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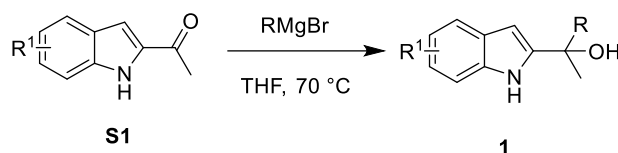
1. General information

^1H and ^{13}C NMR spectra were measured at 400 and 100 MHz, respectively. The solvents used for NMR spectroscopy were CDCl_3 , using tetramethylsilane as the internal reference. HRMS (ESI) was determined by a HRMS/MS instrument. Enantiomeric excesses (*ee*) were determined by chiral high-performance liquid chromatography (chiral HPLC). The chiral columns used for the determination of enantiomeric excesses by chiral HPLC were Chiralpak columns. Optical rotation values were measured with instruments operating at $\lambda = 589$ nm, corresponding to the sodium D line at the temperatures indicated. The X-ray source used for the single crystal X-ray diffraction analysis of compound **3aa** were $\text{GaK}\alpha$ ($\lambda = 1.34139$), and the thermal ellipsoid was drawn at the 30% probability level. Analytical grade solvents for the column chromatography were distilled before use. All starting materials commercially available were used directly. Substrates **1-2** were synthesized according to the literature methods.¹

2. Synthetic procedures and characterization data of substrates **1** and **8**

Substrates **1a**¹ and **2** are known compounds. Substrates **1b-1g**, **8** were prepared following the **Typical Procedure A**.

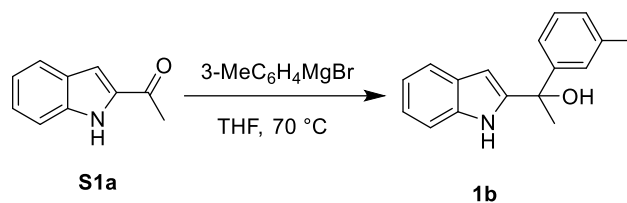
Synthesis of substrate **1b-1g**:



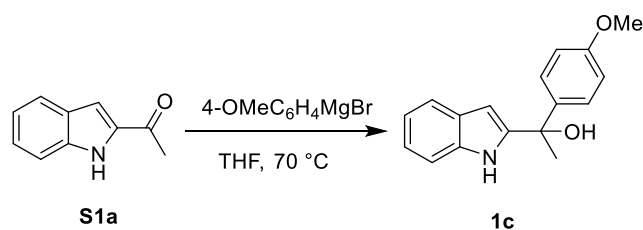
Typical Procedure A: Under argon atmosphere, RMgBr (20 mmol) was added to a flame-dried Schlenk bottle. The solution of **S1** (10 mmol) in anhydrous THF (20 mL) was added to the

¹ a) Y. Zhou, X.-P. Xu and S.-J. Ji, Cooperation of Mn(III)/Brønsted Acid for the Synthesis of Quindoline Derivatives via Dehydroxylation/Azidation/Cyclization Cascade of Diaryl(1*H*-indol-2-yl)methanols with Trimethylsilyl Azide, *Org. Lett.* 2019, **21**, 2039; b) J. Mao, H. Zhang, X.-F. Ding, X. Luo and W.-P. Deng, Synergistic Catalysis for Asymmetric [3 + 2] Cycloadditions of 2-Indolylmethanols with α,β -Unsaturated Aldehydes, *J. Org. Chem.* 2019, **84**, 11186; c) Z. Tang, G. Hong, C. Hu, Q. Wang, Y. Zhong, Y. Gong, P. Yang and L. Wang, $\text{La}(\text{OTf})_3$ Facilitated Self-Condensation of 2-Indolylmethanol: Construction of Highly Substituted Indeno[1,2-*b*]indoles, *Org. Biomol. Chem.* 2021, **19**, 10337; d) T.-Z. Li, S.-J. Liu, Y.-W. Sun, S. Deng, W. Tan, Y. Jiao, Y.-C. Zhang and F. Shi, Regio- and Enantioselective (3+3) Cycloaddition of Nitrones with 2-Indolylmethanols Enabled by Cooperative Organocatalysis, *Angew. Chem. Int. Ed.* 2021, **60**, 2355.

mixture at 0 °C, then the reaction mixture was stirred at 70 °C overnight. After the completion of the reaction indicated by TLC, the reaction mixture was quenched by saturated ammonium chloride solution and was extracted by ethyl acetate for three times. The combined organic layer was dried by anhydrous sodium sulfate, which was concentrated under the reduced pressure. The resulted residue was purified through flash chromatography on silica gel (petroleum ether/ethyl acetate = 20/1) to afford the pure **1**.

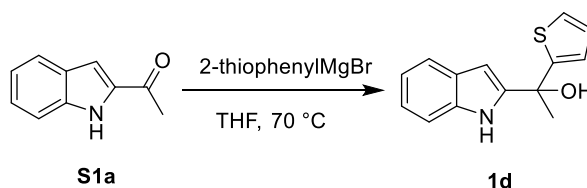


Typical Procedure A: Under argon atmosphere, 3-MeC₆H₄MgBr (20 mL, 1.0mol/L in THF) was added to a flame-dried Schlenk bottle. The solution of **S1a** (1.59 g, 10 mmol) in anhydrous THF (20 mL) was added to the mixture at 0 °C, then the reaction mixture was stirred at 70 °C overnight. After the completion of the reaction indicated by TLC, the reaction mixture was quenched by saturated ammonium chloride solution and was extracted by ethyl acetate for three times. The combined organic layer was dried by anhydrous sodium sulfate, which was concentrated under the reduced pressure. The resulted residue was purified through flash chromatography on silica gel (petroleum ether/ethyl acetate = 20/1) to afford the pure **1b** (1.8 g, 72% yield) as a brown solid; m.p. 156.9 – 157.3 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.16 (s, 1H), 7.60 (d, *J* = 7.6 Hz, 1H), 7.30 – 7.26 (m, 2H), 7.26 – 7.20 (m, 2H), 7.19 – 7.13 (m, 1H), 7.12 – 7.07 (m, 2H), 6.50 (s, 1H), 2.33 (s, 3H), 2.28 (s, 1H), 2.01 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 145.7, 144.2, 138.0, 136.0, 128.3, 128.2, 128.0, 125.9, 122.4, 122.1, 120.6, 119.8, 111.0, 99.6, 73.3, 30.9, 21.6; IR (KBr): 3496, 3319, 2981, 1605, 1456, 1417, 1291, 1142, 923, 746 cm⁻¹; ESI FTMS exact mass calcd for (C₁₇H₁₇NO+Na)⁺ requires m/z 274.1202, found m/z 274.1199.

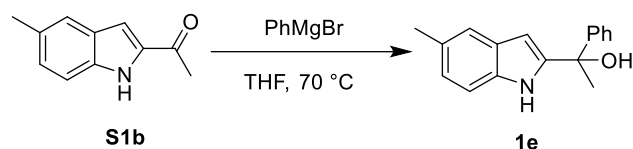


Typical Procedure A: Under argon atmosphere, 4-OMeC₆H₄MgBr (20 mL, 1.0mol/L in THF) was added to a flame-dried Schlenk bottle. The solution of **S1a** (1.59 g, 10 mmol) in anhydrous

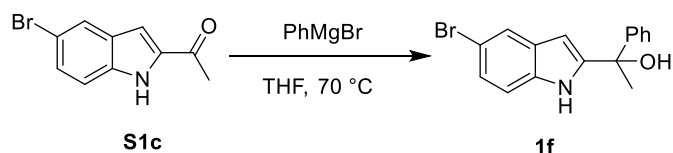
THF (20 mL) was added to the mixture at 0 °C, then the reaction mixture was stirred at 70 °C overnight. After the completion of the reaction indicated by TLC, the reaction mixture was quenched by saturated ammonium chloride solution and was extracted by ethyl acetate for three times. The combined organic layer was dried by anhydrous sodium sulfate, which was concentrated under the reduced pressure. The resulted residue was purified through flash chromatography on silica gel (petroleum ether/ethyl acetate = 20/1) to afford the pure **1c** (2.1 g, 79% yield) as a brown solid; m.p. 117.1 – 117.8 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.20 (s, 1H), 7.59 (d, *J* = 7.6 Hz, 1H), 7.37 (d, *J* = 8.4 Hz, 2H), 7.29 – 7.26 (m, 1H), 7.18 – 7.13 (m, 1H), 7.12 – 7.07 (m, 1H), 6.85 (d, *J* = 8.8 Hz, 2H), 6.49 – 6.43 (m, 1H), 3.79 (s, 3H), 2.31 (s, 1H), 2.00 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 159.9, 153.2, 140.1, 136.3, 135.6, 132.6, 128.9, 128.0, 127.9, 124.7, 119.4, 116.8, 116.3, 112.3, 61.9, 39.3, 21.7; IR (KBr): 3334, 2931, 1608, 1508, 1457, 1339, 1290, 1249, 1176, 748 cm⁻¹; ESI FTMS exact mass calcd for (C₁₇H₁₇NO₂+Na)⁺ requires *m/z* 290.1151, found *m/z* 290.1146.



Typical Procedure A: Under argon atmosphere, 2-thiophenylMgBr (20 mL, 1.0 mol/L in THF) was added to a flame-dried Schlenk bottle. The solution of **S1a** (1.59 g, 10 mmol) in anhydrous THF (20 mL) was added to the mixture at 0 °C, then the reaction mixture was stirred at 70 °C overnight. After the completion of the reaction indicated by TLC, the reaction mixture was quenched by saturated ammonium chloride solution and was extracted by ethyl acetate for three times. The combined organic layer was dried by anhydrous sodium sulfate, which was concentrated under the reduced pressure. The resulted residue was purified through flash chromatography on silica gel (petroleum ether/ethyl acetate = 20/1) to afford the pure **1d** (1.8 g, 74% yield) as a brown solid; m.p. 102.6 – 102.8 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.37 (s, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.32 (d, *J* = 8.0 Hz, 1H), 7.27 (s, 1H), 7.21 – 7.17 (m, 1H), 7.13 – 7.09 (m, 1H), 6.96 – 6.93 (m, 2H), 6.48 – 6.46 (m, 1H), 2.58 (s, 1H), 2.11 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 150.9, 143.3, 135.7, 128.1, 126.8, 125.0, 124.1, 122.2, 120.7, 119.9, 111.1, 99.2, 72.0, 31.7; IR (KBr): 3400, 3055, 2978, 1456, 1373, 1290, 1233, 1098, 793, 745 cm⁻¹; ESI FTMS exact mass calcd for (C₁₄H₁₃NOS+Na)⁺ requires *m/z* 266.0610, found *m/z* 266.0605.

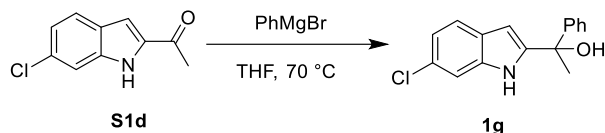


Typical Procedure A: Under argon atmosphere, PhMgBr (7.1 mL, 2.8 mol/L in THF) was added to a flame-dried Schlenk bottle. The solution of **S1b** (1.72 g, 10 mmol) in anhydrous THF (20 mL) was added to the mixture at 0 °C, then the reaction mixture was stirred at 70 °C overnight. After the completion of the reaction indicated by TLC, the reaction mixture was quenched by saturated ammonium chloride solution and was extracted by ethyl acetate for three times. The combined organic layer was dried by anhydrous sodium sulfate, which was concentrated under the reduced pressure. The resulted residue was purified through flash chromatography on silica gel (petroleum ether/ethyl acetate = 20/1) to afford the pure **1e** (1.5 g, 60% yield) as a brown solid; m.p. 154.3 – 154.6 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.07 (s, 1H), 7.48 – 7.42 (m, 2H), 7.38 (s, 1H), 7.35 – 7.26 (m, 3H), 7.16 (d, *J* = 8.4 Hz, 1H), 6.99 (d, *J* = 8.4 Hz, 1H), 6.42 (s, 1H), 2.43 (s, 3H), 2.30 (s, 1H), 2.01 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 145.9, 144.1, 134.3, 129.1, 128.3, 128.2, 127.4, 125.3, 123.7, 120.2, 110.6, 99.2, 73.4, 30.9, 21.4; IR (KBr): 3852, 3438, 3025, 2918, 1669, 1447, 1312, 1293, 1026, 738 cm⁻¹; ESI FTMS exact mass calcd for (C₁₇H₁₇NO+Na)⁺ requires m/z 274.1202, found m/z 274.1201.



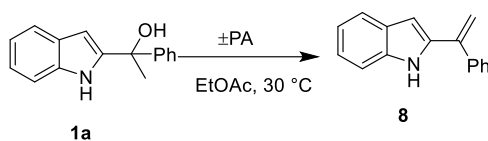
Typical Procedure A: Under argon atmosphere, PhMgBr (7.1 mL, 2.8 mol/L in THF) was added to a flame-dried Schlenk bottle. The solution of **S1c** (2.37 g, 10 mmol) in anhydrous THF (20 mL) was added to the mixture at 0 °C, then the reaction mixture was stirred at 70 °C overnight. After the completion of the reaction indicated by TLC, the reaction mixture was quenched by saturated ammonium chloride solution and was extracted by ethyl acetate for three times. The combined organic layer was dried by anhydrous sodium sulfate, which was concentrated under the reduced pressure. The resulted residue was purified through flash chromatography on silica gel (petroleum ether/ethyl acetate = 20/1) to afford the pure **1f** (2.3 g, 73% yield); brown solid; m.p. 92.4 – 93.3 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.29 (s, 1H), 7.71 (s, 1H), 7.45 – 7.39 (m, 2H), 7.36 – 7.27 (m, 3H), 7.23 (d, *J* = 8.4 Hz, 1H), 7.09 (d, *J* = 8.4 Hz, 1H), 6.40 (s, 1H), 2.48 (s, 1H), 1.99 (s, 3H); ¹³C NMR

(100 MHz, CDCl₃) δ 145.5, 145.4, 134.5, 129.7, 128.6, 128.5, 128.4, 127.6, 125.2, 124.9, 123.1, 112.4, 99.2, 73.3, 30.8; IR (KBr): 3649, 3420, 2978, 1749, 1576, 1446, 1405, 1305, 1050, 700 cm⁻¹; ESI FTMS exact mass calcd for (C₁₆H₁₄BrNO+H)⁺ requires m/z 316.0332, found m/z 316.0351.



Typical Procedure A: Under argon atmosphere, PhMgBr (7.1 mL, 2.8 mol/L in THF) was added to a flame-dried Schlenk bottle. The solution of **S1d** (1.93 g, 10 mmol) in anhydrous THF (20 mL) was added to the mixture at 0 °C, then the reaction mixture was stirred at 70 °C overnight. After the completion of the reaction indicated by TLC, the reaction mixture was quenched by saturated ammonium chloride solution and was extracted by ethyl acetate for three times. The combined organic layer was dried by anhydrous sodium sulfate, which was concentrated under the reduced pressure. The resulted residue was purified through flash chromatography on silica gel (petroleum ether/ethyl acetate = 20/1) to afford the pure **1g** (1.6 g, 59% yield); brown solid; m.p. 100.4 – 100.7 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.14 (s, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.43 – 7.36 (m, 2H), 7.32 – 7.27 (m, 3H), 7.21 – 7.14 (m, 1H), 7.15 – 7.07 (m, 1H), 6.49 (s, 1H), 2.29 (s, 1H), 2.00 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 144.4, 143.5, 136.1, 133.3, 128.4, 127.9, 126.9, 122.4, 120.7, 120.0, 111.0, 99.9, 73.1, 31.0; IR (KBr): 3745, 3056, 1701, 1610, 1508, 1447, 1321, 1240, 1061, 699 cm⁻¹; ESI FTMS exact mass calcd for (C₁₆H₁₄ClNO-H)⁻ requires m/z 270.0691, found m/z 270.0706.

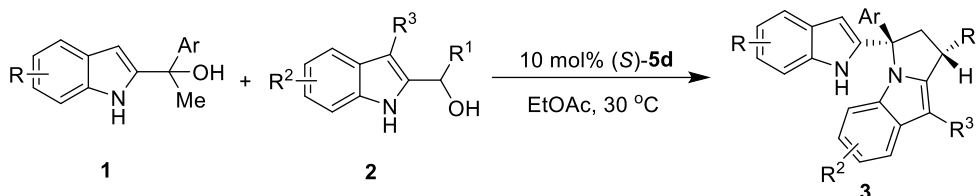
Synthesis of substrate **8**:



2-Indole methanol **1a** (47.4 mg, 0.2 mmol), 1,1'-Binaphthyl-2,2'-diyl hydrogenphosphate (7.0 mg, 0.1 mmol) were added to a reaction tube. Then, ethyl acetate (2 mL) was added to the reaction mixture, which was stirred at 30 °C for 1 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was concentrated under reduced pressure and the residue was purified through flash column chromatography (petroleum ether/dichloromethane = 2:1) on silica gel to afford pure compound **8** in 98% yield (42.9 mg); ¹H NMR (400 MHz, CDCl₃) δ 8.12 (s, 1H), 7.59 (d, *J* = 7.9 Hz, 1H), 7.54 – 7.48 (m, 2H), 7.45 – 7.39 (m, 3H), 7.34 (d, *J* = 8.1 Hz, 1H), 7.24 – 7.18 (m, 1H), 7.15 – 7.09 (m, 1H), 6.53 (s, 1H), 5.62 (s, 1H), 5.39 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 141.7,

140.1, 137.8, 136.5, 128.7, 128.6, 128.4, 128.3, 122.7, 120.9, 120.2, 112.8, 110.8, 103.4; ESI FTMS exact mass calcd for (C₁₆H₁₃NO+H)⁺ requires m/z 220.1121, found m/z 220.1110.

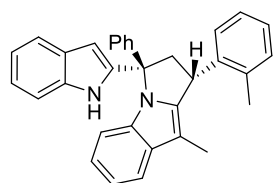
3. General procedure for the synthesis of products 3



Methyl-substituted 2-indolylmethanol **1** (0.1 mmol), 3-alkyl(aryl)-2-indolylmethanol **2** (0.2 mmol), and catalyst (*S*)-**5d** (0.01 mmol) were added to a reaction tube. Then, ethyl acetate (1 mL) was added to the reaction mixture, which was stirred at 30 °C for 5 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography on silica gel to afford pure products **3**.

4. Synthetic procedures and characterization data of products 3

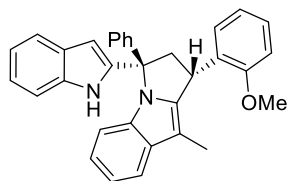
(1*R*,3*R*)-3-(1*H*-indol-2-yl)-9-methyl-3-phenyl-1-(*o*-tolyl)-2,3-dihydro-1*H*-pyrrolo[1,2-*a*]indole (3aa):



Following the general procedure, methyl-substituted 2-indolylmethanol **1a** (23.7 mg, 0.1 mmol), 3-alkyl(aryl)-2-indolylmethanol **2a** (50.2 mg, 0.2 mmol), catalyst (*S*)-**5d** (7.1 mg, 0.01 mmol) were added to a reaction tube. Then, EtOAc (1 mL) was added to the reaction mixture, which was stirred at 30 °C for 5 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (petroleum ether/dichloromethane = 2:1) on silica gel to afford pure compound **3aa** in 95% yield (42.9 mg) as a white solid. m.p. 122.6 – 122.9 °C; > 95:5 dr; [α]_D²⁰ = 39.5 (c = 0.86, acetone); ¹H NMR (400 MHz, CDCl₃) δ 8.09 (s, 1H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.39 – 7.33 (m, 4H), 7.25 – 7.17 (m, 5H), 7.14 – 7.08 (m, 4H), 6.93 – 6.88 (m, 1H), 6.62 (d, *J* = 8.4 Hz, 1H), 6.42 (s, 1H), 4.63 – 4.56 (m, 1H), 3.61 – 3.54 (m, 1H), 3.25 – 3.14 (m, 1H), 2.36 (s, 3H), 2.00 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 141.6, 141.1, 139.3, 136.5, 135.9, 133.6, 132.9, 130.6, 128.6, 128.0, 127.9, 127.0, 126.9, 126.6, 122.5, 121.3, 120.8, 120.1, 119.2, 118.8, 111.2, 110.6, 104.4, 103.1, 68.0, 56.6, 38.8, 19.7, 8.7; IR (KBr):

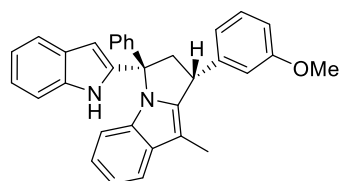
3566, 3055, 1558, 1540, 1489, 1455, 1338, 1312, 1298, 746 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{33}\text{H}_{28}\text{N}_2\text{-H})^+$ requires m/z 451.2179, found m/z 451.2199; The enantiomeric excess: 93%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 90/10, flow rate 1.0 mL/min, T = 30 $^{\circ}\text{C}$, 254 nm): t_{R} = 4.877 (minor), t_{R} = 11.777 (major).

(1*R*,3*R*)-3-(1*H*-indol-2-yl)-1-(2-methoxyphenyl)-9-methyl-3-phenyl-2,3-dihydro-1*H*-pyrrolo[1,2-*a*]indole (3ab):



Following the general procedure, methyl-substituted 2-indolylmethanol **1a** (23.7 mg, 0.1 mmol), 3-alkyl(aryl)-2-indolylmethanol **2b** (53.4 mg, 0.2 mmol), catalyst (*S*)-**5d** (7.1 mg, 0.01 mmol) were added to a reaction tube. Then, EtOAc (1 mL) was added to the reaction mixture, which was stirred at 30 $^{\circ}\text{C}$ for 5 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (petroleum ether/dichloromethane = 2:1) on silica gel to afford pure compound **3ab** in 69% yield (32.3 mg) as a white solid. m.p. 81.5 – 82.0 $^{\circ}\text{C}$; > 95:5 dr; $[\alpha]_{\text{D}}^{20}$ = 37.3 (c = 0.65, acetone); ^1H NMR (400 MHz, CDCl_3) δ 8.17 (s, 1H), 7.57 – 7.52 (m, 2H), 7.38 – 7.32 (m, 3H), 7.31 – 7.26 (m, 2H), 7.21 (d, J = 8.0 Hz, 1H), 7.17 – 7.12 (m, 1H), 7.12 – 7.03 (m, 4H), 6.97 – 6.85 (m, 3H), 6.63 (d, J = 8.0 Hz, 1H), 6.39 (s, 1H), 4.80 – 4.72 (m, 1H), 3.81 (s, 3H), 3.61 – 3.53 (m, 1H), 3.37 – 3.27 (m, 1H), 2.00 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 157.3, 141.6, 141.5, 139.9, 136.4, 133.6, 132.7, 129.1, 128.8, 128.4, 128.1, 127.8, 127.7, 126.9, 122.3, 120.9, 120.7, 119.9, 119.0, 118.5, 111.1, 111.0, 110.6, 104.0, 102.5, 67.9, 56.0, 55.7, 36.3, 8.5; IR (KBr): 3392, 3055, 2961, 2836, 1491, 1455, 1338, 1242, 1028, 746 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{33}\text{H}_{28}\text{N}_2\text{O-H})^+$ requires m/z 467.2129, found m/z 467.2134; The enantiomeric excess: 90%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 90/10, flow rate 1.0 mL/min, T = 30 $^{\circ}\text{C}$, 254 nm): t_{R} = 5.526 (minor), t_{R} = 7.033 (major).

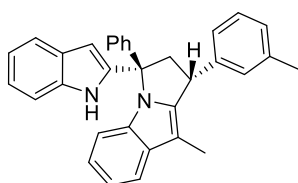
(1*R*,3*R*)-3-(1*H*-indol-2-yl)-1-(3-methoxyphenyl)-9-methyl-3-phenyl-2,3-dihydro-1*H*-pyrrolo[1,2-*a*]indole (3ac):



Following the general procedure, methyl-substituted 2-indolylmethanol **1a** (23.7 mg, 0.1 mmol), 3-alkyl(aryl)-2-indolylmethanol **2c** (53.4 mg, 0.2 mmol), catalyst (*S*)-**5d** (7.1 mg, 0.01 mmol) were added to a reaction tube. Then, EtOAc (1 mL)

was added to the reaction mixture, which was stirred at 30 °C for 5 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (petroleum ether/dichloromethane = 2:1) on silica gel to afford pure compound **3ac** in 92% yield (43.1 mg) as a white solid. m.p. 117.6 – 118.2 °C; > 95:5 dr; $[\alpha]_D^{20} = 42.9$ (c = 0.86, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.12 (s, 1H), 7.60 – 7.53 (m, 2H), 7.40 – 7.33 (m, 3H), 7.31 – 7.27 (m, 1H), 7.24 (s, 1H), 7.21 – 7.15 (m, 1H), 7.14 – 7.03 (m, 4H), 6.94 (d, $J = 7.6$ Hz, 1H), 6.92 – 6.87 (m, 2H), 6.86 – 6.81 (m, 1H), 6.57 (d, $J = 8.0$ Hz, 1H), 6.44 (s, 1H), 4.35 – 4.28 (m, 1H), 3.77 (s, 3H), 3.56 – 3.49 (m, 1H), 3.30 – 3.22 (m, 1H), 2.00 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 160.0, 142.5, 141.4, 140.9, 139.1, 136.5, 133.5, 132.9, 129.8, 128.6, 128.1, 128.0, 127.0, 122.6, 121.4, 120.9, 120.5, 120.2, 119.2, 118.9, 113.7, 112.4, 111.2, 110.5, 104.5, 103.4, 68.0, 58.4, 55.3, 42.3, 8.6; IR (KBr): 3648, 3054, 2935, 1599, 1490, 1455, 1337, 1264, 1155, 741 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{33}\text{H}_{28}\text{N}_2\text{O}-\text{H})^-$ requires m/z 467.2129, found m/z 467.2148; The enantiomeric excess: 94%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 90/10, flow rate 1.0 mL/min, T = 30 °C, 254 nm): $t_R = 5.437$ (minor), $t_R = 9.803$ (major).

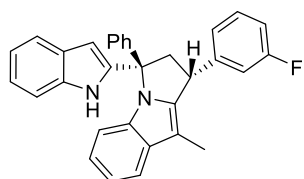
(1*R*,3*R*)-3-(1*H*-indol-2-yl)-9-methyl-3-phenyl-1-(*m*-tolyl)-2,3-dihydro-1*H*-pyrrolo[1,2-*a*]indole (3ad**):**



Following the general procedure, methyl-substituted 2-indolylmethanol **1a** (23.7 mg, 0.1 mmol), 3-alkyl(aryl)-2-indolylmethanol **2d** (50.2 mg, 0.2 mmol), catalyst (*S*)-**5d** (7.1 mg, 0.01 mmol) were added to a reaction tube. Then, EtOAc (1 mL) was added to the reaction mixture, which was stirred at 30 °C for 5 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (petroleum ether/dichloromethane = 2:1) on silica gel to afford pure compound **3ad** in 90% yield (40.7 mg) as a white solid. m.p. 70.4 – 71.1 °C; > 95:5 dr; $[\alpha]_D^{20} = 36.2$ (c = 0.81, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.12 (s, 1H), 7.60 – 7.53 (m, 2H), 7.39 – 7.31 (m, 3H), 7.27 (s, 1H), 7.25 – 7.23 (m, 1H), 7.20 – 7.13 (m, 3H), 7.13 – 7.04 (m, 5H), 6.92 – 6.86 (m, 1H), 6.57 (d, $J = 8.0$ Hz, 1H), 6.44 (s, 1H), 4.33 – 4.26 (m, 1H), 3.55 – 3.47 (m, 1H), 3.30 – 3.20 (m, 1H), 2.33 (s, 3H), 1.97 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 141.7, 140.9, 140.8, 139.2, 138.5, 136.5, 133.5, 132.8, 128.8, 128.7, 128.6, 128.1, 128.0, 127.9, 127.0, 125.1, 122.6, 121.4,

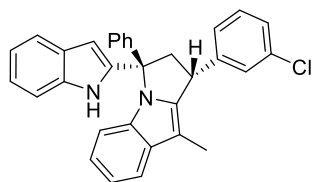
120.9, 120.2, 119.2, 118.8, 111.2, 110.5, 104.5, 103.3, 68.0, 58.5, 42.1, 21.5, 8.5; IR (KBr): 3440, 3382, 3052, 2916, 2862, 1606, 1455, 1338, 1010, 740 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{33}\text{H}_{28}\text{N}_2\text{-H})^+$ requires m/z 451.2179, found m/z 451.2202; The enantiomeric excess: 94%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 90/10, flow rate 1.0 mL/min, T = 30 $^{\circ}\text{C}$, 254 nm): t_{R} = 4.433 (minor), t_{R} = 5.557 (major).

(1*R*,3*R*)-1-(3-fluorophenyl)-3-(1*H*-indol-2-yl)-9-methyl-3-phenyl-2,3-dihydro-1*H*-pyrrolo[1,2-*a*]indole (3ae):



Following the general procedure, methyl-substituted 2-indolylmethanol **1a** (23.7 mg, 0.1 mmol), 3-alkyl(aryl)-2-indolylmethanol **2e** (51.0 mg, 0.2 mmol), catalyst (*S*)-**5d** (7.1 mg, 0.01 mmol) were added to a reaction tube. Then, EtOAc (1 mL) was added to the reaction mixture, which was stirred at 30 $^{\circ}\text{C}$ for 5 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (petroleum ether/dichloromethane = 2:1) on silica gel to afford pure compound **3ae** in 53% yield (24.2 mg) as a white solid. m.p. 77.9 – 78.4 $^{\circ}\text{C}$; > 95:5 dr; $[\alpha]_{\text{D}}^{20}$ = 1.7 (c = 0.48, acetone); ^1H NMR (400 MHz, CDCl_3) δ 8.10 (s, 1H), 7.60 – 7.54 (m, 2H), 7.40 – 7.26 (m, 5H), 7.21 – 7.17 (m, 1H), 7.15 – 7.08 (m, 3H), 7.08 – 7.04 (m, 3H), 7.03 – 6.96 (m, 1H), 6.93 – 6.87 (m, 1H), 6.57 (d, J = 8.0 Hz, 1H), 6.47 – 6.41 (m, 1H), 4.37 – 4.30 (m, 1H), 3.58 – 3.50 (m, 1H), 3.30 – 3.20 (m, 1H), 1.99 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 163.2 (d, J = 244.7 Hz), 143.6, 143.5, 140.7 (d, J = 15.2 Hz), 138.8, 136.5, 133.4, 132.9, 130.3 (d, J = 8.3 Hz), 128.6, 128.1, 127.9, 126.9, 123.7 (d, J = 2.7 Hz), 122.6, 121.6, 120.9, 120.2, 119.3, 118.9, 114.9 (d, J = 21.6 Hz), 114.1 (d, J = 21.0 Hz), 111.2, 110.5, 104.5, 103.5, 67.9, 58.3, 41.9, 8.5; ^{19}F NMR (376 MHz, CDCl_3) δ -112.7; IR (KBr): 3648, 3308, 3056, 2926, 1699, 1616, 1521, 1456, 1263, 747 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{32}\text{H}_{25}\text{FN}_2\text{-H})^+$ requires m/z 455.1929, found m/z 455.1938; The enantiomeric excess: 92%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 90/10, flow rate 1.0 mL/min, T = 30 $^{\circ}\text{C}$, 254 nm): t_{R} = 4.500 (minor), t_{R} = 6.397 (major).

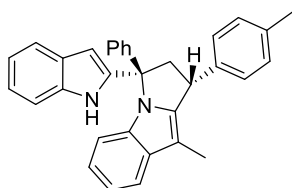
(1*R*,3*R*)-1-(3-chlorophenyl)-3-(1*H*-indol-2-yl)-9-methyl-3-phenyl-2,3-dihydro-1*H*-pyrrolo[1,2-*a*]indole (3af):



Following the general procedure, methyl-substituted 2-indolylmethanol **1a** (23.7 mg, 0.1 mmol), 3-alkyl(aryl)-2-indolylmethanol **2f** (54.2 mg, 0.2 mmol), catalyst (*S*)-**5d** (7.1 mg, 0.01 mmol) were added to a reaction tube. Then, EtOAc (1 mL) was added to the reaction mixture, which was stirred at 30 °C for 5 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (petroleum ether/dichloromethane = 2:1) on silica gel to afford pure compound **3af** in 57% yield (26.9 mg) as a white solid. m.p. 101.9 – 102.8 °C; > 95:5 dr; $[\alpha]_{\text{D}}^{20} = 20.3$ (c = 0.54, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.11 (s, 1H), 7.60 – 7.54 (m, 2H), 7.39 – 7.33 (m, 4H), 7.30 – 7.26 (m, 3H), 7.23 – 7.16 (m, 2H), 7.14 – 7.07 (m, 2H), 7.07 – 7.02 (m, 2H), 6.94 – 6.86 (m, 1H), 6.56 (d, $J = 8.0$ Hz, 1H), 6.44 (s, 1H), 4.34 – 4.28 (m, 1H), 3.57 – 3.47 (m, 1H), 3.29 – 3.16 (m, 1H), 1.99 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 143.0, 140.7, 140.6, 138.8, 136.5, 134.7, 133.4, 132.9, 130.1, 128.6, 128.1, 127.9, 127.4, 126.9, 126.3, 122.7, 121.7, 120.9, 120.2, 119.3, 119.0, 111.2, 110.5, 104.6, 103.6, 68.0, 58.4, 41.9, 8.6; IR (KBr): 3734, 3056, 2917, 1596, 1521, 1455, 1338, 1311, 1010, 739 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{32}\text{H}_{25}\text{ClN}_2\text{-H})^+$ requires m/z 471.1633, found m/z 471.1625; The enantiomeric excess: 94%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 90/10, flow rate 1.0 mL/min, T = 30 °C, 254 nm): $t_{\text{R}} = 4.900$ (minor), $t_{\text{R}} = 7.373$ (major).

(1*R*,3*R*)-3-(1*H*-indol-2-yl)-9-methyl-3-phenyl-1-(*p*-tolyl)-2,3-dihydro-1*H*-pyrrolo[1,2-*a*]indole

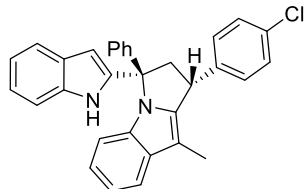
(3ag):



Following the general procedure, methyl-substituted 2-indolylmethanol **1a** (23.7 mg, 0.1 mmol), 3-alkyl(aryl)-2-indolylmethanol **2g** (50.2 mg, 0.2 mmol), catalyst (*S*)-**5d** (7.1 mg, 0.01 mmol) were added to a reaction tube. Then, EtOAc (1 mL) was added to the reaction mixture, which was stirred at 30 °C for 5 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (petroleum ether/dichloromethane = 2:1) on silica gel to afford pure compound **3ag** in 80% yield (36.2 mg) as a white solid. m.p. 89.2 – 90.5 °C; > 95:5 dr; $[\alpha]_{\text{D}}^{20} = 27.1$ (c = 0.72, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.11 (s, 1H), 7.61 – 7.52 (m, 2H), 7.39 – 7.32 (m, 3H), 7.26 – 7.22 (m, 3H), 7.21 – 7.15 (m, 3H), 7.15 – 7.05 (m, 4H), 6.92 – 6.85 (m, 1H), 6.57 (d, $J = 8.4$ Hz, 1H), 6.45 (s, 1H), 4.34 – 4.27 (m, 1H), 3.57 – 3.46 (m, 1H), 3.30 – 3.19 (m, 1H),

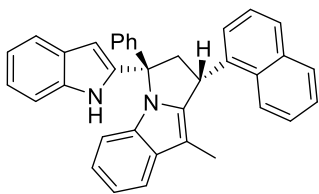
2.38 (s, 3H), 1.97 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 141.7, 140.8, 139.2, 137.7, 136.7, 136.5, 133.4, 132.8, 129.5, 128.5, 128.0, 127.9, 126.9, 122.5, 121.3, 120.8, 120.1, 119.1, 118.7, 111.1, 110.4, 104.4, 103.2, 67.9, 58.6, 41.8, 21.1, 8.4; IR (KBr): 3648, 3050, 2916, 2862, 1699, 1558, 1455, 1339, 1299, 748 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{33}\text{H}_{28}\text{N}_2\text{-H})^-$ requires m/z 451.2179, found m/z 451.2179; The enantiomeric excess: 85%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 90/10, flow rate 1.0 mL/min, $T = 30^\circ\text{C}$, 254 nm): $t_{\text{R}} = 4.350$ (minor), $t_{\text{R}} = 4.953$ (major).

(1*R*,3*R*)-1-(4-chlorophenyl)-3-(1*H*-indol-2-yl)-9-methyl-3-phenyl-2,3-dihydro-1*H*-pyrrolo[1,2-*a*]indole (3ah):



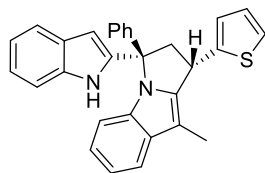
Following the general procedure, methyl-substituted 2-indolylmethanol **1a** (23.7 mg, 0.1 mmol), 3-alkyl(aryl)-2-indolylmethanol **2h** (54.2 mg, 0.2 mmol), catalyst (*S*)-**5d** (7.1 mg, 0.01 mmol) were added to a reaction tube. Then, EtOAc (1 mL) was added to the reaction mixture, which was stirred at 30°C for 5 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (petroleum ether/dichloromethane = 2:1) on silica gel to afford pure compound **3ah** in 78% yield (36.8 mg) as a white solid. m.p. $98.7 - 99.9^\circ\text{C}$; $> 95:5$ dr; $[\alpha]_{\text{D}}^{20} = 3.5$ ($c = 0.74$, acetone); ^1H NMR (400 MHz, CDCl_3) δ 8.10 (s, 1H), 7.61 – 7.53 (m, 2H), 7.39 – 7.31 (m, 5H), 7.31 – 7.27 (m, 2H), 7.25 (s, 1H), 7.22 – 7.16 (m, 1H), 7.15 – 7.07 (m, 2H), 7.07 – 7.01 (m, 2H), 6.93 – 6.86 (m, 1H), 6.57 (d, $J = 8.4$ Hz, 1H), 6.45 (s, 1H), 4.37 – 4.26 (m, 1H), 3.56 – 3.47 (m, 1H), 3.28 – 3.15 (m, 1H), 1.97 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 141.0, 140.6, 139.4, 138.8, 136.5, 133.4, 132.9, 132.8, 129.3, 129.0, 128.6, 128.1, 127.9, 126.9, 122.6, 121.6, 120.8, 120.2, 119.3, 118.9, 111.1, 110.5, 104.5, 103.4, 67.9, 58.4, 41.6, 8.5; IR (KBr): 3734, 3056, 1733, 1489, 1456, 1338, 1262, 1089, 1013, 747 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{32}\text{H}_{25}\text{ClN}_2\text{-H})^-$ requires m/z 471.1633, found m/z 471.1633; The enantiomeric excess: 81%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 90/10, flow rate 1.0 mL/min, $T = 30^\circ\text{C}$, 254 nm): $t_{\text{R}} = 4.866$ (minor), $t_{\text{R}} = 6.276$ (major).

(1*R*,3*R*)-3-(1*H*-indol-2-yl)-9-methyl-1-(naphthalen-1-yl)-3-phenyl-2,3-dihydro-1*H*-pyrrolo[1,2-*a*]indole (3ai):



Following the general procedure, methyl-substituted 2-indolylmethanol **1a** (23.7 mg, 0.1 mmol), 3-alkyl(aryl)-2-indolylmethanol **2i** (57.4 mg, 0.2 mmol), catalyst (*S*)-**5d** (7.1 mg, 0.01 mmol) were added to a reaction tube. Then, EtOAc (1 mL) was added to the reaction mixture, which was stirred at 30 °C for 5 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (petroleum ether/dichloromethane = 2:1) on silica gel to afford pure compound **3ai** in 84% yield (41.0 mg) as a white solid. m.p. 142.6 – 142.9 °C; > 95:5 dr; $[\alpha]_D^{20} = 114.1$ (c = 0.82, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.09 (s, 1H), 8.04 – 7.96 (m, 1H), 7.96 – 7.88 (m, 1H), 7.80 (d, $J = 8.0$ Hz, 1H), 7.63 (d, $J = 8.0$ Hz, 1H), 7.58 – 7.48 (m, 4H), 7.44 – 7.35 (m, 4H), 7.22 – 7.05 (m, 6H), 6.99 – 6.90 (m, 1H), 6.69 (d, $J = 8.4$ Hz, 1H), 6.35 (s, 1H), 5.37 – 5.06 (m, 1H), 3.89 – 3.64 (m, 1H), 3.48 – 3.11 (m, 1H), 2.06 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 141.3, 141.1, 139.1, 136.3, 133.7, 133.0, 131.5, 129.1, 128.7, 128.0, 127.8, 126.9, 126.3, 125.7, 122.4, 121.3, 120.8, 120.0, 119.3, 118.9, 111.1, 110.7, 104.2, 103.6, 68.1, 57.4, 30.6, 9.0; IR (KBr): 3441, 3054, 2914, 1558, 1540, 1455, 1396, 1338, 1302, 746 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{36}\text{H}_{28}\text{N}_2\text{-H})^-$ requires m/z 487.2179, found m/z 487.2176; The enantiomeric excess: 93%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 90/10, flow rate 1.0 mL/min, T = 30 °C, 254 nm): $t_{\text{R}} = 6.717$ (minor), $t_{\text{R}} = 20.137$ (major).

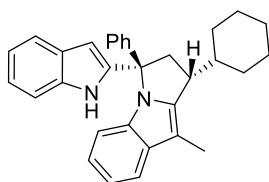
(1S,3R)-3-(1H-indol-2-yl)-9-methyl-3-phenyl-1-(thiophen-2-yl)-2,3-dihydro-1H-pyrrolo[1,2-a]indole (3aj):



Following the general procedure, methyl-substituted 2-indolylmethanol **1a** (23.7 mg, 0.1 mmol), 3-alkyl(aryl)-2-indolylmethanol **2j** (48.6 mg, 0.2 mmol), catalyst (*S*)-**5d** (7.1 mg, 0.01 mmol) were added to a reaction tube. Then, EtOAc (1 mL) was added to the reaction mixture, which was stirred at 30 °C for 5 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (petroleum ether/dichloromethane = 2:1) on silica gel to afford pure compound **3aj** in 93% yield (41.3 mg) as a white solid. m.p. 123.6 – 124.0 °C; > 95:5 dr; $[\alpha]_D^{20} = 12.7$ (c = 0.83, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.12 (s, 1H), 7.60 – 7.54 (m, 2H), 7.39 – 7.32 (m, 3H), 7.26 – 7.22 (m, 2H), 7.20 – 7.16 (m, 1H), 7.14 – 7.04 (m, 4H), 7.02 – 6.96 (m, 2H), 6.93 – 6.84 (m, 1H), 6.55 (d, $J = 8.0$ Hz, 1H), 6.43 (s, 1H), 4.73 – 4.63 (m,

1H), 3.63 – 3.53 (m, 1H), 3.40 – 3.31 (m, 1H), 2.08 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 144.6, 140.9, 140.6, 138.8, 136.5, 133.4, 132.6, 128.5, 128.0, 127.8, 126.9, 126.7, 125.4, 124.5, 122.5, 121.6, 120.8, 120.1, 119.2, 118.9, 111.2, 110.5, 104.5, 103.8, 67.7, 58.9, 37.3, 8.4; IR (KBr): 3648, 3566, 3055, 2915, 1683, 1558, 1455, 1338, 1303, 745 cm⁻¹; ESI FTMS exact mass calcd for (C₃₀H₂₄N₂S-H)⁻ requires m/z 443.1587, found m/z 443.1584; The enantiomeric excess: 85%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 90/10, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 5.356 (minor), t_R = 6.566 (major).

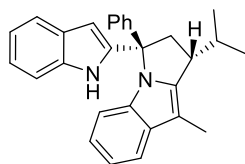
(1R,3R)-1-cyclohexyl-3-(1H-indol-2-yl)-9-methyl-3-phenyl-2,3-dihydro-1H-pyrrolo[1,2-a]indole (3ak):



Following the general procedure, methyl-substituted 2-indolylmethanol **1a** (23.7 mg, 0.1 mmol), 3-alkyl(aryl)-2-indolylmethanol **2k** (48.6 mg, 0.2 mmol), catalyst (*S*)-**5d** (7.1 mg, 0.01 mmol) were added to a reaction tube.

Then, EtOAc (1 mL) was added to the reaction mixture, which was stirred at 30 °C for 5 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (petroleum ether/dichloromethane = 2:1) on silica gel to afford pure compound **3ak** in 95% yield (42.2 mg) as a white solid. m.p. 117.7 – 118.3 °C; > 95:5 dr; [α]_D²⁰ = 16.7 (c = 0.84, acetone); ¹H NMR (400 MHz, CDCl₃) δ 8.03 (s, 1H), 7.62 – 7.56 (m, 2H), 7.34 – 7.28 (m, 3H), 7.24 – 7.21 (m, 1H), 7.21 – 7.11 (m, 2H), 7.09 – 7.04 (m, 1H), 7.04 – 6.98 (m, 2H), 6.87 – 6.78 (m, 1H), 6.53 – 6.45 (m, 2H), 3.30 – 3.22 (m, 1H), 3.20 – 3.12 (m, 1H), 3.11 – 3.03 (m, 1H), 2.38 (s, 3H), 2.22 – 2.10 (m, 1H), 1.82 – 1.68 (m, 4H), 1.38 – 1.07 (m, 6H); ¹³C NMR (100 MHz, CDCl₃) δ 141.7, 141.4, 140.2, 136.4, 133.6, 132.6, 128.3, 128.0, 127.7, 126.9, 122.3, 120.9, 120.7, 120.1, 118.9, 118.3, 111.1, 110.3, 103.8, 102.2, 67.5, 49.3, 42.0, 38.3, 32.0, 27.7, 26.8, 26.6, 26.5, 8.9; IR (KBr): 3437, 3377, 3055, 2923, 2851, 1455, 1339, 1313, 1237, 739 cm⁻¹; ESI FTMS exact mass calcd for (C₃₂H₃₂N₂-H)⁻ requires m/z 443.2492, found m/z 443.2490; The enantiomeric excess: 93%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 90/10, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 4.426 (minor), t_R = 7.963 (major).

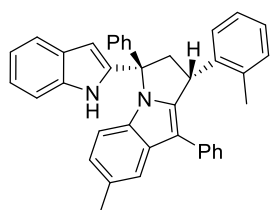
(1R,3R)-3-(1H-indol-2-yl)-1-isopropyl-9-methyl-3-phenyl-2,3-dihydro-1H-pyrrolo[1,2-a]indole (3al):



Following the general procedure, methyl-substituted 2-indolylmethanol **1a** (23.7 mg, 0.1 mmol), 3-alkyl(aryl)-2-indolylmethanol **2l** (40.6 mg, 0.2 mmol), catalyst (*S*)-**5d** (7.1 mg, 0.01 mmol) were added to a reaction tube.

Then, EtOAc (1 mL) was added to the reaction mixture, which was stirred at 30 °C for 5 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (petroleum ether/dichloromethane = 2:1) on silica gel to afford pure compound **3al** in 91% yield (36.8 mg) as a white solid. m.p. 98.4 – 98.7 °C; > 95:5 dr; $[\alpha]_D^{20} = 15.8$ ($c = 0.74$, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.04 (s, 1H), 7.63 – 7.56 (m, 2H), 7.34 – 7.27 (m, 3H), 7.25 – 7.21 (m, 1H), 7.21 – 7.16 (m, 1H), 7.16 – 7.11 (m, 1H), 7.10 – 7.05 (m, 1H), 7.03 – 6.98 (m, 2H), 6.89 – 6.82 (m, 1H), 6.52 – 6.46 (m, 2H), 3.31 – 3.22 (m, 1H), 3.17 – 3.02 (m, 2H), 2.59 – 2.47 (m, 1H), 2.38 (s, 3H), 1.02 (d, $J = 6.8$ Hz, 6H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 142.3, 141.5, 140.1, 136.3, 133.6, 132.5, 128.3, 128.0, 127.7, 126.9, 122.3, 121.0, 120.7, 120.1, 118.9, 118.4, 111.2, 110.3, 103.8, 102.2, 67.4, 48.4, 42.5, 28.0, 21.3, 17.2, 8.9; IR (KBr): 3648, 3055, 2958, 2869, 1558, 1455, 1339, 1305, 1238, 748 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{29}\text{H}_{28}\text{N}_2\text{-H})^+$ requires m/z 403.2179, found m/z 403.2176; The enantiomeric excess: 90%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 90/10, flow rate 1.0 mL/min, T = 30 °C, 254 nm): $t_R = 4.417$ (minor), $t_R = 9.393$ (major).

(1R,3R)-3-(1H-indol-2-yl)-6-methyl-3,9-diphenyl-1-(*o*-tolyl)-2,3-dihydro-1H-pyrrolo[1,2-*a*]indole (3am):

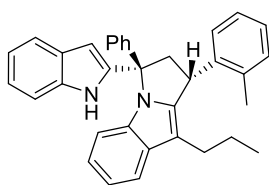


Following the general procedure, methyl-substituted 2-indolylmethanol **1a** (23.7 mg, 0.1 mmol), 3-alkyl(aryl)-2-indolylmethanol **2m** (65.4 mg, 0.2 mmol), catalyst (*S*)-**5d** (7.1 mg, 0.01 mmol) were added to a reaction tube. Then, EtOAc (1 mL) was added to the reaction mixture, which was

stirred at 30 °C for 5 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (petroleum ether/dichloromethane = 2:1) on silica gel to afford pure compound **3am** in 94% yield (49.6 mg) as a white solid. m.p. 119.7 – 120.2 °C; > 95:5 dr; $[\alpha]_D^{20} = 47.9$ ($c = 0.99$, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.11 (s, 1H), 7.72 (s, 1H), 7.54 (d, $J = 7.6$ Hz, 1H), 7.42 – 7.36 (m, 3H), 7.30 – 7.27 (m, 2H), 7.24 (s, 1H), 7.20 – 7.14 (m, 5H), 7.13 – 7.09 (m, 1H), 7.08 – 7.03 (m, 2H), 7.01 – 6.94 (m, 2H), 6.83 – 6.76 (m, 2H), 6.59 (d, $J = 8.0$ Hz, 1H), 6.41 (s, 1H), 4.89 – 4.78 (m, 1H), 3.69 – 3.57

(m, 1H), 3.35 – 3.20 (m, 1H), 2.45 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 142.3, 141.1, 138.9, 136.4, 135.3, 134.5, 131.5, 131.3, 130.2, 129.6, 128.7, 128.3, 128.1, 127.9, 127.8, 126.9, 126.7, 126.0, 125.2, 123.3, 122.5, 120.8, 120.1, 119.7, 111.1, 110.5, 109.5, 104.4, 68.2, 56.4, 53.5, 21.6, 19.7; IR (KBr): 3648, 3442, 3055, 3026, 2920, 1506, 1456, 1294, 1265, 743 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{39}\text{H}_{32}\text{N}_2+\text{Na})^+$ requires m/z 551.2457, found m/z 551.2437; The enantiomeric excess: 91%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 90/10, flow rate 1.0 mL/min, $T = 30\text{ }^\circ\text{C}$, 254 nm): $t_{\text{R}} = 5.380$ (major), $t_{\text{R}} = 6.443$ (minor).

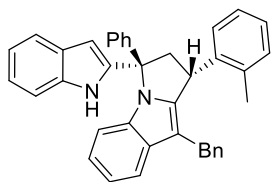
(1R,3R)-3-(1H-indol-2-yl)-3-phenyl-9-propyl-1-(*o*-tolyl)-2,3-dihydro-1H-pyrrolo[1,2-*a*]indole (3an):



Following the general procedure, methyl-substituted 2-indolylmethanol **1a** (23.7 mg, 0.1 mmol), 3-alkyl(aryl)-2-indolylmethanol **2n** (55.8 mg, 0.2 mmol), catalyst (*S*)-**5d** (7.1 mg, 0.01 mmol) were added to a reaction tube. Then, EtOAc (1 mL) was added to the reaction mixture, which was stirred

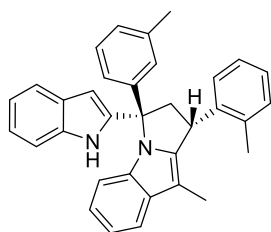
at 30 $^\circ\text{C}$ for 5 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (petroleum ether/dichloromethane = 2:1) on silica gel to afford pure compound **3an** in 86% yield (41.3 mg) as a white solid. m.p. 220.7 – 220.9 $^\circ\text{C}$; > 95:5 dr; $[\alpha]_{\text{D}}^{20} = 44.4$ ($c = 0.83$, acetone); ^1H NMR (400 MHz, CDCl_3) δ 8.13 (s, 1H), 7.63 (d, $J = 8.0$ Hz, 1H), 7.56 (d, $J = 8.0$ Hz, 1H), 7.40 – 7.31 (m, 4H), 7.24 (s, 1H), 7.23 – 7.14 (m, 4H), 7.14 – 7.00 (m, 4H), 6.93 – 6.85 (m, 1H), 6.61 (d, $J = 8.0$ Hz, 1H), 6.45 (s, 1H), 4.64 – 4.47 (m, 1H), 3.62 – 3.47 (m, 1H), 3.22 (s, 1H), 2.61 – 2.48 (m, 1H), 2.35 (s, 3H), 2.31 – 2.19 (m, 1H), 1.60 – 1.53 (m, 1H), 1.51 – 1.43 (m, 1H), 0.75 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 141.9, 141.1, 139.2, 136.4, 135.7, 133.1, 133.0, 130.5, 128.6, 128.0, 127.9, 126.9, 126.8, 126.5, 122.5, 121.1, 120.8, 120.1, 119.2, 119.1, 111.1, 110.7, 108.2, 104.3, 68.0, 56.9, 53.5, 25.9, 23.2, 19.7, 14.0; IR (KBr): 3055, 2955, 2928, 2867, 1490, 1473, 1336, 1265, 1011, 747 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{35}\text{H}_{32}\text{N}_2-\text{H})^-$ requires m/z 479.2492, found m/z 479.2494; The enantiomeric excess: 94%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 90/10, flow rate 1.0 mL/min, $T = 30\text{ }^\circ\text{C}$, 254 nm): $t_{\text{R}} = 4.590$ (minor), $t_{\text{R}} = 8.730$ (major).

(1R,3R)-9-benzyl-3-(1H-indol-2-yl)-3-phenyl-1-(*o*-tolyl)-2,3-dihydro-1H-pyrrolo[1,2-*a*]indole (3ao):



Following the general procedure, methyl-substituted 2-indolylmethanol **1a** (23.7 mg, 0.1 mmol), 3-alkyl(aryl)-2-indolylmethanol **2o** (65.4 mg, 0.2 mmol), catalyst (*S*)-**5d** (7.1 mg, 0.01 mmol) were added to a reaction tube. Then, EtOAc (1 mL) was added to the reaction mixture, which was stirred at 30 °C for 5 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (petroleum ether/dichloromethane = 2:1) on silica gel to afford pure compound **3ao** in 98% yield (51.7 mg) as a white solid. m.p. 80.9 – 81.2 °C; > 95:5 dr; $[\alpha]_D^{20} = 40.6$ ($c = 1.03$, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.13 (s, 1H), 7.60 – 7.51 (m, 2H), 7.42 – 7.35 (m, 3H), 7.35 – 7.26 (m, 2H), 7.22 – 7.09 (m, 8H), 7.08 – 7.03 (m, 3H), 6.98 – 6.94 (m, 2H), 6.93 – 6.87 (m, 1H), 6.64 (d, $J = 8.0$ Hz, 1H), 6.46 (s, 1H), 4.46 – 4.36 (m, 1H), 4.02 – 3.91 (m, 1H), 3.67 – 3.57 (m, 1H), 3.58 – 3.46 (m, 1H), 3.32 – 3.13 (m, 1H), 2.15 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 142.8, 141.2, 141.0, 139.1, 136.4, 135.9, 133.1, 133.0, 130.5, 128.6, 128.4, 128.1, 128.0, 127.9, 126.9, 126.8, 126.5, 125.5, 122.5, 121.3, 120.8, 120.1, 119.5, 119.3, 111.2, 110.7, 106.7, 104.4, 68.2, 56.8, 38.3, 30.1, 19.5; IR (KBr): 3440, 3057, 3024, 2926, 1602, 1453, 1298, 1166, 1048, 745 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{39}\text{H}_{32}\text{N}_2\text{-H})^+$ requires m/z 527.2492, found m/z 527.2500; The enantiomeric excess: 93%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 90/10, flow rate 1.0 mL/min, $T = 30$ °C, 254 nm): $t_R = 5.146$ (minor), $t_R = 9.416$ (major).

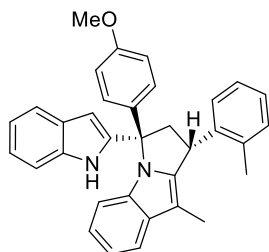
(1*R*,3*R*)-3-(1*H*-indol-2-yl)-9-methyl-3-(*m*-tolyl)-1-(*o*-tolyl)-2,3-dihydro-1*H*-pyrrolo[1,2-*a*]indole (3ba**):**



Following the general procedure, methyl-substituted 2-indolylmethanol **1b** (25.1 mg, 0.1 mmol), 3-alkyl(aryl)-2-indolylmethanol **2a** (50.2 mg, 0.2 mmol), catalyst (*S*)-**5d** (7.1 mg, 0.01 mmol) were added to a reaction tube. Then, EtOAc (1 mL) was added to the reaction mixture, which was stirred at 30 °C for 5 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (petroleum ether/dichloromethane = 2:1) on silica gel to afford pure compound **3ba** in 64% yield (29.8 mg) as a white solid. m.p. 102.8 – 103.7 °C; > 95:5 dr; $[\alpha]_D^{20} = 25.3$ ($c = 0.60$, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.09 (s, 1H), 7.63 – 7.55 (m, 2H), 7.37 – 7.33 (m, 1H), 7.25 – 7.16 (m, 7H), 7.15 – 7.09 (m, 2H), 7.07 (s, 1H), 6.95 – 6.89 (m, 1H), 6.82 (d, $J = 7.2$ Hz, 1H), 6.65 (d, $J = 8.0$ Hz, 1H), 6.44

(s, 1H), 4.68 – 4.60 (m, 1H), 3.64 – 3.56 (m, 1H), 3.28 – 3.18 (m, 1H), 2.40 (s, 3H), 2.37 (s, 3H), 2.03 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 141.6, 141.1, 139.5, 138.9, 138.2, 136.4, 135.8, 133.6, 132.9, 130.6, 128.8, 128.5, 127.9, 127.6, 126.9, 126.5, 123.9, 122.4, 121.2, 120.8, 120.1, 119.1, 118.8, 111.1, 110.6, 104.2, 103.0, 67.9, 56.6, 38.5, 21.8, 19.7, 8.6; IR (KBr): 3648, 3049, 2921, 2860, 1699, 1473, 1455, 1338, 1299, 740 cm⁻¹; ESI FTMS exact mass calcd for (C₃₄H₃₀N₂+Na)⁺ requires m/z 489.2301, found m/z 489.2291; The enantiomeric excess: 92%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 90/10, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 4.783 (minor), t_R = 6.310 (major).

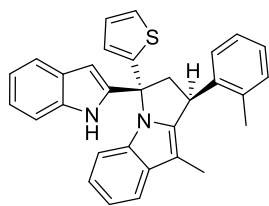
(1R,3R)-3-(1H-indol-2-yl)-3-(4-methoxyphenyl)-9-methyl-1-(o-tolyl)-2,3-dihydro-1H-pyrrolo[1,2-a]indole (3ca):



Following the general procedure, methyl-substituted 2-indolylmethanol **1c** (26.7 mg, 0.1 mmol), 3-alkyl(aryl)-2-indolylmethanol **2a** (50.2 mg, 0.2 mmol), catalyst (*S*)-**5d** (7.1 mg, 0.01 mmol) were added to a reaction tube. Then, EtOAc (1 mL) was added to the reaction mixture, which was stirred at 30 °C for 5 h. After the completion of the reaction which was indicated

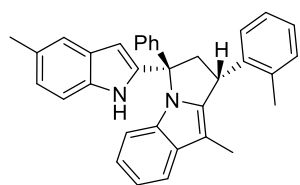
by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (petroleum ether/dichloromethane = 2:1) on silica gel to afford pure compound **3ca** in 98% yield (47.2 mg) as a white solid. m.p. 231.2 – 231.4 °C; > 95:5 dr; [α]_D²⁰ = 30.9 (c = 0.94, acetone); ¹H NMR (400 MHz, CDCl₃) δ 8.08 (s, 1H), 7.58 – 7.52 (m, 2H), 7.34 – 7.30 (m, 1H), 7.25 – 7.22 (m, 1H), 7.22 – 7.14 (m, 4H), 7.12 – 7.06 (m, 2H), 7.00 (d, *J* = 8.4 Hz, 2H), 6.92 – 6.85 (m, 3H), 6.61 (d, *J* = 8.4 Hz, 1H), 6.40 (s, 1H), 4.61 – 4.54 (m, 1H), 3.82 (s, 3H), 3.55 – 3.48 (m, 1H), 3.19 – 3.10 (m, 1H), 2.36 (s, 3H), 1.98 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 159.2, 141.6, 139.7, 136.4, 135.8, 133.6, 133.0, 132.9, 130.6, 128.1, 128.0, 126.9, 126.6, 122.5, 121.2, 120.8, 120.1, 119.1, 118.8, 113.9, 111.2, 110.6, 104.2, 103.0, 67.5, 56.5, 55.3, 38.5, 19.7, 8.6; IR (KBr): 3648, 3049, 2931, 2860, 1699, 1615, 1507, 1456, 1252, 747 cm⁻¹; ESI FTMS exact mass calcd for (C₃₄H₃₀N₂O+Na)⁺ requires m/z 505.2250, found m/z 505.2235; The enantiomeric excess: 89%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 90/10, flow rate 1.0 mL/min, T = 30 °C, 254 nm): t_R = 5.726 (minor), t_R = 7.073 (major).

(1S,3R)-3-(1H-indol-2-yl)-9-methyl-3-(thiophen-2-yl)-1-(o-tolyl)-2,3-dihydro-1H-pyrrolo[1,2-a]indole (3da):



Following the general procedure, methyl-substituted 2-indolylmethanol **1d** (48.6 mg, 0.2 mmol), 3-alkyl(aryl)-2-indolylmethanol **2a** (25.1 mg, 0.1 mmol), catalyst (*R*)-**4e** (14.0 mg, 0.02 mmol) were added to a reaction tube. Then, EtOAc (1 mL) was added to the reaction mixture, which was stirred at 30 °C for 5 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (petroleum ether/dichloromethane = 2:1) on silica gel to afford pure compound **3da** in 52% yield (23.8 mg) as a white solid. m.p. 103.3 – 103.7 °C; > 95:5 dr; $[\alpha]_D^{20} = -78.2$ ($c = 0.48$, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.18 (s, 1H), 7.59 – 7.53 (m, 2H), 7.36 – 7.31 (m, 1H), 7.29 – 7.27 (m, 1H), 7.25 (s, 1H), 7.24 – 7.15 (m, 4H), 7.14 – 7.09 (m, 2H), 7.01 – 6.93 (m, 3H), 6.85 (d, $J = 8.0$ Hz, 1H), 6.50 (s, 1H), 4.84 – 4.76 (m, 1H), 3.70 – 3.62 (m, 1H), 3.11 – 3.01 (m, 1H), 2.44 (s, 3H), 1.97 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 144.9, 141.4, 139.2, 138.7, 136.3, 135.8, 134.1, 132.2, 130.6, 128.0, 126.9, 126.8, 126.6, 125.7, 125.1, 122.5, 121.1, 120.8, 120.1, 119.4, 118.8, 111.1, 111.0, 103.6, 65.3, 57.0, 39.1, 19.6, 8.6; IR (KBr): 3436, 3050, 2916, 2859, 1616, 1489, 1455, 1336, 1238, 741 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{31}\text{H}_{26}\text{N}_2\text{S}+\text{Na})^+$ requires m/z 481.1709, found m/z 481.1695; The enantiomeric excess: 82%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 90/10, flow rate 1.0 mL/min, $T = 30$ °C, 254 nm): $t_R = 5.036$ (major), $t_R = 9.140$ (minor).

