

Dearomative, aminocatalytic formal normal-electron-demand aza-Diels-Alder cycloaddition in the synthesis of tetrahydrofuropyridines

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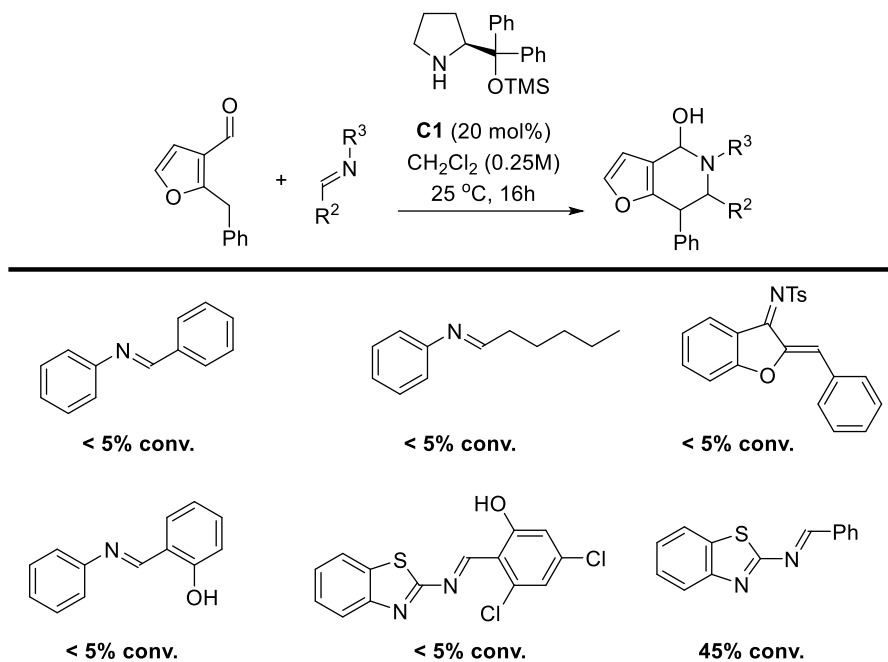
1. General methods

NMR spectra were acquired on a Bruker Ultra Shield 700 instrument, running at 700 MHz for ^1H and 176 MHz for ^{13}C . Chemical shifts (δ) are reported in ppm relative to residual solvent signals (CDCl_3 : 7.26 ppm for ^1H NMR, 77.16 ppm for ^{13}C NMR). Mass spectra were recorded on a Bruker Maxis Impact spectrometer using chemical ionization (APCI) and electrospray (ESI) referenced to the mass of the charged species. Optical rotations were measured on a Perkin-Elmer 241 polarimeter and $[\alpha]_D$ values are given in $\text{deg}\cdot\text{cm}\cdot\text{g}^{-1}\cdot\text{dm}^{-1}$; concentration c is listed in $\text{g}\cdot(100\text{ mL})^{-1}$. Analytical thin layer chromatography (TLC) was performed using pre-coated aluminium-backed plates (Merck Kieselgel 60 F254) and visualized by ultraviolet irradiation or Hanessian's stain. The enantiomeric ratio (er) of the products was determined by chiral stationary phase HPLC (Daicel Chiralpak IA, IB, ID columns). Unless otherwise noted, analytical grade solvents and commercially available reagents were used without further purification. For flash chromatography (FC) silica gel (60, 35-70 μm , Merck KGaA) was used. 2-benzyl-3-furfurals **1** and imines **2** were obtained using literature procedures.^{1,2} The racemic samples of products **4** for chiral HPLC separation studies were prepared using mixture of (*S*)-(-)- α,α -diphenyl-2-pyrrolidinemethanol trimethylsilyl ether and (*R*)-(+)- α,α -diphenyl-2-pyrrolidinemethanol trimethylsilyl ether C1 under the general reaction condition.

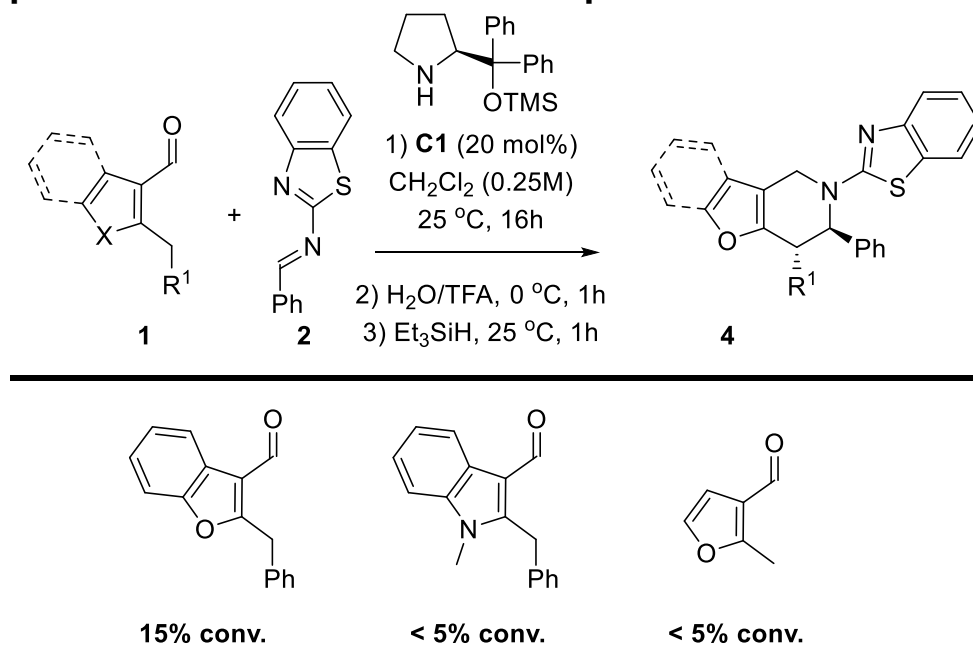
¹ J. Bojanowski, A. Skrzyńska and A. Albrecht, *Asian J. Org. Chem.* 2019, **8**, 844.

² P. Vicini, A. Geronikaki, M. Incerti, B. Busonera, G. Poni, C. A. Cabras and P. La Colla, *Bioorg. Med. Chem.* 2003, **11**, 4785.

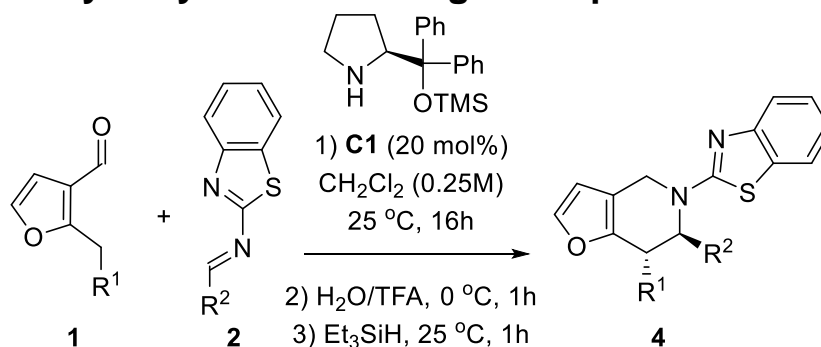
2. Optimization studies



3. Scope studies – unsuccessful attempts

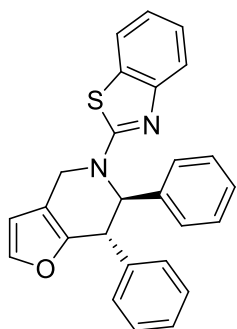


4. Organocatalytic synthesis of 4 – general procedure



To the mixture of the corresponding 2-alkylfuran-3-carbaldehyde **1** (1 equiv., 0.1 mmol) and (*E*)-*N*-benzylidenebenzo[d]thiazol-2-amine **2** (2.5 equiv., 0.25 mmol) in CH₂Cl₂ (0.4 mL) (*S*)-(-)- α,α -diphenyl-2-pyrrolidinemethanol trimethylsilyl ether **C1** (3.9 mg, 0.02 mmol) was added and the resulting mixture was stirred at 25 °C for 16 hours. Reaction mixture was then cooled down to 0 °C, H₂O (5.6 equiv., 0.56 mmol, 10 μ L) and trifluoroacetic acid (10 equiv., 10 mmol, 76,5 μ L) were added, and the mixture was stirred at 25 °C for an additional hour. Next, Et₃SiH (10 equiv., 10 mmol, 156 μ L) was added and the resulting mixture was stirred at 25 °C for 1 hours. The reaction mixture was then washed with saturated sodium bicarbonate (2 mL), aqueous phase was washed with CH₂Cl₂ (5 mL), organic phases were combined, dried over Na₂SO₄, and concentrated *in vacuo*. The residue was subjected to column chromatography on silica gel (hexanes:ethyl acetate 100:0 to 80:20) to furnish pure compounds **4**.

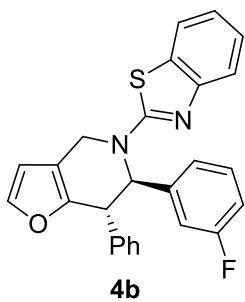
(6*R*,7*S*)-5-(Benzo[*d*]thiazol-2-yl)-6,7-diphenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4a



4a

Following the general procedure, product **4a** (>20:1 dr in a crude reaction mixture) was isolated in 66% (28,0 mg) yield as a light-yellow oil. ¹H NMR (700 MHz, CDCl₃) δ 7.60 – 7.57 (m, 2H), 7.50 – 7.47 (m, 1H), 7.44 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.40 (d, *J* = 1.9 Hz, 1H), 7.35 – 7.32 (m, 2H), 7.29 – 7.26 (m, 2H), 7.25 – 7.21 (m, 4H), 7.11 (td, *J* = 7.5, 1.1 Hz, 1H), 7.00 (ddd, *J* = 8.2, 7.3, 1.1 Hz, 1H), 6.33 (d, *J* = 1.9 Hz, 1H), 5.51 (d, *J* = 6.8 Hz, 1H), 4.66 (d, *J* = 6.9 Hz, 1H), 4.32 (d, *J* = 14.4 Hz, 1H), 4.21 (d, *J* = 14.4 Hz, 1H). ¹³C NMR (176 MHz, CDCl₃) δ 168.8, 152.7, 148.3, 143.0, 141.2, 139.1, 130.7, 129.0 (2C), 128.9 (2C), 128.2, 127.7 (2C), 127.5, 126.9 (2C), 126.1, 121.6, 120.8, 119.4, 115.3, 108.1, 67.2, 44.4, 43.2. The er was determined by HPLC using chiral Chiralpack ID column [hexane/*i*-PrOH (90:10)]; flow rate 1.0 mL/min; *T*_{minor}=8.3 min; *T*_{major}=12.4 min (1:99 er). [α]_D²⁰ = -43.2 (c=1.0, CHCl₃). HRMS calculated for [C₂₆H₂₀N₂OS+H⁺]: 409.1369; found: 409.1370.

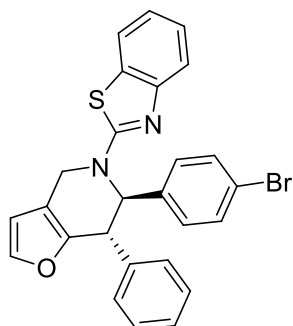
(6*R*,7*S*)-5-(Benzo[*d*]thiazol-2-yl)-6-(3-fluorophenyl)-7-phenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4b



4b

Following the general procedure, product **4b** (10:1 dr in a crude reaction mixture) was isolated in 69% (29.4 mg) yield as a light-yellow oil. ¹H NMR (700 MHz, CDCl₃) δ 7.55 (ddd, *J* = 9.4, 8.0, 1.3 Hz, 2H), 7.41 (d, *J* = 1.9 Hz, 1H), 7.32 – 7.26 (m, 4H), 7.26 – 7.20 (m, 3H), 7.13 (ddt, *J* = 7.8, 1.7, 0.8 Hz, 1H), 7.09 – 7.04 (m, 1H), 7.04 – 7.01 (m, 1H), 6.97 (tdd, *J* = 8.4, 2.5, 1.0 Hz, 1H), 6.38 (d, *J* = 2.0 Hz, 1H), 5.65 (s, 1H), 5.14 (d, *J* = 15.7 Hz, 1H), 4.61 (s, 1H), 4.27 (dd, *J* = 15.7, 1.7 Hz, 1H). ¹³C NMR (176 MHz, CDCl₃) δ 168.6, 163. (d, *J* = 246.7 Hz), 152.6, 148.1, 143.2, 141.7 (d, *J* = 6.4 Hz), 140.9, 130.7, 130.4 (d, *J* = 8.1 Hz), 129.0 (2C), 127.6 (2C), 126.2, 122.7 (d, *J* = 3.1 Hz), 121.8, 120.2 (d, *J* = 221.9 Hz), 115.2 (d, *J* = 21.0 Hz), 115.1, 114.0 (d, *J* = 22.2 Hz), 108.1, 66.2, 44.4, 43.4. ¹⁹F NMR (376 MHz, CDCl₃) δ -111.70 (td, *J* = 9.2, 5.8 Hz). The er was determined by HPLC using a chiral Chiralpack ID column [hexane/*i*-PrOH (90:10)]; flow rate 1.0 mL/min; *T*_{minor}=7.5 min; *T*_{major}=9.2 min (2:98 er). [α]_D²⁰ = -9.6 (c=1.0, CHCl₃). HRMS calculated for [C₂₆H₁₉FN₂OS+H⁺]: 427.1275; found: 427.1278

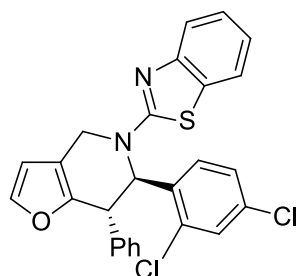
(6*R*,7*S*)-5-(Benzo[*d*]thiazol-2-yl)-6-(4-bromophenyl)-7-phenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4c



4c

Following the general procedure, product **4c** (>20:1 dr in a crude reaction mixture) was isolated in 75% (36.7 mg) yield as a light-yellow oil. ¹H NMR (700 MHz, CDCl₃) δ 7.58 (d, *J* = 8.1 Hz, 1H), 7.52 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.43 – 7.39 (m, 3H), 7.32 – 7.27 (m, 3H), 7.25 – 7.19 (m, 5H), 7.07 (td, *J* = 7.6, 1.1 Hz, 1H), 6.37 (d, *J* = 2.0 Hz, 1H), 5.61 (s, 1H), 5.14 (d, *J* = 15.7 Hz, 1H), 4.60 (s, 1H), 4.22 (dd, *J* = 15.7, 1.7 Hz, 1H). ¹³C NMR (176 MHz, CDCl₃) δ 168.6, 152.6, 148.1, 143.2, 140.9, 138.1, 132.0 (2C), 130.7, 129.0 (2C), 128.7 (2C), 127.6 (2C), 126.2, 122.2, 121.8, 120.8, 119.5, 115.1, 108.1, 66.0, 44.3, 43.3. The er was determined by HPLC using a chiral Chiralpack ID column [hexane/*i*-PrOH (90:10)]; flow rate 1.0 mL/min; *T*_{minor}=7.7 min; *T*_{major}=12.3 min (95:5 er). [α]_D²⁰ = -53.8 (c=1.0, CHCl₃). HRMS calculated for [C₂₆H₁₉BrN₂OS+H⁺]: 487.0474; found: 487.0473.

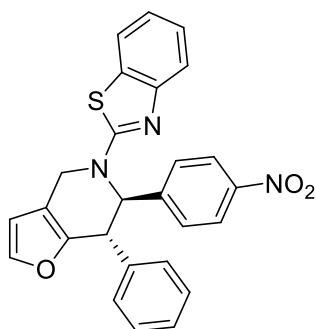
(6*R*,7*S*)-5-(Benzo[*d*]thiazol-2-yl)-6-(2,4-dichlorophenyl)-7-phenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4d



4d

Following the general procedure, product **4d** (15:1 dr in a crude reaction mixture) was isolated in 68% (29.3 mg) yield as a light-yellow oil. ¹H NMR (700 MHz, CDCl₃) δ 7.60 (d, *J* = 8.1 Hz, 1H), 7.50 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.46 (d, *J* = 2.2 Hz, 1H), 7.38 (d, *J* = 2.0 Hz, 1H), 7.32 – 7.27 (m, 3H), 7.26 – 7.22 (m, 3H), 7.09 (dd, *J* = 8.5, 2.2 Hz, 1H), 7.08 – 7.03 (m, 1H), 6.97 (d, *J* = 8.5 Hz, 1H), 6.48 (d, *J* = 1.9 Hz, 1H), 5.70 (s, 1H), 5.29 (d, *J* = 16.0 Hz, 1H), 4.97 (dd, *J* = 16.0, 1.3 Hz, 1H), 4.40 (s, 1H). ¹³C NMR (176 MHz, CDCl₃) δ 168.0, 147.1, 143.4, 140.8, 138.1, 134.4, 133.8, 129.8, 129.1 (2C), 127.9, 127.8, 127.8, 127.3 (2C), 126.2, 122.0, 120.8, 119.6, 114.0, 108.2, 64.8, 46.3, 45.6. The er was determined by HPLC using a chiral Chiralpack IB column [hexane/*i*-PrOH (90:10)]; flow rate 1.0 mL/min; *T*_{minor}=7.1 min; *T*_{major}=11.3 min (2:98 er). [α]_D²⁰ = -29.0 (c=1.0, CHCl₃). HRMS calculated for [C₂₆H₁₈Cl₂N₂OS+H⁺]: 478.4123; found: 478.4131.

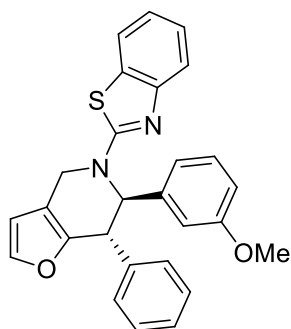
(6*R*,7*S*)-5-(Benzo[*d*]thiazol-2-yl)-6-(4-nitrophenyl)-7-phenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4e



4e

Following the general procedure, product **4e** (10:1 dr in a crude reaction mixture) was isolated in 66% (30.1 mg) yield as a light-yellow oil. ¹H NMR (700 MHz, CDCl₃) δ 8.16 – 8.12 (m, 2H), 7.58 – 7.54 (m, 2H), 7.51 (d, *J* = 8.9 Hz, 2H), 7.43 (d, *J* = 2.0 Hz, 1H), 7.33 – 7.28 (m, 3H), 7.27 – 7.21 (m, 4H), 6.39 (d, *J* = 2.0 Hz, 1H), 5.91 (s, 1H), 5.06 (d, *J* = 15.6 Hz, 1H), 4.63 (s, 1H), 4.25 (dd, *J* = 15.5, 1.7 Hz, 1H). ¹³C NMR (176 MHz, CDCl₃) δ 168.3, 152.4, 147.8, 147.7, 146.5, 143.5, 140.4, 130.7, 129.1 (2C), 128.0 (2C), 127.8, 127.6 (2C), 126.3, 124.1 (2C), 122.0, 120.9, 119.7, 115.0, 108.1, 65.2, 44.2, 43.7. The er was determined by HPLC using a chiral Chiralpack IB column [hexane/*i*-PrOH (90:10)]; flow rate 1.0 mL/min; *T*_{major}=9.8 min; *T*_{minor}=10.9 min (15:85 er). [α]_D²⁰ = –23.3 (c=1.0, CHCl₃). HRMS calculated for [C₂₆H₁₉N₃O₃S+H⁺]: 454.1219; found: 454.1211.

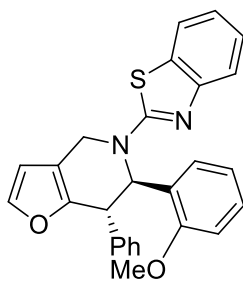
(6*R*,7*S*)-5-(Benzo[*d*]thiazol-2-yl)-6-(3-methoxyphenyl)-7-phenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4f



4f

Following the general procedure, product **4f** (10:1 dr in a crude reaction mixture) was isolated in 72% (31.6 mg) yield as a light-yellow oil. ¹H NMR (700 MHz, CDCl₃) δ 7.56 – 7.54 (m, 1H), 7.53 – 7.50 (m, 1H), 7.40 (d, *J* = 1.9 Hz, 1H), 7.30 – 7.26 (m, 3H), 7.24 – 7.19 (m, 4H), 7.07 – 7.03 (m, 1H), 6.91 (ddt, *J* = 7.8, 1.7, 0.8 Hz, 1H), 6.89 (t, *J* = 2.2 Hz, 1H), 6.81 (ddd, *J* = 8.2, 2.5, 0.9 Hz, 1H), 6.37 (d, *J* = 1.9 Hz, 1H), 5.55 (s, 1H), 5.19 (d, *J* = 15.6 Hz, 1H), 4.62 (s, 1H), 4.30 (dd, *J* = 15.7, 1.8 Hz, 1H), 3.72 (s, 3H). ¹³C NMR (176 MHz, CDCl₃) δ 168.8, 159.9, 152.7, 148.3, 143.0, 141.2, 140.7, 130.7, 129.9, 129.0 (2C), 127.6 (2C), 127.5, 126.1, 121.6, 120.7, 119.4, 119.2, 115.16, 113.1 (2C), 108.1, 67.0, 55.3, 44.6, 43.4. The er was determined by HPLC using a chiral Chiralpack ID column [hexane/*i*-PrOH (85:15)]; flow rate 1.0 mL/min; *T*_{minor}=10.9 min; *T*_{major}=15.2 min (1:99 er). [α]_D²⁰ = –19.1 (c=1.0, CHCl₃). HRMS calculated for [C₂₇H₂₂N₂O₂S+H⁺]: 439.1474; found: 439.1471.

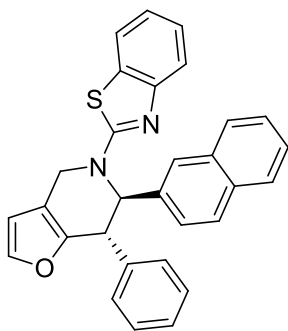
(6*R*,7*S*)-5-(Benzo[*d*]thiazol-2-yl)-6-(2-methoxyphenyl)-7-phenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4g



4g

Following the general procedure, product **4g** (15:1 dr in a crude reaction mixture) was isolated in 68% (29.3 mg) yield as a light-green oil. ¹H NMR (700 MHz, CDCl₃) δ 7.58 – 7.54 (m, 1H), 7.45 (ddd, *J* = 7.8, 1.3, 0.5 Hz, 1H), 7.36 (d, *J* = 1.9 Hz, 1H), 7.29 (tt, *J* = 6.6, 1.3 Hz, 2H), 7.26 – 7.20 (m, 5H), 7.02 – 6.98 (m, 2H), 6.94 (dd, *J* = 8.2, 1.1 Hz, 1H), 6.81 (td, *J* = 7.5, 1.1 Hz, 1H), 6.45 – 6.43 (m, 1H), 5.61 (s, 1H), 5.36 (d, *J* = 16.0 Hz, 1H), 4.80 (dd, *J* = 16.1, 1.4 Hz, 1H), 4.51 (s, 1H), 3.96 (s, 3H). ¹³C NMR (176 MHz, CDCl₃) δ 168.9, 156.8, 152.5, 147.9, 142.9, 141.8, 131.0, 129.3, 129.0, 128.9 (2C), 127.5 (2C), 127.4, 126.2, 125.9, 121.4, 120.8, 120.6, 119.2, 114.6, 110.5, 108.2, 63.6, 55.6, 45.4, 45.3. The er was determined by HPLC using a chiral Chiralpack IA column [hexane/*i*-PrOH (90:10)]; flow rate 1.0 mL/min; *T*_{minor}=11.0 min; *T*_{major}=26.4 min (1:99 er). $[\alpha]_D^{20} = -27.5$ (c=1.0, CHCl₃). HRMS calculated for [C₂₇H₂₂N₂O₂S+H⁺]: 439.1474; found: 439.1471.

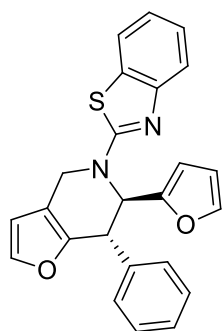
(6*R*,7*S*)-5-(Benzo[*d*]thiazol-2-yl)-6-(naphthalen-2-yl)-7-phenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4h



4h

Following the general procedure, product **4h** (>20:1 dr in a crude reaction mixture) was isolated in 64% (29,2 mg) yield as a light-yellow oil. ¹H NMR (700 MHz, CDCl₃) δ 7.79 – 7.72 (m, 4H), 7.56 (dd, *J* = 8.2, 1.1 Hz, 1H), 7.52 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.49 – 7.44 (m, 3H), 7.41 (d, *J* = 2.0 Hz, 1H), 7.32 – 7.27 (m, 4H), 7.26 – 7.23 (m, 2H), 7.04 – 7.07 (m, 1H), 6.36 (d, *J* = 2.0 Hz, 1H), 5.74 (s, 1H), 5.23 (d, *J* = 15.8 Hz, 1H), 4.81 (s, 1H), 4.28 (dd, *J* = 15.8, 1.7 Hz, 1H). ¹³C NMR (176 MHz, CDCl₃) δ 168.9, 152.7, 148.3, 143.1, 141.2, 136.5, 133.3, 133.1, 130.8, 129.0 (2C), 128.8, 128.4, 127.7 (2C), 127.7, 127.6, 126.5, 126.4, 126.1, 125.7, 125.0, 121.6, 120.8, 119.4, 115.3, 108.1, 67.2, 44.4, 43.4. The er was determined by HPLC using a chiral Chiralpack ID column [hexane/*i*-PrOH (90:10)]; flow rate 1.0 mL/min; *T*_{minor}=9.2 min; *T*_{major}=16.6 min (2:98 er). $[\alpha]_D^{20} = -23.7$ (c=1.0, CHCl₃). HRMS calculated for [C₃₀H₂₂N₂OS+H⁺]: 459.1525; found: 459.1524.

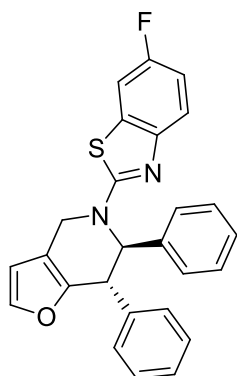
(6*R*,7*S*)-5-(Benzo[*d*]thiazol-2-yl)-6-(furan-2-yl)-7-phenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4i



4i

Following the general procedure, product **4i** (18:1 dr in a crude reaction mixture) was isolated in 73% (29.1 mg) yield as a light-yellow oil. ¹H NMR (700 MHz, CDCl₃) δ 7.57 (dd, *J* = 8.2, 1.1 Hz, 1H), 7.54 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.37 (d, *J* = 1.9 Hz, 1H), 7.32 (d, *J* = 1.8 Hz, 1H), 7.31 – 7.27 (m, 3H), 7.23 (ddt, *J* = 6.7, 4.0, 1.8 Hz, 3H), 7.07 (td, *J* = 7.6, 1.2 Hz, 1H), 6.35 (d, *J* = 1.9 Hz, 1H), 6.27 (dd, *J* = 3.3, 1.8 Hz, 1H), 6.14 (dt, *J* = 3.4, 1.0 Hz, 1H), 5.60 (s, 1H), 5.13 (d, *J* = 15.3 Hz, 1H), 4.69 (s, 1H), 4.30 (dd, *J* = 15.4, 1.8 Hz, 1H). ¹³C NMR (176 MHz, CDCl₃) δ 168.9, 152.5, 151.7, 148.0, 142.9, 142.3, 140.4, 130.9, 128.9, 127.7, 127.6, 126.1, 121.8, 120.8, 119.6, 114.7, 110.5, 108.1, 107.2, 62.0, 43.5, 43.4. The er was determined by HPLC using a chiral Chiralpack ID column [hexane/*i*-PrOH (90:10)]; flow rate 1.0 mL/min; *T*_{minor}=7.4 min; *T*_{major}=11.0 min (3:97 er). $[\alpha]_D^{20} = -11.4$ (*c*=1.0, CHCl₃). HRMS calculated for [C₂₄H₁₈N₂O₂S+H⁺]: 399.1161; found: 399.1163

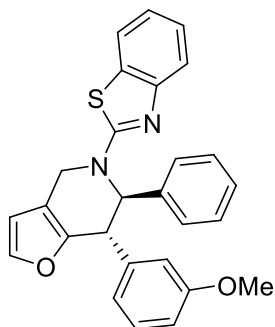
(6*R*,7*S*)-5-(6-Fluorobenzo[*d*]thiazol-2-yl)-6,7-diphenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4j



4j

Following the general procedure, product **4j** (10:1 dr in a crude reaction mixture) was isolated in 94% (40.0 mg) yield as a light-yellow oil¹. ¹H NMR (700 MHz, CDCl₃) δ 7.45 (dd, *J* = 8.8, 4.7 Hz, 1H), 7.40 (d, *J* = 1.9 Hz, 1H), 7.35 – 7.27 (m, 7H), 7.25 – 7.19 (m, 4H), 7.00 (td, *J* = 9.0, 2.6 Hz, 1H), 6.37 (d, *J* = 1.9 Hz, 1H), 5.52 (s, 1H), 5.15 (d, *J* = 15.6 Hz, 1H), 4.65 (s, 1H), 4.24 (dd, *J* = 15.7, 1.7 Hz, 1H). ¹³C NMR (176 MHz, CDCl₃) δ 168.3, 158.3 (d, *J* = 240.3 Hz), 149.1 (d, *J* = 1.9 Hz), 148.2, 143.1, 141.2, 139.0, 131.4 (d, *J* = 10.8 Hz), 129.0 (2C), 129.0 (2C), 128.3, 127.7 (2C), 127.6, 126.8 (2C), 119.8 (d, *J* = 8.6 Hz), 115.2, 113.7 (d, *J* = 23.6 Hz), 108.1, 107.5 (d, *J* = 26.8 Hz), 67.2, 44.4, 43.3. ¹⁹F NMR (376 MHz, CDCl₃) δ -121.07. The er was determined by HPLC using a chiral Chiralpack ID column [hexane/*i*-PrOH (90:10)]; flow rate 1.0 mL/min; *T*_{minor}=7.2 min; *T*_{major}=9.0 min (1:99 er). $[\alpha]_D^{20} = -33.7$ (*c*=1.0, CHCl₃). HRMS calculated for [C₂₆H₁₉FN₂OS+H⁺]: 427.1275; found: 427.1278.

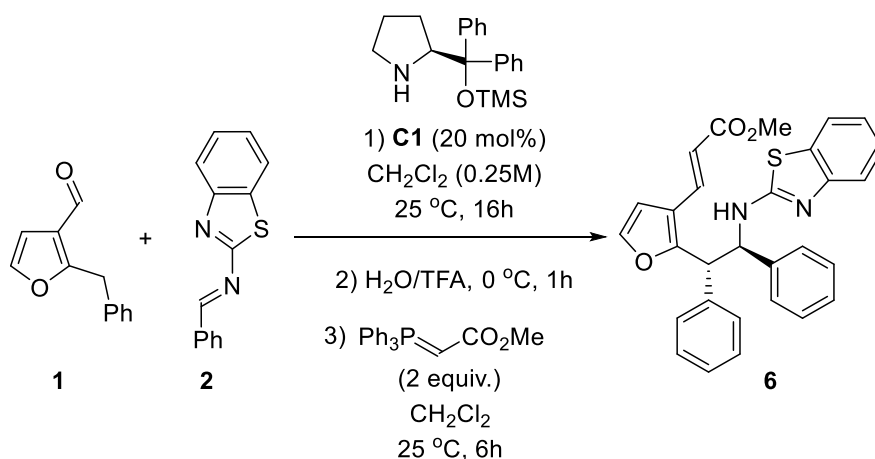
(6*R*,7*S*)-5-(Benzo[*d*]thiazol-2-yl)-7-(3-methoxyphenyl)-6-phenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4k



4

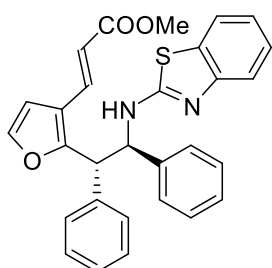
Following the general procedure, product **4k** (15:1 dr in a crude reaction mixture) in 58% (25.6 mg) yield as a light-yellow oil. ¹H NMR (700 MHz, CDCl₃) δ 7.57 – 7.51 (m, 2H), 7.40 (d, J = 1.9 Hz, 1H), 7.34 – 7.31 (m, 2H), 7.30 – 7.26 (m, 4H), 7.22 – 7.18 (m, 1H), 7.06 (td, J = 7.6, 1.2 Hz, 1H), 6.83 (dt, J = 7.7, 1.3 Hz, 1H), 6.78 – 6.76 (m, 2H), 6.36 (d, J = 2.0 Hz, 1H), 5.62 (s, 1H), 5.17 (d, J = 15.7 Hz, 1H), 4.62 (s, 1H), 4.24 (dd, J = 15.7, 1.8 Hz, 1H), 3.69 (s, 3H). ¹³C NMR (176 MHz, CDCl₃) δ 168.8, 160.0, 152.7, 148.3, 143.0, 142.8, 139.1, 130.7, 130.0, 128.9 (2C), 128.2, 126.9 (2C), 126.1, 121.6, 120.8, 120.1, 119.4, 115.2, 113.5, 112.9, 108.1, 66.8, 55.3, 44.3, 43.2. The er was determined by HPLC using a chiral Chiralpack ID column [hexane/*i*-PrOH (90:10)]; flow rate 1.0 mL/min; T_{minor}=10.5 min; T_{major}=18.5 min (1:99 er). [α]_D²⁰ = –55.1 (c=1.0, CHCl₃). HRMS calculated for [C₂₇H₂₂N₂O₂S+H⁺]: 439.1474; found: 439.1471.

