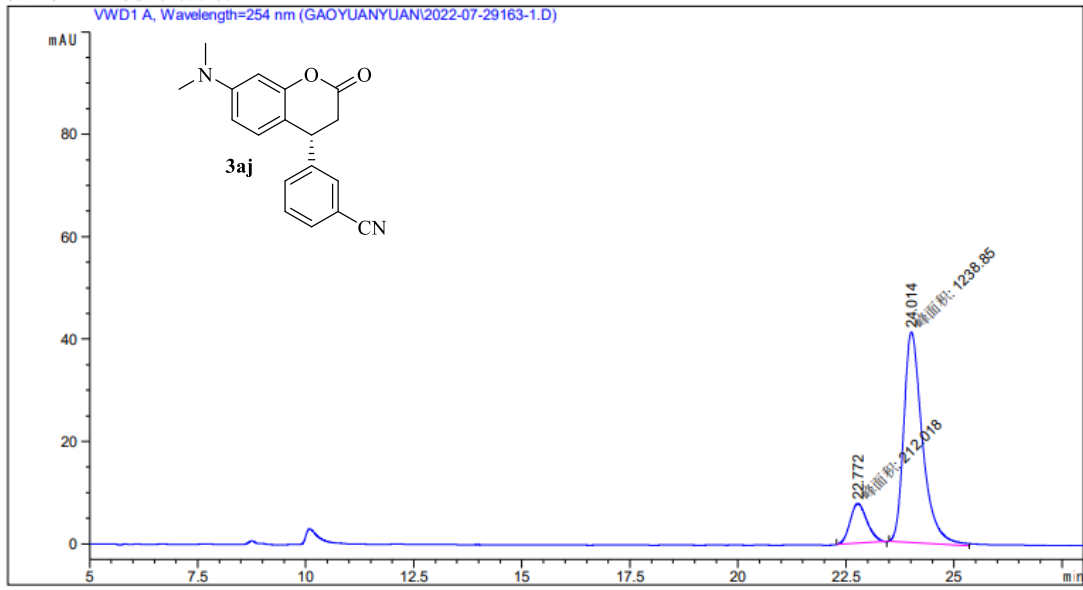
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.861	VV	0.1954	2014.46899	155.25610	49.9855
2	15.048	BV	0.2885	2015.63611	106.65786	50.0145



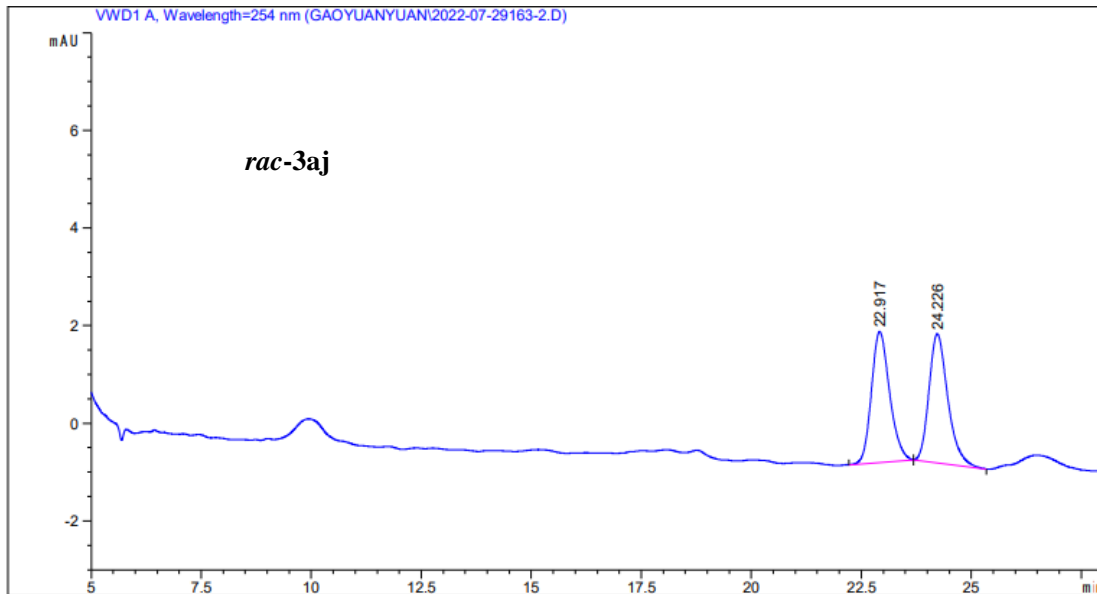
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	8.253	MM	0.1484	5398.14990	606.11841	94.1485
2	9.358	BB	0.1540	335.50391	32.62458	5.8515



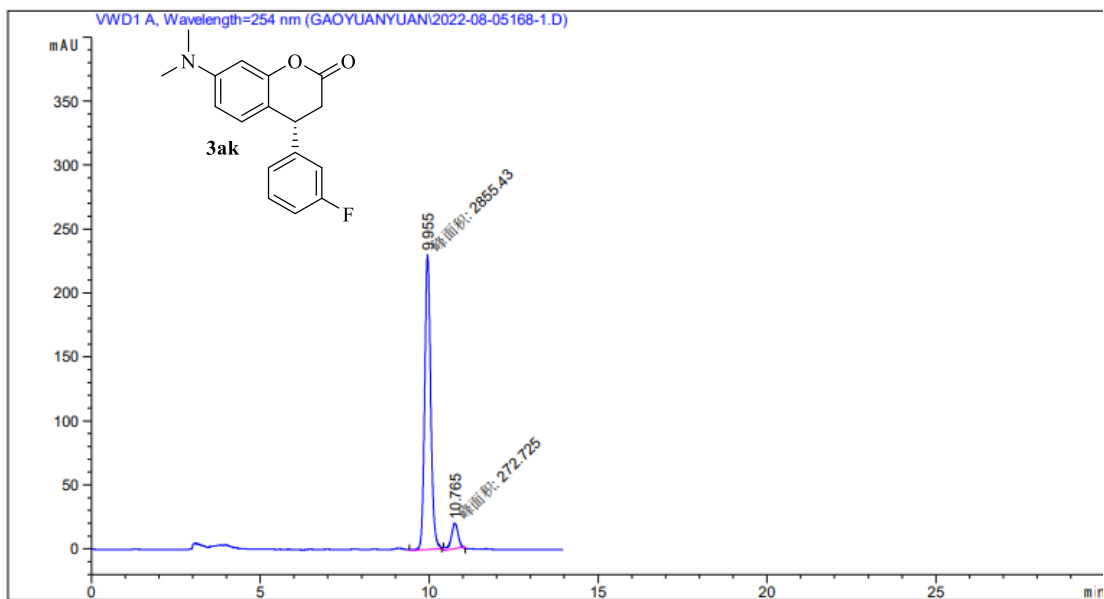
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	8.235	BB	0.1328	1225.46594	139.09288	49.8705
2	9.329	BB	0.1507	1231.83203	123.15009	50.1295



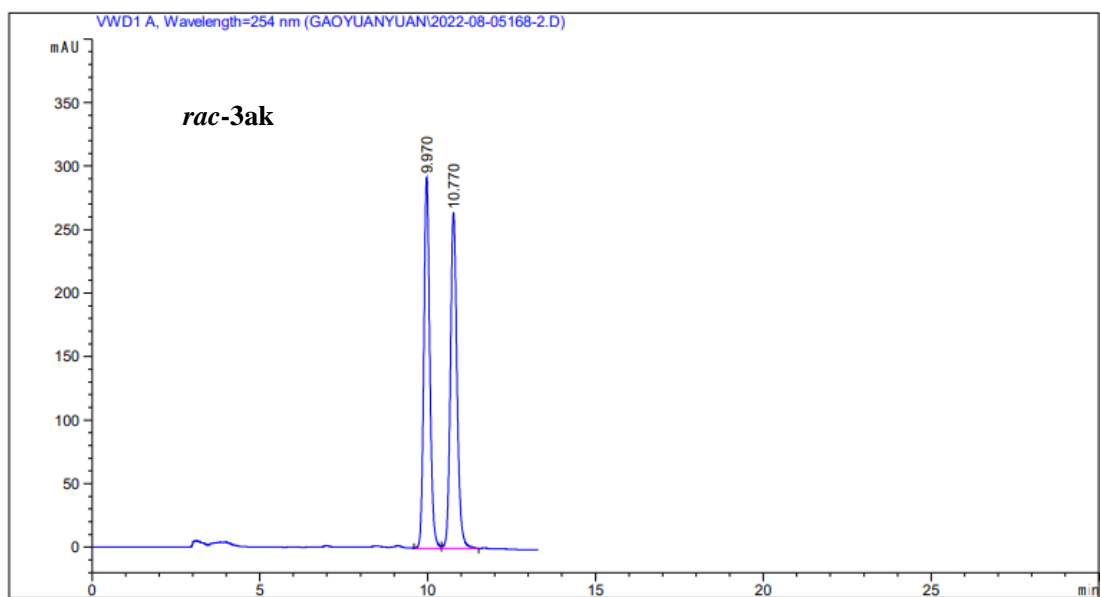
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	22.772	MM	0.4554	212.01811	7.75949	14.6132
2	24.014	MM	0.5019	1238.84705	41.13690	85.3868



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	22.917	BB	0.4394	77.05459	2.68051	49.4075
2	24.226	BB	0.4424	78.90276	2.64188	50.5925

