BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

# Supporting Information

for

# *N*-Sulfinylpyrrolidine-containing ureas and thioureas as bifunctional organocatalysts

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## Characterization data, copies of spectra, and DFT computational details

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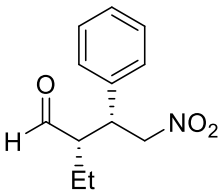
# 1. General considerations

All commercially available chemicals were purchased from Merck, Alfa Aesar or TCI and were used without further purification. Solvents were distilled and dried according to the standard procedures. Thin-layer chromatography was performed on silica gel 60, F-254 nm plates. Compounds were visualized by irradiation with UV light and/or by treatment with $KMnO_4$ or *p*-anisaldehyde solution. NMR spectra were recorded on Varian NMR System 300 and Varian NMR System 600 (300 or 600 MHz for $^{1}H$, 75 or 151 MHz for $^{13}C$). Chemical shifts (δ ppm) are given in ppm relative to tetramethylsilane. Products of Michael additions were purified by flash chromatography using Isolera Biotage FSKO-1107-0010. Enantiomeric purity was determined by chiral HPLC column (Chiralcel AS-H, Chiralpak IC Chiralcel ODH). Specific optical rotations were measured on Jasco P-2000 polarimeter. High-resolution mass spectra were recorded with Thermo Velos Pro Orbitrap spectrometer. Melting points were measured on Büchi Melting Point M-565. Infrared spectroscopy spectra were recorded with Agilent Technologies Cary 630 FTIR. Frequencies are given in wavenumbers ($cm^{-1}$) and only selected peaks were reported. Mechanochemical reactions were carried out in a ball mill Retsch MM 400.

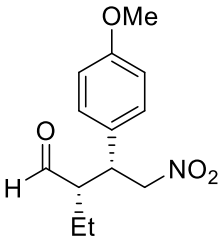
# 2. Characterization data

**2-Ethyl-4-nitro-3-phenylbutanal** (**8a**)[1]



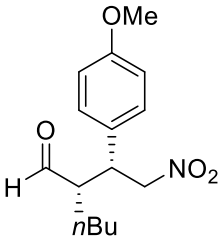

Colourless oil, RF = 0.44 (Hexanes/EtOAc, 5:1), **$^1$H NMR** (600 MHz, $CDCl_3$) δ 9.72 (d, *J* = 2.6 Hz, 0.84H); 9.49 (d, *J* = 2.9 Hz, 0.16H); 7.36–7.28 (m, 3H); 7.19–7.17 (m, 2H); 4.83–4.75 (m, 0.32H); 4.72 (dd, *J* = 12.7; 4.9 Hz, 0.84H); 4.63 (dd, *J* = 12.7; 9.7 Hz, 0.84H); 3.79 (td, *J*= 9.8; 4.9 Hz, 1H); 2.7–2.66 (m, 1H); 1.54–1.49 (m, 2H); 0.99 (t, *J* = 7.5 Hz, 0.5H); 0.84 (t, *J* = 7.5 Hz, 2.5H) ppm. **HPLC:** Chiralcel ODH, Hexane/iPrOH 80:20, 0.8 ml/min, λ = 211 nm, $t_R$ = 18.4 min and 32.3 min (minor), $t_R$ = 17.1 min and 21.0 min (major).

**2-Ethyl-3-(4-methoxyphenyl)-4-nitrobutanal** (**8b**)[2]




Colourless oil, RF = 0.35 (Hexanes/EtOAc, 4:1), **$^1$H NMR** (600 MHz, $CDCl_3$) δ 9.71 (d, *J* = 2.6 Hz, 0.84 H); 9.47 (d, *J* = 3 Hz, 0.16 H); 7.09 (d, *J* = 8.6 Hz, 2H); 6.87 (d, *J* = 8.7 Hz, 2H); 4.8–4.71 (m, 0.32H); 4.69 (dd, *J* = 12.6; 4.9 Hz, 0.84H); 4.58 (dd, *J* = 12.5; 9.9 Hz, 0.84H); 3.79 (s, 2.5H); 3.78 (s, 0.5H); 3.74 (td, *J* = 9.9; 4.9 Hz, 1H); 2.65–2.61 (m, 1H); 1.55–1.47 (m, 2H); 0.99 (t, *J* = 7.5 Hz, 0.5H); 0.83 (t, *J* = 7.5 Hz, 2.5H) ppm. **HPLC:** Chiralpak IC, Hexane/iPrOH 80:20, 1 ml/min, λ = 210 nm, $t_R$ = 18.2 min and 23.8 min (minor), $t_R$ = 28.7 min and 30.8 min (major).

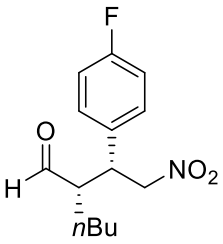
**2-[1-(4-Methoxyphenyl)-2-nitroethyl]hexanal** (**8c**)[3]




Colourless oil, RF = 0.36 (Hexanes/EtOAc, 4:1), **$^1$H NMR** (300 MHz, $CDCl_3$) δ 9.70 (d, *J* = 2.8 Hz, 0.63H); 9.46 (d, *J* = 3.1 Hz, 0.37H); 7.08 (d, *J* = 8.7 Hz, 2H); 6.87 (d, *J* = 8.7 Hz, 1H); 6.85 (d, *J* = 8.7 Hz, 1H); 4.78 (dd, *J* = 12.8; 6.0 Hz, 0.37H); 4.71 (dd, *J* = 12.8; 9.4 Hz, 0.37H); 4.67 (dd, *J* = 12.6; 5.0 Hz, 0.63H); 4.59 (dd, *J* = 12.6; 9.8 Hz, 0.63H); 3.79 (s, 1.1H); 3.78 (s, 1.9H); 3.74–3.70 (m, 1H); 2.67–2.62 (m, 0.63H); 2.60–2.56 (m, 0.37H); 1.52–1.37 (m, 2.4H); 1.26–1.12 (m, 3.6H); 0.89 (m,1.1H); 0.79 (t, *J* = 6.9 Hz, 1.9H) ppm. **$^{13}$C NMR** (151 MHz, $CDCl_3$) δ 203.5; 203.4; 159.3; 159.2; 129.3; 129.0; 128.5; 127.9; 114.5; 114.4; 78.7; 78.2; 55.22; 55.21; 54.0; 53.5; 43.8; 42.5; 29.1; 28.5; 27.3; 27.0; 22.6; 22.5; 13.8; 13.7 ppm. **HRMS (ESI):** $C_{14}H_{21}NO_4$ calculated $[M+Na]^+$ = 302.1363, found 302.1362. **IR (ATR):** 2930.2; 2859.8;1719.0; 1610.9; 1549.3; 1512.7; 1464.0; 1377.8; 1249.5; 1179.6; 1032.2; 830.5;

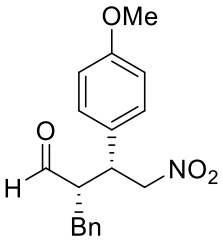
755.6 $cm^{-1}$. **HPLC:** Chiralpak IC, Hexane/iPrOH 80:20, 1 ml/min, λ = 210 nm, $t_R$ = 15.0 min and 20.8 min (minor), $t_R$ = 22.2 min and 24.9 min (major).

**2-[1-(4-Fluorophenyl)-2-nitroethyl]hexanal** (**8d**)[3]



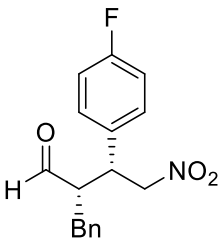

Colourless oil, RF = 0.36 (Hexanes/EtOAc, 4:1), **$^1$H NMR** (600 MHz, $CDCl_3$) δ 9.71 (d, *J* = 2.6 Hz, 0.8H); 9.48 (d, *J* = 2.8 Hz, 0.2H); 7.17–7.15 (m, 2H); 7.06–7.02 (m, 2H); 4.80 (dd, *J* = 12.9; 5.8 Hz, 0.2H); 4.75–4.71 (m, 0.2H); 4.70 (dd, *J* = 12.8; 4.8 Hz, 0.8H); 4,61 (dd, *J* = 12.8; 9.9 Hz, 0.8H); 3.77(td, *J* = 9.8; 4.8 Hz, 1H); 2.70–2.65 (m, 0.8H); 2.64–2.60 (m, 0.2H); 1.49–1.45 (m, 1H); 1.43–1.38 (m, 1H); 1.26–1.22 (m, 2H); 1.18–1.13 (m, 2H); 0.90–0.89 (m, 0.6H), 0.79 (t, *J* = 6.9 Hz, 2.4H) ppm. **$^{13}$C NMR** (151 MHz, $CDCl_3$) δ 203.0; 202.9; 162.3 (d, *J* = 247.4 Hz); 132.5 (d, *J* = 3.4 Hz); 129.9 (d, *J* = 8.1 Hz); 129.6 (d, *J* = 8.2 Hz); 116.2 (d, *J* = 21.5 Hz); 116.1 (d, *J* = 21.5 Hz); 78.4; 77.9; 53.8; 53.5; 43.6; 42.4; 29.1; 28.4; 27.2; 27.0; 22.6; 22.5; 13.7; 13.6 ppm. **HRMS (ESI):** $C_{14}H_{18}FNO_3$ calculated $[M+H]^+$ = 268.1343, found 268.1352. **IR (ATR):** 2956.5; 2927.8; 2860.3; 1685.7 1636.9; 1458.2; 1413.5; 1378.4 1274.1; 1213.2; 933.4; 720.0; 659.7 $cm^{-1}$. **HPLC:** Chiralpak IC, Hexane/iPrOH 95:5, 1 ml/min, λ= 210 nm, $t_R$ = 18.7 min and 28.6 min (minor), $t_R$ = 30.1 min: and 35.4 min (major).