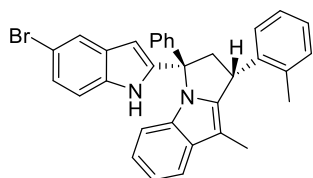
(1R,3R)-9-methyl-3-(5-methyl-1H-indol-2-yl)-3-phenyl-1-(*o*-tolyl)-2,3-dihydro-1H-pyrrolo[1,2-*a*]indole (3ea):



Following the general procedure, methyl-substituted 2-indolylmethanol **1e** (25.1 mg, 0.1 mmol), 3-alkyl(aryl)-2-indolylmethanol **2a** (50.2 mg, 0.2 mmol), catalyst (*S*)-**5d** (7.1 mg, 0.01 mmol) were added to a reaction tube. Then, EtOAc (1 mL) was added to the reaction mixture, which was stirred at 30 °C for 5 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (petroleum ether/dichloromethane = 2:1) on silica gel to afford pure compound **3ea** in 80% yield (37.3 mg) as a white solid. m.p. 123.4 – 124.2 °C; > 95:5 dr; $[\alpha]_D^{20} = 88.5$ ($c = 0.75$, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.00 (s, 1H), 7.59 (d, $J = 8.0$ Hz, 1H), 7.40 – 7.32 (m, 5H), 7.24 – 7.16 (m, 3H), 7.16 – 7.06 (m, 4H), 7.00 (d, $J = 8.4$ Hz, 1H), 6.94 – 6.86 (m,

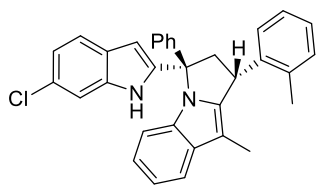
1H), 6.62 (d, $J = 8.0$ Hz, 1H), 6.33 (s, 1H), 4.62 – 4.52 (m, 1H), 3.61 – 3.51 (m, 1H), 3.25 – 3.13 (m, 1H), 2.44 (s, 3H), 2.35 (s, 3H), 1.99 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 141.6, 141.1, 139.5, 139.4, 139.3, 135.9, 134.8, 133.7, 133.6, 133.0, 132.9, 130.6, 129.4, 128.6, 128.2, 128.0, 126.9, 126.6, 124.2, 121.3, 120.4, 119.2, 118.8, 110.8, 110.6, 103.9, 103.1, 68.0, 56.6, 38.3, 21.5, 19.7, 8.7; IR (KBr): 3567, 3022, 2918, 2859, 1733, 1558, 1455, 1339, 1311, 743 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{34}\text{H}_{30}\text{N}_2+\text{Na})^+$ requires m/z 489.2301, found m/z 489.2283; The enantiomeric excess: 90%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 90/10, flow rate 1.0 mL/min, $T = 30$ °C, 254 nm): $t_{\text{R}} = 5.233$ (minor), $t_{\text{R}} = 11.520$ (major).

(1*R*,3*R*)-3-(5-bromo-1*H*-indol-2-yl)-9-methyl-3-phenyl-1-(*o*-tolyl)-2,3-dihydro-1*H*-pyrrolo[1,2-*a*]indole (3fa):



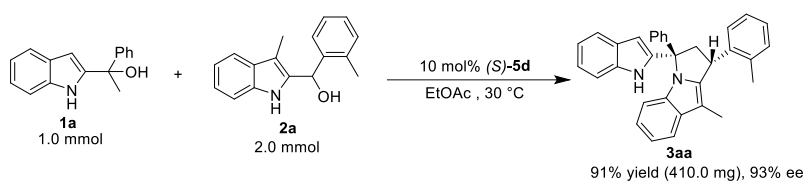
Following the general procedure, methyl-substituted 2-indolylmethanol **1f** (31.5 mg, 0.1 mmol), 3-alkyl(aryl)-2-indolylmethanol **2a** (50.2 mg, 0.2 mmol), catalyst (*S*)-**5d** (7.1 mg, 0.01 mmol) were added to a reaction tube. Then, EtOAc (1 mL) was added to the reaction mixture, which was stirred at 30 °C for 5 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (petroleum ether/dichloromethane = 2:1) on silica gel to afford pure compound **3fa** in 67% yield (35.5 mg) as a white solid. m.p. 254.8 – 255.0 °C; > 95:5 dr; $[\alpha]_{\text{D}}^{20} = 88.3$ ($c = 0.71$, acetone); ^1H NMR (400 MHz, CDCl_3) δ 8.10 (s, 1H), 7.63 (s, 1H), 7.59 (d, $J = 8.0$ Hz, 1H), 7.41 – 7.33 (m, 3H), 7.30 – 7.27 (m, 1H), 7.25 – 7.20 (m, 2H), 7.20 – 7.12 (m, 2H), 7.12 – 7.00 (m, 4H), 6.95 – 6.86 (m, 1H), 6.55 (d, $J = 8.4$ Hz, 1H), 6.33 (s, 1H), 4.65 – 4.51 (m, 1H), 3.63 – 3.49 (m, 1H), 3.23 – 3.05 (m, 1H), 2.35 (s, 3H), 2.00 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 141.5, 140.8, 140.7, 138.7, 135.8, 135.0, 133.6, 132.8, 130.6, 129.5, 128.6, 128.1, 126.9, 126.8, 126.5, 125.3, 123.2, 121.3, 119.3, 118.9, 113.2, 112.5, 110.3, 103.7, 103.3, 67.8, 56.5, 38.4, 19.6, 8.6; IR (KBr): 3437, 3372, 3055, 2917, 2860, 1558, 1490, 1455, 1307, 740 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{33}\text{H}_{27}\text{BrN}_2+\text{H})^+$ requires m/z 531.1431, found m/z 531.1434; The enantiomeric excess: 91%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 90/10, flow rate 1.0 mL/min, $T = 30$ °C, 254 nm): $t_{\text{R}} = 5.583$ (minor), $t_{\text{R}} = 16.930$ (major).

(1*R*,3*R*)-3-(6-chloro-1*H*-indol-2-yl)-9-methyl-3-phenyl-1-(*o*-tolyl)-2,3-dihydro-1*H*-pyrrolo[1,2-*a*]indole (3ga):



Following the general procedure, methyl-substituted 2-indolymethanol **1g** (27.1 mg, 0.1 mmol), 3-alkyl(aryl)-2-indolymethanol **2a** (50.2 mg, 0.2 mmol), catalyst (*S*)-**5d** (7.1 mg, 0.01 mmol) were added to a reaction tube. Then, EtOAc (1 mL) was added to the reaction mixture, which was stirred at 30 °C for 5 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified through preparative thin layer chromatography (petroleum ether/dichloromethane = 2:1) on silica gel to afford pure compound **3ga** in 69% yield (33.5 mg) as a white solid. m.p. 121.3 – 121.7 °C; > 95:5 dr; $[\alpha]_D^{20} = 49.7$ ($c = 0.67$, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.04 (s, 1H), 7.59 (d, $J = 8.0$ Hz, 1H), 7.41 (d, $J = 8.4$ Hz, 1H), 7.39 – 7.32 (m, 3H), 7.32 – 7.28 (m, 1H), 7.23 – 7.12 (m, 4H), 7.11 – 7.03 (m, 4H), 6.93 – 6.85 (m, 1H), 6.56 (d, $J = 8.0$ Hz, 1H), 6.35 (s, 1H), 4.63 – 4.53 (m, 1H), 3.61 – 3.50 (m, 1H), 3.18 – 3.06 (m, 1H), 2.35 (s, 3H), 2.00 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 141.5, 140.8, 140.2, 136.7, 135.8, 133.7, 132.8, 130.6, 128.7, 128.3, 128.1, 127.0, 126.8, 126.6, 126.4, 121.7, 121.4, 120.9, 119.3, 119.0, 111.1, 110.4, 104.3, 103.3, 67.8, 56.5, 38.6, 19.7, 8.7; IR (KBr): 3587, 3055, 2916, 2860, 1716, 1616, 1455, 1339, 1311, 741 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{33}\text{H}_{27}\text{ClN}_2+\text{Na})^+$ requires m/z 509.1755, found m/z 509.1733; The enantiomeric excess: 85%, determined by HPLC (Daicel Chiralpak IB, hexane/isopropanol = 90/10, flow rate 1.0 mL/min, $T = 30$ °C, 254 nm): $t_R = 5.453$ (minor), $t_R = 15.290$ (major).

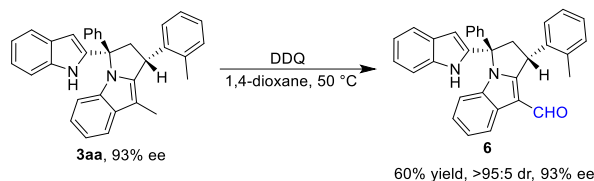
5. Procedure for one-mmol-scale reaction



Methyl-substituted 2-indolymethanol **1a** (237.1 mg, 1.0 mmol), 3-alkyl(aryl)-2-indolymethanol **2a** (502.3 mg, 2.0 mmol), and catalyst (*S*)-**5d** (70.8 mg, 0.1 mmol) were added to a reaction tube. Then, ethyl acetate (10 mL) was added to the reaction mixture, which was stirred at 30 °C for 5 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was concentrated under reduced pressure and the residue was purified through flash column chromatography (petroleum ether/dichloromethane = 2:1) on silica gel to afford pure compound **3aa**

in 91% yield (410.0 mg) with 93% ee.

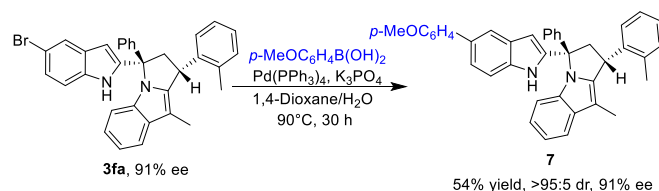
6. Synthetic procedures and characterization data of products 6-7



Compound **3aa** (45.2 mg, 0.1 mmol), DDQ (45.4 mg, 0.2 mmol) and 1,4-dioxane (1.0 mL) were added to a reaction tube. Then, the reaction mixture was stirred at 50 °C for 3 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was directly purified by preparative thin layer chromatography (petroleum ether/acetone = 5:1) on silica gel to afford pure product **6** (27.8 mg, 60% yield) with 93% ee.

(1*R*,3*R*)-3-(1*H*-indol-2-yl)-3-phenyl-1-(*o*-tolyl)-2,3-dihydro-1*H*-pyrrolo[1,2-*a*]indole-9-

carbaldehyde (6): white solid; m.p. 298.6 – 299.7 °C; $[\alpha]_D^{20} = 67.3$ ($c = 0.56$, acetone); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 9.46 (s, 1H), 8.39 – 8.25 (m, 2H), 7.57 (d, $J = 7.6$ Hz, 1H), 7.46 – 7.36 (m, 4H), 7.33 – 7.27 (m, 1H), 7.24 – 7.19 (m, 4H), 7.17 – 7.09 (m, 4H), 7.02 – 6.96 (m, 1H), 6.65 (d, $J = 8.0$ Hz, 1H), 6.52 (s, 1H), 4.93 – 4.80 (m, 1H), 3.71 – 3.59 (m, 1H), 3.52 – 3.31 (m, 1H), 2.38 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 184.5, 156.4, 139.4, 137.2, 136.5, 135.6, 133.4, 129.6, 129.0, 128.7, 127.7, 127.1, 126.6, 123.8, 123.3, 123.0, 122.7, 121.0, 120.5, 111.3, 111.2, 105.1, 70.0, 56.3, 39.2, 19.7; IR (KBr): 3054, 1643, 1537, 1452, 1413, 1384, 1301, 1263, 1162, 749 cm^{-1} ; ESI FTMS exact mass calcd for $(\text{C}_{33}\text{H}_{26}\text{N}_2\text{O}+\text{Na})^+$ requires m/z 489.1937, found m/z 489.1935; The enantiomeric excess: 93%, determined by HPLC (Daicel Chiralpak IC, hexane/isopropanol = 90/10, flow rate 1.0 mL/min, $T = 30$ °C, 254 nm): $t_R = 8.893$ (minor), $t_R = 11.037$ (major).



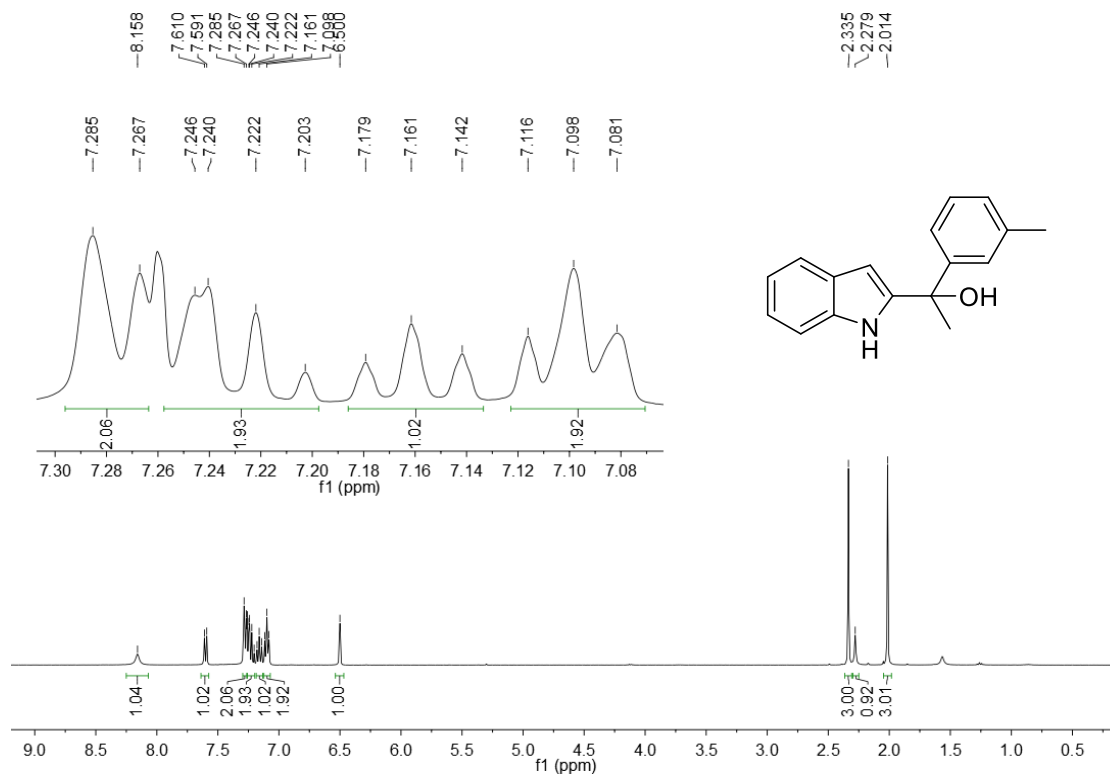
To a solution of **3fa** (53.0 mg, 0.1 mmol) in 1,4-dioxane/ H_2O (1 mL, 4:1 v/v) was added $\text{Pd(PPh}_3)_4$ (11.6 mg, 0.01 mmol), (*p*-methoxyphenyl)boronic acid (18.2 mg, 0.12 mmol) and K_3PO_4 (42.5 mg, 0.2 mmol). Then, the reaction mixture was stirred at 90 °C for 30 hours under argon atmosphere. After the completion of the reaction which was indicated by TLC, water (5 mL) was

added to the mixture and the aqueous layer was extracted with EtOAc (3 × 10.0 mL). The combined organic layers were dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. Finally, the residue was purified by preparative thin layer chromatography (petroleum ether/ethyl acetate = 4:1) on silica gel to afford pure product **7** (30.2 mg, 54% yield) with 91% ee.

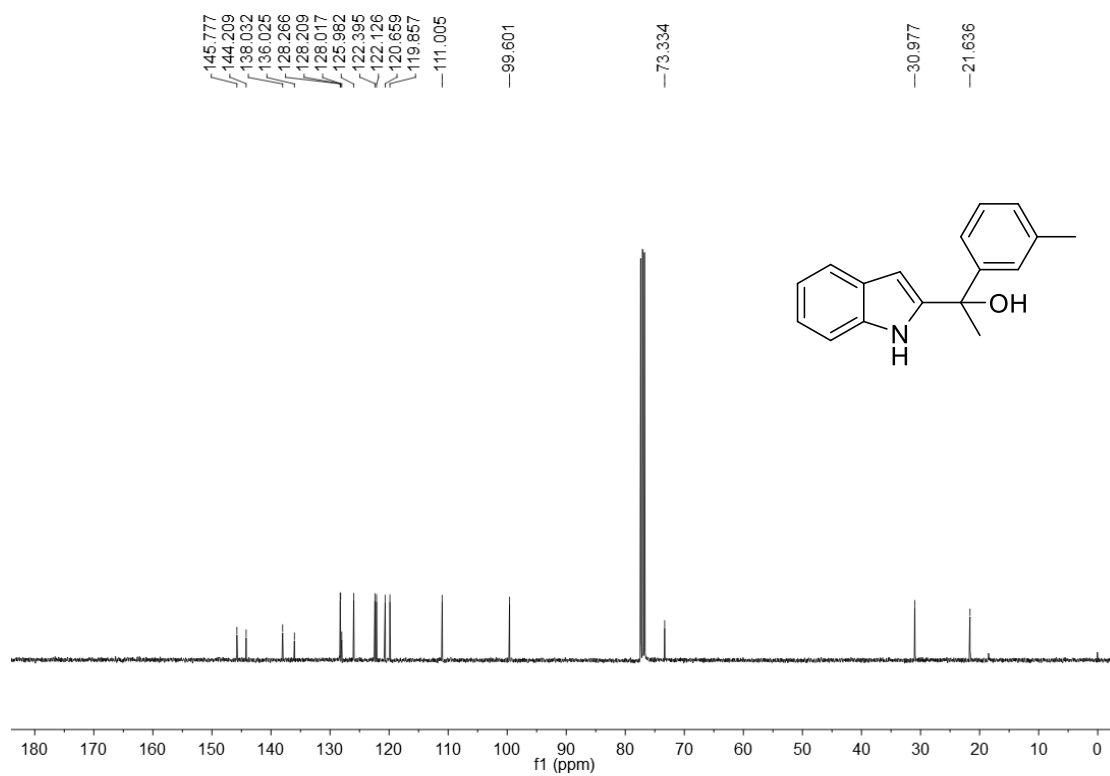
(1*R*,3*R*)-3-(5-(4-methoxyphenyl)-1*H*-indol-2-yl)-9-methyl-3-phenyl-1-(*o*-tolyl)-2,3-dihydro-1*H*-pyrrolo[1,2-*a*]indole (7): white solid; m.p. 107.4 – 108.4 °C; [α]_D²⁰ = 127.0 (c = 0.60, acetone); ¹H NMR (400 MHz, CDCl₃) δ 8.10 (s, 1H), 7.69 (s, 1H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.56 (s, 1H), 7.54 (s, 1H), 7.40 – 7.32 (m, 5H), 7.28 (s, 1H), 7.24 – 7.17 (m, 3H), 7.13 – 7.07 (m, 3H), 6.99 (s, 1H), 6.97 (s, 1H), 6.95 – 6.89 (m, 1H), 6.65 (d, *J* = 8.4 Hz, 1H), 6.44 (s, 1H), 4.64 – 4.54 (m, 1H), 3.86 (s, 3H), 3.62 – 3.52 (m, 1H), 3.29 – 3.11 (m, 1H), 2.35 (s, 3H), 2.00 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 158.5, 141.6, 141.0, 140.0, 135.9, 135.7, 135.1, 133.6, 133.4, 132.9, 130.6, 128.6, 128.5, 128.3, 128.0, 127.0, 126.9, 126.6, 122.2, 121.3, 119.2, 118.9, 118.8, 114.2, 111.3, 110.6, 104.6, 103.2, 68.0, 56.6, 55.4, 38.9, 19.7, 8.7; IR (KBr): 3024, 2930, 2834, 1608, 1514, 1455, 1313, 1273, 1242, 742 cm⁻¹; ESI FTMS exact mass calcd for (C₄₀H₃₄N₂O+Na)⁺ requires *m/z* 581.2563, found *m/z* 581.2546; The enantiomeric excess: 91%, determined by HPLC (Daicel Chiralpak AD-H, hexane/isopropanol = 90/10, flow rate 1.0 mL/min, T = 30 °C, 254 nm): *t*_R = 5.623 (minor), *t*_R = 6.510 (major).

7. NMR spectra of substrates 1b-1g and 8

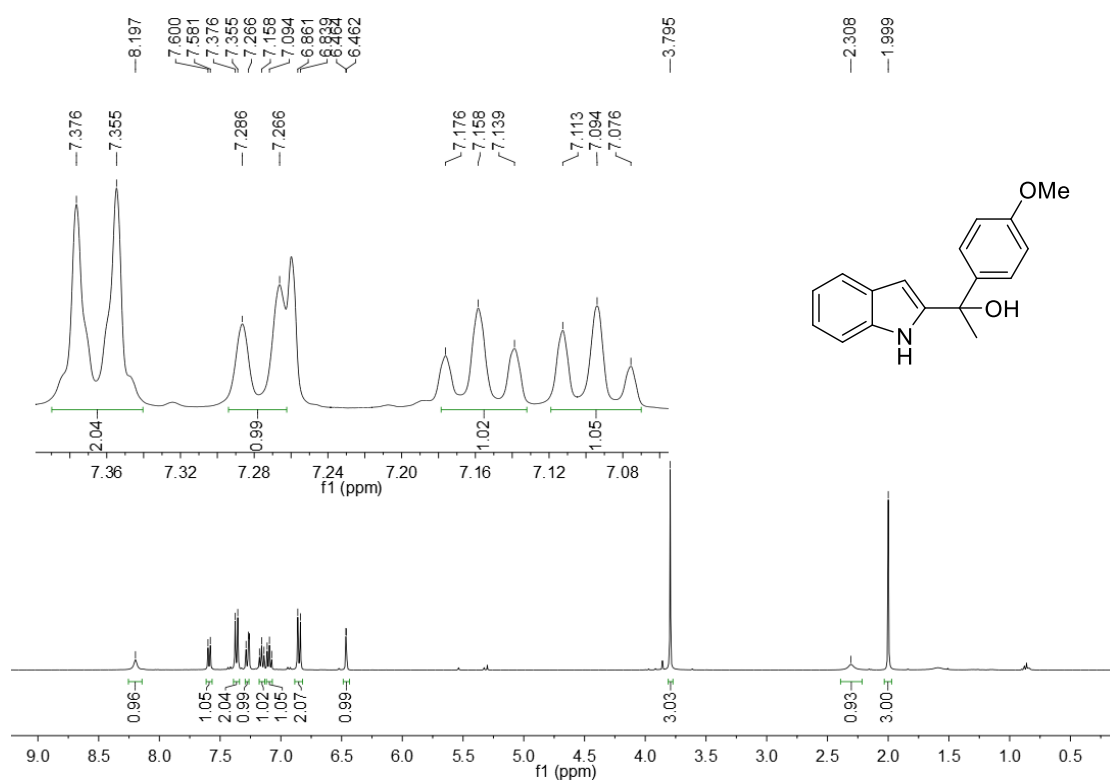
^1H NMR (400 MHz, CDCl_3) of compound **1b**:



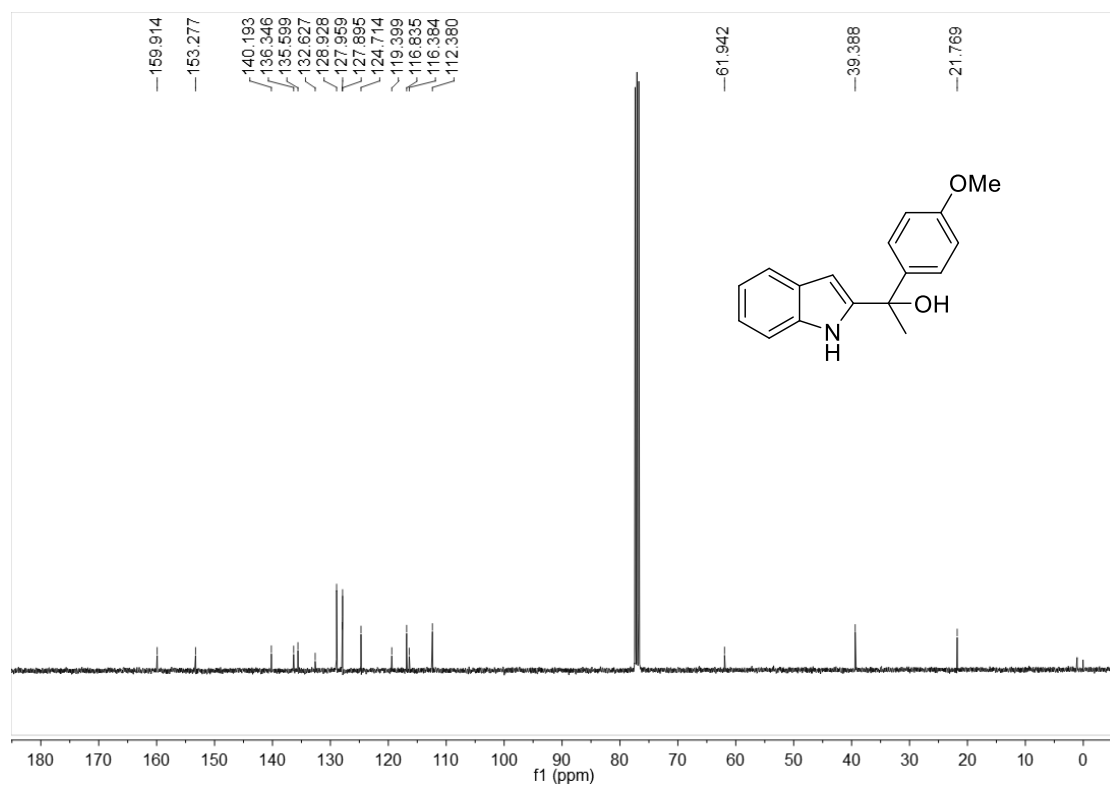
^{13}C NMR (100 MHz, CDCl_3) of compound **1b**:



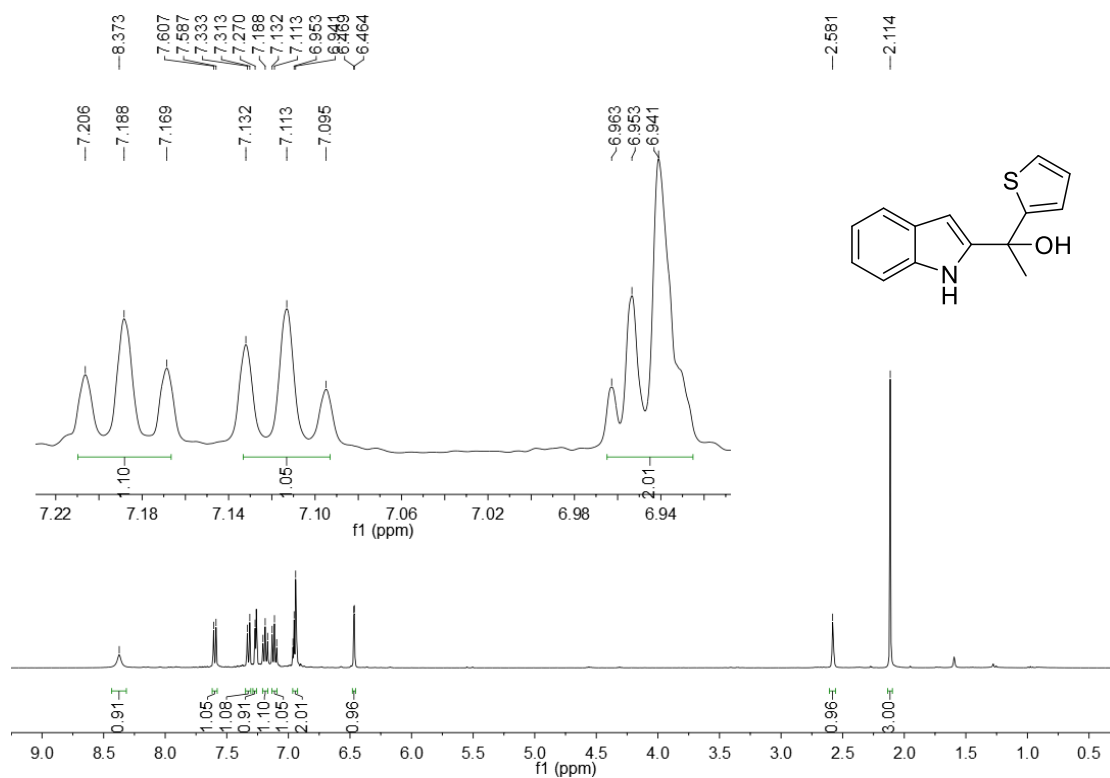
¹H NMR (400 MHz, CDCl₃) of compound **1c**:



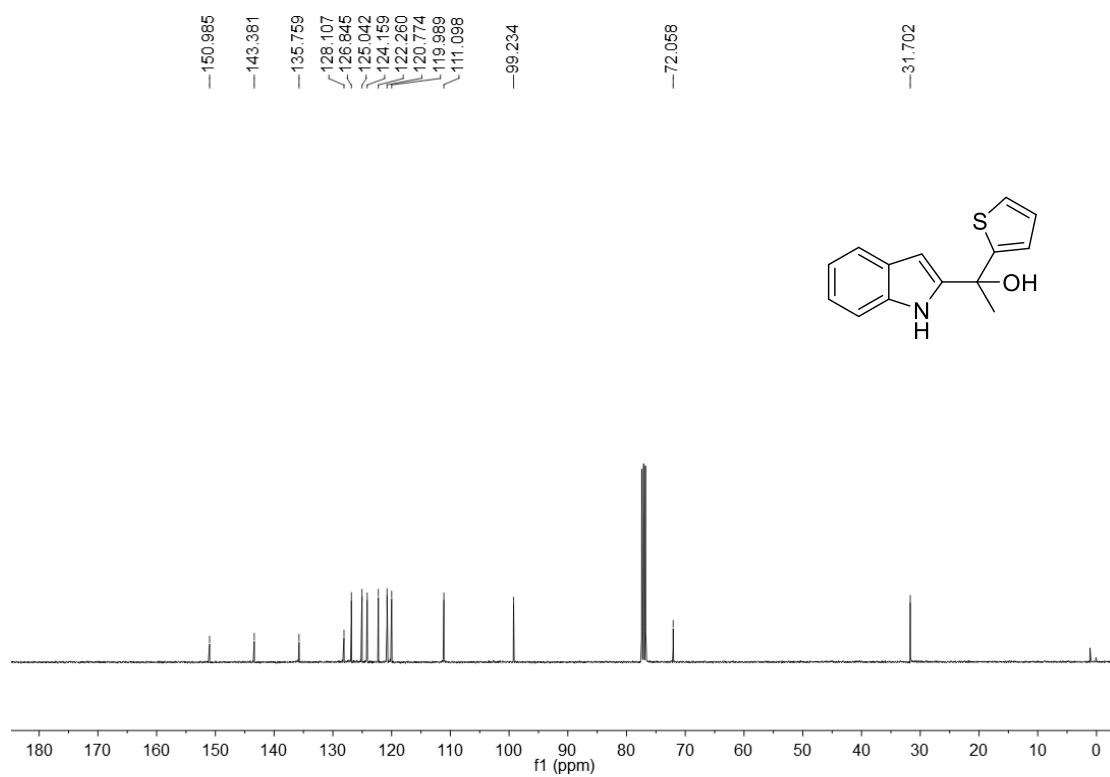
¹³C NMR (100 MHz, CDCl₃) of compound **1c**:



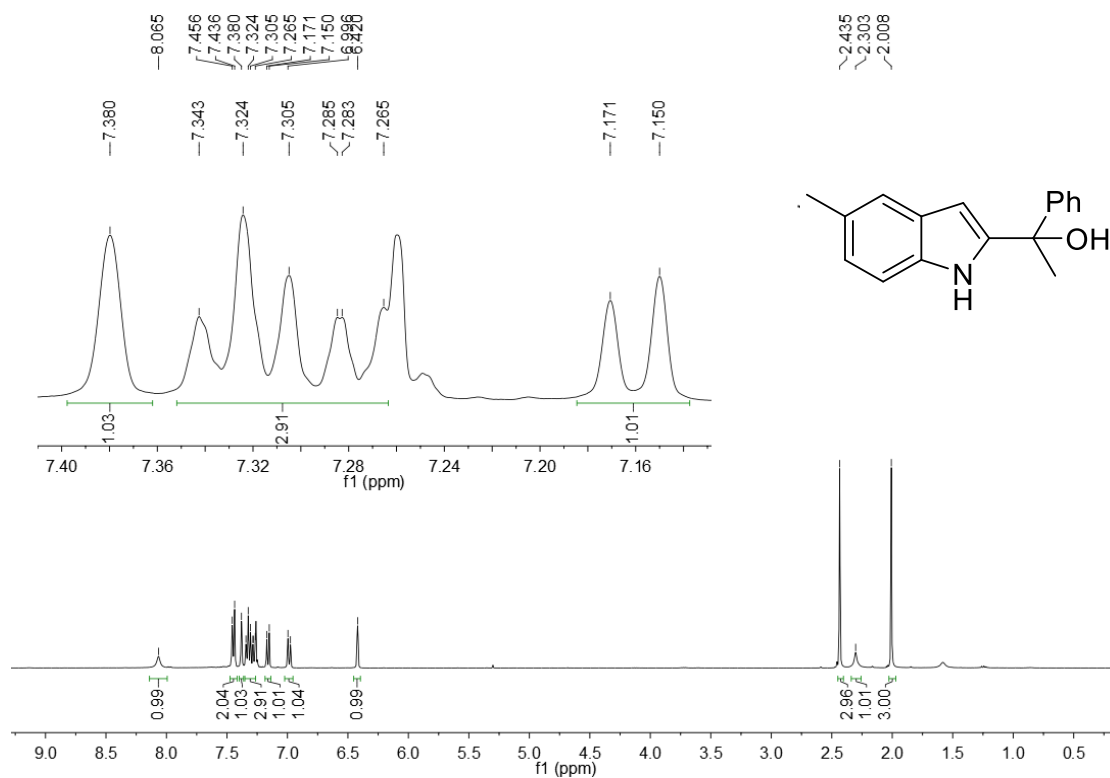
¹H NMR (400 MHz, CDCl₃) of compound **1d**:



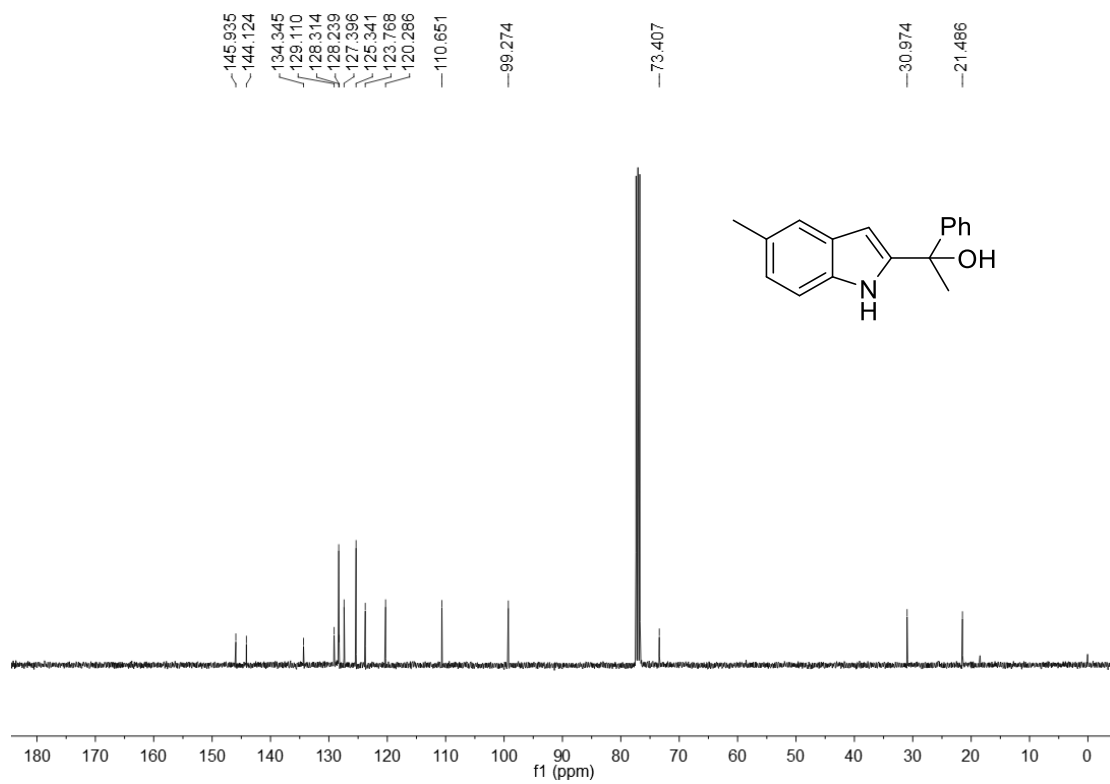
¹³C NMR (100 MHz, CDCl₃) of compound **1d**:



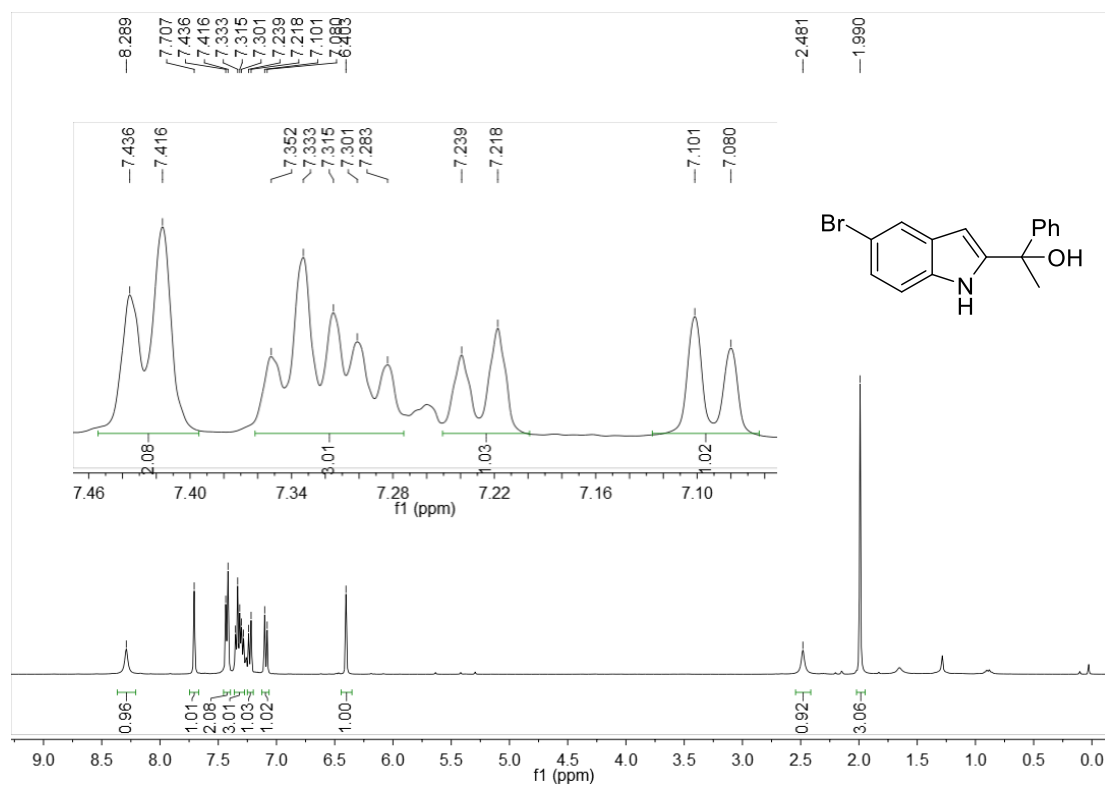
¹H NMR (400 MHz, CDCl₃) of compound **1e**:



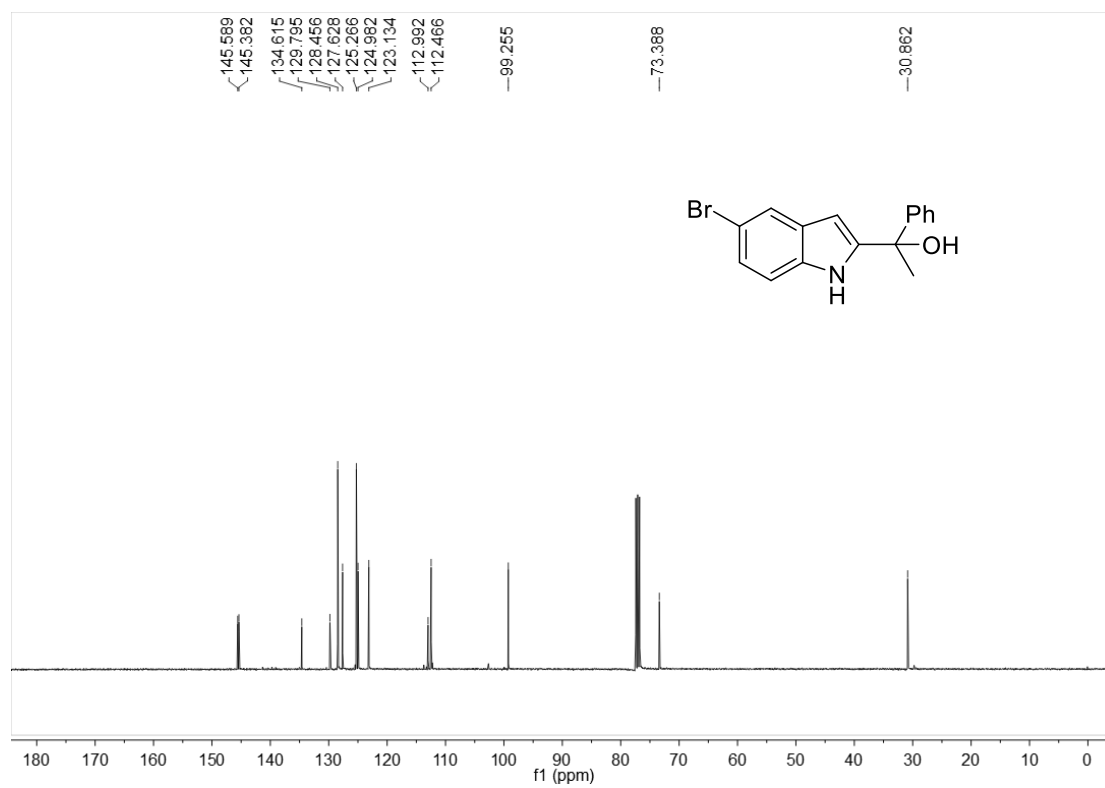
¹³C NMR (100 MHz, CDCl₃) of compound **1e**:



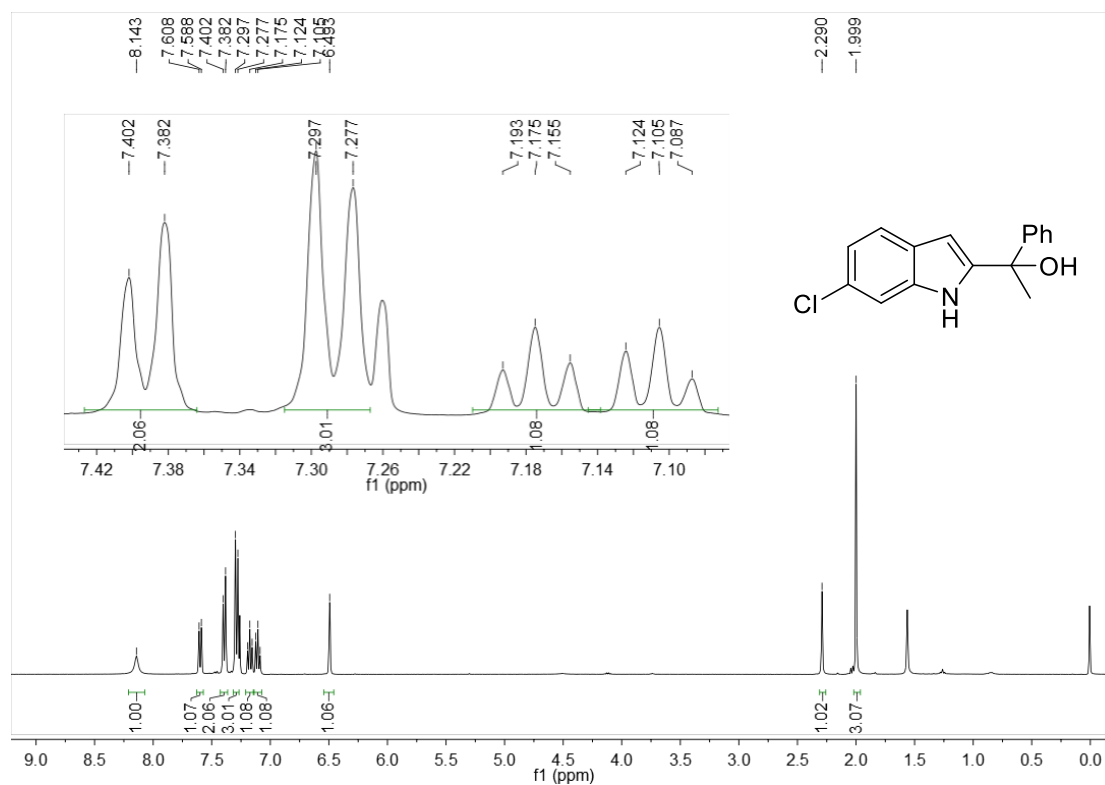
¹H NMR (400 MHz, CDCl₃) of compound **1f**:



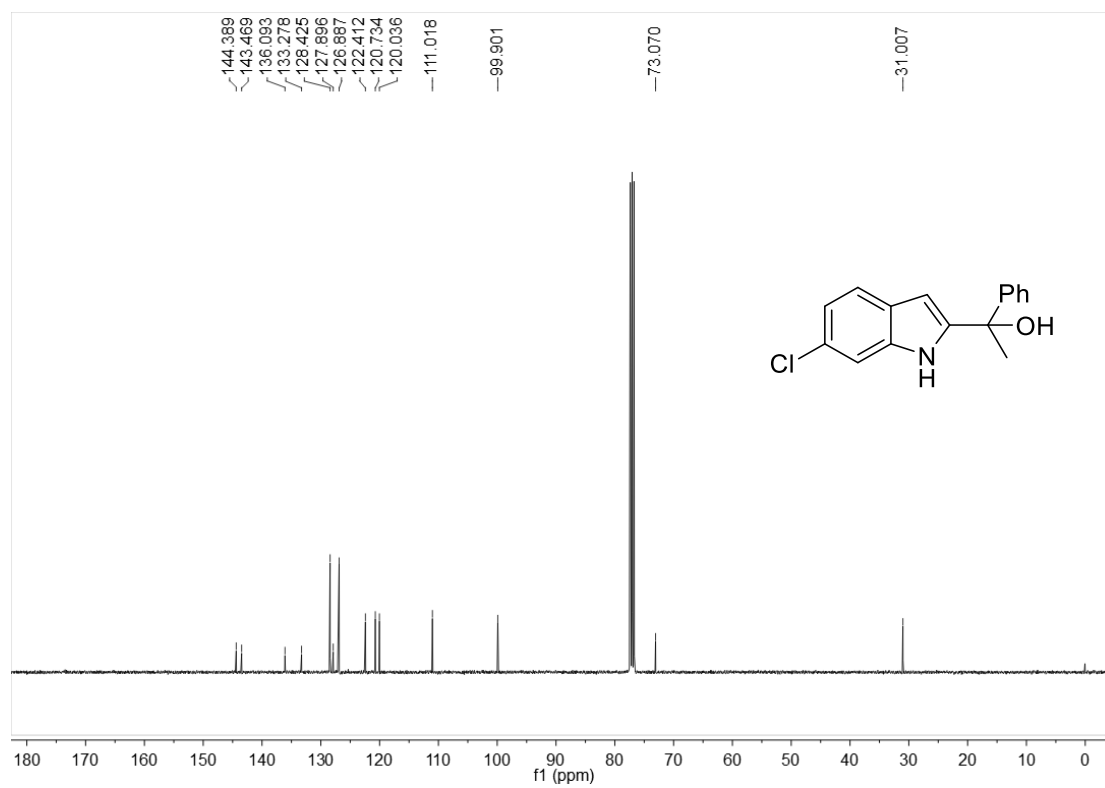
¹³C NMR (100 MHz, CDCl₃) of compound **1f**:



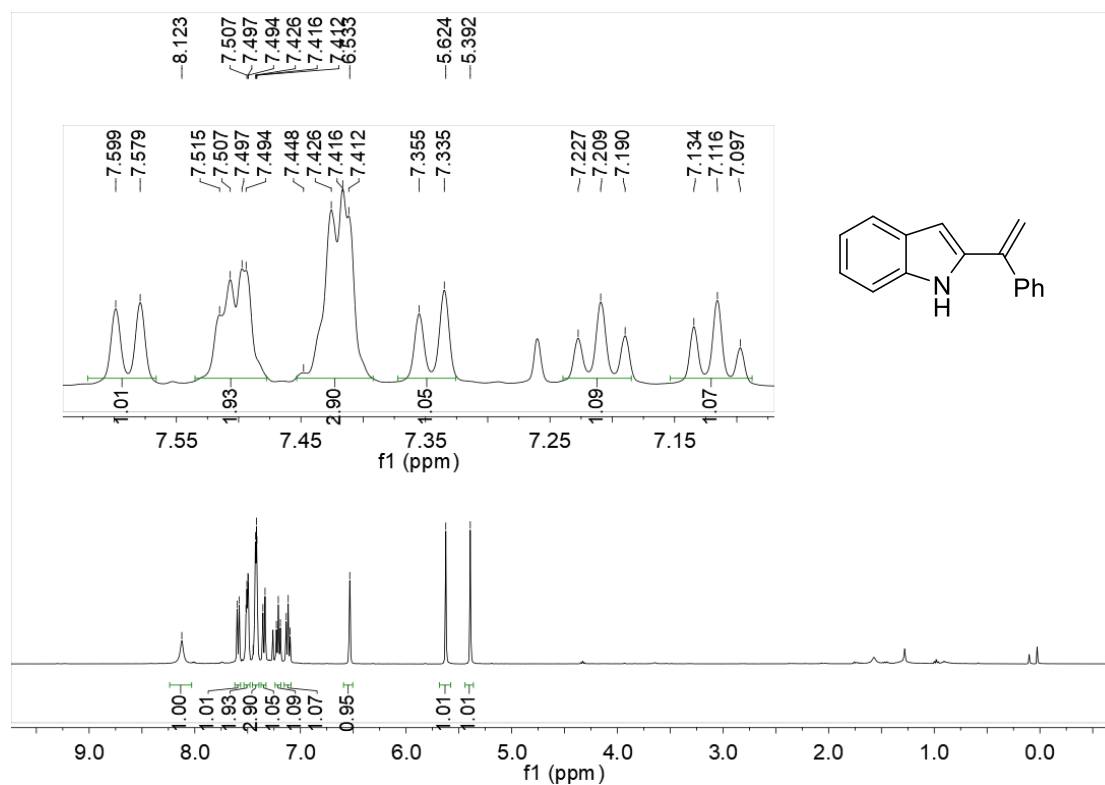
¹H NMR (400 MHz, CDCl₃) of compound **1g**:



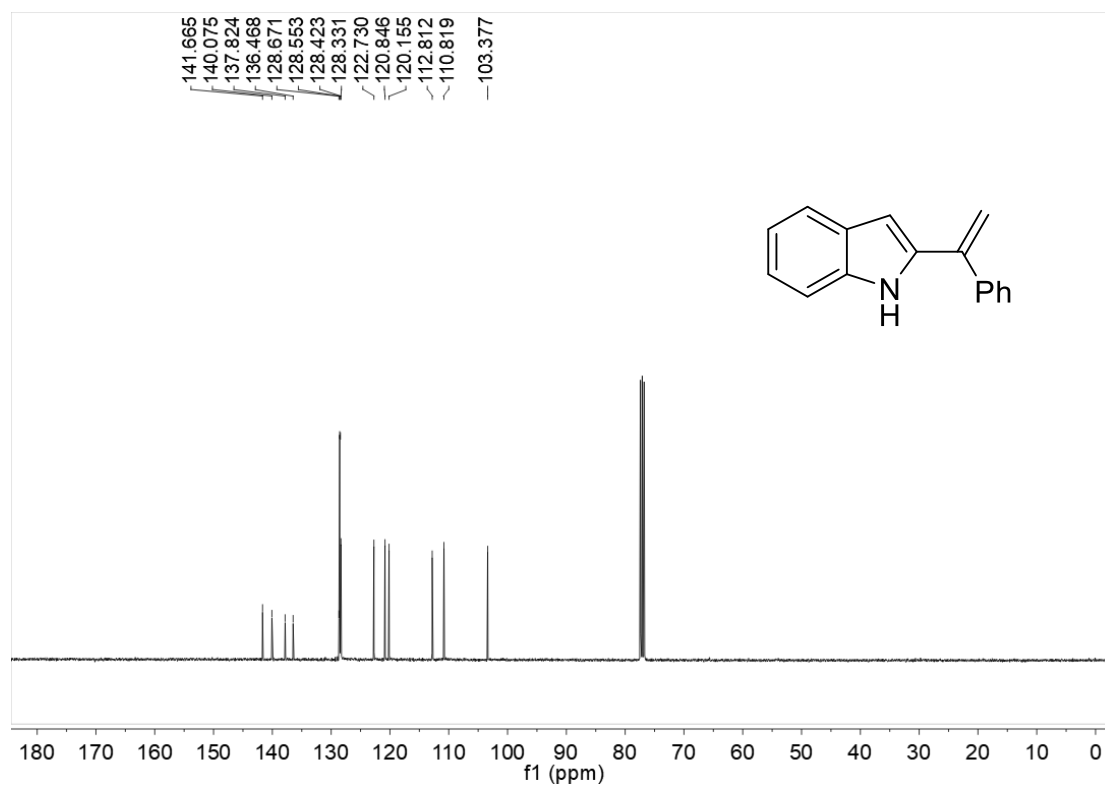
¹³C NMR (100 MHz, CDCl₃) of compound **1g**:



^1H NMR (400 MHz, CDCl_3) of compound **8**:

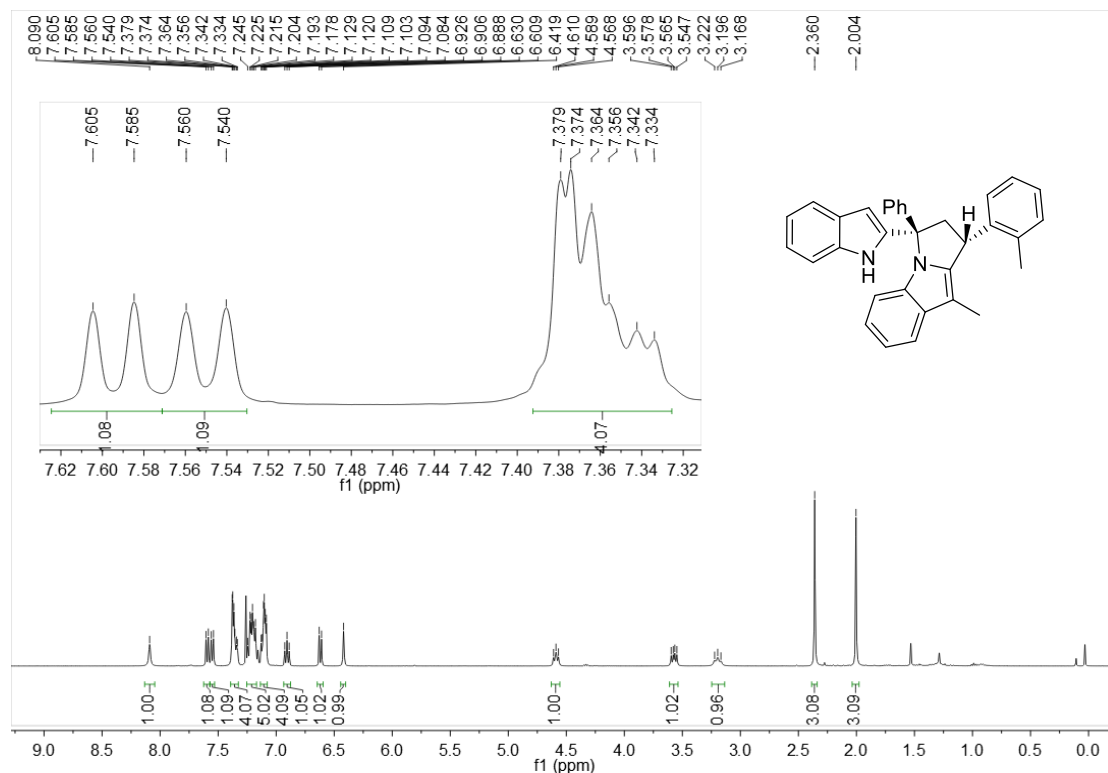


^{13}C NMR (100 MHz, CDCl_3) of compound **8**:

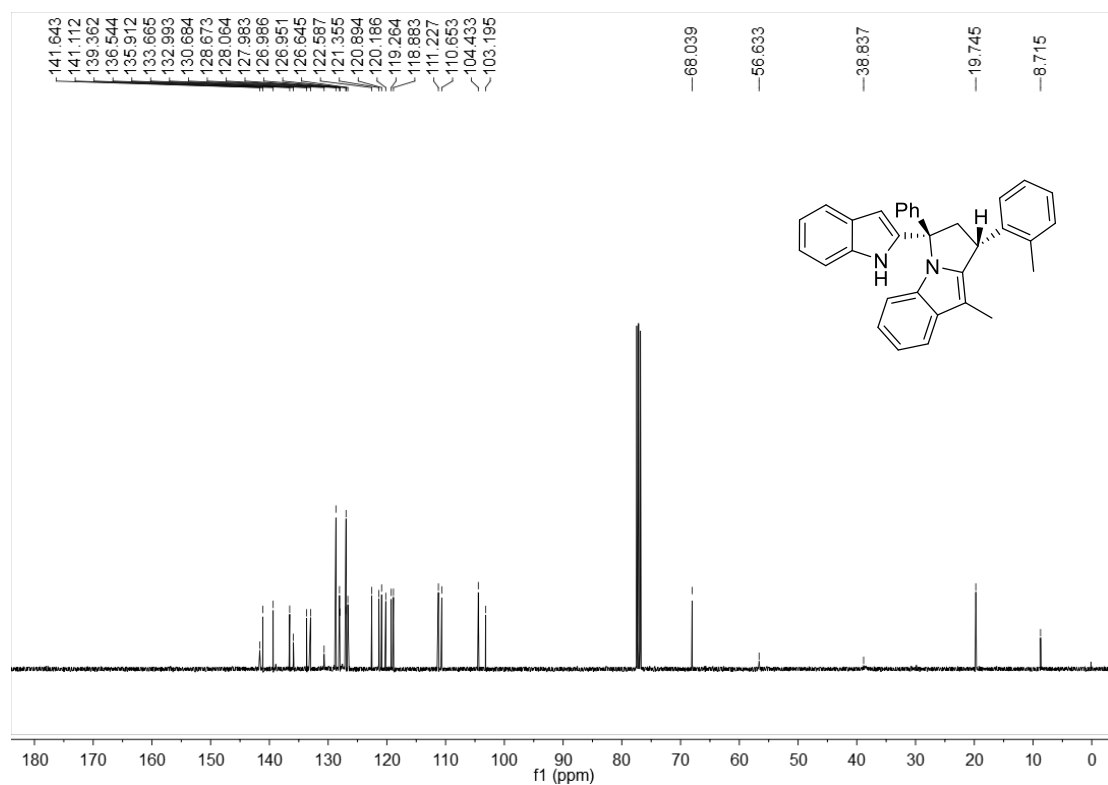


8. NMR spectra of products 3 and 6-7

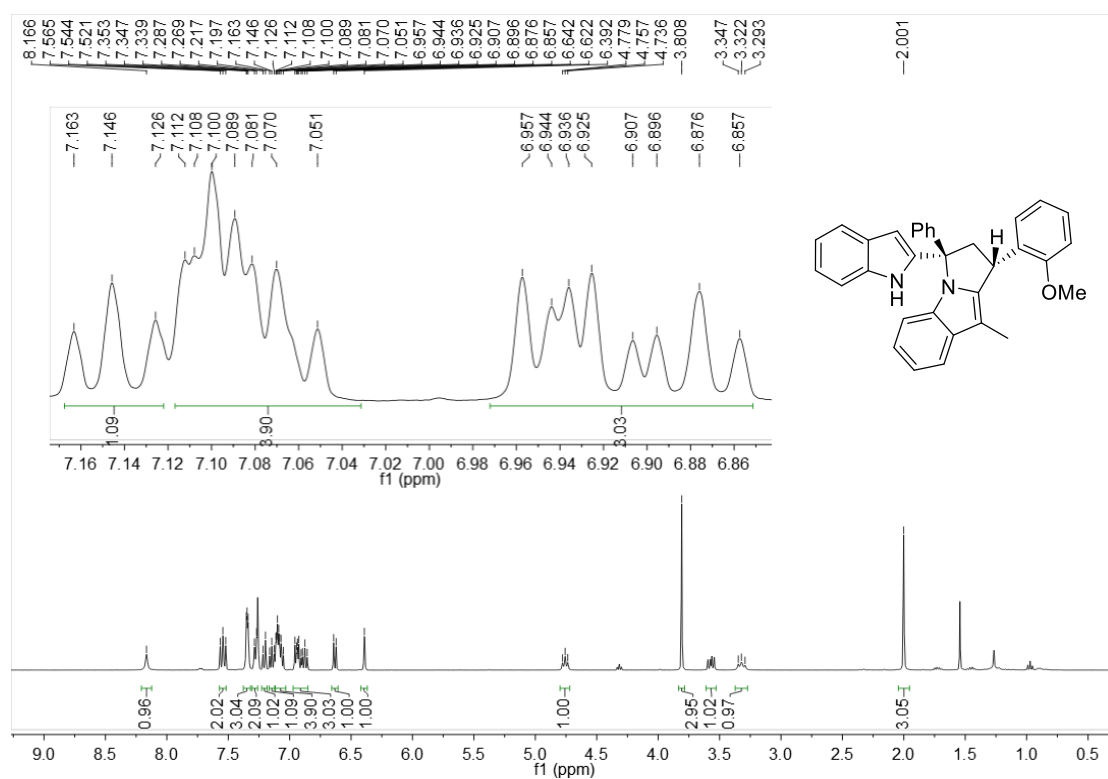
^1H NMR (400 MHz, CDCl_3) of compound **3aa**:



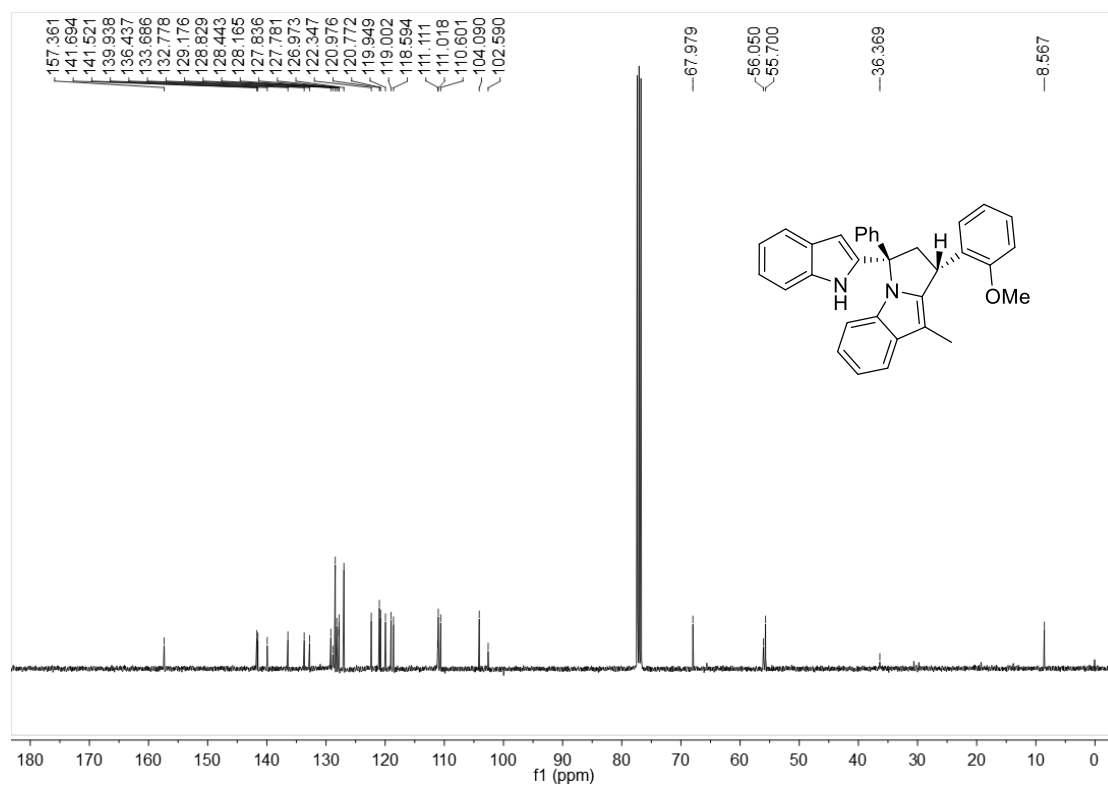
^{13}C NMR (100 MHz, CDCl_3) of compound **3aa**:



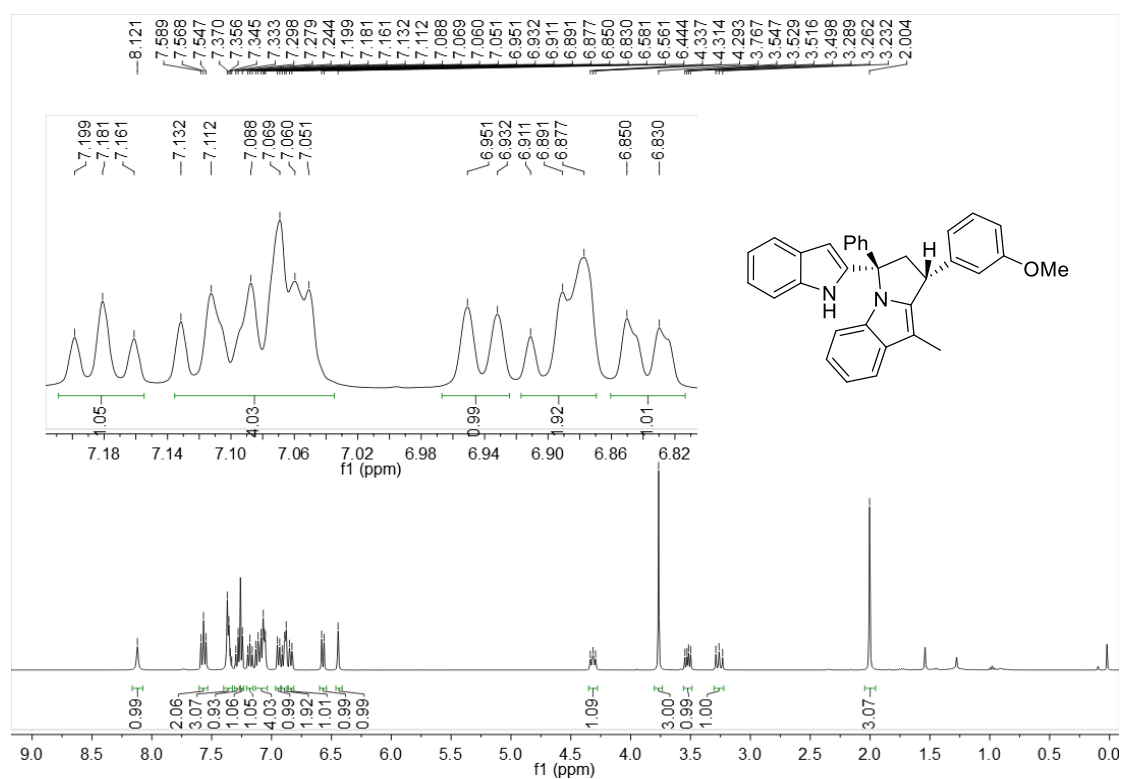
¹H NMR (400 MHz, CDCl₃) of compound **3ab**:



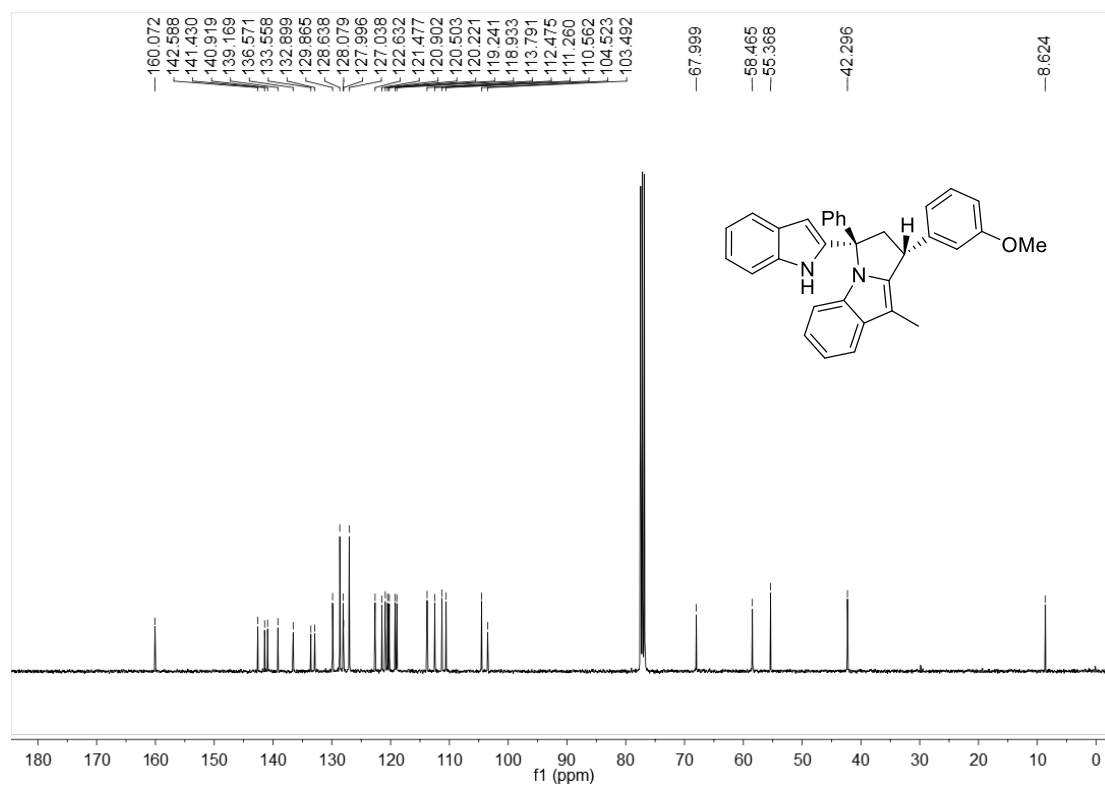
¹³C NMR (100 MHz, CDCl₃) of compound **3ab**:



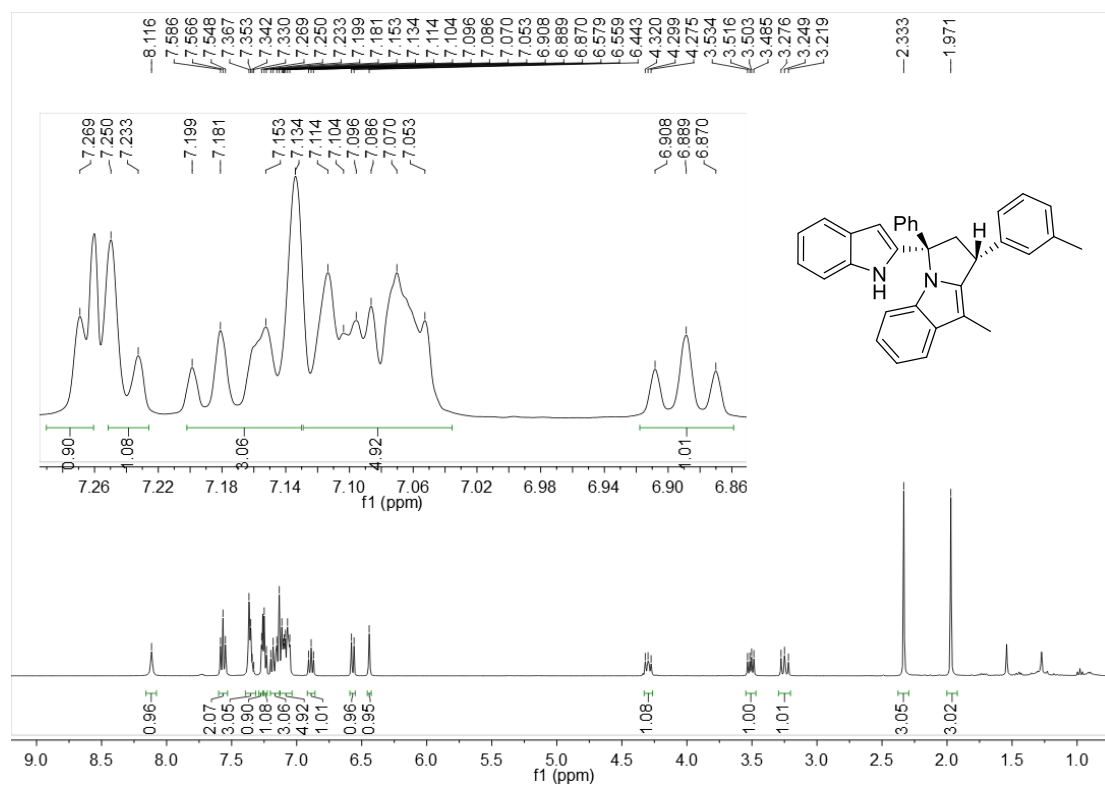
¹H NMR (400 MHz, CDCl₃) of compound **3ac**:



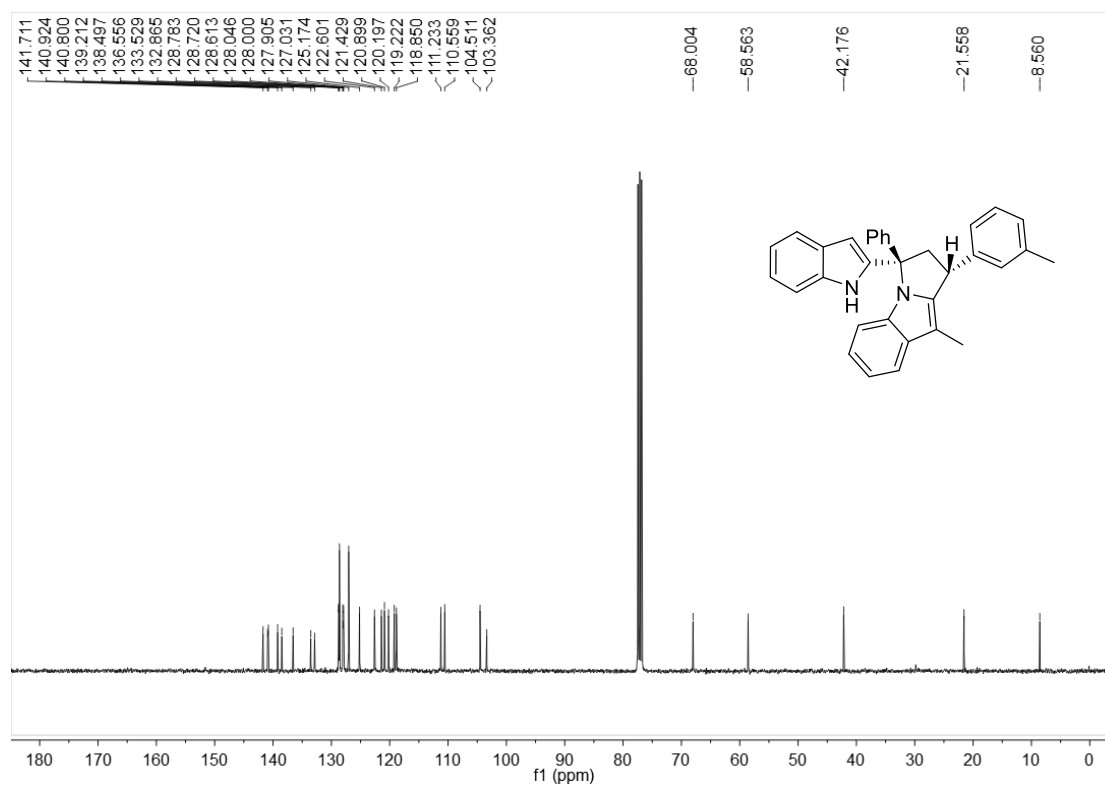
¹³C NMR (100 MHz, CDCl₃) of compound **3ac**:



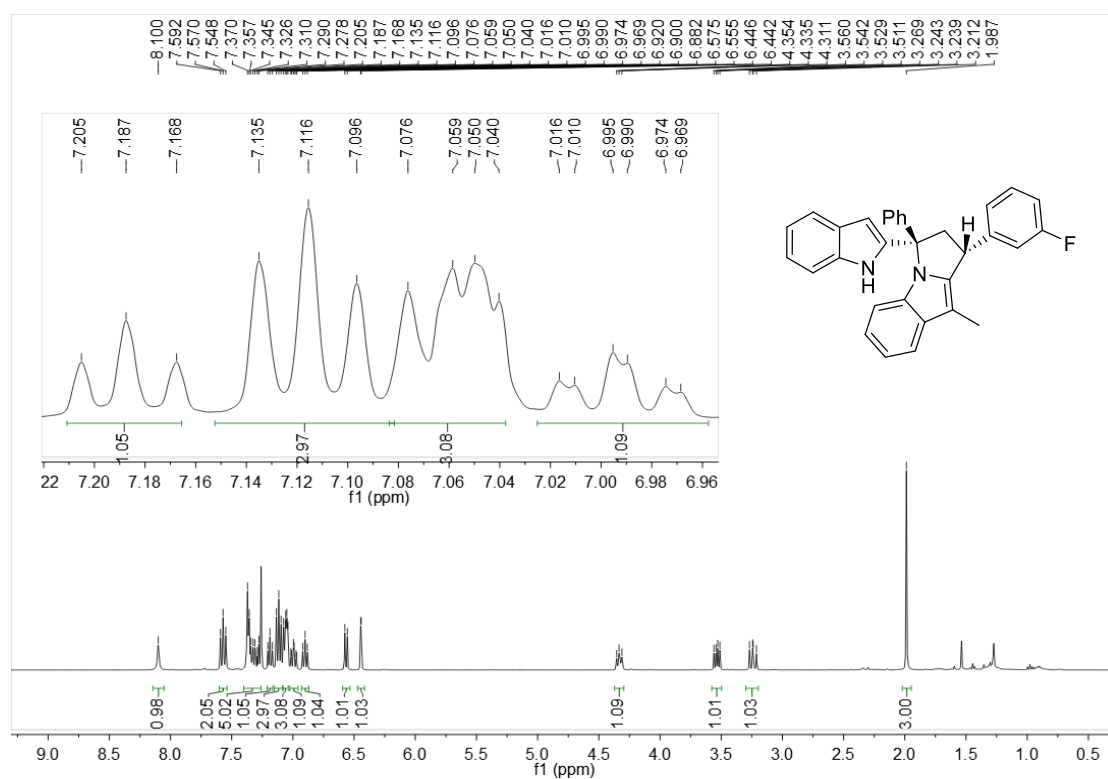
¹H NMR (400 MHz, CDCl₃) of compound **3ad**:



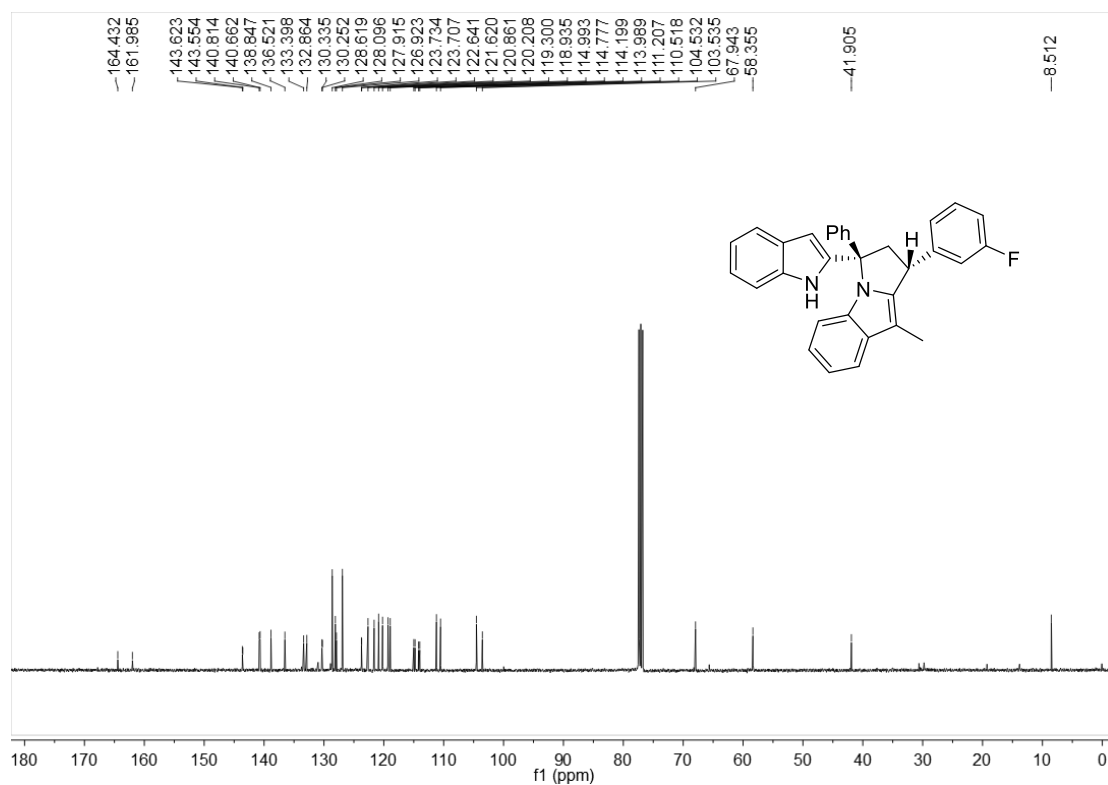
¹³C NMR (100 MHz, CDCl₃) of compound **3ad**:



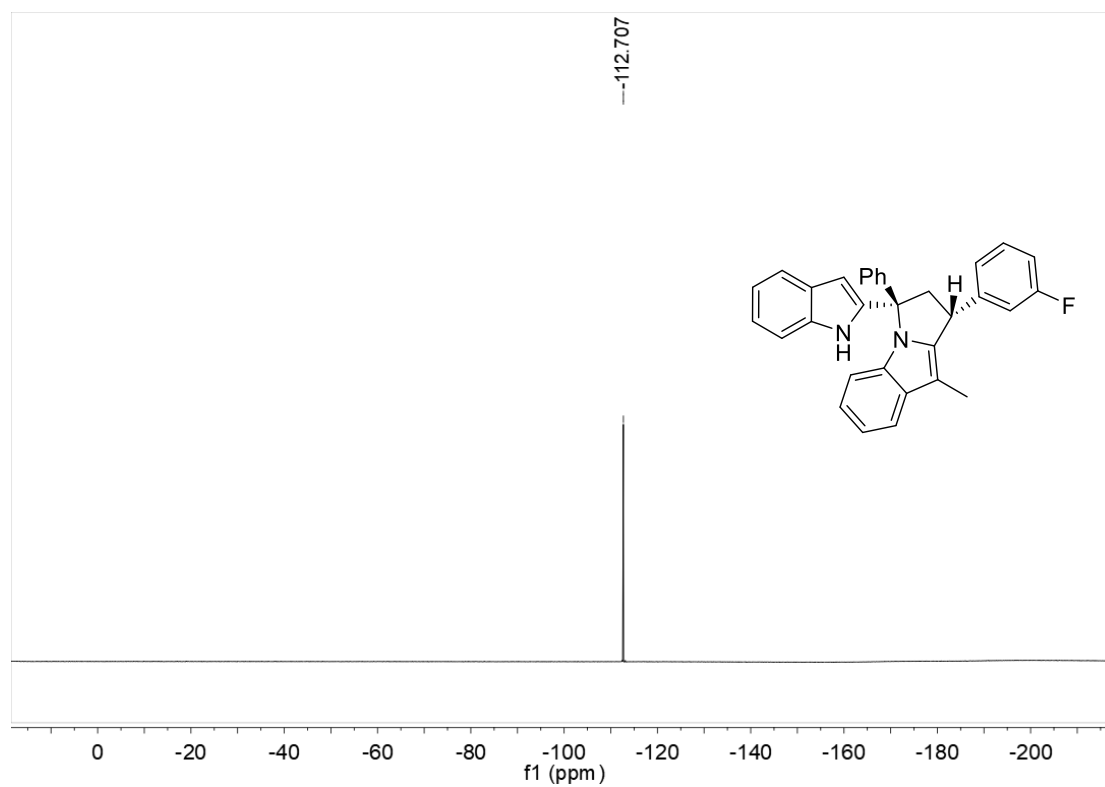
¹H NMR (400 MHz, CDCl₃) of compound **3ae**:



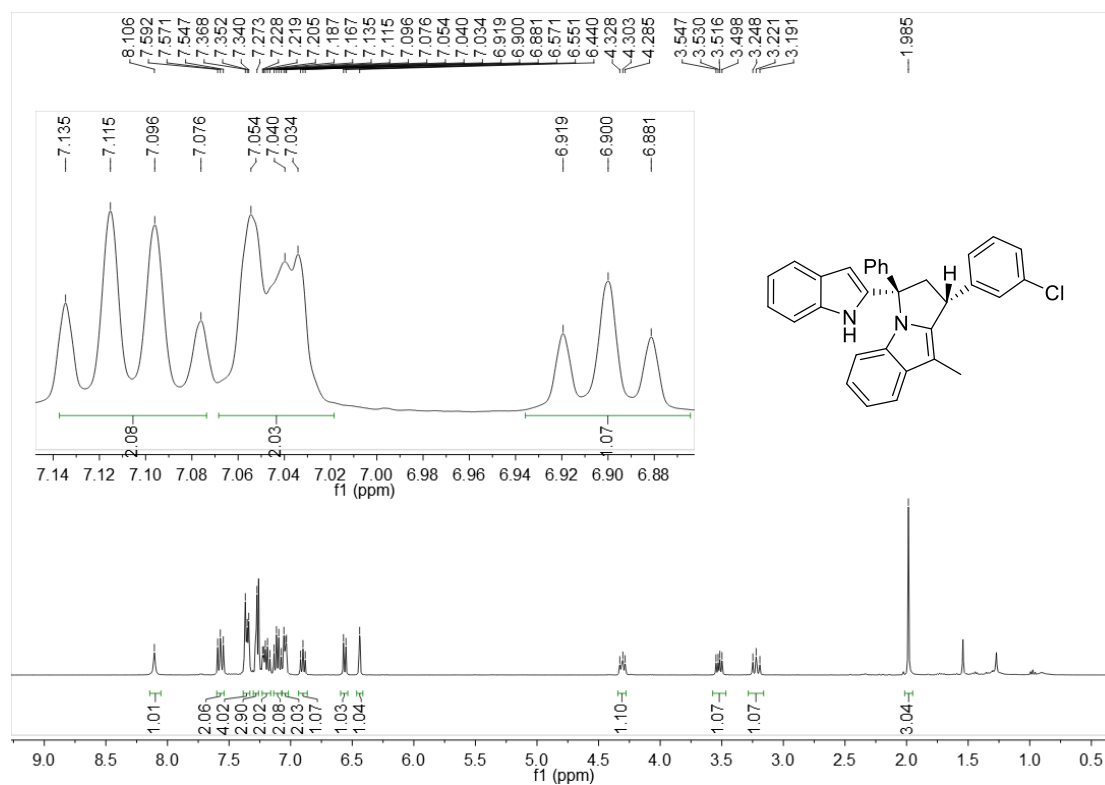
¹³C NMR (100 MHz, CDCl₃) of compound **3ae**:



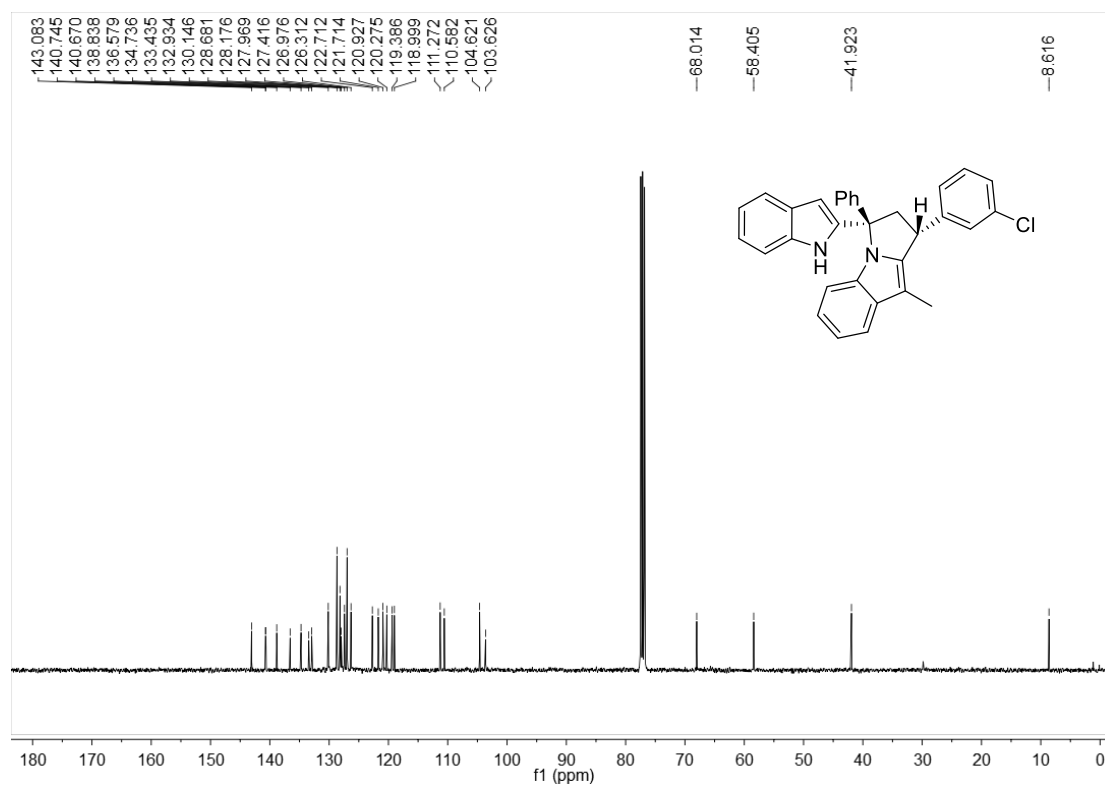
^{19}F NMR (376 MHz, CDCl_3) of compound **3ae**:



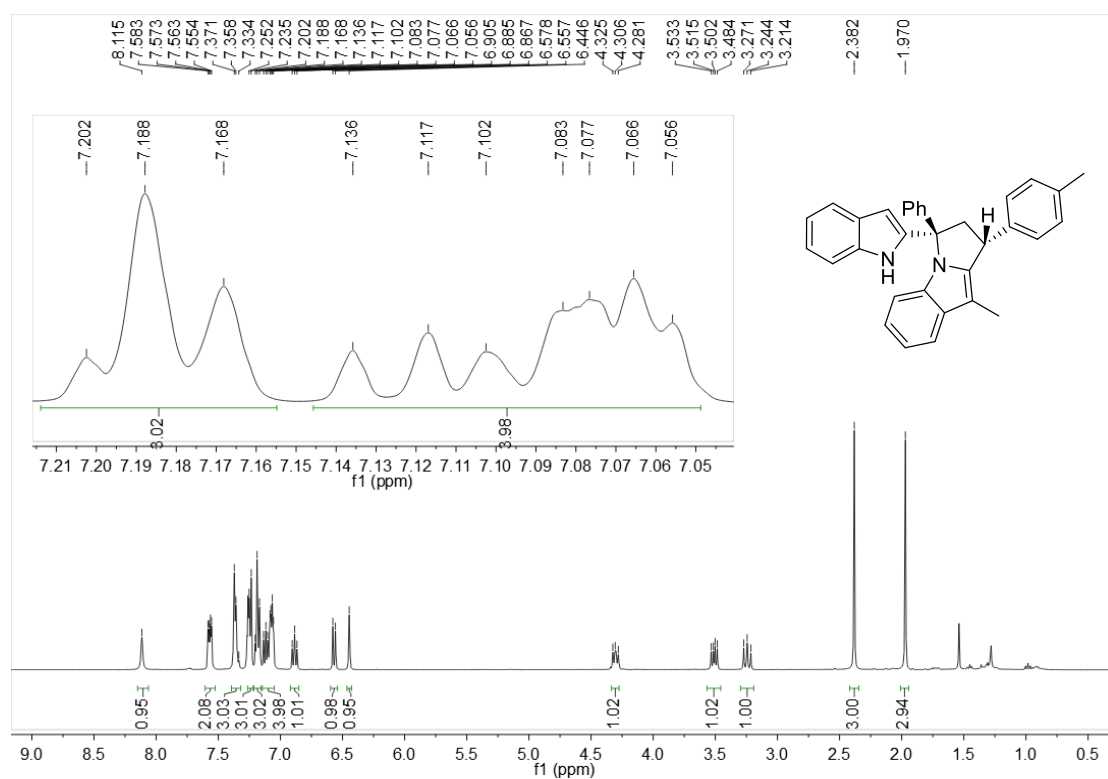
¹H NMR (400 MHz, CDCl₃) of compound **3af**:



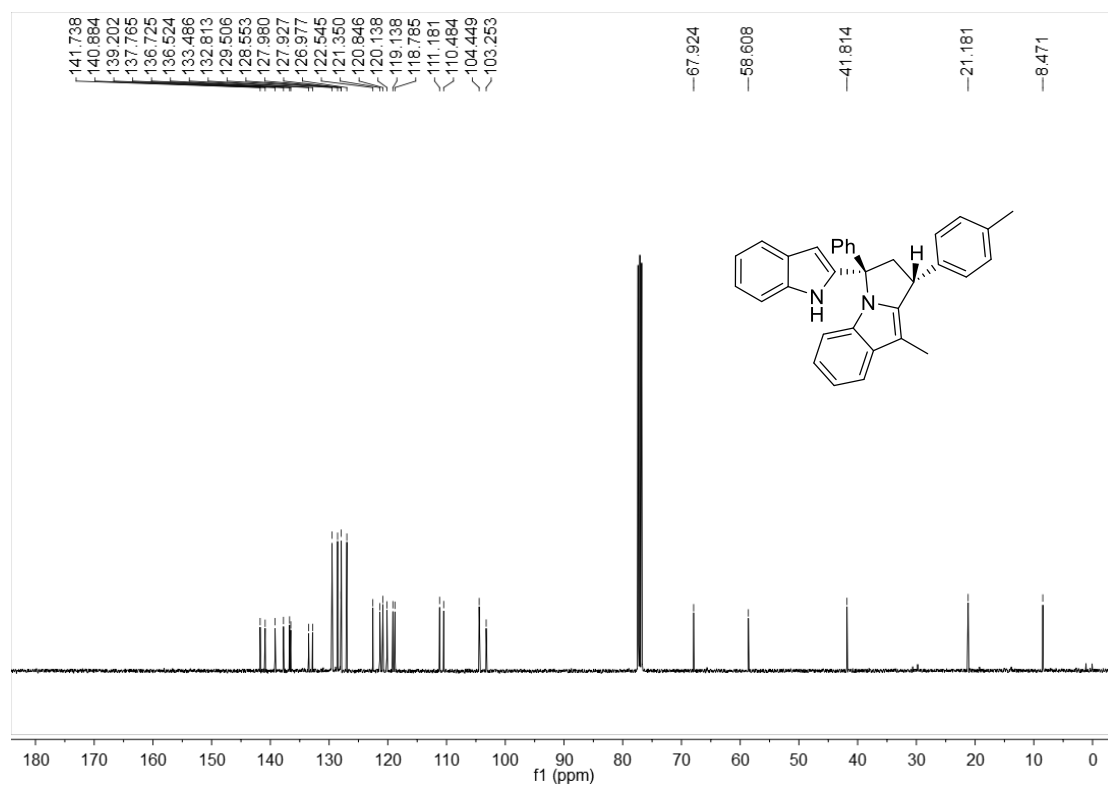
¹³C NMR (100 MHz, CDCl₃) of compound **3af**:



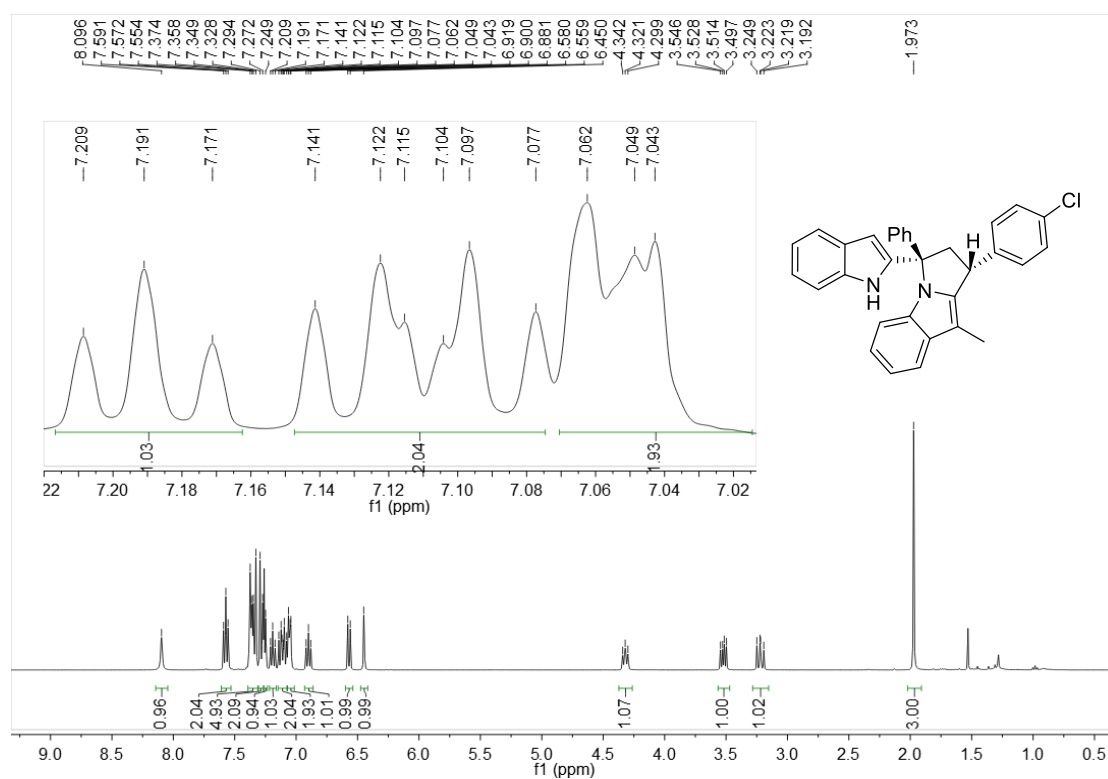
¹H NMR (400 MHz, CDCl₃) of compound **3ag**:



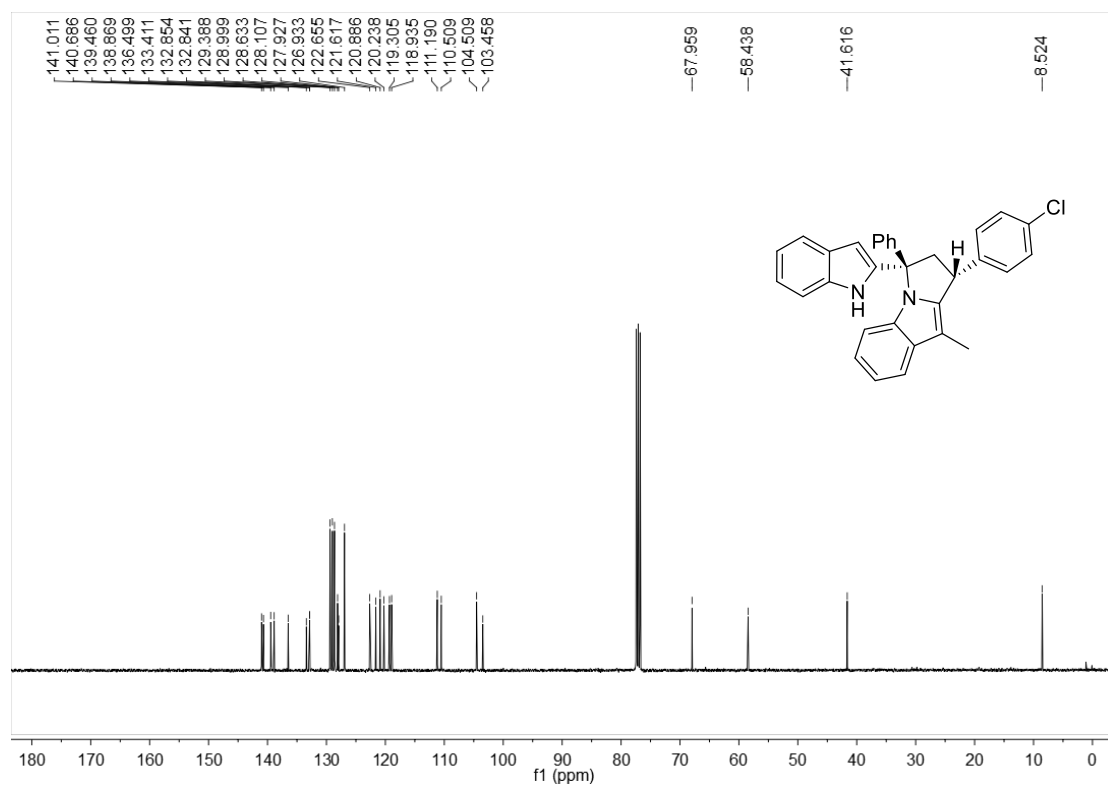
¹³C NMR (100 MHz, CDCl₃) of compound **3ag**:



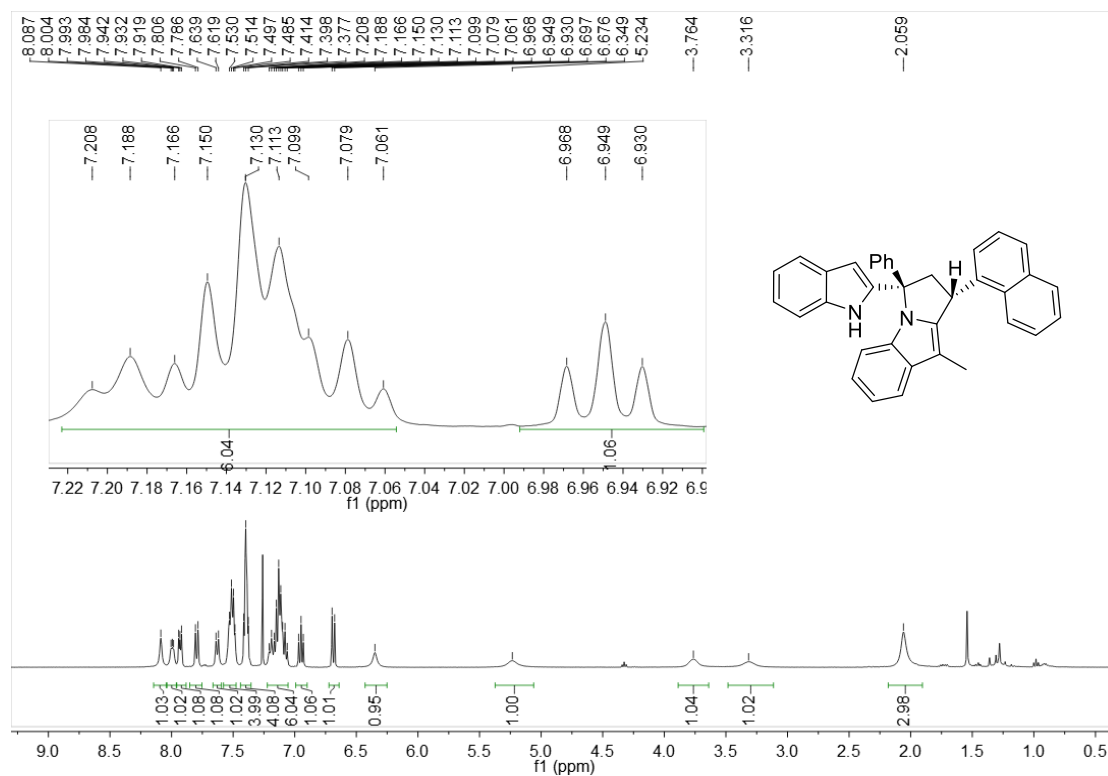
¹H NMR (400 MHz, CDCl₃) of compound **3ah**:



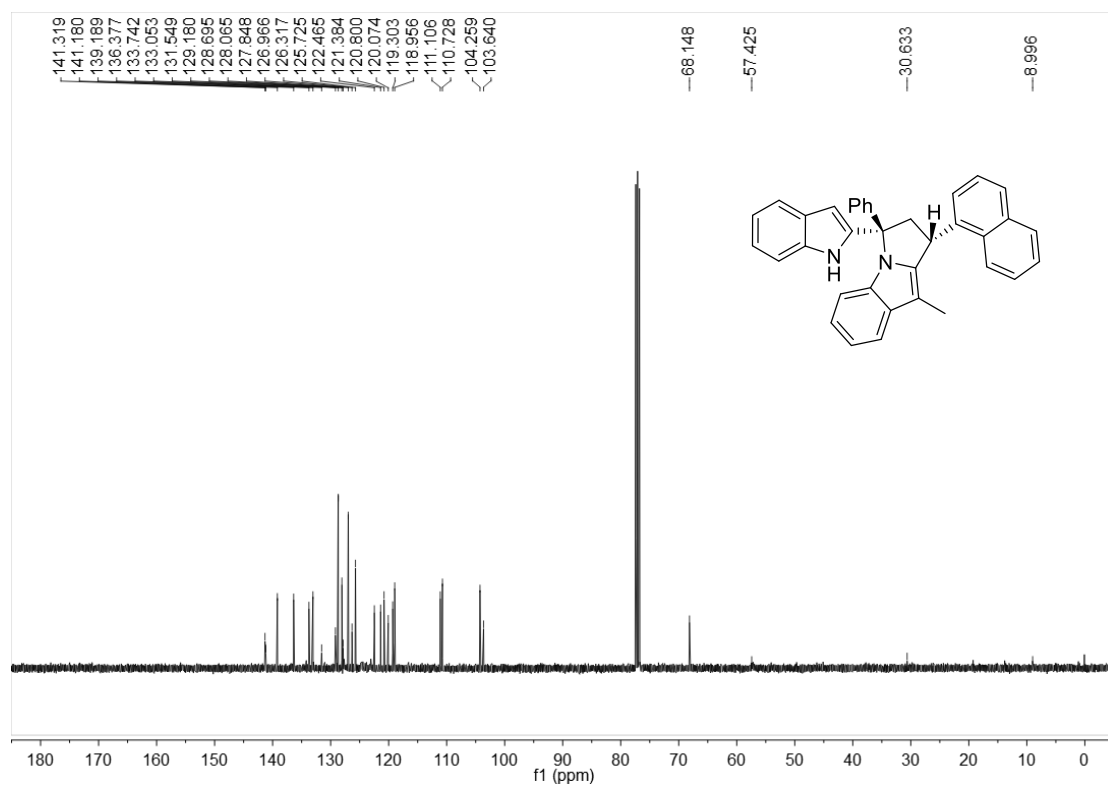
¹³C NMR (100 MHz, CDCl₃) of compound **3ah**:



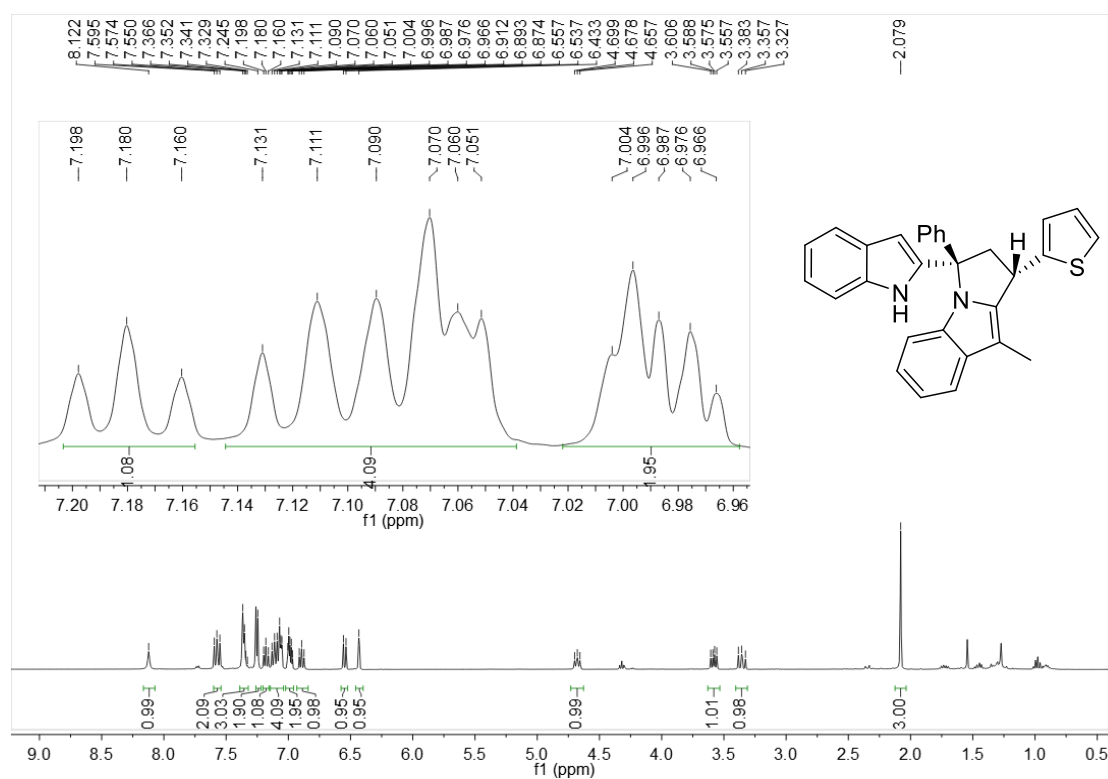
¹H NMR (400 MHz, CDCl₃) of compound **3ai**:



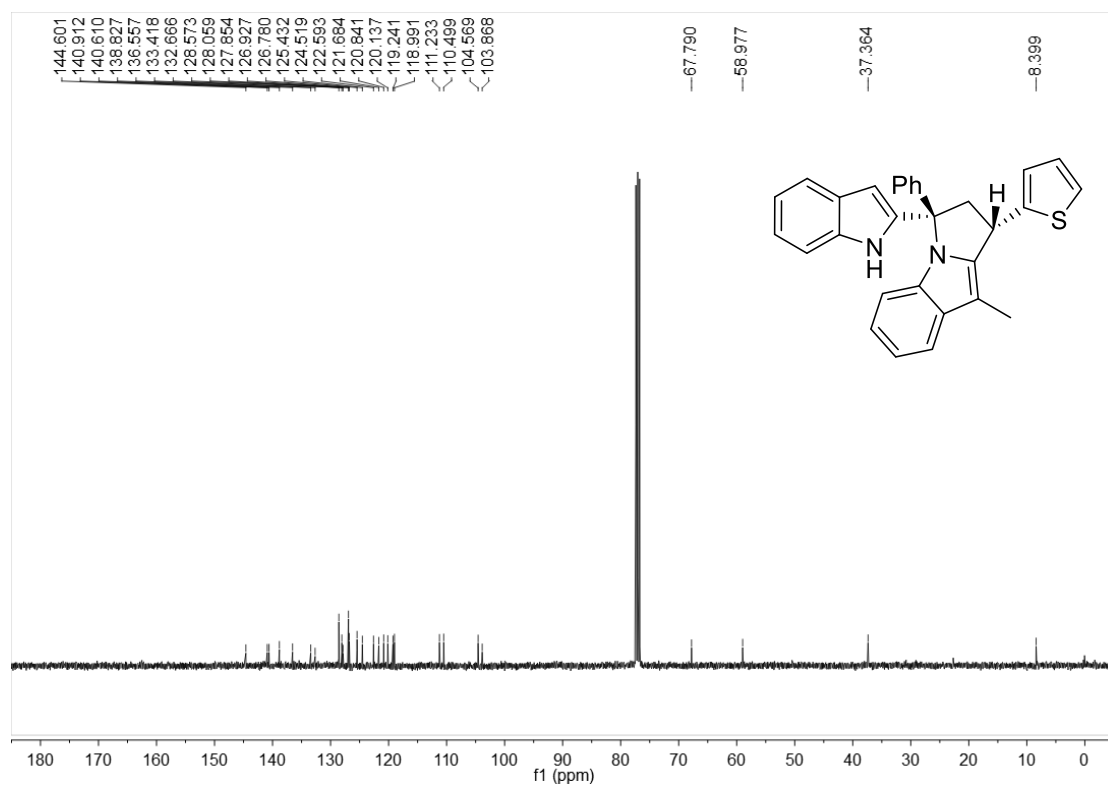
¹³C NMR (100 MHz, CDCl₃) of compound **3ai**:



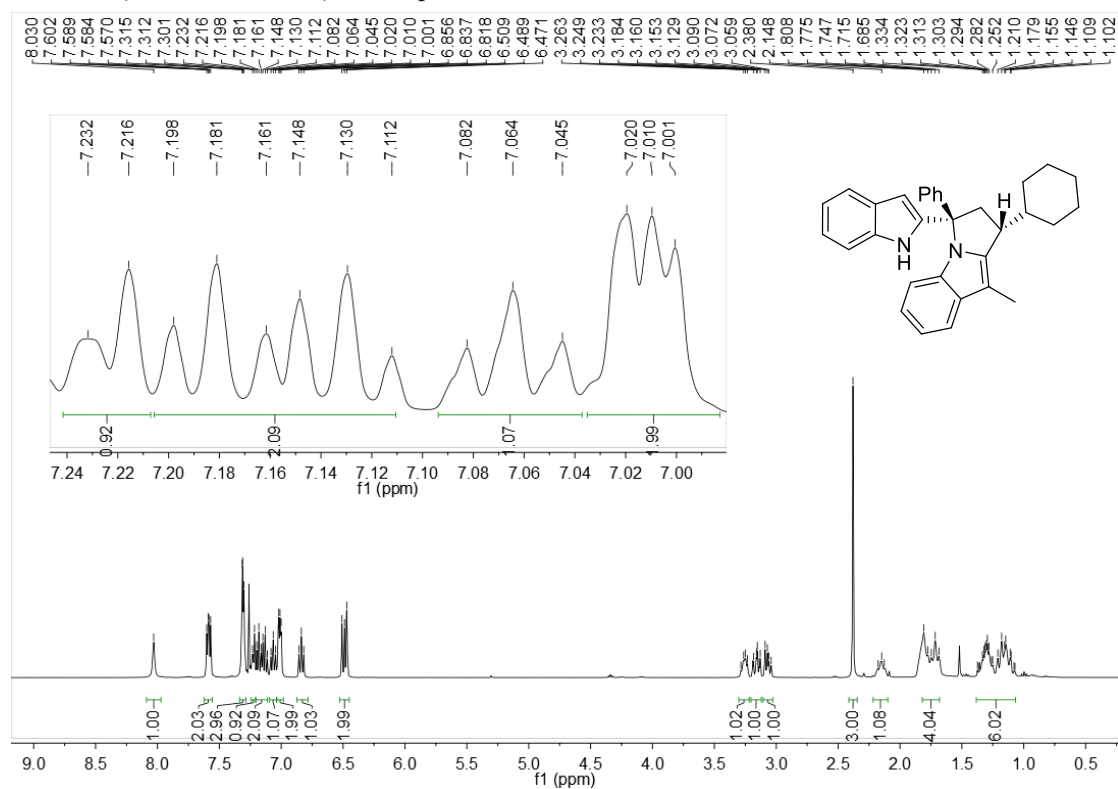
¹H NMR (400 MHz, CDCl₃) of compound **3aj**:



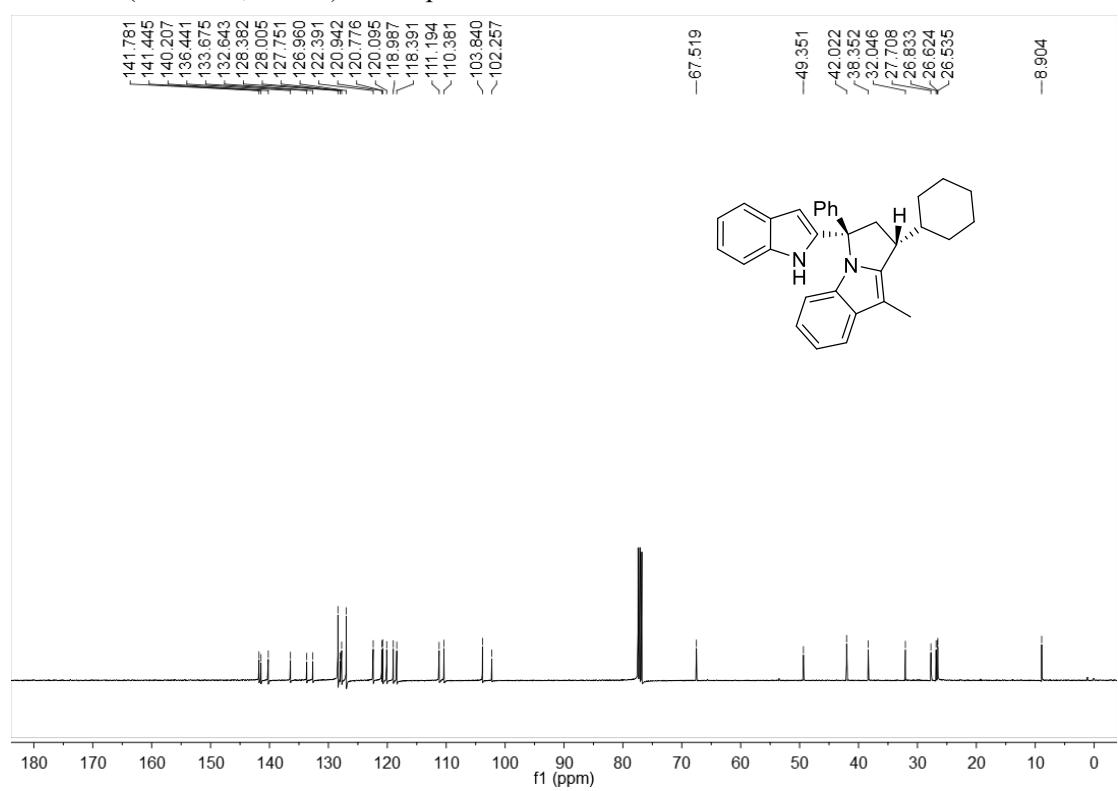
¹³C NMR (100 MHz, CDCl₃) of compound **3aj**:



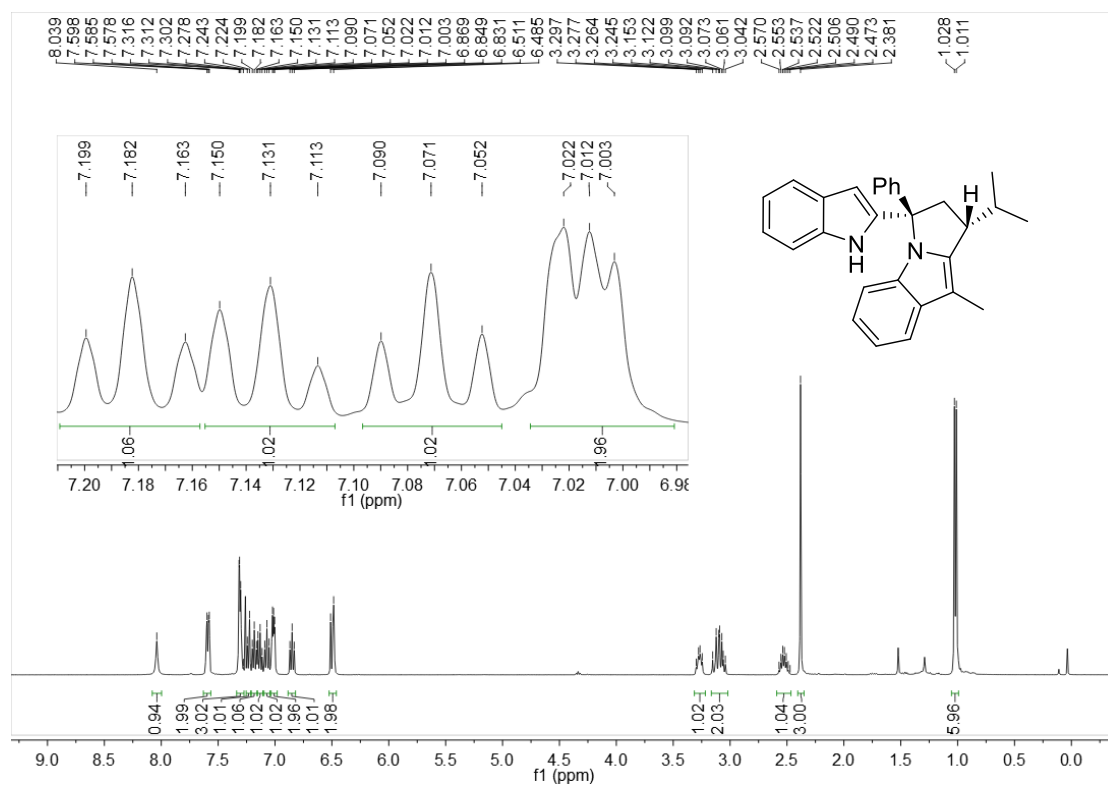
¹H NMR (400 MHz, CDCl₃) of compound **3ak**:



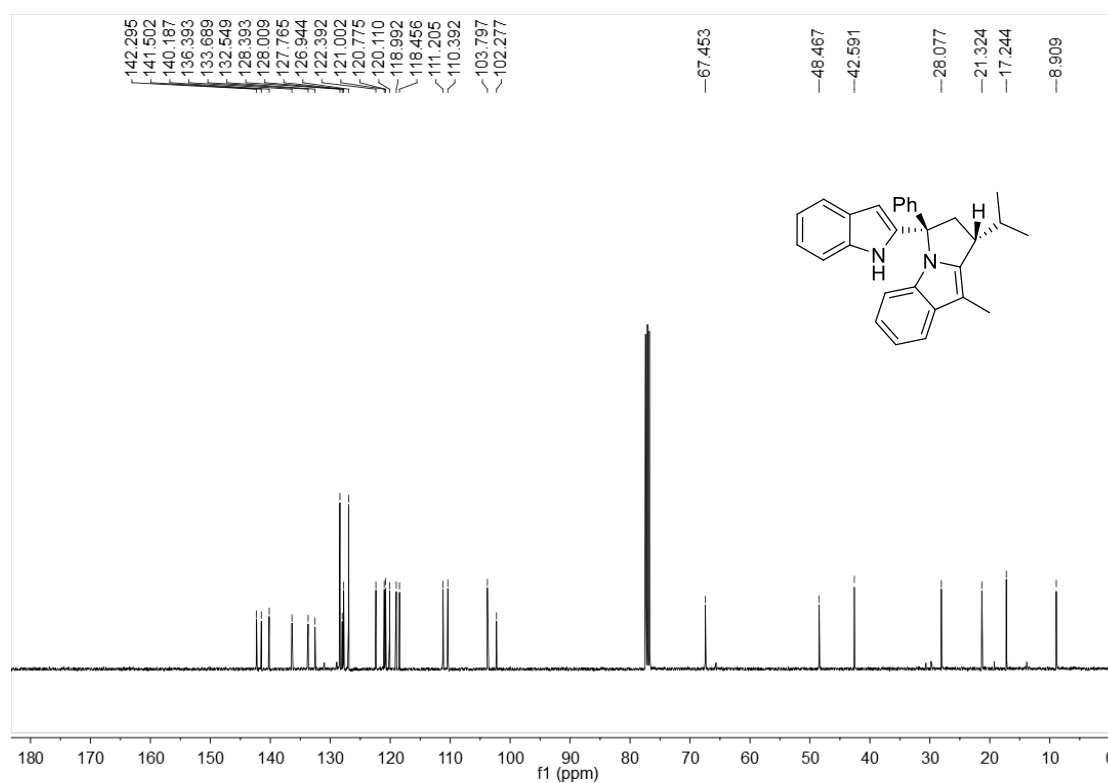
¹³C NMR (100 MHz, CDCl₃) of compound **3ak**:



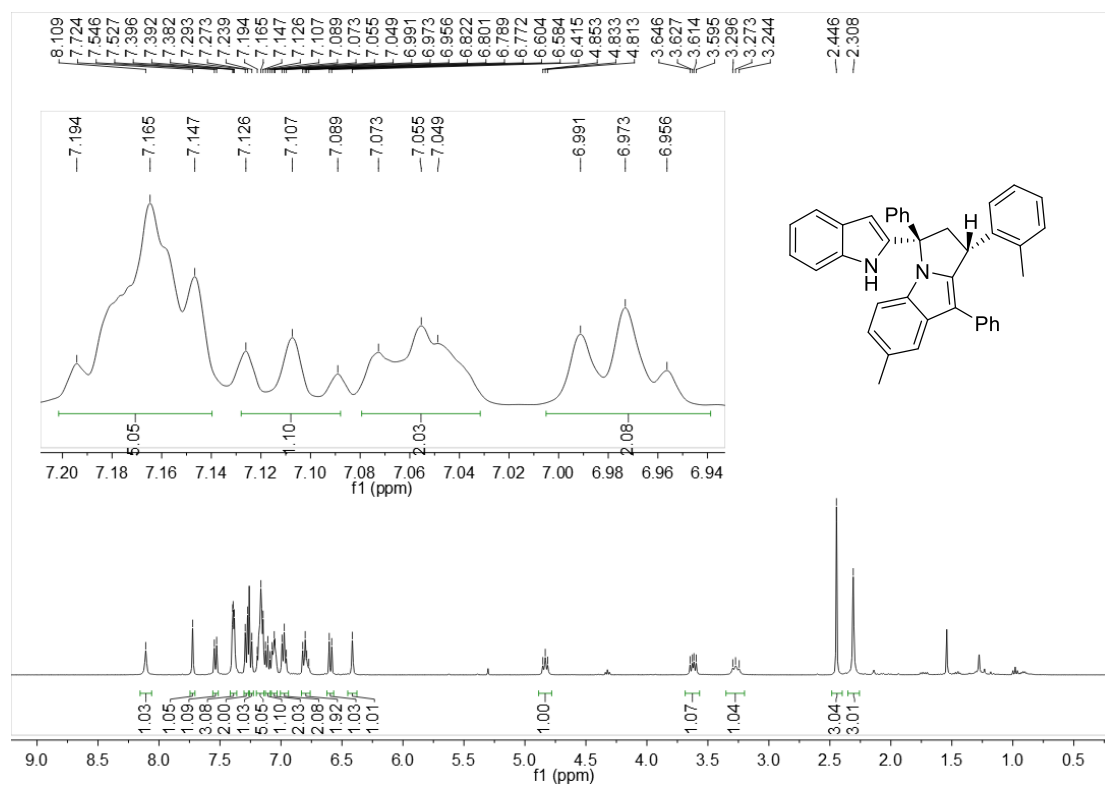
¹H NMR (400 MHz, CDCl₃) of compound **3al**:



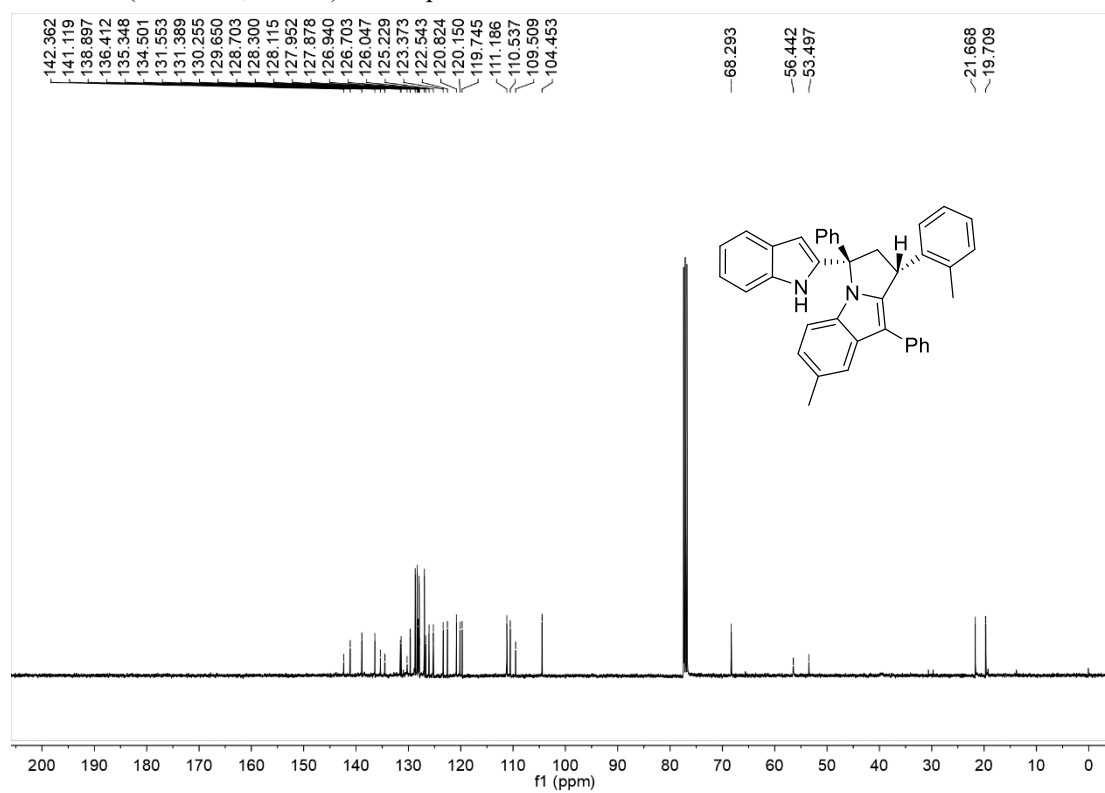
¹³C NMR (100 MHz, CDCl₃) of compound **3al**:



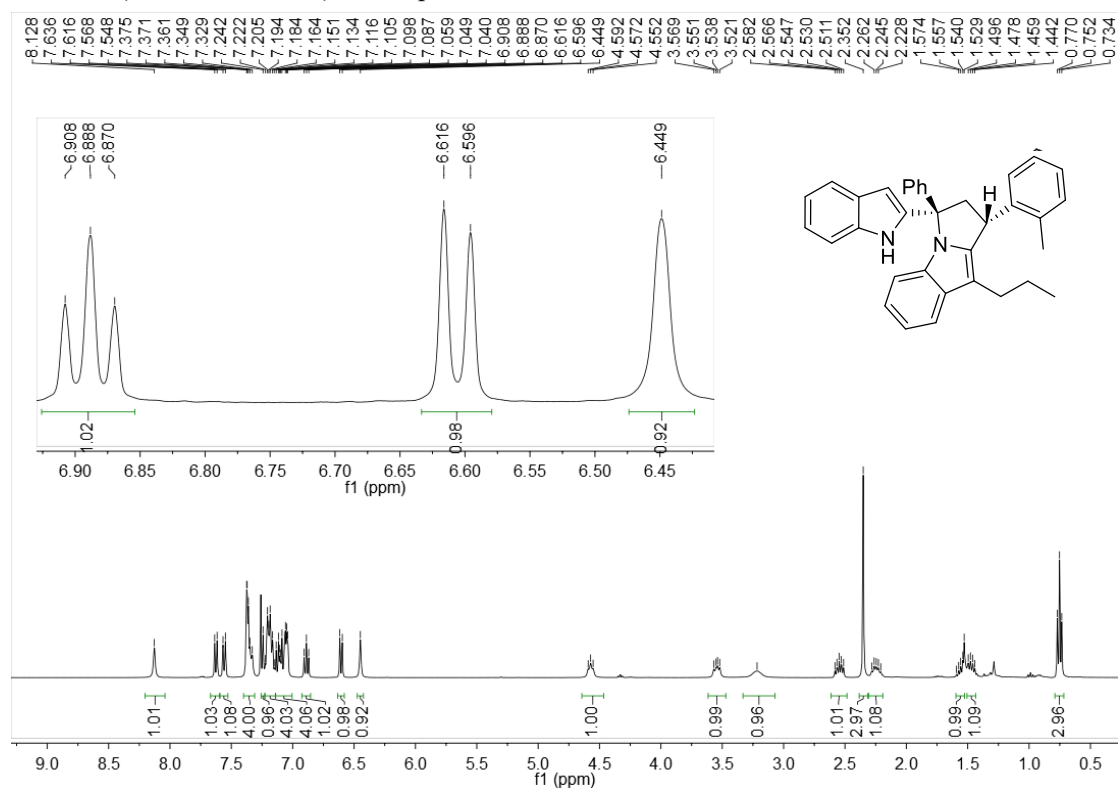
¹H NMR (400 MHz, CDCl₃) of compound **3am**:



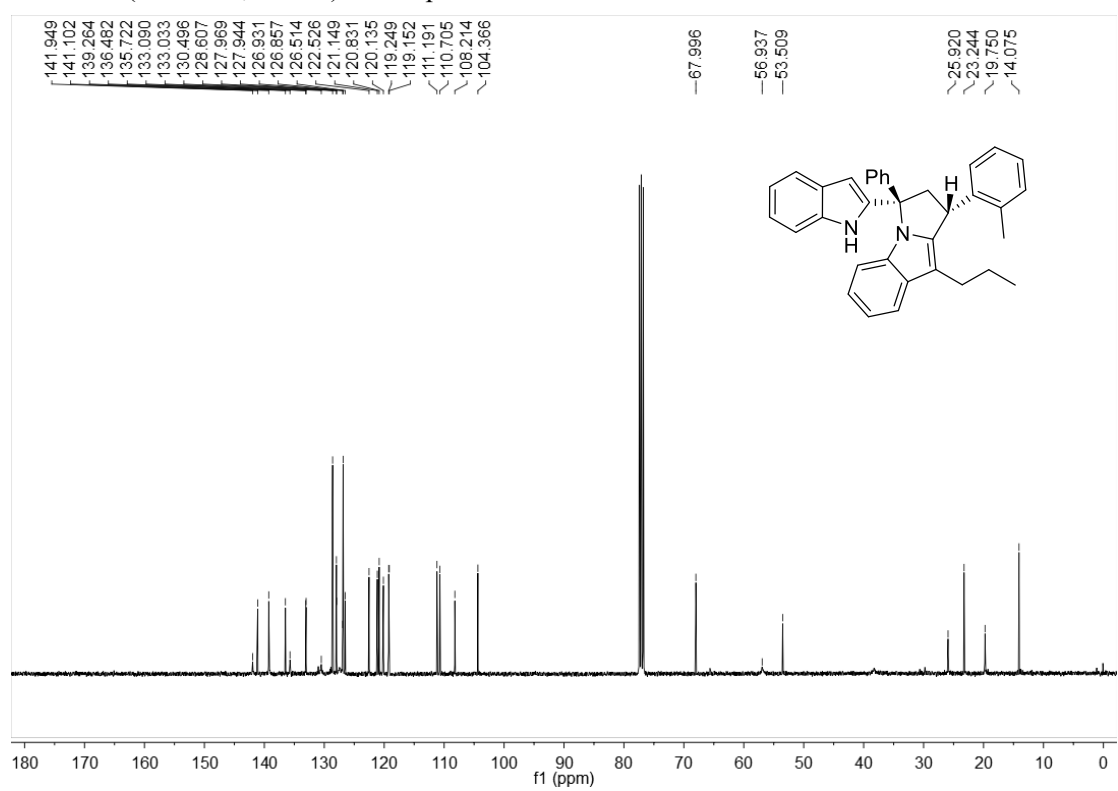
¹³C NMR (100 MHz, CDCl₃) of compound **3am**:



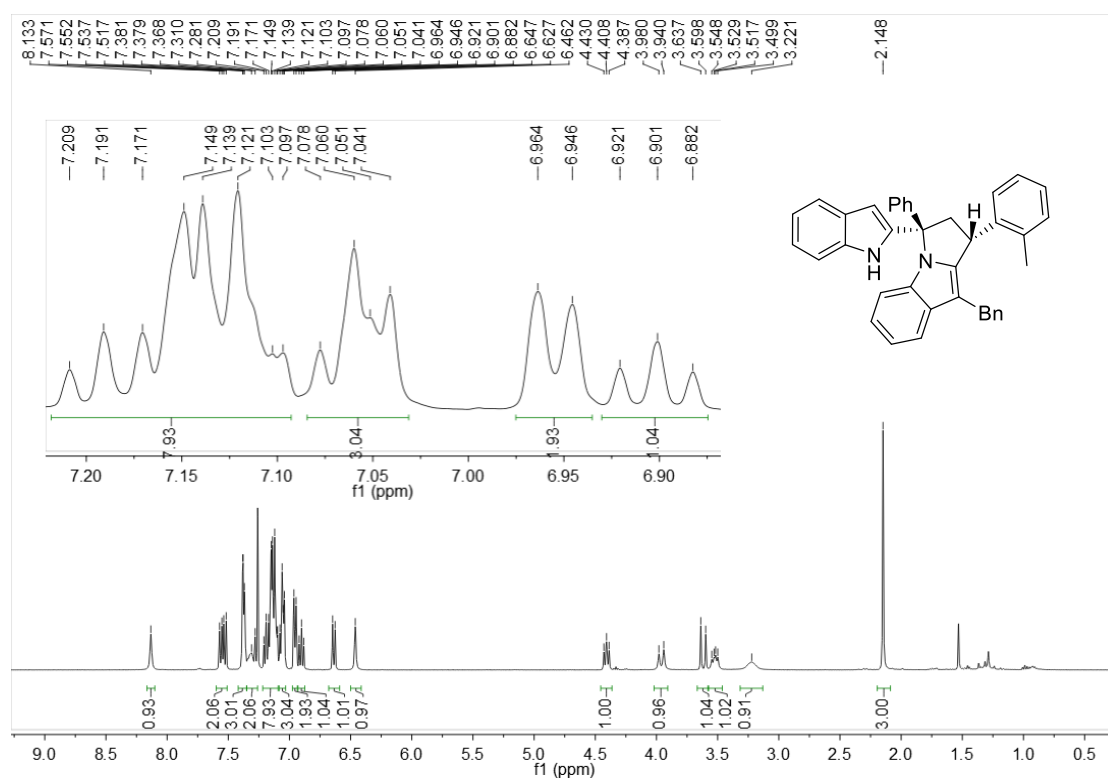
¹H NMR (400 MHz, CDCl₃) of compound **3an**:



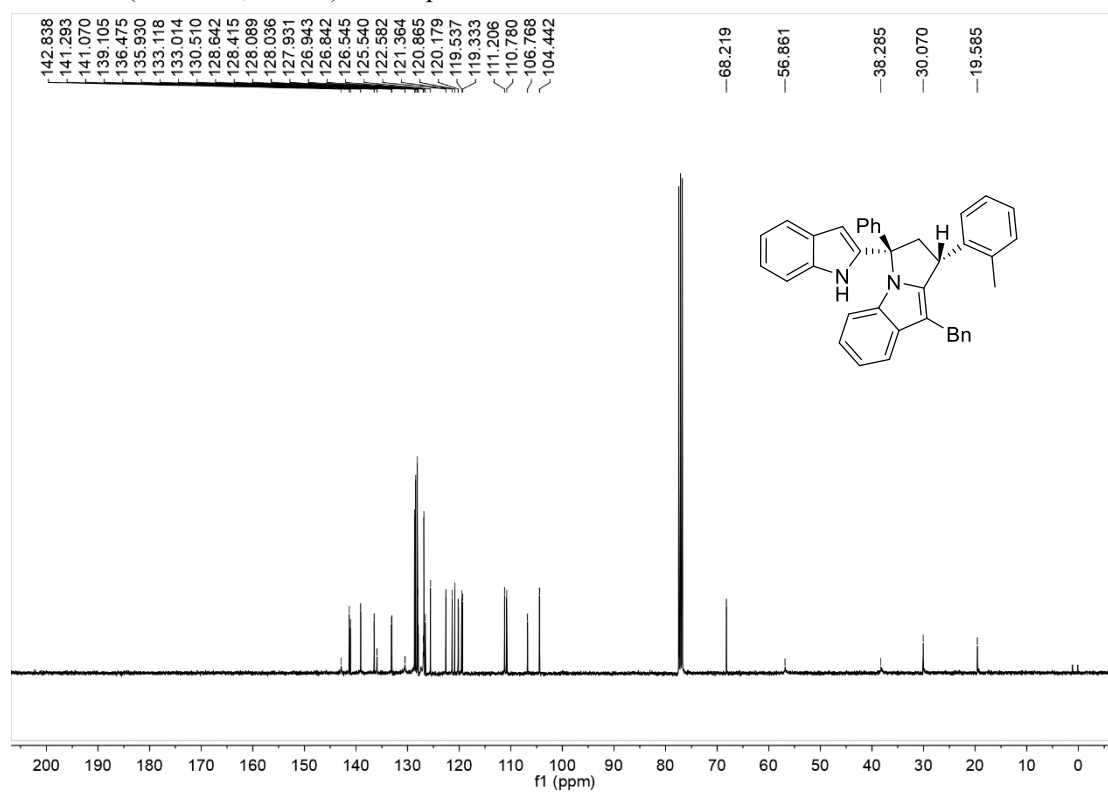
¹³C NMR (100 MHz, CDCl₃) of compound **3an**:



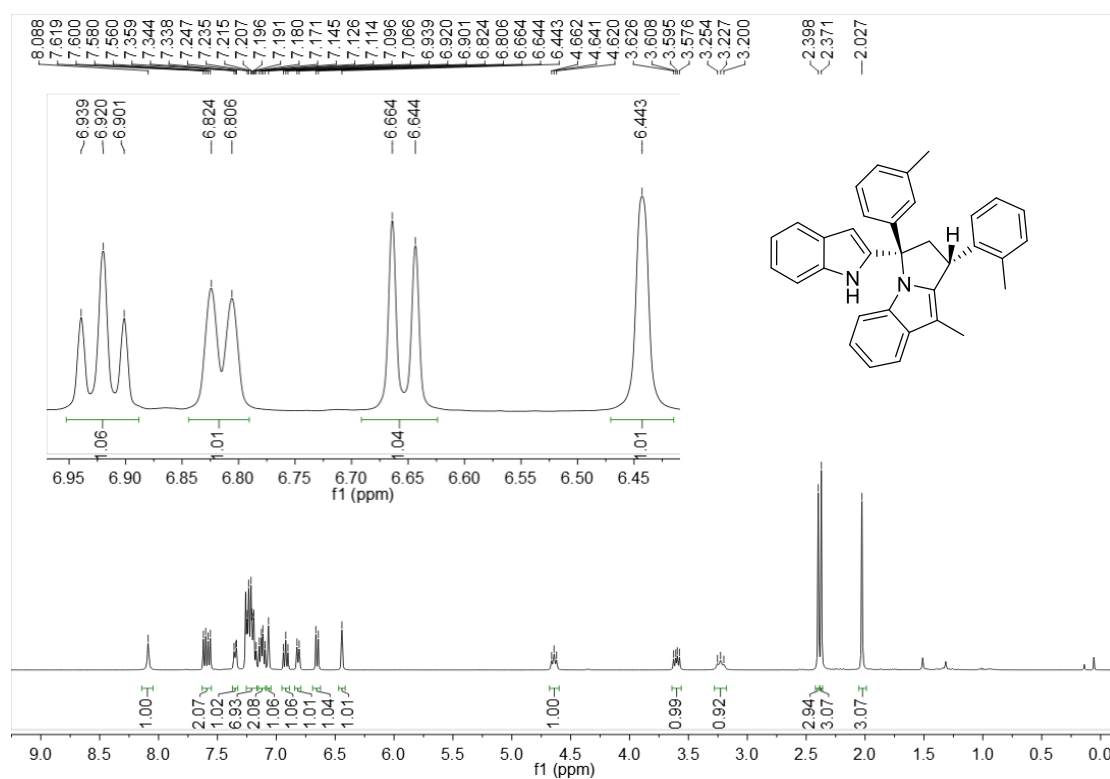
¹H NMR (400 MHz, CDCl₃) of compound **3ao**:



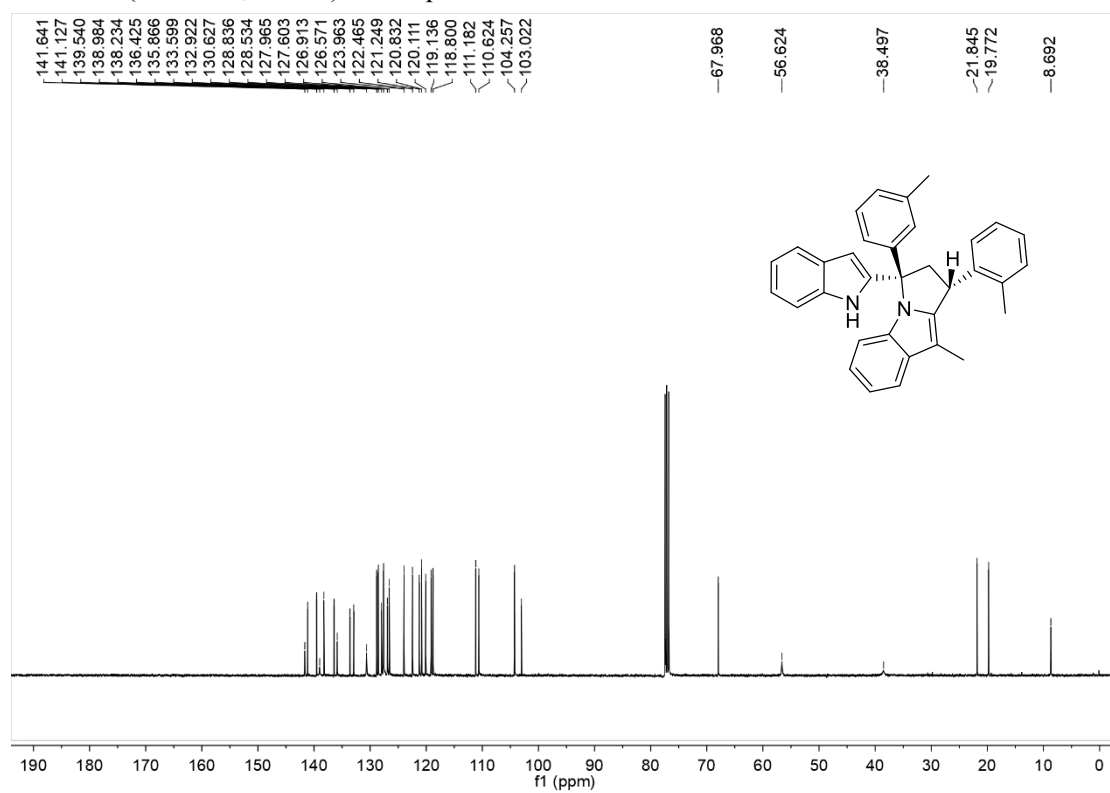
¹³C NMR (100 MHz, CDCl₃) of compound **3ao**:



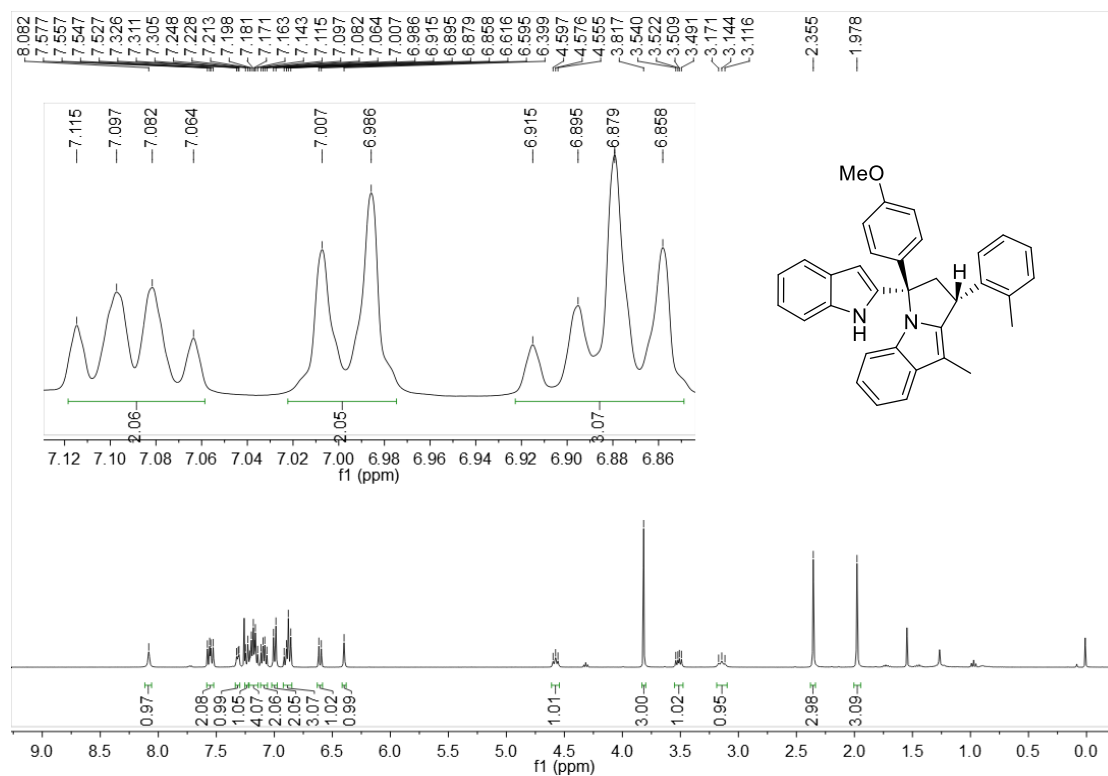
¹H NMR (400 MHz, CDCl₃) of compound **3ba**:



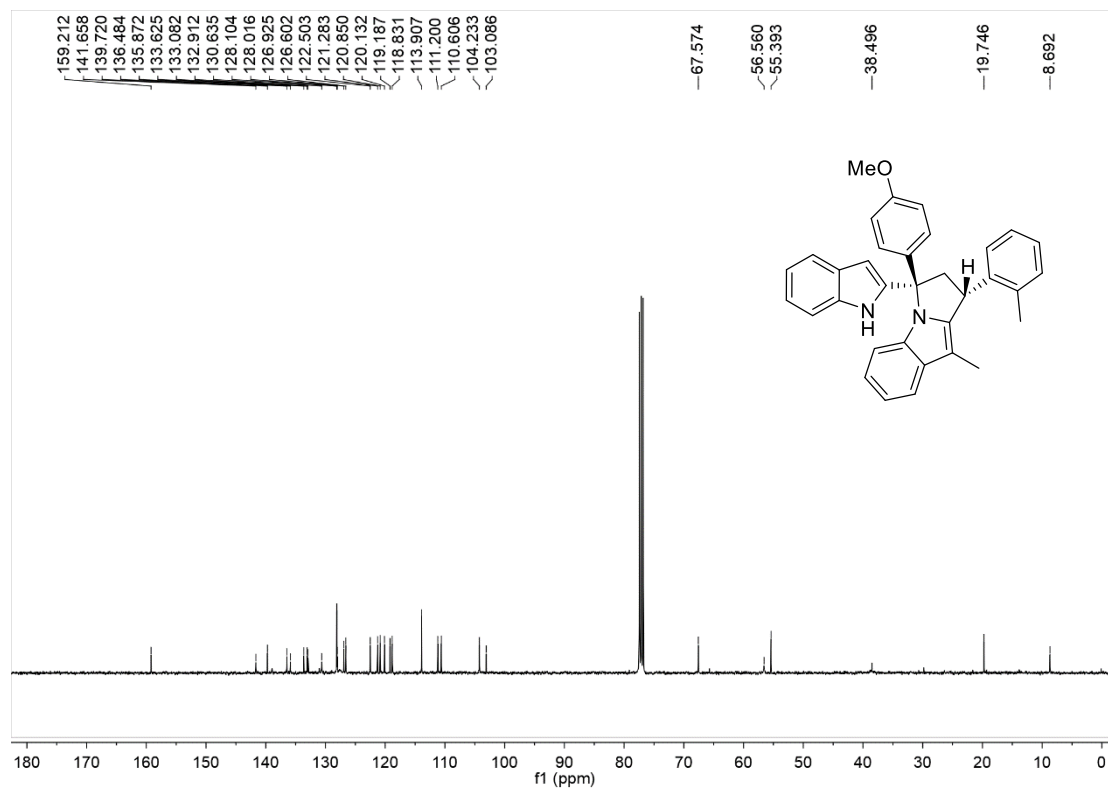
¹³C NMR (100 MHz, CDCl₃) of compound **3ba**:



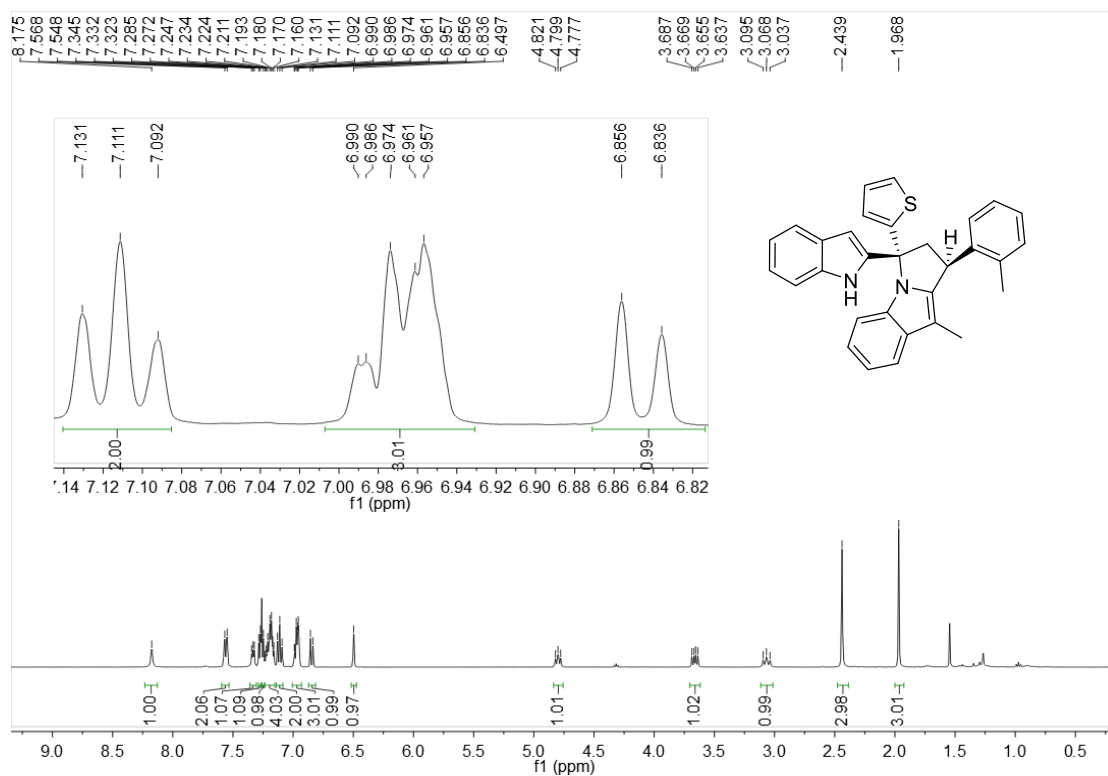
¹H NMR (400 MHz, CDCl₃) of compound **3ca**:



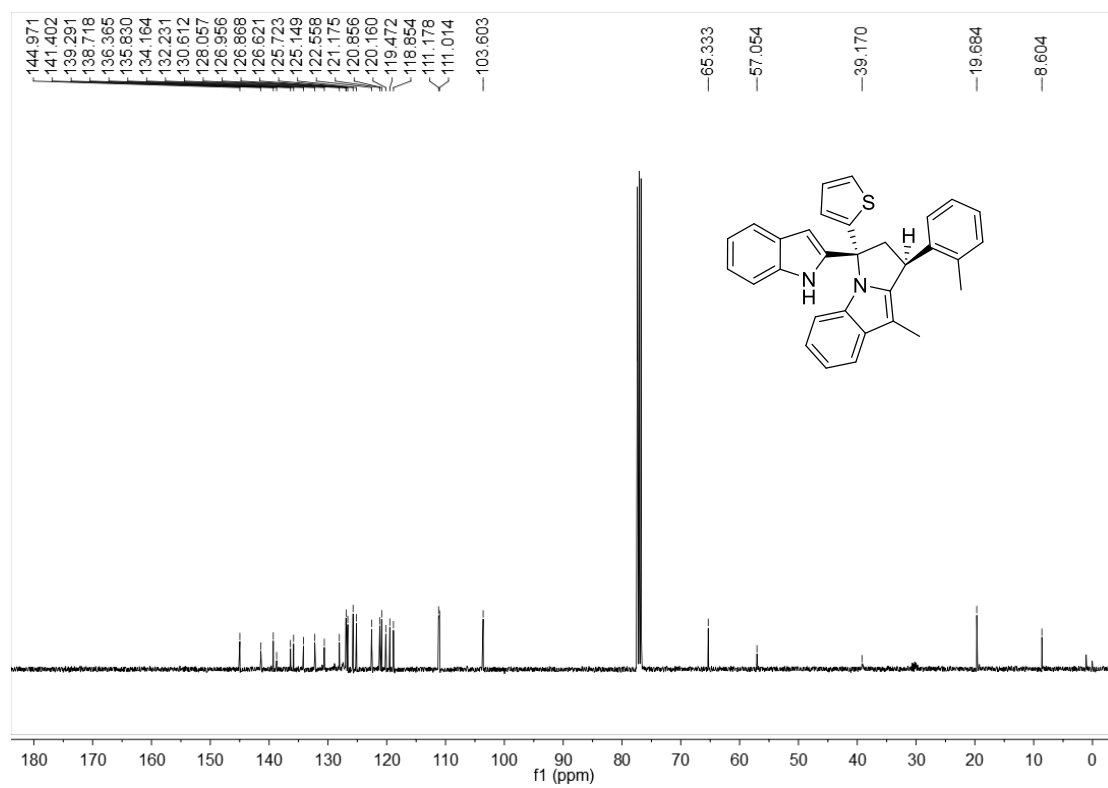
¹³C NMR (100 MHz, CDCl₃) of compound **3ca**:



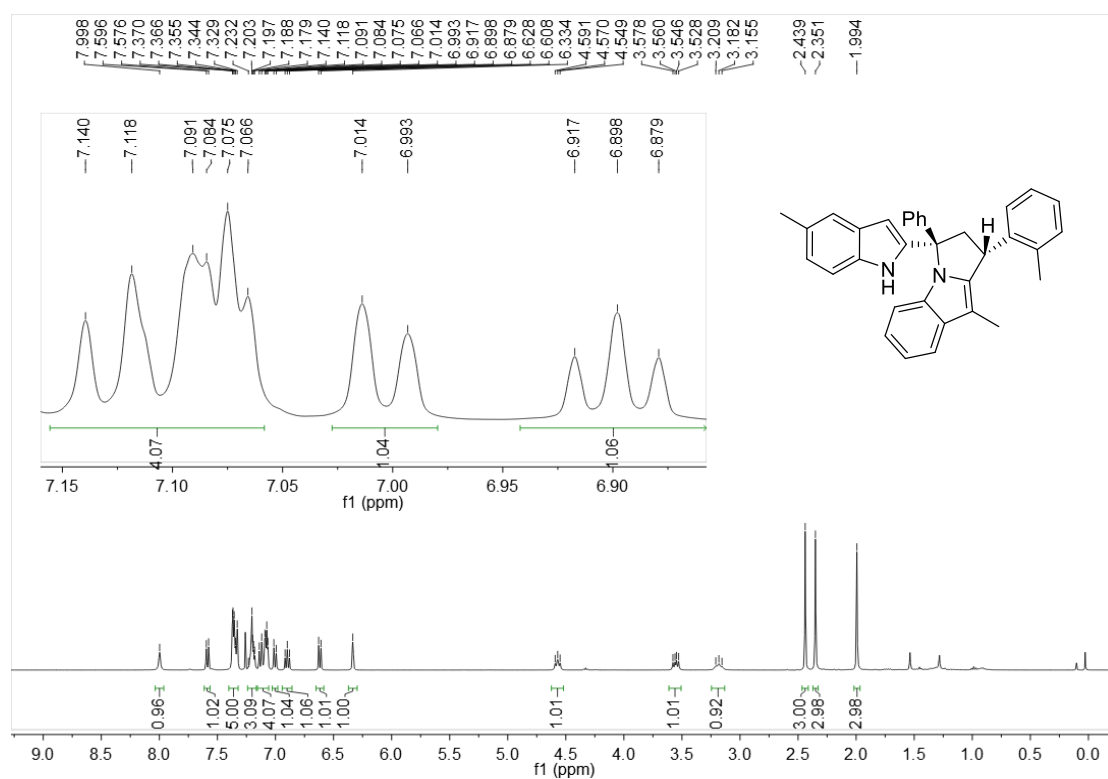
¹H NMR (400 MHz, CDCl₃) of compound **3da**:



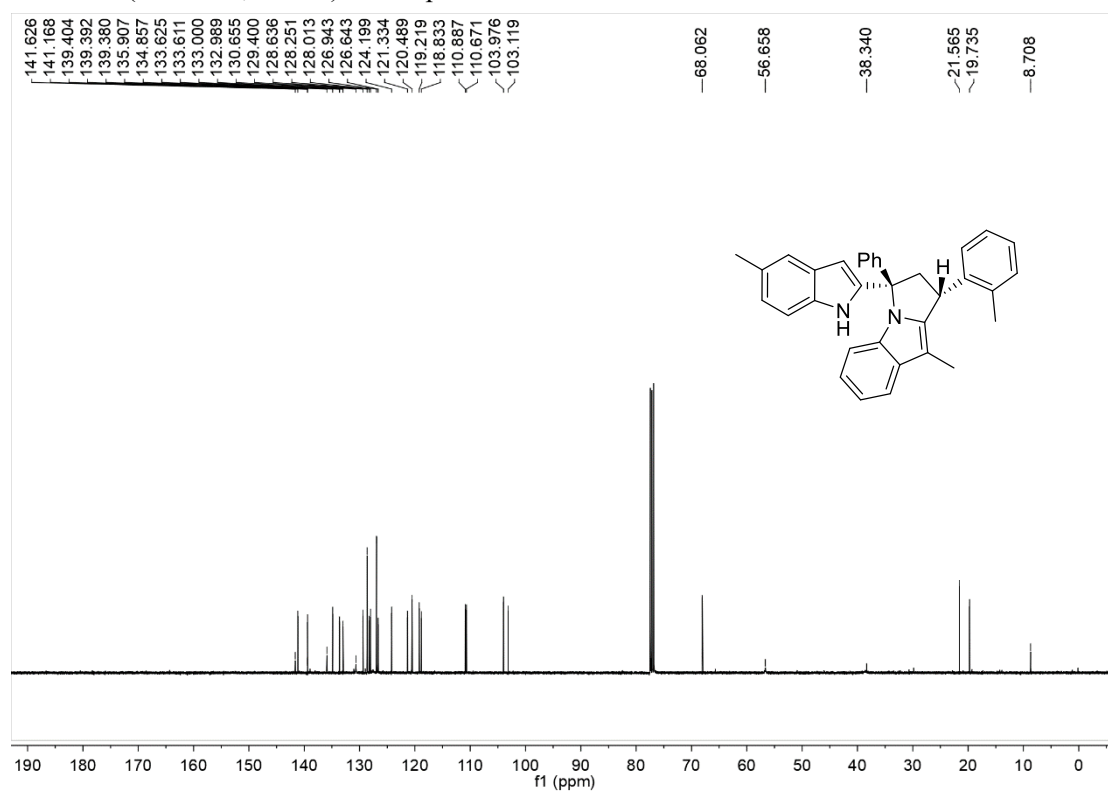
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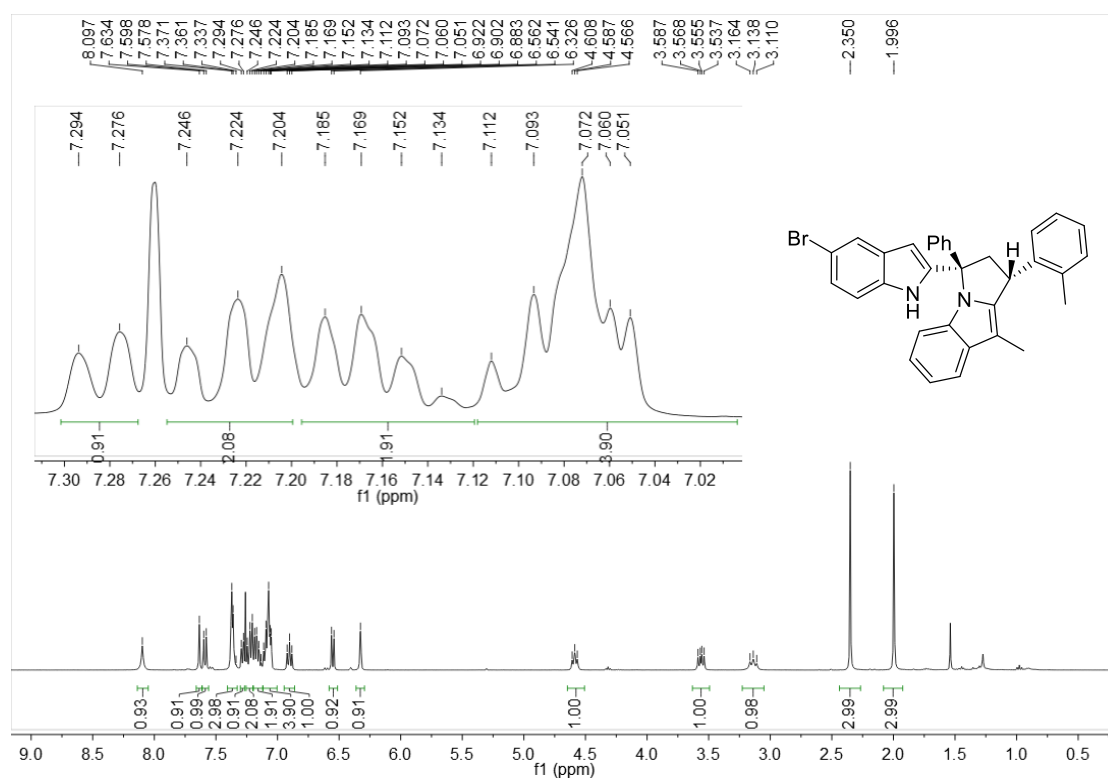
¹H NMR (400 MHz, CDCl₃) of compound **3ea**:



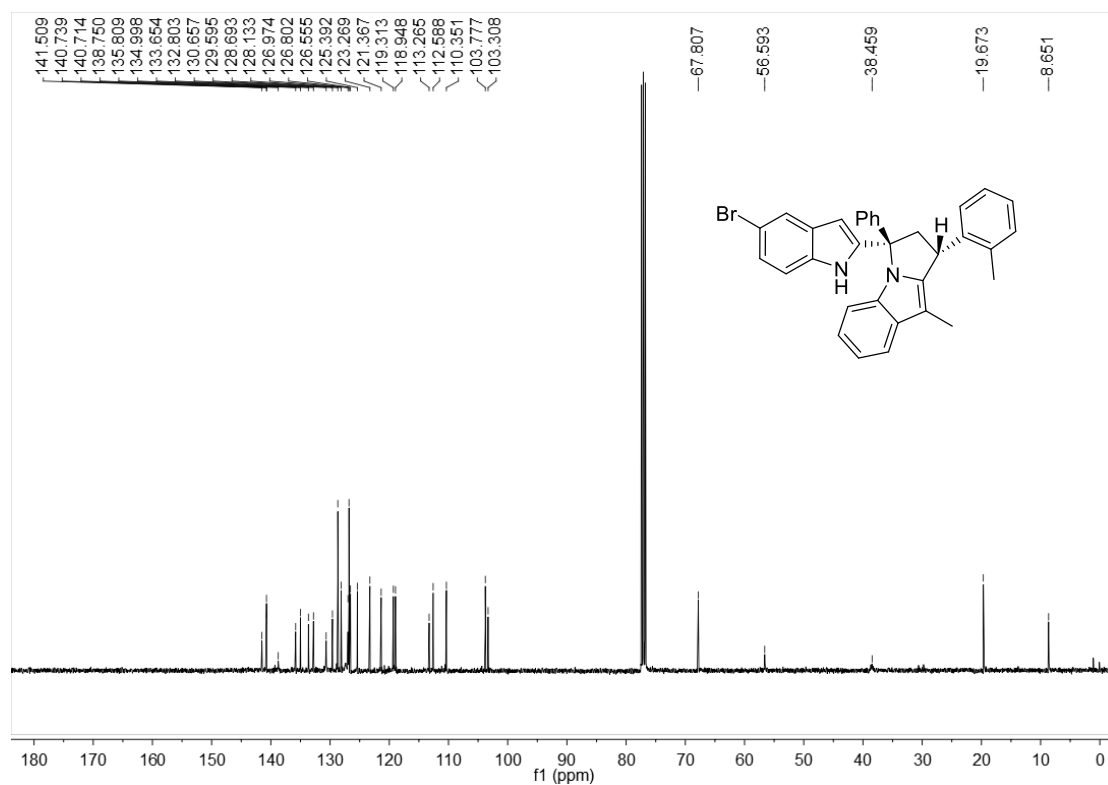
¹³C NMR (100 MHz, CDCl₃) of compound **3ea**:



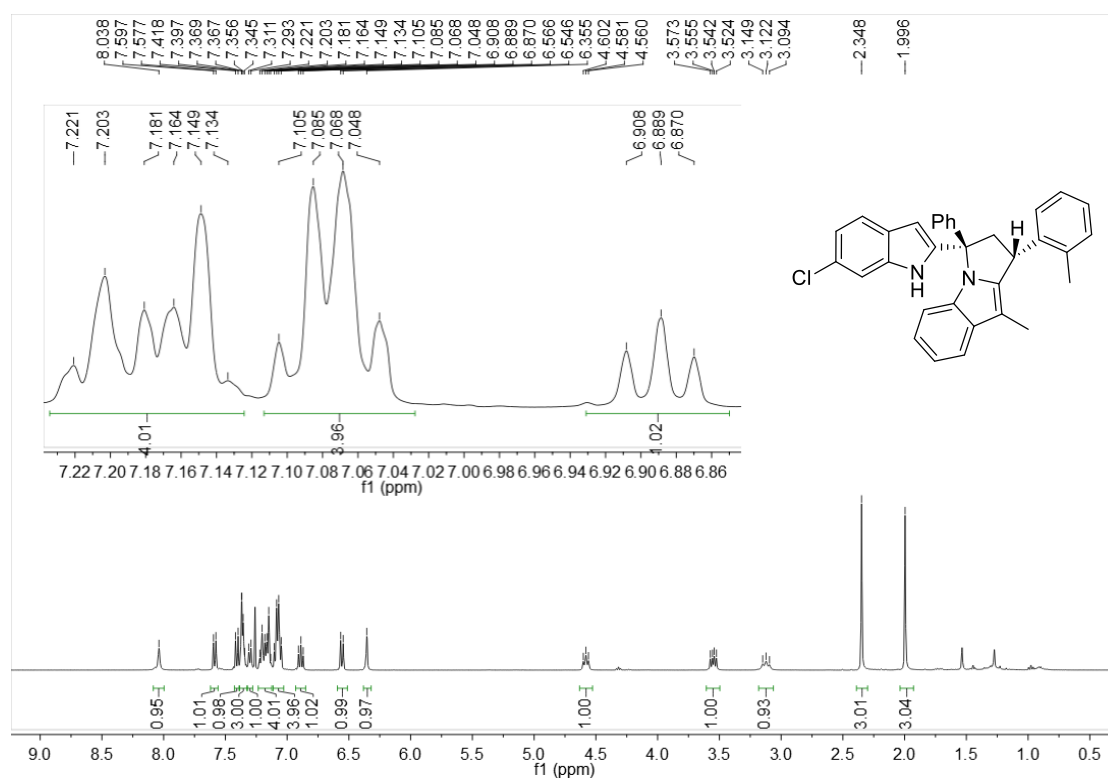
^1H NMR (400 MHz, CDCl_3) of compound **3fa**:



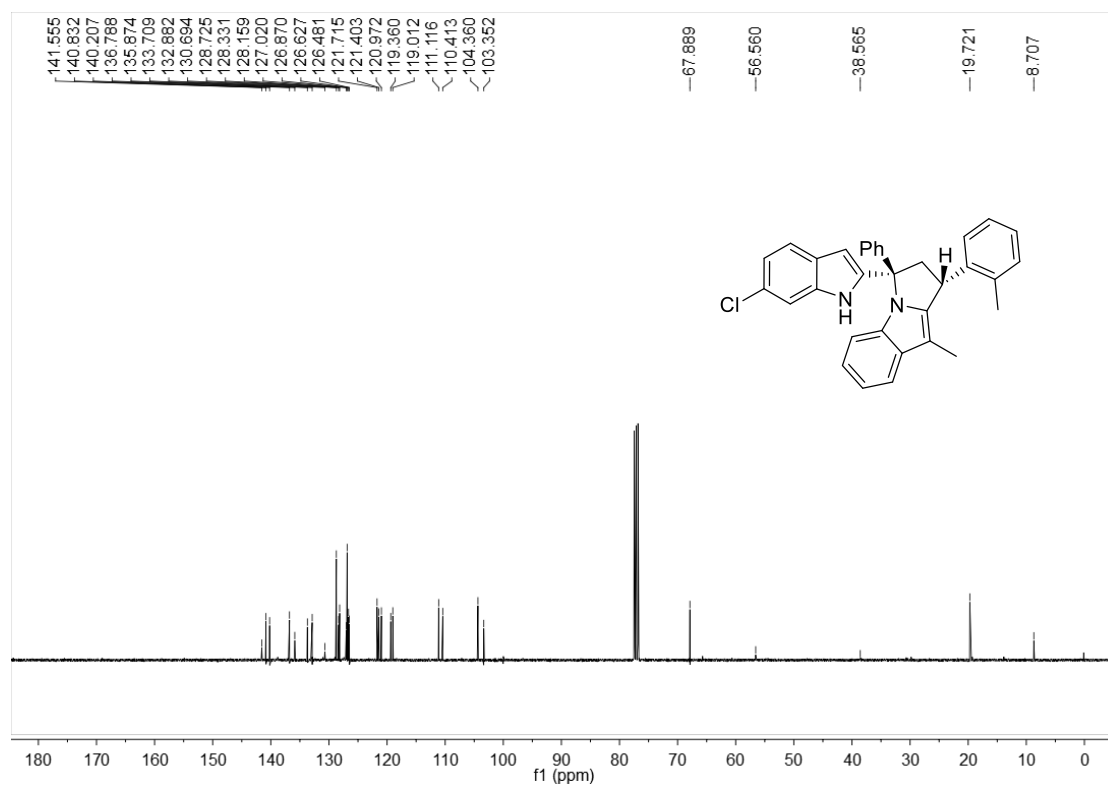
^{13}C NMR (100 MHz, CDCl_3) of compound **3fa**:



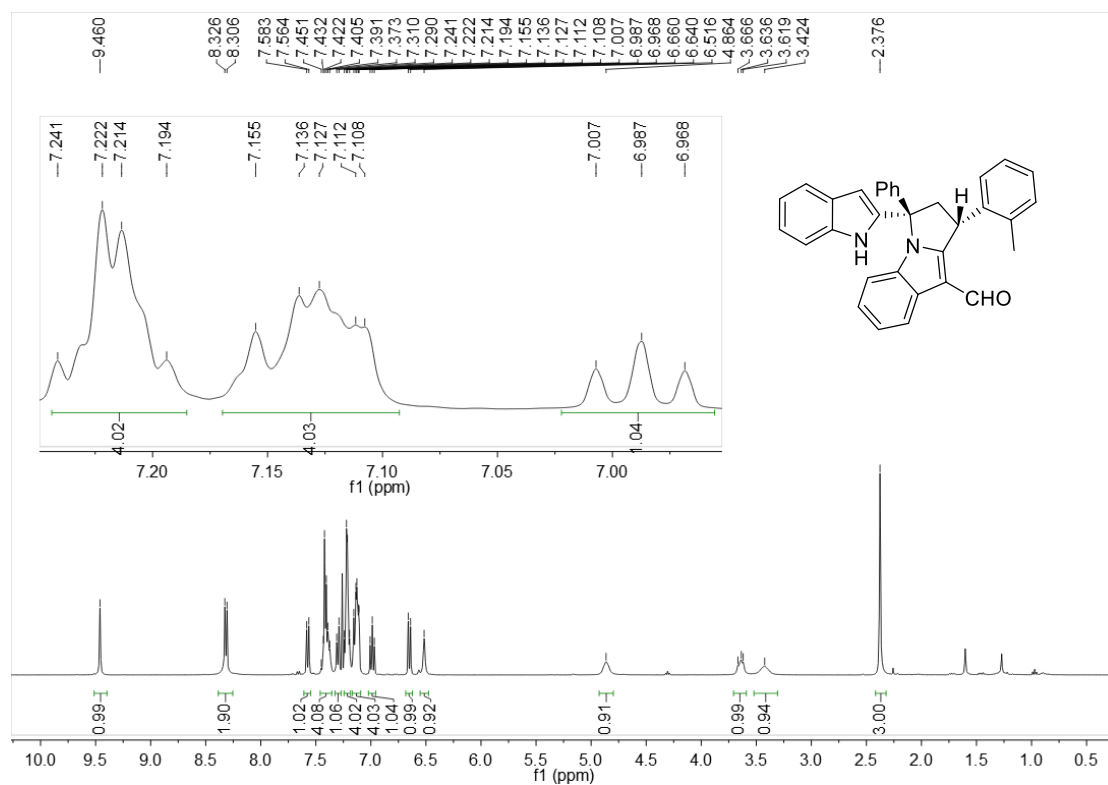
¹H NMR (400 MHz, CDCl₃) of compound **3ga**:



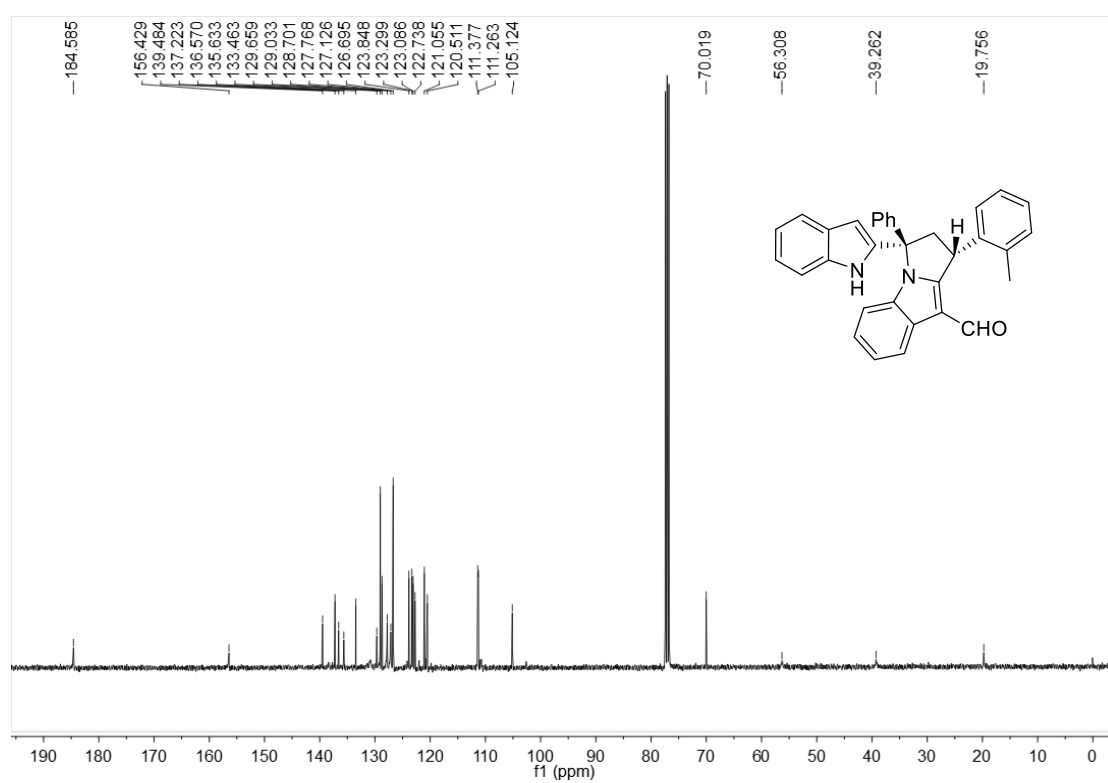
¹³C NMR (100 MHz, CDCl₃) of compound **3ga**:



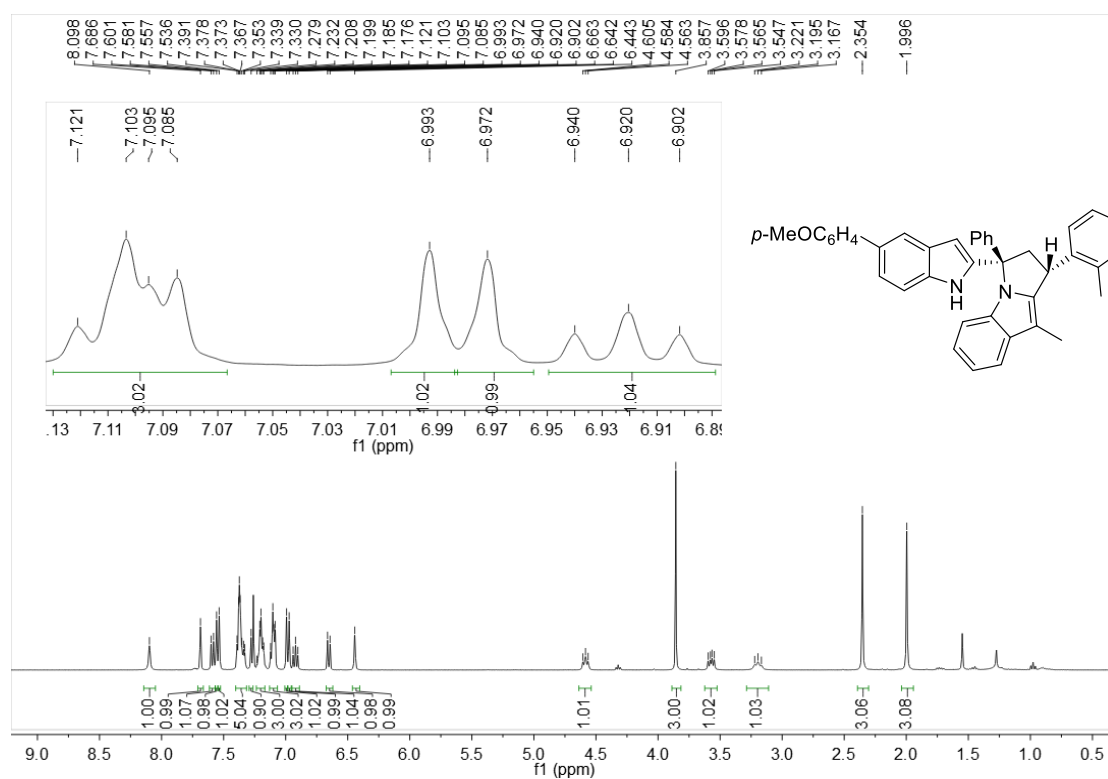
¹H NMR (400 MHz, CDCl₃) of compound **6**:



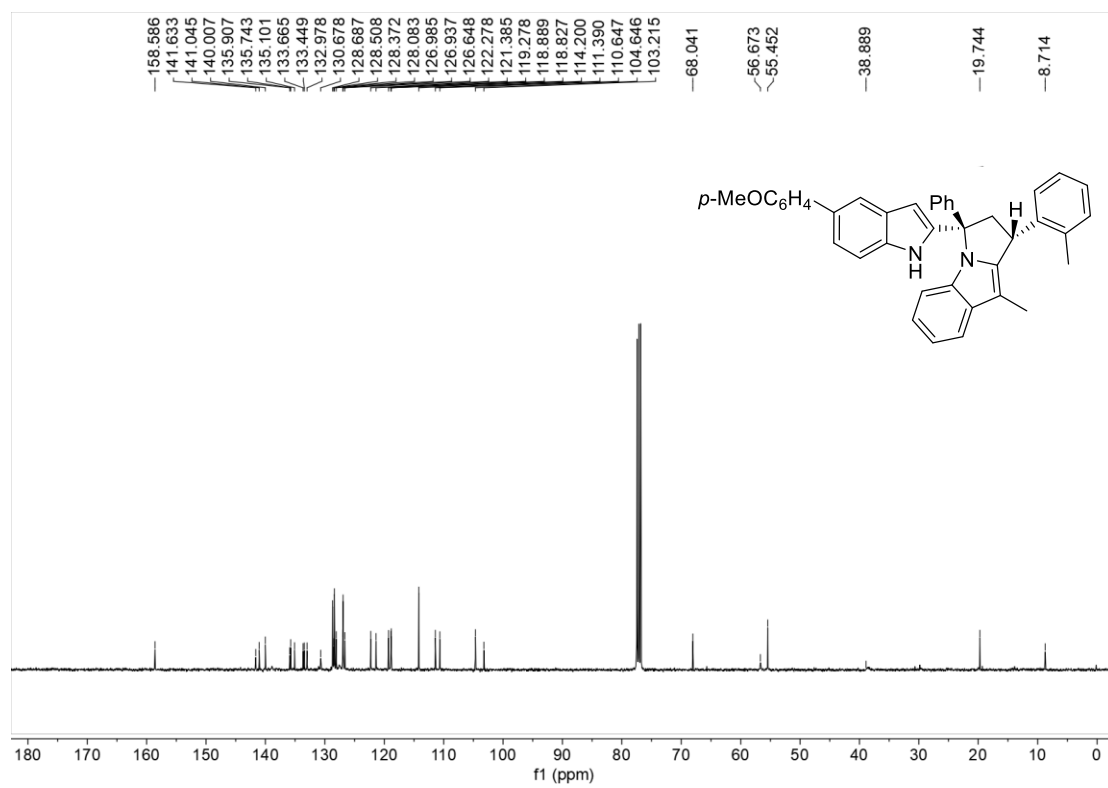
¹³C NMR (100 MHz, CDCl₃) of compound **6**:



¹H NMR (400 MHz, CDCl₃) of compound 7:



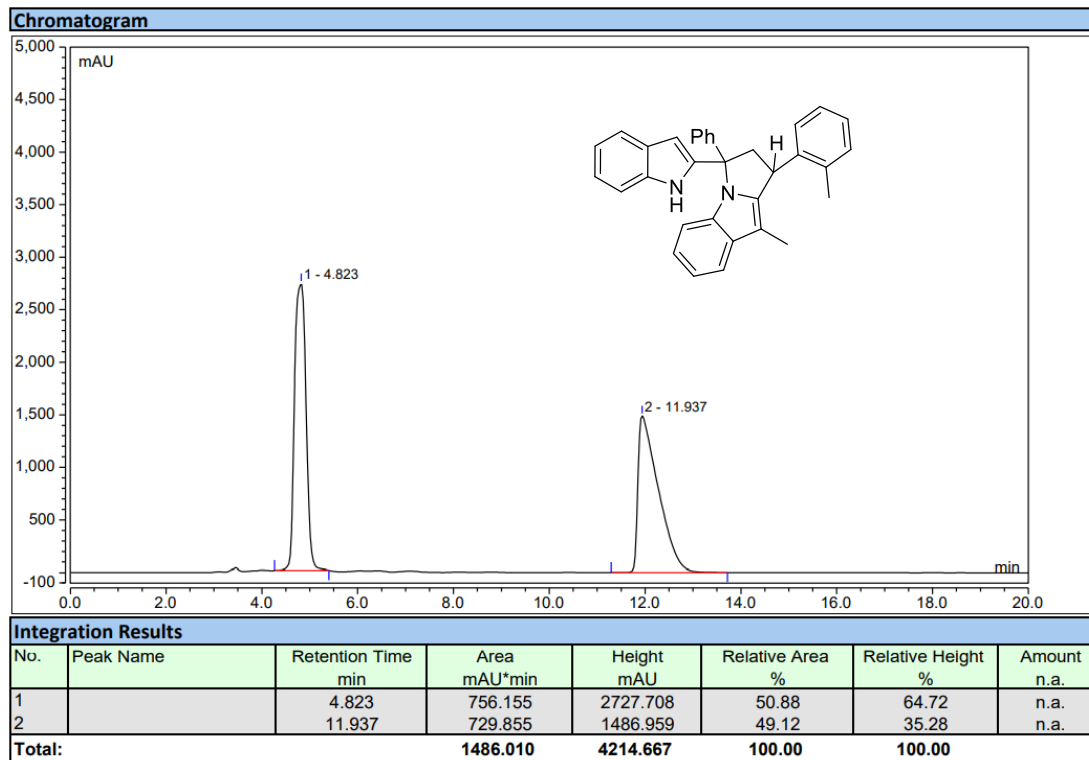
¹³C NMR (100 MHz, CDCl₃) of compound 7:



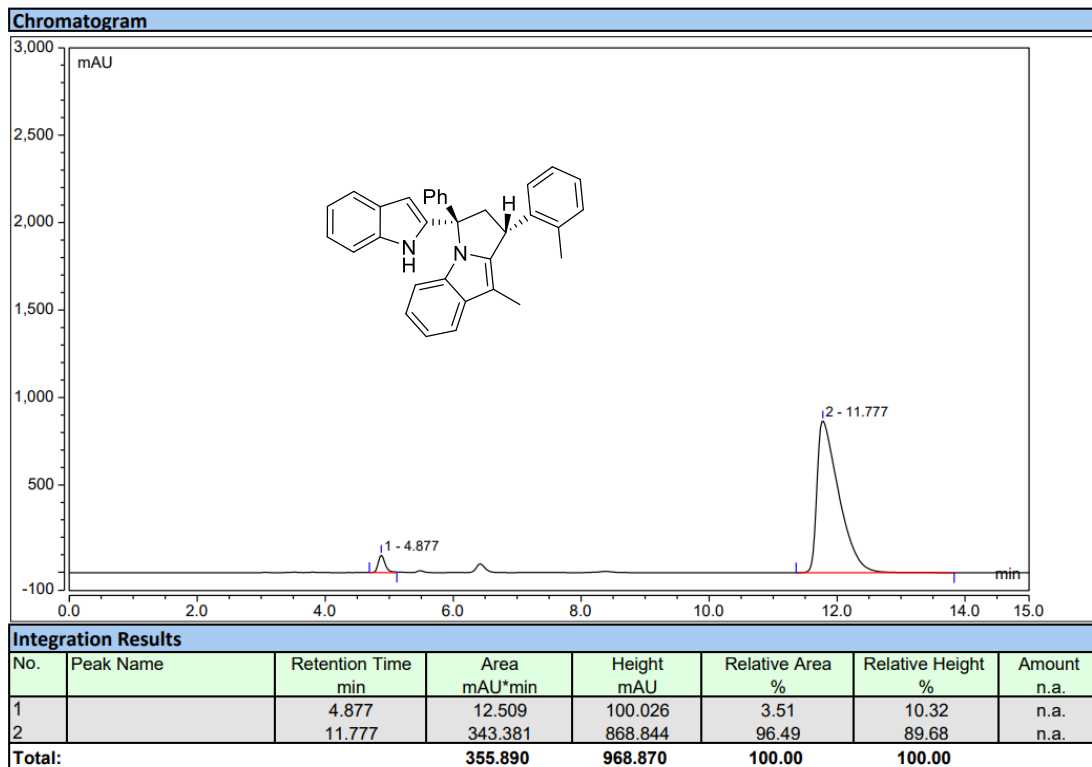
9. HPLC traces of products 3 and 6-7

3aa

Racemic:

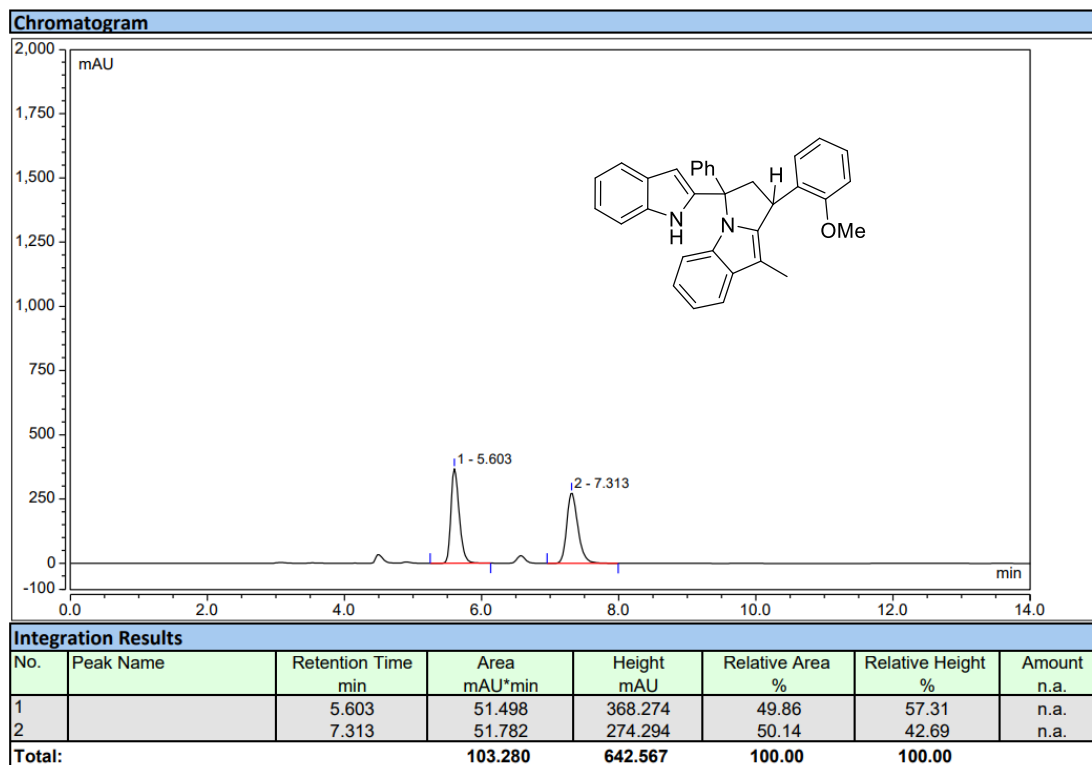


Enantioselective:

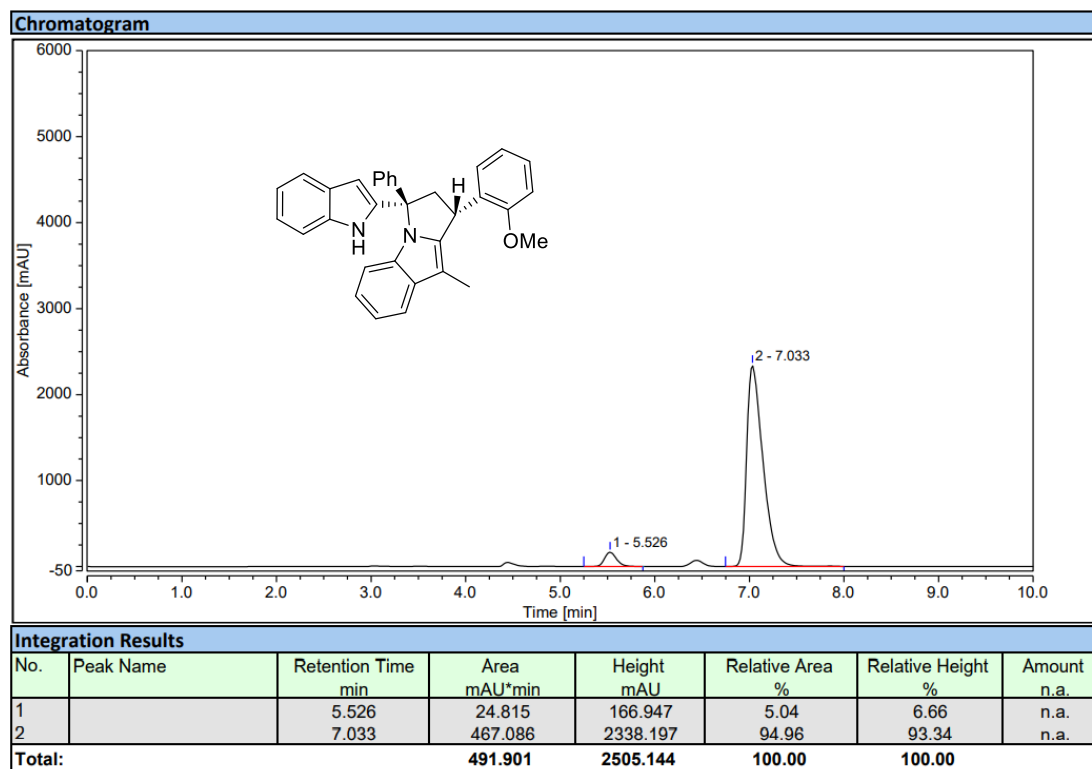


3ab

Racemic:

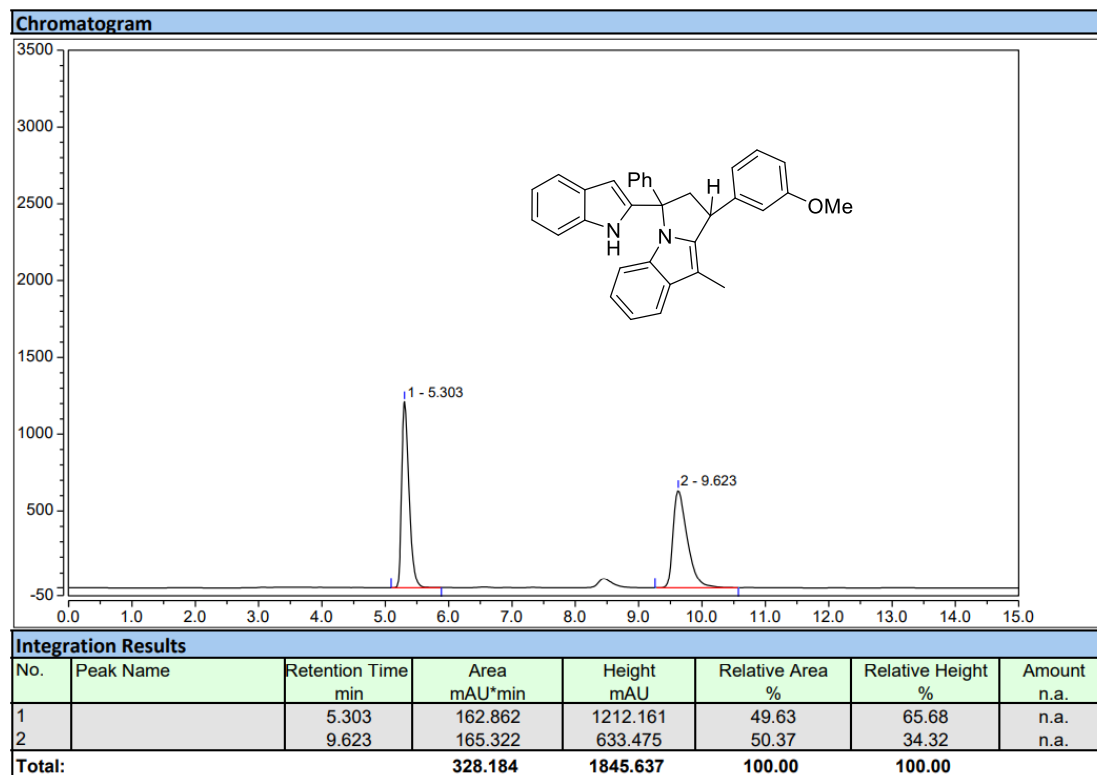


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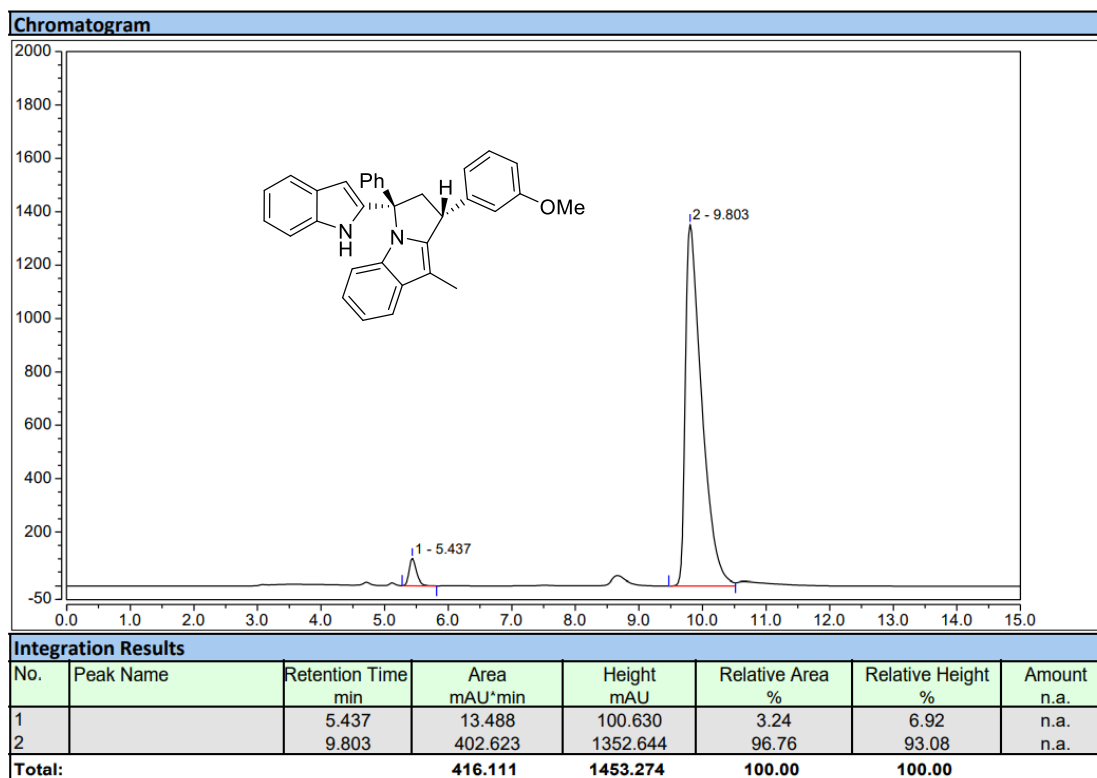


3ac

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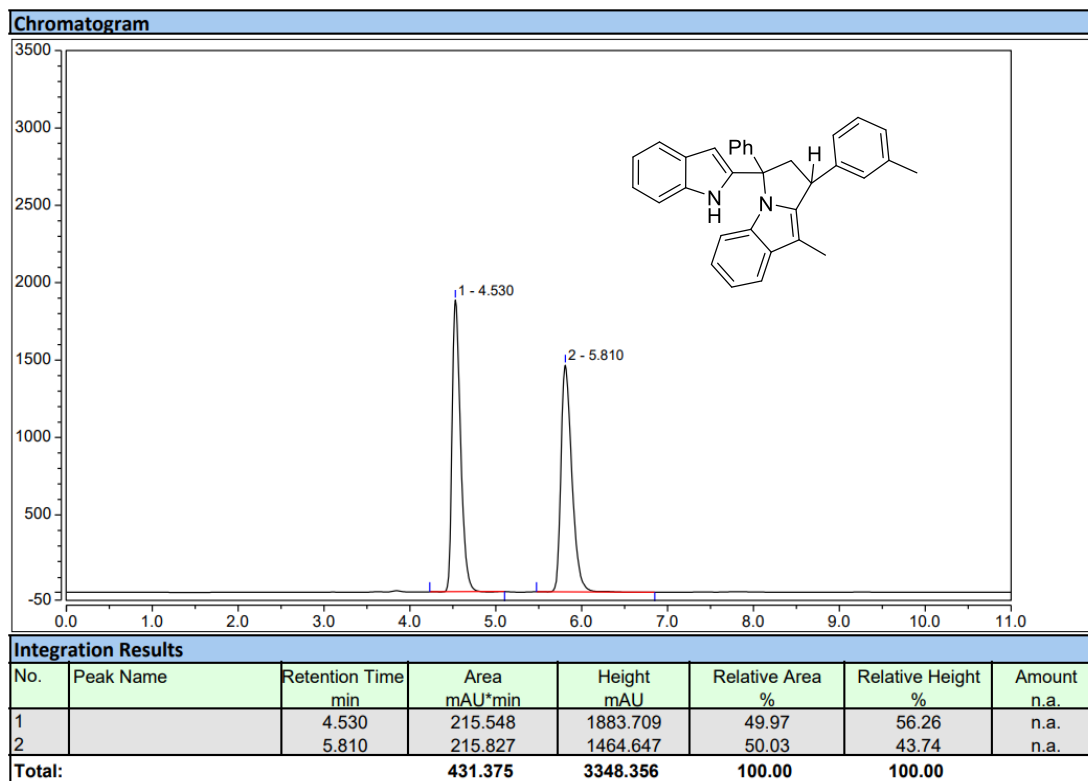


Enantioselective:

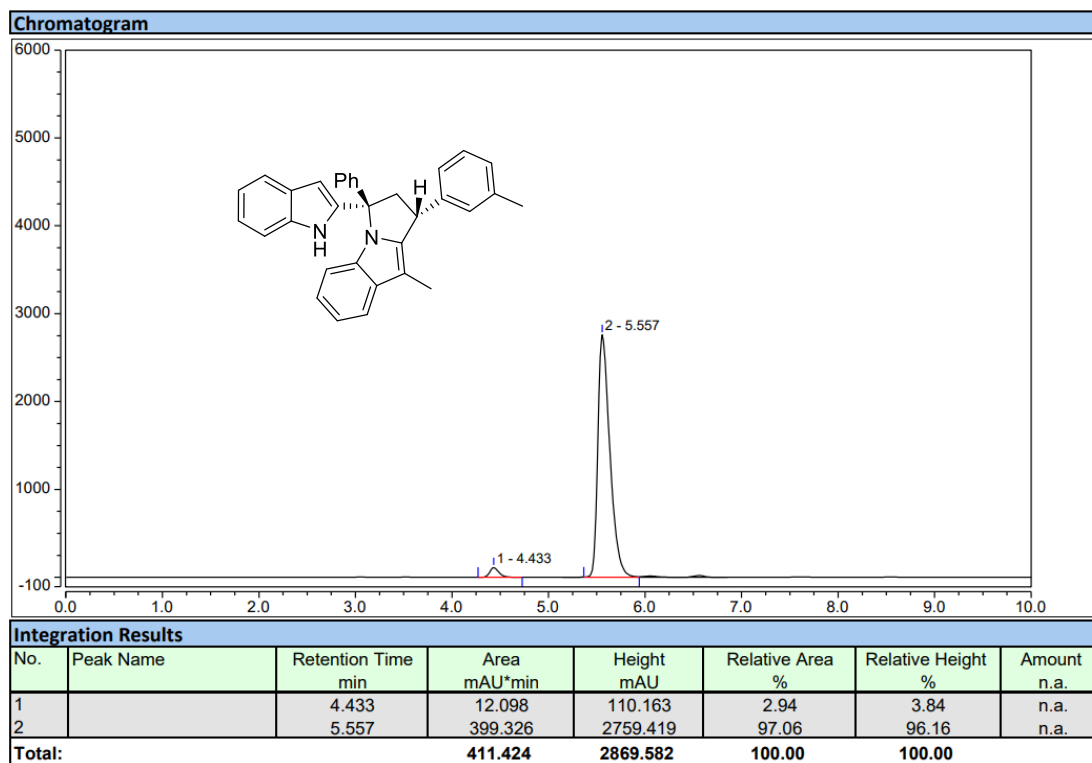


3ad

Racemic:

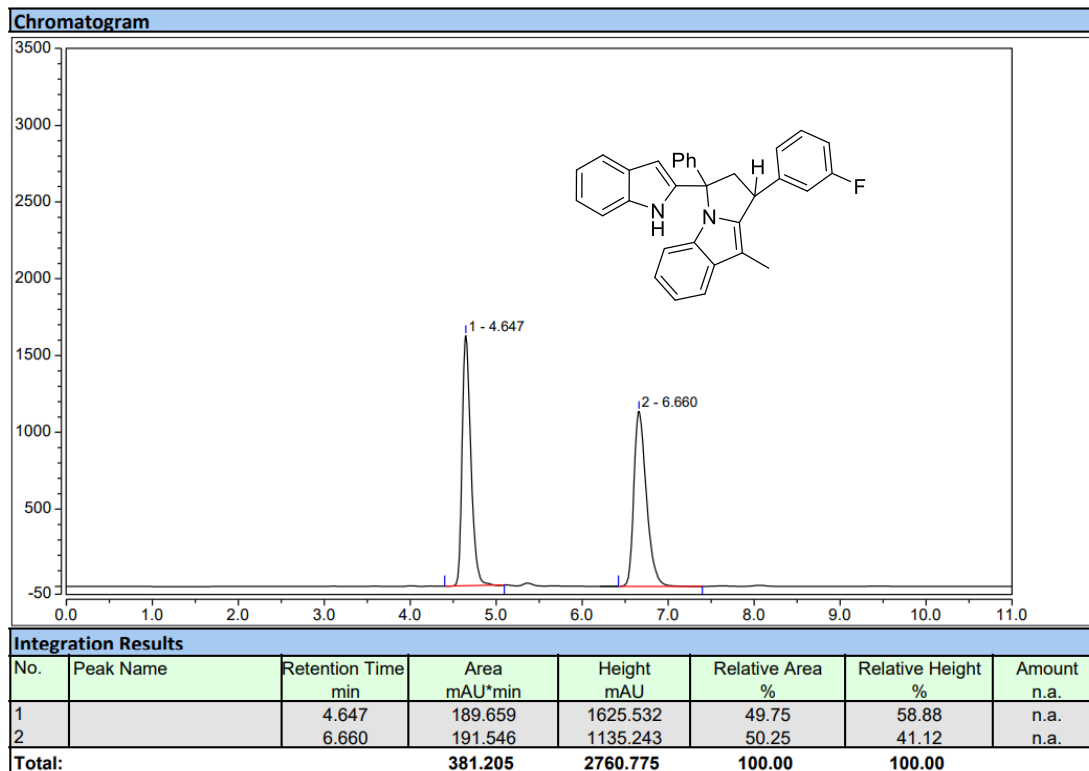


Enantioselective:

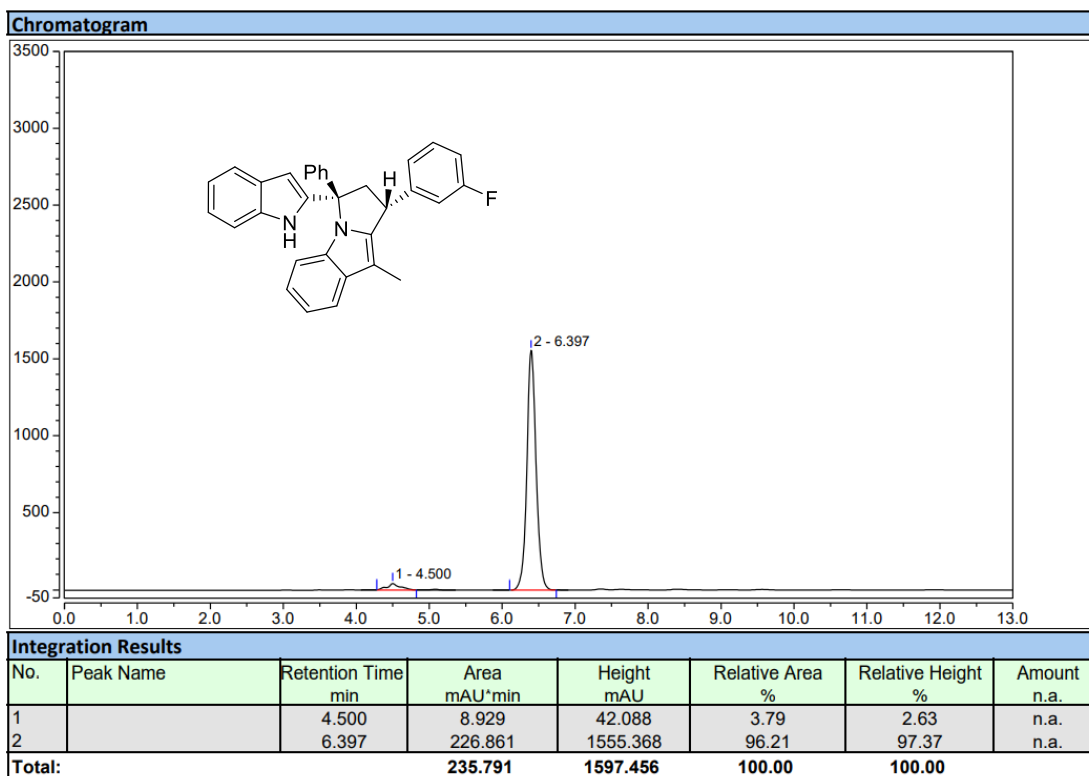


3ae

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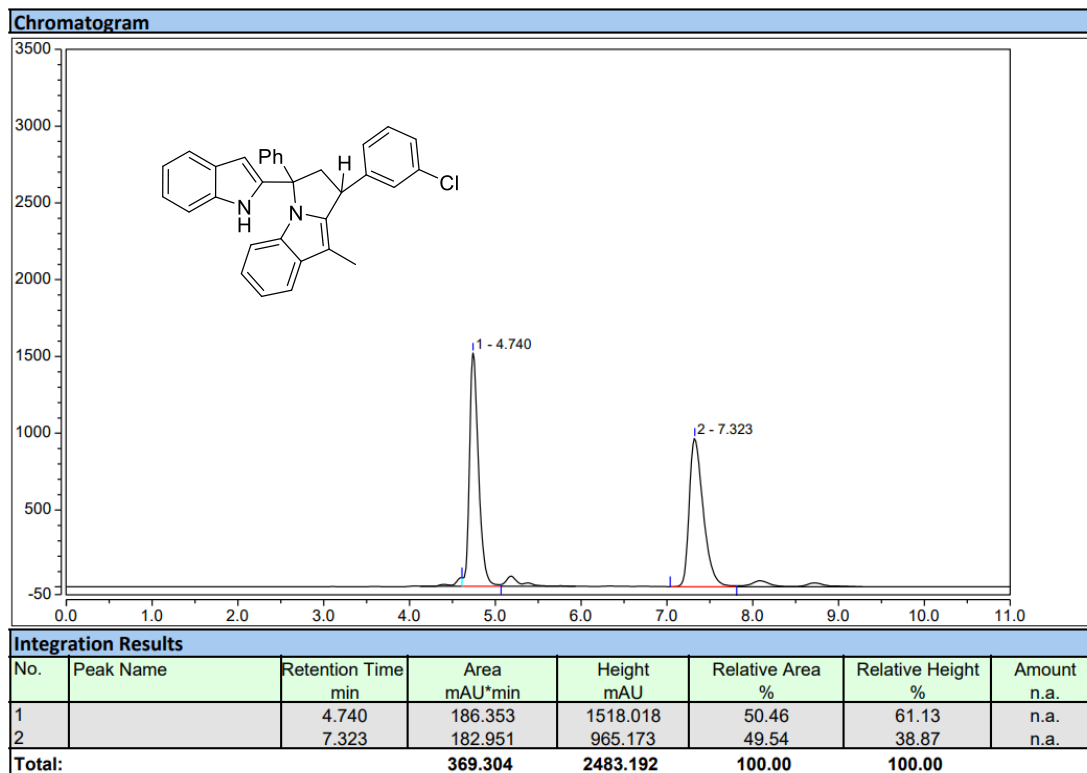


Enantioselective:

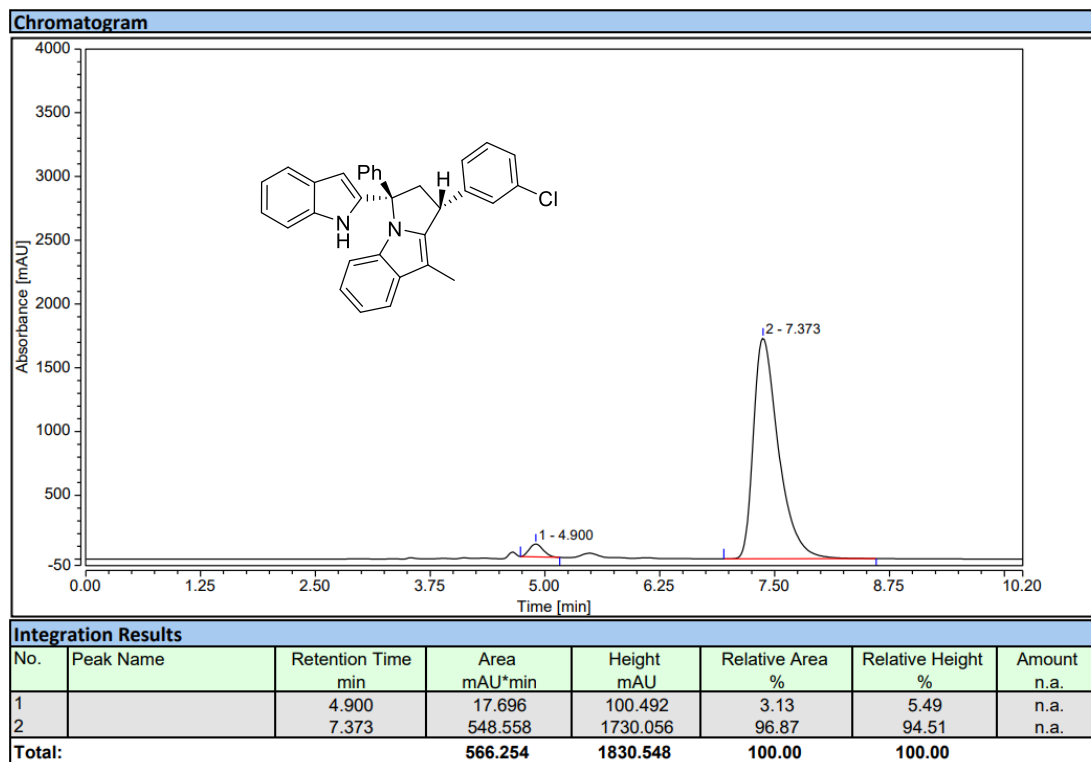


3af

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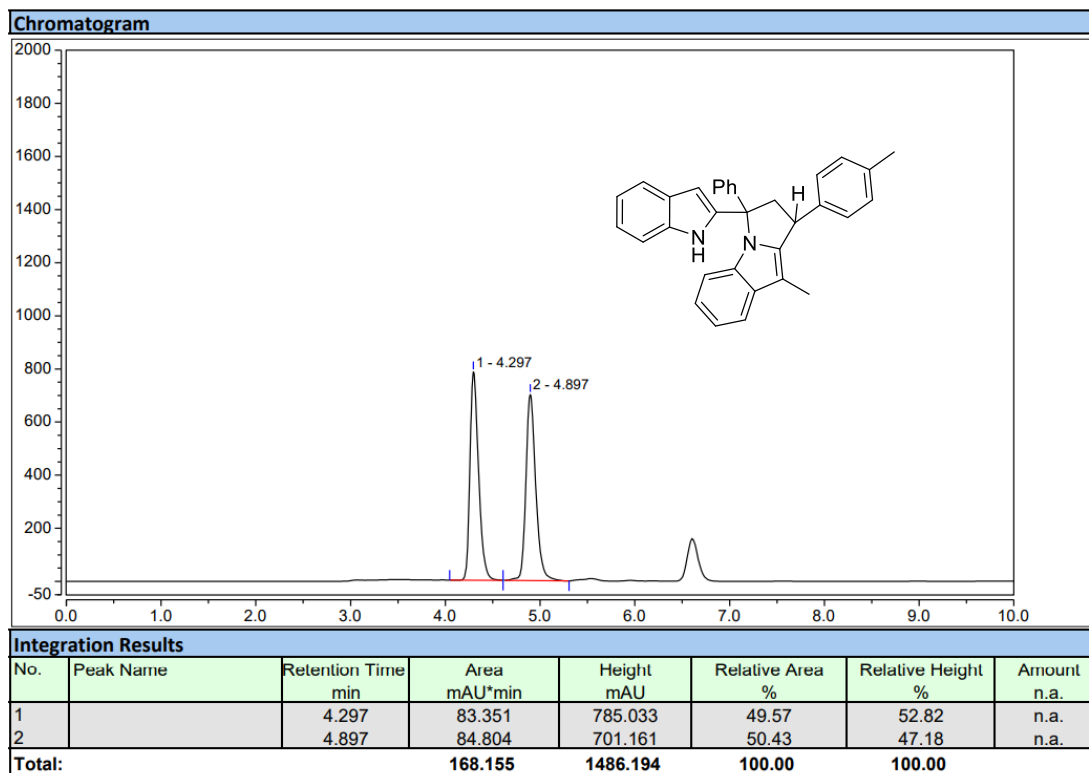


Enantioselective:

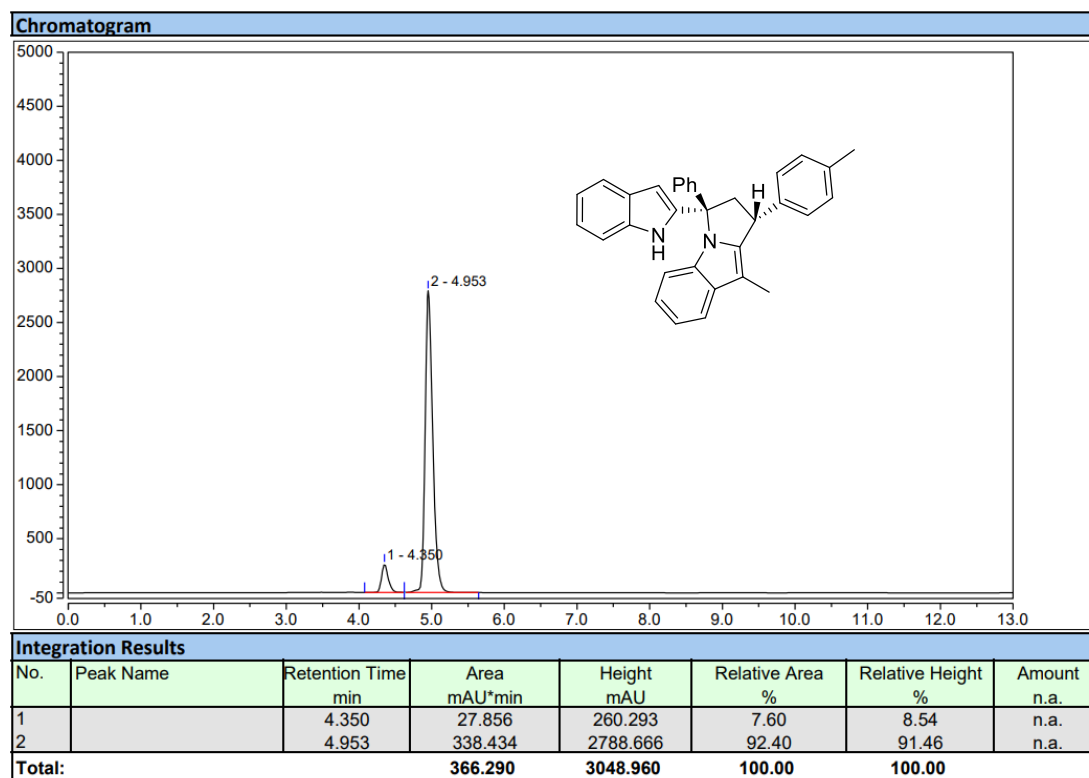


3ag

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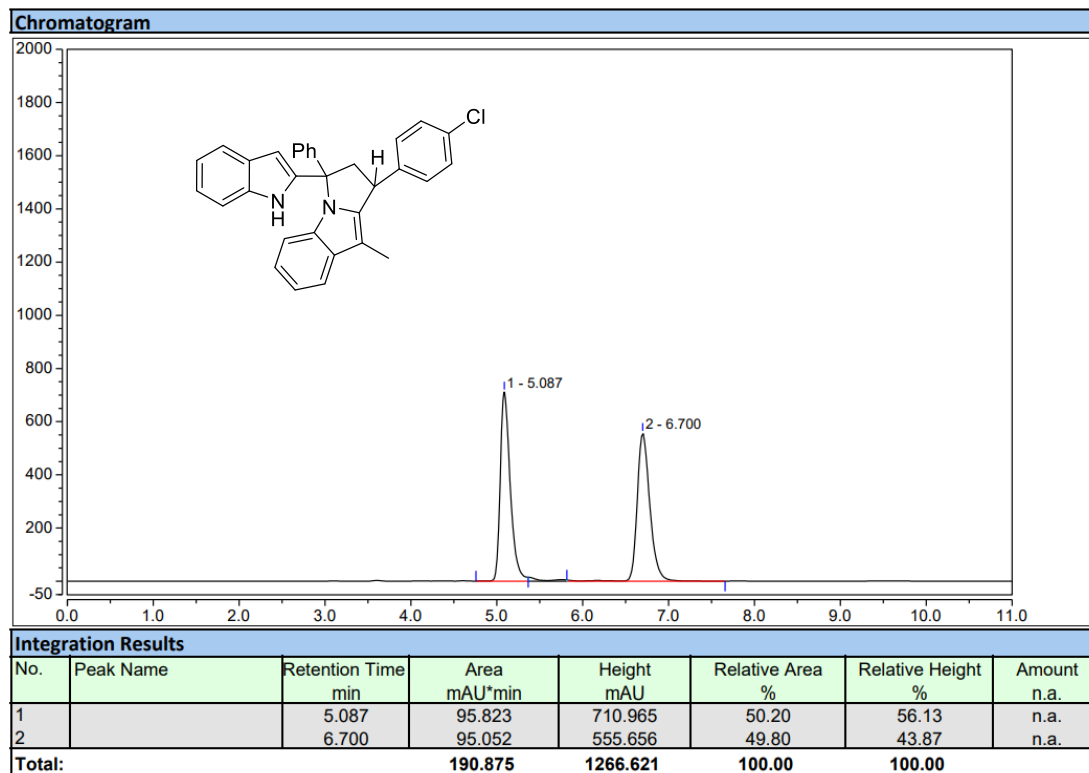


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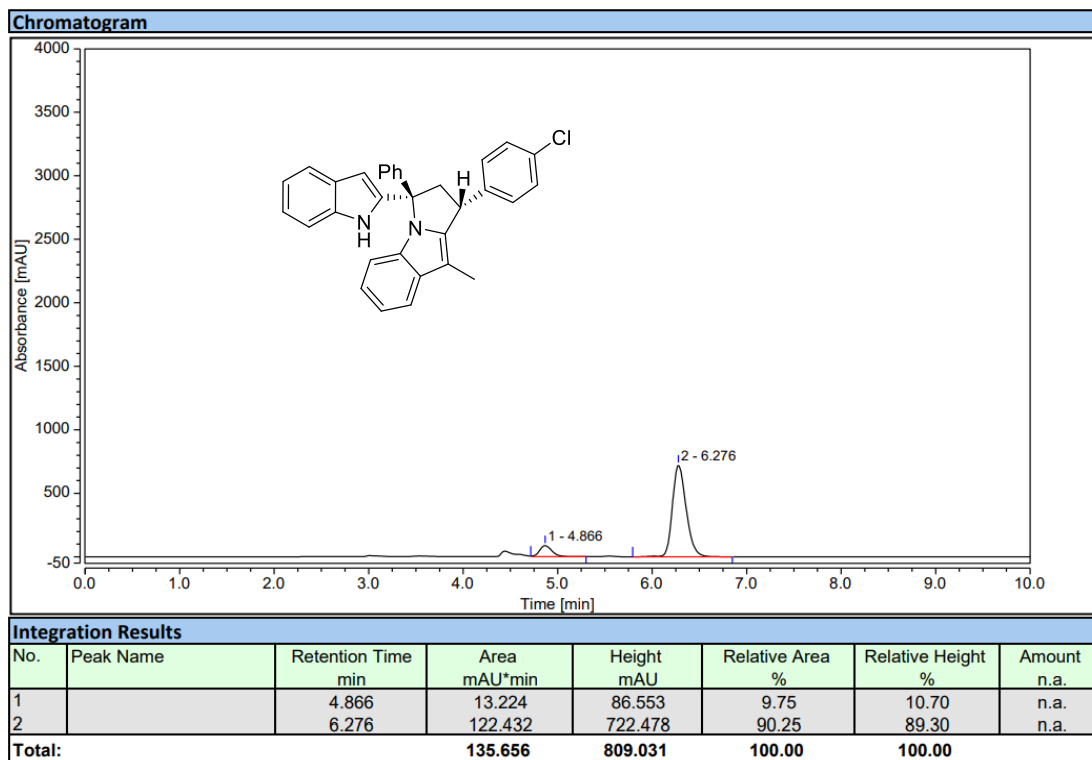


3ah

Racemic:

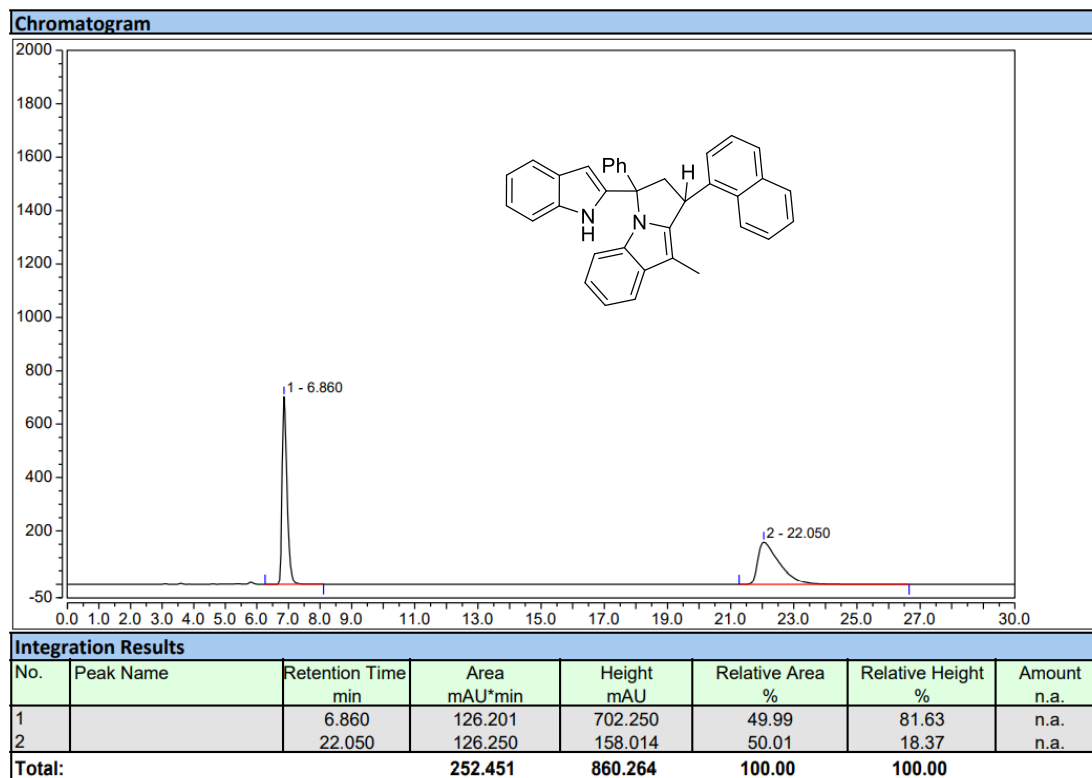


Enantioselective:

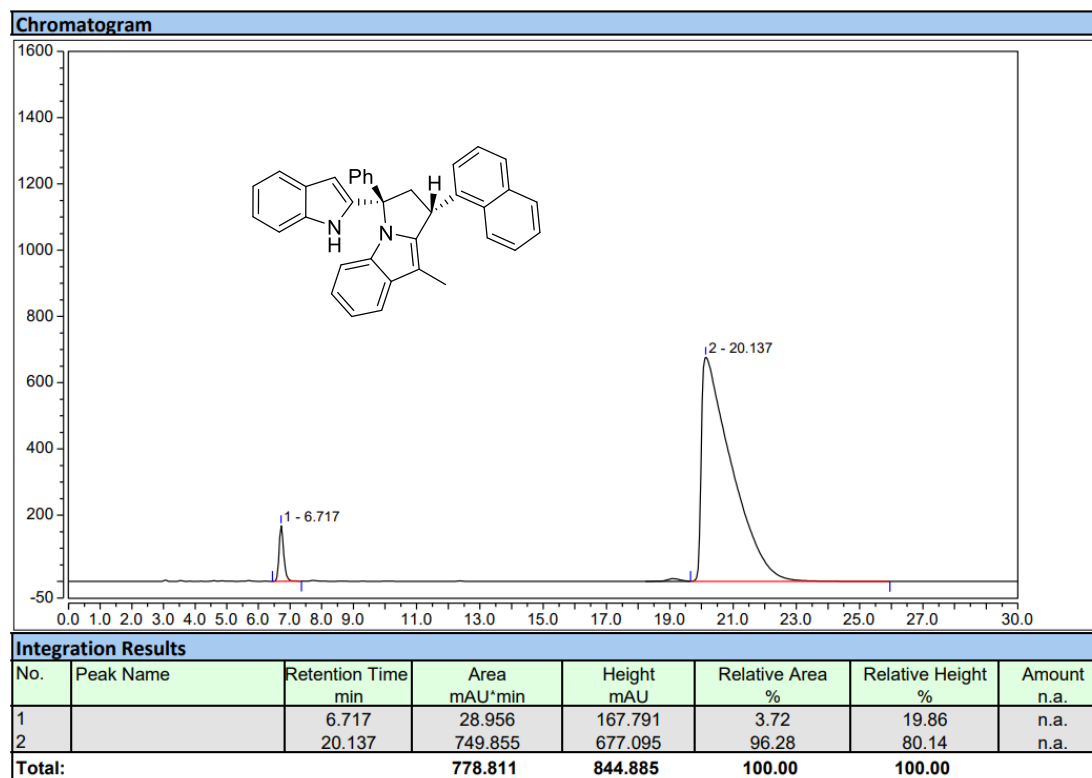


3ai

Racemic:

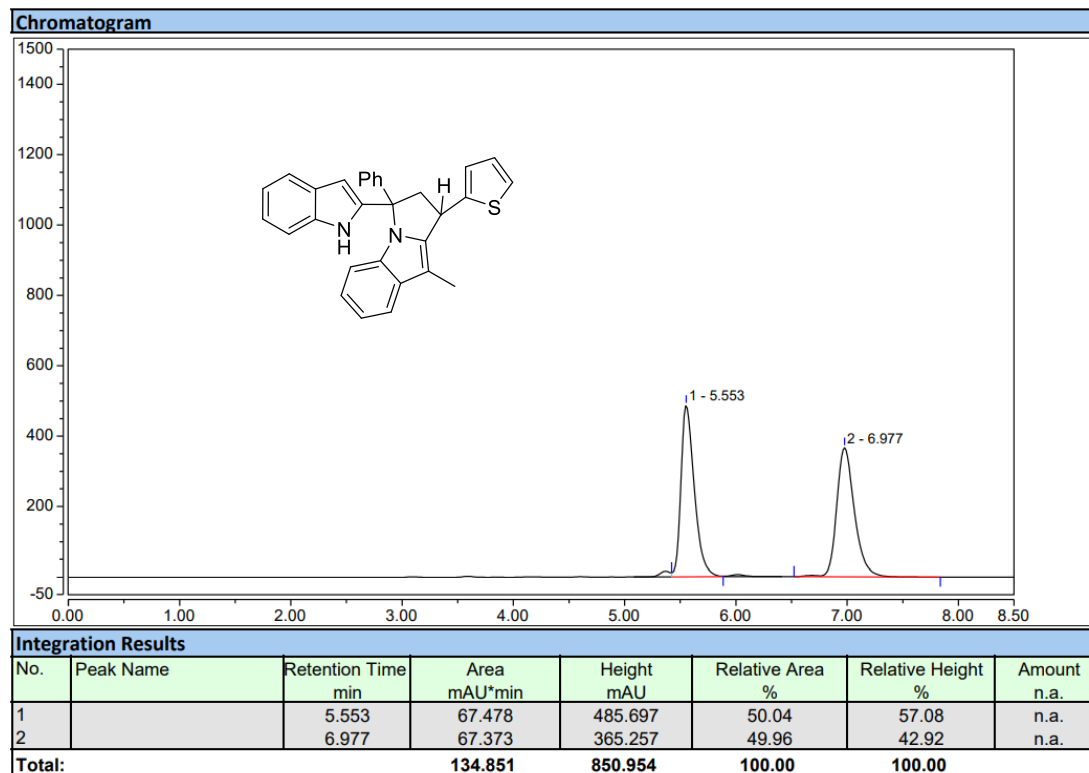


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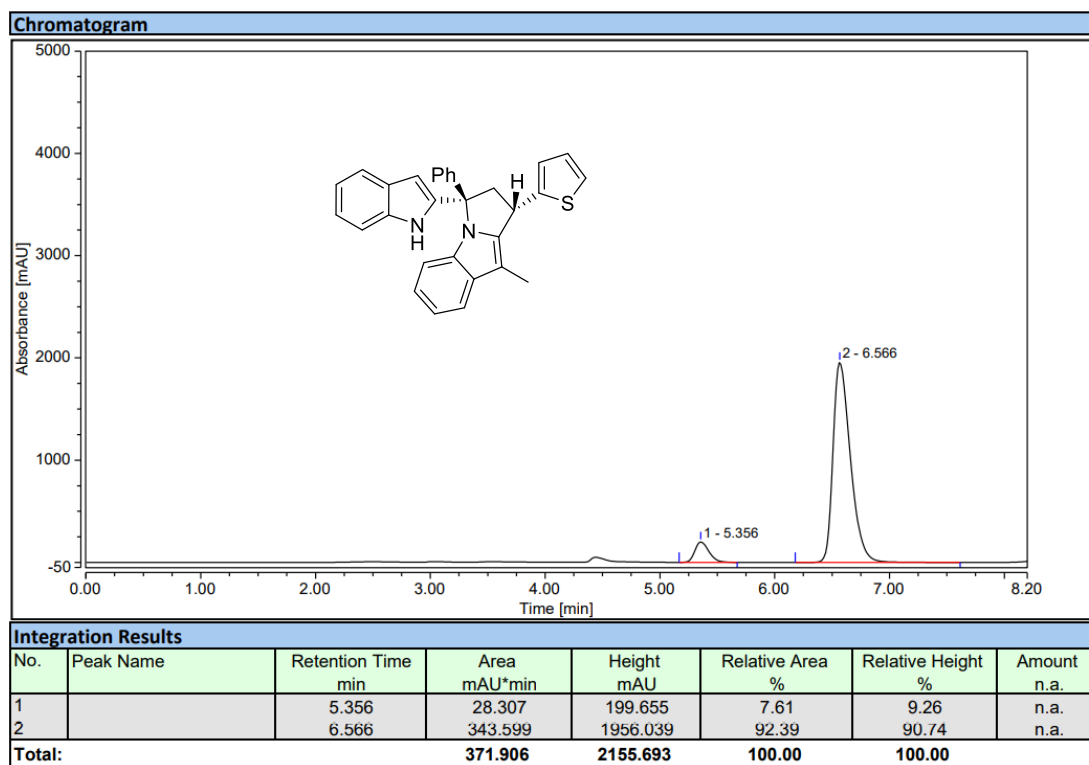


3aj

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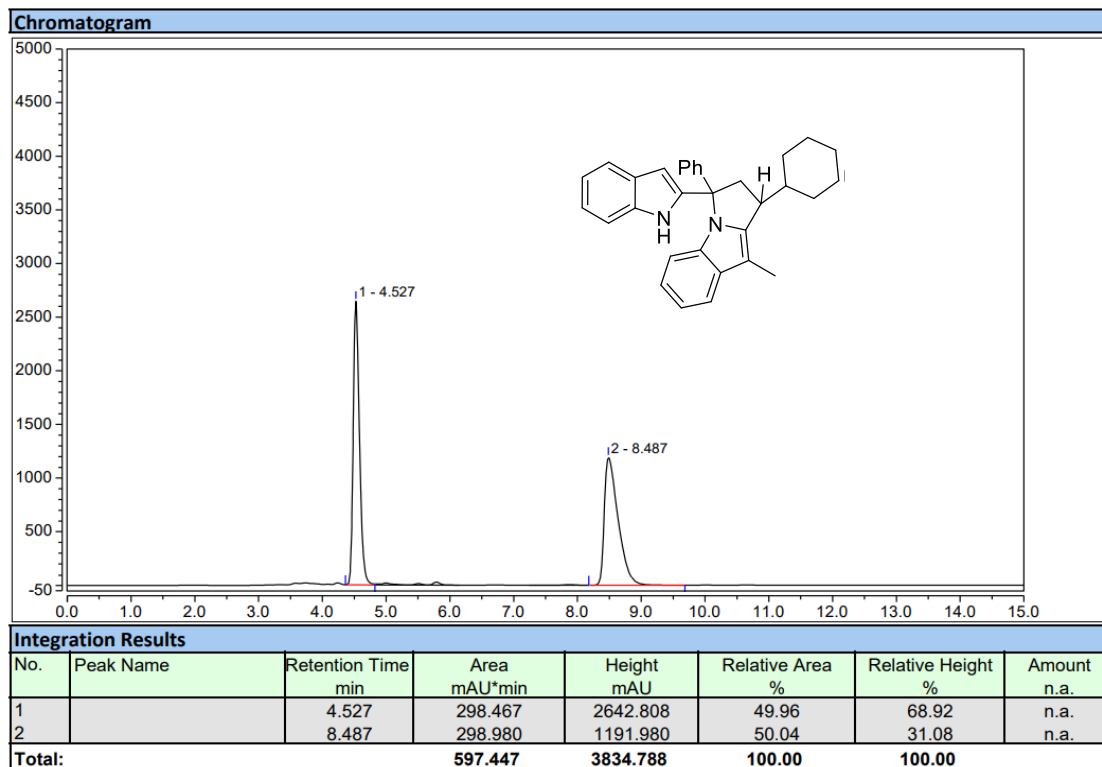


Enantioselective:

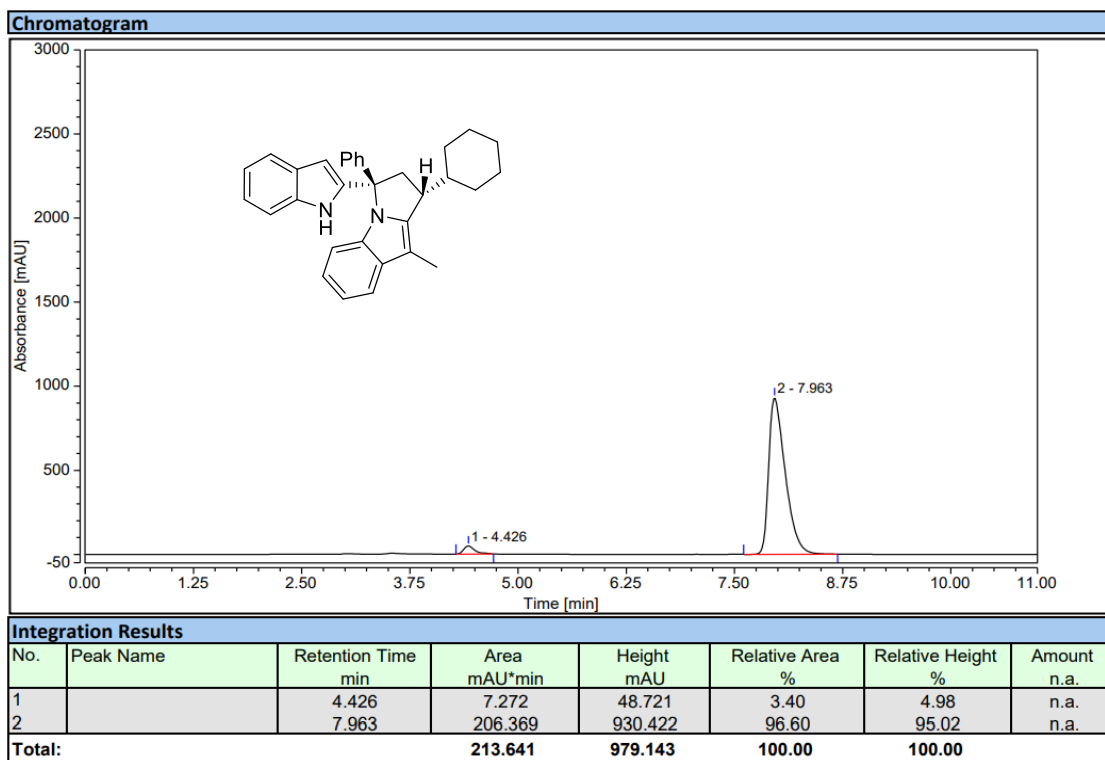


3ak

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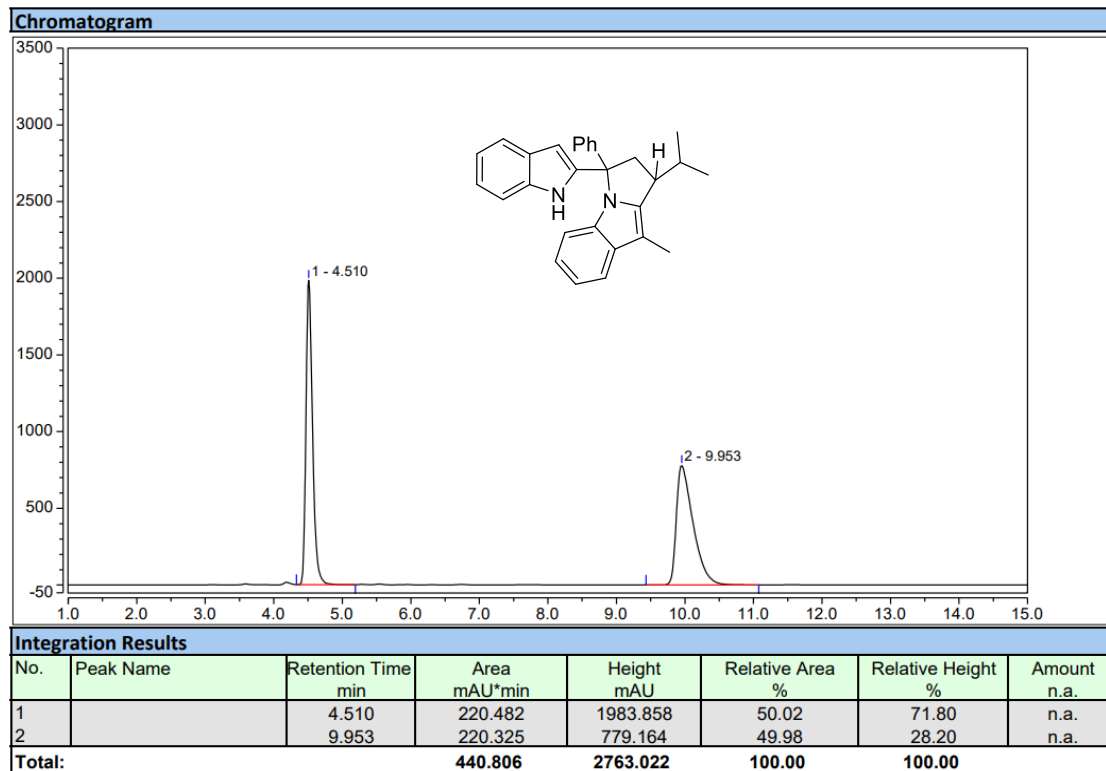


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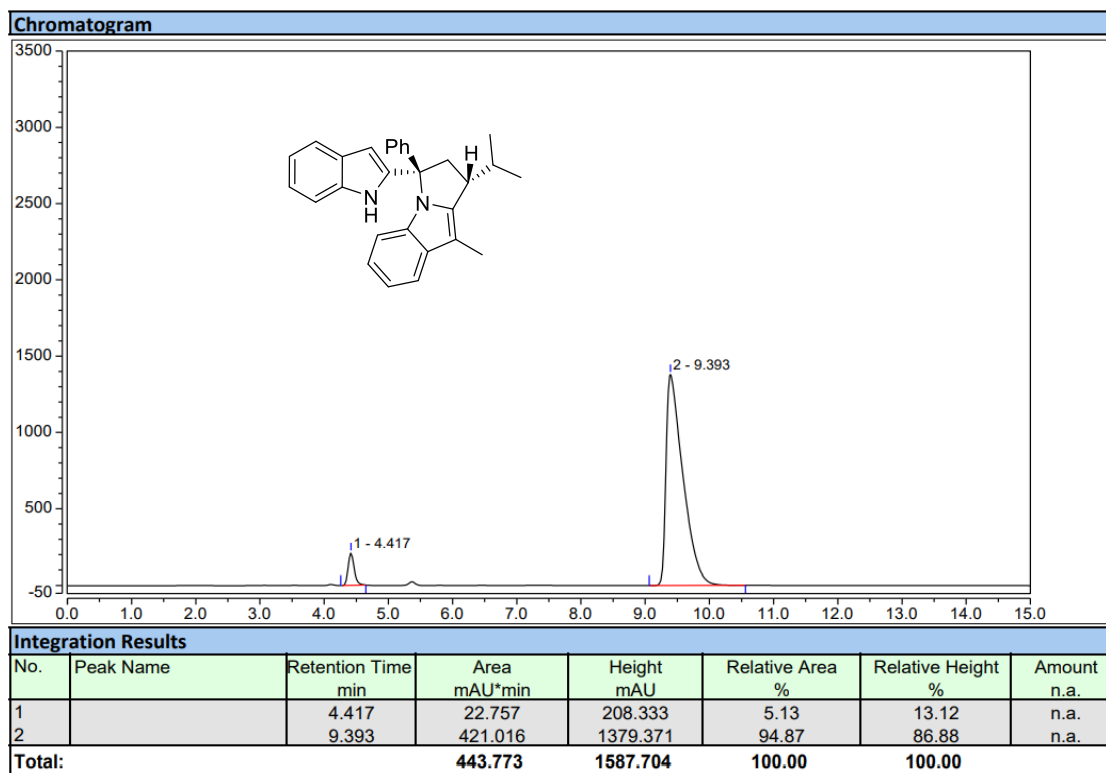


3al

Racemic:

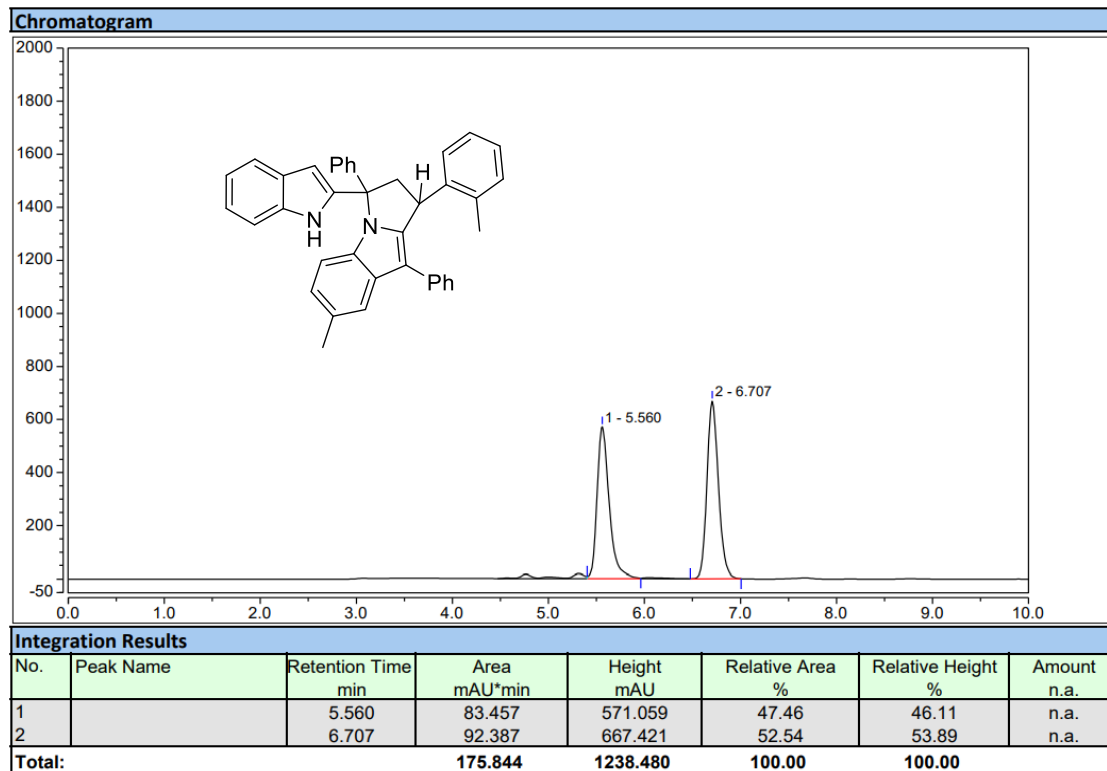


Enantioselective:

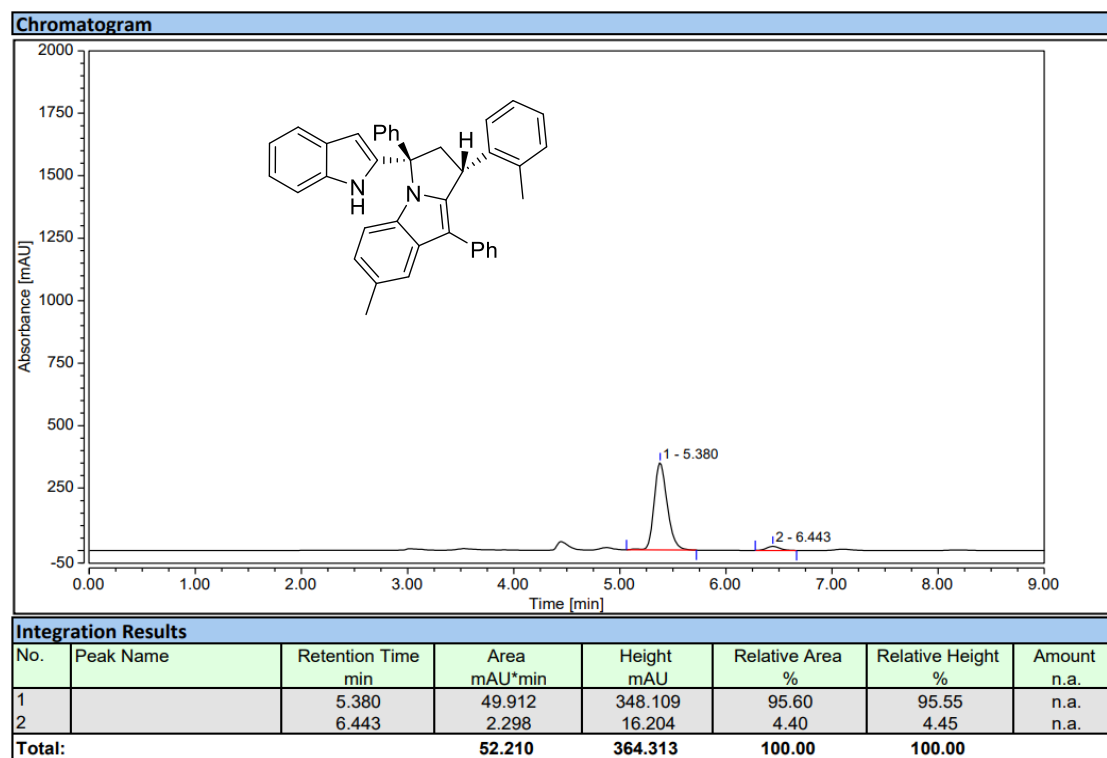


3am

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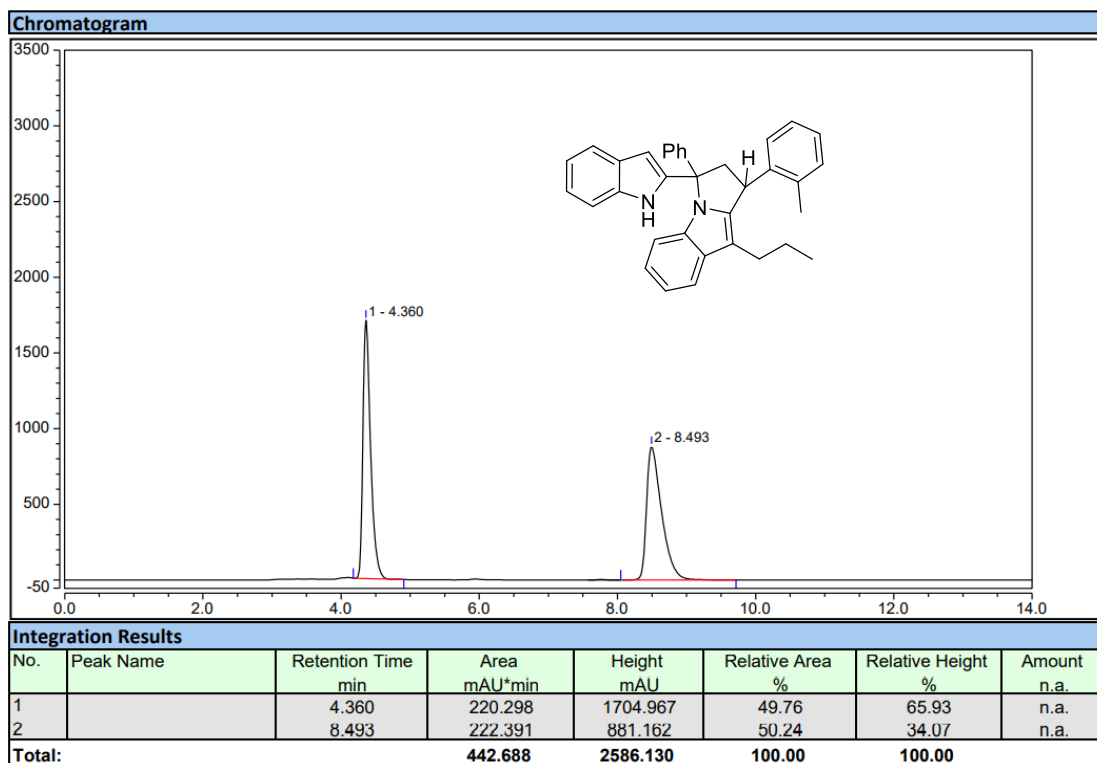


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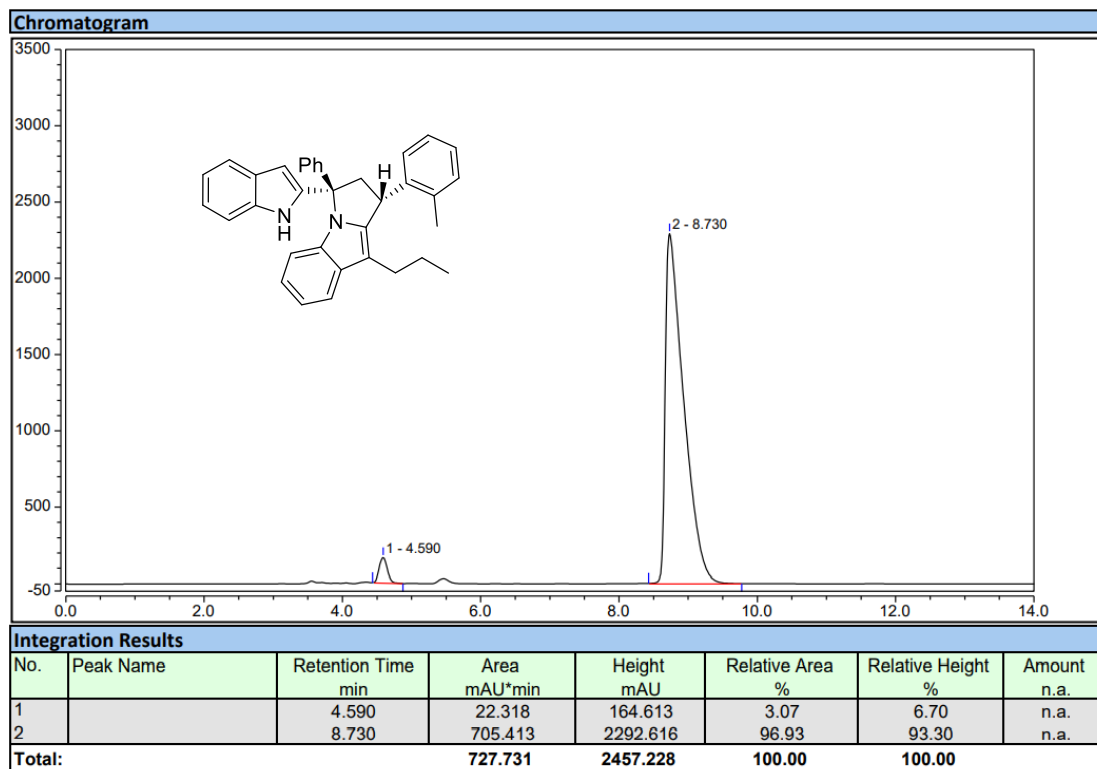