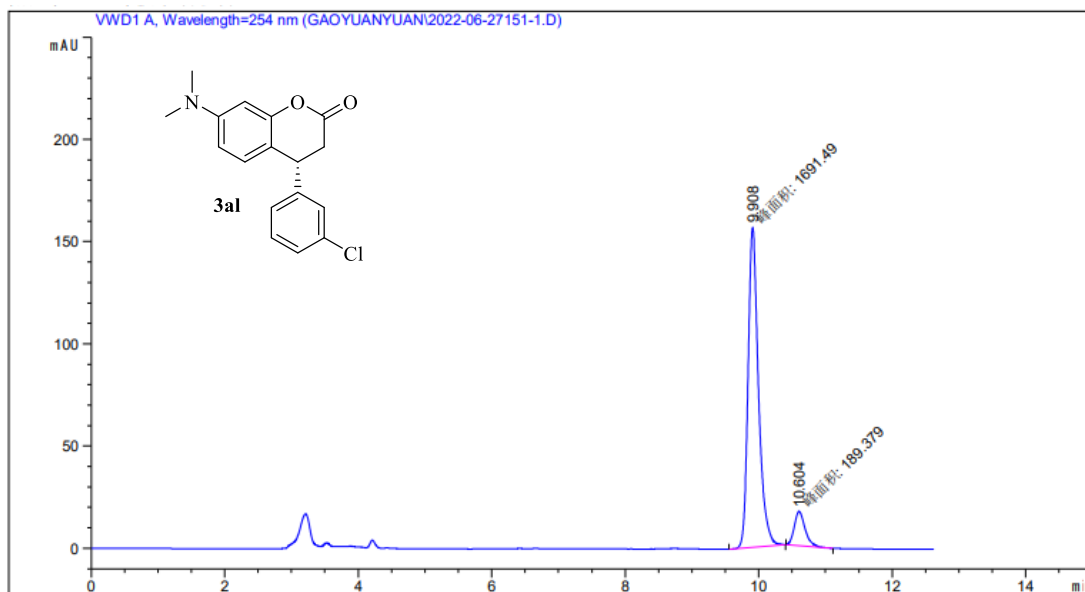


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.955	MM	0.2067	2855.42676	230.18752	91.2816
2	10.765	MM	0.2301	272.72491	19.75656	8.7184

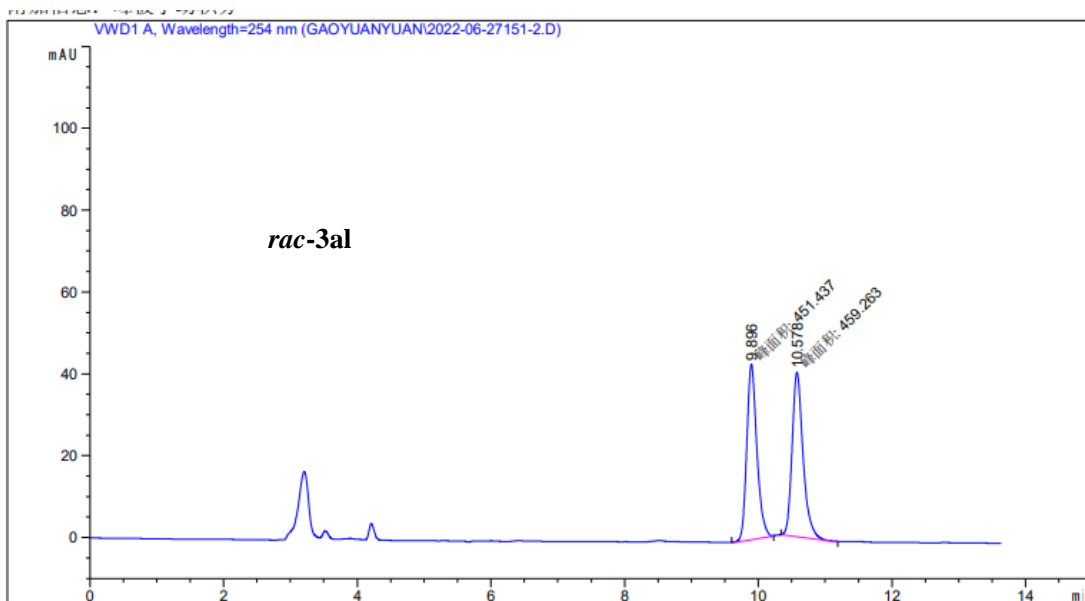


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.970	BV	0.1886	3612.25854	291.49619	50.0279
2	10.770	VB	0.2116	3608.22949	263.82230	49.9721

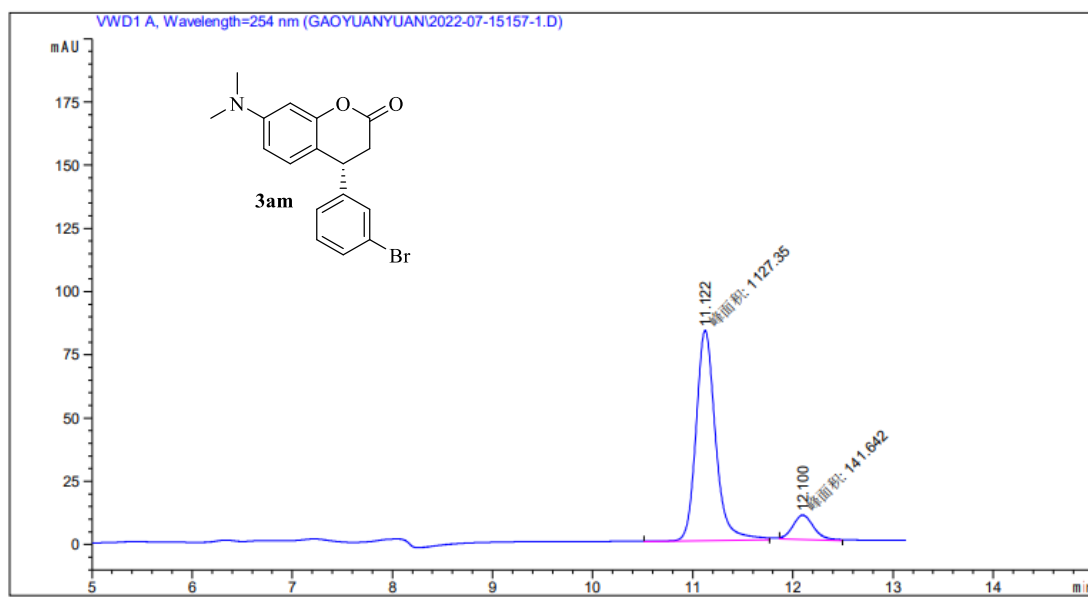




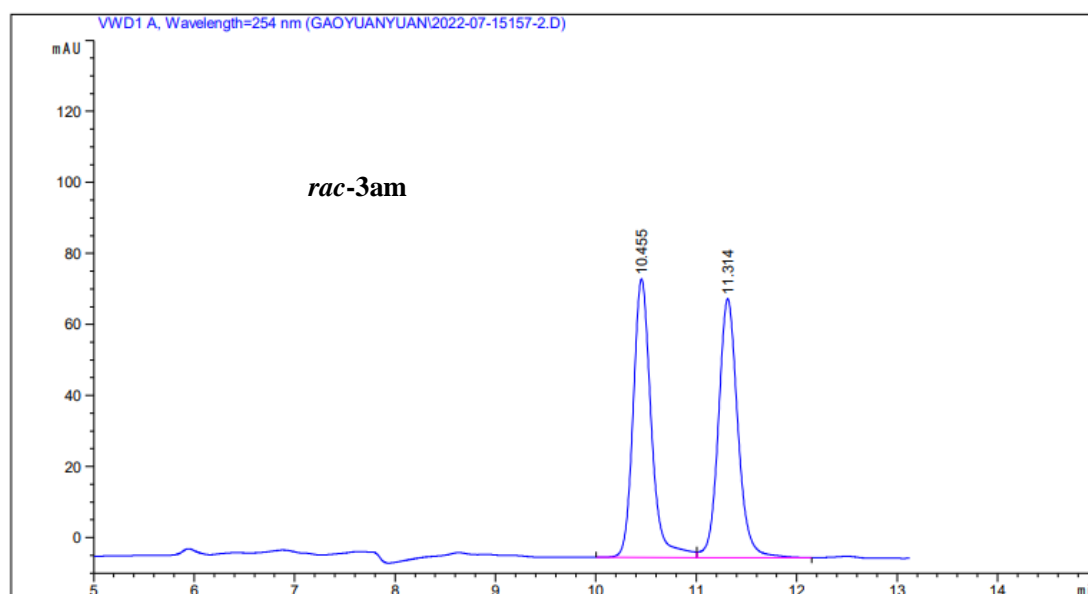
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.908	MM	0.1801	1691.49292	156.55855	89.9313
2	10.604	MM	0.1873	189.37907	16.84866	10.0687



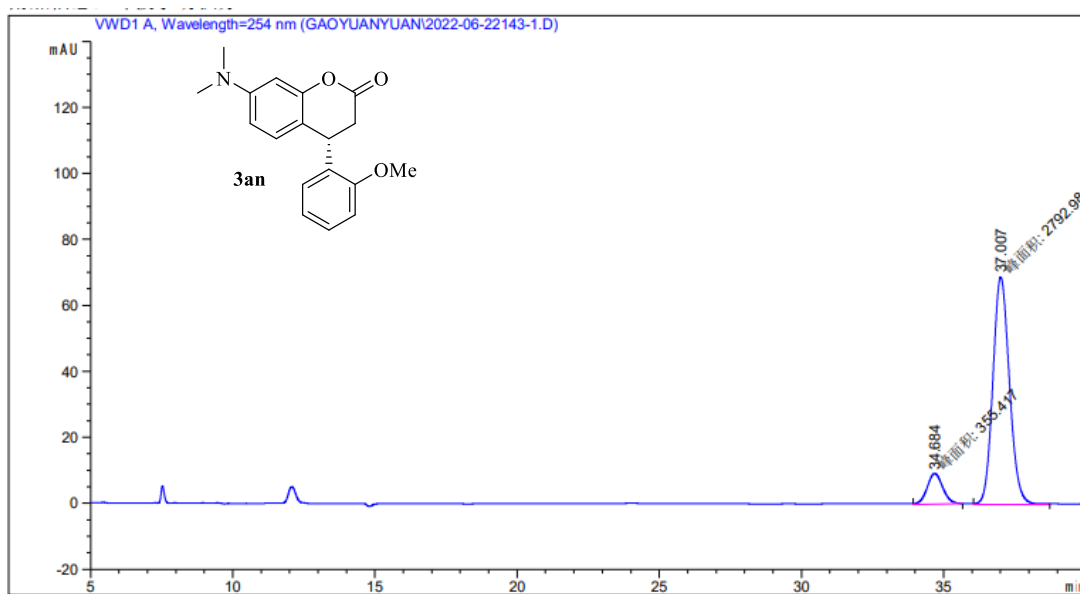
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.896	MM	0.1753	451.43683	42.91893	49.5703
2	10.578	MM	0.1901	459.26288	40.26058	50.4297