**2-Benzyl-3-(4-methoxyphenyl)-4-nitrobutanal** (**8e**)



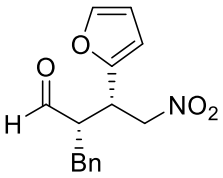

Colourless oil, RF = 0.35 (Hexanes/EtOAc, 3:1), **$^1$H NMR** (600 MHz, $CDCl_3$) δ 9.71 (d, *J* = 2.3 Hz, 0.8H); 9.55 (d, *J* = 1.9 Hz, 0.2H); 7.32–7.24 (m, 2H); 7.21–7.19 (m, 1H); 7.13 (d, *J* = 8.6 Hz, 2H); 7.09 (d, *J* = 8.7 Hz, 0.4H); 7.03 (d, *J* = 7.2 Hz, 1.6H); 6.9 (d, *J* = 8.7 Hz, 1.6H); 6.87 (d, *J* = 8.7 Hz, 0.4H); 4.84 (dd, *J* = 13.0, 6.3 Hz, 0.2 H), 4.75 (dd, *J* = 12.9, 9.1 Hz, 0,2 H), 4.70 (dd, *J* = 12.7, 5.4 Hz, 0,8 H), 4.65 (dd, *J* = 12.6, 9.3 Hz, 0,8 H); 3.81 (s, 2.4H); 3.80 (s, 0.6H); 3.79–3.75 (m, 1H); 3.09–2.99 (m, 1H); 2.76 (d, *J* = 7.3 Hz, 2H) ppm. **$^{13}$C NMR** (151 MHz, $CDCl_3$) δ 202.2; 202.1; 158.4; 136.3; 136.2; 128.1; 127.9; 127.85; 127.8; 127.7; 127.35; 127.3; 126.0; 125.9; 113.6; 113.5; 77.3; 76.9; 54.5; 54.2; 53.4; 42.8; 41.8; 33.2; 32.7 ppm. **HRMS (ESI):** $C_{18}H_{19}NO_4$ calculated $[M-H]^-$ = 312.1241, found 312.1245. **IR (ATR):** 3026.6; 2925.8; 2836.5; 1719.6; 1610.0; 1548.6; 1512.4; 1540.0; 1438.1; 1377.7; 1249.5; 1179.3; 1029.8; 830.1; 749.4 $cm^{-1}$. **HPLC:** Chiralpak IC, Hexane/iPrOH 80:20, 1 ml/min, λ = 210 nm, $t_R$ = 15.6 min and 20.8 min (minor), $t_R$ =19.9 min and 26.1 min (major).

**2-Benzyl-3-(4-fluorophenyl)-4-nitrobutanal** (**8f**)[3]



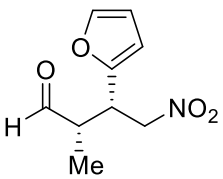
Colourless oil, RF = 0.34 (Hexanes/EtOAc, 3:1), **$^{1}$H NMR** (600 MHz, $CDCl_3$) δ 9.72 (d, *J* = 2.1 Hz, 0.62H); 9.55 (d, *J* = 2.0 Hz, 0.38H); 7.23–7.18 (m, 5H); 7.08–7.04 (m, 2H); 7.02–7.01 (m, 2H); 4.85 (dd, *J* = 13.1; 6.2 Hz, 0.38H); 4.78 (dd, *J* = 13.1; 9.2 Hz, 0.38H); 4.72 (dd, *J* = 12.8; 5.2 Hz, 0.62H); 4.68 (dd, *J*= 12.8; 9.4 Hz, 0.62H); 3.82 (td, *J* = 9.2; 5.2 Hz, 1H); 3.12–3.07 (m,1H); 2.8–2.73 (m, 2H) ppm. **$^{13}$C NMR** (151 MHz, $CDCl_3$) δ 202.8; 202.7; 162.42 (d, *J* = 247.8 Hz); 162.4 (d, *J* = 247.9 Hz); 137.0; 136.9; 132.5 (d, *J* = 3.4 Hz); 131.6 (d, *J* = 3.4 Hz); 130.2 (d, *J* = 8.1 Hz); 129.7 (d, *J* = 8.2 Hz); 128.9; 128.8; 128.7; 127.1; 127.0; 116.3 (d, *J* = 21.5 Hz); 116.1 (d, *J* = 21.5 Hz) 78.0; 77.7; 55.2; 54.3; 43.7; 42.7; 34.2 33.7 ppm. **HRMS (ESI):** $C_{17}H_{16}FNO_3$ calculated $[M+H]^+$ = 302.1187, found 302.1192. **IR (ATR):** 3026.2; 2921.7; 1720.8; 1602.6; 1553.7; 1509.8; 1453.8; 1377.5; 1225.3; 1161.0; 835.4; 746.5; 699.6 $cm^{-1}$. **HPLC:** Chiralpak IC, Hexane/iPrOH 80:20, 1 ml/min, λ = 210 nm, $t_R$ = 10.2 min and 14.7 min (minor), $t_R$ =13.3 and 16.5 (major).

**2-Benzyl-3-(furan-2-yl)-4-nitrobutanal** (**10a**)[4]



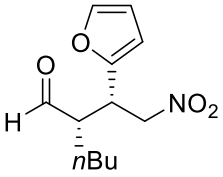
Pale yellow oil, $R_F$ = 0.48 (Hexanes/EtOAc, 3:1), **$^{1}$H NMR** (600 MHz, $CDCl_3$) δ 9.71 (d, *J* = 1.1 Hz, 0.75H); 9.69 (d, *J* = 1.9 Hz, 0.25H); 7.40 (s, 1H); 7.34–7.27 (m, 2H); 7.25–7.22 (m, 1H); 7.15 (d, *J* = 7.4 Hz, 0.5H); 7.12 (d, *J* = 7.4 Hz, 1.5H); 6.36–6.33 (m, 1H); 6.24–6.21 (m, 1H), 4.76–4.60 (m, 2H); 4.10–4.05 (m, 0.75H); 3.98–3.93 (m, 0.25H); 3.20–3.14 (m, 0.75H); 3.05 (dd, *J* = 13.9; 7.9 Hz, 0.25H); 3.00–2.95 (m, 0.25H); 2.88 (dd, *J* = 14.4; 8.9 Hz, 0.75H); 2.81 (dd, *J* = 14.0; 7.1 Hz, 0.25H); 2.76 (dd, *J* = 14.4; 5.6 Hz, 0.75H) ppm. **HPLC:** Chiralcel AS-H, heptane/iPrOH 90:10, 0.7 mL/min, λ = 220 nm, $t_R$ = 29.2 min, $t_R$ = 39.5 min.

**3-(Furan-2-yl)-2-methyl-4-nitrobutanal** (**10b**)[5]



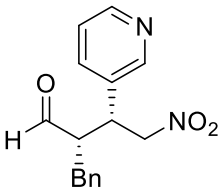
Brown oil, RF = 0.32 (Hexanes/EtOAc, 3:1), **$^{1}$H NMR** (600 MHz, $CDCl_3$) δ 9.71 (d, *J* = 0.8 Hz, 0.59H); 9.64 (d, *J* = 1.3 Hz, 0.41H); 7.37–7.36 (m, 1H); 6.32–6.3 (m, 1H); 6.2 (dd, *J* = 12.6; 3.3 Hz, 1H); 4.77–4.68 (m, 2H); 4.09 (dt, *J* = 8.5; 6.7 Hz, 0.59H); 4.01 (dt, *J* = 8.8; 5.6 Hz, 0.41H); 2.87–2.78 (m, 1H); 1.22 (d, *J* = 7.3 Hz, 1.75H); 1.08 (d, *J* = 7.3 Hz, 1.25H) ppm. **HPLC:** Chiralcel AS-H, Hexane/iPrOH 90:10, 0.8 ml/min, λ = 210 nm, $t_R$ = 23.1 min and 27.8 min (minor), $t_R$ = 20.0 min and 21.4 min (major).

**2-[1-(Furan-2-yl)-2-nitroethyl]hexanal** (**10c**)[3]




Brown oil, RF = 0.47 ($CH_2Cl_2$/ Hexanes, 3:1), **$^1$H NMR** (300 MHz, $CDCl_3$) δ 9.71 (d, *J* = 1.9 Hz, 0.5H); 9.6 (d, *J* = 2.7 Hz, 0.5H); 7.37–7.36 (m, 1H); 6.32–6.30 (m, 1H); 6.21–6.19 (m, 1H); 4.78–4.62 (m, 2H); 4.04–3.93 (m, 1H); 2.78 (tdd, *J* = 8.1; 4.6; 1.9 Hz, 0.5H); 2.60 (dtd, *J* = 8.3; 5.4; 2.7 Hz, 0.5H); 1.74–1.64 (m, 1H); 1.55–1.44 (m, 2H); 1.35–1.28 (m, 3H); 0.89–0.85 (m, 3H) ppm. **$^{13}$C NMR** (151 MHz, $CDCl_3$) δ 202.3; 202.8; 150.1; 149.6; 142.7; 142.6; 110.5; 110.4; 108.9; 108.7; 76.1; 75.9; 52.2; 52.1; 38.0; 36.9; 29.2; 28.7; 26.9; 26.5; 22.6; 22.5; 13.7; 13.6 ppm. **HRMS (ESI):** $C_{12}H_{17}NO_4$ calculated $[M+H]^+$ = 240.1230, found 240.1229. **IR (ATR):** 2930.5; 2861.5; 2729.0; 1719.4; 1551.0; 1505.7; 1430.9; 1376.0; 1190.8; 1148.0; 1072.9; 1013.6; 913.7; 735.2 $cm^{-1}$. **HPLC:** Chiralpak IC, Hexane/iPrOH 95:5, 0.6 ml/min, λ = 217 nm, $t_R$ = 50.1 min and 60.2 min (minor), $t_R$ = 44.8 min and 57.3 (major).