3an

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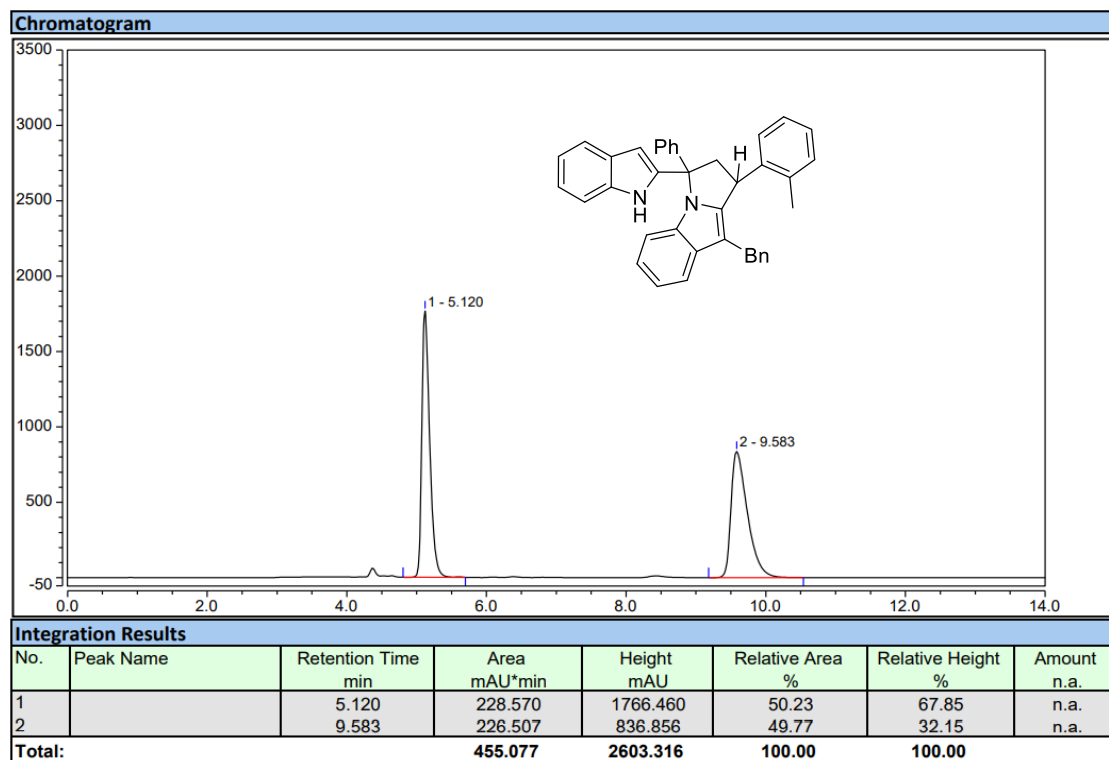


Enantioselective:

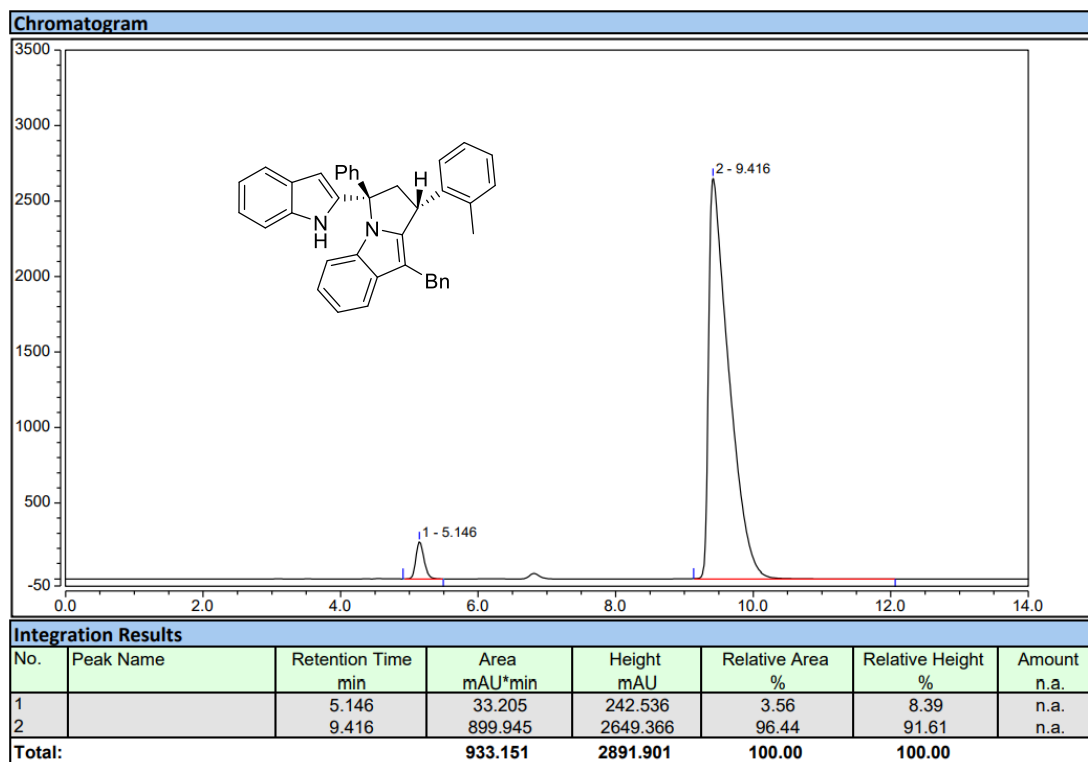


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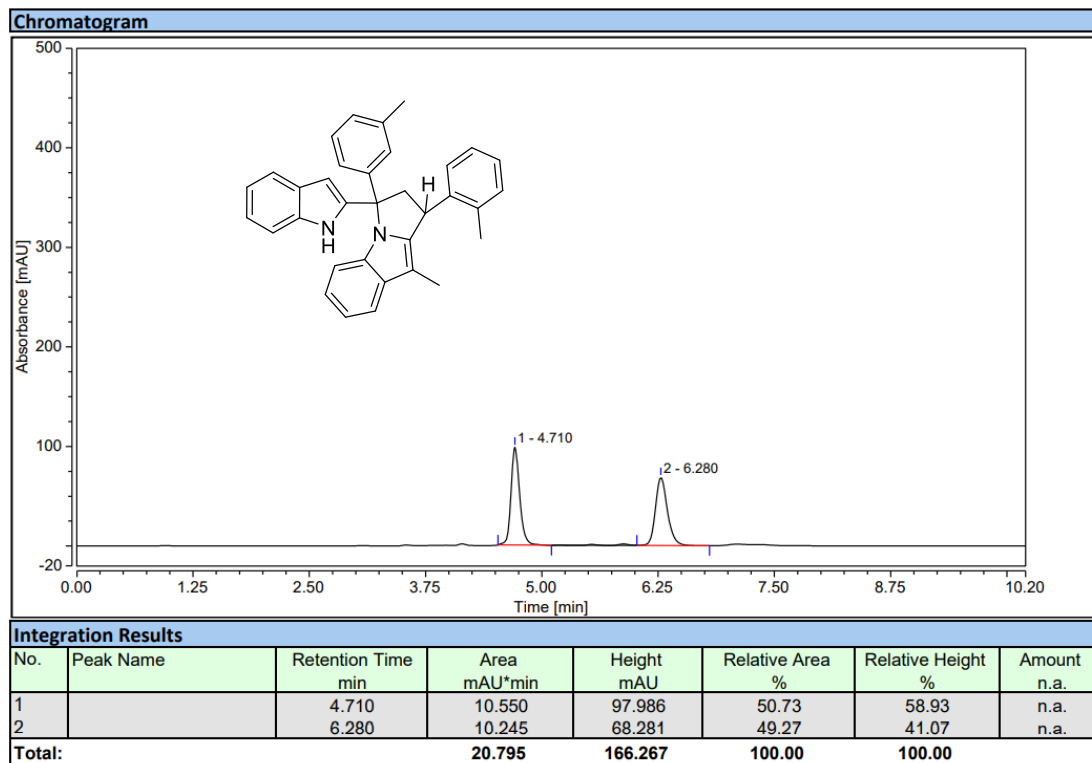


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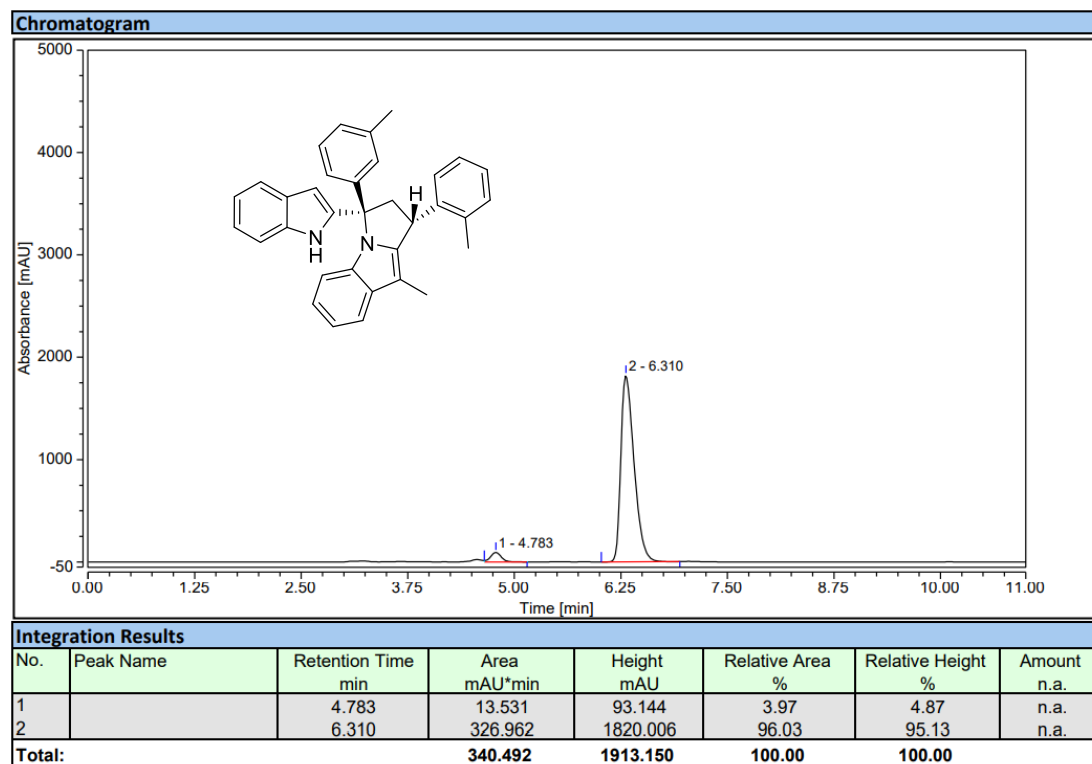


3ba

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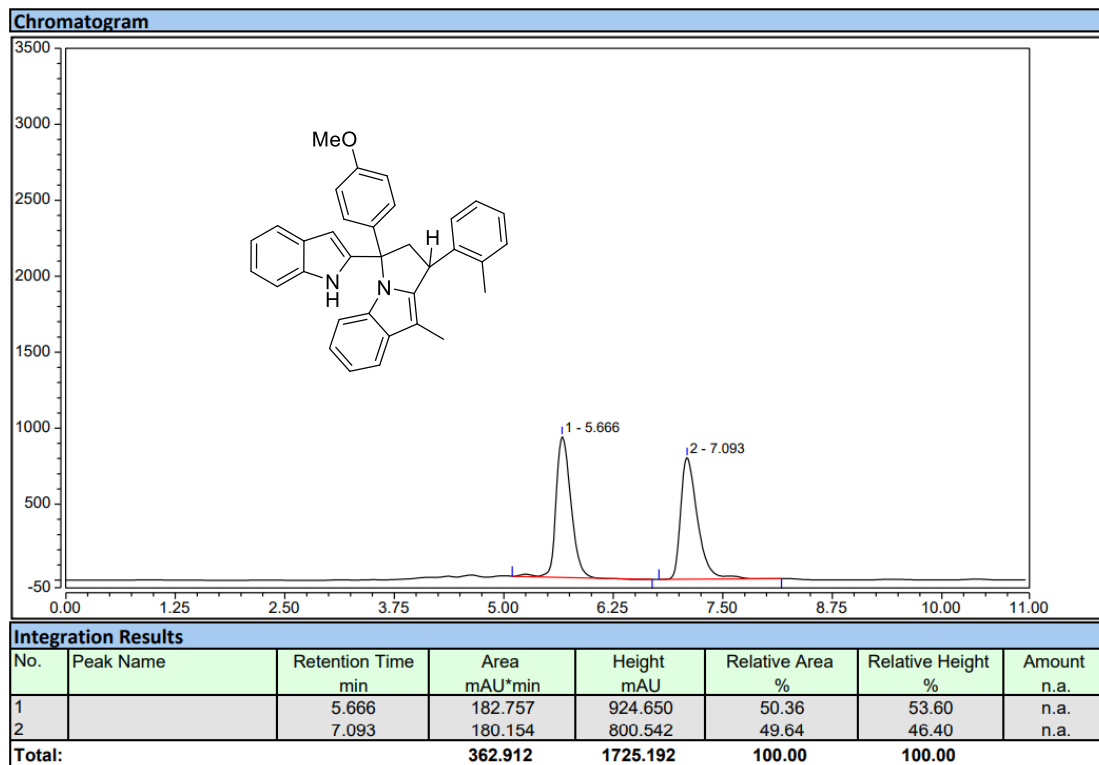


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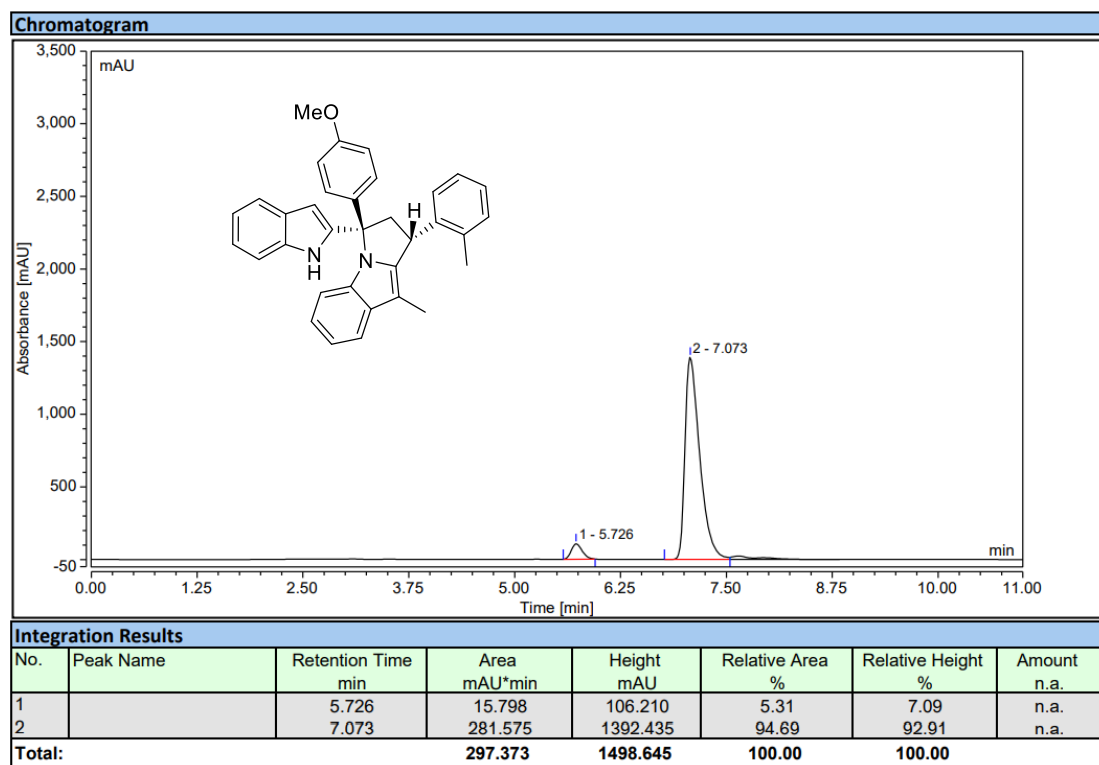


3ca

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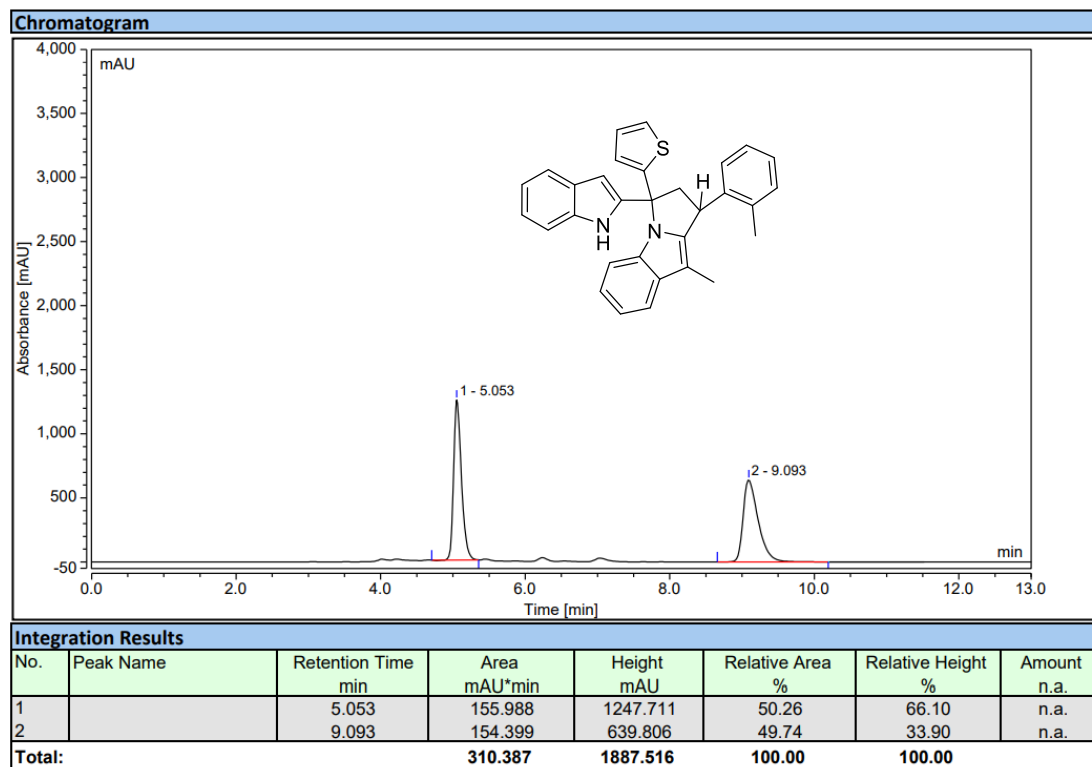


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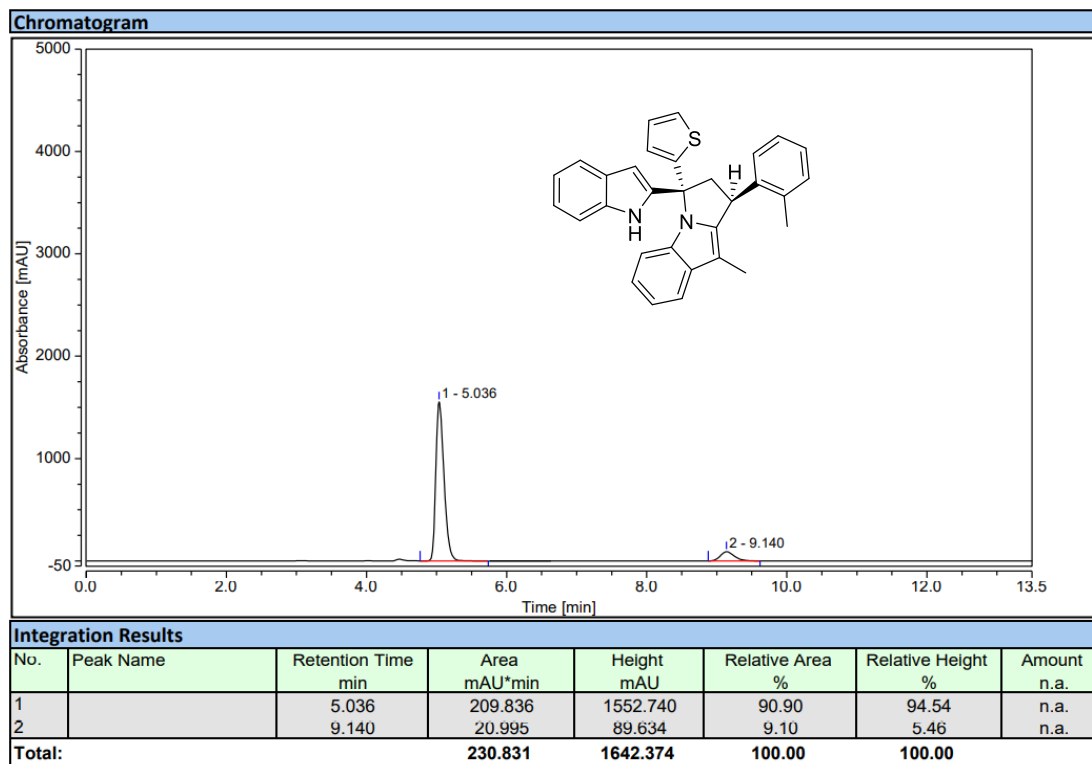


3da

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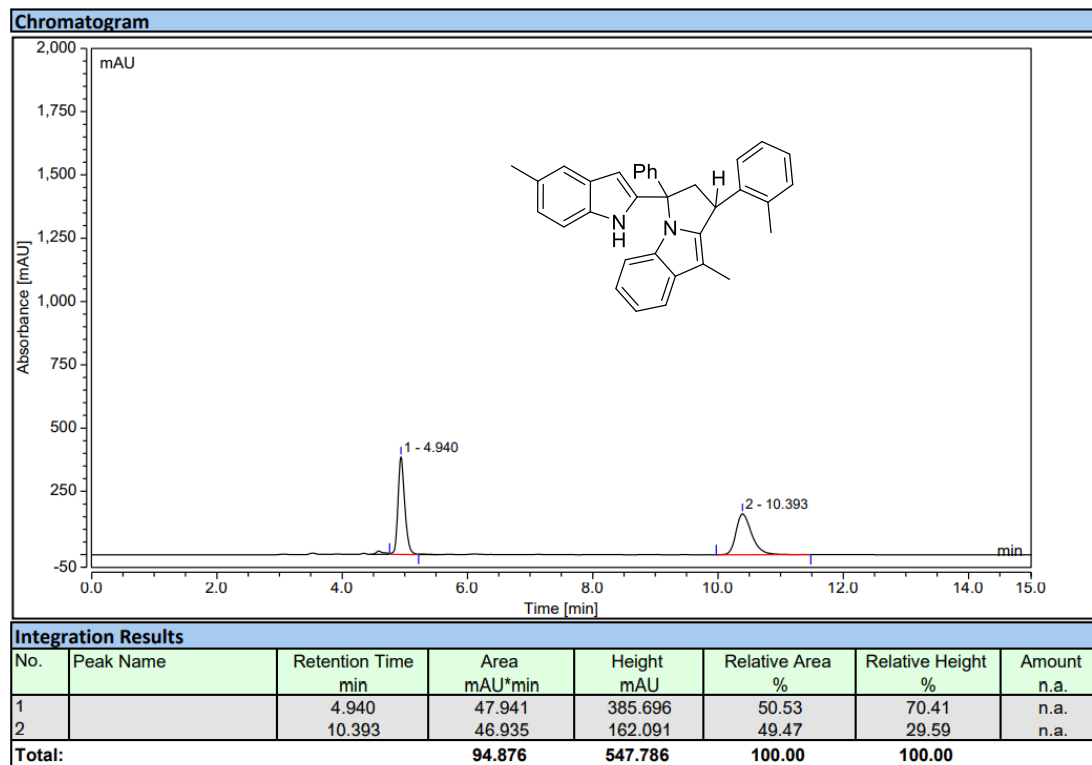


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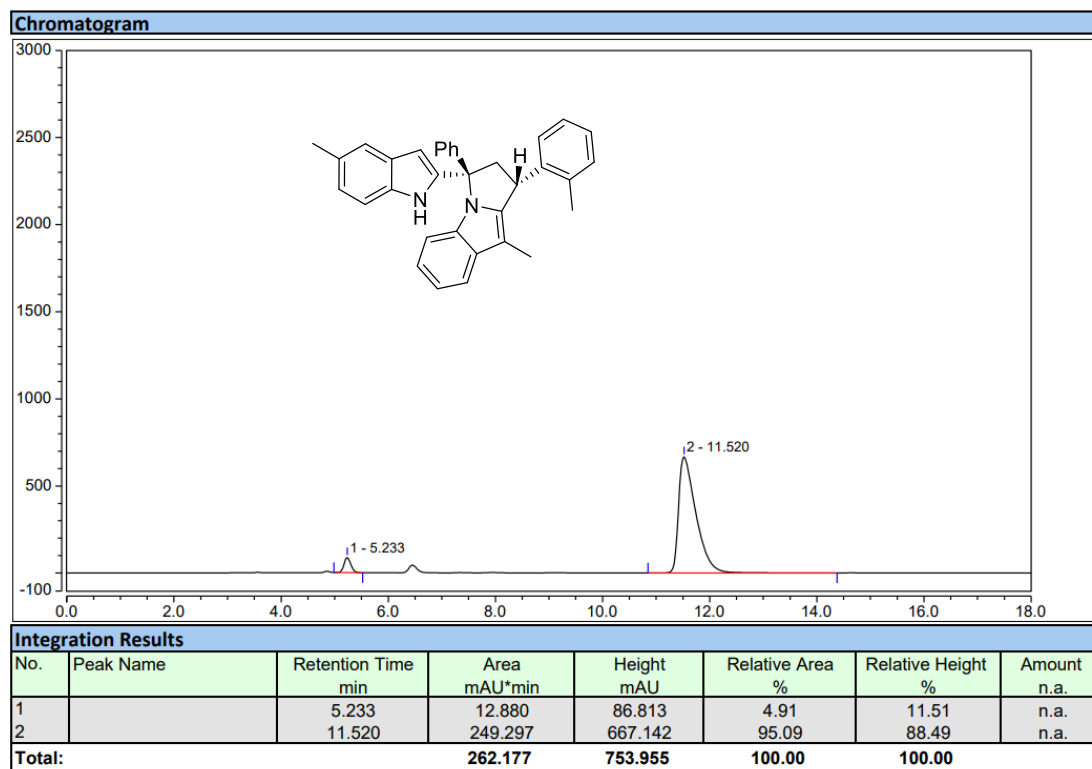


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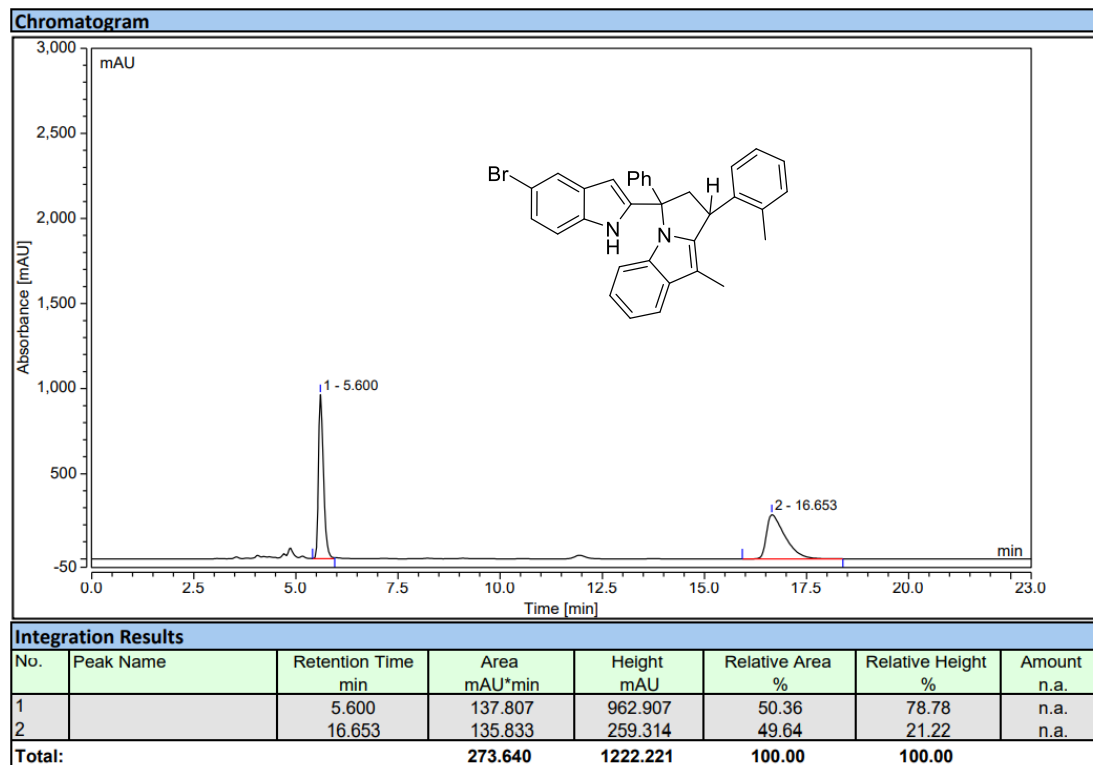


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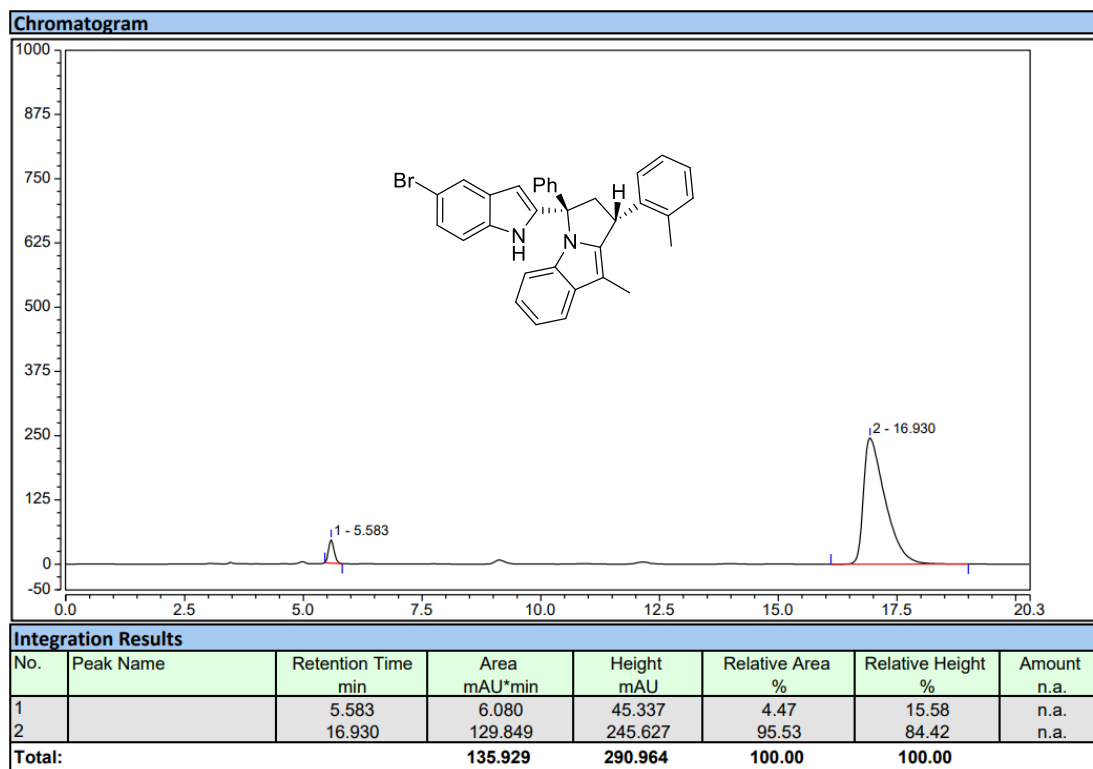


3fa

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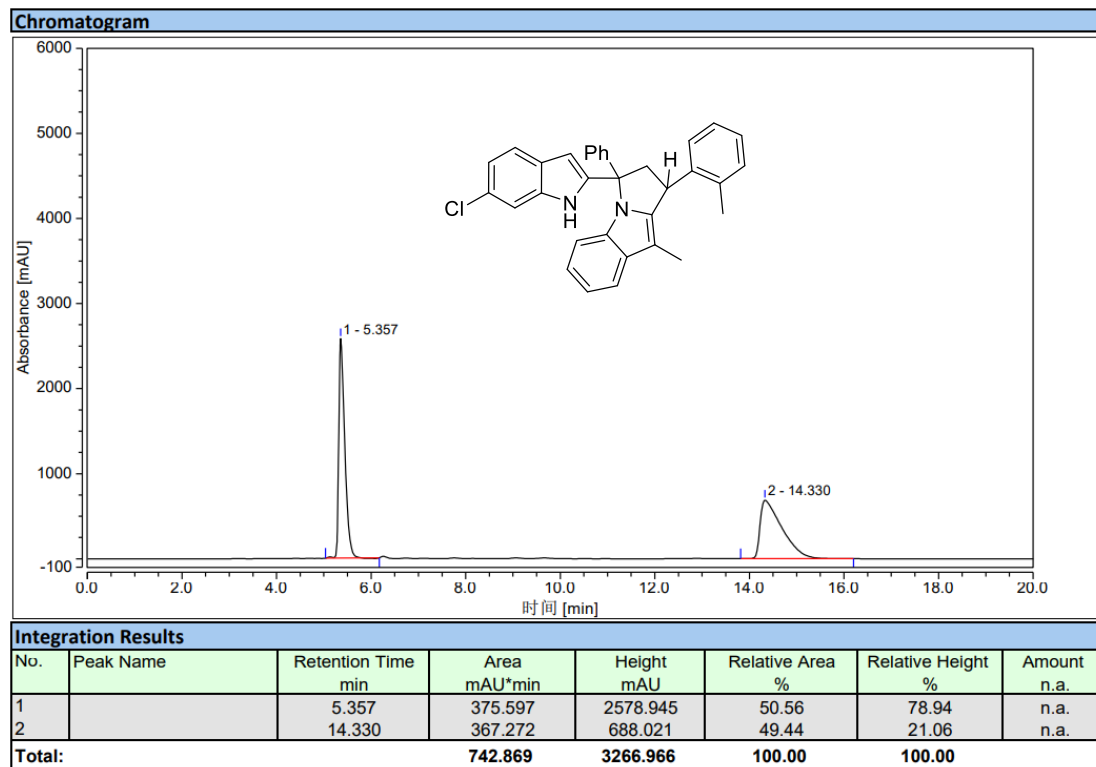


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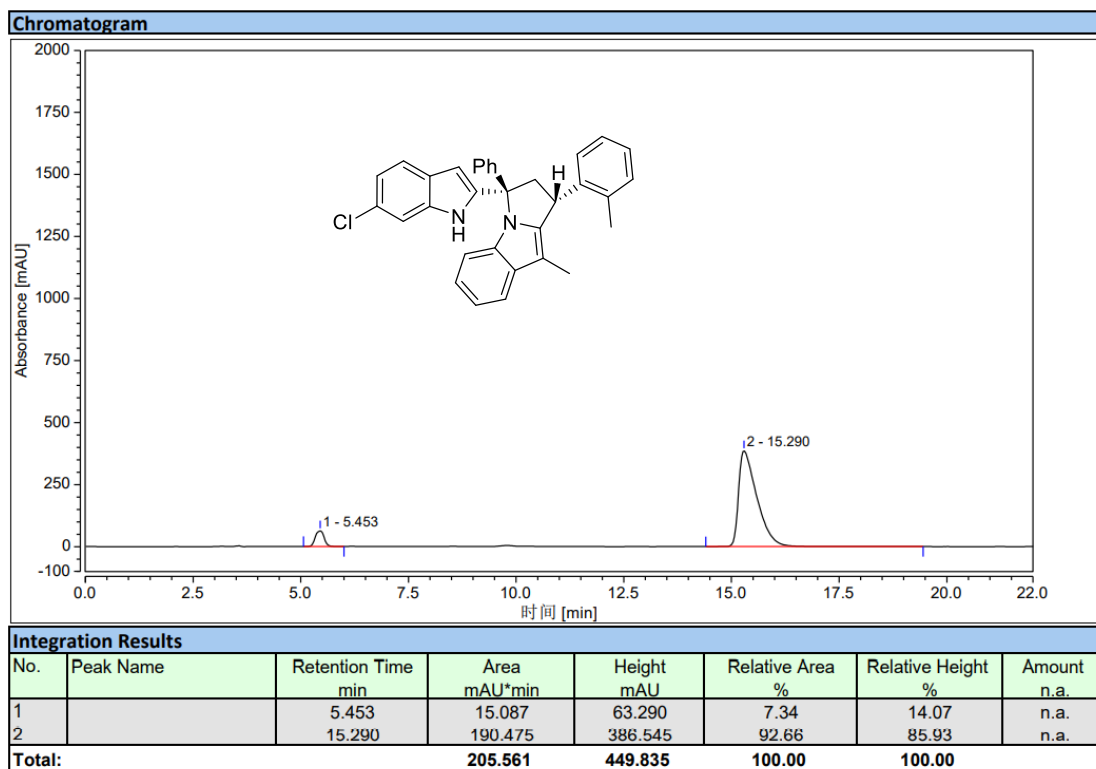


3ga

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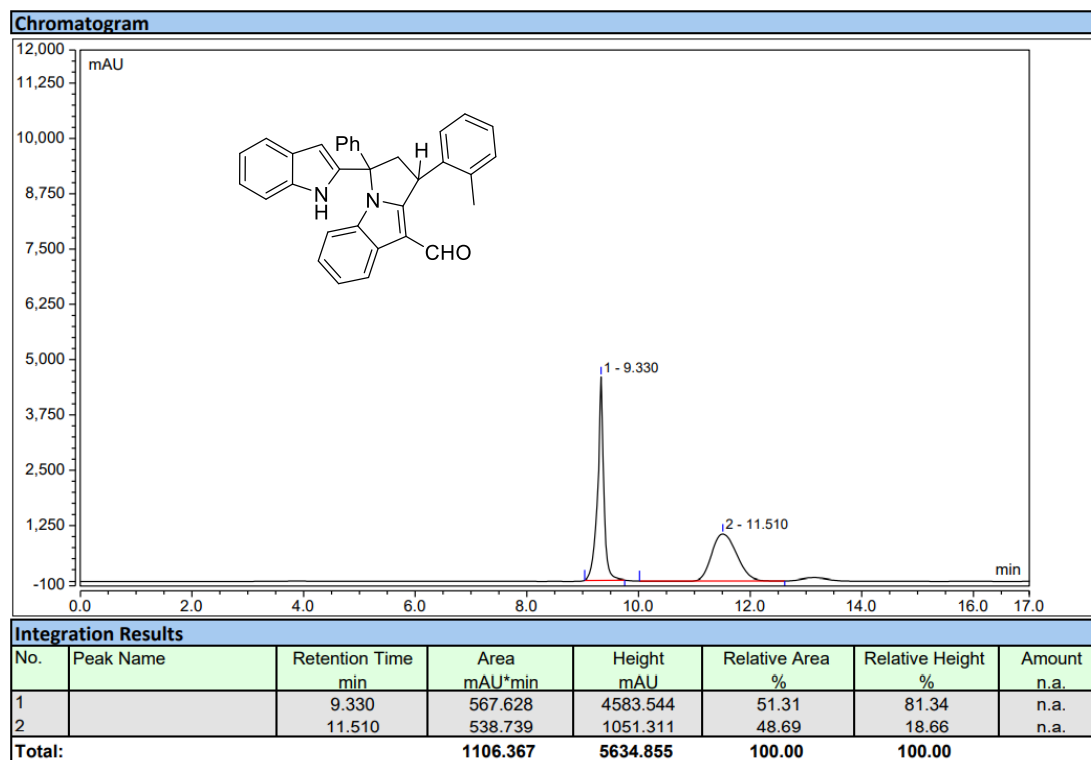


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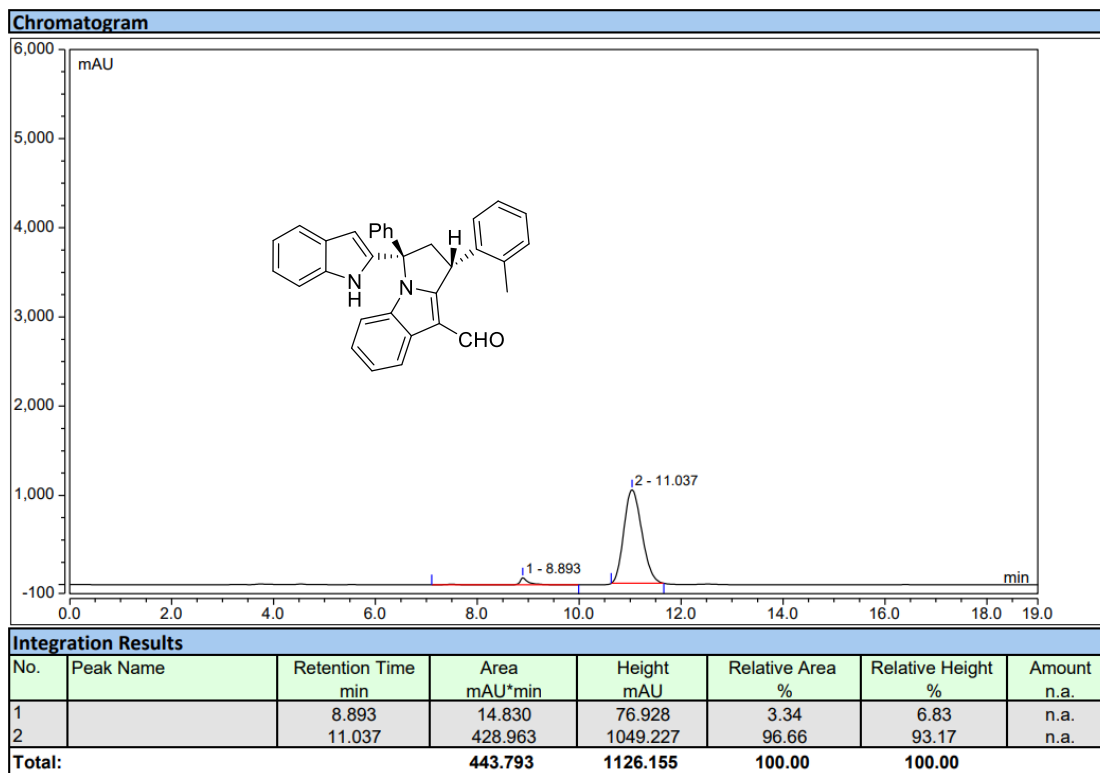


6

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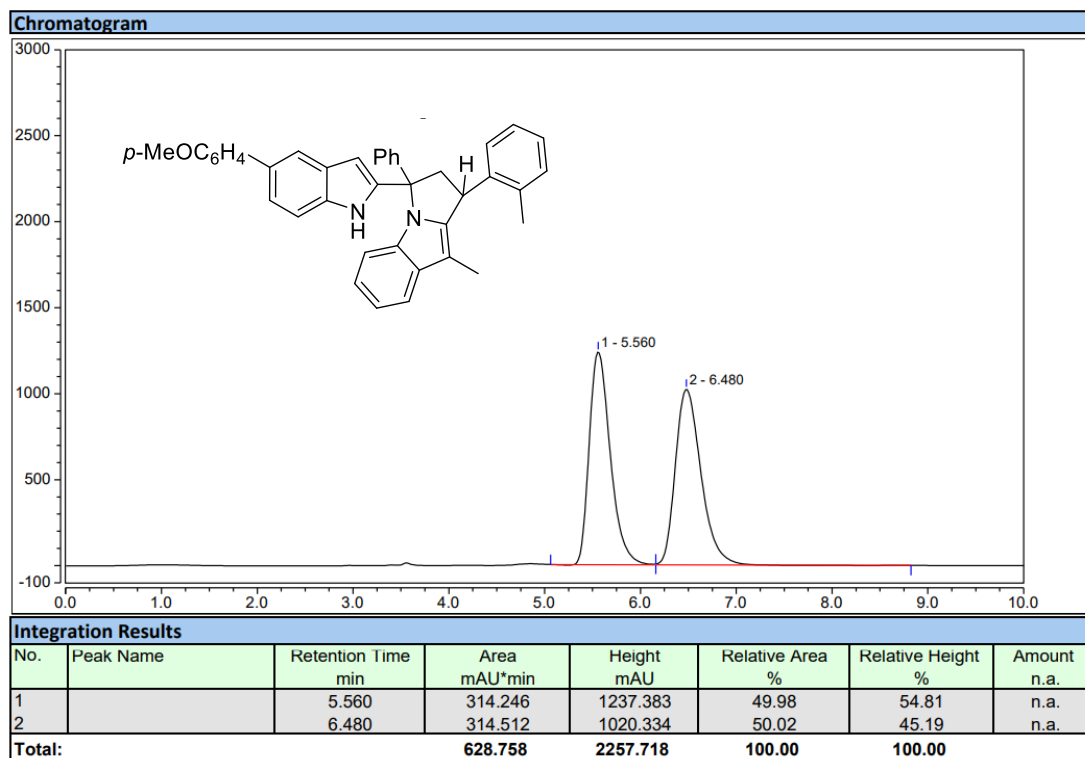


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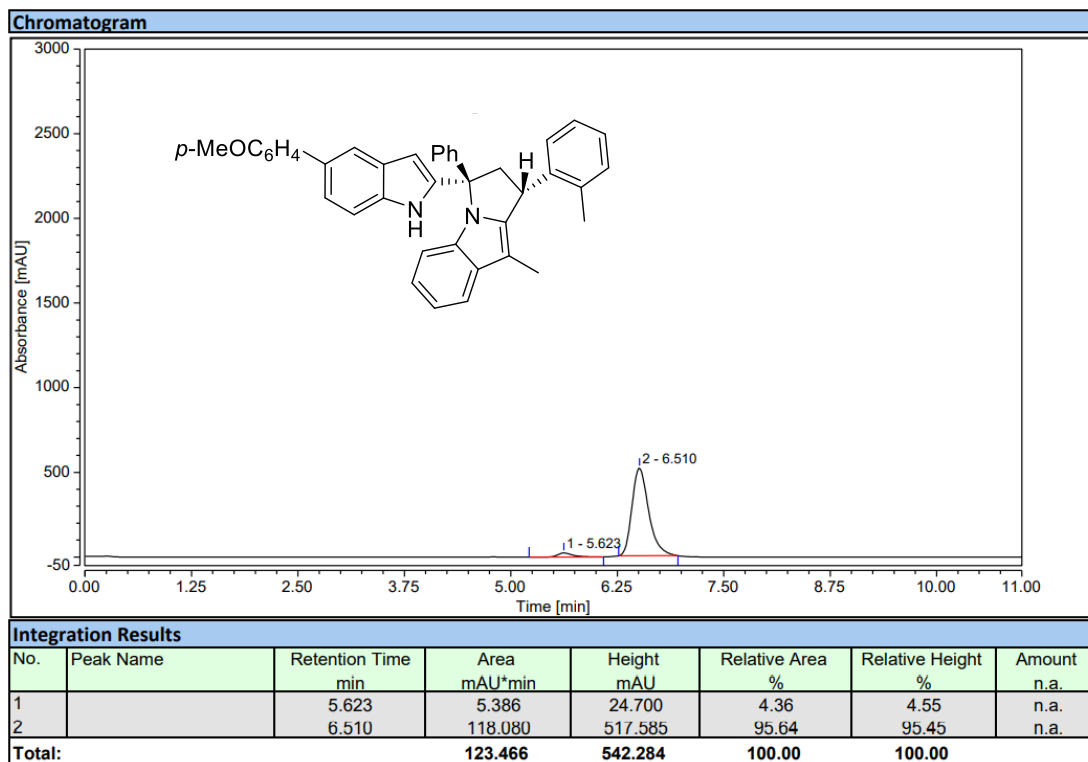


7

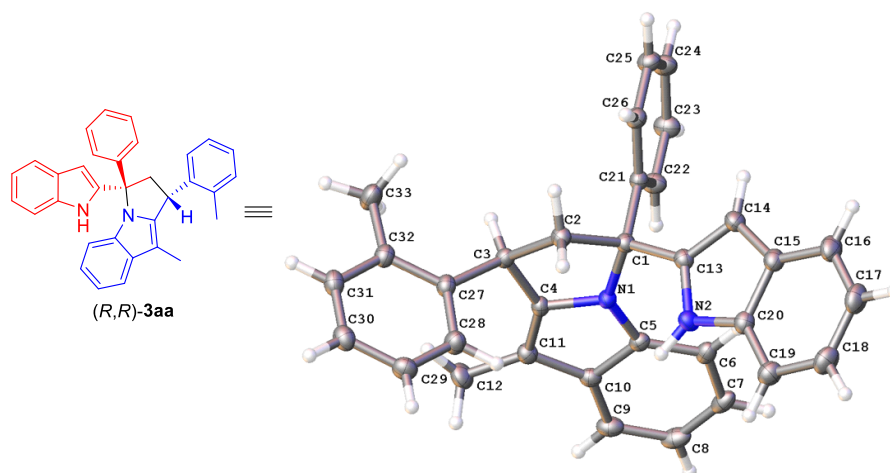
Racemic:



Enantioselective:



10. X-ray single-crystal data for compounds 3aa



Empirical formula	C ₃₉ H ₄₂ N ₂
Formula weight	538.74
Temperature/K	173.01
Crystal system	orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁
a/Å	9.3855(7)
b/Å	14.3714(11)
c/Å	23.0972(18)
α/°	90
β/°	90
γ/°	90
Volume/Å ³	3115.4(4)
Z	4
ρ _{calc} /cm ³	1.149
μ/mm ⁻¹	0.321
F(000)	1160.0
Crystal size/mm ³	0.08 × 0.06 × 0.05
Radiation	GaKα (λ = 1.34139)
2θ range for data collection/°	6.302 to 109.946
Index ranges	-11 ≤ h ≤ 8, -17 ≤ k ≤ 17, -28 ≤ l ≤ 28
Reflections collected	32572
Independent reflections	5870 [R _{int} = 0.0305, R _{sigma} = 0.0178]
Data/restraints/parameters	5870/0/374
Goodness-of-fit on F ²	1.053
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0429, wR ₂ = 0.1175
Final R indexes [all data]	R ₁ = 0.0437, wR ₂ = 0.1188
Largest diff. peak/hole / e Å ⁻³	0.28/-0.26
Flack parameter	0.08(13)

11. Theoretical calculations

Theoretical calculations of catalytic asymmetric formal (2 + 3) cycloaddition

Computational Methods: The DFT calculations of the possible transition states and intermediates in the reactions were performed by using the Gaussian 16 package.² The geometry optimizations of minima and transition states were carried out at the B3LYP-D3³ with a Becke–Johnson (BJ)⁴ damping function and the 6-31G(d)⁵ basis set. The vibrational frequencies were computed at the same level to check whether each optimized structure is an energy minimum (zero imaginary frequency) or a transition state (one imaginary frequency) and to evaluate its zero-point vibration energy (ZPE) and thermal corrections at 298 K in kcal·mol⁻¹. The single-point energies and solvent effects in ethylethanoate were computed with the dispersion-corrected density functional method B3LYP-D3 with a Becke–Johnson (BJ) damping function and the 6-311+G (d,p) basis set using the SDM solvation model.⁶ DFT-optimized structures are illustrated using CYLView.⁷

To explain the observed high diastereoselectivity of the catalytic asymmetric formal (2 + 3)

² In Gaussian 16, rev. C.01.

³ a) S. Grimme, J. Antony, S. Ehrlich and H. Krieg, A Consistent and Accurate *ab Initio* Parametrization of Density Functional Dispersion Correction (DFT-D) for the 94 Elements H-Pu, *J. Chem. Phys.* 2010, **132**, 154104; b) C. Lee, W. Yang and R. G. Parr, Development of the Colle-Salvetti Correlation-Energy Formula into a Functional of the Electron Density, *Phys. Rev. B*, 1988, **37**, 785.

⁴ a) T. Korona, M. Przybytek and B. Jeziorski, Time-Independent Coupled Cluster Theory of the Polarization Propagator. Implementation and Application of the Singles and Doubles Model to Dynamic Polarizabilities and Van Der Waals Constants, *Mol. Phys.* 2006, **104**, 2303; b) S. Grimme, S. Ehrlich and L. Goerigk, Effect of the Damping Function in Dispersion Corrected Density Functional Theory, *J. Comput. Chem.* 2011, **32**, 1456.

⁵ a) A. V. Marenich, C. J. Cramer and D. G. Truhlar, Universal Solvation Model Based on the Generalized Born Approximation with Asymmetric Descreening, *Theory Comput.* 2009, **5**, 2447; b) A. V. Marenich, C. J. Cramer and D. G. Truhlar, Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions, *J. Phys. Chem. B*, 2009, **113**, 6378.

⁶ a) H. Puthoff, Source of Vacuum Electromagnetic Zero-Point Energy, *Phys. Rev. A*, 1989, **40**, 4857; b) A. V. Marenich, C. J. Cramer and D. G. Truhlar, Performance of SM6, SM8, and SMD on the SAMPL1 Test Set for the Prediction of Small-Molecule Solvation Free Energies, *J. Phys. Chem. B*, 2009, **113**, 4538.

⁷ C. Y. Legault, CYLView, 1.0b, Université de Sherbrook, 2009; www.cylview.org.

cycloaddition, the key transition states **TS5** and **TS5'** of the diastereoselectivity-determining step were compared. Obviously, the H-bonds between CPA (*S*)-**5d** and the intermediate in **TS5** (1.589 Å and 1.770 Å) are shorter than those in **TS5'** (1.688 Å and 1.790 Å), which implied that the hydrogen-bonding interactions between (*S*)-**5d** and the intermediate in **TS5** are stronger than those in **TS5'**. Additionally, the Gibbs free energy of **TS5'** (-0.46 kcal·mol⁻¹) is higher than that of **TS5** (-6.93 kcal·mol⁻¹), and the energy difference between the two transition states is 6.47 kcal·mol⁻¹. These results explained the excellent diastereoselectivity during the step of intramolecular addition and the formation of (1*R*,3*R*)-**3aa** as a major product.

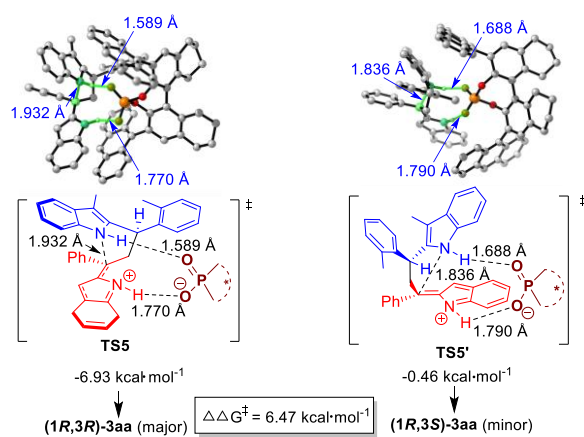
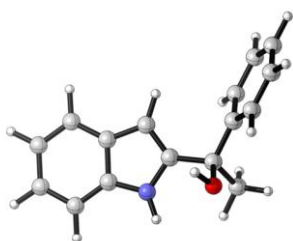


Figure S1. Key transition states leading to the diastereomers of **3aa**

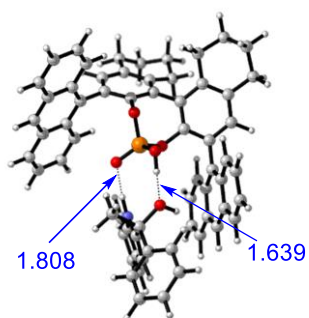
Table S1. Electronic energies, enthalpies and free energies (in hartrees) computed at the level of

B3LYP-D3(BJ)-SMD(ethylethanoate)/6-311+G(d,p)//B3LYP-D3(BJ)/6-31G(d)

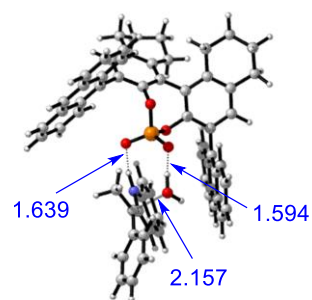
Structure	ZPE	$\Delta H_{0\rightarrow T}$	$\Delta G_{0\rightarrow T}$	E	H	G	Imaginary Frequency
1a	0.272377	0.288020	0.230317	-749.007080	-748.719060	-748.776763	
Int1	1.002933	1.060280	0.909864	-3243.705696	-3242.645416	-3242.795832	
TS1	1.000217	1.057557	0.908166	-3243.683473	-3242.625916	-3242.775307	-79.00i
Int2'	0.999461	1.057293	0.905237	-3243.688104	-3242.630811	-3242.782867	
Int2	0.973841	1.029945	0.882417	-3167.207399	-3166.177454	-3166.324982	
TS2	0.969677	1.024988	0.880132	-3167.194131	-3166.169143	-3166.313999	-1187.43i
8a	0.244868	0.258839	0.204627	-672.532841	-672.274002	-672.328214	
2a	0.300123	0.317932	0.254986	-788.343487	-788.025555	-788.088501	
Int3	1.030585	1.089793	0.936358	-3283.039044	-3281.949251	-3282.102686	
TS3	1.027671	1.086723	0.933698	-3283.015688	-3281.928965	-3282.08199	-148.47i
Int4'	1.028426	1.088649	0.935010	-3283.029723	-3281.941074	-3282.094713	
Int4	1.002629	1.060337	0.911422	-3206.549355	-3205.489018	-3205.637933	
Int5	1.250427	1.322583	1.141519	-3879.126127	-3877.803544	-3877.984608	
TS4	1.251219	1.322193	1.144858	-3879.115803	-3877.79361	-3877.970945	-286.68i
Int6	1.253166	1.324067	1.146770	-3879.133032	-3877.808965	-3877.986262	
TS5	1.253523	1.323454	1.150284	-3879.118791	-3877.795337	-3877.968507	-256.04i
(R,R)-3aa	0.523116	0.552317	0.462920	-1384.440947	-1383.88863	-1383.978027	
Int5'	1.250589	1.322616	1.143563	-3879.125286	-3877.80267	-3877.981723	
TS4'	1.251740	1.322375	1.147856	-3879.109409	-3877.787034	-3877.961553	-196.19i
(S)-5d	0.727462	0.769444	0.652644	-2494.655748	-2493.886304	-2494.003104	
H₂O	0.021169	0.024947	0.003502	-76.465854	-76.440907	-76.462352	
TS5'	1.254621	1.324337	1.148641	-3879.106835	-3877.782498	-3877.958194	-189.61i
(R,S)-3aa	0.523154	0.552310	0.462965	-1384.440702	-1383.888392	-1383.977737	



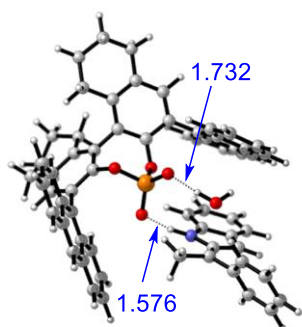
1a



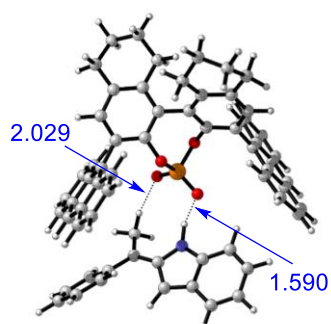
Int1



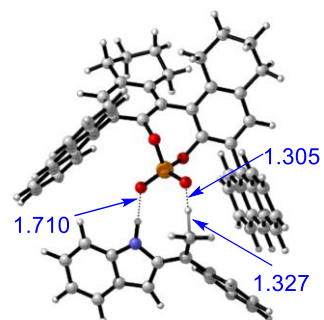
TS1



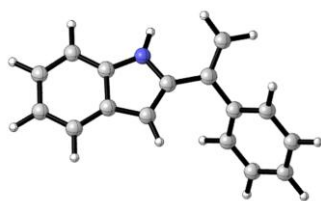
Int2'



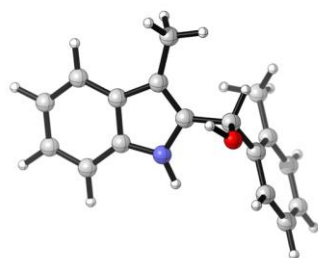
Int2



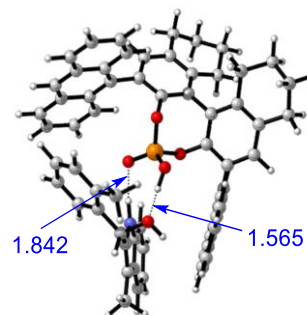
TS2



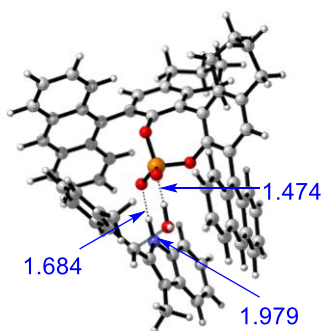
8a



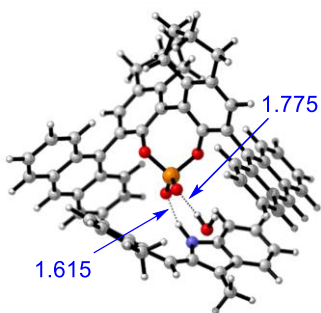
2a



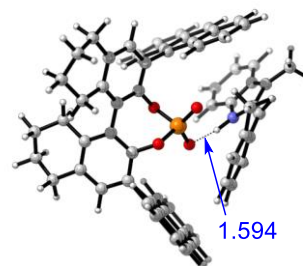
Int3



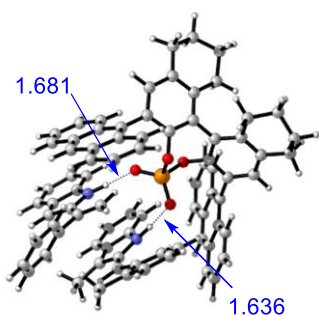
TS3



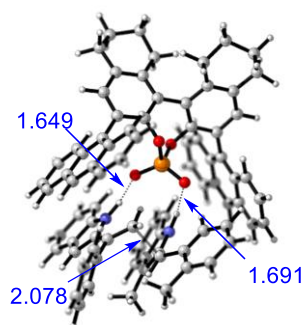
Int4'



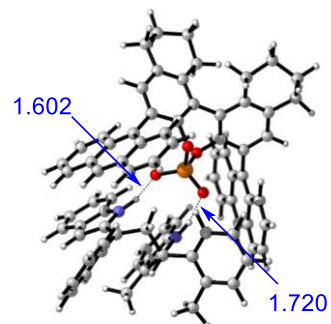
Int4



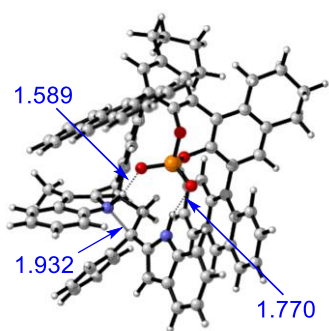
Int5



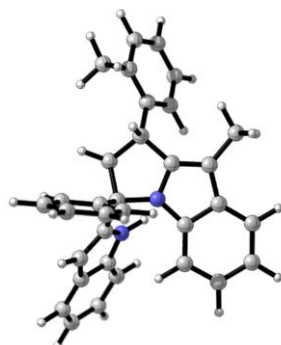
TS4



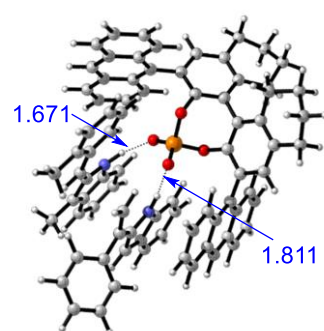
Int6



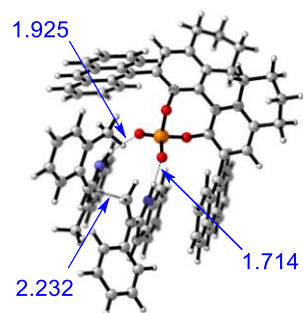
TS5



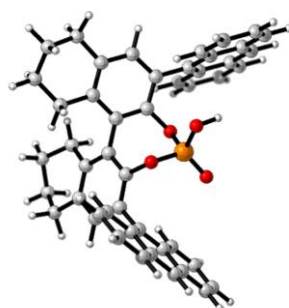
(R,R)-3aa



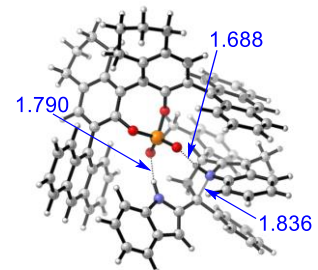
Int5'



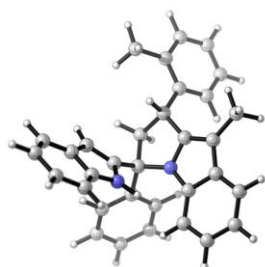
TS4'



(S)-5d



TS5'



(R,S)-3aa

Figure S2. Quantum chemistry method-optimized structures (distances are shown in angstroms).