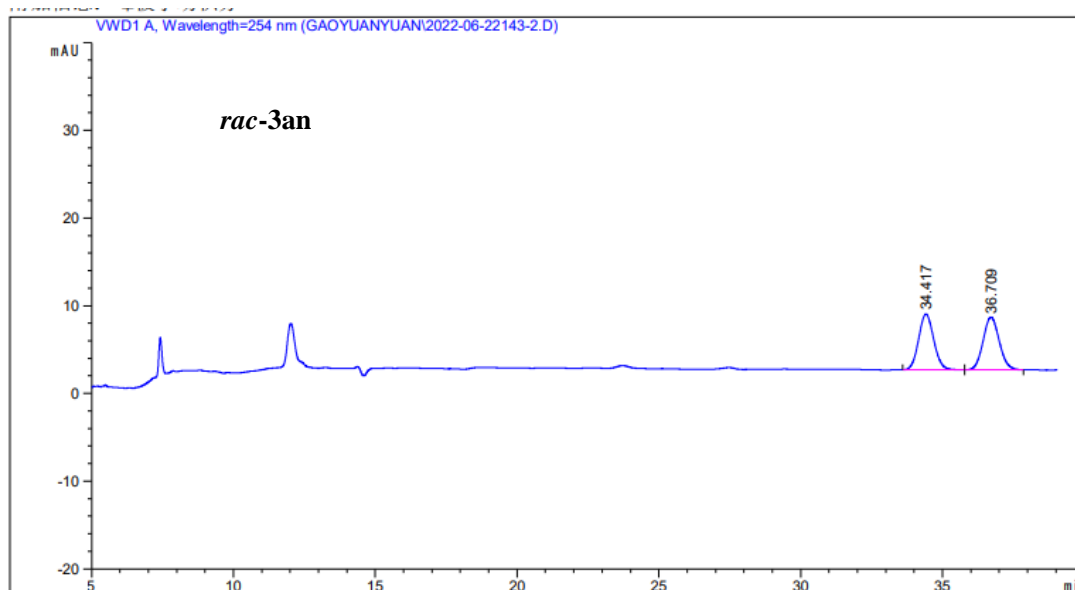
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.122	MM	0.2257	1127.34790	83.23850	88.8382
2	12.100	MM	0.2447	141.64246	9.64810	11.1618



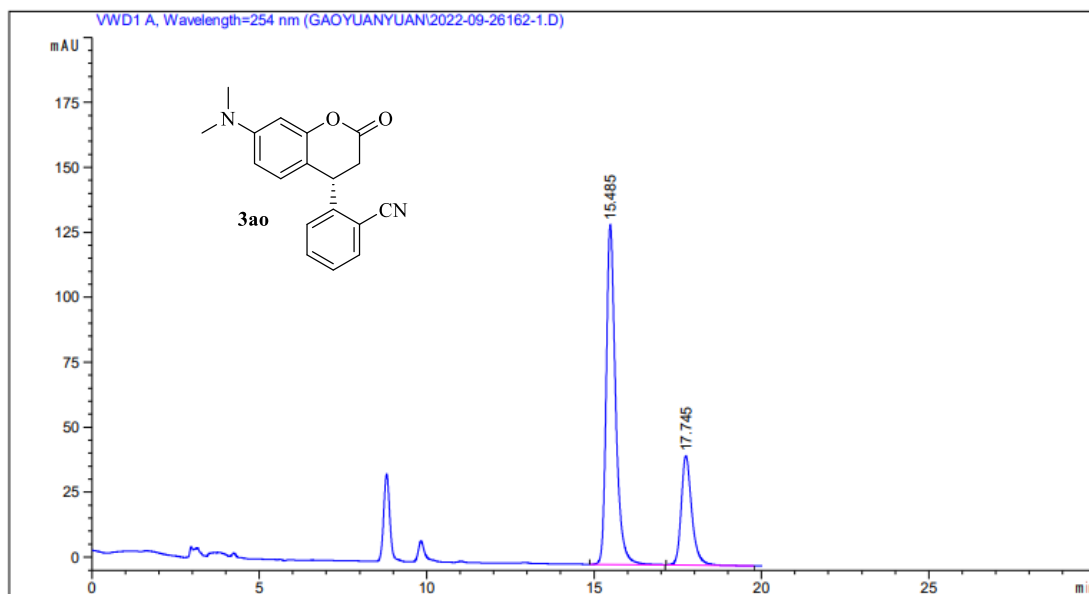
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.455	BV	0.1908	980.01318	78.43313	50.0568
2	11.314	VB	0.2045	977.79028	72.87521	49.9432



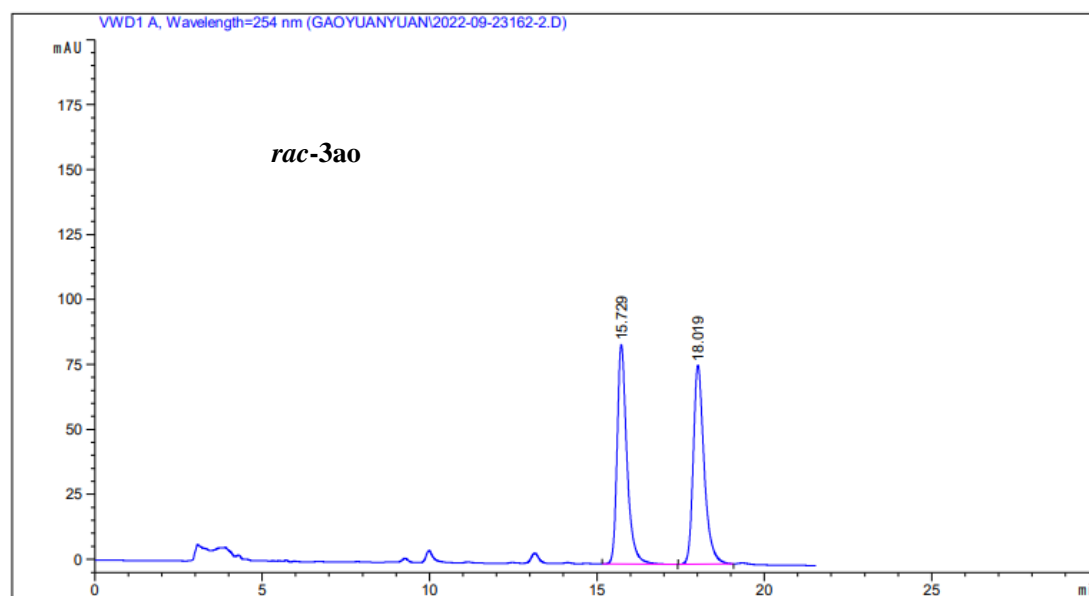
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	34.684	MM	0.6358	355.41727	9.31702	11.2888
2	37.007	MM	0.6752	2792.97998	68.93867	88.7112



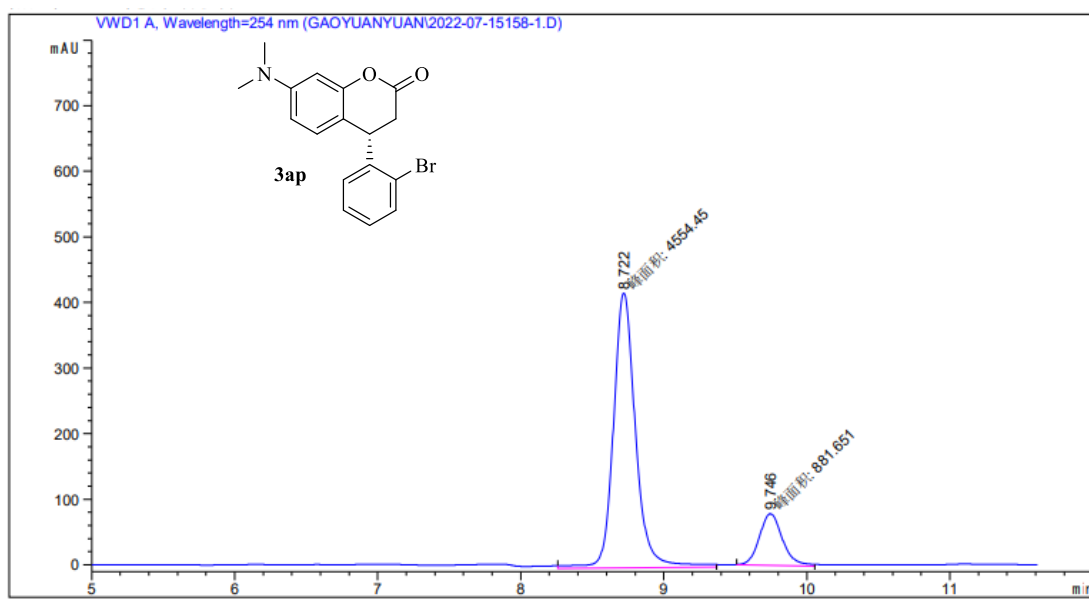
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	34.417	BB	0.5604	234.51306	6.34248	49.6130
2	36.709	BB	0.6101	238.17120	6.02611	50.3870



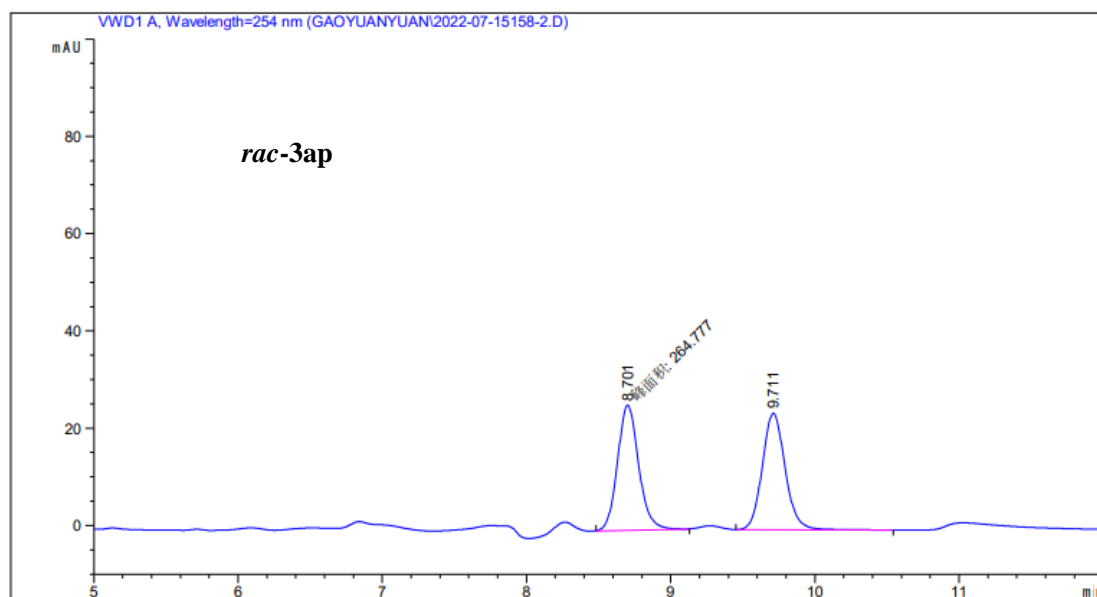
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	15.485	BB	0.2930	2532.69019	130.75598	73.2841
2	17.745	BB	0.3310	923.29987	42.07044	26.7159



