# Enantioselective assembly of 3,3-disubstituted succinimides *via* three-component reaction of vinyl diazosuccinimides with alcohols and imines

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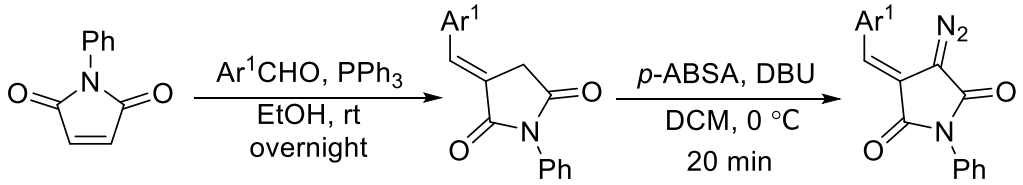
**General Information**

All reactions were carried out in oven-dried glassware. Flash column chromatography was performed using silica gel (300-400 mesh). Analytical thin-layer chromatography was performed using glass plates pre-coated with 200-300 mesh silica gel impregnated with a fluorescent indicator (254 nm). $^{1}H$ NMR and $^{13}C$ NMR spectra were recorded in $CDCl_3$ on a 400 MHz spectrometer; chemical shifts were reported in ppm with the solvent signal as reference, and coupling constants (*J*) were given in Hertz. The peak information was described as: br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, comp = composite. Enantioselectivity was determined on HPLC using Chiralpak IA, IB-3, IC, and AD-H column. High-resolution mass spectra (HRMS) were recorded on a commercial apparatus (ESI Source) and (CI Source).

**General Procedure for the Synthesis of Diazo Compounds 1.[1]**

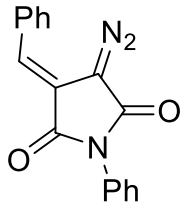



**S1** **S2** **1**

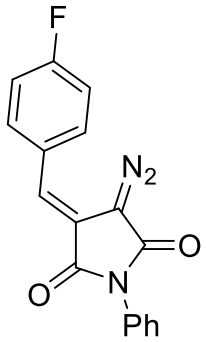
***Synthesis of S2:*** To a solution of *N*-phenylmaleimide (1.73 g, 10mmol, 1.0 equiv.) in EtOH (100 mL), was added triphenylphosphine (2.75 g, 10.5 mmol, 1.05 equiv.) at room temperature under argon atmosphere, then aldehyde (11 mmol, 1.1 equiv.) was added to the reaction mixture after stirring for 20 min. The reaction mixture was stirred at room temperature overnight. When the reaction was completed (monitored by TLC), the reaction mixture was filtered, the precipitation was wash with ethanol and dry by air to afford **S2** in >80% yields, which was used in the next step without further purification.

***Synthesis of 1:*** To a 50-mL oven-dried flask containing a magnetic stirring bar, **S2** (1.5 mmol), and *p*-ABSA (4-acetamidobenzenesulfonyl azide, 468 mg, 1.95 mmol,

1.3 equiv.) in DCM (10 mL), was added DBU (1,8-diazabicyclo[5.4.0]undec-7-ene, 342 mg, 2.25 mmol, 1.5 equiv.) in DCM (2.0 mL) slowly at 0 ℃, and the resulting reaction mixture was stirred at room temperature for 20 min. The reaction mixture was diluted with ethyl acetate (10 mL) and washed with saturated aqueous $NH_4Cl$ (20 mL), saturated aqueous $NaHCO_3$ (20 mL), and saturated aqueous NaCl (20 mL) in sequence, and the separated organic phase was dried with anhydrous $Na_2SO_4$. The solvent was evaporated in vacuo after filtration, and the residue was purified by column chromatography on silica gel (Hexanes : EtOAc = 5:1) to provide diazo compounds **1** as orange solid (> 90% yield).

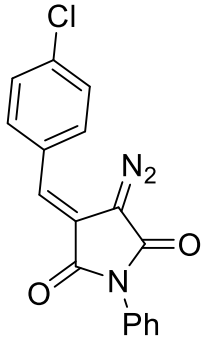



**(*E*)-3-Benzylidene-4-diazo-1-phenylpyrrolidine-2,5-dione (1a).** Orange solid. $^1$H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.76 (s, 1H), 7.52 – 7.35 (comp, 10H); $^{13}$C NMR (100 MHz, $CDCl_3$) (δ, ppm) 166.3, 164.1, 133.5, 131.9, 129.7, 129.3, 129.1, 128.9, 128.6, 128.3, 126.6, 116.7. HRMS (TOF MS ESI$^+$) calculated for $C_{17}H_{12}N_3O_2$ [M + H]$^+$: 290.0924, found: 290.0919.

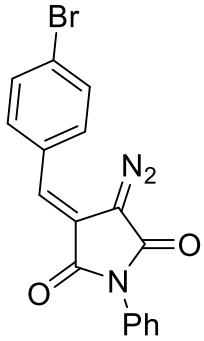



**(*E*)-3-Diazo-4-(4-fluorobenzylidene)-1-phenylpyrrolidine-2,5-dione (1k).** Orange solid. $^1$H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.70 (s, 1H), 7.51 – 7.47 (m, 2H), 7.42 –

7.40 (comp, 3H), 7.34 (m, 2H), 7.14 (t, $J$ = 8.6 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) (δ, ppm) 166.1, 164.0, 163.3 (d, $J$ = 252.0 Hz), 131.9, 131.0 (d, $J$ = 8.5 Hz), 129.7 (d, $J$ = 3.4 Hz), 129.3, 128.7, 127.1, 126.6, 116.7, 116.2 (d, $J$ = 22.0 Hz); $^{19}$F NMR (376 MHz, $CDCl_3$) (δ, ppm) -109.70; HRMS (TOF MS ESI$^+$) calculated for $C_{17}H_{11}FN_3O_2$ $[M + H]^+$: 308.0830, found: 308.0826.

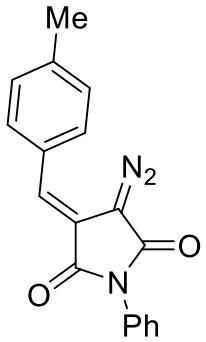



**(*E*)-3-(4-Chlorobenzylidene)-4-diazo-1-phenylpyrrolidine-2,5-dione (1l).** Orange solid. $^1$H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.67 (s, 1H), 7.50 (d, $J$ = 7.8 Hz, 2H), 7.44 (s, 1H), 7.41 (d, $J$ = 3.1 Hz, 3H), 7.40 (s, 1H), 7.29 (d, $J$ = 8.4 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) (δ, ppm) 166.0, 163.9, 135.8, 131.94, 131.85, 130.3, 129.32, 129.25, 128.7, 126.7, 126.6, 117.3; HRMS (TOF MS ESI$^+$) calculated for $C_{17}H_{11}ClN_3O_2$ $[M + H]^+$: 324.0534, found: 324.0541.

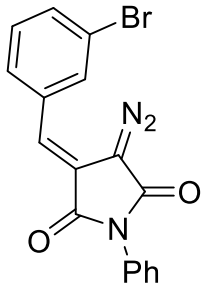



**(*E*)-3-(4-Bromobenzylidene)-4-diazo-1-phenylpyrrolidine-2,5-dione (1m).** Orange solid. $^1$H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.64 (s, 1H), 7.58 (d, $J$ = 8.4 Hz, 2H), 7.51 – 7.47 (m, 2H), 7.45 - 7.42 (comp, 3H), 7.21 (d, $J$ = 8.3 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) (δ, ppm) 166.0, 163.9, 132.4, 132.2, 131.8, 130.5, 129.3, 128.7, 126.7,

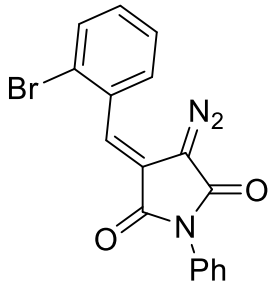
126.5, 124.0, 117.3; HRMS (TOF MS ESI$^+$) calculated for $C_{17}H_{11}BrN_3O_2$ [M + H]$^+$: 368.0029, found: 368.0039.




**(*E*)-3-Diazo-4-(4-methylbenzylidene)-1-phenylpyrrolidine-2,5-dione (1n).** Orange solid. $^1$H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.72 (s, 1H), 7.54 - 7.50 (m, 2H), 7.46 - 7.43 (comp, 3H), 7.24 (s, 4H), 2.39 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) (δ, ppm) 166.4, 164.2, 140.2, 132.0, 130.7, 129.6, 129.2, 129.1, 128.6, 128.5, 126.6, 115.8, 21.6; HRMS (TOF MS ESI$^+$) calculated for $C_{18}H_{14}N_3O_2$ [M + H]$^+$: 304.1081, found: 304.1078.




**(*E*)-3-(3-Bromobenzylidene)-4-diazo-1-phenylpyrrolidine-2,5-dione (1o).** Orange solid. $^1$H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.64 (s, 1H), 7.51 – 7.47 (comp, 4H), 7.42 – 7.38 (comp, 3H), 7.30 (m, 2H).; $^{13}$C NMR (100 MHz, $CDCl_3$) δ 165.8, 163.8, 135.5, 132.6, 131.8, 131.7, 130.3, 129.3, 128.7, 127.5, 126.5, 126.0, 123.0, 118.1; HRMS (TOF MS ESI$^+$) calculated for $C_{17}H_{11}BrN_3O_2$ [M + H]$^+$: 368.0029, found: 368.0015.

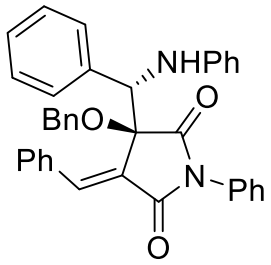



**(*E*)-3-(2-Bromobenzylidene)-4-diazo-1-phenylpyrrolidine-2,5-dione (1p).**

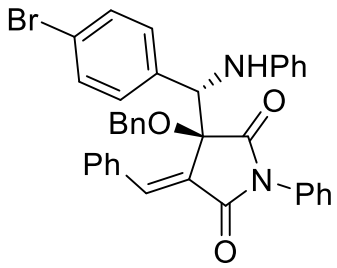
Orange solid. $^{1}$H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.77 (s, 1H), 7.67 (d, *J* = 7.9 Hz, 1H), 7.52 – 7.47 (m, 2H), 7.41 - 7.46 (comp, 4H), 7.30 – 7.27 (m, 1H), 7.26 – 7.22 (m, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) (δ, ppm) 165.8, 163.6, 133.8, 133.6, 131.8, 131.0, 129.8, 129.3, 128.7, 127.1, 126.9, 126.6, 125.0, 118.8; HRMS (TOF MS ESI$^+$) calculated for $C_{17}H_{11}BrN_3O_2$ $[M + H]^+$: 368.0029, found: 368.0023.

**General Procedure for the Asymmetric Three-component Reaction**

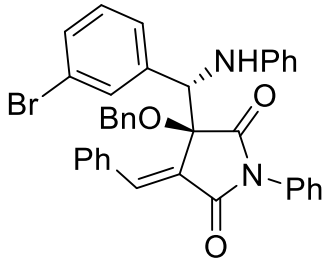
To a 10-mL oven-dried vial containing a magnetic stirring bar, $Rh_2(OAc)_4$ (0.50 mg, 1.0 mol%), **5e** (7.2 mg, 10 mol%), **2** (0.10 mmol, 1.0 equiv.), imine **3** (0.10 mmol, 1.0 equiv.), and 5 Å MS (100 mg) in DCM (1.0 mL), was added as a solution of diazo compound **1** (0.12 mmol, 1.2 equiv.) in DCM (1.0 mL) *via* a syringe pump in 2 h under argon atmosphere at 0 °C. After addition, the reaction mixture was stirred for additional 1 h under these conditions. Until consumption of the material (monitored by TLC), the crued reaction mixture was subjected to proton NMR analysis to determine the *dr* values, and the product was purified by column chromatography on silica gel without any additional treatment (Hexanes : EtOAc = 10:1) to give the pure products **4** in good to high yields with excellent enantioselectivity.




**(*S*)-4-((*E*)-Benzylidene)-3-(benzyloxy)-1-phenyl-3-((*S*)-phenyl(phenylamino)methyl)pyrrolidine-2,5-dione (4a).** Yellow oil. 46.8 mg, 85% yield. >20:1 *dr*, 88% *ee*, $[\alpha]_D^{20}$ = -135.1 (c = 0.033, DCM); $^1$H NMR (500 MHz, $CDCl_3$) (δ, ppm) 8.11 (d, *J* = 7.3 Hz, 2H), 8.07 (s, 1H), 7.50 – 7.44 (comp, 3H), 7.39 - 7.34 (comp, 4H), 7.31 – 7.25 (comp, 6H), 7.23 (s, 2H), 7.21 (s, 1H), 7.03 (t, *J* = 7.7 Hz, 2H), 6.85 (d, *J* = 7.6 Hz, 2H), 6.62 (t, *J* = 7.3 Hz, 1H), 6.46 (d, *J* = 8.0 Hz, 2H), 5.74 (d, *J* = 4.4 Hz, 1H), 5.31 (d, *J* = 4.4 Hz, 1H), 4.51 (d, *J* = 10.0 Hz, 1H), 4.48 (d, *J* = 10.0 Hz, 1H); $^{13}$C NMR (125 MHz, $CDCl_3$) (δ, ppm) 173.3, 167.7, 147.2, 141.6, 137.2, 136.2, 133.2, 132.4, 131.8, 131.1, 129.6, 129.12, 129.06, 128.9, 128.7, 128.62, 128.55, 128.4, 128.3, 126.3, 124.1, 117.5, 113.7, 83.4, 68.7, 61.1; HRMS (TOF MS ESI$^+$) calculated for $C_{37}H_{31}N_2O_3$ $[M + H]^+$: 551.2329, found: 551.2333; HPLC conditions for determination of enantiomeric excess: Daicel Chiralcel IB-3, λ = 300 nm, hexane : 2-propanol = 97:3, flow rate = 1.0 mL/min, $t_{major}$ = 11.4 min, $t_{minor}$ = 13.4 min.

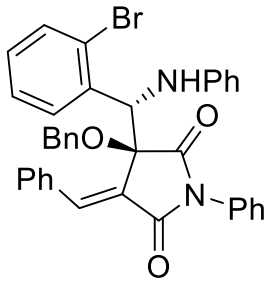



**(*S*)-4-((*E*)-Benzylidene)-3-(benzyloxy)-3-((*S*)-(4-bromophenyl)(phenylamino)methyl)-1-phenylpyrrolidine-2,5-dione (4b).** Yellow solid. mp = 86 – 89 ºC. 53.4 mg, 85% yield. >20:1 *dr*, 72% *ee*, $[\alpha]_D^{20}$ = -175.6 (c = 0.033, DCM); $^1$H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.09 (s, 1H), 8.07 (d, *J* = 6.9 Hz, 2H), 7.50 – 7.46 (m, 2H), 7.44 (d, *J* = 6.5 Hz, 2H), 7.41 (d, *J* = 7.8 Hz, 2H), 7.37 (d, *J* = 7.1 Hz, 1H), 7.34 (s, 1H), 7.32 (s, 1H), 7.30 (d, *J* = 2.8 Hz, 2H), 7.28 – 7.25 (m, 2H), 7.10 (d, *J* = 8.2 Hz, 2H), 7.04 (t, *J* = 7.8 Hz, 2H), 6.87 (d, *J* = 8.0 Hz, 2H), 6.64 (t, *J* = 7.3 Hz, 1H), 6.43 (d, *J* = 8.0 Hz, 2H), 5.68 (d, *J* = 4.1 Hz, 1H), 5.25 (d, *J* = 4.1 Hz, 1H), 4.52 (d, *J* = 10.1 Hz, 1H), 4.48 (d, *J* = 10.1 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) (δ, ppm) 173.1, 167.6, 146.8, 142.0, 136.5, 136.0, 133.1, 132.2, 132.0, 131.9, 131.0, 130.0, 129.7, 129.2, 129.0, 128.7, 128.6, 128.5, 126.24, 126.17, 123.6, 122.8, 117.9, 113.7, 83.1, 68.8, 60.7; HRMS (TOF MS ESI$^+$) calculated for $C_{37}H_{30}BrN_2O_3$ $[M + H]^+$: 629.1434, found: 629.1429; HPLC conditions for determination of enantiomeric excess: Daicel Chiralcel IB-3, λ = 300 nm, hexane : 2-propanol = 97:3, flow rate = 1.0 mL/min, $t_{major}$ = 12.9 min, $t_{minor}$ = 17.9 min.



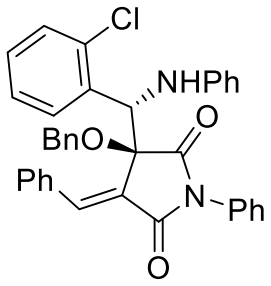

**(*S*)-4-((*E*)-Benzylidene)-3-(benzyloxy)-3-((*S*)-(3-bromophenyl)(phenylamino)methyl)-1-phenylpyrrolidine-2,5-dione (4c).** Yellow oil. 55.3 mg, 88% yield. >20:1 *dr*, 77% *ee*, $[\alpha]_D^{20}$ = -223.2 (c = 0.033, DCM); $^1$H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.09 – 8.08 (comp, 3H), 7.51 - 7.47 (comp, 3H), 7.45 – 7.42 (comp, 4H), 7.38 (t, *J* = 6.9

Hz, 2H), 7.30 (d, *J* = 1.6 Hz, 1H), 7.27 – 7.25 (comp, 3H), 7.10 – 7.03 (comp, 4H), 6.97 (d, *J* = 7.8 Hz, 2H), 6.66 (t, *J* = 7.3 Hz, 1H), 6.46 (d, *J* = 7.7 Hz, 2H), 5.72 (d, *J* = 4.0 Hz, 1H), 5.25 (d, *J* = 4.0 Hz, 1H), 4.58 (d, *J* = 10.0 Hz, 1H), 4.48 (d, *J* = 10.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) (δ, ppm) 173.2, 167.5, 147.0, 142.1, 134.0, 136.0, 133.1, 132.3, 132.00, 131.97, 131.02, 130.96, 130.2, 129.7, 129.2, 129.4, 128.7, 128.6, 128.5, 127.3, 126.3, 123.7, 123.1, 117.9, 113.7, 83.1, 68.8, 60.8; HRMS (TOF MS ESI$^+$) calculated for $C_{37}H_{30}BrN_2O_3$ $[M + H]^+$: 629.1434, found: 629.1429; HPLC conditions for determination of enantiomeric excess: Daicel Chiralcel IB-3, λ = 300 nm, hexane : 2-propanol = 97:3, flow rate = 1.0 mL/min, $t_{major}$ = 12.2 min, $t_{minor}$ = 16.1 min.

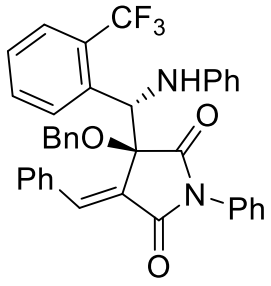



**(*S*)-4-((*E*)-Benzylidene)-3-(benzyloxy)-3-((*S*)-(2-bromophenyl)(phenylamino)methyl)-1-phenylpyrrolidine-2,5-dione (4d).** Yellow solid. mp = 181 – 183 °C. 55.3 mg, 88% yield. >20:1 *dr*, 94% *ee*, $[\alpha]_D^{20}$ = -222.2 (c = 0.033, DCM); $^1$H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.09 (d, *J* = 7.0 Hz, 2H), 7.99 (s, 1H), 7.51 (d, *J* = 2.2 Hz, 1H), 7.50 – 7.48 (m, 1H), 7.47 (d, *J* = 2.1 Hz, 1H), 7.43 (s, 2H), 7.41 (s, 1H), 7.40 (s, 1H), 7.30 – 7.26 (comp, 3H), 7.21 (m, 2H), 7.14 – 7.08 (comp, 3H), 7.08 – 7.03 (comp, 4H), 6.64 (t, *J* = 7.4 Hz, 1H), 6.51 (d, *J* = 8.0 Hz, 2H), 5.86 (d, *J* = 4.6 Hz, 1H), 5.82 (d, *J* = 4.6 Hz, 1H), 4.43 (d, *J* = 10.0 Hz, 1H), 4.38 (d, *J* = 10.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) (δ, ppm) 173.5, 167.8, 146.7, 143.4, 136.7, 136.1, 133.6, 133.3, 133.1, 131.7, 131.2, 130.02, 129.96, 129.30, 129.28, 129.1, 128.9, 128.7, 128.5, 128.4, 128.0, 126.2, 126.0, 121.6, 117.8, 113.5, 83.5, 68.3, 60.7; HRMS (TOF MS ESI$^+$) calculated for $C_{37}H_{30}BrN_2O_3$ $[M + H]^+$: 629.1434, found: 629.1434; HPLC conditions for

determination of enantiomeric excess: Daicel Chiralcel IB-3, λ = 300 nm, hexane : 2-propanol = 97:3, flow rate = 1.0 mL/min, $t_{major}$ = 11.4 min, $t_{minor}$ = 14.5 min.

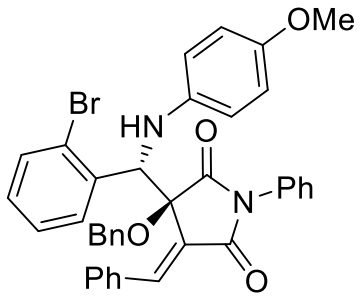



**(*S*)-4-((*E*)-Benzylidene)-3-(benzyloxy)-3-((*S*)-(2-chlorophenyl)(phenylamino)methyl)-1-phenylpyrrolidine-2,5-dione (4e).** Yellow solid. mp = 84 – 85 °C. 50.2 mg, 86% yield. >20:1 *dr*, 92% *ee*, $[\alpha]_D^{20}$ = -225.2 (c = 0.033, DCM); $^1$H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.09 (d, *J* = 6.4 Hz, 2H), 7.99 (s, 1H), 7.50 (d, *J* = 9.4 Hz, 1H), 7.47 – 7.34 (comp, 7H), 7.29 - 7.27 (comp, 4H), 7.23 – 7.14 (comp, 3H), 7.12 – 7.01 (comp, 4H), 6.64 (t, *J* = 7.3 Hz, 1H), 6.49 (d, *J* = 8.0 Hz, 2H), 5.93 (d, *J* = 4.8 Hz, 1H), 5.81 (d, *J* = 4.8 Hz, 1H), 4.44 (d, *J* = 10.0 Hz, 1H), 4.41 (d, *J* = 10.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) (δ, ppm) 173.6, 167.8, 146.8, 143.3, 136.1, 135.3 135.2, 133.2, 133.0, 132.0, 131.2, 130.2, 129.7, 129.6, 129.33, 129.29, 129.1, 128.9, 128.7, 128.5, 128.4, 127.4, 126.2, 121.7, 117.8, 113.4, 83.3, 68.4, 58.0; HRMS (TOF MS ESI$^+$) calculated for $C_{37}H_{30}ClN_2O_3$ $[M + H]^+$: 585.1939, found: 585.1939; HPLC conditions for determination of enantiomeric excess: Daicel Chiralcel IB-3, λ = 300 nm, hexane : 2-propanol = 97:3, flow rate = 1.0 mL/min, $t_{major}$ = 10.1 min, $t_{minor}$ = 11.7 min.



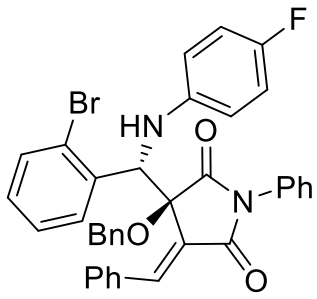

**(*S*)-4-((*E*)-Benzylidene)-3-(benzyloxy)-1-phenyl-3-((*S*)-(phenylamino)(2-(trifluoromethyl)phenyl)methyl)pyrrolidine-2,5-dione (4f).** Yellow oil. 56.2 mg, 91%

yield. >20:1 *dr*, 97% *ee*, $[\alpha]_D^{20}$ = -223.5 (c = 0.033, DCM). $^1$H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.01 (s, 1H), 7.83 (d, *J* = 7.3 Hz, 2H), 7.71 (d, *J* = 7.3 Hz, 1H), 7.58 (d, *J* = 7.7 Hz, 1H), 7.44 – 7.35 (comp, 5H), 7.32 – 7.21 (comp, 6H), 7.18 – 7.13 (m, 2H), 7.10 – 7.03 (comp, 4H), 6.69 (t, *J* = 7.3 Hz, 1H), 6.60 (d, *J* = 7.7 Hz, 2H), 5.99 (d, *J* = 6.7 Hz, 1H), 5.28 (d, *J* = 6.7 Hz, 1H), 4.44 (d, *J* = 10.0 Hz, 1H), 4.32 (d, *J* = 10.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) (δ, ppm) 173.8, 168.1, 146.6, 143.7, 136.5, 136.1, 133.1, 132.6, 132.0, 131.4, 131.3, 129.6, 129.3, 129.1, 129.0, 128.9, 128.8, 128.7, 128.5, 128.4, 128.2, 127.4 (q, J = 5.4 Hz), 126.2, 125.9, 123.1, 122.0, 118.6, 114.2, 85.1, 68.4, 58.6, 58.52, 58.49; $^{19}$F NMR (376 MHz, $CDCl_3$) (δ, ppm) -54.78; HRMS (TOF MS ESI$^+$) calculated for $C_{38}H_{30}F_3N_2O_3$ $[M + H]^+$: 619.2203, found: 619.2204; HPLC conditions for determination of enantiomeric excess: Daicel Chiralpak IB-3, λ = 300 nm, hexane : 2-propanol = 97:3, flow rate = 1.0 mL/min, $t_{major}$ = 11.9 min, $t_{minor}$ = 20.9 min.

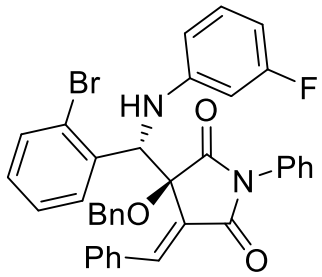



**(*S*)-4-((*E*)-Benzylidene)-3-(benzyloxy)-3-((*S*)-(2-bromophenyl)((4-methoxyphenyl)amino)methyl)-1-phenylpyrrolidine-2,5-dione (4g).** Yellow oil. 60.4 mg, 92% yield. >20:1 *dr*, 90% *ee*, $[\alpha]_D^{20}$ = -189.2 (c = 0.033, DCM); $^1$H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.07 (d, *J* = 7.6 Hz, 2H), 7.98 (s, 1H), 7.54 – 7.35 (comp, 9H), 7.24 – 7.22 (comp, 3H), 7.14 – 7.03 (comp, 4H), 6.67 (d, *J* = 8.4 Hz, 2H), 6.48 (d, *J* = 8.4 Hz, 2H), 5.81 (d, *J* = 4.4 Hz, 1H), 5.51 (d, *J* = 4.4 Hz, 1H), 4.42 (d, *J* = 10.0 Hz, 1H), 4.37 (d, *J* = 10.0 Hz, 1H), 3.67 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) (δ, ppm) 173.4, 167.8, 152.4, 143.3, 141.1, 137.0, 136.2, 133.6, 133.3, 133.1, 131.6, 131.2, 130.1, 130.0, 129.3, 129.1, 128.9, 128.7, 128.5, 128.3, 128.0, 126.2, 126.0, 121.8, 114.89, 114.87, 83.8, 68.3, 61.5, 55.8; HRMS (TOF MS ESI$^+$) calculated for $C_{38}H_{32}BrN_2O_4$

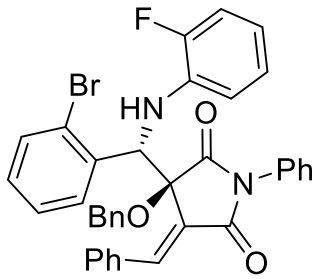
[M + H]$^+$: 659.1540, found: 659.1532; HPLC conditions for determination of enantiomeric excess: Daicel Chiralcel IB-3 λ = 300 nm, hexane : 2-propanol = 97:3, flow rate = 1.0 mL/min, $t_{major}$ = 18.1 min, $t_{minor}$ = 23.3 min.




**(*S*)-4-((*E*)-Benzylidene)-3-(benzyloxy)-3-((*S*)-(2-bromophenyl)((4-fluorophenyl)amino)methyl)-1-phenylpyrrolidine-2,5-dione (4h).** Yellow oil. 61.9 mg, 96% yield. >20:1 *dr*, 90% *ee*, $[\alpha]_D^{20}$ = -231.2 (c = 0.033, DCM); $^1$H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.08 (d, *J* = 7.6 Hz, 2H), 7.99 (s, 1H), 7.51 – 7.44 (comp, 4H), 7.45 – 7.42 (comp, 5H), 7.24 (s, 2H), 7.23 – 7.19 (m, 2H), 7.13 (m, 2H), 7.04 (d, *J* = 7.8 Hz, 2H), 6.77 (t, *J* = 8.4 Hz, 2H), 6.48 – 6.37 (m, 2H), 5.81 (d, *J* = 4.8 Hz, 1H), 5.68 (d, *J* = 4.8Hz, 1H), 4.42 (d, *J* = 10.0 Hz, 1H), 4.38 (d, *J* = 10.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) (δ, ppm) 173.5, 167.7, 156.1 (d, *J* = 235.3 Hz) , 143.4, 143.2 (d, *J* = 1.8 Hz), 136.6, 136.1, 133.7, 133.3, 133.1, 131.7, 131.2, 130.1, 129.9, 129.3, 129.1, 128.9, 128.7, 128.5, 128.4, 128.0, 126.2, 126.0, 121.6, 115.7 (d, *J* = 22.3 Hz) , 114.6 (d, *J* = 7.4 Hz) , 83.6, 68.4, 61.3; $^{19}$F NMR (376 MHz, $CDCl_3$) (δ, ppm) -127.6; HRMS (TOF MS ESI$^+$) calculated for $C_{37}H_{29}BrFN_2O_3$ [M + H]$^+$: 647.1340, found: 647.1330; HPLC conditions for determination of enantiomeric excess: Daicel Chiralcel IB-3, λ = 300 nm, hexane : 2-propanol = 97:3, flow rate = 1.0 mL/min, $t_{major}$ = 13.6 min, $t_{minor}$ = 18.9 min.

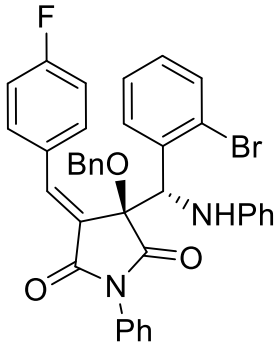



**(*S*)-4-((*E*)-Benzylidene)-3-(benzyloxy)-3-((*S*)-(2-bromophenyl)((3-fluorophenyl)amino)methyl)-1-phenylpyrrolidine-2,5-dione (4i).** Yellow oil. 53.9 mg, 84% yield. >20:1 *dr*, 86% *ee*, $[\alpha]_D^{20}$ = -201.2 (c = 0.033, DCM); $^1$H NMR (500 MHz, $CDCl_3$) (δ, ppm) 8.10 (d, *J* = 7.5 Hz, 2H), 8.00 (s, 1H), 7.52 – 7.42 (comp, 8H), 7.40 (d, *J* = 7.3 Hz, 1H), 7.29 – 7.29 (m, 1H), 7.25 (s, 1H), 7.22 (s, 2H), 7.14 (t, *J* = 7.1 Hz, 2H), 7.04 (d, *J* = 7.5 Hz, 2H), 6.99 (t, *J* = 7.3 Hz, 1H), 6.32 (m, 2H), 6.19 (d, *J* = 11.6 Hz, 1H), 5.96 (d, *J* = 4.8 Hz, 1H), 5.83 (d, *J* = 4.8 Hz, 1H), 4.43 (d, *J* = 10.0 Hz, 1H), 4.39 (d, *J* = 10.0 Hz, 1H); $^{13}$C NMR(125 MHz, $CDCl_3$) (δ, ppm) 173.6, 167.7, 164.0 (d, *J* = 242.9 Hz) , 148.5 (d, *J* = 10.8 Hz) , 143.6, 136.2, 136.0, 133.8, 133.3, 133.1, 131.8, 131.1, 130.3 (d, *J* = 10.1 Hz) , 130.2, 129.7, 129.4, 129.1, 129.0, 128.7, 128.54, 128.47, 128.0, 126.2, 126.0, 121.4, 109.4 (d, *J* = 2.2 Hz) , 104.3 (d, *J* = 21.6 Hz) , 100.4 (d, *J* = 25.6 Hz) , 83.3, 68.4, 60.5; $^{19}$F NMR (471 MHz, $CDCl_3$) (δ, ppm) -112.63. HRMS (TOF MS ESI$^+$) calculated for $C_{37}H_{29}BrFN_2O_3$ $[M + H]^+$: 647.1340, found: 647.1343; HPLC conditions for determination of enantiomeric excess: Chiralpak IB-3, λ = 300 nm, hexane : 2-propanol = 97:3, flow rate = 1.0 mL/min, $t_{major}$ = 13.1 min, $t_{minor}$ = 15.9 min.



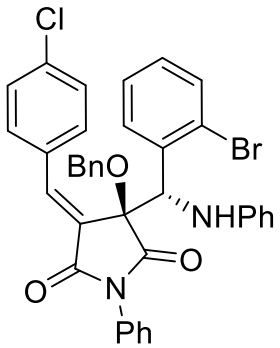

**(*S*)-4-((*E*)-Benzylidene)-3-(benzyloxy)-3-((*S*)-(2-bromophenyl)((2-fluorophenyl)amino)methyl)-1-phenylpyrrolidine-2,5-dione (4j).** Yellow oil. 52.8 mg, 82% yield. >20:1 *dr*, 95% *ee*, $[\alpha]_D^{20}$ = -264.3 (c = 0.033, DCM); $^1$H NMR (400 MHz,

$CDCl_3$) (δ, ppm) 8.08 (d, *J* = 6.6 Hz, 2H), 8.00 (s, 1H), 7.51 – 7.37 (comp, 9H), 7.29 – 7.28 (comp, 3H), 7.25 – 7.23 (m, 1H), 7.14 - 7.12 (m, 2H), 7.06 (d, *J* = 7.3 Hz, 2H), 6.95 – 6.91 (m, 1H), 6.79 (t, *J* = 7.7 Hz, 1H), 6.58 – 6.53 (m, 1H), 6.32 (t, *J* = 8.4 Hz, 1H), 6.17 (t, *J* = 1.8 Hz, 1H), 5.87 (d, *J* = 5.1 Hz, 1H), 4.47 (d, *J* = 10.0 Hz, 1H), 4.37 (d, *J* = 10.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) (δ, ppm) 173.4, 167.7, 151.9 (d, *J* = 239.7 Hz), 143.5, 136.4, 136.1, 135.5 (d, *J* = 11.0 Hz) , 133.7, 133.3, 133.1, 131.7, 131.2, 130.2, 129.9, 129.3, 129.1, 128.9, 128.7, 128.5, 128.4, 128.1, 126.2, 125.9, 124.5 (d, *J* = 3.5 Hz) , 121.6, 117.3 (d, *J* = 6.8 Hz) , 114.6 (d, *J* = 18.4 Hz) , 112.7 (d, *J* = 2.7 Hz) , 83.4, 68.4, 60.5; $^{19}$F NMR (471 MHz, $CDCl_3$) (δ, ppm) -135.40. HRMS (TOF MS ESI$^+$) calculated for $C_{37}H_{29}BrFN_2O_3$ $[M + H]^+$: 647.1340, found: 647.1340; HPLC conditions for determination of enantiomeric excess: Daicel Chiralcel AD-H, λ = 300 nm, hexane : 2-propanol = 97:3, flow rate = 1.0 mL/min, $t_{major}$ = 41.1 min, $t_{minor}$ = 46.3 min.

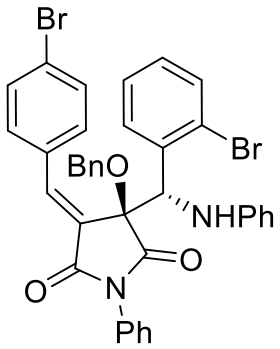



**(*S*)-3-(Benzyloxy)-3-((*S*)-(2-bromophenyl)(phenylamino)methyl)-4-((*E*)-4-fluorobenzylidene)-1-phenylpyrrolidine-2,5-dione (4k).** Yellow oil. 62.6 mg, 97% yield. >20:1 *dr*, 95% *ee*, $[\alpha]_D^{20}$ = -210.2 (c = 0.033, DCM); $^1$H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.09 (d, *J* = 8.7, 2H), 7.94 (s, 1H), 7.49 (t, *J* = 6.7 Hz, 2H), 7.44 – 7.38 (comp, 3H), 7.33 – 7.27 (comp, 3H), 7.22 – 7.18 (m, 1H), 7.15 – 7.09 (comp, 3H), 7.09 – 7.03 (comp, 6H), 6.65 (t, *J* = 7.3 Hz, 1H), 6.52 (d, *J* = 8.0 Hz, 2H), 5.80 (t, *J* = 3.7 Hz, 2H), 4.46 (d, *J* = 10.0 Hz, 1H), 4.35 (d, *J* = 10.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) (δ, ppm) 173.4, 167.7, 164.6 (d, *J* = 255.3 Hz), 146.7, 141.9, 136.6, 136.0, 135.7 (d, *J* = 8.8 Hz) , 133.6, 131.1, 130.1, 130.0, 129.5 (d, *J* = 3.2 Hz) , 129.3,

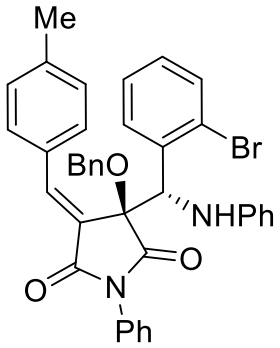
129.1, 128.9, 128.6, 128.54, 128.47, 128.0, 126.2, 125.9, 117.9, 116.6 (d, $J$ = 21.7 Hz) , 113.6, 83.5, 68.4, 60.7; $^{19}$F NMR (376 MHz, $CDCl_3$) (δ, ppm) -106.38; HRMS (TOF MS ESI$^+$) calculated for $C_{37}H_{29}BrFN_2O_3$ [M + H]$^+$: 647.1340, found: 647.1333; HPLC conditions for determination of enantiomeric excess: Daicel Chiralcel IB-3, λ = 300 nm, hexane : 2-propanol = 97:3, flow rate = 1.0 mL/min, $t_{major}$ = 14.5 min, $t_{minor}$ = 19.5 min.