**2-Benzyl-4-nitro-3-(pyridin-3-yl)butanal** (**12**)[6]




Pale yellov oil, $R_F$ = 0.21 (Hexanes/EtOAc, 1:1), $[\boldsymbol{\alpha}]_{\boldsymbol{D}}^{\boldsymbol{20}}$ = 3.58 (*c* = 0.5, MeCN), **$^1$H NMR** (600 MHz, $CDCl_3$) δ 9.71 (d, *J* = 1.6 Hz, 0.6H); 9.57 (d, *J* = 1.1 Hz, 0.4H), 8.58–8.53 (m, 1H); 8.48 (dd, *J* = 9.8 Hz; 1.9 Hz, 1H); 7.59–7.54 (m, 1H); 7.35–7.18 (m, 4H); 7.12 (d, *J* = 7.3 Hz, 1H); 7.01 (d, *J* = 7.2 Hz, 1H); 4.91–4.83 (m, 1H); 4.76 (d, *J* = 6.8 Hz, 1H); 3.88–3.82 (m, 1H); 3.21–3.13 (m, 1H); 3.0 (dd, *J* = 19.5; 11.3 Hz, 0.6H); 2.85–2.74 (m, 2H) ppm. **$^{13}$C NMR** (151 MHz, $CDCl_3$) δ 202.3, 202.2, 150.0, 149.6, 149.51, 149.5, 136.5, 136.4, 136.1, 135.7, 132.8, 132,1, 129.1, 129.0, 128.73, 128.5, 128.3, 127.3, 127.2, 124.0, 123.9, 54.7, 54.1, 53.4, 41.6, 40.9, 34.2, 33.5 ppm. **IR (ATR):** 1721.0; 1550.5; 1377.0; 1495.9 $cm^{-1}$. **HRMS (ESI):** $C_{16}H_{15}N_2O_3$ calculated $[M-H]^-$ = 283.1077, found 283.1088. **HPLC:** Chiralcel AS-H, hexane/iPrOH, 70:30, 0.75 mL/min, λ = 218 nm, $t_R$ = 27.0 min and 29.2 (major), $t_R$ =34.4 and 43.4 min (minor).

