

## Supporting Information

# **Dinuclear zinc-catalyzed asymmetric [3+2] cyclization reaction for direct assembly of chiral $\alpha$ -amino- $\gamma$ -butyrolactones bearing three stereocenters**

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## General Information

All reactions were carried out under an atmosphere of argon using oven-dried glassware. Super dry solvents, metal catalysts, were purchased from chemical companies and used without further treatment. Flash column chromatography was performed using silica gel (300-400 mesh).  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR,  $^{19}\text{F}$  NMR spectra were recorded in  $\text{CDCl}_3$  or  $\text{DMSO-d}_6$  on a 400 MHz spectrometer; chemical shifts are reported in ppm with the solvent signals as reference, and coupling constants ( $J$ ) are given in Hertz. The peak information is described as: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. High-resolution mass spectra (HRMS) were recorded on a commercial apparatus (ESI Source).  $\alpha$ -Hydroxy-1-indanone<sup>1</sup>,  $\alpha$ -hydroxyacetophenone<sup>2</sup>, 3-hydroxychroman-4-one<sup>3</sup> and alkylidene azlactone<sup>4</sup> were synthesized according to the literature.

## General Procedure for optimization of the reaction conditions.

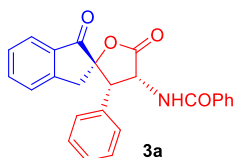
Under a nitrogen atmosphere, a solution of diethylzinc (40  $\mu\text{L}$ , 1.0 M in hexane, 0.04 mmol) was added dropwise to a solution of **L** (0.02 mmol) in solvent (2 mL). After the mixture was stirred for 30 min at room temperature, then,  $\alpha$ -hydroxy-1-indanone **1a** (0.2 mmol) and alkylidene azlactone **2a** (0.2 mmol) were added. The reaction mixture was stirred for 24 h at the same temperature. The reaction was quenched with HCl solution (1 M, 2 mL), and the organic layer was extracted with  $\text{CH}_2\text{Cl}_2$  (3  $\times$  5 mL). The combined organic layer was washed with brine and dried over  $\text{Na}_2\text{SO}_4$ . The solvent was removed under reduced pressure by using a rotary evaporator. The residue was purified by flash chromatography with petroleum ether/ethyl acetate (4/1) to afford the desired product **3a**.

## Synthesis of chiral $\alpha$ -amino- $\gamma$ -butyrolactones.

Under a nitrogen atmosphere, a solution of diethylzinc (40  $\mu\text{L}$ , 1.0 M in hexane, 0.04 mmol) was added dropwise to a solution of **L4** (0.02 mmol) in THF (2 mL). After the mixture was stirred for 30 min at room temperature, then,  $\alpha$ -hydroxy-1-indanone **1** or  $\alpha$ -hydroxyacetophenone **1** or 3-hydroxychroman-4-one **1** (0.2 mmol) and alkylidene azlactone **2** (0.2 mmol) were added. The reaction mixture was stirred for 24 h at the same temperature. The reaction was quenched with HCl solution (1 M, 2 mL), and the organic layer was extracted with  $\text{CH}_2\text{Cl}_2$  (3  $\times$  5 mL). The combined organic layer was washed with brine and dried over  $\text{Na}_2\text{SO}_4$ . The solvent was removed under reduced pressure by using a rotary evaporator. The residue was purified by flash chromatography with petroleum ether/ethyl acetate (4/1) to afford the desired product **3**.

## Characterization of **3**

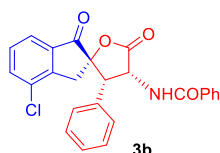
*N*-((2*S*,3*S*,4*R*)-1',5-dioxo-3-phenyl-1',3',4,5-tetrahydro-3*H*-spiro[furan-2,2'-inden]-4-yl)benzamide (**3a**):



Yellow solid in 70% isolated yield (83mg, >20:1 dr);  $[\alpha]_{\text{D}}^{20} = +125$  ( $c = 1.0$ ,  $\text{DMSO}$ , 99% ee); **m.p.** = 112.6-113.4  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-d}_6$ )  $\delta$  8.70 (d,  $J = 7.6$  Hz, 1H), 7.84 (d,  $J = 7.6$  Hz, 1H), 7.79-7.73 (m, 1H), 7.56-7.43 (m, 5H), 7.39-7.30 (m, 5H), 7.20-7.13 (m, 2H), 6.04-5.97 (m, 1H), 4.35 (d,  $J = 8.8$  Hz, 1H), 3.36 (d,  $J = 18.1$  Hz, 1H), 3.01 (d,  $J = 18.2$  Hz, 1H);  $^{13}\text{C}$  NMR (101 MHz,

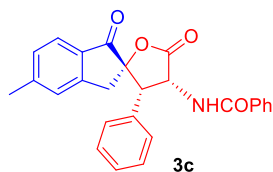
DMSO- $d_6$ )  $\delta$  201.5, 173.9, 167.1, 151.1, 136.9, 134.7, 133.3, 132.3, 131.5, 129.2, 128.6, 128.0, 127.4, 126.9, 124.8, 88.6, 52.5, 49.9, 36.3; **IR** (neat): 3386, 2919, 1788, 1716, 1655, 1160, 747, 699, 467  $\text{cm}^{-1}$ ; **HRMS** (ESI):  $m/z$  for  $[M+H]^+$ : calcd 398.1387, found 398.1384; **HPLC**: Daicel Chiralpak IA, *n*-hexane/*i*-PrOH = 50/50, flow rate = 1 mL/min,  $\lambda$  = 254 nm,  $t_{\text{major}}$  = 15.50 min and  $t_{\text{minor}}$  = 9.28 min.

***N*-((2*S*,3*S*,4*R*)-6'-chloro-1',5-dioxo-3-phenyl-1',3',4,5-tetrahydro-3*H*-spiro[furan-2,2'-inden]-4-yl) benzamide (3b):**



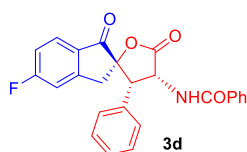
Major diastereoisomer of **3b**: Yellow solid in 80% isolated yield (103mg, 5:1 dr);  $[\alpha]_D^{20} = +79$  ( $c = 1.0$ ,  $\text{CDCl}_3$ , 94% ee); **m.p.** = 222.8-223.6 °C; **<sup>1</sup>H NMR** (400 MHz,  $\text{DMSO-}d_6$ )  $\delta$  8.74 (d,  $J = 7.5$  Hz, 1H), 7.91-7.81 (m, 2H), 7.62-7.56 (m, 1H), 7.53-7.42 (m, 3H), 7.40-7.28 (m, 5H), 7.23-7.01 (m, 3H), 6.07-5.89 (m, 1H), 4.43 (d,  $J = 8.8$  Hz, 1H), 3.31 (d,  $J = 18.1$  Hz, 1H), 2.94 (d,  $J = 18.2$  Hz, 1H); **<sup>13</sup>C NMR** (101 MHz,  $\text{DMSO-}d_6$ )  $\delta$  200.6, 173.7, 167.0, 148.2, 136.2, 134.6, 133.3, 131.4, 130.6, 129.3, 128.9, 128.4, 128.0, 127.5, 127.3, 123.7, 88.2, 52.4, 49.8, 35.4; **IR** (neat): 3392, 2926, 1797, 1715, 1667, 1523, 1156, 713, 509  $\text{cm}^{-1}$ ; **HRMS** (ESI):  $m/z$  for  $[M+H]^+$ : calcd 432.0997, found 432.0995; **HPLC**: Daicel Chiralpak IB, *n*-hexane/*i*-PrOH = 80/20, flow rate = 1 mL/min,  $\lambda$  = 254 nm,  $t_{\text{major}}$  = 14.89 min and  $t_{\text{minor}}$  = 10.98 min.

***N*-((2*S*,3*S*,4*R*)-5'-methyl-1',5-dioxo-3-phenyl-1',3',4,5-tetrahydro-3*H*-spiro[furan-2,2'-inden]-4-yl) benzamide (3c):**

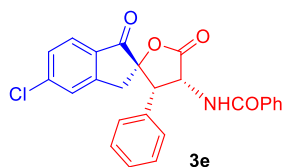


Yellow solid in 80% isolated yield (99mg, >20:1 dr);  $[\alpha]_D^{20} = +77$  ( $c = 1.0$ ,  $\text{DMSO}$ , 95% ee); **m.p.** = 235.5-236.3 °C; **<sup>1</sup>H NMR** (400 MHz,  $\text{DMSO-}d_6$ )  $\delta$  8.69 (d,  $J = 7.2$  Hz, 1H), 7.73 (d,  $J = 7.7$  Hz, 1H), 7.53-7.42 (m, 3H), 7.39-7.27 (m, 7H), 7.16 (d,  $J = 5.9$  Hz, 2H), 6.08 – 5.93 (m, 1H), 4.30 (d,  $J = 8.6$  Hz, 1H), 3.31 (d,  $J = 22.4$  Hz, 1H), 2.95 (d,  $J = 18.2$  Hz, 1H), 2.39 (s, 3H); **<sup>13</sup>C NMR** (101 MHz,  $\text{DMSO-}d_6$ )  $\delta$  200.7, 173.9, 167.0, 151.4, 148.2, 134.8, 133.3, 131.5, 129.9, 129.7, 129.3, 128.7, 128.0, 127.5, 127.0, 124.77, 88.77, 52.5, 50.15, 36.1, 21.8; **IR** (neat): 3399, 2926, 1783, 1712, 1671, 1609, 1123, 1085, 709, 496  $\text{cm}^{-1}$ ; **HRMS** (ESI):  $m/z$  for  $[M+H]^+$ : calcd 412.1543, found 432.1542; **HPLC**: Daicel Chiralpak IB, *n*-hexane/*i*-PrOH = 80/20, flow rate = 1 mL/min,  $\lambda$  = 254 nm,  $t_{\text{major}}$  = 16.07 min and  $t_{\text{minor}}$  = 12.64 min.

***N*-((2*S*,3*S*,4*R*)-5'-fluoro-1',5-dioxo-3-phenyl-1',3',4,5-tetrahydro-3*H*-spiro[furan-2,2'-inden]-4-yl) benzamide (3d):**

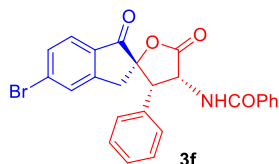


Yellow solid in 76% isolated yield (94mg, >20:1 dr);  $[\alpha]_{\text{D}}^{20} = +90$  (c = 1.0, DMSO, 99% ee); **m.p.** = 239.1-240.2 °C; **<sup>1</sup>H NMR** (400 MHz, DMSO-*d*<sub>6</sub>) δ 8.71 (d, *J* = 7.4 Hz, 1H), 7.98-7.85 (m, 1H), 7.52-7.43 (m, 3H), 7.41-7.29 (m, 7H), 7.17 (d, *J* = 6.6 Hz, 2H), 6.05-5.92 (m, 1H), 4.38 (d, *J* = 8.8 Hz, 1H), 3.36 (d, *J* = 17.9 Hz, 1H), 3.02 (d, *J* = 18.4 Hz, 1H); **<sup>13</sup>C NMR** (101 MHz, DMSO-*d*<sub>6</sub>) δ 199.7, 173.8, 167.40 (d, *J* = 256.0 Hz), 167.0, 154.46 (d, *J* = 11.3 Hz), 134.7, 133.3, 131.5, 129.2, 128.7, 128.2, 128.3, 127.4, 127.3, 117.0, 116.7, 113.8, 113.6, 88.6, 52.5, 50.0, 36.3; **<sup>19</sup>F NMR** (376 MHz, DMSO-*d*<sub>6</sub>) δ -99.98; **IR** (neat): 3383, 2929, 1799, 1713, 1662, 1264, 1139, 714, 646, 498 cm<sup>-1</sup>; **HRMS** (ESI): *m/z* for [M+H]<sup>+</sup>: calcd 416.1293, found 416.1292; **HPLC**: Daicel Chiralpak IB, *n*-hexane/*i*-PrOH = 80/20, flow rate = 1 mL/min, λ = 254 nm, *t*<sub>major</sub> = 14.65 min and *t*<sub>minor</sub> = 18.34 min.  
***N*-((2*S*,3*S*,4*R*)-5'-chloro-1',5-dioxo-3-phenyl-1',3',4,5-tetrahydro-3*H*-spiro[furan-2,2'-inden]-4-yl) benzamide (3e):**



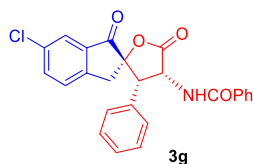
Yellow solid in 78% isolated yield (100mg, >20:1 dr);  $[\alpha]_{\text{D}}^{20} = +97$  (c = 1.0, DMSO, 98% ee); **m.p.** = 232.2-233.4 °C; **<sup>1</sup>H NMR** (400 MHz, DMSO-*d*<sub>6</sub>) δ 8.72 (d, *J* = 7.4 Hz, 1H), 7.85 (d, *J* = 8.2 Hz, 1H), 7.65 (s, 1H), 7.59 (d, *J* = 8.1 Hz, 1H), 7.52-7.42 (m, 3H), 7.40-7.29 (m, 5H), 7.17 (d, *J* = 6.5 Hz, 2H), 6.05-5.95 (m, 1H), 4.39 (d, *J* = 8.8 Hz, 1H), 3.35 (d, *J* = 18.3 Hz, 1H), 3.02 (d, *J* = 18.4 Hz, 1H); **<sup>13</sup>C NMR** (101 MHz, DMSO-*d*<sub>6</sub>) δ 200.3, 173.8, 167.0, 152.9, 141.7, 134.7, 133.3, 131.5, 131.2, 129.3, 129.0, 128.7, 128.0, 127.5, 127.0, 126.4, 88.5, 52.5, 49.9, 36.2; **IR** (neat): 3399, 2988, 1787, 1717, 1667, 1629, 1102, 1084, 713, 464 cm<sup>-1</sup>; **HRMS** (ESI): *m/z* for [M+H]<sup>+</sup>: calcd 432.0997, found 432.0996; **HPLC**: Daicel Chiralpak IB, *n*-hexane/*i*-PrOH = 80/20, flow rate = 1 mL/min, λ = 254 nm, *t*<sub>major</sub> = 11.54 min and *t*<sub>minor</sub> = 15.50 min.

***N*-((2*S*,3*S*,4*R*)-5'-bromo-1',5-dioxo-3-phenyl-1',3',4,5-tetrahydro-3*H*-spiro[furan-2,2'-inden]-4-yl) benzamide (3f):**



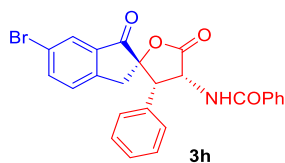
Yellow solid in 40% isolated yield (57mg, >20:1 dr);  $[\alpha]_{\text{D}}^{20} = +66$  (c = 1.0, DMSO, 97% ee); **m.p.** = 258.0-259.1 °C; **<sup>1</sup>H NMR** (400 MHz, DMSO-*d*<sub>6</sub>) δ 8.69 (d, *J* = 7.5 Hz, 1H), 7.83-7.70 (m, 3H), 7.52-7.43 (m, 3H), 7.40-7.29 (m, 5H), 7.16 (d, *J* = 6.6 Hz, 2H), 6.07-5.90 (m, 1H), 4.38 (d, *J* = 8.8 Hz, 1H), 3.35 (d, *J* = 19.0 Hz, 1H), 3.02 (d, *J* = 18.4 Hz, 1H); **<sup>13</sup>C NMR** (101 MHz, DMSO-*d*<sub>6</sub>) δ 200.5, 173.8, 167.0, 153.0, 134.7, 133.4, 131.9, 131.5, 131.2, 130.0, 129.3, 128.7, 128.0, 127.5, 126.4, 88.5, 52.4, 49.9, 36.1; **IR** (neat): 3425, 2918, 1779, 1719, 1667, 1207, 1140, 913, 714, 489 cm<sup>-1</sup>; **HRMS** (ESI): *m/z* for [M+H]<sup>+</sup>: calcd 498.0311, found 498.0309; **HPLC**: Daicel Chiralpak IB, *n*-hexane/*i*-PrOH = 80/20, flow rate = 1 mL/min, λ = 254 nm, *t*<sub>major</sub> = 15.73 min and *t*<sub>minor</sub> = 21.68 min.

***N*-((2*S*,3*S*,4*R*)-4'-chloro-1',5-dioxo-3-phenyl-1',3',4,5-tetrahydro-3*H*-spiro[furan-2,2'-inden]-4-yl) benzamide (3g):**



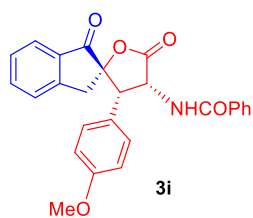
Yellow solid in 78% isolated yield (101mg, >20:1 dr);  $[\alpha]_{\text{D}}^{20} = +109$  (c = 1.0, DMSO, 99% ee); **m.p.** = 180.5-181.7 °C; **<sup>1</sup>H NMR** (400 MHz, DMSO- $d_6$ )  $\delta$  8.71 (d,  $J$  = 7.0 Hz, 1H), 7.85 (d,  $J$  = 8.0 Hz, 1H), 7.65 (s, 1H), 7.59 (d,  $J$  = 7.8 Hz, 1H), 7.52-7.43 (m, 3H), 7.41-7.27 (m, 5H), 7.21-7.11 (m, 2H), 6.08-5.91 (m, 1H), 4.39 (d,  $J$  = 8.4 Hz, 1H), 3.35 (d,  $J$  = 17.9 Hz, 1H), 3.02 (d,  $J$  = 18.3 Hz, 1H); **<sup>13</sup>C NMR**(101 MHz, DMSO- $d_6$ )  $\delta$  200.3, 173.8, 167.0, 153.0, 141.7, 134.7, 133.3, 131.5, 131.2, 129.3, 129.0, 128.7, 128.0, 127.5, 127.0, 126.4, 88.5, 52.5, 49.9, 36.2; **IR** (neat): 3399, 2923, 1788, 1717, 1667, 1519, 1101, 702, 635, 493  $\text{cm}^{-1}$ ; **HRMS** (ESI):  $m/z$  for  $[M+H]^+$ : calcd 432.0997, found 432.0995; **HPLC**: Daicel Chiralpak IB, *n*-hexane/*i*-PrOH = 80/20, flow rate = 1 mL/min,  $\lambda$  = 254 nm,  $t_{\text{major}}$  = 17.12 min and  $t_{\text{minor}}$  = 13.33 min.

**((2S,3S,4R)-4'-bromo-1',5-dioxo-3-phenyl-1',3',4,5-tetrahydro-3H-spiro[furan-2,2'-inden]-4-yl)benzamide (3h):**



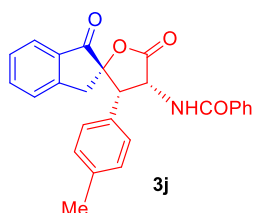
Yellow solid in 39% isolated yield (56mg, >20:1 dr);  $[\alpha]_{\text{D}}^{20} = +172$  (c = 1.0, DMSO, 99% ee); **m.p.** = 236.1-237.4 °C; **<sup>1</sup>H NMR** (400 MHz, DMSO- $d_6$ )  $\delta$  8.71 (d,  $J$  = 7.3 Hz, 1H), 7.99 (s, 1H), 7.92 (d,  $J$  = 7.8 Hz, 1H), 7.52-7.43 (m, 4H), 7.41-7.28 (m, 5H), 7.19-7.10 (m, 2H), 6.02-5.90 (m, 1H), 4.39 (d,  $J$  = 8.7 Hz, 1H), 3.31 (d,  $J$  = 17.6 Hz, 1H), 2.96 (d,  $J$  = 18.3 Hz, 1H); **<sup>13</sup>C NMR** (101 MHz, DMSO- $d_6$ )  $\delta$  200.3, 173.8, 167.0, 150.1, 139.1, 134.6, 133.3, 131.5, 129.3, 129.1, 128.7, 128.0, 127.5, 127.1, 121.5, 88.7, 52.4, 49.8, 36.1; **IR** (neat): 3384, 2933, 1798, 1714, 1662, 1524, 1132, 1084, 633, 509  $\text{cm}^{-1}$ ; **HRMS** (ESI):  $m/z$  for  $[M+H]^+$ : calcd 476.0492, found 476.0491; **HPLC**: Daicel Chiralpak IB, *n*-hexane/*i*-PrOH = 80/20, flow rate = 1 mL/min,  $\lambda$  = 254 nm,  $t_{\text{major}}$  = 13.19 min and  $t_{\text{minor}}$  = 17.52 min.

***N*-((2S,3S,4R)-3-(4-methoxyphenyl)-1',5-dioxo-1',3',4,5-tetrahydro-3H-spiro[furan-2,2'-inden]-4-yl)benzamide (3i):**



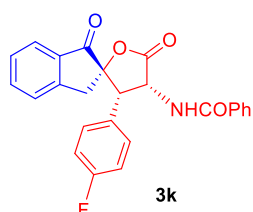
Yellow solid in 85% isolated yield (109mg, >20:1 dr);  $[\alpha]_{\text{D}}^{20} = +147$  (c = 1.0, DMSO, 99% ee); **m.p.** = 207.1-208.4 °C; **<sup>1</sup>H NMR** (400 MHz, DMSO- $d_6$ )  $\delta$  8.69 (d,  $J$  = 7.6 Hz, 1H), 7.84 (d,  $J$  = 7.6 Hz, 1H), 7.76 (t,  $J$  = 7.9 Hz, 1H), 7.60-7.45 (m, 5H), 7.41-7.33 (m, 2H), 7.10 (d,  $J$  = 8.7 Hz, 2H), 6.91 (d,  $J$  = 8.7 Hz, 2H), 6.05-5.97 (m, 1H), 4.30 (d,  $J$  = 8.8 Hz, 1H), 3.74 (s, 3H), 3.33 (d,  $J$  = 18.2 Hz, 1H), 3.03 (d,  $J$  = 18.2 Hz, 1H); **<sup>13</sup>C NMR**(101 MHz, DMSO- $d_6$ )  $\delta$  201.5, 174.0, 167.0, 158.7, 151.0, 136.8, 133.3, 132.4, 131.5, 130.4, 128.5, 128.1, 127.5, 126.9, 126.6, 124.8, 114.1, 88.8, 55.0, 52.4, 49.4, 36.3; **IR** (neat): 3360, 2917, 1791, 1708, 1662, 1258, 1185, 931, 754, 471  $\text{cm}^{-1}$ ; **HRMS** (ESI):  $m/z$  for  $[M+H]^+$ : calcd 428.1492, found 428.1491; **HPLC**: Daicel Chiralpak IB, *n*-hexane/*i*-PrOH = 80/20, flow rate = 1 mL/min,  $\lambda$  = 254 nm,  $t_{\text{major}}$  = 17.64 min and  $t_{\text{minor}}$  = 26.98 min.

***N*-((2*S*,3*S*,4*R*)-1',5-dioxo-3-(*p*-tolyl)-1',3',4,5-tetrahydro-3*H*-spiro[furan-2,2'-inden]-4-yl)benzamide (3j):**



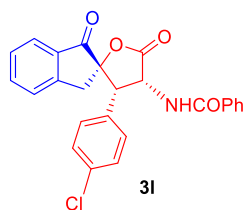
Yellow solid in 70% isolated yield (86mg, >20:1 dr);  $[\alpha]_{\text{D}}^{20} = +120$  (c = 1.0, DMSO, 97% ee); **m.p.** = 239.5-240.9 °C; **<sup>1</sup>H NMR** (400 MHz, DMSO-*d*<sub>6</sub>) δ 8.68 (d, *J* = 7.6 Hz, 1H), 7.83 (d, *J* = 7.7 Hz, 1H), 7.76 (t, *J* = 7.3 Hz, 1H), 7.56-7.45 (m, 5H), 7.39-7.33 (m, 2H), 7.16 (d, *J* = 7.9 Hz, 2H), 7.05 (d, *J* = 7.9 Hz, 2H), 6.03-5.93 (m, 1H), 4.29 (d, *J* = 8.8 Hz, 1H), 3.28 (d, *J* = 18.2 Hz, 1H), 2.98 (d, *J* = 18.2 Hz, 1H), 2.29 (s, 3H); **<sup>13</sup>C NMR** (101 MHz, DMSO-*d*<sub>6</sub>) δ 201.5, 174.0, 167.0, 151.1, 136.9, 133.3, 132.4, 132.2, 131.9, 131.6, 129.2, 128.5, 128.1, 127.5, 126.9, 124.8, 88.7, 52.4, 49.6, 36.3, 20.7; **IR** (neat): 3336, 2926, 1796, 1709, 1661, 1340, 1124, 998, 748, 567 cm<sup>-1</sup>; **HRMS** (ESI): *m/z* for [M+H]<sup>+</sup>: calcd 412.1543, found 412.1542; **HPLC**: Daicel Chiralpak IA, *n*-hexane/*i*-PrOH = 50/50, flow rate = 1 mL/min, λ = 254 nm, *t*<sub>major</sub> = 14.53 min and *t*<sub>minor</sub> = 10.41 min.

***N*-((2*S*,3*S*,4*R*)-3-(4-fluorophenyl)-1',5-dioxo-1',3',4,5-tetrahydro-3*H*-spiro[furan-2,2'-inden]-4-yl)benzamide (3k):**



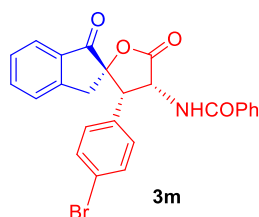
Yellow solid in 80% isolated yield (100mg, >20:1 dr);  $[\alpha]_{\text{D}}^{20} = +148$  (c = 1.0, DMSO, 99% ee); **m.p.** = 200.3-201.5 °C; **<sup>1</sup>H NMR** (400 MHz, DMSO-*d*<sub>6</sub>) δ 8.78 (d, *J* = 7.5 Hz, 1H), 7.85 (d, *J* = 7.6 Hz, 1H), 7.78 (t, *J* = 7.5 Hz, 1H), 7.57-7.47 (m, 5H), 7.41-7.35 (m, 2H), 7.24-7.17 (m, 4H), 6.07-5.95 (m, 1H), 4.43 (d, *J* = 8.8 Hz, 1H), 3.39 (d, *J* = 18.1 Hz, 1H), 3.03 (d, *J* = 18.2 Hz, 1H); **<sup>13</sup>C NMR** (101 MHz, DMSO-*d*<sub>6</sub>) δ 201.3, 173.8, 167.0, 161.58 (d, *J* = 244.1 Hz), 151.1, 136.9, 133.3, 132.4, 131.9, 131.1, 131.1, 128.6, 128.1, 127.5, 126.9, 124.8, 115.6, 115.4, 88.5, 52.5, 49.1, 36.3; **<sup>19</sup>F NMR** (376 MHz, DMSO) δ -114.39. **IR** (neat): 3349, 2921, 1793, 1698, 1337, 1224, 1195, 921, 732, 453 cm<sup>-1</sup>; **HRMS** (ESI): *m/z* for [M+H]<sup>+</sup>: calcd 416.1293, found 416.1290; **HPLC**: Daicel Chiralpak IA, *n*-hexane/*i*-PrOH = 50/50, flow rate = 1 mL/min, λ = 254 nm, *t*<sub>major</sub> = 18.92 min and *t*<sub>minor</sub> = 9.89 min.

***N*-((2*S*,3*S*,4*R*)-3-(4-chlorophenyl)-1',5-dioxo-1',3',4,5-tetrahydro-3*H*-spiro[furan-2,2'-inden]-4-yl)benzamide (3l):**

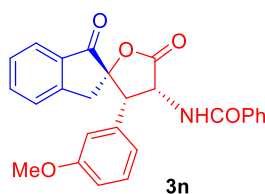


Yellow solid in 72% isolated yield (93mg, >20:1 dr);  $[\alpha]_{\text{D}}^{20} = +152$  (c = 1.0, DMSO, 99% ee); **m.p.** = 216.3-217.4 °C; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.87 (d, *J* = 7.7 Hz, 1H), 7.70-7.64 (m, 1H), 7.50-7.39

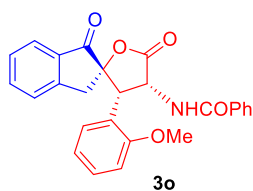
(m, 4H), 7.37-7.29 (m, 5H), 7.09 (d,  $J = 8.4$  Hz, 2H), 6.33 (d,  $J = 5.2$  Hz, 1H), 6.06-5.98 (m, 1H), 4.31 (d,  $J = 8.3$  Hz, 1H), 3.42 (d,  $J = 18.0$  Hz, 1H), 3.13 (d,  $J = 18.0$  Hz, 1H);  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  200.2, 174.8, 167.3, 150.2, 136.9, 134.5, 133.2, 132.7, 132.0, 130.1, 129.5, 128.7, 126.8, 126.5, 125.7, 89.0, 53.7, 51.2, 36.6; **IR** (neat): 3350, 2923, 1795, 1703, 1663, 1326, 1220, 1192, 726, 522  $\text{cm}^{-1}$ ; **HRMS** (ESI):  $m/z$  for  $[\text{M}+\text{H}]^+$ : calcd 432.0997 found 432.0995; **HPLC**: Daicel Chiralpak IA,  $n$ -hexane/ $i$ -PrOH = 50/50, flow rate = 1 mL/min,  $\lambda = 254$  nm,  $t_{\text{major}} = 23.54$  min and  $t_{\text{minor}} = 10.71$  min.  
***N*-((2S,3S,4R)-3-(4-bromophenyl)-1',5-dioxo-1',3',4,5-tetrahydro-3H-spiro[furan-2,2'-inden]-4-yl)benzamide (3m):**



Yellow solid in 80% isolated yield (111mg, >20:1 dr);  $[\alpha]_{\text{D}}^{20} = +158$  ( $c = 1.0$ ,  $\text{CDCl}_3$ , 99% ee); **m.p.** = 204.1-205.5  $^{\circ}\text{C}$ ;  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.87 (d,  $J = 7.7$  Hz, 1H), 7.69-7.64 (m, 1H), 7.50-7.39 (m, 6H), 7.37-7.31 (m, 3H), 7.03 (d,  $J = 8.5$  Hz, 2H), 6.33 (d,  $J = 5.5$  Hz, 1H), 6.05-5.98 (m, 1H), 4.30 (d,  $J = 8.3$  Hz, 1H), 3.41 (d,  $J = 18.0$  Hz, 1H), 3.13 (d,  $J = 18.0$  Hz, 1H);  $^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  200.1, 174.8, 167.3, 150.2, 136.9, 133.7, 133.1, 132.7, 132.5, 132.0, 130.4, 128.7, 126.8, 126.5, 125.7, 122.6, 88.9, 53.7, 51.3, 36.6; **IR**(neat): 3337, 2923, 1795, 1660, 1157, 1069, 725, 515  $\text{cm}^{-1}$ ; **HRMS** (ESI):  $m/z$  for  $[\text{M}+\text{H}]^+$ : calcd 476.0492, found 476.0490; **HPLC**: Daicel Chiralpak IB,  $n$ -hexane/ $i$ -PrOH = 70/30, flow rate = 1 mL/min,  $\lambda = 254$  nm,  $t_{\text{major}} = 12.43$  min and  $t_{\text{minor}} = 26.42$  min.  
***N*-((2S,3S,4R)-3-(3-methoxyphenyl)-1',5-dioxo-1',3',4,5-tetrahydro-3H-spiro[furan-2,2'-inden]-4-yl)benzamide (3n):**

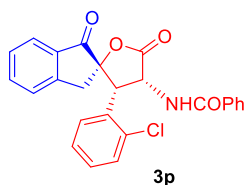


Yellow solid in 75% isolated yield (96mg, >20:1 dr);  $[\alpha]_{\text{D}}^{20} = +148$  ( $c = 1.0$ , DMSO, 99% ee); **m.p.** = 180.0-181.4  $^{\circ}\text{C}$ ;  $^1\text{H NMR}$  (400 MHz,  $\text{DMSO-d}_6$ )  $\delta$  8.73 (d,  $J = 7.7$  Hz, 1H), 7.84 (d,  $J = 7.5$  Hz, 1H), 7.77 (t,  $J = 7.5$  Hz, 1H), 7.56-7.45 (m, 5H), 7.39-7.33 (m, 2H), 7.27 (t,  $J = 7.9$  Hz, 1H), 6.92-6.87 (m, 1H), 6.76-6.68 (m, 2H), 6.02 (t,  $J = 8.2$  Hz, 1H), 4.31 (d,  $J = 8.8$  Hz, 1H), 3.72 (s, 3H), 3.41 (d,  $J = 18.3$  Hz, 1H), 3.06 (d,  $J = 18.3$  Hz, 1H);  $^{13}\text{C NMR}$  (101 MHz,  $\text{DMSO-d}_6$ )  $\delta$  202.0, 174.4, 167.6, 159.7, 151.7, 137.4, 136.7, 133.9, 132.8, 132.0, 130.3, 129.0, 128.6, 128.0, 127.4, 125.3, 121.9, 115.3, 113.8, 89.0, 55.4, 53.0, 50.4, 36.8; **IR** (neat): 3266, 2922, 1783, 1716, 1665, 1326, 1227, 1173, 719, 472  $\text{cm}^{-1}$ ; **HRMS** (ESI):  $m/z$  for  $[\text{M}+\text{H}]^+$ : calcd 428.1492, found 428.1490; **HPLC**: Daicel Chiralpak IA,  $n$ -hexane/ $i$ -PrOH = 50/50, flow rate = 1 mL/min,  $\lambda = 254$  nm,  $t_{\text{major}} = 11.01$  min and  $t_{\text{minor}} = 8.60$  min.  
***N*-((2S,3S,4R)-3-(2-methoxyphenyl)-1',5-dioxo-1',3',4,5-tetrahydro-3H-spiro[furan-2,2'-inden]-4-yl)benzamide (3o):**



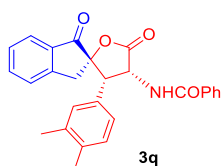
Yellow solid in 88% isolated yield (113mg, >20:1 dr);  $[\alpha]_{\text{D}}^{20} = +138$  (c = 1.0, DMSO, 99% ee); **m.p.** = 126.9-128.6 °C; **<sup>1</sup>H NMR** (400 MHz, DMSO-*d*<sub>6</sub>) δ 8.17 (d, *J* = 14.0 Hz, 1H), 7.87-7.80 (m, 1H), 7.78-7.71 (m, 1H), 7.57- 7.28 (m, 8H), 7.13-6.96 (m, 2H), 6.90-6.75 (m, 1H), 5.87-5.61 (m, 1H), 4.36 (d, *J* = 6.2 Hz, 1H), 3.76 (s, 3H), 3.31 (d, *J* = 22.7 Hz, 2H), 2.90 (d, *J* = 18.1 Hz, 1H); **<sup>13</sup>C NMR** (101 MHz, DMSO-*d*<sub>6</sub>) δ 202.1, 173.9, 167.3, 157.2, 151.1, 136.8, 133.5 132.3, 131.4, 129.7, 128.5, 128.0, 127.3, 126.8, 124.8, 122.7, 120.6, 110.9, 87.4, 55.0, 51.3, 36.0; **IR** (neat): 3339, 2937, 1783, 1718, 1664, 1334, 1226, 1021, 749, 491 cm<sup>-1</sup>; **HRMS**. (ESI): *m/z* for [M+H]<sup>+</sup>: calcd 428.1492, found 428.1491; **HPLC**: Daicel Chiralpak IB, *n*-hexane/*i*-PrOH = 80/20, flow rate = 1 mL/min, λ = 254 nm, *t*<sub>major</sub> = 13.92 min and *t*<sub>minor</sub> = 15.61 min.

***N*-((3S,4R)-3-(2-chlorophenyl)-1',5-dioxo-1',3',4,5-tetrahydro-3H-spiro[furan-2,2'-inden]-4-yl)benzamide (3p):**



Yellow solid in 75% isolated yield (97mg, >20:1 dr);  $[\alpha]_{\text{D}}^{20} = +175$  (c = 1.0, DMSO, 98% ee); **m.p.** = 212.1-213.8 °C; **<sup>1</sup>H NMR** (400 MHz, DMSO-*d*<sub>6</sub>) δ 8.85 (d, *J* = 7.2 Hz, 1H), 7.87 (d, *J* = 7.6 Hz, 1H), 7.79 (t, *J* = 7.4 Hz, 1H), 7.59-7.34 (m, 11H), 6.23-6.05 (m, 1H), 4.76 (d, *J* = 8.8 Hz, 1H), 3.54 (d, *J* = 18.1 Hz, 1H), 3.06 (d, *J* = 18.2 Hz, 1H); **<sup>13</sup>C NMR** (101 MHz, DMSO-*d*<sub>6</sub>) δ 201.2, 173.5, 167.1, 151.1, 137.1, 134.6, 133.3, 131.8, 131.6, 130.0, 129.7, 128.7, 128.1, 127.8, 127.5, 126.9, 124.9, 87.8, 52.0, 46.0, 36.2; **IR** (neat): 3375, 2926, 1789, 1713, 1667, 1328, 1119, 879, 744, 457 cm<sup>-1</sup>; **HRMS** (ESI): *m/z* for [M+H]<sup>+</sup>: calcd 432.0997, found 432.0996; **HPLC**: Daicel Chiralpak IA, *n*-hexane/*i*-PrOH = 50/50, flow rate = 1 mL/min, λ = 254 nm, *t*<sub>major</sub> = 10.78 min and *t*<sub>minor</sub> = 8.78 min.

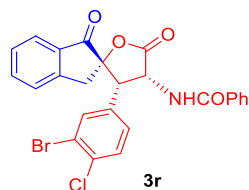
***N*-((3S,4R)-3-(3,4-dimethylphenyl)-1',5-dioxo-1',3',4,5-tetrahydro-3H-spiro[furan-2,2'-inden]-4-yl)benzamide (3q):**



Yellow solid in 74% isolated yield (94mg, >20:1 dr);  $[\alpha]_{\text{D}}^{20} = +115$  (c = 1.0, DMSO, 98% ee); **m.p.** = 204.8-206.4 °C; **<sup>1</sup>H NMR** (400 MHz, DMSO-*d*<sub>6</sub>) δ 8.70 (d, *J* = 7.7 Hz, 1H), 7.83 (d, *J* = 7.6 Hz, 1H), 7.78-7.71 (m, 1H), 7.59 -7.44 (m, 6H), 7.40-7.33 (m, 2H), 7.10 (d, *J* = 7.7 Hz, 1H), 6.94 (s, 1H), 6.88 (d, *J* = 7.7 Hz, 1H), 6.05-5.98 (m, 1H), 4.24 (d, *J* = 8.8 Hz, 1H), 3.31 (d, *J* = 18.2 Hz, 1H), 3.01 (d, *J* = 18.2 Hz, 1H), 2.19 (s, 3H), 2.18 (s, 3H); **<sup>13</sup>C NMR** (101 MHz, DMSO-*d*<sub>6</sub>) δ 201.6, 174.1, 167.0, 151.1, 136.8, 136.5, 135.7, 133.3, 132.3, 132.0, 131.5, 130.2, 129.7, 128.5, 128.1, 127.6, 126.9, 126.7, 124.8, 88.7, 52.3, 49.7, 36.3, 19.4, 19.0; **IR** (neat): 3364, 2923, 1791, 1707, 1668, 1320, 1227, 1168, 756, 466 cm<sup>-1</sup>; **HRMS** (ESI): *m/z* for [M+H]<sup>+</sup>: calcd 426.1700, found 426.1701; **HPLC**: Daicel Chiralpak IB, *n*-hexane/*i*-PrOH = 80/20, flow rate = 1 mL/min, λ = 254 nm, *t*<sub>major</sub> = 15.48 min and *t*<sub>minor</sub> = 13.85 min.

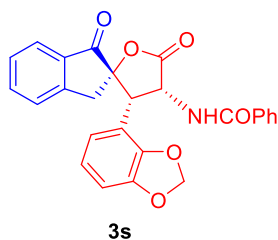


***N*-((2*S*,3*S*,4*R*)-3-(3-bromo-4-chlorophenyl)-1',5-dioxo-1',3',4,5-tetrahydro-3*H*-spiro[furan-2,2'-inden]-4-yl)benzamide (3r):**



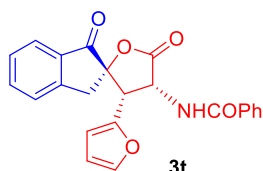
Yellow solid in 80% isolated yield (122mg, >20:1 dr);  $[\alpha]_D^{20} = +115$  (c = 1.0, DMSO, 99% ee); **m.p.** = 158.7-160.4 °C; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.87 (d, *J* = 7.7 Hz, 1H), 7.71-7.65 (m, 1H), 7.50-7.44 (m, 4H), 7.44-7.39 (m, 2H), 7.38 – 7.33 (m, 3H), 7.08 – 7.03 (m, 1H), 6.44 (d, *J* = 5.2 Hz, 1H), 6.04 – 5.95 (m, 1H), 4.33 (d, *J* = 8.3 Hz, 1H), 3.44 (d, *J* = 18.0 Hz, 1H), 3.13 (d, *J* = 18.0 Hz, 1H); **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>) δ 199.9, 174.5, 167.5, 150.1, 137.0, 135.0, 134.8, 134.0, 132.9, 132.6, 132.1, 131.0, 128.8, 128.7, 128.5, 126.9, 126.5, 125.7, 123.4, 88.8, 53.9, 51.0, 36.6; **IR** (neat): 3364, 2923, 1791, 1707, 1668, 1320, 1227, 1168, 756, 466 cm<sup>-1</sup>; **HRMS** (ESI): *m/z* for [M+H]<sup>+</sup>: calcd 510.0102, found 510.0103; **HPLC**: Daicel Chiralpak IB, *n*-hexane/*i*-PrOH = 80/20, flow rate = 1 mL/min, λ = 254 nm, *t*<sub>major</sub> = 11.45min and *t*<sub>minor</sub> = 24.14min.

***N*-((2*S*,3*S*,4*R*)-3-(benzo[*d*][1,3]dioxol-4-yl)-1',5-dioxo-1',3',4,5-tetrahydro-3*H*-spiro[furan-2,2'-inden]-4-yl)benzamide (3s):**



Yellow solid in 80% isolated yield (105mg, >20:1 dr);  $[\alpha]_D^{20} = +74$  (c = 1.0, DMSO, 97% ee); **m.p.** = 253.1-254.4 °C; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.78 (d, *J* = 7.6 Hz, 1H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.44-7.34 (m, 4H), 7.31- 7.23 (m, 3H), 6.67 (d, *J* = 7.9 Hz, 1H), 6.57-6.47 (m, 2H), 6.22 (d, *J* = 5.9 Hz, 1H), 6.02-5.94 (m, 1H), 5.88 (d, *J* = 6.1 Hz, 2H), 4.10 (d, *J* = 8.3 Hz, 1H), 3.34 (d, *J* = 18.0 Hz, 1H), 3.14 (d, *J* = 18.0 Hz, 1H); **<sup>13</sup>C NMR**(101 MHz, CDCl<sub>3</sub>) δ 199.4, 174.0, 166.3, 149.3, 147.4, 146.7, 135.7, 132.4, 131.7, 130.8, 127.6, 127.1, 125.9, 125.4, 124.6, 121.7, 107.9, 107.4, 106.6, 100.4, 88.1, 52.5, 50.4, 35.5; **IR** (neat): 3396, 2930, 1790, 1718, 1660, 1331, 1218, 873, 562, 471 cm<sup>-1</sup>; **HRMS** (ESI): *m/z* for [M+H]<sup>+</sup>: calcd 442.1285, found 442.1285; **HPLC**: Daicel Chiralpak IB, *n*-hexane/*i*-PrOH = 80/20, flow rate = 1 mL/min, λ = 254 nm, *t*<sub>major</sub> = 24.00 min and *t*<sub>minor</sub> = 57.42 min.

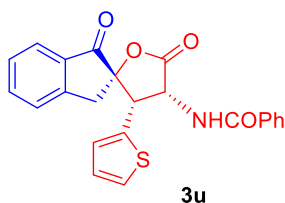
***N*-((3*R*,4*R*)-3-(furan-2-yl)-1',5-dioxo-1',3',4,5-tetrahydro-3*H*-spiro[furan-2,2'-inden]-4-yl)benzamide (3t):**



Yellow solid in 74% isolated yield (86mg, >20:1 dr);  $[\alpha]_D^{20} = +140$  (c = 1.0, DMSO, 90% ee); **m.p.** = 188.7-190.1 °C; **<sup>1</sup>H NMR** (400 MHz, DMSO-*d*<sub>6</sub>) δ 8.77 (d, *J* = 7.7 Hz, 1H), 7.87-7.75 (m, 2H), 7.71 (s, 1H), 7.66 (d, *J* = 7.4 Hz, 2H), 7.60-7.48 (m, 3H), 7.45-7.37 (m, 2H), 6.49-6.26 (m, 2H), 5.96-5.84 (m, 1H), 4.53 (d, *J* = 8.8 Hz, 1H), 3.38 (d, *J* = 17.2 Hz, 1H), 3.03 (d, *J* = 18.2 Hz, 1H); **<sup>13</sup>C NMR**(101 MHz,

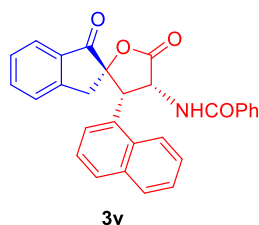
DMSO- $d_6$ )  $\delta$  201.0, 173.2, 167.3, 151.0, 148.9, 143.9, 136.9, 133.3, 132.4, 131.6, 128.6, 128.1, 127.7, 126.9, 124.8, 111.0, 110.1, 87.5, 51.3, 44.1, 36.0; **IR** (neat): 3441, 2925, 1784, 1707, 1668, 1232, 1164, 786, 597, 467  $\text{cm}^{-1}$ ; **HRMS** (ESI):  $m/z$  for  $[M+H]^+$ : calcd 408.1206, found 410.0998; **HPLC**: Daicel Chiralpak IB, *n*-hexane/*i*-PrOH = 50/50, flow rate = 1 mL/min,  $\lambda$  = 254 nm,  $t_{\text{major}}$  = 12.64 min and  $t_{\text{minor}}$  = 13.57 min.

***N*-((3*S*,4*R*)-1',5-dioxo-3-(thiophen-2-yl)-1',3',4,5-tetrahydro-3*H*-spiro[furan-2,2'-inden]-4-yl)benzamide (3u):**



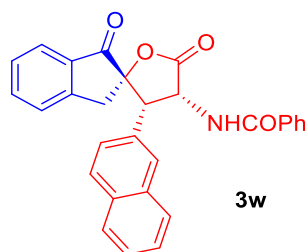
Yellow solid in 74% isolated yield (89mg, >20:1 dr);  $[\alpha]_{\text{D}}^{20} = +207$  ( $c = 1.0$ , DMSO, 99% ee); **m.p.** = 212.6-213.9  $^{\circ}\text{C}$ ;  **$^1\text{H NMR}$**  (400 MHz, DMSO- $d_6$ )  $\delta$  8.78 (d,  $J = 7.5$  Hz, 1H), 7.83 (d,  $J = 7.6$  Hz, 1H), 7.79-7.73 (m, 1H), 7.67-7.61 (m, 2H), 7.58-7.48 (m, 4H), 7.45-7.36 (m, 2H), 7.08-7.01 (m, 1H), 6.99-6.92 (m, 1H), 5.96-5.85 (m, 1H), 4.76 (d,  $J = 8.6$  Hz, 1H), 3.43 (d,  $J = 18.3$  Hz, 1H), 3.27 (d,  $J = 18.3$  Hz, 1H);  **$^{13}\text{C NMR}$** (101 MHz, DMSO- $d_6$ )  $\delta$  201.0, 173.3, 167.2, 151.2, 136.9, 135.7, 133.3, 132.6, 131.6, 128.6, 128.1, 127.6, 127.3, 126.9, 126.3, 124.7, 88.6, 52.7, 45.6, 36.4; **IR** (neat): 3433, 2926, 1778, 1708, 1670, 1327, 1234, 1128, 909, 702, 466  $\text{cm}^{-1}$ ; **HRMS** (ESI):  $m/z$  for  $[M+H]^+$ : calcd 402.1158, found 404.0950; **HPLC**: Daicel Chiralpak IB, *n*-hexane/*i*-PrOH = 50/50, flow rate = 1 mL/min,  $\lambda$  = 254 nm,  $t_{\text{major}}$  = 10.28 min and  $t_{\text{minor}}$  = 9.33 min.