**(*S*)-3-(Benzyloxy)-3-((*S*)-(2-bromophenyl)(phenylamino)methyl)-4-((*E*)-4-chlorobenzylidene)-1-phenylpyrrolidine-2,5-dione (4l).** Yellow solid. mp = 82 – 83 °C. 50.2 mg, 76% yield. >20:1 *dr*, 92% *ee*, $[\alpha]_D^{20}$ = -285.3 (c = 0.033, DCM); $^1$H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.01 (d, J = 8.6 Hz, 2H), 7.92 (s, 1H), 7.51 – 7.46 (m, 2H), 7.43 (t, J = 7.3 Hz, 2H), 7.40 – 7.37 (m, 2H), 7.36 – 7.25 (m, 1H), 7.30 – 7.29 (m, 3H) 7.21 – 7.19 (m, 2H), 7.15 – 7.04 (comp, 6H), 6.66 (t, J = 7.4 Hz, 1H), 6.52 (d, J = 7.5 Hz, 2H), 5.80 (d, J = 2.9 Hz, 1H), 5.77 (d, J = 4.3 Hz, 1H), 4.45 (d, $J$ = 10.0 Hz, 1H), 4.34 (d, $J$ = 10.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) (δ, ppm) 173.3, 167.6, 146.7, 141.7, 138.0 136.6, 135.9, 134.5, 134.4, 133.6, 131.6, 131.1, 130.1, 130.0, 129.6, 129.3, 129.1, 129.0, 128.6, 128.5, 128.1, 126.2, 126.0, 122.3, 118.0, 113.6, 83.6, 68.4, 60.8; HRMS (TOF MS ESI$^+$) calculated for $C_{37}H_{29}BrClN_2O_3$ [M + H]$^+$: 663.1045, found: 663.1035; HPLC conditions for determination of enantiomeric excess: Daicel Chiralcel IB-3, λ = 300 nm, hexane : 2-propanol = 97:3, flow rate = 1.0 mL/min, $t_{major}$ = 13.8 min, $t_{minor}$ = 17.7 min.

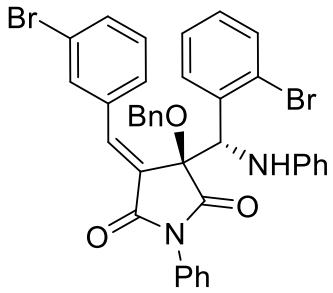



**(*S*)-3-(Benzyloxy)-4-((*E*)-4-bromobenzylidene)-3-((*S*)-(2-bromophenyl)(phenylamino)methyl)-1-phenylpyrrolidine-2,5-dione (4m).** Yellow solid. mp = 88 – 89 °C. 50.5 mg, 72% yield. >20:1 *dr*, 91% *ee*, $[\alpha]_D^{20}$ = -168.6 (c = 0.033, DCM); $^1$H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.93 (d, *J* = 8.5 Hz, 2H), 7.90 (s, 1H), 7.53 (d, *J* = 8.5 Hz, 2H), 7.50 – 7.46 (m, 2H), 7.43 (d, *J* = 7.7 Hz, 2H), 7.38 (m, 1H), 7.32 – 7.26 (comp, 3H), 7.23 – 7.16 (m, 2H), 7.15 – 7.10 (comp, 3H), 7.08 (s, 1H), 7.06 (d, *J* = 3.7 Hz, 1H), 7.04 (s, 1H), 6.66 (t, *J* = 7.3 Hz, 1H), 6.51 (d, *J* = 7.7 Hz, 2H), 5.80 (s, 1H), 5.78 (s, 1H), 4.45 (d, *J* = 10.0 Hz, 1H), 4.33 (d, *J* = 10.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) (δ, ppm) 173.3, 167.6, 146.7, 141.8, 136.6, 135.9, 134.6, 133.7, 132.6, 132.0, 131.1, 130.1, 130.0, 129.3, 129.1, 129.0, 128.6, 128.5, 128.1, 126.7, 126.1, 125.9, 122.5, 118.0, 113.6, 83.6, 68.4, 60.7; HRMS (TOF MS ESI$^+$) calculated for $C_{37}H_{29}Br_2N_2O_3$ $[M + H]^+$: 707.0539, found: 707.0529; HPLC conditions for determination of enantiomeric excess: Daicel Chiralcel IB-3, λ = 300 nm, hexane : 2-propanol = 97:3, flow rate = 1.0 mL/min, $t_{major}$ = 15.3 min, $t_{minor}$ = 19.8 min.



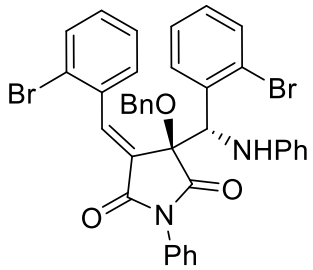

**(*S*)-3-(Benzyloxy)-3-((*S*)-(2-bromophenyl)(phenylamino)methyl)-4-((*E*)-4-methylbenzylidene)-1-phenylpyrrolidine-2,5-dione (4n).** Yellow solid. mp = 86 – 88 °C.

46.4 mg, 72% yield. >20:1 *dr*, 93% *ee*, $[\alpha]_D^{20}$ = -210.2 (c = 0.033, DCM); $^1$H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.00 (s, 1H), 7.97 (d, *J* = 3.2 Hz, 2H), 7.51 – 7.30 (comp, 7H), 7.25 – 7.22 (comp, 5H), 7.14 – 6.99 (comp, 6H), 6.65 (t, *J* = 6.7 Hz, 1H), 6.52 (d, *J* = 5.4 Hz, 2H), 5.89 – 5.75 (m, 2H), 4.45 – 4.33 (m, 2H), 2.40 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) (δ, ppm) 173.7, 167.9, 146.8, 143.5, 142.6, 136.8, 136.2, 133.6, 133.4, 131.2, 130.5, 130.1, 130.0, 129.3, 129.1, 128.8, 128.6, 128.5, 128.3, 128.0, 126.2, 126.1, 120.3, 117.7, 113.5, 83.5, 68.3, 60.6, 21.9; HRMS (TOF MS ESI$^+$) calculated for $C_{38}H_{32}BrN_2O_3$ $[M + H]^+$: 643.1591, found: 643.1598; HPLC conditions for determination of enantiomeric excess: Chiralpak IB-3, λ = 300 nm, hexane : ethanol= 97:3, flow rate = 0.5 mL/min, $t_{major}$ = 20.7 min, $t_{minor}$ = 21.7 min.

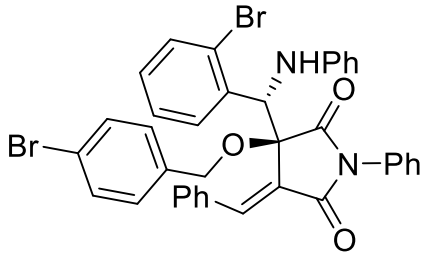



**(*S*)-3-(Benzyloxy)-4-((*E*)-3-bromobenzylidene)-3-((*S*)-(2-bromophenyl)(phenylamino)methyl)-1-phenylpyrrolidine-2,5-dione (4o).** Yellow solid. mp = 71 – 72 $^o$C. 48.0 mg, 68% yield. >20:1 *dr*, 92% *ee*, $[\alpha]_D^{20}$ = -201.2 (c = 0.033, DCM); $^1$H NMR (500 MHz, $CDCl_3$) (δ, ppm) 8.09 (d, *J* = 2.6 Hz, 2H), 7.88 (s, 1H), 7.54 (d, *J* = 7.9 Hz, 1H), 7.51 – 7.36 (comp, 7H), 7.28 (d, *J* = 3.2 Hz, 2H), 7.21 (m, 2H), 7.10- 7.06 (comp, 6H), 6.66 (t, *J* = 7.3 Hz, 1H), 6.54 (d, *J* = 8.0 Hz, 2H), 5.84 (d, *J* = 4.5 Hz, 1H), 5.68 (d, *J* = 5.0 Hz, 1H), 4.46 (d, *J* = 10.0 10.0 Hz, 1H), 4.34 (d, *J* = 10.0 Hz, 1H); $^{13}$C NMR (125 MHz, $CDCl_3$) (δ, ppm) 173.2, 167.4, 146.7, 141.5, 136.6, 136.1, 135.9, 135.0, 134.3, 133.7, 131.13, 131.07, 130.7, 130.1, 129.9, 129.4, 129.1, 129.0, 128.5, 128.42, 128.35, 128.0, 126.2, 125.9, 123.5, 123.2, 118.1, 113.8, 83.7, 68.3, 60.9; HRMS (TOF MS ESI$^+$) calculated for $C_{37}H_{29}Br_2N_2O_3$ $[M + H]^+$: 707.0539, found: 707.0543; HPLC conditions for determination of enantiomeric excess: Daicel

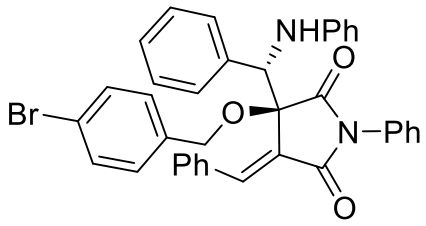
Chiralcel IB-3, λ = 300 nm, hexane : 2-propanol = 97:3, flow rate = 1.0 mL/min, $t_{major}$ = 14.2 min, $t_{minor}$ = 21.8 min.




**(*S*)-3-(Benzyloxy)-4-((*E*)-2-bromobenzylidene)-3-((*S*)-(2-bromophenyl)(phenylamino)methyl)-1-phenylpyrrolidine-2,5-dione (4p).** Yellow solid. mp = 153 – 154 ºC. 53.7 mg, 76% yield. >20:1 *dr*, 95% *ee*, $[\alpha]_D^{20}$ = -183.2 (c = 0.033, DCM); $^1$H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.56 (d, *J* = 9.6 Hz, 1H), 8.52 (s, 1H), 7.73 – 7.66 (m, 1H), 7.52 – 7.48 (m, 2H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.38 (d, *J* = 7.0 Hz, 1H), 7.27 (m, 2H), 7.25 – 7.21 (comp, 3H), 7.15 (m, 2H), 7.11 (m, 2H), 7.09 – 7.05 (comp, 4H), 6.65 (t, *J* = 7.4 Hz, 1H), 6.50 (d, *J* = 8.0 Hz, 2H), 5.80 (d, *J* = 3.9 Hz, 1H), 5.72 (d, *J* = 4.7 Hz, 1H), 4.47 (d, *J* = 10.0 Hz, 1H), 4.31 (d, *J* = 10.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) (δ, ppm) 173.1, 167.3, 146.6, 141.2, 136.5, 135.9, 133.9, 133.8, 132.9, 132.5, 132.3, 131.1, 130.1, 123.0, 129.3, 129.10, 129.05, 128.9, 128.48, 128.45, 128.37, 128.2, 128.1, 126.1, 125.7, 124.0, 117.9, 113.6, 83.7, 68.3, 61.1; HRMS (TOF MS ESI$^+$) calculated for $C_{37}H_{29}Br_2N_2O_3$ $[M + H]^+$: 707.0539, found: 707.0549; HPLC conditions for determination of enantiomeric excess: Daicel Chiralcel IB-3, λ = 300 nm, hexane : 2-propanol = 97:3, flow rate = 1.0 mL/min, $t_{major}$ = 11.4 min, $t_{minor}$ = 15.4 min.

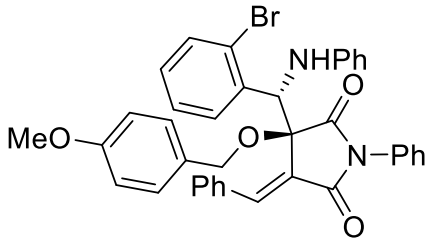



**(*S*)-4-((*E*)-Benzylidene)-3-((4-bromobenzyl)oxy)-3-((*S*)-(2-bromophenyl)(phenylamino)methyl)-1-phenylpyrrolidine-2,5-dione (4q).** Yellow oil. 50.8 mg, 72% yield. >20:1 *dr*, 96% *ee*, $[\alpha]_D^{20}$ = -237.2 (c = 0.033, DCM); $^1$H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.05 (d, *J* = 2.8 Hz, 2H), 7.98 (s, 1H), 7.54 – 7.35 (comp, 10H), 7.18 – 6.96 (comp, 8H), 6.73 – 6.59 (m, 1H), 6.53 (s, 2H), 5.88 (d, *J* = 5.2 Hz, 1H), 5.75 (d, *J* = 5.2 Hz, 1H), 4.37 (d, *J* = 10.2 Hz, 1H), 4.31 (d, *J* = 10.2 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) (δ, ppm) 173.5, 167.7, 146.7, 143.4, 136.6, 135.1, 133.7, 133.3, 133.0, 131.8, 131.6, 131.1, 130.2, 130.1, 129.9, 129.3, 129.1, 129.0, 128.0, 126.1, 126.0, 122.4, 121.5, 117.9, 113.6, 83.7, 67.5, 60.8; HRMS (TOF MS ESI$^+$) calculated for $C_{37}H_{29}Br_2N_2O_3$ $[M + H]^+$: 707.0539, found: 707.0538; HPLC conditions for determination of enantiomeric excess: Daicel Chiralcel IB-3, λ =300 nm, hexane : 2-propanol = 97:3, flow rate = 1.0 mL/min, $t_{major}$ = 16.5 min, $t_{minor}$ = 22.1 min.

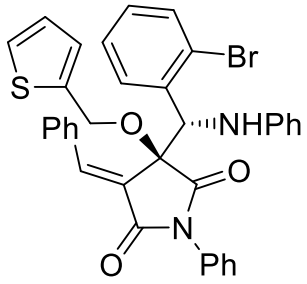



**(*S*)-4-((*E*)-Benzylidene)-3-((4-bromobenzyl)oxy)-1-phenyl-3-((*S*)-phenyl(phenylamino)methyl)pyrrolidine-2,5-dione (4r).** Yellow solid. mp = 86 – 89 ºC. 51.5 mg, 82% yield. >20:1 *dr*, 92% *ee*, $[\alpha]_D^{20}$ = -195.2 (c = 0.033, DCM); $^1$H NMR (500 MHz, $CDCl_3$) (δ, ppm) 8.08 (s, 1H), 8.06 (d, *J* = 3.8 Hz, 2H), 7.52 – 7.45 (comp, 3H), 7.44 – 7.33 (comp, 5H), 7.24 (d, *J* = 5.8 Hz, 2H), 7.21 (d, *J* = 4.1 Hz, 3H), 7.11 (d, *J* = 8.1 Hz, 2H), 7.06 (t, *J* = 7.7 Hz, 2H), 6.85 (t, *J* = 4.6 Hz, 2H), 6.65 (t, *J* = 7.3 Hz, 1H), 6.49 (d, *J* = 8.0 Hz, 2H), 5.69 (d, *J* = 5.0 Hz, 1H), 5.32 (d, *J* = 5.0 Hz, 1H), 4.46 (d, *J* = 9.6 Hz, 1H), 4.31 (d, *J* = 9.6 Hz, 1H); $^{13}$C NMR (126 MHz, $CDCl_3$) (δ, ppm) 173.3,

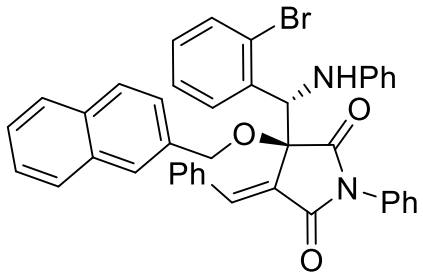
167.6, 147.3, 141.6, 137.1, 135.2, 133.1, 132.3, 131.9, 131.7, 131.0, 130.2, 129.7, 129.2, 129.1, 129.0, 128.8, 128.7, 128.3, 126.3, 123.9, 122.5, 117.0, 113.8, 83.6, 67.9, 61.2; HRMS (TOF MS ESI$^+$) calculated for $C_{37}H_{30}BrN_2O_3$ [M + H]$^+$: 629.1434, found: 629.1430; HPLC conditions for determination of enantiomeric excess: Chiralpak IB-3, λ = 300 nm, hexane : 2-propanol = 98:2, flow rate = 1.0 mL/min, $t_{major}$ = 19.4 min, $t_{minor}$ = 21.8 min.




**(*S*)-4-((*E*)-Benzylidene)-3-((*S*)-(2-bromophenyl)(phenylamino)methyl)-3-((4-methoxybenzyl)oxy)-1-phenylpyrrolidine-2,5-dione (4s).** Yellow oil. 53.7 mg, 82% yield. >20:1 *dr*, 95% *ee*, $[\alpha]_D^{20}$ = -207.2 (c = 0.033, DCM); $^1$H NMR (500 MHz, $CDCl_3$) (δ, ppm) 8.10 (d, *J* = 7.4 Hz, 2H), 7.99 (s, 1H), 7.50 – 7.41 (comp, 8H), 7.16 – 6.98 (comp, 8H), 6.80 (d, *J* = 8.0 Hz, 2H), 6.63 (t, *J* = 7.3 Hz, 1H), 6.49 (d, *J* = 8.0 Hz, 2H), 5.83 (s, 1H), 5.80 (s, 1H), 4.58 (d, *J* = 10.0 Hz, 1H), 4.54 (d, *J* = 10.0 Hz, 1H), 3.78 (s, 3H); $^{13}$C NMR (125 MHz, $CDCl_3$) (δ, ppm) 173.6, 167.8, 159.8, 146.7, 143.3, 136.7, 133.6, 133.4, 133.1, 131.6, 131.2, 130.5, 123.0, 129.3, 129.2, 129.0, 128.9, 128.3, 128.0, 126.2, 126.0, 121.8, 117.7, 113.9, 113.5, 83.3, 68.1, 60.7, 55.4; HRMS (TOF MS ESI$^+$) calculated for $C_{38}H_{32}BrN_2O_4$ [M + H]$^+$: 659.1540, found: 659.1530; HPLC conditions for determination of enantiomeric excess: Daicel Chiralcel IB-3, λ = 300 nm, hexane : 2-propanol = 97:3, flow rate = 1.0 mL/min, $t_{major}$ = 17.7 min, $t_{minor}$ = 21.6 min.

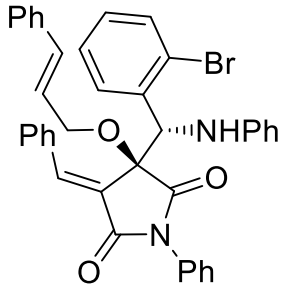



**(*S*)-4-((*E*)-Benzylidene)-3-((*S*)-(2-bromophenyl)(phenylamino)methyl)-1-phenyl-3-(thiophen-2-ylmethoxy)pyrrolidine-2,5-dione (4t).** Brown oil. 32.3 mg, 51% yield. >20:1 *dr*, 92% *ee*, $[\alpha]_D^{20}$ = -170.6 (c = 0.033, DCM); $^1$H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.10 (d, *J* = 9.1 Hz, 2H), 7.98 (s, 1H), 7.49 – 7.45 (comp, 5H), 7.44 – 7.37 (comp, 3H), 7.29 (d, *J* = 4.5 Hz, 1H), 7.14 – 7.08 (comp, 3H), 7.07 (d, *J* = 1.3 Hz, 1H), 7.05 (s, 1H), 7.02 (d, *J* = 1.1 Hz, 1H), 6.90 (m, 1H), 6.81 (d, *J* = 3.5 Hz, 1H), 6.64 (t, *J* = 7.2 Hz, 1H), 6.53 – 6.47 (m, 2H), 5.83 (s, 1H), 5.82 (s, 1H), 4.59 (s, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) (δ, ppm) 173.1, 167.7, 146.7, 143.5, 138.1, 136.6, 133.7, 133.4, 133.0, 131.7, 131.2, 130.1, 129.4, 129.3, 129.1, 128.9, 128.03, 127.96, 127.0, 126.7, 126.2, 126.0, 121.4, 117.8, 113.6, 83.3, 62.8, 60.7; HRMS (TOF MS ESI$^+$) calculated for $C_{35}H_{28}BrN_2O_3S$ $[M + H]^+$: 635.0999, found: 635.0998; HPLC conditions for determination of enantiomeric excess: Daicel Chiralcel IB-3, λ = 300 nm, hexane : 2-propanol = 97:3, flow rate = 1.0 mL/min, $t_{major}$ = 15.2 min, $t_{minor}$ = 19.5 min.

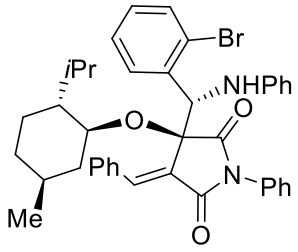



**(*S*)-4-((*E*)-Benzylidene)-3-((*S*)-(2-bromophenyl)(phenylamino)methyl)-3-(naphthalen-2-ylmethoxy)-1-phenylpyrrolidine-2,5-dione (4u).** Yellow solid. mp = 109 - 110 ºC. 50.6 mg, 75% yield. >20:1 *dr*, 93% *ee*, $[\alpha]_D^{20}$ = -192.2 (c = 0.033, DCM); $^1$H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.12 (d, *J* = 7.3 Hz, 2H), 8.03 (s, 1H), 7.84 – 7.75 (comp, 3H), 7.70 (m, 1H), 7.56 (s, 1H), 7.52 – 7.38 (comp, 10H), 7.14 – 7.05 (comp,

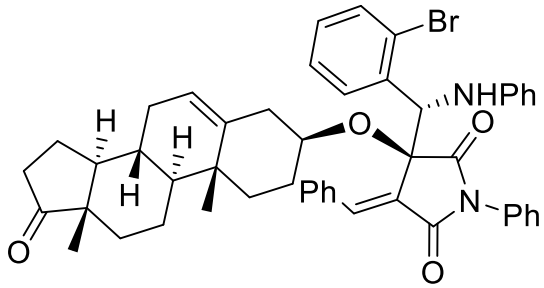
4H), 7.04 – 6.96 (m, 2H), 6.65 (t, *J* = 7.3 Hz, 1H), 6.54 (d, *J* = 7.6 Hz, 2H), 5.91 (s, 1H), 5.84 (s, 1H), 4.56 (q, *J* = 10.0 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) (δ, ppm) 173.6, 167.8, 146.8, 143.4, 136.7, 133.62, 133.56, 133.4, 133.3, 133.2, 133.1, 131.7, 131.1, 130.02, 129.97, 129.3, 129.1, 128.9, 128.2, 128.1, 128.0, 127.8, 127.6, 126.4, 126.32, 126.25, 126.2, 126.0, 121.7, 117.9, 113.6, 83.6, 68.5, 60.8; HRMS (TOF MS ESI$^+$) calculated for $C_{41}H_{32}BrN_2O_3$ [M + H]$^+$: 679.1591, found: 679.1580; HPLC conditions for determination of enantiomeric excess: Daicel Chiralcel IB-3, λ = 300 nm, hexane : 2-propanol = 97:3, flow rate = 1.0 mL/min, $t_{minor}$ = 17.5 min, $t_{major}$ = 30.2 min.




**(*S*)-4-((*E*)-Benzylidene)-3-((*S*)-(2-bromophenyl)(phenylamino)methyl)-3-(cinnamyloxy)-1-phenylpyrrolidine-2,5-dione (4v).** Yellow oil. 23.4 mg, 36% yield. >20:1 *dr*, 94% *ee*, $[\alpha]_D^{20}$ = -195.2 (c = 0.033, DCM); $^1$H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.12 (d, *J* = 3.7 Hz, 2H), 7.98 (s, 1H), 7.54 – 7.43 (comp, 5H), 7.40 – 7.31 (m, 3H), 7.29 – 7.28 (comp, 4H), 7.17 – 7.04 (comp, 5H), 7.01 – 6.89 (m, 2H), 6.67 (t, *J* = 7.3 Hz, 1H), 6.56 (d, *J* = 8.0 Hz, 2H), 6.40 (d, *J* = 15.9 Hz, 1H), 6.24 (t, *J* = 11.1 Hz, 1H), 5.87 (d, *J* = 4.4 Hz, 1H), 5.83 (d, *J* = 3.7 Hz, 1H), 4.12 (dd, *J* = 6.6, 2.3 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) (δ, ppm) 173.8, 167.8, 146.8, 143.4, 136.7, 136.3, 134.2, 133.6, 133.4, 133.1, 131.7, 131.1, 130.0, 129.34, 129.32, 129.0, 128.8, 128.7, 128.2, 128.0, 126.8, 126.2, 126.1, 124.5, 121.7, 117.8, 113.6, 83.2, 67.2, 60.7; HRMS (TOF MS ESI$^+$) calculated for $C_{39}H_{32}BrN_2O_3$ [M + H]$^+$: 655.1591, found: 655.1578; HPLC conditions for determination of enantiomeric excess: Daicel Chiralcel IB-3, λ = 300 nm, hexane : 2-propanol = 97:3, flow rate = 1.0 mL/min, $t_{major}$ = 15.2 min, $t_{minor}$ = 27.2 min.



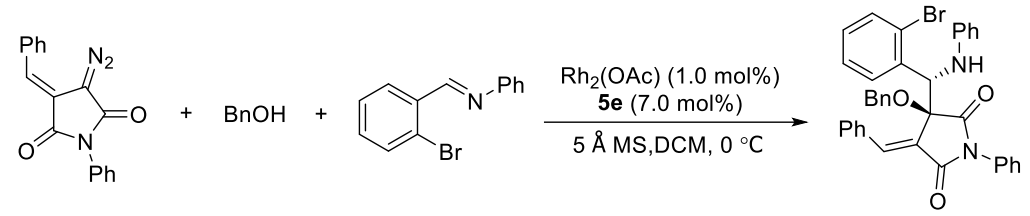

**(*S*)-4-((*E*)-Benzylidene)-3-((*S*)-(2-bromophenyl)(phenylamino)methyl)-3-(((1*S*,2*R*,5*S*)-2-isopropyl-5-methylcyclohexyl)oxy)-1-phenylpyrrolidine-2,5-dione (4w).** Yellow solid. mp = 70 – 73 ºC. 31.1 mg, 46% yield. >20:1 *dr*. $[\alpha]_D^{20}$ = -166.6 (c = 0.033, DCM); $^1$H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.02 (d, J = 8.7 Hz, 2H), 7.94 (s, 1H), 7.49 (d, J = 7.7 Hz, 1H), 7.46 – 7.37 (comp, 7H), 7.16 – 7.12 (comp, 3H), 7.09 (d, J = 8.2 Hz, 1H), 6.89 (d, J = 7.6 Hz, 2H), 6.70 (t, J = 7.3 Hz, 1H), 6.60 (d, J = 8.0 Hz, 2H), 5.88 (d, J = 5.2 Hz, 1H), 5.79 (d, J = 5.5 Hz, 1H), 3.42 (m, 1H), 2.15 (m, 1H), 1.81 (d, J = 11.0 Hz, 1H), 1.64 – 1.50 (m, 1H), 1.45 (t, J = 9.4 Hz, 1H), 1.38 – 1.20 (m, 3H), 0.86 (d, J = 6.2 Hz, 3H), 0.84 – 0.79 (m, 2H), 0.78 (d, J = 6.9 Hz, 3H), 0.40 (d, J = 6.9 Hz, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) (δ, ppm) 176.2, 168.2, 147.9, 143.0, 137.4, 133.49, 133.46, 133.2, 131.4, 130.9, 129.8, 129.5, 129.3, 129.2, 129.0, 127.8, 126.2, 125.5, 122.6, 117.9, 113.7, 80.7, 77.4, 60.9, 49.4, 42.2, 33.9, 31.9, 24.3, 23.0, 22.5, 22.1, 17.4; HRMS (TOF MS ESI$^+$) calculated for $C_{40}H_{42}BrN_2O_3$ $[M + H]^+$: 677.2373, found: 677.2365.




**(*S*)-4-((*E*)-Benzylidene)-3-((*S*)-(2-bromophenyl)(phenylamino)methyl)-3-(((3*S*,8*R*,9*S*,10*R*,13*S*,14*S*)-10,13-dimethyl-17-oxo-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[a]phenanthren-3-yl)oxy)-1-phenylpyrrolidine-2,5-dione (4x).** Yellow solid. mp = 101 – 105 ºC. 42.0 mg, 52% yield. >20:1 *dr*, $[\alpha]_D^{20}$ = -149.2 (c = 0.33, DCM); $^1$H NMR (500 MHz, $CDCl_3$) (δ, ppm) 8.09 (s, 2H), 7.92 (s, 1H),

7.52 – 7.34 (comp, 9H), 7.17 – 7.05 (comp, 3H), 6.98 (d, J = 7.8 Hz, 2H), 6.66 (t, J = 7.2 Hz, 1H), 6.55 (d, J = 7.8 Hz, 2H), 5.81 (s, 1H), 4.99 (s, 1H), 3.38 (dd, J = 10.1, 5.5 Hz, 1H), 2.42 (dd, J = 19.2, 8.6 Hz, 1H), 2.30 (t, J = 11.8 Hz, 1H), 2.16 – 1.92 (comp, 3H), 1.88 – 1.68 (comp, 4H), 1.70 – 1.40 (comp, 7H), 1.33 – 1.15 (comp, 4H), 0.96 (s, 3H), 0.84 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) (δ, ppm) 221.2, 179.4, 174.5, 170.2, 168.0, 147.0, 145.2, 143.5, 142.7, 140.5, 137.6, 136.9, 136.1, 133.9, 133.6, 133.4, 131.6, 131.2, 130.2, 129.9, 129.3, 129.1, 129.0, 128.9, 127.9, 126.8, 126.2, 126.0, 123.1, 121.6, 117.7, 113.6, 82.4, 78.2, 60.4, 51.8, 50.1, 47.6, 40.1, 37.4, 36.7, 35.9, 31.5, 30.8, 29.6, 22.0, 20.4, 19.4, 13.6; HRMS (TOF MS ESI$^+$) calculated for $C_{49}H_{50}BrN_2O_4$ $[M + H]^+$: 809.2948, found: 809.2930.

**General Procedure for the Scale Up**




**1a,** 635.8 mg
2.2 mmol

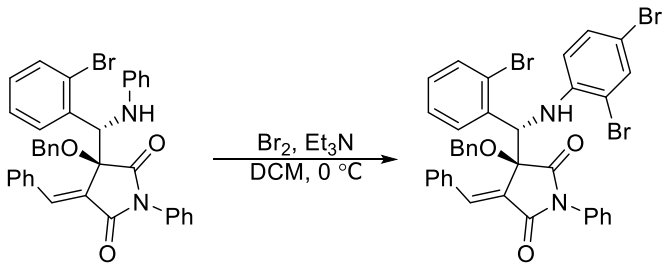
**2a,** 216 mg
2.0 mmol

**3d,** 518 mg
2.0 mmol

**4d**, 0.97 g
77% yield
>20:1 *dr,* 92% *ee*

To a 50-mL oven-dried vial containing a magnetic stirring bar, $Rh_2(OAc)_4$ (8.8 mg, 1.0 mol%), BnOH **2a** (216 mg, 2.0 mmol, 1.0 equiv.), imine **3d** (518 mg, 2.0 mmol, 1.0 equiv.), CPA **5e** (100 mg, 0.14mmol, 7.0 mol%), and 5 Å MS (1.0 g) in DCM (10 mL), was added as a solution of diazo compound **1a** (635.8 mg, 2.4 mmol, 1.2 equiv.) in DCM (20 mL) *via* a syringe pump over 2 h under argon atmosphere at 0 °C. After addition, the reaction mixture was stirred at 0 °C for additional 1 h. Then the solvent was evaporated in vacuo, the residue was purified by column chromatography on silica gel (Hexanes : EtOAc = 10:1) to give 0.97 g of pure product **4d** in 77% yield with 92% *ee*.

**General Procedure for the Synthesis of 6**



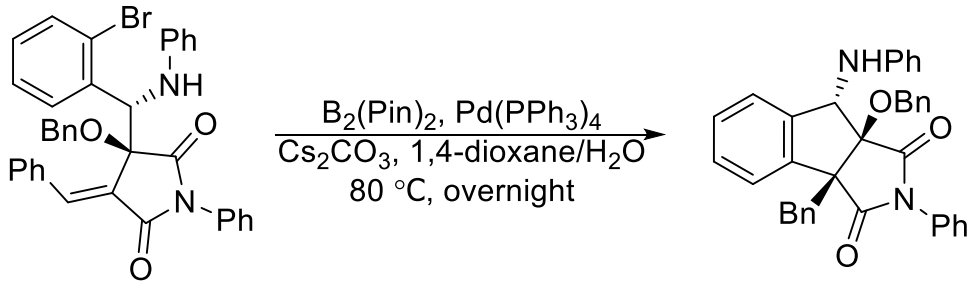

**4d**, 92% *ee*

**6**, 91%
> 20:1 *dr*, 92% *ee*

To a 10-mL oven-dried vial containing a magnetic stirring bar, **4d** (92% *ee*, 50 mg, 0.08 mmol, 1.0 equiv.) in anhydrous DCM (1.0 mL), was added $Br_2$ (8.5 μL, 0.16 mmol, 2.0 equiv.) at 0 °C, and the reaction mixture was stirred for additional 15 min under these conditions, followed by the addition of $Et_3N$ (22.3 μL, 0.16 mmol, 2.0

equiv.). Then, the reaction mixture was quenched with saturated aqueous $Na_2S_2O_3$ (5.0 mL), and extracted with ethyl acetate (2 X 5.0 mL). The combined organic phase was washed with brine, dried with anhydrous $Na_2SO_4$. The solvent was evaporated in vacuo after filtration. The crude product was purified by flash chromatography on silica gel (Hexanes : EtOAc = 10:1) to give 57.0 mg pure product **6** in 91% yield. Yellow solid, mp = 153 – 154 °C. 92% *ee*, $[\alpha]_D^{20}$ = -240.2 (c = 0.033, DCM). $^1$H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.09 (d, *J* = 6.8 Hz, 2H), 8.01 (s, 1H), 7.51 (d, *J* = 2.2 Hz, 1H), 7.50 – 7.36 (comp, 9H), 7.30 (s, 4H), 7.18 – 7.10 (m, 2H), 7.08 – 6.99 (comp, 3H), 6.74 (d, *J* = 4.8 Hz, 1H), 6.07 (d, *J* = 8.8 Hz, 1H), 5.81 (d, *J* = 4.8 Hz, 1H), 4.49 (d, *J* = 9.9 Hz, 1H), 4.38 (d, *J* = 9.9 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) (δ, ppm) 173.5, 167.6, 143.8, 142.9, 136.0, 135.5, 134.5, 133.7, 133.3, 133.0, 131.8, 131.2, 131.0, 130.4, 129.7, 129.4, 129.1, 129.0, 128.9, 128.5, 128.2, 126.2, 126.0, 121.2, 112.6, 110.7, 108.6, 83.1, 68.6, 60.5; HRMS (TOF MS ESI$^+$) calculated for $C_{37}H_{27}Br_3N_2O_3Na$ $[M + Na]^+$: 806.9464, found: 806.9458; HPLC conditions for determination of enantiomeric excess: Daicel Chiralcel IC, λ = 300 nm, hexane : 2-propanol = 99:1, flow rate = 1.0 mL/min, $t_{minor}$ = 13.1 min, $t_{major}$ = 17.0 min.

**General Procedure for the Synthesis of 7**



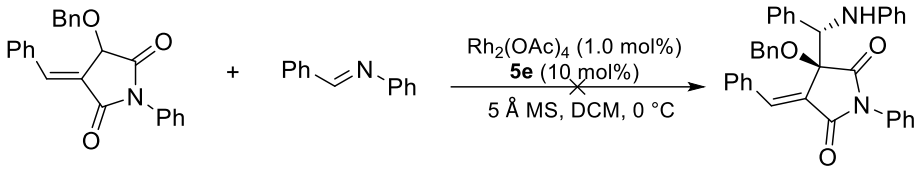

**4d,** 92% *ee*

**7**, 51%, 92% *ee*

To a 10-mL oven-dried vial containing a magnetic stirring bar, **4d** (92% *ee*, 62.8 mg, 0.10 mmol, 1.0 equiv.), $B_2(Pin)_2$ (38.0 mg, 0.15 mmol, 1.5 equiv.), $Pd(PPh_3)_4$ (12 mg, 10 mol%), $Cs_2CO_3$ (48.8 mg, 0.15 mmol, 1.5 equiv.), and a combined solvent (1,4-Dioxane/$H_2O$ = 5:1, 1.0 mL) were added in sequence at room temperature, then

the reaction mixture was stirred at 80 ℃ overnight. When the reaction was completed (monitored by TLC), quenched with $H_2O$ (15 mL) and extracted with ethyl acetate (3 X 10 mL). The combined organic phase was washed successively with water and brine, dried over anhydrous $Na_2SO_4$, and then concentrated under reduced pressure after filtration. The crude product was purified by flash chromatography on silica gel (Hexanes : EtOAc = 15:1 to 10:1) to give 28.1 mg pure product **7** in 51% yield. Colorless oil., 92% *ee*, $[\alpha]_D^{20}$ = 18.56 (c = 0.033, DCM). $^1$H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.54 (d, *J* = 7.6 Hz, 1H), 7.45 – 7.34 (comp, 7H), 7.32 (m, 2H), 7.27 (m, 1H), 7.25 (m, 1H), 7.16 (m, 3H), 7.08 (m, 4H), 6.89 (d, *J* = 7.5 Hz, 2H), 6.72 (t, *J* = 7.3 Hz, 1H), 6.46 (d, *J* = 8.0 Hz, 2H), 5.46 (d, *J* = 9.2 Hz, 1H), 5.15 (d, J = 11.1 Hz, 1H), 4.82 (d, *J* = 11.1 Hz, 1H), 4.63 (d, *J* = 9.2 Hz, 1H), 3.58 (d, *J* = 13.6 Hz, 1H), 3.52 (d, *J* = 13.6 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) (δ, ppm) 176.4, 174.5, 147.2, 142.3, 137.8, 137.5, 135.5, 131.4, 131.3, 130.0, 129.7, 129.3, 129.2, 129.0, 128.7, 128.3, 128.2, 127.7, 126.9, 126.4, 124.9, 124.1, 118.0, 112.6, 85.9, 69.7, 62.3, 62.0, 35.5; HRMS (TOF MS ESI$^+$) calculated for $C_{37}H_{31}N_2O_3$ $[M + H]^+$: 551.2329, found: 551.2333; HPLC conditions or determination of enantiomeric excess: Daicel Chiralcel IB-3, λ = 254 nm, hexane : 2-propanol = 99:1, flow rate = 1.0 mL/min, $t_{minor}$ = 8.5 min, $t_{major}$ = 9.3 min.

## Control Experiments




**8** **3a** **4a**, ND

To a 10-mL oven-dried vial containing a magnetic stirring bar, **8** (36.9 mg, 0.10 mmol), **3a** (18.1 mg, 0.10 mmol), **5e** (7.0 mg, 10 mol%), 5 Å MS (100 mg), $Rh_2(OAc)_4$ (0.5 mg, 1.0 mol%), and DCM (2.0 mL) were added in sequence, and the reaction mixture was stirred at 0 °C under argon atmosphere for 3 h. Then the reaction crude mixture was subjected to proton NMR analysis in $CDCl_3$ after the solvent was evaporated (see Figure S1). No reaction was occurred under these conditions.