# 3. Copies of $^{1}$H, $^{13}$C NMR and HRMS spectra

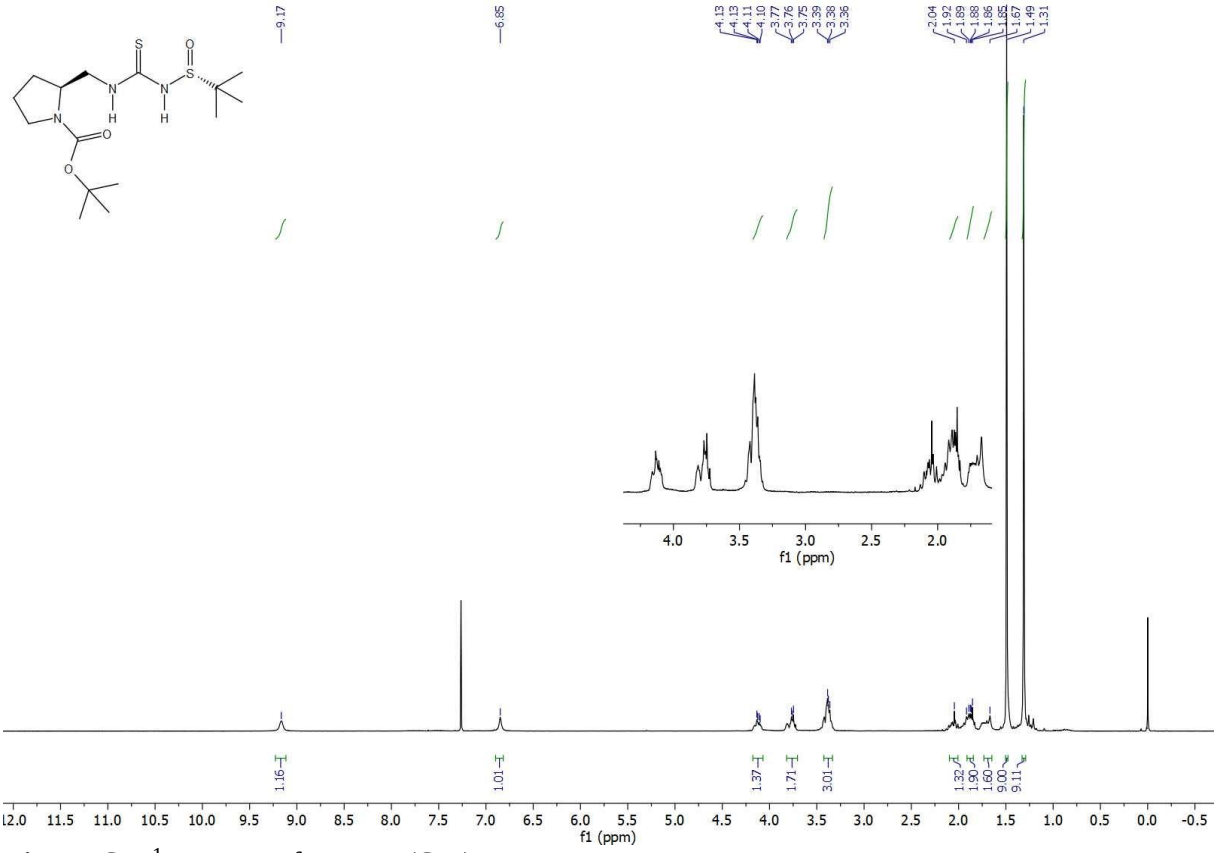



**Figure S1.** $^{1}$H NMR of ***N*-Boc-(*S*,*R*)-5a**

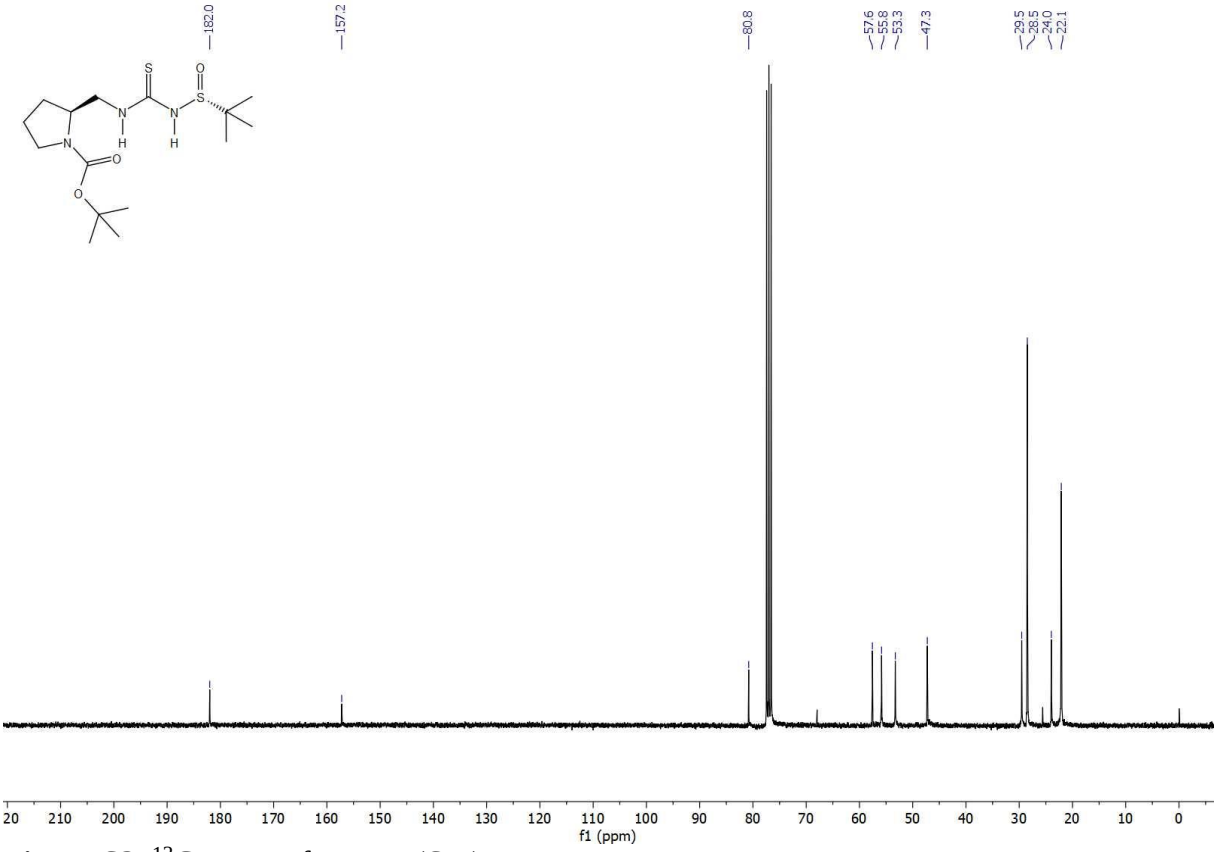



**Figure S2.** $^{13}$C NMR of ***N*-Boc-(*S*,*R*)-5a**

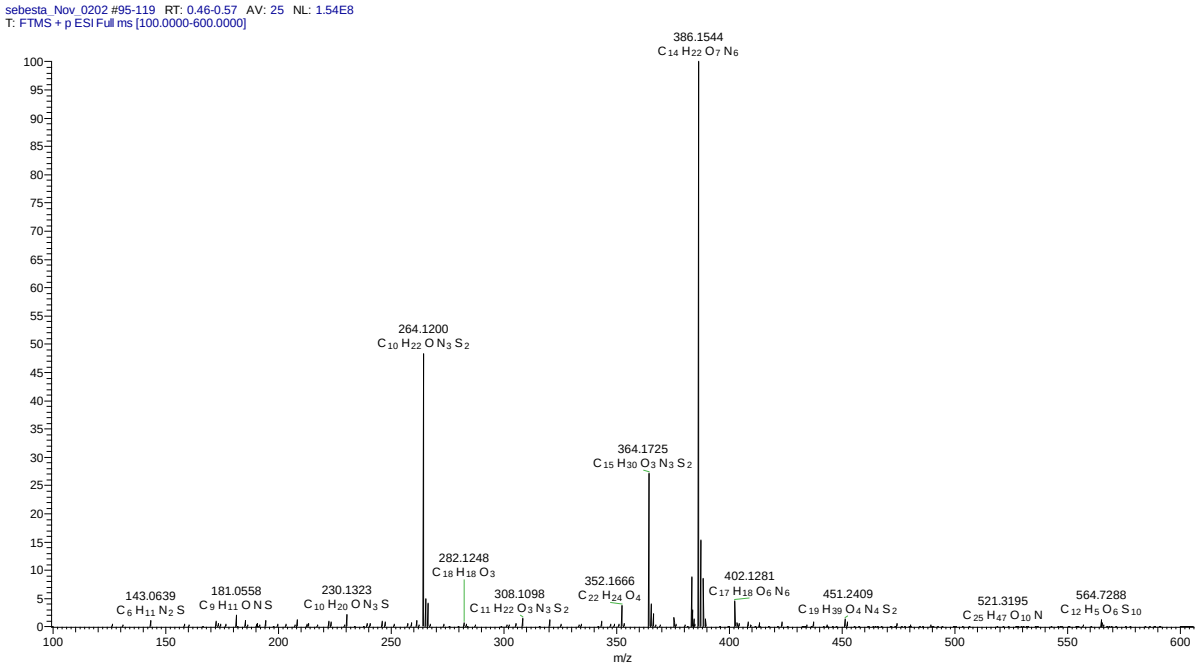



**Figure S3.** HRMS of ***N*-Boc-(*S*,*R*)-5a**

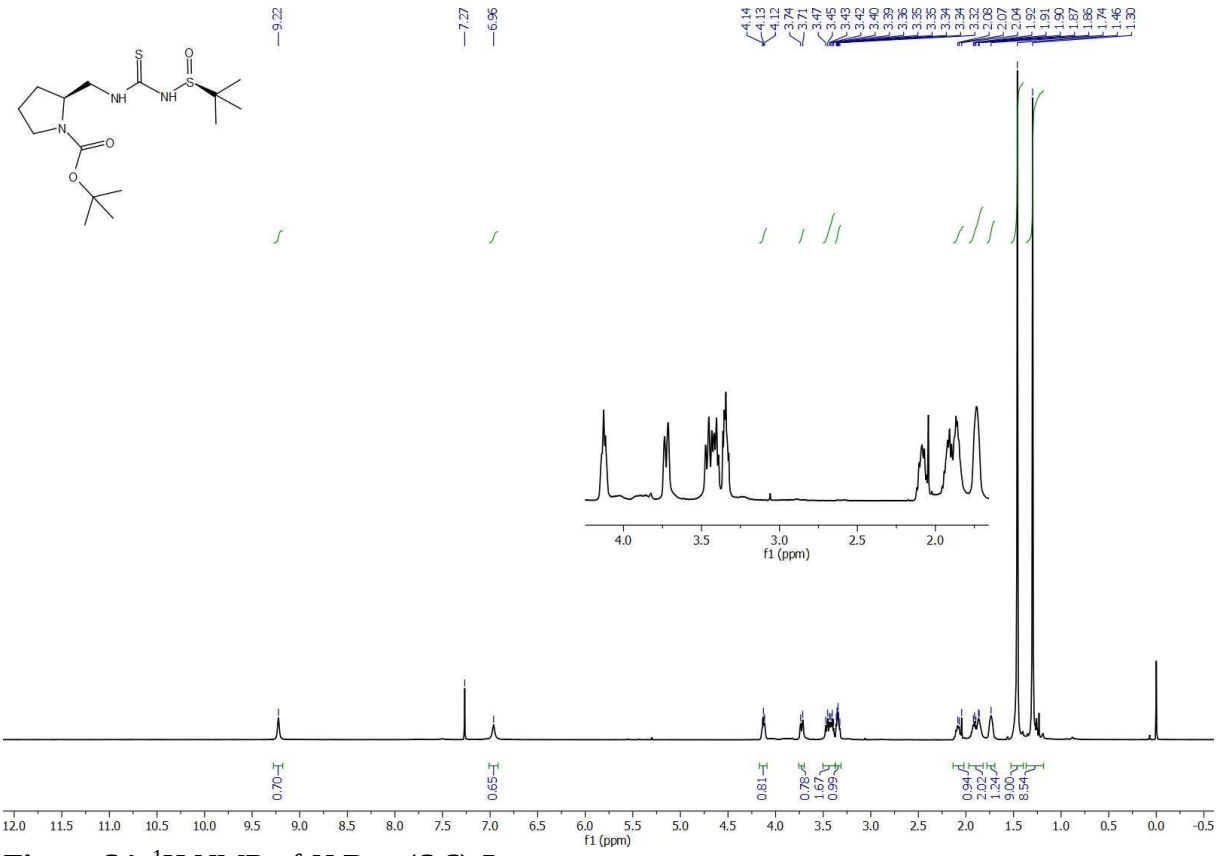