***N*-((3*S*,4*R*)-3-(naphthalen-1-yl)-1',5-dioxo-1',3',4,5-tetrahydro-3*H*-spiro[furan-2,2'-inden]-4-yl)benzamide (3v):**



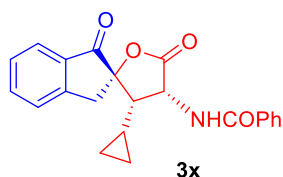
Yellow solid in 72% isolated yield (97mg, >20:1 dr);  $[\alpha]_{\text{D}}^{20} = +136$  ( $c = 1.0$ , DMSO, 99% ee); **m.p.** = 167.6-168.9  $^{\circ}\text{C}$ ;  **$^1\text{H NMR}$**  (400 MHz, DMSO- $d_6$ )  $\delta$  8.60 (d,  $J = 8.1$  Hz, 1H), 7.98-7.85 (m, 4H), 7.75-7.69 (m, 1H), 7.66-7.60 (m, 1H), 7.57-7.51 (m, 2H), 7.44-7.29 (m, 4H), 7.23-7.15 (m, 4H), 6.42-6.33 (m, 1H), 5.30 (d,  $J = 8.7$  Hz, 1H), 3.56 (d,  $J = 18.3$  Hz, 1H), 3.11 (d,  $J = 18.3$  Hz, 1H);  **$^{13}\text{C NMR}$** (101 MHz, DMSO- $d_6$ )  $\delta$  201.5, 174.2, 167.4, 151.0, 136.8, 133.4, 132.4, 131.2, 130.8, 128.5, 128.2, 127.8, 127.3, 126.8, 126.2, 125.6, 124.9, 123.2, 88.5, 52.9, 44.0, 36.50; **IR** (neat): 3399, 2970, 1789, 1717, 1662, 1513, 1087, 902, 785, 575  $\text{cm}^{-1}$ ; **HRMS** (ESI):  $m/z$  for  $[M+H]^+$ : calcd 468.1570, found 470.1360; **HPLC**: Daicel Chiralpak IB, *n*-hexane/*i*-PrOH = 80/20, flow rate = 1 mL/min,  $\lambda$  = 254 nm,  $t_{\text{major}}$  = 16.22 min and  $t_{\text{minor}}$  = 20.35min.

***N*-((3*S*,4*R*)-3-(naphthalen-2-yl)-1',5-dioxo-1',3',4,5-tetrahydro-3*H*-spiro[furan-2,2'-inden]-4-yl)benzamide (3w):**



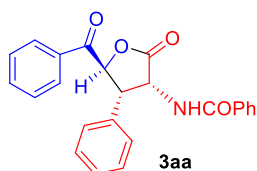
Yellow solid in 71% isolated yield (95mg, >20:1 dr);  $[\alpha]_{\text{D}}^{20} = +142$  ( $c = 1.0$ , DMSO, 99% ee); **m.p.** = 207.6-208.9 °C; **<sup>1</sup>H NMR** (400 MHz, DMSO- $d_6$ )  $\delta$  8.83 (d,  $J = 7.2$  Hz, 1H), 7.97-7.89 (m, 2H), 7.89-7.81 (m, 2H), 7.79-7.69 (m, 2H), 7.57-7.44 (m, 6H), 7.42-7.36 (m, 1H), 7.35-7.30 (m, 1H), 7.30-7.19 (m, 2H), 6.17-6.06 (m, 1H), 4.54 (d,  $J = 8.7$  Hz, 1H), 3.39 (d,  $J = 18.3$  Hz, 1H), 3.02 (d,  $J = 18.2$  Hz, 1H); **<sup>13</sup>C NMR** (101 MHz, DMSO- $d_6$ )  $\delta$  201.5, 174.0, 167.0, 151.2, 136.9, 133.2, 132.8, 132.6, 132.2, 131.4, 128.6, 128.2, 128.0, 127.5, 126.8, 126.3, 124.8, 88.6, 52.6, 50.2, 36.3; **IR** (neat): 3349, 2917, 1791, 1705, 1661, 1345, 1211, 1185, 931, 749, 646, 480  $\text{cm}^{-1}$ ; **HRMS** (ESI):  $m/z$  for  $[M+H]^+$ : calcd 468.1570, found 470.1363; **HPLC**: Daicel Chiralpak IA, *n*-hexane/*i*-PrOH = 60/40, flow rate = 1 mL/min,  $\lambda = 254$  nm,  $t_{\text{major}} = 28.66$  min and  $t_{\text{minor}} = 46.62$  min.

***N*-((3S,4R)-3-cyclopropyl-1',5-dioxo-1',3',4,5-tetrahydro-3H-spiro[furan-2,2'-inden]-4-yl)benzamide (3x):**



Yellow solid in 70% isolated yield (76mg, >20:1 dr);  $[\alpha]_{\text{D}}^{20} = +58$  ( $c = 1.0$ , DMSO, 73% ee); **m.p.** = 245.6-246.9 °C; **<sup>1</sup>H NMR** (400 MHz, DMSO- $d_6$ )  $\delta$  9.14 (d,  $J = 8.5$  Hz, 1H), 7.93 (d,  $J = 7.2$  Hz, 2H), 7.86-7.75 (m, 2H), 7.70-7.64 (m, 1H), 7.62-7.48 (m, 4H), 5.59-5.48 (m, 1H), 4.08 (d,  $J = 17.8$  Hz, 1H), 3.45 (d,  $J = 17.8$  Hz, 1H), 2.23 – 2.08 (m, 1H), 0.97 – 0.81 (m, 1H), 0.58 – 0.43 (m, 2H), 0.00 (d,  $J = 2.5$  Hz, 2H); **<sup>13</sup>C NMR** (101 MHz, DMSO- $d_6$ )  $\delta$  202.1, 174.2, 166.7, 151.3, 136.8, 133.5, 132.4, 131.7, 128.4, 127.5, 126.8, 124.6, 88.9, 54.9, 51.5, 48.5, 34.6, 8.4, 3.8, 3.4, 2.7; **IR** (neat): 3350, 2922, 1788, 1709, 1661, 1334, 1232, 1073, 998, 713, 572  $\text{cm}^{-1}$ ; **HRMS** (ESI):  $m/z$  for  $[M+H]^+$ : calcd 382.1414, found 384.1205; **HPLC**: Daicel Chiralpak IB, *n*-hexane/*i*-PrOH = 80/20, flow rate = 1 mL/min,  $\lambda = 254$  nm,  $t_{\text{major}} = 10.16$  min and  $t_{\text{minor}} = 15.48$  min.

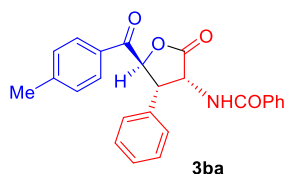
***N*-((3R,4S,5S)-5-benzoyl-2-oxo-4-phenyltetrahydrofuran-3-yl)benzamide (3aa)**



Yellow solid in 70% isolated yield (81mg, >20:1 dr);  $[\alpha]_{\text{D}}^{20} = +36$  ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ , 98% ee); **m.p.** = 90.6-91.9 °C; **<sup>1</sup>H NMR** (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.85 (d,  $J = 7.6$  Hz, 2H), 7.59 (t,  $J = 7.4$  Hz, 1H), 7.48-7.40 (m, 2H), 7.38-7.27 (m, 6H), 7.25-7.16 (m, 4H), 6.07 (s, 1H), 6.00 (d,  $J = 5.9$  Hz, 1H), 5.18-5.10 (m, 1H), 4.26 (d,  $J = 8.6$  Hz, 1H); **<sup>13</sup>C NMR** (101 MHz,  $\text{CDCl}_3$ )  $\delta$  192.5, 174.3, 167.7, 135.4, 134.8, 133.1, 132.9, 132.0, 129.5, 129.3, 128.6, 127.6, 126.9, 82.7, 52.2, 47.7; **IR** (neat): 3345, 3030, 1792, 1654, 1562, 1151, 694, 510,  $\text{cm}^{-1}$ ; **HRMS** (ESI):  $m/z$  for  $[M+H]^+$ : calcd 386.1387, found

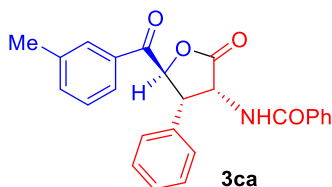
386.1386; **HPLC**: Daicel Chiralpak IB, *n*-hexane/*i*-PrOH = 80/20, flow rate = 1 mL/min,  $\lambda$  = 254 nm,  $t_{\text{major}}$  = 12.22 min and  $t_{\text{minor}}$  = 33.33 min.

***N*-((3*R*,4*S*,5*S*)-5-(4-methylbenzoyl)-2-oxo-4-phenyltetrahydrofuran-3-yl)benzamide (3ba)**



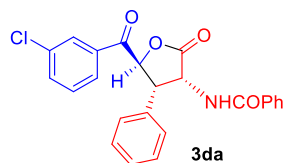
Yellow solid in 68% isolated yield (81mg, >20:1 dr);  $[\alpha]_{\text{D}}^{20}$  = +56 ( $c$  = 1.0,  $\text{CH}_2\text{Cl}_2$ , 99% ee); **m.p.** = 76.6-77.9 °C; **<sup>1</sup>H NMR** (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.75 (d,  $J$  = 8.2 Hz, 2H), 7.39-7.33 (m, 1H), 7.33-7.27 (m, 5H), 7.26-7.21 (m, 4H), 7.20-7.17 (m, 2H), 6.05 (d,  $J$  = 0.6 Hz, 1H), 5.94 (d,  $J$  = 6.2 Hz, 1H), 5.18-5.11 (m, 1H), 4.25 (d,  $J$  = 8.7 Hz, 1H), 2.37 (s, 3H); **<sup>13</sup>C NMR** (101 MHz,  $\text{CDCl}_3$ )  $\delta$  192.1, 174.4, 167.6, 146.0, 135.5, 133.2, 132.0, 130.4, 129.9, 129.5, 128.9, 128.5, 127.6, 126.8, 82.6, 52.2, 47.8, 21.9; **IR** (neat): 3356, 2927, 1800, 1667, 1494, 1137, 723, 634  $\text{cm}^{-1}$ ; **HRMS** (ESI):  $m/z$  for  $[\text{M}+\text{H}]^+$ : calcd 400.1543, found 400.1542; **HPLC**: Daicel Chiralpak IB, *n*-hexane/*i*-PrOH = 80/20, flow rate = 1 mL/min,  $\lambda$  = 254 nm,  $t_{\text{major}}$  = 10.97 min and  $t_{\text{minor}}$  = 21.07 min.

***N*-((3*R*,4*S*,5*S*)-5-(3-methylbenzoyl)-2-oxo-4-phenyltetrahydrofuran-3-yl)benzamide (3ca)**



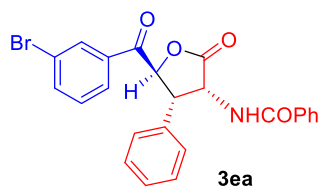
Yellow solid in 67% isolated yield (81mg, >20:1 dr);  $[\alpha]_{\text{D}}^{20}$  = +36 ( $c$  = 1.0,  $\text{CH}_2\text{Cl}_2$ , 92% ee); **m.p.** = 77.6-78.9 °C; **<sup>1</sup>H NMR** (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.78 (s, 1H), 7.67 (d,  $J$  = 7.7 Hz, 1H), 7.50-7.35 (m, 8H), 7.34-7.28 (m, 2H), 7.28-7.24 (m, 2H), 6.12 (s, 1H), 6.03 (d,  $J$  = 6.1 Hz, 1H), 5.26-5.18 (m, 1H), 4.33 (d,  $J$  = 8.7 Hz, 1H), 2.42 (s, 3H); **<sup>13</sup>C NMR** (101 MHz,  $\text{CDCl}_3$ )  $\delta$  192.7, 174.3, 167.6, 139.3, 135.5, 133.2, 132.9, 132.0, 129.5, 129.2, 129.0, 128.6, 127.6, 126.8, 125.8, 82.7, 52.2, 47.7, 21.4; **IR** (neat): 3337, 2921, 1786, 1656, 1157, 1149, 696, 511  $\text{cm}^{-1}$ ; **HRMS** (ESI):  $m/z$  for  $[\text{M}+\text{H}]^+$ : calcd 400.1543, found 400.1540; **HPLC**: Daicel Chiralpak IB, *n*-hexane/*i*-PrOH = 80/20, flow rate = 1 mL/min,  $\lambda$  = 254 nm,  $t_{\text{major}}$  = 11.74 min and  $t_{\text{minor}}$  = 25.07 min.

***N*-((3*R*,4*S*,5*S*)-5-(3-chlorobenzoyl)-2-oxo-4-phenyltetrahydrofuran-3-yl)benzamide (3da)**



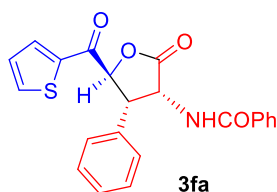
Yellow solid in 65% isolated yield (82mg, 10:1 dr);  $[\alpha]_{\text{D}}^{20}$  = +36 ( $c$  = 1.0,  $\text{CH}_2\text{Cl}_2$ , 97% ee); **m.p.** = 100.6-101.9 °C; **<sup>1</sup>H NMR** (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.98-7.92 (m, 1H), 7.79-7.74 (m, 1H), 7.66-7.61 (m, 1H), 7.49-7.42 (m, 2H), 7.41-7.35 (m, 5H), 7.32-7.24 (m, 4H), 6.13-6.05 (m, 2H), 5.23-5.15 (m, 1H), 4.34 (d,  $J$  = 8.9 Hz, 1H); **<sup>13</sup>C NMR** (101 MHz,  $\text{CDCl}_3$ )  $\delta$  191.6, 174.0, 167.7, 135.8, 135.1, 134.7, 134.5, 133.0, 132.0, 130.5, 129.6, 128.9, 128.6, 127.6, 126.8, 82.6, 52.2, 47.4; **IR** (neat): 3327, 2919, 1792, 1654, 1533, 1156, 700, 496  $\text{cm}^{-1}$ ; **HRMS** (ESI):  $m/z$  for  $[\text{M}+\text{H}]^+$ : calcd 420.0997, found 420.0993; **HPLC**: Daicel Chiralpak IB, *n*-hexane/*i*-PrOH = 80/20, flow rate = 1 mL/min,  $\lambda$  = 254 nm,  $t_{\text{major}}$  = 11.96 min and  $t_{\text{minor}}$  = 25.84 min.

***N*-((3*R*,4*S*,5*S*)-5-(3-bromobenzoyl)-2-oxo-4-phenyltetrahydrofuran-3-yl)benzamide (3ea)**



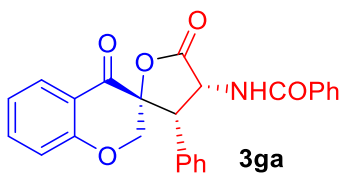
Yellow solid in 68% isolated yield (95mg, >20:1 dr);  $[\alpha]_{\text{D}}^{20} = +36$  ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ , 97% ee); **m.p.** = 102.6-103.9 °C; **<sup>1</sup>H NMR** (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.13-8.08 (m, 1H), 7.85-7.76 (m, 2H), 7.46-7.35 (m, 7H), 7.33-7.28 (m, 2H), 7.27-7.24 (m, 2H), 6.12-6.03 (m, 2H), 5.22-5.15 (m, 1H), 4.34 (d,  $J = 9.2$  Hz, 1H); **<sup>13</sup>C NMR** (101 MHz,  $\text{CDCl}_3$ )  $\delta$  191.5, 174.0, 167.7, 137.6, 135.1, 134.7, 133.0, 132.0, 131.8, 130.7, 129.6, 128.8, 128.6, 127.6, 127.1, 126.9, 123.7, 82.6, 52.1, 47.4; **IR** (neat): 3309, 2927, 1782, 1656, 1527, 1152, 688  $\text{cm}^{-1}$ ; **HRMS** (ESI):  $m/z$  for  $[\text{M}+\text{H}]^+$ : calcd 464.0492, found 464.0493; **HPLC**: Daicel Chiralpak IB,  $n$ -hexane/ $i$ -PrOH = 80/20, flow rate = 1 mL/min,  $\lambda = 254$  nm,  $t_{\text{major}} = 13.10$  min and  $t_{\text{minor}} = 28.54$  min.

***N*-((3R,4S,5S)-2-oxo-4-phenyl-5-(thiophene-2-carbonyl)tetrahydrofuran-3-yl)benzamide (3fa)**



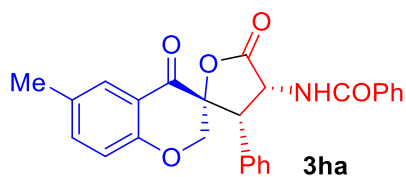
Yellow solid in 65% isolated yield (76mg, >20:1 dr);  $[\alpha]_{\text{D}}^{20} = +56$  ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ , 93% ee); **m.p.** = 111.6-112.9 °C; **<sup>1</sup>H NMR** (400 MHz,  $\text{DMSO}-d_6$ )  $\delta$  8.88 (d,  $J = 7.6$  Hz, 1H), 8.17 (d,  $J = 4.6$  Hz, 1H), 7.90 (d,  $J = 3.3$  Hz, 1H), 7.56 (d,  $J = 7.4$  Hz, 2H), 7.52-7.46 (m, 1H), 7.42-7.36 (m, 2H), 7.31-7.21 (m, 6H), 6.30 (d,  $J = 6.0$  Hz, 1H), 5.02 (t,  $J = 8.6$  Hz, 1H), 4.29-4.17 (m, 1H); **<sup>13</sup>C NMR** (101 MHz,  $\text{DMSO}-d_6$ )  $\delta$  188.0, 173.8, 167.5, 140.6, 137.7, 135.7, 135.2, 133.6, 132.1, 129.7, 129.3, 128.8, 128.1, 127.8, 82.6, 52.4, 48.1; **IR** (neat): 3327, 2923, 1786, 1660, 1409, 700, 503  $\text{cm}^{-1}$ ; **HRMS** (ESI):  $m/z$  for  $[\text{M}+\text{H}]^+$ : calcd 392.0951, found 392.0948; **HPLC**: Daicel Chiralpak IB,  $n$ -hexane/ $i$ -PrOH = 80/20, flow rate = 1 mL/min,  $\lambda = 254$  nm,  $t_{\text{major}} = 13.69$  min and  $t_{\text{minor}} = 28.28$  min.

***N*-((3R,3'S,4'R)-4,5'-dioxo-3'-phenyl-4',5'-dihydro-3'H-spiro[chromane-3,2'-furan]-4'-yl)benzamide (3ga)**

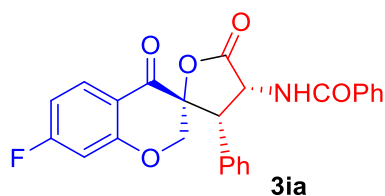


Yellow solid in 88% isolated yield (109mg, 7:1 dr);  $[\alpha]_{\text{D}}^{20} = +156$  ( $c = 1.0$ ,  $\text{CH}_2\text{Cl}_2$ , 92% ee); **m.p.** = 178.6-179.9 °C; **<sup>1</sup>H NMR** (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.02 (d,  $J = 7.6$  Hz, 1H), 7.65-7.50 (m, 1H), 7.46-7.26 (m, 8H), 7.22-7.07 (m, 3H), 6.96 (d,  $J = 8.3$  Hz, 1H), 6.40 (d,  $J = 5.5$  Hz, 1H), 5.66-5.53 (m, 1H), 4.46 (d,  $J = 11.9$  Hz, 1H), 4.35 (d,  $J = 8.2$  Hz, 1H), 4.25 (d,  $J = 11.9$  Hz, 1H); **<sup>13</sup>C NMR** (101 MHz,  $\text{CDCl}_3$ )  $\delta$  188.6, 174.2, 167.3, 161.3, 137.3, 133.1, 132.2, 131.9, 129.3, 128.9, 128.5, 126.9, 122.7, 118.1, 117.9, 82.0, 69.0, 52.2, 49.6; **IR** (neat): 3360, 2917, 1800, 1467, 1154, 1020, 717, 501  $\text{cm}^{-1}$ ; **HRMS** (ESI):  $m/z$  for  $[\text{M}+\text{H}]^+$ : calcd 414.1336, found 414.1334; **HPLC**: Daicel Chiralpak IB,  $n$ -hexane/ $i$ -PrOH = 80/20, flow rate = 1 mL/min,  $\lambda = 254$  nm,  $t_{\text{major}} = 11.05$  min and  $t_{\text{minor}} = 9.35$  min.

***N*-((3R,3'S,4'R)-6-methyl-4,5'-dioxo-3'-phenyl-4',5'-dihydro-3'H-spiro[chromane-3,2'-furan]-4'-yl)benzamide (3ha)**

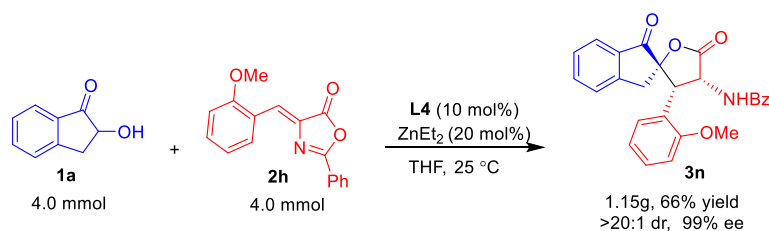


Yellow solid in 70% isolated yield (90mg, 10:1 dr);  $[\alpha]_D^{20} = +171$  (c = 1.0, CH<sub>2</sub>Cl<sub>2</sub>, 96% ee); **m.p.** = 168.6-169.9 °C; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 7.81 (d, *J* = 1.1 Hz, 1H), 7.44-7.34 (m, 7H), 7.32-7.26 (m, 2H), 7.16-7.09 (m, 2H), 6.86 (d, *J* = 8.5 Hz, 1H), 6.32 (d, *J* = 5.7 Hz, 1H), 5.65-5.55 (m, 1H), 4.43 (d, *J* = 11.9 Hz, 1H), 4.33 (d, *J* = 8.3 Hz, 1H), 4.22 (d, *J* = 11.9 Hz, 1H), 2.37 (s, 3H); **<sup>13</sup>C NMR** (101MHz, CDCl<sub>3</sub>) δ 188.7, 174.2, 167.3, 159.3, 138.5, 133.1, 132.3, 131.9, 129.3, 128.8, 128.5, 128.0, 126.8, 117.7, 82.0, 69.0, 52.1, 49.6, 20.5; **IR** (neat): 3311, 2921, 1798, 1663, 1489, 1156, 696, 504 cm<sup>-1</sup>; **HRMS** (ESI): *m/z* for [M+H]<sup>+</sup>: calcd 428.1492, found 428.1490; **HPLC**: Daicel Chiralpak IB, *n*-hexane/*i*-PrOH = 80/20, flow rate = 1 mL/min, λ = 254 nm, *t*<sub>major</sub> = 12.56 min and *t*<sub>minor</sub> = 25.39 min. ***N*-((3*R*,3'*S*,4'*R*)-7-fluoro-4,5'-dioxo-3'-phenyl-4',5'-dihydro-3'*H*-spiro[chromane-3,2'-furan]-4-yl)benzamide (3ia)**



Yellow solid in 75% isolated yield (97mg, 9:1 dr);  $[\alpha]_D^{20} = +80$  (c = 1.0, CH<sub>2</sub>Cl<sub>2</sub>, 97% ee); **m.p.** = 182.6-183.2 °C; **<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ 8.12-8.00 (m, 1H), 7.42-7.32 (m, 6H), 7.32-7.24 (m, 2H), 7.21-7.07 (m, 2H), 6.96-6.84 (m, 1H), 6.71-6.61 (m, 1H), 6.37 (d, *J* = 6.0 Hz, 1H), 5.68-5.52 (m, 1H), 4.47 (d, *J* = 12.0 Hz, 1H), 4.35 (d, *J* = 8.3 Hz, 1H), 4.26 (d, *J* = 12.0 Hz, 1H); **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>) δ 187.2, 174.0, 168.24 (d, *J* = 259.2 Hz), 167.3, 162.88 (d, *J* = 13.8 Hz), 133.1, 132.0, 131.3, 129.4, 129.0, 128.5, 126.8, 115.1, 111.6, 111.4, 105.0, 104.7, 81.6, 69.5, 52.2, 49.5; **<sup>19</sup>F NMR** (376 MHz, CDCl<sub>3</sub>) δ -97.41; **IR** (neat): 3296, 2917, 1792, 1613, 1250, 1071, 698, 496, cm<sup>-1</sup>; **HRMS** (ESI): *m/z* for [M+H]<sup>+</sup>: calcd 432.1242, found 432.1240; **HPLC**: Daicel Chiralpak IB, *n*-hexane/*i*-PrOH = 80/20, flow rate = 1 mL/min, λ = 254 nm, *t*<sub>major</sub> = 16.95 min and *t*<sub>minor</sub> = 28.86 min.

## Gram-scale reaction



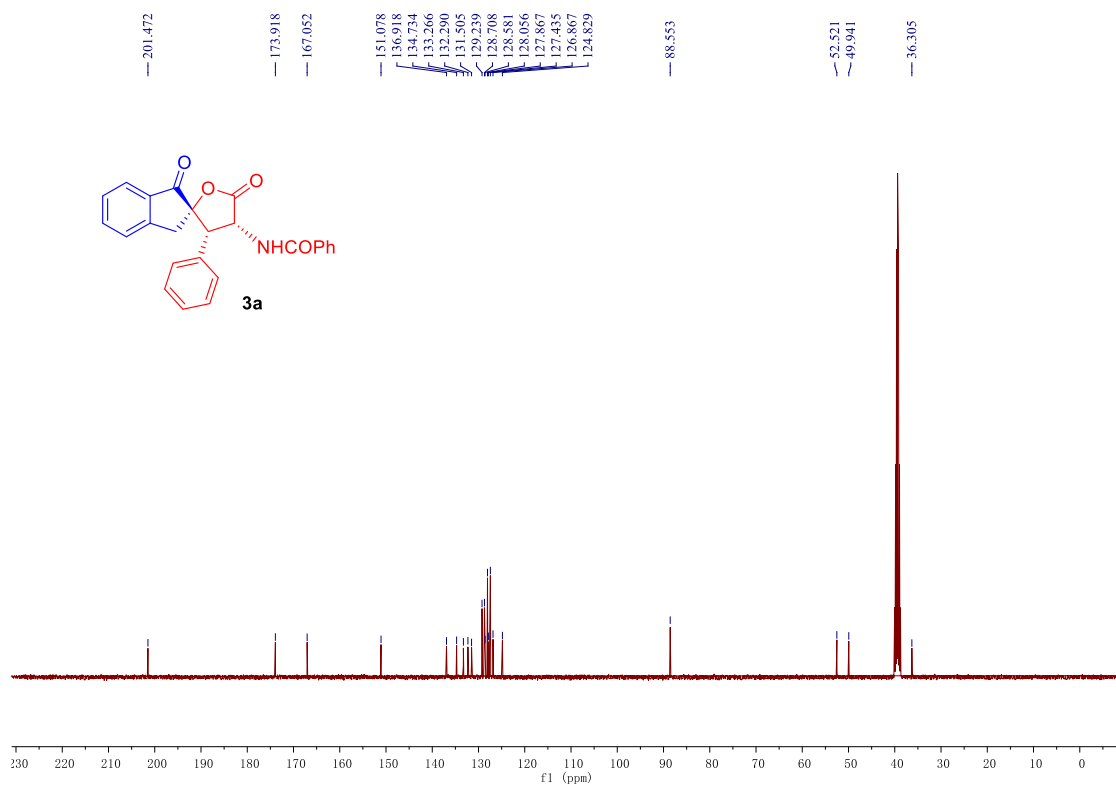
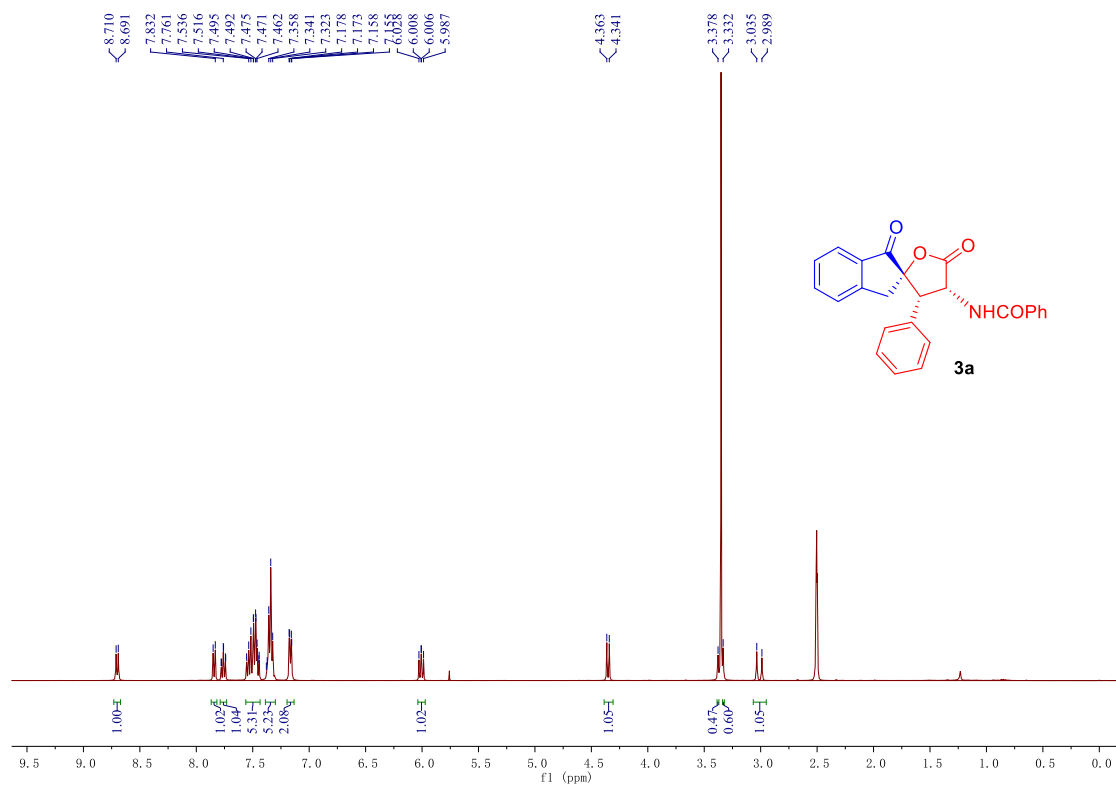
Under a nitrogen atmosphere, a solution of diethylzinc (800 μL, 1.0 M in hexane, 0.8 mmol) was added dropwise to a solution of **L4** (0.4 mmol) in MeCN (10 mL). After the mixture was stirred for 30 min at room temperature, then, α-hydroxy-1-indanone **1a** (4.0 mmol) and isatylydene malononitriles **2h** (4.0 mmol) were added. The reaction mixture was stirred for 24 h at the same temperature. The reaction was quenched with HCl solution (1 M, 2 mL), and the organic layer was extracted with EA (3 × 5 mL). The combined organic layer was washed with brine and dried over Na<sub>2</sub>SO<sub>4</sub>. The solvent was removed under

reduced pressure by using a rotary evaporator. The residue was purified by flash chromatography with petroleum ether/ethyl acetate (4/1) to afford the desired product 1.15g of **3n**.

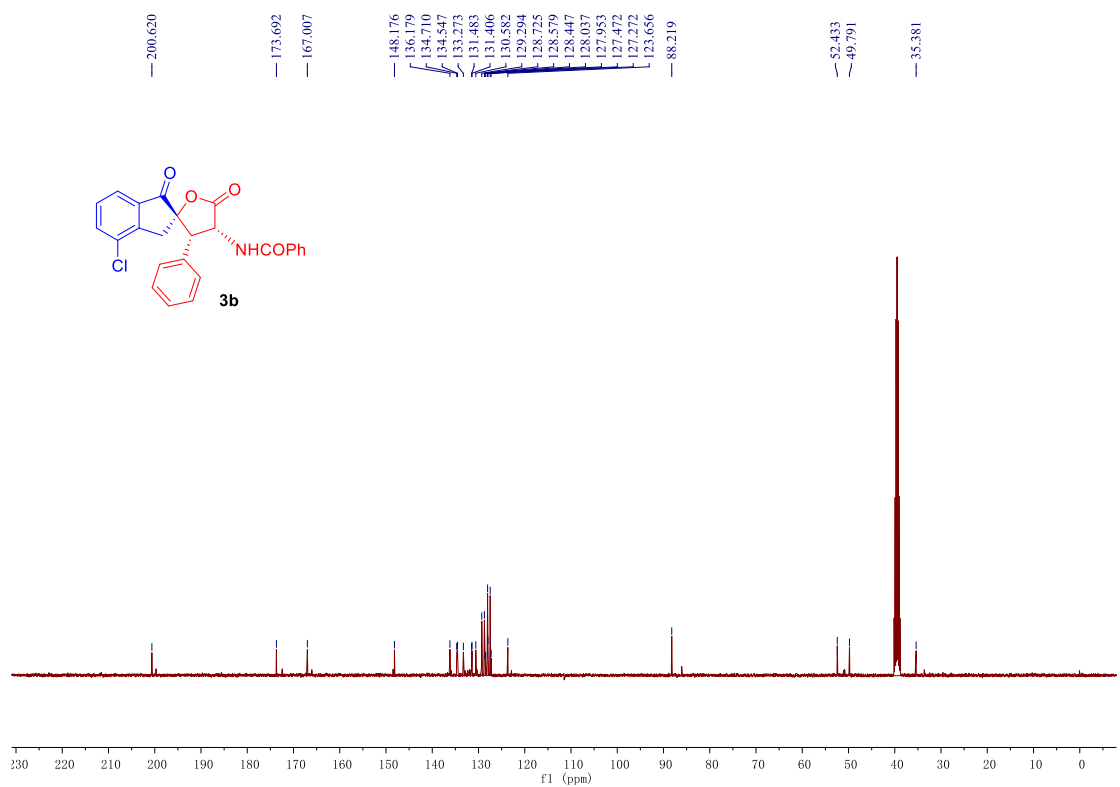
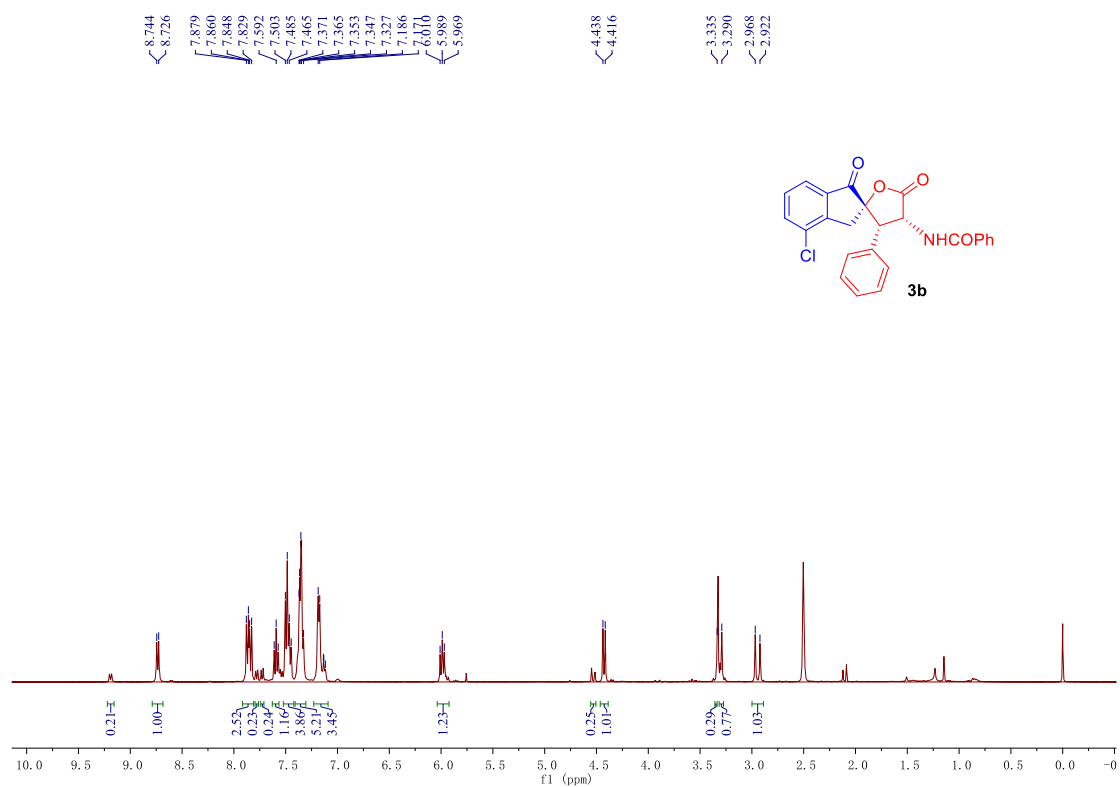
## References

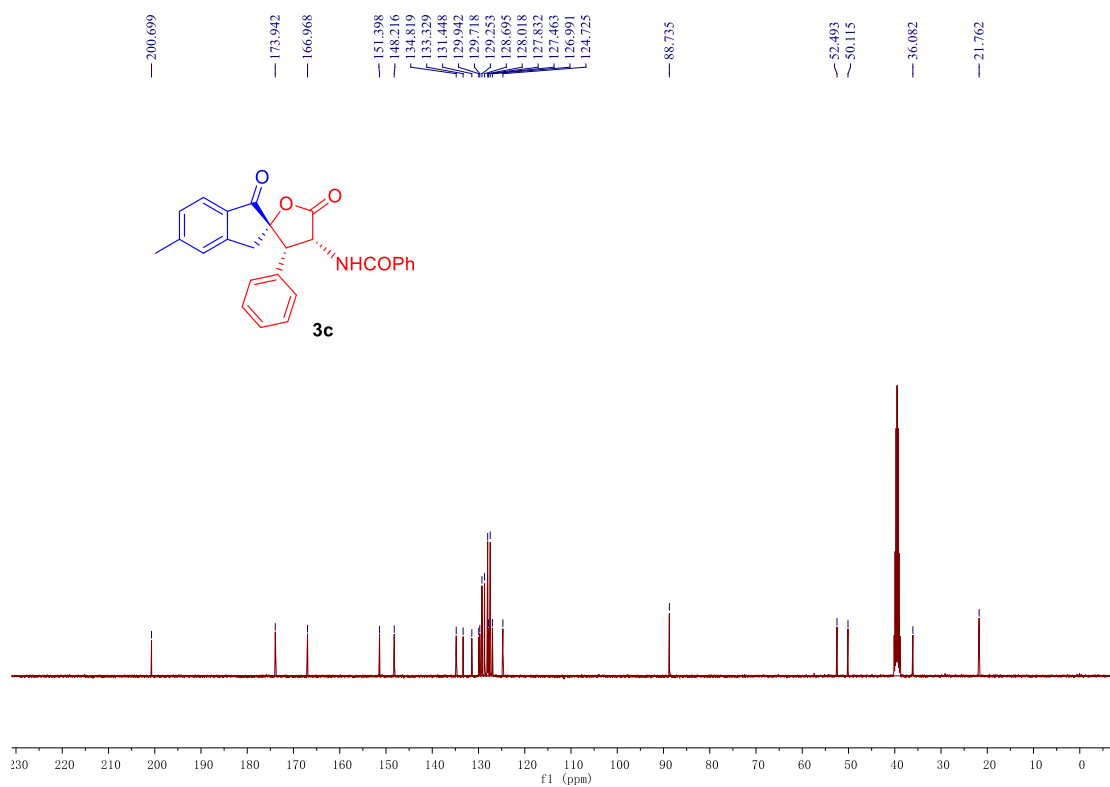
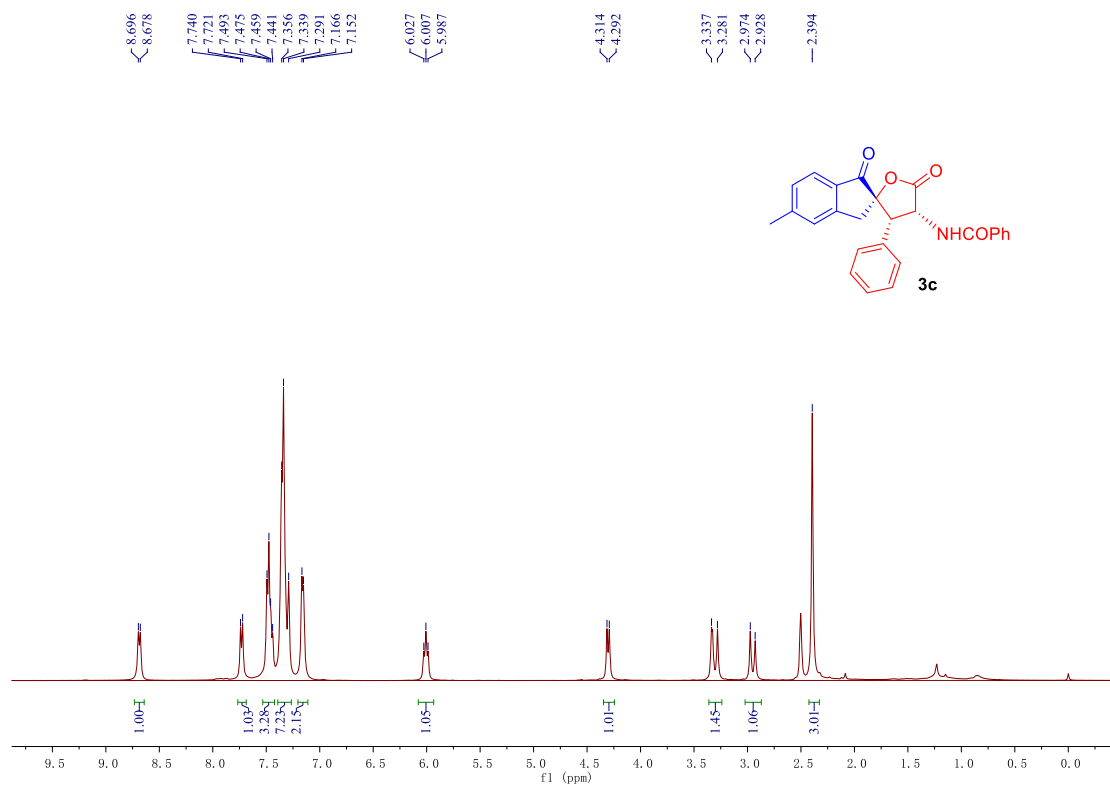
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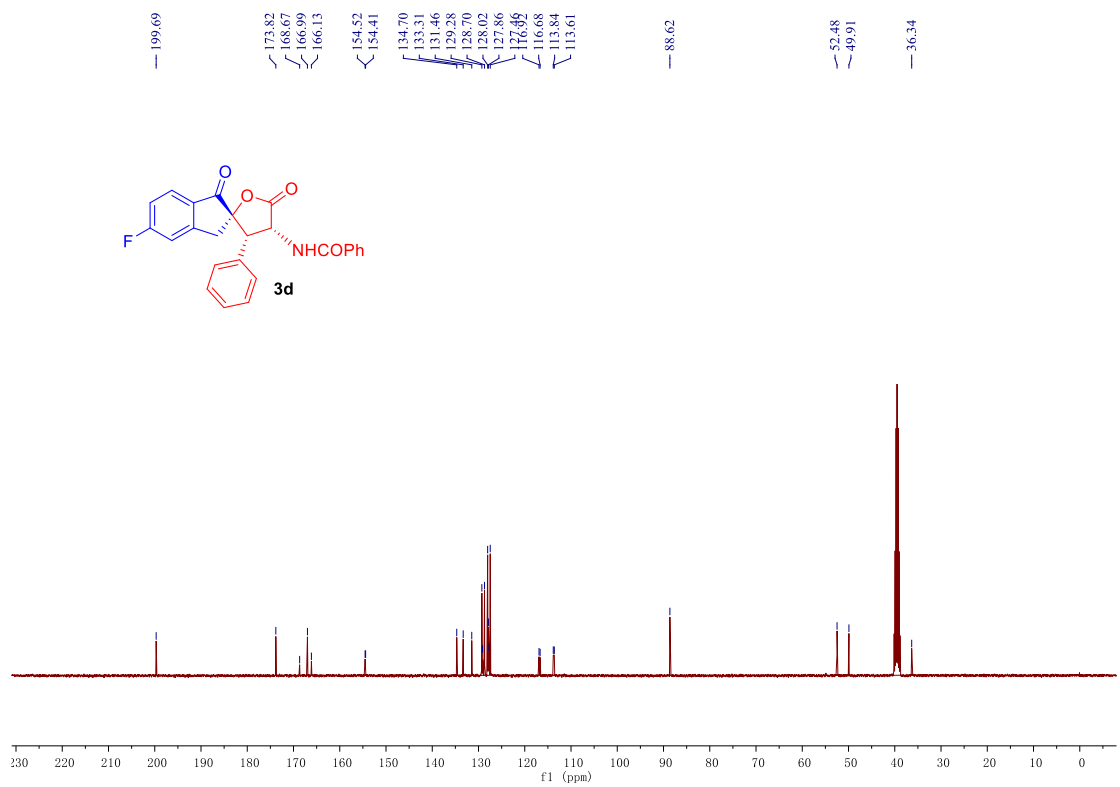
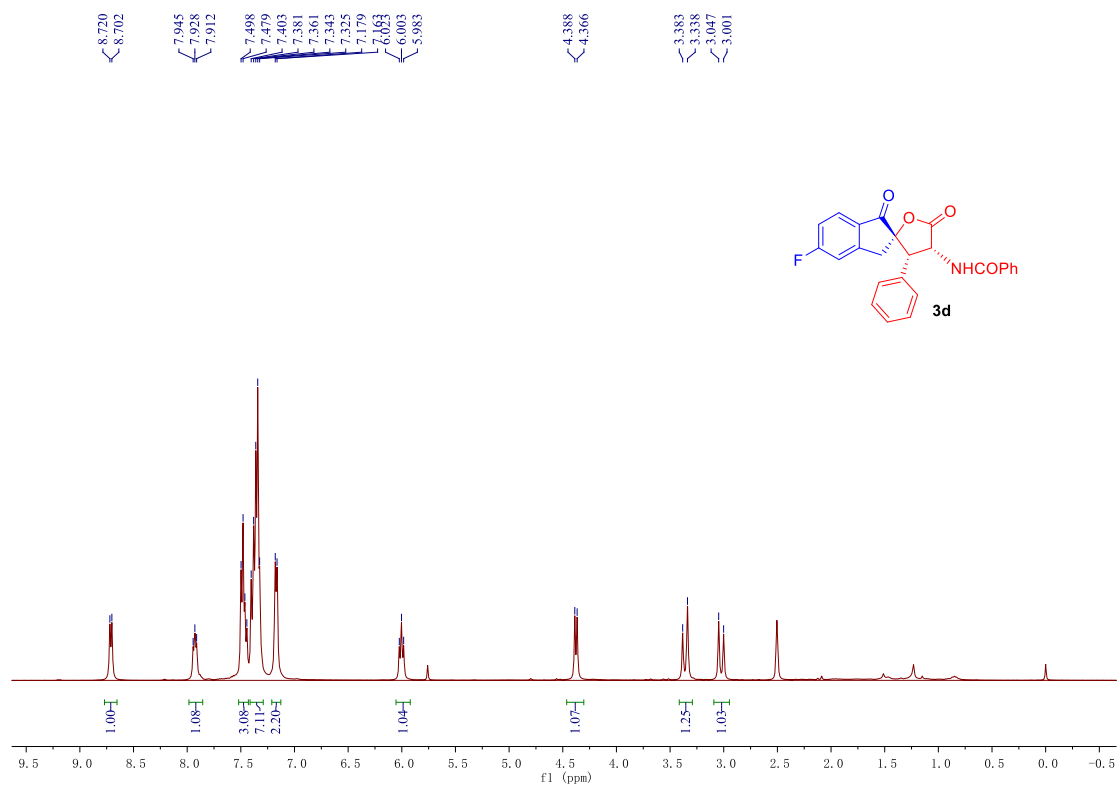
# NMR Spectra of compounds