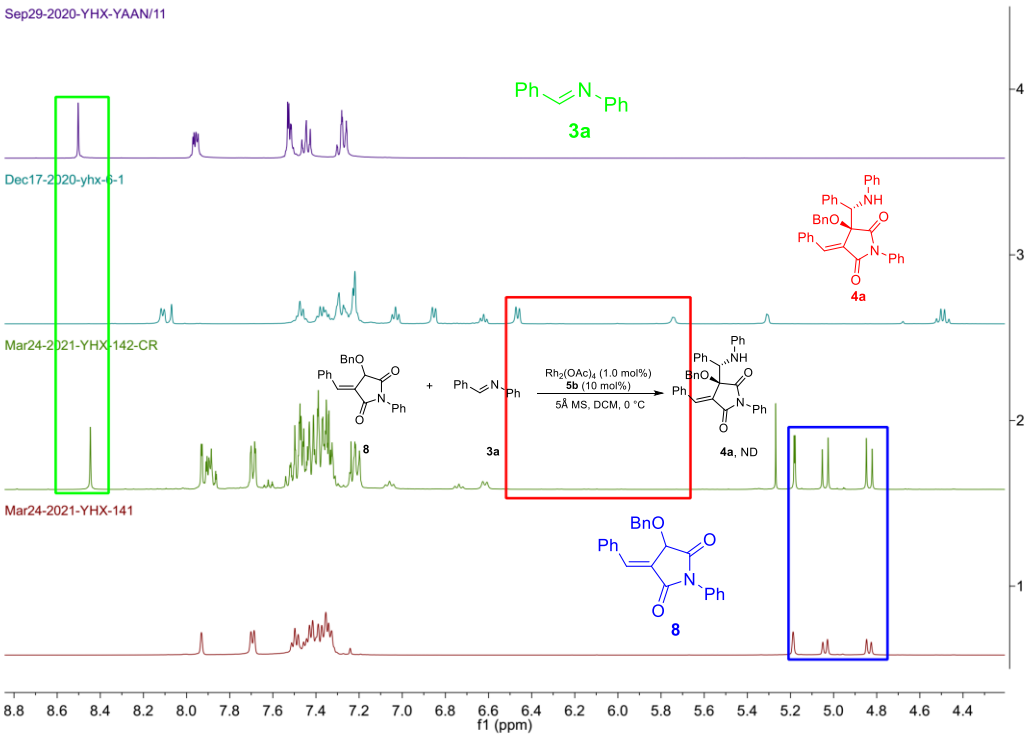
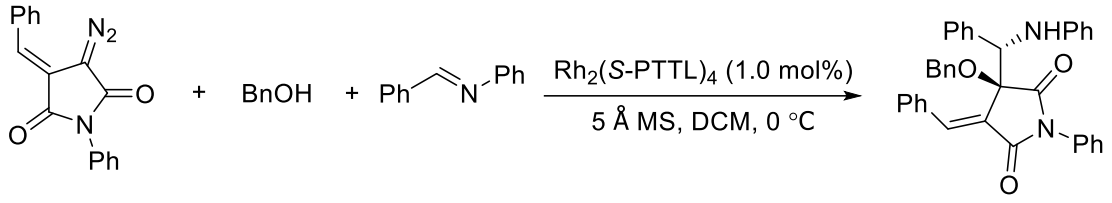



***Figure S1.*** Proton NMR spectrum of crude reaction mixture of **8** with **3a** under standard conditions.

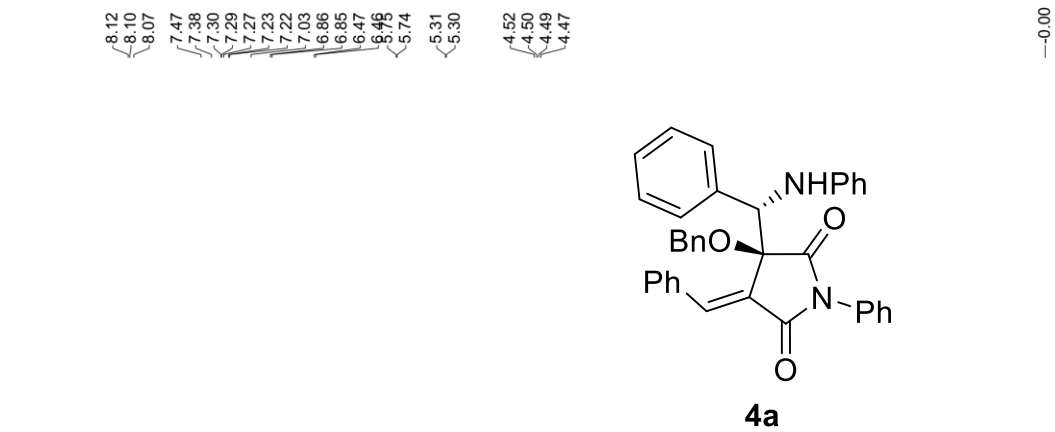



**1a** **2a** **3a** **4a**, 91%
> 20:1 *dr,* 2% *ee*

To a 10-mL oven-dried vial containing a magnetic stirring bar, $Rh_2$(*S*-PTTL)$_4$ (1.3 mg, 1.0 mol%), BnOH **2a** (10.8 mg, 0.1 mmol, 1.0 equiv.), imine **3a** (18.1 mg, 0.10 mmol, 1.0 equiv.), and 5 Å MS (100 mg) in DCM (1.0 mL), was added as a solution of diazo compound **1a** (34.4 mg, 0.12 mmol, 1.2 equiv.) in DCM (1.0 mL) *via* a syringe pump over 2 h under argon atmosphere at 0 °C. After addition, the reaction mixture was stirred at 0 °C for additional 1 h. Then the solvent was evaporated in vacuo, the residue was purified by column chromatography on silica gel (Hexanes : EtOAc = 10:1) to give pure **4a** in 91% yield with 2% *ee*.

**References:**

(1) (*a*) E. G. Chupakhin, G. P. Kantin, D. V. Dar'in and M. Krasavin, *Mendeleev Commun.*, 2021, **31**, 36-38; (*b*) E. Chupakhin, M. Gecht, A. Ivanov, G. Kantin, D. Dar'in and M. Krasavin, *Synthesis*, 2020, **52**, 36-38; (*c*) D. Laha and R. G. Bhat, *Asian J. Org. Chem.*, 2020, **9**, 918-921.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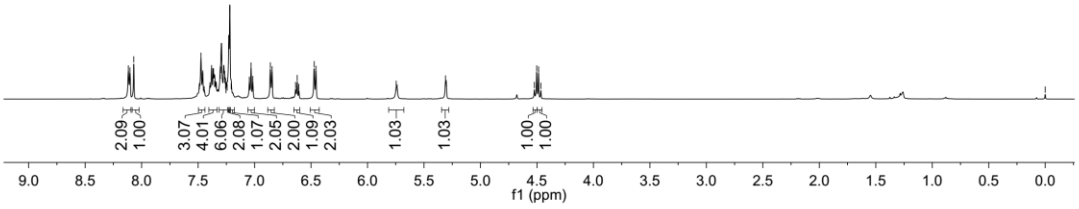
8.10
8.07
7.47
7.38
7.30
7.29
7.27
7.23
7.22
7.03
6.86
6.85
6.47
5.74
5.31
5.30
4.52
4.50
4.49
4.47
0.00
NHPh
O
BnO
Ph
N
Ph
O

**4a**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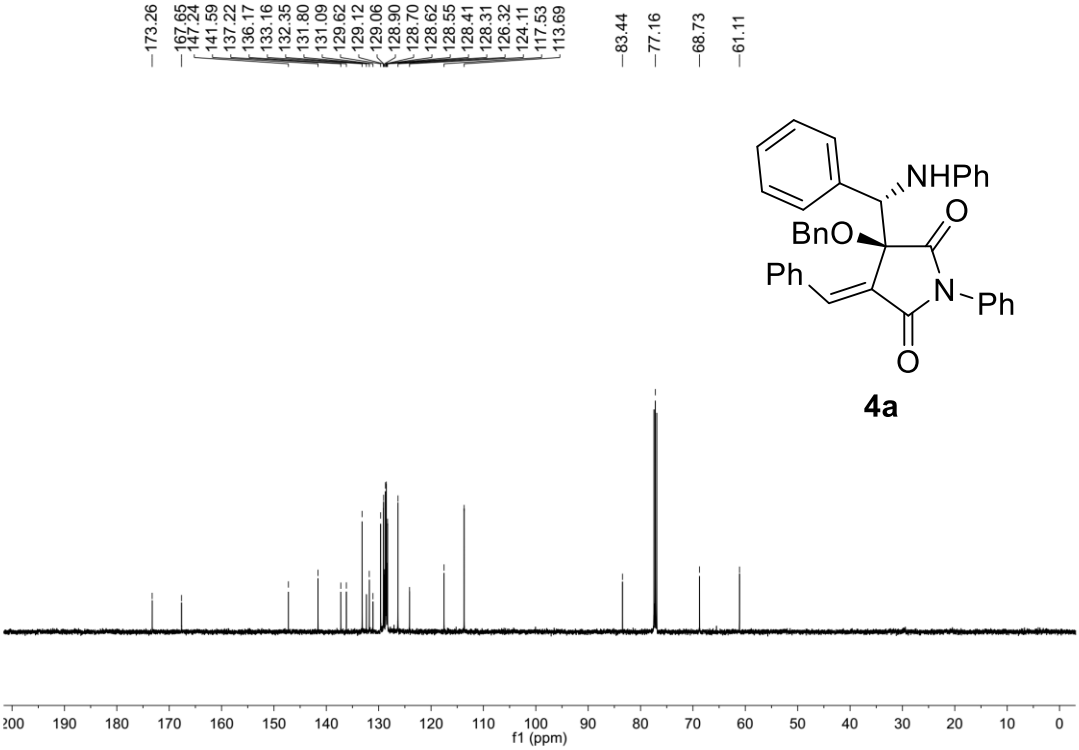
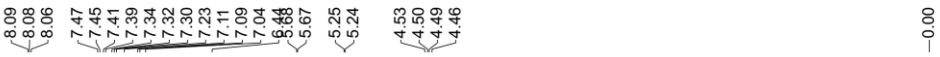
1.00
3.07
4.01
6.06
2.08
1.07
2.05
2.00
1.09
2.03
1.03
1.03
1.00
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


173.26
167.65
147.24
141.59
137.22
136.17
133.16
132.35
131.80
131.09
129.62
129.12
129.06
128.90
128.70
128.62
128.55
128.41
128.31
126.32
124.11
117.53
113.69
83.44
77.16
68.73
61.11
NHPh
O
BnO
Ph
N
Ph
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

**4a**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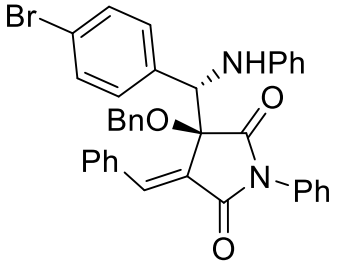
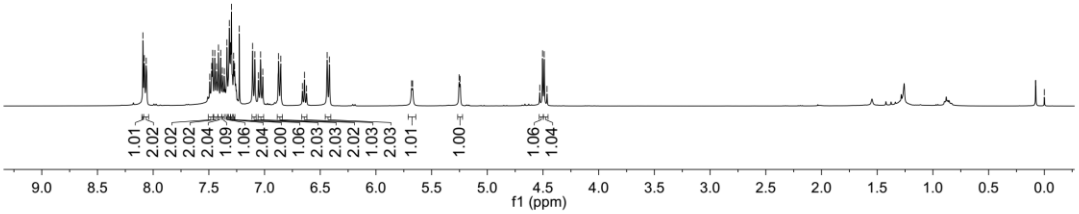
8.08
8.06
7.47
7.45
7.41
7.39
7.34
7.32
7.30
7.23
7.11
7.09
7.04
5.68
5.67
5.25
5.24
4.53
4.50
4.49
4.46
0.00


Br
NHPh
O
BnO
Ph
N
Ph
O

**4b**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2.02
2.02
2.02
2.04
1.09
1.06
2.04
2.00
1.06
2.03
2.03
2.02
1.03
2.03
1.01
1.00
1.06
1.04
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
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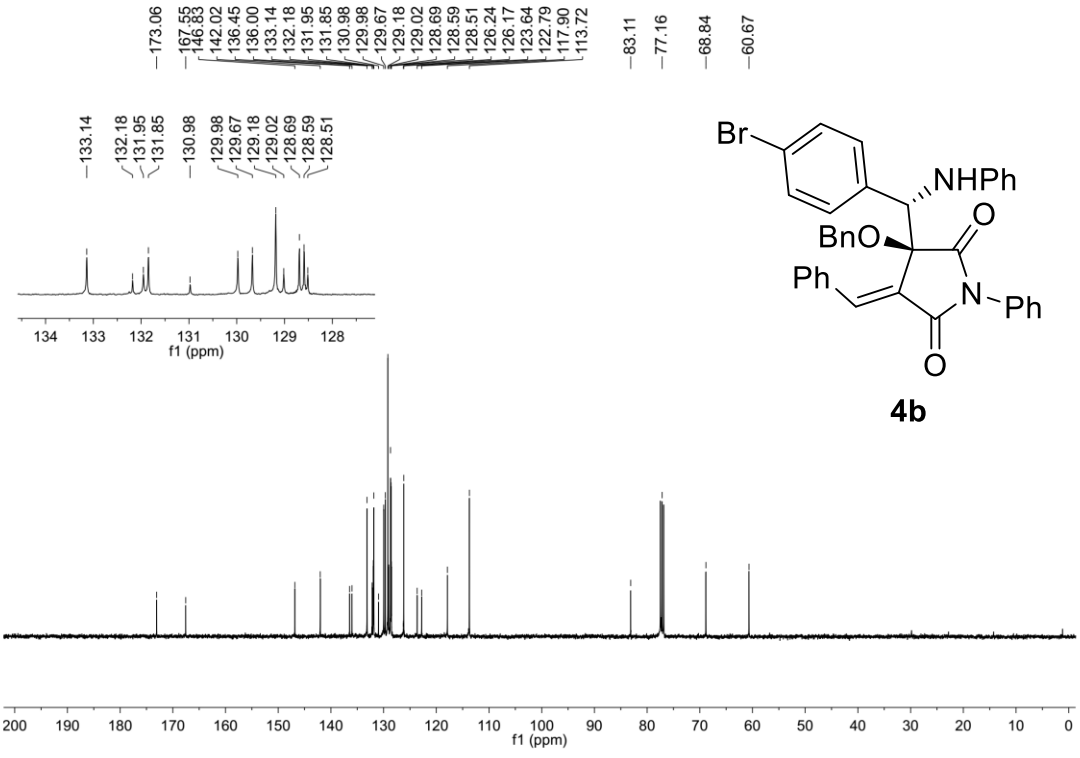
1.5
1.0
0.5
0.0
f1 (ppm)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132.18
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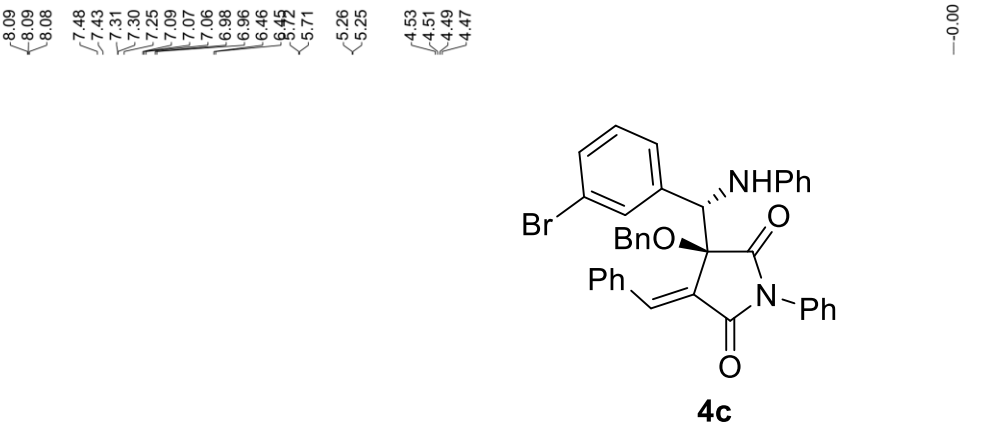
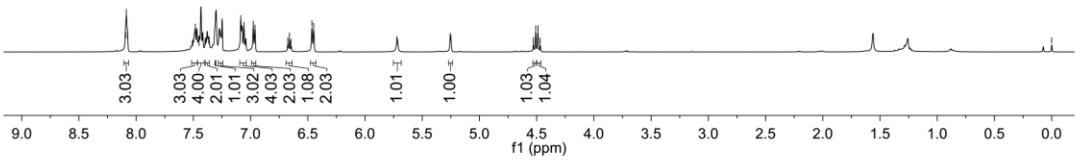
131.85
130.98
129.98
129.67
129.18
129.02
128.69
128.59
128.51
126.24
126.17
123.64
122.79
117.90
113.72
83.11
77.16
68.84
60.67
133.14
132.18
131.95
131.85
130.98
129.98
129.67
129.18
129.02
128.69
128.59
128.51
134
133
132
131
130
129
128
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

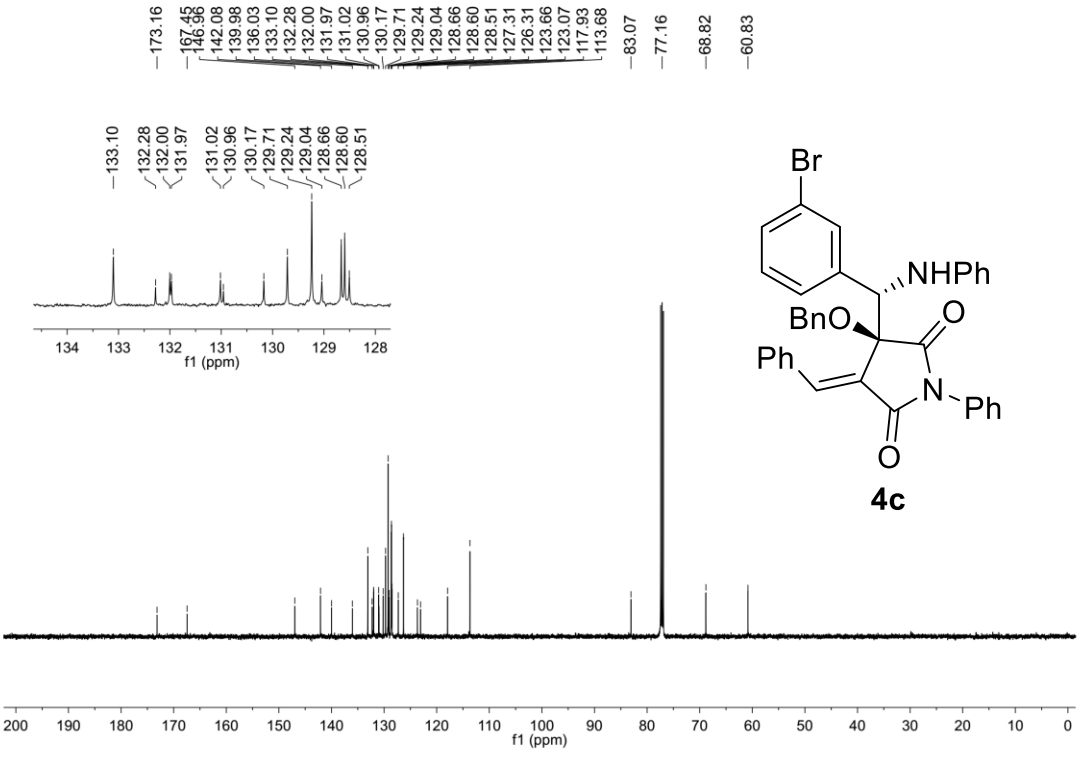

Br
NHPh
O
BnO
Ph
N
Ph
O

**4b**

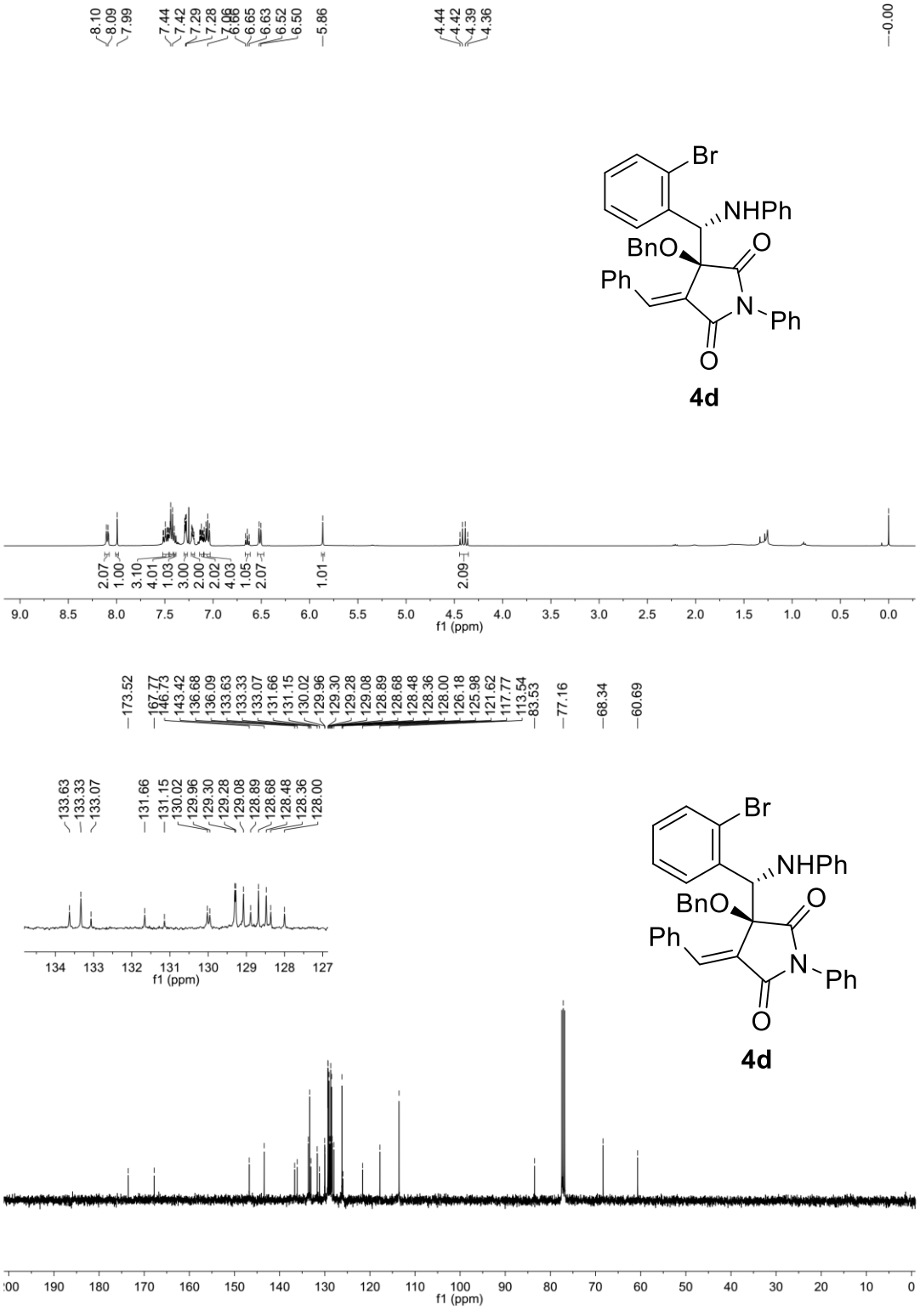



**4c**




**4c**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4.42
4.39
4.36
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BnO
O
Ph
N
Ph
O
4d
2.07
1.00
3.10
4.01
1.03
3.00
2.00
2.02
4.03
1.05
2.07
1.01
2.09
f1 (ppm)
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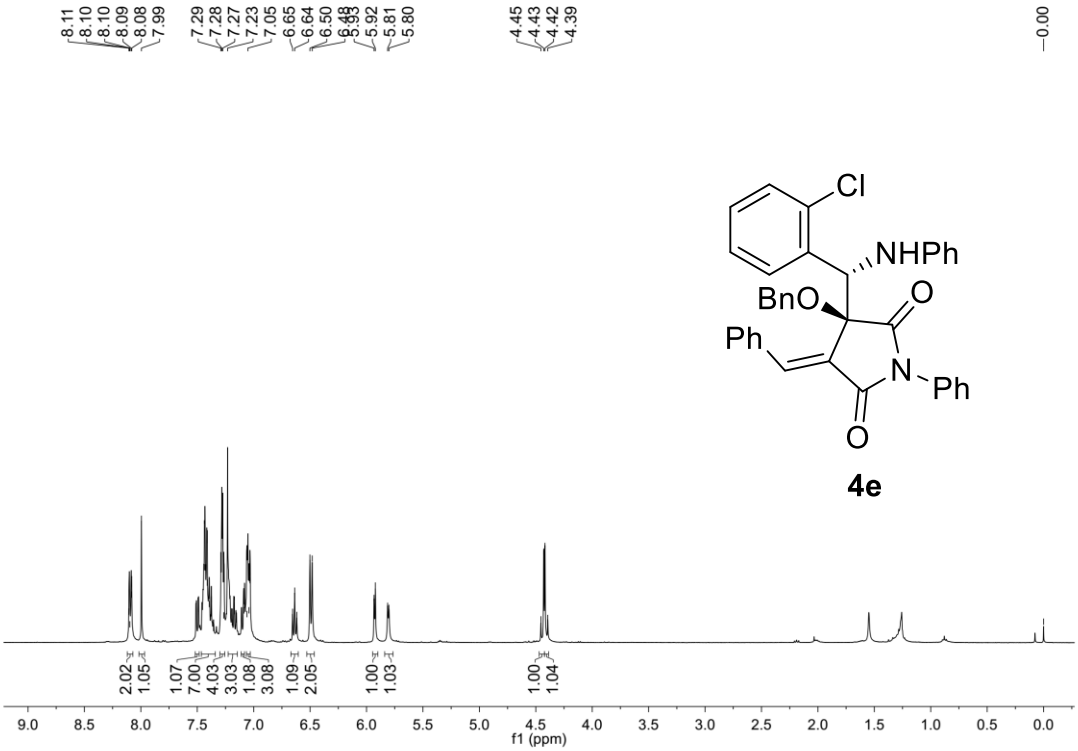
167.77
166.73
143.42
136.68
136.09
133.63
133.33
133.07
131.66
131.15
130.02
129.96
129.30
129.28
129.08
128.89
128.68
128.48
128.36
128.00
126.18
125.98
121.62
117.77
113.54
83.53
77.16
68.34
60.69
f1 (ppm)
Br
NHPh
BnO
O
Ph
N
Ph
O
4d
f1 (ppm)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6.50
6.48
5.93
5.92
5.81
5.80
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4.43
4.42
4.39
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BnO
O
Ph
N
Ph
O
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1.05
1.07
7.00
4.03
3.03
1.08
3.08
1.09
2.05
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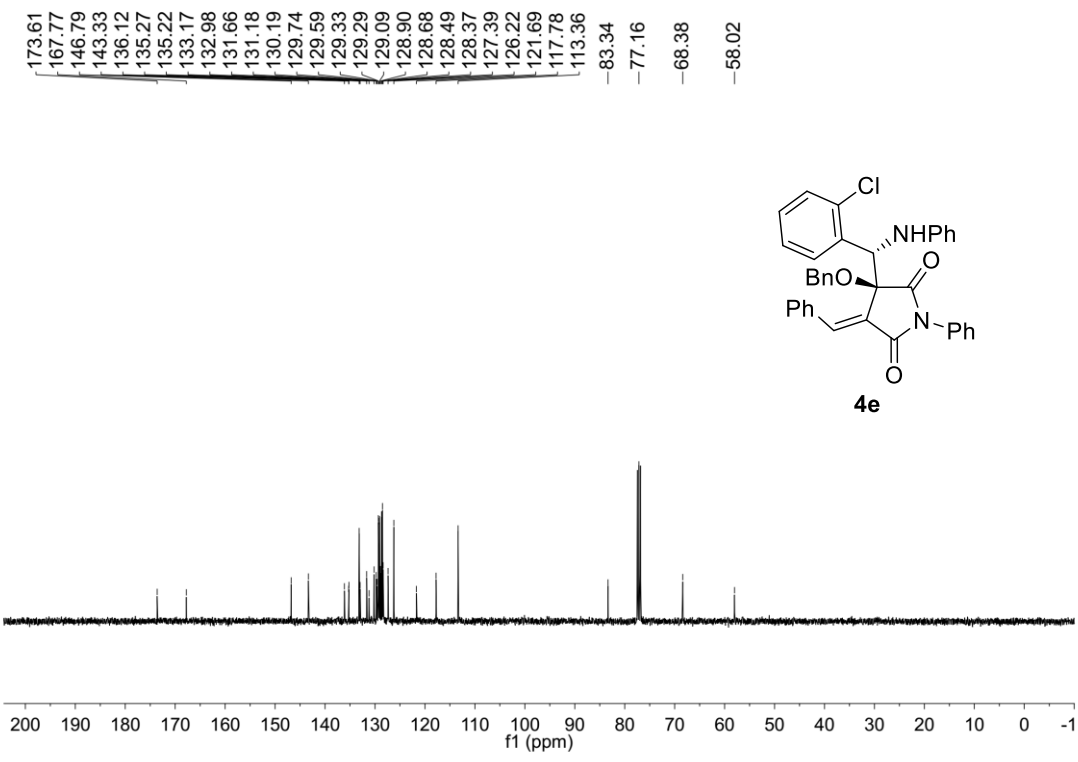
1.03
1.00
1.04
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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129.59
129.33
129.29
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128.49
128.37
127.39
126.22
121.69
117.78
113.36
83.34
77.16
68.38
58.02
Cl
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BnO
O
Ph
N
Ph
O
4e
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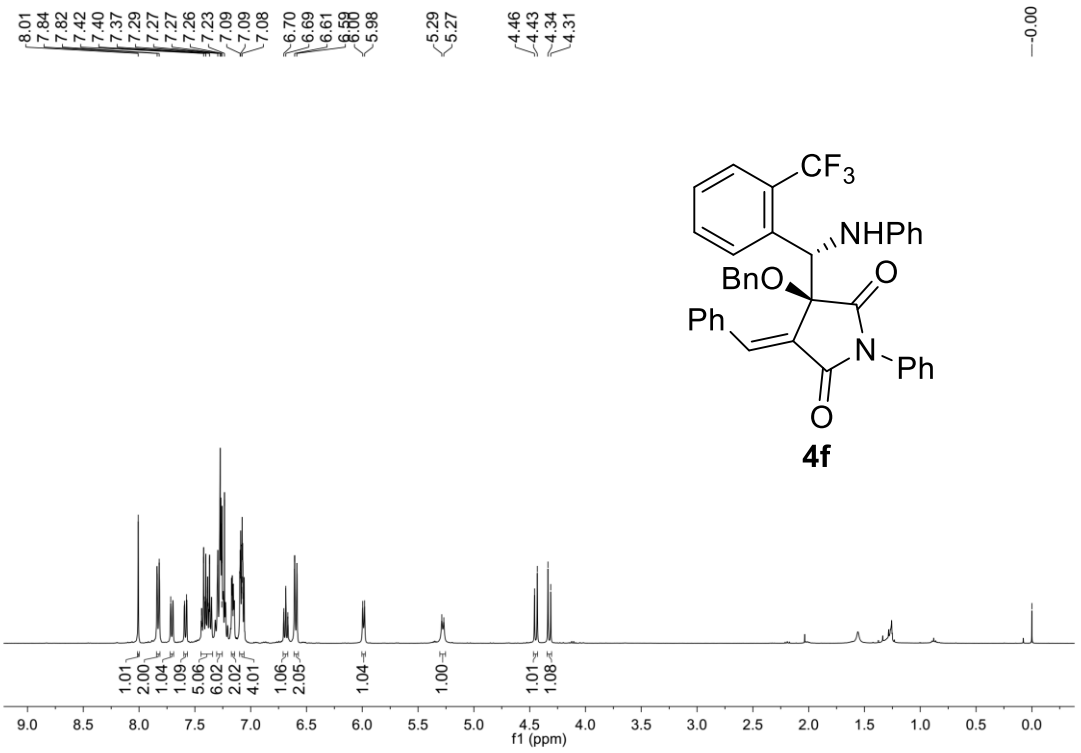
f1 (ppm)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7.09
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6.70
6.69
6.61
6.59
6.00
5.98
5.29
5.27
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4.43
4.34
4.31
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NHPh
BnO
O
Ph
N
Ph
O
4f
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2.00
1.04
1.09
5.06
6.02
2.02
4.01
1.06
2.05
1.04
1.00
1.01
1.08
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
3.0
2.5
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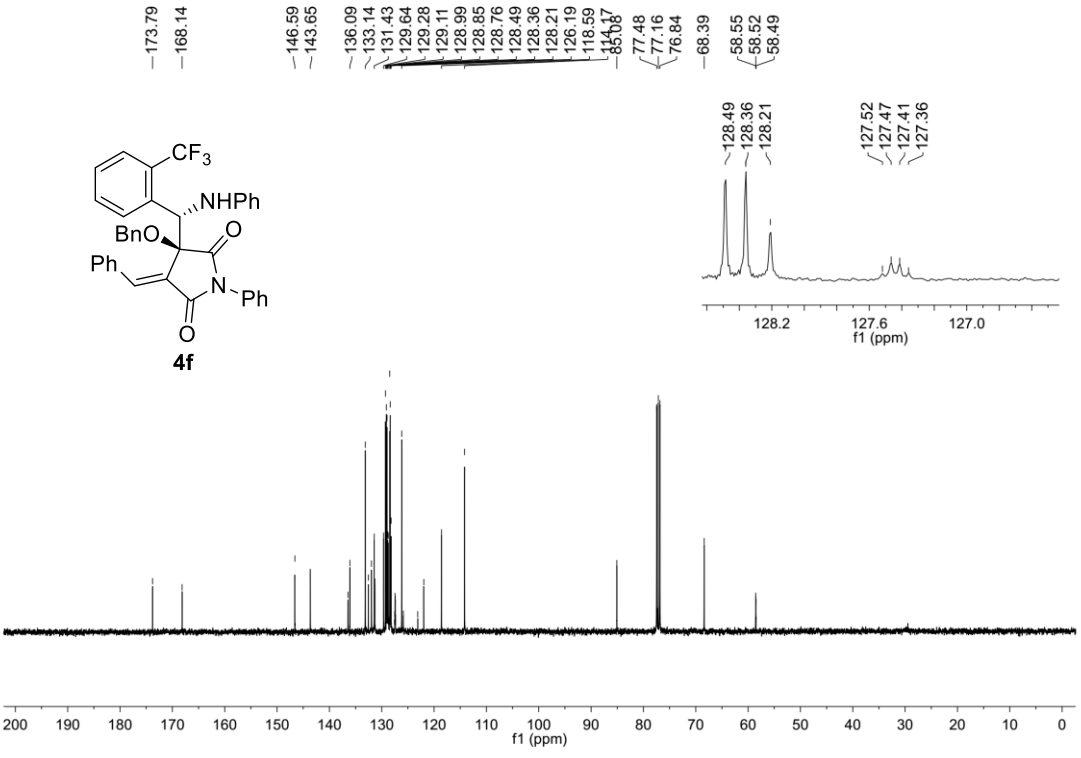
1.0
0.5
0.0
f1 (ppm)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128.85
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128.49
128.36
128.21
126.19
118.59
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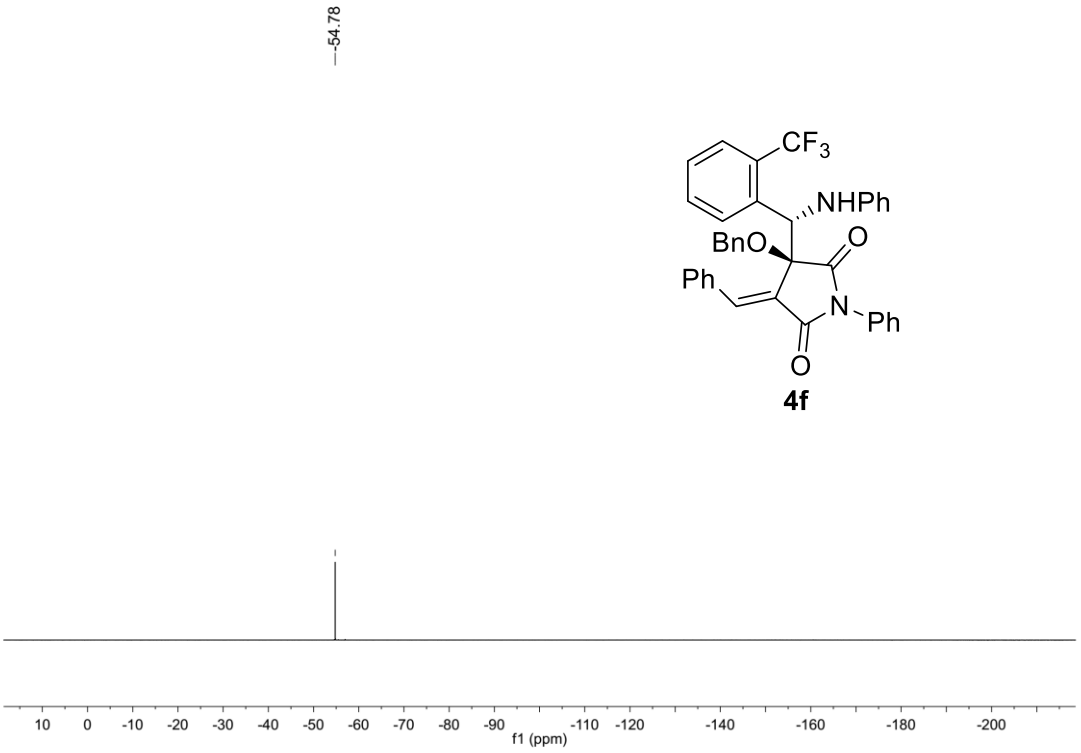
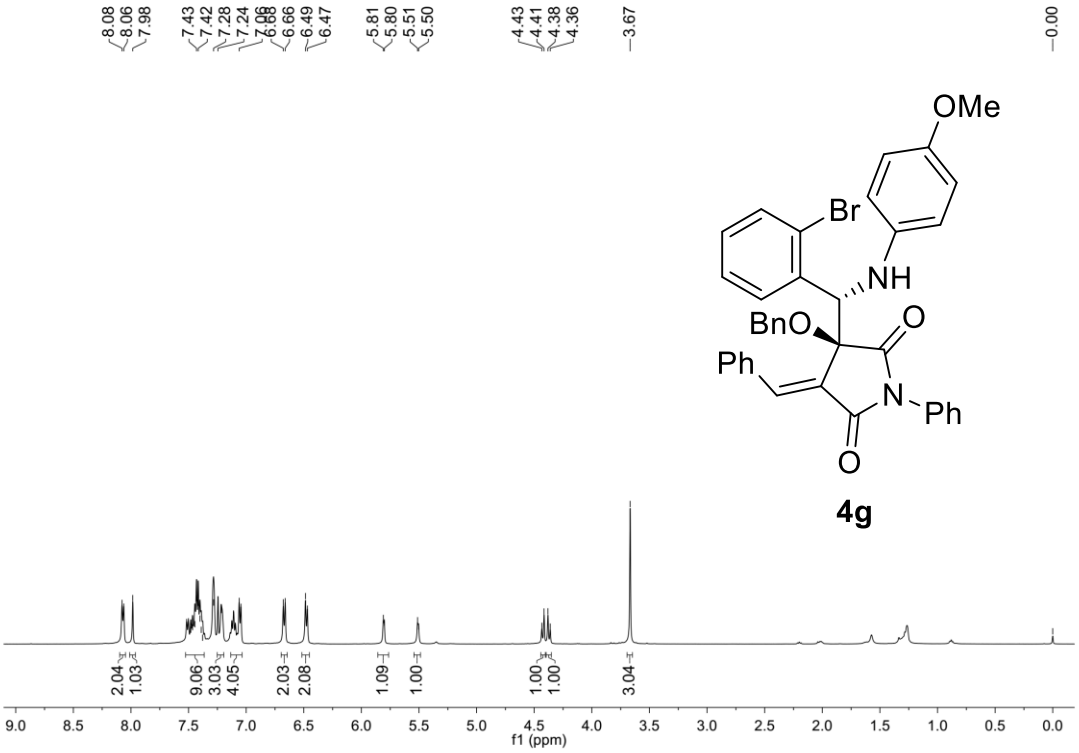
77.16
76.84
68.39
58.55
58.52
58.49
128.49
128.36
128.21
127.52
127.47
127.41
127.36
CF3
NHPh
BnO
O
Ph
N
Ph
O
4f
128.2
127.6
127.0
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-54.78
CF3
NHPh
BnO
O
Ph
N
Ph
O
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-120
-140
-160
-180
-200
f1 (ppm)