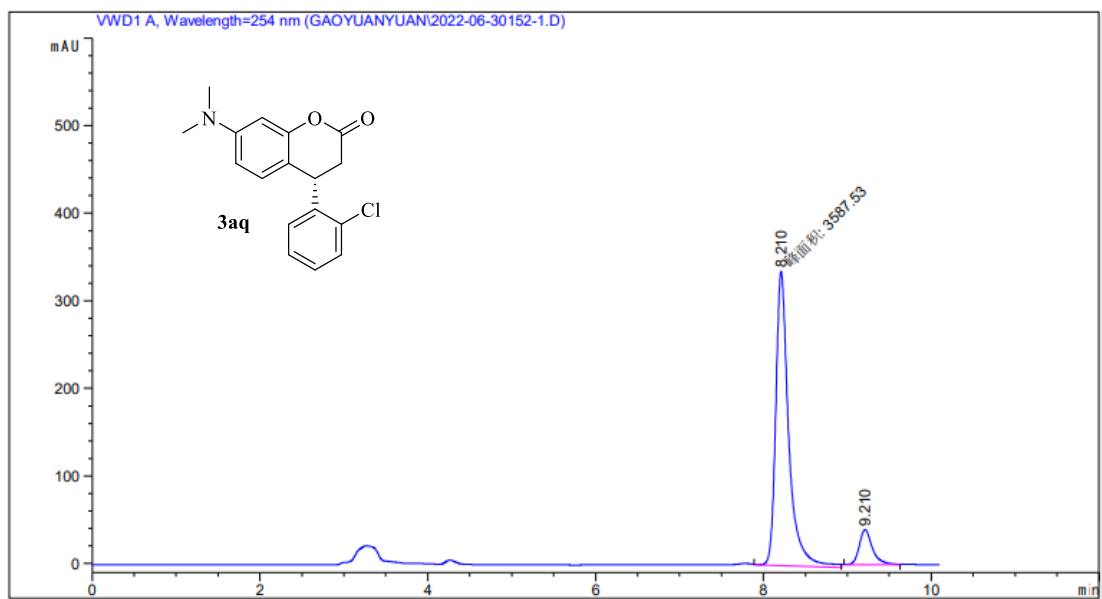
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	15.729	BB	0.3051	1718.01880	84.52218	49.7850
2	18.019	BB	0.3411	1732.85925	76.55825	50.2150



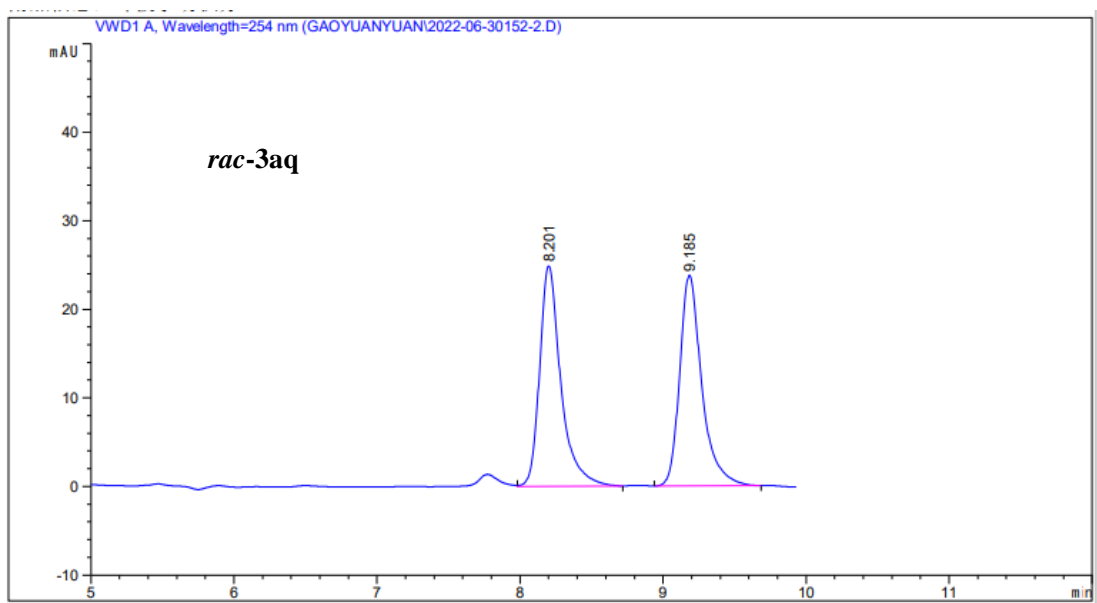
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	8.722	MM	0.1812	4554.45068	418.95493	83.7816
2	9.746	MM	0.1872	881.65118	78.49992	16.2184



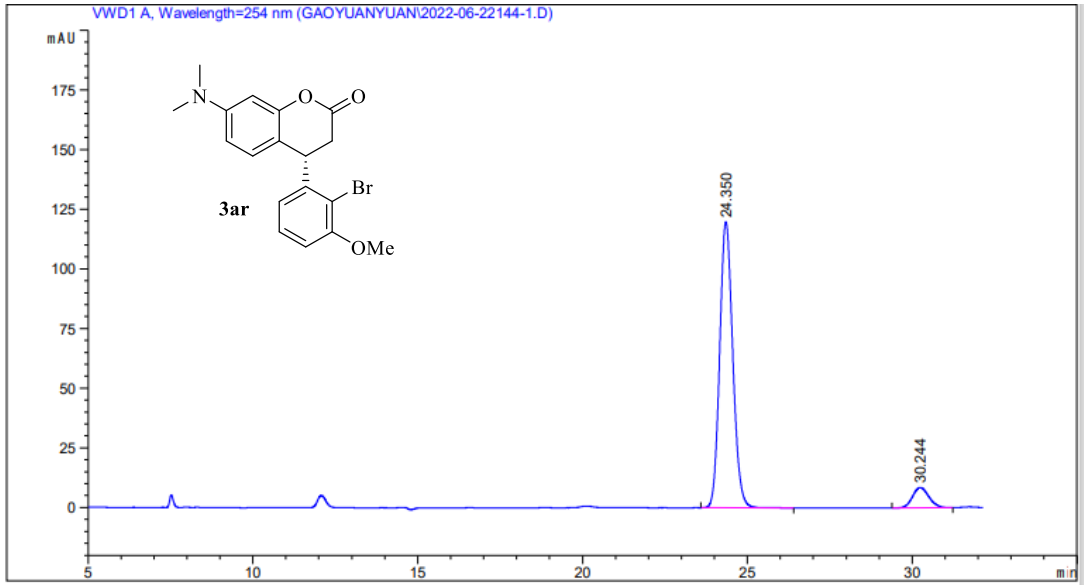
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	8.701	MM	0.1711	264.77740	25.78514	50.0641
2	9.711	BB	0.1697	264.09961	23.94738	49.9359



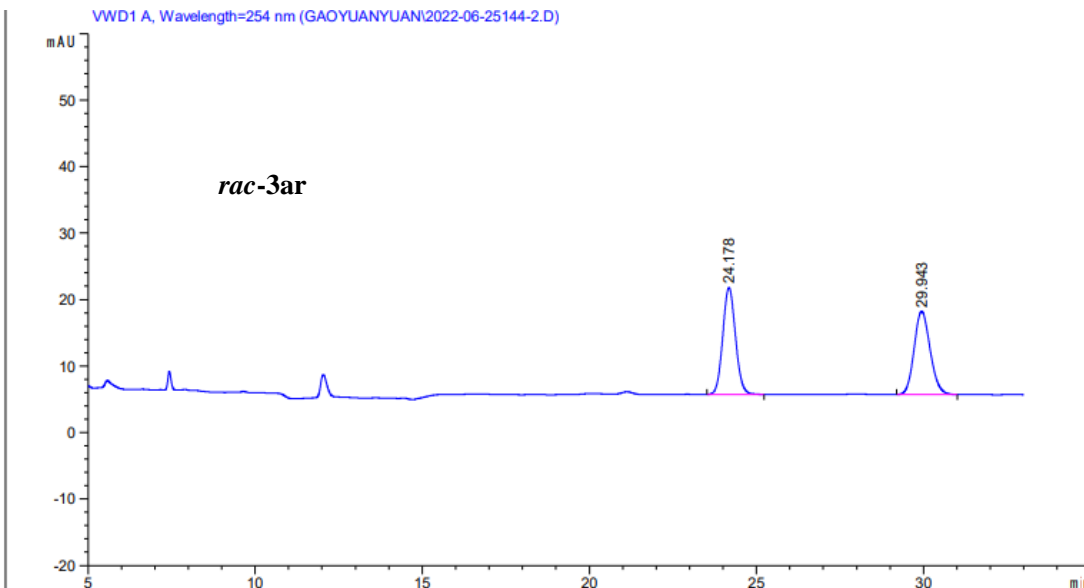
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	8.210	MM	0.1781	3587.52759	335.79007	88.9391
2	9.210	VV	0.1655	446.16412	40.20618	11.0609