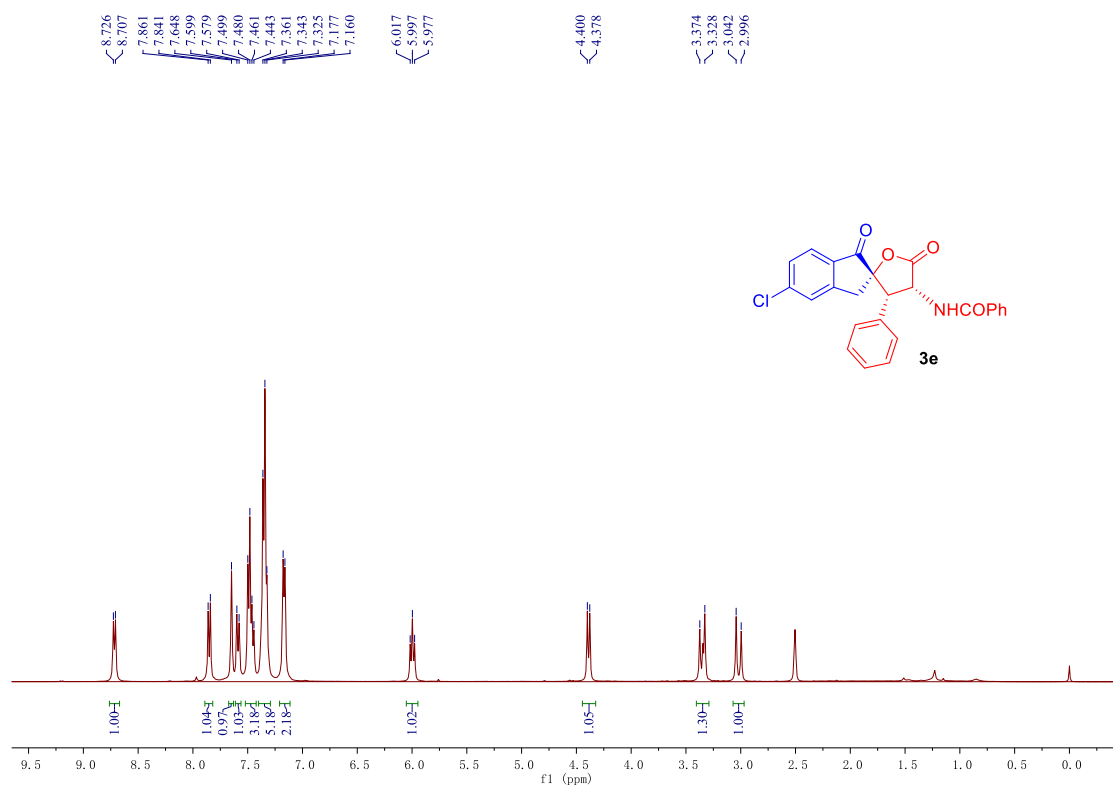
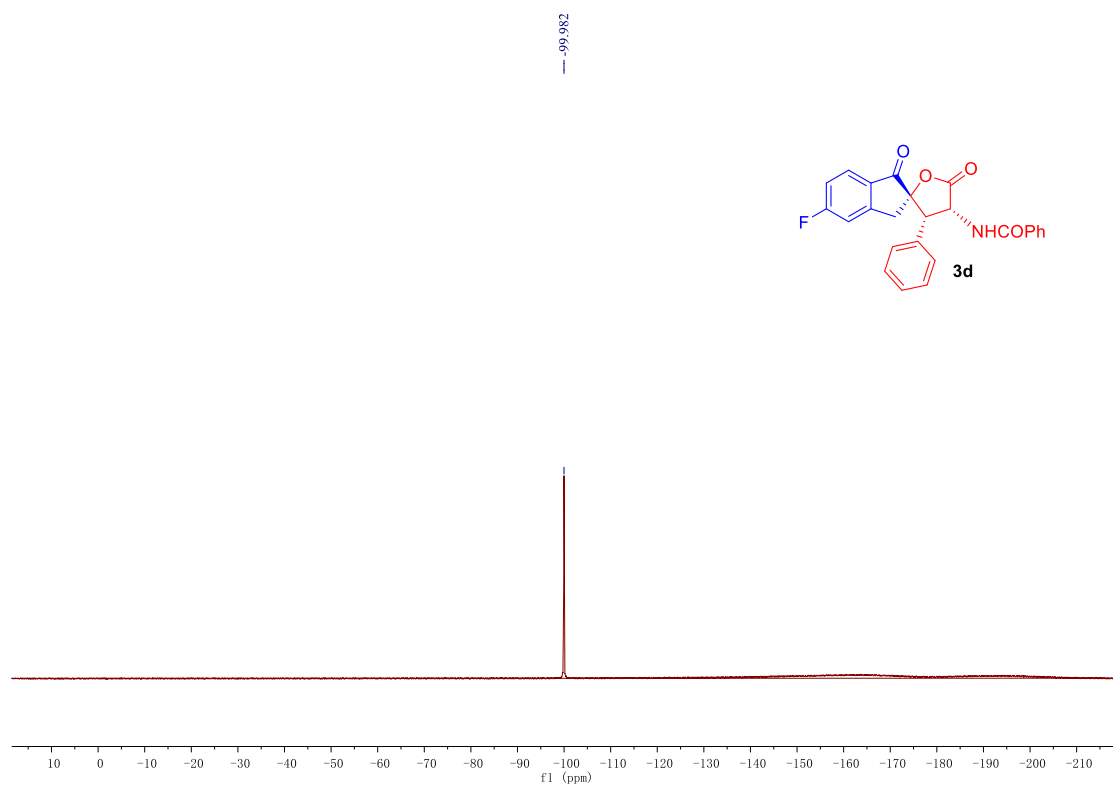


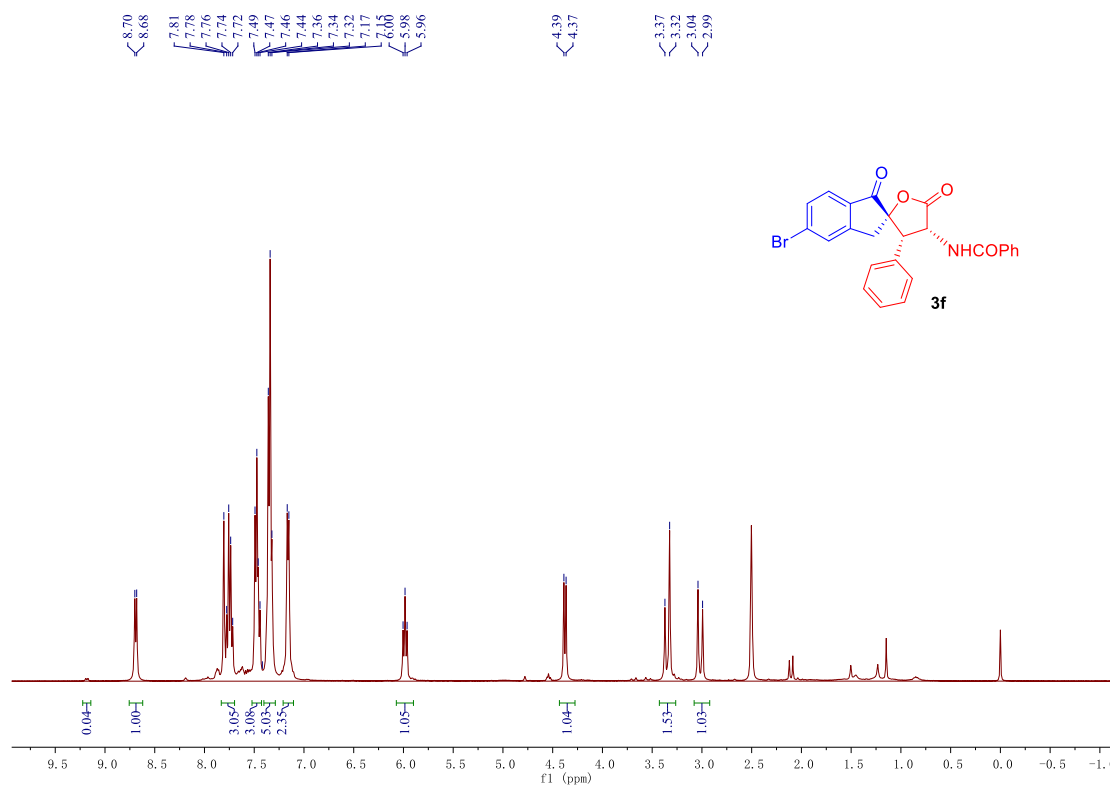
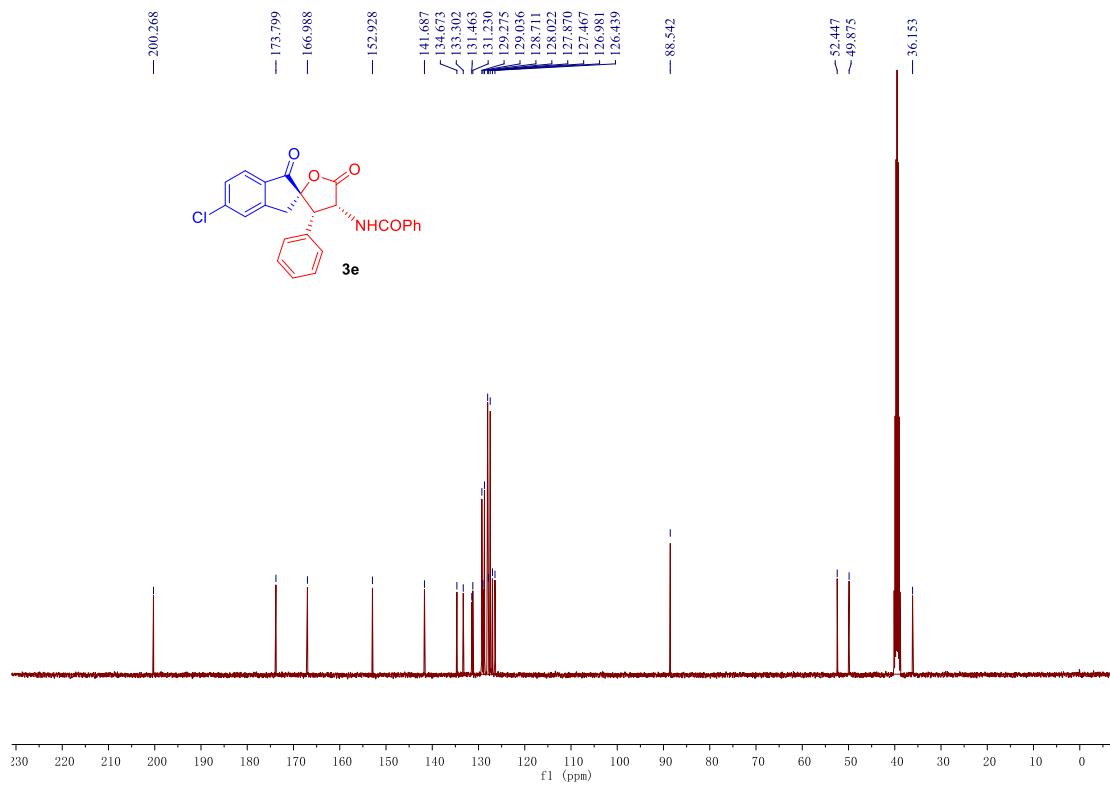


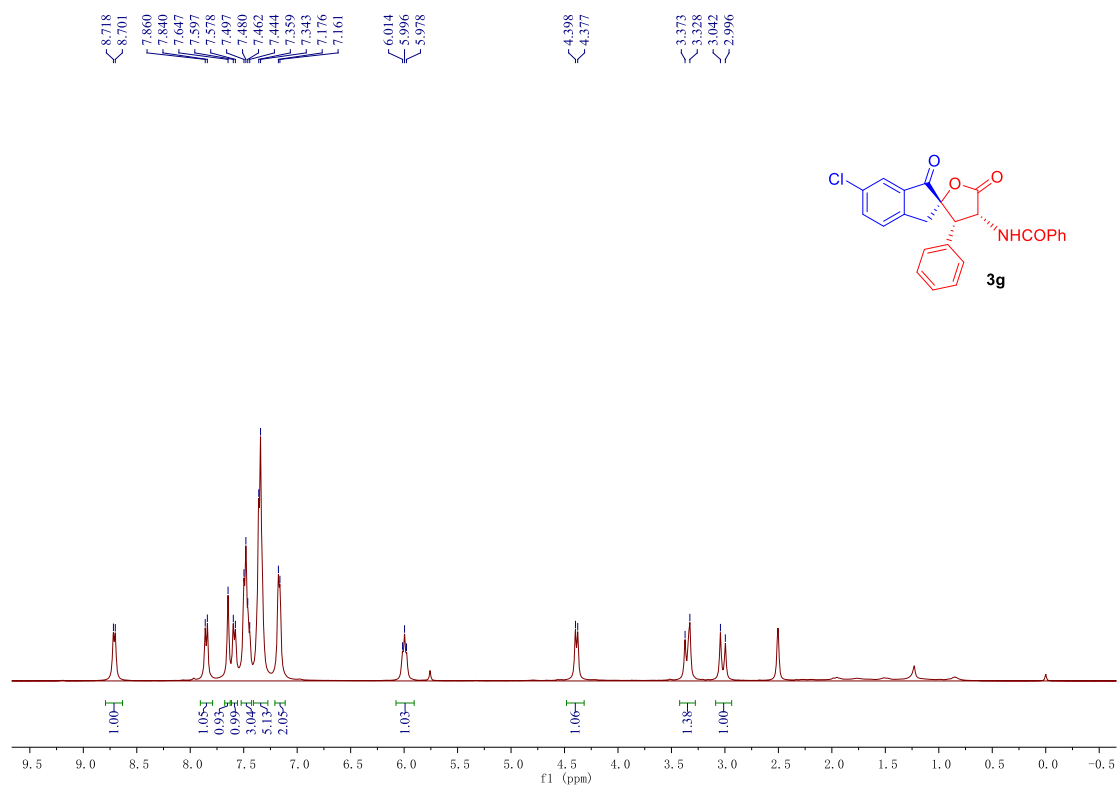
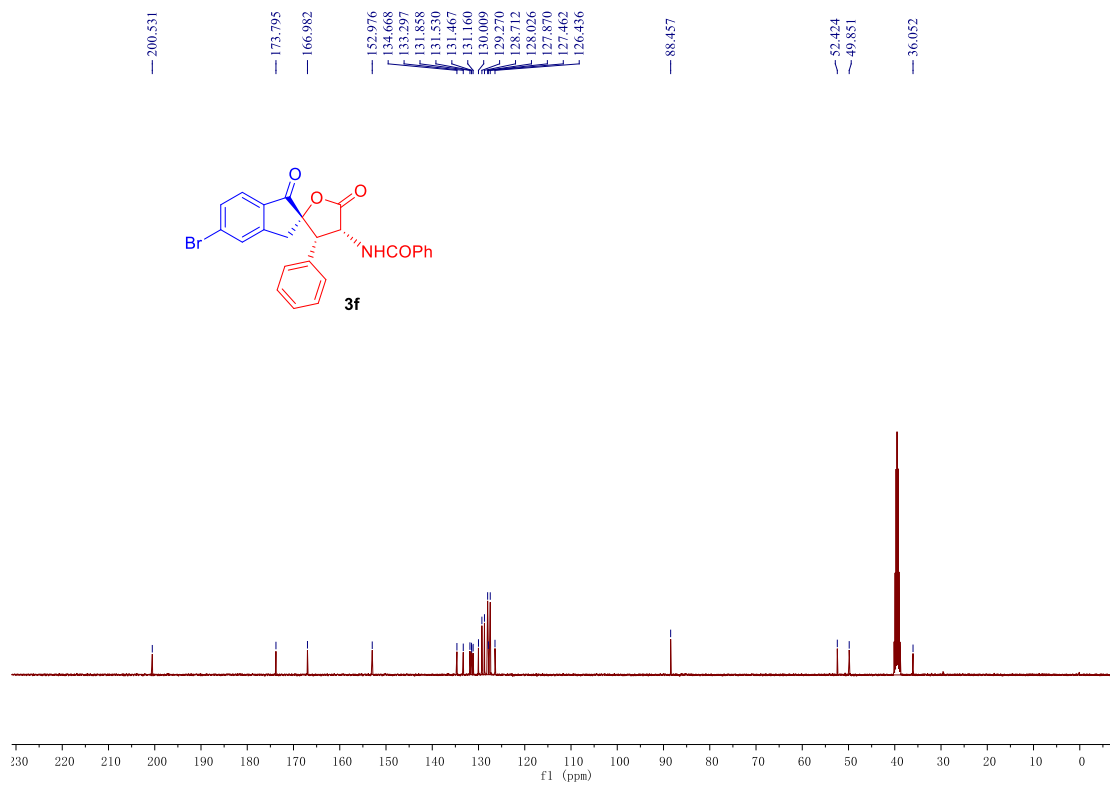


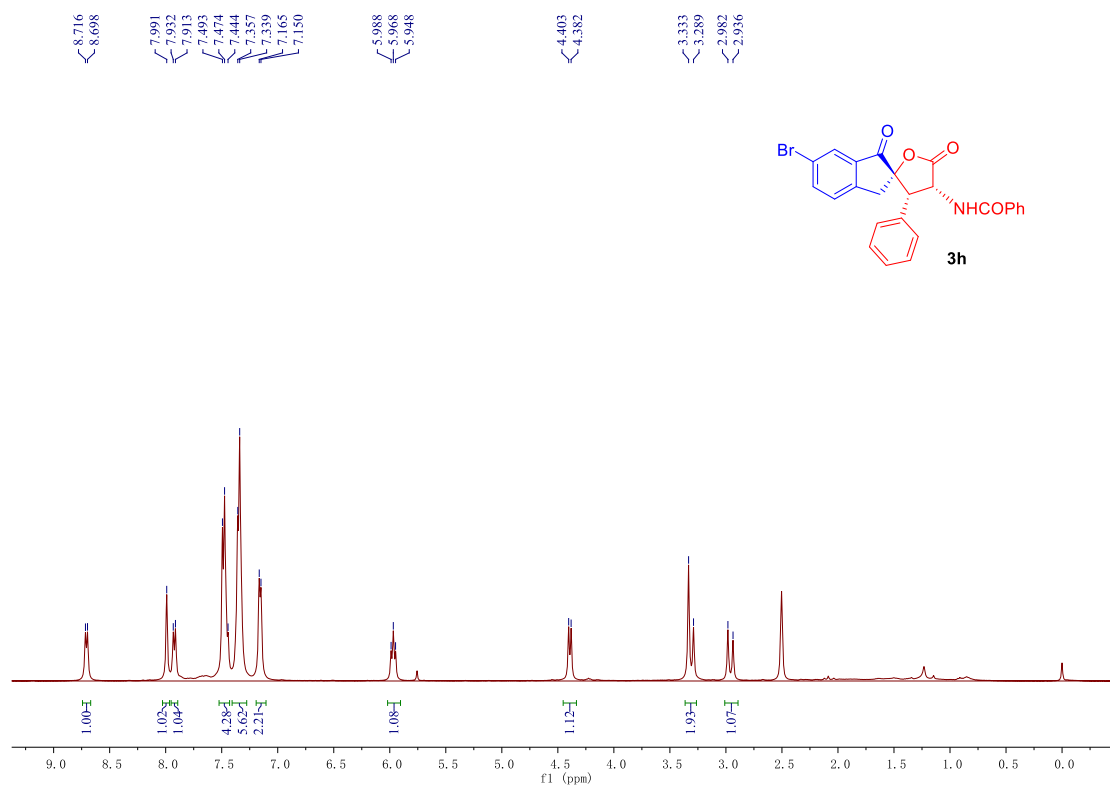
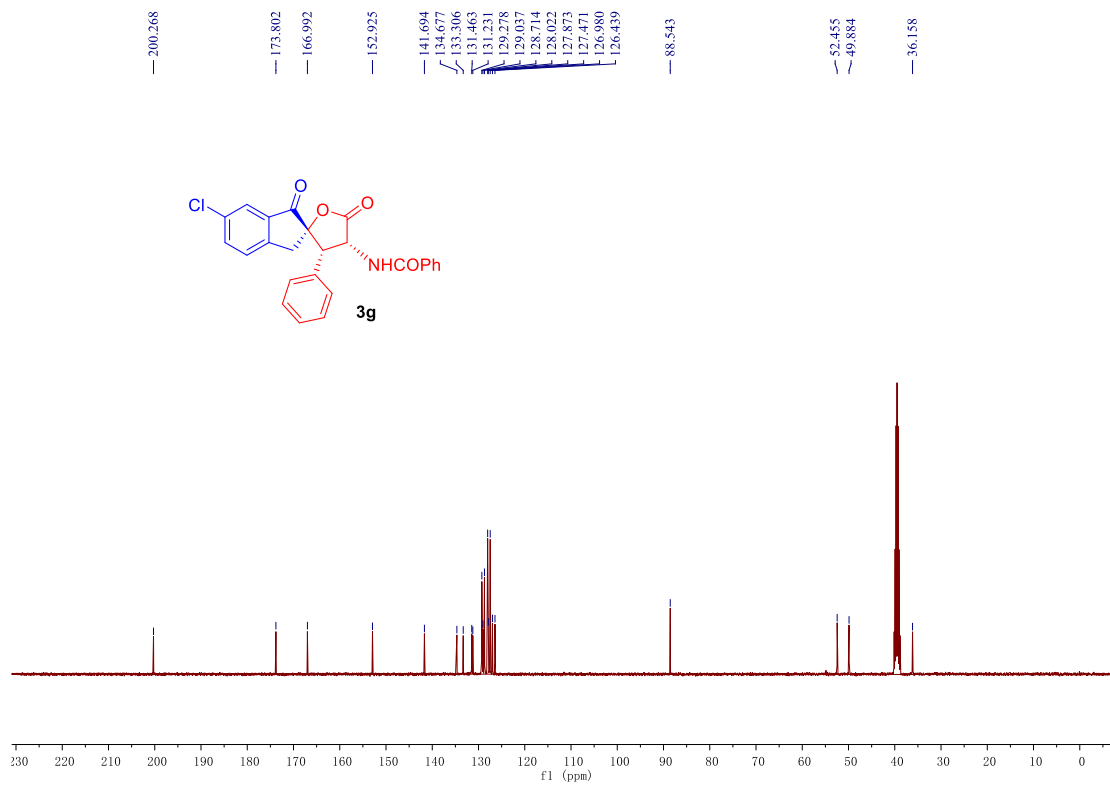


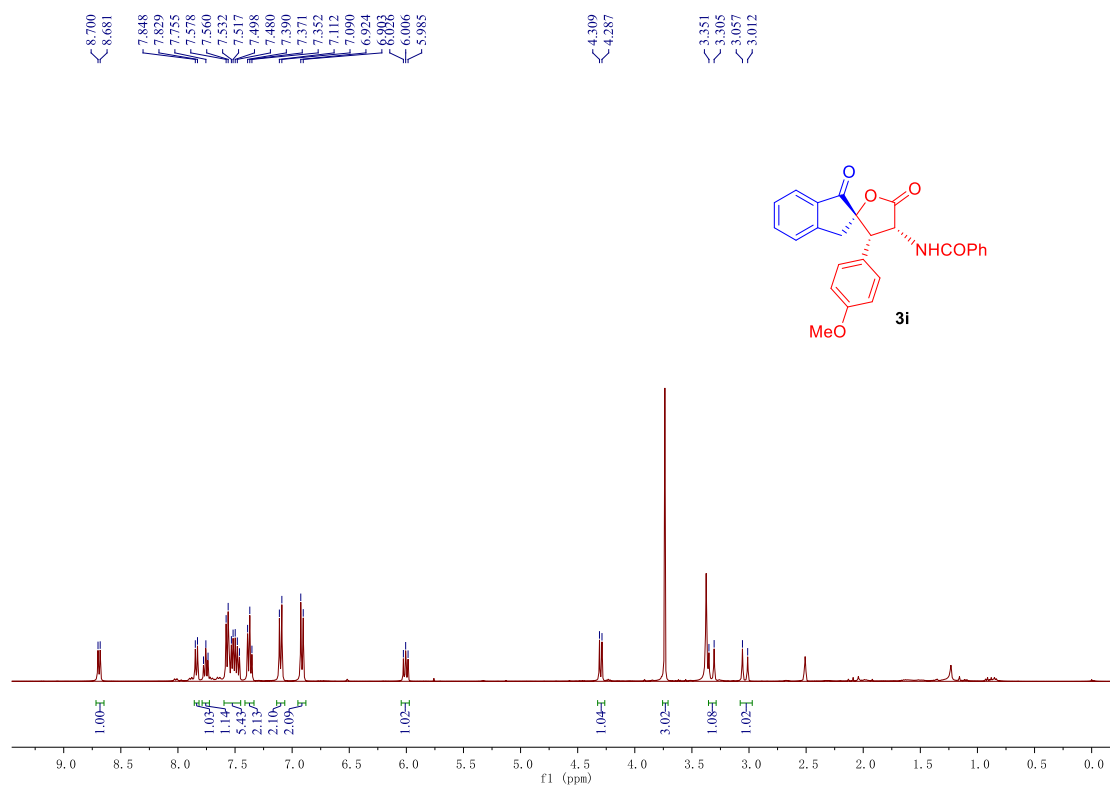
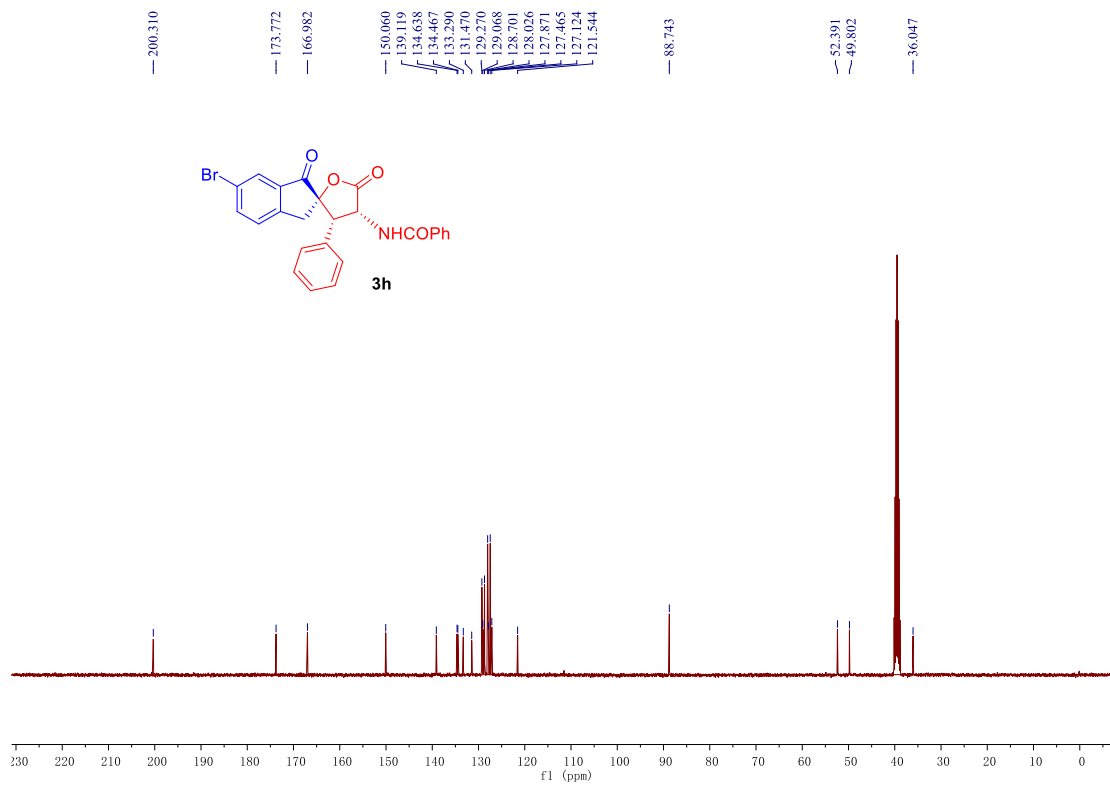




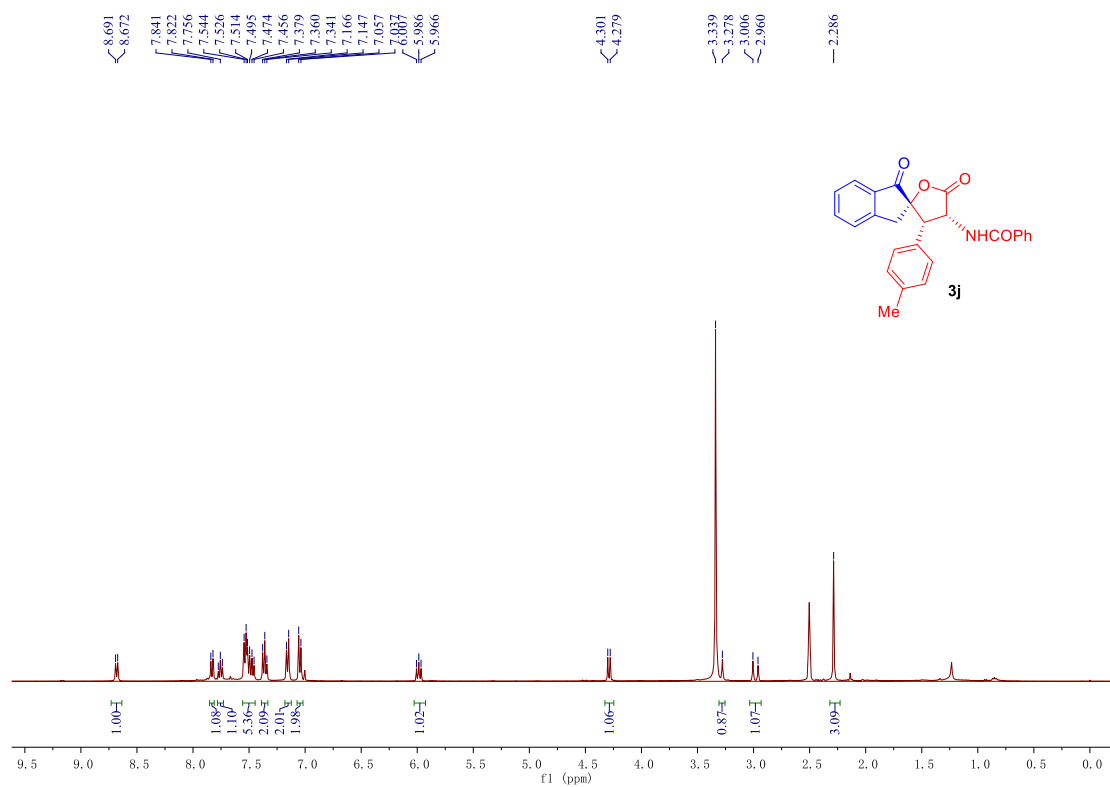
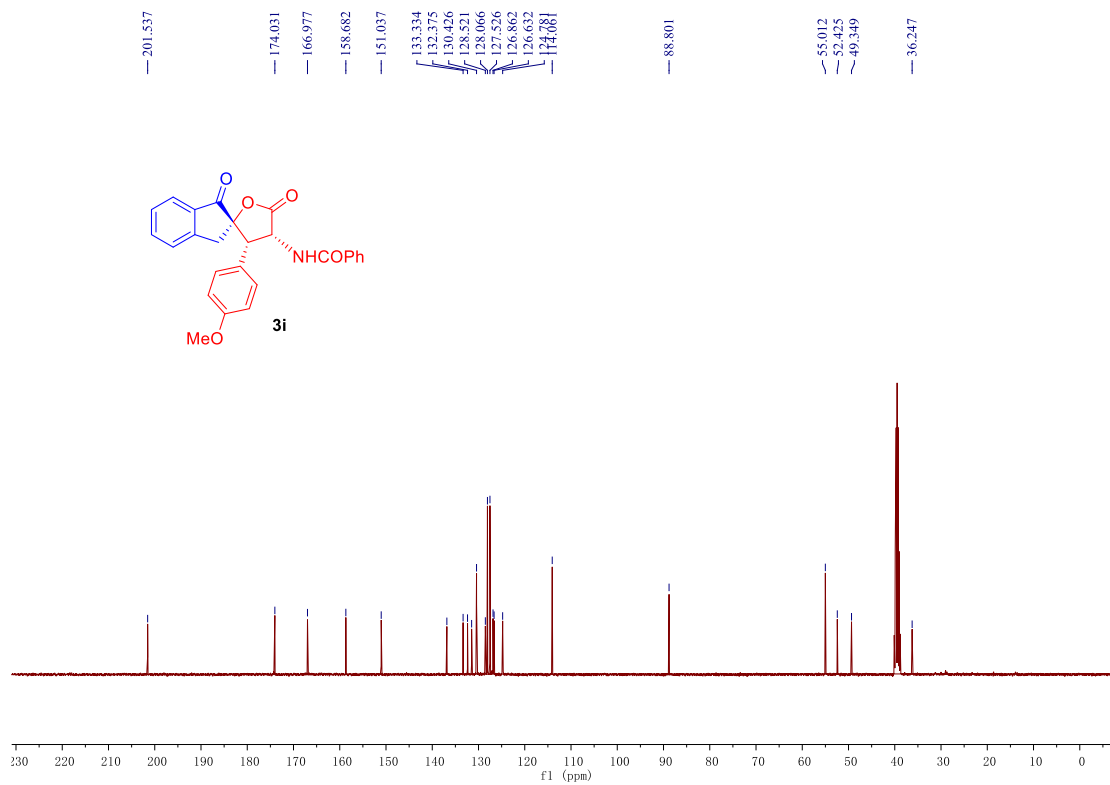


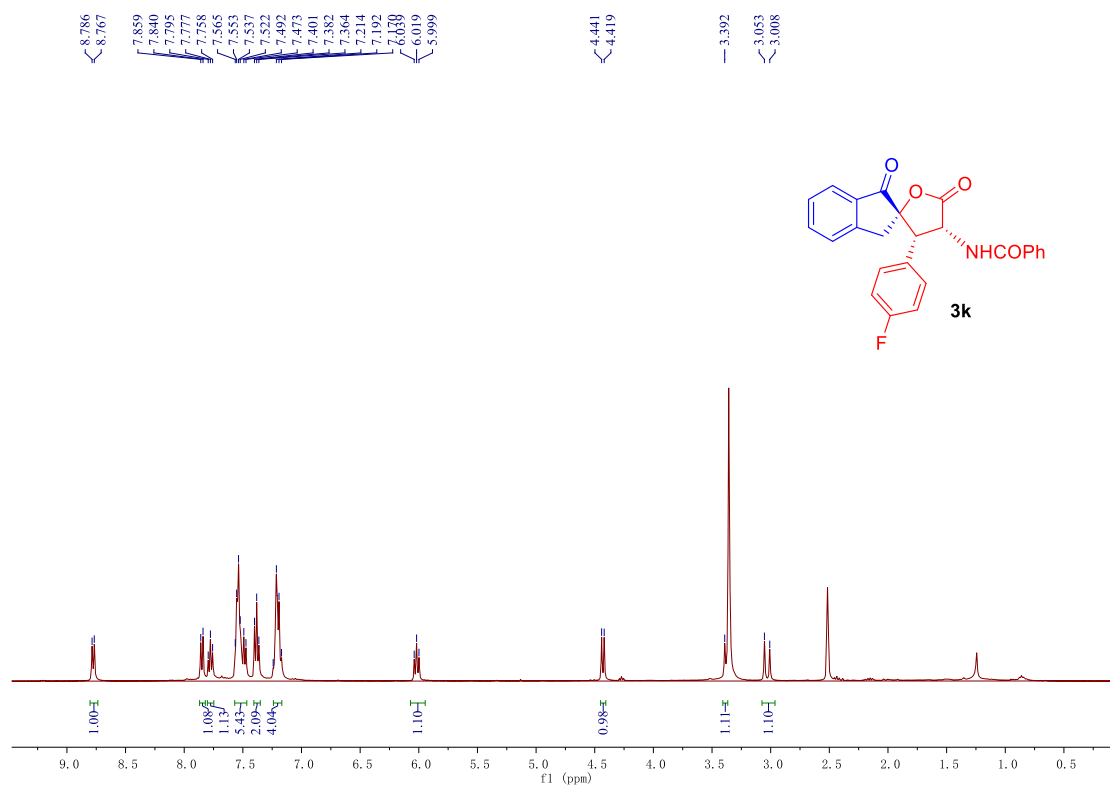
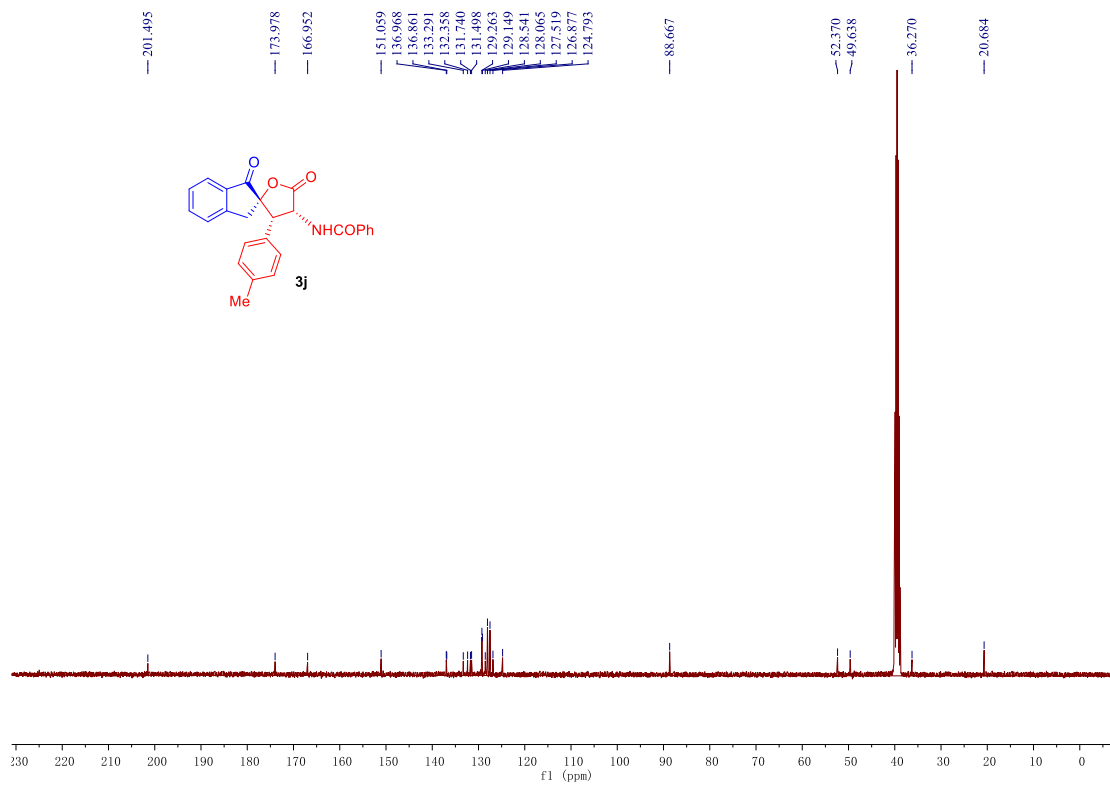


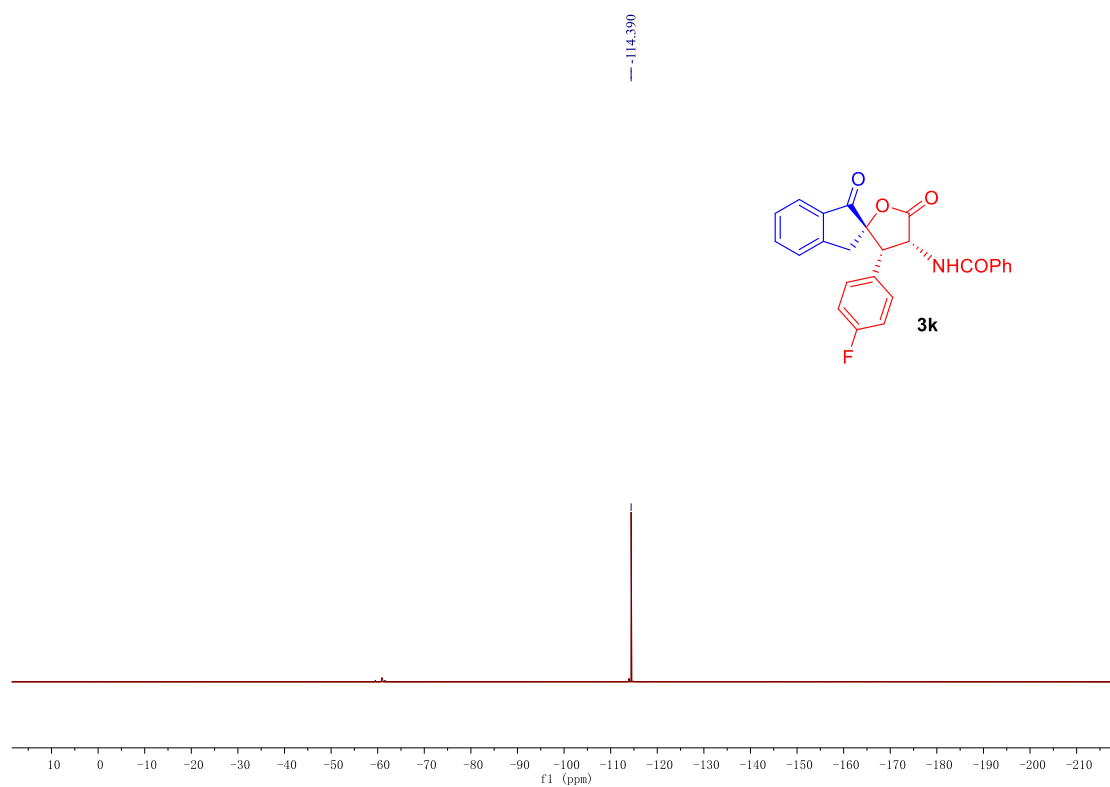
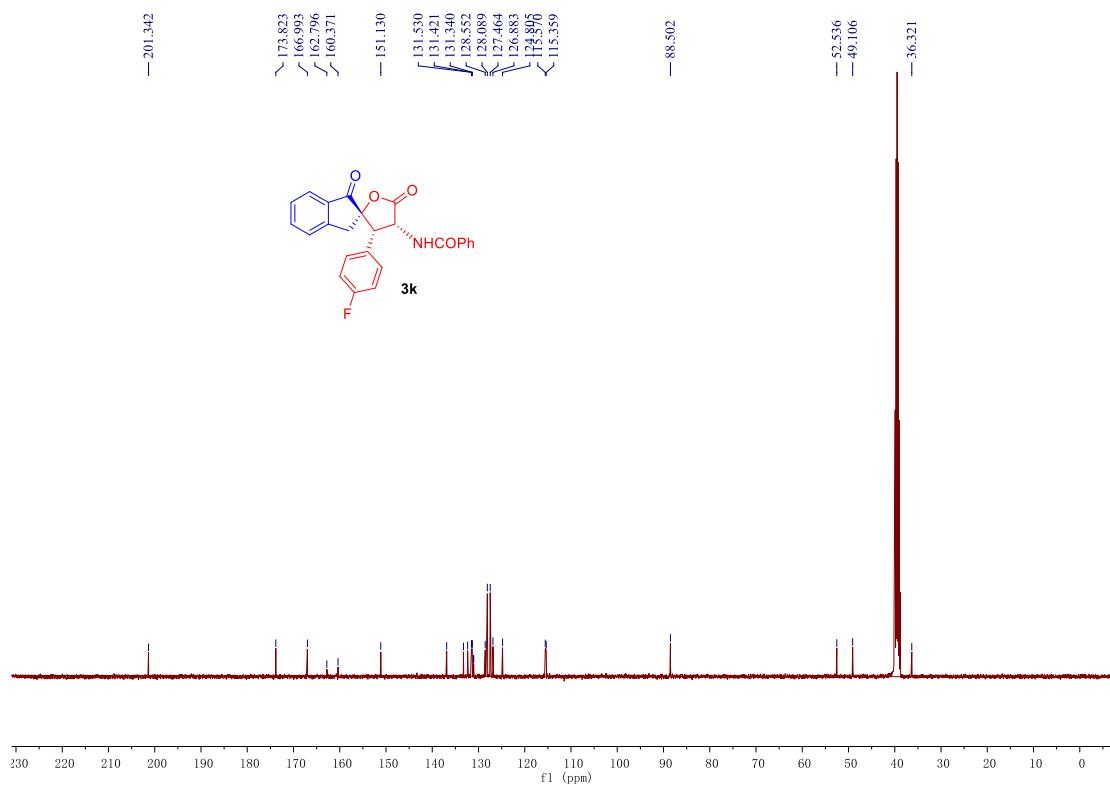


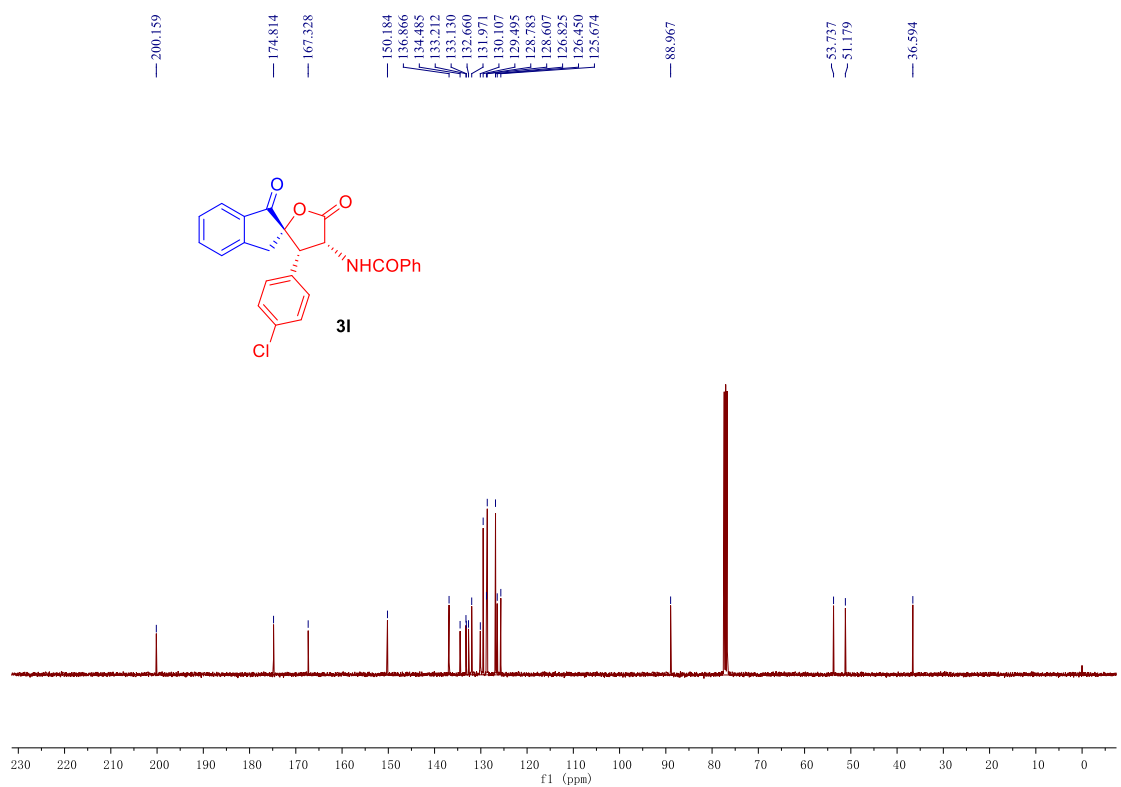
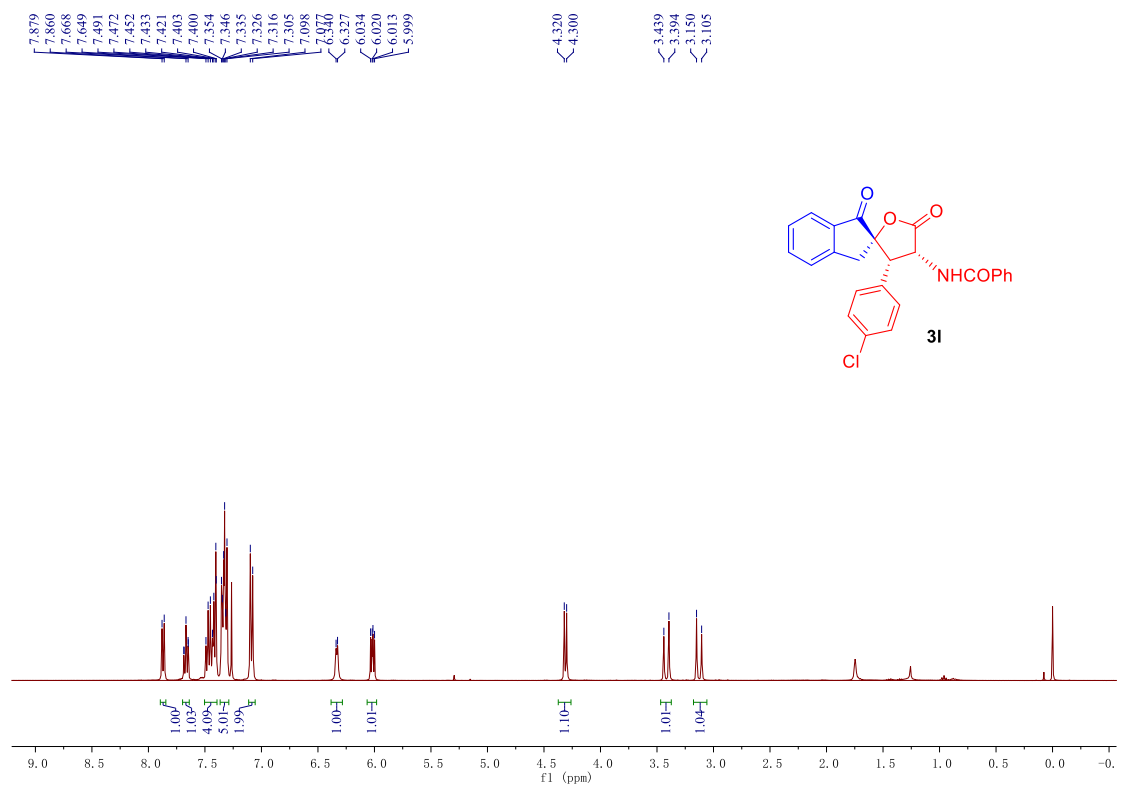