**4f**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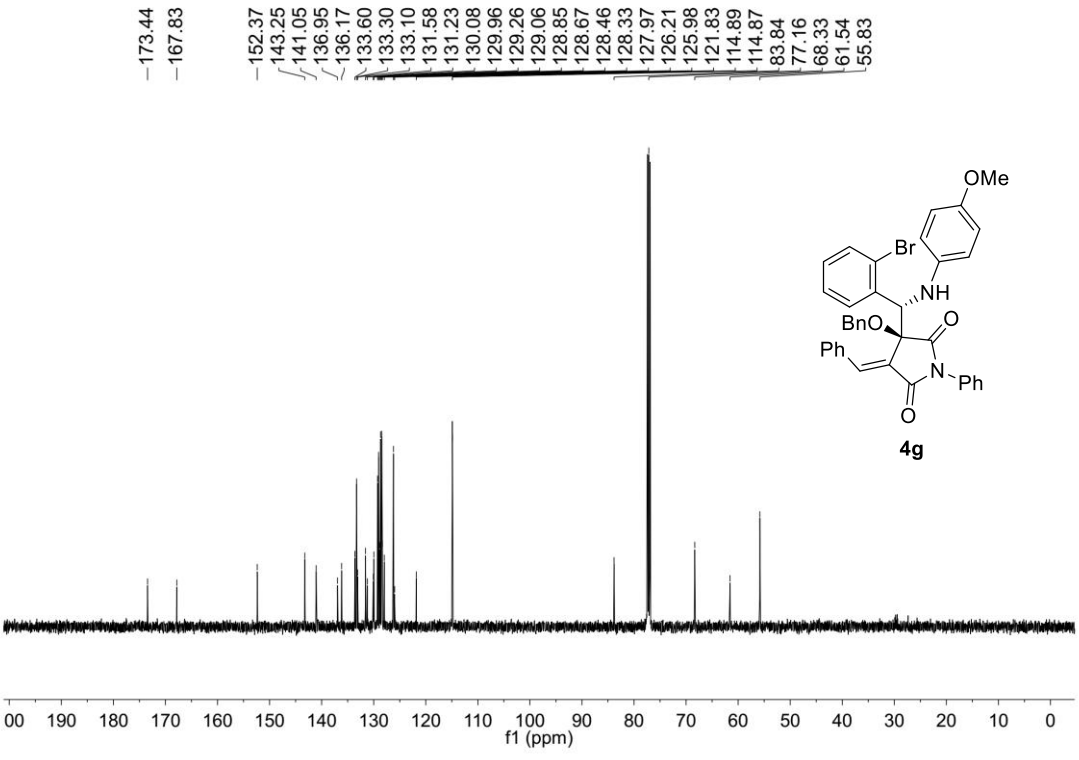
6.49
6.47
5.81
5.80
5.51
5.50
4.43
4.41
4.38
4.36
3.67
0.00
OMe
Br
NH
BnO
O
Ph
N
Ph
O
4g
2.04
1.03
9.06
3.03
4.05
2.03
2.08
1.09
1.00
1.00
1.00
3.04
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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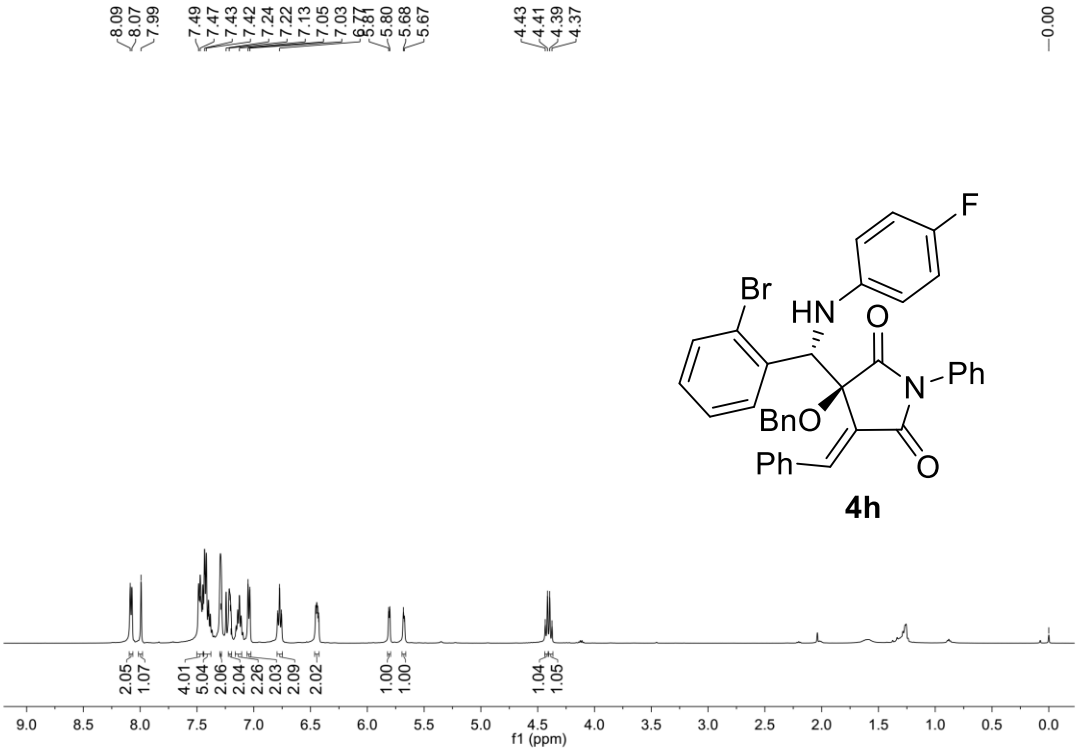
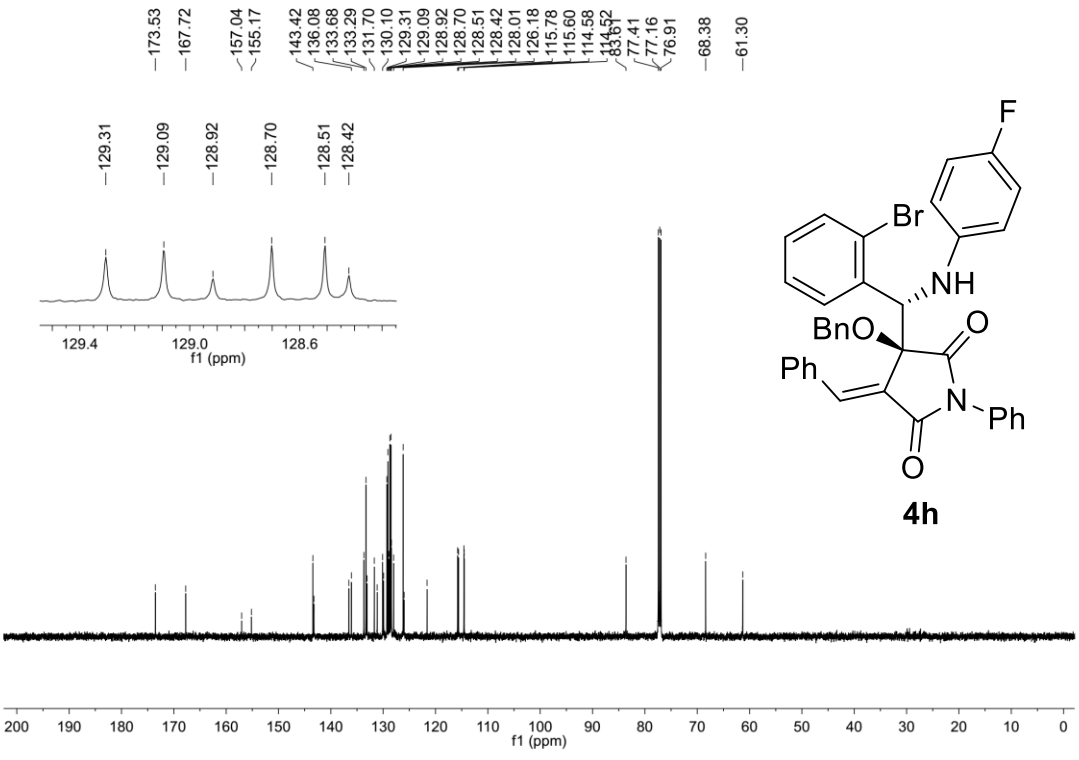
131.58
131.23
130.08
129.96
129.26
129.06
128.85
128.67
128.46
128.33
127.97
126.21
125.98
121.83
114.89
114.87
83.84
77.16
68.33
61.54
55.83
OMe
Br
NH
BnO
O
Ph
N
Ph
O
4g
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.09
8.07
7.99
7.49
7.47
7.43
7.42
7.24
7.22
7.13
7.05
7.03
6.77
5.81
5.80
5.68
5.67
4.43
4.41
4.39
4.37
0.00
F
Br
HN
O
N
Ph
BnO
Ph
O
4h
2.05
1.07
4.01
5.04
2.06
2.04
2.26
2.03
2.09
2.02
1.00
1.00
1.04
1.05
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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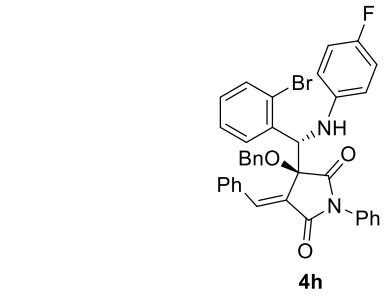
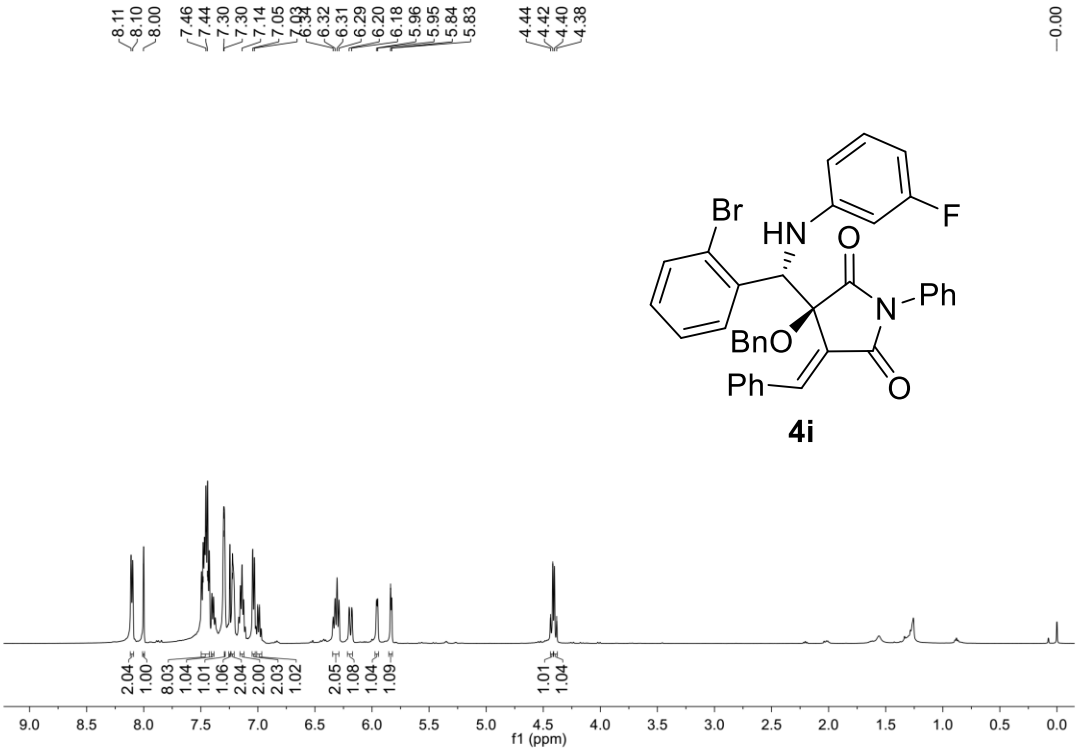
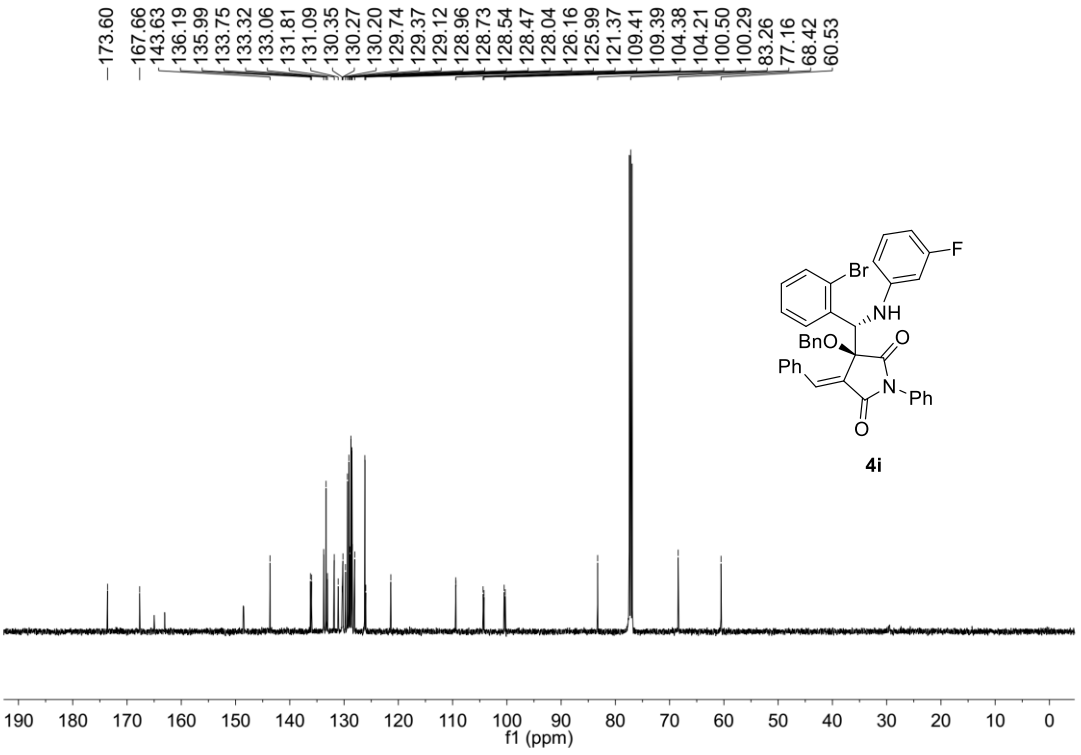
167.72
157.04
155.17
143.42
136.08
133.68
133.29
131.70
130.10
129.31
129.09
128.92
128.70
128.51
128.42
128.01
126.18
115.78
115.60
114.58
114.52
83.61
77.41
77.16
76.91
68.38
61.30
129.31
129.09
128.92
128.70
128.51
128.42
129.4
129.0
128.6
f1 (ppm)
F
Br
NH
BnO
O
Ph
N
Ph
O
4h
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

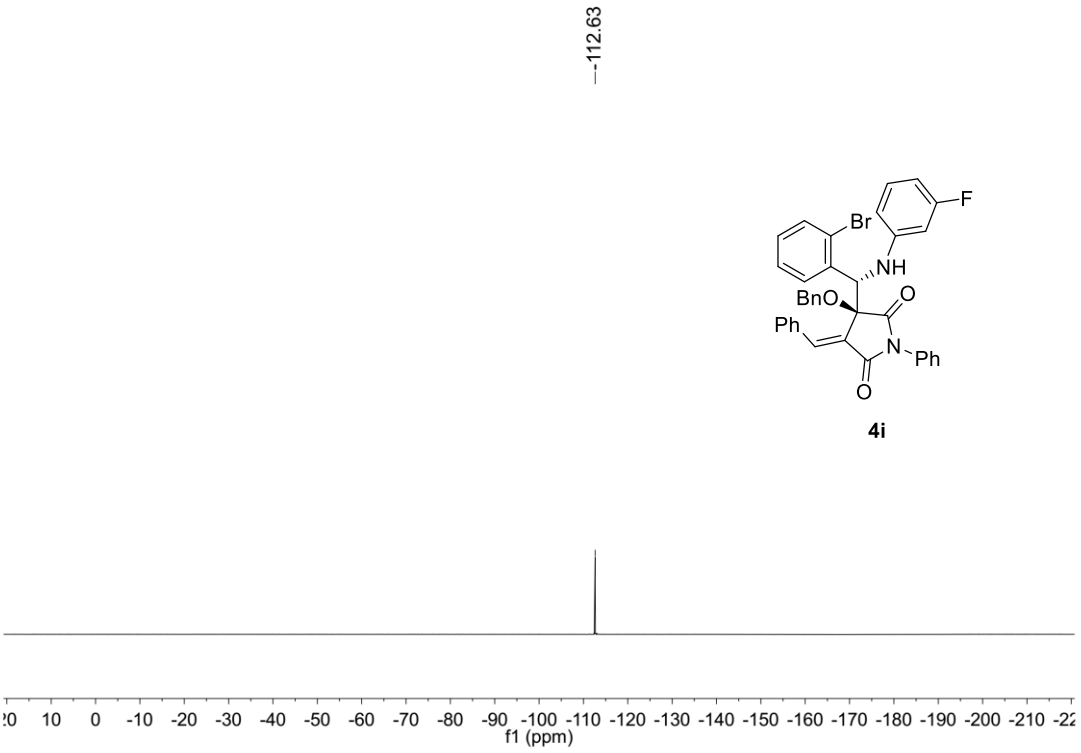

F
Br
NH
BnO
O
Ph
N
Ph
O

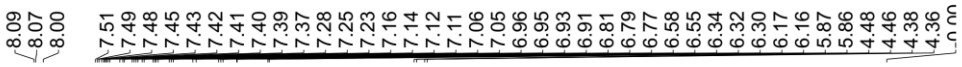
**4h**

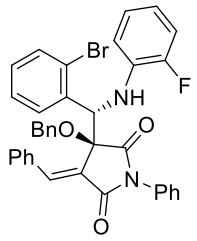

-127.67
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


8.11
8.10
8.00
7.46
7.44
7.30
7.30
7.14
7.05
6.32
6.31
6.29
6.20
6.18
5.96
5.95
5.84
5.83
4.44
4.42
4.40
4.38
0.00
Br
HN
F
O
N
Ph
BnO
Ph
O
4i
2.04
1.00
8.03
1.04
1.01
1.06
2.04
2.00
2.03
1.02
2.05
1.08
1.04
1.09
1.01
1.04
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

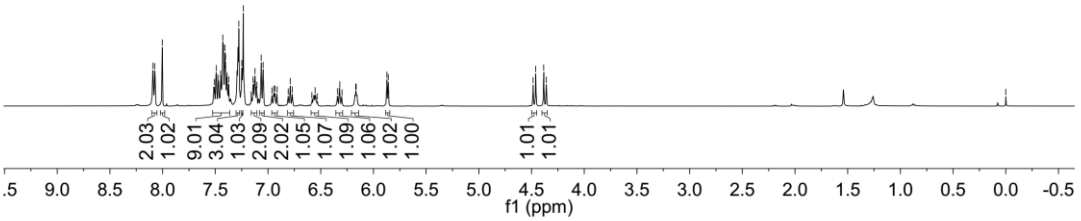

173.60
167.66
143.63
136.19
135.99
133.75
133.32
133.06
131.81
131.09
130.35
130.27
130.20
129.74
129.37
129.12
128.96
128.73
128.54
128.47
128.04
126.16
125.99
121.37
109.41
109.39
104.38
104.21
100.50
100.29
83.26
77.16
68.42
60.53
F
Br
NH
BnO
O
Ph
N
Ph
O
4i
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

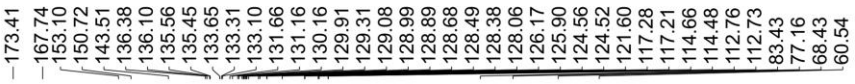

-112.63
Br
F
NH
BnO
O
Ph
N
Ph
O
4i
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

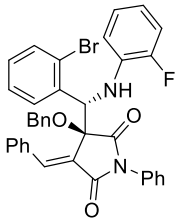

8.09
8.07
8.00
7.51
7.49
7.48
7.45
7.43
7.42
7.41
7.40
7.39
7.37
7.28
7.25
7.23
7.16
7.14
7.12
7.11
7.06
7.05
6.96
6.95
6.93
6.91
6.81
6.79
6.77
6.58
6.55
6.34
6.32
6.30
6.17
6.16
5.87
5.86
4.48
4.46
4.38
4.36


Br
F
NH
BnO
O
Ph
N
Ph
O

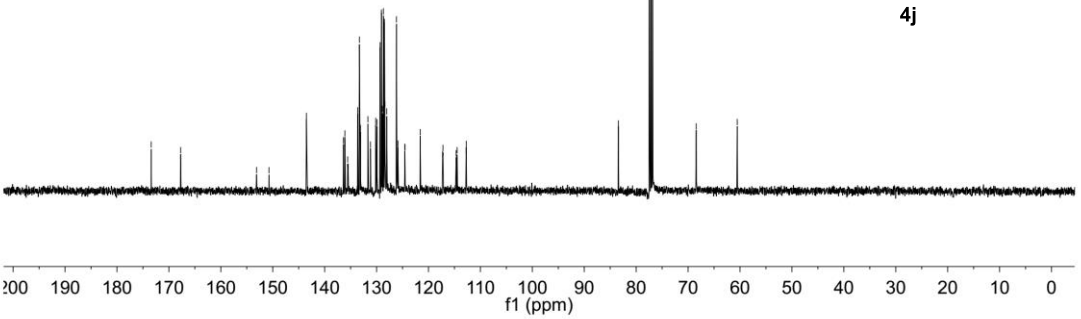
**4j**

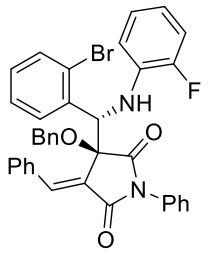

2.03
1.02
9.01
3.04
1.03
2.09
2.02
1.05
1.07
1.09
1.06
1.02
1.00
1.01
1.01
f1 (ppm)


173.41
167.74
153.10
150.72
143.51
136.38
136.10
135.56
135.45
133.65
133.31
133.10
131.66
131.16
130.16
129.91
129.31
129.08
128.99
128.89
128.68
128.49
128.38
128.06
126.17
125.90
124.56
124.52
121.60
117.28
117.21
114.66
114.48
112.76
112.73
83.43
77.16
68.43
60.54


Br
F
NH
BnO
O
Ph
N
Ph
O

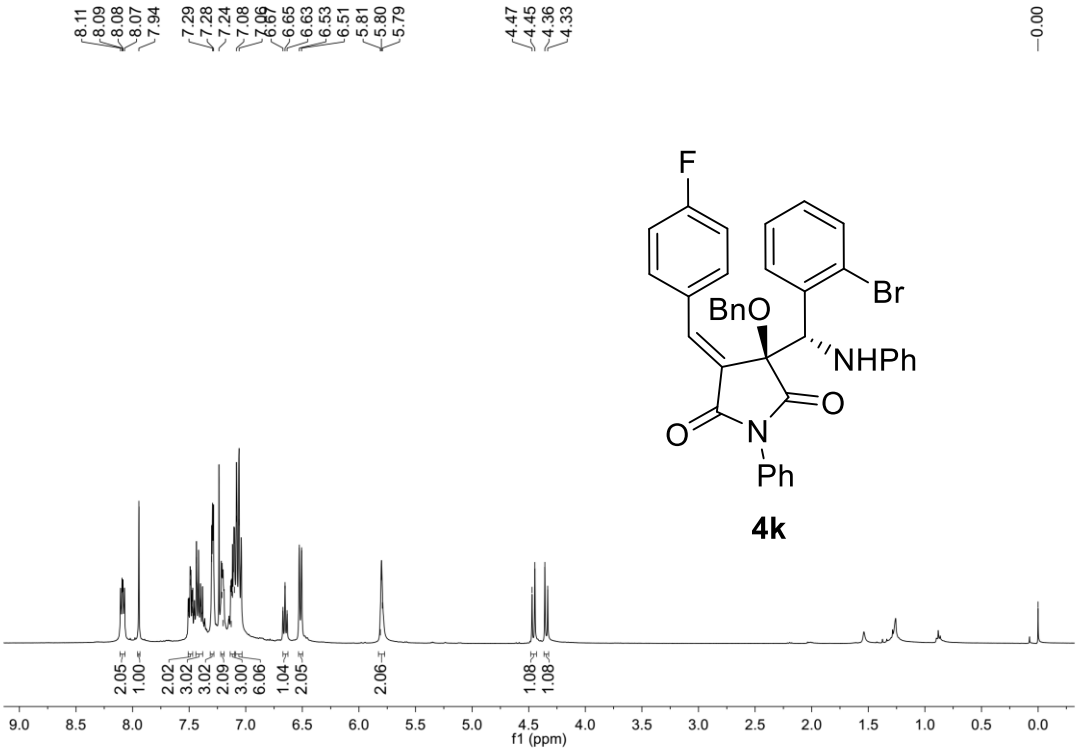
**4j**

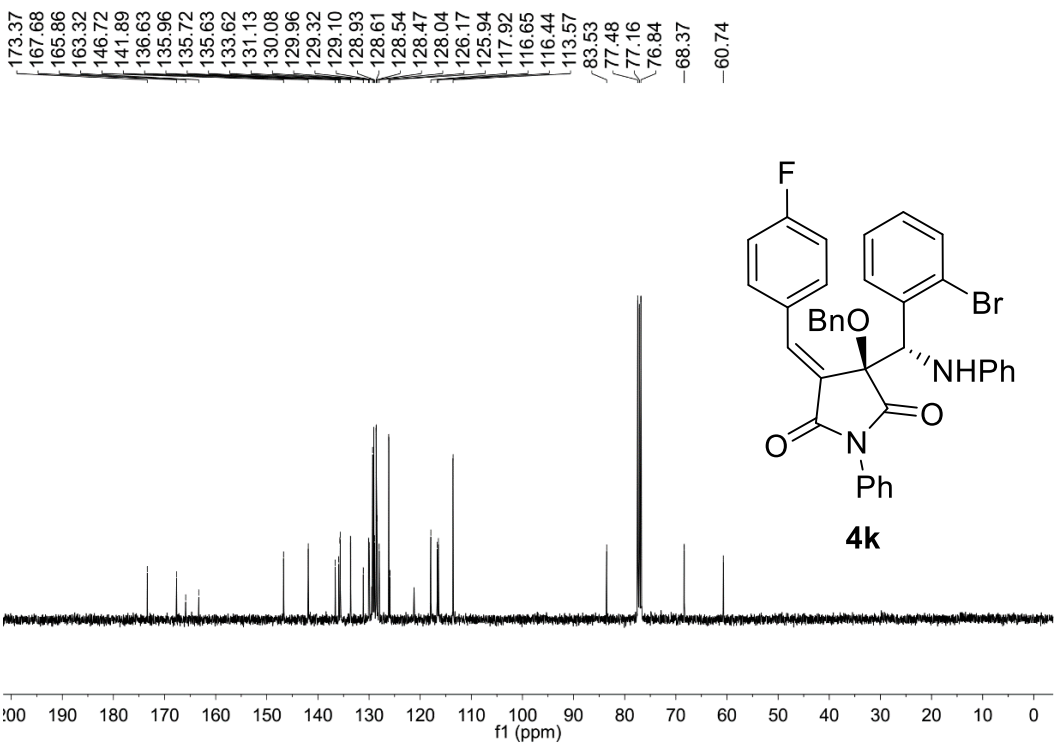

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

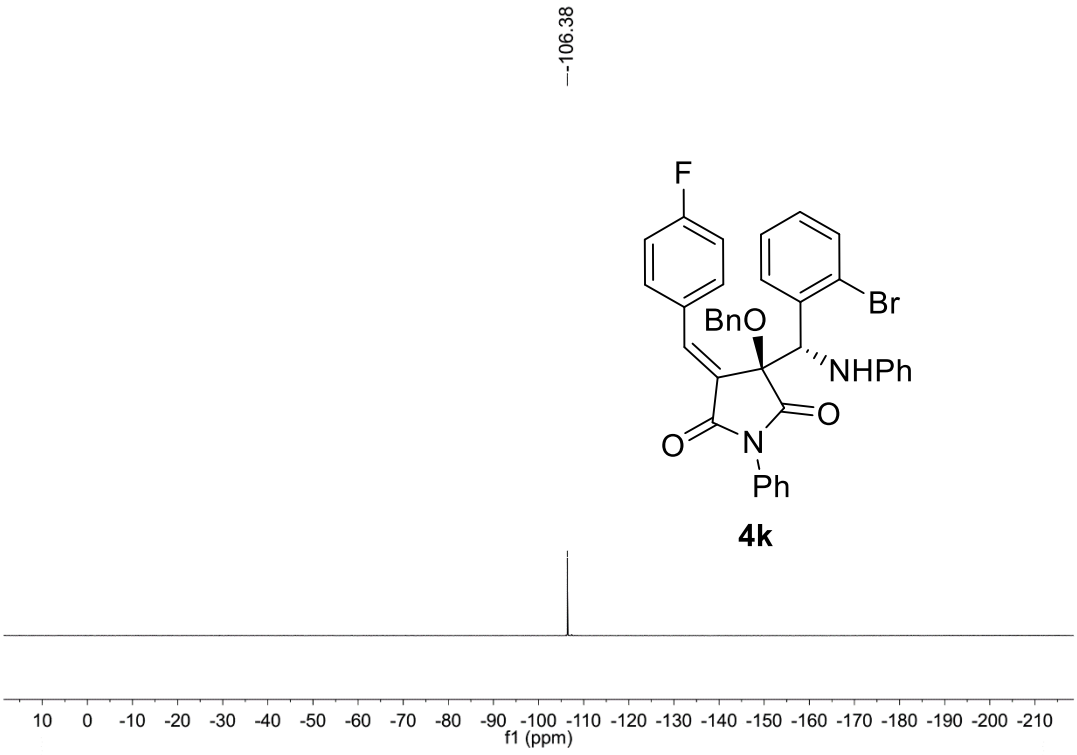

Br
F
NH
BnO
O
Ph
N
Ph
O

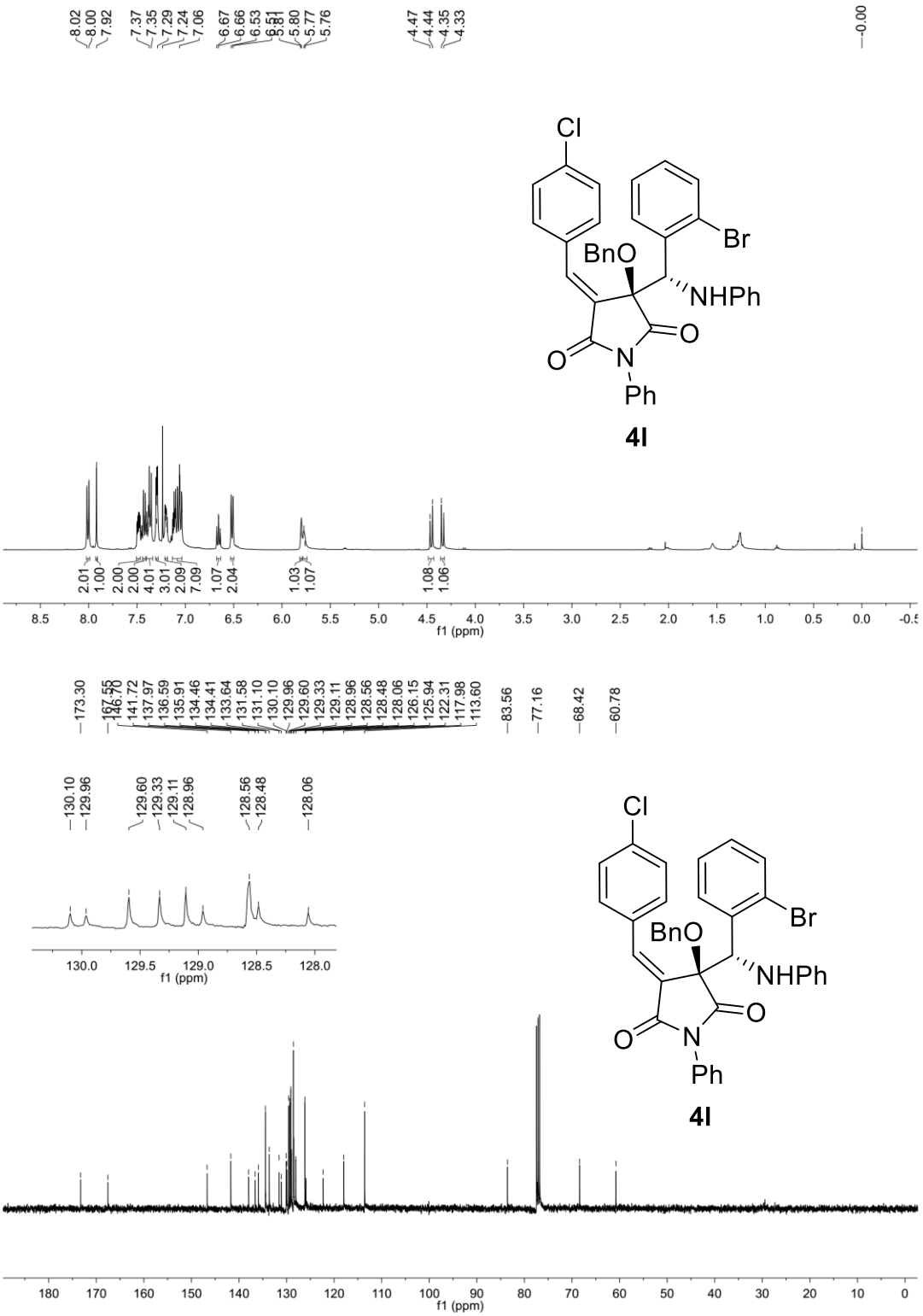
**4j**

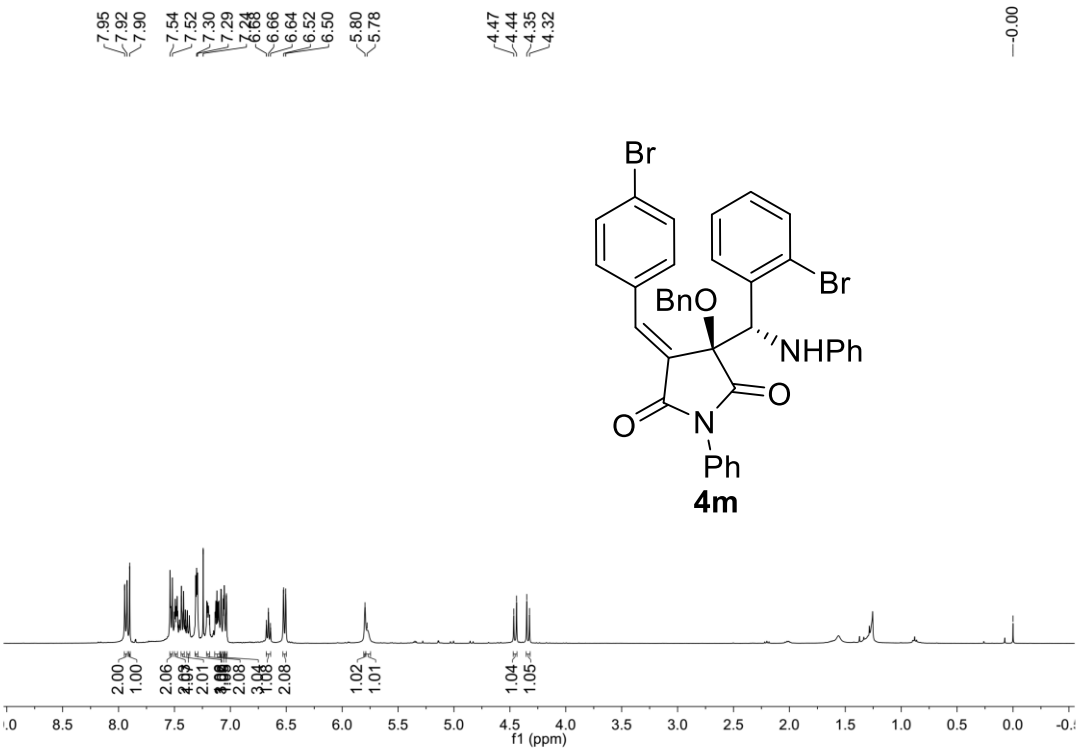

135.40
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


8.11
8.09
8.08
8.07
7.94
7.29
7.28
7.24
7.08
7.06
6.67
6.65
6.63
6.53
6.51
5.81
5.80
5.79
4.47
4.45
4.36
4.33
0.00
F
Br
BnO
NHPh
O
O
N
Ph
4k
2.05
1.00
2.02
3.02
3.02
2.09
3.00
6.06
1.04
2.05
2.06
1.08
1.08
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


173.37
167.68
165.86
163.32
146.72
141.89
136.63
135.96
135.72
135.63
133.62
131.13
130.08
129.96
129.32
129.10
128.93
128.61
128.54
128.47
128.04
126.17
125.94
117.92
116.65
116.44
113.57
83.53
77.48
77.16
76.84
68.37
60.74
F
Br
BnO
NHPh
O
O
N
Ph
4k
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-106.38
F
Br
BnO
NHPh
O
O
N
Ph
4k
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