Wittig olefination



To the mixture of 2-benzylfuran-3-carbaldehyde **1a** (1 equiv., 0.1 mmol) and (*E*)-*N*-benzylidenebenzo[*d*]thiazol-2-amine **2a** (2 equiv., 0.2 mmol) in CH_2Cl_2 (0.4 mL) (*S*)-(-)- α,α -diphenyl-2-pyrrolidinemethanol trimethylsilyl ether **C1** (3.9 mg, 0.02 mmol) was added and the resulting mixture was stirred at 25°C for 16 hours. Reaction mixture was then cooled down to 0°C , H_2O (5.6 equiv., 0.56 mmol, $10\mu\text{L}$) and trifluoroacetic acid (10 equiv., 10 mmol, $76.5\mu\text{L}$) were added, and the mixture was stirred at 25°C for an additional hour. Afterwards, the reaction mixture was washed with saturated NaHCO_3 solution, dried over Na_2SO_4 , filtered and concentrated *in vacuo*. The residue was dissolved in CH_2Cl_2 (0.4 mL), (carbethoxymethylene)triphenylphosphorane (2 equiv., 0.2 mmol) was added and the resulting mixture was stirred at 25°C for 6 hours. The reaction mixture was directly subjected to column chromatography on silica gel (hexanes:ethyl acetate 100:0 to 80:20) to furnish pure compound **6**.

(*E*)-Methyl 3-(2-((1*S*,2*R*)-2-(benzo[*d*]thiazol-2-ylamino)-1,2-diphenylethyl)furan-3-yl)acrylate **6**



Product **6** (20:1 dr in a crude reaction mixture) was isolated in 55% (26.5 mg) yield as a light-yellow oil. ^1H NMR (700 MHz, CDCl_3) δ 7.49 (td, $J = 8.0, 1.2$ Hz, 2H), 7.44 (d, $J = 2.0$ Hz, 1H), 7.34 (d, $J = 15.6$ Hz, 1H), 7.28 – 7.15 (m, 11H), 7.03 (ddd, $J = 8.2, 7.4, 1.2$ Hz, 1H), 6.50 (d, $J = 2.0$ Hz, 1H), 6.23 (s, 1H), 6.03 (d, $J = 15.6$ Hz, 1H), 5.39 (d, $J = 7.2$ Hz, 1H), 4.66 (d, $J = 7.2$ Hz, 1H), 3.76 (s, 3H). ^{13}C NMR (176 MHz, CDCl_3) δ 167.4, 166.7, 154.1, 152.0, 143.4, 139.4, 137.7, 133.7, 130.9, 128.8 (2C), 128.6 (2C), 128.5 (2C), 128.1, 127.6, 127.0 (2C), 126.0, 121.7, 120.9, 120.6, 119.2, 118.0, 108.2, 63.3, 51.7, 49.8. The er was determined by HPLC

using a chiral Chiralpack IC column [hexane/*i*-PrOH (90:10)]; flow rate 1.0 mL/min; $\tau_{\text{minor}}=5.3$ min; $\tau_{\text{major}}=6.1$ min (1:99 er). $[\alpha]_D^{20} = -41.1$ (c=1.0, CHCl₃). HRMS calculated for [C₂₉H₂₄N₂O₃S+H⁺]: 481.1580; found: 481.1579.

5. X-Ray crystallography of 4g

The crystal structure of the compound **4g**, $C_{27}H_{22}N_2O_2S$, was established by single-crystal X-ray diffraction at 100 K. The compound crystallizes in the non-centrosymmetric monoclinic space group $P2_1$ ($Z = 4$), with two crystallographically independent formula units per unit cell (Figure 1).

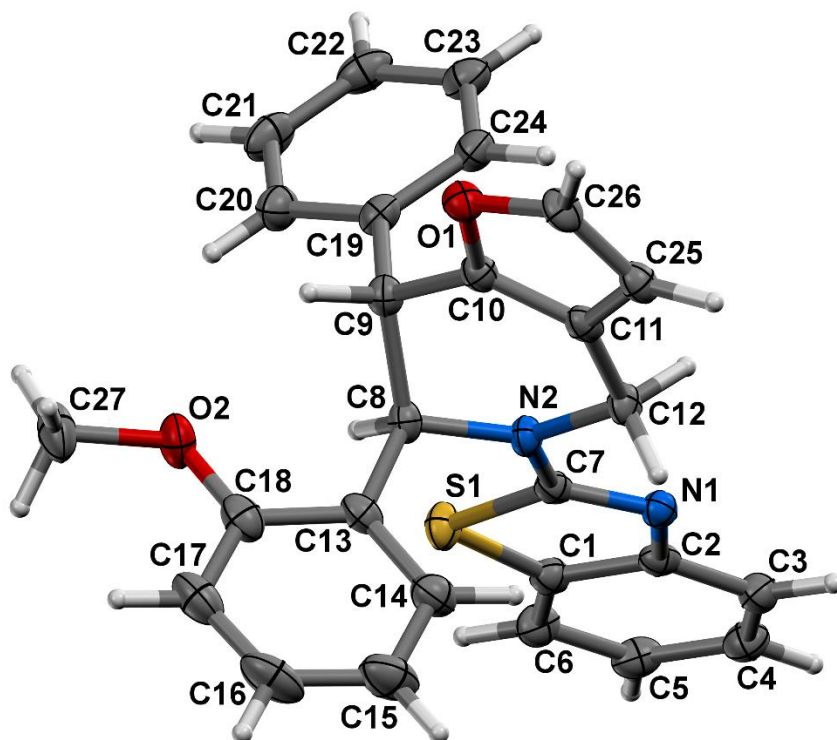


Figure 1. The molecular structure of the compound 4f at 100 K, showing 50% probability displacement ellipsoids. One of two independent molecules is shown. Hydrogen atoms are drawn with an arbitrary radius.

Single crystal X-ray diffraction data were collected at 100 K by the ω -scan technique using a RIGAKU XtaLAB Synergy, Dualflex, Pilatus 300K diffractometer³ with PhotonJet micro-focus X-ray Source Cu-K α ($\lambda = 1.54184 \text{ \AA}$). Data collection, cell refinement, data reduction and absorption correction were performed using CrysAlis PRO software. The crystal structure was solved using direct methods and the SHELXT 2018/2 program⁴ with atomic scattering factors taken from the International Tables for X-ray Crystallography. Positional parameters of non-H-atoms were refined by a full-matrix least-squares method on F^2 with anisotropic thermal parameters by using the

³ Rigaku OD. CrysAlis PRO. Rigaku Oxford Diffraction Ltd, Yarnton, Oxfordshire, England, 2019

⁴ G.M. Sheldrick, *Acta Cryst.* 2015, **A71**, 3.

SHELXL 2019/2 program⁵. All hydrogen atoms were found from the difference Fourier maps and for further calculations they were positioned geometrically in calculated positions (C–H = 0.95–1.00 Å) and constrained to ride on their parent atoms with isotropic displacement parameters set to 1.2–1.5 times the U_{eq} of the parent atom.

4f: Formula $C_{27}H_{22}N_2O_2S$, monoclinic, space group $P2_1$, $Z = 4$, unit cell constants $a = 9.3277(1)$, $b = 26.9016(1)$, $c = 9.3909(1)$ Å, $\beta = 107.691(1)^\circ$, $V = 2245.02(4)$ Å³. The integration of the data yielded a total of 112889 reflections with θ angles in the range of 3.29 to 67.74°, of which 8120 were unique ($R_{int} = 2.90\%$). The final anisotropic full-matrix least-squares refinement on F^2 with 580 parameters. The final R_1 was 0.0222 (for $I > 2\sigma(I)$) and wR_2 was 0.0600 (all data). The largest peak in the final difference electron density synthesis was 0.197 eÅ⁻³ and the largest hole was -0.159 eÅ⁻³. The goodness-of-fit was 1.034. The absolute configuration was unambiguously established from anomalous scattering, by calculating the x Flack parameter⁶ of 0.005(4) using 3911 quotients.

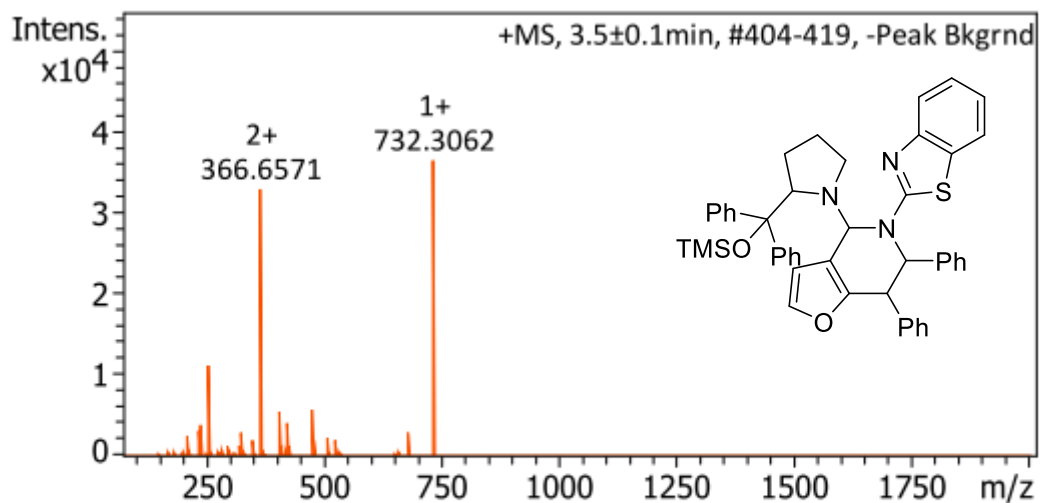
CCDC 2265527 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures

⁵ G.M. Sheldrick *Acta Cryst.* 2015, **C71**, 3.

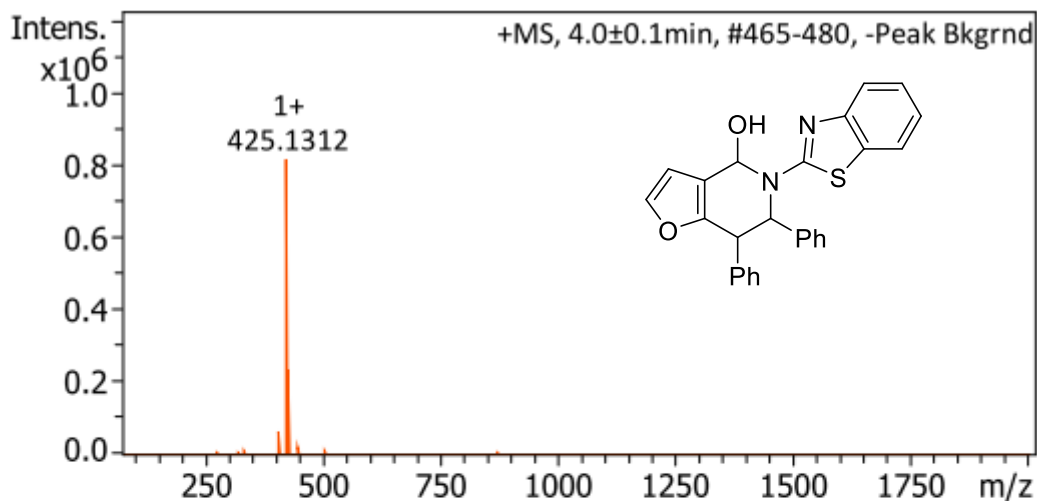
⁶ S. Parsons; H.D. Flack, T. Wagner *Acta Cryst.* 2013, **B69**, 249.

6. Mechanistic studies

6.1. HRMS experiments of a reaction mixture



#	m/z	Res.	S/N	I	I %	FWHM	z
1	213.1460	26167	106.8	2478	6.8	0.0081	
2	236.1435	28991	128.3	3181	8.7	0.0081	1+
3	239.0634	27650	155.2	3891	10.7	0.0086	1+
4	255.1195	27101	427.6	11270	30.9	0.0094	1+
5	256.1221	26356	80.4	2126	5.8	0.0097	1+
6	326.3776	32007	88.3	2900	7.9	0.0102	1+
7	366.6571	30791	901.9	33001	90.4	0.0119	2+
8	367.1584	32285	520.0	19054	52.2	0.0114	2+
9	367.6590	27481	206.3	7570	20.7	0.0134	2+
10	368.1593	28632	66.1	2428	6.6	0.0129	2+
11	407.1206	33766	136.4	5504	15.1	0.0121	1+
12	409.1358	30103	63.0	2553	7.0	0.0136	1+
13	425.1314	33543	99.9	4187	11.5	0.0127	1+
14	478.1945	33839	127.1	5880	16.1	0.0141	1+
15	510.2450	33132	46.0	2258	6.2	0.0154	1+
16	680.3191	38154	46.4	2835	7.8	0.0178	1+
17	732.3062	35950	573.2	36508	100.0	0.0204	1+
18	733.3090	36080	319.5	20360	55.8	0.0203	1+
19	734.3107	29089	124.5	7936	21.7	0.0252	1+
20	735.3116	28906	40.4	2576	7.1	0.0254	1+



#	m/z	Res.	S/N	I	I %	FWHM	z
1	249.1090	28485	142.6	2399	0.3	0.0087	
2	275.1060	27849	304.4	5406	0.7	0.0099	1+
3	292.2230	33036	170.3	3172	0.4	0.0088	
4	294.2425	29083	124.9	2338	0.3	0.0101	
5	320.2541	32646	340.6	6756	0.8	0.0098	1+
6	334.2346	29814	540.6	11056	1.4	0.0112	1+
7	407.1205	31079	2926.2	68116	8.4	0.0131	1+
8	408.1236	31029	819.3	19098	2.3	0.0132	1+
9	409.1211	20831	171.9	4013	0.5	0.0196	1+
10	425.1312	30540	33935.7	815264	100.0	0.0139	1+
11	426.1343	30227	9751.7	234474	28.8	0.0141	1+
12	427.1323	19740	2078.8	50040	6.1	0.0216	1+

6.2. Computational data

All DFT calculations were carried out using ORCA 5.0 package⁷. Visualization of calculated structures were done using ChemCraft (v. b648b) graphical software. All calculations utilized RIJCOSX approximation with def2/J⁸, auxiliary basis set and included PCM solvation model⁹ to account for the effects exerted by CH₂Cl₂. The ground-state structures of minima and transition states were found assuming the ω B97X-D3 long-range corrected hybrid functional¹⁰ and the def2-SVP basis set.¹¹ The harmonic vibrational frequencies were computed for located structures at the same level of theory to confirm the character of the located stationary points. For each located transition state intrinsic reaction coordinate (IRC) analysis was performed to confirm the connection between reactants and products. Single-point energy calculations were performed assuming DSD-BLYP double hybrid functional¹² with def2-TZVPP/C correlation fitting set¹³ and Domain-based Local Pair Natural Orbital (DLPNO) scheme for the treatment of MP2 part of the double hybrid, def2-TZVPP basis set, and applying counterpoise¹⁴ and D3BJ dispersion corrections¹⁵.

⁷a) F. Neese, *WIREs Comput Mol Sci.* 2012, **2**, 73; b) F. Neese, *WIREs Comput Mol Sci.* 2018, **8**, e1327; c) F. Neese, *WIREs Comput Mol Sci.* 2022, **12**, e1606.

⁸ F. Weigend, *Phys. Chem. Chem. Phys.* 2006, **8**, 1057

⁹ S. Miertuš, E. Scrocco and J. Tomasi, *Chem. Phys.* 1981, **55**, 117.

¹⁰ J.-D. Chai and M. Head-Gordon, *Phys. Chem. Chem. Phys.* 2008, **10**, 6615.

¹¹ a) F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.* 2005, **7**, 3297; b) F. Weigend, *Phys. Chem. Chem. Phys.* 2006, **8**, 1057.

¹² S. Kozuch, D. Gruzman and J. M. L. Martin, *J. Phys. Chem. C* 2010, **114**, 20801.

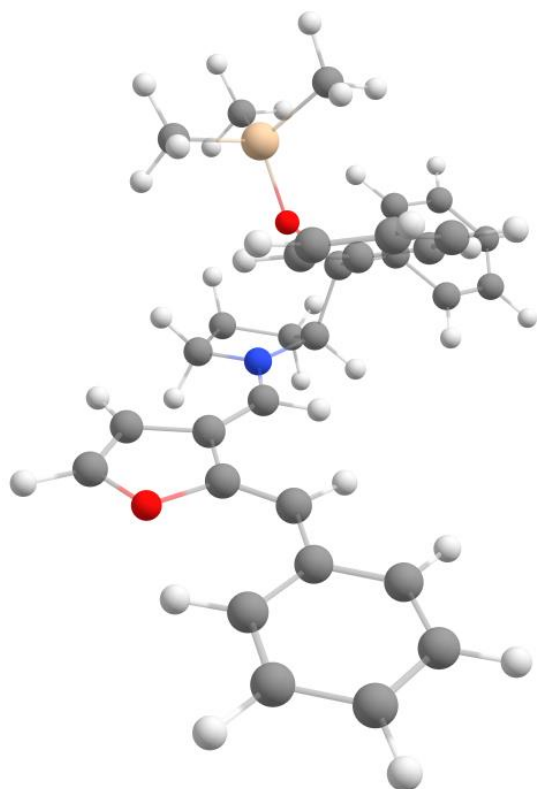
¹³ A. Hellweg, C. Hattig, S. Hofener and W. Klopper *Theor. Chem. Acc.* 2007, **117**, 587.

¹⁴ H. Kruse and S. Grimme, *J. Chem. Phys.* 2012, **136**, 154101.

¹⁵ a) S. Grimme, S. Ehrlich and L. Goerigk, *J Comput Chem* 2011, **32**, 1456; b) S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.* 2010, **132**, 154104.

Cartesian coordinates

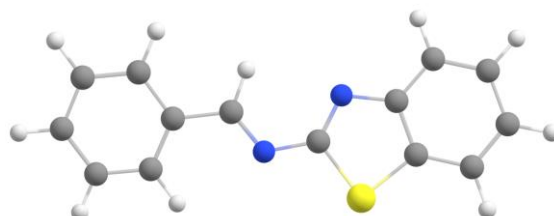
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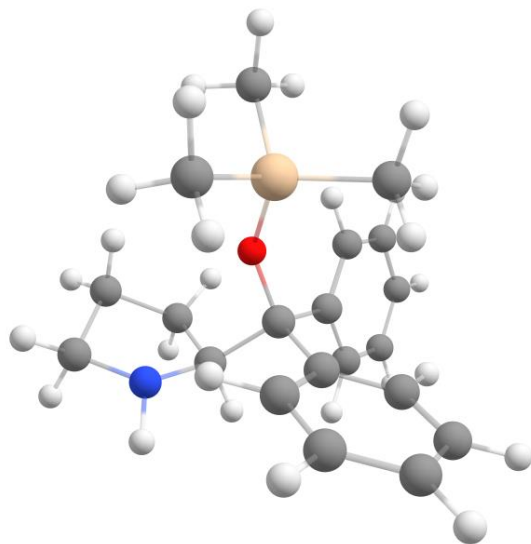
Imine 2



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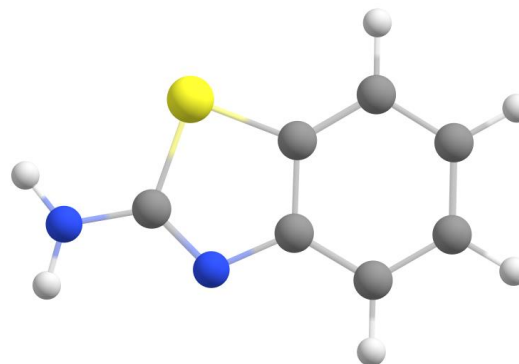
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H	-3.190696000	-0.205916000	2.651767000
C	-3.150394000	-3.416998000	1.545697000
H	-2.819219000	-4.015575000	-0.505801000
H	-3.456861000	-2.500961000	3.477380000
H	-3.277845000	-4.438072000	1.915040000
C	-2.870176000	1.712764000	1.112559000
C	-3.974853000	2.566682000	1.141744000
C	-1.890961000	1.869877000	2.105834000
C	-4.112247000	3.537956000	2.135982000
H	-4.735458000	2.481370000	0.365895000
C	-2.020451000	2.841071000	3.096542000
H	-1.014449000	1.216690000	2.122473000
C	-3.135533000	3.680743000	3.118352000
H	-4.990975000	4.188462000	2.135617000
H	-1.243897000	2.940889000	3.859619000
H	-3.239999000	4.441623000	3.896209000
O	-3.700051000	0.847151000	-0.976230000
Si	-5.224967000	0.237755000	-1.359887000
C	-6.148511000	1.715994000	-2.053031000
H	-7.133616000	1.403361000	-2.435297000
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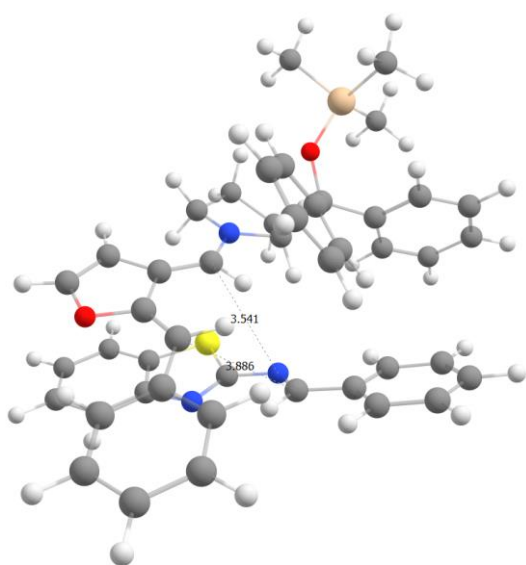
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H	-7.175144000	-0.657529000	-0.135952000
H	-5.674886000	-1.402388000	-0.476910000
C	-5.073588000	-1.050709000	-2.715233000
H	-4.710035000	-2.016664000	-2.335413000
H	-6.055974000	-1.215952000	-3.186498000
H	-4.376141000	-0.702542000	-3.493821000
C	-1.331368000	0.904135000	-0.684950000
H	-0.567063000	0.796127000	0.101640000
H	-0.376037000	-0.720787000	-1.546536000

Benzo[d]thiazol-2-amine



C	-2.596081000	0.802578000	-0.234227000
C	-1.250171000	0.455574000	-0.342927000
C	-0.215280000	1.400310000	-0.167323000
C	-0.555305000	2.728088000	0.125515000
C	-1.896983000	3.080016000	0.234479000
C	-2.911596000	2.128076000	0.057071000
H	-3.381826000	0.056242000	-0.373740000
H	0.238106000	3.466056000	0.264662000
H	-2.163773000	4.115252000	0.462687000
H	-3.959243000	2.425360000	0.146884000
C	1.057176000	-0.358270000	-0.573287000
N	1.071261000	0.910907000	-0.305047000
N	2.156720000	-1.121421000	-0.729702000
H	2.088879000	-2.055728000	-1.110311000
H	3.050655000	-0.650200000	-0.798967000
S	-0.544383000	-1.106095000	-0.692721000

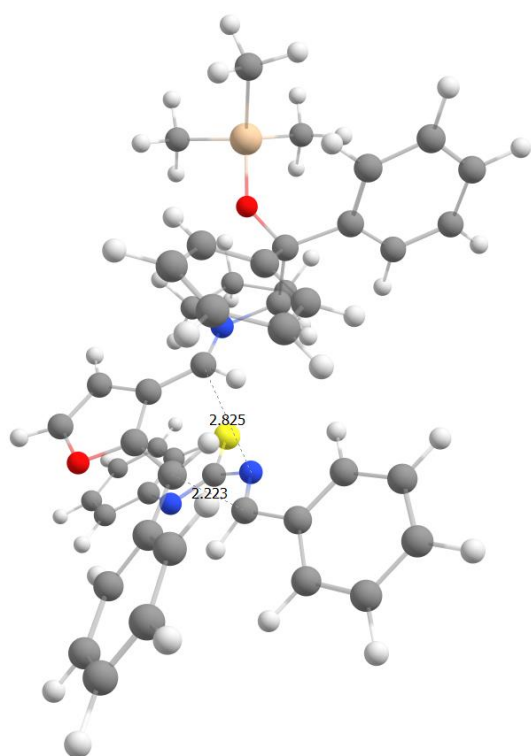
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H	-0.320623000	-3.648167000	-0.248898000
H	0.552266000	-3.428107000	-1.788518000
H	3.163189000	-2.528835000	1.316705000
H	1.527564000	-2.812146000	1.950753000
H	2.681576000	-3.664924000	-0.745367000
H	1.749978000	-4.659154000	0.398593000
N	0.543105000	-1.749718000	-0.499235000
C	2.690393000	-0.396676000	-0.236891000
C	2.025366000	0.628237000	-1.167623000
C	1.861112000	0.338893000	-2.524004000
C	1.482812000	1.817451000	-0.665695000
C	1.157894000	1.208656000	-3.359025000
H	2.275568000	-0.589782000	-2.920148000
C	0.783356000	2.689946000	-1.497903000
H	1.601591000	2.066907000	0.391457000
C	0.613315000	2.386514000	-2.849197000
H	1.030107000	0.958702000	-4.415607000
H	0.365720000	3.611237000	-1.083301000
H	0.053341000	3.063879000	-3.499176000
C	3.529232000	0.333823000	0.831034000
C	4.391391000	1.357969000	0.413354000
C	3.516644000	0.007533000	2.191605000
C	5.242259000	2.001607000	1.307323000
H	4.388852000	1.666050000	-0.634526000
C	4.367843000	0.649291000	3.093683000
H	2.840630000	-0.752392000	2.582510000
C	5.242315000	1.640115000	2.655563000
H	5.907039000	2.791978000	0.949281000
H	4.337884000	0.369243000	4.149816000
H	5.909519000	2.140876000	3.361840000
O	3.491913000	-1.262050000	-1.004717000
Si	5.129819000	-1.541429000	-1.311465000
C	6.085878000	-1.854757000	0.270674000
H	7.117548000	-2.153754000	0.022837000
H	6.133377000	-0.958504000	0.907874000
H	5.627131000	-2.669516000	0.852740000
C	5.908479000	-0.148345000	-2.301365000
H	6.181475000	0.716444000	-1.679956000
H	6.827825000	-0.519521000	-2.783098000
H	5.225585000	0.195393000	-3.094720000
C	5.102568000	-3.087894000	-2.367585000
H	4.511123000	-2.927057000	-3.282743000
H	6.126811000	-3.360565000	-2.668487000

H	4.669334000	-3.942519000	-1.825349000
C	1.574366000	-1.273809000	0.431459000
H	1.085787000	-0.647499000	1.195474000
C	-0.522759000	-0.986456000	-0.812064000
H	-0.430234000	0.046513000	-0.470164000
C	-1.676139000	-1.301195000	-1.477790000
C	-2.726901000	-0.301831000	-1.716904000
C	-2.236834000	-2.554904000	-1.990269000
O	-3.807385000	-0.956109000	-2.246564000
C	-3.481065000	-2.282187000	-2.406313000
H	-1.770970000	-3.535635000	-2.015771000
H	-4.264020000	-2.906872000	-2.830944000
C	-2.724611000	1.039024000	-1.502977000
H	-1.778174000	1.451357000	-1.145829000
C	-3.807574000	2.006199000	-1.649367000
C	-3.522551000	3.365721000	-1.396314000
C	-5.132745000	1.680343000	-2.008722000
C	-4.503129000	4.348034000	-1.495564000
H	-2.501594000	3.645718000	-1.117390000
C	-6.112444000	2.667512000	-2.104869000
H	-5.393329000	0.641818000	-2.212937000
C	-5.809993000	4.006086000	-1.850893000
H	-4.245507000	5.391586000	-1.293172000
H	-7.131541000	2.382663000	-2.382474000
H	-6.583246000	4.774584000	-1.930737000
C	-3.859532000	-1.566330000	1.341140000
C	-3.124550000	-2.739284000	1.624305000
C	-3.647017000	-4.010903000	1.368007000
C	-4.918053000	-4.093117000	0.814197000
C	-5.657530000	-2.932472000	0.519794000
C	-5.141553000	-1.672073000	0.780428000
C	-2.023322000	-0.607986000	2.090333000
H	-3.070036000	-4.911146000	1.591053000
H	-5.347921000	-5.074983000	0.601116000
H	-6.651703000	-3.027748000	0.076179000
H	-5.700938000	-0.763728000	0.546357000
N	-1.057865000	0.326951000	2.432264000
N	-3.210464000	-0.384182000	1.635152000
S	-1.577971000	-2.295068000	2.278794000
C	-1.237191000	1.538195000	2.052520000
H	-2.132921000	1.822643000	1.473996000
C	-0.257252000	2.593967000	2.321672000
C	0.906033000	2.339231000	3.064896000
C	-0.465917000	3.867818000	1.775694000
C	1.852596000	3.341363000	3.240841000
H	1.059927000	1.343638000	3.486472000
C	0.485585000	4.870782000	1.952063000
H	-1.373789000	4.063640000	1.197531000
C	1.646160000	4.605822000	2.679809000
H	2.762750000	3.136315000	3.809331000
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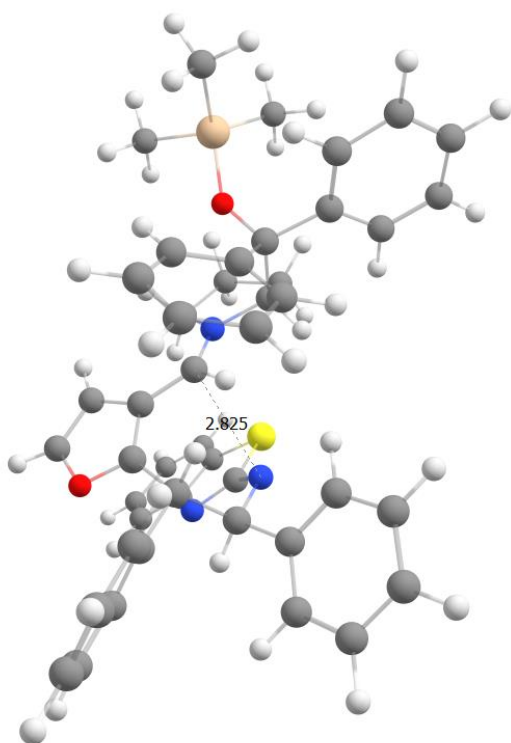
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C	2.674828000	1.789805000	-1.498058000
C	2.472974000	2.984470000	-0.555076000
H	0.433462000	3.195914000	0.230091000
H	1.624357000	2.665607000	1.451145000
H	3.734401000	1.633343000	-1.733332000
H	2.144985000	1.954324000	-2.448191000
H	3.387749000	3.191537000	0.013027000
H	2.222644000	3.895826000	-1.114618000
N	1.029754000	1.198541000	0.057314000
C	3.045629000	-0.287627000	0.042797000
C	2.230994000	-1.302965000	0.860899000
C	1.977750000	-1.085822000	2.216059000
C	1.649639000	-2.412991000	0.234402000
C	1.147124000	-1.951341000	2.931226000
H	2.423527000	-0.218160000	2.705592000
C	0.816433000	-3.274965000	0.944355000
H	1.839500000	-2.601452000	-0.826276000
C	0.558985000	-3.044374000	2.297678000
H	0.951575000	-1.761388000	3.989817000
H	0.358118000	-4.126725000	0.434728000
H	-0.099965000	-3.714857000	2.855410000
C	4.035960000	-1.059620000	-0.844811000
C	4.921046000	-1.940019000	-0.206825000
C	4.105689000	-0.950650000	-2.236760000
C	5.884265000	-2.643535000	-0.922239000
H	4.842454000	-2.085801000	0.872965000
C	5.064633000	-1.663881000	-2.961797000
H	3.414206000	-0.314081000	-2.789774000
C	5.966310000	-2.499677000	-2.308886000
H	6.567066000	-3.315077000	-0.395437000
H	5.101383000	-1.559023000	-4.049094000
H	6.719790000	-3.050646000	-2.877477000
O	3.696507000	0.593489000	0.918798000
Si	5.244292000	1.077560000	1.394683000
C	6.298507000	1.527595000	-0.087054000
H	7.276015000	1.902635000	0.257612000
H	6.477090000	0.657918000	-0.738249000