Cartesian coordinates of DFT-computed structures:

1a

C	-2.58190500	0.49027200	0.00171000
C	-2.12754300	-0.85801800	-0.05595900
C	-3.07587100	-1.88921500	-0.15707200
C	-4.42469800	-1.56221000	-0.20759500
C	-4.85083500	-0.21932000	-0.15748000
C	-3.93808600	0.82391900	-0.05158600
C	-0.31776700	0.50210600	0.09996000
C	-0.69180900	-0.81680600	-0.00025800
H	-2.75559000	-2.92682800	-0.19849500
H	-5.16679000	-2.35140700	-0.28750800
H	-5.91278500	0.00503500	-0.20044100
H	-4.26748600	1.85849600	-0.00928200
H	-0.02112000	-1.66205600	-0.02815100
N	-1.46359500	1.28972200	0.11628300
H	-1.44239600	2.29287300	0.01422200
C	1.02497100	1.19506800	0.14390200
C	2.18022200	0.20119300	0.02662100
C	2.32598200	-0.83252500	0.96236700
C	3.13601900	0.33242500	-0.98295300
C	3.39049900	-1.72696500	0.87358800
H	1.59754800	-0.94311200	1.75992100
C	4.20371200	-0.56297700	-1.07317100
H	3.05353100	1.15270200	-1.68710100
C	4.33292400	-1.59779600	-0.14883700
H	3.48488300	-2.52472500	1.60513100
H	4.93704900	-0.44527000	-1.86626700
H	5.16312000	-2.29489300	-0.21859100
O	1.04650400	2.16942400	-0.91959700
H	0.82734400	1.69223000	-1.73758600
C	1.19162900	2.02984500	1.42483200
H	0.37513500	2.75091400	1.52538800
H	1.19735400	1.38413900	2.30602000
H	2.13868000	2.57447400	1.37712300

Int1

H	-1.31058300	0.04709300	-1.80431700
C	3.26907800	0.90516800	0.31922700
C	3.00267500	-0.31288900	-0.31451400
C	3.68856600	-1.49070500	-0.01446100
C	4.70887500	-1.40363200	0.93251000
H	5.26390700	-2.30547600	1.17715100

C	2.43597800	2.09722300	-0.01599000
C	1.04941900	1.99746500	0.13225700
C	0.18175600	3.07554200	-0.06190200
C	0.76565300	4.29180200	-0.42296200
H	0.12050400	5.15549500	-0.56094300
O	1.96851000	-0.36585000	-1.26089700
O	0.50237200	0.75961800	0.47530100
P	0.46041100	-0.39038800	-0.67666400
O	-0.32153900	0.17627000	-1.92474800
O	-0.01752200	-1.65762000	-0.07424900
C	4.98945000	-0.21902100	1.62073100
C	6.09769600	-0.22567100	2.65897000
C	4.24042600	0.93984200	1.34634100
C	5.94945500	0.87565600	3.71052000
H	7.06076200	-0.09449800	2.14268500
H	6.14392900	-1.21190900	3.13550100
C	4.37027300	2.16329500	2.24079900
C	5.68445700	2.21518500	3.02280200
H	6.85084800	0.92276800	4.33227500
H	5.11030800	0.63926300	4.37910600
H	4.23234000	3.08593700	1.67521200
H	3.53176300	2.13520200	2.95379200
H	5.64319400	3.03108200	3.75354900
H	6.51359400	2.44259100	2.33761600
C	2.98314100	3.30946100	-0.49026800
C	4.43821700	3.37604800	-0.92246400
C	2.13792900	4.42061000	-0.66108400
C	4.98968500	4.80201800	-0.98345500
H	4.50038100	2.92685800	-1.92542000
H	5.06584900	2.74745500	-0.28770700
C	2.68087400	5.77699300	-1.07582200
C	4.04015800	5.70239100	-1.77586700
H	5.98808200	4.79141000	-1.43548700
H	5.10500800	5.19947900	0.03516400
H	1.94709300	6.28541200	-1.71247500
H	2.78105900	6.40089800	-0.17474000
H	4.45587700	6.71009900	-1.88965300
H	3.91468100	5.29178700	-2.78717900
C	-1.29072200	2.91167200	0.07315900
C	-1.84915800	2.52893000	1.31546600
C	-2.12042200	3.11483000	-1.05441500
C	-3.27312800	2.31945800	1.42163500
C	-3.55302100	2.97334200	-0.91590400
C	-4.08726200	2.55666100	0.30827100

C	3.27434500	-2.79354200	-0.60619100
C	3.64199300	-3.12432000	-1.92535600
C	2.48058000	-3.66928200	0.16457200
C	3.21119900	-4.38161300	-2.48712100
C	2.04935500	-4.92118700	-0.40948100
C	2.43049100	-5.24530000	-1.71397600
C	-1.05764500	2.32622200	2.48839500
C	-3.82265700	1.87407300	2.66112900
C	-1.62435500	1.90117700	3.65974500
C	-3.02319800	1.66211700	3.74914200
H	-4.89038500	1.68575800	2.71268800
H	-3.44619700	1.28317100	4.67248800
H	-1.00039400	1.73392800	4.53262500
H	0.00919800	2.50754200	2.43817200
H	-5.16081000	2.40761800	0.39499000
C	-1.60529000	3.40797600	-2.35787100
C	-2.44102300	3.60823700	-3.42400100
C	-4.39089900	3.21340200	-2.04958200
C	-3.85440100	3.52959200	-3.26760300
H	-5.46566400	3.11733200	-1.92126800
H	-4.50076200	3.70429200	-4.12292300
H	-2.02328700	3.82061000	-4.40375700
H	-0.53222000	3.45073900	-2.49659400
C	3.59076100	-4.70655500	-3.82537100
C	4.43315600	-2.25670800	-2.74041600
C	1.22662900	-5.79316900	0.36824800
C	2.04821700	-3.35383900	1.49140000
C	4.34753900	-3.84568100	-4.57340400
C	4.77324300	-2.60406900	-4.02082200
C	0.83764200	-5.45237100	1.63480600
C	1.25434200	-4.21380700	2.20073200
H	3.26016600	-5.65664700	-4.23766300
H	4.62698100	-4.10405600	-5.59085200
H	5.37298600	-1.92861400	-4.62443500
H	4.76172400	-1.31001300	-2.32505800
H	0.90955900	-6.73312300	-0.07660400
H	0.20456800	-6.11977400	2.21245200
H	0.92500600	-3.94740400	3.20122400
H	2.34147600	-2.40446500	1.92333600
H	2.10232100	-6.18971000	-2.14277600
C	-2.79940000	-1.61747700	2.56798500
C	-4.20531500	-1.44159600	2.72633700
C	-4.74345900	-1.41946000	4.02444500
C	-3.88843800	-1.55869200	5.11052300

C	-2.49733500	-1.72237400	4.92863700
C	-1.93511200	-1.75581400	3.65859400
C	-3.70052000	-1.40760500	0.51589500
C	-4.74929000	-1.30006300	1.40668200
H	-5.81248700	-1.29144700	4.17539500
H	-4.29318100	-1.54527700	6.11892300
H	-1.85614200	-1.82751500	5.79961900
H	-0.86656600	-1.87831600	3.50731900
H	-5.78445900	-1.13864200	1.14636900
N	-2.52646800	-1.60069100	1.22311000
H	-1.59371200	-1.67209700	0.81119200
C	-3.65375000	-1.28230700	-0.98811900
C	-5.04945700	-1.15380100	-1.59593700
C	-6.02365500	-2.12870400	-1.34210500
C	-5.35944000	-0.10037500	-2.45897500
C	-7.28873000	-2.03449000	-1.91873300
H	-5.79353300	-2.95648200	-0.67877100
C	-6.62757800	-0.00475700	-3.03531600
H	-4.60455100	0.64089000	-2.68777500
C	-7.59835900	-0.96745000	-2.76506600
H	-8.03391400	-2.79606800	-1.70597300
H	-6.85023400	0.82487500	-3.70131100
H	-8.58546100	-0.89332900	-3.21281500
O	-2.86717000	-0.09991700	-1.31279500
H	-3.20296200	0.65230500	-0.79142000
C	-2.90451800	-2.44764300	-1.65196400
H	-1.89045100	-2.54247800	-1.25757700
H	-3.44213400	-3.38253200	-1.47537200
H	-2.85546800	-2.27387800	-2.73129400

TS1

H	2.17643300	0.89399500	-1.81756200
C	-3.27875000	-0.53055500	0.04732500
C	-2.80056900	0.77775700	-0.07864800
C	-3.36927700	1.85398600	0.60832500
C	-4.45209800	1.57747100	1.44254300
H	-4.91654800	2.40050700	1.98011600
C	-2.60198000	-1.61322800	-0.72633300
C	-1.23045600	-1.81307200	-0.52314800
C	-0.54579000	-2.88774000	-1.09937000
C	-1.26131000	-3.72398500	-1.95531500
H	-0.74765300	-4.57102100	-2.40382400
O	-1.71469500	1.00764000	-0.90562800
O	-0.53673800	-0.92732300	0.28120000

P	-0.22376300	0.58491700	-0.34721800
O	0.65339800	0.49771700	-1.56319500
O	0.18271800	1.40929400	0.84691100
C	-4.92387400	0.27578700	1.64484300
C	-6.09224100	0.06353800	2.59139900
C	-4.31767300	-0.79706200	0.96700000
C	-6.17322400	-1.36129200	3.14382200
H	-7.02678100	0.28599100	2.05379300
H	-6.03607600	0.79146100	3.40958200
C	-4.67992600	-2.23121900	1.31976900
C	-6.04318900	-2.36930700	2.00129700
H	-7.11588200	-1.49981900	3.68627200
H	-5.36086600	-1.52592100	3.86542500
H	-4.62831800	-2.87821000	0.44211700
H	-3.90067200	-2.60761800	2.00076400
H	-6.17000100	-3.39552200	2.36596000
H	-6.84256700	-2.19124700	1.26764400
C	-3.28328200	-2.42056200	-1.66359400
C	-4.69739800	-2.06341000	-2.09060900
C	-2.60381400	-3.48945300	-2.27381300
C	-5.44027300	-3.21992100	-2.76215600
H	-4.62492200	-1.22532400	-2.80048000
H	-5.27441300	-1.67637900	-1.24838000
C	-3.29857100	-4.42993200	-3.24351300
C	-4.57128400	-3.84115100	-3.85712800
H	-6.39077400	-2.85948400	-3.17261200
H	-5.68631800	-3.98706500	-2.01374700
H	-2.59519300	-4.72724700	-4.03075600
H	-3.55988900	-5.35600300	-2.70878200
H	-5.11799500	-4.62006400	-4.40155200
H	-4.30557700	-3.06555400	-4.58857500
C	0.87488000	-3.17095900	-0.74374600
C	1.14160100	-3.92986700	0.41590900
C	1.93282500	-2.73197300	-1.56499800
C	2.50187900	-4.28066900	0.74308600
C	3.29597800	-3.02581700	-1.18777800
C	3.54436600	-3.79637000	-0.04966200
C	-2.80932700	3.22758800	0.47183000
C	-3.05374000	3.96929700	-0.70293200
C	-2.03057200	3.77202500	1.51410800
C	-2.51003900	5.29979200	-0.83118100
C	-1.49727000	5.10687500	1.37942700
C	-1.75149600	5.83369000	0.21391500
C	0.10094300	-4.39555100	1.28024600

C	2.74745000	-5.12295800	1.86920100
C	0.38044400	-5.18481000	2.36446700
C	1.72026500	-5.56861900	2.65619800
H	3.77517800	-5.39822400	2.08900300
H	1.92180100	-6.21091000	3.50913400
H	-0.42631500	-5.53170500	3.00415400
H	-0.92283100	-4.11897900	1.05551200
H	4.57038000	-4.03615400	0.21811500
C	1.70688700	-2.00339700	-2.77409300
C	2.75286000	-1.59212900	-3.55771800
C	4.36002200	-2.54195100	-2.01011000
C	4.09954300	-1.85552200	-3.16808000
H	5.38253700	-2.75347400	-1.70730400
H	4.91675900	-1.50765000	-3.79423700
H	2.55991500	-1.03122600	-4.46675500
H	0.68935200	-1.75744900	-3.04782600
C	-2.76492100	6.03959800	-2.02648000
C	-3.83164800	3.45354200	-1.78580100
C	-0.71294600	5.65060800	2.44324000
C	-1.72034000	3.04108700	2.70356800
C	-3.51152000	5.50563200	-3.04163200
C	-4.05197600	4.19412900	-2.91646400
C	-0.45603900	4.92219500	3.57254800
C	-0.96362200	3.59741100	3.69892900
H	-2.34920500	7.04087400	-2.11003000
H	-3.69638000	6.07860400	-3.94607000
H	-4.64320800	3.78018800	-3.72852600
H	-4.24619500	2.45558200	-1.69788600
H	-0.32399400	6.65991200	2.33140800
H	0.14171200	5.34711700	4.37447100
H	-0.73339600	3.02017300	4.59010300
H	-2.07693400	2.02259500	2.79338600
H	-1.34676300	6.83893900	0.11605800
C	2.88195700	-0.51502600	2.13923000
C	4.25157900	-0.91832800	1.97866200
C	4.73378700	-2.02754300	2.71905100
C	3.86100900	-2.68820200	3.55192900
C	2.49176200	-2.30389900	3.64965500
C	1.98225700	-1.23017100	2.95197100
C	3.83414100	0.92700600	0.71674900
C	4.82454000	-0.02335000	1.05866800
H	5.77079600	-2.33843600	2.63021700
H	4.20443400	-3.53916100	4.13126600
H	1.83032500	-2.89240400	4.27670700

H	0.93727300	-0.94472600	2.99994100
H	5.83286200	-0.04083000	0.67297100
N	2.66855100	0.59891500	1.39923300
H	1.72182500	1.01773200	1.25279900
C	3.90428700	2.00748200	-0.19012900
C	5.23282300	2.43418900	-0.70024000
C	6.31702200	2.54801600	0.18730400
C	5.40150300	2.84740700	-2.03241900
C	7.54435300	3.04085200	-0.25413700
H	6.18554100	2.28196100	1.22989800
C	6.63326300	3.32328000	-2.47017700
H	4.57072200	2.74466100	-2.71907100
C	7.70918700	3.42237100	-1.58453300
H	8.36856900	3.13027900	0.44748500
H	6.75390200	3.61901500	-3.50827500
H	8.66705000	3.80116400	-1.92922500
O	3.15701700	1.07707500	-1.98690000
H	3.56177400	0.19155900	-1.99709100
C	2.82447100	3.05066000	-0.22498400
H	1.82569700	2.65715700	-0.03175700
H	3.05953500	3.78402400	0.55956500
H	2.83956800	3.57729700	-1.18078100

Int2'

H	2.34087500	0.64891000	-2.04689200
C	-3.26811100	0.01921400	0.26488500
C	-2.58938600	1.21616900	0.02236000
C	-2.85265900	2.39135500	0.73435500
C	-3.83519100	2.32982000	1.72098200
H	-4.06596300	3.23159000	2.28300100
C	-2.91066100	-1.17962200	-0.55223800
C	-1.58321300	-1.63112200	-0.53191800
C	-1.20449100	-2.83573500	-1.13666100
C	-2.17927700	-3.53895000	-1.84288500
H	-1.90436100	-4.48202100	-2.30929500
O	-1.59894400	1.22143400	-0.94379800
O	-0.62856300	-0.89054900	0.13468600
P	-0.14612000	0.58084300	-0.50217600
O	0.64864400	0.42092200	-1.75727300
O	0.40963300	1.30423900	0.70145800
C	-4.49645800	1.13733700	2.03992600
C	-5.53202700	1.15514500	3.15082900
C	-4.19836600	-0.03801700	1.32756000
C	-5.78363200	-0.22360900	3.76503200

H	-6.48079400	1.53769800	2.74416100
H	-5.22602600	1.87103800	3.92311500
C	-4.76198800	-1.37610900	1.77953500
C	-6.01027100	-1.25152800	2.65607500
H	-6.64331400	-0.18035300	4.44410300
H	-4.91468600	-0.52560000	4.36628300
H	-4.96254400	-2.02632500	0.92598800
H	-3.97266700	-1.88822700	2.35152800
H	-6.26529600	-2.23226700	3.07480600
H	-6.86469200	-0.93714200	2.03954800
C	-3.85605100	-1.86115300	-1.35060700
C	-5.22328100	-1.24636600	-1.60135200
C	-3.48408400	-3.05538600	-1.99166900
C	-6.25789400	-2.24913200	-2.11631700
H	-5.09259100	-0.45057100	-2.35046300
H	-5.59421300	-0.74003200	-0.70784400
C	-4.47365000	-3.86551000	-2.81114600
C	-5.68191600	-3.05317500	-3.28325400
H	-7.16865800	-1.71806500	-2.41690200
H	-6.54222600	-2.93673200	-1.30662100
H	-3.95655600	-4.31663800	-3.66664000
H	-4.83225300	-4.70708400	-2.19867900
H	-6.43698500	-3.72203100	-3.71283800
H	-5.37561500	-2.36198600	-4.08055600
C	0.17069200	-3.38412800	-0.94788500
C	0.39980300	-4.27298500	0.12479100
C	1.22070700	-3.04044900	-1.82299800
C	1.71348400	-4.83835000	0.31662900
C	2.54699600	-3.56015500	-1.58277100
C	2.75816100	-4.44453200	-0.52193200
C	-2.08119300	3.63307100	0.44201900
C	-2.37440700	4.37069700	-0.72479300
C	-1.03818500	4.03795400	1.30092200
C	-1.59892200	5.54596100	-1.03979700
C	-0.25805700	5.20667500	0.96875400
C	-0.56064500	5.92989000	-0.18728100
C	-0.63389800	-4.65143500	1.03924700
C	1.91239400	-5.78656600	1.36584100
C	-0.39859400	-5.55390800	2.04358600
C	0.88886200	-6.14194100	2.20304500
H	2.90225700	-6.21969800	1.48439700
H	1.05381800	-6.86875100	2.99379400
H	-1.20118900	-5.83205800	2.72108300
H	-1.61840000	-4.21408800	0.91812700

H	3.75420000	-4.84864800	-0.35579700
C	1.02019100	-2.19568600	-2.95797600
C	2.05696300	-1.87578900	-3.79252900
C	3.60868300	-3.17642600	-2.45906800
C	3.37088000	-2.36505700	-3.53793300
H	4.60554500	-3.56331200	-2.26204800
H	4.18299700	-2.08971000	-4.20544000
H	1.88670600	-1.21709800	-4.63794800
H	0.03327400	-1.78914100	-3.13499300
C	-1.90829200	6.28394000	-2.22323500
C	-3.42397000	3.99862200	-1.62138700
C	0.81979600	5.58881500	1.82668800
C	-0.69052400	3.31330900	2.48383700
C	-2.92153200	5.89140600	-3.05522400
C	-3.68876600	4.73218600	-2.74716000
C	1.11485300	4.86680500	2.95137500
C	0.34532400	3.71469200	3.28268500
H	-1.31536300	7.16713200	-2.44837500
H	-3.14504200	6.46051200	-3.95331700
H	-4.49039500	4.42915500	-3.41492500
H	-4.01361500	3.11758900	-1.39401300
H	1.39823300	6.47133900	1.56385900
H	1.93469100	5.16976000	3.59750000
H	0.59627500	3.14220500	4.17139300
H	-1.24657700	2.41555100	2.72207600
H	0.03014200	6.80981800	-0.43329800
C	2.70123300	-1.01631500	1.98149000
C	4.04183400	-1.55147000	1.91516000
C	4.31522800	-2.81060700	2.51955700
C	3.28406000	-3.47431600	3.13270200
C	1.95385600	-2.94560500	3.14062500
C	1.64041700	-1.73311000	2.57290700
C	3.94927600	0.47671300	0.88327600
C	4.80372400	-0.62137800	1.20917100
H	5.31874700	-3.22463900	2.49378300
H	3.45812500	-4.43727100	3.60043300
H	1.16496100	-3.54410800	3.58256600
H	0.62881600	-1.34568400	2.53948400
H	5.84284800	-0.70167100	0.92689700
N	2.68333500	0.19358600	1.39049300
H	1.79329600	0.72077200	1.18102800
C	4.22976000	1.61172200	0.13408200
C	5.61067600	1.87411000	-0.30266500
C	6.67237700	1.82177900	0.61842800

C	5.87437300	2.24018600	-1.63496300
C	7.97016100	2.12897400	0.21521900
H	6.46629300	1.58168100	1.65624700
C	7.17672000	2.52241400	-2.03372500
H	5.05876200	2.22211200	-2.34861500
C	8.22612500	2.47467500	-1.11186100
H	8.77865500	2.10360900	0.93994400
H	7.37547800	2.77885800	-3.07020500
H	9.23890600	2.70859000	-1.42718300
O	3.32610800	0.64941700	-2.14999900
H	3.53802600	-0.29705300	-2.17424900
C	3.22006600	2.68871200	-0.08991200
H	2.18611000	2.35480300	-0.00290300
H	3.38654500	3.46513000	0.67327000
H	3.38038700	3.15835200	-1.06234000

Int2

C	2.81684900	-1.55942500	-0.60940700
C	2.86482100	-0.39437000	0.16975200
C	3.80905700	0.61257500	-0.06321600
C	4.73681600	0.39827900	-1.08493300
H	5.49010500	1.16066900	-1.26779300
C	1.76042300	-2.56929200	-0.30927400
C	0.42468800	-2.14447500	-0.32828800
C	-0.63690100	-3.03184000	-0.12207300
C	-0.31707900	-4.36823900	0.12595300
H	-1.12878600	-5.07479000	0.28125400
O	1.95964000	-0.24206800	1.19826000
O	0.16271300	-0.80180700	-0.51500800
P	0.38563600	0.14495000	0.84941400
O	-0.46036300	-0.35196700	1.97543100
O	0.29231900	1.56779000	0.35263300
C	4.69388900	-0.72777300	-1.91064500
C	5.73154800	-0.86805300	-3.00983900
C	3.69972800	-1.70032200	-1.70238500
C	5.28202800	-1.78070800	-4.15333700
H	6.65454500	-1.28021400	-2.57374400
H	5.99750200	0.12519300	-3.39124500
C	3.49463600	-2.81314100	-2.71813500
C	4.72537700	-3.08759900	-3.58574900
H	6.12101600	-1.97187100	-4.83294800
H	4.49998200	-1.28040600	-4.74135200
H	3.15980900	-3.73284900	-2.23536200
H	2.66000200	-2.51067200	-3.36968900

H	4.46038900	-3.78392500	-4.39024600
H	5.50129600	-3.57980200	-2.98177100
C	2.05839900	-3.90464900	0.03672900
C	3.49171600	-4.31730800	0.32898200
C	1.00370100	-4.81408900	0.22992400
C	3.71269300	-5.83101200	0.28580200
H	3.73803400	-3.94978100	1.33693400
H	4.19107400	-3.81009700	-0.33846200
C	1.25928600	-6.28087000	0.52945400
C	2.64712400	-6.54697400	1.11760400
H	4.71923400	-6.06716200	0.65081600
H	3.66019300	-6.18397300	-0.75437400
H	0.47841500	-6.65873200	1.20055400
H	1.15693300	-6.85469000	-0.40447600
H	2.83626400	-7.62632800	1.15640400
H	2.68870900	-6.17676500	2.15131900
C	-2.06054900	-2.59428300	-0.14573700
C	-2.66611000	-2.20607100	-1.36219900
C	-2.82303600	-2.63434700	1.04301400
C	-4.08070800	-1.91867000	-1.39597600
C	-4.24190200	-2.37176600	0.99167800
C	-4.83561600	-2.03660000	-0.22636400
C	3.78857900	1.89491800	0.69134400
C	4.09549900	1.92661600	2.06849600
C	3.48076300	3.09067000	0.00300200
C	4.09573500	3.18714600	2.77155500
C	3.52113100	4.35013700	0.70810700
C	3.81731800	4.36423100	2.07292300
C	-1.93145600	-2.09644500	-2.58401200
C	-4.67976500	-1.52604300	-2.63273400
C	-2.53970500	-1.70340400	-3.74664200
C	-3.93308800	-1.41176100	-3.77439000
H	-5.74751300	-1.32352600	-2.64255700
H	-4.40011900	-1.10905900	-4.70776100
H	-1.95696200	-1.61570200	-4.65914700
H	-0.87186200	-2.32154700	-2.57425000
H	-5.90392900	-1.83965900	-0.25961200
C	-2.23170200	-2.88706900	2.32099100
C	-2.99371800	-2.91599100	3.45847200
C	-5.00505100	-2.43579500	2.19877100
C	-4.40101200	-2.70284500	3.39817600
H	-6.07499100	-2.25498300	2.13899100
H	-4.98954600	-2.74324300	4.31107400
H	-2.51987100	-3.08615200	4.42067200

H	-1.15780700	-3.00389700	2.37872100
C	4.40143400	3.20383400	4.16718300
C	4.42856800	0.74797700	2.80567700
C	3.26787700	5.55854300	-0.01172500
C	3.11242800	3.11253000	-1.37997200
C	4.70068000	2.04899700	4.83680100
C	4.71804700	0.80583100	4.14248100
C	2.97723200	5.53660800	-1.34918400
C	2.87858900	4.29254200	-2.03599600
H	4.39226100	4.16028300	4.68416900
H	4.92998100	2.07441800	5.89851500
H	4.96180400	-0.10443800	4.68291300
H	4.44395700	-0.20272500	2.28654400
H	3.32306200	6.50000900	0.52936000
H	2.81325800	6.46581400	-1.88910200
H	2.60210200	4.28082600	-3.08658500
H	3.01029300	2.17083500	-1.90443500
H	3.83932800	5.31441800	2.60232300
C	-1.75252100	3.86760500	-0.63966300
C	-3.00430200	4.39867300	-1.12589400
C	-2.99851600	5.58613100	-1.91051900
C	-1.78823900	6.16436900	-2.19922700
C	-0.55952300	5.59762400	-1.73060900
C	-0.51383300	4.45681500	-0.96070700
C	-3.36272000	2.51476700	0.10943000
C	-3.99942000	3.53920500	-0.66537000
H	-3.92996600	6.00952100	-2.27392700
H	-1.74885600	7.06799200	-2.79985200
H	0.37302800	6.08819500	-1.98824600
H	0.41425100	4.01611200	-0.61628100
H	-5.06762100	3.65416900	-0.77518800
N	-1.99759800	2.77978800	0.12318000
H	-1.18659900	2.14986300	0.39027900
C	-3.96979600	1.51340600	0.86596800
C	-5.35214700	1.14428300	0.58049000
C	-6.22349700	0.76908100	1.62348200
C	-5.83861800	1.12790400	-0.74449900
C	-7.54417800	0.43254500	1.35394600
H	-5.86674200	0.76844100	2.64677300
C	-7.15783200	0.77752000	-1.00924300
H	-5.15372600	1.31654800	-1.56206800
C	-8.01585400	0.43496100	0.03766100
H	-8.20825200	0.16390700	2.16982300
H	-7.51035000	0.74917800	-2.03583200

H	-9.04475300	0.15671200	-0.17076100
C	-3.22394700	0.84798200	1.96417900
H	-2.78496200	1.58743100	2.64351400
H	-3.83625000	0.13761100	2.51758700
H	-2.34911600	0.28202600	1.59401300

TS2

C	2.92693400	-1.36854900	-0.58205600
C	2.74733700	-0.16728000	0.11519000
C	3.56319100	0.94885300	-0.09157200
C	4.59169700	0.81605800	-1.02793000
H	5.24975400	1.66489700	-1.19481700
C	2.01254900	-2.50603900	-0.27416000
C	0.63356400	-2.29695000	-0.39719700
C	-0.30288000	-3.29551400	-0.11805600
C	0.19351600	-4.54235000	0.26765600
H	-0.51628800	-5.33852700	0.47763700
O	1.70063500	-0.08003800	1.02777300
O	0.18587600	-1.03517200	-0.77236300
P	0.19819200	0.12474800	0.39549300
O	-0.73171700	-0.30002000	1.53947300
O	0.00647800	1.44908800	-0.26528700
C	4.76870500	-0.34255300	-1.78880600
C	5.89958300	-0.38626100	-2.80174000
C	3.90989900	-1.43895000	-1.59246500
C	5.68880200	-1.42831400	-3.90237900
H	6.83595900	-0.61761000	-2.27141100
H	6.03939100	0.61070500	-3.23648000
C	3.95209400	-2.62605500	-2.54082700
C	5.28304700	-2.76640300	-3.28251900
H	6.60242700	-1.53105600	-4.49945900
H	4.89597100	-1.09181900	-4.58465000
H	3.70430700	-3.55417200	-2.02264700
H	3.14670000	-2.48434500	-3.27792000
H	5.19664900	-3.54457000	-4.04984600
H	6.06435300	-3.09474400	-2.58194000
C	2.48143800	-3.74595700	0.21140000
C	3.94042000	-3.91643700	0.60321100
C	1.55885000	-4.78092000	0.44775200
C	4.37774100	-5.37912600	0.70875500
H	4.07445200	-3.43324200	1.58332900
H	4.59829500	-3.37132900	-0.07595100
C	2.00569400	-6.16313100	0.89023000
C	3.38271900	-6.17154500	1.55804700

H	5.38652900	-5.43151400	1.13460300
H	4.43228500	-5.82271100	-0.29584700
H	1.25057400	-6.59464600	1.55811700
H	2.03783800	-6.82016300	0.00761600
H	3.72192300	-7.20394900	1.70256900
H	3.31441800	-5.71385700	2.55463100
C	-1.76863900	-3.03839100	-0.16274600
C	-2.42407700	-2.84791200	-1.39773900
C	-2.49915900	-3.00606000	1.04591000
C	-3.85456100	-2.65866500	-1.42258400
C	-3.93206200	-2.83883900	1.00615500
C	-4.57204200	-2.67823900	-0.22432100
C	3.34125100	2.23928200	0.61616900
C	3.54955700	2.33336800	2.00975700
C	2.97058300	3.38177600	-0.12870800
C	3.39193300	3.60795200	2.66915300
C	2.86822700	4.66117600	0.53336100
C	3.07024100	4.73798700	1.91334500
C	-1.72410600	-2.83977700	-2.64436100
C	-4.50586500	-2.45735300	-2.67824500
C	-2.38418200	-2.63726700	-3.82689800
C	-3.79469500	-2.44060000	-3.84726700
H	-5.58306300	-2.31585600	-2.67833400
H	-4.30085000	-2.28289900	-4.79567900
H	-1.82980100	-2.62565700	-4.76101400
H	-0.65084900	-2.99063000	-2.63870700
H	-5.64886900	-2.54061400	-0.24741200
C	-1.87020400	-3.09335000	2.32828500
C	-2.60445100	-3.04886900	3.48287700
C	-4.66397700	-2.81973500	2.23397300
C	-4.02275300	-2.92194700	3.43878400
H	-5.74331000	-2.71069400	2.18397600
H	-4.58971300	-2.90190800	4.36567900
H	-2.10185500	-3.10000100	4.44441600
H	-0.79100300	-3.16262600	2.37321600
C	3.59310100	3.68966600	4.08146000
C	3.93324200	1.21084900	2.80791200
C	2.56957400	5.82412600	-0.24305100
C	2.67393600	3.32916900	-1.52792500
C	3.94138600	2.58484900	4.80936500
C	4.11835900	1.33048600	4.15925100
C	2.35298500	5.73515900	-1.59174700
C	2.38053700	4.46489400	-2.23505000
H	3.46410500	4.65544500	4.56377400

H	4.08992700	2.65948000	5.88296300
H	4.40344800	0.46095300	4.74473300
H	4.07431900	0.25132000	2.32507400
H	2.52011900	6.78322800	0.26637600
H	2.13838800	6.62755400	-2.17323600
H	2.15217800	4.39776100	-3.29467600
H	2.66682300	2.36554900	-2.02181900
H	2.98096100	5.70142900	2.41051700
C	-2.09139100	4.21547600	-0.45789000
C	-3.42521700	4.54191100	-0.86133900
C	-3.65695700	5.74818800	-1.56126400
C	-2.57562500	6.55214900	-1.86427700
C	-1.25670600	6.18502400	-1.48652500
C	-0.99301000	5.02093900	-0.78711600
C	-3.41590900	2.54247400	0.22160200
C	-4.24252600	3.46518800	-0.44173400
H	-4.66298300	6.02609800	-1.86255700
H	-2.72895700	7.48040500	-2.40688300
H	-0.42926500	6.83662600	-1.75063300
H	0.01369100	4.73758400	-0.50545900
H	-5.31614700	3.38505500	-0.53225500
N	-2.11893800	3.04008100	0.24035800
H	-1.28215100	2.43103300	0.28049000
C	-3.80085500	1.36426700	0.92908300
C	-5.05634400	0.71813200	0.51338800
C	-5.94648300	0.21700100	1.47923300
C	-5.41133400	0.63195300	-0.84576600
C	-7.17257400	-0.31935800	1.09950800
H	-5.68450800	0.28386200	2.52924300
C	-6.63384700	0.08355600	-1.22286200
H	-4.71032500	0.97102000	-1.59942300
C	-7.52109900	-0.38479200	-0.25227100
H	-7.86088800	-0.68099900	1.85782700
H	-6.88922300	0.01527300	-2.27590200
H	-8.47912600	-0.80382900	-0.54675500
C	-3.01969400	0.85444700	1.98999700
H	-2.48438000	1.60399100	2.57597100
H	-3.46302200	0.04977400	2.57565200
H	-1.91649900	0.24505800	1.57508200

8a

C	2.50100100	0.57522400	0.18071800
C	2.06819000	-0.68251800	-0.33090500
C	3.02790400	-1.67729600	-0.58681300

C	4.36335200	-1.40939000	-0.31978200
C	4.76664700	-0.16143000	0.19905500
C	3.84404400	0.84640700	0.45527000
C	0.24603300	0.64855100	-0.04940500
C	0.64387100	-0.60877700	-0.45996200
H	2.72462400	-2.64167000	-0.98509100
H	5.11362500	-2.17109400	-0.51134300
H	5.81907500	0.01721100	0.39978900
H	4.15686500	1.80911600	0.85014200
H	-0.01489100	-1.37572400	-0.84020900
N	1.38044800	1.36716400	0.31744300
H	1.34941700	2.24814100	0.80638600
C	-1.08428600	1.25428400	-0.02263100
C	-2.25694400	0.34050300	0.03002500
C	-3.39735400	0.60872500	-0.74213900
C	-2.26271200	-0.78801200	0.86487100
C	-4.51641900	-0.21853100	-0.67349000
H	-3.39040600	1.46093200	-1.41495800
C	-3.38258600	-1.61428200	0.93469000
H	-1.38662800	-1.00764000	1.46591500
C	-4.51370700	-1.33286700	0.16675000
H	-5.38707100	0.00126600	-1.28513100
H	-3.37225700	-2.47861800	1.59291500
H	-5.38413800	-1.98087000	0.21800400
C	-1.25276100	2.59221000	-0.04523000
H	-0.41820200	3.27671600	-0.16404400
H	-2.23879500	3.03527000	0.03937500

2a

C	2.46048200	0.32845300	0.09080800
C	1.89731800	-0.93212000	-0.25580600
C	2.63885000	-2.11630100	-0.20528700
C	3.96638900	-2.02506600	0.19680300
C	4.54555100	-0.78607700	0.53990000
C	3.80539400	0.38823000	0.48972200
C	1.42348500	1.31869300	-0.06098300
C	0.29479700	0.64600500	-0.48194000
H	2.19464600	-3.07165700	-0.47040100
H	4.56966600	-2.92701800	0.24695700
H	5.58675100	-0.75398300	0.84765800
H	4.25843100	1.33957800	0.75565700
N	0.58705000	-0.70543600	-0.61069300
H	-0.10745200	-1.40621700	-0.82269000
C	1.57483000	2.78477700	0.20559600

H	2.32895900	3.23885200	-0.45029100
H	1.89835400	2.96947300	1.23794000
H	0.63638800	3.32699300	0.05416400
C	-1.06620100	1.15752300	-0.85787500
H	-1.17641900	2.16327900	-0.42902200
O	-1.20875600	1.22913700	-2.28297400
H	-0.36822300	1.57127500	-2.62484200
C	-2.16170000	0.26029500	-0.30721000
C	-2.82576700	-0.62803800	-1.15716400
C	-2.46718900	0.28001000	1.06901100
C	-3.79445100	-1.50178000	-0.66029300
H	-2.58599800	-0.61094800	-2.21398700
C	-3.44302000	-0.59986200	1.54650800
C	-4.10433700	-1.48775100	0.69719900
H	-4.30541000	-2.18351900	-1.33447900
H	-3.68565400	-0.58746300	2.60630400
H	-4.85782800	-2.16057900	1.09708600
C	-1.76121400	1.21423700	2.02160600
H	-0.68015000	1.03419200	2.03509300
H	-2.14086000	1.08967600	3.03973900
H	-1.90380500	2.26564700	1.74017900

Int3

C	5.21585400	1.16807100	1.39507500
C	3.87238800	0.92758600	1.80364700
C	3.56314900	0.33847400	3.03320200
C	4.62274400	-0.00942200	3.86079900
C	5.96186000	0.20841500	3.47263700
C	6.26685300	0.78807600	2.24672700
C	5.15694200	1.80594500	0.10503300
C	3.81672700	1.93852400	-0.20526600
H	2.53247400	0.15100400	3.31812400
H	4.41633200	-0.47450500	4.82044500
H	6.76410400	-0.08036000	4.14627300
H	7.30094200	0.95815300	1.95745700
N	3.04686900	1.38620800	0.80820300
H	2.02452700	1.41246800	0.84359200
C	6.34251100	2.21936900	-0.71100600
H	6.05015600	2.71059800	-1.64436000
H	6.98504400	2.91824800	-0.16033300
H	6.96797500	1.35596200	-0.97673900
C	3.17510600	2.44960300	-1.45541900
H	3.95025300	2.92516700	-2.07093200
O	2.67607800	1.31433000	-2.21837400

H	1.29153200	0.67288800	-1.86898300
C	2.01923500	3.42235000	-1.26151900
C	1.86197200	4.06375200	-0.02768600
C	1.12202900	3.71478300	-2.31256700
C	0.80533600	4.93742100	0.20814900
H	2.56630900	3.85920800	0.76993600
C	0.05945600	4.58872000	-2.05052900
C	-0.11269300	5.18824400	-0.80632100
H	0.68665700	5.39410300	1.18497100
H	-0.64757300	4.80063000	-2.84881800
H	-0.95735700	5.84681600	-0.63499400
C	1.24653100	3.14930000	-3.71048200
H	0.69526100	3.78064300	-4.41479800
H	2.28692500	3.09256400	-4.04424900
H	0.83824900	2.13622300	-3.77459900
H	3.39602700	0.66262600	-2.30635700
C	-2.70906800	-1.68641200	0.40661700
C	-2.70193500	-0.30375000	0.19498800
C	-3.55085900	0.57327800	0.87071000
C	-4.42520600	0.01499600	1.80262200
H	-5.10266200	0.67589700	2.33706300
C	-1.76723200	-2.54808800	-0.36945200
C	-0.40036300	-2.27664800	-0.28506800
C	0.57787400	-3.08645700	-0.86840500
C	0.13171600	-4.18331800	-1.60322500
H	0.86792800	-4.84032100	-2.05959800
O	-1.80675800	0.23301200	-0.73085300
O	0.01356900	-1.13682600	0.40044900
P	-0.23833400	0.30470200	-0.32463500
O	0.37536900	0.25093900	-1.77109100
O	0.19863200	1.37206900	0.60445000
C	-4.42369100	-1.35206300	2.09974900
C	-5.39454500	-1.86865600	3.14689300
C	-3.54247400	-2.21263600	1.42052800
C	-4.96988800	-3.20295100	3.76434400
H	-6.38105400	-1.99605300	2.67568300
H	-5.52949600	-1.10846100	3.92535100
C	-3.38976800	-3.65907800	1.86451600
C	-4.58687100	-4.18695100	2.65821800
H	-5.78049800	-3.60267600	4.38445300
H	-4.10637600	-3.04789700	4.42580100
H	-3.18155200	-4.31353300	1.01643400
H	-2.49017300	-3.71268200	2.49694800
H	-4.34484900	-5.17164000	3.07460800

H	-5.44411400	-4.32809500	1.98447200
C	-2.19454800	-3.60983600	-1.19845400
C	-3.66904700	-3.77489400	-1.52696500
C	-1.23167200	-4.43860200	-1.80191600
C	-4.02121800	-5.16463700	-2.06144100
H	-3.91967500	-3.02478700	-2.29258400
H	-4.29246900	-3.52487700	-0.66607200
C	-1.62945400	-5.63731900	-2.64567700
C	-3.05974500	-5.55668400	-3.18461400
H	-5.05927700	-5.17183200	-2.41325200
H	-3.95447000	-5.90277400	-1.24927900
H	-0.91491300	-5.75701300	-3.46883200
H	-1.53374000	-6.54470900	-2.03020400
H	-3.34452600	-6.51656800	-3.63053900
H	-3.11337400	-4.80380000	-3.98290200
C	2.01689800	-2.75357300	-0.66815700
C	2.60399300	-2.98070200	0.59663900
C	2.76744100	-2.16461600	-1.70617300
C	3.96827600	-2.57691100	0.83356200
C	4.12784000	-1.74913100	-1.45038700
C	4.68706600	-1.95128600	-0.18792800
C	-3.51106900	2.04168600	0.61554700
C	-4.16312900	2.56852700	-0.51837000
C	-2.83283900	2.89047900	1.51406500
C	-4.16038100	3.99451600	-0.74048300
C	-2.85343600	4.31683600	1.29395500
C	-3.52114500	4.82936400	0.17950100
C	1.89526700	-3.60763500	1.66772200
C	4.55564800	-2.82085500	2.11078900
C	2.49724200	-3.83068800	2.87818100
C	3.84450900	-3.43450400	3.10520300
H	5.57270400	-2.48249900	2.28015800
H	4.29998700	-3.60839000	4.07573700
H	1.94106500	-4.31455400	3.67638700
H	0.86879800	-3.91586300	1.50469400
H	5.69996500	-1.61135000	0.00870200
C	2.22611800	-1.93065900	-3.01069100
C	2.97690800	-1.35239700	-3.99950300
C	4.87154400	-1.12808600	-2.50382400
C	4.32010400	-0.94480200	-3.74660100
H	5.89032200	-0.81160900	-2.29536100
H	4.89753000	-0.47620600	-4.53833800
H	2.54246200	-1.17909300	-4.97923000
H	1.19518800	-2.20471700	-3.19874700

C	-4.81890600	4.51669300	-1.89543800
C	-4.83818800	1.74090400	-1.46871000
C	-2.17759100	5.16980800	2.21891200
C	-2.10192600	2.39250500	2.63738000
C	-5.44630800	3.68758600	-2.78551100
C	-5.45559000	2.28066100	-2.56571200
C	-1.49768700	4.65139500	3.28744000
C	-1.45423600	3.24281600	3.49212800
H	-4.80809200	5.59268000	-2.05119200
H	-5.94101600	4.09730000	-3.66159500
H	-5.95789900	1.63236200	-3.27822600
H	-4.85032900	0.66836500	-1.30896800
H	-2.20913200	6.24307300	2.04730600
H	-0.98219800	5.31027700	3.98070700
H	-0.89145400	2.84236900	4.33028300
H	-2.04935100	1.32111800	2.79000400
H	-3.53586700	5.90530600	0.01807000

TS3

C	-4.75078200	-1.66269900	2.00732200
C	-3.34905700	-1.51535300	2.24869000
C	-2.85259500	-1.04546500	3.47509600
C	-3.77717000	-0.75208600	4.46045200
C	-5.17234000	-0.90935600	4.24966500
C	-5.66525600	-1.35598000	3.03894000
C	-4.89688400	-2.10401100	0.66377000
C	-3.59772700	-2.24819900	0.14861500
H	-1.78606200	-0.91439400	3.62461400
H	-3.42985900	-0.38503800	5.42213700
H	-5.85791800	-0.66779800	5.05674000
H	-6.73423500	-1.46985400	2.88071300
N	-2.67537800	-1.89778800	1.13050600
H	-1.66093300	-1.73090600	0.96623200
C	-6.19090700	-2.35775900	-0.03934000
H	-6.05724900	-2.50637300	-1.11500100
H	-6.69982900	-3.24684000	0.35509400
H	-6.87334700	-1.51002500	0.09482100
C	-3.22637700	-2.50963900	-1.20040300
H	-4.06849500	-2.64788600	-1.87060200
O	-3.06982300	-0.61055200	-1.73404800
H	-2.05479500	-0.40227300	-1.69239800
C	-1.96052700	-3.12268100	-1.60863200
C	-1.18392400	-3.80273900	-0.65117900
C	-1.51596400	-3.08299800	-2.95636100

C	0.02311300	-4.39691400	-0.99021200
H	-1.53431700	-3.86903400	0.36970900
C	-0.29390600	-3.67621100	-3.26981800
C	0.48254200	-4.31361700	-2.30159700
H	0.61036800	-4.89025500	-0.22592000
H	0.06676300	-3.61934900	-4.29330200
H	1.44621400	-4.73409200	-2.57065400
C	-2.25900800	-2.35288300	-4.04575700
H	-1.99329400	-2.75966000	-5.02577400
H	-3.34788900	-2.42110000	-3.94458900
H	-1.98367500	-1.29150100	-4.04725300
H	-3.36135600	-0.37841200	-2.63331800
C	2.61517200	1.67739500	0.57197600
C	2.62094700	0.33035600	0.18474100
C	3.48078700	-0.60974000	0.75888900
C	4.34773700	-0.15965500	1.75529800
H	5.03086100	-0.87292000	2.20995700
C	1.66451600	2.61272500	-0.10195400
C	0.30053400	2.30018600	-0.06523400
C	-0.67904600	3.13750200	-0.61063900
C	-0.24094000	4.31485700	-1.21909000
H	-0.98183300	4.98935100	-1.64150900
O	1.73635700	-0.09068600	-0.79157500
O	-0.08592900	1.11208300	0.52034000
P	0.15687300	-0.27623100	-0.35546000
O	-0.59308200	-0.21665700	-1.66584700
O	-0.04633500	-1.38294600	0.63637100
C	4.33126400	1.16024600	2.21652400
C	5.29616500	1.55749400	3.32000400
C	3.43911400	2.08543700	1.64475600
C	4.85826300	2.80488900	4.09105500
H	6.28308400	1.74921400	2.87171700
H	5.43682100	0.71180600	4.00382800
C	3.26478300	3.46288600	2.26473900
C	4.45888200	3.90887000	3.11091800
H	5.66607800	3.13798300	4.75326900
H	3.99856500	2.56256800	4.73121600
H	3.03763500	4.21264800	1.50502200
H	2.36976700	3.42184100	2.90466400
H	4.20814400	4.83425900	3.64276300
H	5.31128000	4.13905900	2.45553600
C	2.08546700	3.76166500	-0.80629900
C	3.56163700	3.98851400	-1.08861700
C	1.11685600	4.62922600	-1.34332400

C	3.89439600	5.43208800	-1.47150400
H	3.84130400	3.32546700	-1.92171600
H	4.17670500	3.66434400	-0.24680600
C	1.50370700	5.92076800	-2.04293300
C	2.94286900	5.92281900	-2.56400500
H	4.93774900	5.49502400	-1.80223700
H	3.80004100	6.08070800	-0.58863800
H	0.79896900	6.11930500	-2.85946000
H	1.38493300	6.75445200	-1.33393100
H	3.21626700	6.92916100	-2.90247200
H	3.02281100	5.25885100	-3.43594600
C	-2.11768200	2.75390800	-0.57271400
C	-2.79645700	2.65805900	0.66282200
C	-2.79146600	2.44573300	-1.77558600
C	-4.18467000	2.26316900	0.68798100
C	-4.19436400	2.10467000	-1.74097400
C	-4.85382000	2.02730000	-0.51431800
C	3.45754800	-2.04245700	0.34913000
C	3.98754200	-2.42991800	-0.90012500
C	2.92844900	-3.00984700	1.22967000
C	4.03259400	-3.82897800	-1.25261900
C	3.00608500	-4.40866900	0.88137700
C	3.56420700	-4.78153500	-0.34384900
C	-2.15664400	2.92732100	1.91280400
C	-4.84290900	2.11094300	1.94631800
C	-2.82471500	2.77614400	3.09803700
C	-4.18363200	2.35347700	3.11894500
H	-5.87825200	1.78154300	1.95004600
H	-4.68990700	2.21512500	4.06876600
H	-2.31313900	2.97497600	4.03563200
H	-1.12128400	3.24646000	1.90949800
H	-5.90241900	1.73845400	-0.49078200
C	-2.11457900	2.36697500	-3.03377800
C	-2.77650300	2.00227200	-4.17743700
C	-4.85673300	1.76446200	-2.96087100
C	-4.17114500	1.70622500	-4.14636100
H	-5.91666000	1.52452200	-2.92024400
H	-4.68395800	1.43267500	-5.06459600
H	-2.23450800	1.92923000	-5.11595200
H	-1.04917600	2.55731700	-3.06028200
C	4.56041100	-4.20661300	-2.52579400
C	4.49330600	-1.48346400	-1.84434500
C	2.47874500	-5.37912800	1.78890700
C	2.28006800	-2.65617900	2.45433000

C	5.01739400	-3.26473000	-3.40748100
C	4.98471200	-1.88480700	-3.05792300
C	1.87803800	-4.99647200	2.95783100
C	1.77037400	-3.61514900	3.28765600
H	4.58997700	-5.26427200	-2.77734000
H	5.41224900	-3.56482200	-4.37417500
H	5.35400100	-1.14607300	-3.76360100
H	4.47247000	-0.43109900	-1.58619300
H	2.55621900	-6.43027300	1.52106500
H	1.47308100	-5.74350300	3.63501600
H	1.26619100	-3.32304500	4.20444900
H	2.16926400	-1.60665100	2.69586500
H	3.61863600	-5.83676500	-0.60433700

Int4'

C	-3.98633400	-2.88116000	1.63879200
C	-2.68215200	-2.44473200	2.06199700
C	-2.50409100	-1.63647800	3.19980100
C	-3.63225000	-1.32924000	3.92880500
C	-4.93113800	-1.79484000	3.55893000
C	-5.12055900	-2.54883400	2.42721800
C	-3.81713000	-3.54344600	0.41618000
C	-2.40795500	-3.53183800	0.13375300
H	-1.51975200	-1.26198400	3.45678600
H	-3.53995600	-0.69753600	4.80602300
H	-5.77841000	-1.52266800	4.18020800
H	-6.11131600	-2.88292800	2.13408800
N	-1.75204700	-2.89035900	1.18681400
H	-0.82215700	-2.40496900	1.11568700
C	-4.87993600	-4.05349500	-0.49463800
H	-4.91052800	-3.40495800	-1.37947300
H	-4.68521300	-5.07831300	-0.82855100
H	-5.85969000	-4.03534000	-0.01005600
C	-1.84545700	-3.94688700	-1.05489700
H	-2.57216800	-4.26023700	-1.79387200
O	-3.17968900	-1.76688400	-2.17603300
H	-2.36941500	-1.39185100	-1.75736100
C	-0.48072200	-3.90127200	-1.47730100
C	0.58620600	-3.89779000	-0.54944700
C	-0.19853300	-3.80540400	-2.87440800
C	1.89562000	-3.76626800	-0.97302400
H	0.37928300	-4.01752600	0.50586700
C	1.12829400	-3.65069500	-3.26724500
C	2.16714800	-3.62162200	-2.33583400

H	2.69897100	-3.76075800	-0.24976800
H	1.35275300	-3.53614900	-4.32405100
H	3.19029000	-3.48723200	-2.67121600
C	-1.29651700	-3.78227200	-3.90369900
H	-0.87865800	-3.65573500	-4.90613700
H	-1.87520100	-4.71614900	-3.90226800
H	-1.99652200	-2.96485400	-3.69374400
H	-3.47067400	-1.05996200	-2.77133100
C	1.94904900	2.30528600	0.25098100
C	2.31905100	0.96656600	0.04963000
C	3.47648600	0.43365200	0.62658000
C	4.24007100	1.27762600	1.43674200
H	5.14499200	0.87765400	1.88746000
C	0.71530500	2.81905200	-0.41068300
C	-0.49368100	2.16905500	-0.13518500
C	-1.71911100	2.65249600	-0.60936400
C	-1.68836300	3.80339500	-1.40080700
H	-2.62996500	4.20774900	-1.76410500
O	1.51409600	0.16410800	-0.73640200
O	-0.46260600	1.02937700	0.63933300
P	0.08161500	-0.37367300	-0.08176100
O	-0.79682900	-0.76284800	-1.22742300
O	0.35744100	-1.30269800	1.07562200
C	3.86179800	2.59058400	1.72203600
C	4.73973000	3.42042200	2.64155800
C	2.69065900	3.11002100	1.14426600
C	3.99415500	4.58459800	3.29674300
H	5.58101800	3.82501200	2.05815300
H	5.18696100	2.77049800	3.40318900
C	2.15761800	4.46549300	1.58346700
C	3.21413100	5.36090500	2.23529500
H	4.70271400	5.23675100	3.82089800
H	3.29369700	4.19953500	4.05088300
H	1.67912100	4.99059400	0.75523000
H	1.35047700	4.27904000	2.30880400
H	2.72924000	6.24285400	2.67033800
H	3.91175800	5.72773200	1.46858400
C	0.72816400	3.91635000	-1.29786000
C	2.04603100	4.46949600	-1.81431100
C	-0.49290700	4.42403200	-1.77460700
C	1.92790500	5.87837000	-2.39960000
H	2.40343800	3.78614500	-2.59996400
H	2.81404900	4.44001700	-1.03873100
C	-0.55429000	5.65557500	-2.66122600

C	0.76149100	5.94689900	-3.38705300
H	2.87045400	6.15645500	-2.88567500
H	1.76124200	6.60345800	-1.58981700
H	-1.37499500	5.54887900	-3.38106100
H	-0.81252600	6.52519400	-2.03766900
H	0.71169700	6.92918200	-3.87151500
H	0.91860800	5.20474300	-4.18206500
C	-3.00616500	1.97624100	-0.29439700
C	-3.47869900	1.93222400	1.03752000
C	-3.78993600	1.44103400	-1.34174400
C	-4.76403200	1.34009700	1.32040800
C	-5.07360400	0.84938100	-1.04569000
C	-5.52040800	0.80291100	0.27604900
C	3.94126500	-0.96919300	0.43292600
C	4.55118000	-1.35509700	-0.77987300
C	3.89296800	-1.86692500	1.52116400
C	5.20677000	-2.63866300	-0.87142500
C	4.56315700	-3.14258800	1.42627000
C	5.22036400	-3.48551100	0.24079900
C	-2.74970100	2.49698800	2.13053300
C	-5.25786900	1.35705800	2.66001600
C	-3.25539900	2.48885400	3.40330900
C	-4.53052200	1.91808600	3.67423000
H	-6.23254200	0.91703600	2.85191500
H	-4.92272100	1.93235900	4.68767200
H	-2.68324300	2.93016400	4.21454500
H	-1.78452200	2.94760600	1.93580100
H	-6.49064100	0.36261300	0.49476300
C	-3.36164100	1.45530300	-2.70762200
C	-4.16756300	0.98107100	-3.71185200
C	-5.87446100	0.35069800	-2.11868000
C	-5.44874100	0.42876900	-3.41693900
H	-6.84016500	-0.08654500	-1.87762000
H	-6.07240600	0.05514400	-4.22399400
H	-3.82080200	1.00993500	-4.74104200
H	-2.37526900	1.83768300	-2.93837600
C	5.82477600	-3.01414500	-2.10437800
C	4.55449000	-0.51434000	-1.93578500
C	4.52193900	-4.03076500	2.54510000
C	3.17651500	-1.56715300	2.72214100
C	5.78986900	-2.18393600	-3.19289600
C	5.14277800	-0.91818600	-3.10493900
C	3.84005900	-3.69593600	3.68339500
C	3.14946900	-2.45284100	3.76580800

H	6.31734300	-3.98191800	-2.15905600
H	6.25739900	-2.48478000	-4.12635800
H	5.11875200	-0.26883500	-3.97538500
H	4.06441800	0.45025900	-1.87715700
H	5.03817800	-4.98431600	2.46549200
H	3.81113900	-4.38270600	4.52492200
H	2.58417000	-2.21479300	4.66234300
H	2.61892500	-0.64075100	2.77196500
H	5.73131900	-4.44355100	0.17352700

Int4

C	-4.58407800	-2.32497800	1.15312100
C	-3.27065700	-2.07040400	1.68940100
C	-3.08717100	-1.45239900	2.94102000
C	-4.22185700	-1.15555100	3.66327300
C	-5.53355700	-1.45221800	3.17880800
C	-5.72546200	-2.01825800	1.94240400
C	-4.40644800	-2.82003700	-0.14441600
C	-2.98702500	-2.88986900	-0.36345200
H	-2.08954600	-1.21295000	3.29190200
H	-4.12374300	-0.66822500	4.62800200
H	-6.38776200	-1.20306800	3.80070700
H	-6.72444500	-2.22369800	1.56926200
N	-2.33970800	-2.47729500	0.80157300
H	-1.33189600	-2.15621900	0.85570600
C	-5.46560900	-3.25314000	-1.10208000
H	-5.23562300	-2.93543000	-2.12355400
H	-5.57876800	-4.34504700	-1.10596300
H	-6.43210100	-2.81965700	-0.83155200
C	-2.36042600	-3.20180800	-1.55219000
H	-3.02512100	-3.25264900	-2.40970000
C	-0.96665500	-3.38964800	-1.79860600
C	-0.10120300	-3.86728500	-0.78727000
C	-0.43410100	-3.04470700	-3.07673800
C	1.25686300	-3.99738200	-1.01873000
H	-0.51289200	-4.14574900	0.17498100
C	0.93470700	-3.17664200	-3.27688500
C	1.77770800	-3.64062200	-2.26482000
H	1.91357000	-4.34373400	-0.23007500
H	1.35973200	-2.87783000	-4.23086700
H	2.84388700	-3.71615600	-2.44739600
C	-1.29408900	-2.40502600	-4.12973600
H	-0.72926900	-2.25810200	-5.05436700
H	-2.18349100	-3.00054300	-4.37360900

H	-1.63295100	-1.42880200	-3.76662800
C	2.19644500	2.08472700	0.25046800
C	2.42833500	0.70592700	0.11505900
C	3.49656200	0.07445100	0.75910800
C	4.33444100	0.86169900	1.55052100
H	5.17242400	0.38393000	2.05241100
C	1.01585600	2.68436800	-0.43991400
C	-0.24141000	2.14707700	-0.14366000
C	-1.42552400	2.67225000	-0.67026600
C	-1.31160300	3.76124600	-1.53449300
H	-2.21775700	4.19522900	-1.95072800
O	1.59047400	-0.04848400	-0.67519300
O	-0.30127100	1.02838200	0.65819800
P	0.04864300	-0.39535200	-0.14533600
O	-0.80286600	-0.55488600	-1.35785800
O	0.08428400	-1.43128500	0.95617900
C	4.10390100	2.22443500	1.75446100
C	5.05369500	2.99967600	2.65061600
C	3.00775900	2.84122800	1.12434400
C	4.43585200	4.27565100	3.22651200
H	5.94639100	3.27363200	2.06747800
H	5.41042100	2.34660400	3.45625200
C	2.61879400	4.26513700	1.49209100
C	3.76187600	5.07360500	2.10967500
H	5.20674400	4.87222000	3.72858400
H	3.68625100	4.01446300	3.98633100
H	2.20200700	4.79610400	0.63477500
H	1.79407300	4.20153300	2.21895400
H	3.37570600	6.02824300	2.48622300
H	4.50549000	5.31342600	1.33603000
C	1.11101900	3.72633300	-1.38640000
C	2.46948300	4.15267900	-1.91758100
C	-0.06858300	4.28025500	-1.91614400
C	2.45605200	5.52619200	-2.59136400
H	2.78586200	3.39793100	-2.65388200
H	3.22576300	4.11836000	-1.13039600
C	-0.03330100	5.45423100	-2.87939000
C	1.30846000	5.60954900	-3.59953800
H	3.42088400	5.70840000	-3.07929400
H	2.33000400	6.31088300	-1.83137500
H	-0.84962800	5.35710300	-3.60557800
H	-0.23988100	6.37800400	-2.31726600
H	1.33171100	6.55991800	-4.14591600
H	1.42445900	4.80907300	-4.34342600

C	-2.74223000	2.06815900	-0.32161700
C	-3.26019300	2.22111400	0.98406200
C	-3.47226800	1.34864600	-1.29334300
C	-4.55855800	1.68055700	1.30693400
C	-4.77031200	0.81284300	-0.95895700
C	-5.28273900	0.99933700	0.32624400
C	3.74037900	-1.39300200	0.65190300
C	4.37323000	-1.92508200	-0.49079500
C	3.40453700	-2.23256300	1.73451600
C	4.75115500	-3.31826800	-0.51467700
C	3.78334300	-3.62570900	1.70231800
C	4.46392500	-4.12683900	0.58873600
C	-2.54776300	2.90968100	2.01519500
C	-5.07990000	1.86420300	2.62339400
C	-3.07377900	3.04878400	3.27239400
C	-4.35963000	2.52337400	3.58293900
H	-6.06464100	1.46279700	2.84513800
H	-4.76740800	2.65467000	4.58169200
H	-2.50971300	3.57117900	4.03994900
H	-1.57280700	3.32275300	1.78514700
H	-6.26256300	0.59881500	0.57300900
C	-2.96329100	1.10499300	-2.60698500
C	-3.69896900	0.41542300	-3.53500600
C	-5.50364400	0.09826700	-1.95511700
C	-4.98949800	-0.09138300	-3.20971700
H	-6.48700600	-0.28440300	-1.69276200
H	-5.56254300	-0.62745700	-3.96214000
H	-3.29384700	0.24616300	-4.52859000
H	-1.96611600	1.45016100	-2.84461200
C	5.40305800	-3.83842200	-1.67556200
C	4.65825800	-1.13004200	-1.64388200
C	3.44517200	-4.46082000	2.81151800
C	2.67708800	-1.75648100	2.86984200
C	5.64928100	-3.04274200	-2.76288500
C	5.26579900	-1.67089700	-2.74612400
C	2.75922300	-3.96017200	3.88463800
C	2.36504100	-2.59184700	3.90824900
H	5.68990600	-4.88729300	-1.67842700
H	6.13867300	-3.45306000	-3.64191900
H	5.46078200	-1.05096000	-3.61658800
H	4.36895600	-0.08548800	-1.63565000
H	3.74240900	-5.50627300	2.77914200
H	2.50456300	-4.60650800	4.72023400
H	1.79862400	-2.21393800	4.75461500

H	2.34949900	-0.72459900	2.87856300
H	4.76147000	-5.17335900	0.57305600

Int5

C	-4.16246200	-0.47166700	0.35882300
C	-3.46431900	0.72971600	0.18427800
C	-3.81363000	1.90948400	0.85040100
C	-4.91497300	1.85664100	1.70483800
H	-5.21601000	2.76268500	2.22538000
C	-3.70879700	-1.66267000	-0.42228300
C	-2.37211400	-2.06798100	-0.29802600
C	-1.84649500	-3.15092800	-1.00971500
C	-2.72062200	-3.84580500	-1.84673700
H	-2.33891000	-4.70011700	-2.40042900
O	-2.36659300	0.73970000	-0.65492800
O	-1.53806600	-1.34687300	0.53915700
P	-0.96771900	0.09193500	-0.04670200
O	-0.08312800	-0.10147100	-1.23918900
O	-0.49950900	0.85694000	1.16189800
C	-5.60628800	0.66490300	1.95197300
C	-6.78335800	0.69213600	2.91176600
C	-5.21139900	-0.51962200	1.30246500
C	-7.12112600	-0.67967500	3.50085400
H	-7.66604900	1.07132500	2.37434800
H	-6.58669400	1.41610200	3.71192200
C	-5.81452100	-1.85452500	1.70833200
C	-7.17993900	-1.72595500	2.38640100
H	-8.07136100	-0.62875900	4.04538900
H	-6.35035200	-0.97137600	4.22770400
H	-5.87315400	-2.53479700	0.85653800
H	-5.11235500	-2.33126500	2.40959500
H	-7.48980600	-2.70115700	2.78004800
H	-7.93540600	-1.42654500	1.64572400
C	-4.54453600	-2.32748800	-1.34580700
C	-5.90967600	-1.75729100	-1.69645700
C	-4.04887300	-3.45009000	-2.03369100
C	-6.84385700	-2.77404000	-2.35614700
H	-5.74606000	-0.92022800	-2.39271600
H	-6.38815300	-1.31145200	-0.82259900
C	-4.92363600	-4.26044800	-2.97423200
C	-6.12886700	-3.48222600	-3.50793600
H	-7.75001800	-2.26753200	-2.70891700
H	-7.16362400	-3.51906100	-1.61342400
H	-4.31451100	-4.64188000	-3.80252000