**Figure S4.** $^{1}$H NMR of ***N*-Boc-(*S*,*S*)-5a**

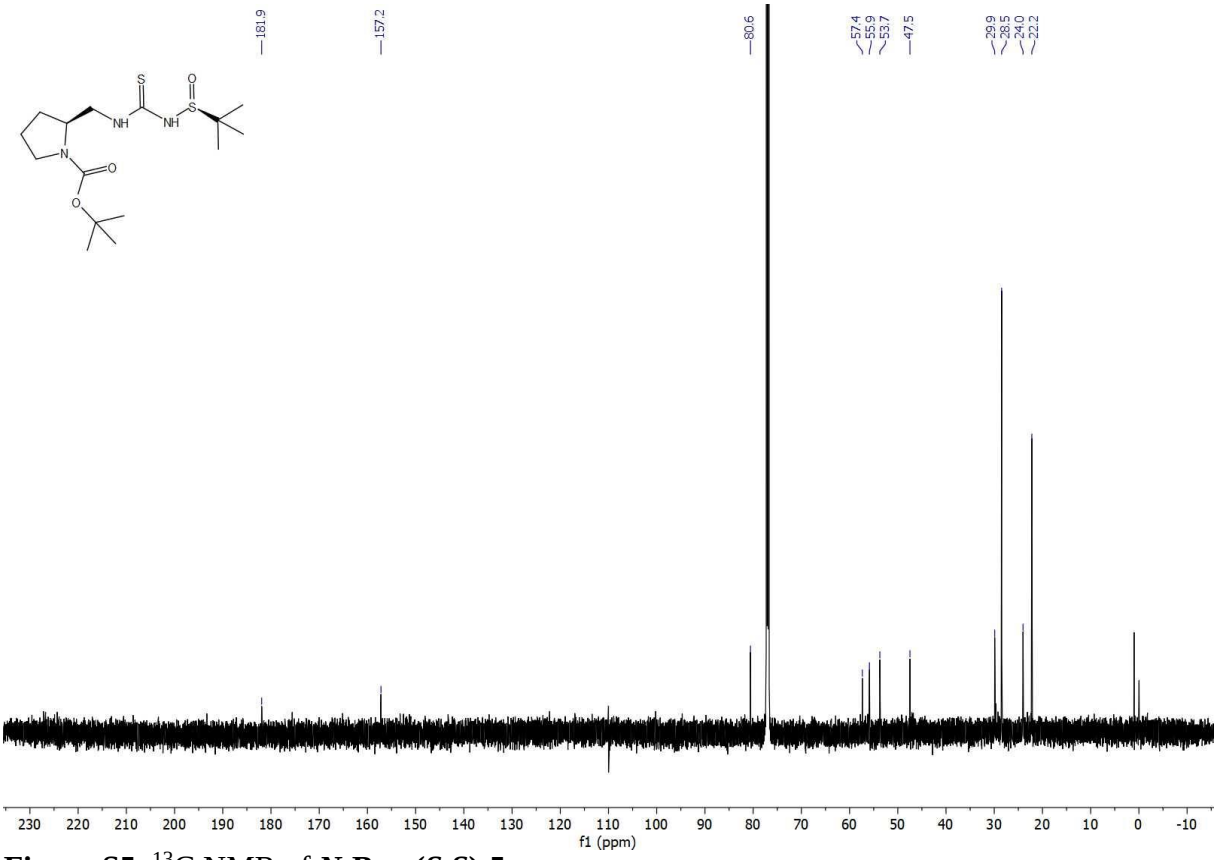



**Figure S5.** $^{13}$C NMR of ***N*-Boc-(*S*,*S*)-5a**

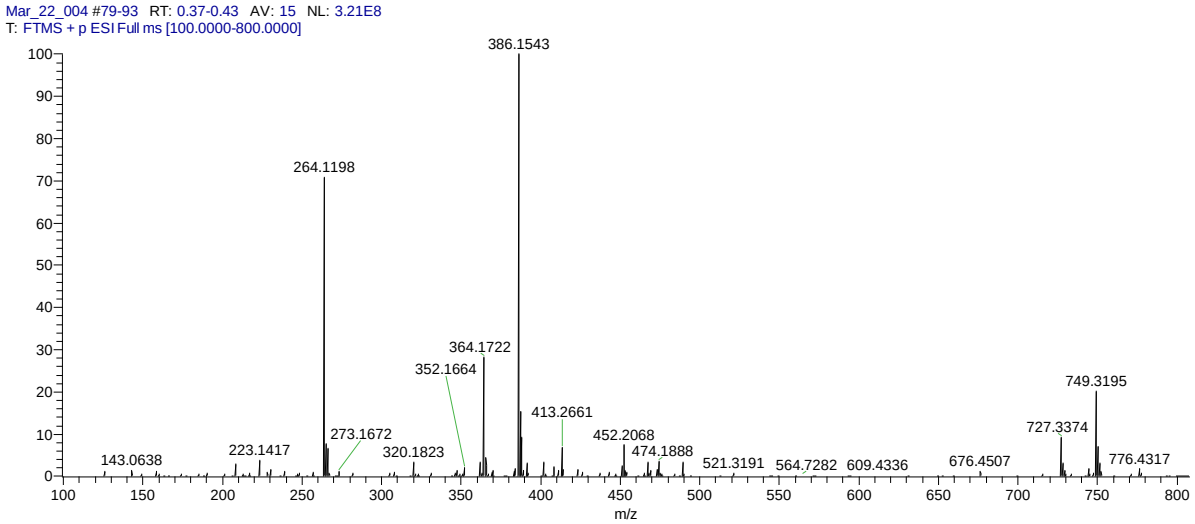



**Figure S6.** HRMS of ***N*-Boc-(*S*,*S*)-5a**

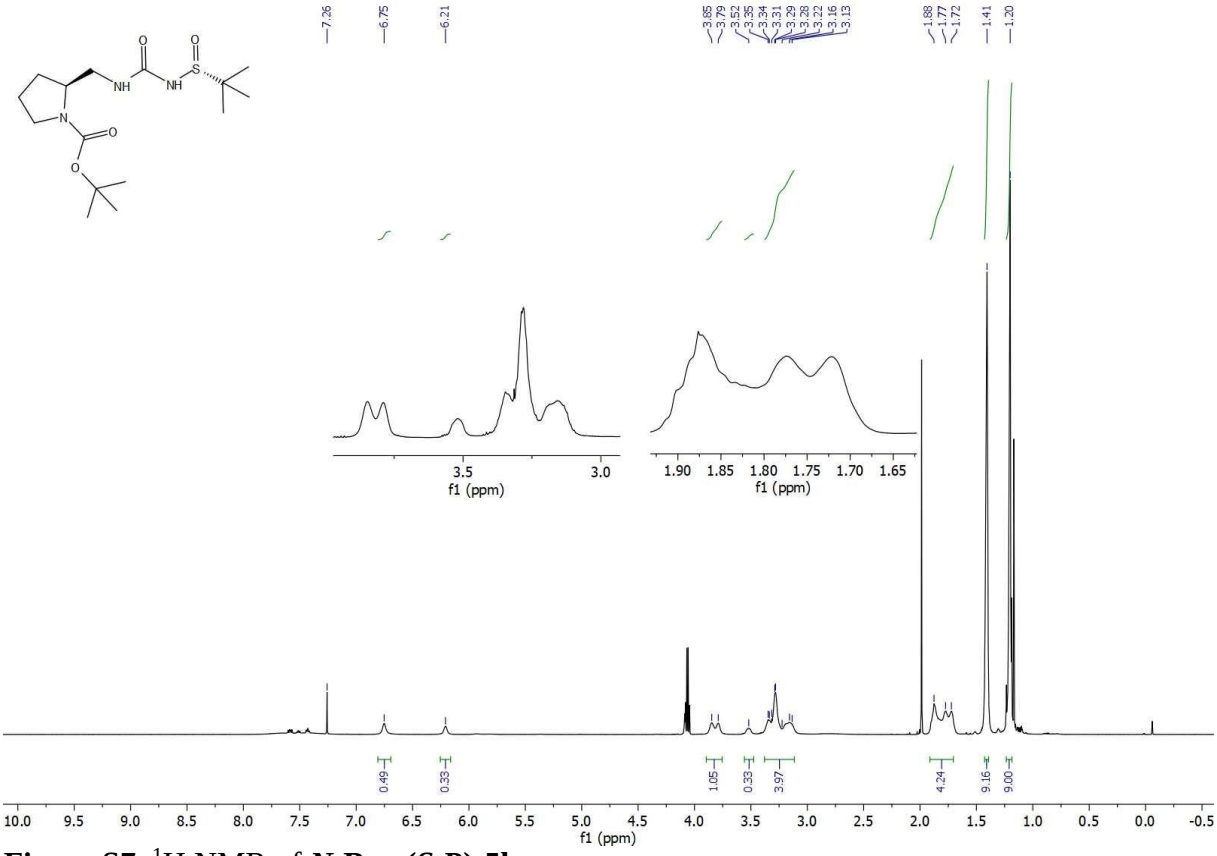



**Figure S7.** $^{1}$H NMR of ***N*-Boc-(*S*,*R*)-5b**

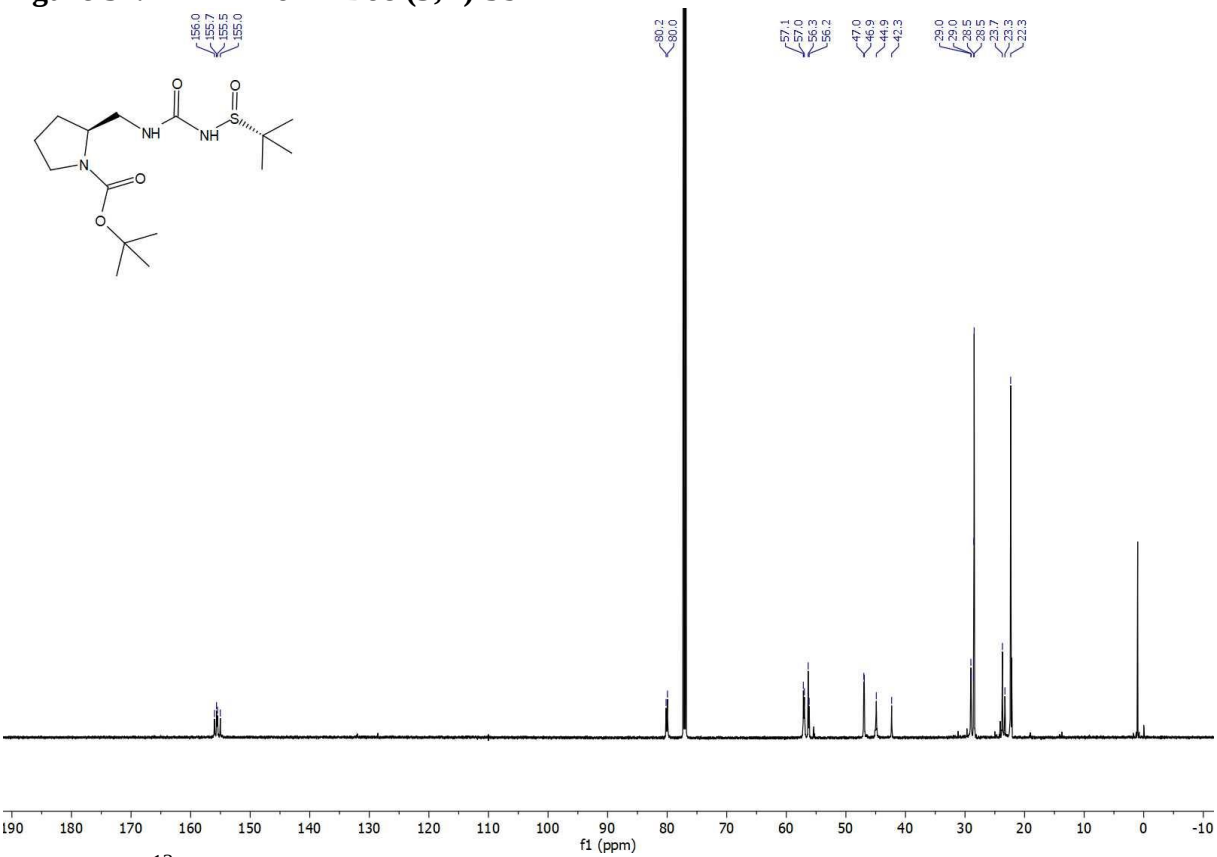