H	5.824964000	2.320154000	-0.687200000
C	6.100001000	-0.207459000	2.462974000
H	6.577451000	-1.008952000	1.881758000
H	6.885622000	0.292427000	3.053102000
H	5.388327000	-0.664027000	3.169563000
C	4.895352000	2.573296000	2.466359000
H	4.251201000	2.290525000	3.314345000
H	5.834685000	2.978746000	2.875175000
H	4.391502000	3.378334000	1.910572000
C	2.047567000	0.576129000	-0.796010000
H	1.533321000	-0.085364000	-1.508264000
C	-0.060912000	0.549900000	0.421188000
H	-0.131193000	-0.462572000	0.026112000
C	-1.106813000	0.969195000	1.242289000
C	-2.263282000	0.155622000	1.411415000
C	-1.386816000	2.195075000	1.974420000
O	-3.150576000	0.824187000	2.174774000
C	-2.617595000	2.043065000	2.497856000
H	-0.753157000	3.068625000	2.096961000
H	-3.244143000	2.682147000	3.115263000
C	-2.545768000	-1.109479000	0.873725000
H	-1.651017000	-1.706235000	0.684874000
C	-3.733995000	-1.897878000	1.235447000
C	-3.612895000	-3.287871000	1.406578000
C	-5.016956000	-1.329515000	1.339647000
C	-4.723774000	-4.078921000	1.691897000
H	-2.626528000	-3.751250000	1.308187000
C	-6.127398000	-2.121556000	1.624824000
H	-5.142301000	-0.256040000	1.182717000
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H	-4.600194000	-5.157580000	1.822491000
H	-7.114609000	-1.657266000	1.700751000
H	-6.861597000	-4.117621000	2.029282000
C	-3.534564000	3.303624000	-0.792068000
C	-2.470805000	3.998909000	-1.414073000
C	-2.417884000	5.393298000	-1.433466000
C	-3.445774000	6.103076000	-0.816942000
C	-4.507473000	5.427746000	-0.194800000
C	-4.560146000	4.038461000	-0.178890000
C	-2.374849000	1.528950000	-1.451354000
H	-1.589327000	5.915206000	-1.918487000
H	-3.423007000	7.195687000	-0.819060000
H	-5.304742000	6.001805000	0.284789000
H	-5.381261000	3.506673000	0.307814000
N	-1.942175000	0.267785000	-1.667552000
N	-3.454770000	1.927397000	-0.835914000
S	-1.350310000	2.839363000	-2.080556000
C	-2.758819000	-0.715529000	-1.303400000
H	-3.820412000	-0.498539000	-1.121251000
C	-2.446665000	-2.089995000	-1.763358000
C	-1.146645000	-2.437452000	-2.157895000
C	-3.452080000	-3.064184000	-1.808659000
C	-0.853640000	-3.736105000	-2.562405000
H	-0.370835000	-1.668706000	-2.144928000
C	-3.161121000	-4.363583000	-2.224634000
H	-4.471618000	-2.798791000	-1.515438000
C	-1.860608000	-4.705320000	-2.594448000
H	0.166383000	-3.996365000	-2.858026000
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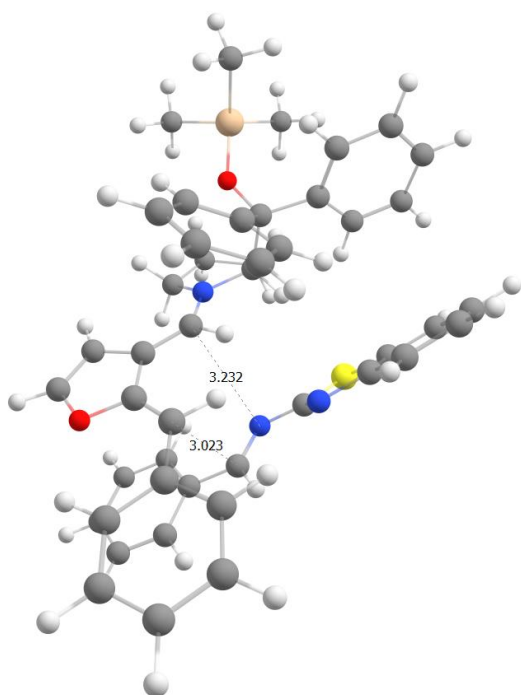
INT1



C	1.496889000	2.514604000	0.517119000
C	2.803066000	1.715438000	-1.391947000
C	2.692353000	2.856782000	-0.373134000
H	0.633288000	3.170828000	0.333723000
H	1.747412000	2.544890000	1.587634000
H	3.850053000	1.488081000	-1.624449000
H	2.301112000	1.985892000	-2.332129000
H	3.605915000	2.925225000	0.229694000
H	2.549732000	3.826003000	-0.869131000
N	1.119018000	1.147459000	0.145210000
C	2.998074000	-0.493458000	-0.012240000
C	2.110326000	-1.498358000	0.740957000
C	1.877965000	-1.352866000	2.109695000
C	1.446554000	-2.518737000	0.046428000
C	0.991704000	-2.203551000	2.774092000
H	2.385080000	-0.552644000	2.651658000
C	0.560040000	-3.366619000	0.706824000
H	1.617078000	-2.648858000	-1.026423000
C	0.328613000	-3.210321000	2.075634000
H	0.815869000	-2.071517000	3.844726000
H	0.043086000	-4.151679000	0.148991000
H	-0.366553000	-3.874609000	2.595467000
C	3.912750000	-1.275873000	-0.970043000
C	4.711135000	-2.287156000	-0.417432000
C	3.982620000	-1.062329000	-2.349897000
C	5.589783000	-3.026109000	-1.202721000
H	4.625638000	-2.513826000	0.647517000
C	4.856459000	-1.809165000	-3.144860000
H	3.352596000	-0.320301000	-2.841149000
C	5.671861000	-2.782873000	-2.575325000
H	6.203521000	-3.804843000	-0.742660000
H	4.892435000	-1.623274000	-4.221245000
H	6.354958000	-3.364684000	-3.199340000
O	3.715655000	0.276863000	0.911065000
Si	5.289457000	0.528030000	1.480433000
C	6.439847000	0.998245000	0.079634000
H	7.436224000	1.239946000	0.484264000
H	6.557470000	0.177199000	-0.644700000

H	6.069419000	1.884884000	-0.458052000
C	5.954328000	-0.948250000	2.431307000
H	6.427287000	-1.698120000	1.781005000
H	6.714481000	-0.597314000	3.148208000
H	5.152981000	-1.440490000	3.005259000
C	5.053532000	1.949822000	2.674221000
H	4.364455000	1.658706000	3.483065000
H	6.015158000	2.231621000	3.131935000
H	4.639121000	2.839785000	2.176670000
C	2.076246000	0.509594000	-0.777651000
H	1.490943000	-0.043910000	-1.526089000
C	0.017777000	0.554658000	0.496038000
H	-0.138614000	-0.429688000	0.058694000
C	-1.010144000	1.040906000	1.349167000
C	-2.244146000	0.403435000	1.361072000
C	-1.146271000	2.185435000	2.223499000
O	-3.068196000	1.050405000	2.178357000
C	-2.411419000	2.128000000	2.696746000
H	-0.403908000	2.934193000	2.484492000
H	-2.981230000	2.743561000	3.387691000
C	-2.691766000	-0.800889000	0.608177000
H	-1.841335000	-1.500074000	0.636420000
C	-3.877063000	-1.499585000	1.239589000
C	-3.748803000	-2.812885000	1.701130000
C	-5.129386000	-0.876736000	1.318265000
C	-4.845297000	-3.495073000	2.229048000
H	-2.777746000	-3.312043000	1.633443000
C	-6.225884000	-1.554776000	1.847123000
H	-5.248696000	0.148389000	0.957423000
C	-6.087972000	-2.867248000	2.303171000
H	-4.726966000	-4.523673000	2.579799000
H	-7.197084000	-1.055713000	1.899807000
H	-6.950009000	-3.398420000	2.715210000
C	-2.824760000	3.602498000	-0.888173000
C	-1.669525000	4.032024000	-1.595004000
C	-1.324873000	5.376279000	-1.699696000
C	-2.143184000	6.331177000	-1.090471000
C	-3.288186000	5.929089000	-0.391204000
C	-3.632236000	4.582781000	-0.286619000
C	-2.087886000	1.566342000	-1.462459000
H	-0.429435000	5.679502000	-2.249151000
H	-1.887366000	7.391259000	-1.162632000
H	-3.923208000	6.683088000	0.082653000
H	-4.522449000	4.268857000	0.264863000
N	-1.910869000	0.275649000	-1.549522000
N	-3.041642000	2.250787000	-0.836544000
S	-0.851147000	2.628631000	-2.246514000
C	-2.944007000	-0.515673000	-0.942980000
H	-3.920534000	-0.002671000	-0.991314000
C	-3.064371000	-1.865653000	-1.630821000
C	-1.916446000	-2.562488000	-2.025584000
C	-4.312683000	-2.459416000	-1.839299000
C	-2.012246000	-3.828801000	-2.600415000
H	-0.940130000	-2.091690000	-1.885688000
C	-4.414294000	-3.727173000	-2.414964000
H	-5.218478000	-1.924254000	-1.539196000
C	-3.263647000	-4.418189000	-2.794068000
H	-1.104318000	-4.358472000	-2.902928000
H	-5.399571000	-4.176242000	-2.566991000
H	-3.340990000	-5.410788000	-3.245910000

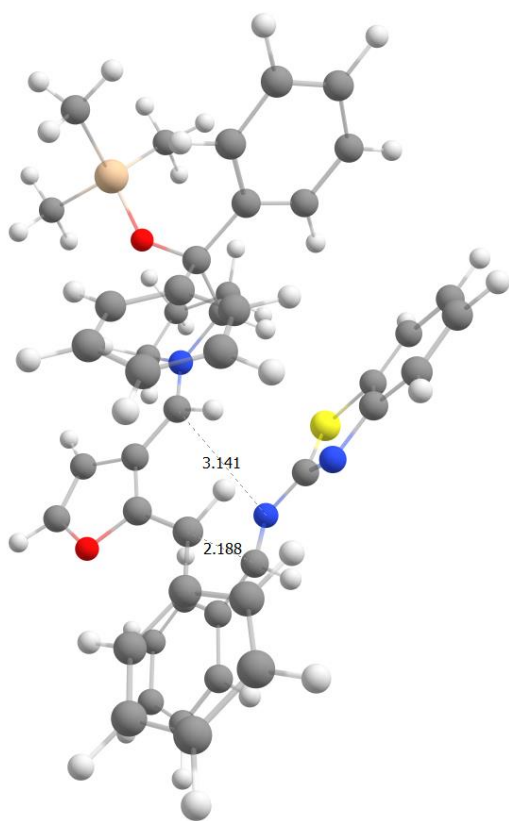
dr-RC



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H	0.167165000	-3.116317000	-1.986044000
H	-0.820765000	-3.768519000	-0.656048000
H	-3.376399000	-1.115041000	-2.371526000
H	-1.794981000	-0.819293000	-3.120776000
H	-2.826468000	-3.350046000	-1.780458000
H	-1.840634000	-3.218298000	-3.248162000
N	-0.607814000	-1.658945000	-0.699735000
C	-2.732317000	-0.641115000	0.214215000
C	-1.930585000	-0.419263000	1.503500000
C	-1.626646000	-1.489286000	2.346110000
C	-1.392228000	0.840555000	1.791389000
C	-0.787164000	-1.309857000	3.447175000
H	-2.037807000	-2.474797000	2.119875000
C	-0.550509000	1.021764000	2.886511000
H	-1.622756000	1.691447000	1.143871000
C	-0.239555000	-0.056608000	3.716899000
H	-0.551221000	-2.160451000	4.092107000
H	-0.131787000	2.011029000	3.089482000
H	0.428399000	0.082012000	4.570988000
C	-3.718545000	0.526464000	0.024208000
C	-4.528876000	0.883884000	1.112129000
C	-3.870835000	1.241661000	-1.167578000
C	-5.489585000	1.884330000	1.003701000
H	-4.394089000	0.375317000	2.069599000
C	-4.832669000	2.248865000	-1.281527000
H	-3.238447000	1.038809000	-2.032019000
C	-5.651570000	2.568713000	-0.202659000
H	-6.109439000	2.136631000	1.867925000
H	-4.932800000	2.789114000	-2.226319000
H	-6.403774000	3.356276000	-0.295610000
O	-3.399530000	-1.876831000	0.280611000
Si	-4.975472000	-2.464368000	0.445186000
C	-6.124749000	-1.737104000	-0.845428000
H	-7.092883000	-2.263098000	-0.811358000
H	-6.312125000	-0.665693000	-0.676462000
H	-5.707090000	-1.860643000	-1.857207000
C	-5.650106000	-2.195854000	2.177675000
H	-6.059056000	-1.185994000	2.325067000

H	-6.462073000	-2.917745000	2.363988000
H	-4.866853000	-2.367036000	2.933323000
C	-4.765104000	-4.304425000	0.167243000
H	-4.029705000	-4.721663000	0.873185000
H	-5.723052000	-4.825030000	0.325989000
H	-4.425203000	-4.528318000	-0.855501000
C	-1.713195000	-0.740091000	-0.969043000
H	-1.296852000	0.266839000	-1.120111000
C	0.508846000	-1.259046000	-0.068641000
H	0.495167000	-0.203927000	0.215733000
C	1.631856000	-1.972047000	0.265143000
C	2.796009000	-1.342546000	0.894265000
C	2.005603000	-3.379789000	0.113065000
O	3.756597000	-2.306477000	1.040506000
C	3.256045000	-3.501054000	0.579738000
H	1.408611000	-4.190433000	-0.294912000
H	3.930965000	-4.350539000	0.658936000
C	3.003630000	-0.051290000	1.270977000
H	2.164362000	0.628037000	1.105292000
C	4.216964000	0.575634000	1.784816000
C	4.223554000	1.980643000	1.929135000
C	5.404057000	-0.112984000	2.113164000
C	5.356064000	2.664288000	2.360481000
H	3.317095000	2.539555000	1.676225000
C	6.535055000	0.576092000	2.548721000
H	5.439461000	-1.197683000	2.017737000
C	6.525295000	1.966082000	2.672712000
H	5.326295000	3.753841000	2.451570000
H	7.440657000	0.013295000	2.793690000
H	7.417533000	2.499720000	3.010338000
C	0.086050000	3.297140000	-0.439201000
C	-0.745189000	3.356877000	-1.578295000
C	-1.856362000	4.202604000	-1.630574000
C	-2.135483000	4.984397000	-0.516313000
C	-1.314277000	4.936725000	0.624334000
C	-0.203981000	4.105261000	0.670338000
C	1.141520000	1.793874000	-1.668552000
H	-2.492833000	4.238726000	-2.517227000
H	-3.007501000	5.642759000	-0.527706000
H	-1.554803000	5.564529000	1.485742000
H	0.441117000	4.062703000	1.550855000
N	1.999985000	0.795016000	-2.070236000
N	1.137314000	2.402606000	-0.525783000
S	-0.153669000	2.238809000	-2.774796000
C	3.202386000	0.805799000	-1.621183000
H	3.578129000	1.651109000	-1.020597000
C	4.144129000	-0.284694000	-1.888703000
C	3.730493000	-1.452143000	-2.547527000
C	5.464847000	-0.174964000	-1.434436000
C	4.626602000	-2.496811000	-2.742053000
H	2.695403000	-1.526997000	-2.888017000
C	6.361639000	-1.222856000	-1.630764000
H	5.781553000	0.731361000	-0.910338000
C	5.942052000	-2.384220000	-2.281035000
H	4.299023000	-3.408632000	-3.247670000
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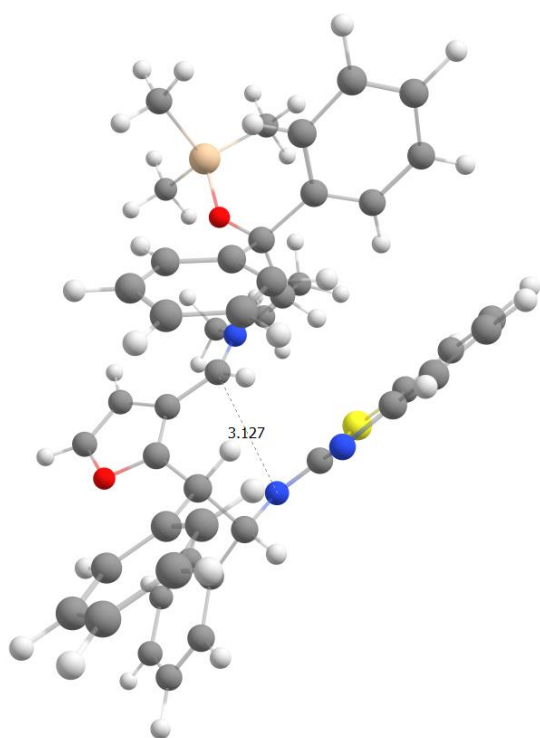
dr-TS1



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C	-2.455141000	-1.828631000	-2.789296000
H	-0.318263000	-2.369433000	-2.755449000
H	-1.292206000	-3.163914000	-1.488068000
H	-3.850034000	-0.247431000	-2.189162000
H	-2.421546000	0.337224000	-3.058072000
H	-3.269299000	-2.514509000	-2.525945000
H	-2.330707000	-1.875249000	-3.879237000
N	-0.865317000	-1.122221000	-1.170838000
C	-2.791351000	-0.480857000	0.292140000
C	-1.806592000	-0.441034000	1.471124000
C	-1.341977000	-1.619648000	2.055015000
C	-1.288294000	0.783760000	1.912475000
C	-0.361361000	-1.579841000	3.049304000
H	-1.738851000	-2.575228000	1.707334000
C	-0.303929000	0.824676000	2.896842000
H	-1.646282000	1.718597000	1.470737000
C	0.167673000	-0.360467000	3.466761000
H	-0.000002000	-2.513390000	3.488326000
H	0.099468000	1.788053000	3.220185000
H	0.947897000	-0.329029000	4.231686000
C	-3.884211000	0.570874000	0.544473000
C	-4.612780000	0.470155000	1.738115000
C	-4.175575000	1.631942000	-0.316554000
C	-5.634049000	1.364531000	2.040029000
H	-4.359867000	-0.315612000	2.453501000
C	-5.193277000	2.540557000	-0.012755000
H	-3.607536000	1.786518000	-1.234120000
C	-5.935096000	2.403994000	1.156907000
H	-6.189071000	1.258177000	2.975685000
H	-5.399448000	3.362534000	-0.702960000
H	-6.733163000	3.113266000	1.390604000
O	-3.311540000	-1.778077000	0.170697000
Si	-4.789640000	-2.599510000	0.205697000
C	-6.047859000	-1.781283000	-0.916399000

H	-6.983596000	-2.363741000	-0.905180000
H	-6.280571000	-0.758631000	-0.580711000
H	-5.693659000	-1.731737000	-1.957776000
C	-5.477895000	-2.770209000	1.944548000
H	-6.057861000	-1.891963000	2.262519000
H	-6.147714000	-3.645226000	1.975036000
H	-4.671087000	-2.939298000	2.675432000
C	-4.322587000	-4.306713000	-0.406439000
H	-3.565541000	-4.753375000	0.257947000
H	-5.205195000	-4.966267000	-0.408523000
H	-3.910529000	-4.285813000	-1.426563000
C	-1.989995000	-0.190391000	-1.018029000
H	-1.585713000	0.829504000	-0.948474000
C	0.282777000	-0.943701000	-0.547968000
H	0.349124000	0.003229000	-0.009225000
C	1.382546000	-1.794458000	-0.443396000
C	2.541365000	-1.395745000	0.285835000
C	1.629735000	-3.172779000	-0.842699000
O	3.399337000	-2.434054000	0.320916000
C	2.841157000	-3.492346000	-0.352850000
H	0.981093000	-3.836694000	-1.407477000
H	3.442045000	-4.397712000	-0.384389000
C	2.870981000	-0.136948000	0.803328000
H	2.020784000	0.546962000	0.857934000
C	3.913612000	0.162211000	1.793225000
C	3.869622000	1.428750000	2.410453000
C	4.974191000	-0.696493000	2.136633000
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H	3.055268000	2.112715000	2.151067000
C	5.938800000	-0.301681000	3.063478000
H	5.045496000	-1.679933000	1.672987000
C	5.880901000	0.956107000	3.663616000
H	4.774349000	2.811129000	3.791652000
H	6.750892000	-0.989645000	3.315127000
H	6.641675000	1.259962000	4.387245000
C	0.076327000	3.209088000	-0.660406000
C	-0.599620000	3.103852000	-1.899365000
C	-1.771720000	3.815334000	-2.160597000
C	-2.281546000	4.640202000	-1.161457000
C	-1.629486000	4.748235000	0.076528000
C	-0.458875000	4.042676000	0.333535000
C	1.461820000	1.760955000	-1.626887000
H	-2.279014000	3.724816000	-3.124304000
H	-3.199362000	5.204385000	-1.343546000
H	-2.046550000	5.398350000	0.849861000
H	0.053454000	4.123855000	1.295168000
N	2.454039000	0.892159000	-1.881636000
N	1.223031000	2.450419000	-0.538995000
S	0.268353000	1.992848000	-2.925695000
C	3.486918000	0.862433000	-1.042521000
H	3.690936000	1.737144000	-0.407063000
C	4.662292000	0.041962000	-1.409766000
C	4.539291000	-0.998303000	-2.342188000
C	5.908080000	0.280617000	-0.815698000
C	5.634924000	-1.794039000	-2.660493000
H	3.565299000	-1.168916000	-2.807000000
C	7.007617000	-0.515875000	-1.137369000
H	6.015129000	1.097327000	-0.096531000
C	6.872673000	-1.557571000	-2.054870000
H	5.525494000	-2.605042000	-3.385613000
H	7.974929000	-0.322643000	-0.666281000
H	7.733532000	-2.183827000	-2.303909000

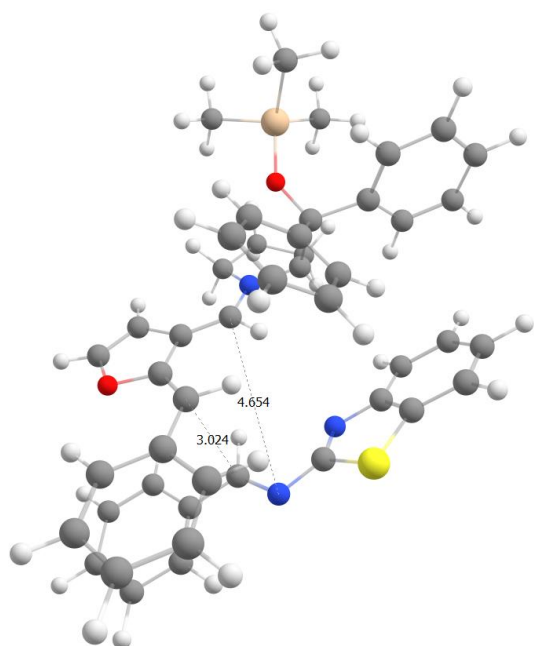
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H	-0.239341000	-2.395348000	-2.676119000
H	-1.725518000	-2.843647000	-1.774231000
H	-3.806204000	-0.569340000	-2.142287000
H	-2.880030000	0.756682000	-2.864255000
H	-2.685021000	-1.871330000	-3.809799000
H	-1.360671000	-0.688978000	-3.923274000
N	-0.867688000	-1.011649000	-1.219486000
C	-2.790055000	-0.454484000	0.247557000
C	-1.810652000	-0.465843000	1.430921000
C	-1.331912000	-1.667712000	1.954008000
C	-1.307640000	0.741833000	1.933343000
C	-0.347899000	-1.666898000	2.946032000
H	-1.720471000	-2.609083000	1.561301000
C	-0.319476000	0.743461000	2.914116000
H	-1.674014000	1.693780000	1.537489000
C	0.169668000	-0.463780000	3.420704000
H	0.024188000	-2.616951000	3.337982000
H	0.074751000	1.693997000	3.283044000
H	0.952527000	-0.461933000	4.183459000
C	-3.910051000	0.548494000	0.557820000
C	-4.631790000	0.359896000	1.745422000
C	-4.239584000	1.636012000	-0.252328000
C	-5.679125000	1.205192000	2.093275000
H	-4.357049000	-0.458208000	2.415891000
C	-5.285864000	2.494421000	0.098089000
H	-3.680148000	1.850340000	-1.162941000
C	-6.015967000	2.277193000	1.262544000
H	-6.229686000	1.034108000	3.021782000
H	-5.522401000	3.341406000	-0.550896000
H	-6.835242000	2.948265000	1.532701000
O	-3.275552000	-1.749866000	0.031840000
Si	-4.723712000	-2.627843000	-0.000117000
C	-6.154154000	-1.656264000	-0.722318000
H	-7.035897000	-2.316514000	-0.769949000
H	-6.419167000	-0.779250000	-0.113340000
H	-5.937159000	-1.315722000	-1.746813000

C	-5.129551000	-3.243293000	1.722371000
H	-5.480047000	-2.438984000	2.385593000
H	-5.925069000	-4.003901000	1.665138000
H	-4.245596000	-3.710553000	2.184331000
C	-4.314408000	-4.079756000	-1.108601000
H	-3.452157000	-4.643694000	-0.719564000
H	-5.172204000	-4.768389000	-1.170165000
H	-4.074962000	-3.743416000	-2.129814000
C	-1.992611000	-0.068630000	-1.046767000
H	-1.572512000	0.938815000	-0.923808000
C	0.240269000	-0.882100000	-0.562357000
H	0.324670000	0.045293000	0.010929000
C	1.326168000	-1.799166000	-0.462728000
C	2.522044000	-1.408244000	0.122332000
C	1.463473000	-3.206508000	-0.766051000
O	3.341894000	-2.456575000	0.176029000
C	2.705196000	-3.543202000	-0.350376000
H	0.728318000	-3.880879000	-1.197947000
H	3.267822000	-4.472981000	-0.343556000
C	2.958611000	-0.051993000	0.537288000
H	2.042963000	0.496574000	0.798866000
C	3.860739000	0.048293000	1.749295000
C	3.606155000	1.096208000	2.645954000
C	4.956822000	-0.787940000	1.996047000
C	4.410520000	1.299870000	3.764744000
H	2.761973000	1.765012000	2.451845000
C	5.761203000	-0.588191000	3.119360000
H	5.188904000	-1.600603000	1.307190000
C	5.492462000	0.452683000	4.007528000
H	4.188751000	2.122372000	4.449889000
H	6.610090000	-1.253665000	3.297965000
H	6.125808000	0.605251000	4.885342000
C	0.110246000	3.214793000	-0.470191000
C	-0.549873000	3.158608000	-1.727773000
C	-1.719621000	3.868582000	-1.981331000
C	-2.264491000	4.656554000	-0.964064000
C	-1.633979000	4.721355000	0.283873000
C	-0.459773000	4.012989000	0.536246000
C	1.535096000	1.783537000	-1.457592000
H	-2.206059000	3.807150000	-2.958711000
H	-3.184319000	5.218048000	-1.144897000
H	-2.067888000	5.337460000	1.076397000
H	0.029691000	4.065258000	1.512315000
N	2.495524000	0.949236000	-1.719571000
N	1.245389000	2.456557000	-0.339690000
S	0.340640000	2.089814000	-2.790127000
C	3.501424000	0.778774000	-0.710403000
H	3.785180000	1.747382000	-0.256454000
C	4.743521000	0.131464000	-1.291942000
C	4.628377000	-0.861888000	-2.271819000
C	6.019082000	0.482513000	-0.839453000
C	5.758633000	-1.505801000	-2.771130000
H	3.632560000	-1.114186000	-2.645030000
C	7.155052000	-0.156144000	-1.340714000
H	6.125349000	1.266695000	-0.083812000
C	7.027697000	-1.156512000	-2.303984000
H	5.649198000	-2.281642000	-3.534083000
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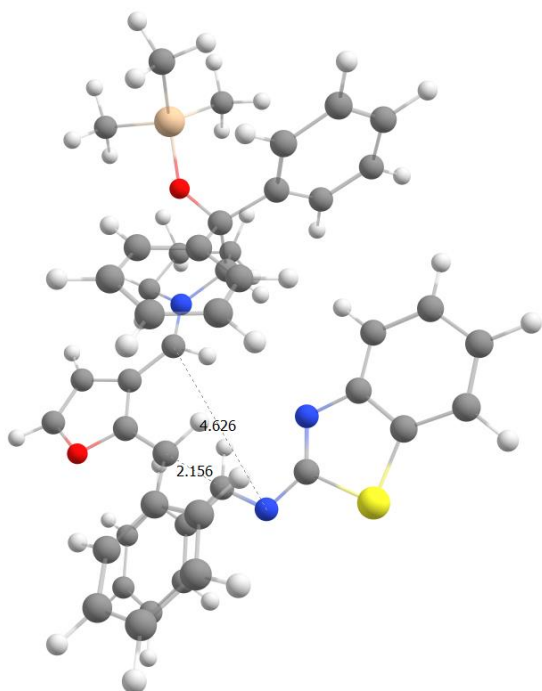
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C	-1.510065000	-2.596867000	-2.083349000
C	-3.034568000	-0.753774000	-2.517525000
C	-2.852298000	-2.258781000	-2.732314000
H	-0.724430000	-2.776446000	-2.835919000
H	-1.573994000	-3.493502000	-1.444174000
H	-4.093552000	-0.490456000	-2.415321000
H	-2.634928000	-0.187449000	-3.373048000
H	-3.661900000	-2.815411000	-2.245623000
H	-2.866283000	-2.527215000	-3.797375000
N	-1.157824000	-1.424478000	-1.295542000
C	-3.007593000	-0.417948000	0.076453000
C	-2.017964000	-0.175290000	1.227719000
C	-1.628559000	-1.210284000	2.076826000
C	-1.452006000	1.094523000	1.404467000
C	-0.687212000	-0.984894000	3.084909000
H	-2.062329000	-2.202028000	1.936597000
C	-0.509202000	1.319770000	2.404333000
H	-1.750250000	1.921006000	0.752143000
C	-0.123410000	0.278100000	3.251292000
H	-0.389955000	-1.807823000	3.740111000
H	-0.072295000	2.315234000	2.520863000
H	0.621302000	0.451992000	4.032349000
C	-4.080678000	0.683312000	0.159118000
C	-4.768006000	0.819653000	1.374576000
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H	-4.492774000	0.181608000	2.217511000
C	-5.403467000	2.525079000	-0.716165000
H	-3.860927000	1.538517000	-1.822043000
C	-6.104932000	2.619809000	0.481762000
H	-6.296699000	1.843210000	2.493478000
H	-5.631838000	3.204345000	-1.541654000
H	-6.892703000	3.367650000	0.603690000
O	-3.564721000	-1.700432000	0.204375000
Si	-5.058209000	-2.459227000	0.419965000
C	-6.339563000	-1.804393000	-0.781480000
H	-7.277416000	-2.371443000	-0.664426000
H	-6.560197000	-0.741613000	-0.596463000
H	-6.007610000	-1.912727000	-1.825774000
C	-5.682412000	-2.329593000	2.186514000
H	-6.190941000	-1.377543000	2.394878000
H	-6.404741000	-3.142569000	2.367449000
H	-4.855951000	-2.448686000	2.905257000

C	-4.664466000	-4.259678000	0.083013000
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H	-5.569402000	-4.876562000	0.203169000
H	-4.275703000	-4.420309000	-0.933823000
C	-2.207210000	-0.401549000	-1.268909000
H	-1.739609000	0.590814000	-1.366230000
C	0.026142000	-1.281952000	-0.674913000
H	0.160025000	-0.304687000	-0.204720000
C	1.060332000	-2.175829000	-0.546033000
C	2.265230000	-1.878140000	0.241741000
C	1.281671000	-3.534671000	-1.052282000
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C	2.489901000	-3.921489000	-0.620927000
H	0.623756000	-4.136268000	-1.672206000
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C	3.823419000	-0.484344000	1.700144000
C	3.961041000	0.800704000	2.266244000
C	4.901015000	-1.380488000	1.859475000
C	5.116258000	1.178778000	2.944099000
H	3.142542000	1.517540000	2.149528000
C	6.054175000	-0.999992000	2.543491000
H	4.834448000	-2.381312000	1.434222000
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C	-0.712414000	4.651719000	0.215490000
C	-1.909157000	4.698815000	-0.489938000
C	-2.081675000	3.953356000	-1.669247000
C	-1.070524000	3.135419000	-2.153224000
C	2.205938000	2.451475000	-0.970831000
H	-0.574621000	5.234883000	1.128664000
H	-2.724881000	5.328015000	-0.125662000
H	-3.028265000	4.017874000	-2.210399000
H	-1.196049000	2.549880000	-3.067028000
N	3.448219000	1.854012000	-1.014501000
N	1.231046000	2.292411000	-1.806425000
S	1.911148000	3.575878000	0.348177000
C	3.517562000	0.674819000	-1.512513000
H	2.613157000	0.163683000	-1.883484000
C	4.775662000	-0.069000000	-1.611783000
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C	7.123206000	-1.573516000	-1.741269000
H	8.086909000	0.131181000	-0.821437000
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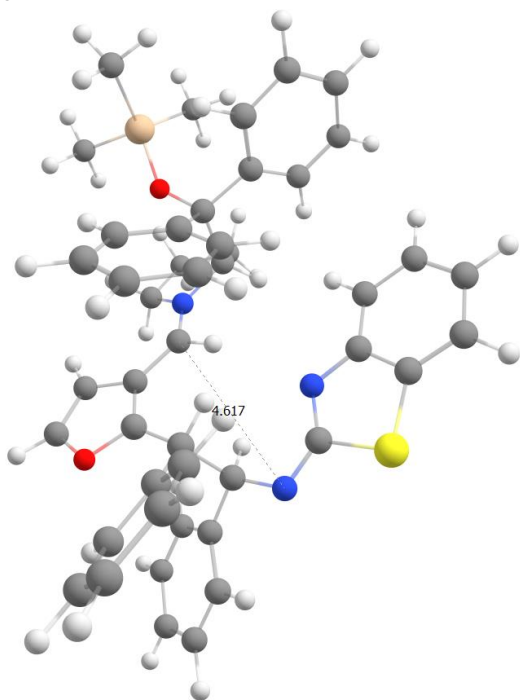
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H	-0.895599000	-3.397696000	-2.306876000
H	-1.907660000	-3.666603000	-0.862237000
H	-4.076760000	-0.750009000	-2.483864000
H	-2.579974000	-0.687187000	-3.430180000
H	-3.835273000	-3.061344000	-2.026204000
H	-2.883171000	-3.037402000	-3.517475000
N	-1.232227000	-1.686263000	-1.153849000
C	-3.061510000	-0.403208000	0.003119000
C	-2.094935000	-0.309590000	1.196020000
C	-1.839527000	-1.430338000	1.989308000
C	-1.380782000	0.867968000	1.449488000
C	-0.874948000	-1.383779000	2.997990000
H	-2.393257000	-2.351781000	1.800508000
C	-0.414374000	0.916255000	2.451896000
H	-1.572771000	1.761287000	0.851359000
C	-0.152309000	-0.214325000	3.227593000
H	-0.681017000	-2.274457000	3.601267000
H	0.139952000	1.842975000	2.623258000
H	0.614188000	-0.180921000	4.006170000
C	-3.902704000	0.884420000	-0.072735000
C	-4.533173000	1.324004000	1.099765000
C	-4.083164000	1.640224000	-1.236220000
C	-5.345190000	2.454016000	1.106122000
H	-4.369401000	0.779323000	2.032240000
C	-4.891178000	2.779973000	-1.233895000
H	-3.593910000	1.366986000	-2.171521000
C	-5.532158000	3.186942000	-0.066863000
H	-5.824876000	2.770846000	2.035747000
H	-5.012709000	3.351499000	-2.157408000
H	-6.163805000	4.078875000	-0.066355000
O	-3.860959000	-1.547838000	0.154576000
Si	-5.482443000	-1.959720000	0.414012000
C	-6.574439000	-1.248564000	-0.932676000
H	-7.616559000	-1.569598000	-0.771995000
H	-6.554007000	-0.147443000	-0.929049000
H	-6.261964000	-1.598761000	-1.929015000
C	-6.103906000	-1.448305000	2.109155000
H	-6.433485000	-0.400339000	2.144646000
H	-6.965923000	-2.082256000	2.374513000