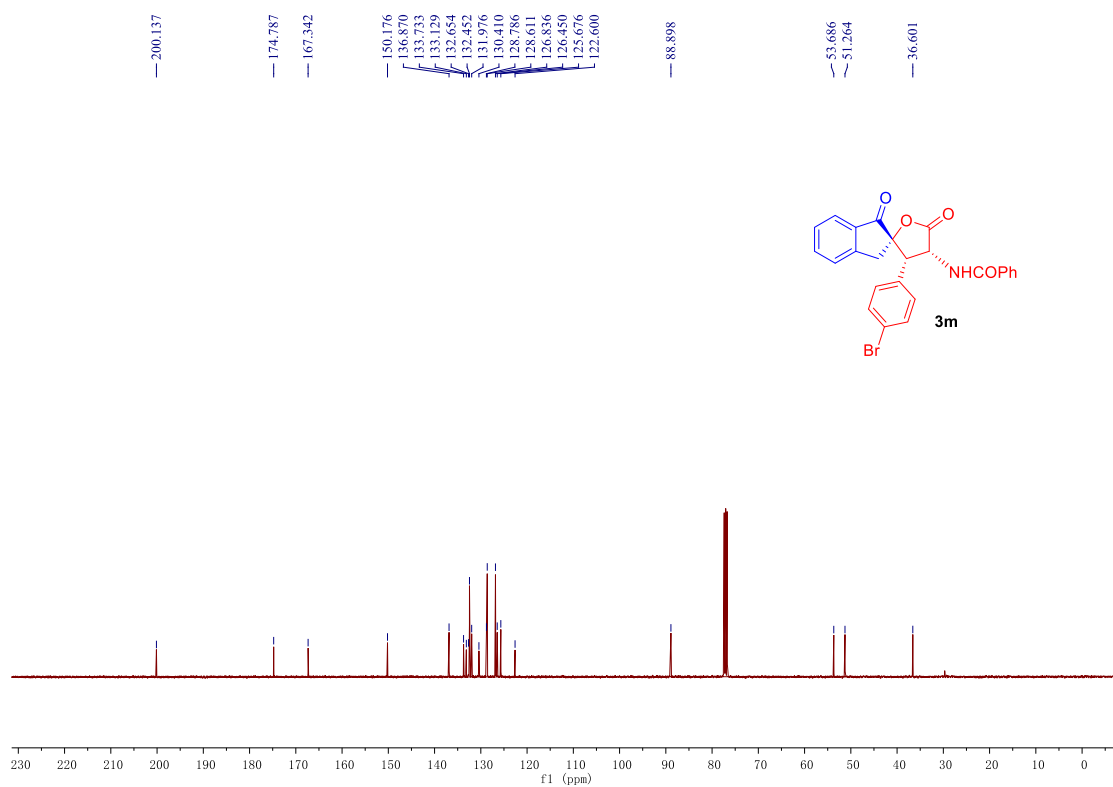
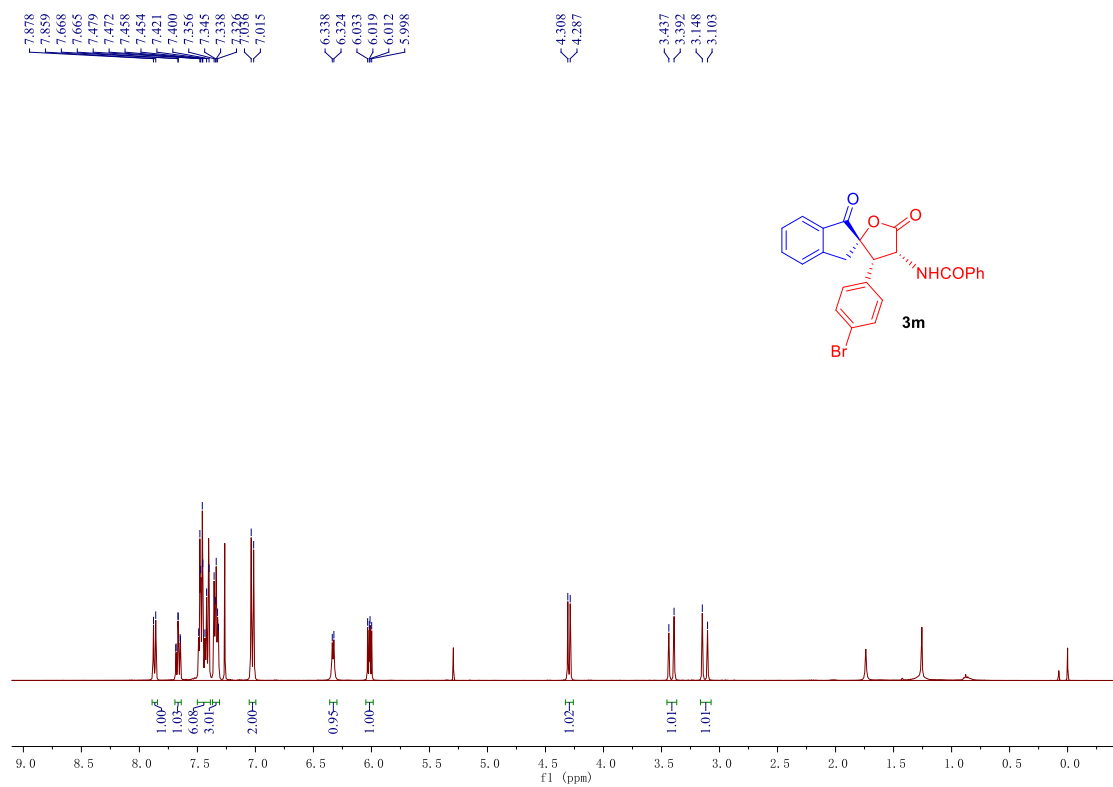


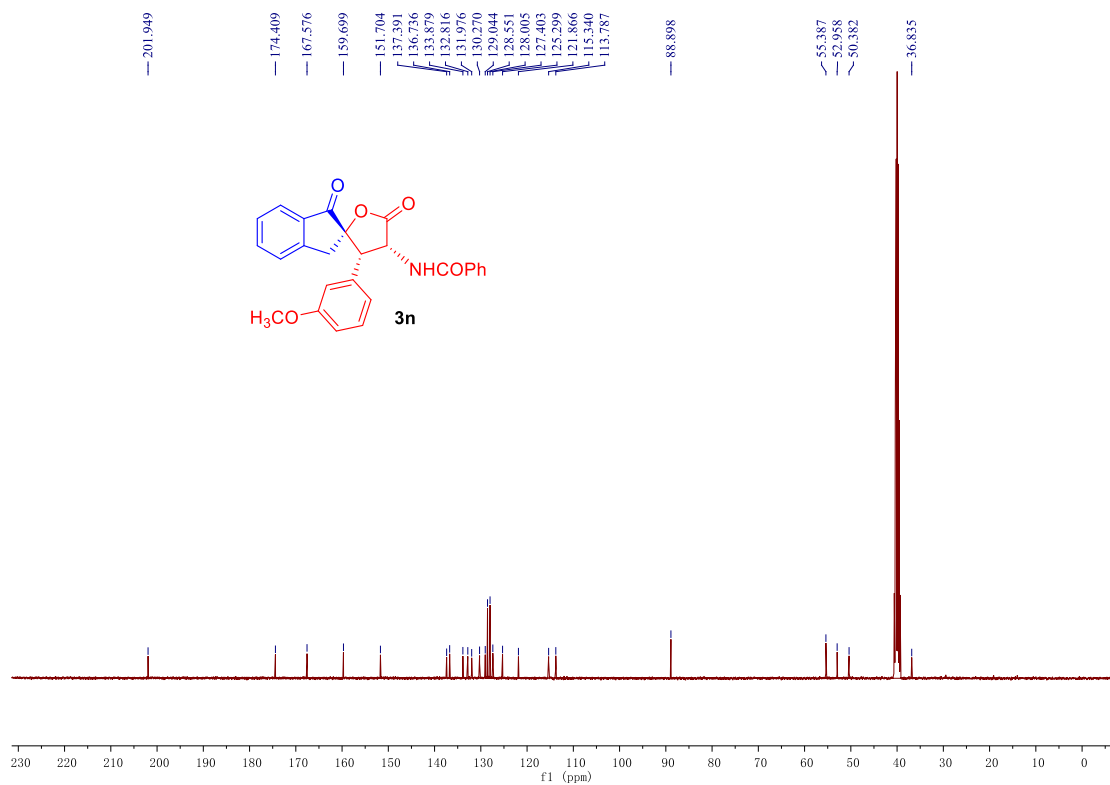
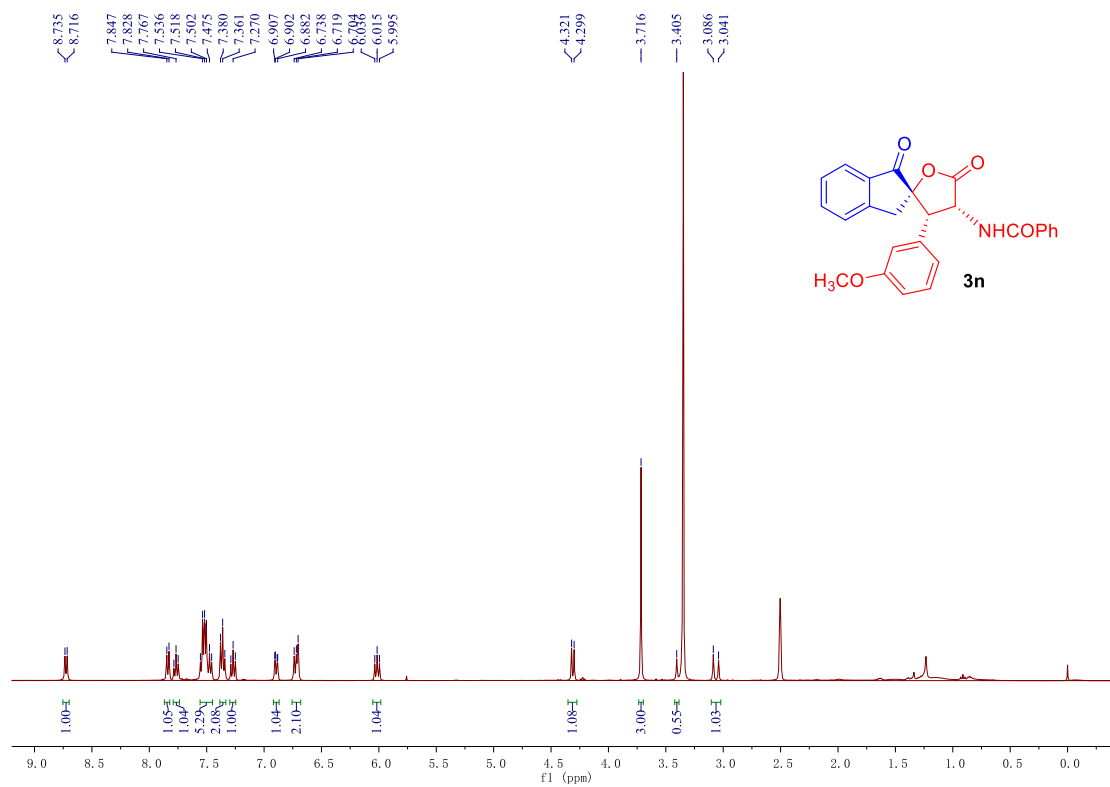


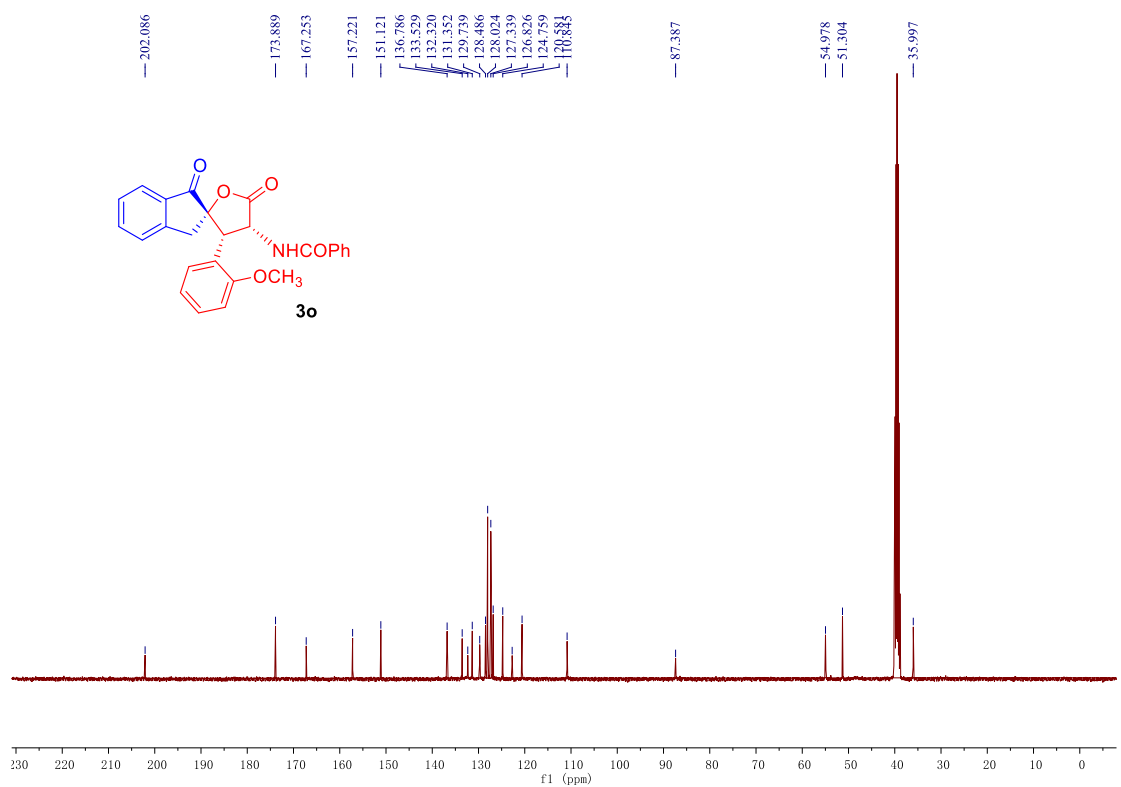
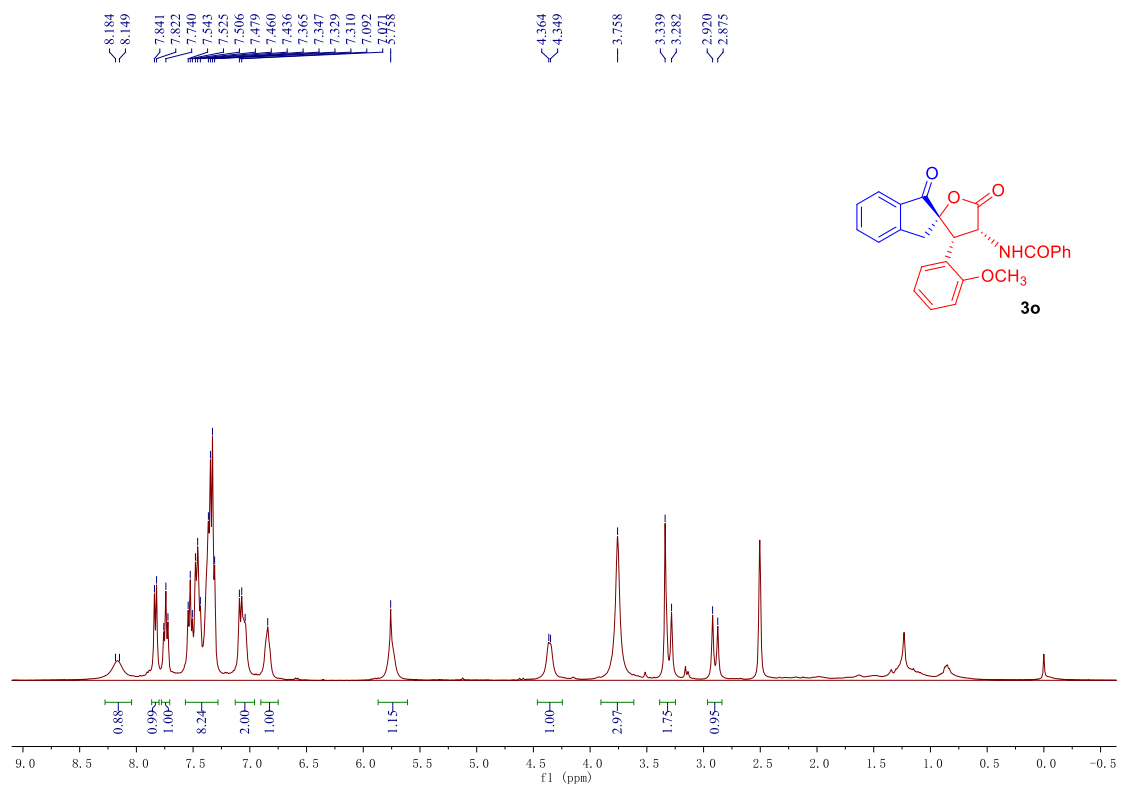


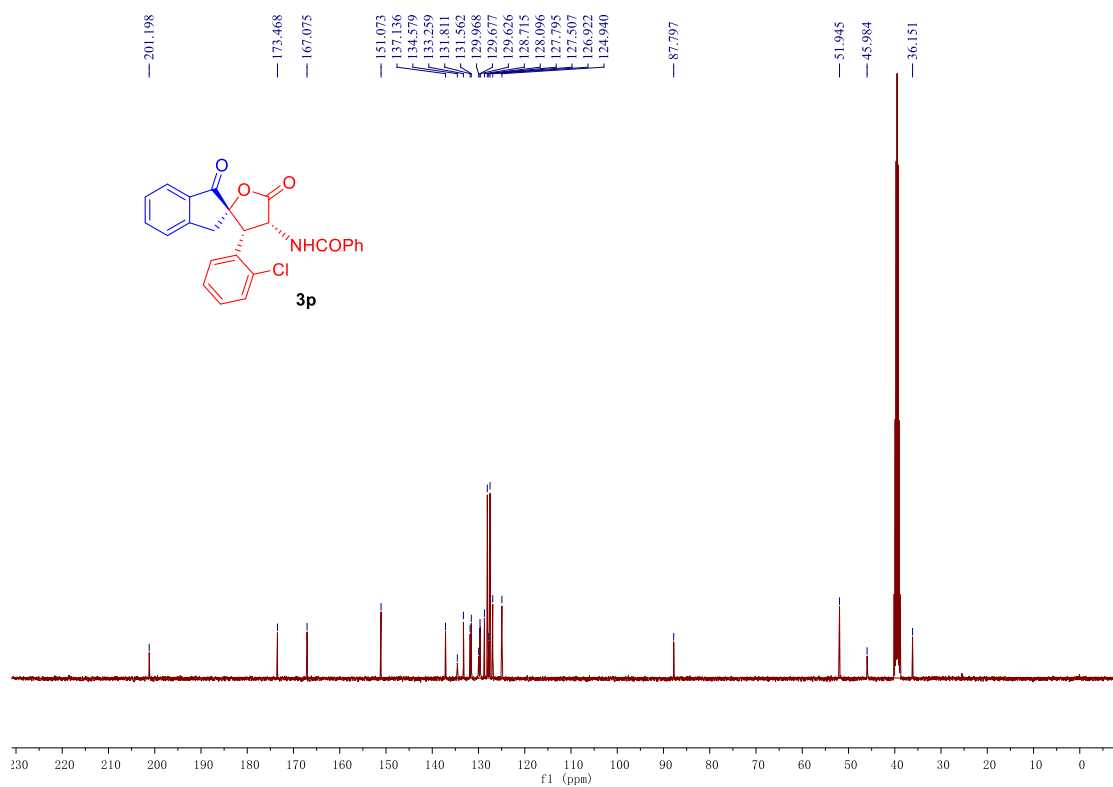
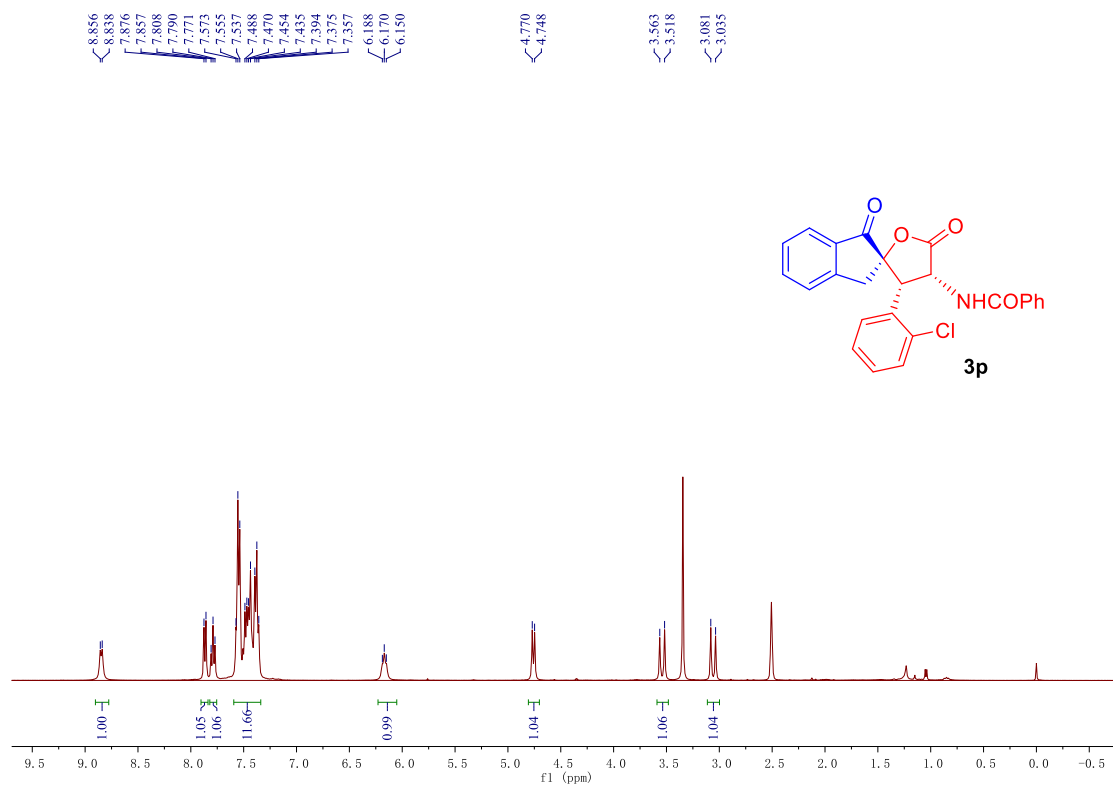




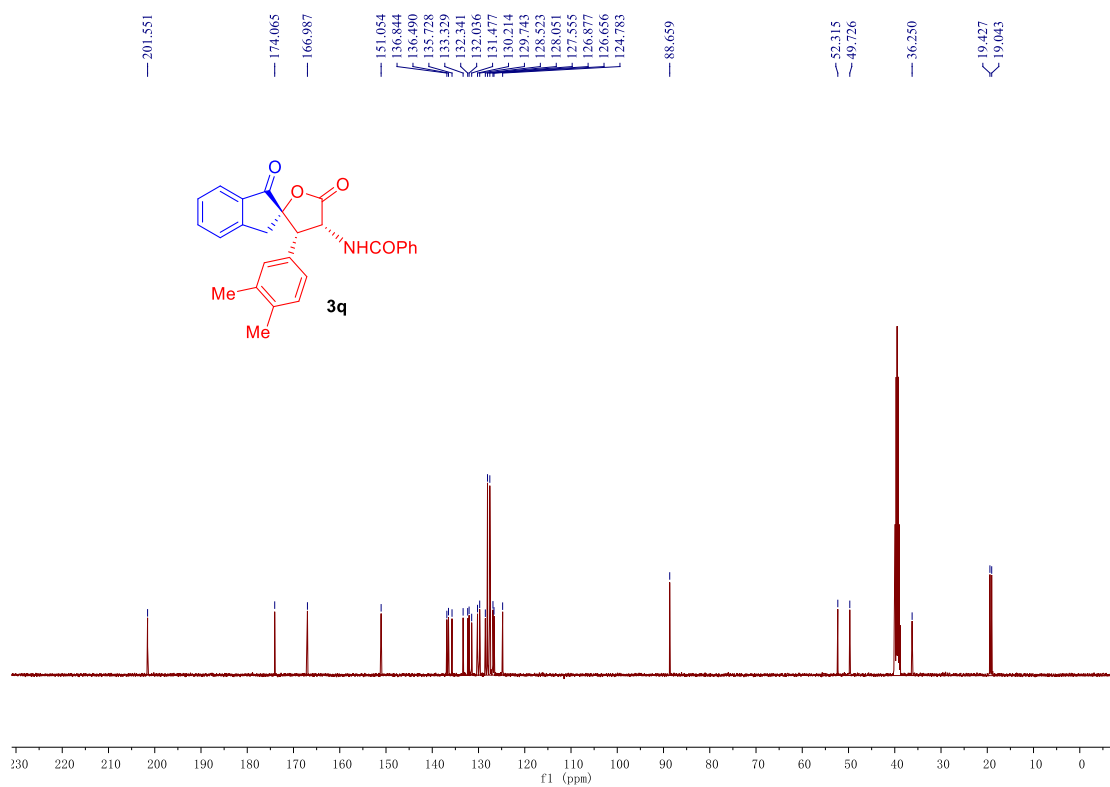
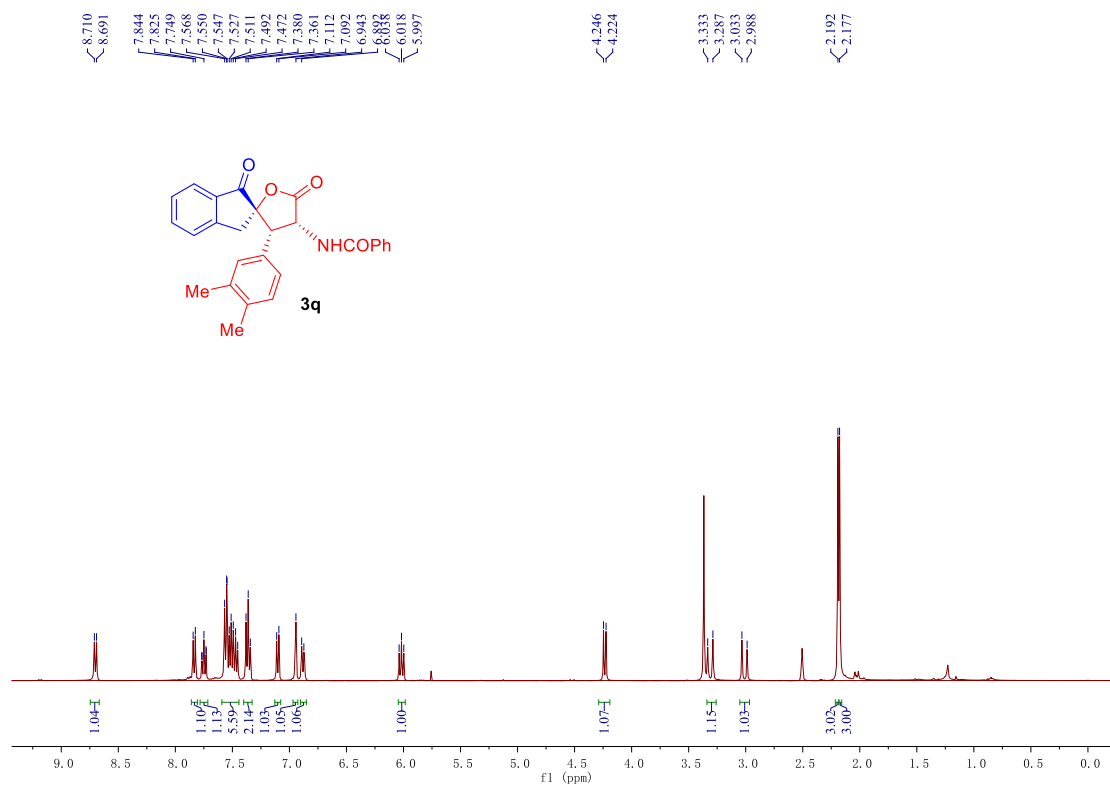


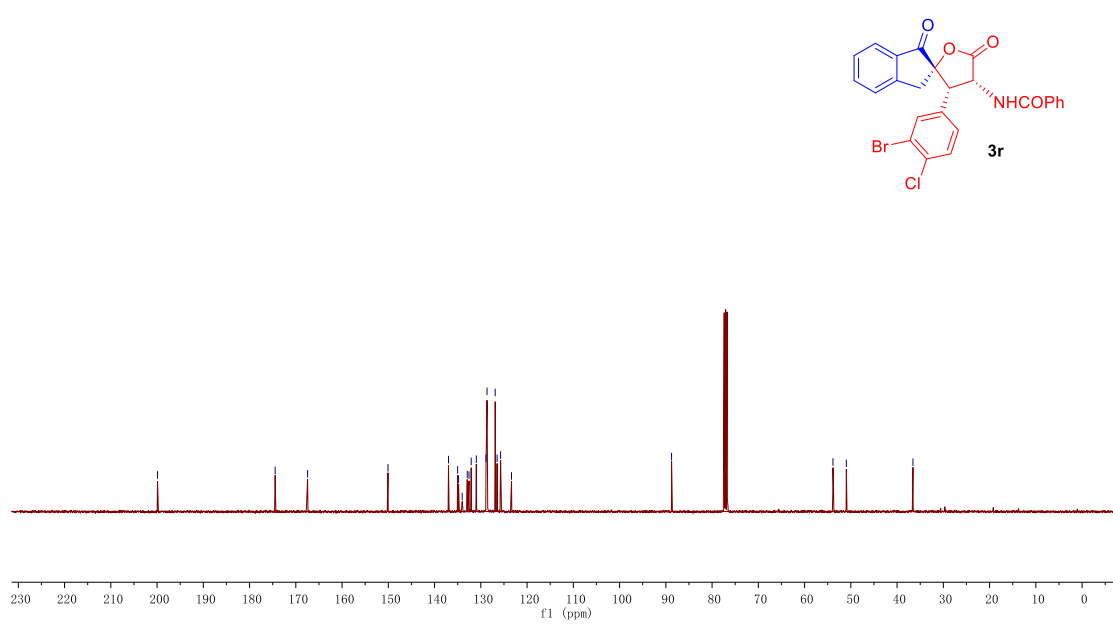
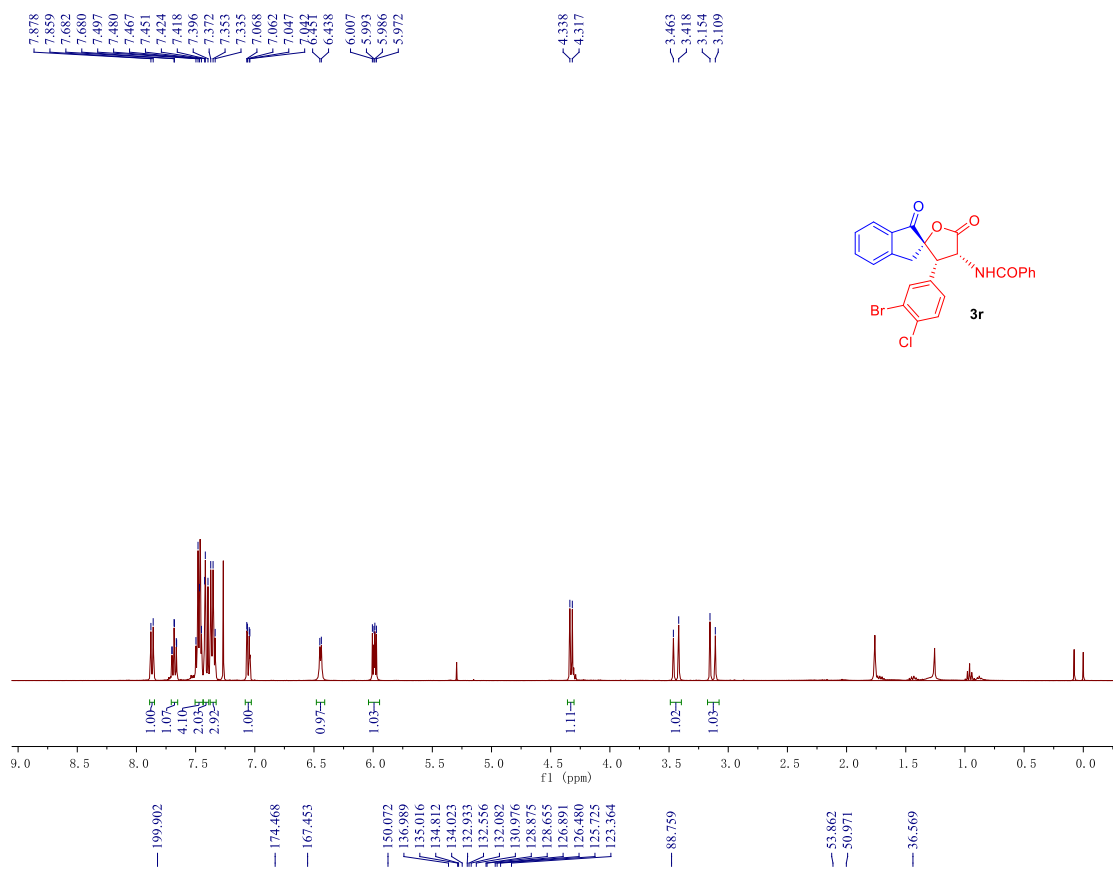


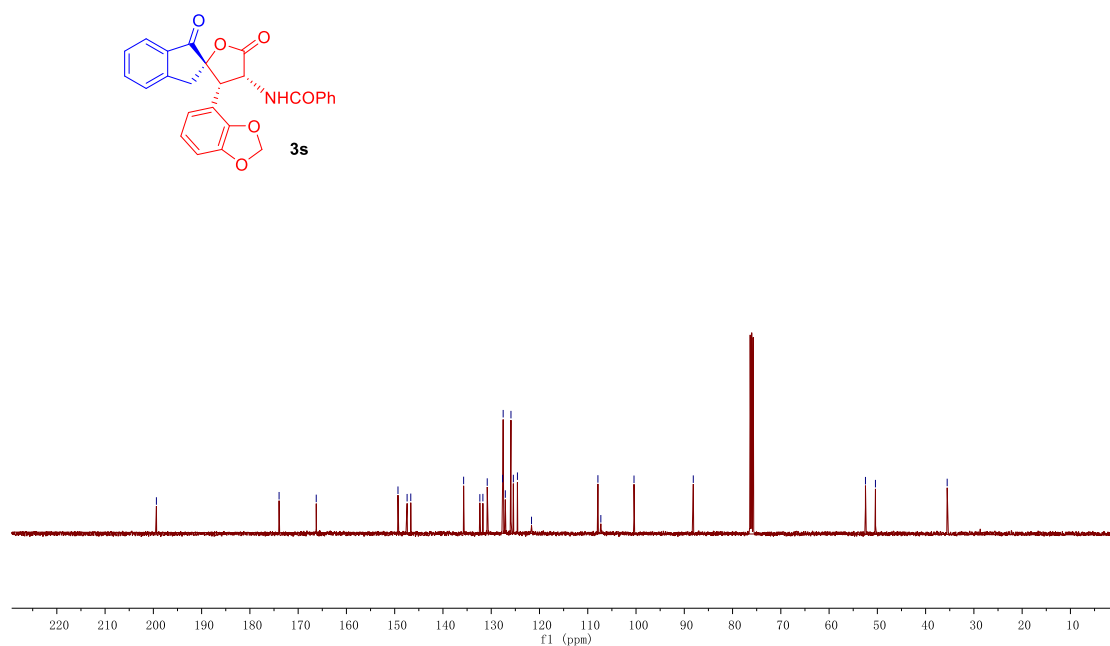
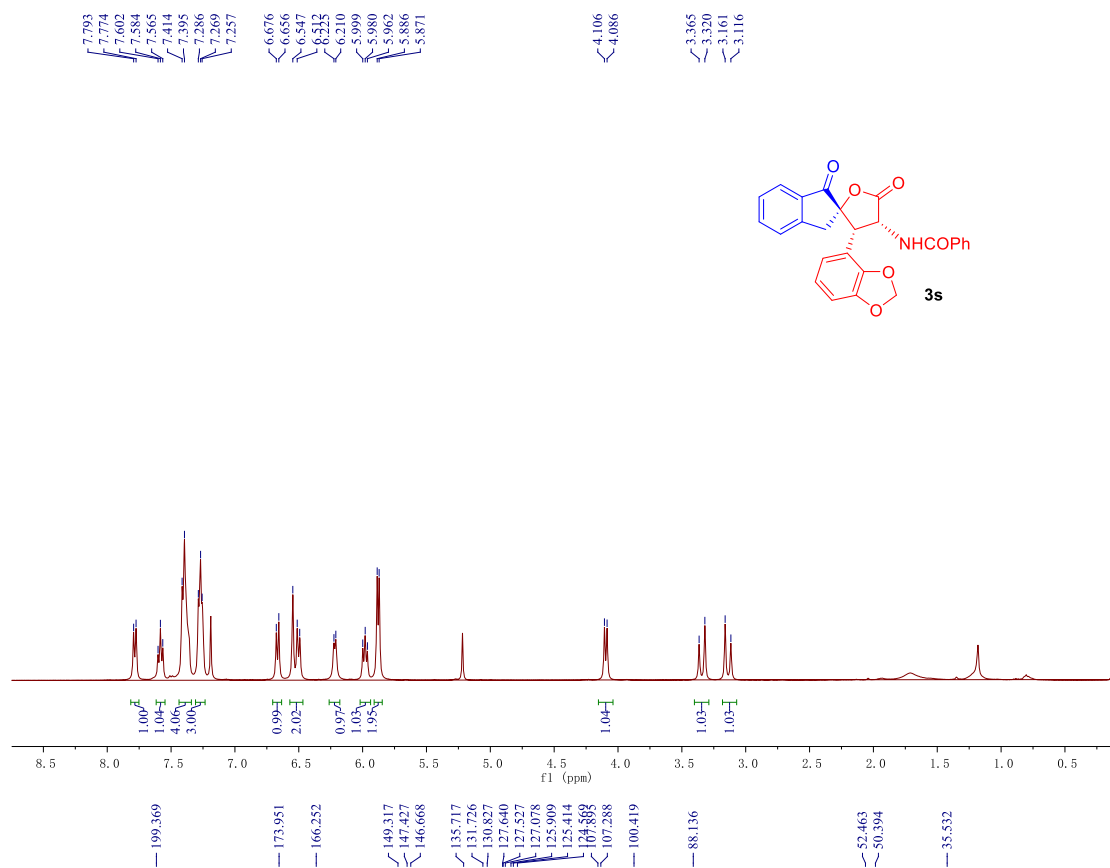


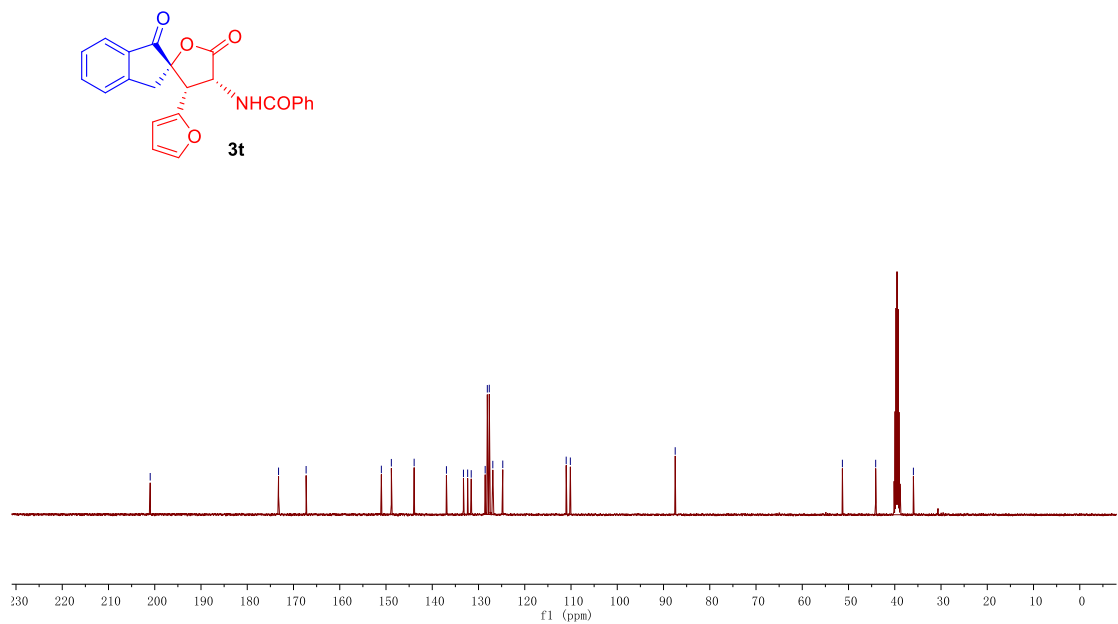
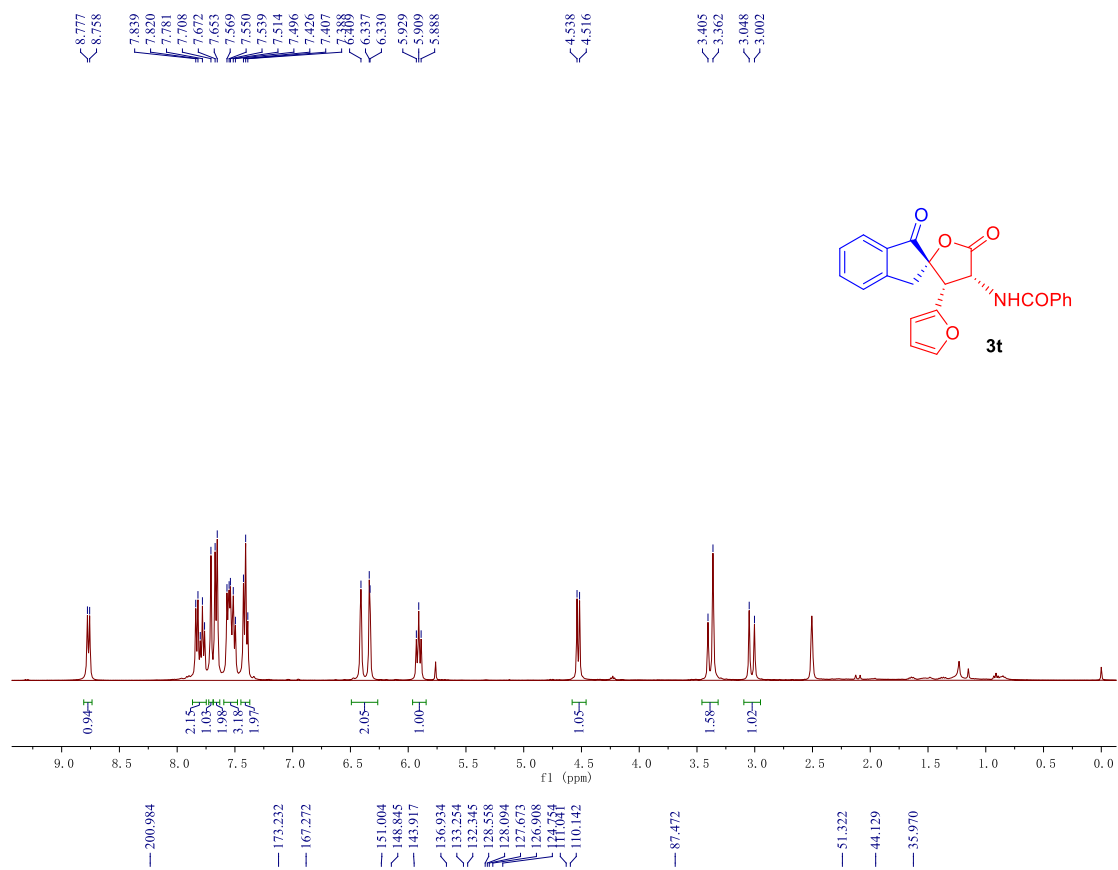


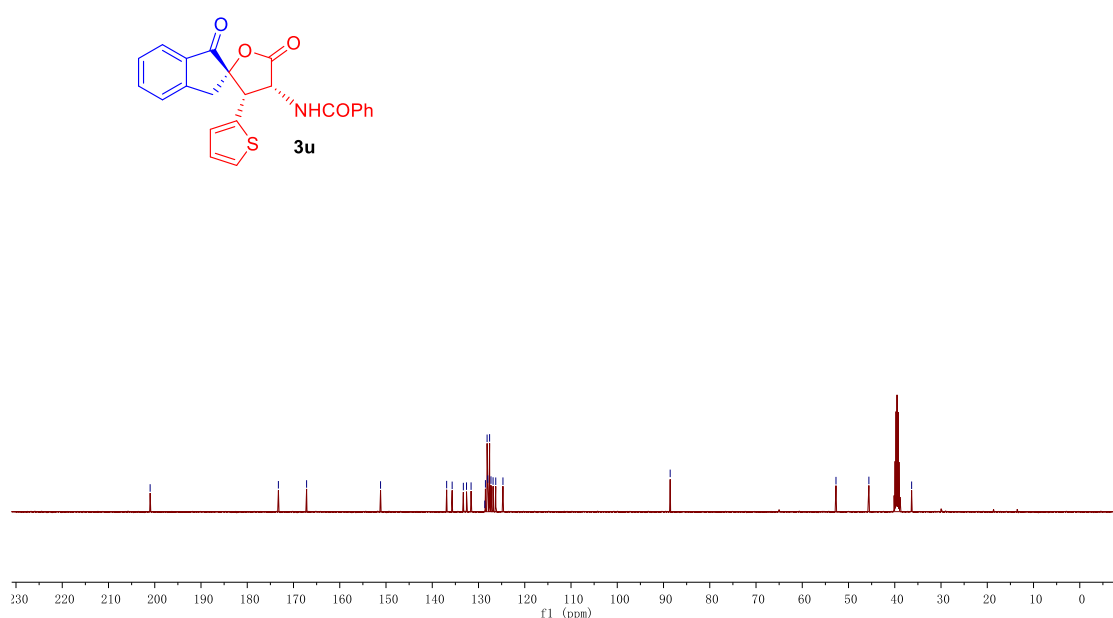
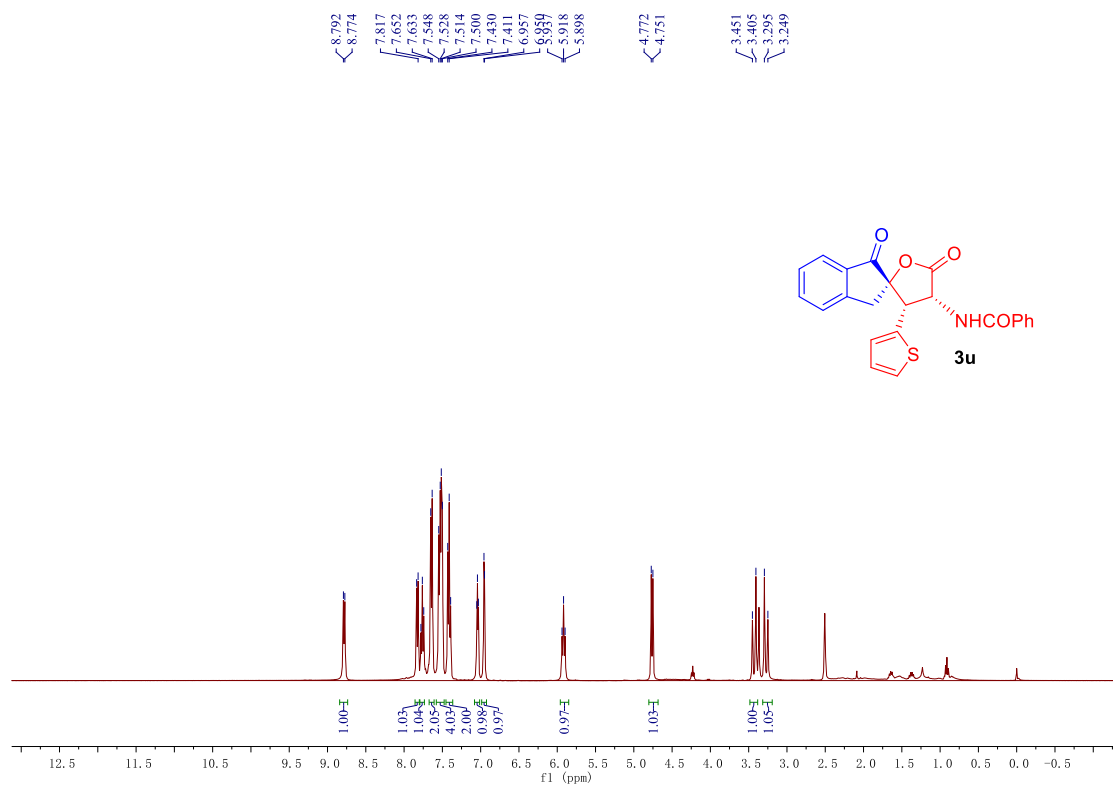