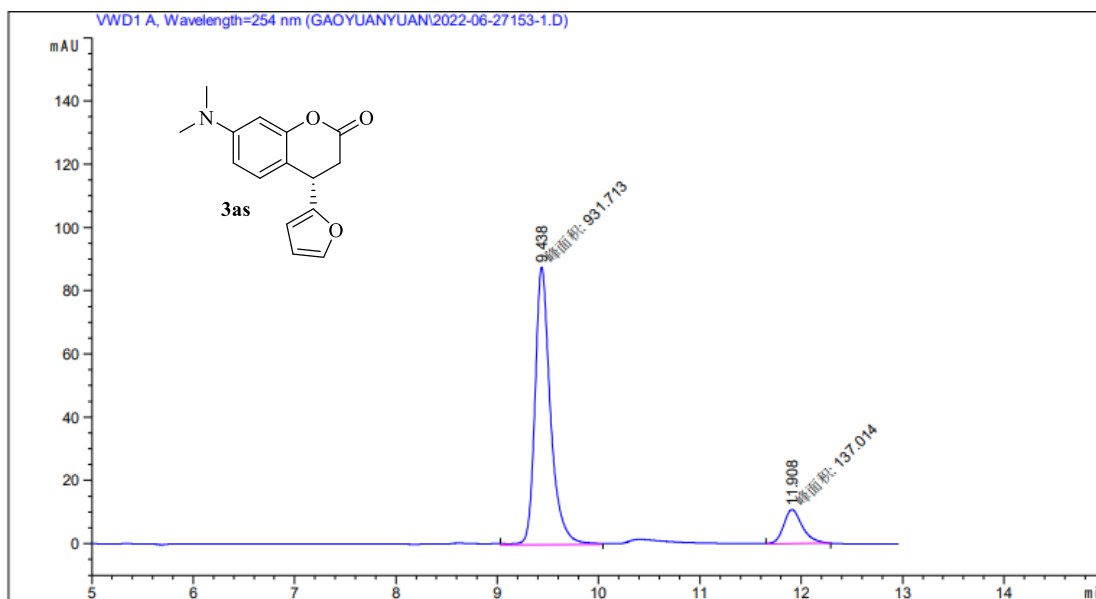
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	8.201	VB	0.1543	256.14182	24.84493	50.1059
2	9.185	BB	0.1612	255.05911	23.77225	49.8941



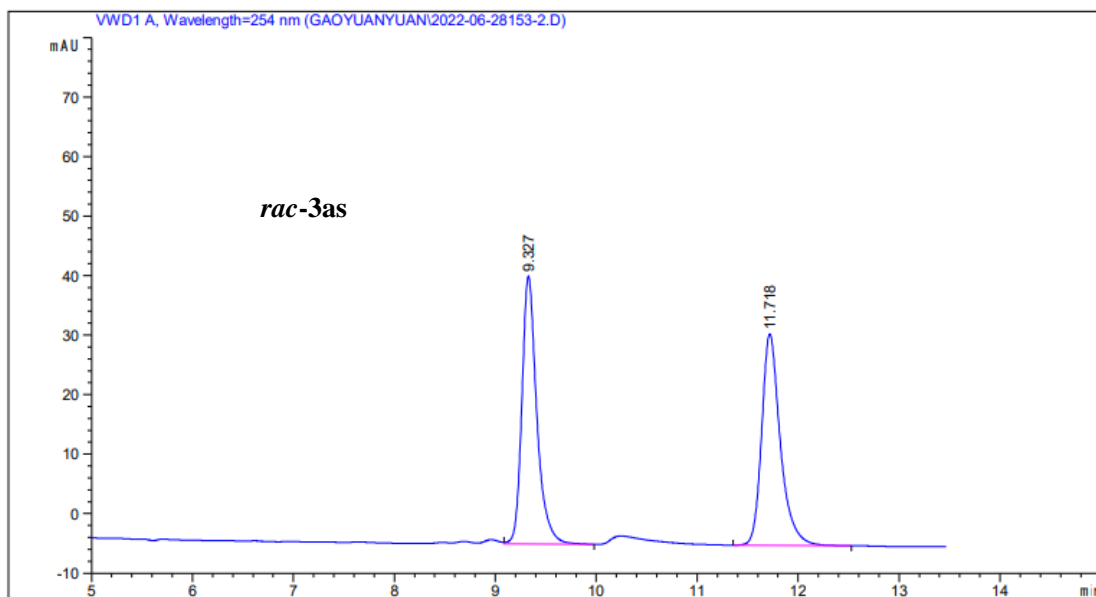
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	24.350	BB	0.4249	3294.20190	119.77538	91.8115
2	30.244	BB	0.5293	293.80368	8.54070	8.1885



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	24.178	BB	0.4099	425.42981	16.06873	50.5380
2	29.943	BB	0.5160	416.37149	12.52117	49.4620

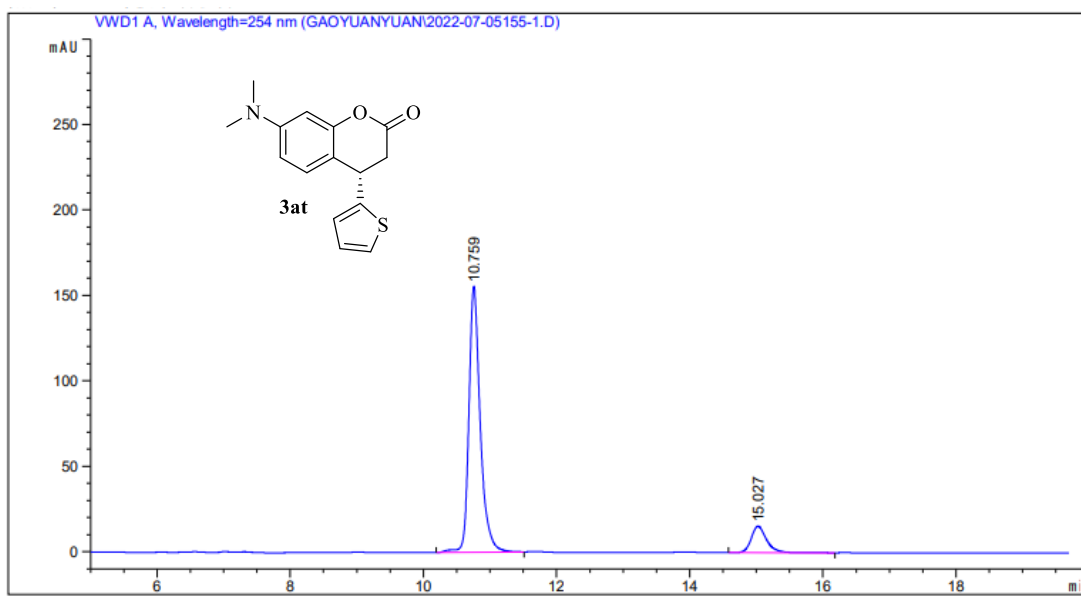


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.438	MM	0.1768	931.71338	87.80967	87.1797
2	11.908	MM	0.2127	137.01357	10.73601	12.8203

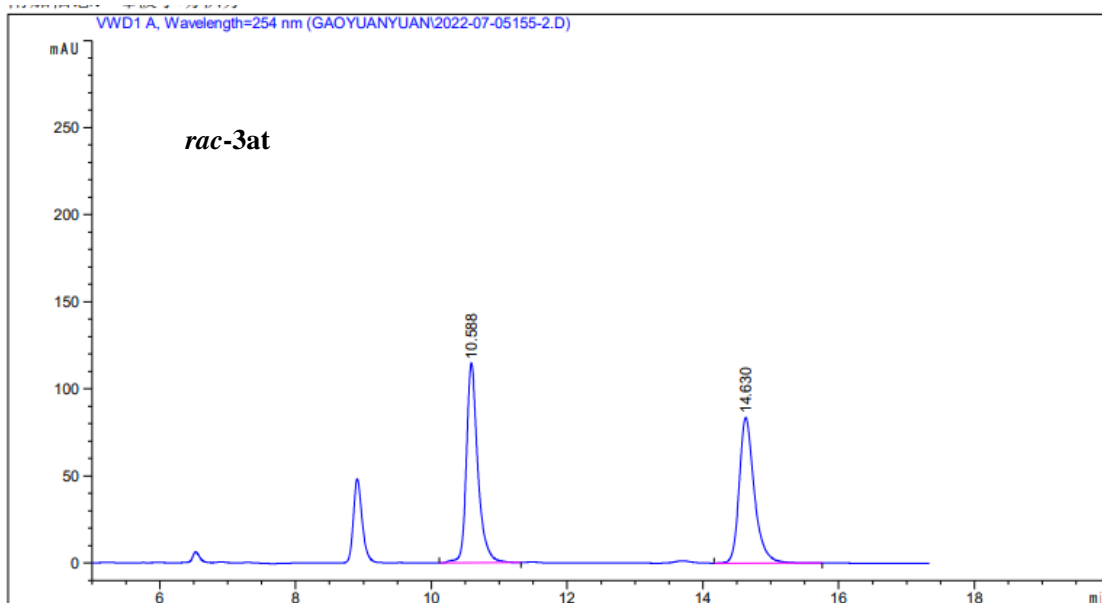


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.327	VB	0.1545	461.33395	45.02203	50.2253
2	11.718	BB	0.1931	457.19550	35.52795	49.7747