H	-5.327445000	-1.597469000	2.876417000
C	-5.441120000	-3.830246000	0.342601000
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H	-1.674525000	0.314824000	-1.516766000
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H	0.354913000	-4.532348000	-0.795515000
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C	3.680462000	-0.294969000	1.588485000
C	3.657600000	0.994695000	2.154173000
C	4.779310000	-1.121886000	1.889612000
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H	4.627918000	2.445892000	3.414881000
H	6.637225000	-1.340213000	2.953704000
H	6.556198000	0.946103000	3.947903000
C	0.552203000	3.212897000	-0.900919000
C	1.311849000	4.362031000	-0.576486000
C	0.714142000	5.606760000	-0.372651000
C	-0.669105000	5.709615000	-0.500577000
C	-1.436085000	4.586234000	-0.844183000
C	-0.836195000	3.349533000	-1.051913000
C	2.558027000	2.247874000	-0.911090000
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H	-1.156271000	6.674678000	-0.341260000
H	-2.520093000	4.680109000	-0.953000000
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N	3.574546000	1.377182000	-1.011693000
N	1.269364000	2.043588000	-1.054967000
S	2.996692000	3.924023000	-0.509838000
C	3.263775000	0.102658000	-1.238646000
H	2.281518000	-0.146463000	-1.672496000
C	4.351907000	-0.846019000	-1.566120000
C	5.682785000	-0.560736000	-1.234207000
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C	6.389496000	-2.674707000	-2.171810000
H	7.729435000	-1.239063000	-1.268910000
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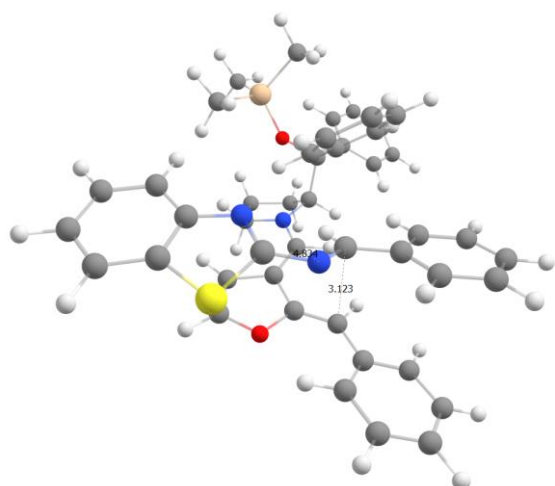
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H	-0.917318000	-3.319665000	-2.390170000
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N	-1.223860000	-1.568432000	-1.286493000
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C	-1.741786000	-1.503924000	1.873699000
C	-1.343630000	0.826623000	1.419533000
C	-0.753222000	-1.479517000	2.859710000
H	-2.282918000	-2.427762000	1.660364000
C	-0.358337000	0.852980000	2.403536000
H	-1.562601000	1.738568000	0.858409000
C	-0.053776000	-0.303432000	3.124339000
H	-0.525489000	-2.390197000	3.419605000
H	0.175519000	1.785634000	2.604082000
H	0.727078000	-0.284605000	3.888868000
C	-3.929876000	0.848283000	0.002706000
C	-4.531173000	1.193544000	1.221095000
C	-4.184587000	1.658661000	-1.108483000
C	-5.390059000	2.283572000	1.320838000
H	-4.307519000	0.605715000	2.114199000
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H	-3.718082000	1.462804000	-2.074453000
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H	-6.326094000	3.928769000	0.271129000
O	-3.797893000	-1.589911000	0.073622000
Si	-5.393352000	-2.074000000	0.387152000
C	-6.583599000	-1.272274000	-0.816682000
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H	-6.307152000	-1.490745000	-1.860151000
C	-5.907646000	-1.743760000	2.160557000
H	-6.254911000	-0.713206000	2.320601000
H	-6.736314000	-2.422798000	2.420179000

H	-5.076917000	-1.944824000	2.855605000
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C	2.713912000	-0.527653000	0.308990000
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C	3.634210000	-0.363233000	1.501475000
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C	5.562588000	-0.946160000	2.859603000
H	4.952471000	-2.033063000	1.105760000
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C	5.810386000	-0.278637000	-1.209741000
C	4.332346000	-1.853818000	-2.271583000
C	6.908687000	-1.036499000	-1.615994000
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H	3.320395000	-2.172010000	-2.545160000
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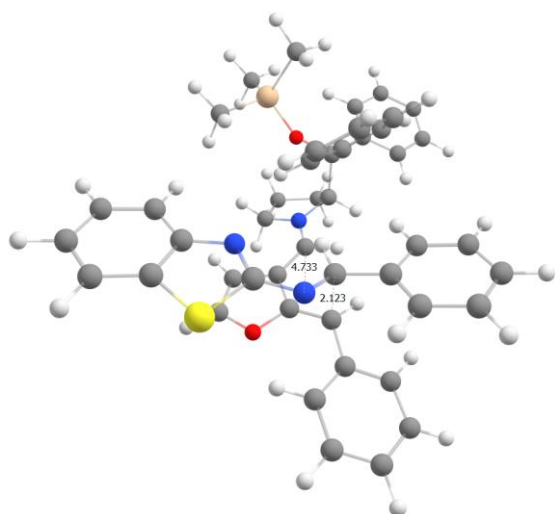
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H	-1.318757000	1.537565000	3.525827000
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H	-3.304576000	-0.932351000	3.757971000
H	-4.126876000	1.696229000	2.444308000
H	-3.608488000	1.424922000	4.122287000
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C	-3.353172000	-0.652007000	0.306735000
C	-2.375024000	-0.849248000	-0.871445000
C	-1.427599000	0.151523000	-1.137122000
C	-2.475303000	-1.908072000	-1.783260000
C	-0.639301000	0.115695000	-2.284894000
H	-1.320721000	0.993133000	-0.451525000
C	-1.673867000	-1.956745000	-2.925521000
H	-3.211278000	-2.697707000	-1.631337000
C	-0.759666000	-0.939845000	-3.188344000
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H	-1.783592000	-2.792403000	-3.621607000
H	-0.140907000	-0.969977000	-4.088898000
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C	-5.783040000	-1.419439000	0.098994000
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C	-6.775581000	-2.400737000	0.143054000
H	-6.063943000	-0.385148000	-0.094921000
C	-5.108364000	-4.055863000	0.658209000
H	-3.083220000	-3.365273000	0.789802000
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H	-7.817163000	-2.121782000	-0.036770000
H	-4.830695000	-5.089243000	0.881603000
H	-7.219060000	-4.492890000	0.462208000
O	-3.927026000	0.626789000	0.216589000
Si	-4.405160000	1.708306000	-0.995567000
C	-6.023087000	2.420817000	-0.369553000
H	-6.820436000	1.665151000	-0.298703000
H	-5.884837000	2.863456000	0.629856000
H	-6.372602000	3.216714000	-1.046592000
C	-4.633089000	0.876221000	-2.658692000
H	-3.674716000	0.526353000	-3.071326000
H	-5.315989000	0.014943000	-2.594553000
H	-5.064872000	1.602644000	-3.366740000
C	-3.161976000	3.108380000	-1.114738000
H	-2.260642000	2.820750000	-1.675324000
H	-3.622548000	3.967322000	-1.629387000
H	-2.854992000	3.439963000	-0.109779000
C	-2.659850000	-0.728141000	1.712789000
H	-2.260135000	-1.745574000	1.820300000
C	-0.277399000	-0.179137000	1.833250000

H	-0.155482000	-1.216549000	1.502538000
C	0.860610000	0.535979000	2.095358000
C	2.204403000	-0.053206000	2.020999000
C	1.097659000	1.962022000	2.339351000
O	3.110838000	0.968866000	2.125735000
C	2.424807000	2.142674000	2.330461000
H	0.360446000	2.751862000	2.453665000
H	3.042604000	3.032286000	2.435048000
C	2.588805000	-1.347762000	1.881879000
H	1.778272000	-2.080519000	1.905003000
C	3.923052000	-1.896329000	1.648160000
C	4.076156000	-3.297963000	1.652470000
C	5.063123000	-1.118989000	1.359042000
C	5.302617000	-3.897492000	1.384306000
H	3.202867000	-3.923679000	1.860922000
C	6.289461000	-1.723219000	1.085940000
H	4.979113000	-0.032540000	1.329545000
C	6.421623000	-3.112511000	1.096943000
H	5.384918000	-4.988072000	1.392566000
H	7.154721000	-1.095171000	0.854916000
H	7.386042000	-3.579730000	0.881433000
C	1.883003000	3.538013000	-0.785737000
C	3.186011000	4.033410000	-0.564396000
C	3.411674000	5.371042000	-0.226325000
C	2.310130000	6.211302000	-0.112895000
C	1.006817000	5.729219000	-0.330170000
C	0.784240000	4.401509000	-0.667066000
C	2.987802000	1.652185000	-1.101347000
H	4.423574000	5.745083000	-0.054782000
H	2.461728000	7.261553000	0.148086000
H	0.158162000	6.410624000	-0.230846000
H	-0.224076000	4.015881000	-0.833370000
N	3.288821000	0.335204000	-1.389807000
N	1.812601000	2.193111000	-1.092118000
S	4.329737000	2.736019000	-0.766319000
C	2.389321000	-0.540777000	-1.128732000
H	1.445790000	-0.249828000	-0.642679000
C	2.534873000	-1.961175000	-1.457442000
C	3.709832000	-2.471967000	-2.025993000
C	1.464627000	-2.822179000	-1.180513000
C	3.812024000	-3.830274000	-2.307801000
H	4.539198000	-1.791000000	-2.230490000
C	1.566289000	-4.181014000	-1.467546000
H	0.546789000	-2.415413000	-0.744317000
C	2.741654000	-4.684948000	-2.027111000
H	4.731230000	-4.230114000	-2.743032000
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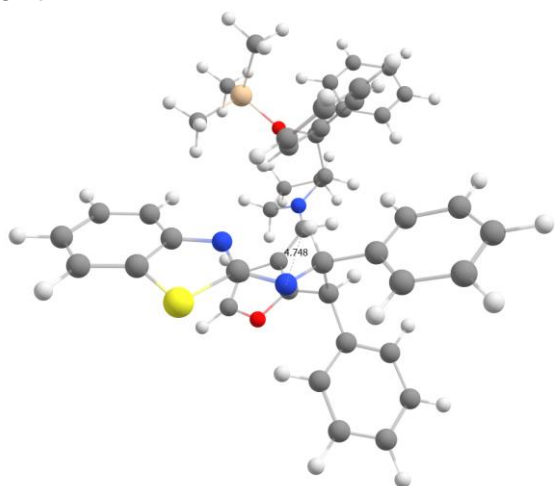
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H	-1.423582000	1.389712000	3.622090000
H	-2.070342000	2.161229000	2.150726000
H	-4.724035000	-0.867449000	2.635287000
H	-3.359184000	-1.222882000	3.710561000
H	-4.259304000	1.492724000	2.658497000
H	-3.670349000	1.082453000	4.284349000
N	-1.643734000	0.092217000	1.997838000
C	-3.415110000	-0.598885000	0.291584000
C	-2.432687000	-0.731604000	-0.893303000
C	-1.446230000	0.249731000	-1.073369000
C	-2.550983000	-1.720513000	-1.879330000
C	-0.617916000	0.250925000	-2.193434000
H	-1.329228000	1.051319000	-0.343042000
C	-1.720971000	-1.725078000	-3.001129000
H	-3.317959000	-2.490419000	-1.799227000
C	-0.752258000	-0.738175000	-3.166308000
H	0.148305000	1.025210000	-2.279577000
H	-1.844187000	-2.507389000	-3.754535000
H	-0.103071000	-0.740965000	-4.045535000
C	-4.541653000	-1.643644000	0.203283000
C	-5.863633000	-1.258756000	-0.023531000
C	-4.271848000	-3.009346000	0.382185000
C	-6.887626000	-2.205770000	-0.093752000
H	-6.105393000	-0.202374000	-0.132271000
C	-5.290104000	-3.957049000	0.315119000
H	-3.249404000	-3.352839000	0.561339000
C	-6.605934000	-3.559135000	0.072748000
H	-7.913967000	-1.876337000	-0.275313000
H	-5.052045000	-5.014995000	0.452185000
H	-7.405897000	-4.301834000	0.017426000
O	-3.938833000	0.702711000	0.324247000
Si	-4.349943000	1.917157000	-0.789601000
C	-5.951573000	2.626672000	-0.122263000
H	-6.783362000	1.906538000	-0.158998000
H	-5.821469000	2.944086000	0.924684000
H	-6.246100000	3.510853000	-0.709889000
C	-4.569645000	1.248398000	-2.525850000
H	-3.610002000	0.929349000	-2.959988000
H	-5.260061000	0.391090000	-2.549568000
H	-4.988435000	2.041340000	-3.166889000
C	-3.057108000	3.275933000	-0.755963000
H	-2.136111000	2.999346000	-1.289123000
H	-3.469179000	4.177223000	-1.238481000
H	-2.792821000	3.541817000	0.279985000
C	-2.735416000	-0.834532000	1.687628000

H	-2.323018000	-1.851477000	1.691700000
C	-0.376216000	-0.216021000	1.791417000
H	-0.223214000	-1.208897000	1.356681000
C	0.757428000	0.551167000	2.046053000
C	2.080495000	0.048887000	1.828819000
C	0.939095000	1.940403000	2.445590000
O	2.954880000	1.027841000	2.100638000
C	2.264095000	2.162012000	2.451088000
H	0.178443000	2.683691000	2.665536000
H	2.873645000	3.036318000	2.664097000
C	2.523329000	-1.192503000	1.331830000
H	1.756346000	-1.968340000	1.389605000
C	3.894033000	-1.711866000	1.474229000
C	4.070652000	-3.103187000	1.589172000
C	5.045503000	-0.905750000	1.410509000
C	5.340375000	-3.670239000	1.652320000
H	3.187161000	-3.748477000	1.620739000
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C	6.474129000	-2.857398000	1.597010000
H	5.445133000	-4.755017000	1.741889000
H	7.197272000	-0.830262000	1.422004000
H	7.473269000	-3.298271000	1.646257000
C	2.201031000	3.330549000	-0.785421000
C	3.534386000	3.774580000	-0.951481000
C	3.862002000	5.130707000	-0.940861000
C	2.839577000	6.059977000	-0.758941000
C	1.511841000	5.635216000	-0.595326000
C	1.185895000	4.283389000	-0.608635000
C	3.143836000	1.324161000	-1.000958000
H	4.896727000	5.457296000	-1.071178000
H	3.076013000	7.126868000	-0.745014000
H	0.722533000	6.378403000	-0.453574000
H	0.154545000	3.946164000	-0.477323000
N	3.360971000	0.004329000	-1.104399000
N	2.017565000	1.966783000	-0.813507000
S	4.570261000	2.384247000	-1.153277000
C	2.363615000	-0.809599000	-0.749819000
H	1.353176000	-0.398008000	-0.621456000
C	2.387487000	-2.213612000	-1.232321000
C	3.562481000	-2.792012000	-1.725069000
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H	4.470605000	-2.186051000	-1.755701000
C	1.213779000	-4.297797000	-1.642584000
H	0.287927000	-2.526920000	-0.823475000
C	2.392599000	-4.869924000	-2.127277000
H	4.488953000	-4.556127000	-2.550438000
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H	2.395203000	-5.906024000	-2.476272000

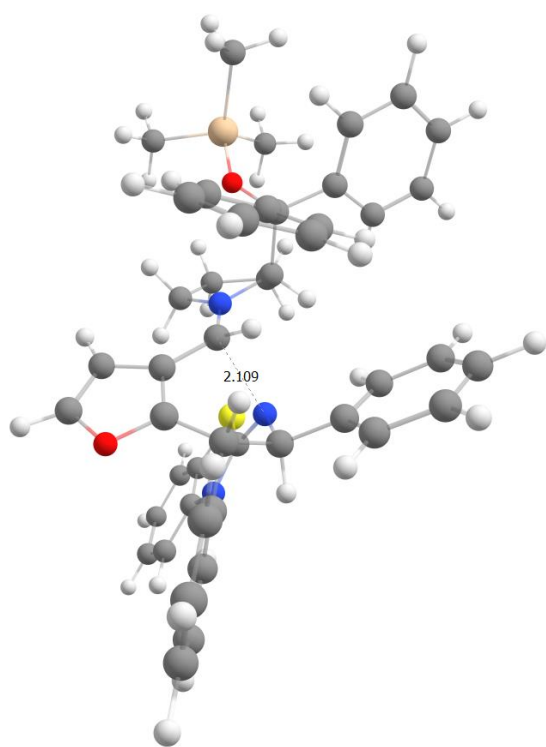
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H	-2.076864000	1.866979000	2.448565000
H	-4.714274000	-1.246364000	2.493179000
H	-3.333908000	-1.690777000	3.512791000
H	-4.283474000	1.116371000	2.771782000
H	-3.744937000	0.523885000	4.360424000
N	-1.645661000	-0.153534000	2.006488000
C	-3.381813000	-0.584951000	0.193862000
C	-2.389187000	-0.666584000	-0.988074000
C	-1.366931000	0.289281000	-1.084519000
C	-2.506721000	-1.594733000	-2.031610000
C	-0.498287000	0.320612000	-2.173593000
H	-1.248162000	1.051138000	-0.312540000
C	-1.636360000	-1.570017000	-3.121695000
H	-3.302415000	-2.338544000	-2.023492000
C	-0.628181000	-0.612207000	-3.200213000
H	0.293516000	1.073434000	-2.186160000
H	-1.759326000	-2.307318000	-3.919250000
H	0.053212000	-0.593379000	-4.054439000
C	-4.589032000	-1.519220000	-0.006313000
C	-5.879469000	-1.006003000	-0.141312000
C	-4.431277000	-2.914103000	0.008132000
C	-6.980836000	-1.852047000	-0.287544000
H	-6.040428000	0.070183000	-0.109742000
C	-5.526844000	-3.761695000	-0.136409000
H	-3.439932000	-3.359427000	0.126168000
C	-6.809866000	-3.233583000	-0.289607000
H	-7.979376000	-1.419994000	-0.392114000
H	-5.375075000	-4.844062000	-0.126993000
H	-7.670305000	-3.897922000	-0.402474000
O	-3.786964000	0.743061000	0.381564000
Si	-4.182260000	2.079342000	-0.596554000
C	-5.702665000	2.814516000	0.216503000
H	-6.571100000	2.138636000	0.198997000
H	-5.486860000	3.064817000	1.267607000
H	-5.989958000	3.744565000	-0.299523000
C	-4.508394000	1.582896000	-2.372657000
H	-3.589144000	1.229686000	-2.864355000
H	-5.268011000	0.790466000	-2.451640000
H	-4.874948000	2.462381000	-2.926971000
C	-2.812938000	3.355574000	-0.510006000
H	-1.947483000	3.089820000	-1.133969000
H	-3.199430000	4.323847000	-0.867613000
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C	-2.733614000	-1.039490000	1.554378000
H	-2.313354000	-2.043415000	1.414584000
C	-0.396803000	-0.381516000	1.727323000

H	-0.219395000	-1.273865000	1.119642000
C	0.739708000	0.379552000	2.104151000
C	2.029536000	-0.022436000	1.750255000
C	0.899727000	1.655710000	2.773664000
O	2.901127000	0.872501000	2.183867000
C	2.227129000	1.897142000	2.784064000
H	0.137513000	2.317094000	3.174141000
H	2.838664000	2.711433000	3.162865000
C	2.504070000	-1.200274000	0.970646000
H	1.745820000	-1.980979000	1.122639000
C	3.823501000	-1.781161000	1.440184000
C	3.864582000	-3.122460000	1.838646000
C	5.015528000	-1.042710000	1.449462000
C	5.060863000	-3.718073000	2.238953000
H	2.943672000	-3.713612000	1.826778000
C	6.211207000	-1.636213000	1.851793000
H	5.008933000	-0.003341000	1.122196000
C	6.239703000	-2.974020000	2.248403000
H	5.069069000	-4.768185000	2.542763000
H	7.131647000	-1.046067000	1.851445000
H	7.179615000	-3.434617000	2.564202000
C	2.071780000	3.256253000	-0.637739000
C	3.303396000	3.813524000	-1.078584000
C	3.490027000	5.186855000	-1.195349000
C	2.436184000	6.045212000	-0.863883000
C	1.217647000	5.516684000	-0.422240000
C	1.029995000	4.140103000	-0.307153000
C	3.151063000	1.307915000	-0.933804000
H	4.445569000	5.589834000	-1.542272000
H	2.568060000	7.126691000	-0.950827000
H	0.397320000	6.192331000	-0.162607000
H	0.079654000	3.730034000	0.043809000
N	3.474058000	0.051246000	-0.988254000
N	2.006453000	1.892929000	-0.567353000
S	4.424171000	2.509137000	-1.410408000
C	2.465544000	-0.879173000	-0.581918000
H	1.450166000	-0.479616000	-0.748931000
C	2.551400000	-2.197457000	-1.332856000
C	3.746629000	-2.646444000	-1.899841000
C	1.411902000	-3.005161000	-1.436478000
C	3.807027000	-3.884015000	-2.542429000
H	4.626603000	-2.003434000	-1.835669000
C	1.466342000	-4.240273000	-2.080687000
H	0.462075000	-2.652229000	-1.019068000
C	2.668865000	-4.686343000	-2.632534000
H	4.751087000	-4.225076000	-2.976544000
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H	2.716267000	-5.654395000	-3.138627000

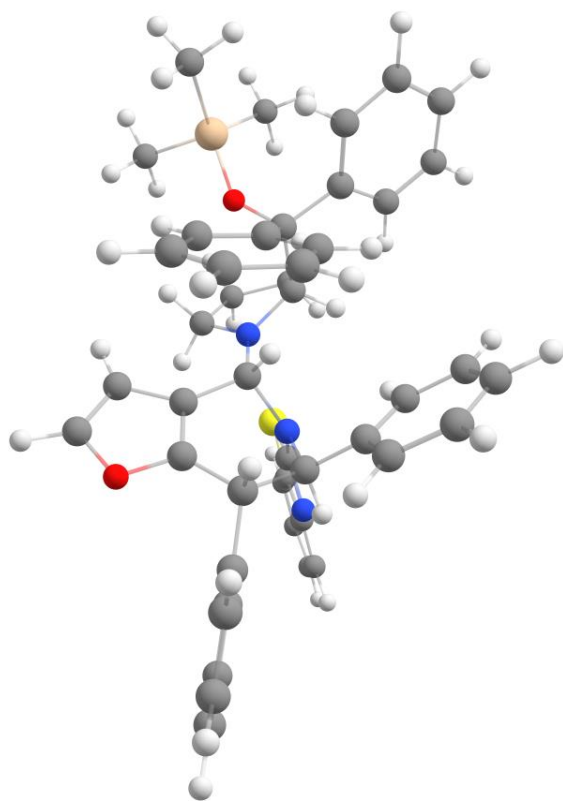
TS2



C	0.886939000	2.461149000	0.913807000
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H	-0.106241000	2.925221000	0.947481000
H	1.306844000	2.447463000	1.931914000
H	3.272838000	2.175292000	-1.399455000
H	1.623777000	2.245835000	-2.040333000
H	2.712343000	3.548477000	0.446569000
H	1.327716000	4.022618000	-0.545827000
N	0.776685000	1.088699000	0.415096000
C	3.037491000	0.012610000	0.195905000
C	2.446557000	-1.167929000	0.982032000
C	2.181194000	-1.053240000	2.348412000
C	2.051593000	-2.332683000	0.312838000
C	1.510215000	-2.071948000	3.028169000
H	2.488099000	-0.146925000	2.873903000
C	1.377895000	-3.348723000	0.987740000
H	2.250810000	-2.443493000	-0.756233000
C	1.098351000	-3.218483000	2.349449000
H	1.300433000	-1.962242000	4.095437000
H	1.062230000	-4.241070000	0.440679000
H	0.565321000	-4.012072000	2.879556000
C	4.061860000	-0.523284000	-0.817868000
C	5.122411000	-1.297613000	-0.327642000
C	3.991725000	-0.301223000	-2.196820000
C	6.110549000	-1.788755000	-1.175433000
H	5.164247000	-1.534660000	0.738065000
C	4.976303000	-0.799824000	-3.053621000
H	3.165334000	0.257975000	-2.636711000
C	6.045538000	-1.533385000	-2.546617000
H	6.930282000	-2.383905000	-0.764847000
H	4.898797000	-0.609397000	-4.127063000
H	6.817130000	-1.919116000	-3.217796000
O	3.607668000	0.925380000	1.098077000
Si	5.079069000	1.689244000	1.429862000
C	5.801362000	2.488520000	-0.103764000
H	6.753454000	2.980083000	0.154619000
H	6.006993000	1.741084000	-0.886196000
H	5.128752000	3.253594000	-0.521505000

C	6.336357000	0.527356000	2.201268000
H	6.889746000	-0.059299000	1.453711000
H	7.067858000	1.125622000	2.769108000
H	5.853618000	-0.169760000	2.904612000
C	4.594960000	2.971597000	2.705739000
H	4.141138000	2.487318000	3.585045000
H	5.482965000	3.528345000	3.045165000
H	3.870711000	3.698025000	2.307296000
C	1.855721000	0.745674000	-0.513925000
H	1.436036000	0.063785000	-1.266810000
C	-0.231318000	0.253966000	0.613096000
H	-0.010697000	-0.780881000	0.353360000
C	-1.291306000	0.444117000	1.589702000
C	-2.379588000	-0.390218000	1.539334000
C	-1.575675000	1.402702000	2.629496000
O	-3.282629000	-0.029298000	2.458590000
C	-2.792928000	1.052762000	3.120061000
H	-0.957366000	2.222107000	2.986639000
H	-3.419861000	1.452622000	3.912897000
C	-2.594753000	-1.535651000	0.613617000
H	-1.856933000	-2.295599000	0.922600000
C	-3.975297000	-2.146771000	0.770445000
C	-4.138082000	-3.352565000	1.460312000
C	-5.108919000	-1.501736000	0.260038000
C	-5.404748000	-3.914465000	1.626781000
H	-3.259515000	-3.860260000	1.870754000
C	-6.374562000	-2.061842000	0.425120000
H	-4.983131000	-0.546055000	-0.258874000
C	-6.527024000	-3.270993000	1.106364000
H	-5.512428000	-4.860496000	2.163981000
H	-7.250360000	-1.548443000	0.018799000
H	-7.520035000	-3.710886000	1.231720000
C	-4.022564000	2.595948000	-1.105942000
C	-3.025295000	3.546741000	-1.429358000
C	-3.322319000	4.898392000	-1.595948000
C	-4.644592000	5.312396000	-1.437987000
C	-5.645006000	4.384295000	-1.116094000
C	-5.345810000	3.035056000	-0.949847000
C	-2.291490000	1.187981000	-1.138863000
H	-2.537805000	5.616832000	-1.846519000
H	-4.899350000	6.367167000	-1.567699000
H	-6.676547000	4.725144000	-0.992949000
H	-6.123670000	2.310568000	-0.695820000
N	-1.523476000	0.109800000	-1.047745000
N	-3.587518000	1.297579000	-0.948709000
S	-1.489855000	2.727938000	-1.574515000
C	-2.211242000	-1.146892000	-0.892967000
H	-3.175494000	-1.082177000	-1.423545000
C	-1.401272000	-2.268671000	-1.548986000
C	-0.340338000	-1.970426000	-2.410700000
C	-1.713827000	-3.618629000	-1.331871000
C	0.408086000	-2.983854000	-3.011501000
H	-0.107051000	-0.921831000	-2.601763000
C	-0.971777000	-4.633980000	-1.933144000
H	-2.550164000	-3.891577000	-0.684322000
C	0.101093000	-4.321710000	-2.769973000
H	1.241615000	-2.721694000	-3.669393000
H	-1.232521000	-5.678373000	-1.741625000
H	0.688000000	-5.117800000	-3.235553000

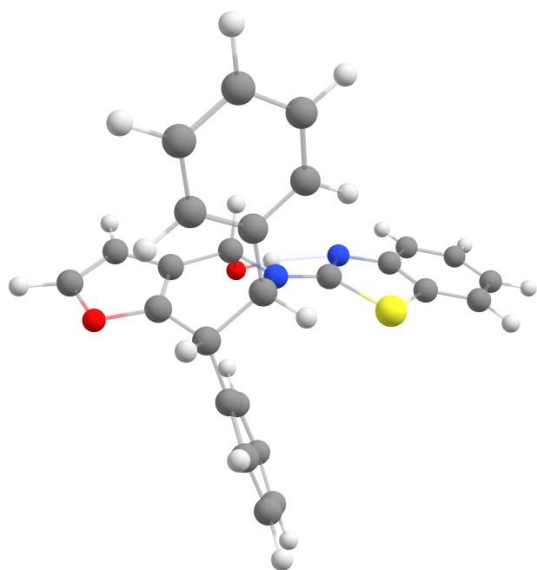
INT2



C	0.919382000	1.892648000	1.705158000
C	2.152284000	2.462448000	-0.344746000
C	1.774562000	2.993026000	1.052253000
H	-0.006871000	2.288813000	2.147137000
H	1.490438000	1.392345000	2.506201000
H	3.222782000	2.584129000	-0.551023000
H	1.599821000	3.003042000	-1.127699000
H	2.666052000	3.199227000	1.657724000
H	1.209609000	3.933016000	0.972819000
N	0.621220000	0.993326000	0.600674000
C	2.910403000	0.022483000	-0.014451000
C	2.365925000	-1.357902000	0.377261000
C	2.178044000	-1.685728000	1.721366000
C	1.971913000	-2.280345000	-0.601040000
C	1.587462000	-2.897594000	2.083422000
H	2.483062000	-0.970913000	2.487471000
C	1.380568000	-3.489625000	-0.243377000
H	2.113220000	-2.046347000	-1.659285000
C	1.178559000	-3.800411000	1.103440000
H	1.435212000	-3.128751000	3.141066000
H	1.067899000	-4.188567000	-1.023349000
H	0.708829000	-4.746161000	1.386245000
C	3.879781000	-0.135743000	-1.201468000
C	4.880075000	-1.114408000	-1.108687000
C	3.839999000	0.649976000	-2.358021000
C	5.832174000	-1.278874000	-2.109687000
H	4.904661000	-1.772078000	-0.236954000
C	4.788827000	0.484350000	-3.370975000
H	3.066644000	1.405870000	-2.497588000
C	5.794066000	-0.471259000	-3.247961000
H	6.602514000	-2.047269000	-2.003402000
H	4.735112000	1.111607000	-4.264537000
H	6.537584000	-0.597525000	-4.039177000
O	3.563465000	0.588399000	1.097288000
Si	5.114797000	0.860216000	1.697158000
C	6.144550000	1.871966000	0.500665000
H	7.091151000	2.166221000	0.982897000

H	6.387995000	1.303544000	-0.410211000
H	5.614792000	2.790803000	0.203322000
C	5.998733000	-0.735189000	2.149604000
H	6.474081000	-1.219615000	1.284619000
H	6.788982000	-0.512915000	2.885239000
H	5.301744000	-1.454129000	2.608909000
C	4.790523000	1.824482000	3.270582000
H	4.132993000	1.252317000	3.944382000
H	5.735108000	2.020028000	3.802877000
H	4.309858000	2.792748000	3.064213000
C	1.713975000	0.984779000	-0.360149000
H	1.317307000	0.678720000	-1.340853000
C	-0.391072000	0.001740000	0.568953000
H	0.035541000	-0.917240000	0.142985000
C	-1.041784000	-0.390056000	1.873541000
C	-2.144583000	-1.181105000	1.783855000
C	-0.787325000	-0.231927000	3.280228000
O	-2.598339000	-1.514751000	3.007418000
C	-1.771060000	-0.931974000	3.910556000
H	0.011499000	0.319716000	3.768583000
H	-2.012475000	-1.094617000	4.958220000
C	-2.719938000	-1.787968000	0.544853000
H	-2.239781000	-2.775940000	0.453184000
C	-4.217462000	-2.020876000	0.653086000
C	-4.726437000	-3.319608000	0.737212000
C	-5.109615000	-0.941602000	0.698448000
C	-6.099801000	-3.541598000	0.858669000
H	-4.039311000	-4.171176000	0.709549000
C	-6.479855000	-1.160276000	0.821481000
H	-4.725264000	0.079986000	0.621201000
C	-6.980188000	-2.462032000	0.901218000
H	-6.481312000	-4.564202000	0.920246000
H	-7.162565000	-0.306971000	0.853896000
H	-8.055739000	-2.632768000	0.996149000
C	-3.754264000	2.920898000	-1.037465000
C	-2.772079000	3.846920000	-0.637927000
C	-3.006585000	5.222091000	-0.648295000
C	-4.253671000	5.671852000	-1.075497000
C	-5.241911000	4.760668000	-1.479942000
C	-5.004201000	3.390385000	-1.463984000
C	-2.163668000	1.461819000	-0.504900000
H	-2.233838000	5.927062000	-0.332233000
H	-4.462219000	6.744344000	-1.094842000
H	-6.213981000	5.133953000	-1.812555000
H	-5.769778000	2.675080000	-1.773424000
N	-1.535831000	0.263346000	-0.374041000
N	-3.382033000	1.594596000	-0.947172000
S	-1.328245000	2.984602000	-0.167345000
C	-2.301140000	-0.936153000	-0.713803000
H	-3.231361000	-0.560297000	-1.158013000
C	-1.593938000	-1.737796000	-1.806160000
C	-0.718145000	-1.089969000	-2.685230000
C	-1.858093000	-3.096211000	-2.017919000
C	-0.091508000	-1.783137000	-3.719348000
H	-0.519864000	-0.024682000	-2.548835000
C	-1.237808000	-3.791930000	-3.056241000
H	-2.559603000	-3.632932000	-1.375119000
C	-0.343074000	-3.142159000	-3.905966000
H	0.599661000	-1.254017000	-4.380892000
H	-1.456203000	-4.853637000	-3.198137000
H	0.149771000	-3.689755000	-4.713362000