8.02
8.00
7.92
7.37
7.35
7.29
7.24
7.06
6.67
6.66
6.53
6.51
5.81
5.80
5.77
5.76
4.47
4.44
4.35
4.33
0.00
Cl
Br
BnO
NHPh
O
O
N
Ph
4l
2.01
1.00
2.00
2.00
4.01
3.01
2.09
7.09
1.07
2.04
1.03
1.07
1.08
1.06
f1 (ppm)
173.30
167.55
166.70
141.72
137.97
136.59
135.91
134.46
134.41
133.64
131.58
131.10
130.10
129.96
129.60
129.33
129.11
128.96
128.56
128.48
128.06
126.15
125.94
122.31
117.98
113.60
83.56
77.16
68.42
60.78
f1 (ppm)
Cl
Br
BnO
NHPh
O
O
N
Ph
4l
f1 (ppm)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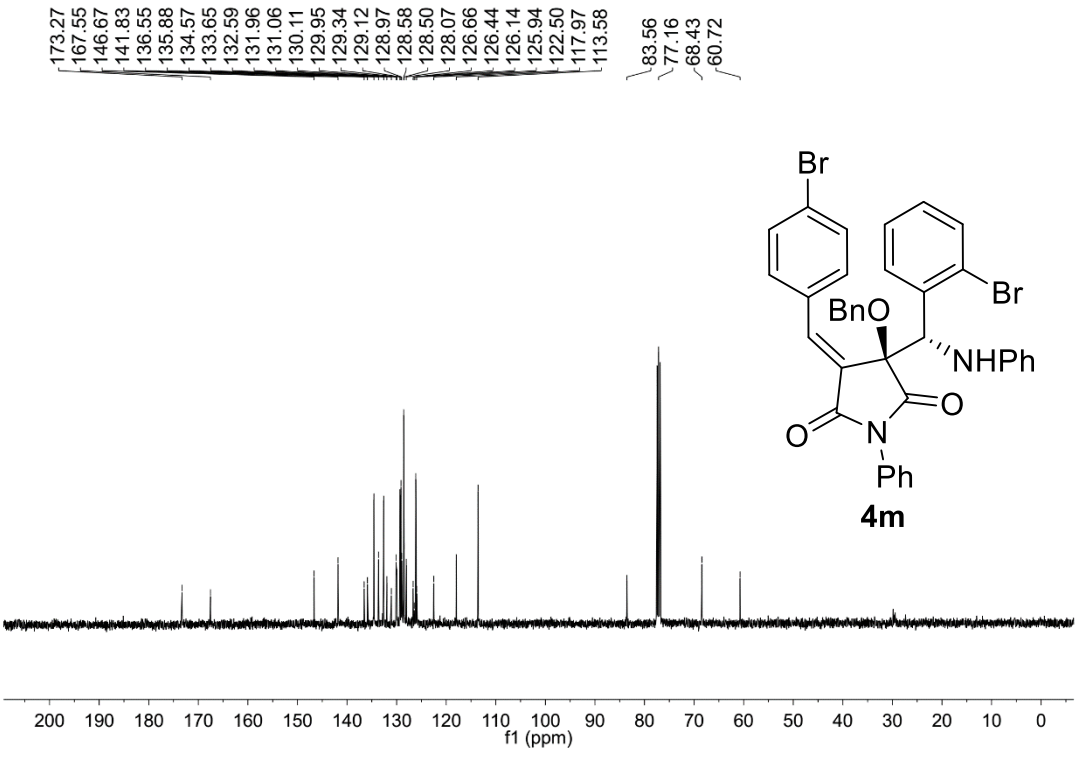
7.92
7.90
7.54
7.52
7.30
7.29
6.66
6.64
6.52
6.50
5.80
5.78
4.47
4.44
4.35
4.32
0.00
Br
Br
BnO
NHPh
O
O
N
Ph
4m
f1 (ppm)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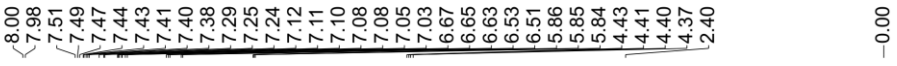
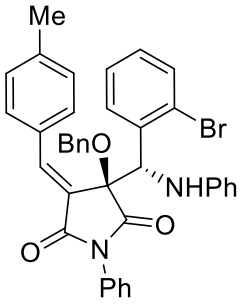
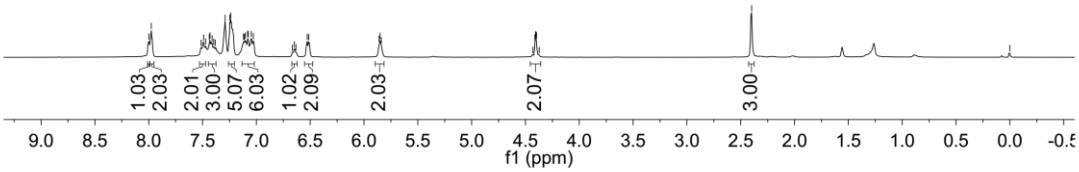
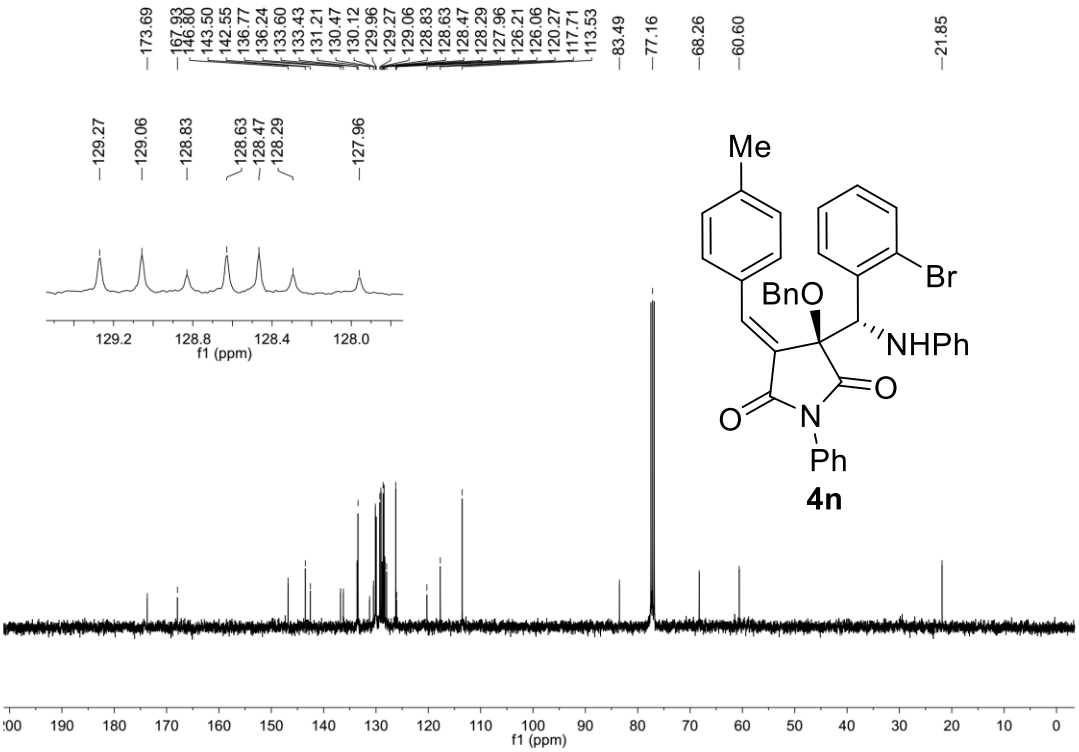
167.55
146.67
141.83
136.55
135.88
134.57
133.65
132.59
131.96
131.06
130.11
129.95
129.34
129.12
128.97
128.58
128.50
128.07
126.66
126.44
126.14
125.94
122.50
117.97
113.58
83.56
77.16
68.43
60.72
Br
Br
BnO
NHPh
O
O
N
Ph
4m
f1 (ppm)


8.00
7.98
7.51
7.49
7.47
7.44
7.43
7.41
7.40
7.38
7.29
7.25
7.24
7.12
7.11
7.10
7.08
7.08
7.05
7.03
6.67
6.65
6.63
6.53
6.51
5.86
5.85
5.84
4.43
4.41
4.40
4.37
2.40
0.00


Me
Br
BnO
NHPh
O
O
N
Ph

**4n**


1.03
2.03
2.01
3.00
5.07
6.03
1.02
2.09
2.03
2.07
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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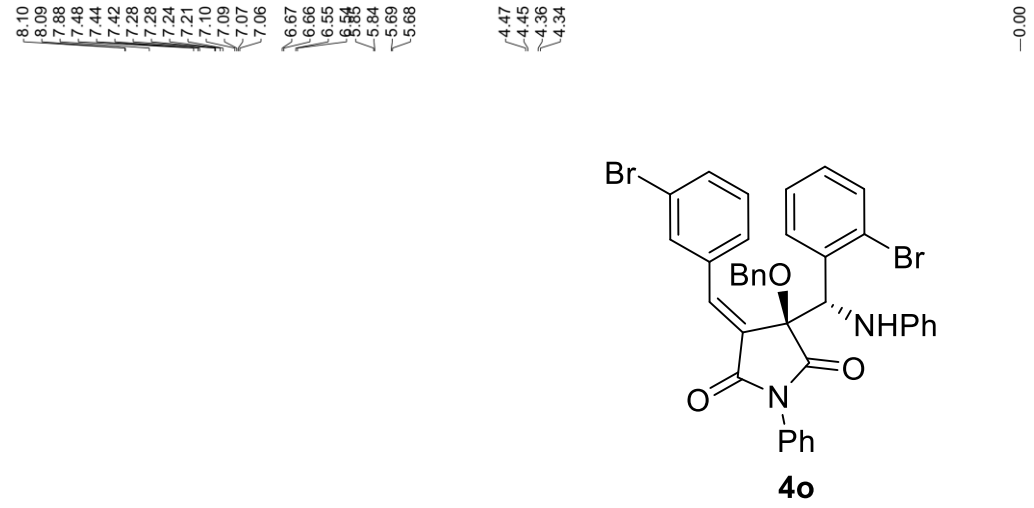
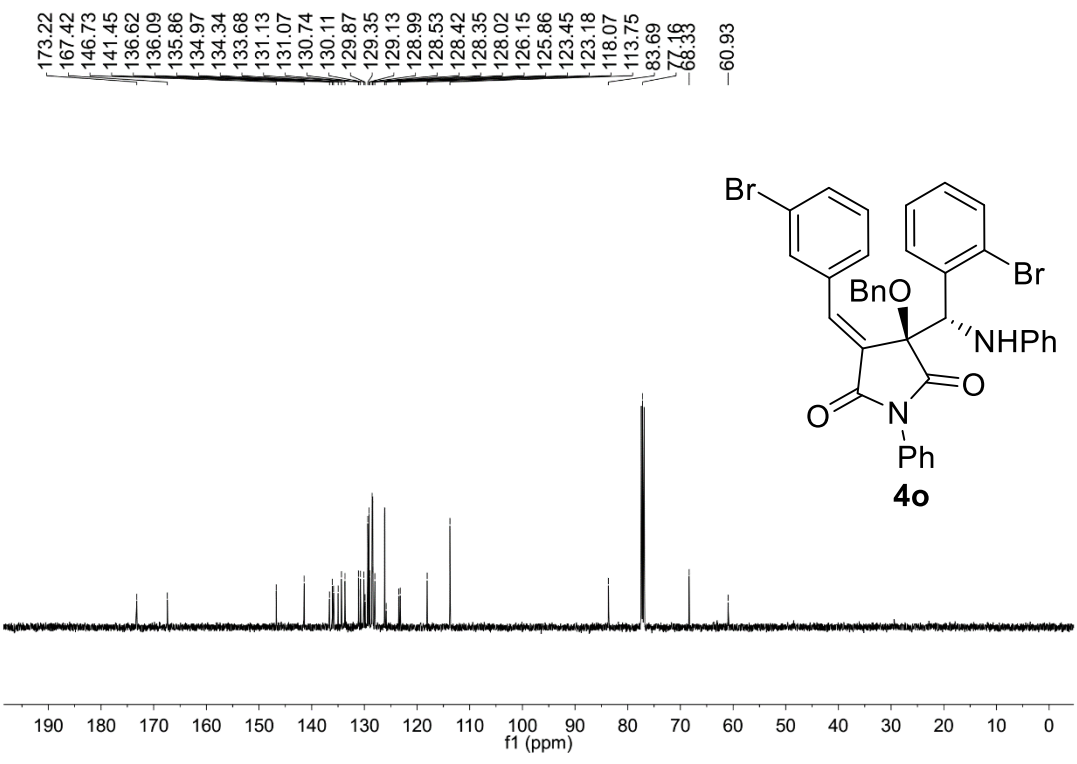
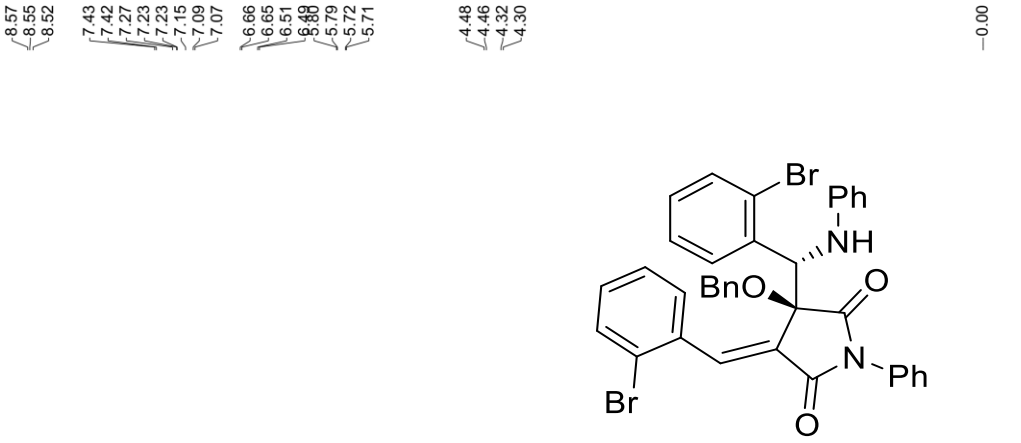
167.93
146.80
143.50
142.55
136.77
136.24
133.60
133.43
131.21
130.47
130.12
129.96
129.27
129.06
128.83
128.63
128.47
128.29
127.96
126.21
126.06
120.27
117.71
113.53
83.49
77.16
68.26
60.60
21.85
129.27
129.06
128.83
128.63
128.47
128.29
127.96
129.2 128.8 128.4 128.0
f1 (ppm)
Me
Br
BnO
NHPh
O
O
N
Ph
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

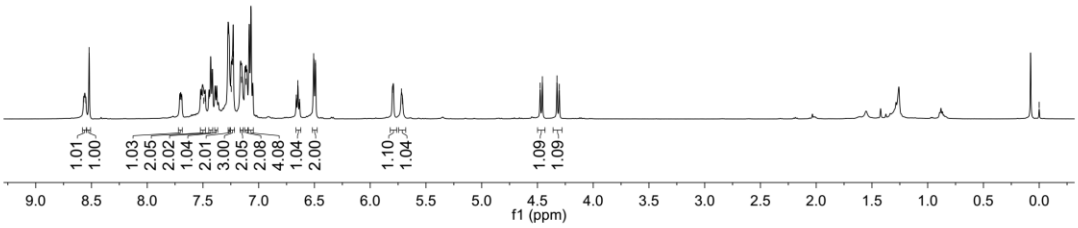
**4n**

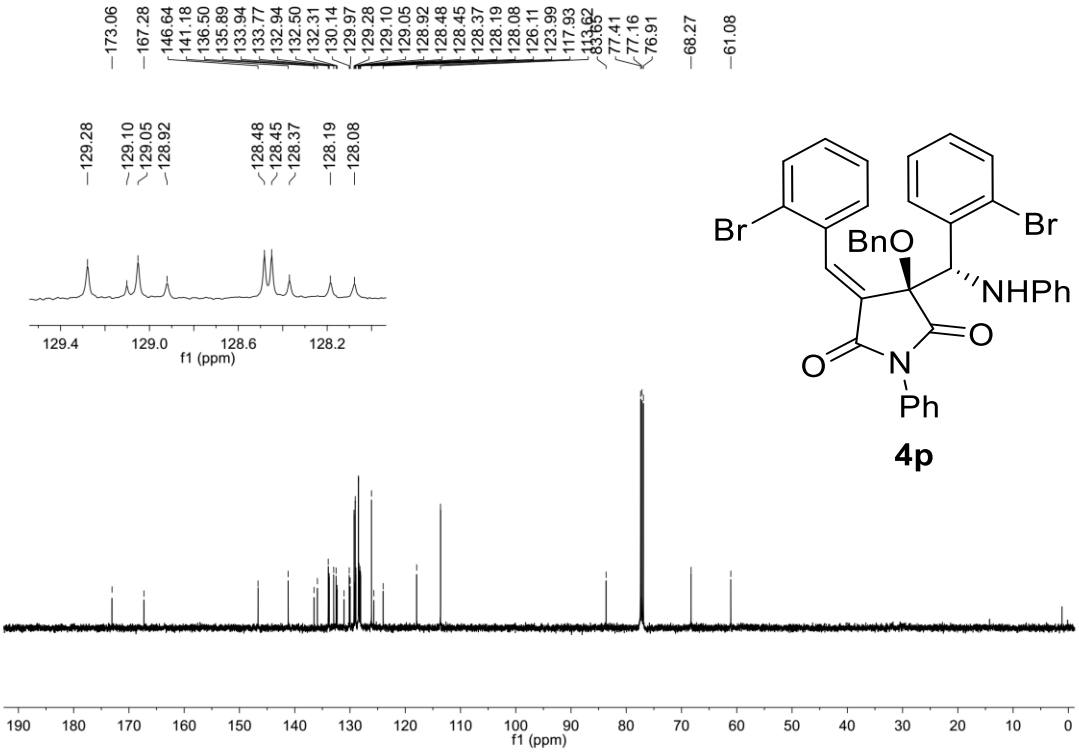

8.10
8.09
7.88
7.48
7.44
7.42
7.28
7.28
7.24
7.21
7.10
7.09
7.07
7.06
6.67
6.66
6.55
6.54
5.84
5.69
5.68
4.47
4.45
4.36
4.34
0.00
Br
Br
BnO
NHPh
O
O
N
Ph
4o
2.05
1.00
1.08
7.02
2.06
2.04
6.06
1.02
2.04
1.04
1.02
1.03
1.02
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


173.22
167.42
146.73
141.45
136.62
136.09
135.86
134.97
134.34
133.68
131.13
131.07
130.74
130.11
129.87
129.35
129.13
128.99
128.53
128.42
128.35
128.02
126.15
125.86
123.45
123.18
118.07
113.75
83.69
77.16
68.33
60.93
Br
Br
BnO
NHPh
O
O
N
Ph
4o
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



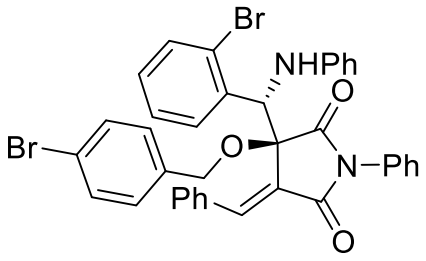

**4p**



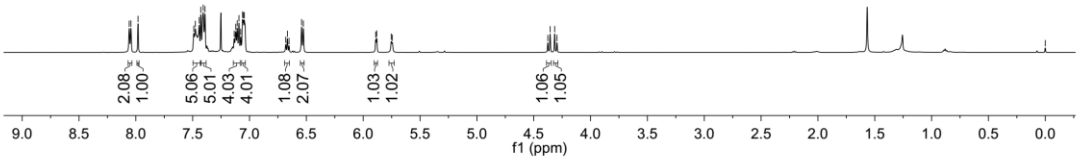



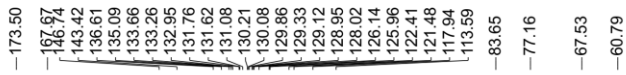

**4p**

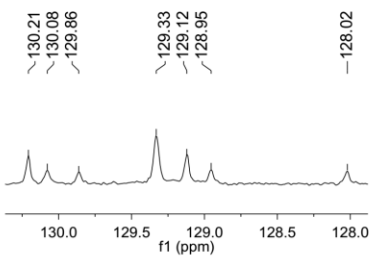

8.06
8.04
7.98
7.43
7.41
7.39
7.06
7.05
6.68
6.67
6.54
5.88
5.75
5.74
4.38
4.36
4.32
4.30
0.00

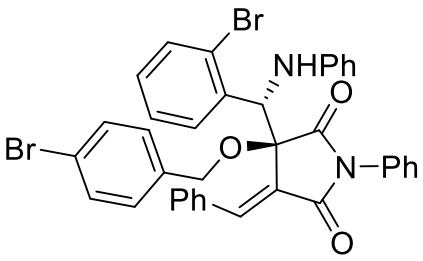

Br
NHPh
O
Br
O
N–Ph
Ph
O

**4q**

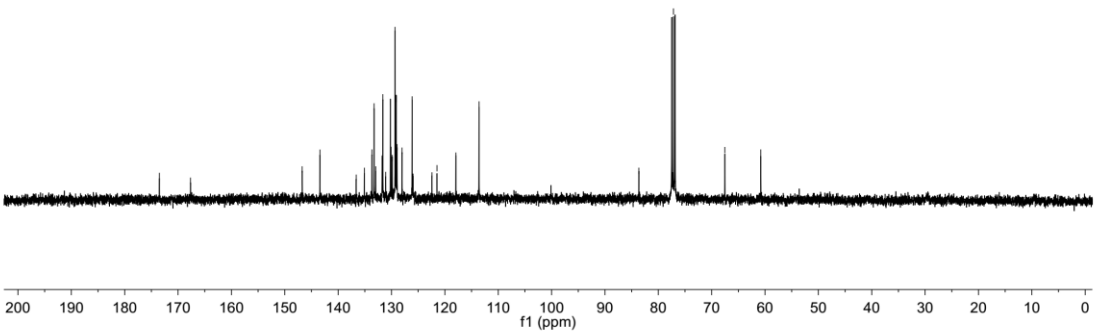

2.08
1.00
5.06
5.01
4.03
4.01
1.08
2.07
1.03
1.02
1.06
1.05
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

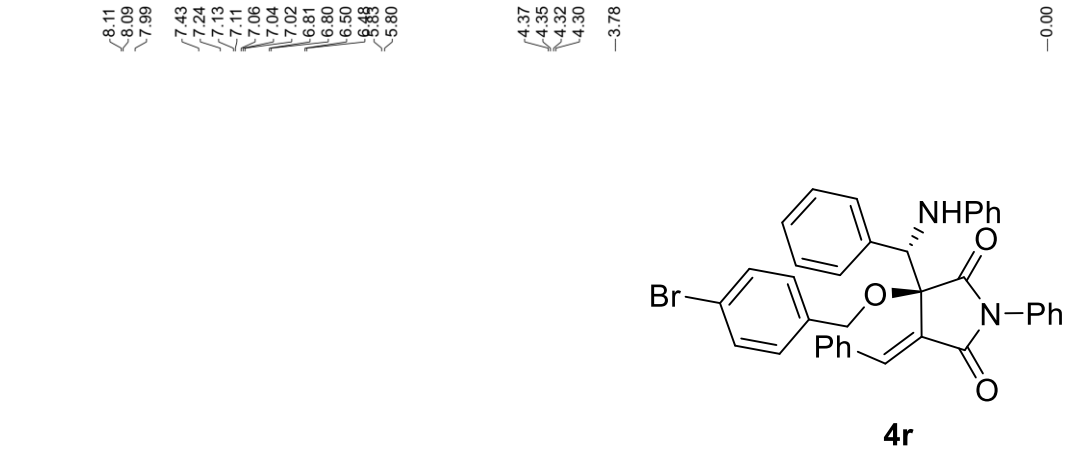

173.50
167.67
146.74
143.42
136.61
135.09
133.66
133.26
132.95
131.76
131.62
131.08
130.21
130.08
129.86
129.33
129.12
128.95
128.02
126.14
125.96
122.41
121.48
117.94
113.59
83.65
77.16
67.53
60.79

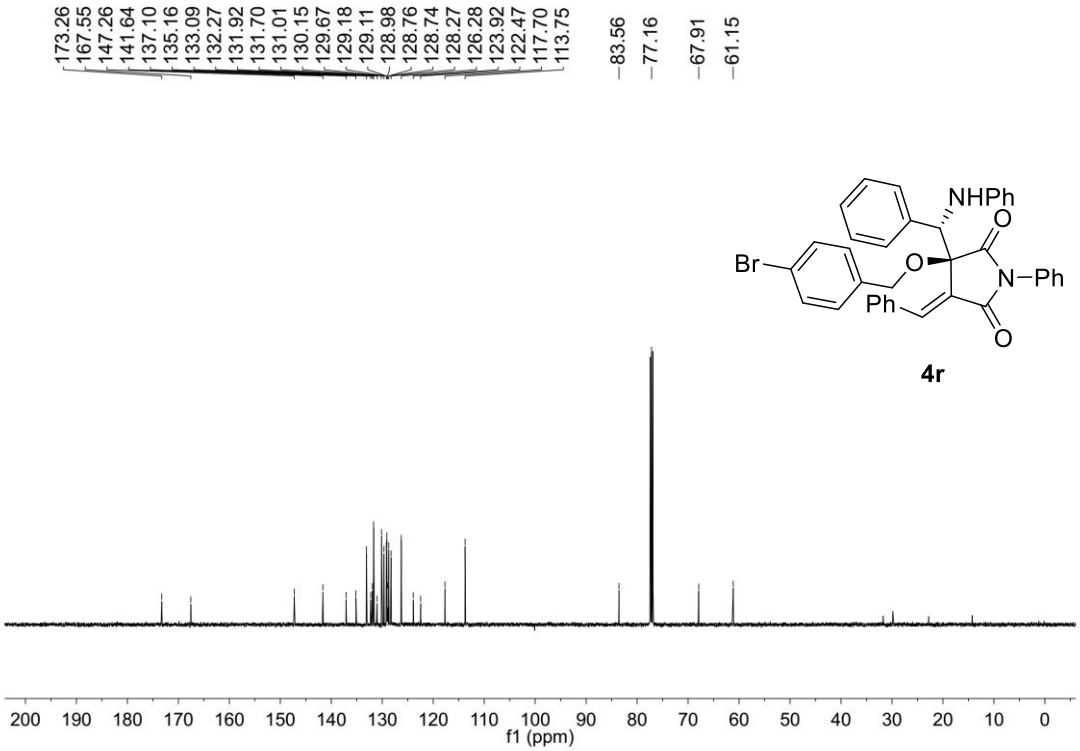

130.21
130.08
129.86
129.33
129.12
128.95
128.02
130.0 129.5 129.0 128.5 128.0
f1 (ppm)


Br
NHPh
O
Br
O
N–Ph
Ph
O

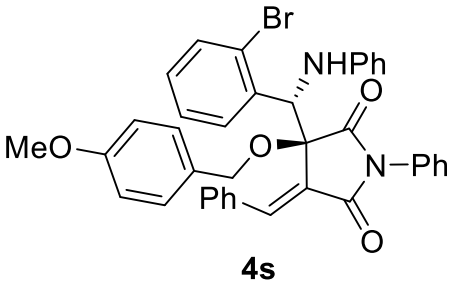
**4q**


200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

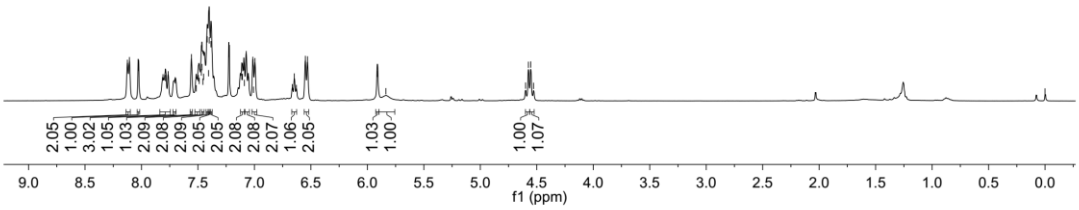

8.11
8.09
7.99
7.43
7.24
7.13
7.11
7.06
7.04
7.02
6.81
6.80
6.50
5.83
5.80
4.37
4.35
4.32
4.30
3.78
0.00
NHPh
O
Br
O
N–Ph
Ph
O
4r
2.08
1.01
8.01
8.05
2.08
1.07
2.02
2.00
1.01
1.01
3.04
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

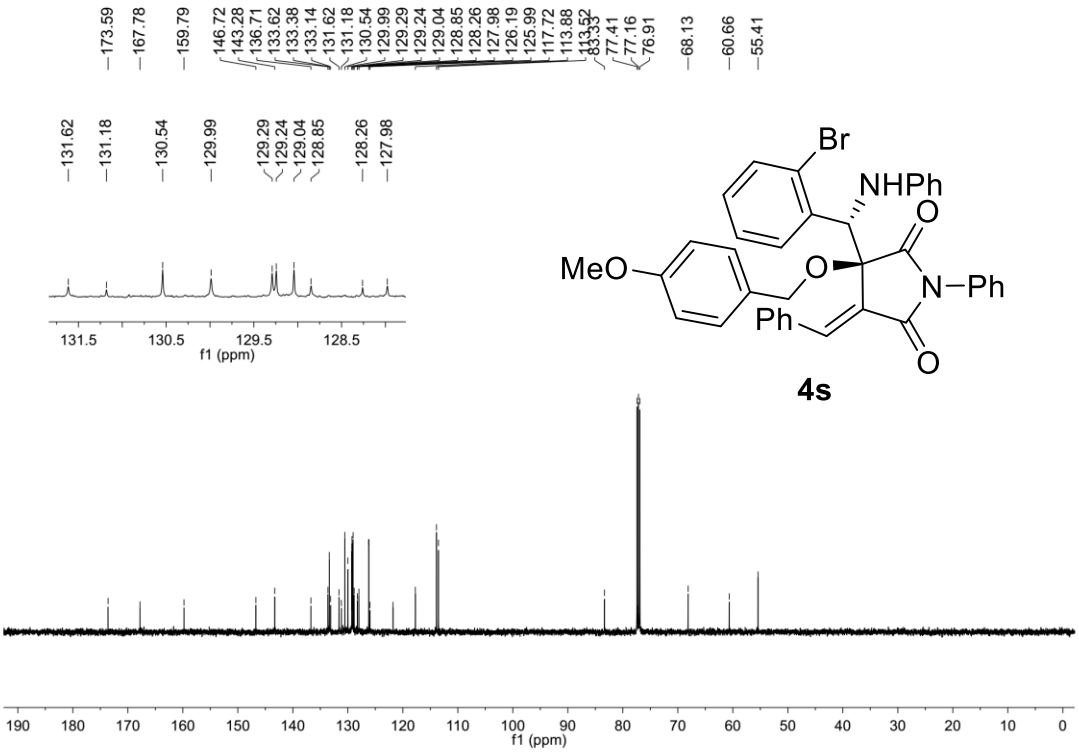

173.26
167.55
147.26
141.64
137.10
135.16
133.09
132.27
131.92
131.70
131.01
130.15
129.67
129.18
129.11
128.98
128.76
128.74
128.27
126.28
123.92
122.47
117.70
113.75
83.56
77.16
67.91
61.15
NHPh
O
Br
O
N–Ph
Ph
O
4r
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.12
8.11
8.03
7.56
7.47
7.46
7.42
7.40
7.38
7.23
7.09
7.07
7.01
7.00
6.66
6.65
6.55
6.53
5.84
4.60
4.57
4.55
4.53
0.00


Br
NHPh
O
MeO
O
N–Ph
Ph
O

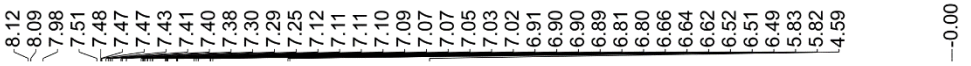
**4s**

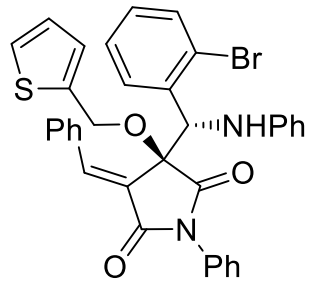

2.05
1.00
3.02
1.05
1.03
2.09
2.08
2.09
2.05
2.05
2.08
2.08
2.07
1.06
2.05
1.03
1.00
1.00
1.07
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


173.59
167.78
159.79
146.72
143.28
136.71
133.62
133.38
133.14
131.62
131.18
130.54
129.99
129.29
129.24
129.04
128.85
128.26
127.98
126.19
125.99
117.72
113.88
113.52
83.33
77.41
77.16
76.91
68.13
60.66
55.41
131.62
131.18
130.54
129.99
129.29
129.24
129.04
128.85
128.26
127.98
131.5
130.5
129.5
128.5
f1 (ppm)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

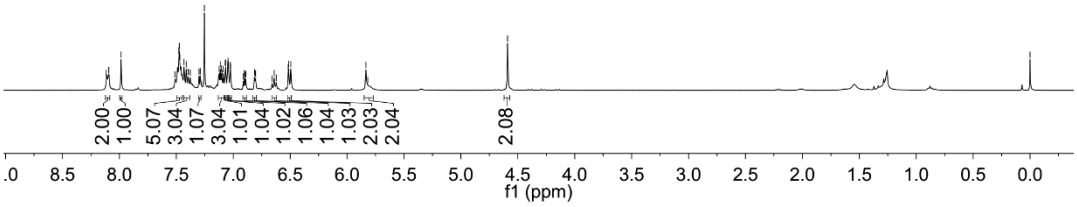

Br
NHPh
O
MeO
O
N–Ph
Ph
O

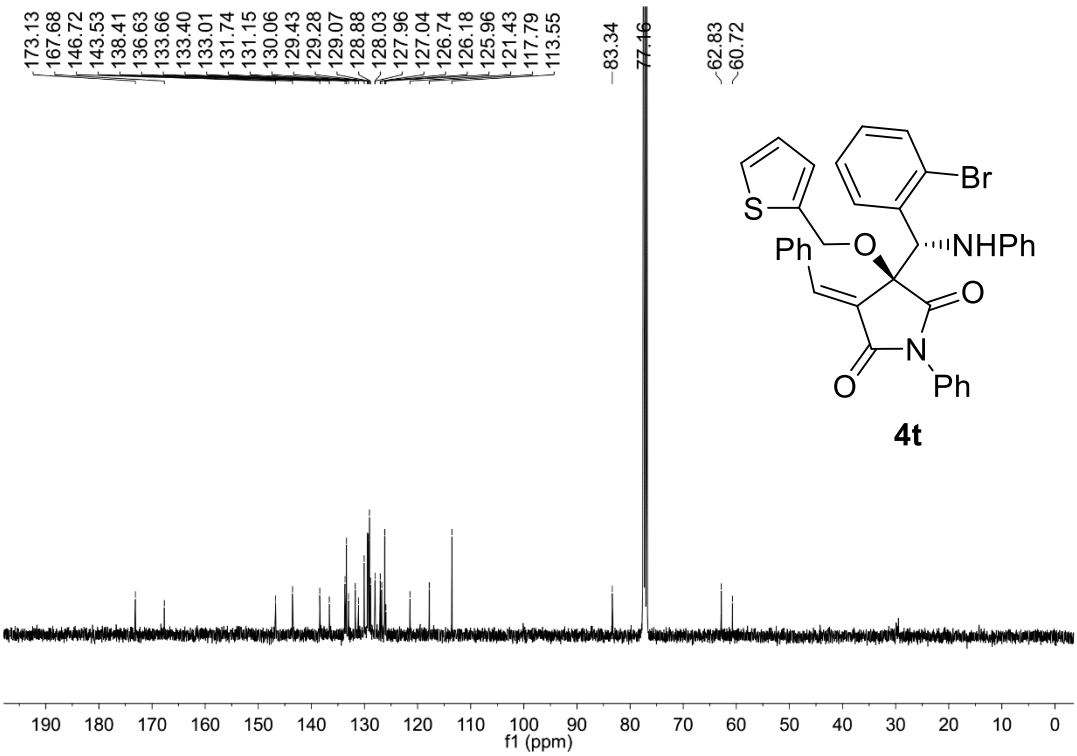
**4s**


8.12
8.09
7.98
7.51
7.48
7.47
7.47
7.43
7.41
7.40
7.38
7.30
7.29
7.25
7.12
7.11
7.11
7.10
7.09
7.07
7.07
7.05
7.03
7.02
6.91
6.90
6.90
6.89
6.81
6.80
6.66
6.64
6.62
6.52
6.51
6.49
5.83
5.82
4.59
0.00


Br
S
Ph
O
NHPh
O
N
O
Ph

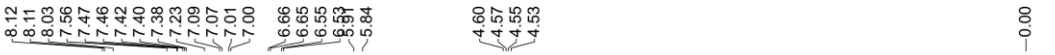
**4t**

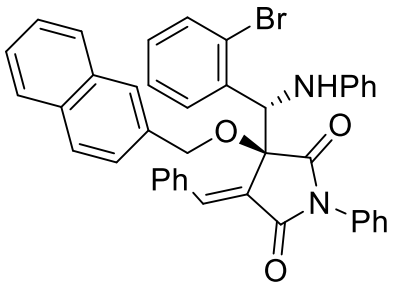

2.00
1.00
5.07
3.04
1.07
3.04
1.01
1.04
1.02
1.06
1.04
1.03
2.03
2.04
2.08
f1 (ppm)


173.13
167.68
146.72
143.53
138.41
136.63
133.66
133.40
133.01
131.74
131.15
130.06
129.43
129.28
129.07
128.88
128.03
127.96
127.04
126.74
126.18
125.96
121.43
117.79
113.55
83.34
77.16
62.83
60.72
f1 (ppm)

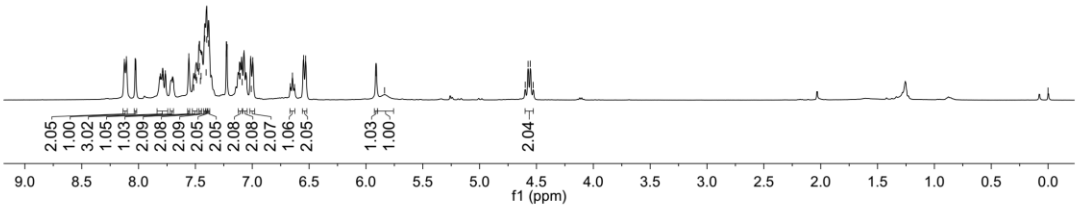

Br
S
Ph
O
NHPh
O
N
O
Ph

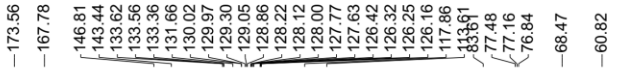
**4t**


8.12
8.11
8.03
7.56
7.47
7.46
7.42
7.40
7.38
7.23
7.09
7.07
7.01
7.00
6.66
6.65
6.55
6.53
5.91
5.84
4.60
4.57
4.55
4.53
0.00


Br
NHPh
O
O
Ph
N
Ph
O

**4u**


2.05
1.00
3.02
1.05
1.03
2.09
2.08
2.09
2.05
2.05
2.08
2.07
1.06
2.05
1.03
1.00
2.04
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