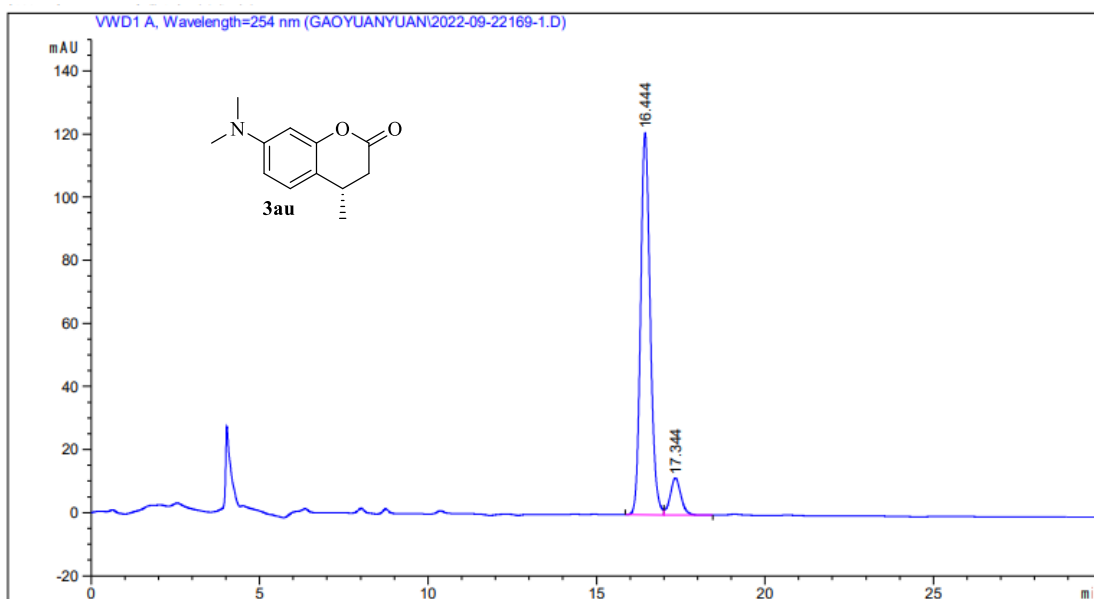




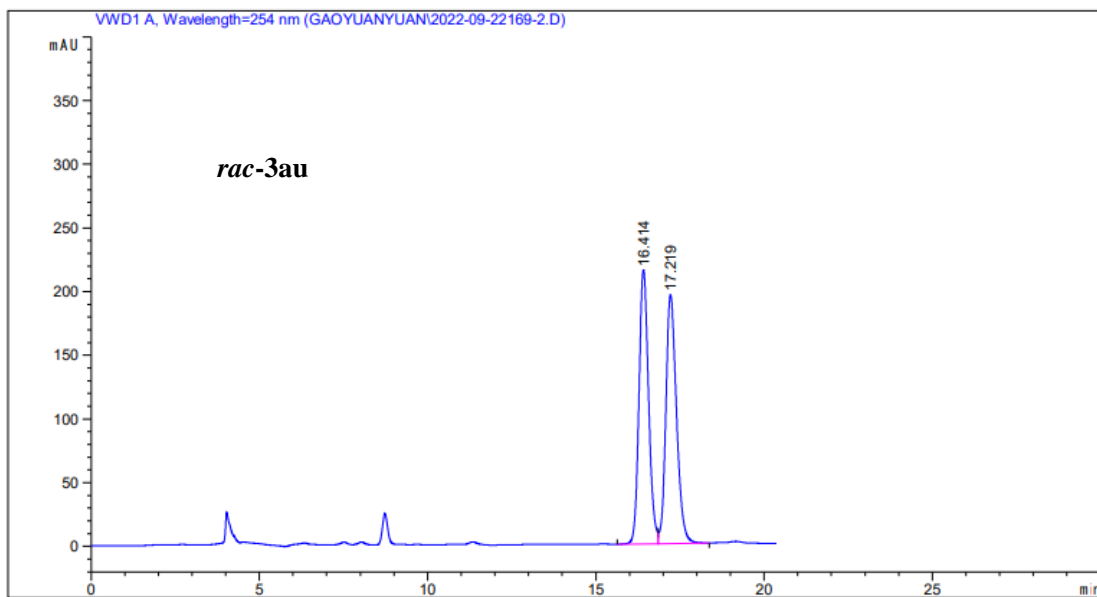
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.759	BB	0.1774	1847.10168	155.69687	88.1676
2	15.027	BB	0.2409	247.88731	15.47609	11.8324



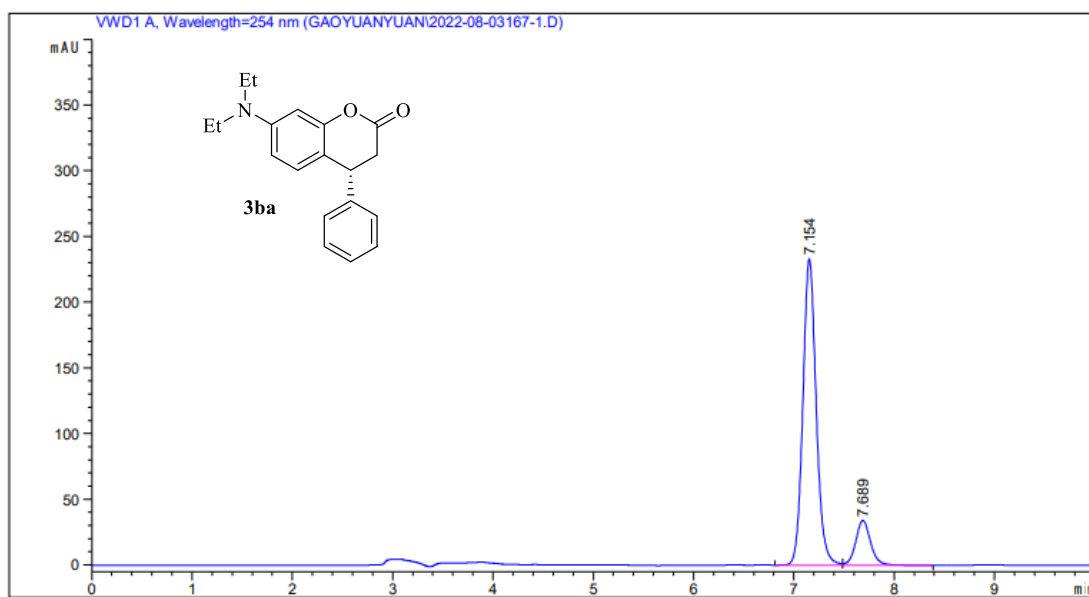
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.588	BB	0.1750	1345.30969	114.59695	50.9932
2	14.630	BB	0.2321	1292.90186	83.75344	49.0068



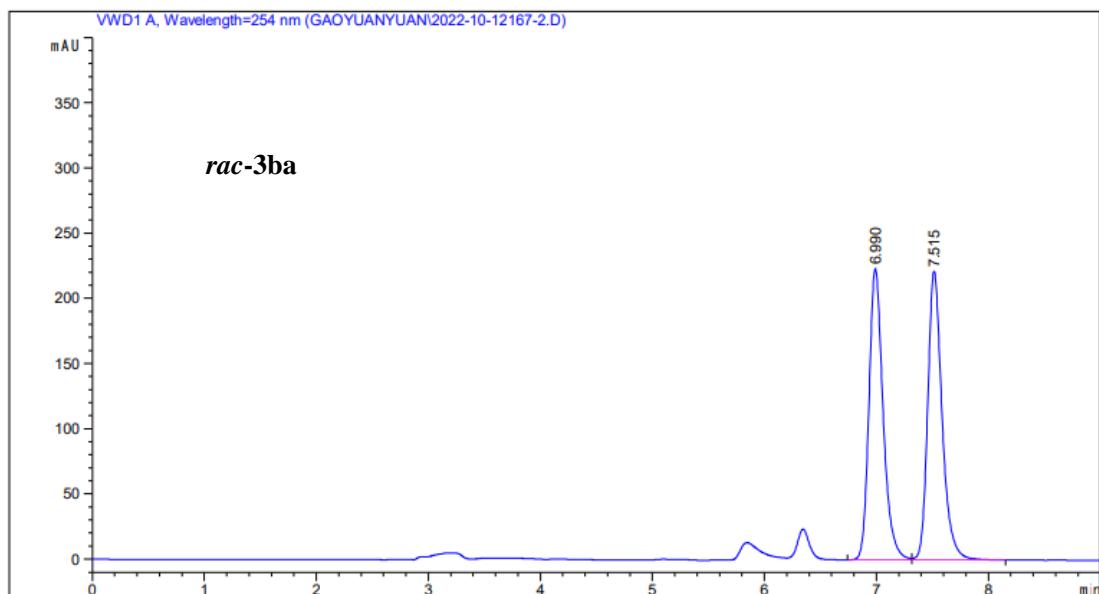
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	16.444	BV	0.3072	2398.81885	121.06214	90.2806
2	17.344	VB	0.3362	258.25137	11.76237	9.7194



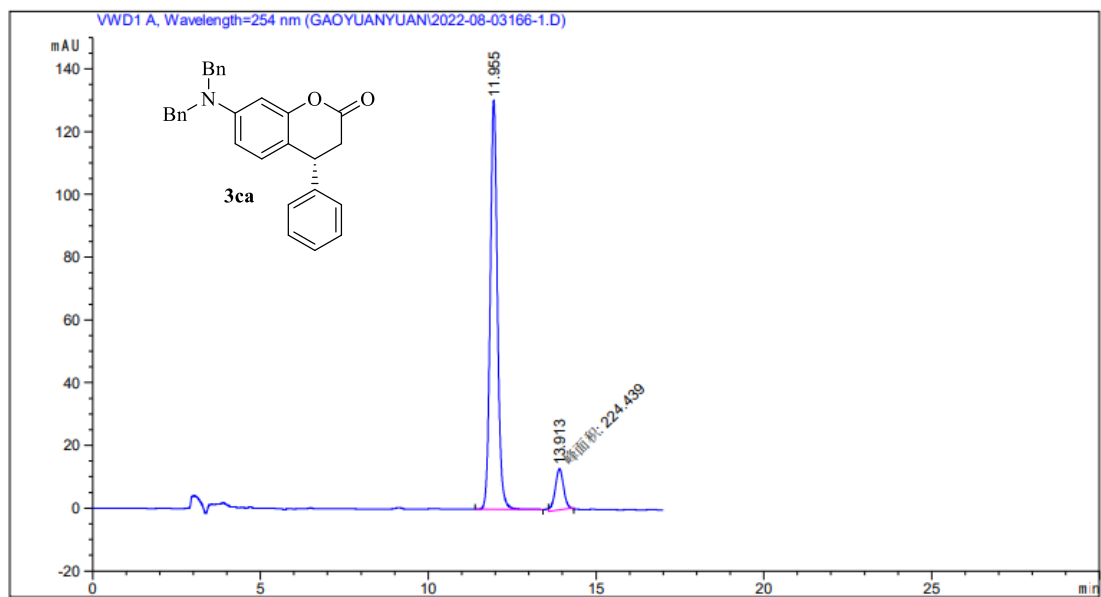
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	16.414	BV	0.3031	4263.84424	215.25920	49.8747
2	17.219	VB	0.3361	4285.26416	195.23238	50.1253