**Figure S8.** $^{13}$C NMR of ***N*-Boc-(*S*,*R*)-5b**

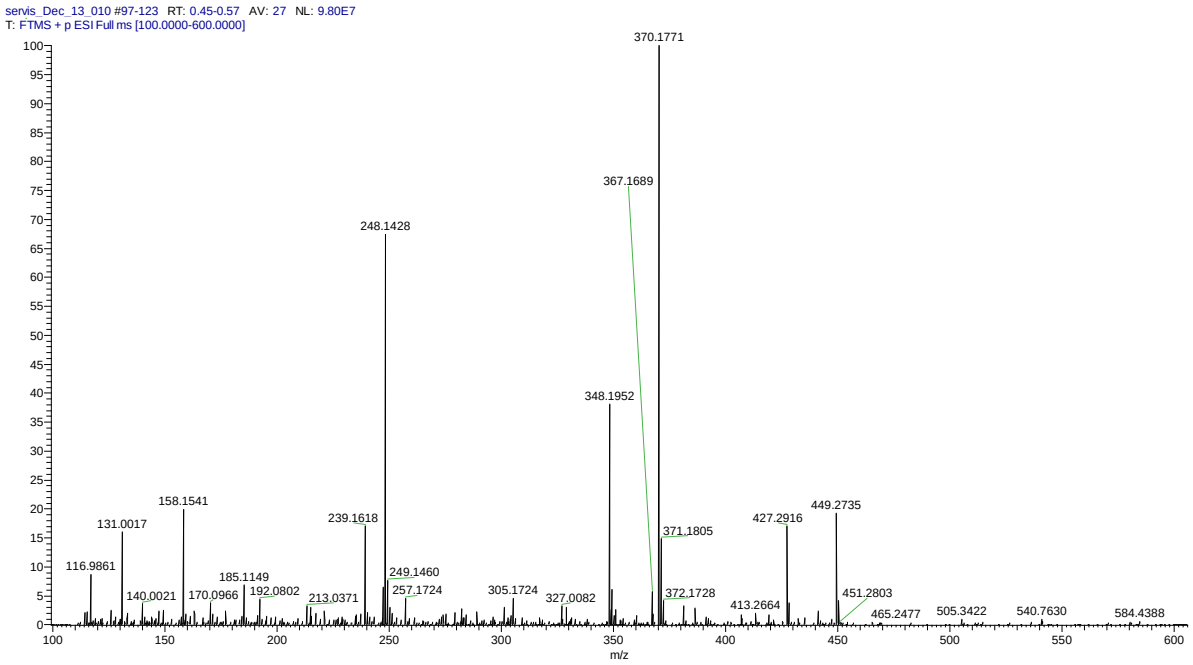



**Figure S9.** HRMS of ***N*-Boc-(*S*,*R*)-5b**

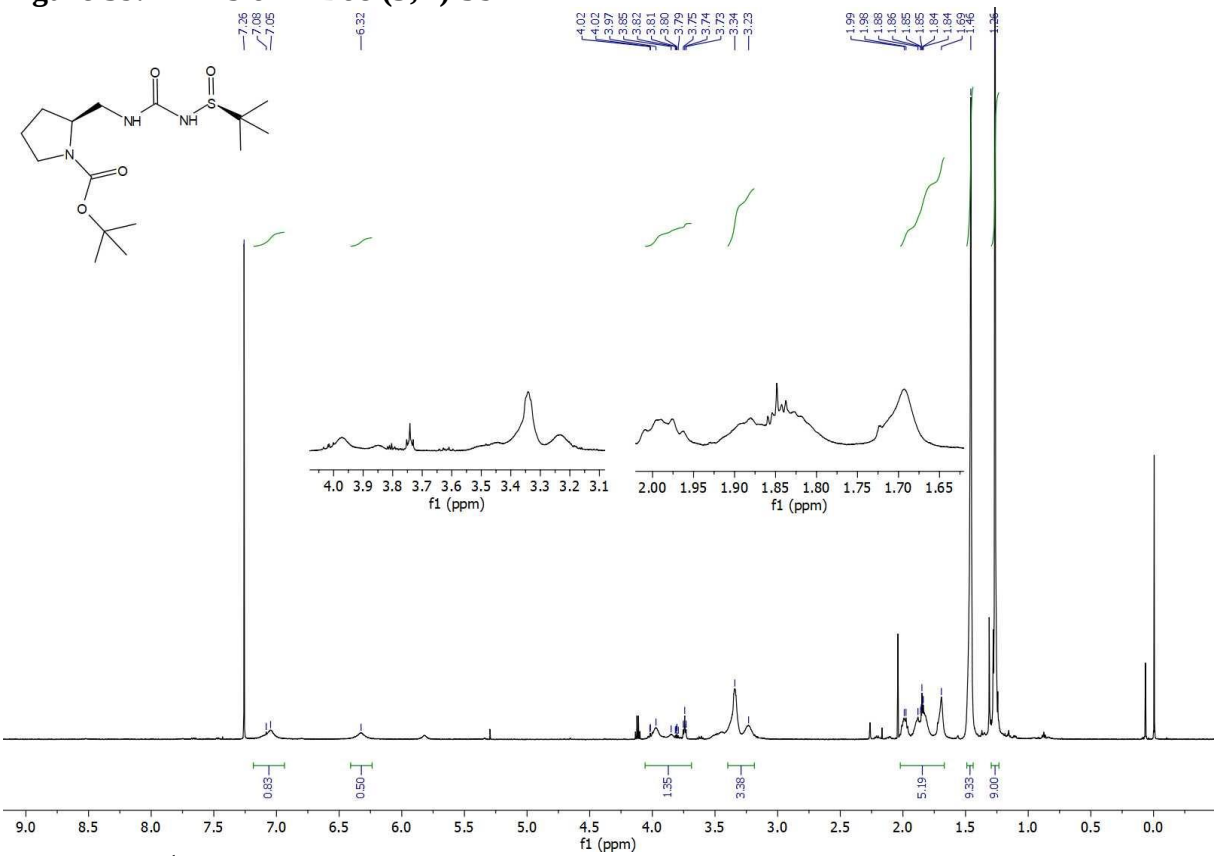



**Figure S10.** $^{1}$H NMR of ***N*-Boc-(*S*,*S*)-5b**

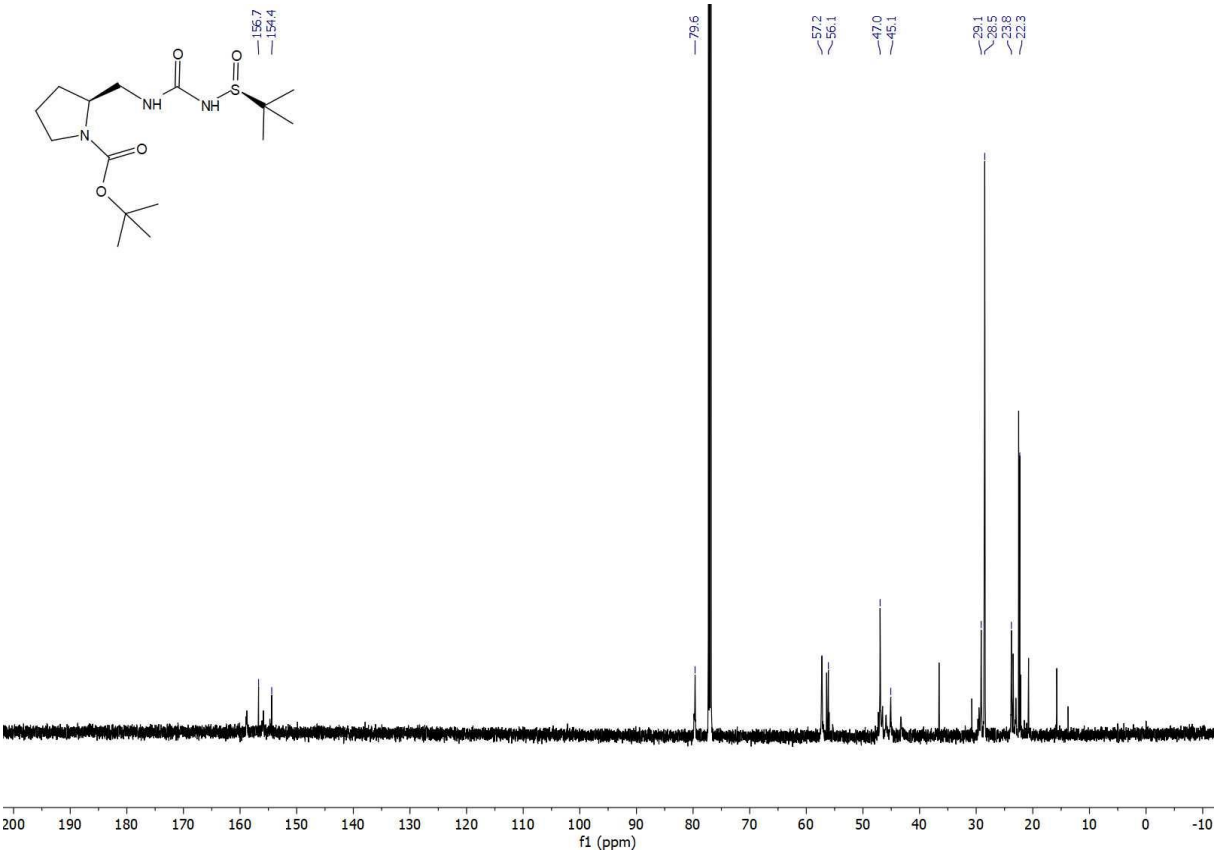