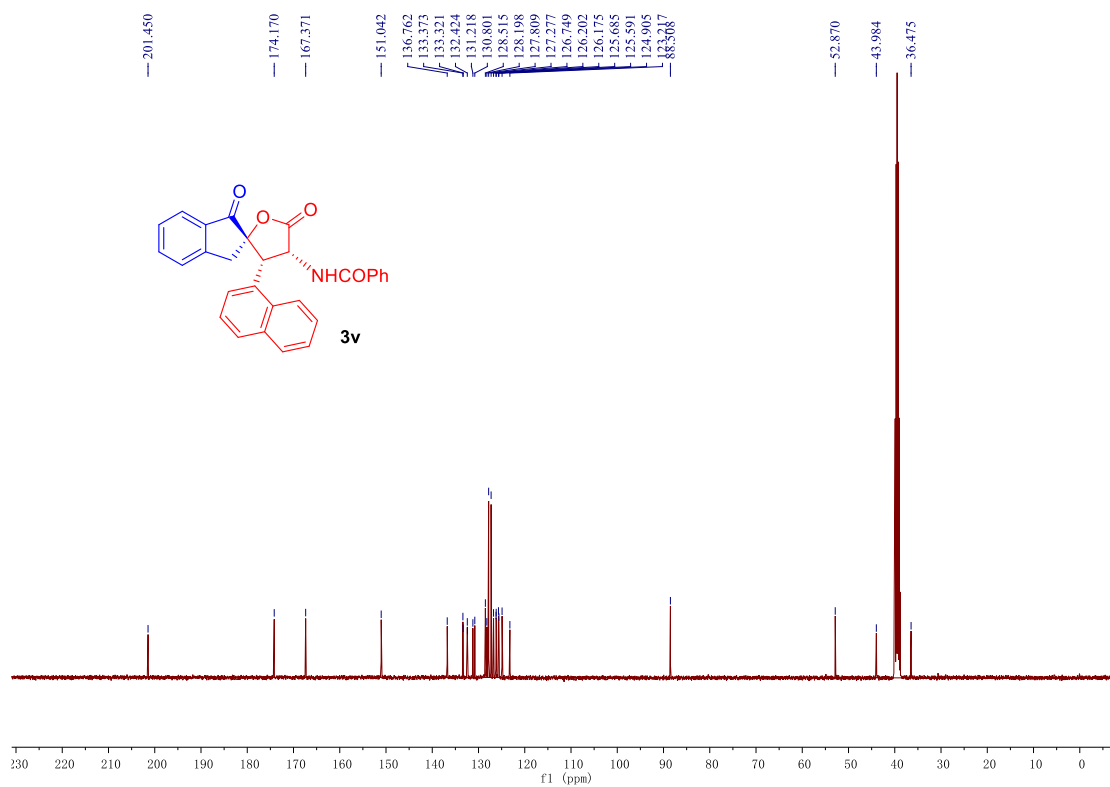
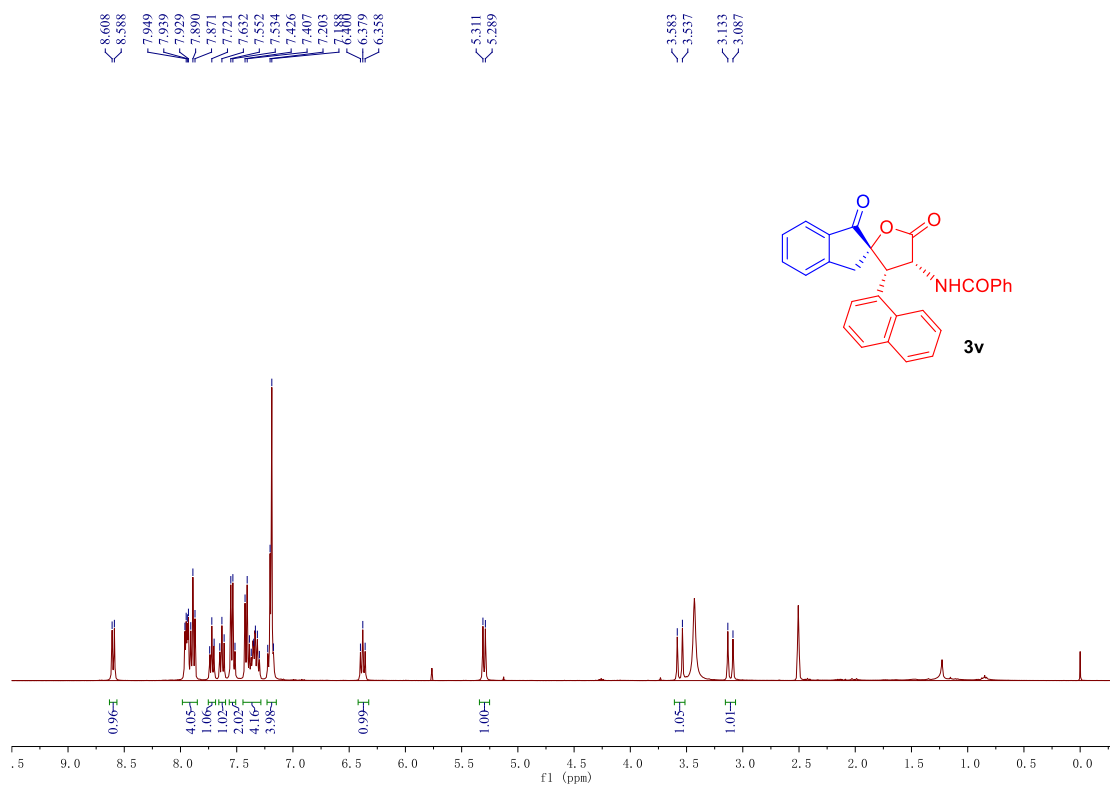


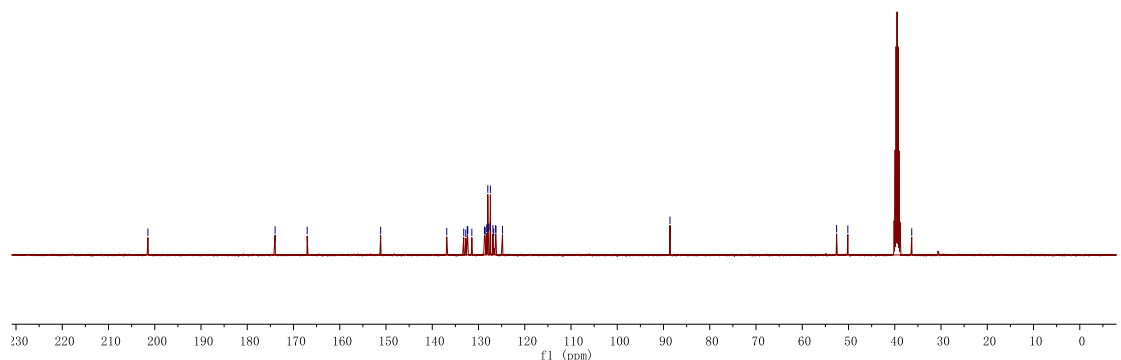
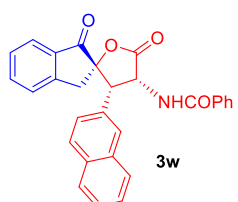
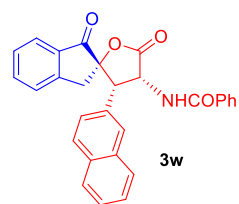
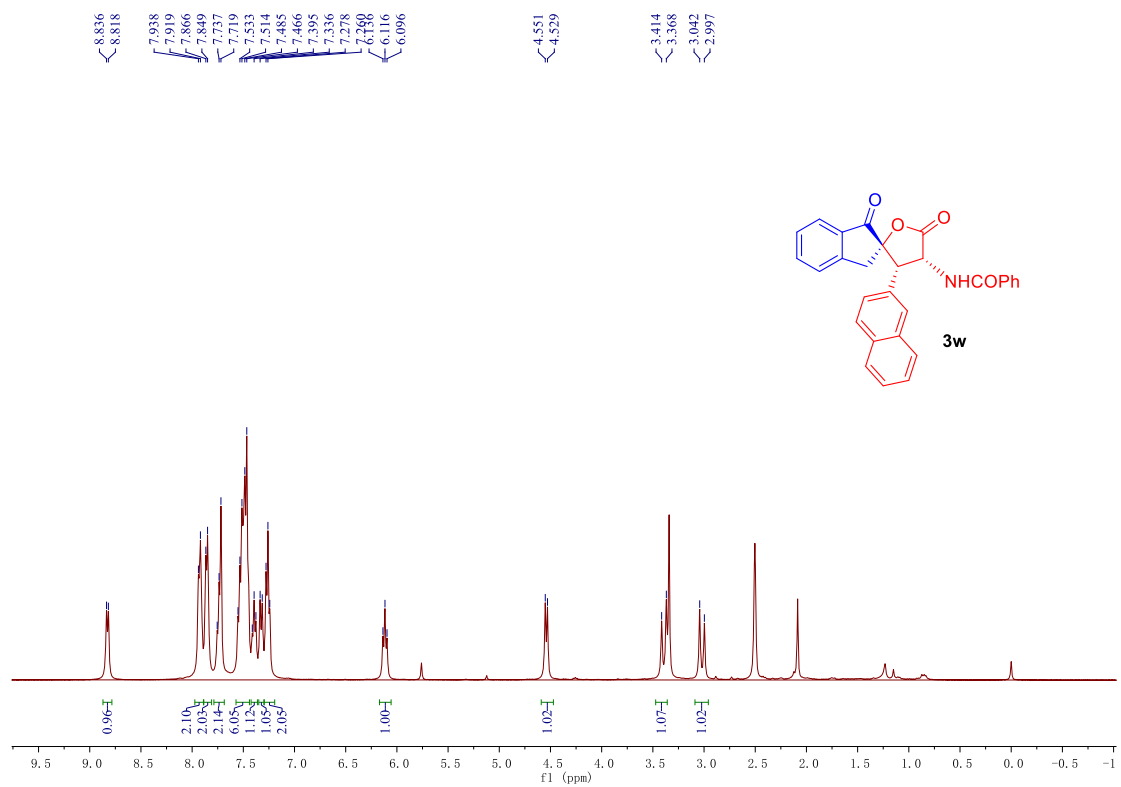


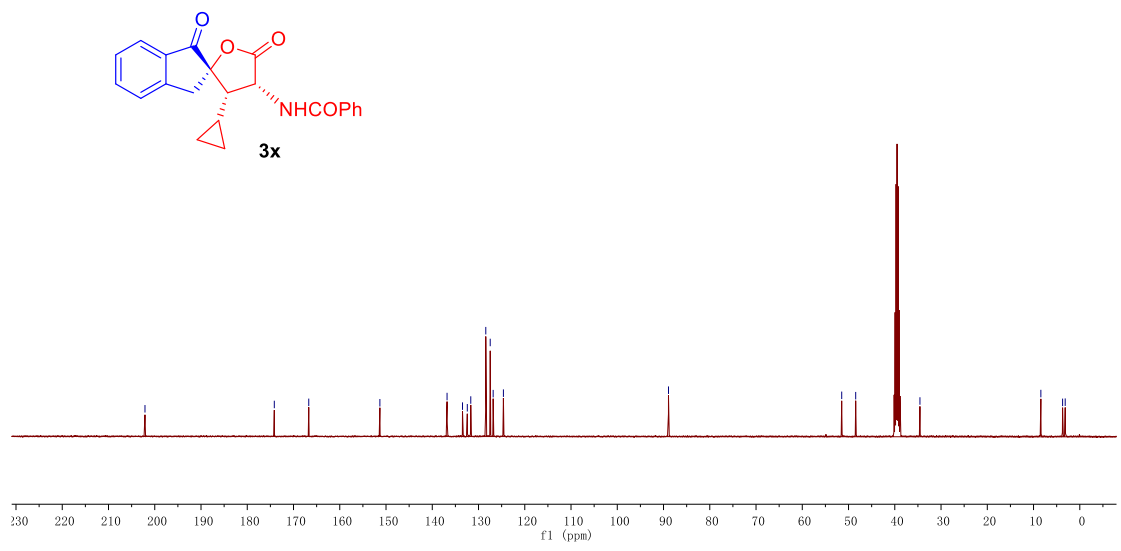
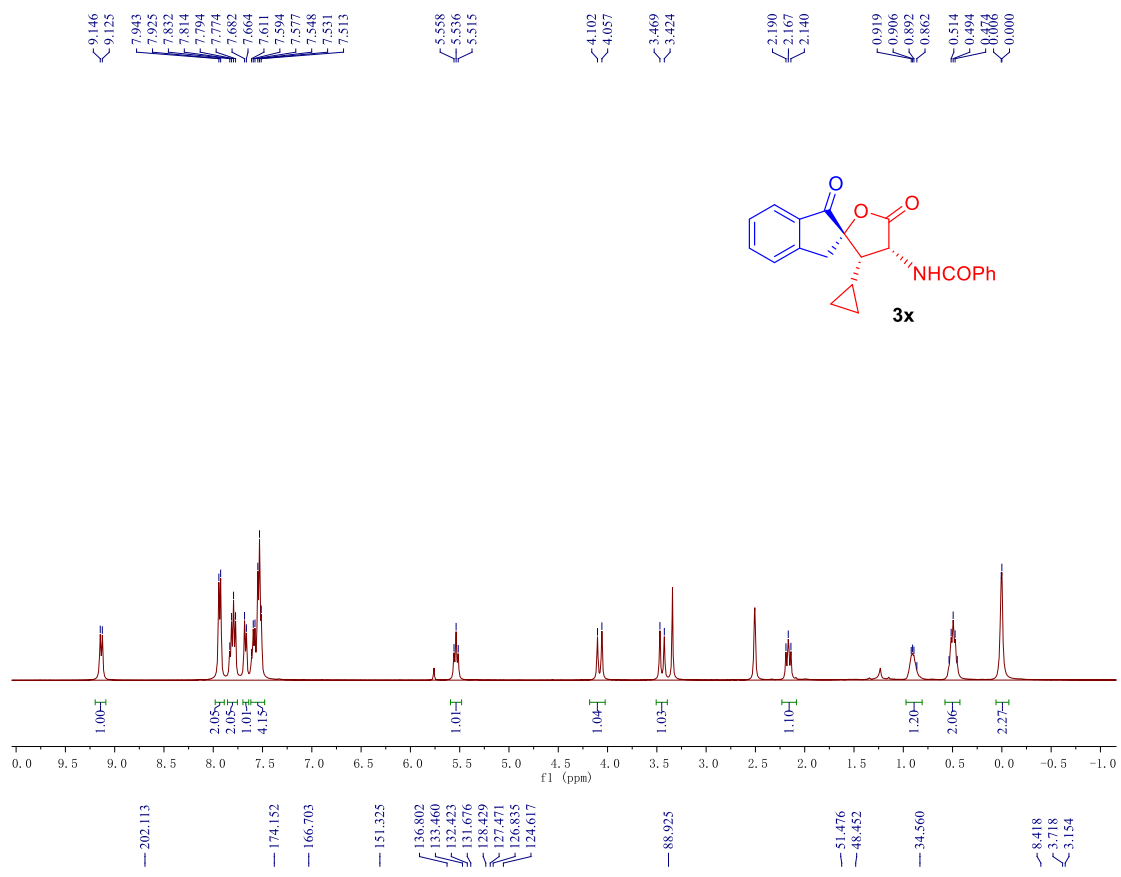




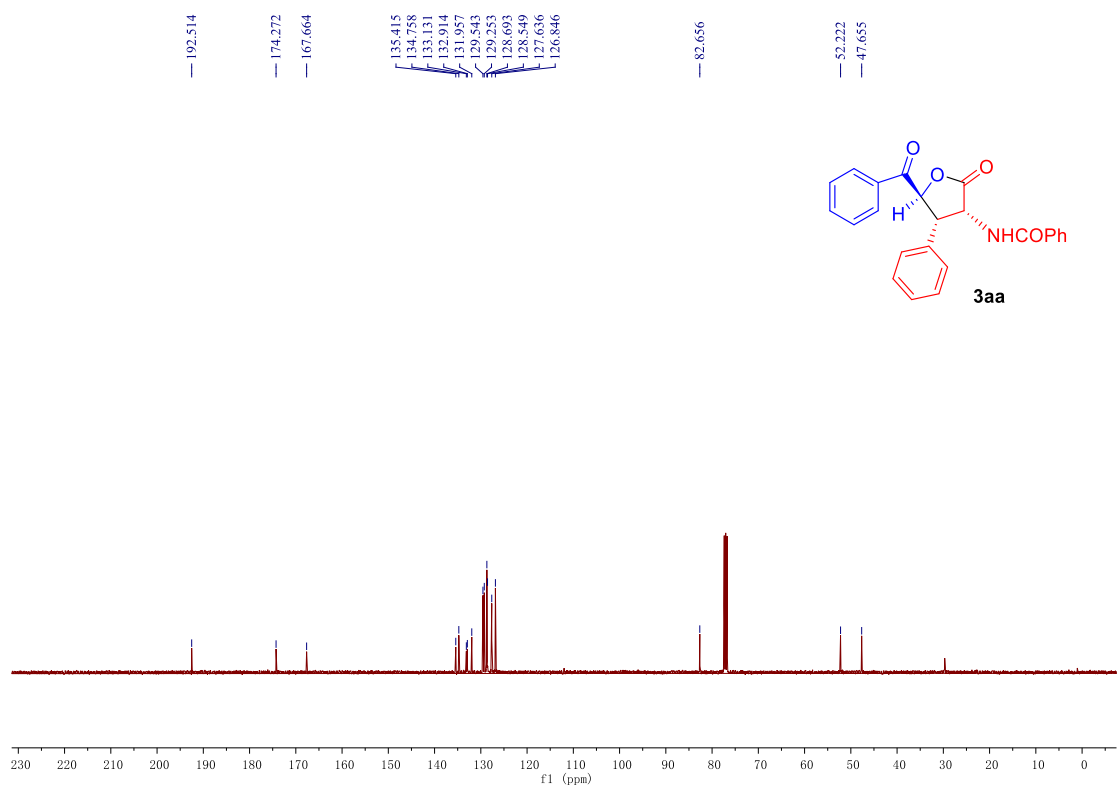
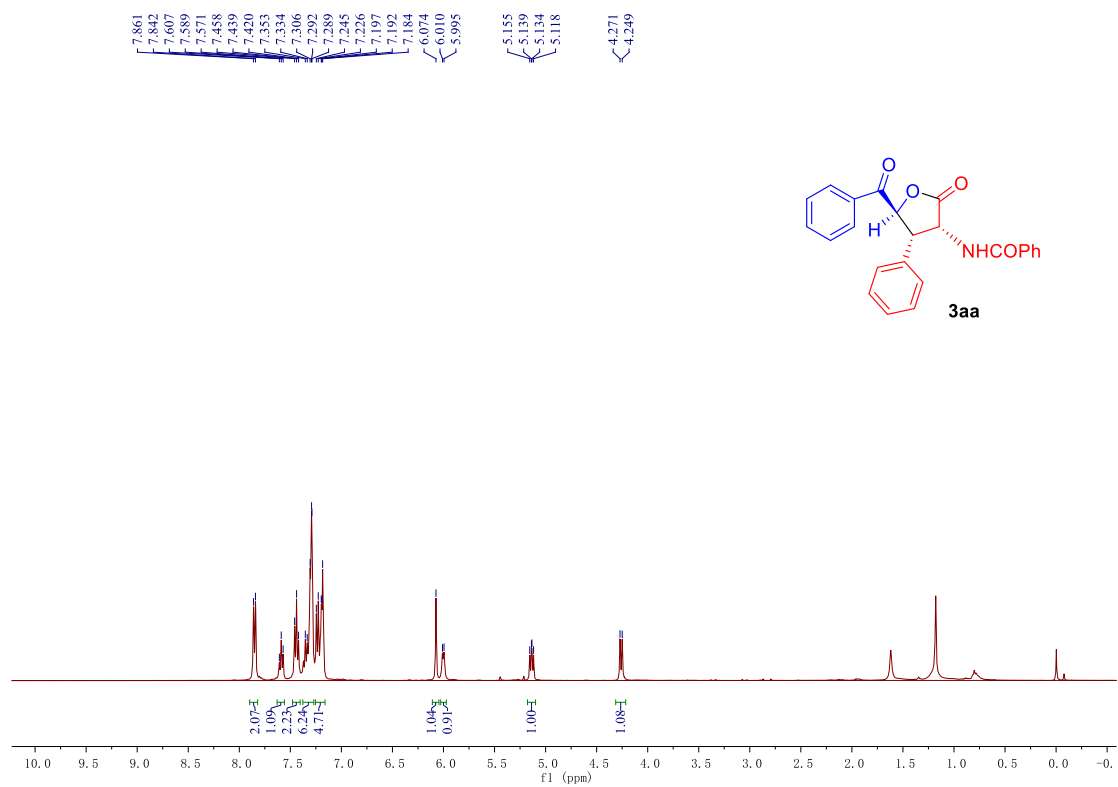


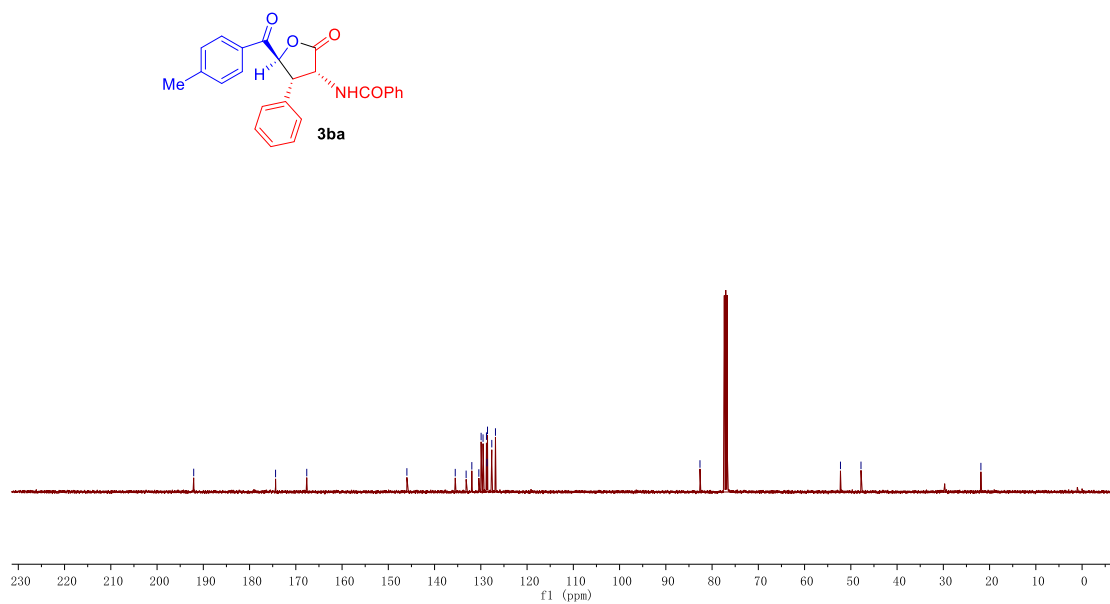
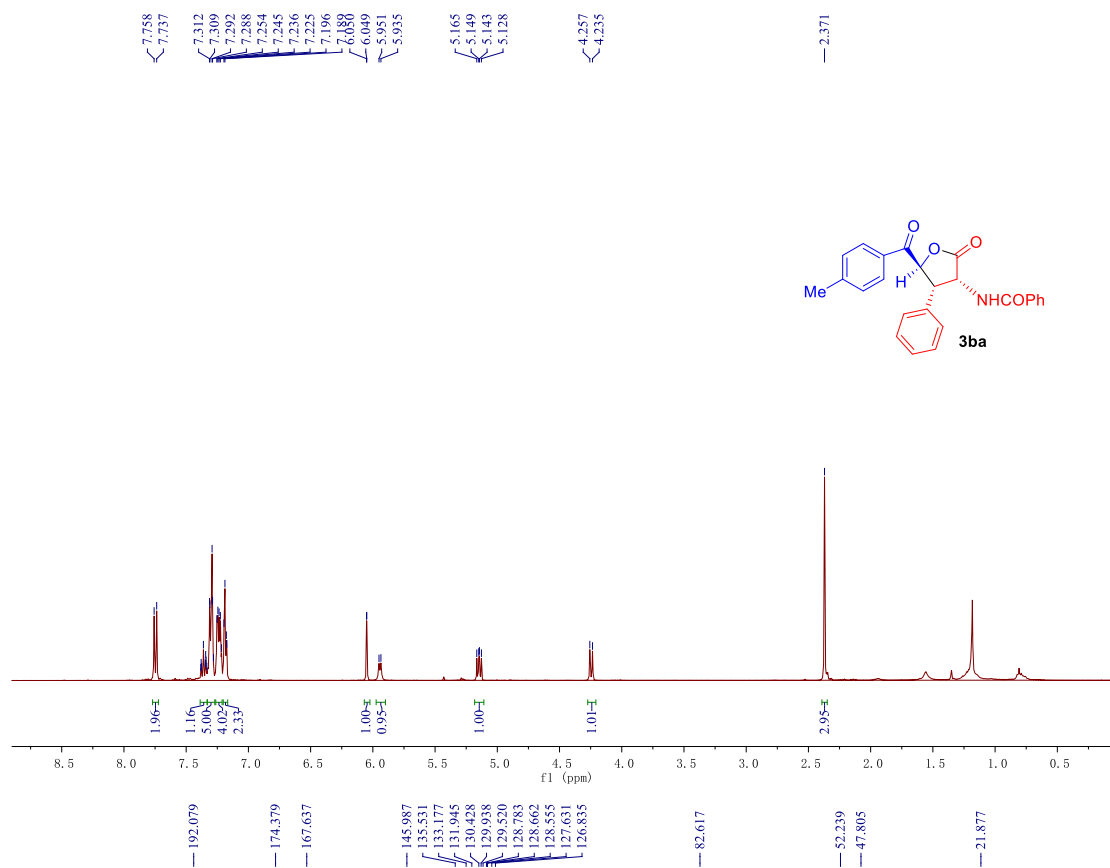


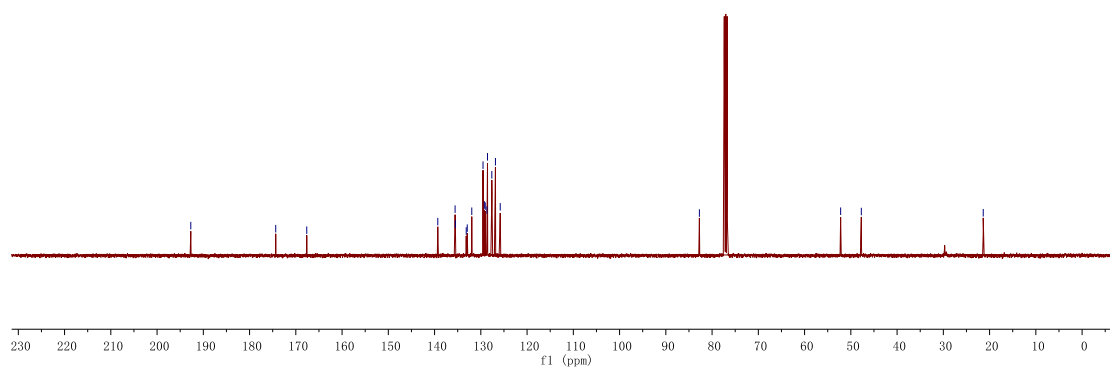
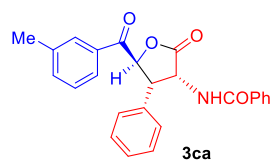
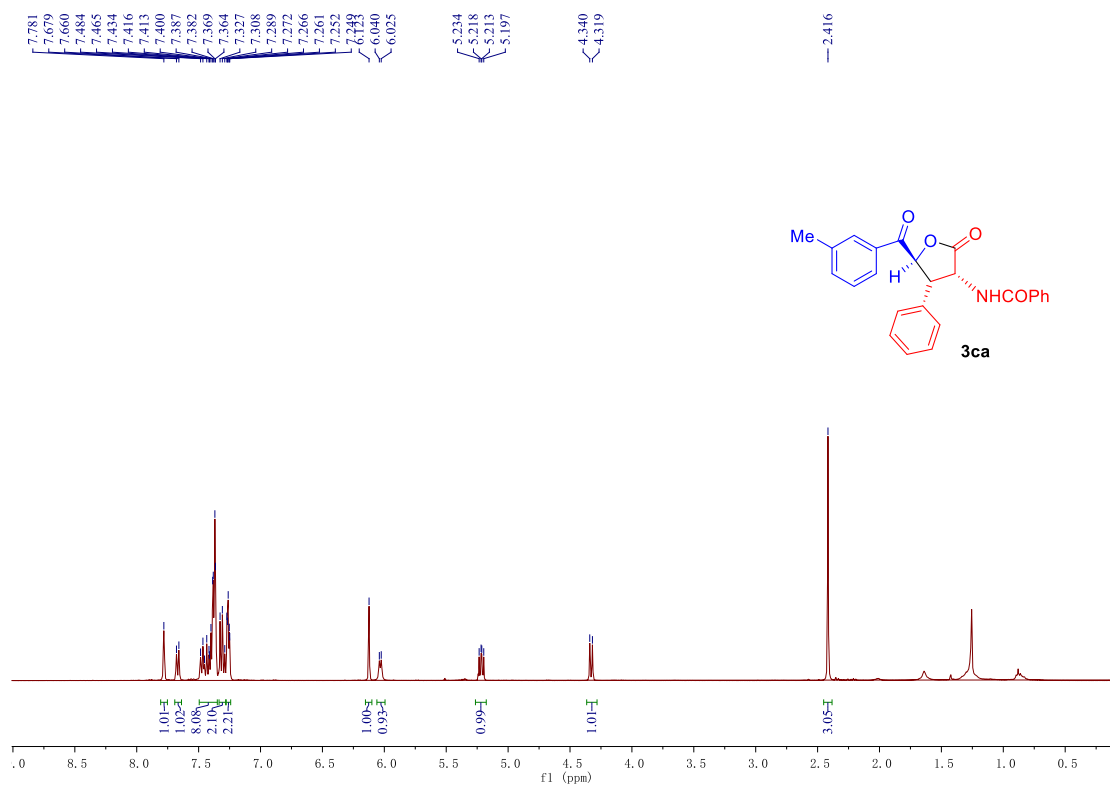


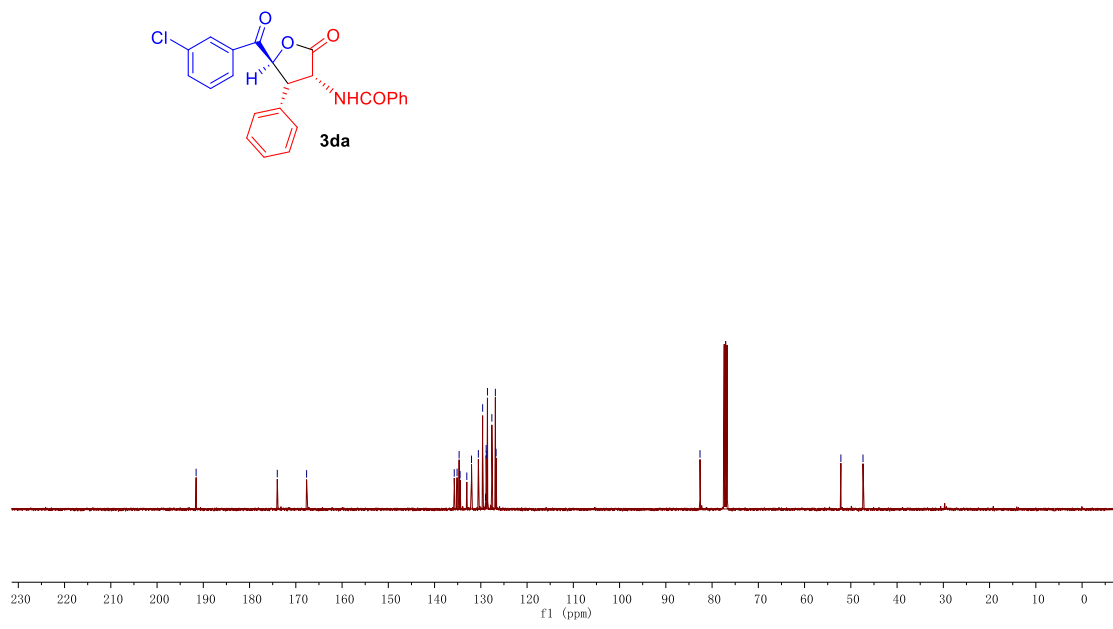
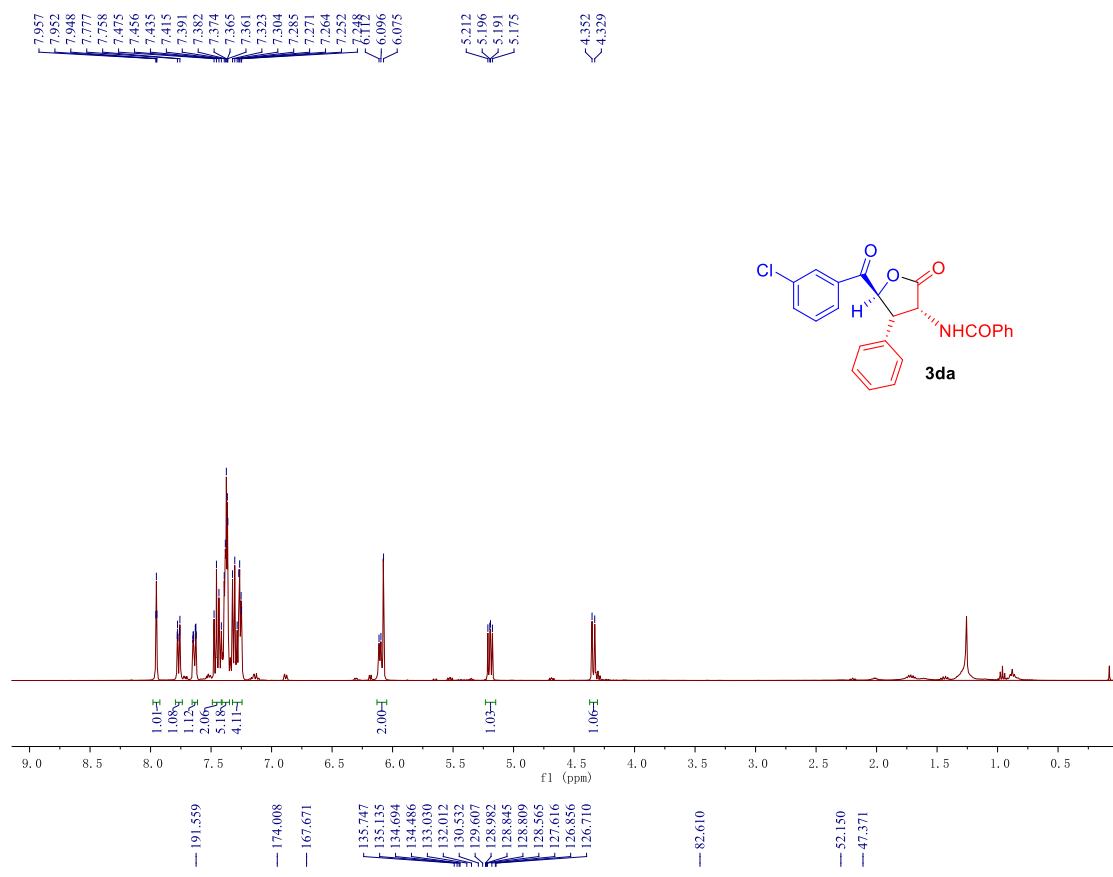


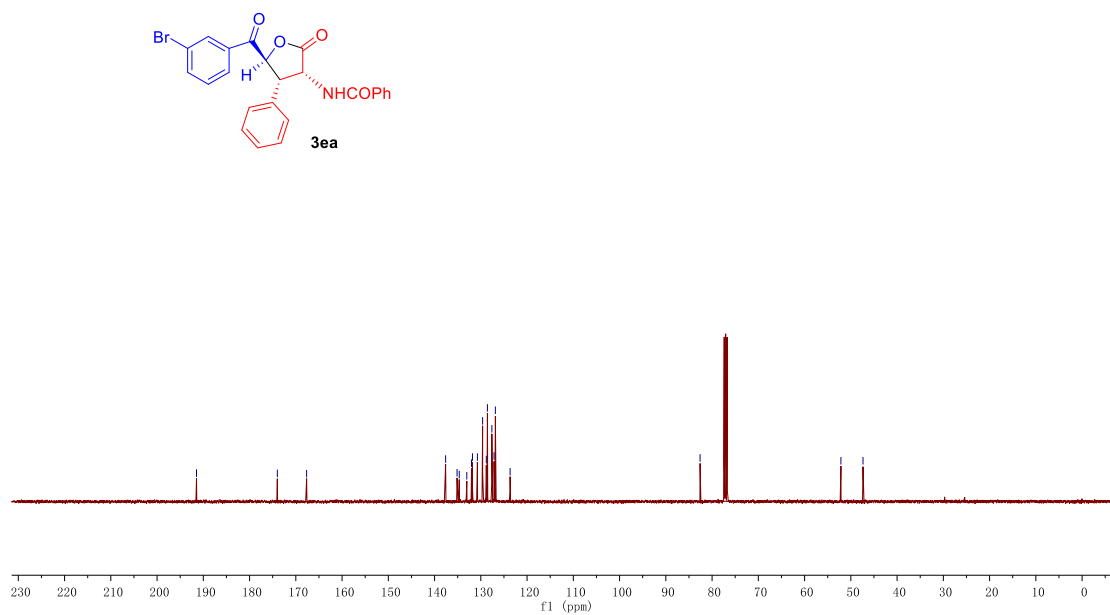
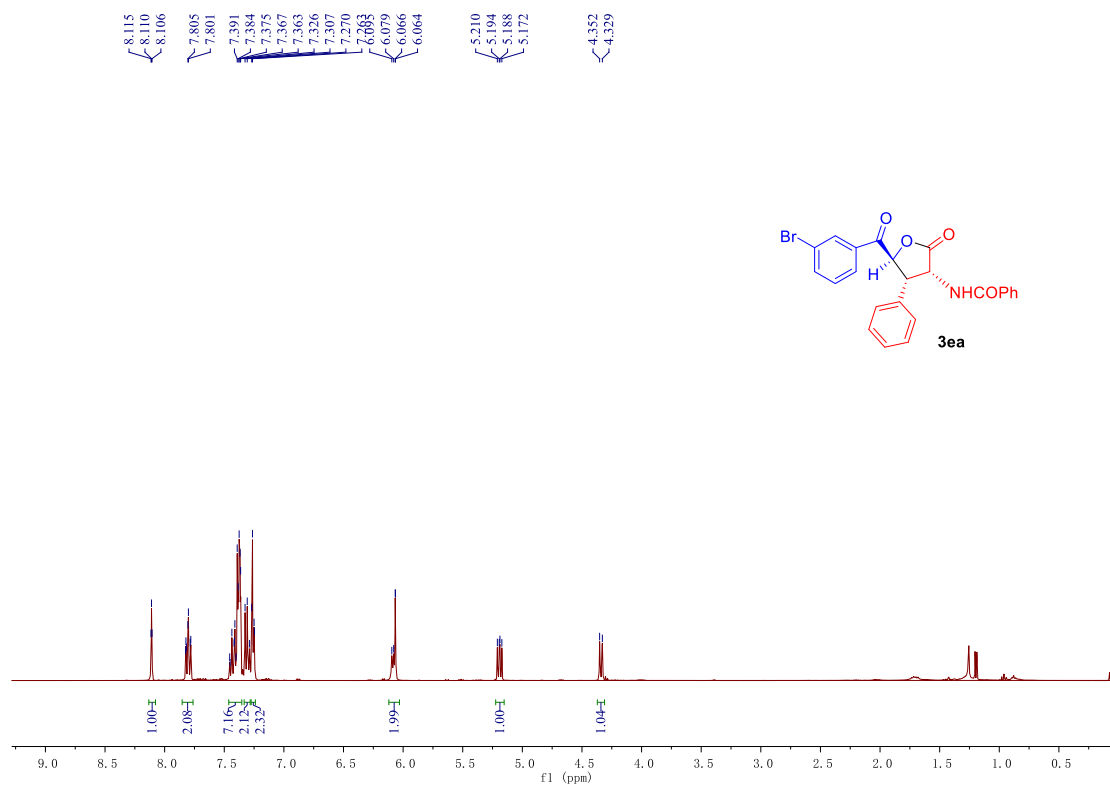


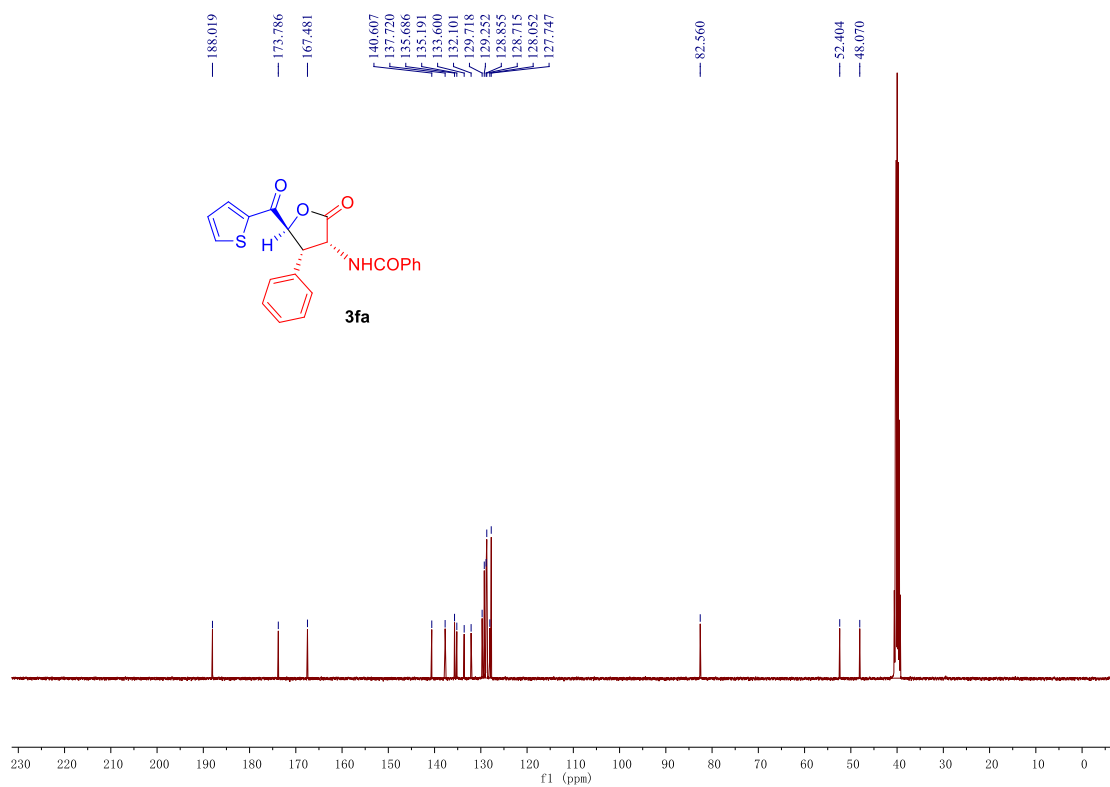
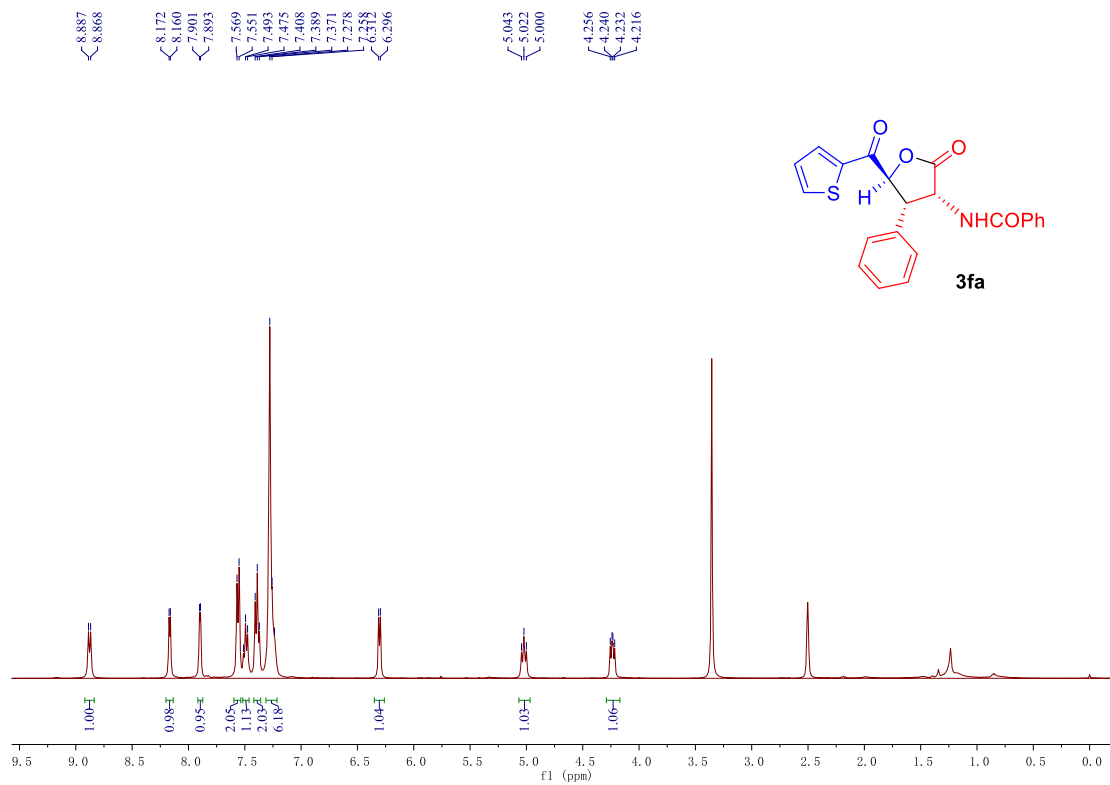


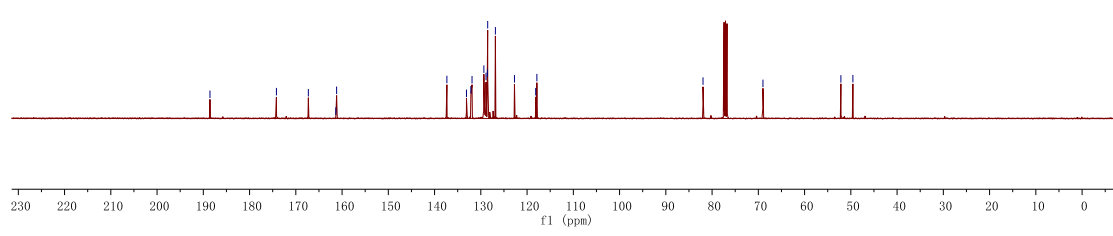
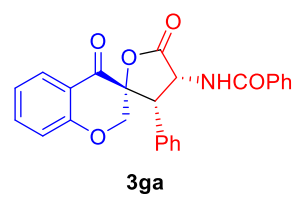
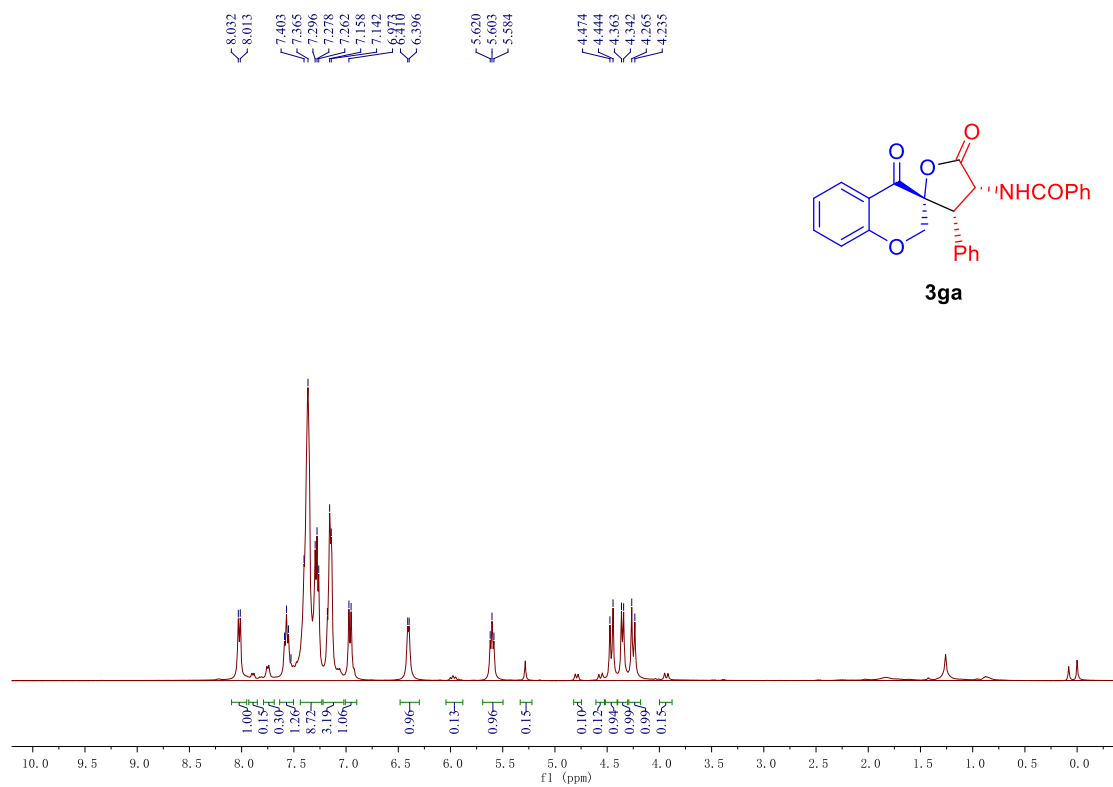