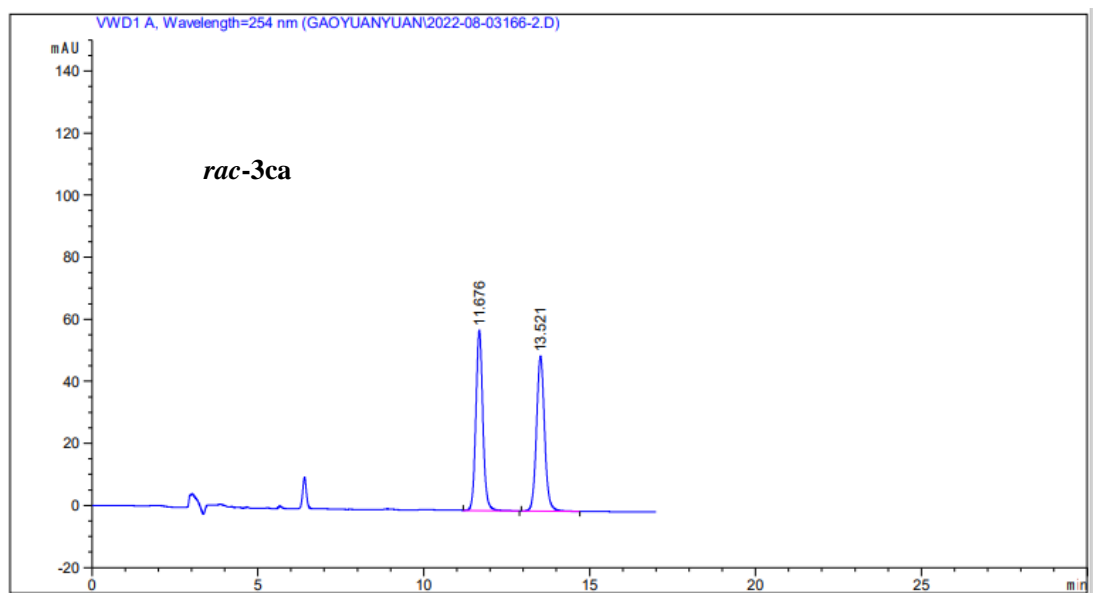
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.154	BV	0.1404	2144.98975	232.93689	85.9566
2	7.689	VB	0.1569	350.44247	34.10397	14.0434



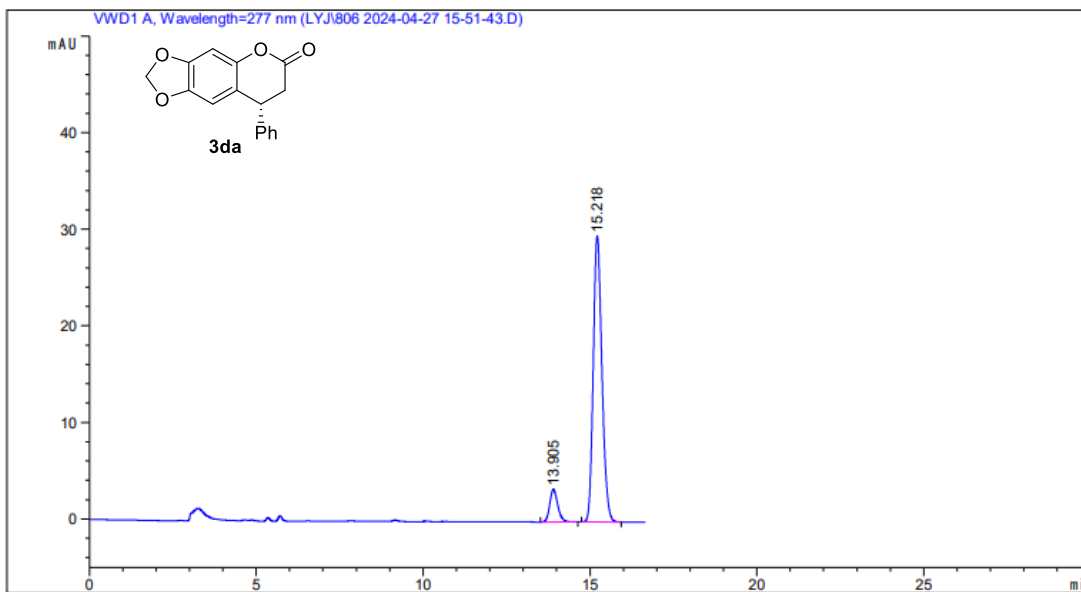
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	6.990	BV	0.1332	1956.85742	223.27641	49.8348
2	7.515	VB	0.1348	1969.82813	221.43661	50.1652



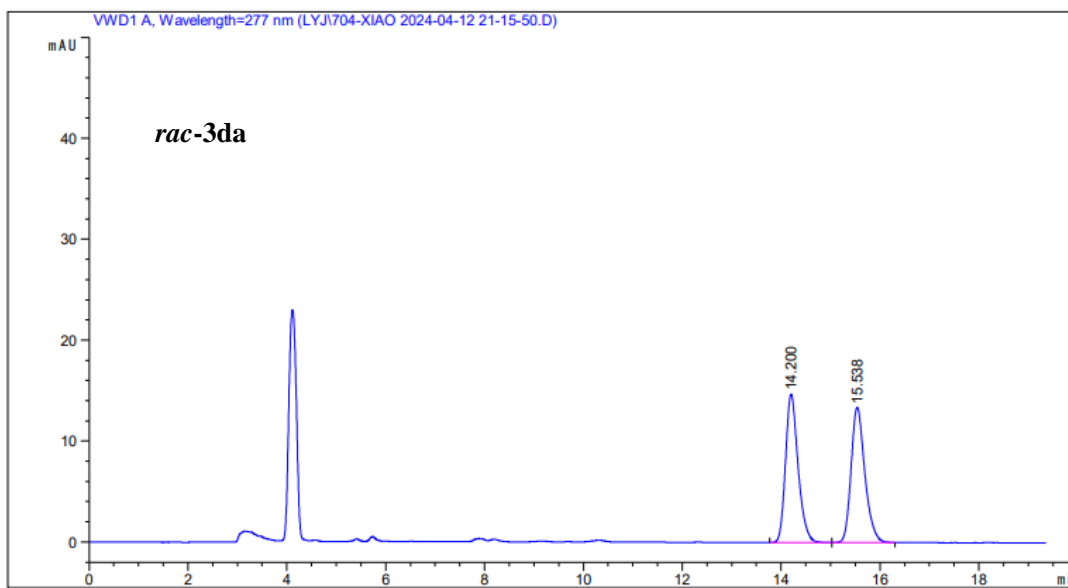
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.955	BV	0.2268	1950.97095	130.19565	89.6829
2	13.913	MM	0.2855	224.43913	13.09992	10.3171



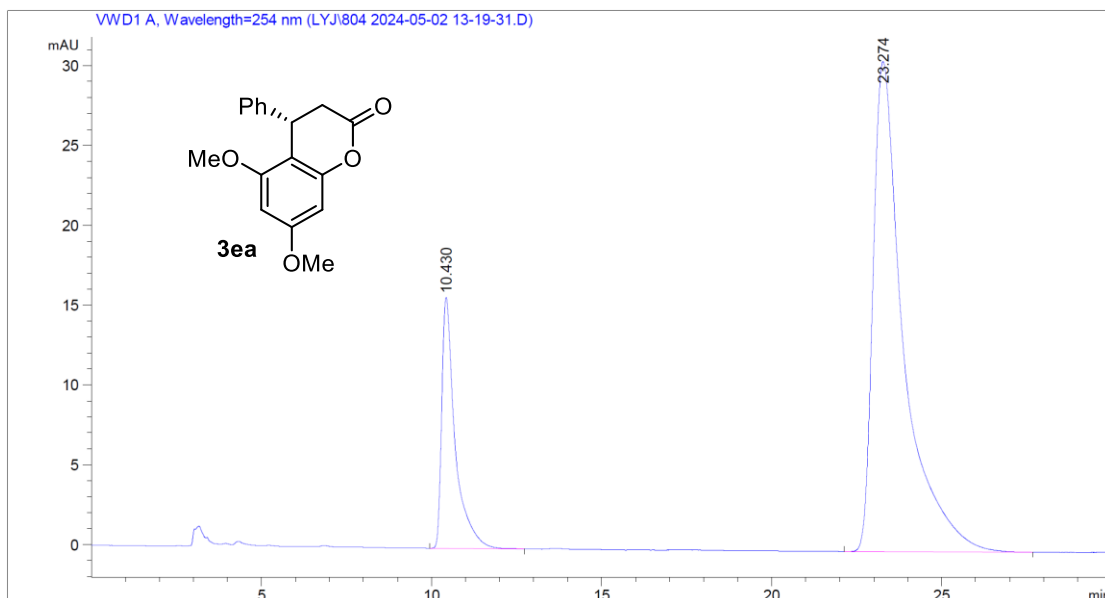
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.676	VB	0.2230	851.83667	58.11563	50.1140
2	13.521	BB	0.2623	847.96136	49.89349	49.8860



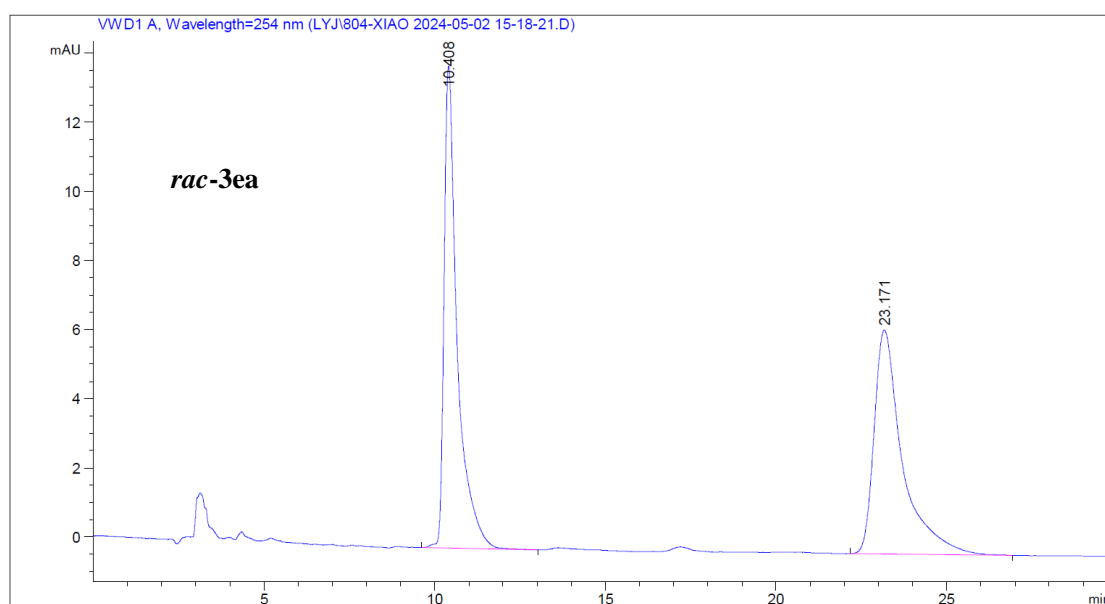
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	13.905	BB	0.2544	55.80571	3.36636	9.4615
2	15.218	BB	0.2774	534.01392	29.61370	90.5385