173.56
167.78
146.81
143.44
133.62
133.56
133.36
131.66
130.02
129.97
129.30
129.05
128.86
128.22
128.12
128.00
127.77
127.63
126.42
126.32
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126.16
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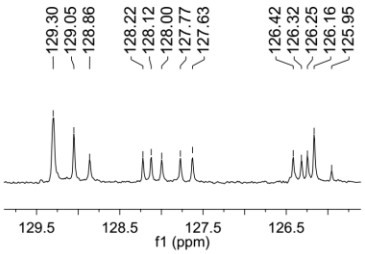
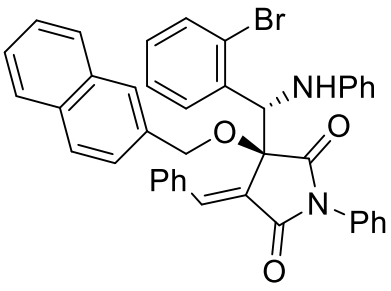
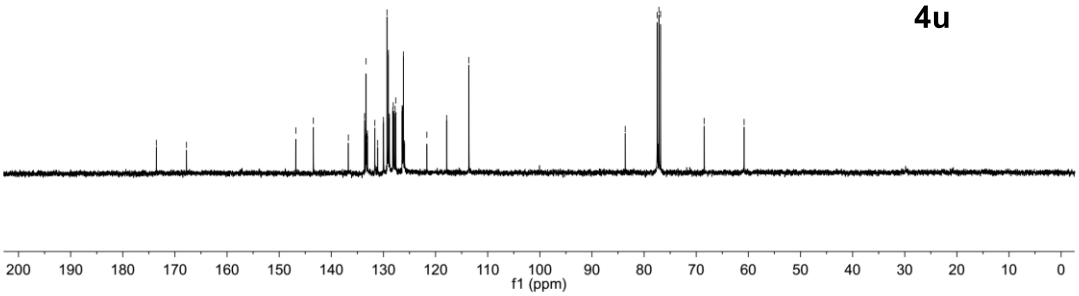
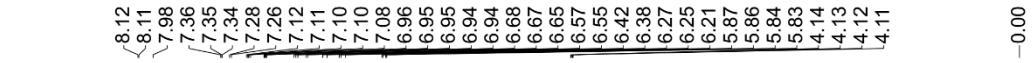
83.61
77.48
77.16
76.84
68.47
60.82


129.30
129.05
128.86
128.22
128.12
128.00
127.77
127.63
126.42
126.32
126.25
126.16
125.95
129.5
128.5
127.5
126.5
f1 (ppm)


Br
NHPh
O
O
Ph
N
Ph
O

**4u**


200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.12
8.11
7.98
7.36
7.35
7.34
7.28
7.26
7.12
7.11
7.10
7.10
7.08
6.96
6.95
6.94
6.94
6.68
6.67
6.65
6.57
6.55
6.42
6.38
6.27
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5.87
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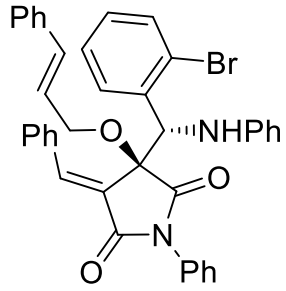
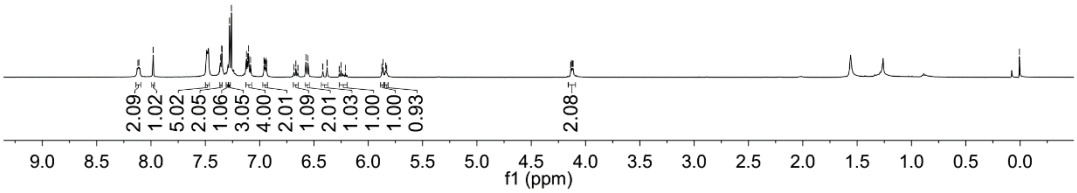
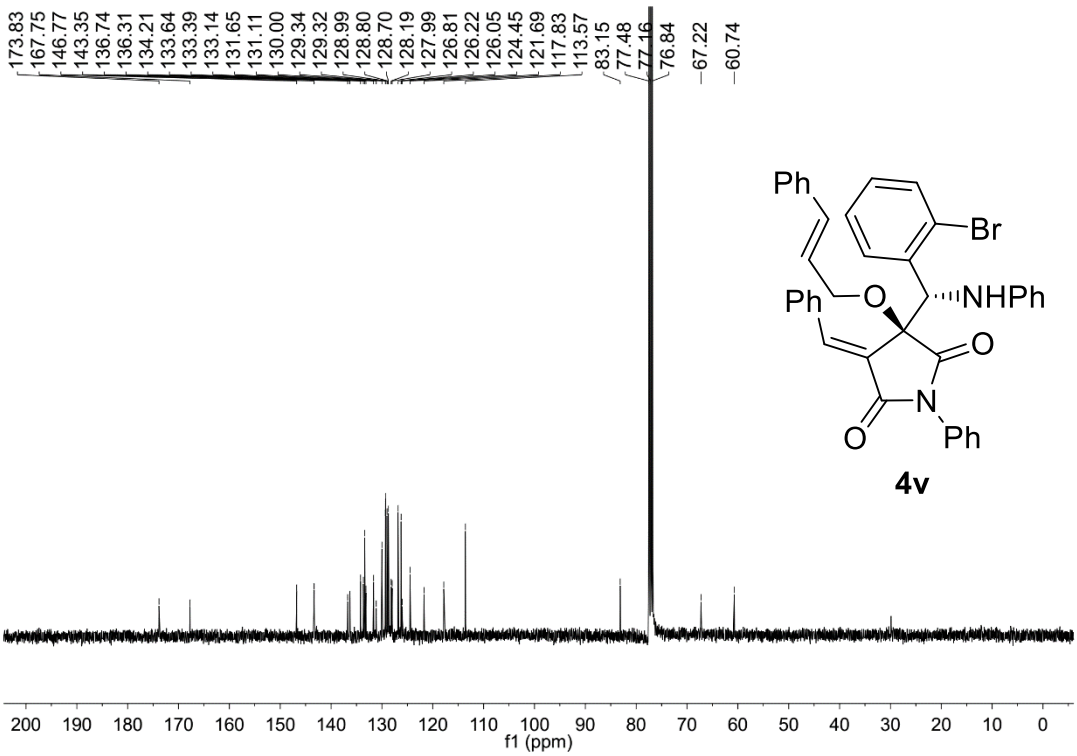
5.83
4.14
4.13
4.12
4.11
0.00


Ph
Br
Ph
O
NHPh
O
N
O
Ph

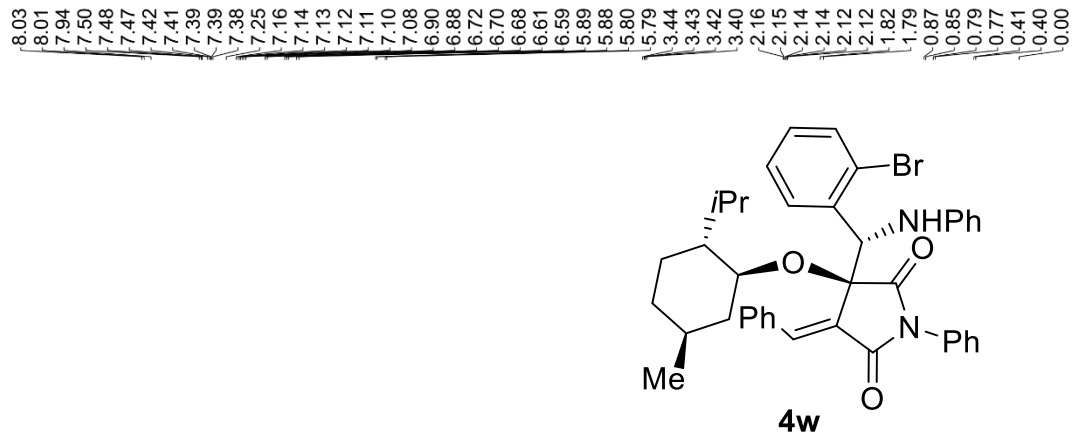
**4v**

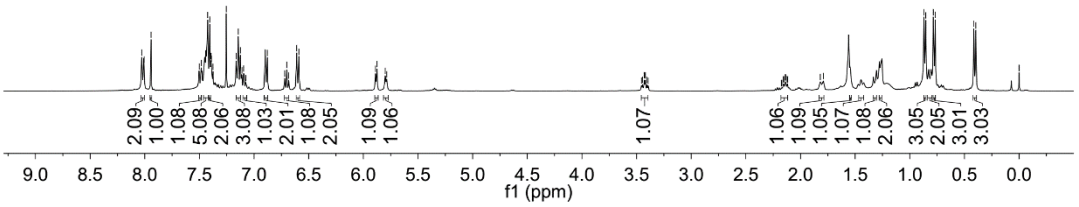

2.09
1.02
5.02
2.05
1.06
3.05
4.00
2.01
1.09
2.01
1.03
1.00
1.00
0.93
2.08
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

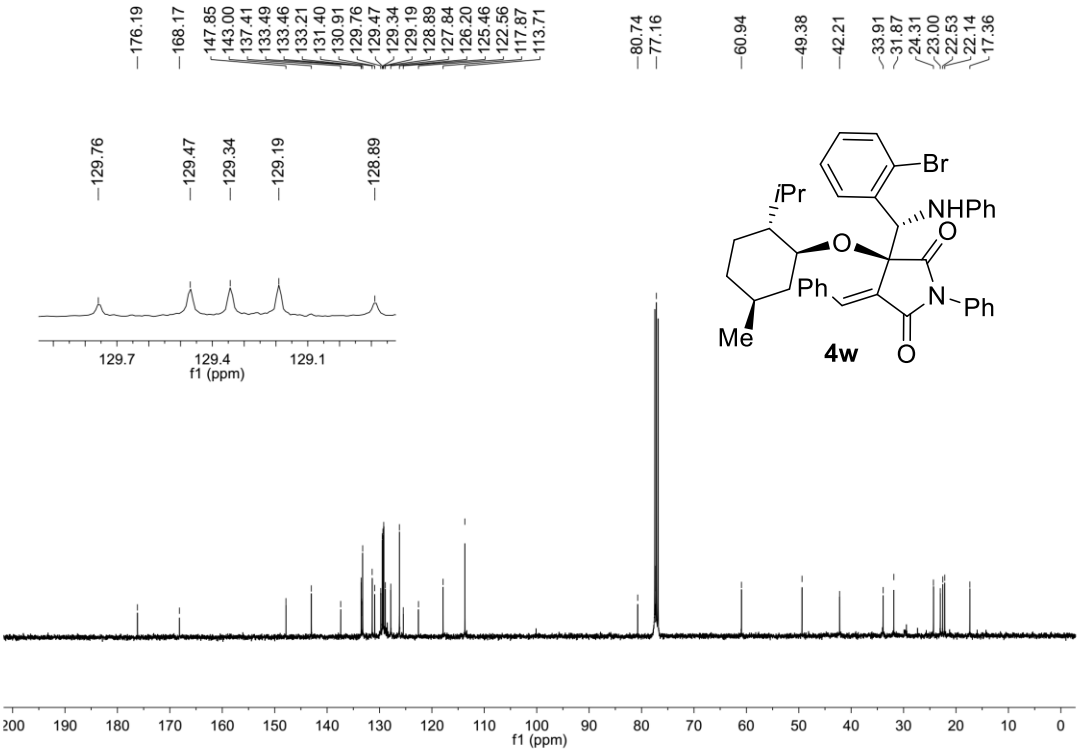

173.83
167.75
146.77
143.35
136.74
136.31
134.21
133.64
133.39
133.14
131.65
131.11
130.00
129.34
129.32
128.99
128.80
128.70
128.19
127.99
126.81
126.22
126.05
124.45
121.69
117.83
113.57
83.15
77.48
77.16
76.84
67.22
60.74
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

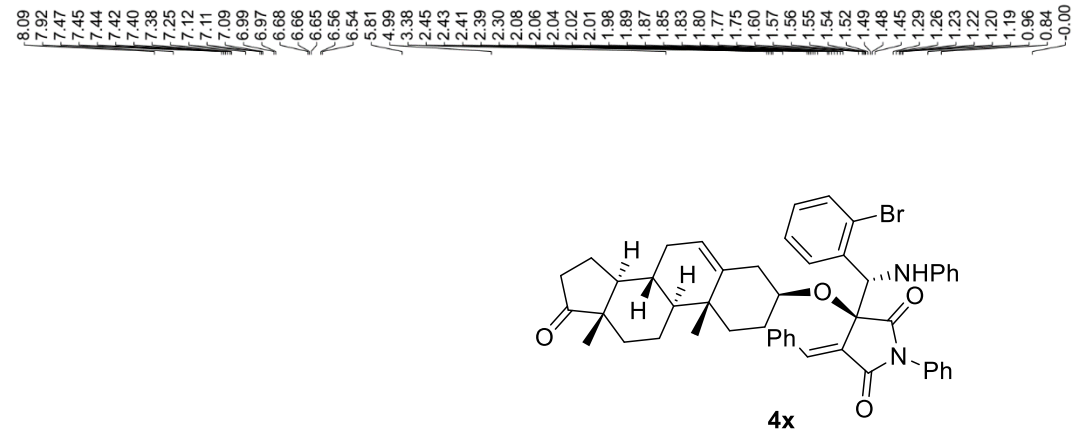

Ph
Br
Ph
O
NHPh
O
N
O
Ph

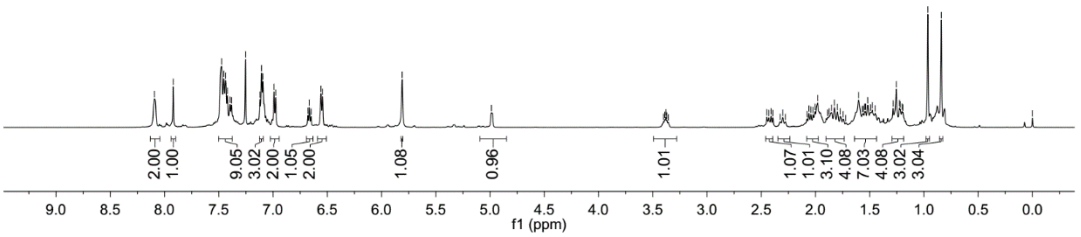
**4v**

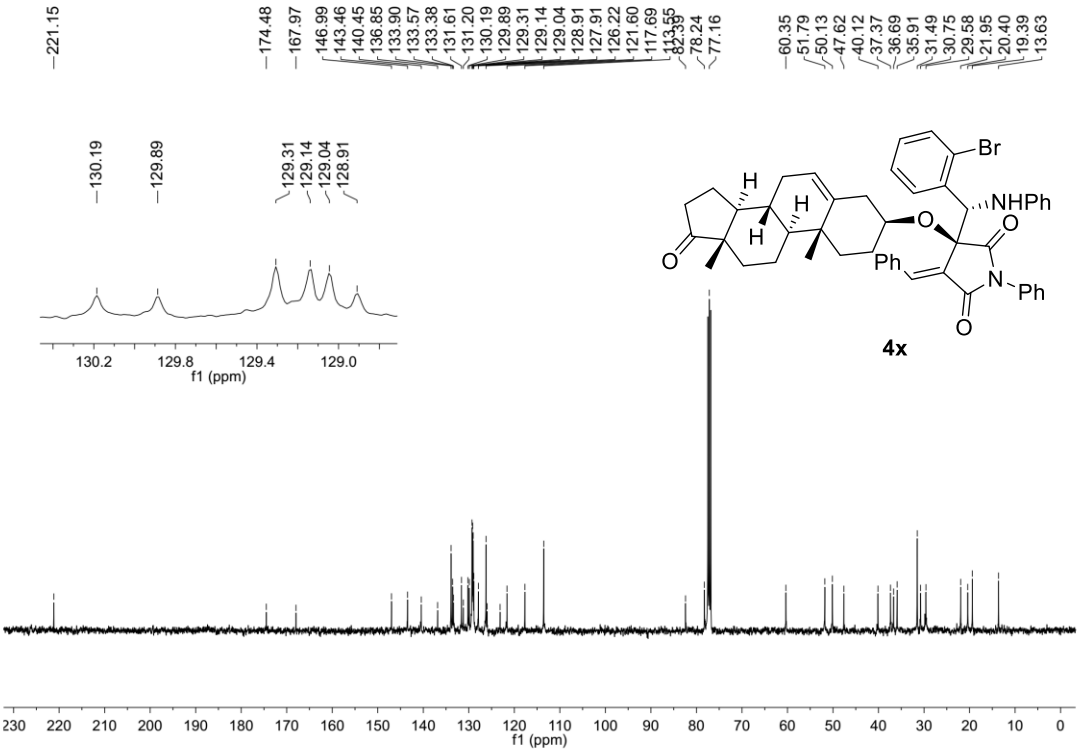

8.03 8.01 7.94 7.50 7.48 7.47 7.42 7.41 7.39 7.39 7.38 7.25 7.16 7.14 7.13 7.12 7.11 7.10 7.08 6.90 6.88 6.72 6.70 6.68 6.61 6.59 5.89 5.88 5.80 5.79 3.44 3.43 3.42 3.40 2.16 2.15 2.14 2.14 2.12 2.12 1.82 1.79 0.87 0.85 0.79 0.77 0.41 0.40 0.00
Br
iPr
NHPh
O
O
Ph
N
Ph
Me
O
4w

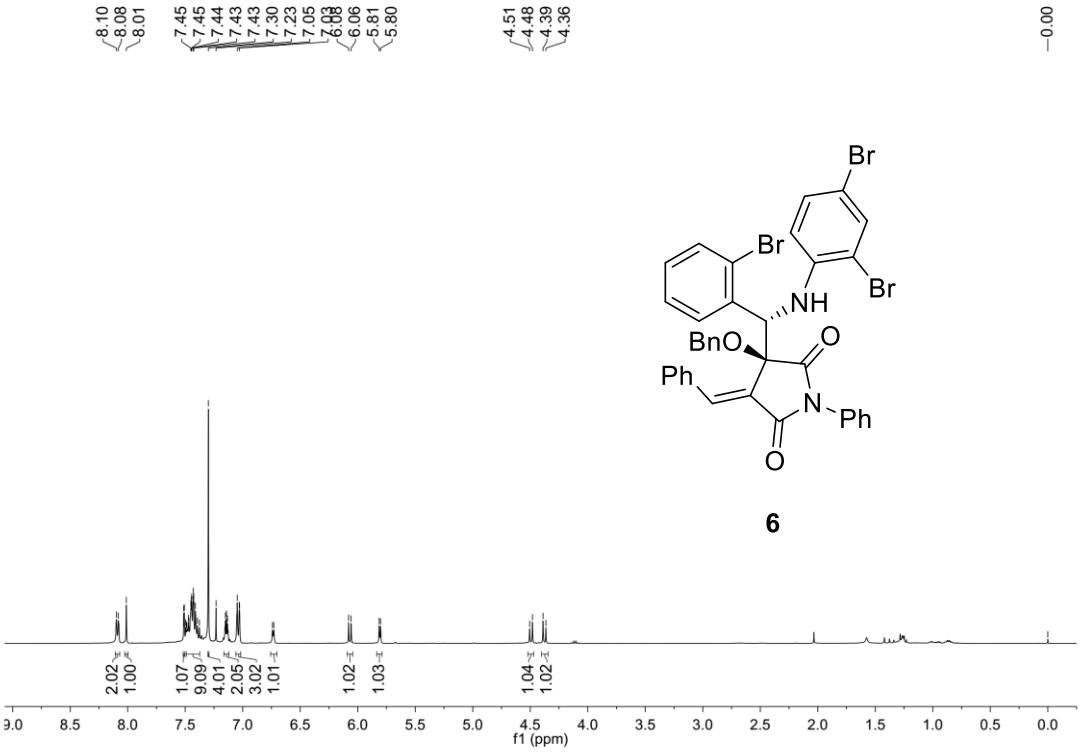

2.09 1.00 1.08 5.08 2.06 3.08 1.03 2.01 1.08 2.05 1.09 1.06 1.07 1.06 1.09 1.05 1.07 1.08 2.06 3.05 2.05 3.01 3.03
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


176.19 168.17 147.85 143.00 137.41 133.49 133.46 133.21 131.40 130.91 129.76 129.47 129.34 129.19 128.89 127.84 126.20 125.46 122.56 117.87 113.71 80.74 77.16 60.94 49.38 42.21 33.91 31.87 24.31 23.00 22.53 22.14 17.36
129.76 129.47 129.34 129.19 128.89
129.7 129.4 129.1
f1 (ppm)
Br
iPr
NHPh
O
O
Ph
N
Ph
Me
4w
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

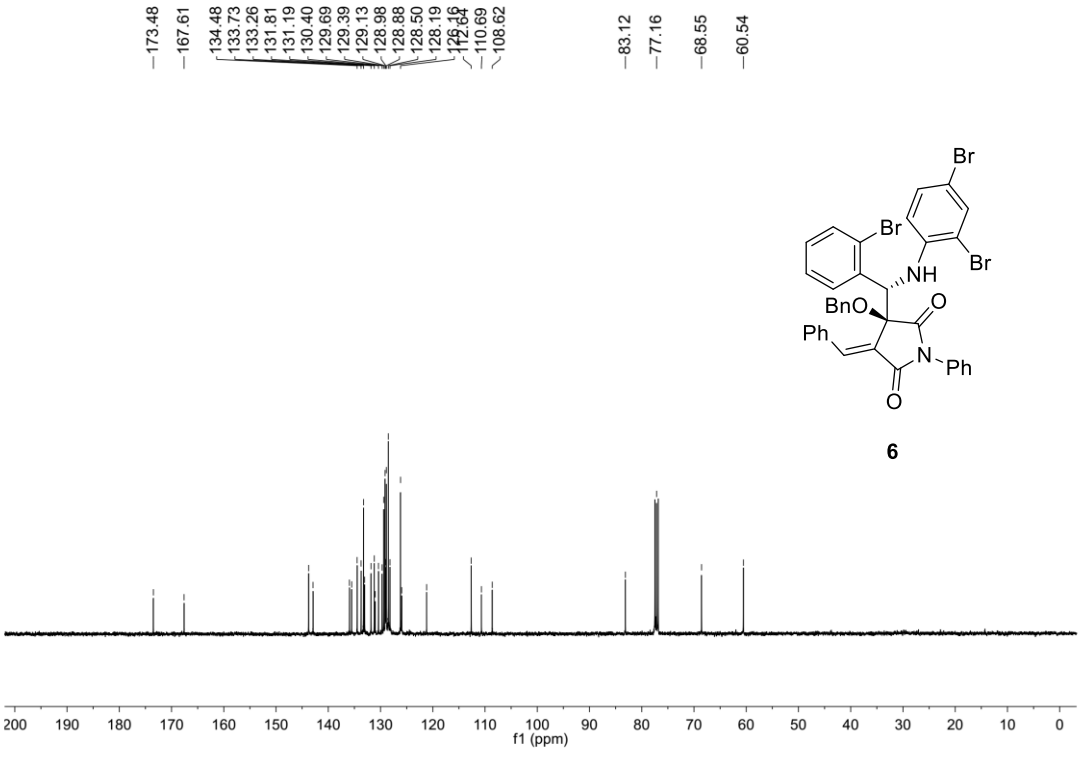

Br
NHPh
Ph
N
Ph
4x


f1 (ppm)

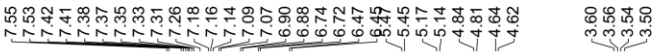

Br
NHPh
Ph
N
Ph
4x
f1 (ppm)
f1 (ppm)

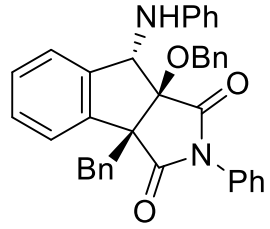

8.10
8.08
8.01
7.45
7.45
7.44
7.43
7.43
7.30
7.23
7.05
6.08
6.06
5.81
5.80
4.51
4.48
4.39
4.36
0.00
Br
Br
Br
NH
BnO
O
Ph
N
Ph
O
2.02
1.00
1.07
9.09
4.01
2.05
3.02
1.01
1.02
1.03
1.04
1.02
f1 (ppm)

**6**

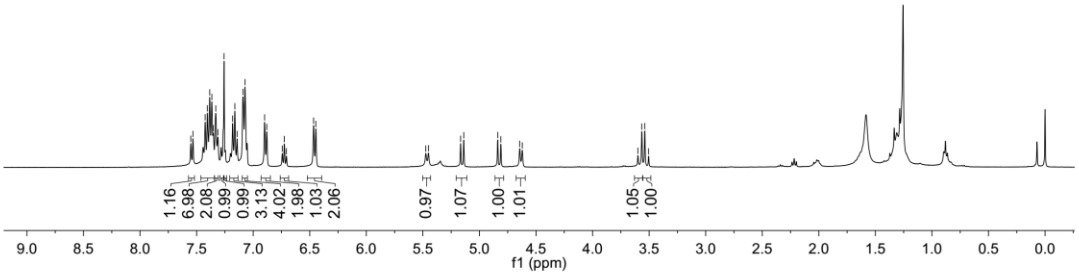

173.48
167.61
134.48
133.73
133.26
131.81
131.19
130.40
129.69
129.39
129.13
128.98
128.88
128.50
128.19
112.64
110.69
108.62
83.12
77.16
68.55
60.54
Br
Br
Br
NH
BnO
O
Ph
N
Ph
O
f1 (ppm)

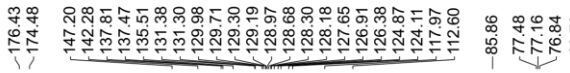
**6**

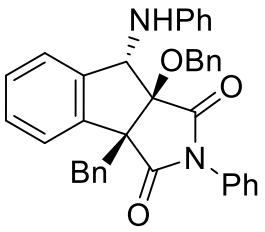

7.55
7.53
7.42
7.41
7.38
7.37
7.35
7.33
7.31
7.26
7.18
7.16
7.14
7.09
7.07
6.90
6.88
6.74
6.72
6.47
6.45
5.47
5.45
5.17
5.14
4.84
4.81
4.64
4.62
3.60
3.56
3.54
3.50


NHPh
OBn
O
Bn
N
Ph
O

**7**


1.16
6.98
2.08
0.99
0.99
3.13
4.02
1.98
1.03
2.06
0.97
1.07
1.00
1.01
1.05
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


176.43
174.48
147.20
142.28
137.81
137.47
135.51
131.38
131.30
129.98
129.71
129.30
129.19
128.97
128.68
128.30
128.18
127.65
126.91
126.38
124.87
124.11
117.97
112.60
85.86
77.48
77.16
76.84
69.70
62.29
62.01
35.49

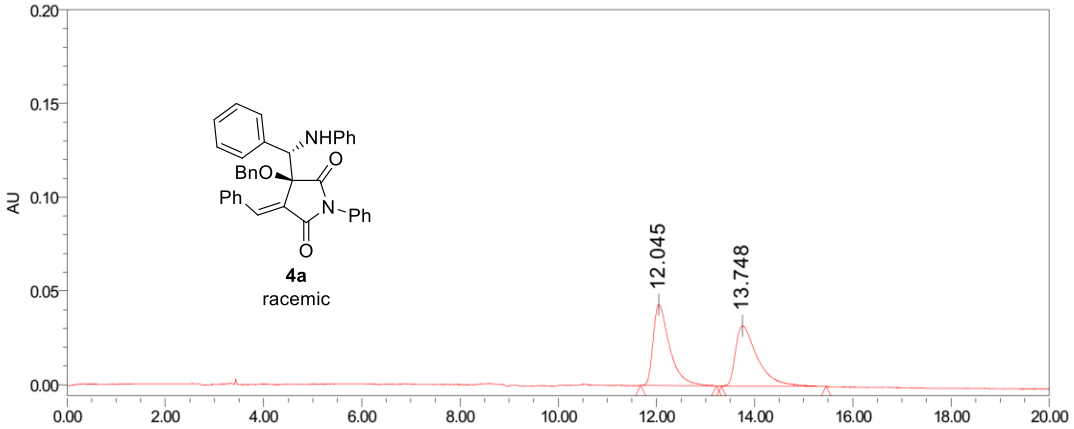

NHPh
OBn
O
Bn
N
Ph
O

**7**

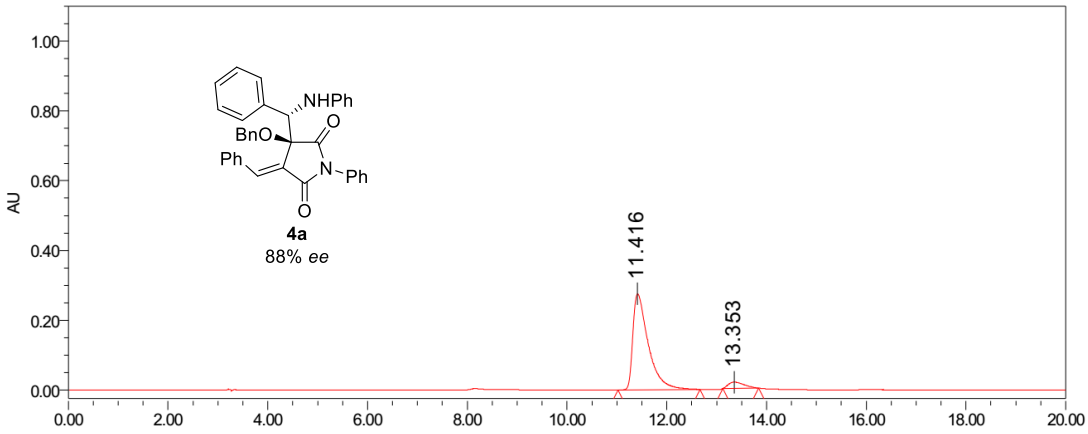

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Condition: hexane: 2-propanol = 97:3

Flow rate = 1.0 mL/min, λ = 300 nm, Chiral IB-3



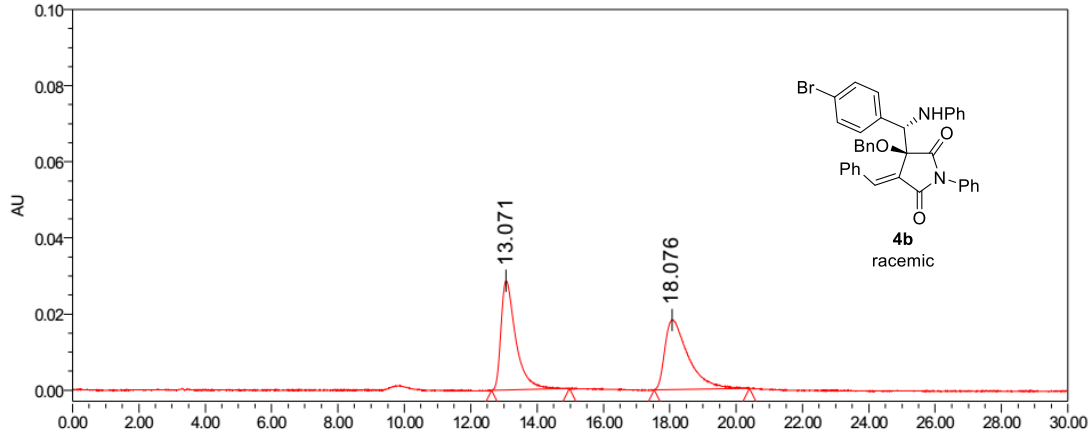

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 12.045 | 1007738 | 43207 | 50.25 |
| 2 | 13.748 | 997599 | 32204 | 49.75 |
| Total | | 2005337 | 75411 | 100.00 |



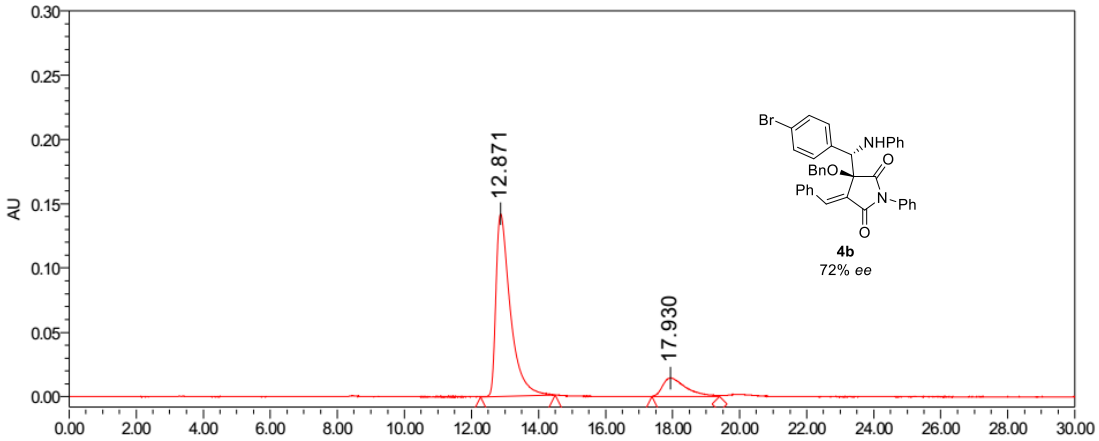

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 11.416 | 5939108 | 275039 | 93.87 |
| 2 | 13.353 | 387552 | 17503 | 6.13 |
| Total | | 6326660 | 292542 | 100.00 |

Condition: hexane: 2-propanol = 97:3

Flow rate = 1.0 mL/min, λ = 300 nm, Chiral IB-3



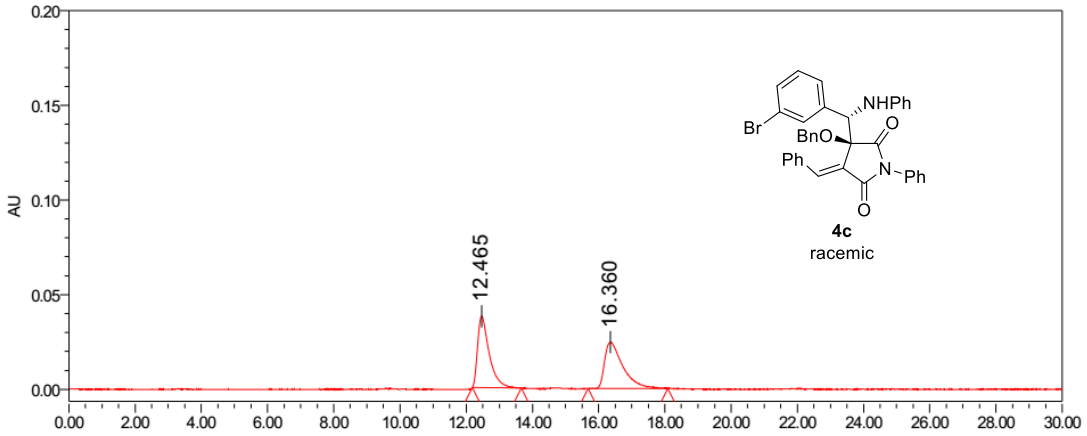

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 13.071 | 894546 | 28698 | 50.11 |
| 2 | 18.076 | 890795 | 18330 | 49.89 |
| Total | | 1785341 | 47028 | 100.00 |



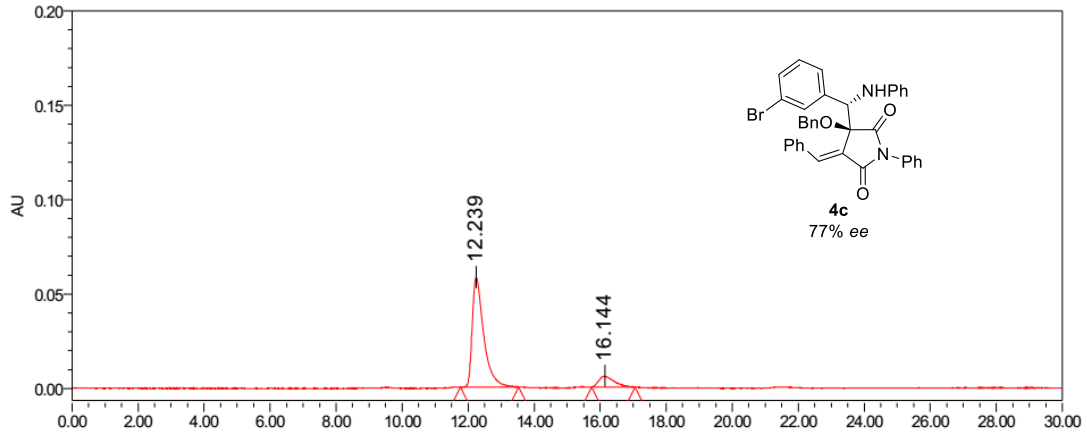

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 12.871 | 4238580 | 141924 | 86.03 |
| 2 | 17.930 | 688481 | 14325 | 13.97 |
| Total | | 4927061 | 156249 | 100.00 |

Condition: hexane: 2-propanol = 97:3

Flow rate = 1.0 mL/min, λ = 300 nm, Chiral IB-3



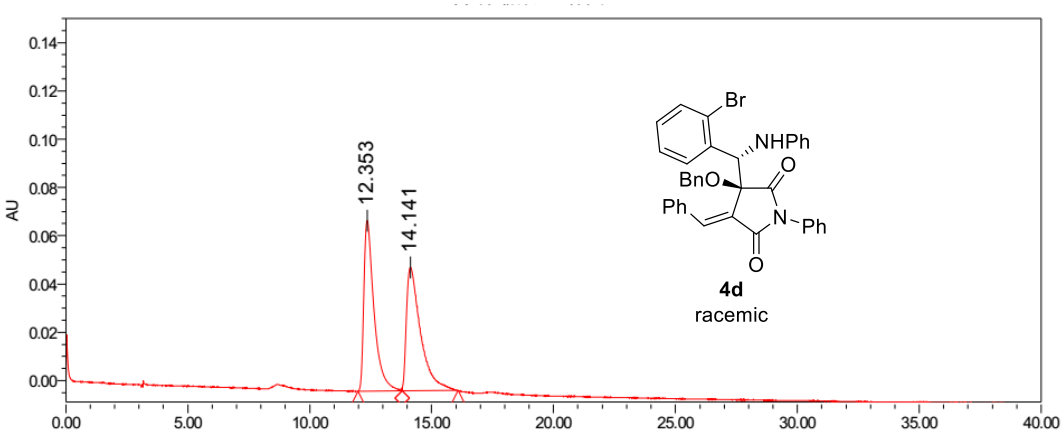

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 12.465 | 928814 | 37783 | 49.93 |
| 2 | 16.360 | 931564 | 24432 | 50.07 |
| Total | | 1860378 | 62215 | 100.00 |