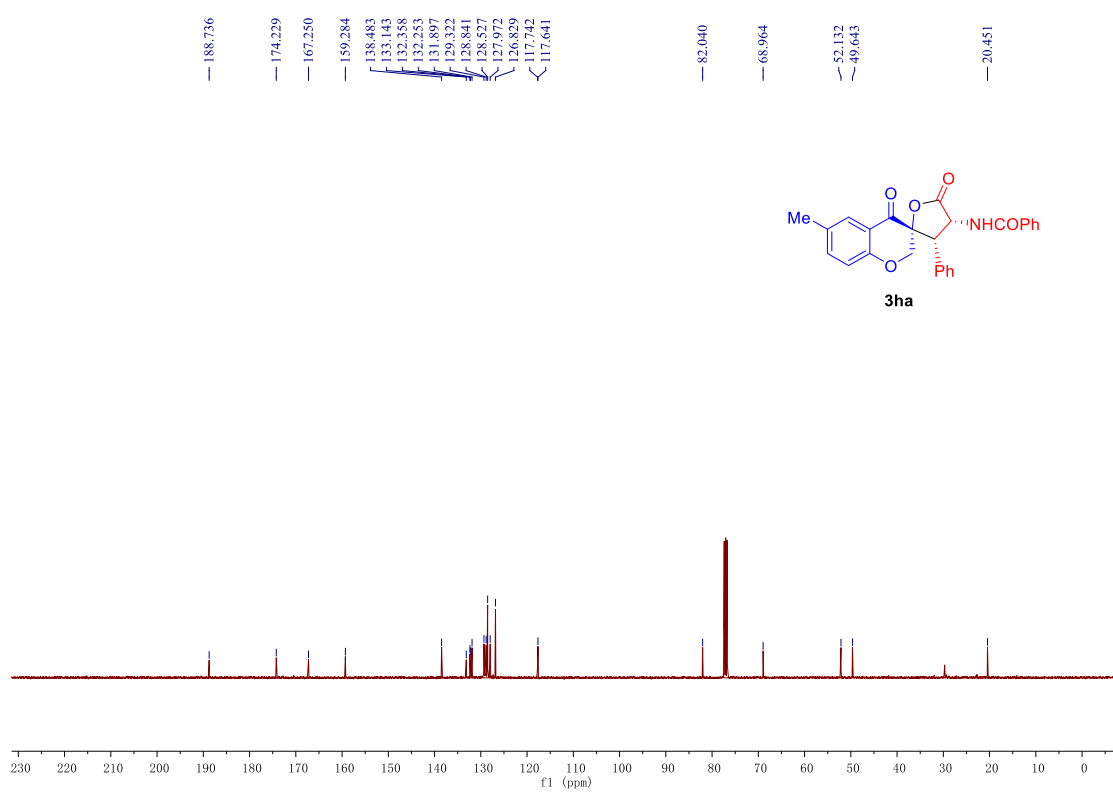
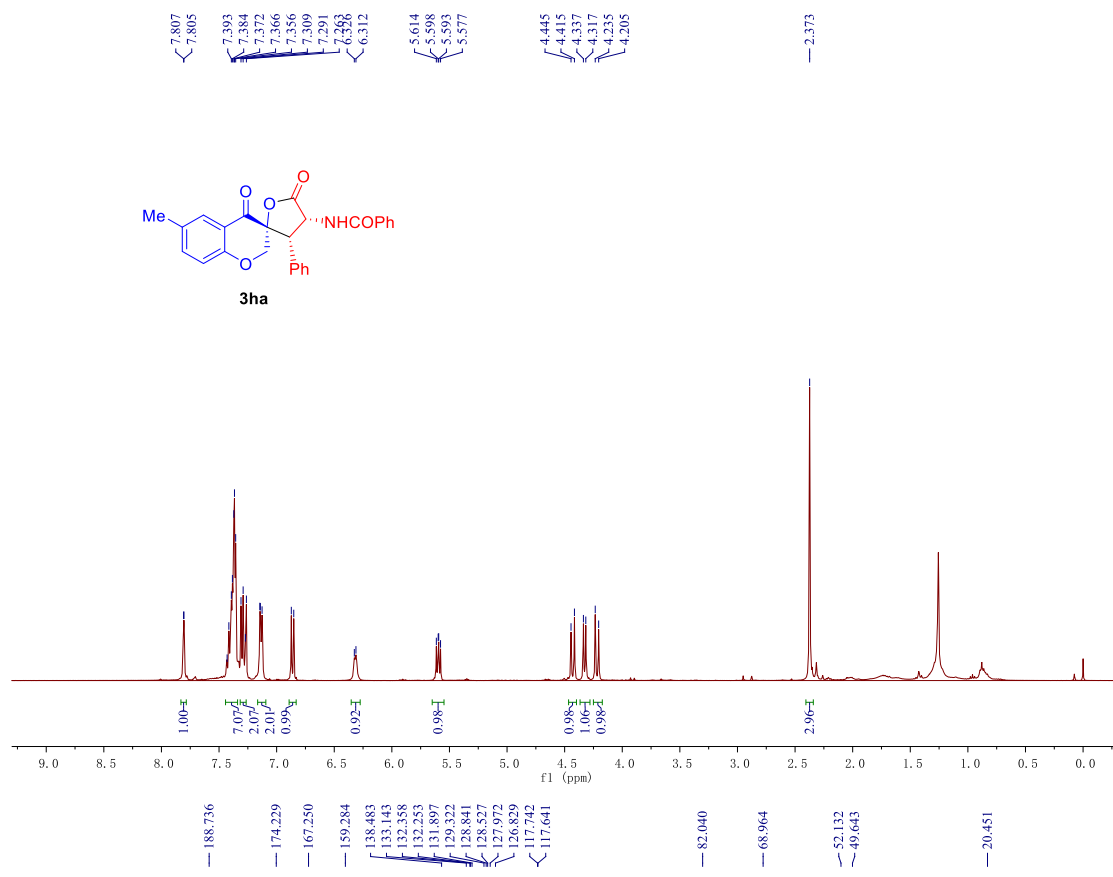




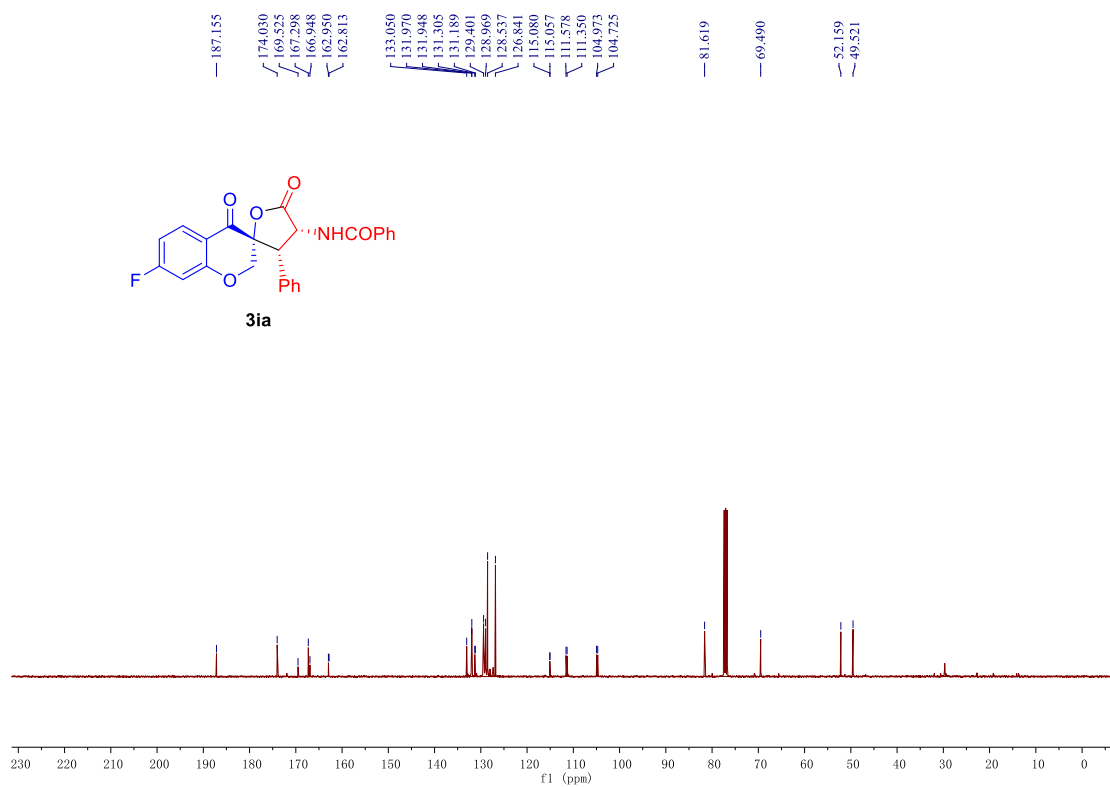
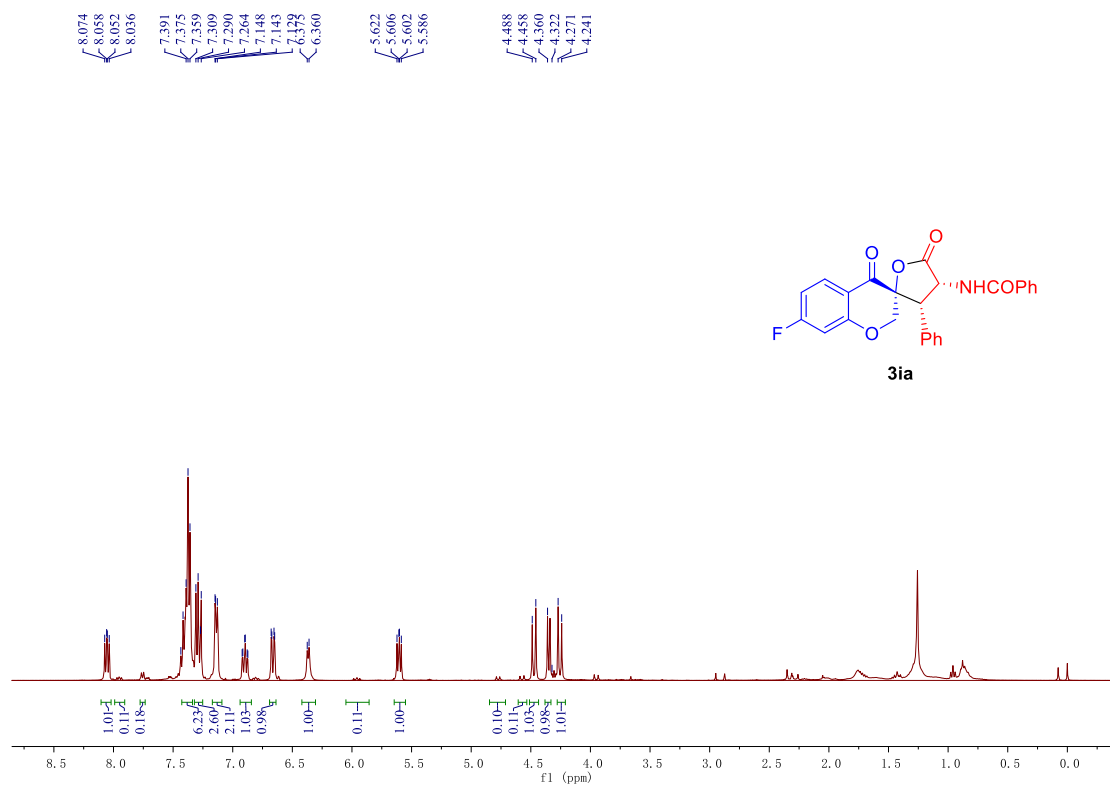




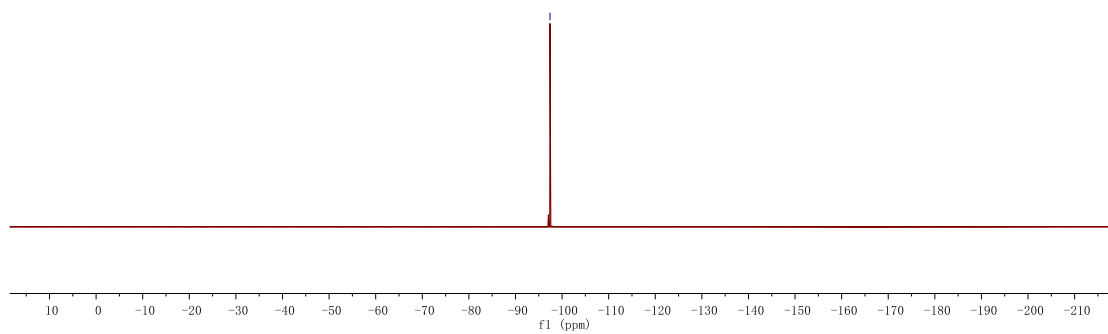
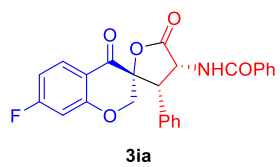




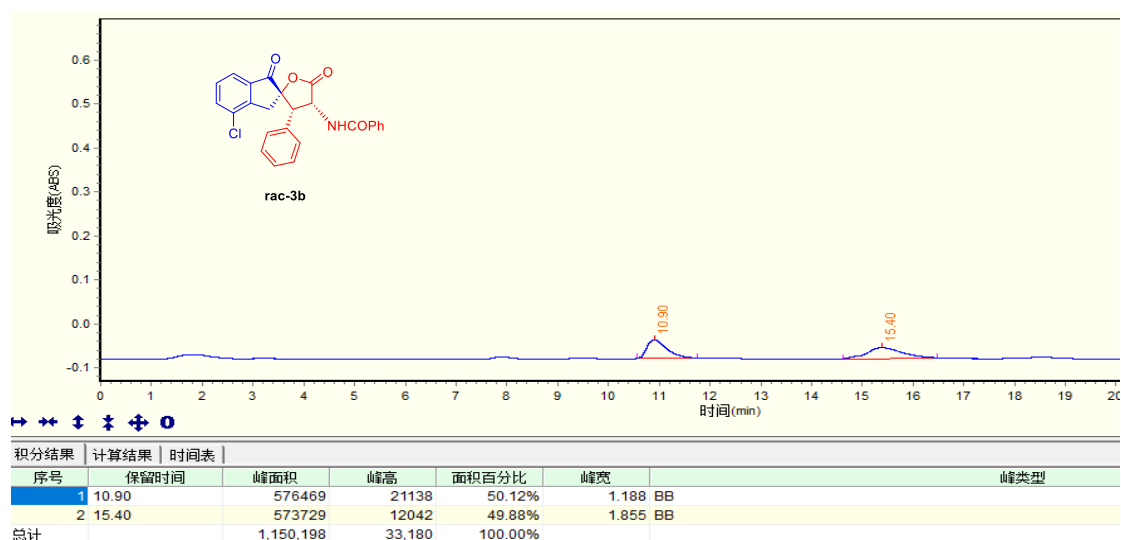
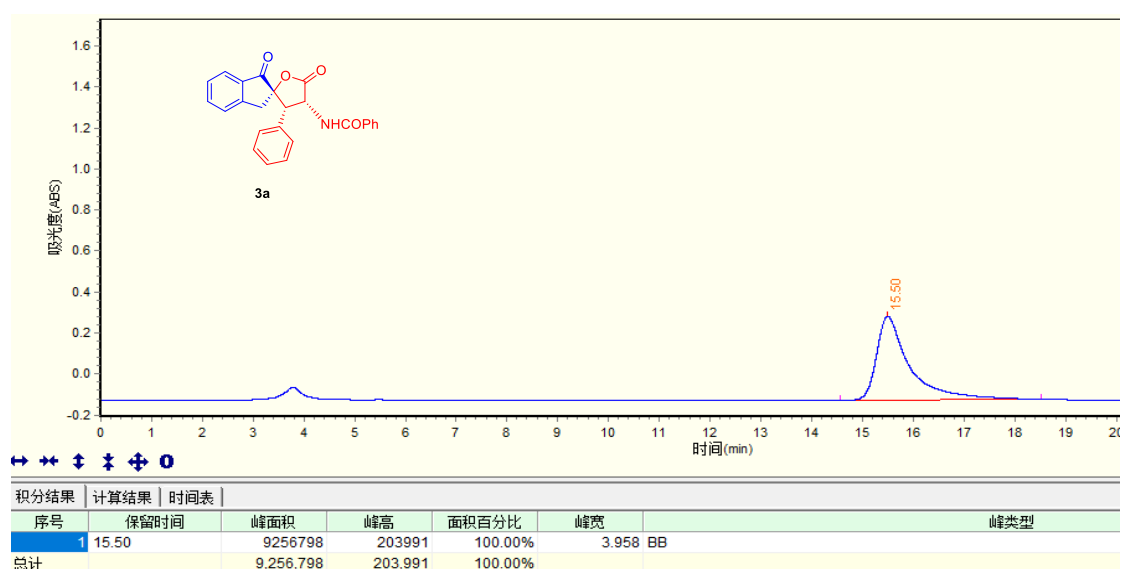
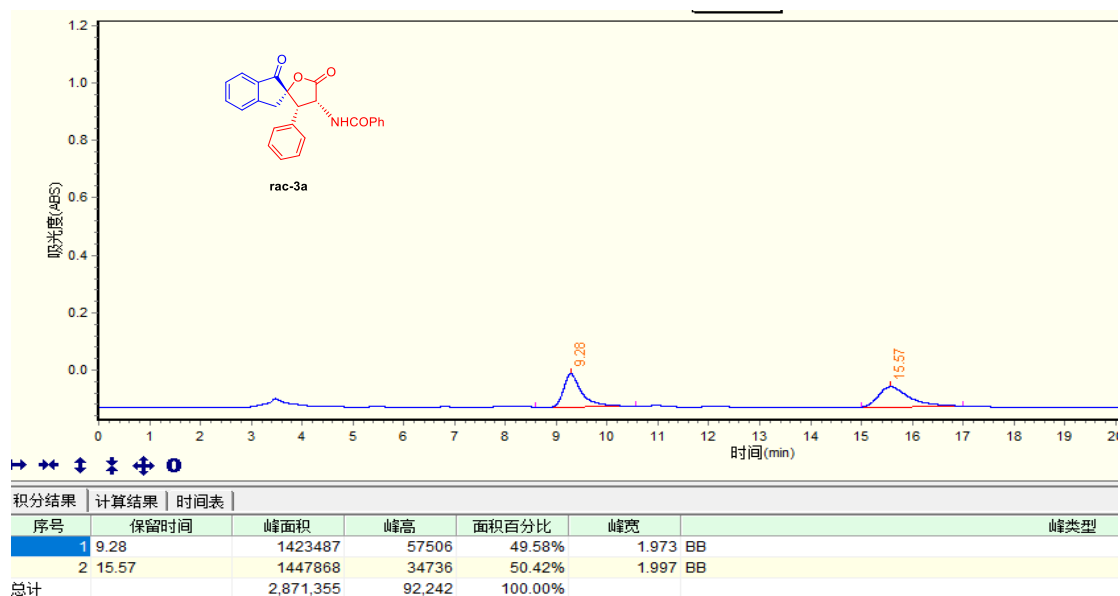


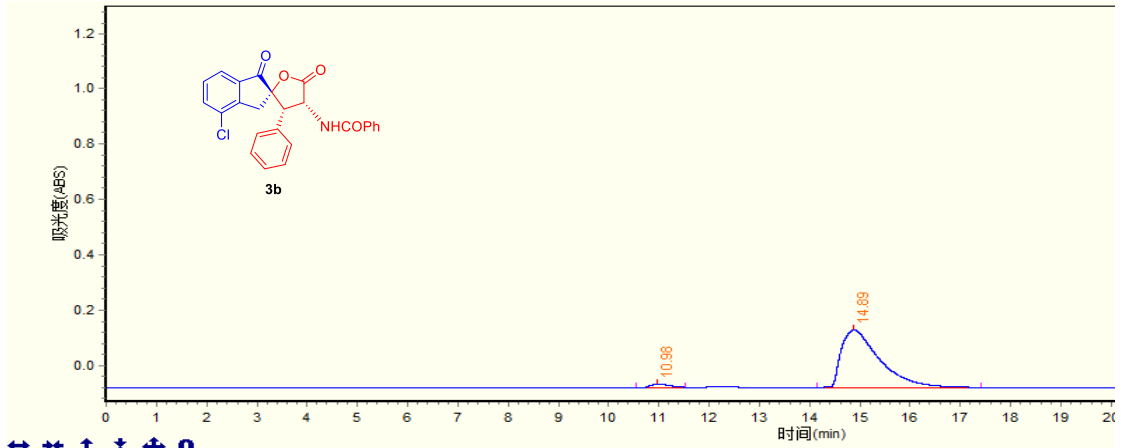


— 97.406

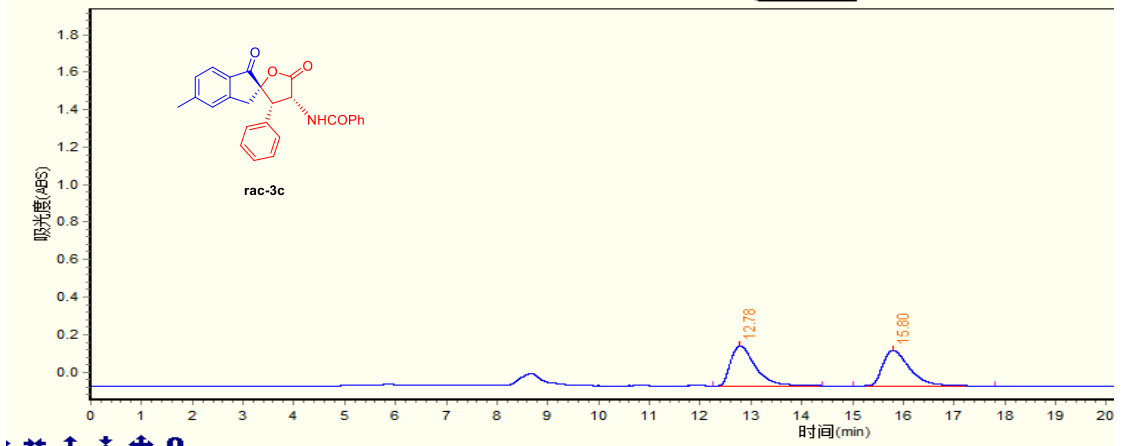


## HPLC spectra of compounds

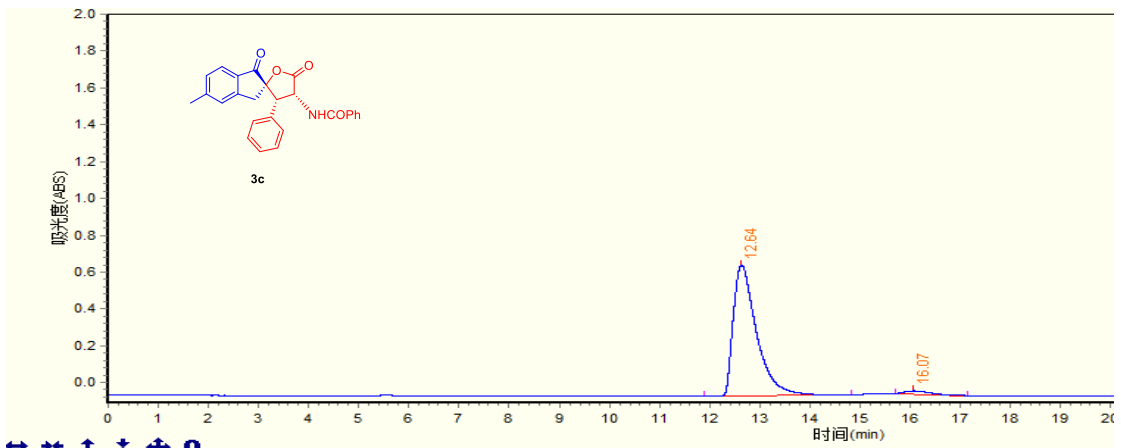




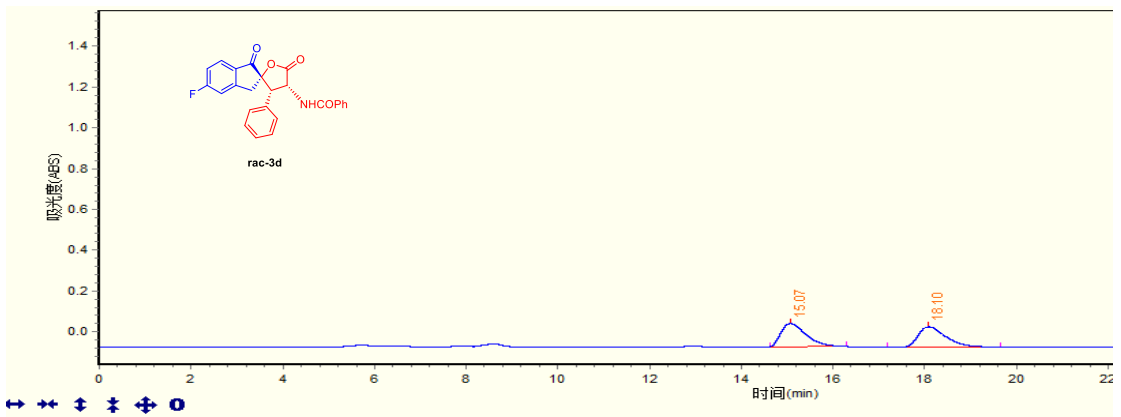
序号	保留时间	峰面积	峰高	面积百分比	峰宽
1	10.98	169777	6717	2.97%	0.977 BB
2	14.89	5537069	103735	97.03%	3.265 BB
总计		5,706,846	110,452	100.00%	



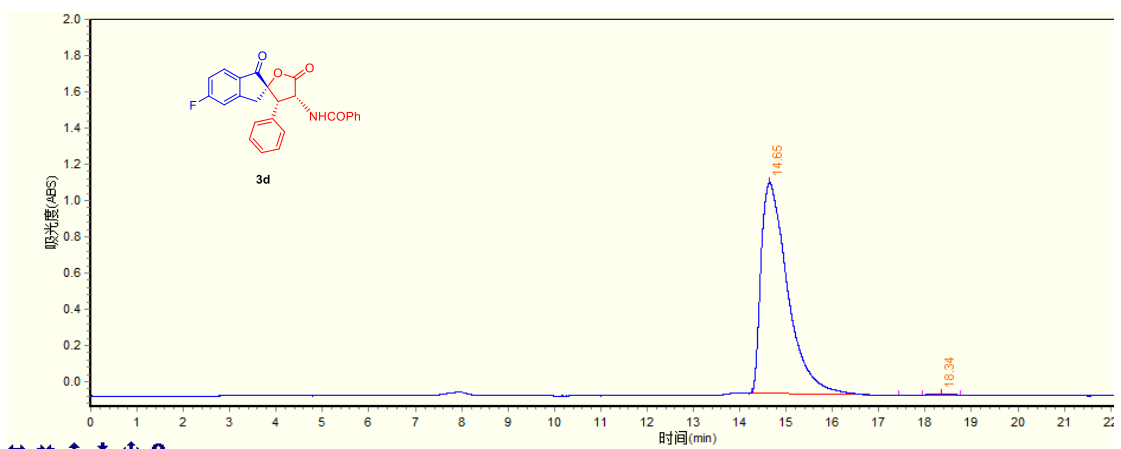
序号	保留时间	峰面积	峰高	面积百分比	峰宽
1	12.78	3567288	106861	50.65%	2.145 BB
2	15.80	3475793	94401	49.35%	2.792 BB
总计		7,043,081	201,262	100.00%	



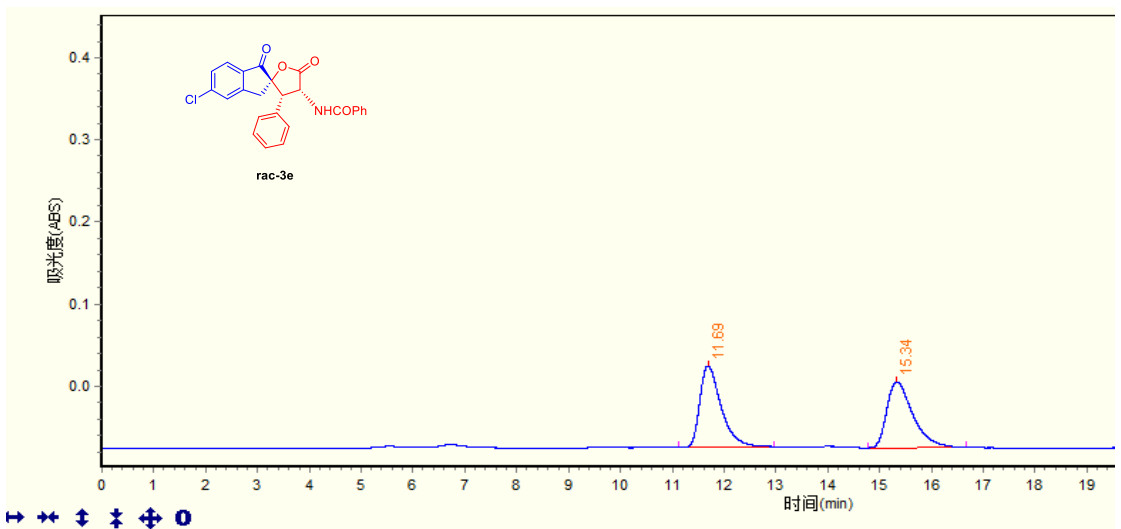
序号	保留时间	峰面积	峰高	面积百分比	峰宽
1	12.64	11440314	353878	97.37%	2.936 BB
2	16.07	308541	8940	2.63%	1.438 BB
总计		11,748,855	362,818	100.00%	



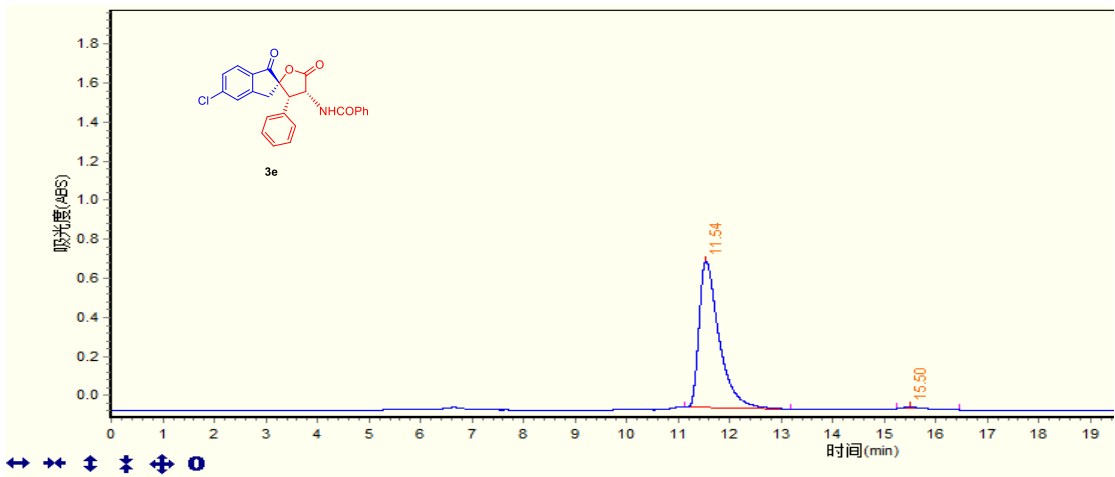
序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类
1	15.07	2157008	56660	50.57%	1.666	BB
2	18.10	2108625	49870	49.43%	2.468	BB
总计		4,265,633	106,530	100.00%		



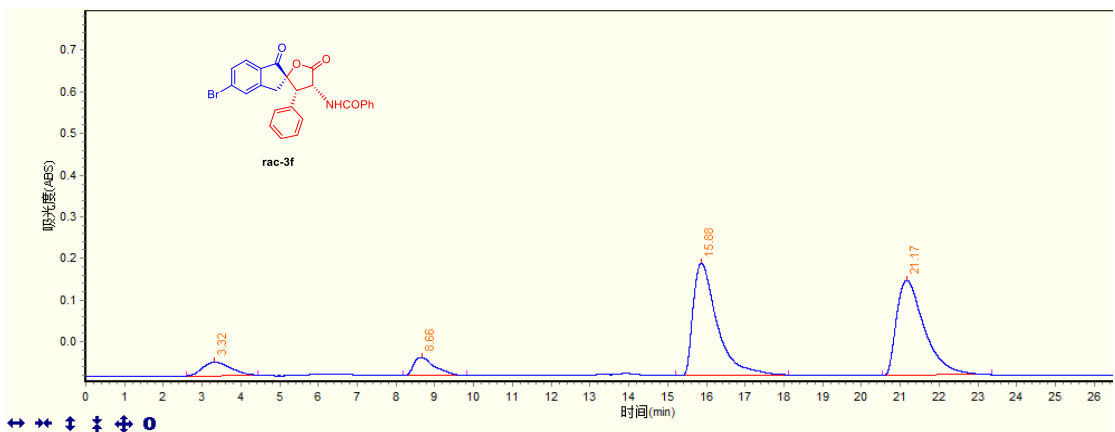
序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	14.65	23072111	580581	99.64%	3.173	BB
2	18.34	82933	2854	0.36%	0.819	BB
总计		23,155,044	583,435	100.00%		



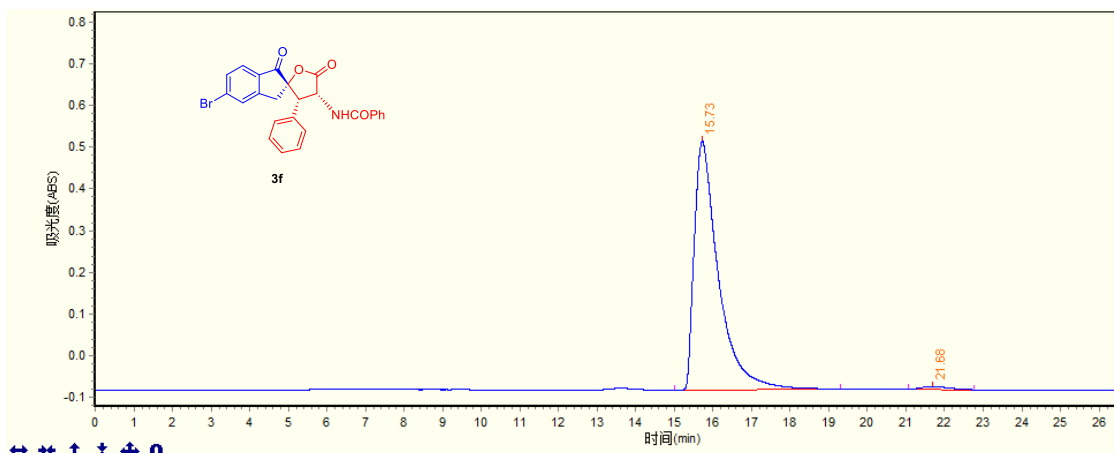
序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类
1	11.69	1408981	49401	50.27%	1.84	BB
2	15.34	1393842	39714	49.73%	1.895	BB
总计		2,802,823	89,115	100.00%		



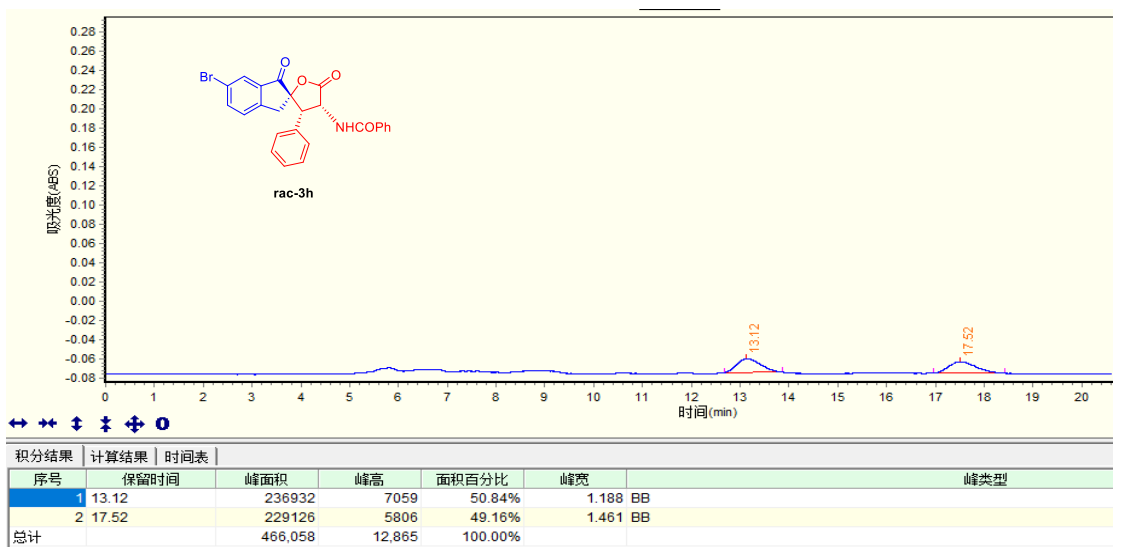
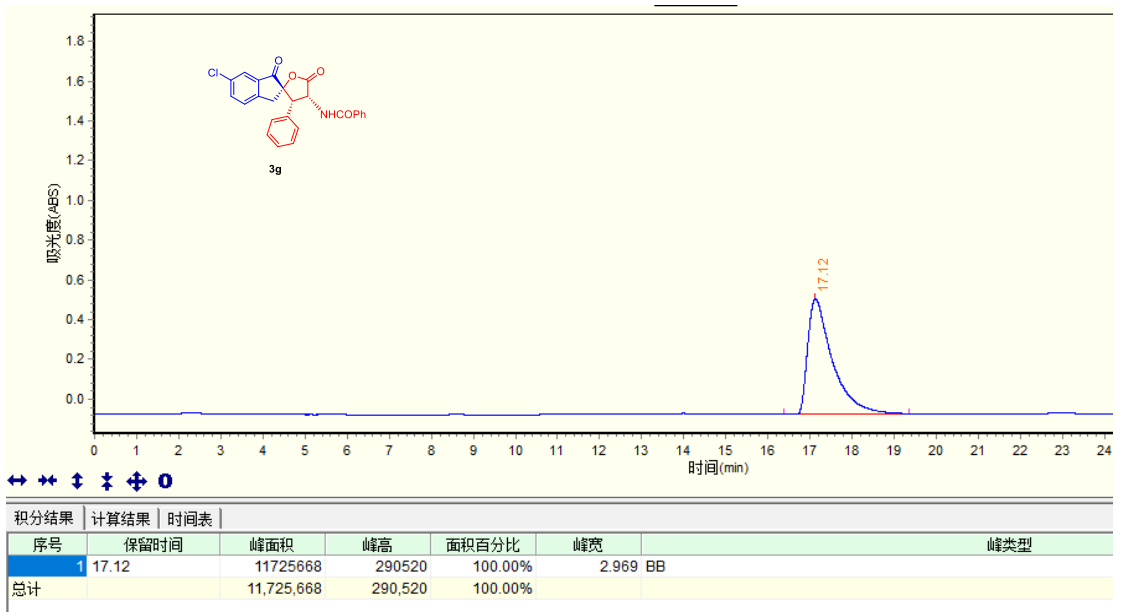
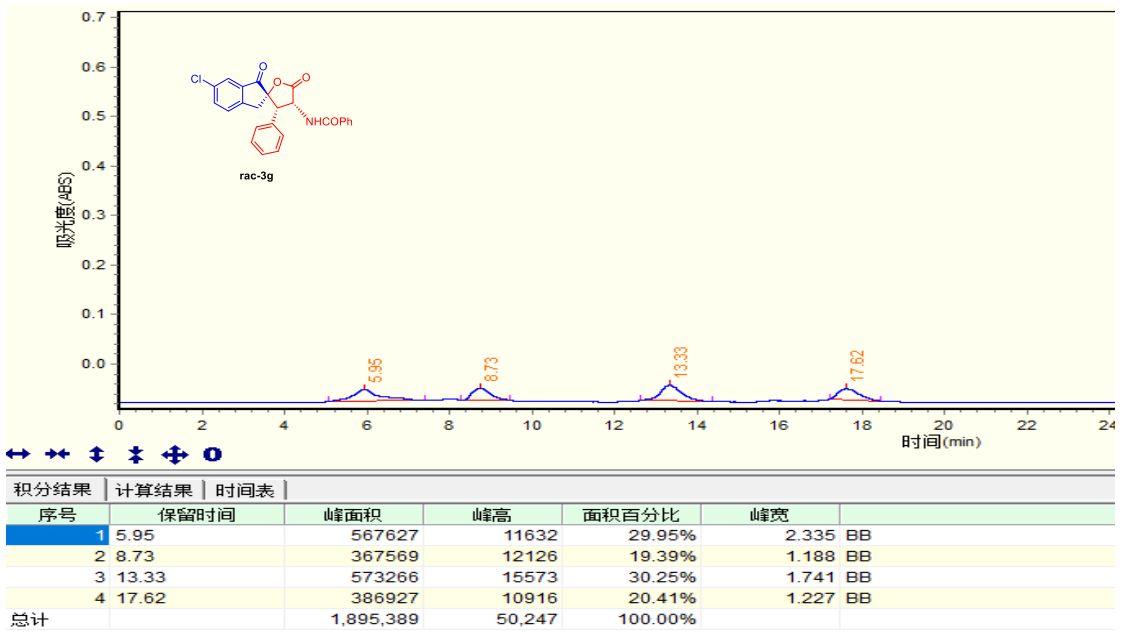
序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	11.54	10019761	373700	98.81%	2.057	BB
2	15.50	120906	4530	1.19%	1.217	BB
总计		10,140,667	378,230	100.00%		

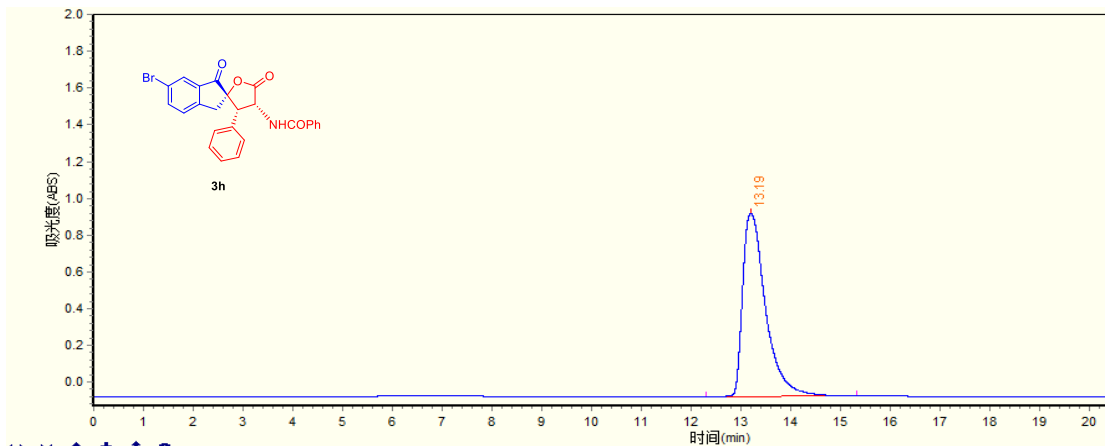


序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	3.32	796050	15969	6.09%	1.832	BB
2	8.66	805306	21530	6.16%	1.625	BB
3	15.88	5764145	134818	44.07%	2.903	BB
4	21.17	5713296	114096	43.68%	2.834	BB
总计		13,078,797	286,413	100.00%		

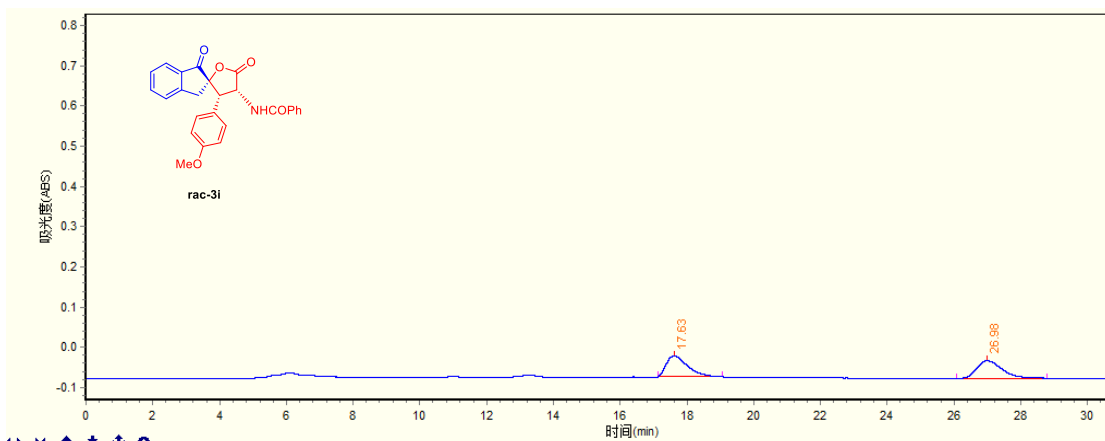


序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	15.73	12925032	297827	98.56%	4.296	BB
2	21.68	189270	3894	1.44%	1.718	BB
总计		13,114,302	301,721	100.00%		

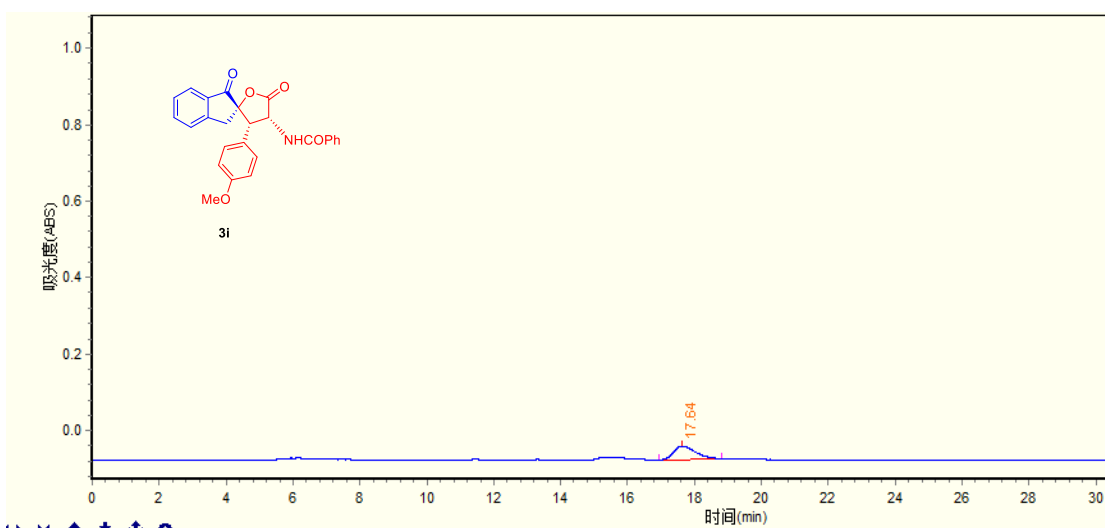




序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	13.19	15952700	497708	100.00%	3.023	BB
总计		15,952,700	497,708	100.00%		

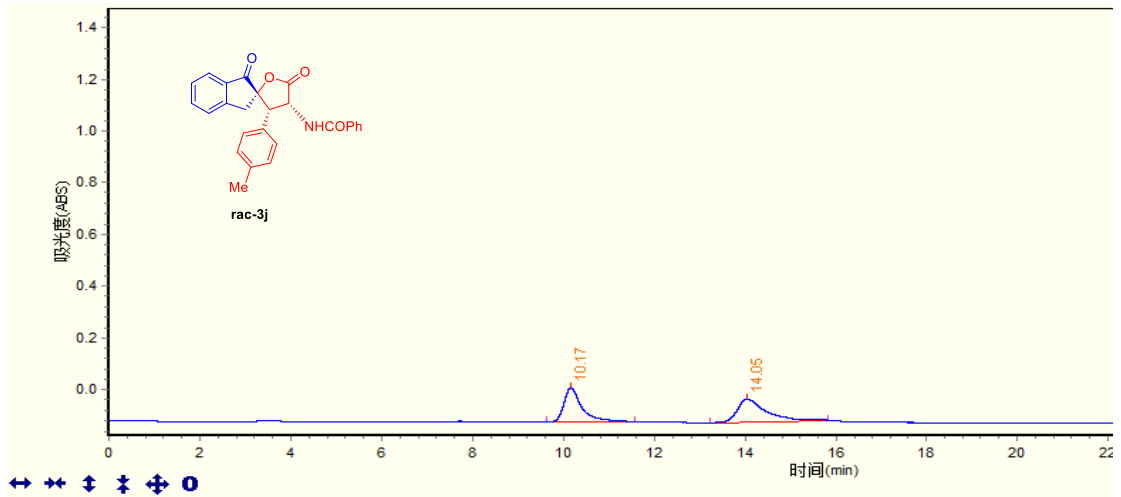


序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	17.63	1152897	25861	50.57%	1.926	BB
2	26.98	1126885	21725	49.43%	2.709	BB
总计		2,279,782	47,586	100.00%		