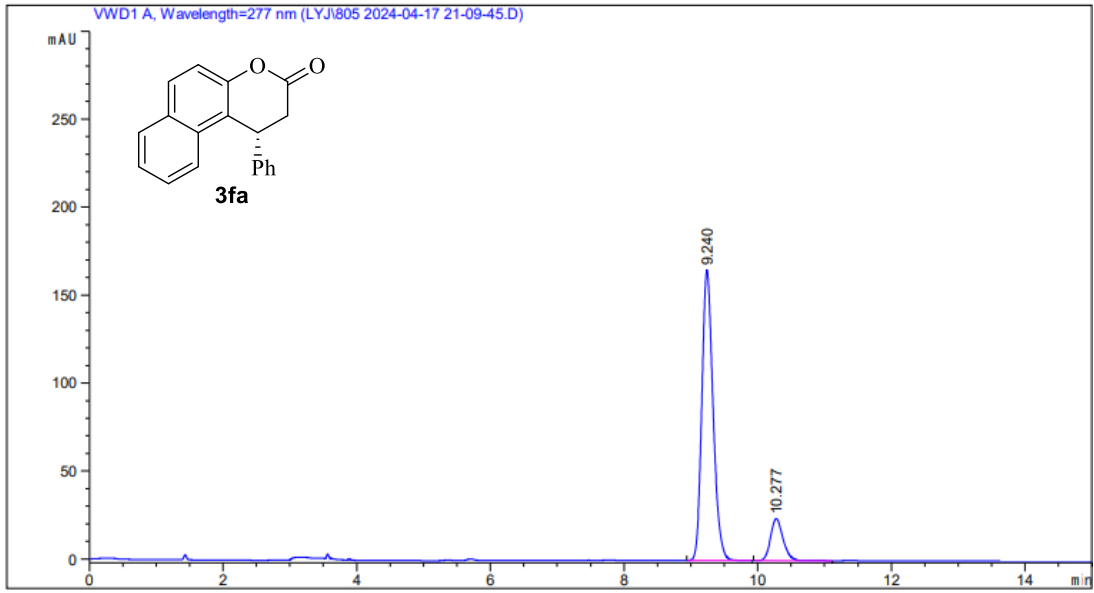
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	4	BB	0.2678	259.20071	14.69171	50.0468
2	14.200	BB	0.2945	258.71643	13.38516	49.9532



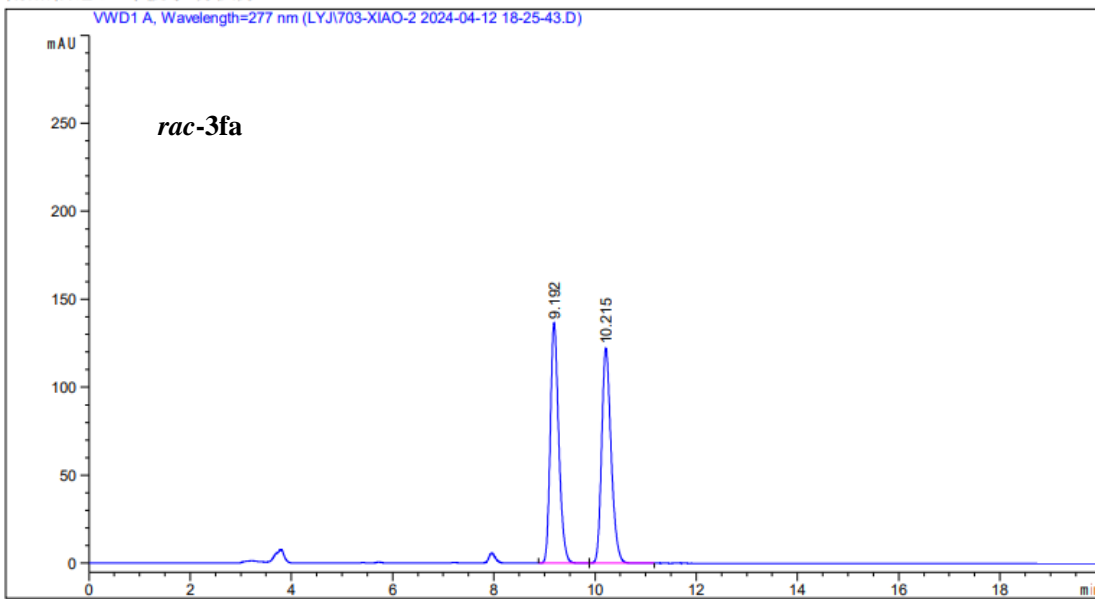
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.430	BB	0.3984	428.48227	15.70181	18.3727
2	23.274	BB	0.9074	1903.68701	30.69971	81.6273



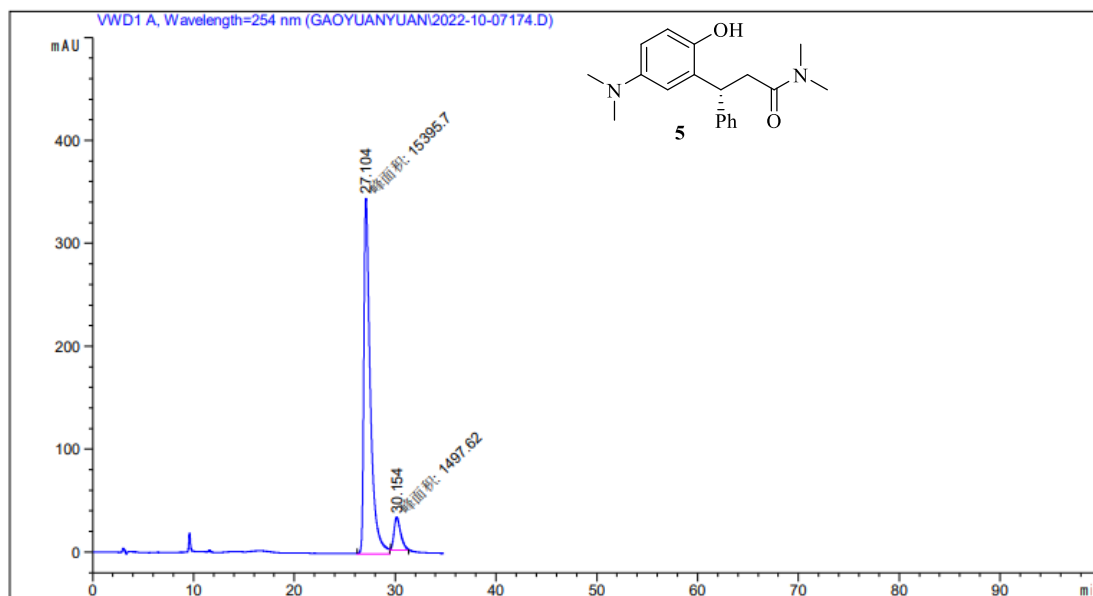
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.408	BB	0.3898	375.20584	13.95162	50.1417
2	23.171	BB	0.8430	373.08466	6.48728	49.8583



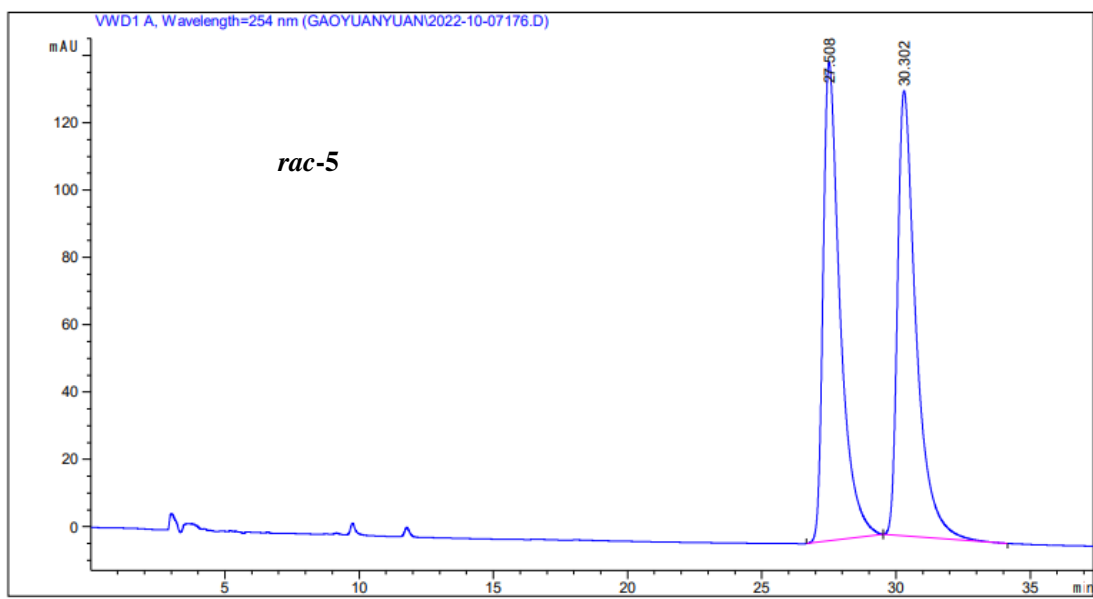
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.240	BB	0.1786	1919.80151	165.21605	86.1638
2	10.277	BB	0.1980	308.28311	23.82517	13.8362



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.192	BB	0.1763	1583.23328	136.53323	49.9885
2	10.215	BB	0.1983	1583.96228	122.10886	50.0115



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	27.104	MM	0.7419	1.53957e4	345.84125	91.1348
2	30.154	MM	0.7753	1497.61755	32.19588	8.8652



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	27.104	MM	0.7419	1.53957e4	345.84125	91.1348
2	30.154	MM	0.7753	1497.61755	32.19588	8.8652