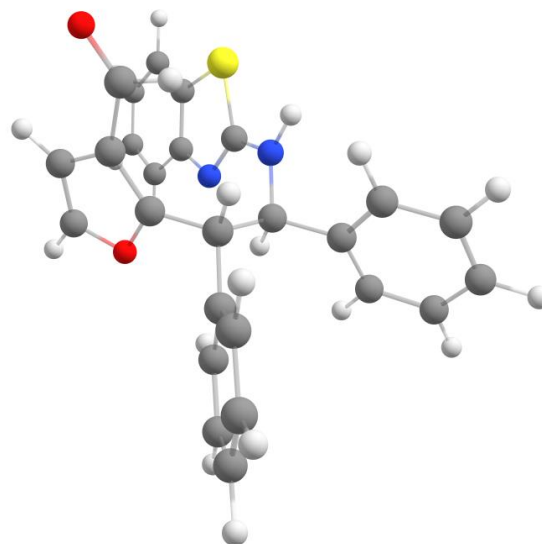
INT3



C	1.806634000	-0.838383000	-1.757425000
C	2.395601000	-2.146230000	-2.183633000
C	3.378289000	-2.773832000	-1.491262000
C	2.171078000	-2.933212000	-3.363546000
O	3.776024000	-3.888600000	-2.132511000
C	3.039153000	-3.977056000	-3.271034000
H	1.463291000	-2.743223000	-4.168124000
H	3.246736000	-4.832697000	-3.909028000
C	3.915793000	-2.365473000	-0.164866000
H	4.118606000	-3.257138000	0.445201000
C	5.192694000	-1.538663000	-0.219979000
C	6.176828000	-1.729963000	0.756075000
C	5.380498000	-0.541796000	-1.185221000
C	7.326987000	-0.941065000	0.772102000
H	6.038827000	-2.506780000	1.514697000
C	6.529144000	0.249329000	-1.168224000
H	4.616892000	-0.372707000	-1.949581000
C	7.505528000	0.052448000	-0.191012000
H	8.087492000	-1.105647000	1.539995000
H	6.662403000	1.025702000	-1.926268000
H	8.407085000	0.670602000	-0.182085000
C	1.522012000	2.903299000	-0.012132000
C	2.168363000	2.912488000	1.239725000
C	2.237557000	4.061534000	2.026424000
C	1.647976000	5.225279000	1.538387000
C	1.005069000	5.233070000	0.291501000
C	0.936628000	4.082978000	-0.488020000
C	2.150454000	0.770909000	0.024963000
H	2.741446000	4.050557000	2.995578000
H	1.688530000	6.140087000	2.134454000
H	0.551448000	6.157525000	-0.074888000
H	0.436101000	4.081845000	-1.458860000
N	2.331810000	-0.499689000	-0.406349000
N	1.523858000	1.682740000	-0.664187000
S	2.808862000	1.320543000	1.574849000
C	2.769586000	-1.568656000	0.498808000
H	3.197027000	-1.084259000	1.389348000
C	1.580605000	-2.413111000	0.970597000
C	1.511139000	-3.800844000	0.814662000
C	0.513710000	-1.760271000	1.604414000
C	0.404961000	-4.516823000	1.276566000
H	2.315479000	-4.348779000	0.320487000
C	-0.590045000	-2.471883000	2.067180000
H	0.545250000	-0.676473000	1.748135000
C	-0.648763000	-3.856940000	1.903997000

H	0.371023000	-5.600565000	1.139002000
H	-1.408248000	-1.941420000	2.560974000
H	-1.514460000	-4.418039000	2.265137000
H	0.702086000	-0.899833000	-1.681959000
O	2.177568000	0.116399000	-2.697597000
H	1.803726000	0.958860000	-2.370081000

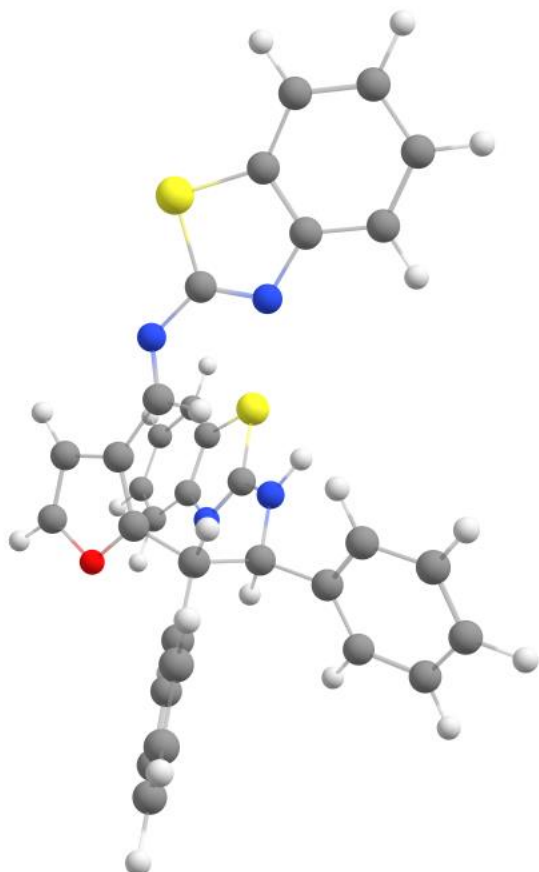
INT4



C	0.175000000	0.700763000	1.296207000
H	0.260413000	-0.283717000	0.778502000
C	-1.182950000	1.118529000	1.641590000
C	-2.351808000	0.444689000	1.369643000
C	-1.565329000	2.343072000	2.296276000
O	-3.391367000	1.162240000	1.816901000
C	-2.916936000	2.310334000	2.370997000
H	-0.900565000	3.126597000	2.653178000
H	-3.664787000	2.989926000	2.771820000
C	-2.632146000	-0.816972000	0.613129000
H	-1.677488000	-1.361402000	0.559545000
C	-3.638283000	-1.724421000	1.300163000
C	-3.231619000	-2.980412000	1.761529000
C	-4.980717000	-1.353060000	1.451163000
C	-4.141931000	-3.850844000	2.361627000
H	-2.187174000	-3.283777000	1.642223000
C	-5.891902000	-2.221573000	2.049723000
H	-5.321635000	-0.376495000	1.099498000
C	-5.476142000	-3.473342000	2.506081000
H	-3.805126000	-4.828958000	2.714711000
H	-6.936443000	-1.918143000	2.158374000
H	-6.193279000	-4.154288000	2.971678000
C	-2.729736000	3.717512000	-1.123928000
C	-1.436744000	4.030040000	-1.595380000
C	-0.983613000	5.344396000	-1.696375000
C	-1.846552000	6.367186000	-1.308511000
C	-3.134201000	6.074298000	-0.835544000
C	-3.582864000	4.760696000	-0.741980000
C	-2.035389000	1.652261000	-1.480283000
H	0.020860000	5.566821000	-2.063998000
H	-1.513338000	7.405807000	-1.373139000
H	-3.795804000	6.891144000	-0.535898000
H	-4.584227000	4.524869000	-0.374598000
N	-2.023466000	0.300307000	-1.524309000
N	-3.036380000	2.369562000	-1.076416000
S	-0.593880000	2.546724000	-1.983581000
C	-3.042167000	-0.495898000	-0.863676000
H	-3.950648000	0.121111000	-0.844504000
C	-3.330160000	-1.765691000	-1.639843000

C	-2.313256000	-2.688148000	-1.914356000
C	-4.631037000	-2.047149000	-2.065395000
C	-2.591378000	-3.862937000	-2.610845000
H	-1.288271000	-2.497771000	-1.579326000
C	-4.913752000	-3.225565000	-2.756364000
H	-5.432754000	-1.335950000	-1.847192000
C	-3.893808000	-4.135134000	-3.032689000
H	-1.787618000	-4.573529000	-2.820007000
H	-5.937452000	-3.433336000	-3.078233000
H	-4.112922000	-5.057978000	-3.575967000
O	1.166166000	1.356211000	1.537917000
H	-1.168891000	-0.161143000	-1.813562000

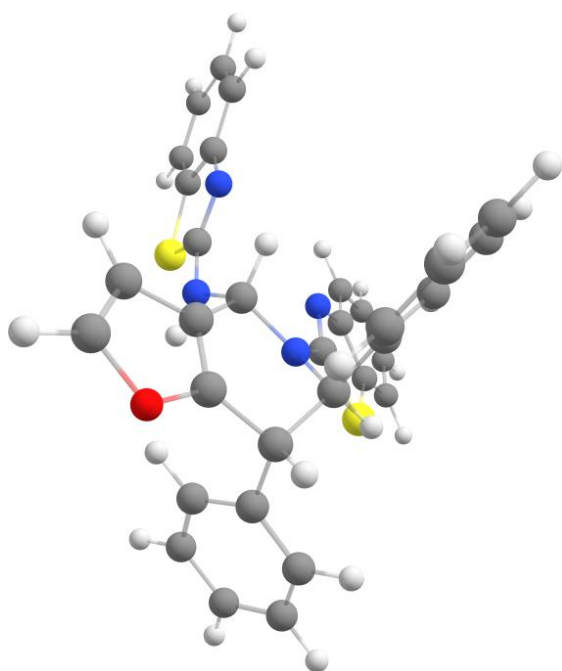
INT5



H	-7.177322000	-1.149547000	2.277917000
H	-6.874492000	-3.439089000	3.216609000
C	-2.818771000	3.514402000	-1.050499000
C	-1.665039000	3.827304000	-1.801344000
C	-1.269189000	5.143858000	-2.032426000
C	-2.045953000	6.167149000	-1.492948000
C	-3.192232000	5.873129000	-0.739614000
C	-3.584107000	4.557572000	-0.513873000
C	-2.187190000	1.449907000	-1.507045000
H	-0.374941000	5.368007000	-2.618669000
H	-1.757352000	7.207623000	-1.660446000
H	-3.786464000	6.690673000	-0.323391000
H	-4.474188000	4.319694000	0.073237000
N	-2.170775000	0.098988000	-1.517949000
N	-3.087288000	2.165312000	-0.907115000
S	-0.902863000	2.342836000	-2.329870000
C	-3.170842000	-0.675059000	-0.809355000
H	-4.079346000	-0.058314000	-0.783501000
C	-3.467871000	-1.962805000	-1.551313000
C	-2.443790000	-2.874740000	-1.837394000
C	-4.774192000	-2.266142000	-1.943446000
C	-2.720790000	-4.060018000	-2.516135000
H	-1.413264000	-2.664332000	-1.530909000
C	-5.054916000	-3.456279000	-2.615274000
H	-5.580298000	-1.562553000	-1.716894000
C	-4.028420000	-4.353941000	-2.906096000
H	-1.911414000	-4.760395000	-2.737677000
H	-6.082270000	-3.681603000	-2.912767000
H	-4.246244000	-5.284496000	-3.436600000
H	-1.432001000	-0.378054000	-2.021434000
N	1.236132000	0.841447000	0.340158000
C	2.116664000	0.241986000	-0.537048000
C	4.148051000	-0.428923000	-1.726227000
C	2.926416000	-0.939626000	-2.216704000
C	5.370693000	-0.757826000	-2.319042000
C	2.932685000	-1.792927000	-3.330393000
C	5.355457000	-1.608186000	-3.418103000
H	6.310184000	-0.358918000	-1.929879000
C	4.145650000	-2.121010000	-3.919280000
H	1.986904000	-2.185447000	-3.710736000
H	6.298100000	-1.880639000	-3.899001000
H	4.162547000	-2.786258000	-4.786193000
S	3.826027000	0.597246000	-0.356558000
N	1.800620000	-0.536535000	-1.523013000

C	0.150237000	0.199638000	0.580458000
H	0.010669000	-0.815293000	0.172964000
C	-0.945574000	0.759242000	1.334325000
C	-2.211295000	0.217006000	1.374041000
C	-1.017695000	2.004577000	2.053410000
O	-3.020148000	1.022036000	2.073514000
C	-2.299189000	2.101504000	2.482249000
H	-0.210323000	2.713651000	2.222430000
H	-2.840056000	2.838014000	3.071280000
C	-2.765280000	-0.985905000	0.677814000
H	-1.938727000	-1.710476000	0.626779000
C	-3.913244000	-1.650805000	1.413335000
C	-3.753546000	-2.935368000	1.941743000
C	-5.155966000	-1.017078000	1.542236000
C	-4.810360000	-3.576549000	2.588883000
H	-2.789672000	-3.442702000	1.839117000
C	-6.213012000	-1.656298000	2.187192000
H	-5.300840000	-0.011800000	1.137762000
C	-6.043586000	-2.938204000	2.712981000
H	-4.668887000	-4.581481000	2.995138000

PR

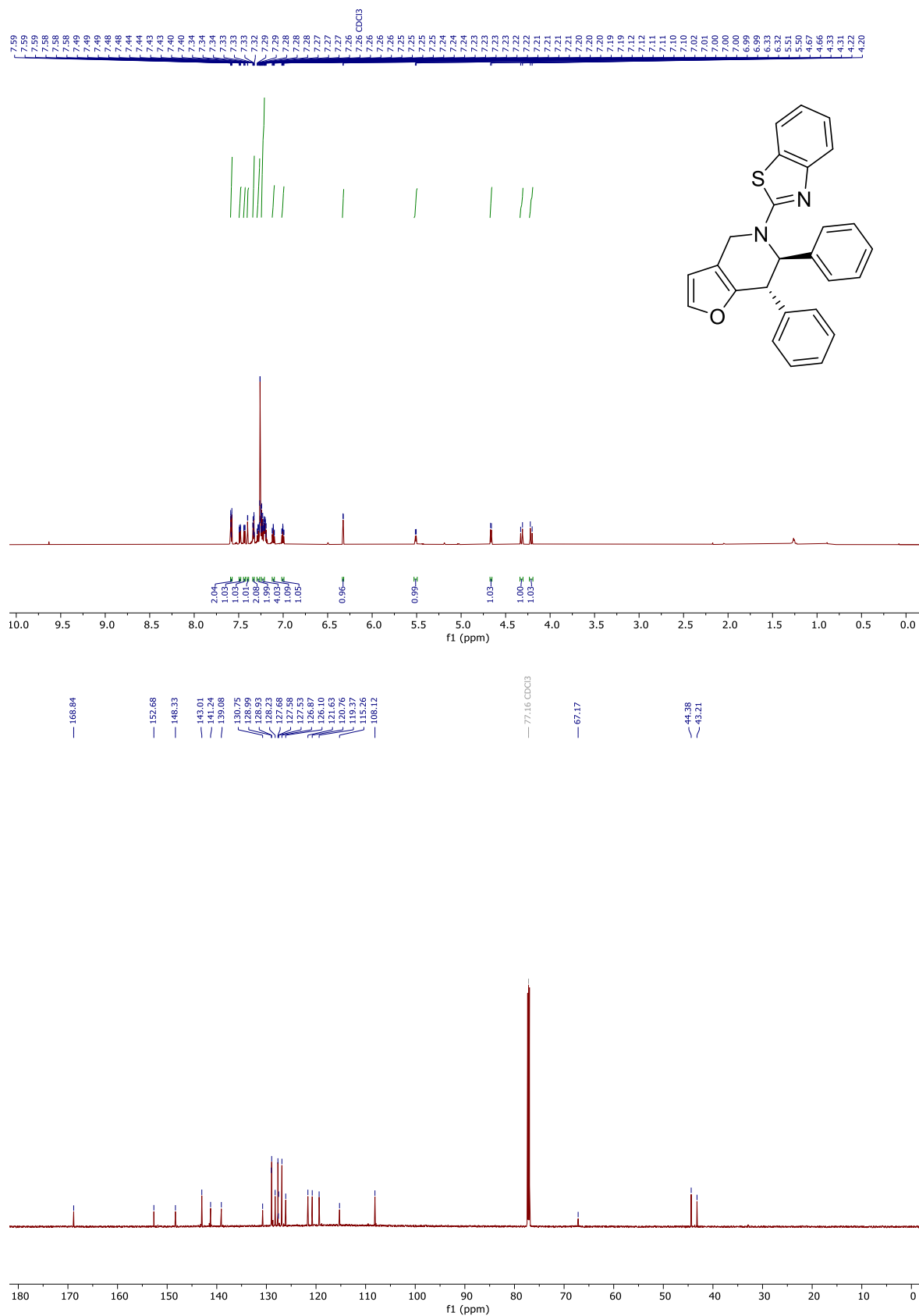


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C	-2.625471000	-0.641643000	1.574771000
C	-3.150550000	-0.334487000	0.361609000
C	-3.737885000	-0.972062000	2.420974000
O	-4.492813000	-0.449143000	0.381767000
C	-4.841021000	-0.836090000	1.636517000
H	-3.714357000	-1.264339000	3.469231000
H	-5.904456000	-0.973198000	1.817317000
C	-2.382577000	0.017520000	-0.862923000
H	-2.831325000	-0.470580000	-1.740832000
C	-2.278714000	1.507312000	-1.157743000
C	-1.949830000	1.917883000	-2.455713000
C	-2.427480000	2.477038000	-0.162686000
C	-1.761343000	3.266487000	-2.750428000
H	-1.832000000	1.167354000	-3.244083000
C	-2.241482000	3.829128000	-0.455532000
H	-2.697022000	2.175838000	0.853158000
C	-1.904401000	4.227662000	-1.748068000
H	-1.502862000	3.568783000	-3.768639000

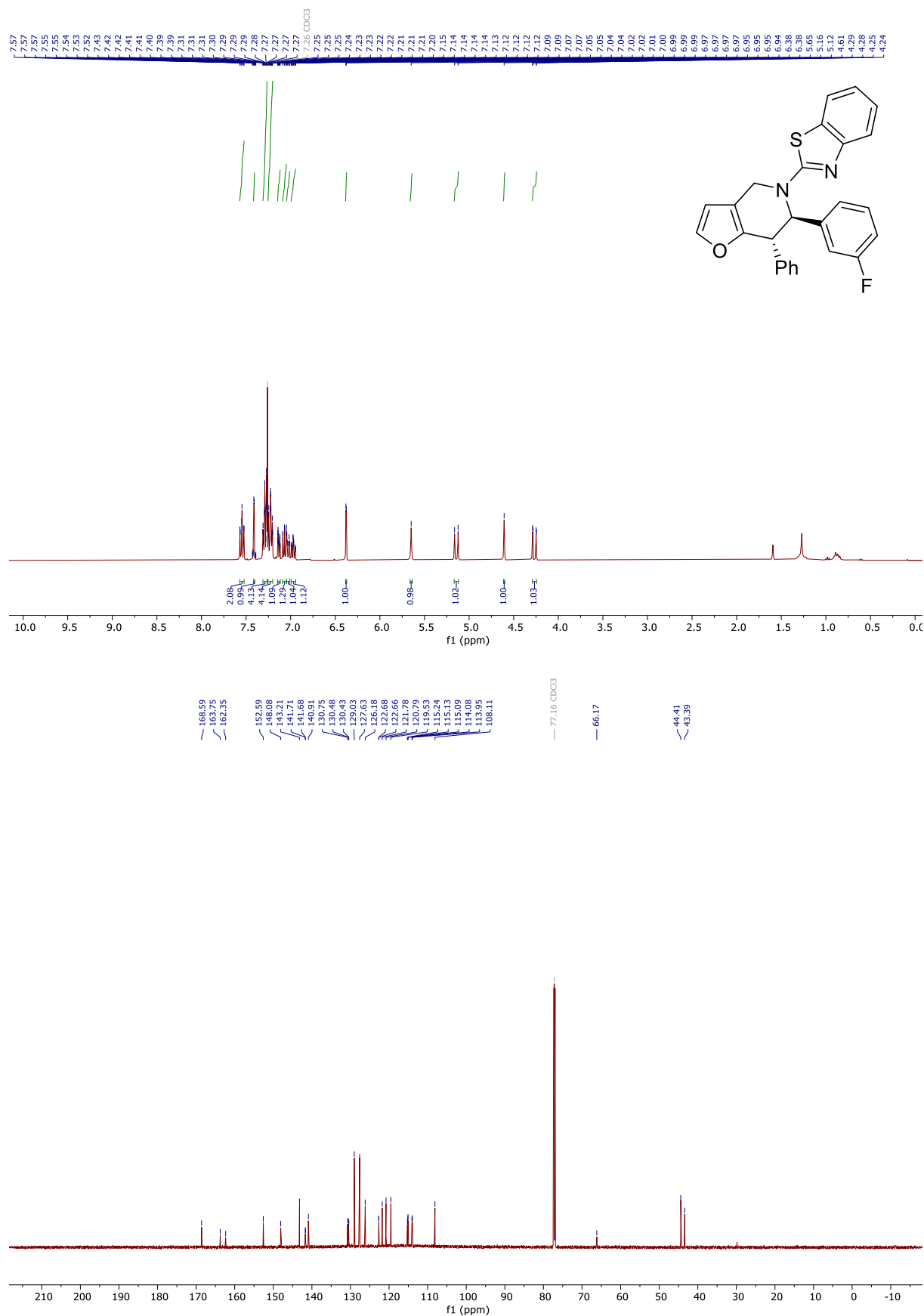
H	-2.362935000	4.575137000	0.334261000
H	-1.757099000	5.286407000	-1.976394000
C	2.796229000	0.867495000	1.622447000
C	2.952450000	1.530953000	0.387666000
C	4.120899000	2.223514000	0.067673000
C	5.138508000	2.263056000	1.017121000
C	4.992068000	1.617770000	2.255258000
C	3.831366000	0.917790000	2.565189000
C	0.826665000	0.347805000	0.759206000
H	4.230807000	2.727494000	-0.895299000
H	6.059486000	2.807443000	0.794445000
H	5.803361000	1.666968000	2.985984000
H	3.707288000	0.411229000	3.525415000
N	-0.456573000	-0.114058000	0.667387000
N	1.599362000	0.194806000	1.783438000
S	1.501654000	1.331143000	-0.561558000
C	-0.978545000	-0.580558000	-0.626668000
H	-0.314099000	-0.171496000	-1.400748000
C	-0.885202000	-2.104875000	-0.735163000
C	-1.975461000	-2.927047000	-1.034473000
C	0.368681000	-2.701950000	-0.541093000
C	-1.816984000	-4.310378000	-1.139194000
H	-2.970417000	-2.502796000	-1.183216000
C	0.528888000	-4.081415000	-0.642246000
H	1.237780000	-2.079553000	-0.308773000
C	-0.566715000	-4.892460000	-0.943506000
H	-2.683101000	-4.934336000	-1.374022000
H	1.515952000	-4.524912000	-0.488419000
H	-0.444195000	-5.975506000	-1.025131000
H	-0.766845000	-1.506630000	2.261063000
N	-0.959277000	0.405026000	2.963816000
C	-0.211883000	0.120280000	4.057482000
N	0.075725000	-1.071778000	4.469966000
S	0.438230000	1.453651000	5.017433000
C	0.876467000	-1.023514000	5.596891000
C	1.179873000	0.271371000	6.071044000
C	1.382980000	-2.133467000	6.285846000
C	1.963107000	0.479029000	7.205702000
C	2.169258000	-1.931704000	7.415515000
H	1.152854000	-3.138343000	5.924531000
C	2.459382000	-0.638035000	7.874028000
H	2.186581000	1.489032000	7.557104000
H	2.568330000	-2.795550000	7.953323000
H	3.080711000	-0.502236000	8.762551000
H	-1.161492000	1.376683000	2.757321000

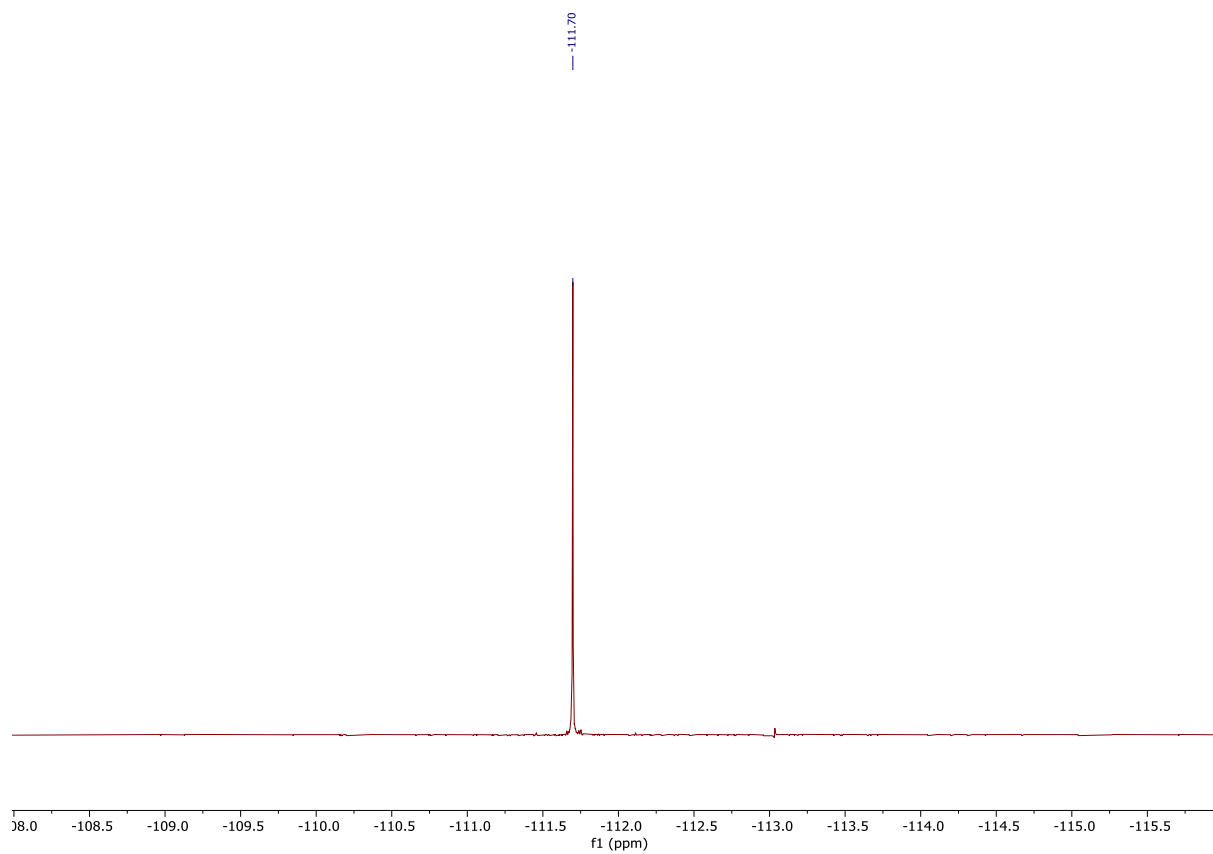
7. NMR spectra

(6*R*,7*S*)-5-(Benzo[*d*]thiazol-2-yl)-6,7-diphenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4a

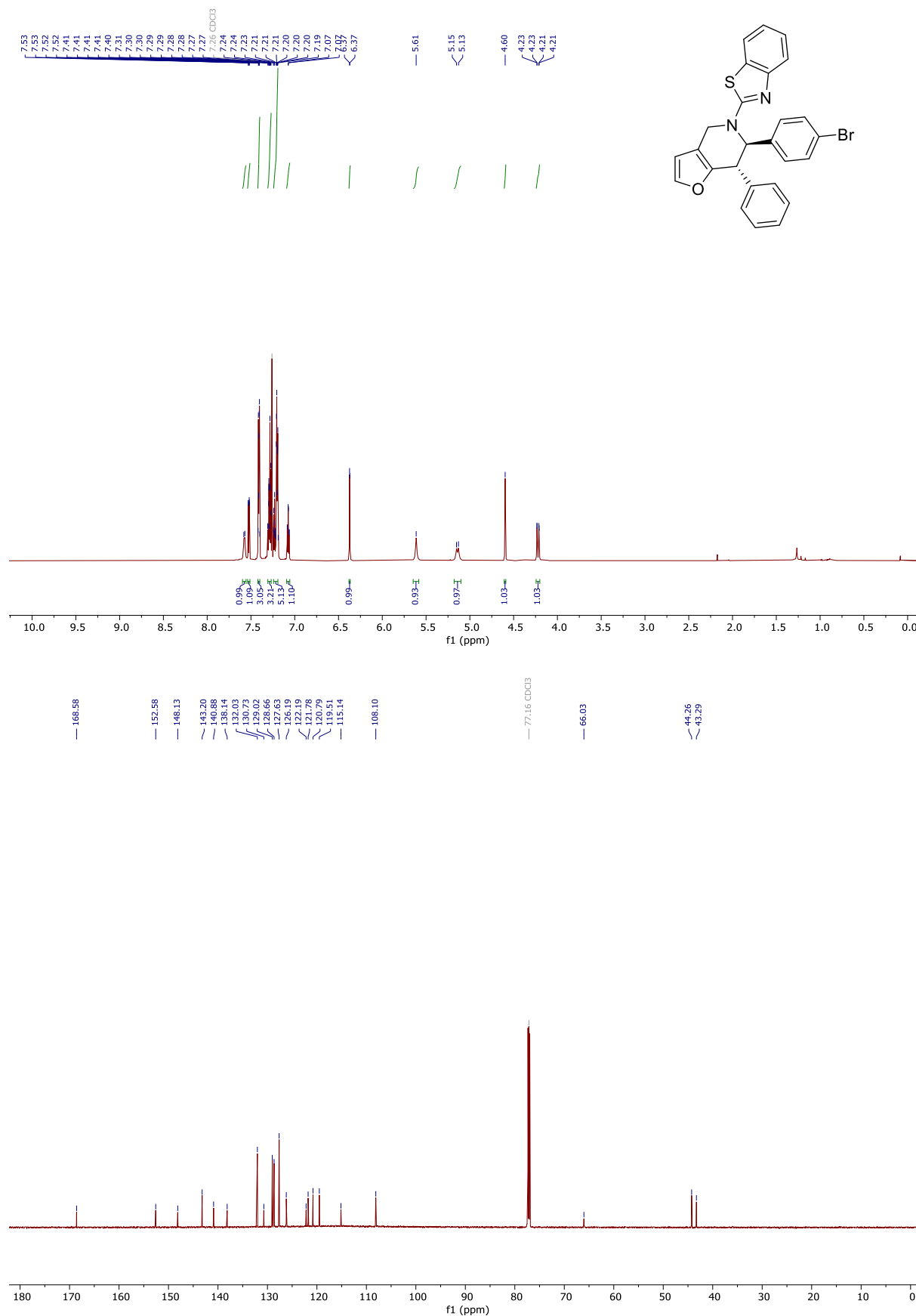


(6*R*,7*S*)-5-(Benzo[*d*]thiazol-2-yl)-6-(3-fluorophenyl)-7-phenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4b