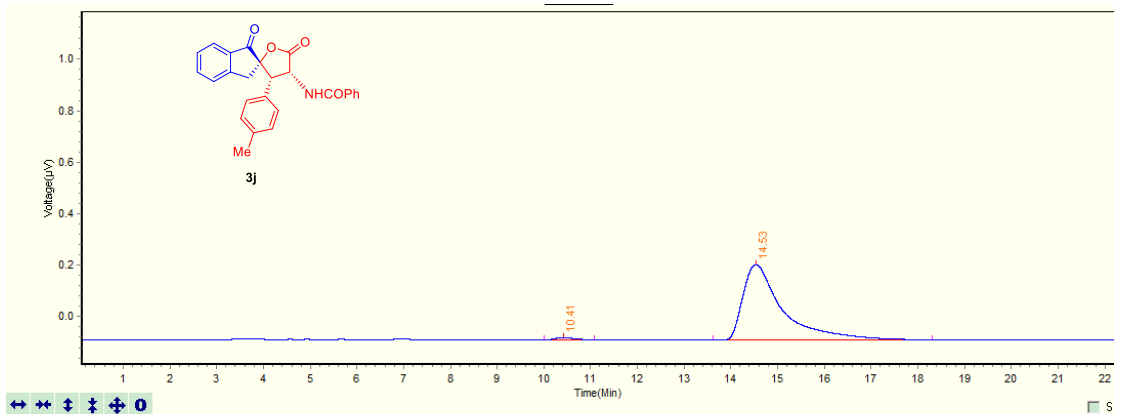


序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	17.64	770497	17383	100.00%	1.873	BB
总计		770,497	17,383	100.00%		

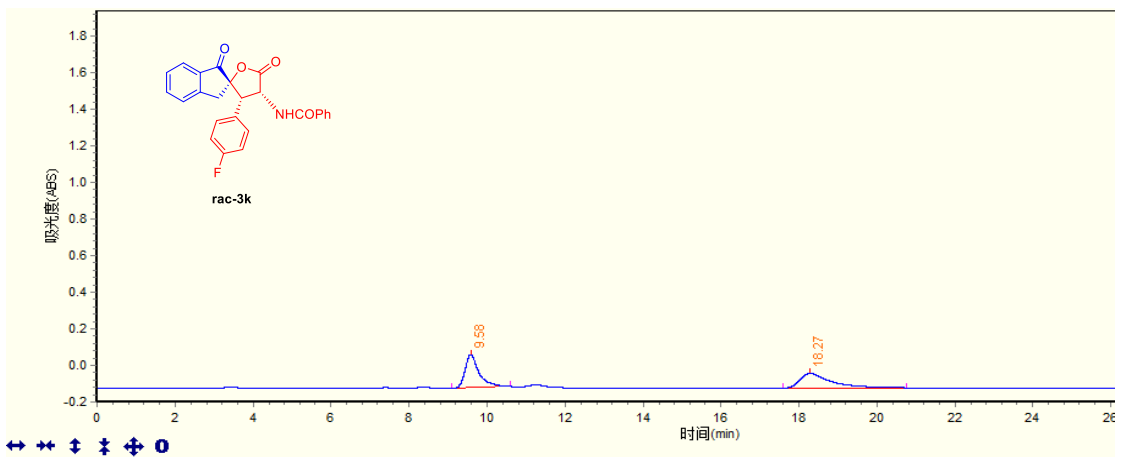




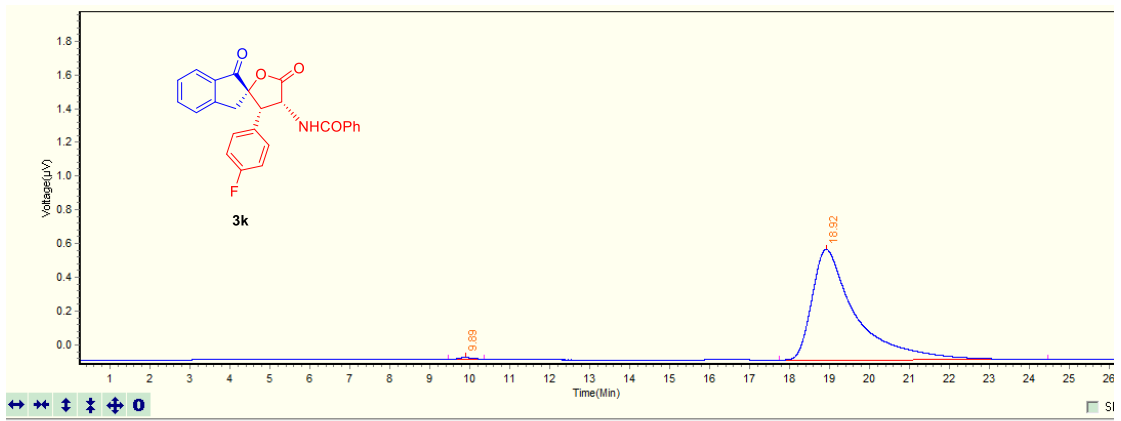
序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	10.17	1843642	66288	49.38%	1.939	BB
2	14.05	1889967	44088	50.62%	2.596	BB
总计		3,733,609	110,376	100.00%		



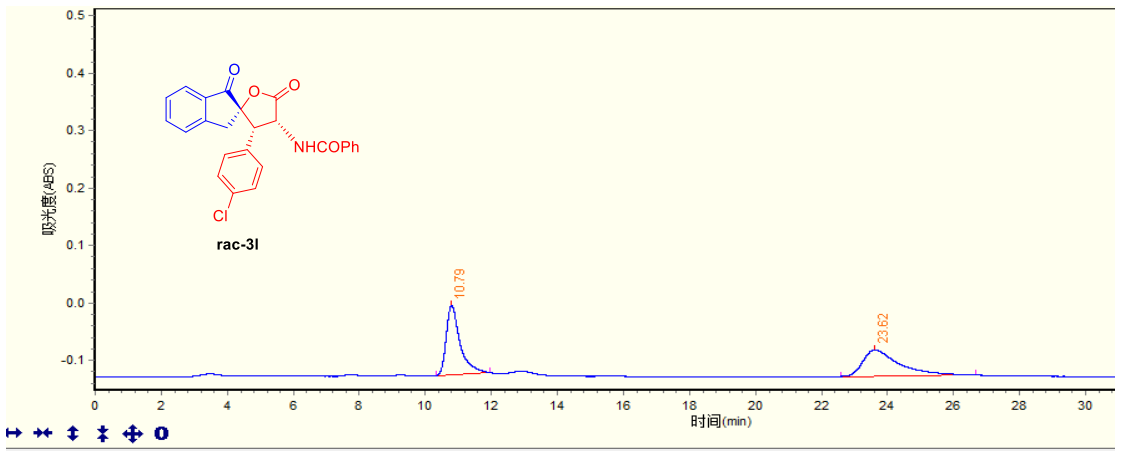
No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	10.41	127951	4675	1.45%	1.083	BB
2	14.53	8667621	146881	98.55%	4.68	BB
Total		8,795,572	151,556	100.00%		



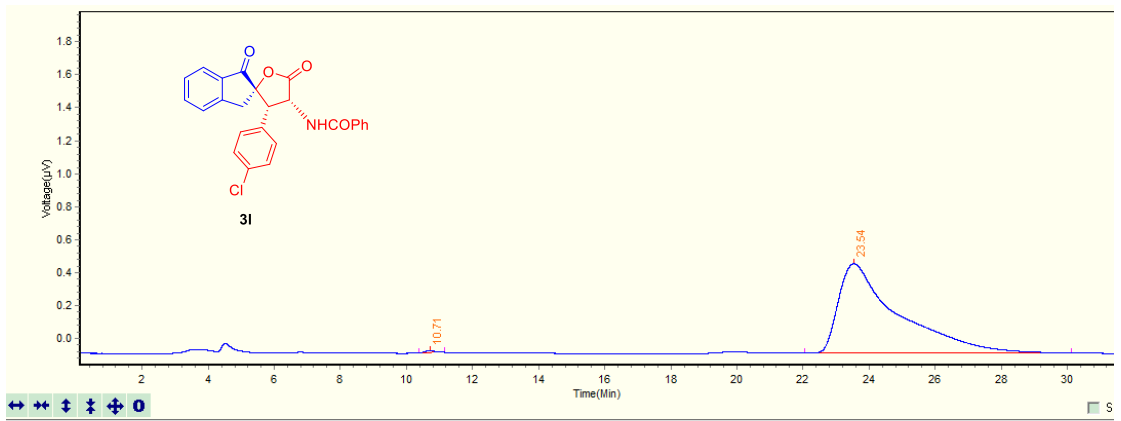
序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	9.58	2242969	90382	50.09%	1.505	BB
2	18.27	2234804	39898	49.91%	3.167	BB
总计		4,477,773	130,280	100.00%		



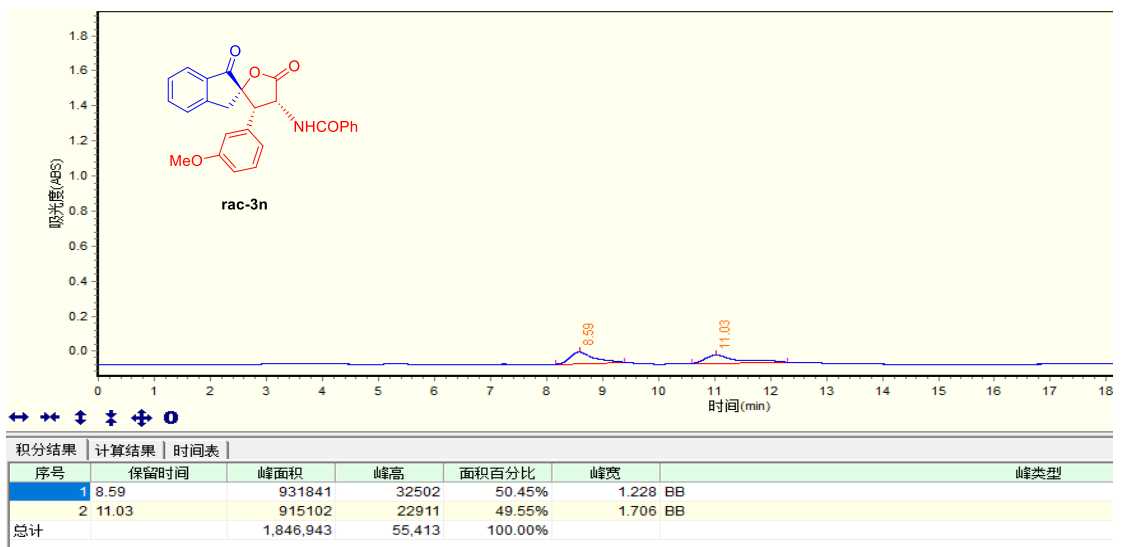
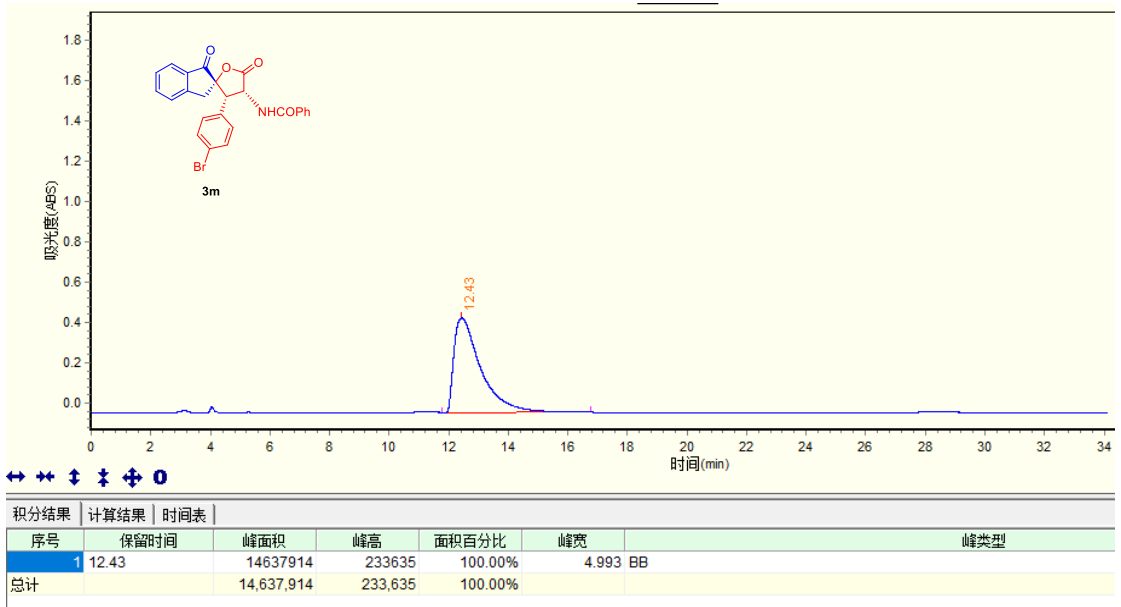
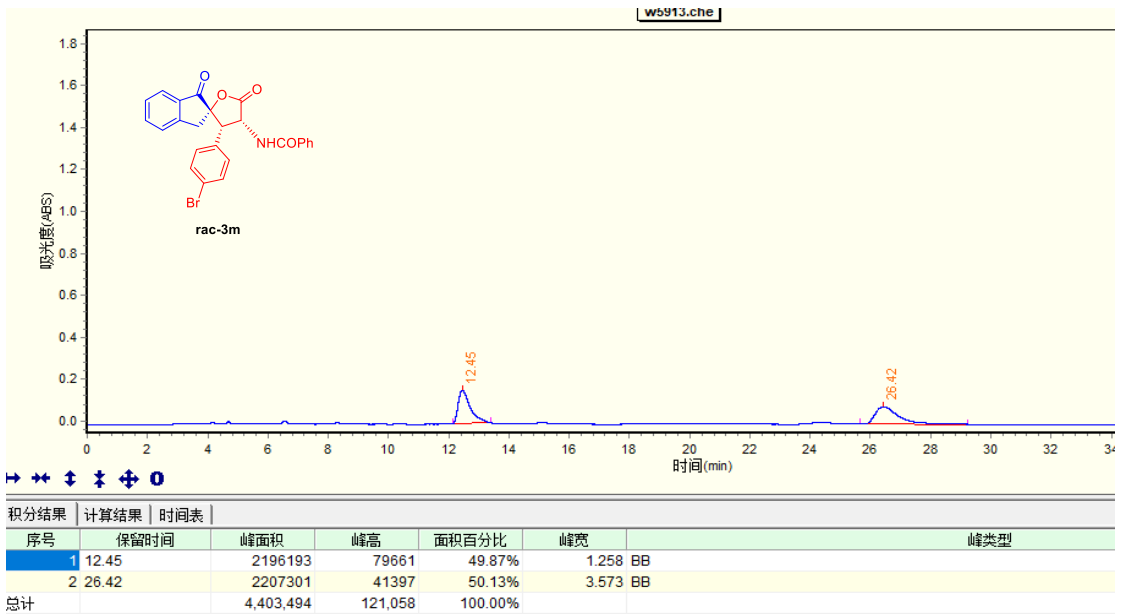
No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	9.89	148592	5741	0.59%	0.911	BB
2	18.92	24853107	328203	99.41%	6.722	BB
Total		25,001,699	333,944	100.00%		

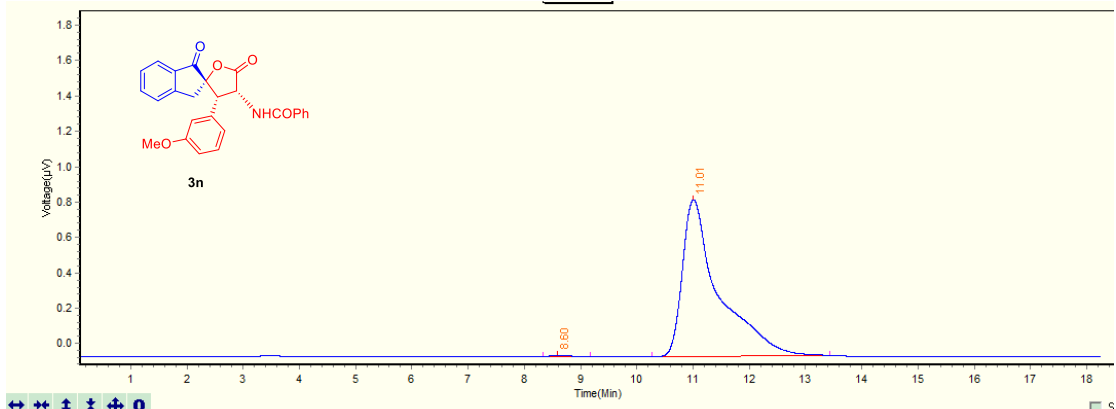


序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	10.79	1753703	60696	50.17%	1.62	BB
2	23.62	1741905	22798	49.83%	4.086	BB
总计		3,495,608	83,494	100.00%		

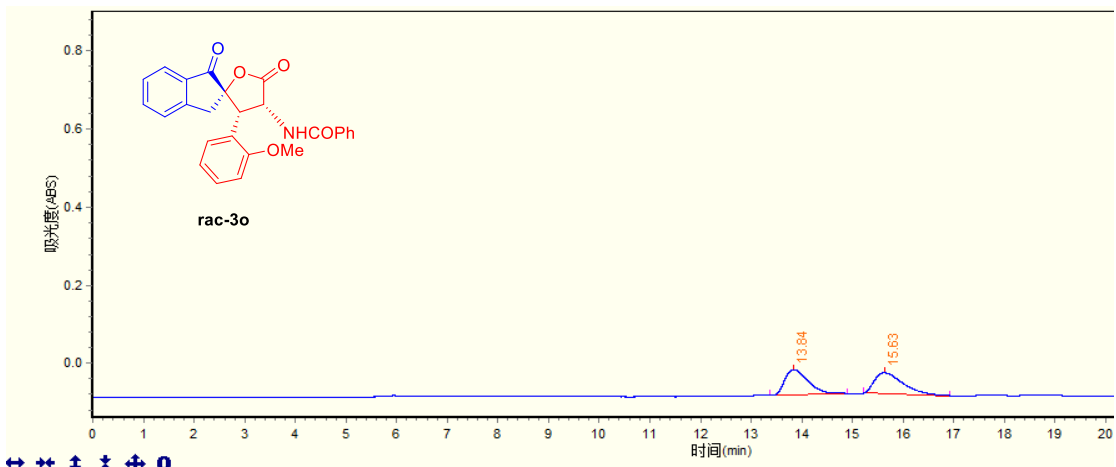


No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	10.71	129008	5375	0.38%	0.781	BB
2	23.54	33810250	270299	99.62%	8.069	BB
Total		33,939,258	275,674	100.00%		

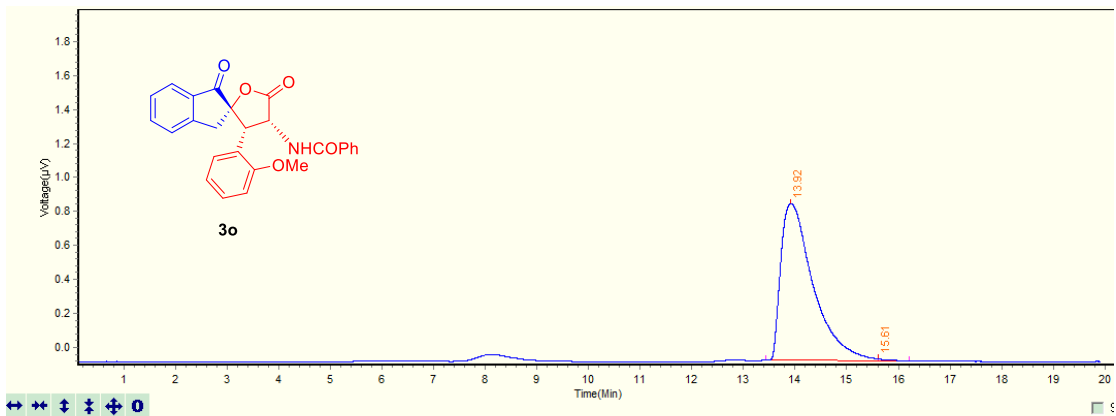




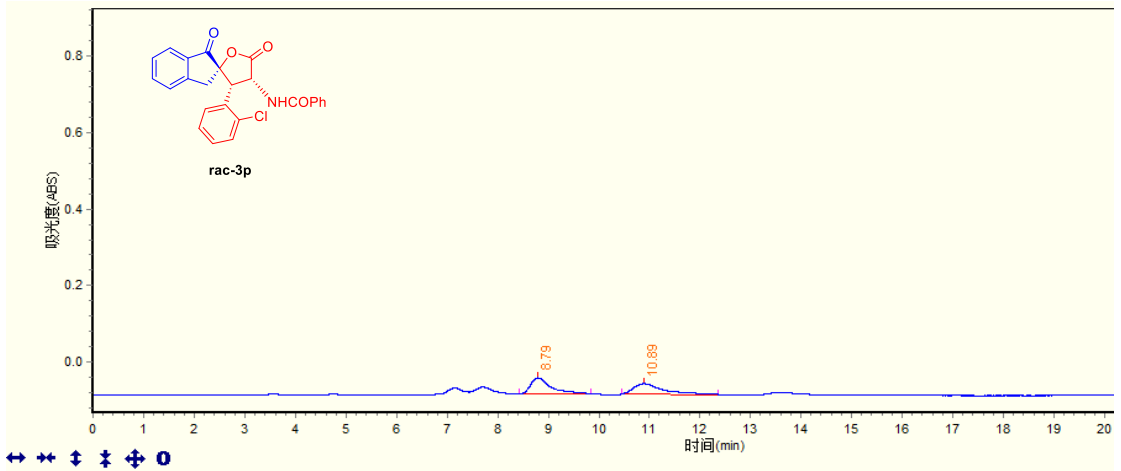
No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	8.60	73877	3139	0.37%	0.85	BB
2	11.01	19929655	442694	99.63%	3.162	BB
Total		20,003,532	445,833	100.00%		



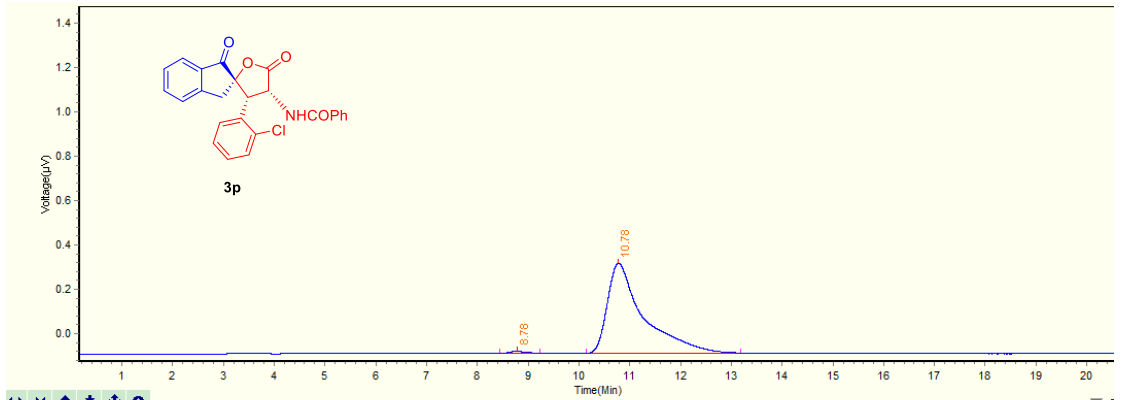
序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	13.84	1014846	31949	49.08%	1.509	BB
2	15.63	1052835	26788	50.92%	1.717	BB
总计		2,067,681	58,737	100.00%		



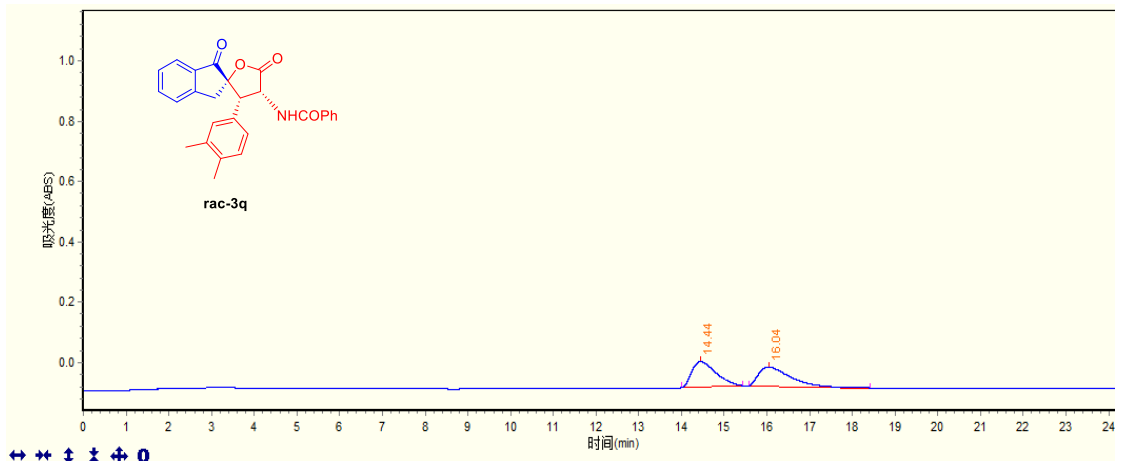
No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	13.92	20060904	460877	99.74%	2.179	BV
2	15.61	52402	4588	0.26%	0.599	VB
Total		20,113,306	465,465	100.00%		



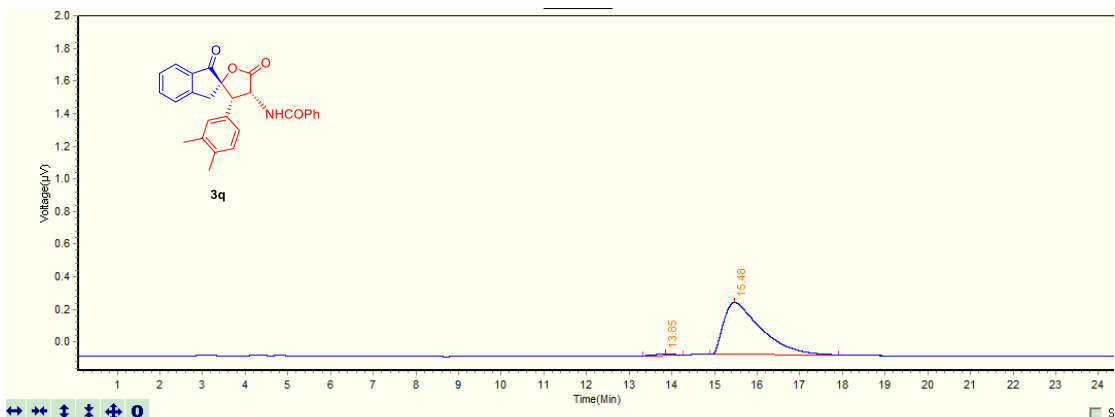
序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	8.79	579688	21022	50.83%	1.417	BB
2	10.89	560661	13741	49.17%	1.905	BB
总计		1,140,349	34,763	100.00%		



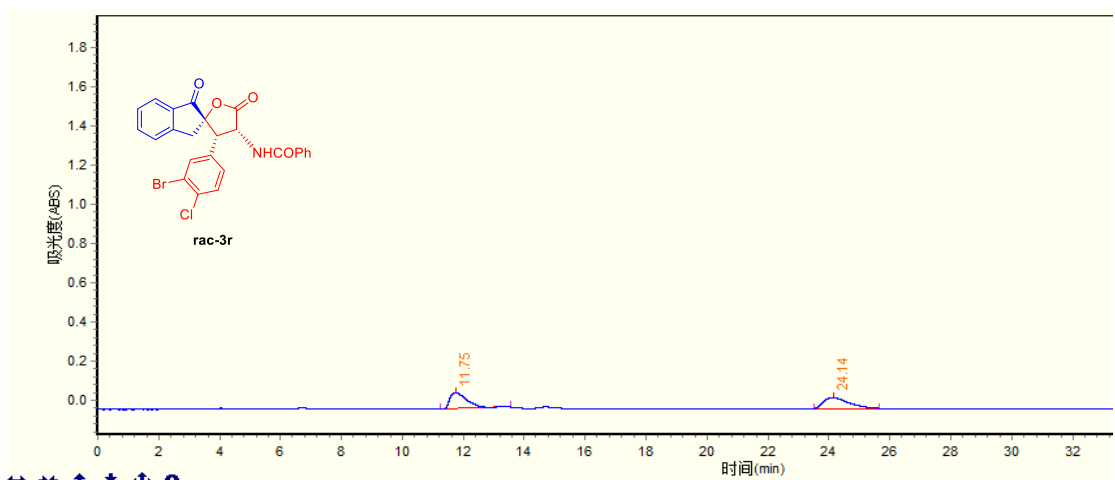
No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	8.78	99349	4522	0.99%	0.798	BB
2	10.78	9968623	202901	99.01%	3.049	BB
Total		10,067,972	207,423	100.00%		



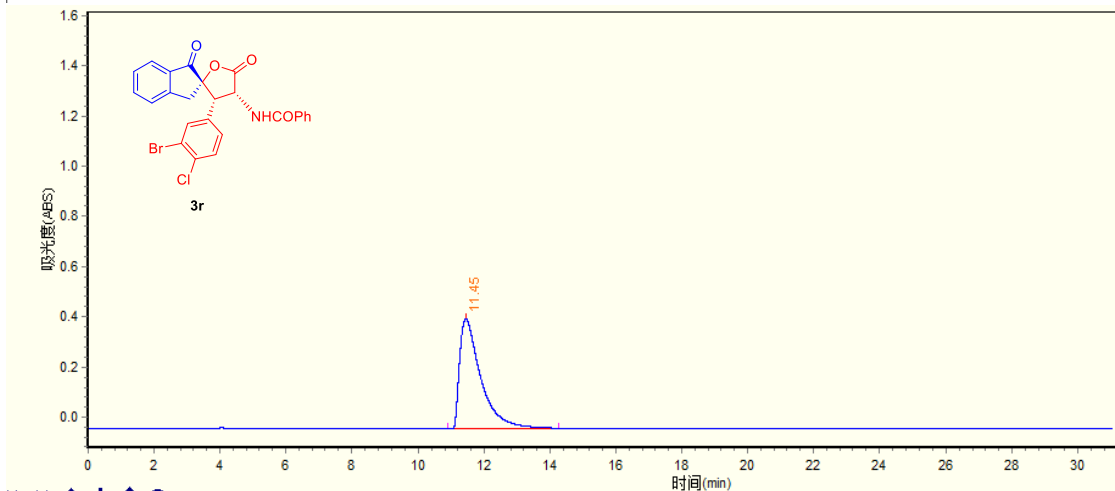
序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	14.44	1661195	42347	50.81%	1.429	BB
2	16.04	1608480	31736	49.19%	2.835	BB
总计		3,269,675	74,083	100.00%		



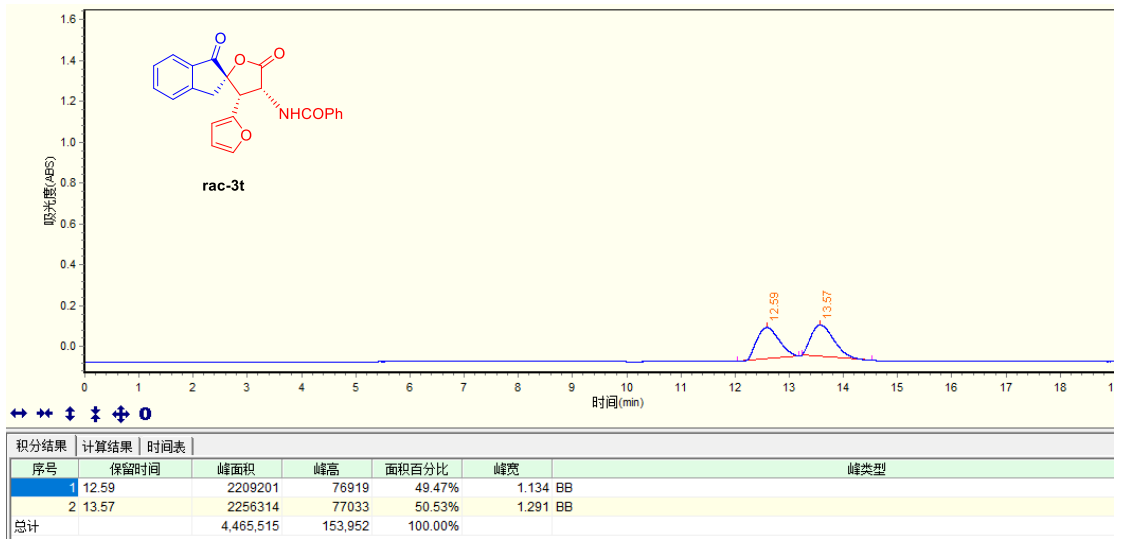
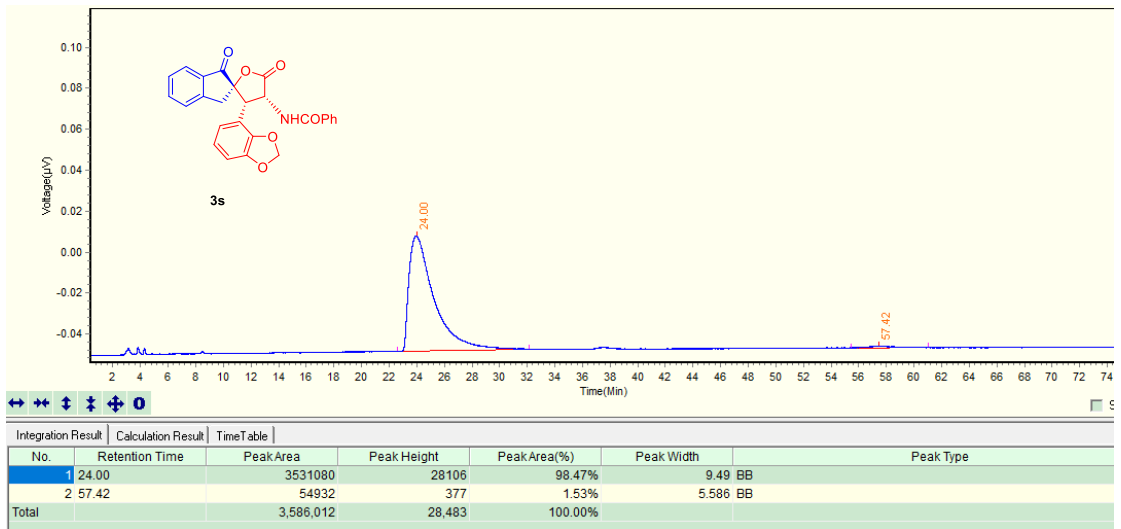
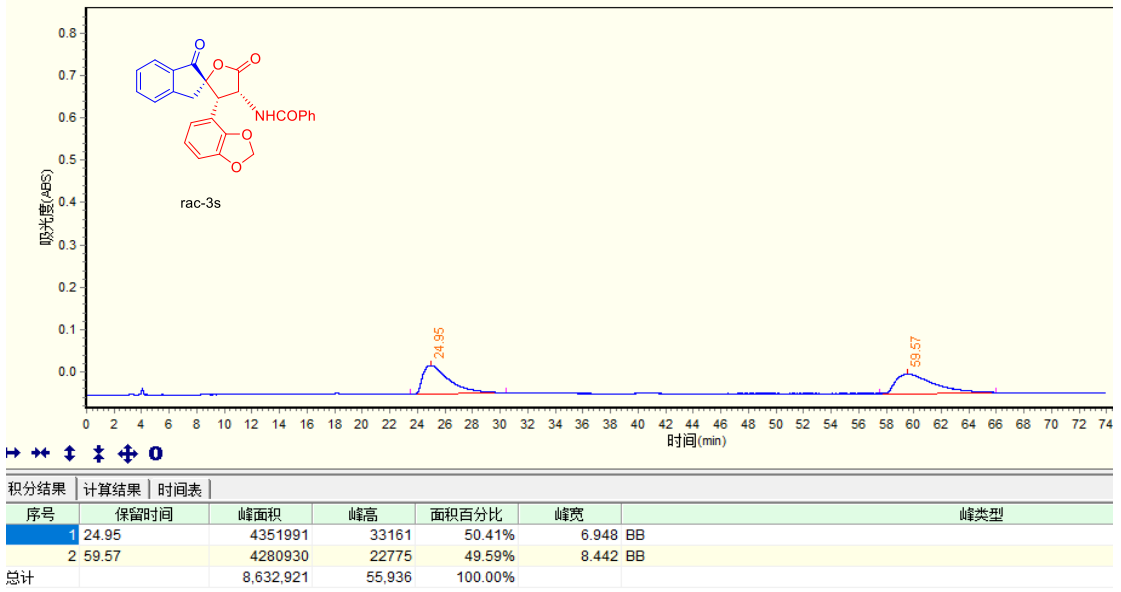
No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	13.85	118369	3865	1.21%	0.945	BB
2	15.48	9625552	158841	98.79%	3.005	BB
Total		9,743,921	162,706	100.00%		

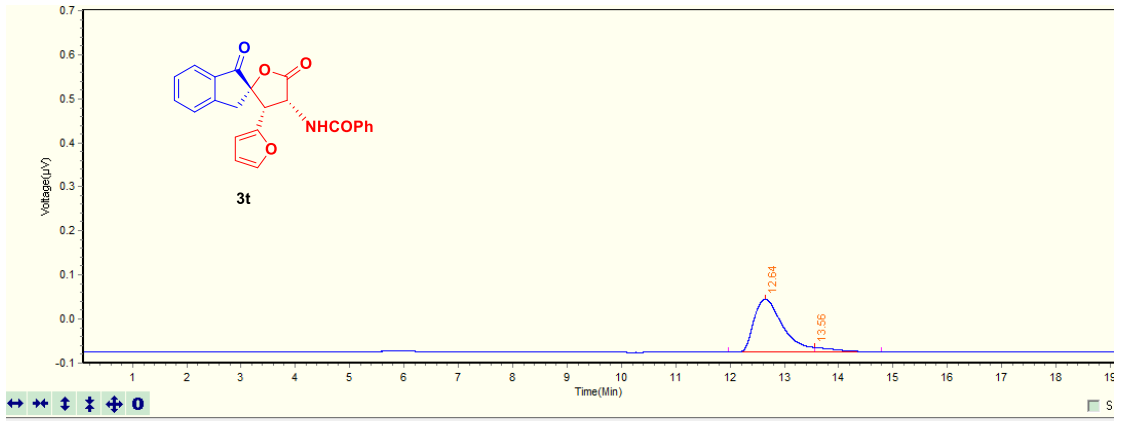


序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	11.75	1635138	41277	50.00%	2.308	BB
2	24.14	1635346	28097	50.00%	2.137	BB
总计		3,270,484	69,374	100.00%		

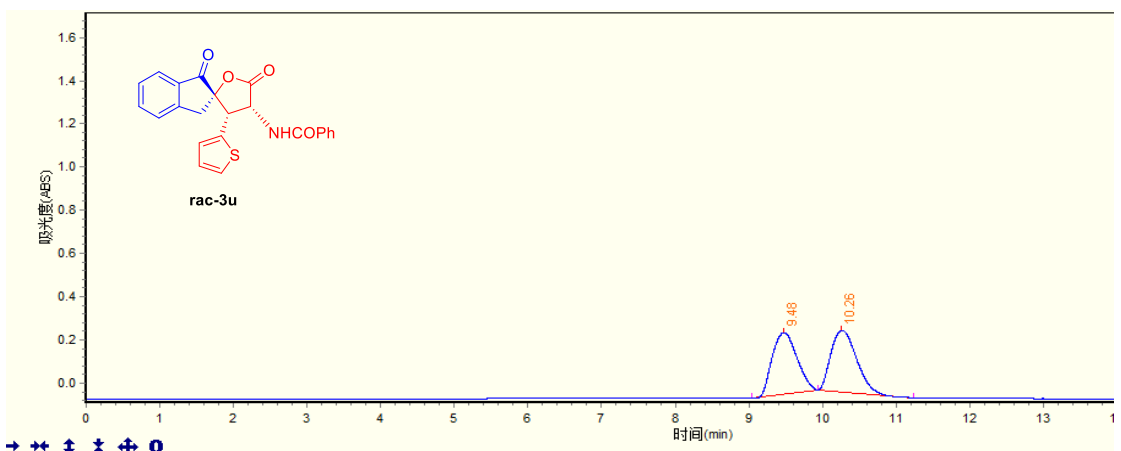


序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	11.45	9728754	219175	100.00%	3.363	BB
总计		9,728,754	219,175	100.00%		

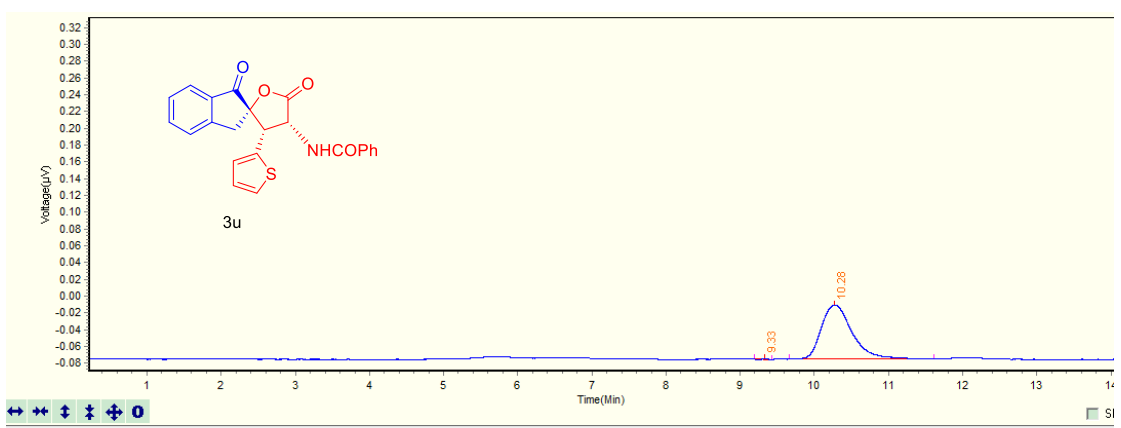




No.	Retention Time	PeakArea	Peak Height	PeakArea(%)	Peak Width	Peak Type
1	12.64	2179844	59877	94.70%	1.583 BV	
2	13.56	122054	4829	5.30%	1.229 VB	
Total		2,301,898	64,706	100.00%		

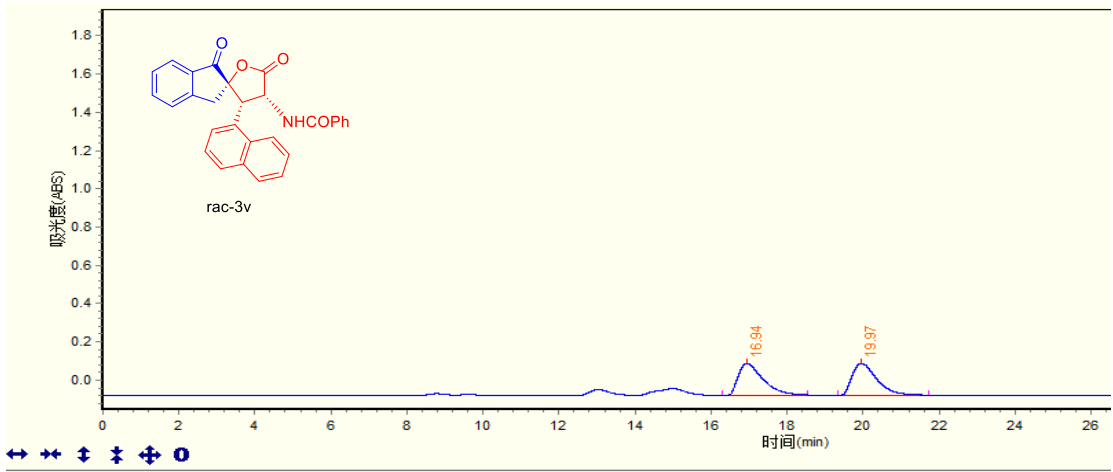


序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	9.48	3317397	142788	49.24%	0.898 BB	
2	10.26	3419769	141783	50.76%	1.299 BB	
总计		6,737,166	284,571	100.00%		

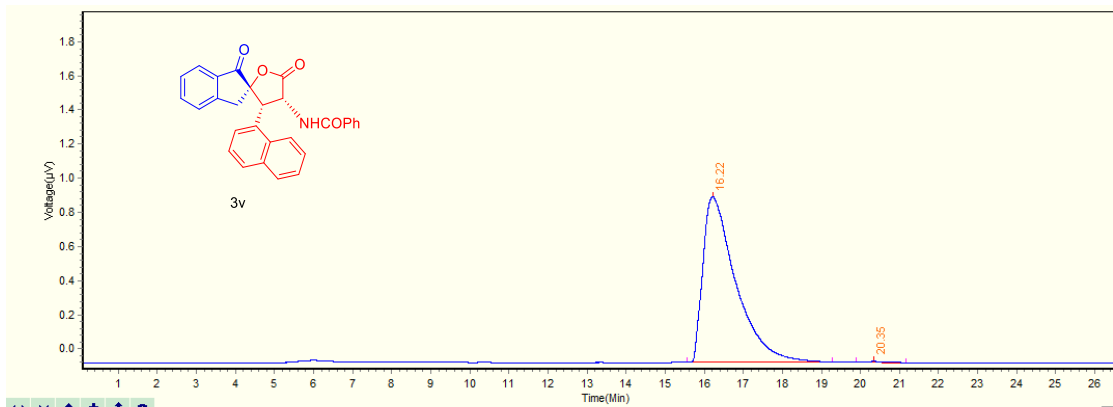


No.	Retention Time	PeakArea	Peak Height	PeakArea(%)	Peak Width	Peak Type
1	9.33	290	95	0.03%	0.231 BB	
2	10.28	932653	32153	99.97%	1.956 BB	
Total		932,943	32,248	100.00%		

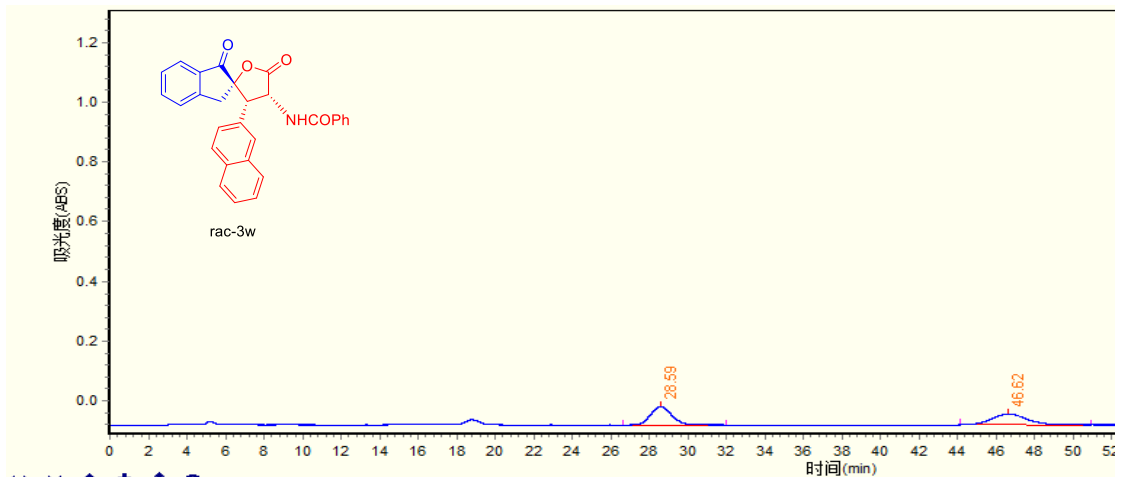




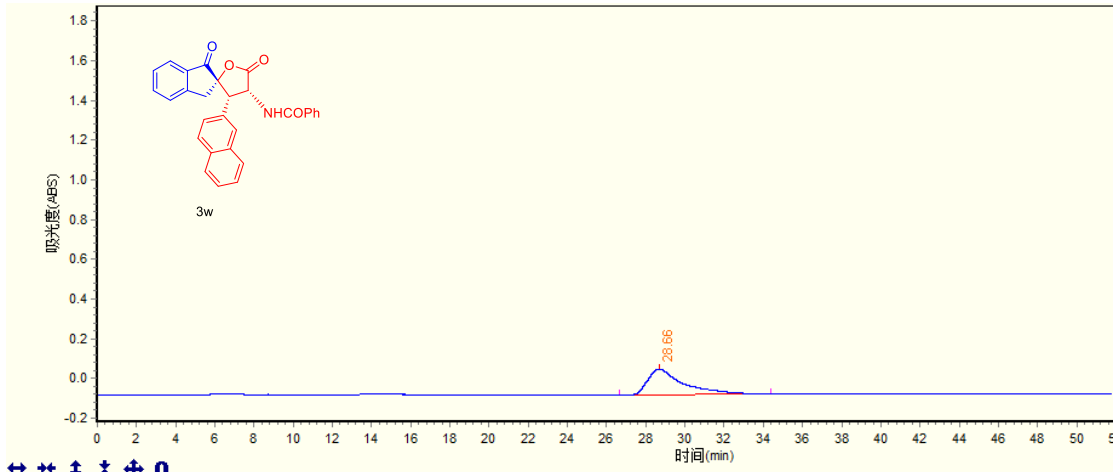
序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰
1	16.94	3661532	81850	49.33%	2.245	BB
2	19.97	3761735	83121	50.67%	2.39	BB
总计		7,423,267	164,971	100.00%		