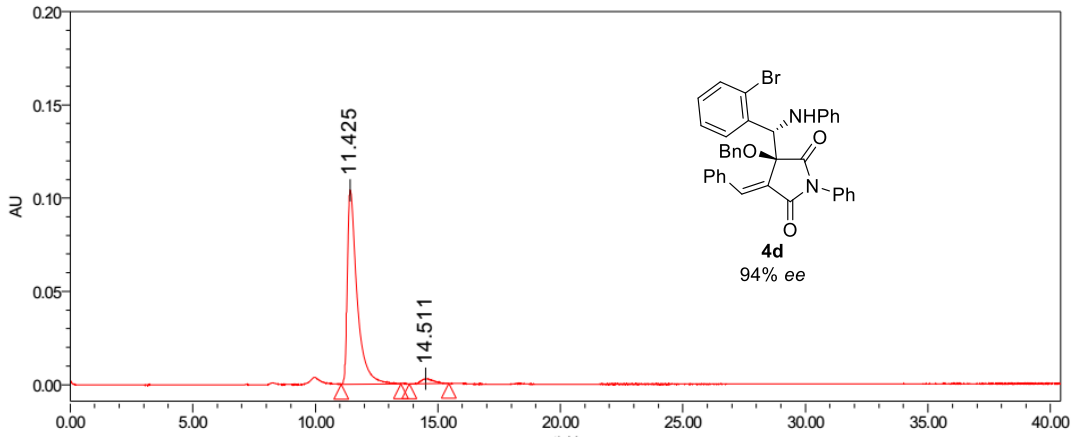

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 12.239 | 1402067 | 58185 | 88.42 |
| 2 | 16.144 | 183670 | 5661 | 11.58 |
| Total | | 1585737 | 63846 | 100.00 |

Condition: hexane: 2-propanol = 97:3

Flow rate = 1.0 mL/min, λ = 300 nm, Chiral IB-3



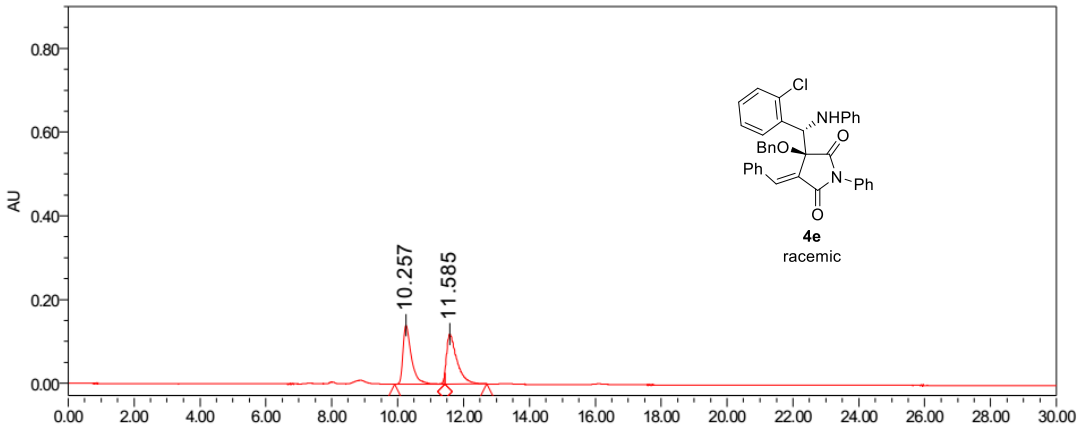

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 12.353 | 2061352 | 70694 | 49.97 |
| 2 | 14.141 | 2063640 | 51205 | 50.03 |
| Total | | 4124992 | 121899 | 100.00 |



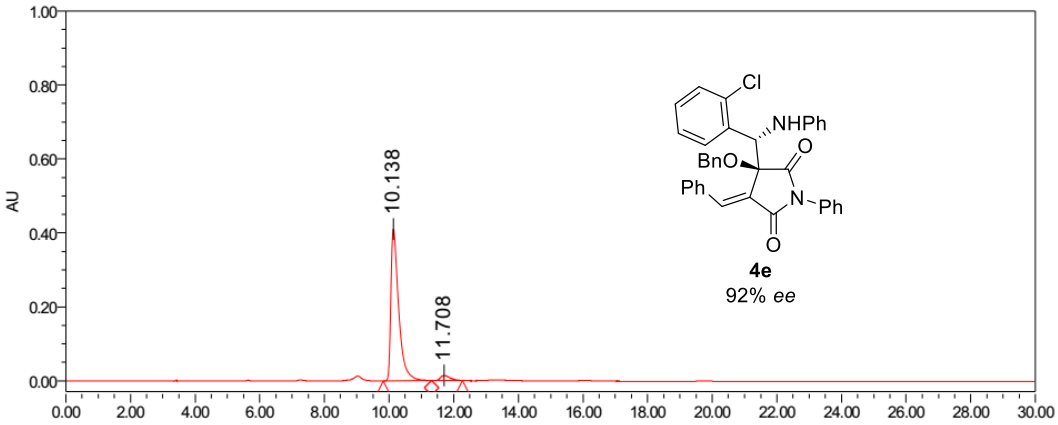

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 11.425 | 2857585 | 103902 | 96.77 |
| 2 | 14.511 | 95318 | 2644 | 3.23 |
| Total | | 2952903 | 106546 | 100 |

Condition: hexane: 2-propanol = 97:3

Flow rate = 1.0 mL/min, λ = 300 nm, Chiral IB-3



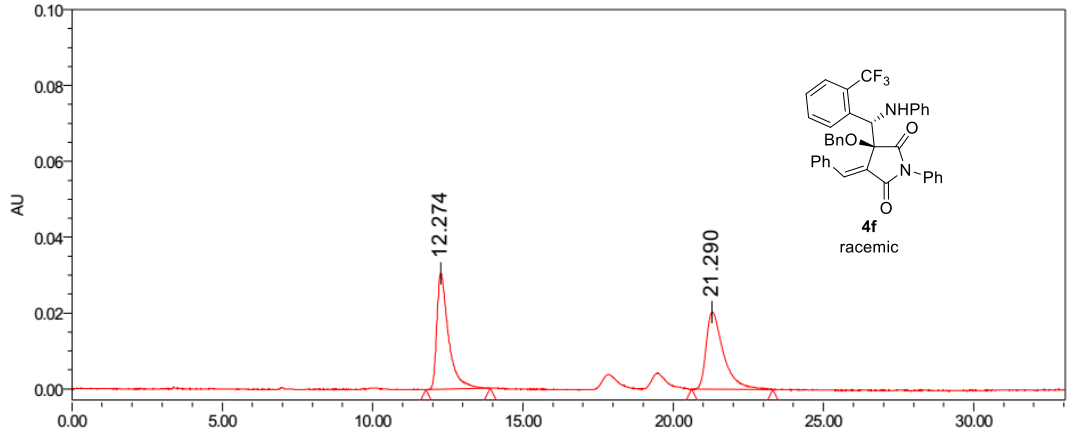

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 10.257 | 2525528 | 140493 | 49.77 |
| 2 | 11.585 | 2549162 | 119388 | 50.23 |
| Total | | 5074690 | 259881 | 100.00 |



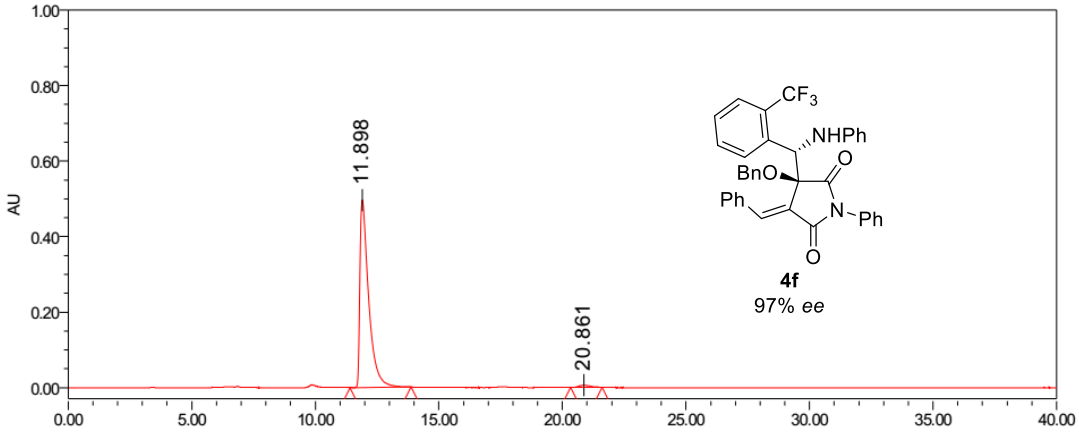

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 10.138 | 6916883 | 411099 | 96.00 |
| 2 | 11.708 | 288341 | 13906 | 4.00 |
| Total | | 7205224 | 425005 | 100.00 |

Condition: hexane: 2-propanol = 97:3

Flow rate = 1.0 mL/min, λ = 300 nm, Chiral IB-3



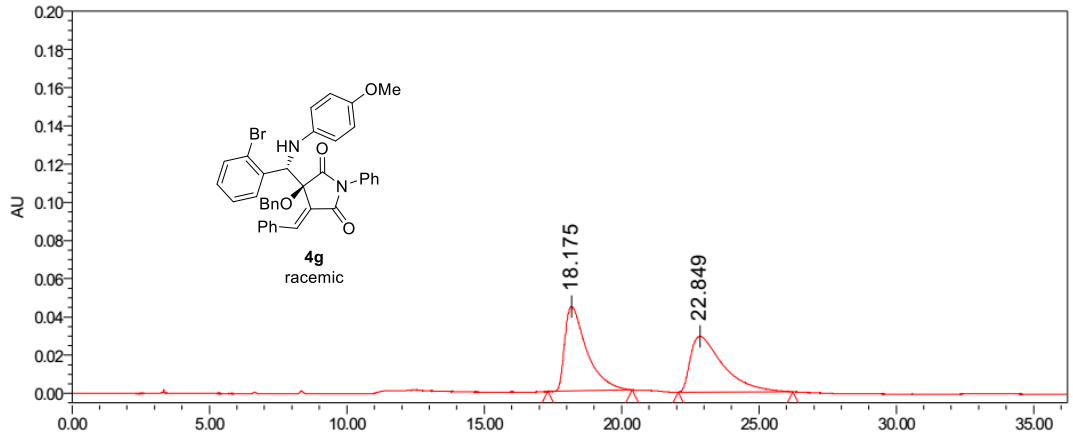

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 12.274 | 824182 | 30573 | 50.28 |
| 2 | 21.290 | 815141 | 20364 | 49.72 |
| Total | | 1639323 | 50937 | 100.00 |



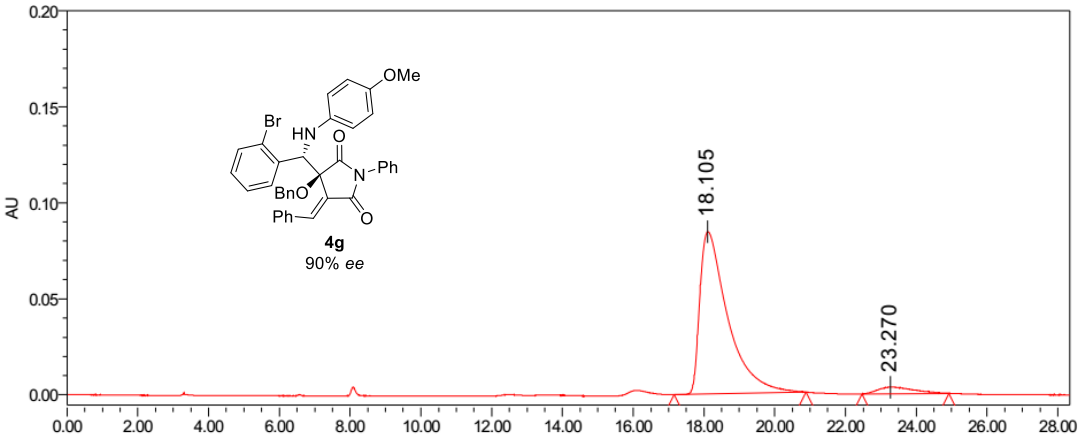

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 11.898 | 12307951 | 496174 | 98.51 |
| 2 | 20.861 | 186767 | 5580 | 1.49 |
| Total | | 12494718 | 501754 | 100.00 |

Condition: hexane: 2-propanol = 97:3

Flow rate = 1.0 mL/min, λ = 300 nm, Chiral IB-3



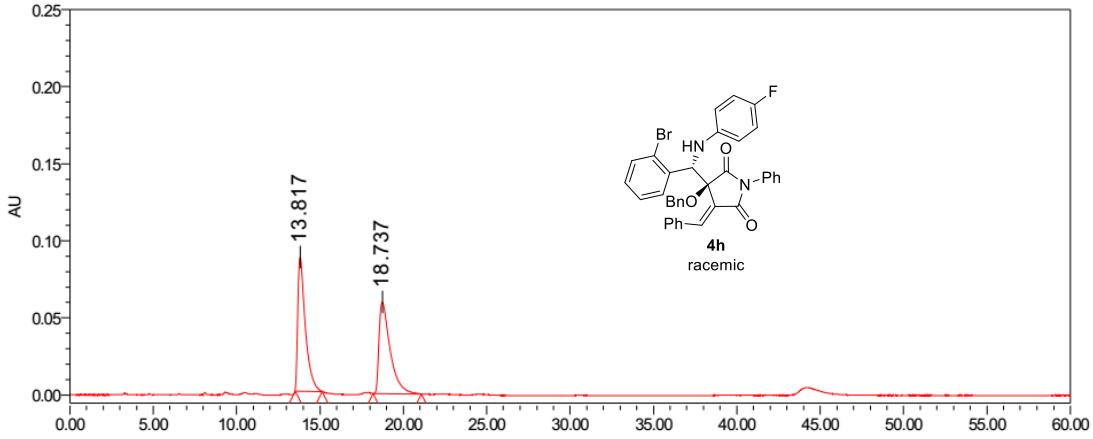

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 18.175 | 2434632 | 44225 | 50.20 |
| 2 | 22.849 | 2414891 | 29191 | 49.80 |
| Total | | 4849523 | 73416 | 100.00 |



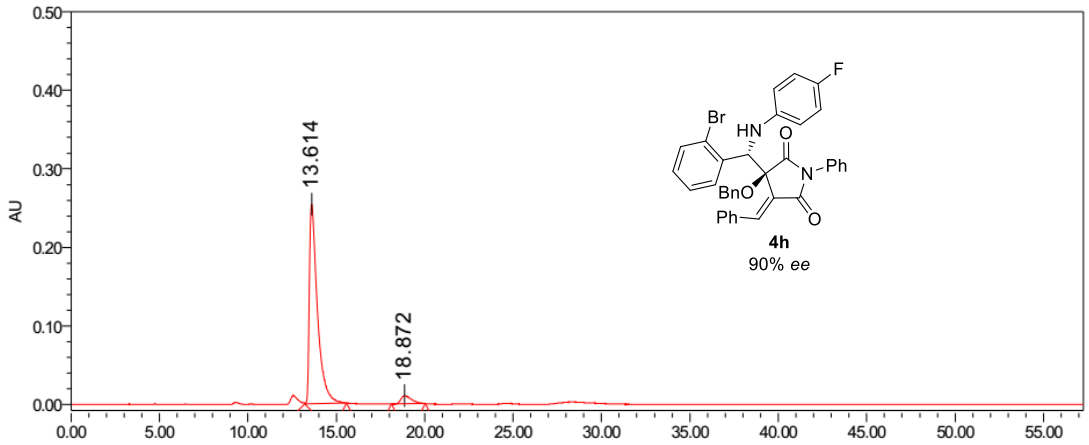

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 18.105 | 4633071 | 84469 | 95.00 |
| 2 | 23.270 | 243957 | 3423 | 5.00 |
| Total | | 4877028 | 87892 | 100.00 |

Condition: hexane: 2-propanol = 97:3

Flow rate = 1.0 mL/min, λ = 300 nm, Chiral IB-3



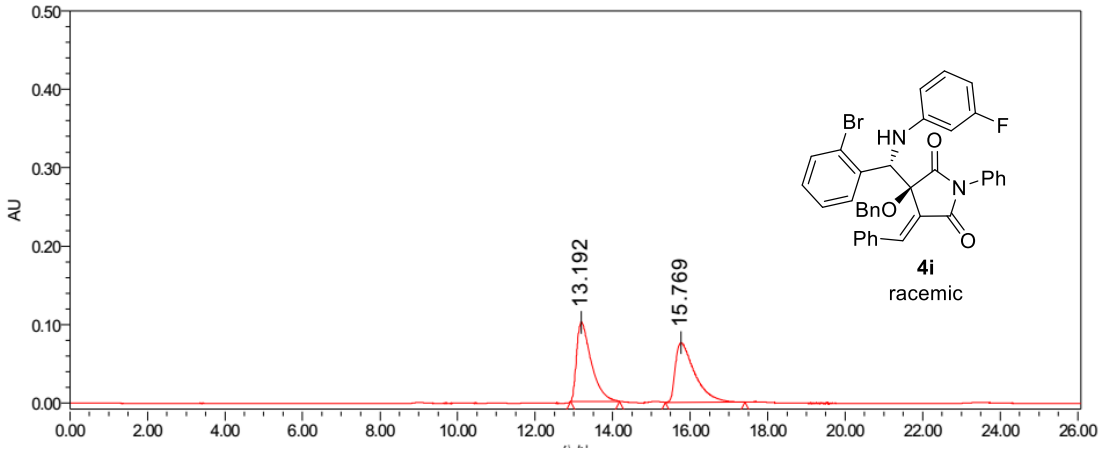

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 13.817 | 2751138 | 86971 | 49.94 |
| 2 | 18.737 | 2757824 | 59369 | 50.06 |
| Total | | 5508962 | 146340 | 100.00 |



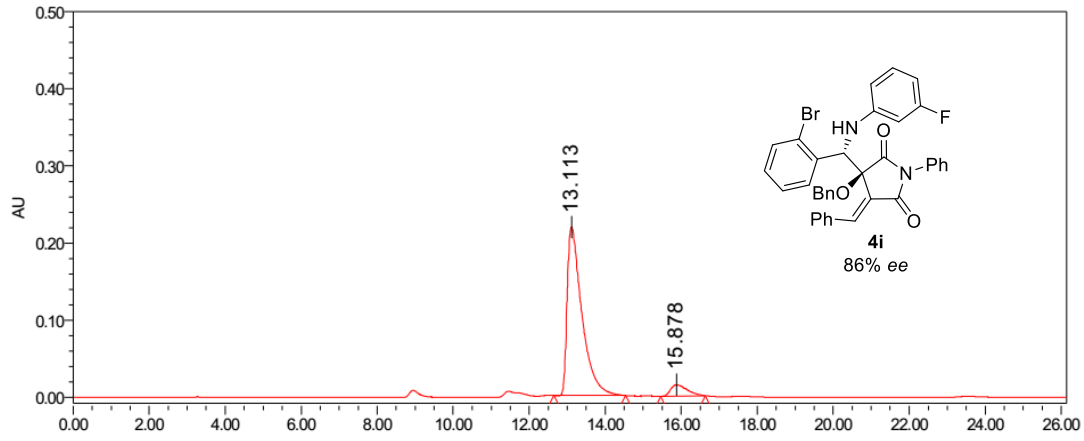

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 13.614 | 8088368 | 86971 | 94.87 |
| 2 | 18.872 | 437236 | 59369 | 5.13 |
| Total | | 8525604 | 146340 | 100.00 |

Condition: hexane: 2-propanol = 97:3

Flow rate = 1.0 mL/min, λ = 300 nm, Chiral IB-3



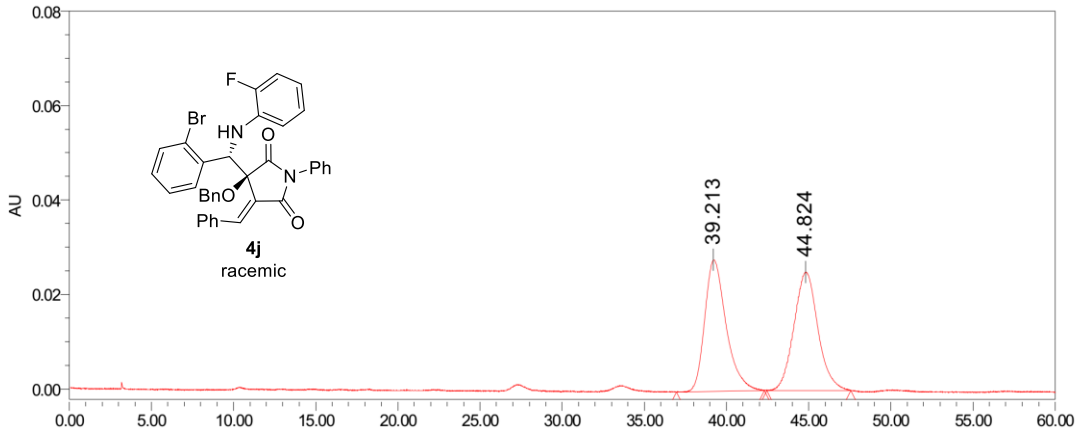

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 13.192 | 2625282 | 101024 | 50.19 |
| 2 | 15.769 | 2605547 | 76001 | 49.81 |
| Total | | 5230829 | 177025 | 100.00 |



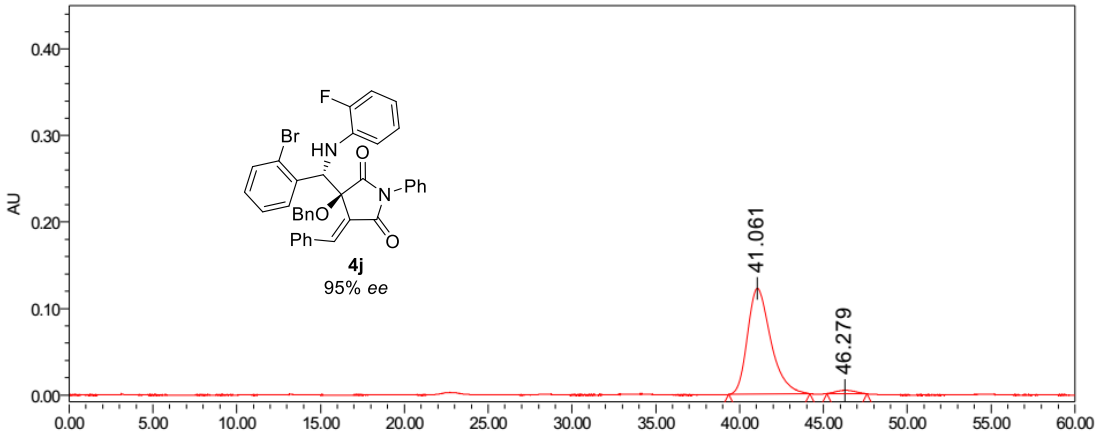

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 13.113 | 5829289 | 21852 | 92.92 |
| 2 | 15.878 | 444287 | 14772 | 7.08 |
| Total | | 6273576 | 36624 | 100.00 |

Condition: hexane: 2-propanol = 97:3

Flow rate = 1.0 mL/min, λ = 300 nm, Chiral AD-H



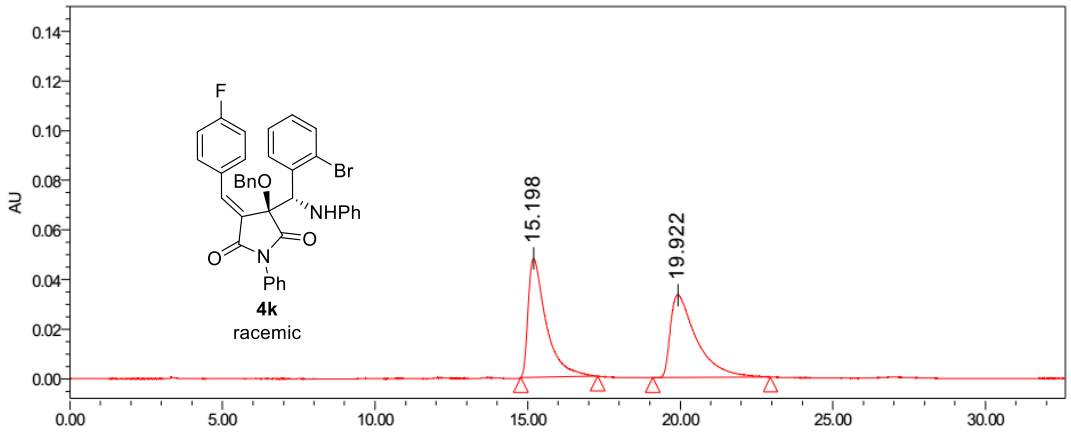

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 39.213 | 2522784 | 27855 | 49.87 |
| 2 | 44.824 | 2536227 | 25056 | 50.13 |
| Total | | 5059011 | 52911 | 100.00 |



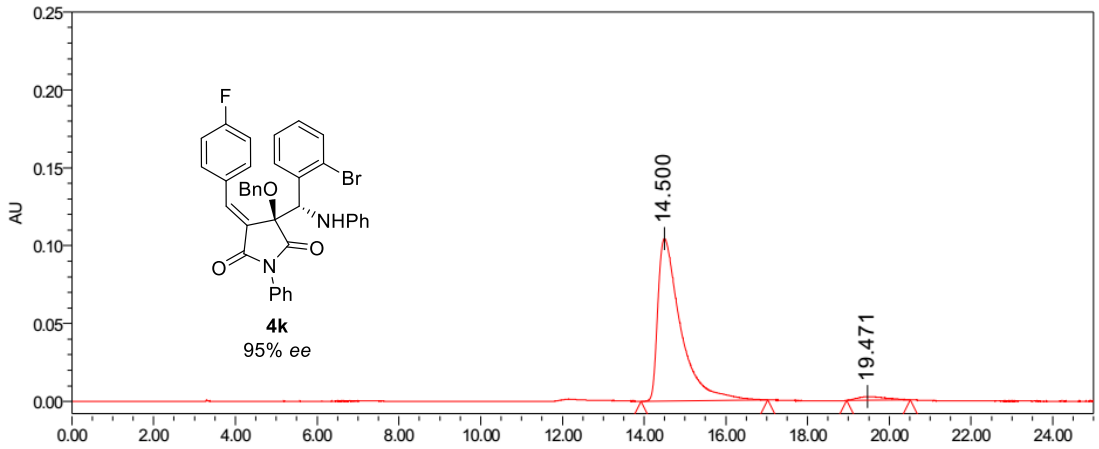

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 41.061 | 11833976 | 122235 | 97.53 |
| 2 | 46.279 | 300053 | 3817 | 2.47 |
| Total | | 12134029 | 126052 | 100.00 |

Condition: hexane: 2-propanol = 97:3

Flow rate = 1.0 mL/min, λ = 300 nm, Chiral IB-3



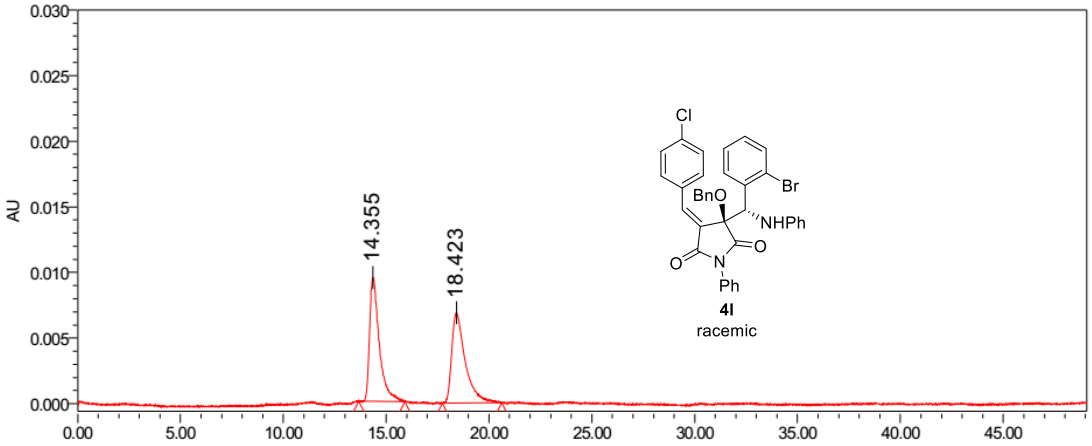

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 15.198 | 1953977 | 47783 | 49.91 |
| 2 | 19.922 | 1961406 | 33249 | 50.09 |
| Total | | 3915383 | 81032 | 100.00 |



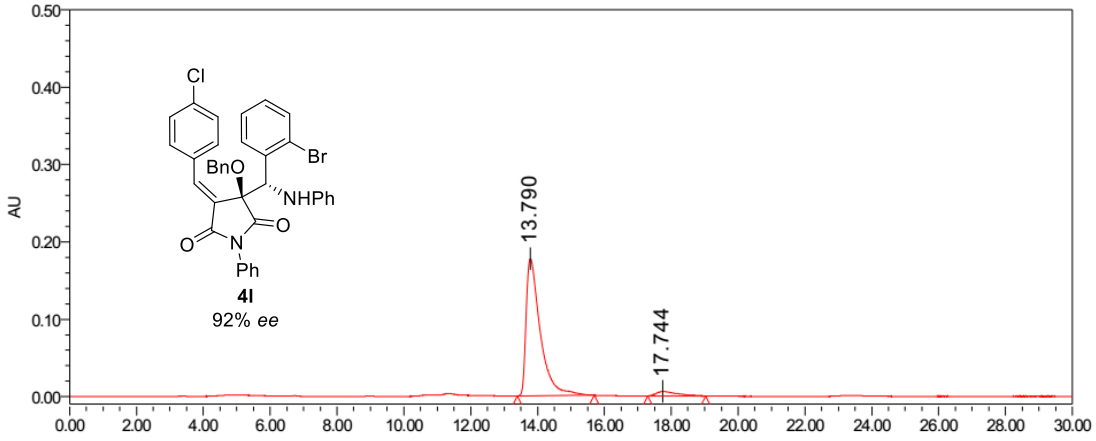

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 14.500 | 4030692 | 104132 | 97.42 |
| 2 | 19.471 | 106642 | 2225 | 2.58 |
| Total | | 4137334 | 106357 | 100.00 |

Condition: hexane: 2-propanol = 97:3

Flow rate = 1.0 mL/min, λ = 300 nm, Chiral IB-3



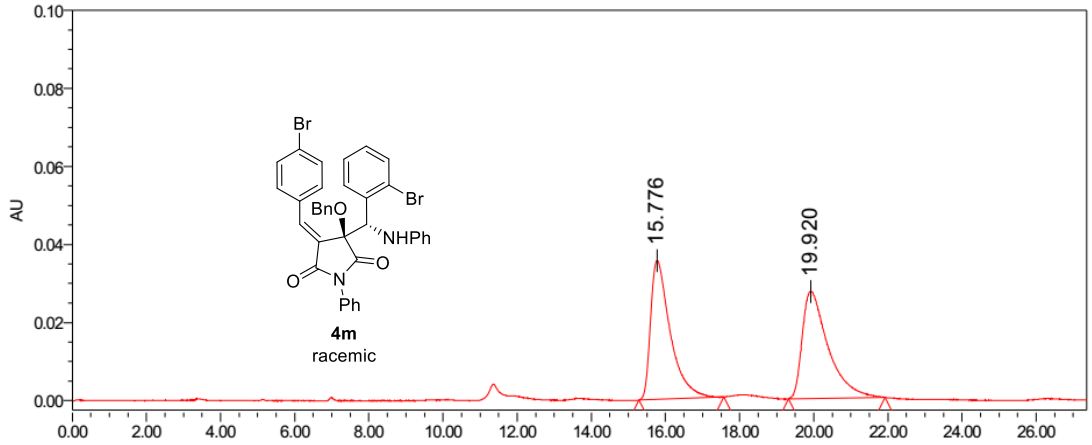

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 14.355 | 310503 | 9428 | 50.07 |
| 2 | 18.423 | 309684 | 6845 | 49.93 |
| Total | | 620187 | 16273 | 100.00 |



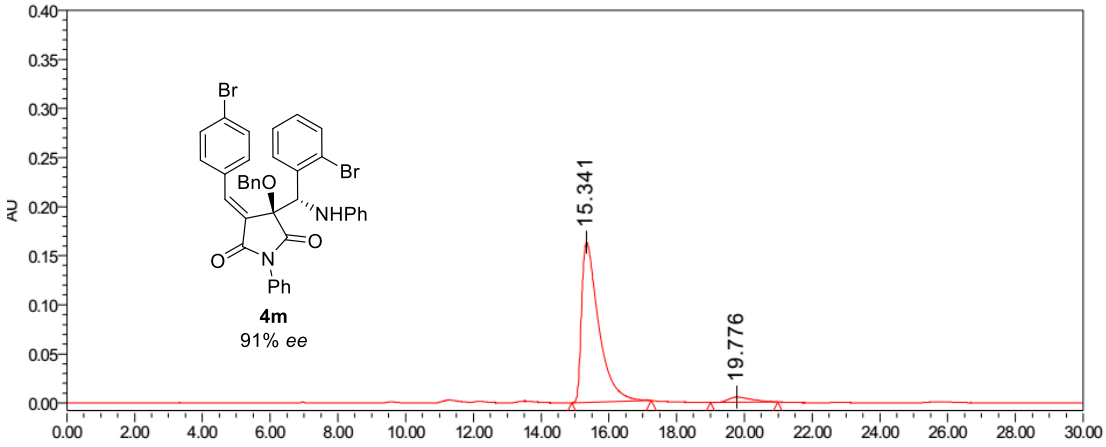

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 13.790 | 5239346 | 177600 | 95.36 |
| 2 | 17.744 | 254772 | 5802 | 4.64 |
| Total | | 5494118 | 183402 | 100.00 |

Condition: hexane: 2-propanol = 97:3

Flow rate = 1.0 mL/min, λ = 300 nm, Chiral IB-3



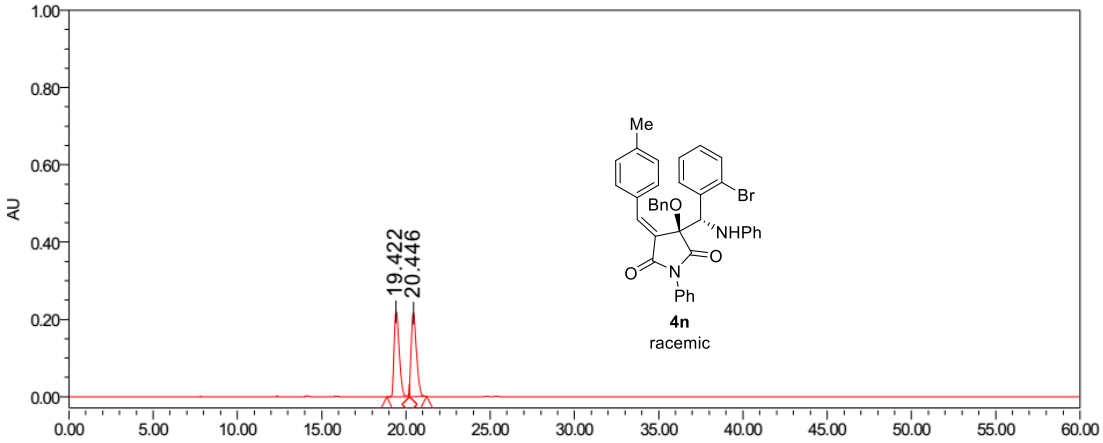

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 15.776 | 1312735 | 35574 | 49.89 |
| 2 | 19.920 | 1318657 | 27412 | 50.11 |
| Total | | 2631392 | 62986 | 100.00 |



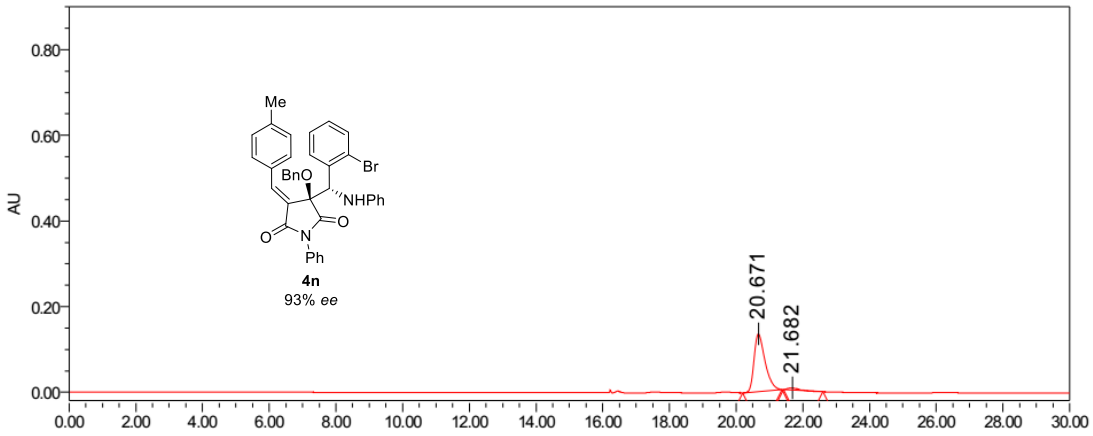

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 15.341 | 5678497 | 35574 | 95.65 |
| 2 | 19.776 | 258408 | 5365 | 4.35 |
| Total | | 5936905 | 40939 | 100.00 |

Condition: hexane: ethanol = 97:3

Flow rate = 0.5 mL/min, λ = 300 nm, Chiral IB-3



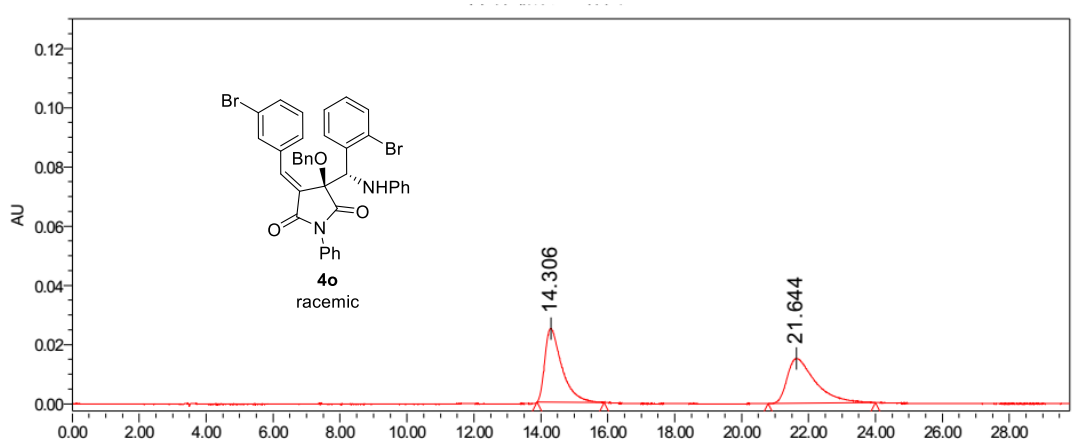

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 19.422 | 4720319 | 219846 | 49.86 |
| 2 | 20.446 | 4746817 | 215787 | 50.14 |
| Total | | 9467136 | 435633 | 100.00 |