**Figure S11.** $^{13}$C NMR of ***N*-Boc-(*S*,*S*)-5b**

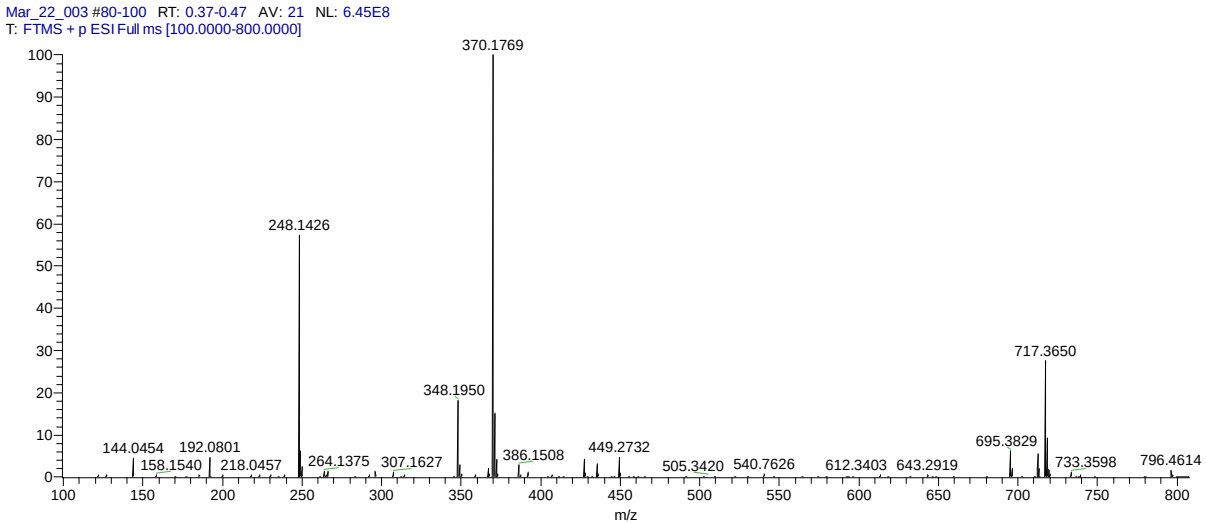



**Figure S12.** HRMS of ***N*-Boc-(*S*,*S*)-5b**

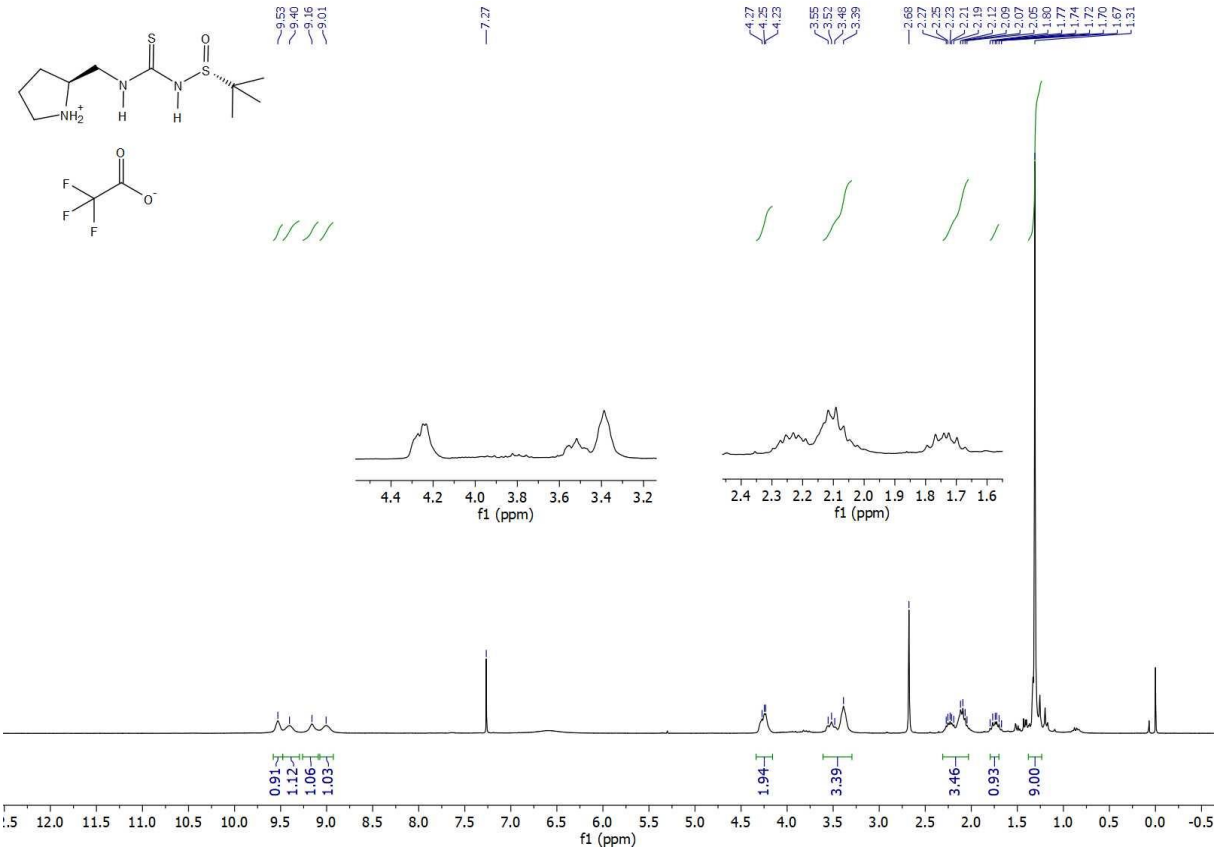



**Figure S13.** $^{1}$H NMR of **(*S*,*R*)-C1**

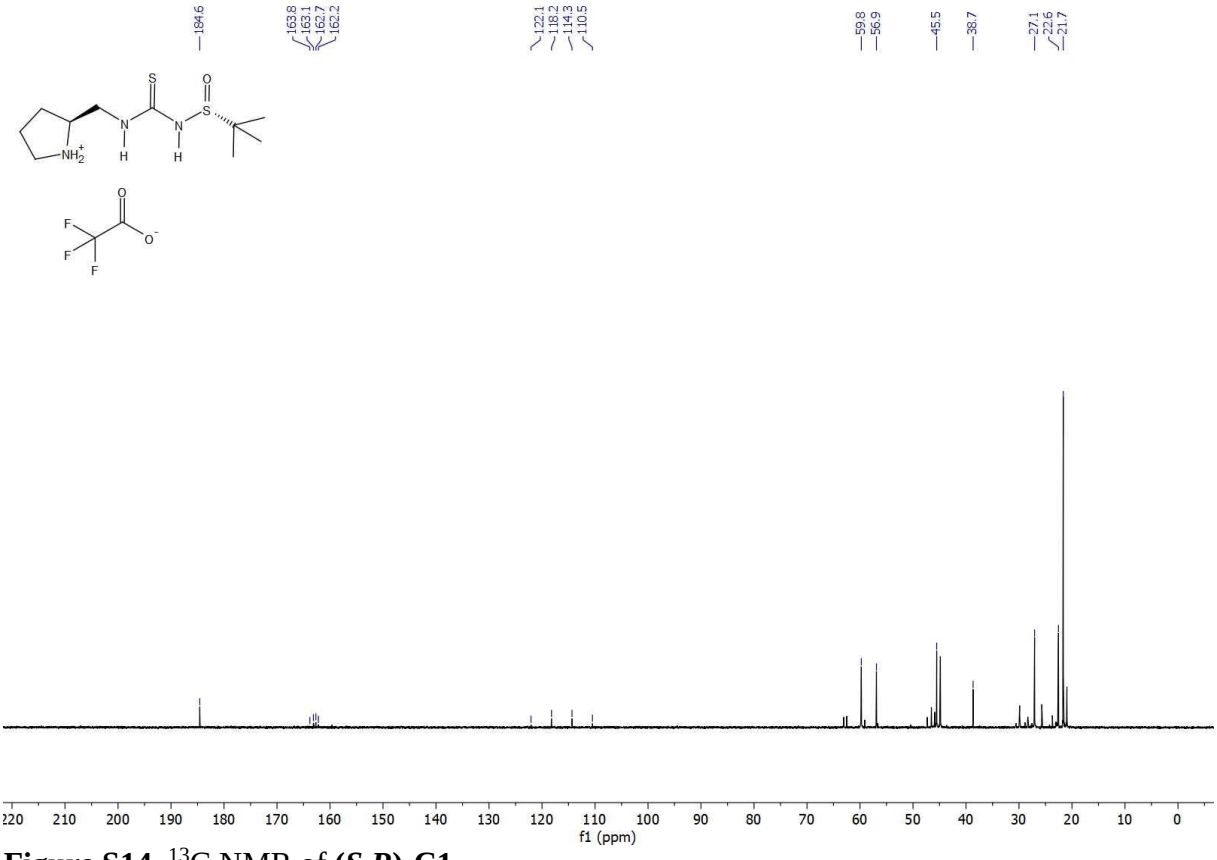



**Figure S14.** $^{13}$C NMR of **(*S*,*R*)-C1**

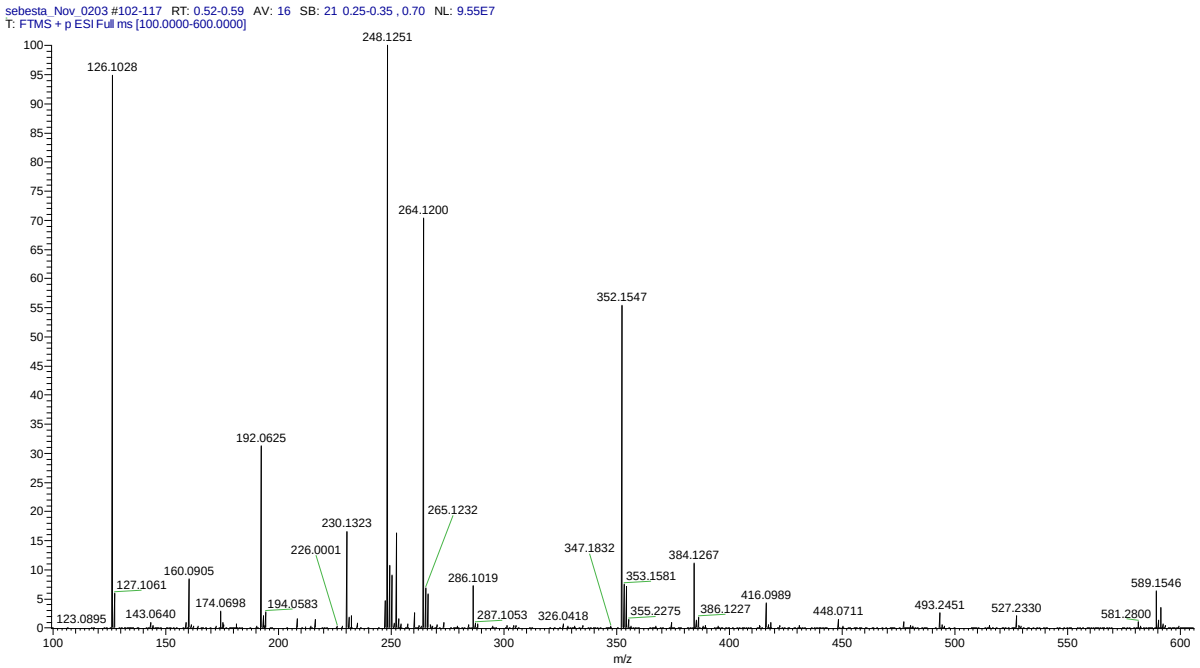