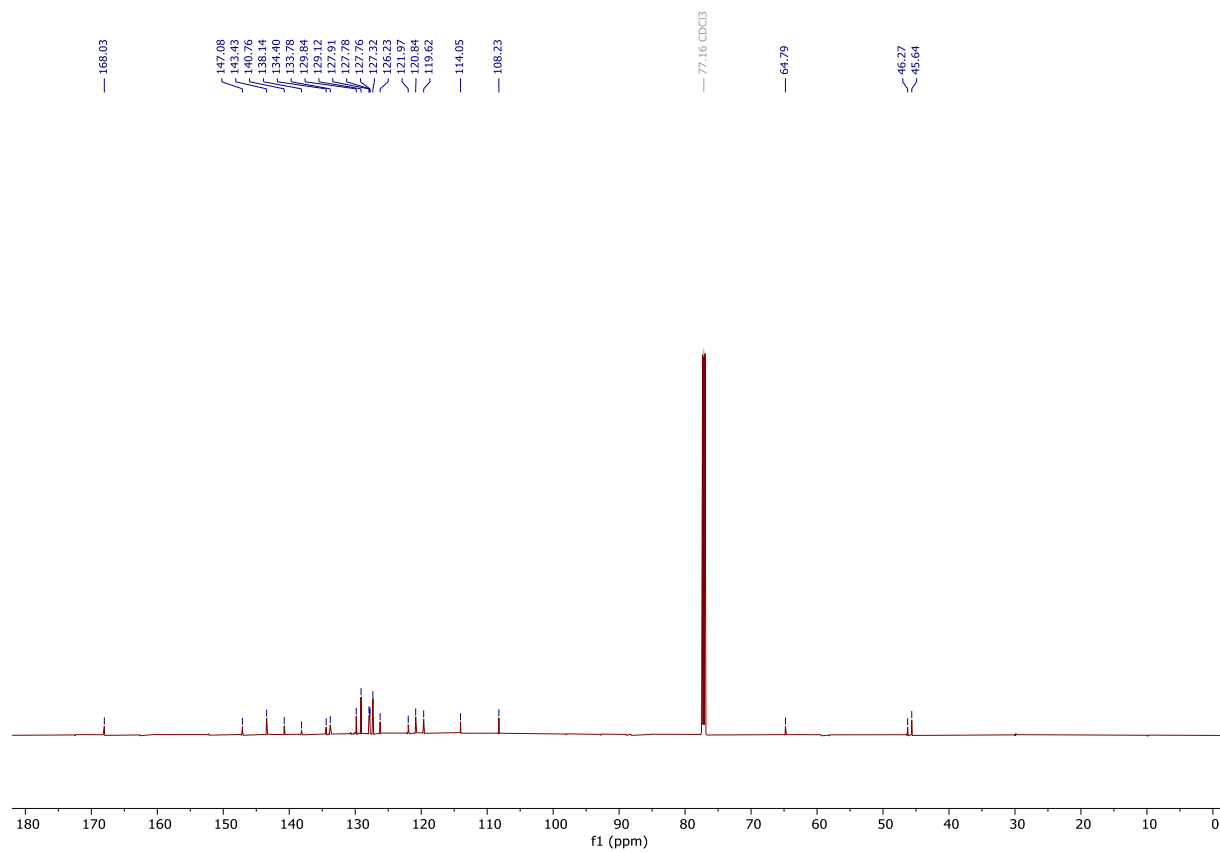
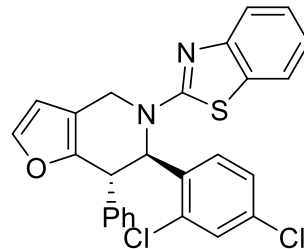
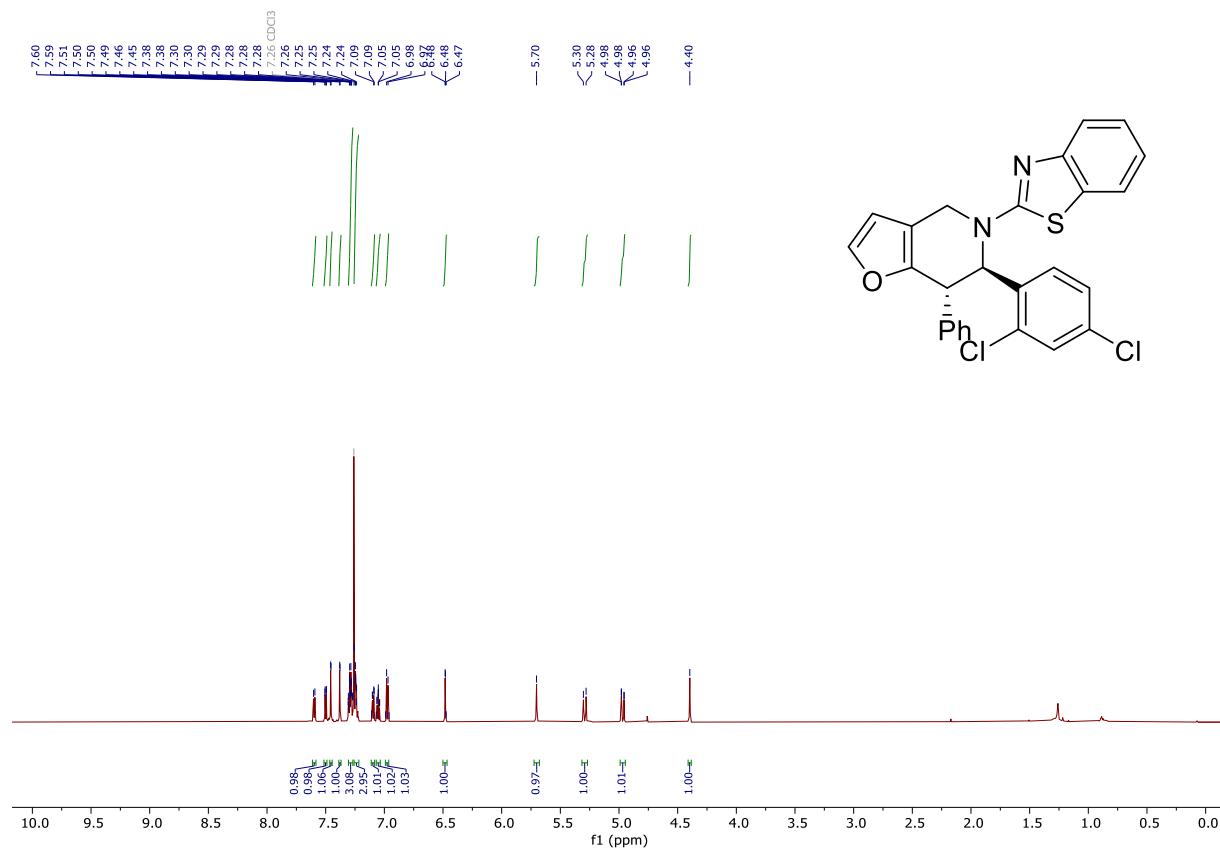




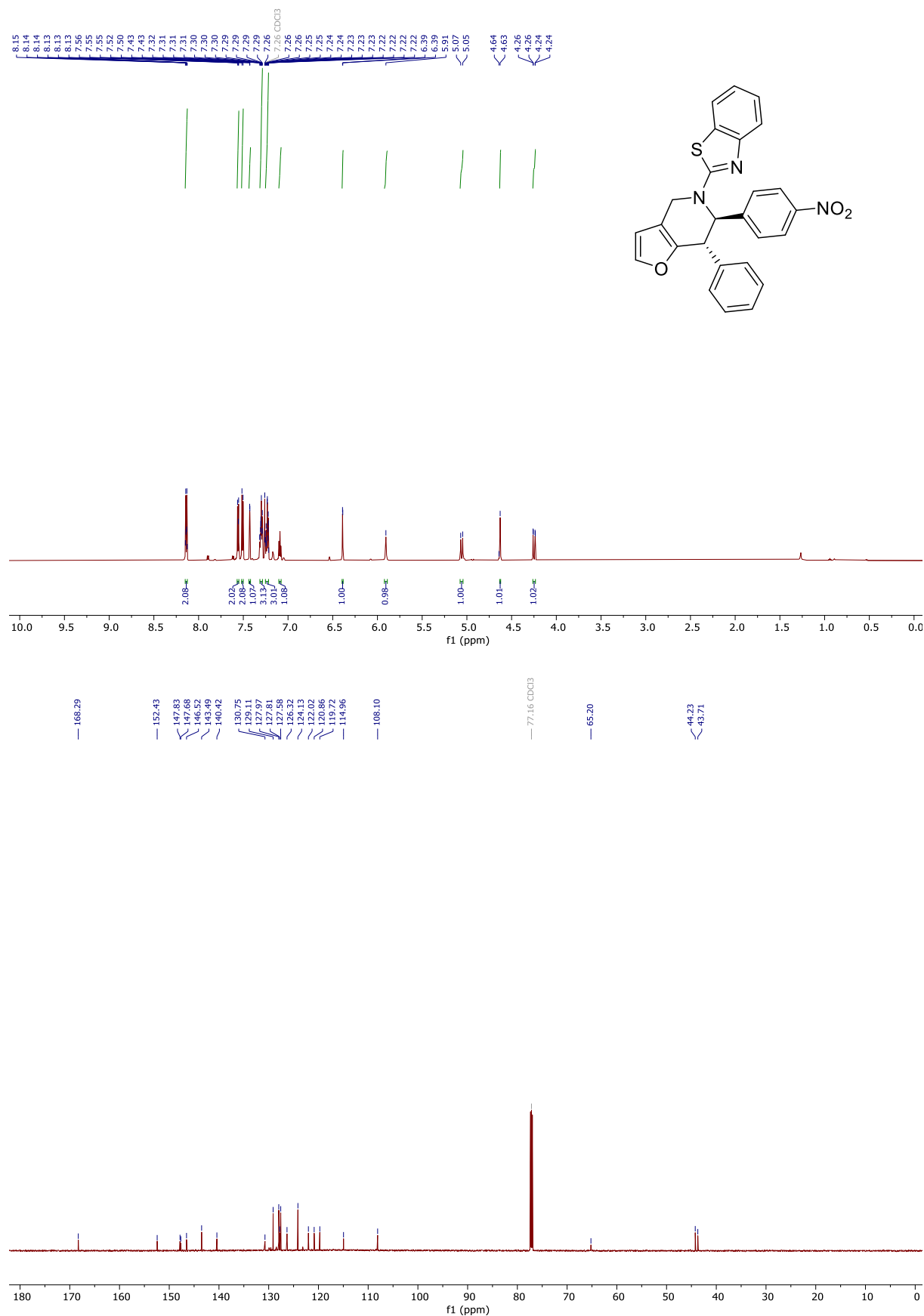
(6*R*,7*S*)-5-(Benzo[*d*]thiazol-2-yl)-6-(4-bromophenyl)-7-phenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4c



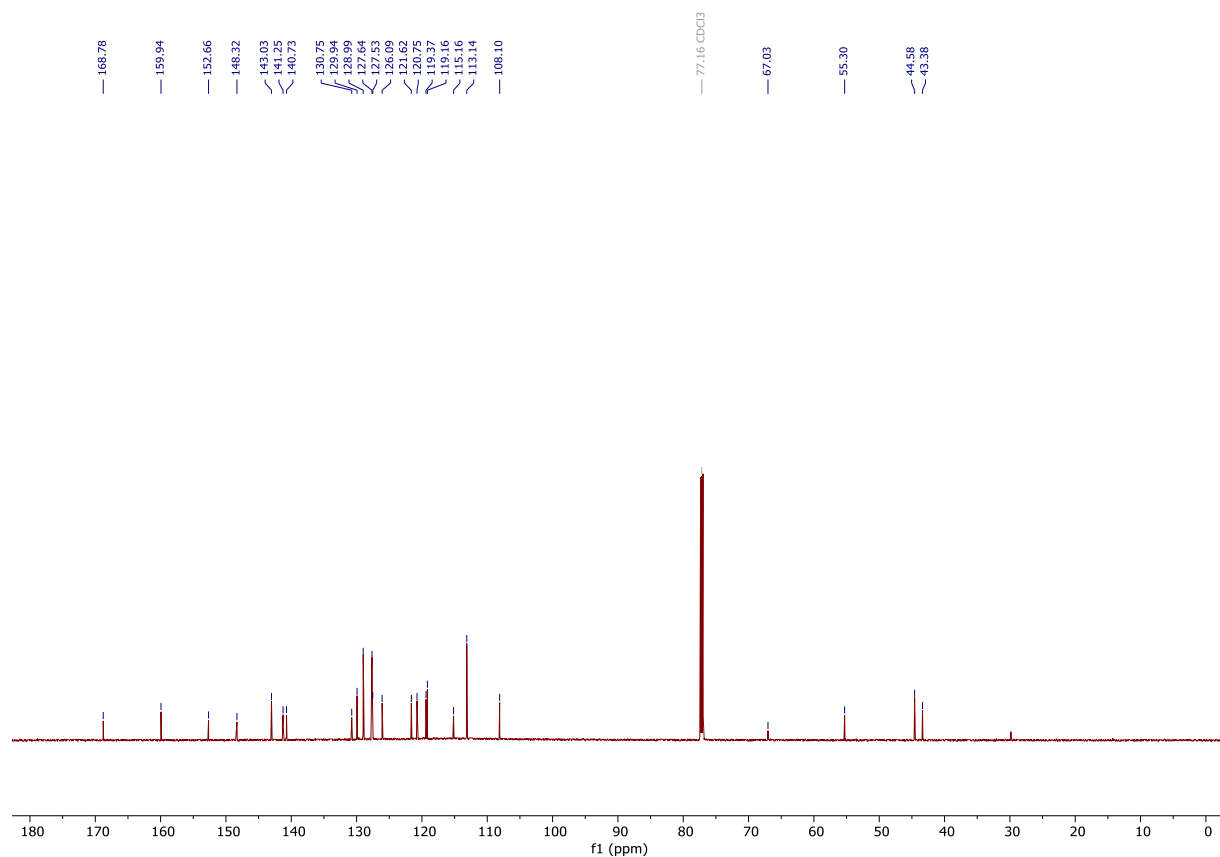
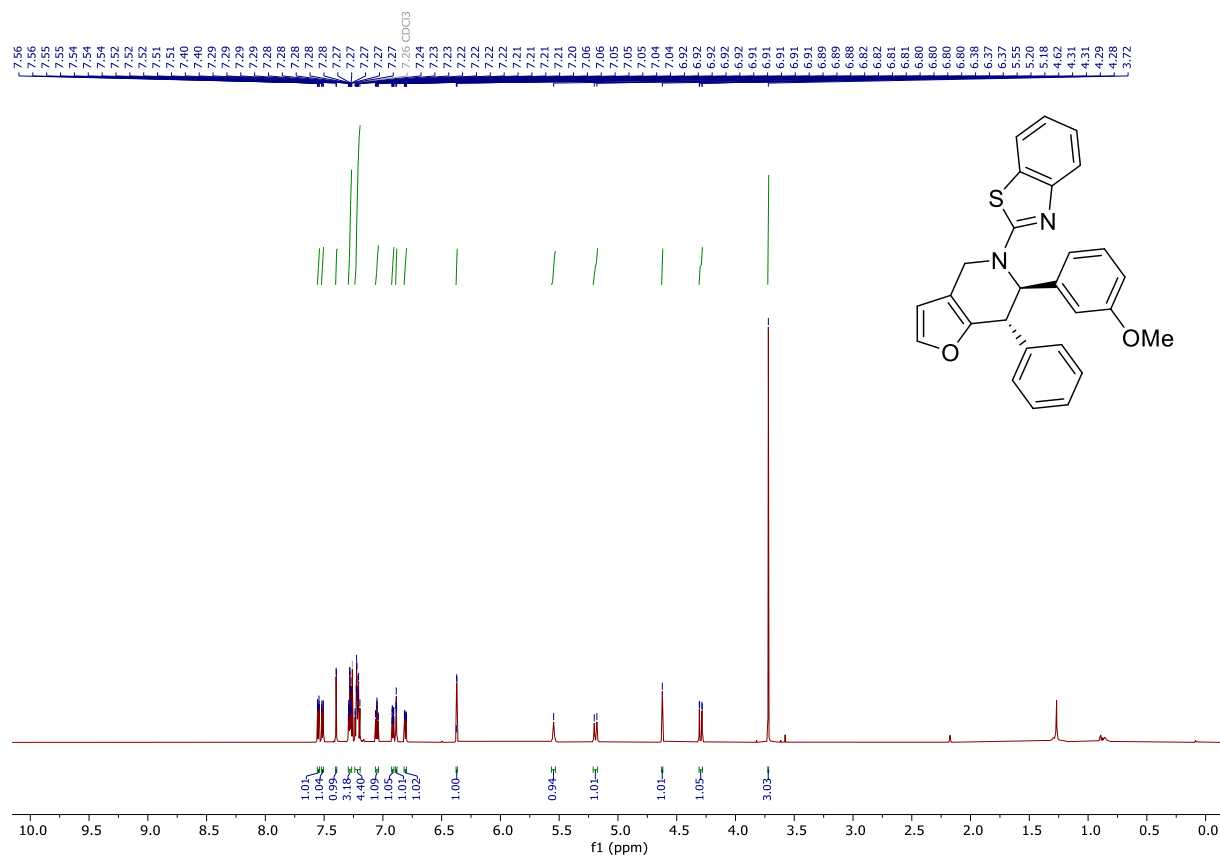
(6*R*,7*S*)-5-(Benzo[d]thiazol-2-yl)-6-(2,4-dichlorophenyl)-7-phenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4d



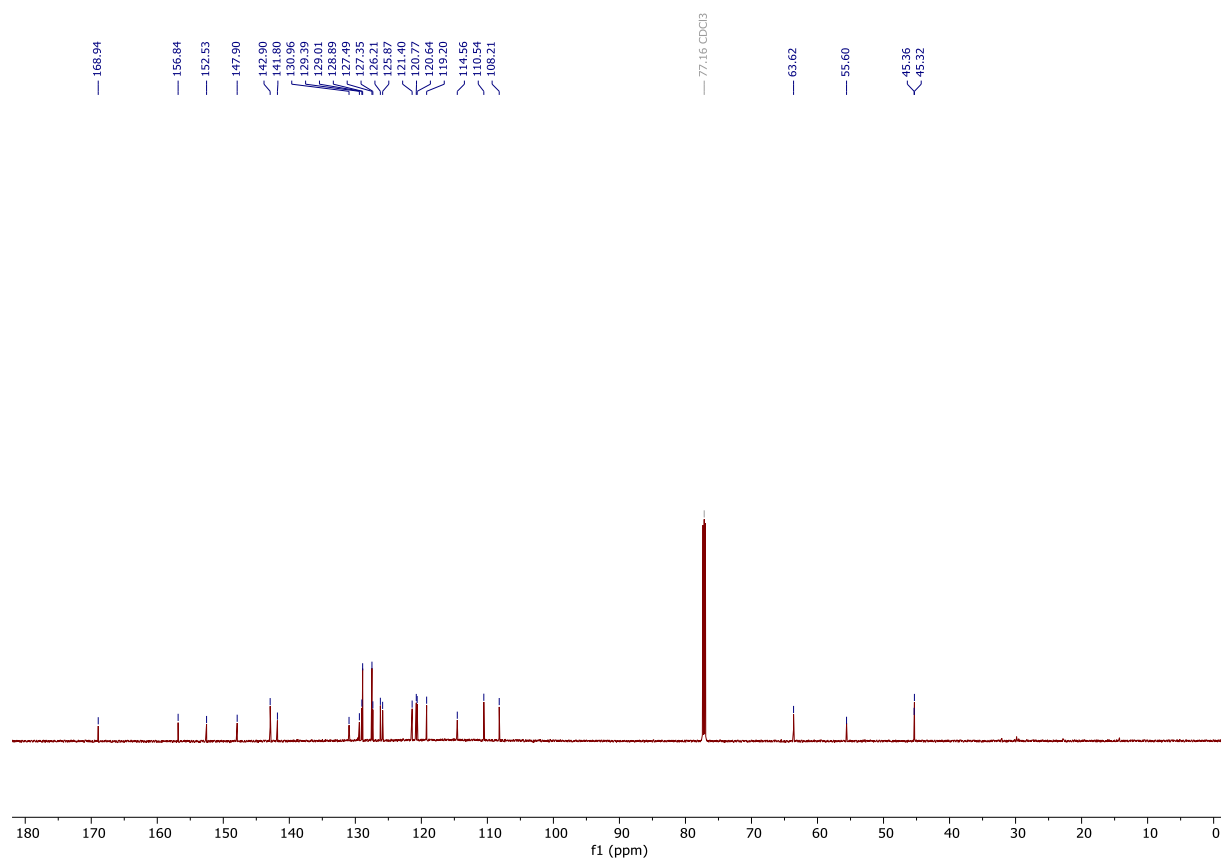
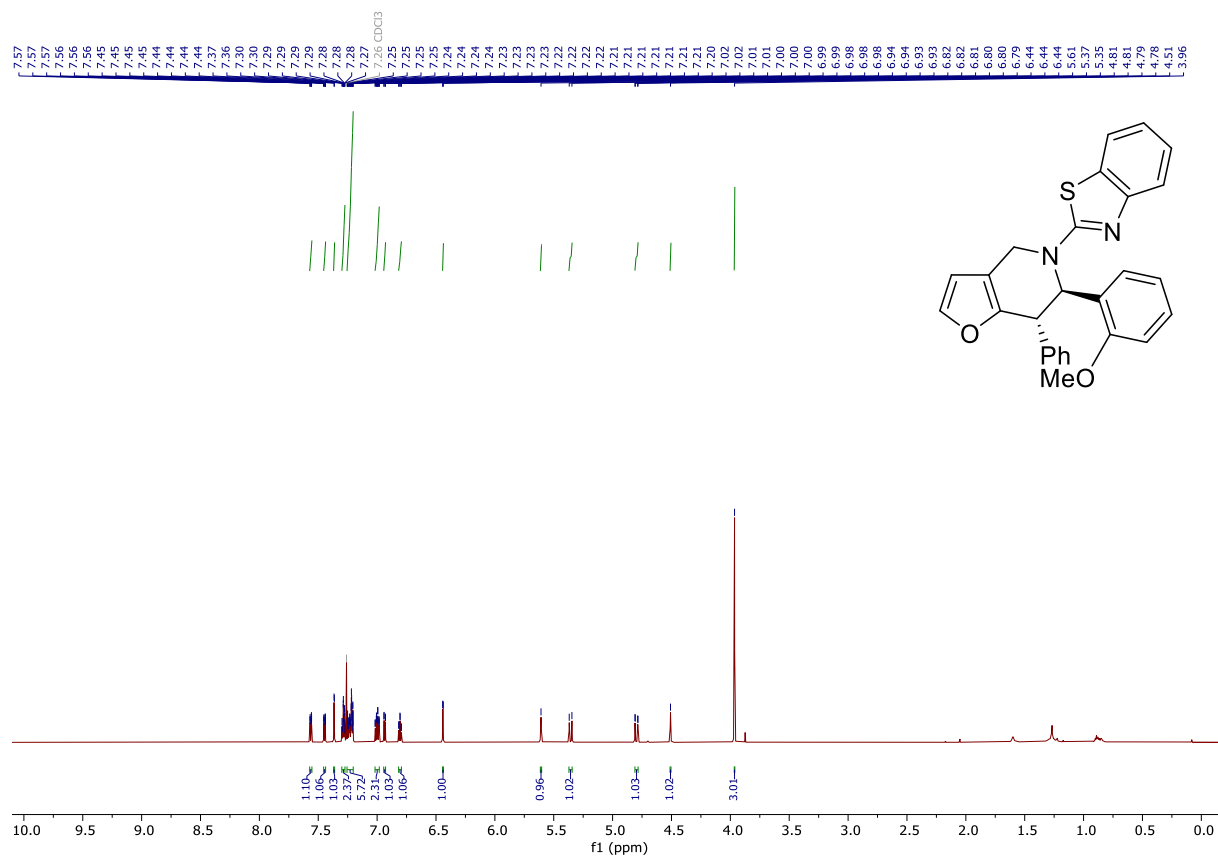
(6*R*,7*S*)-5-(Benzo[*d*]thiazol-2-yl)-6-(4-nitrophenyl)-7-phenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4e



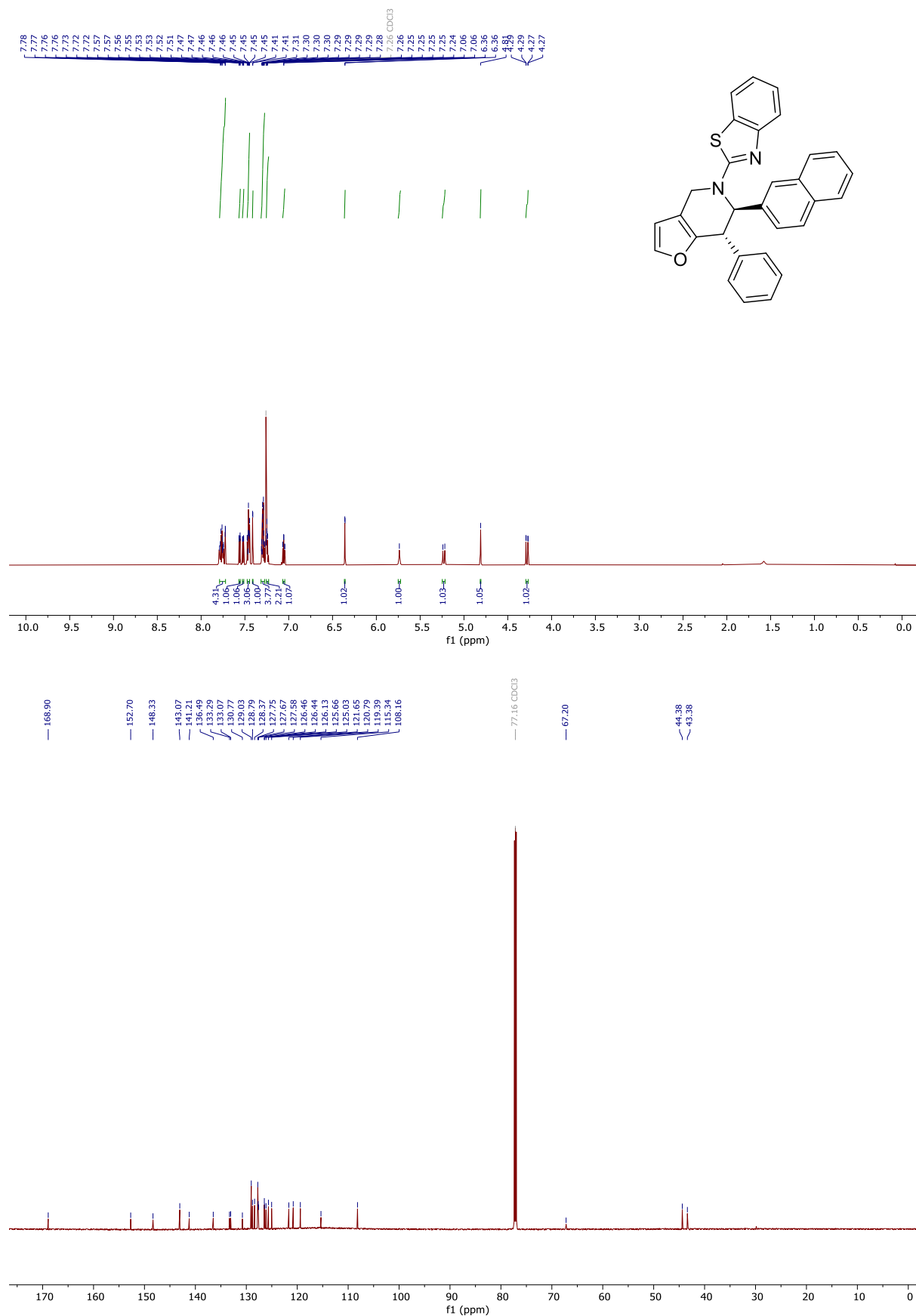
(6*R*,7*S*)-5-(Benzo[*d*]thiazol-2-yl)-6-(3-methoxyphenyl)-7-phenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4f



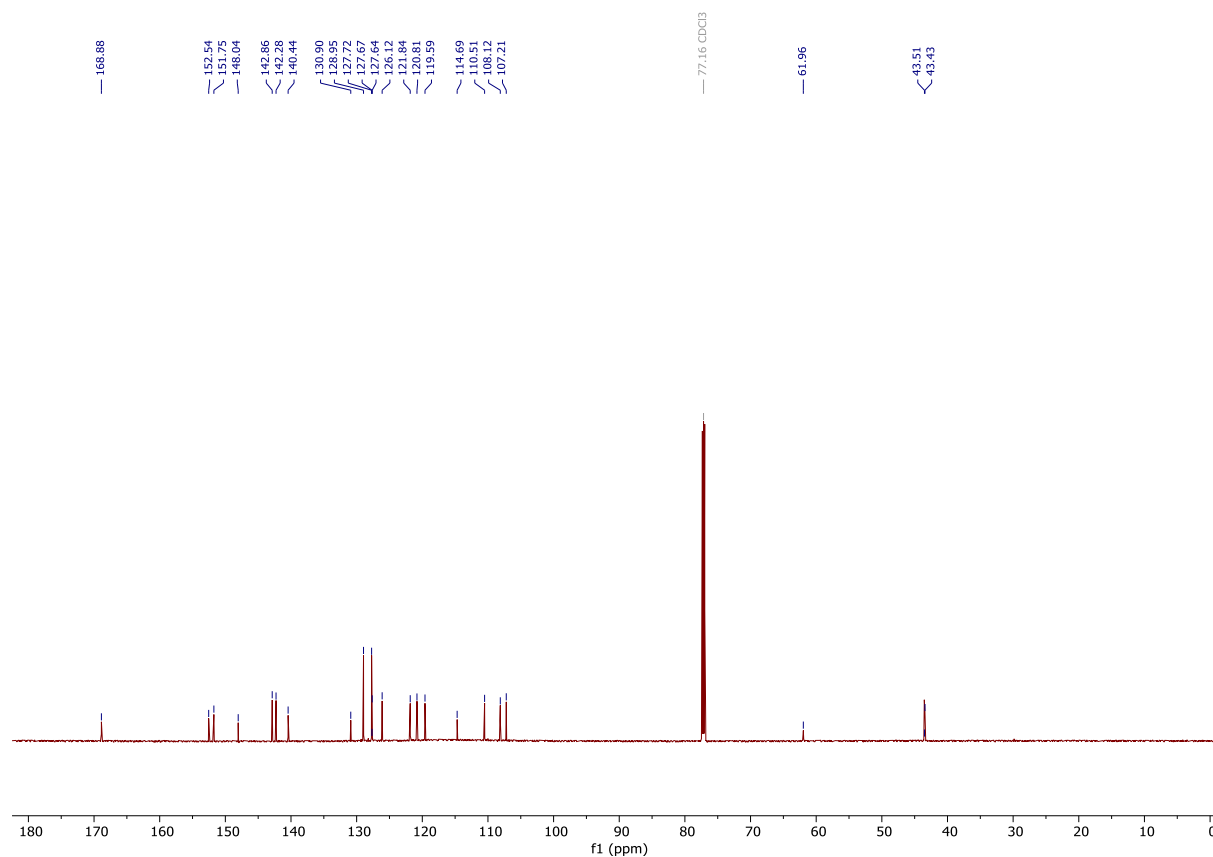
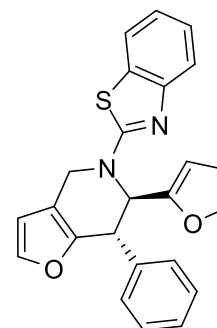
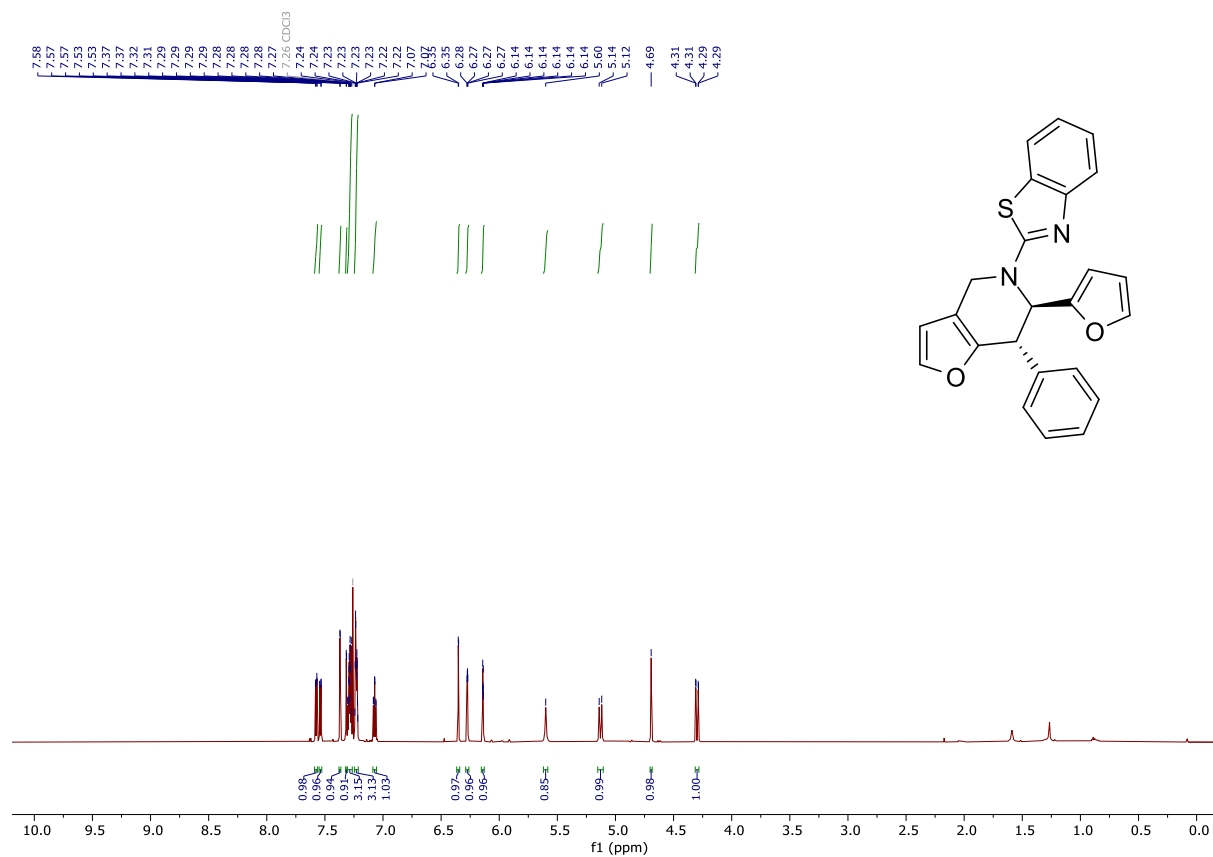
(6*R*,7*S*)-5-(Benzo[*d*]thiazol-2-yl)-6-(2-methoxyphenyl)-7-phenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4g