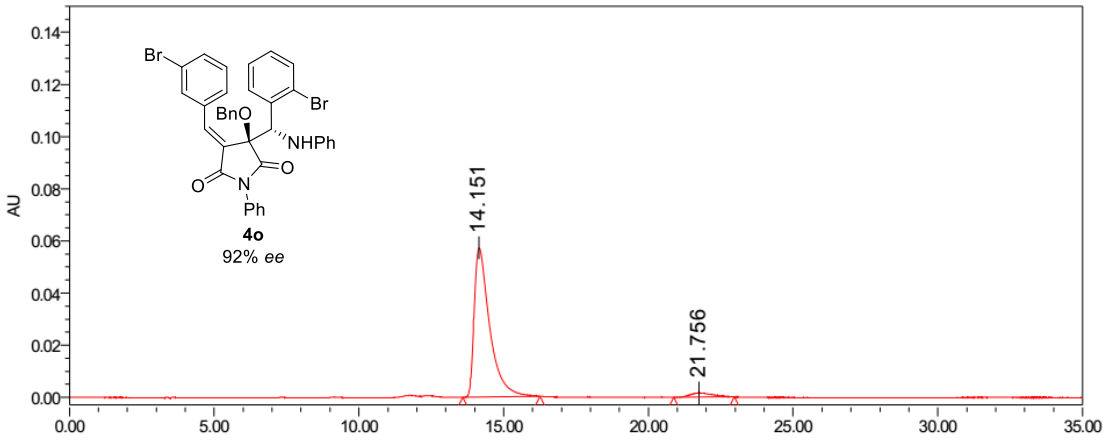

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 20.674 | 3088891 | 134297 | 96.45 |
| 2 | 21.682 | 113691 | 5169 | 3.55 |
| Total | | 3202582 | 139466 | 100.00 |

Condition: hexane: 2-propanol = 97:3

Flow rate = 1.0 mL/min, λ = 300 nm, Chiral IB-3



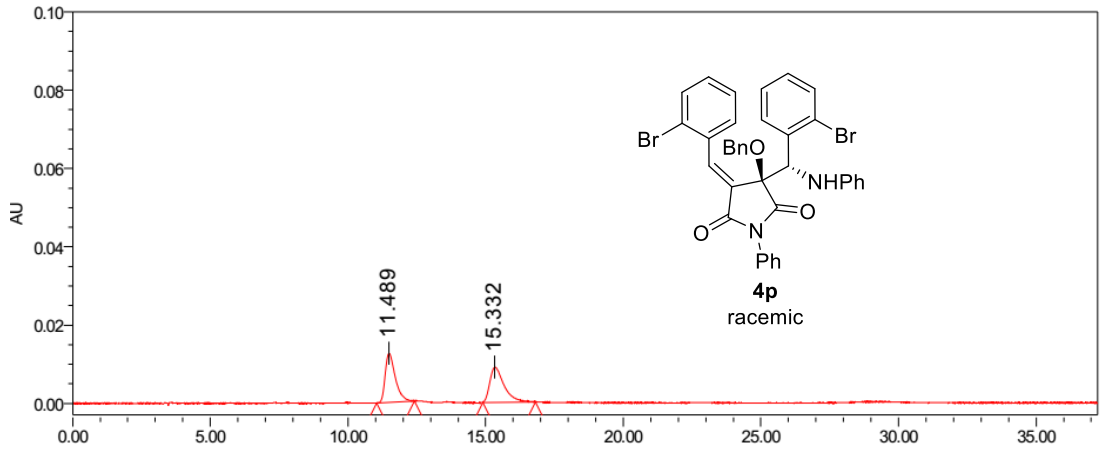

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 14.306 | 878647 | 124950 | 50.06 |
| 2 | 21.644 | 876384 | 15132 | 49.94 |
| Total | | 1755031 | 140082 | 100.00 |



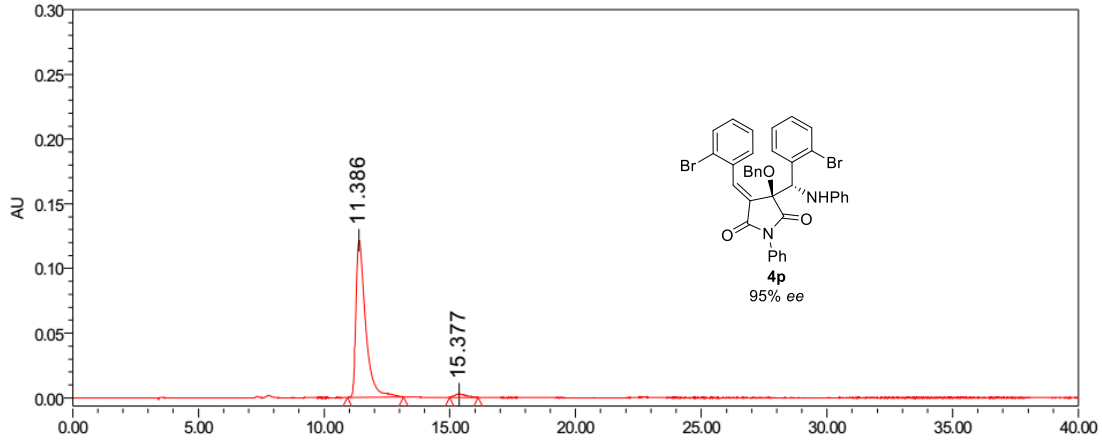

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 14.151 | 2131283 | 57223 | 96.18 |
| 2 | 21.756 | 84622 | 1574 | 3.82 |
| Total | | 2215905 | 58797 | 100.00 |

Condition: hexane: 2-propanol = 97:3

Flow rate = 1.0 mL/min, λ = 300 nm, Chiral IB-3



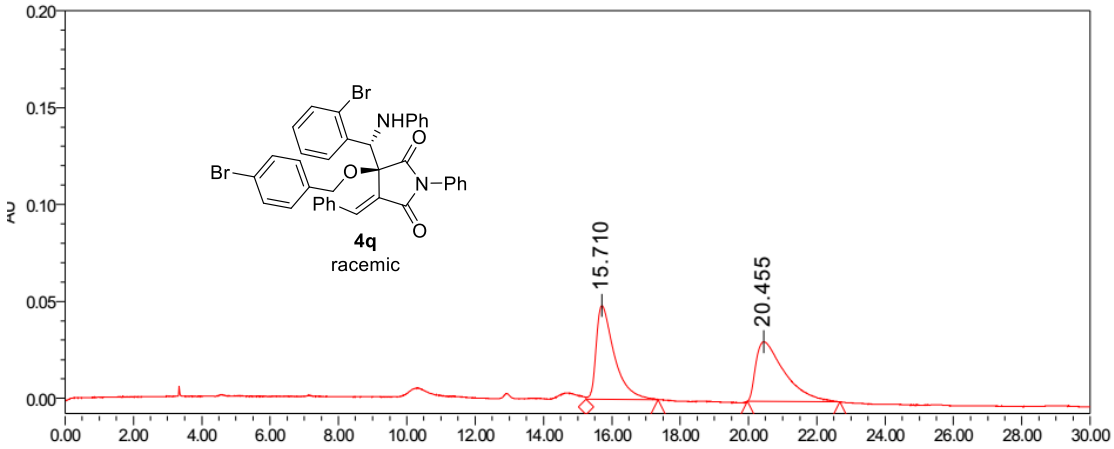

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 11.489 | 320109 | 12558 | 49.85 |
| 2 | 15.332 | 322057 | 8932 | 50.15 |
| Total | | 642166 | 21490 | 100.00 |



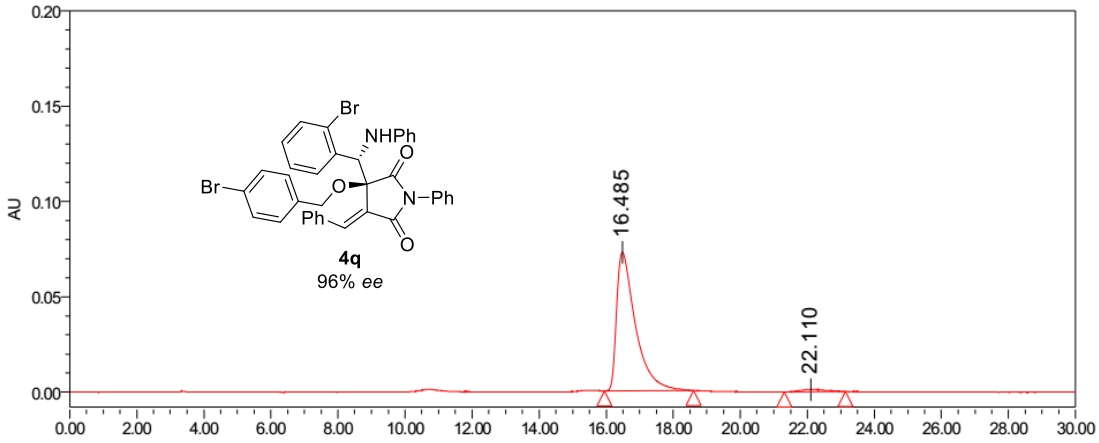

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 11.386 | 3227267 | 121377 | 97.59 |
| 2 | 15.377 | 79718 | 2493 | 2.41 |
| Total | | 3306985 | 123870 | 100.00 |

Condition: hexane: 2-propanol = 97:3

Flow rate = 1.0 mL/min, λ = 300 nm, Chiral IB-3



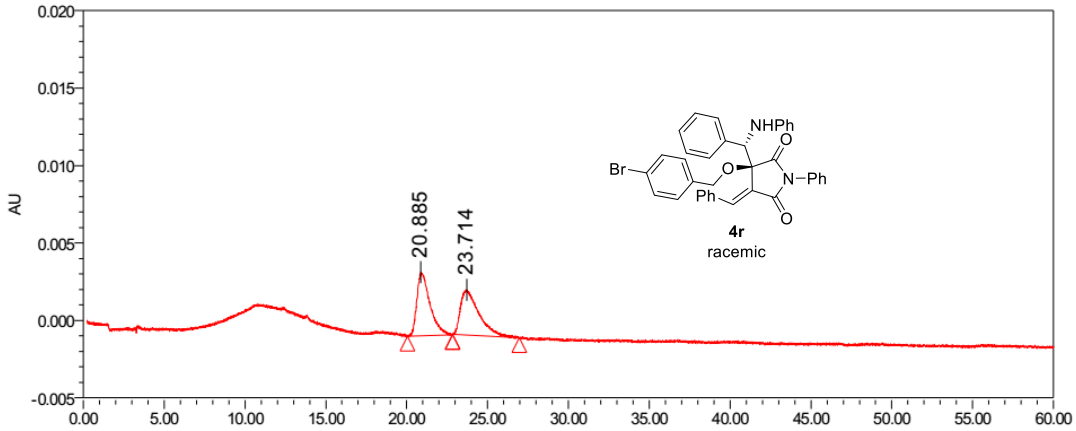

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 15.710 | 1783038 | 48425 | 49.95 |
| 2 | 20.455 | 1786505 | 30665 | 50.05 |
| Total | | 3569543 | 79090 | 100.00 |



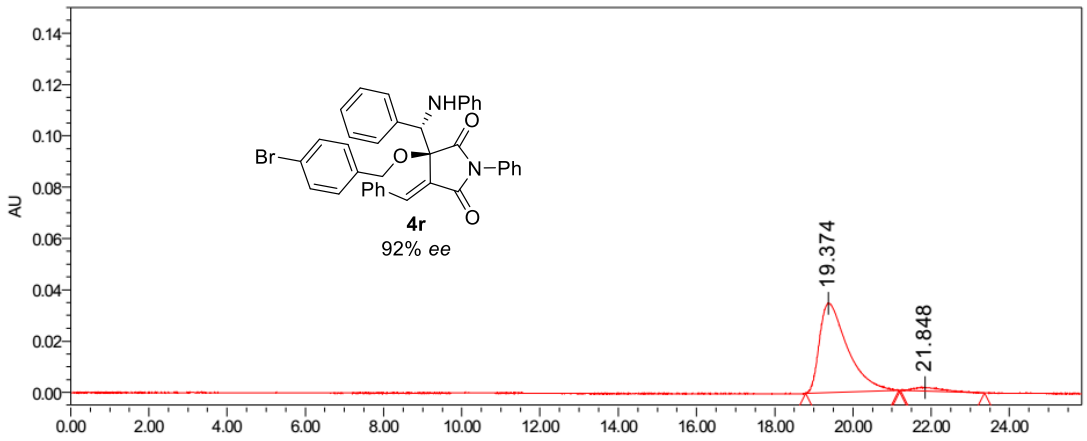

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 16.485 | 2855032 | 72689 | 97.85 |
| 2 | 22.110 | 62613 | 1205 | 2.15 |
| Total | | 2917645 | 73894 | 100.00 |

Condition: hexane: 2-propanol = 98:2

Flow rate = 1.0 mL/min, λ = 300 nm, Chiral IB-3



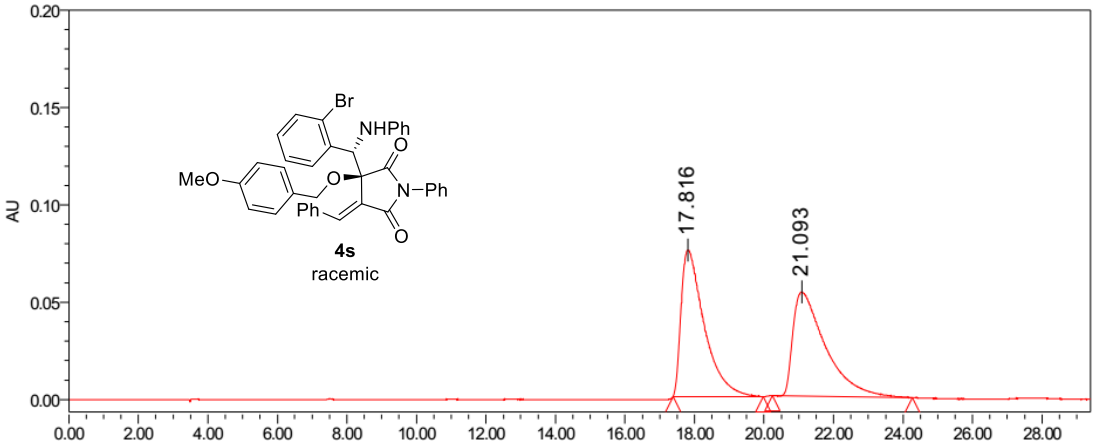

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 20.885 | 229405 | 4092 | 50.10 |
| 2 | 23.714 | 228486 | 2921 | 49.90 |
| Total | | 457891 | 7013 | 100.00 |



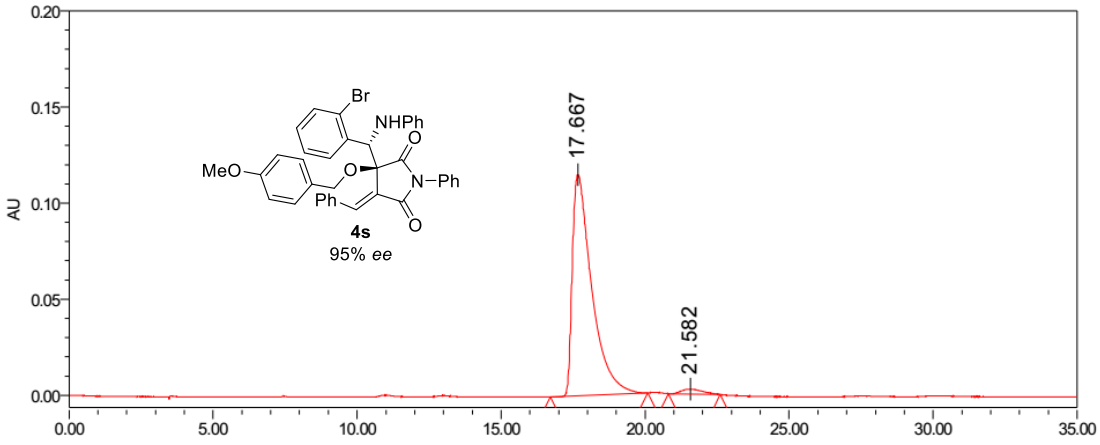

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 19.374 | 1727038 | 34795 | 96.07 |
| 2 | 21.848 | 70703 | 1339 | 3.93 |
| Total | | 1797741 | 36134 | 100.00 |

Condition: hexane: 2-propanol = 97:3

Flow rate = 1.0 mL/min, λ = 300 nm, Chiral IB-3



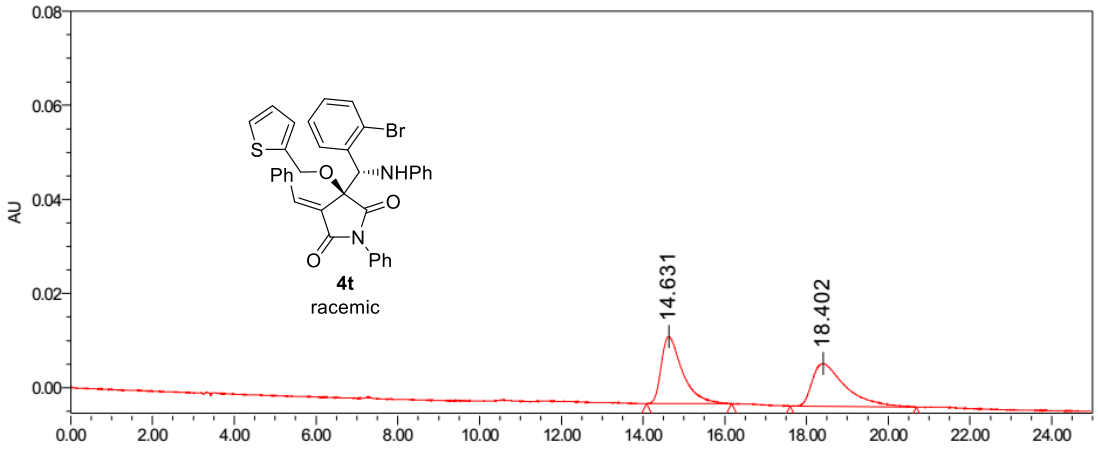

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 17.816 | 3461047 | 75281 | 50.05 |
| 2 | 21.093 | 3453860 | 53377 | 49.95 |
| Total | | 6914907 | 128658 | 100.00 |



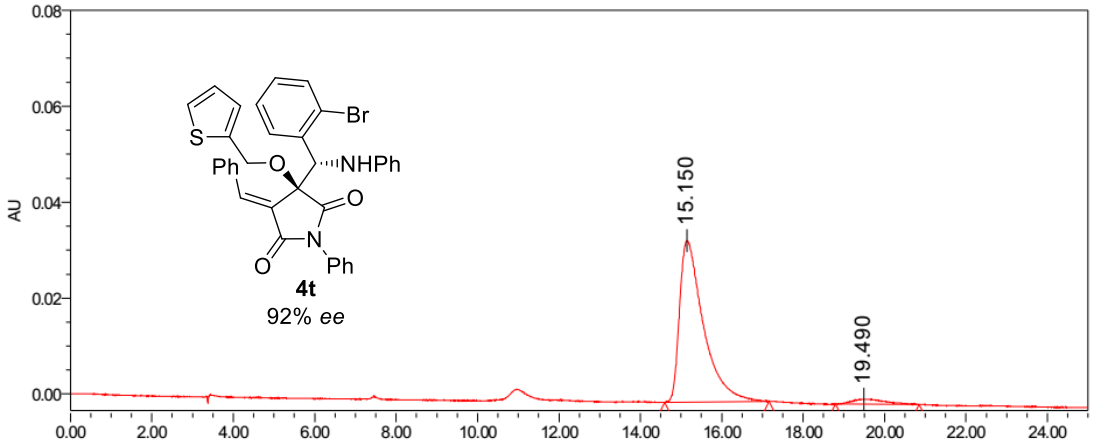

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 17.667 | 5370683 | 115063 | 97.67 |
| 2 | 21.582 | 128267 | 2535 | 2.33 |
| Total | | 5498950 | 117598 | 100.00 |

Condition: hexane: 2-propanol = 97:3

Flow rate = 1.0 mL/min, λ = 300 nm, Chiral IB-3



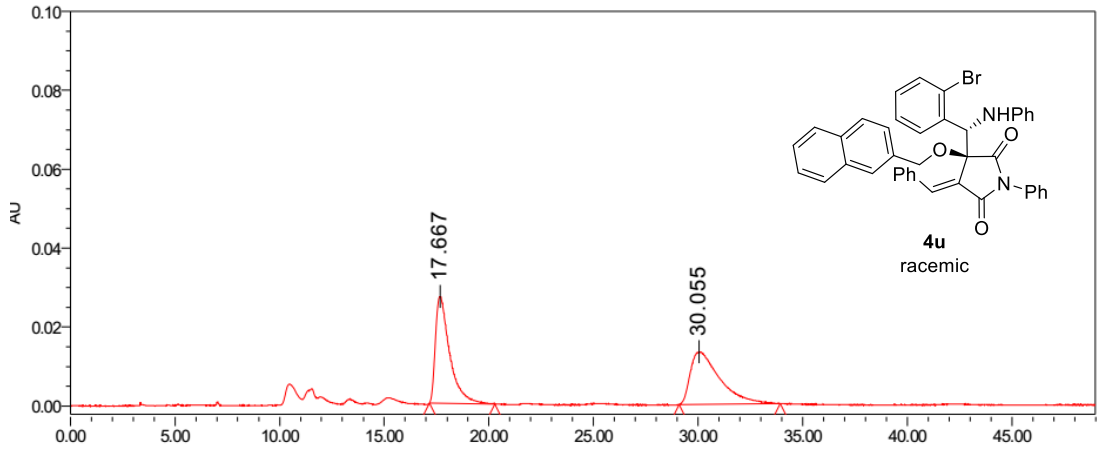

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 14.631 | 513269 | 14257 | 50.16 |
| 2 | 18.402 | 509972 | 9078 | 49.84 |
| Total | | 1023241 | 23335 | 100.00 |



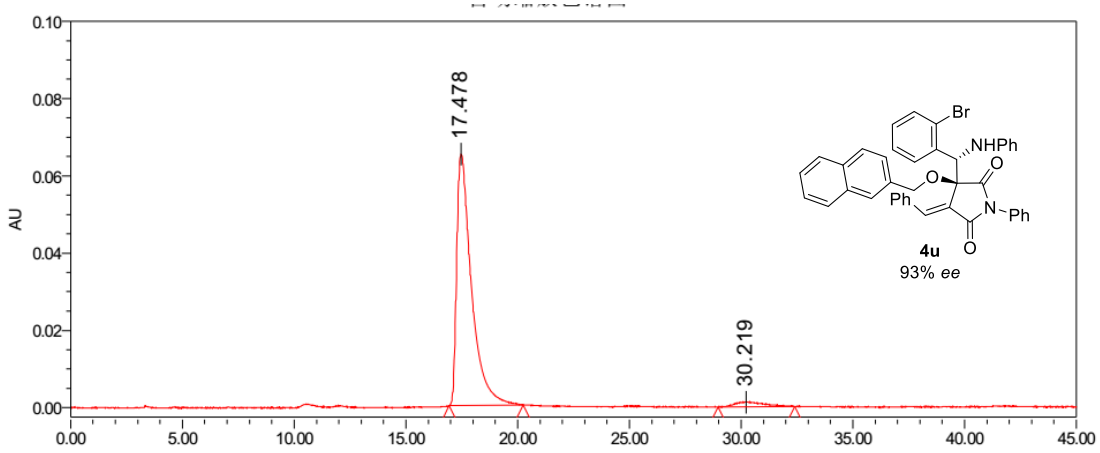

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 15.150 | 1356691 | 33624 | 95.73 |
| 2 | 19.490 | 60493 | 1063 | 4.27 |
| Total | | 1417184 | 34687 | 100.00 |

Condition: hexane: 2-propanol = 97:3

Flow rate = 1.0 mL/min, λ = 300 nm, Chiral IB-3



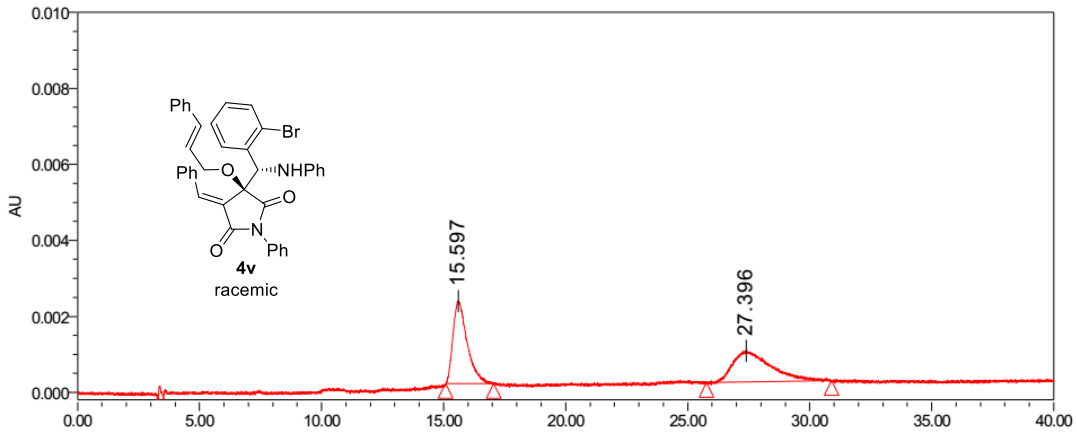

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 17.667 | 1279084 | 27109 | 49.90 |
| 2 | 30.055 | 1284177 | 13301 | 50.10 |
| Total | | 2563261 | 40410 | 100.00 |



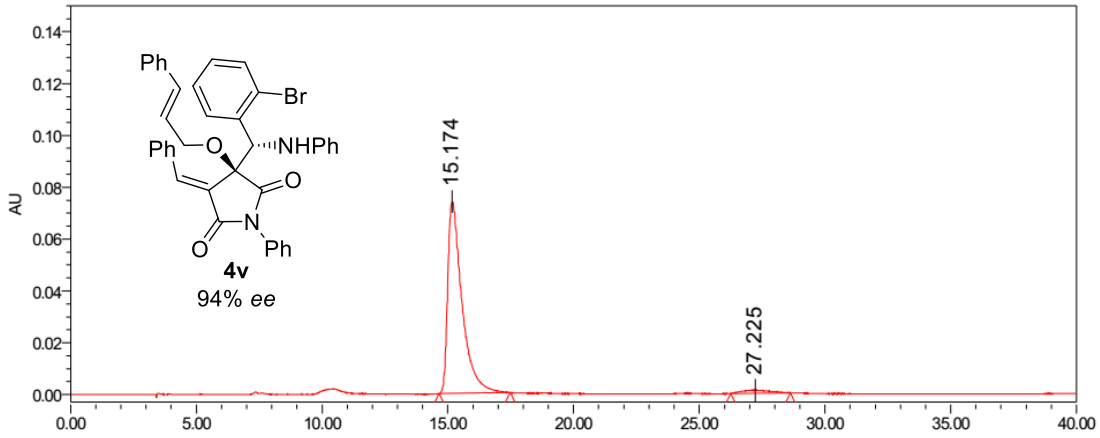

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 17.478 | 2968602 | 65065 | 96.33 |
| 2 | 30.219 | 113038 | 1206 | 3.67 |
| Total | | 3081640 | 66271 | 100.00 |

Condition: hexane: 2-propanol = 97:3

Flow rate = 1.0 mL/min, λ = 300 nm, Chiral IB-3



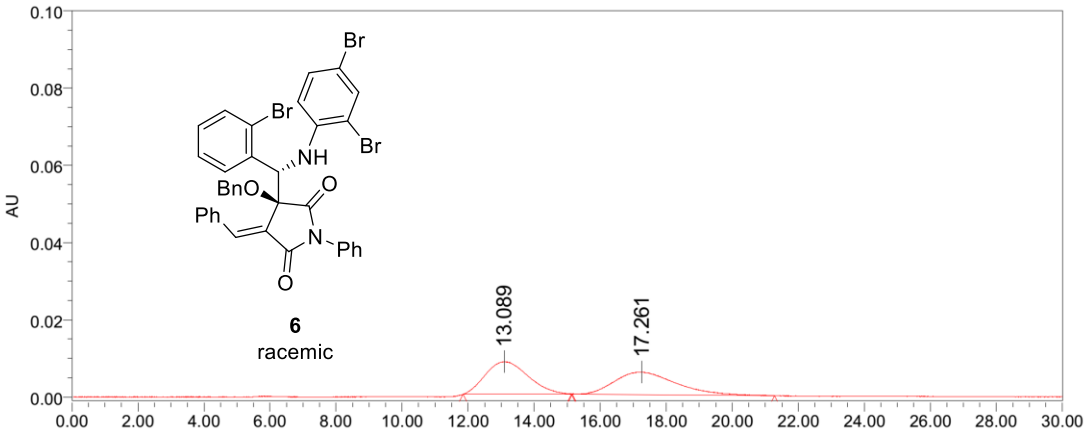

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 15.597 | 88197 | 74014 | 49.80 |
| 2 | 27.396 | 88898 | 1140 | 50.20 |
| Total | | 177095 | 75154 | 100.00 |



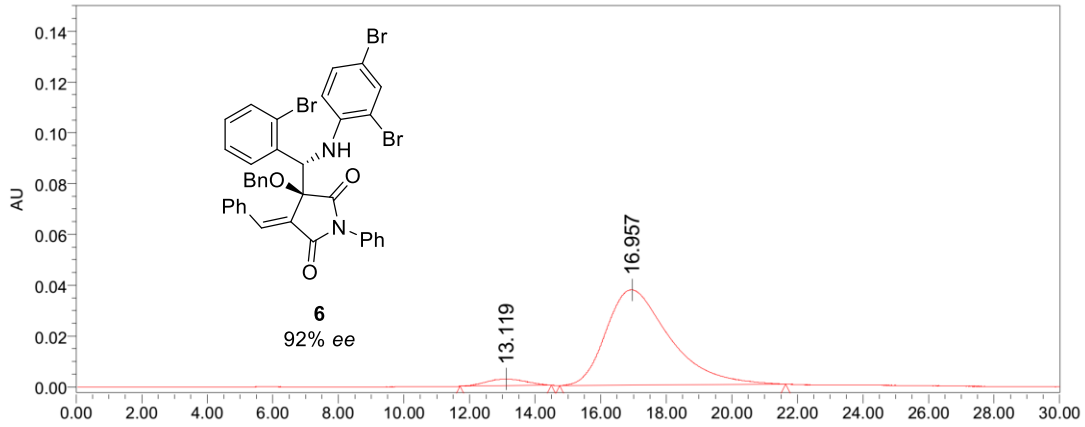

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 15.174 | 2891530 | 74014 | 96.99 |
| 2 | 27.225 | 89745 | 1140 | 3.01 |
| Total | | 2981275 | 75154 | 100.00 |

Condition: hexane: 2-propanol = 99:1

Flow rate = 1.0 mL/min, λ = 300 nm, Chiral IC



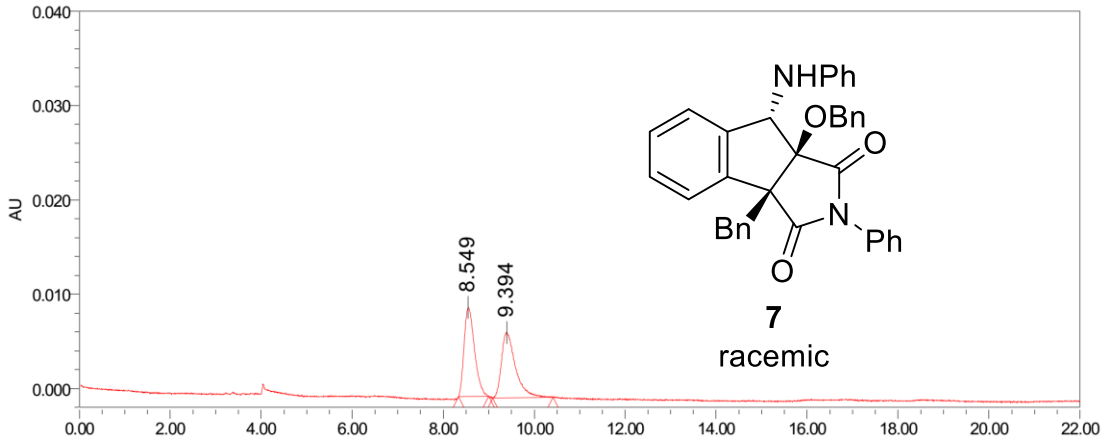

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 13.089 | 752731 | 8402 | 49.97 |
| 2 | 17.261 | 753643 | 5825 | 50.03 |
| Total | | 1506374 | 14227 | 100.00 |



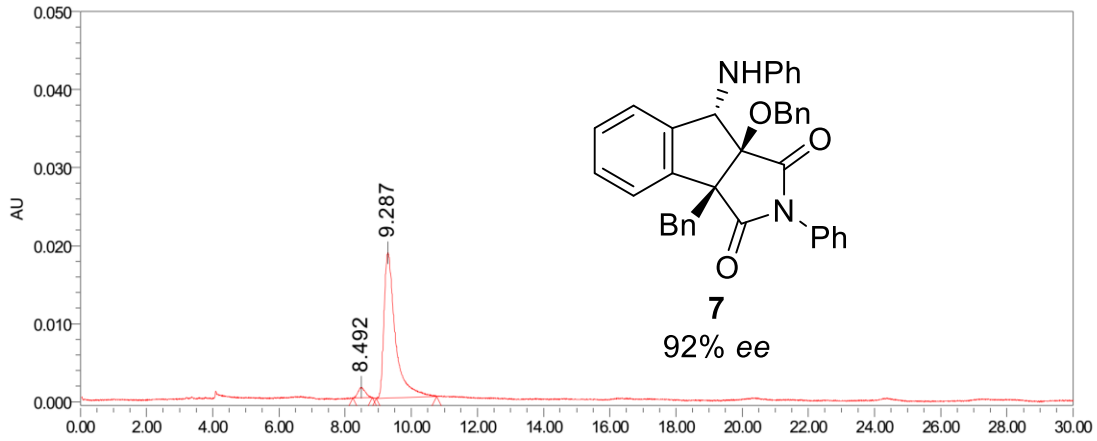

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 13.119 | 218967 | 2648 | 4.17 |
| 2 | 16.957 | 5033265 | 37484 | 95.83 |
| Total | | 5252232 | 40132 | 100.00 |

Condition: hexane: 2-propanol = 99:1

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral IB-3

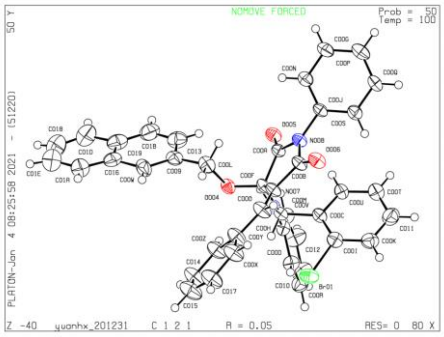


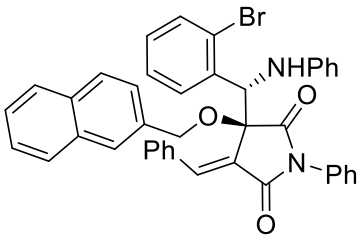

| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 8.549 | 149113 | 9442 | 50.16 |
| 2 | 9.394 | 148144 | 6912 | 49.84 |
| Total | | 297257 | 16354 | 100.00 |




| PDA Ch1 300nm | | | | |
|---|---|---|---|---|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 8.492 | 19734 | 1317 | 4.18 |
| 2 | 9.287 | 451851 | 18649 | 95.82 |
| Total | | 471585 | 19966 | 100.00 |

## Crystallographic Data for 4u.






**(*S*,*S*)-4u**
**CCDC:2070768**

## Datablock: yuanhx_201231

Bond precision: C-C = 0.0103 A Wavelength=1.54184

Cell: a=17.0243(1) b=11.2874(1) c=19.8460(2)
alpha=90 beta=90.530(1) gamma=90
Temperature: 100 K

| | Calculated | Reported |
|---|---|---|
| Volume | 3813.45(6) | 3813.45(6) |
| Space group | C 2 | C 1 2 1 |
| Hall group | C 2y | C 2y |
| Moiety formula | C41 H31 Br N2 O3 [+ solvent] | C41 H31 Br N2 O3 |
| Sum formula | C41 H31 Br N2 O3 [+ solvent] | C41 H31 Br N2 O3 |
| Mr | 679.58 | 679.59 |
| Dx,g cm-3 | 1.184 | 1.184 |
| Z | 4 | 4 |
| Mu (mm-1) | 1.758 | 1.758 |
| F000 | 1400.0 | 1400.0 |
| F000' | 1400.91 | |
| h,k,lmax | 21,14,25 | 21,13,25 |
| Nref | 8025[ 4223] | 7732 |
| Tmin,Tmax | 0.689,0.839 | 0.797,1.000 |
| Tmin' | 0.614 | |

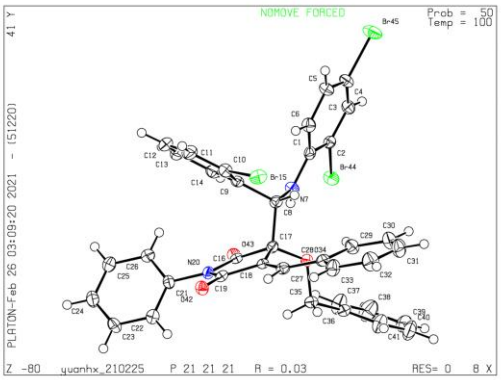
Correction method= # Reported T Limits: Tmin=0.797 Tmax=1.000
AbsCorr = MULTI-SCAN

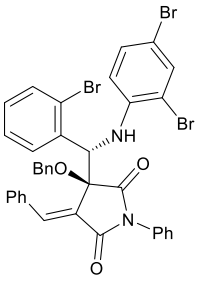
Data completeness= 1.83/0.96 Theta(max)= 76.796

R(reflections)= 0.0545( 7535) wR2(reflections)= 0.1502( 7732)

S = 1.066 Npar= 424

## Crystallographic Data for 6.




**(*S*,*S*)-6**
**CCDC:2070773**

## Datablock: yuanhx_210225

Bond precision: C-C = 0.0063 A Wavelength=1.54184

Cell: a=8.4292(1) b=17.2642(1) c=22.5485(2)
alpha=90 beta=90 gamma=90
Temperature: 100 K

| | Calculated | Reported |
|---|---|---|
| Volume | 3281.34(5) | 3281.33(5) |
| Space group | P 21 21 21 | P 21 21 21 |
| Hall group | P 2ac 2ab | P 2ac 2ab |
| Moiety formula | C37 H27 Br3 N2 O3 | C37 H27 Br3 N2 O3 |
| Sum formula | C37 H27 Br3 N2 O3 | C37 H27 Br3 N2 O3 |
| Mr | 787.31 | 787.33 |
| Dx,g cm-3 | 1.594 | 1.594 |
| Z | 4 | 4 |
| Mu (mm-1) | 4.876 | 4.876 |
| F000 | 1568.0 | 1568.0 |
| F000' | 1563.24 | |
| h,k,lmax | 10,21,28 | 10,21,27 |
| Nref | 6949[ 3913] | 6776 |
| Tmin,Tmax | 0.746,0.784 | 0.807,1.000 |
| Tmin' | 0.614 | |

Correction method= # Reported T Limits: Tmin=0.807 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.73/0.98 Theta(max)= 76.960

R(reflections)= 0.0320( 6367) wR2(reflections)= 0.0741( 6776)

S = 1.067 Npar= 406