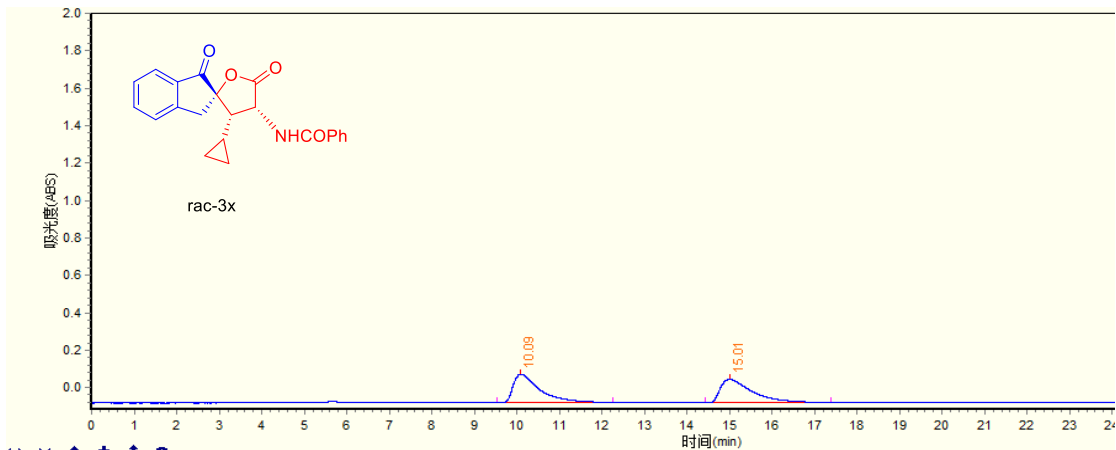
No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	16.22	28189940	483047	99.57%	3.736	BB
2	20.35	121757	3088	0.43%	1.281	BB
Total		28,311,697	486,135	100.00%		



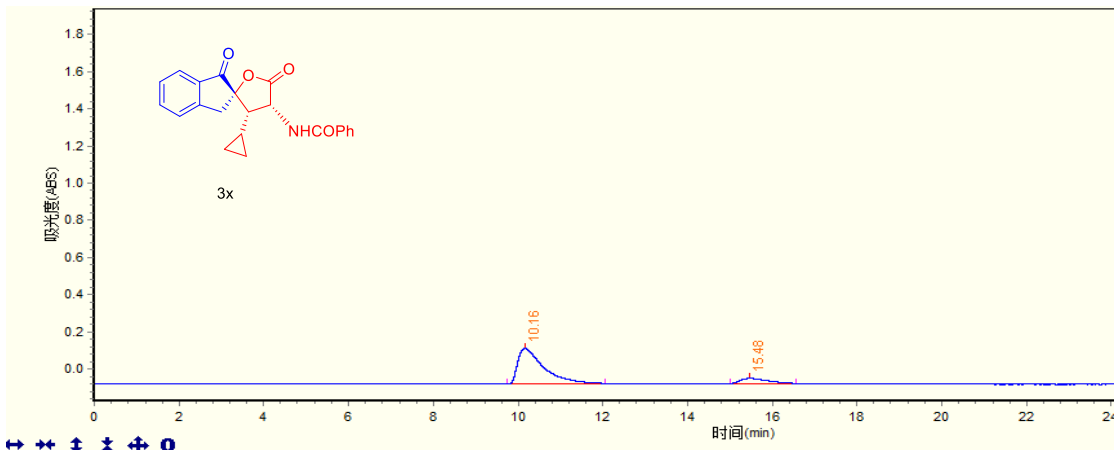
序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰
1	28.59	2333347	30895	50.36%	5.358	BB
2	46.62	2299797	18036	49.64%	6.792	BB
总计		4,633,144	48,931	100.00%		



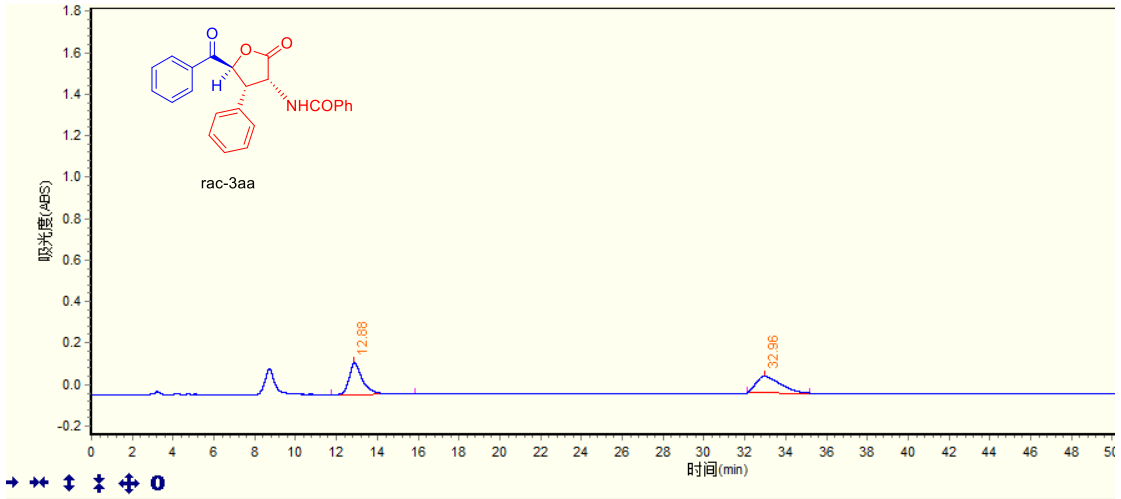
序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	28.66	7961476	63735	100.00%	7.699	BB
总计		7,961,476	63,735	100.00%		



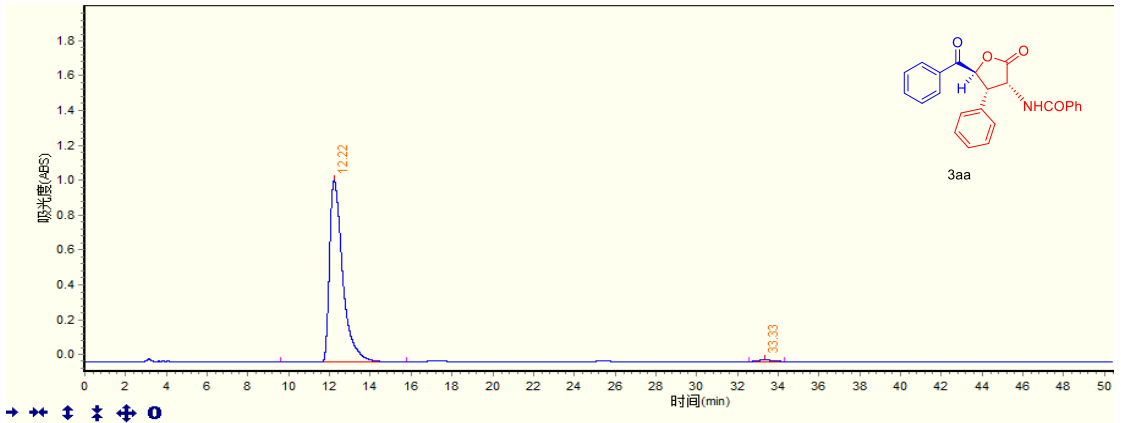
序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	10.09	3245519	75519	49.75%	2.705	BB
2	15.01	3278443	62852	50.25%	2.966	BB
总计		6,523,962	138,371	100.00%		



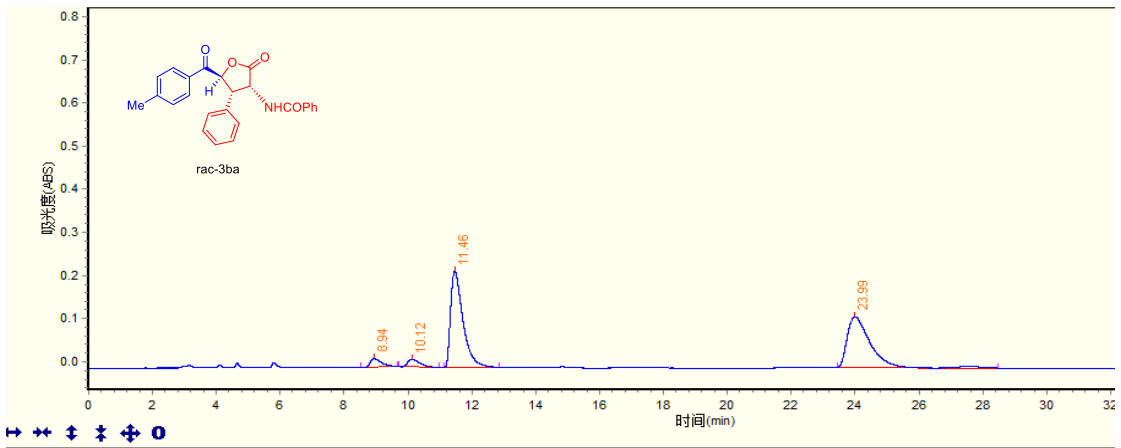
序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	10.16	4062677	95328	86.36%	2.313	BB
2	15.48	641799	14359	13.64%	1.552	BB
总计		4,704,476	109,687	100.00%		



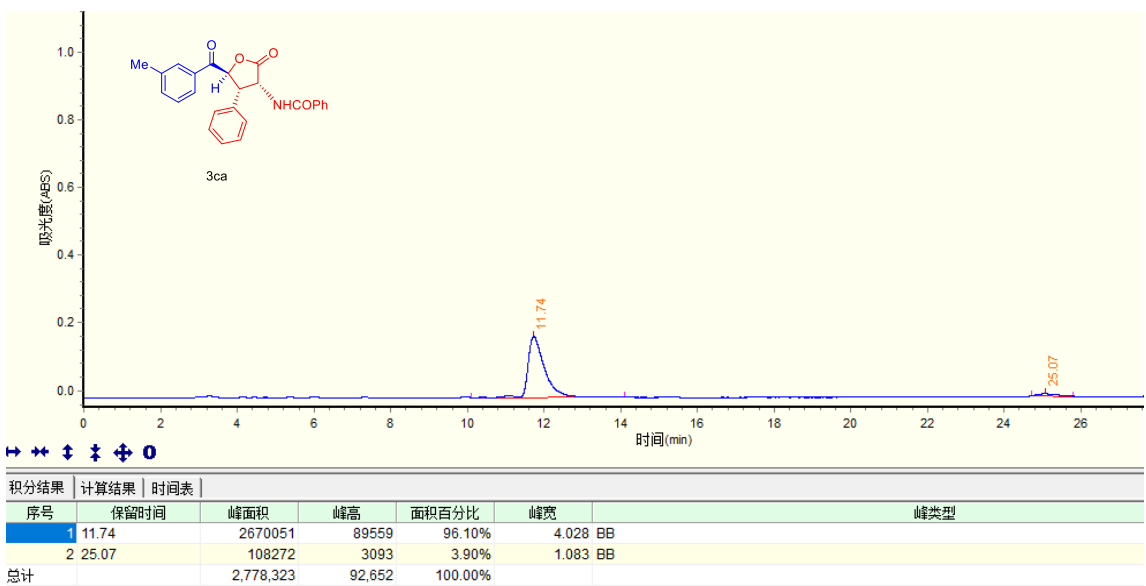
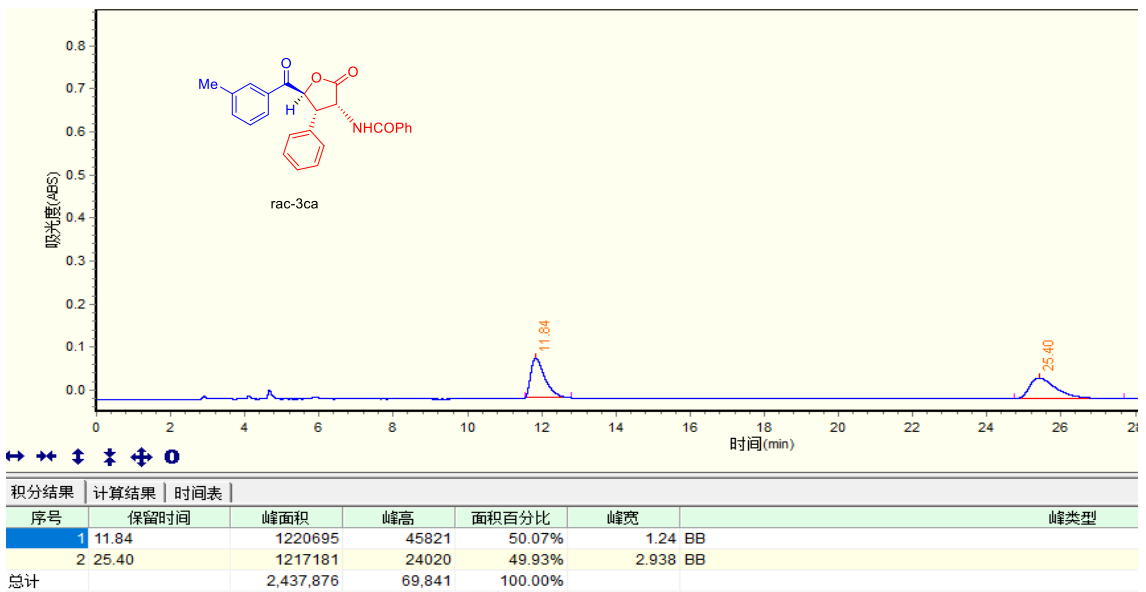
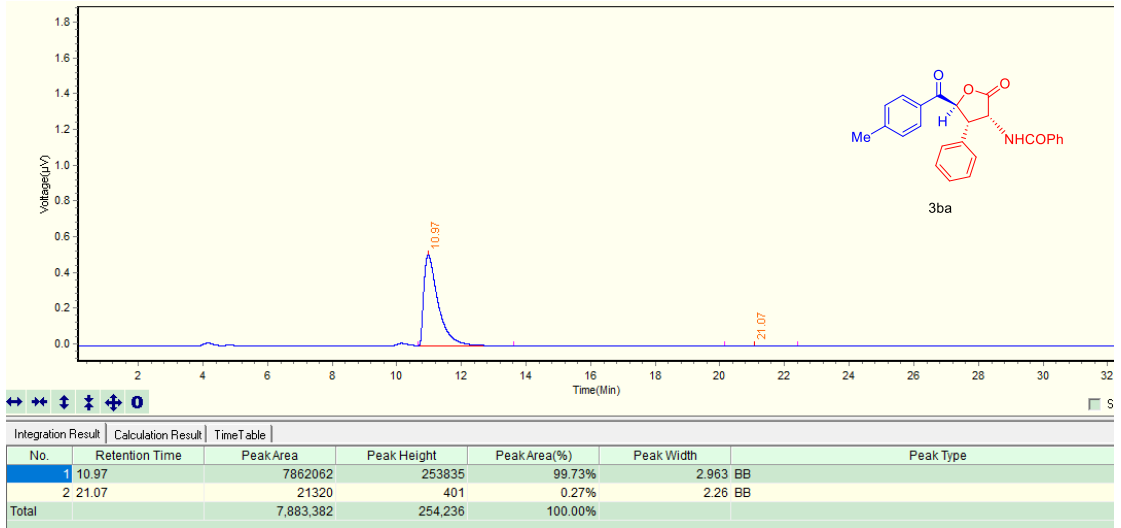
序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	12.88	3420363	75765	50.91%	4.098	BB
2	32.96	3297737	40247	49.09%	3.058	BB
总计		6,718,100	116,012	100.00%		

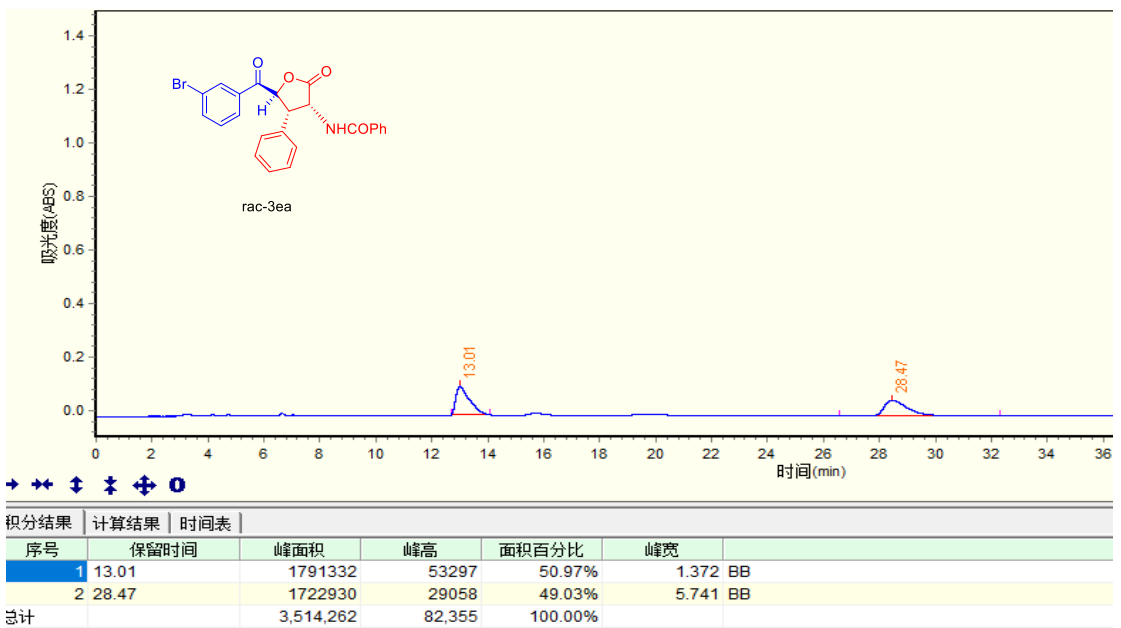
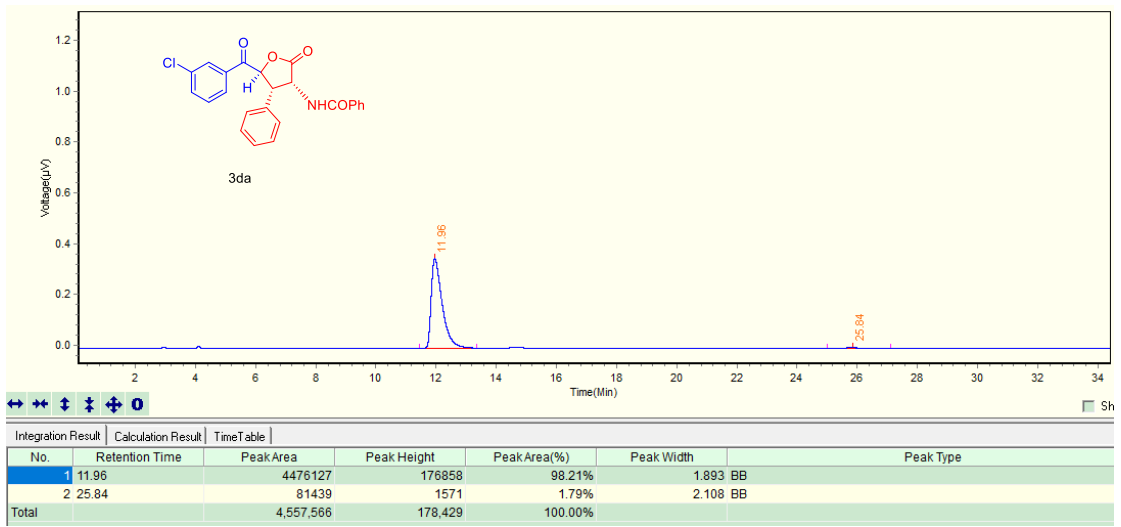
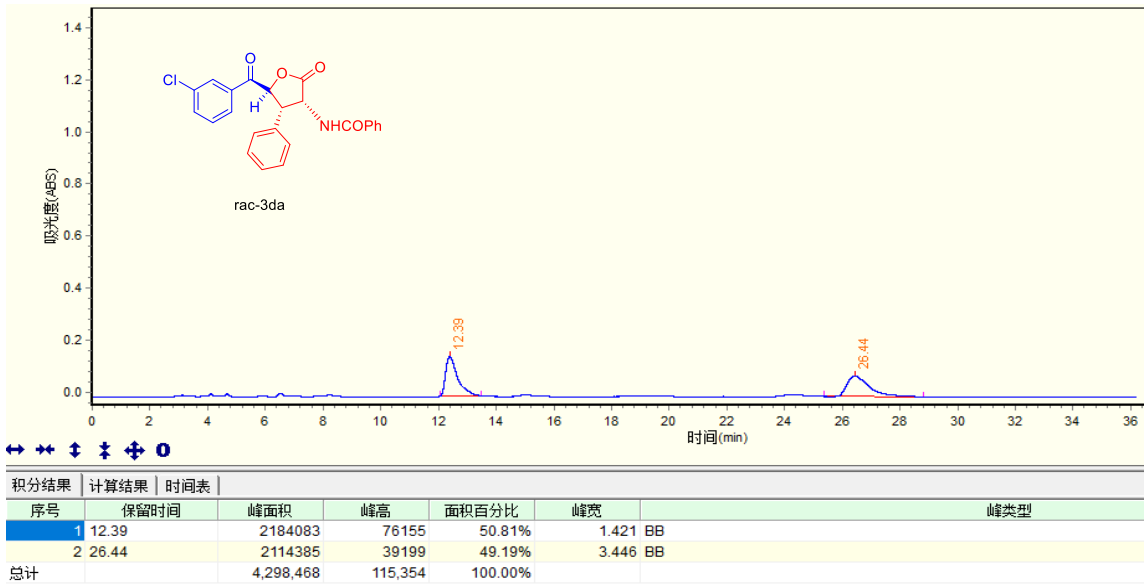


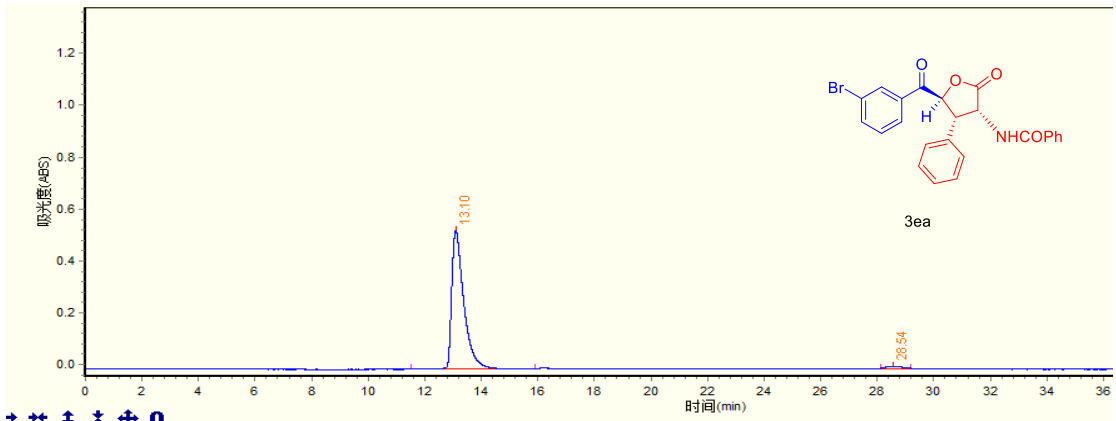
序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	12.22	23439092	521411	98.84%	6.177	BB
2	33.33	274592	4771	1.16%	1.739	BB
总计		23,713,684	526,182	100.00%		



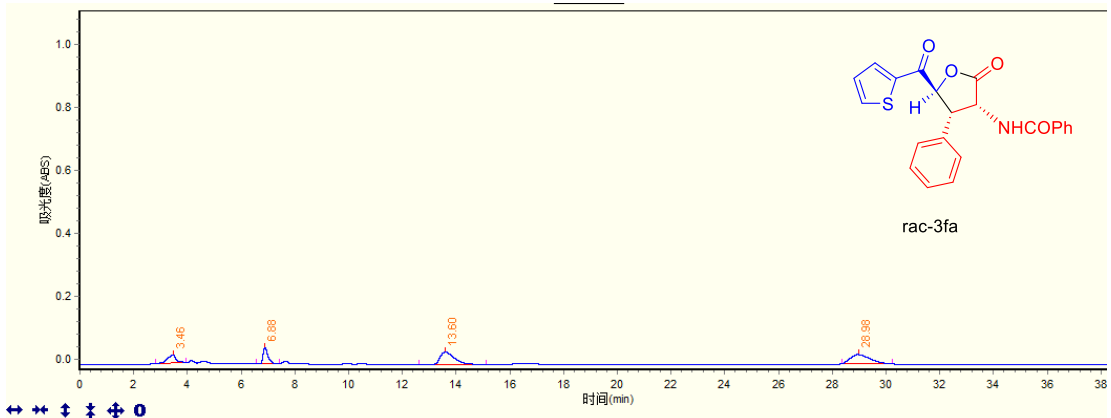
序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	8.94	235323	9907	3.67%	1.156	BB
2	10.12	224802	8677	3.51%	1.272	BB
3	11.46	3000157	111223	46.83%	1.733	BB
4	23.99	2946760	58623	45.99%	5.027	BB
总计		6,407,042	188,430	100.00%		



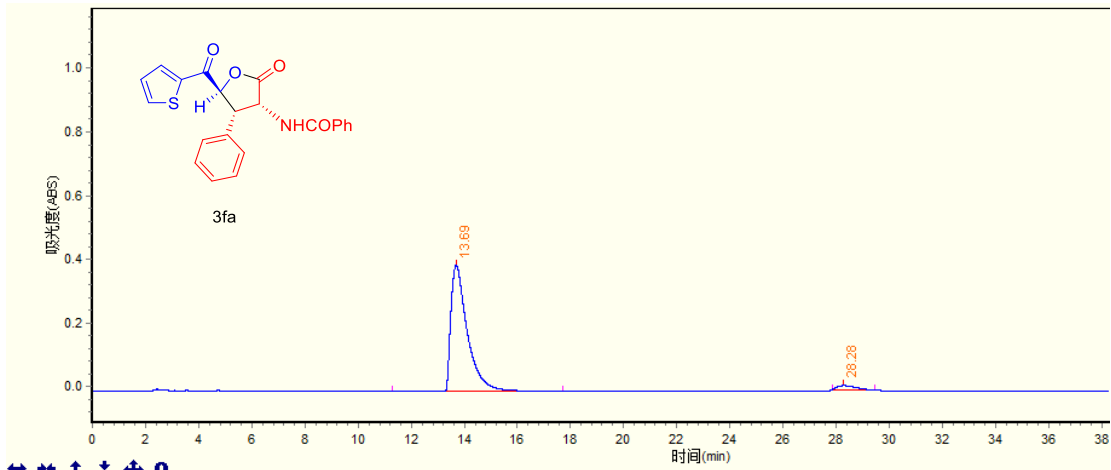




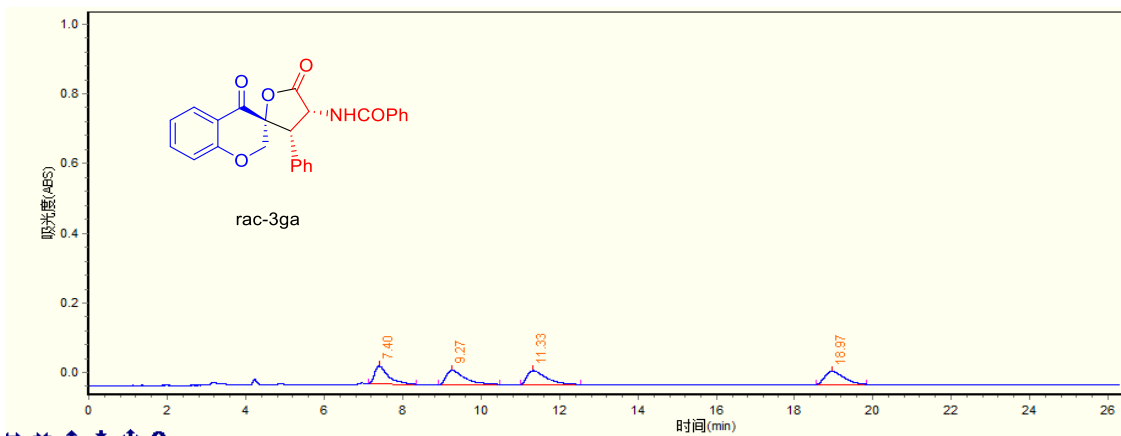
序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	13.10	7899784	266278	98.31%	4.384	BB
2	28.54	136197	3694	1.69%	1.063	BB
总计		8,035,981	269,972	100.00%		



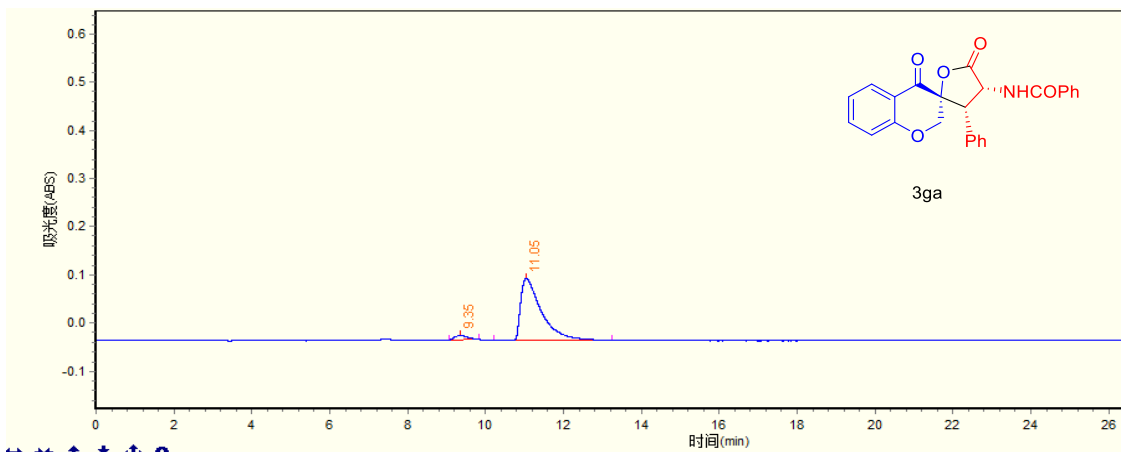
序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	3.46	310535	13411	14.79%	1.133	BB
2	6.88	316462	25068	15.07%	0.859	BB
3	13.60	732353	19445	34.87%	2.5	BB
4	28.98	740794	14555	35.27%	1.875	BB
总计		2,100,144	72,479	100.00%		



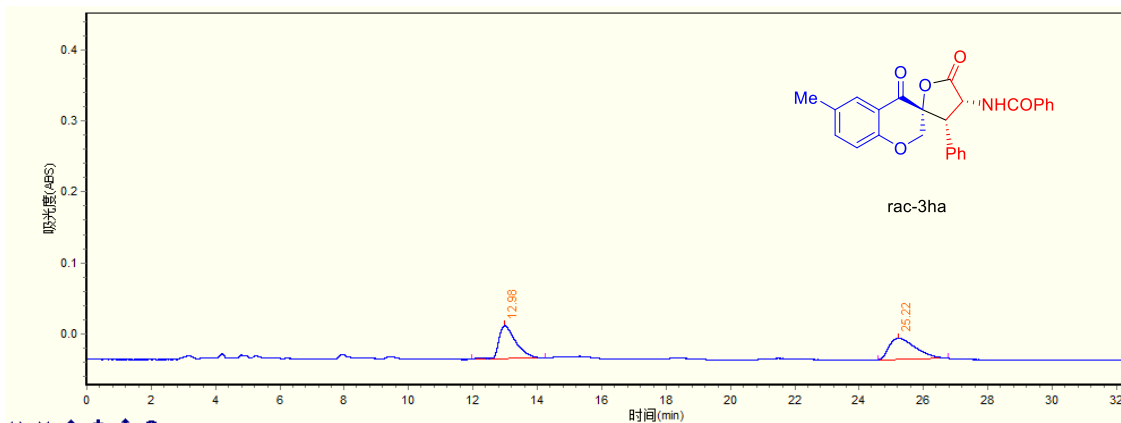
序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	13.69	8481874	197464	96.49%	6.419	BB
2	28.28	308528	6261	3.51%	1.593	BB
总计		8,790,402	203,725	100.00%		



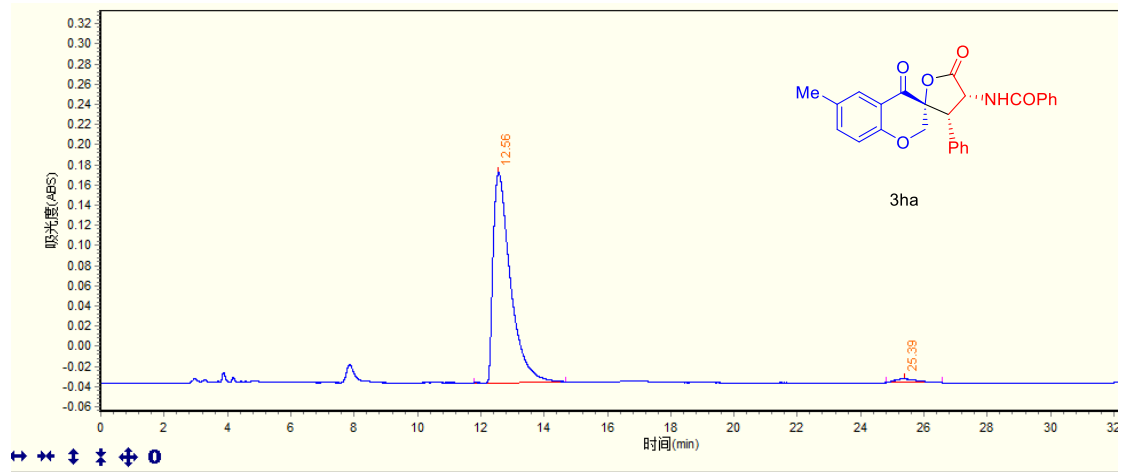
序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	7.40	626896	25783	24.38%	1.22	BB
2	9.27	650179	20442	25.29%	1.563	BB
3	11.33	666977	19840	25.94%	1.533	BB
4	18.97	626947	18524	24.39%	1.282	BB
总计		2,570,999	84,589	100.00%		



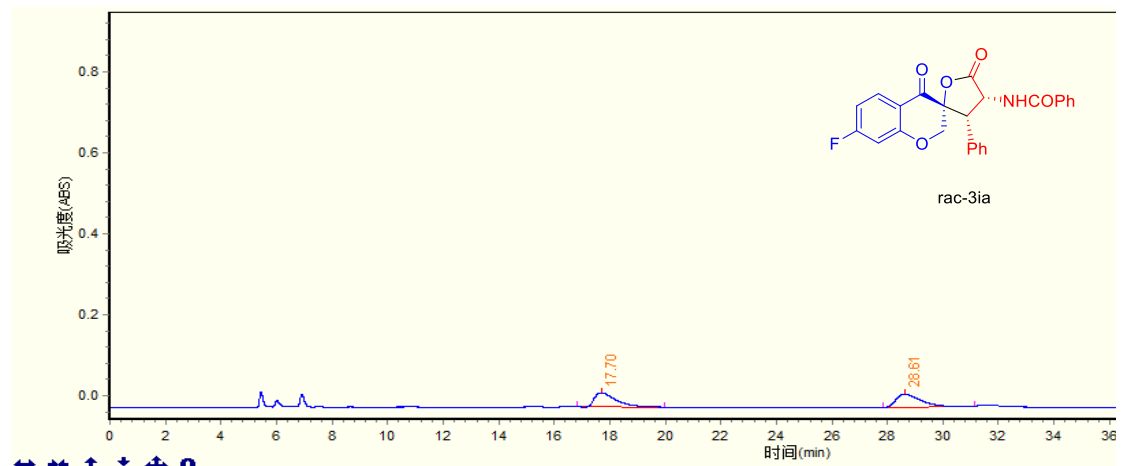
序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	9.35	103722	4275	4.20%	0.766	BB
2	11.05	2367492	64308	95.80%	3.032	BB
总计		2,471,214	68,583	100.00%		



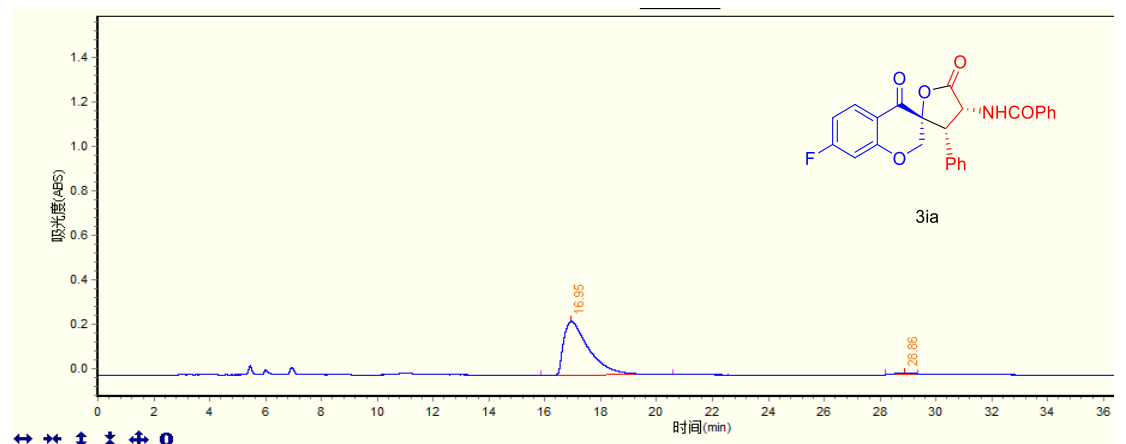
序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	12.98	859244	23231	50.34%	2.271	BB
2	25.22	847690	14901	49.66%	2.18	BB
总计		1,706,934	38,132	100.00%		



序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	12.56	3937640	104054	97.76%	2.9	BB
2	25.39	90190	1828	2.24%	1.772	BB
总计		4,027,830	105,882	100.00%		



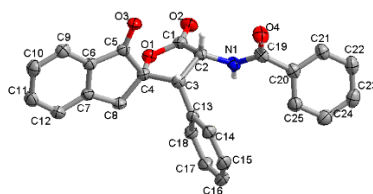
序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	17.70	939142	17448	50.31%	3.148	BB
2	28.61	927395	15762	49.69%	3.296	BB
总计		1,866,537	33,210	100.00%		



序号	保留时间	峰面积	峰高	面积百分比	峰宽	峰类型
1	16.95	7537332	120307	98.54%	4.727	BB
2	28.86	111784	2863	1.46%	1.16	BB
总计		7,649,116	123,170	100.00%		



## Single-crystal X-ray diffraction of 3a (CCDC 2074877)



### Datablock: 202011247

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Bond precision:	C-C = 0.0067 Å	Wavelength=1.54184	
Cell:	a=9.3096 (18)	b=10.340 (3)	c=10.3533 (17)
	alpha=90	beta=91.294 (17)	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	996.4 (4)	996.4 (4)	
Space group	P 21	P 1 21 1	
Hall group	P 2yb	P 2yb	
Moiety formula	C25 H19 N O4	C25 H19 N O4	
Sum formula	C25 H19 N O4	C25 H19 N O4	
Mr	397.41	397.41	
Dx, g cm <sup>-3</sup>	1.325	1.325	
Z	2	2	
Mu (mm <sup>-1</sup> )	0.732	0.732	
F000	416.0	416.0	
F000'	417.30		
h,k,lmax	11,12,12	11,12,12	
Nref	3559 [ 1888]	3218	
Tmin,Tmax	0.896,0.929	0.767,1.000	
Tmin'	0.896		

Correction method= # Reported T Limits: Tmin=0.767 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 1.70/0.90      Theta(max)= 67.074

R(reflections)= 0.0453 ( 2641)      wR2(reflections)= 0.1220 ( 3218)

S = 1.110      Npar= 275

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The following ALERTS were generated. Each ALERT has the format  
**test-name ALERT alert-type alert-level.**  
Click on the hyperlinks for more details of the test.

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**Alert level C**

PLAT089_ALERT_3_C	Poor Data / Parameter Ratio (Zmax < 18) .....	6.87	Note
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.00667	Ang.
PLAT915_ALERT_3_C	No Flack x Check Done: Low Friedel Pair Coverage	80	%

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**Alert level G**

PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF .....	Please	Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature .... (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature .... (K)	293	Check
PLAT791_ALERT_4_G	Model has Chirality at C2 (Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C3 (Sohnke SpGr)	S	Verify
PLAT791_ALERT_4_G	Model has Chirality at C4 (Sohnke SpGr)	S	Verify
PLAT909_ALERT_3_G	Percentage of I>2 $\sigma$ (I) Data at Theta(Max) Still	54%	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	6	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	4.2	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

---

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
10 **ALERT level G** = General information/check it is not something unexpected
- 3 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data  
2 **ALERT type 2** Indicator that the structure model may be wrong or deficient  
5 **ALERT type 3** Indicator that the structure quality may be low  
3 **ALERT type 4** Improvement, methodology, query or suggestion  
0 **ALERT type 5** Informative message, check
- 

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special\_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

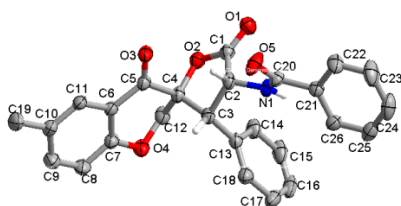
**Publication of your CIF in IUCr journals**

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

**Publication of your CIF in other journals**

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

## Single-crystal X-ray diffraction of 3ha (CCDC 2092642)



### Datablock: 202106179

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Bond precision: C-C = 0.0050 Å      Wavelength=1.54184  
Cell:            a=10.8915(3)      b=13.7026(6)      c=14.8233(10)  
                  alpha=90            beta=90            gamma=90  
Temperature:    293 K

	Calculated	Reported
Volume	2212.26(19)	2212.25(19)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C26 H21 N O5	C26 H21 N O5
Sum formula	C26 H21 N O5	C26 H21 N O5
Mr	427.44	427.44
Dx, g cm <sup>-3</sup>	1.283	1.283
Z	4	4
Mu (mm <sup>-1</sup> )	0.731	0.731
F000	896.0	896.0
F000'	898.87	
h,k,lmax	13,16,18	13,16,17
Nref	4280 [ 2432]	4175
Tmin,Tmax	0.900,0.930	0.944,1.000
Tmin'	0.896	

Correction method= # Reported T Limits: Tmin=0.944 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 1.72/0.98      Theta(max)= 70.932  
R(reflections)= 0.0437( 3651)      wR2(reflections)= 0.1149( 4175)  
S = 1.046                              Npar= 294

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The following ALERTS were generated. Each ALERT has the format  
**test-name\_ALERT\_alert-type\_alert-level.**  
Click on the hyperlinks for more details of the test.

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**Alert level C**

PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C23	Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.00504	Ang.
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .	1	Check

---

**Alert level G**

PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !	
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature .... (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature .... (K)	293	Check
PLAT791_ALERT_4_G	Model has Chirality at C2 (Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C3 (Sohnke SpGr)	S	Verify
PLAT791_ALERT_4_G	Model has Chirality at C4 (Sohnke SpGr)	R	Verify
PLAT912_ALERT_4_G	Missing # of PCF Reflections Above STh/L= 0.600	32	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

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3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
8 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
2 ALERT type 2 Indicator that the structure model may be wrong or deficient  
2 ALERT type 3 Indicator that the structure quality may be low  
4 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check

---

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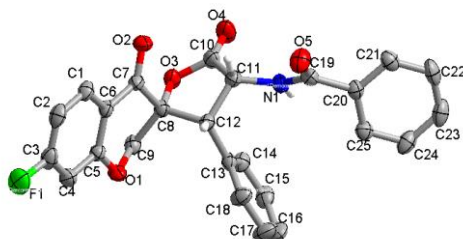
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#### Publication of your CIF in other journals

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## Single-crystal X-ray diffraction of 3ia (CCDC 2097633)



### Datablock: 202106190

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Bond precision: C-C = 0.0054 Å                      Wavelength=1.54184

Cell:                      a=9.9904 (8)              b=9.9960 (6)              c=10.8047 (8)  
                                    alpha=90              beta=104.900 (8)              gamma=90

Temperature:              293 K

	Calculated	Reported
Volume	1042.72 (14)	1042.72 (14)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	C25 H18 F N O5	C25 H18 F N O5
Sum formula	C25 H18 F N O5	C25 H18 F N O5
Mr	431.40	431.40
Dx, g cm <sup>-3</sup>	1.374	1.374
Z	2	2
Mu (mm <sup>-1</sup> )	0.854	0.854
F000	448.0	448.0
F000'	449.55	
h,k,lmax	12,12,13	12,12,13
Nref	4018 [ 2133]	3908
Tmin,Tmax	0.875,0.918	0.923,1.000
Tmin'	0.872	

Correction method= # Reported T Limits: Tmin=0.923 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 1.83/0.97                      Theta(max)= 70.764

R(reflections)= 0.0390 ( 3380)                      wR2(reflections)= 0.1005 ( 3908)

S = 1.057    Npar= 293

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● Alert level C			
PLAT089_ALERT_3_C	Poor Data / Parameter Ratio (Zmax < 18) .....	7.20	Note
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.00538	Ang.
PLAT420_ALERT_2_C	D-H Bond Without Acceptor N1 --H1 .		Please Check

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● Alert level G			
PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF .....		Please Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature .....	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature .....	293	Check
PLAT791_ALERT_4_G	Model has Chirality at C8 (Sohnke SpGr)		R Verify
PLAT791_ALERT_4_G	Model has Chirality at C11 (Sohnke SpGr)		R Verify
PLAT791_ALERT_4_G	Model has Chirality at C12 (Sohnke SpGr)		S Verify
PLAT912_ALERT_4_G	Missing # of PCF Reflections Above STh/L= 0.600	21	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	3.7	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	2	Info

---

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- 

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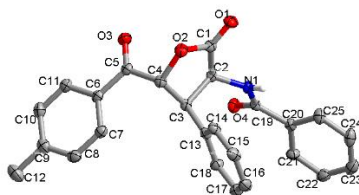
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#### Publication of your CIF in other journals

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## Single-crystal X-ray diffraction of rac-3aa (CCDC 2097681)



### Datablock: 20210717b4-1

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Bond precision:	C-C = 0.0022 Å	Wavelength=1.54184	
Cell:	a=14.9905 (2) alpha=90	b=10.3667 (1) beta=90	c=25.5652 (3) gamma=90
Temperature:	200 K		
	Calculated	Reported	
Volume	3972.88 (8)	3972.88 (8)	
Space group	P b c a	P b c a	
Hall group	-P 2ac 2ab	-P 2ac 2ab	
Moiety formula	C25 H21 N O4	C25 H21 N O4	
Sum formula	C25 H21 N O4	C25 H21 N O4	
Mr	399.43	399.43	
Dx, g cm <sup>-3</sup>	1.336	1.336	
Z	8	8	
Mu (mm <sup>-1</sup> )	0.735	0.735	
F000	1680.0	1680.0	
F000'	1685.22		
h,k,lmax	18,12,31	18,12,31	
Nref	3776	3765	
Tmin,Tmax	0.969,0.978	0.849,1.000	
Tmin'	0.960		
Correction method=	# Reported T Limits: Tmin=0.849 Tmax=1.000		
AbsCorr =	MULTI-SCAN		
Data completeness=	0.997	Theta(max)=	70.066
R(reflections)=	0.0385 ( 3052)	wR2(reflections)=	0.1053 ( 3765)
S =	1.035	Npar=	272

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The following ALERTS were generated. Each ALERT has the format  
**test-name\_ALERT\_alert-type\_alert-level**.  
Click on the hyperlinks for more details of the test.

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**Alert level G**

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	1	Report
PLAT142_ALERT_4_G	s.u. on b - Axis Small or Missing .....	0.00010	Ang.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	51	Note
PLAT793_ALERT_4_G	Model has Chirality at C007 (Centro SPGR)		S Verify
PLAT793_ALERT_4_G	Model has Chirality at C008 (Centro SPGR)		R Verify
PLAT793_ALERT_4_G	Model has Chirality at C00B (Centro SPGR)		R Verify
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	3.2	Low

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0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
7 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
0 ALERT type 2 Indicator that the structure model may be wrong or deficient  
1 ALERT type 3 Indicator that the structure quality may be low  
5 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check

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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special\_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

**Publication of your CIF in IUCr journals**

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

**Publication of your CIF in other journals**

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.