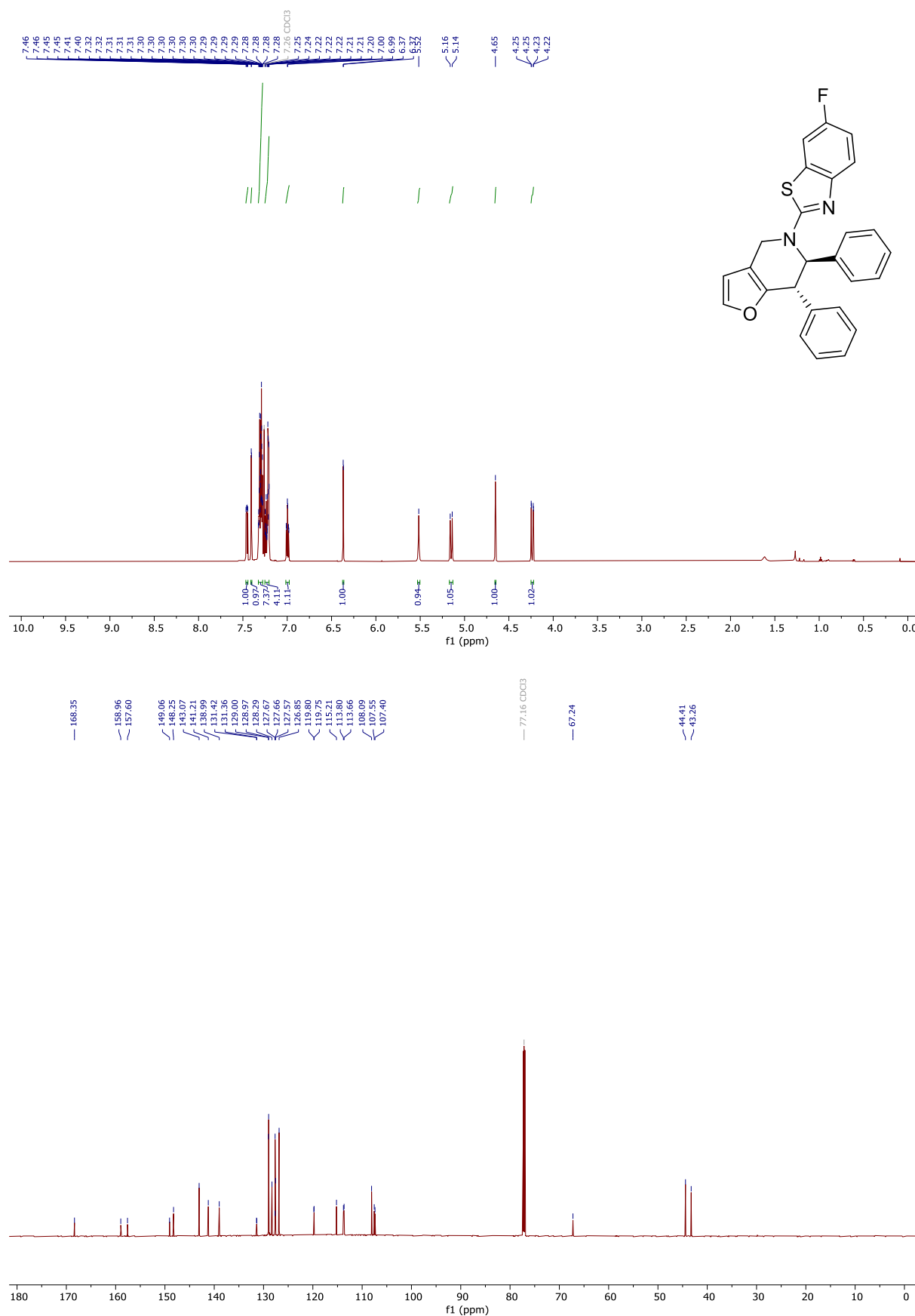
(6*R*,7*S*)-5-(Benzo[*d*]thiazol-2-yl)-6-(naphthalen-2-yl)-7-phenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4h

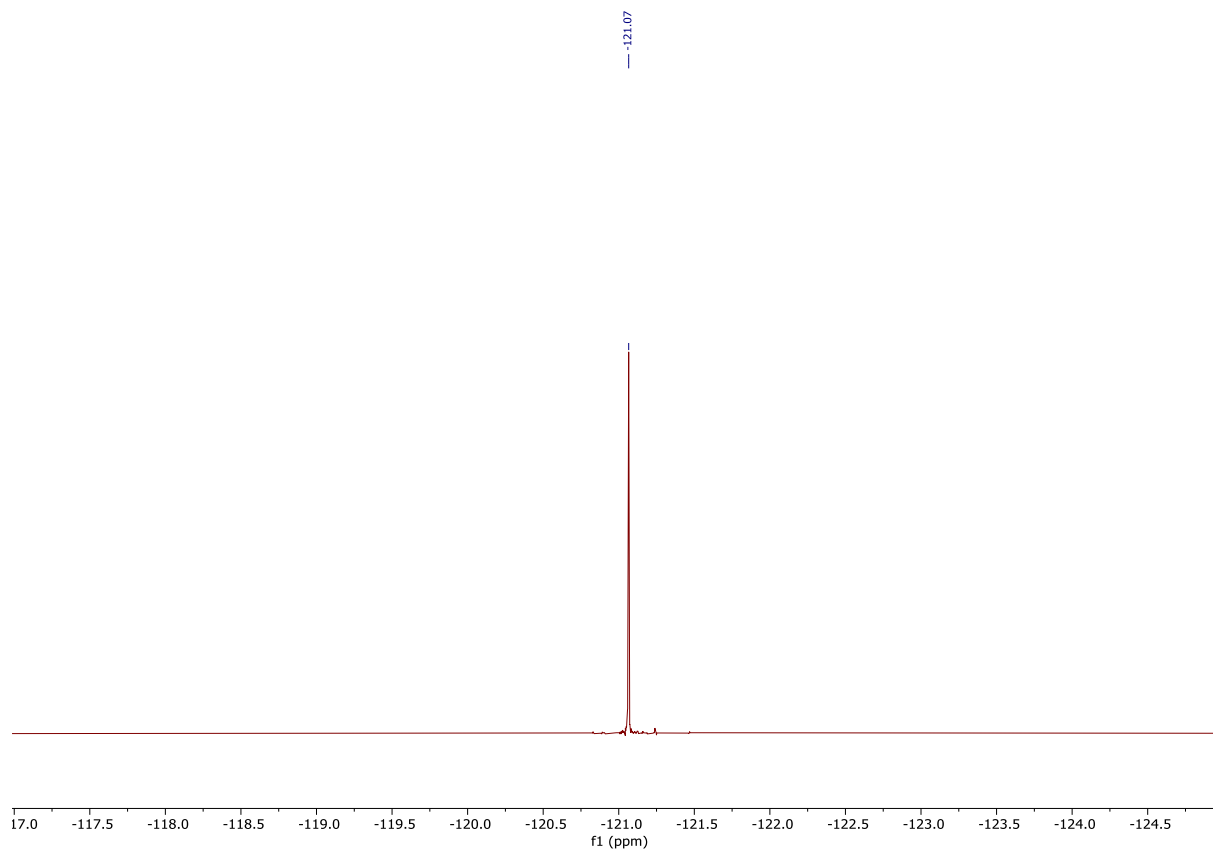


(6*R*,7*S*)-5-(Benzo[*d*]thiazol-2-yl)-6-(furan-2-yl)-7-phenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4i

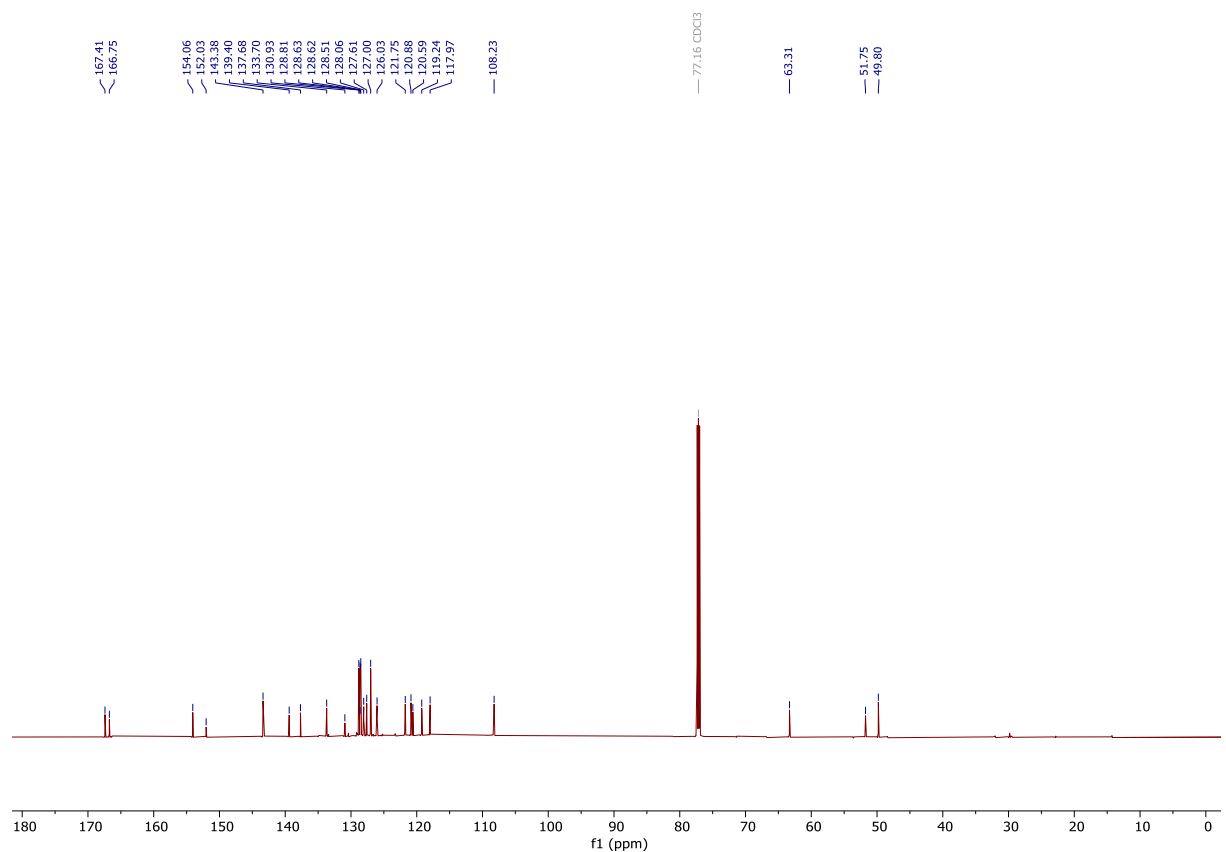
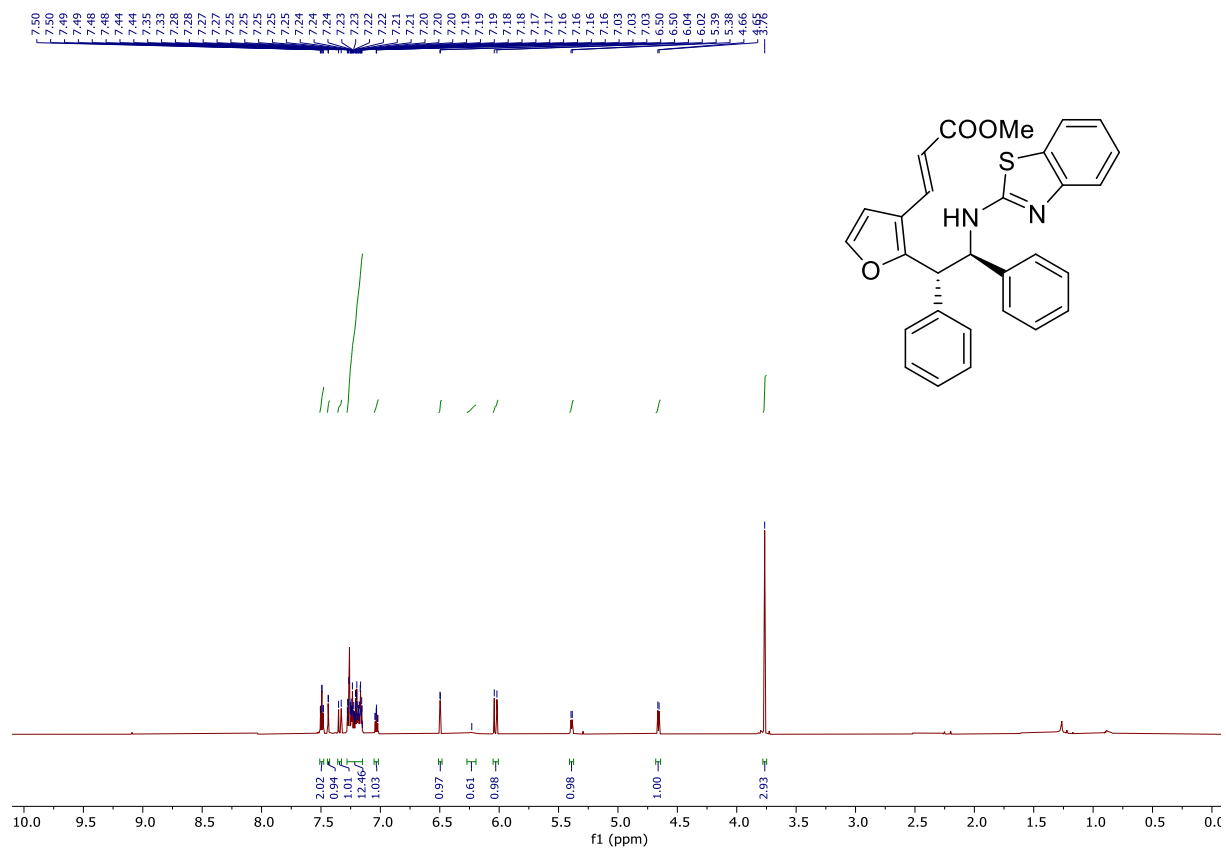


(6*R*,7*S*)-5-(6-Fluorobenzo[*d*]thiazol-2-yl)-6,7-diphenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4j



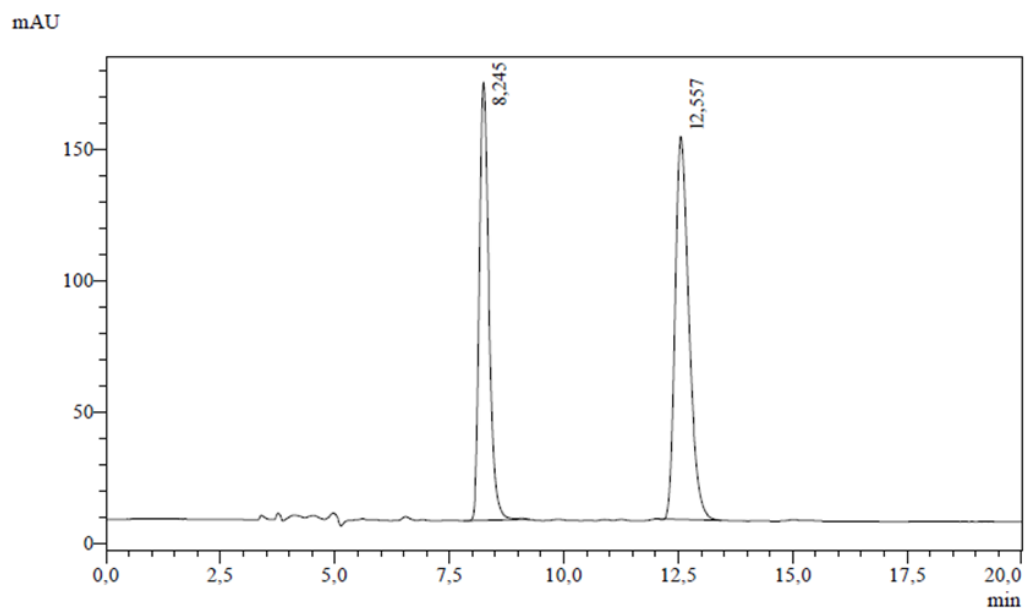


(E)-Methyl 3-(2-((1S,2R)-2-(benzo[d]thiazol-2-ylamino)-1,2-diphenylethyl)furan-3-yl)acrylate 6



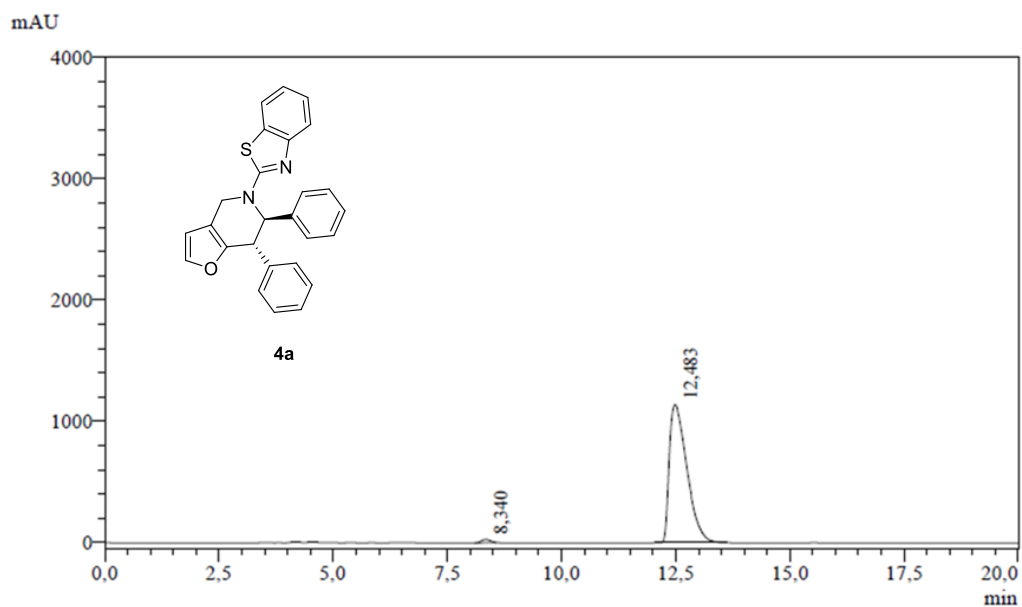
8. HPLC traces

(6*R*,7*S*)-5-(Benzo[*d*]thiazol-2-yl)-6,7-diphenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4a



Peak Table

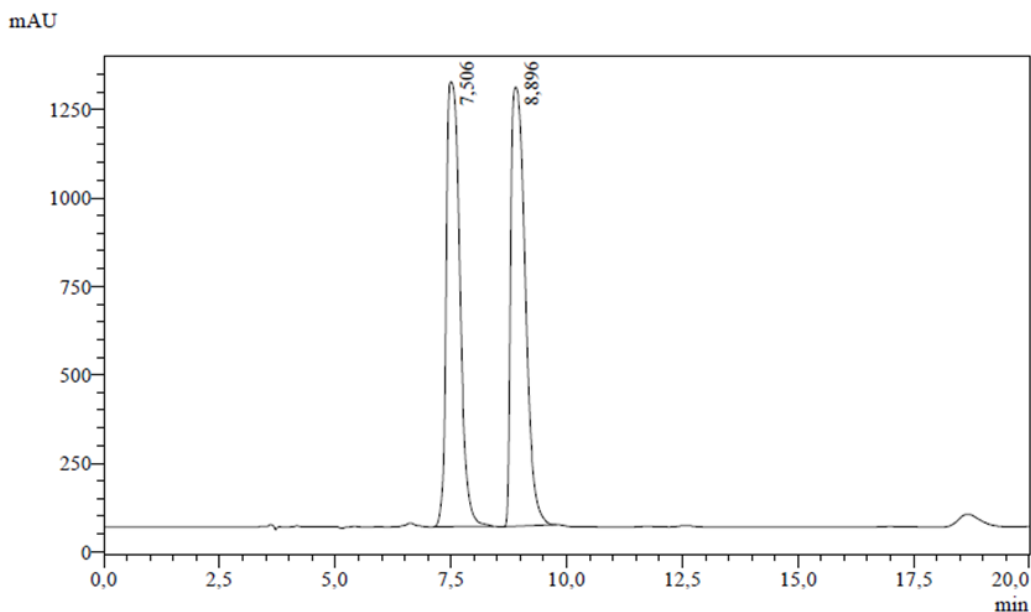
Peak	Ret. Time	Area %
1	8.245	44.113
2	12.557	55.887
Total		100.000



Peak Table

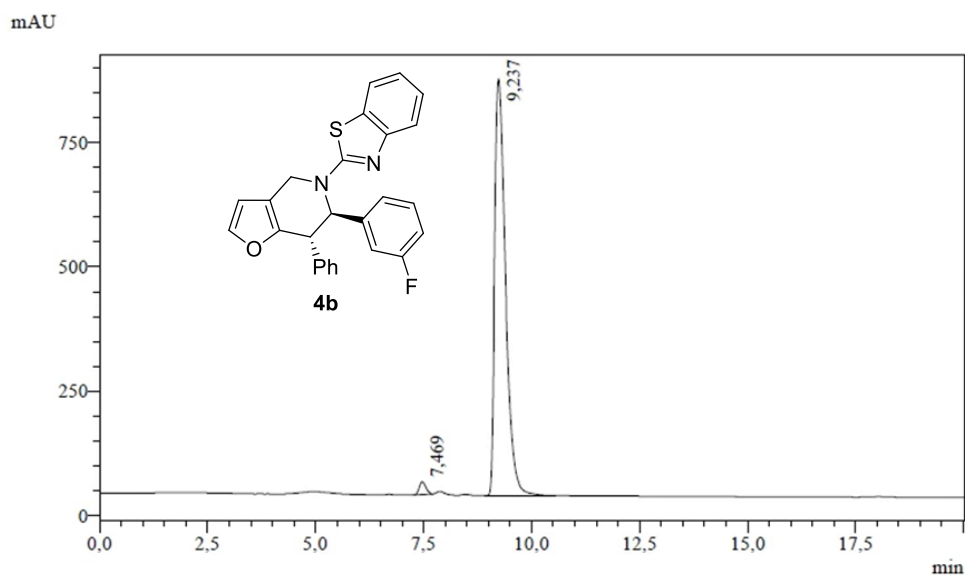
Peak	Ret. Time	Area %
1	8.340	1.125
2	12.483	98.875
Total		100.000

(6*R*,7*S*)-5-(Benzo[*d*]thiazol-2-yl)-6-(3-fluorophenyl)-7-phenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4b



Peak Table

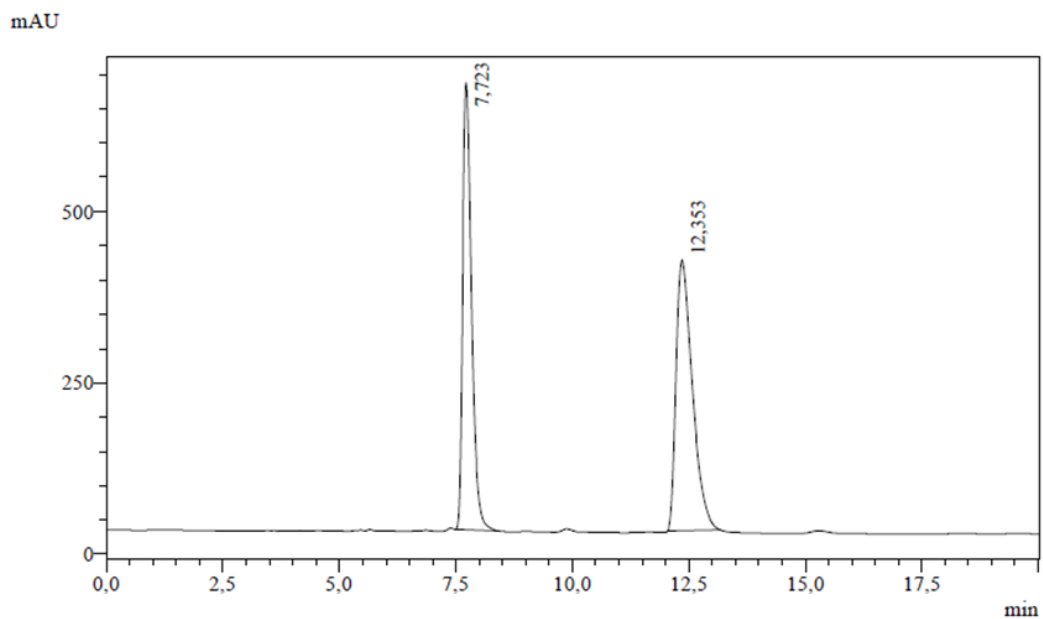
Peak	Ret. Time	Area %
1	7.506	49.022
2	8.896	50.978
Total		100,000



Peak Table

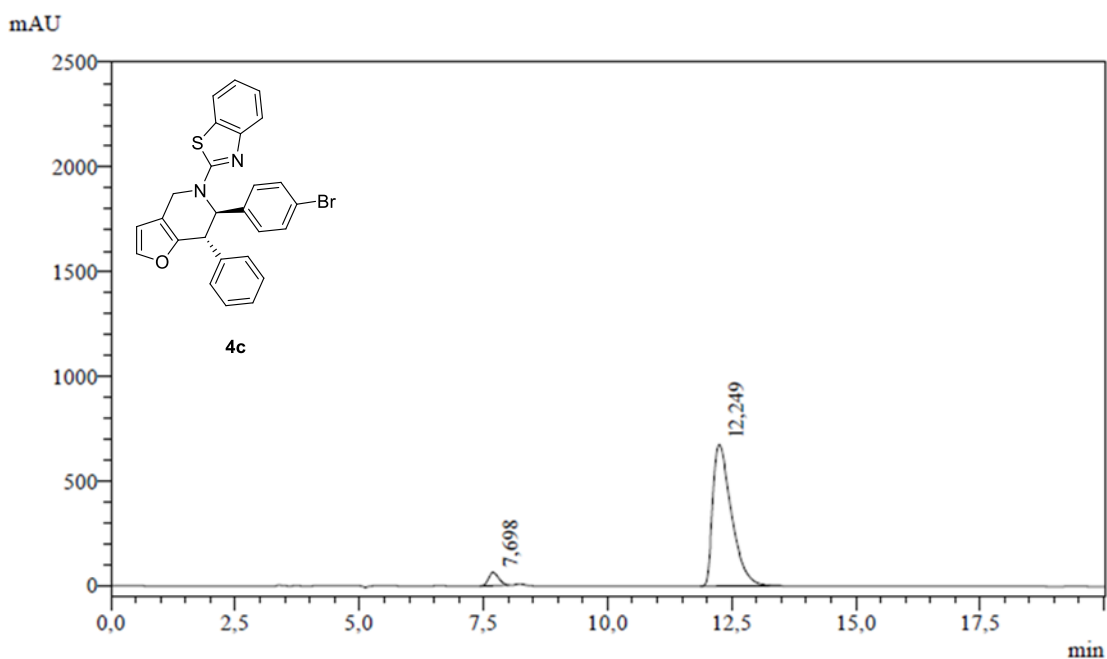
Peak	Ret. Time	Area %
1	7.469	1.824
2	9.237	98.176
Total		100,000

(6*R*,7*S*)-5-(Benzo[*d*]thiazol-2-yl)-6-(4-bromophenyl)-7-phenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4c



Peak Table

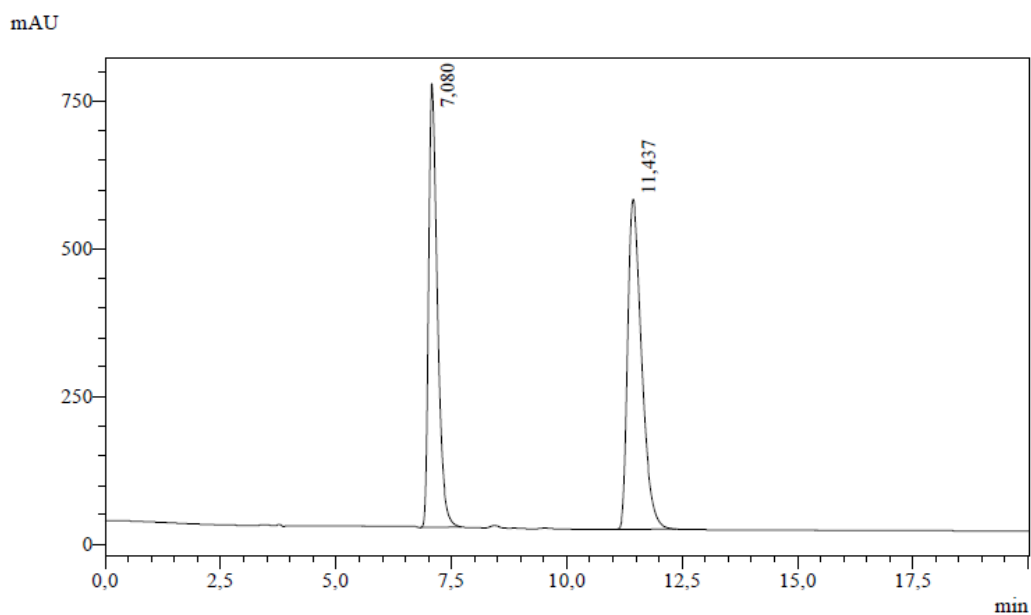
Peak	Ret. Time	Area %
1	7.723	47.172
2	12.353	52.828
Total		100.000



Peak Table

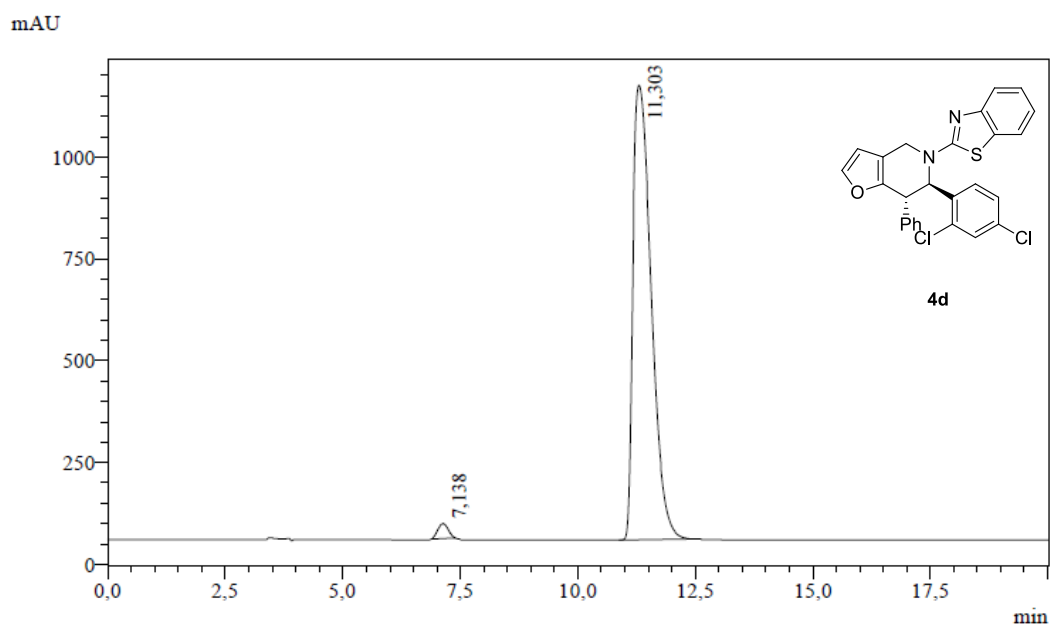
Peak	Ret. Time	Area %
1	7.698	4.820
2	12.249	95.180
Total		100.000

(6*R*,7*S*)-5-(Benzo[*d*]thiazol-2-yl)-6-(2,4-dichlorophenyl)-7-phenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4d



Peak Table

Peak	Ret. Time	Area %
1	7.080	46,242
2	11.437	53,758
Total		100,000

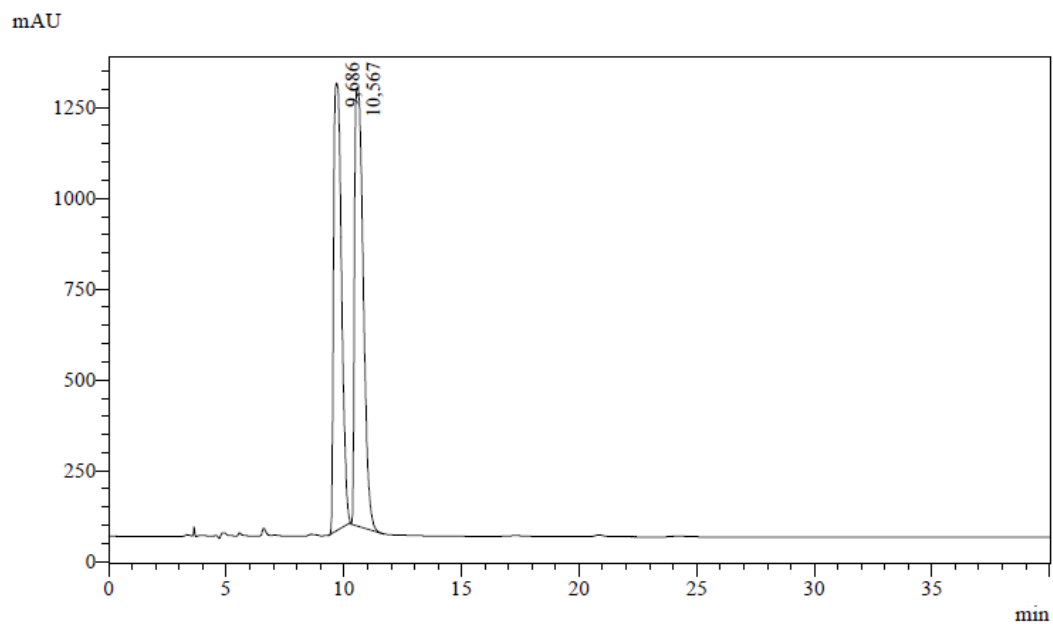


Peak Table

PDA Ch2 269nm

Peak	Ret. Time	Area %
1	7.138	1,828
2	11.303	98,172
Total		100,000

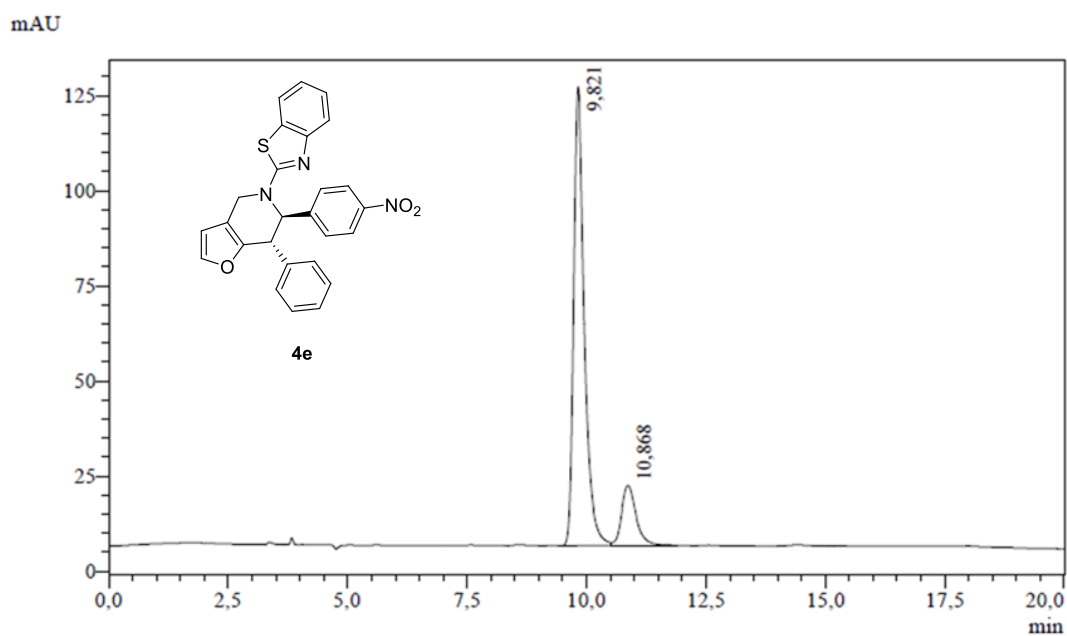
(6*R*,7*S*)-5-(Benzo[*d*]thiazol-2-yl)-6-(4-nitrophenyl)-7-phenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4e