H	-5.28874800	-5.14833700	-2.43561900
H	-6.80865700	-4.16133700	-4.03593500
H	-5.79323600	-2.73294700	-4.23825900
C	-0.40407500	-3.52154500	-0.91520200
C	0.08400100	-4.17029200	0.23987100
C	0.46569000	-3.22462800	-1.98766200
C	1.46884200	-4.57251000	0.30099900
C	1.85385700	-3.61435100	-1.90795500
C	2.31216600	-4.29344100	-0.77746000
C	-2.97623100	3.13099100	0.68100100
C	-2.97225000	3.81927200	-0.55265600
C	-2.13205300	3.55131500	1.73211300
C	-2.10633100	4.95932500	-0.73317200
C	-1.26531400	4.69007300	1.53819400
C	-1.27806900	5.36504400	0.31585600
C	-0.74555800	-4.45006600	1.36978600
C	1.94895700	-5.22645500	1.47681900
C	-0.24329500	-5.06545300	2.48603300
C	1.12335600	-5.46020000	2.54385000
H	2.99115200	-5.53701700	1.50302000
H	1.50382700	-5.95326400	3.43422900
H	-0.89185400	-5.25850700	3.33603700
H	-1.78841000	-4.15642700	1.33201000
H	3.35967800	-4.58142300	-0.72257200
C	0.03922800	-2.50475700	-3.14812900
C	0.91813600	-2.19505300	-4.15019800
C	2.73874400	-3.26565500	-2.97436400
C	2.28815800	-2.57359200	-4.06414500
H	3.78602400	-3.54123600	-2.88409600
H	2.97434300	-2.28440900	-4.85417700
H	0.58006900	-1.62337300	-5.00905500
H	-0.98994300	-2.17356900	-3.20335600
C	-2.09008800	5.62616900	-1.99679900
C	-3.79014100	3.41809700	-1.65456800
C	-0.39271500	5.08970300	2.59754500
C	-2.06569500	2.86723800	2.98713100
C	-2.87970300	5.19860800	-3.03034100
C	-3.74334100	4.08020900	-2.85234500
C	-0.37485800	4.41648800	3.78796400
C	-1.22786200	3.29223300	3.98282700
H	-1.42866700	6.48043900	-2.11827900
H	-2.85610700	5.71234300	-3.98743800
H	-4.36885100	3.75161500	-3.67736600
H	-4.44895600	2.56684500	-1.52755400

H	0.25849800	5.94417500	2.43103300
H	0.29250000	4.72893900	4.58627000
H	-1.19327100	2.75745700	4.92742000
H	-2.68130100	1.98801500	3.12962400
H	-0.61290000	6.21299600	0.16951800
C	3.15274500	3.14678800	-0.85980200
C	1.79459100	2.80422000	-0.53296700
C	0.72538000	3.13685800	-1.38050300
C	1.03770900	3.82650900	-2.53405200
C	2.37703700	4.18086800	-2.87975200
C	3.43033700	3.84332900	-2.06685100
C	3.95979100	2.66287500	0.17380200
C	3.07698800	2.03580800	1.13628800
H	-0.29185000	2.86240800	-1.13701700
H	0.23067900	4.10758900	-3.20362300
H	2.55700800	4.69838300	-3.81578000
H	4.45192700	4.08778300	-2.33812900
N	1.77317500	2.16587000	0.66316200
H	0.93094700	1.62434400	0.96181600
C	5.43333000	2.86809500	0.29100400
H	5.92750300	2.58129800	-0.64320600
H	5.66370300	3.92578400	0.47370200
H	5.87818900	2.29003900	1.10355200
C	3.48995500	1.40532700	2.28960200
H	4.56734400	1.34526400	2.38625800
C	2.74097200	0.77848900	3.34574400
C	1.34644200	0.95710100	3.48693900
C	3.42664900	-0.07593100	4.26432900
C	0.62654800	0.25161200	4.43805600
H	0.81141500	1.65081800	2.86006600
C	2.67672200	-0.76804900	5.21261400
C	1.28923900	-0.62711500	5.29442300
H	-0.44800400	0.38484200	4.49226700
H	3.18902600	-1.43618600	5.89933200
H	0.73320100	-1.19537500	6.03478100
C	4.92127100	-0.27197000	4.22425500
H	5.45968100	0.67990600	4.31259700
H	5.24241800	-0.90759900	5.05353500
H	5.24735300	-0.74808700	3.29707500
C	2.82627700	0.54305100	-2.96641500
C	4.24374200	0.55368100	-3.13562000
C	4.78068100	1.13123100	-4.30494400
C	3.91310800	1.64873500	-5.25551400
C	2.51079400	1.59761400	-5.07387900

C	1.94890300	1.04199700	-3.93207500
C	3.72058400	-0.44299500	-1.15368100
C	4.78817000	-0.08664300	-1.98430100
H	5.85600000	1.15914000	-4.46286900
H	4.31337300	2.09191600	-6.16335600
H	1.86151400	1.99932500	-5.84716900
H	0.87779500	0.99374500	-3.77285600
H	5.82906900	-0.30849000	-1.80665000
N	2.55131500	-0.04581700	-1.76286700
H	1.58574700	-0.17664400	-1.42877900
C	3.70161500	-1.14287100	0.13038600
C	4.98720400	-1.55261400	0.75724600
C	5.07578900	-2.79605600	1.40594600
C	6.11934800	-0.72207600	0.77254300
C	6.24483700	-3.18681300	2.05563200
H	4.21530700	-3.45580900	1.39463400
C	7.29167000	-1.11374700	1.41815500
H	6.07356000	0.24324100	0.28708800
C	7.36067600	-2.34794100	2.06540400
H	6.28609500	-4.15377000	2.54973300
H	8.15072400	-0.44798800	1.42078200
H	8.27354500	-2.65384100	2.56831500
C	2.54183500	-1.43530100	0.75497700
H	1.57406400	-1.21447500	0.32521700
H	2.53266500	-1.92007600	1.72366300

TS4

C	-4.10986800	-0.82572000	0.51526300
C	-3.53802200	0.41364000	0.19997100
C	-4.04741400	1.62117800	0.68772100
C	-5.16231500	1.55341600	1.52291700
H	-5.58281500	2.47993600	1.90640600
C	-3.51427600	-2.04942600	-0.10090500
C	-2.14834400	-2.29135400	0.09675100
C	-1.49025800	-3.38582900	-0.47216800
C	-2.26129300	-4.26675400	-1.23316800
H	-1.77462700	-5.13219400	-1.67602700
O	-2.41577000	0.44358600	-0.60820000
O	-1.42216700	-1.38857500	0.85155400
P	-0.97783100	0.01623900	0.09620900
O	-0.04835900	-0.24774600	-1.05264100
O	-0.59207600	0.95749600	1.20228300
C	-5.72190600	0.33326400	1.91875400
C	-6.92275300	0.35014500	2.84851900

C	-5.17853200	-0.87139100	1.43660400
C	-7.12673500	-0.96558400	3.60354400
H	-7.82499600	0.55796400	2.25307200
H	-6.82927300	1.18639900	3.55195500
C	-5.64678000	-2.20404800	1.99833500
C	-7.03815100	-2.14373700	2.63191700
H	-8.09280100	-0.95326600	4.12183700
H	-6.35091500	-1.07548200	4.37395800
H	-5.60617900	-2.98696600	1.23844000
H	-4.91938300	-2.51009300	2.76588900
H	-7.25269900	-3.09017200	3.14209000
H	-7.79868600	-2.02528500	1.84666300
C	-4.24723200	-2.90330400	-0.95296800
C	-5.64937500	-2.52034000	-1.39958200
C	-3.61694900	-4.04097000	-1.49049200
C	-6.44869100	-3.68765400	-1.98327100
H	-5.54395800	-1.73965900	-2.16878700
H	-6.20701500	-2.04731000	-0.58926200
C	-4.37317000	-5.03893500	-2.34944400
C	-5.61318100	-4.44207400	-3.01862000
H	-7.37786400	-3.31117600	-2.42705200
H	-6.73774800	-4.37785700	-1.17758000
H	-3.69559900	-5.46216000	-3.10066100
H	-4.68731200	-5.88323700	-1.71668800
H	-6.19990900	-5.23548200	-3.49641400
H	-5.30694600	-3.74645500	-3.81218500
C	-0.01788500	-3.57214400	-0.33126800
C	0.54034200	-3.94699800	0.91074500
C	0.81382100	-3.38684000	-1.45841600
C	1.96025700	-4.18848800	1.01208300
C	2.23263100	-3.62920600	-1.34534100
C	2.76647800	-4.03177500	-0.11950500
C	-3.38426200	2.91024300	0.34189600
C	-3.50630200	3.43328900	-0.96425300
C	-2.61090200	3.58439600	1.31076500
C	-2.84388200	4.66991600	-1.30251200
C	-1.94372300	4.81595100	0.95817400
C	-2.08160300	5.32747500	-0.33392200
C	-0.25401100	-4.11316700	2.08720500
C	2.50444200	-4.59172300	2.27048200
C	0.30973500	-4.47790000	3.28122900
C	1.70822400	-4.72407000	3.37669500
H	3.56906000	-4.80723900	2.32580400
H	2.13708700	-5.02781700	4.32761100

H	-0.31395500	-4.58720600	4.16373600
H	-1.32128800	-3.93775500	2.02086900
H	3.83499800	-4.21980800	-0.04366000
C	0.31159500	-2.92698100	-2.71682500
C	1.14393000	-2.74959900	-3.78882500
C	3.06519800	-3.43444400	-2.49025700
C	2.53902400	-3.01089300	-3.67909100
H	4.13224000	-3.61163700	-2.38577000
H	3.18421300	-2.84057400	-4.53569700
H	0.74651700	-2.37386600	-4.72643000
H	-0.74068300	-2.68713600	-2.79884500
C	-2.95999900	5.17740400	-2.63307500
C	-4.26268000	2.77621200	-1.98431700
C	-1.14456700	5.47966900	1.93978200
C	-2.43814300	3.08466700	2.63984500
C	-3.68601900	4.50963600	-3.58259800
C	-4.34741500	3.29312500	-3.24965100
C	-1.01901900	4.97420300	3.20433700
C	-1.68284700	3.76438300	3.55663700
H	-2.45072300	6.10713700	-2.87415600
H	-3.76415900	4.90518800	-4.59153100
H	-4.92326700	2.77276900	-4.00978400
H	-4.76811800	1.84916900	-1.73879400
H	-0.63726300	6.39746400	1.65361200
H	-0.40827400	5.48588400	3.94269600
H	-1.57837000	3.37533600	4.56503200
H	-2.90577600	2.14530600	2.90658400
H	-1.56772600	6.24859100	-0.59854600
C	2.70501600	3.21364800	-1.51178500
C	1.39571100	2.93098800	-1.01615400
C	0.24143800	3.19826200	-1.76165100
C	0.41528900	3.78516700	-3.00499900
C	1.70368400	4.09567500	-3.50989500
C	2.84500200	3.81656500	-2.78051600
C	3.62724900	2.73755500	-0.53965500
C	2.86094000	2.19746800	0.51649100
H	-0.74006900	2.94240400	-1.38339700
H	-0.46220000	4.00662600	-3.60527300
H	1.79013300	4.54780100	-4.49363200
H	3.83018400	4.03664900	-3.18166400
N	1.51769400	2.36011000	0.21956900
H	0.72649000	1.87881100	0.67963400
C	5.11384400	2.88086800	-0.62657200
H	5.48513700	2.49158400	-1.58113900

H	5.41390000	3.93557900	-0.56625000
H	5.63255700	2.35097600	0.17665300
C	3.37649200	1.46903600	1.63930700
H	4.45687800	1.42320600	1.58606600
C	2.89599800	1.51085300	3.03830500
C	1.54666800	1.71636100	3.37278400
C	3.84438200	1.30585100	4.07766000
C	1.13678200	1.73144600	4.70209900
H	0.79150800	1.82635400	2.60896400
C	3.40645900	1.33964100	5.40292600
C	2.06545500	1.54857000	5.72358000
H	0.08600200	1.87607400	4.92692700
H	4.13310800	1.19380900	6.19814300
H	1.75156100	1.55887600	6.76373800
C	5.30828400	1.04768200	3.80110800
H	5.78026500	1.87714400	3.25961500
H	5.85398500	0.92003400	4.74011400
H	5.46487100	0.14243200	3.20461600
C	2.62134200	0.21100700	-2.92454600
C	3.99686900	0.08708000	-3.32493000
C	4.34818200	0.38261500	-4.66729100
C	3.35124000	0.76615700	-5.53659600
C	1.99158500	0.86501700	-5.11457800
C	1.60591100	0.58508800	-3.82133800
C	3.77708800	-0.45733800	-1.12328200
C	4.70064500	-0.36145900	-2.19498200
H	5.38022800	0.30303200	-4.99703700
H	3.59662100	1.00014700	-6.56846800
H	1.24222500	1.17336300	-5.83777800
H	0.58073300	0.65644200	-3.47985400
H	5.75146500	-0.60001000	-2.14088000
N	2.52529600	-0.11797200	-1.61754000
H	1.59662100	-0.19951100	-1.16151500
C	3.97756900	-0.77976400	0.23871800
C	5.30474500	-1.20320400	0.74145700
C	5.37704300	-2.24806600	1.67931700
C	6.49192000	-0.53957600	0.38762700
C	6.59802400	-2.63274000	2.22613800
H	4.46694500	-2.76018400	1.96924600
C	7.71184500	-0.91967400	0.94434000
H	6.45171600	0.30247900	-0.29188300
C	7.77147700	-1.96983100	1.86096600
H	6.63234600	-3.44909700	2.94192600
H	8.61583500	-0.38361100	0.66990800

H	8.72306400	-2.26366000	2.29408200
C	2.97521300	-0.52058900	1.19409300
H	1.93983800	-0.40407700	0.89367300
H	3.10638200	-0.92896200	2.18870300

Int6

C	4.12885200	-0.69805100	-0.48223200
C	3.48378000	0.48592600	-0.09743800
C	3.96351600	1.75139900	-0.45108200
C	5.12198700	1.80191200	-1.22490800
H	5.51842800	2.77490200	-1.50489800
C	3.55863200	-1.99589900	-0.00682500
C	2.21693800	-2.26990200	-0.30095100
C	1.56530100	-3.42349500	0.14664500
C	2.32663100	-4.34027100	0.87464600
H	1.85048600	-5.25351300	1.22293100
O	2.32013600	0.40141300	0.64641300
O	1.49900500	-1.33535900	-1.01830900
P	0.93940600	-0.03143900	-0.16109700
O	-0.00702500	-0.47200300	0.92369900
O	0.52857500	0.96653200	-1.19828800
C	5.75672600	0.64442700	-1.69085900
C	7.00125900	0.79175800	-2.54924500
C	5.24551800	-0.61887500	-1.34264600
C	7.30742000	-0.44537900	-3.39681400
H	7.86081300	0.98878000	-1.89024700
H	6.90304400	1.67907700	-3.18619400
C	5.80260500	-1.87694100	-1.98913400
C	7.22244800	-1.70476100	-2.53264100
H	8.29800500	-0.34796600	-3.85652600
H	6.57972300	-0.52275700	-4.21647600
H	5.75505300	-2.72556000	-1.30379300
H	5.13337200	-2.14225600	-2.82210700
H	7.50902300	-2.59432600	-3.10599700
H	7.93223400	-1.62147600	-1.69700000
C	4.27671200	-2.89560900	0.81015900
C	5.63981200	-2.50972400	1.36121800
C	3.66038100	-4.09474100	1.21596900
C	6.45208700	-3.69987100	1.87662000
H	5.46823100	-1.80799300	2.19202400
H	6.21674100	-1.94523000	0.62655000
C	4.40827900	-5.13973800	2.02541400
C	5.59762500	-4.56816900	2.80111500
H	7.34719800	-3.33715500	2.39535000

H	6.79997100	-4.30649900	1.02805100
H	3.71074500	-5.64304500	2.70580700
H	4.77637300	-5.91931900	1.34080500
H	6.18892400	-5.38363200	3.23397500
H	5.23422300	-3.95556100	3.63781500
C	0.10484000	-3.61780900	-0.07525000
C	-0.40824000	-3.80056800	-1.37964100
C	-0.77176800	-3.60752900	1.03528300
C	-1.82204700	-4.02505000	-1.56786000
C	-2.17902800	-3.86119000	0.83761200
C	-2.66788100	-4.06384000	-0.45457000
C	3.22636500	2.97799100	-0.02762800
C	3.36273200	3.45151700	1.29486000
C	2.35826900	3.62402600	-0.93279700
C	2.62121800	4.61655800	1.71463900
C	1.59642300	4.76966700	-0.49257600
C	1.76058400	5.24410500	0.81064200
C	0.42610600	-3.77860900	-2.54000900
C	-2.32208800	-4.21514500	-2.89279300
C	-0.09590000	-3.93824600	-3.79645000
C	-1.48935500	-4.16064900	-3.97859700
H	-3.38168100	-4.42410000	-3.01861800
H	-1.88527300	-4.30155800	-4.98039500
H	0.55811600	-3.90370700	-4.66275000
H	1.49023400	-3.62345300	-2.41106200
H	-3.72874400	-4.25600900	-0.59716500
C	-0.32906200	-3.30265800	2.36051200
C	-1.20155500	-3.29874900	3.41739800
C	-3.05077700	-3.86941700	1.96892300
C	-2.57731600	-3.60355400	3.22482600
H	-4.10474700	-4.07678300	1.80360800
H	-3.25301900	-3.59064200	4.07490500
H	-0.84701600	-3.03882800	4.41000400
H	0.70906900	-3.03707400	2.51167900
C	2.75428700	5.07365200	3.06164100
C	4.20479300	2.80885600	2.25527000
C	0.66104700	5.36818500	-1.39227700
C	2.16510200	3.16324900	-2.27185300
C	3.56707800	4.42388900	3.95171000
C	4.30262900	3.27627800	3.53911400
C	0.49572200	4.88126800	-2.66000100
C	1.27122200	3.77460000	-3.10673800
H	2.18572300	5.94943600	3.36455200
H	3.65594500	4.78023800	4.97431400

H	4.94533200	2.76853300	4.25307500
H	4.76520500	1.93265000	1.94824000
H	0.07296000	6.21010900	-1.03590400
H	-0.23659300	5.32296900	-3.32961000
H	1.11821900	3.39197000	-4.10936800
H	2.71346800	2.29103100	-2.60452600
H	1.17554200	6.09875400	1.14190900
C	-2.90501500	2.92598900	1.64533600
C	-1.57211100	2.71018300	1.18190100
C	-0.44965300	3.00593100	1.96256500
C	-0.67412300	3.54540400	3.22227200
C	-1.98467100	3.78112300	3.69849400
C	-3.09748200	3.47807100	2.92531600
C	-3.78686800	2.44082000	0.61915800
C	-2.97575800	1.95045100	-0.39704200
H	0.55069200	2.80299900	1.60016600
H	0.17893800	3.78554300	3.85063300
H	-2.11981100	4.20187000	4.69141900
H	-4.10052300	3.65071300	3.30745200
N	-1.65142300	2.14965900	-0.06464800
H	-0.83922000	1.83189700	-0.61576700
C	-5.28285700	2.47258100	0.67595400
H	-5.66620000	1.92569800	1.54817100
H	-5.65983900	3.50081500	0.75717600
H	-5.73482600	2.03328000	-0.21844600
C	-3.31860700	1.14577800	-1.61230400
H	-4.40066700	1.21590400	-1.75994300
C	-2.64896900	1.66054600	-2.88487300
C	-1.53841200	1.02446800	-3.44376000
C	-3.16846100	2.82074200	-3.50040500
C	-0.95243600	1.50292000	-4.61548100
H	-1.08849800	0.17285900	-2.95025200
C	-2.56619700	3.28724700	-4.67239200
C	-1.47150800	2.63378100	-5.23842600
H	-0.08434200	0.99404300	-5.02382300
H	-2.96936400	4.17705300	-5.15017500
H	-1.02476200	3.01454600	-6.15308000
C	-4.34680900	3.56293500	-2.91885200
H	-4.15125800	3.87494400	-1.88704400
H	-4.57426100	4.45483000	-3.50994400
H	-5.25296000	2.94233800	-2.89744500
C	-2.63923600	-0.23468200	2.79531800
C	-3.99578300	-0.52480800	3.21299300
C	-4.33960400	-0.37898700	4.58829800

C	-3.36452200	0.03259500	5.45870700
C	-2.02525100	0.30423800	5.01687500
C	-1.63884500	0.16245400	3.70722100
C	-3.77892600	-0.81576000	0.95946400
C	-4.67856100	-0.93720800	2.07714400
H	-5.35053900	-0.58436100	4.92706800
H	-3.59896000	0.16267200	6.51085400
H	-1.29729900	0.63618600	5.75087300
H	-0.63648700	0.36984600	3.35524900
H	-5.70271400	-1.27128700	2.01897300
N	-2.54173800	-0.42776200	1.47415500
H	-1.60489600	-0.39379600	1.00675400
C	-4.01633700	-0.91486200	-0.39740600
C	-5.32421600	-1.31846100	-0.93748400
C	-5.36750600	-2.18555200	-2.04614600
C	-6.54130500	-0.83670900	-0.41893900
C	-6.58349800	-2.59882600	-2.58009600
H	-4.44093000	-2.55760200	-2.46641700
C	-7.75613500	-1.23774400	-0.96882800
H	-6.52795800	-0.10468600	0.37833800
C	-7.78355300	-2.12861200	-2.04254200
H	-6.59423200	-3.28452100	-3.42222300
H	-8.68304100	-0.84028600	-0.56590100
H	-8.73230800	-2.44151500	-2.46823900
C	-3.01069900	-0.39849300	-1.36789200
H	-1.98427100	-0.51785900	-1.02200400
H	-3.10524700	-0.90272400	-2.33086900

TS5

C	3.78894500	0.26138800	-0.19742200
C	3.08716500	1.11537300	0.66223600
C	3.15655100	2.51004200	0.56182400
C	4.00820100	3.03499000	-0.41035600
H	4.08827400	4.11521500	-0.50191300
C	3.58278500	-1.21252300	-0.06931800
C	2.27326100	-1.70375100	-0.16237300
C	1.98226100	-3.07130700	-0.14934600
C	3.05806200	-3.94948000	-0.01438000
H	2.85860900	-5.01824800	-0.01174700
O	2.27031900	0.55647200	1.63178800
O	1.23161500	-0.79900000	-0.24579800
P	0.80587100	-0.02867700	1.17094400
O	0.35377300	-1.01901000	2.19814900
O	-0.12332500	1.07116000	0.71860200

C	4.70404000	2.22068700	-1.31103400
C	5.56966100	2.87954600	-2.36974200
C	4.56739800	0.82207400	-1.23560300
C	5.75869500	2.01132100	-3.61557800
H	6.55882500	3.09522500	-1.93765000
H	5.13936300	3.85154100	-2.63828800
C	5.10033300	-0.06220700	-2.35181600
C	6.18473100	0.60175300	-3.20335800
H	6.49945200	2.46787800	-4.28246600
H	4.81427700	1.95750800	-4.17563000
H	5.45934900	-1.01676400	-1.96399600
H	4.24378500	-0.31765800	-2.99474700
H	6.39091100	-0.01925800	-4.08306500
H	7.12098000	0.66141900	-2.63017800
C	4.63900000	-2.11896800	0.16588200
C	6.01928200	-1.60518600	0.54163500
C	4.37013400	-3.49938900	0.16673000
C	7.12849400	-2.64224700	0.35201800
H	5.98183400	-1.31514200	1.60281000
H	6.25701400	-0.68609700	0.00192700
C	5.47568500	-4.52705100	0.33270800
C	6.73098000	-3.96714200	1.00572100
H	8.06542100	-2.26140000	0.77522500
H	7.30635200	-2.80418700	-0.72105900
H	5.09248600	-5.38916500	0.89171000
H	5.75004000	-4.91105500	-0.66179900
H	7.54600900	-4.69775500	0.94322400
H	6.53450400	-3.79663900	2.07320600
C	0.58180100	-3.57244400	-0.26207000
C	-0.08699100	-3.51220500	-1.50522600
C	-0.05478200	-4.14415600	0.86083900
C	-1.41758800	-4.06140900	-1.62663600
C	-1.39176900	-4.67654900	0.73089800
C	-2.03793200	-4.61661900	-0.50502200
C	2.26669400	3.36388700	1.39737500
C	1.16795900	4.01297200	0.79139800
C	2.47325100	3.45816400	2.78911900
C	0.23977000	4.75388300	1.61199200
C	1.54580000	4.21067000	3.59866000
C	0.45240200	4.83196200	2.99024000
C	0.50313900	-2.92441000	-2.66749900
C	-2.07188000	-4.02156700	-2.89726400
C	-0.15948300	-2.89544600	-3.86623600
C	-1.46158700	-3.45951400	-3.98825500

H	-3.06601700	-4.45531500	-2.97688300
H	-1.96394800	-3.44773100	-4.95166600
H	0.30672900	-2.42847900	-4.72707700
H	1.49032700	-2.48504000	-2.58621600
H	-3.04271100	-5.02259600	-0.59875300
C	0.57076500	-4.21215900	2.14560300
C	-0.05935200	-4.80628900	3.20518400
C	-2.01998100	-5.26981500	1.86860600
C	-1.36860200	-5.34947800	3.06711400
H	-3.03105900	-5.65201900	1.75813700
H	-1.85921500	-5.79329700	3.92764900
H	0.43221100	-4.84164100	4.17324000
H	1.54769100	-3.76330300	2.27096800
C	-0.88372700	5.38449300	0.99411000
C	0.90291500	3.93669800	-0.61118700
C	1.76660300	4.29544300	5.00769100
C	3.57988900	2.83192700	3.44195600
C	-1.08650200	5.29889200	-0.35596400
C	-0.18288500	4.55717700	-1.16704900
C	2.83828500	3.67747100	5.59254800
C	3.75741700	2.93730000	4.79547200
H	-1.58220200	5.92761300	1.62527600
H	-1.94529900	5.78352900	-0.80931400
H	-0.36350600	4.46742000	-2.23438200
H	1.57160500	3.36415800	-1.23928800
H	1.05884200	4.86448200	5.60563000
H	2.99376500	3.74825400	6.66548100
H	4.60536300	2.45144900	5.27000300
H	4.28433300	2.26670700	2.84205400
H	-0.25245100	5.38780700	3.60501300
H	-1.64557400	1.09338200	0.26475500
N	-2.59896700	1.28815300	-0.17109000
N	-2.31914500	-1.33186400	1.70649300
H	-1.32055200	-1.10447800	1.62898500
C	-3.27629000	-0.49598500	-0.46917600
C	-2.11629100	-0.72699600	-1.43614300
H	-1.17388600	-0.81129900	-0.89528600
H	-2.25139300	-1.66652700	-1.97087000
C	-2.07776500	0.48568600	-2.41963900
H	-2.86765900	0.33812600	-3.15698800
C	-2.52239800	1.64069600	-1.56464100
C	-3.29861500	2.33890500	0.47453200
C	-3.54797400	2.49967400	1.82746200
H	-3.19773500	1.77361000	2.55369600

C	-4.27267700	3.63600400	2.20304500
H	-4.50055600	3.80116400	3.25145500
C	-4.70984500	4.56173100	1.24450400
H	-5.27394500	5.43223000	1.56688500
C	-4.42251700	4.39544100	-0.11352600
H	-4.74528600	5.13358600	-0.84206600
C	-3.69248800	3.27367500	-0.50426000
C	-3.18899000	2.79626700	-1.79431700
C	-3.42799600	3.44375900	-3.11793400
H	-3.04507000	4.47198100	-3.12839300
H	-4.50036200	3.49337100	-3.34571300
H	-2.92807700	2.89459500	-3.92080900
C	-3.36737700	-1.15517300	0.82065300
C	-4.52163700	-1.70325100	1.39554300
H	-5.49458700	-1.73570800	0.93063900
C	-4.16494700	-2.22898900	2.66450700
C	-4.86455900	-2.88974200	3.69812000
H	-5.92010700	-3.12317300	3.58831500
C	-4.18017000	-3.21755000	4.85381500
H	-4.70125000	-3.71974000	5.66407900
C	-2.80630700	-2.89953500	5.01114700
H	-2.30826800	-3.16661300	5.93917700
C	-2.08469700	-2.26673900	4.01437300
H	-1.03170100	-2.02943700	4.10686200
C	-2.77629400	-1.95184800	2.83642500
C	-4.61120600	-0.29676500	-1.12714800
C	-5.60919500	0.47473000	-0.51259900
H	-5.41293200	0.93665400	0.44593400
C	-6.84538800	0.65691600	-1.12857100
H	-7.59849100	1.27118500	-0.64397400
C	-7.11577400	0.04952500	-2.35495200
H	-8.08142200	0.18787100	-2.83274400
C	-6.14243000	-0.74746200	-2.95883400
H	-6.34989400	-1.24238400	-3.90314200
C	-4.89867100	-0.91495500	-2.35423800
H	-4.16062200	-1.55220700	-2.82947400
C	-0.77143900	0.65804300	-3.17156500
C	0.36977100	1.08108100	-2.48745600
H	0.30424200	1.28942300	-1.42693100
C	1.59012600	1.21459900	-3.14574900
H	2.46512400	1.53322200	-2.59122600
C	1.67424600	0.93199200	-4.50785500
H	2.62066400	1.03135100	-5.03344900
C	0.53336900	0.52552100	-5.19945100

H	0.59488200	0.31315500	-6.26435900
C	-0.69970800	0.38349600	-4.55165800
C	-1.90582500	-0.06540700	-5.34506400
H	-2.70228500	0.69008800	-5.35237800
H	-2.33871800	-0.98757500	-4.94106100
H	-1.63081100	-0.25899200	-6.38633300

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N	0.09256900	0.07298600	0.84256300
N	-1.80768000	-1.28795200	-0.80194700
H	-1.16322100	-1.89862900	-0.32213500
C	-0.34462200	0.69306400	-0.41194700
C	0.85433100	0.26291600	-1.32332500
H	0.67405600	-0.74822400	-1.69958500
H	0.97913000	0.92943000	-2.17753600
C	2.09744900	0.24081500	-0.38162900
H	2.47968000	1.26563000	-0.30001200
C	1.46342400	-0.13119700	0.93056300
C	-0.49938600	-0.18492400	2.06391600
C	-1.83278100	-0.11117000	2.47594600
H	-2.61209700	0.21681800	1.79641100
C	-2.11268100	-0.47247100	3.79005500
H	-3.13803000	-0.42676600	4.14546200
C	-1.09409000	-0.89559200	4.66718200
H	-1.35185500	-1.17076100	5.68603700
C	0.23117200	-0.96409700	4.25208700
H	1.00905700	-1.28919700	4.93788900
C	0.55291100	-0.60243300	2.93449800
C	1.79736600	-0.55217000	2.19352600
C	3.15525200	-0.89895500	2.72168200
H	3.20608200	-1.94497400	3.05205700
H	3.41778900	-0.27728900	3.58738600
H	3.92515300	-0.75735900	1.95871000
C	-1.65858200	0.09314900	-0.83809200
C	-2.83325300	0.65688000	-1.27165000
H	-3.01222700	1.71230200	-1.40968600
C	-3.76766700	-0.41274100	-1.49899500
C	-5.10188500	-0.47360400	-1.93305500
H	-5.63574500	0.43551000	-2.19627700
C	-5.72774600	-1.71092500	-2.01343900
H	-6.76061100	-1.77022700	-2.34440400
C	-5.04603400	-2.89604600	-1.67032100
H	-5.56377200	-3.84834500	-1.73993100

C	-3.72235000	-2.86999500	-1.24571600
H	-3.19601200	-3.78340700	-0.98325500
C	-3.09608200	-1.62372200	-1.16969100
C	-0.41525000	2.21838100	-0.31100900
C	-0.22897500	2.88063300	0.90455100
H	-0.05254600	2.31031000	1.80901000
C	-0.27072300	4.27520800	0.96326700
H	-0.12421200	4.77400600	1.91713000
C	-0.49799400	5.02351300	-0.19026500
H	-0.53031400	6.10823300	-0.14235100
C	-0.68075800	4.36852600	-1.40983600
H	-0.85511400	4.94049600	-2.31690600
C	-0.63537300	2.97736300	-1.46891700
H	-0.78124000	2.47474000	-2.42069200
C	3.19923300	-0.66391700	-0.89450000
C	3.17494900	-2.03148000	-0.59997800
H	2.39038800	-2.41222200	0.04773100
C	4.14439200	-2.89677600	-1.10293000
H	4.10844200	-3.95426100	-0.85680300
C	5.15816500	-2.39404900	-1.91631600
H	5.92344300	-3.05455600	-2.31413800
C	5.18714300	-1.03319500	-2.21728100
H	5.97748300	-0.64040600	-2.85233400
C	4.21947100	-0.15225800	-1.72097200
C	4.29030500	1.31447700	-2.07828200
H	4.44146400	1.94395300	-1.19229700
H	3.37289100	1.66520700	-2.56566800
H	5.12174500	1.50548800	-2.76288700

Int5'

C	-3.51812600	-1.58259400	-0.89173300
C	-2.23952300	-2.02574900	-0.53075400
C	-1.64013500	-3.14409900	-1.11871100
C	-2.35206000	-3.78431800	-2.13378000
H	-1.90942700	-4.65989000	-2.60245300
C	-4.10909700	-0.45191900	-0.11536200
C	-3.40791900	0.75895700	-0.06124700
C	-3.87182300	1.85487900	0.67581300
C	-5.08318700	1.70903900	1.35087500
H	-5.46521300	2.55347300	1.91953100
O	-1.54425100	-1.31013200	0.43136700
O	-2.20765900	0.85765000	-0.74707500
P	-0.87807000	0.12792700	-0.06979400
O	-0.47733700	0.83511800	1.19624900

O	0.11610500	-0.08199600	-1.17440500
C	-3.58907300	-3.31644900	-2.59072500
C	-4.27776200	-4.06054600	-3.72116400
C	-4.17739400	-2.19632500	-1.97823500
C	-5.33373300	-3.22236900	-4.44635900
H	-4.76306500	-4.95790500	-3.30752300
H	-3.52481600	-4.42666400	-4.42940200
C	-5.44043200	-1.57664300	-2.55262700
C	-6.24752200	-2.53832500	-3.42771400
H	-5.91028800	-3.85696900	-5.12966000
H	-4.84082300	-2.45558100	-5.06001200
H	-6.06885400	-1.16258100	-1.76091700
H	-5.13506300	-0.71165700	-3.16108900
H	-7.05505900	-1.99195000	-3.92919000
H	-6.72368200	-3.30246800	-2.79644600
C	-5.28832800	-0.60164000	0.64793900
C	-5.92849900	-1.97158900	0.80766700
C	-5.79121500	0.50266600	1.35927400
C	-7.37592500	-1.91656900	1.30078400
H	-5.32385000	-2.53323900	1.53655100
H	-5.86438200	-2.54576200	-0.11800300
C	-7.09318100	0.42672400	2.13708900
C	-7.48863600	-1.00115200	2.52057400
H	-7.72329700	-2.92937000	1.53631800
H	-8.02526300	-1.53528700	0.49954200
H	-7.02273800	1.06004500	3.02967300
H	-7.89633200	0.86133500	1.52231600
H	-8.50618400	-1.01064600	2.92862300
H	-6.82222600	-1.37075800	3.31226700
C	-3.06863700	3.10774900	0.76132700
C	-3.10423800	4.03318500	-0.30117000
C	-2.24755200	3.34005300	1.88454200
C	-2.26881400	5.20905600	-0.25328400
C	-1.40056500	4.50887600	1.91537300
C	-1.43274000	5.40983400	0.84759400
C	-0.31299700	-3.65566700	-0.66771400
C	-0.22523500	-4.37427000	0.54552800
C	0.83422100	-3.46099600	-1.46491500
C	1.04148800	-4.93054800	0.95498300
C	2.09656400	-4.02369400	-1.04522500
C	2.16613100	-4.74319300	0.14863700
C	-3.92272500	3.83405800	-1.45708700
C	-2.28976600	6.11665300	-1.35532000
C	-3.90942700	4.72650600	-2.49697600

C	-3.08118400	5.88424900	-2.44797000
H	-1.64937900	6.99394500	-1.31101500
H	-3.08172000	6.58070600	-3.28178700
H	-4.53648000	4.55393200	-3.36721500
H	-4.55348300	2.95291900	-1.49871900
H	-0.78591300	6.28410000	0.87065700
C	-2.19861100	2.44386400	2.99771200
C	-1.37777800	2.68729400	4.06490400
C	-0.53530400	4.70839600	3.03547400
C	-0.52293500	3.82652700	4.08115800
H	0.11180900	5.58192400	3.03669000
H	0.14159400	3.98609200	4.92546700
H	-1.35805800	1.99408200	4.90117000
H	-2.81467500	1.55361200	2.97366800
C	1.12066200	-5.64631300	2.18712100
C	-1.35081700	-4.56922200	1.40502700
C	3.25147000	-3.82016500	-1.86142900
C	0.80807900	-2.69414600	-2.67218800
C	0.01927600	-5.80532100	2.98361500
C	-1.23191700	-5.25534100	2.58525400
C	3.17904300	-3.09411300	-3.01818100
C	1.94076200	-2.51719600	-3.42058000
H	2.08591700	-6.04591000	2.48638800
H	0.09462200	-6.34566200	3.92320000
H	-2.10097300	-5.38553600	3.22445900
H	-2.30913400	-4.15746700	1.10912200
H	4.19185500	-4.25679200	-1.53421700
H	4.06863700	-2.93115000	-3.61951000
H	1.90240200	-1.91415200	-4.32295300
H	-0.11956100	-2.21872100	-2.96372000
H	3.12211900	-5.15028500	0.46906500
C	3.81072100	1.62832800	2.65526500
C	2.38122800	1.49154600	2.62540700
C	1.66809300	0.91838600	3.69023400
C	2.40209100	0.50910300	4.78318600
C	3.82092100	0.65832200	4.84975000
C	4.52750600	1.20158900	3.80631900
C	4.19468100	2.16138400	1.42224400
C	2.98394300	2.38245100	0.66211700
H	0.59719900	0.78388500	3.61329400
H	1.88982900	0.04416400	5.61975900
H	4.34167100	0.31126900	5.73664700
H	5.60853200	1.29372500	3.84740500
N	1.90903100	1.97614500	1.44920800

H	0.95366700	1.69609200	1.15312900
C	5.58692500	2.44708200	0.96544300
H	6.29299500	2.35157500	1.79436800
H	5.89367000	1.74297100	0.18387000
H	5.68628100	3.45917200	0.55693500
C	2.98385200	2.94123900	-0.60020600
H	3.98594600	3.15791200	-0.94734500
C	1.93632300	3.31954900	-1.51008000
C	0.56863600	3.08096500	-1.25043900
C	2.30641700	3.90911100	-2.75930400
C	-0.39906400	3.34096100	-2.20807800
H	0.24864200	2.67892000	-0.30198100
C	1.30904900	4.19997800	-3.68550900
C	-0.03183400	3.90713200	-3.42660900
H	-1.43044800	3.09186400	-2.00372000
H	1.58778500	4.65160100	-4.63388900
H	-0.79047000	4.12576600	-4.17197800
C	3.74256400	4.20252500	-3.11929200
H	3.79481800	4.72725900	-4.07700400
H	4.24283700	4.83000800	-2.37248100
H	4.32812600	3.28050400	-3.22013400
C	2.39086200	-1.54178300	1.42164800
C	3.74042400	-1.76720500	1.84824800
C	3.96829100	-2.39232600	3.09025200
C	2.87992500	-2.77065500	3.85681100
C	1.55510000	-2.53810900	3.41244800
C	1.29009500	-1.92658200	2.19982500
C	3.75906300	-0.78491600	-0.20168500
C	4.58140300	-1.27619000	0.81153400
H	4.98306600	-2.56950400	3.43672100
H	3.03853700	-3.25964500	4.81424200
H	0.72344300	-2.86437400	4.02903400
H	0.27568200	-1.75449900	1.86705100
H	5.66120900	-1.26441900	0.80223400
N	2.43997500	-0.94393100	0.18983500
H	1.61712600	-0.70968900	-0.37979500
C	4.12003000	-0.17344200	-1.46929600
C	5.54316800	-0.25545200	-1.89781900
C	6.24458100	-1.47114100	-1.85299100
C	6.20739400	0.87544500	-2.39585700
C	7.56317800	-1.55017800	-2.29697400
H	5.73881000	-2.35390800	-1.47970600
C	7.52757400	0.79869200	-2.83764000
H	5.68352500	1.82575900	-2.41954400

C	8.21162900	-0.41623700	-2.78986100
H	8.08500300	-2.50262200	-2.26126100
H	8.02304500	1.69003400	-3.21291400
H	9.24075700	-0.47894200	-3.13190200
C	3.20941200	0.45045500	-2.25189800
H	2.15603300	0.50219900	-2.00270400
H	3.50441200	0.85490800	-3.21474000

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C	-3.47004300	-1.69255500	-0.98845400
C	-2.20053700	-2.09887000	-0.55411000
C	-1.53014000	-3.18280300	-1.12941800
C	-2.17122100	-3.84362100	-2.17964200
H	-1.67033700	-4.69408100	-2.63559500
C	-4.12214000	-0.55010800	-0.28332200
C	-3.44113300	0.67303900	-0.24196500
C	-3.96723800	1.79608900	0.40371300
C	-5.22300800	1.66187000	0.99841900
H	-5.65493700	2.52659400	1.49639000
O	-1.58758900	-1.37277300	0.45551800
O	-2.19397500	0.74968800	-0.83840300
P	-0.92838200	0.08807100	0.00515500
O	-0.65591400	0.84300300	1.26775500
O	0.16562200	-0.13598500	-1.00971300
C	-3.40308700	-3.42439200	-2.68985700
C	-4.01062400	-4.18763100	-3.85356300
C	-4.05495900	-2.32363700	-2.10649100
C	-5.04143000	-3.37358100	-4.63912200
H	-4.49995000	-5.09357000	-3.46410300
H	-3.21128700	-4.53982300	-4.51663000
C	-5.30092800	-1.73732700	-2.75066000
C	-6.02945700	-2.71651200	-3.67419800
H	-5.56100000	-4.01996400	-5.35621200
H	-4.53205100	-2.59293700	-5.22105200
H	-5.98634700	-1.34479100	-1.99679500
H	-4.98515400	-0.86078700	-3.33698700
H	-6.82021400	-2.18884400	-4.22039300
H	-6.52189200	-3.49488300	-3.07356100
C	-5.34820000	-0.68364300	0.40245300
C	-5.98042900	-2.05430400	0.58258000
C	-5.91424000	0.44659700	1.01958000
C	-7.46176700	-1.99762300	0.96169300
H	-5.42671900	-2.56886700	1.38308400
H	-5.83743900	-2.67225500	-0.30576700

C	-7.26879200	0.38767100	1.70352500
C	-7.67605000	-1.02656900	2.12390700
H	-7.81504000	-3.00288600	1.21981200
H	-8.05278400	-1.66460700	0.09634500
H	-7.27165600	1.06236100	2.56816400
H	-8.02901600	0.78188100	1.01184400
H	-8.72127000	-1.03172600	2.45484100
H	-7.06725800	-1.34897900	2.97999800
C	-3.20305000	3.07181500	0.50415700
C	-3.09564900	3.92457200	-0.61409500
C	-2.60133300	3.42545400	1.73084600
C	-2.39585500	5.18086900	-0.48979000
C	-1.88829300	4.67633400	1.84069900
C	-1.81394400	5.52475200	0.73271100
C	-0.18774000	-3.64426100	-0.67037900
C	-0.06848100	-4.37365800	0.53258400
C	0.94416000	-3.42918800	-1.48651700
C	1.20702200	-4.93998200	0.90114800
C	2.21301500	-4.00792300	-1.11261300
C	2.31005800	-4.74947800	0.06658000
C	-3.64986700	3.58671600	-1.88784700
C	-2.29570400	6.03356000	-1.63189800
C	-3.51608100	4.42288000	-2.96456800
C	-2.83289600	5.66627700	-2.83697300
H	-1.77310900	6.98067800	-1.52144200
H	-2.74438400	6.32135900	-3.69924800
H	-3.93633600	4.14053500	-3.92558200
H	-4.17506300	2.64392200	-1.99042200
H	-1.27840000	6.46753600	0.82005300
C	-2.64522500	2.57408500	2.87928100
C	-2.04399800	2.93922000	4.05346500
C	-1.26530700	5.01373900	3.08225400
C	-1.34112000	4.17377600	4.15907500
H	-0.72529500	5.95493200	3.14762400
H	-0.85898700	4.43838300	5.09581800
H	-2.08493300	2.27390900	4.91147600
H	-3.14323100	1.61675300	2.79513500
C	1.31219400	-5.68079000	2.11675700
C	-1.17422100	-4.58086200	1.41488800
C	3.34307700	-3.80429700	-1.96219200
C	0.89276000	-2.62717200	-2.66957800
C	0.22927300	-5.85100400	2.93562300
C	-1.02917300	-5.28788200	2.57919600
C	3.24476600	-3.05117600	-3.10060100

C	2.00590200	-2.44076600	-3.44581200
H	2.28208600	-6.09108500	2.38443400
H	0.32452900	-6.41108700	3.86175700
H	-1.88231800	-5.42603500	3.23768200
H	-2.13641300	-4.15858500	1.14888600
H	4.28593600	-4.26523900	-1.67741800
H	4.11478300	-2.89497300	-3.73159300
H	1.94842100	-1.81259700	-4.32996600
H	-0.03774800	-2.13478500	-2.92001000
H	3.26957900	-5.17505200	0.35017500
C	3.42728900	1.15917700	2.92480200
C	2.03496300	1.40854400	2.73407200
C	1.07969300	1.08514800	3.70610800
C	1.54597300	0.50286400	4.87150800
C	2.92557400	0.24551000	5.08764600
C	3.86611100	0.56853800	4.13258800
C	4.08666000	1.56253600	1.74148900
C	3.08904500	2.07044400	0.85987600
H	0.02863400	1.25335400	3.51443600
H	0.83465100	0.22498000	5.64446100
H	3.23648900	-0.22386900	6.01600300
H	4.91946000	0.36089300	4.29408600
N	1.85702300	1.98503100	1.50350200
H	0.93576600	1.90757000	1.07027100
C	5.56979500	1.57712100	1.53592100
H	6.04402700	0.82785300	2.17589700
H	5.85746400	1.35025600	0.50614500
H	6.00184900	2.55320700	1.79619000
C	3.41084900	2.56536700	-0.42729300
H	4.48568300	2.52613800	-0.55340600
C	2.86042500	3.66594900	-1.24505800
C	1.49997400	3.96920500	-1.49856500
C	3.85234400	4.48168700	-1.83744200
C	1.20375300	5.08162900	-2.29695400
C	3.53631100	5.58386300	-2.61891500
C	2.19464800	5.88929700	-2.84787500
H	0.15865900	5.30168200	-2.49392300
H	4.32713300	6.19367400	-3.04571200
H	1.92072100	6.74161800	-3.46349500
C	2.43726700	-1.65645900	1.47513900
C	3.79356500	-2.03639200	1.76294000
C	4.06491500	-2.77556300	2.94050300
C	3.01483700	-3.09479700	3.77263900
C	1.68463200	-2.68727200	3.47460000

C	1.37403100	-1.97870200	2.33180100
C	3.72695700	-0.85665900	-0.18555500
C	4.58481900	-1.52367700	0.71836300
H	5.08157000	-3.07721800	3.17708600
H	3.19788900	-3.66141100	4.68103400
H	0.88677900	-2.96027100	4.15697400
H	0.36154000	-1.66577800	2.11072600
H	5.66030200	-1.56850400	0.63646500
N	2.43384100	-0.96052800	0.30592700
H	1.57745000	-0.67298600	-0.19986500
C	4.03616900	-0.07861300	-1.33999800
C	5.38958000	-0.14642800	-1.93236800
C	6.10165000	-1.35822700	-1.98869500
C	5.98596700	0.99788600	-2.49448700
C	7.36768200	-1.41732300	-2.56675500
H	5.63741500	-2.25778700	-1.60563000
C	7.25334500	0.93787500	-3.06640300
H	5.45589200	1.94433100	-2.47853600
C	7.95293700	-0.27001700	-3.10321900
H	7.89402100	-2.36688800	-2.60607100
H	7.69633400	1.83761900	-3.48394600
H	8.94054600	-0.31703500	-3.55264600
C	3.11114900	0.84580100	-1.81799900
H	2.06069900	0.74389300	-1.57517200
H	3.32304200	1.36700100	-2.74447800
H	4.89782000	4.24585100	-1.65379600
C	0.35482300	3.14690400	-0.98638500
H	0.07308700	3.43933200	0.03029800
H	-0.53244900	3.28888100	-1.60585200
H	0.57767600	2.08167200	-0.99784900

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H	-1.36830000	-2.69650300	-1.22500700
C	0.70359800	1.65356200	0.30673200
C	1.53998700	0.57785700	-0.00475500
C	2.86592000	0.50009200	0.42353300
C	3.33384000	1.54426500	1.22094300
H	4.36527800	1.51067100	1.56200500
C	-0.67974600	1.67723200	-0.25126700
C	-1.53047900	0.60458600	0.02461800
C	-2.86385800	0.56887300	-0.39013900
C	-3.32384000	1.65381300	-1.13591300
H	-4.36046900	1.65561500	-1.46312000
O	1.02814300	-0.46985900	-0.77848900

O	-1.02558800	-0.48902900	0.73161400
P	-0.00169300	-1.49048000	-0.05034200
O	-0.75096500	-1.96451400	-1.39096700
O	0.51483600	-2.52753100	0.85528400
C	2.51048600	2.59903500	1.62975400
C	3.09754200	3.67485600	2.52648700
C	1.17574000	2.64978400	1.19119100
C	2.03997800	4.46381700	3.30209800
H	3.67308100	4.37421900	1.90137400
H	3.82121600	3.22094500	3.21367900
C	0.21776900	3.68433100	1.75964600
C	0.92200700	4.90488600	2.35644000
H	2.50395600	5.32660700	3.79369600
H	1.61465000	3.83350600	4.09514900
H	-0.51492100	3.99566400	1.01291300
H	-0.36791600	3.18824700	2.54875600
H	0.19038400	5.53227600	2.87851200
H	1.34870400	5.51725800	1.54909700
C	-1.14410900	2.71775800	-1.08735400
C	-0.17372500	3.75883000	-1.62106700
C	-2.48478200	2.70944100	-1.51101300
C	-0.86161400	5.01599600	-2.15748000
H	0.39468800	3.28638300	-2.43669300
H	0.57171100	4.02300300	-0.86882300
C	-3.06160000	3.83332000	-2.35382300
C	-1.99798300	4.63503100	-3.10775300
H	-0.12449800	5.65139700	-2.66166400
H	-1.26816600	5.60173000	-1.32054700
H	-3.80137500	3.42288100	-3.05133300
H	-3.61703400	4.51589600	-1.69294400
H	-2.45150300	5.52586600	-3.55726200
H	-1.59313900	4.03120100	-3.93144100
C	-3.73888100	-0.58763800	-0.04855500
C	-4.21192400	-0.73503900	1.27323700
C	-4.07652700	-1.53377100	-1.04028200
C	-5.04982900	-1.86136300	1.60816600
C	-4.91665500	-2.65749900	-0.69383700
C	-5.38035000	-2.78931800	0.61724300
C	3.73454400	-0.65094000	0.05027100
C	4.29980300	-0.70390800	-1.24068900
C	3.98596800	-1.67059600	0.99040100
C	5.15747500	-1.80937700	-1.59401300
C	4.85372200	-2.76697500	0.62988100
C	5.41530600	-2.80571400	-0.64864700

C	-3.89692100	0.19898800	2.30873200
C	-5.52040800	-2.00175700	2.94965200
C	-4.36777200	0.02836000	3.58321100
C	-5.18947900	-1.08706600	3.91186700
H	-6.14817900	-2.85657600	3.18780600
H	-5.55150900	-1.20593100	4.92899500
H	-4.11333600	0.74939700	4.35479200
H	-3.27398400	1.05305100	2.06842600
H	-6.00977200	-3.63832200	0.87426200
C	-3.59608300	-1.44484200	-2.38662900
C	-3.92461800	-2.39297900	-3.31959600
C	-5.24275700	-3.61696200	-1.70165600
C	-4.76310300	-3.49253800	-2.97718500
H	-5.87866000	-4.45453700	-1.42645400
H	-5.01451900	-4.23164700	-3.73230500
H	-3.54043300	-2.30880600	-4.33204800
H	-2.94694300	-0.61995900	-2.65384700
C	5.72483800	-1.85389500	-2.90431500
C	4.06289800	0.30526600	-2.22534600
C	5.11154500	-3.79073800	1.59218400
C	3.39917600	-1.67577700	2.29425700
C	5.46729000	-0.86937300	-3.81946800
C	4.62488000	0.22479100	-3.47182500
C	4.54033400	-3.74883000	2.83472600
C	3.66811600	-2.67920800	3.18522600
H	6.36766600	-2.69320000	-3.15785500
H	5.90373300	-0.91643100	-4.81314900
H	4.42823100	1.00150600	-4.20562100
H	3.42443100	1.14353300	-1.96878700
H	5.77010400	-4.60824000	1.30961400
H	4.74084100	-4.53566600	3.55641800
H	3.20201900	-2.66990500	4.16615400
H	2.71786200	-0.87715400	2.56259000
H	6.06579200	-3.63531400	-0.91704300

H₂O

O	0.00000000	0.00000000	0.11972000
H	0.00000000	0.76154500	-0.47888000
H	0.00000000	-0.76154500	-0.47888000

TS5'

H	1.70003200	0.49752600	-0.74909100
N	2.73914400	0.61741900	-0.55229900
N	0.74430200	3.01173300	-0.21817500
H	0.19173800	2.28289000	0.25264900

C	2.93055600	2.11225200	0.49676000
C	2.34864600	1.44425500	1.75924600
H	1.28691400	1.65578500	1.84742100
H	2.83265200	1.85365200	2.64500800
C	2.52999400	-0.12430300	1.68028000
H	1.52728300	-0.50769500	1.47696600
C	3.29727000	-0.32517600	0.40655300
C	3.51448700	0.50260400	-1.74112500
C	3.29704700	1.10316100	-2.96724300
H	2.42058200	1.71666100	-3.14553400
C	4.27471800	0.89089500	-3.94785000
H	4.15902200	1.34955000	-4.92490100
C	5.39849200	0.09914400	-3.68184300
H	6.14458900	-0.04141600	-4.45870800
C	5.56535200	-0.54051400	-2.44847900
H	6.42596800	-1.17781400	-2.26902900
C	4.59522600	-0.34925700	-1.46872900
C	4.43262600	-0.86649500	-0.09895200
C	5.43756900	-1.77513200	0.53317900
H	5.83101000	-2.47423400	-0.21068500
H	6.28899700	-1.19816200	0.91756400
H	5.01020300	-2.34965400	1.35360100
C	2.11902600	3.15398300	-0.13170200
C	2.48829600	4.30980400	-0.81769300
H	3.48668600	4.71052100	-0.89275700
C	1.30331400	4.87551200	-1.36909500
C	1.02612500	6.00038000	-2.17353000
H	1.82408700	6.67568800	-2.47061700
C	-0.27680800	6.21347400	-2.58969300
H	-0.50733400	7.06951500	-3.21781300
C	-1.31971400	5.32656800	-2.22562900
H	-2.32780100	5.51097300	-2.58418700
C	-1.08537300	4.22164500	-1.42421900
H	-1.87327600	3.52777000	-1.15789700
C	0.22881300	4.01540600	-0.98970500
C	4.41772700	2.36328300	0.51164400
C	5.09957600	2.74005900	-0.65967300
H	4.55337800	2.87008000	-1.58143400
C	6.47959200	2.92460800	-0.66494700
H	6.97409400	3.20089100	-1.59136800
C	7.21912500	2.74593700	0.50300100
H	8.29614100	2.88719000	0.49916500
C	6.55920400	2.38756200	1.67760800
H	7.11561400	2.25409700	2.60085400

C	5.17871100	2.19653400	1.67916500
H	4.70650700	1.91456300	2.60960300
C	2.99835600	-0.76206400	2.96701600
C	4.34777100	-0.76785900	3.33452700
H	5.07630900	-0.31084100	2.67631200
C	4.77511000	-1.35521100	4.52411900
H	5.83108400	-1.35667100	4.78004100
C	3.83810000	-1.93653800	5.37532900
H	4.15308400	-2.40289900	6.30484300
C	2.48687100	-1.90125100	5.03487700
H	1.75258100	-2.33568700	5.70868800
C	2.04002900	-1.31367400	3.84513200
C	0.56056000	-1.27508000	3.54246500
H	0.20294300	-0.26340700	3.32487400
H	0.30743700	-1.88189300	2.66819400
H	-0.00970900	-1.66287900	4.39235300
C	-3.69656200	-1.39130000	0.27696800
C	-3.37115400	-0.03442700	0.13775200
C	-4.05744000	0.95970700	0.84403000
C	-5.06624700	0.54527000	1.71636600
H	-5.61393500	1.30768800	2.26481000
C	-2.96044000	-2.38590500	-0.55384400
C	-1.56797300	-2.44684200	-0.43041800
C	-0.79711200	-3.36729100	-1.14248300
C	-1.47513700	-4.23238400	-2.00535600
H	-0.89428700	-4.95946700	-2.56706300
O	-2.32552000	0.30649900	-0.71550000
O	-0.94350600	-1.53769600	0.40934100
P	-0.79516400	0.01827400	-0.14758700
O	0.16070000	0.09300000	-1.30991800
O	-0.51992900	0.85821000	1.06924400
C	-5.36325100	-0.80102400	1.94080700
C	-6.45765400	-1.15518400	2.93162100
C	-4.65850900	-1.78728900	1.23065200
C	-6.35217500	-2.58615600	3.46393800
H	-7.43307300	-1.03377300	2.43625100
H	-6.44930500	-0.43475300	3.75832800
C	-4.83635100	-3.25734300	1.57539000
C	-6.14833300	-3.56015600	2.30238900
H	-7.25148700	-2.83917000	4.03769000
H	-5.50009600	-2.66316400	4.15362300
H	-4.74191000	-3.88448000	0.68685700
H	-3.99470000	-3.54699100	2.22340500
H	-6.14110600	-4.59759800	2.65686500

H	-6.99002400	-3.47004900	1.60052300
C	-3.61085000	-3.21203400	-1.49445000
C	-5.07857300	-2.99120000	-1.82302100
C	-2.85575600	-4.16068000	-2.20698900
C	-5.72874400	-4.17429100	-2.54413800
H	-5.13976800	-2.10150700	-2.46841400
H	-5.64710100	-2.73342200	-0.92717000
C	-3.50207600	-5.12323500	-3.18717300
C	-4.85391000	-4.63373100	-3.71145300
H	-6.72851500	-3.88841200	-2.89145900
H	-5.86318300	-5.00857700	-1.84055800
H	-2.81260300	-5.31525600	-4.01797300
H	-3.64778800	-6.09238000	-2.68597400
H	-5.34492200	-5.43076000	-4.28203800
H	-4.70126600	-3.79230800	-4.40135500
C	0.68594000	-3.43544400	-1.04346700
C	1.30982000	-3.92311000	0.12584600
C	1.45997900	-3.08971400	-2.17260400
C	2.73559900	-4.15009800	0.12801300
C	2.87346900	-3.37679500	-2.18074400
C	3.46669700	-3.92297200	-1.04090400
C	-3.78141200	2.41989700	0.70662000
C	-2.98612000	3.08204800	1.66574000
C	-4.41410700	3.14819100	-0.32401900
C	-2.81756700	4.51398200	1.58412600
C	-4.26459000	4.58321500	-0.37709200
C	-3.47318400	5.22617800	0.57750500
C	0.58370000	-4.21516000	1.32209600
C	3.36277600	-4.60519100	1.32839900
C	1.22632200	-4.62980100	2.45905800
C	2.63693600	-4.81680600	2.46936400
H	4.43737300	-4.76880300	1.31759100
H	3.13064100	-5.13042300	3.38413800
H	0.65693600	-4.81420300	3.36540900
H	-0.49162800	-4.07957100	1.32382500
H	4.52874100	-4.15403000	-1.05529300
C	0.89650700	-2.43988900	-3.31559900
C	1.66904900	-2.13335800	-4.40347300
C	3.63353100	-3.07361000	-3.35072000
C	3.05209800	-2.46961200	-4.43104500
H	4.69441900	-3.30790600	-3.34995200
H	3.64809100	-2.22085800	-5.30403200
H	1.22769800	-1.61658300	-5.25074900
H	-0.14749800	-2.15533500	-3.28783400

C	-1.97820900	5.16831600	2.53728900
C	-2.32722400	2.38440700	2.72569300
C	-4.91011100	5.30747600	-1.42571000
C	-5.21169700	2.51658700	-1.32927600
C	-1.35329800	4.45935500	3.52684300
C	-1.53710000	3.05026500	3.62347400
C	-5.65795000	4.66215100	-2.37386400
C	-5.80913100	3.24701300	-2.32205600
H	-1.84616700	6.24393800	2.45343400
H	-0.71391500	4.96777800	4.24332600
H	-1.03345900	2.49749400	4.41167700
H	-2.43664800	1.30997000	2.78385300
H	-4.78832100	6.38754800	-1.45385300
H	-6.13964500	5.22498300	-3.16845600
H	-6.40394500	2.74554700	-3.08028100
H	-5.32981000	1.43918400	-1.29583900
H	-3.34244300	6.30404000	0.51912100

(R,S)-3aa

N	-0.18524400	-0.93416600	-0.24752100
N	2.34061700	0.40407200	-0.50111800
H	2.31130100	-0.47318100	-1.00233200
C	0.32983200	-0.16879800	0.89861400
C	-0.97260200	0.58904700	1.28987800
H	-1.58059100	-0.07098200	1.91407600
H	-0.77235400	1.50048400	1.85423400
C	-1.71841100	0.84744700	-0.05472800
H	-1.28955700	1.74770800	-0.51076200
C	-1.27672400	-0.33899600	-0.86714800
C	0.31121600	-1.94289500	-1.04857200
C	1.39958400	-2.80777700	-0.88384800
H	2.02407100	-2.76414900	0.00249100
C	1.63286400	-3.74241600	-1.89036300
H	2.47016300	-4.42740100	-1.79322500
C	0.79974600	-3.82198000	-3.02235200
H	1.00994200	-4.56620500	-3.78515100
C	-0.28536100	-2.96539100	-3.17814100
H	-0.92164900	-3.03540100	-4.05631000
C	-0.54387100	-2.00118800	-2.19292300
C	-1.54713000	-0.96615900	-2.05709900
C	-2.64011900	-0.65943400	-3.03380300
H	-3.29264700	-1.52758100	-3.19526700
H	-2.23428000	-0.37718900	-4.01395000
H	-3.26769300	0.16242700	-2.67910600

C	1.38955600	0.80149900	0.42526700
C	1.64875800	2.10083300	0.79616000
H	1.09425900	2.67828200	1.52200300
C	2.80244600	2.54061200	0.06015200
C	3.53228300	3.73927000	-0.00065500
H	3.24769400	4.58789300	0.61567800
C	4.61962200	3.82193000	-0.86045400
H	5.19170100	4.74365100	-0.91630100
C	4.99640200	2.72833000	-1.66693900
H	5.85087500	2.82495600	-2.33052400
C	4.29634400	1.52821200	-1.62814300
H	4.58607800	0.68482200	-2.24854100
C	3.20535800	1.44780000	-0.75841600
C	0.82019200	-1.09674600	2.00972000
C	0.10755100	-2.27052500	2.28820800
H	-0.75816400	-2.52402200	1.68421100
C	0.51466100	-3.11850000	3.31494100
H	-0.04386200	-4.02878000	3.51393200
C	1.64025800	-2.80383300	4.07985200
H	1.96038500	-3.46674600	4.87866900
C	2.35222600	-1.63674500	3.80797500
H	3.23083400	-1.38402400	4.39483300
C	1.94564200	-0.78741500	2.77702400
H	2.50424600	0.11877000	2.56766900
C	-3.20936700	1.03995600	0.12927200
C	-4.05984700	-0.07034500	0.16572300
H	-3.63738700	-1.05829800	0.00608600
C	-5.42857300	0.07530000	0.38308400
H	-6.07104600	-0.80047300	0.40283600
C	-5.96301900	1.34874100	0.56951700
H	-7.02843700	1.47960500	0.73688400
C	-5.12105100	2.45948800	0.53936800
H	-5.53720800	3.45319700	0.68634600
C	-3.74446400	2.32908600	0.32365700
C	-2.87014300	3.56162800	0.30250400
H	-2.39717100	3.71033700	-0.67636000
H	-2.06166600	3.50589600	1.04109200
H	-3.45859600	4.45686100	0.52326900