Peak Table

PDA Ch2 268nm

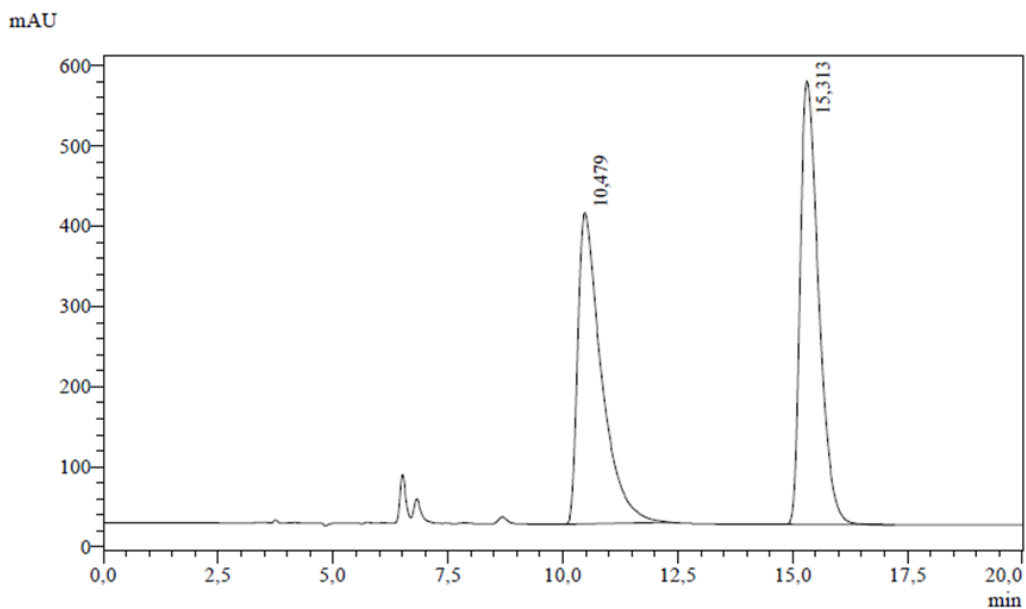
Peak	Ret. Time	Area %
1	9.686	48.122
2	10.567	51.878
Total		100.000



Peak Table

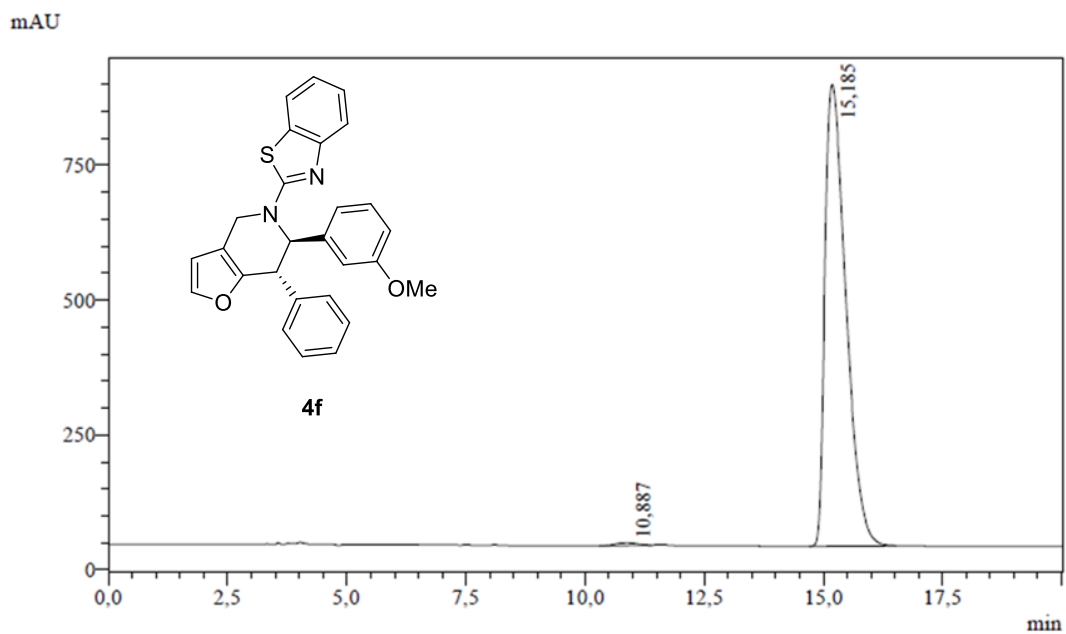
Peak	Ret. Time	Area %
1	9.821	84.906
2	10.868	15.094
Total		100.000

(6*R*,7*S*)-5-(Benzo[*d*]thiazol-2-yl)-6-(3-methoxyphenyl)-7-phenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4f



Peak Table

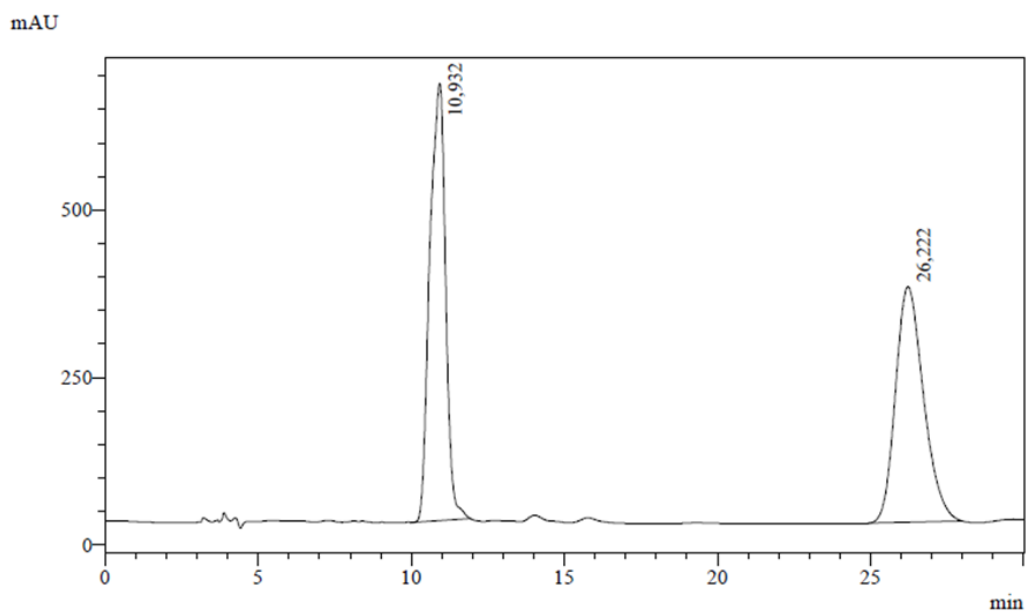
Peak	Ret. Time	Area %
1	10.479	47.287
2	15.313	52.713
Total		100.000



Peak Table

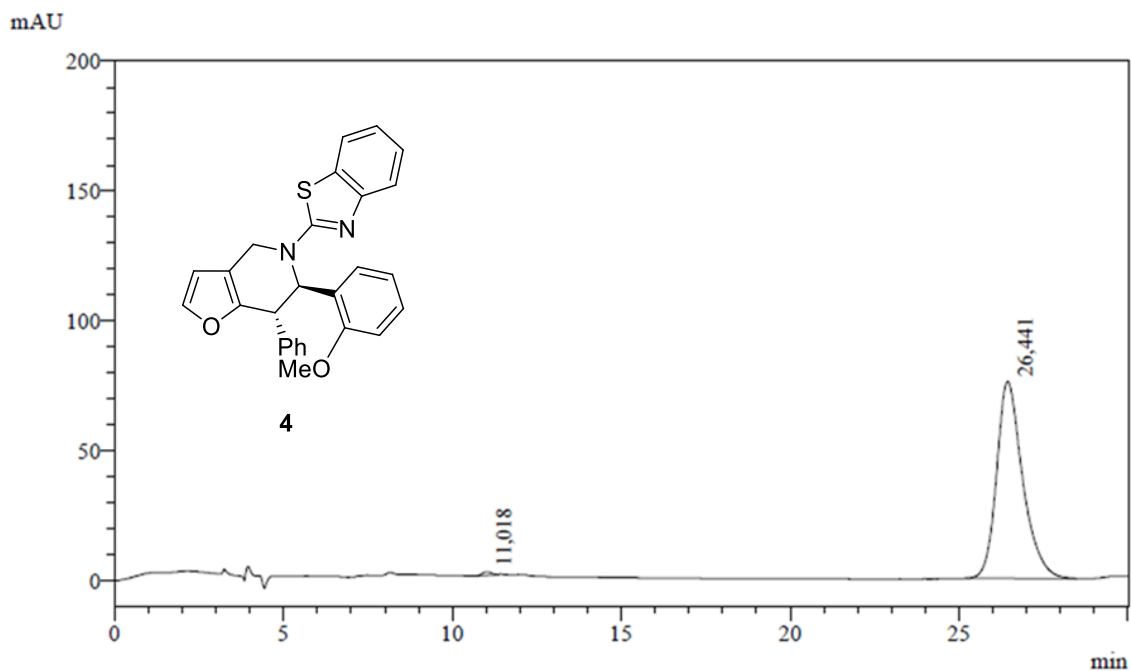
Peak	Ret. Time	Area %
1	10.887	0.559
2	15.185	99.441
Total		100.000

(6*R*,7*S*)-5-(Benzo[*d*]thiazol-2-yl)-6-(2-methoxyphenyl)-7-phenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4g



Peak Table

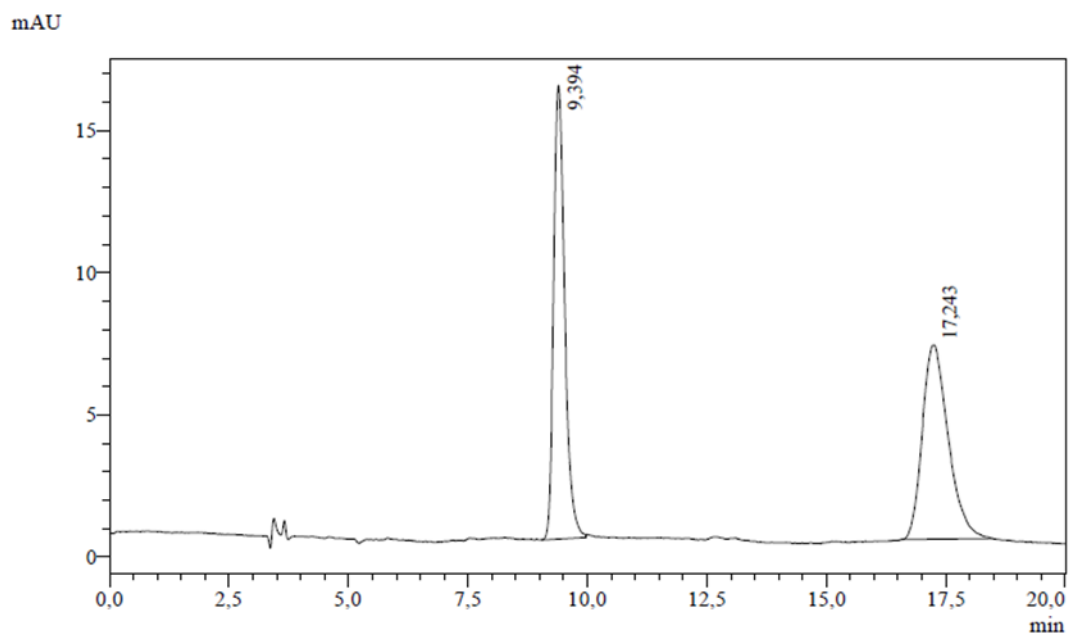
Peak	Ret. Time	Area %
1	10.932	50.994
2	26.222	49.006
Total		100.000



Peak Table

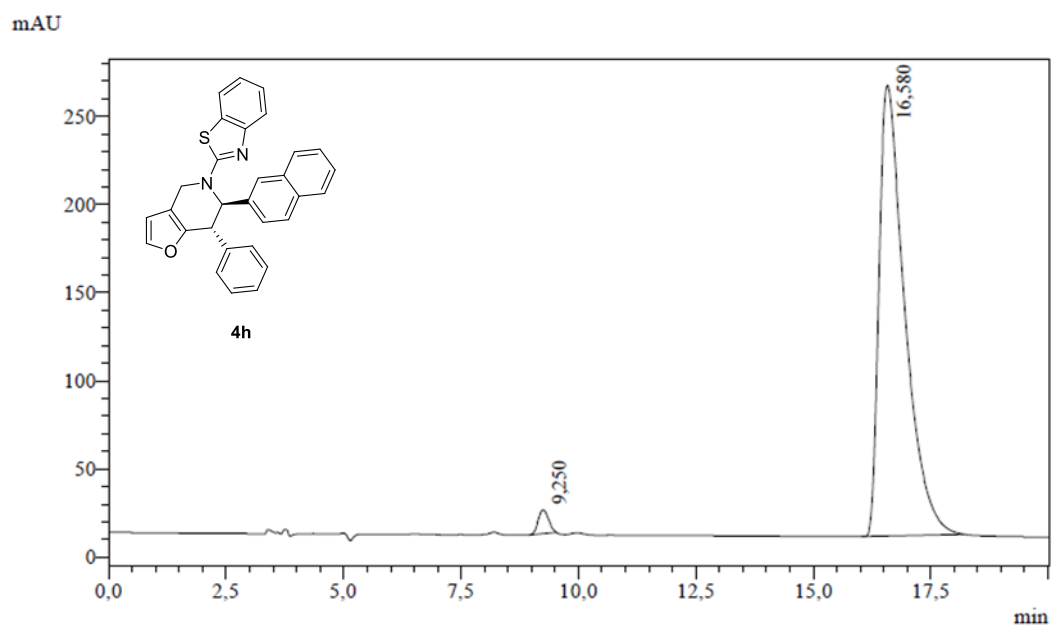
Peak	Ret. Time	Area %
1	11.018	0.604
2	26.441	99.396
Total		100.000

(6*R*,7*S*)-5-(Benzo[*d*]thiazol-2-yl)-6-(naphthalen-2-yl)-7-phenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4h



Peak Table

Peak	Ret. Time	Area %
1	9.394	49.628
2	17.243	50.372
Total		100.000

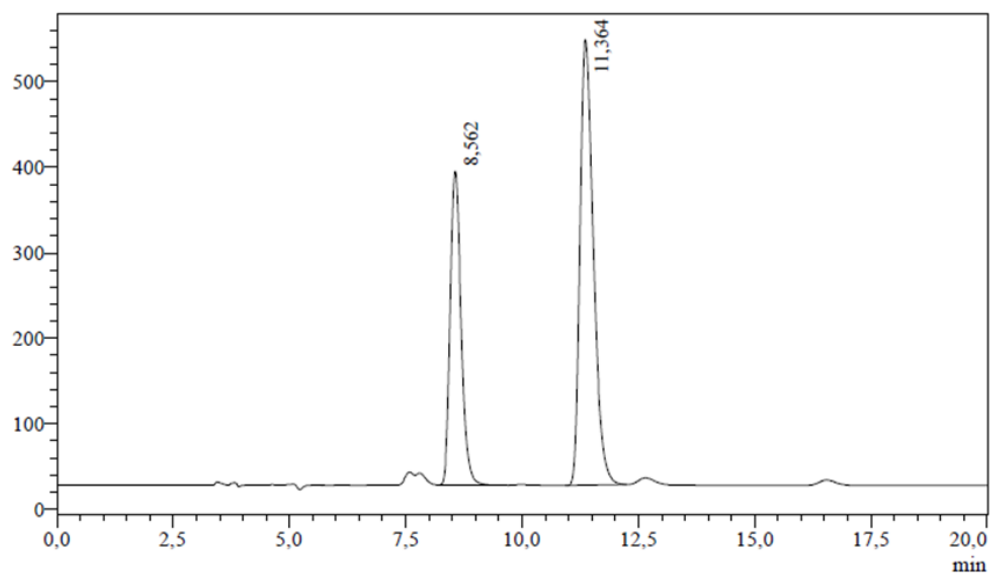


Peak Table

Peak	Ret. Time	Area %
1	9.250	2.056
2	16.580	97.944
Total		100.000

(6*R*,7*S*)-5-(Benzo[*d*]thiazol-2-yl)-6-(furan-2-yl)-7-phenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4i

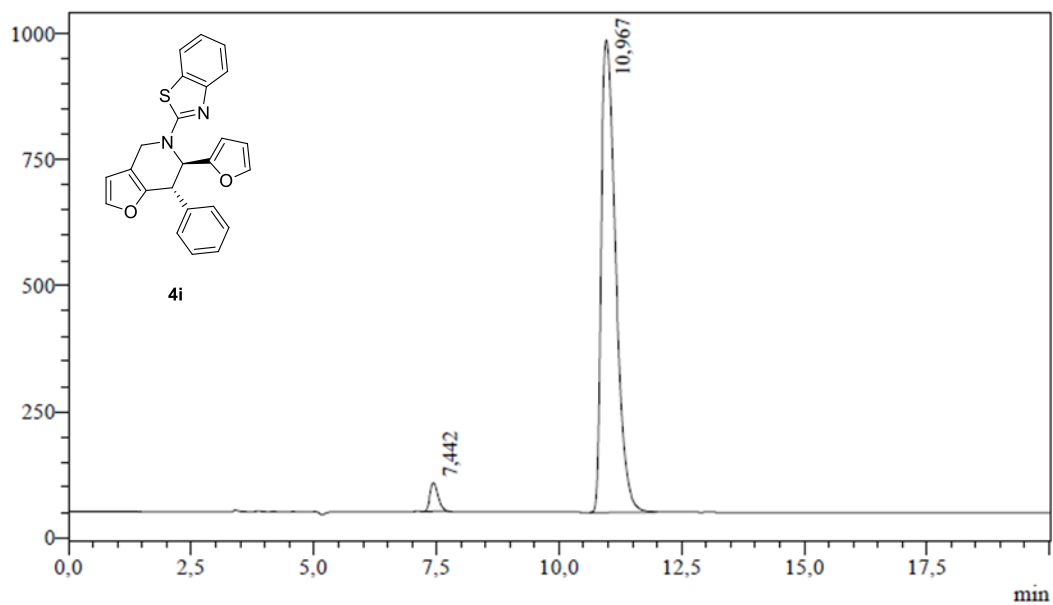
mAU



Peak Table

Peak	Ret. Time	Area %
1	8.562	36.306
2	11.364	63.694
Total		100.000

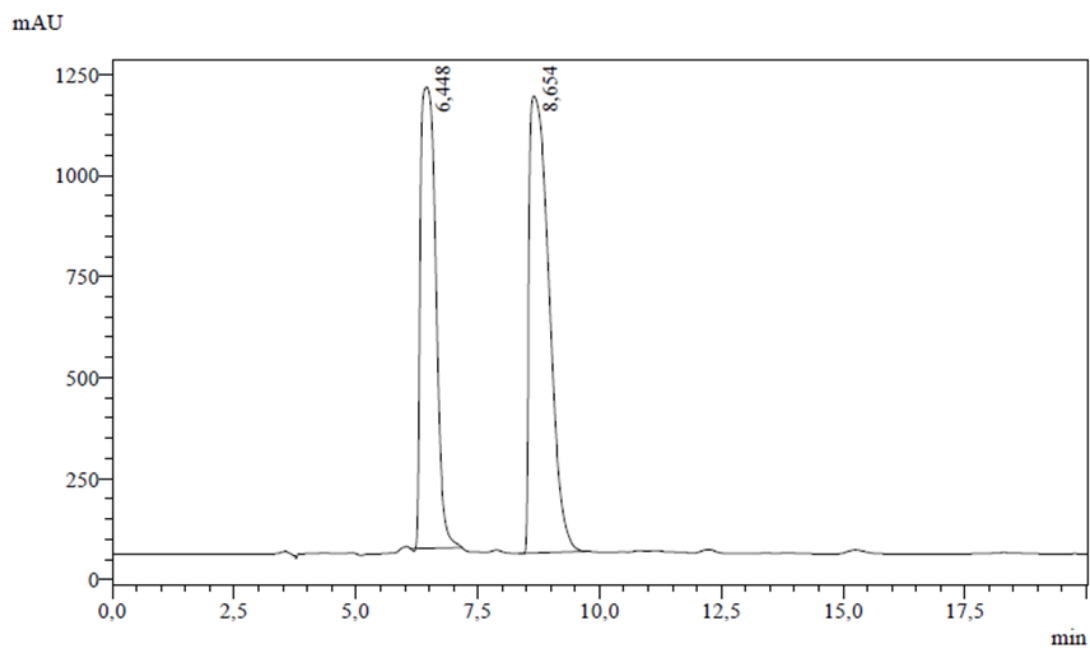
mAU



Peak Table

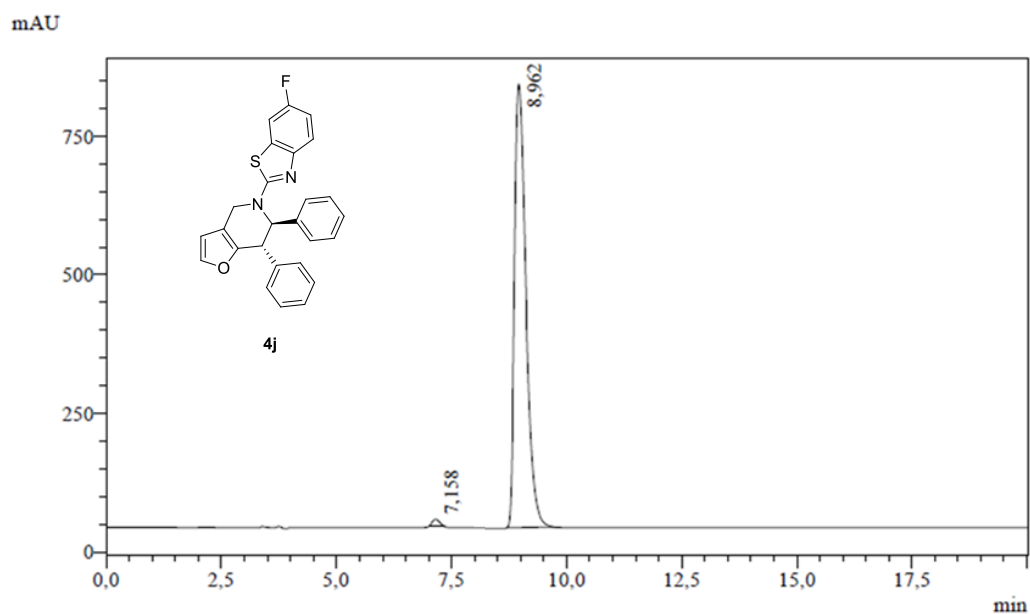
Peak	Ret. Time	Area %
1	7.442	3.267
2	10.967	96.733
Total		100.000

(6*R*,7*S*)-5-(6-Fluorobenzo[*d*]thiazol-2-yl)-6,7-diphenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4j



Peak Table

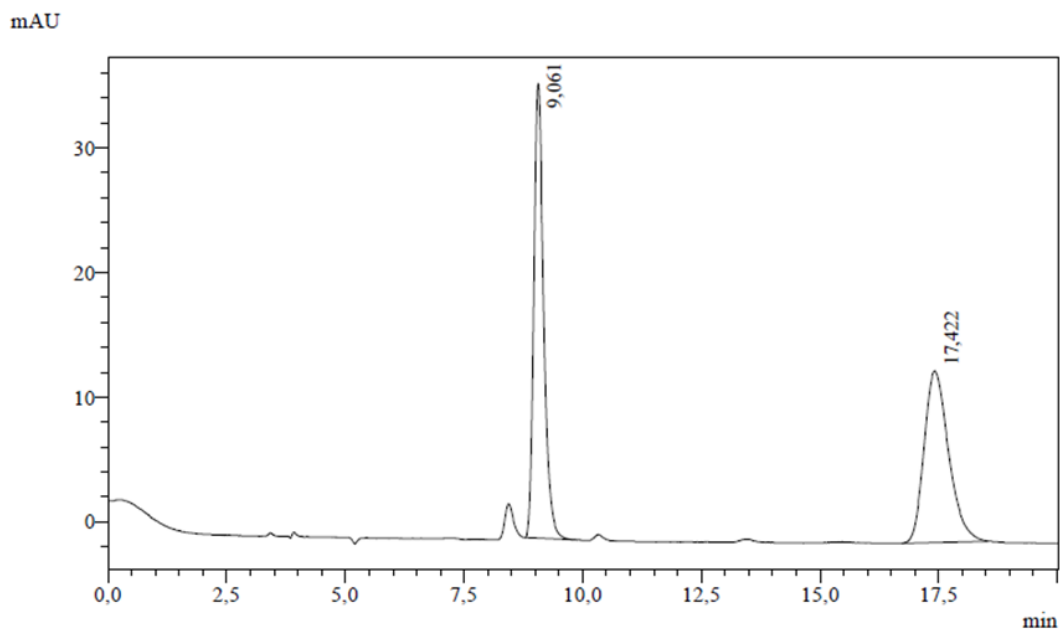
Peak	Ret. Time	Area %
1	6.448	43.813
2	8.654	56.187
Total		100.000



Peak Table

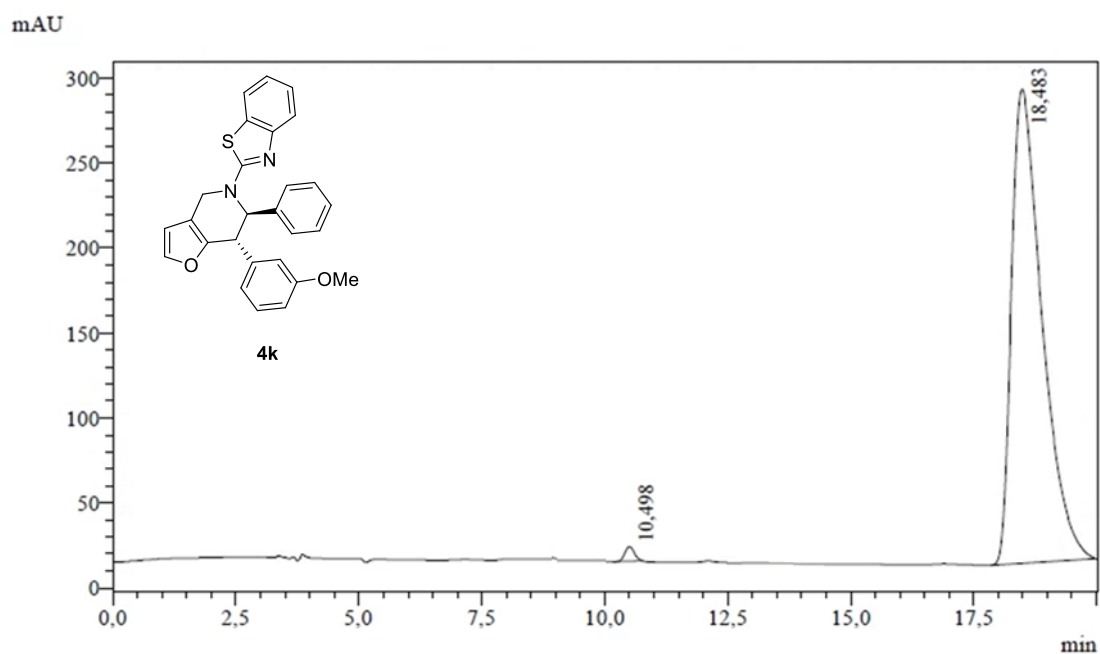
Peak	Ret. Time	Area %
1	7.158	1.019
2	8.962	98.981
Total		100.000

(6*R*,7*S*)-5-(Benzo[*d*]thiazol-2-yl)-7-(3-methoxyphenyl)-6-phenyl-4,5,6,7-tetrahydrofuro[3,2-*c*]pyridine 4k



Peak Table

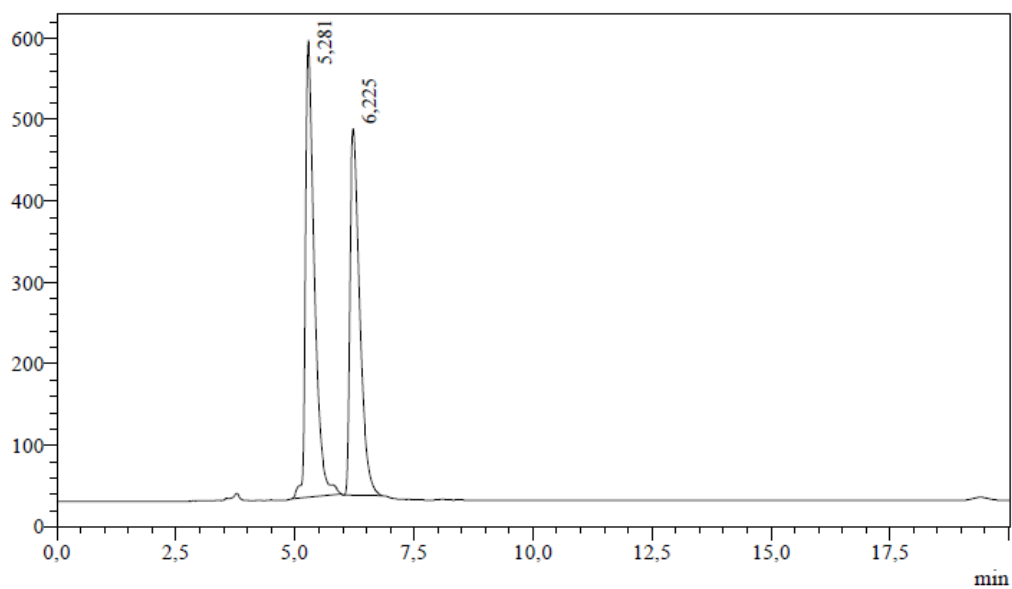
Peak	Ret. Time	Area %
1	9.061	51.380
2	17.422	48.620
Total		100.000



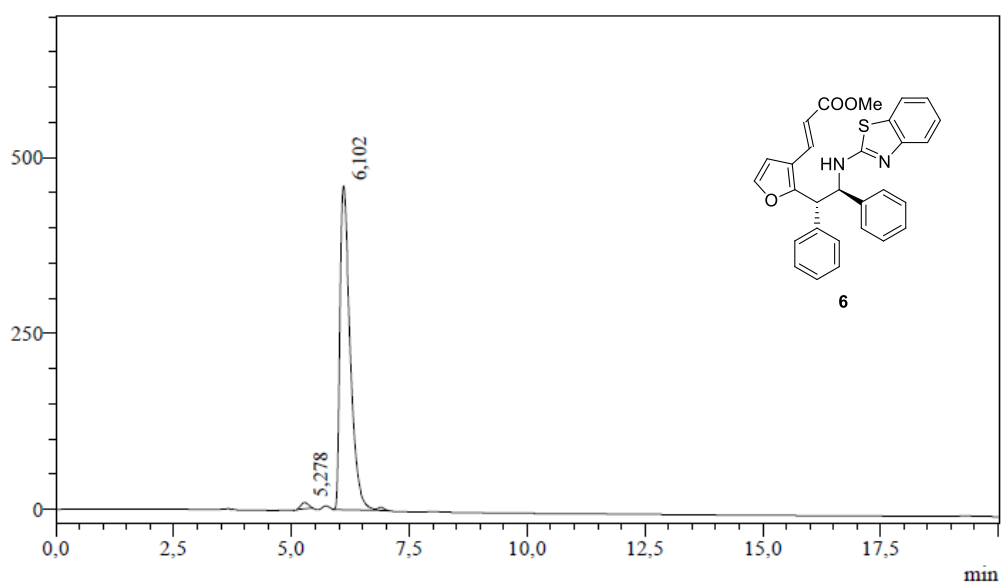
Peak Table

Peak	Ret. Time	Area %
1	10.498	0.960
2	18.483	99.040
Total		100.000

(E)-Methyl 3-(2-((1*S*,2*R*)-2-(benzo[*d*]thiazol-2-ylamino)-1,2-diphenylethyl)furan-3-yl)acrylate 6



Peak	Ret. Time	Area %
1	5,281	53,758
2	6,225	46,242
Total		100,000



Peak	Ret. Time	Area %
1	5,278	1,427
2	6,102	98,573
Total		100,000