**Figure S15.** HRMS of **(*S*,*R*)-C1**

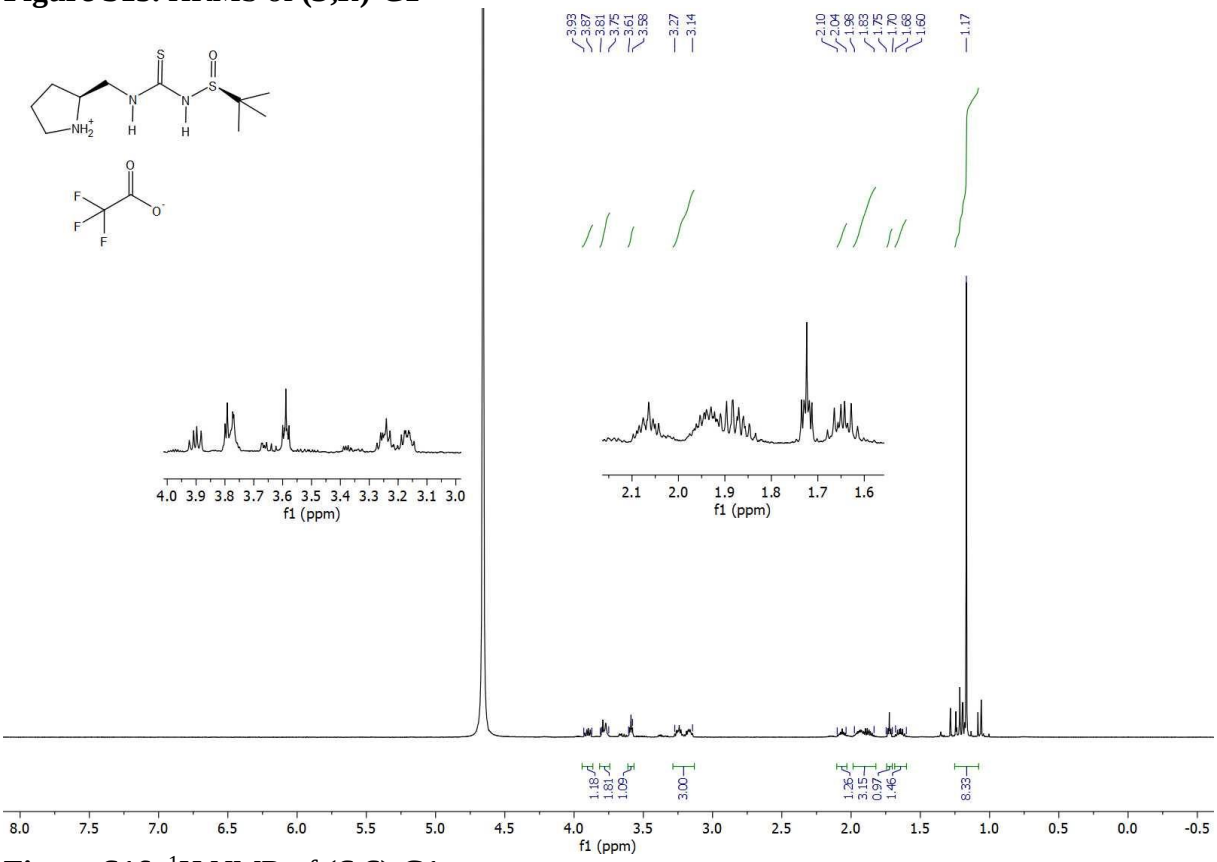



**Figure S16.** $^{1}$H NMR of **(*S*,*S*)-C1**

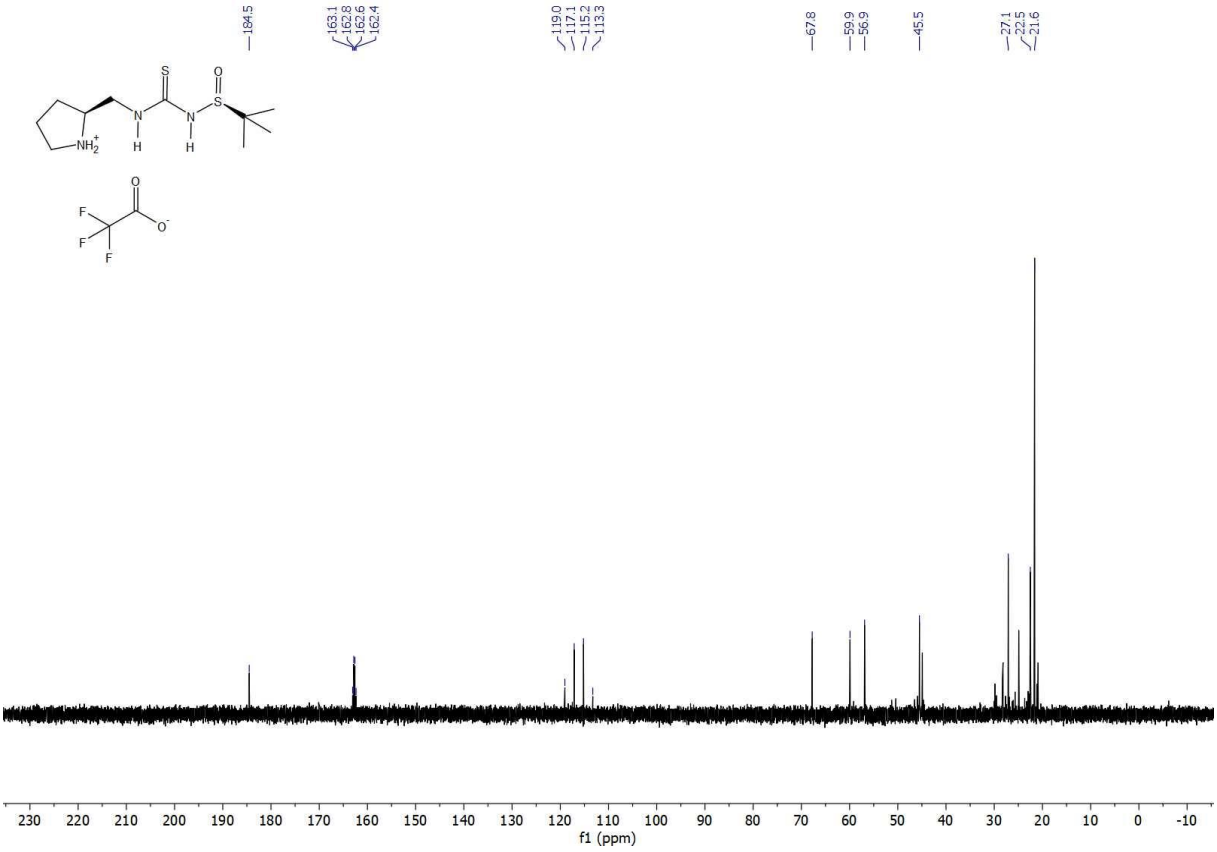



**Figure S17.** $^{13}$C NMR of **(*S*,*S*)-C1**

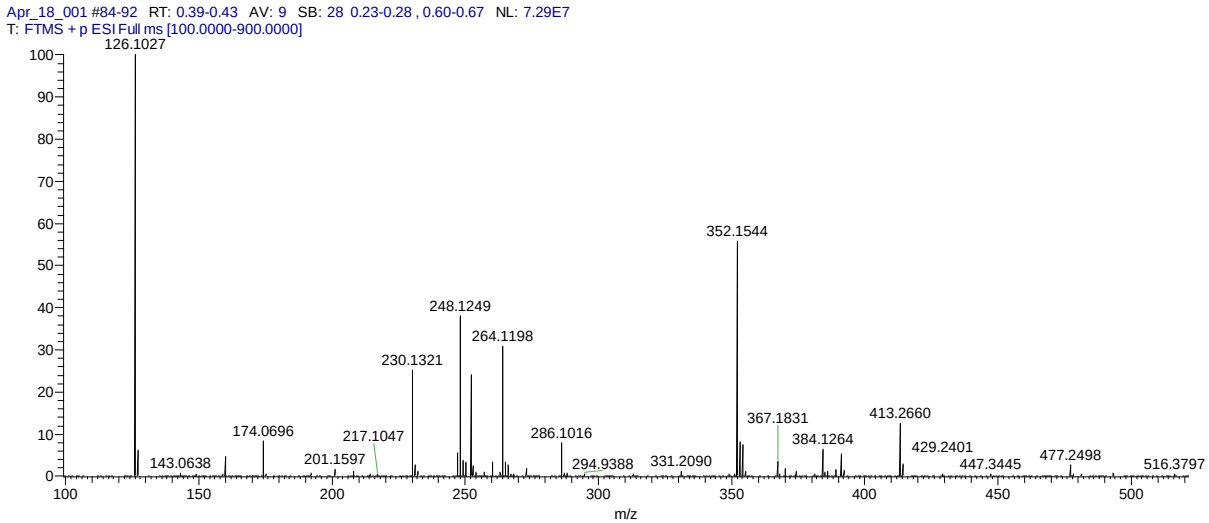



**Figure S18.** HRMS1 of **(*S*,*S*)-C1**

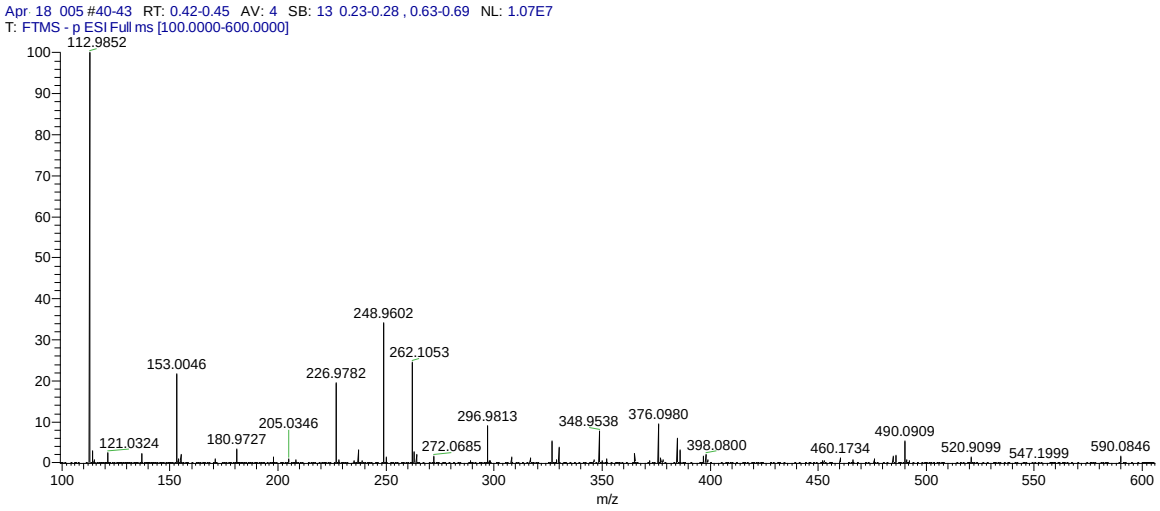



**Figure S19.** HRMS2 of **(*S*,*S*)-C1**

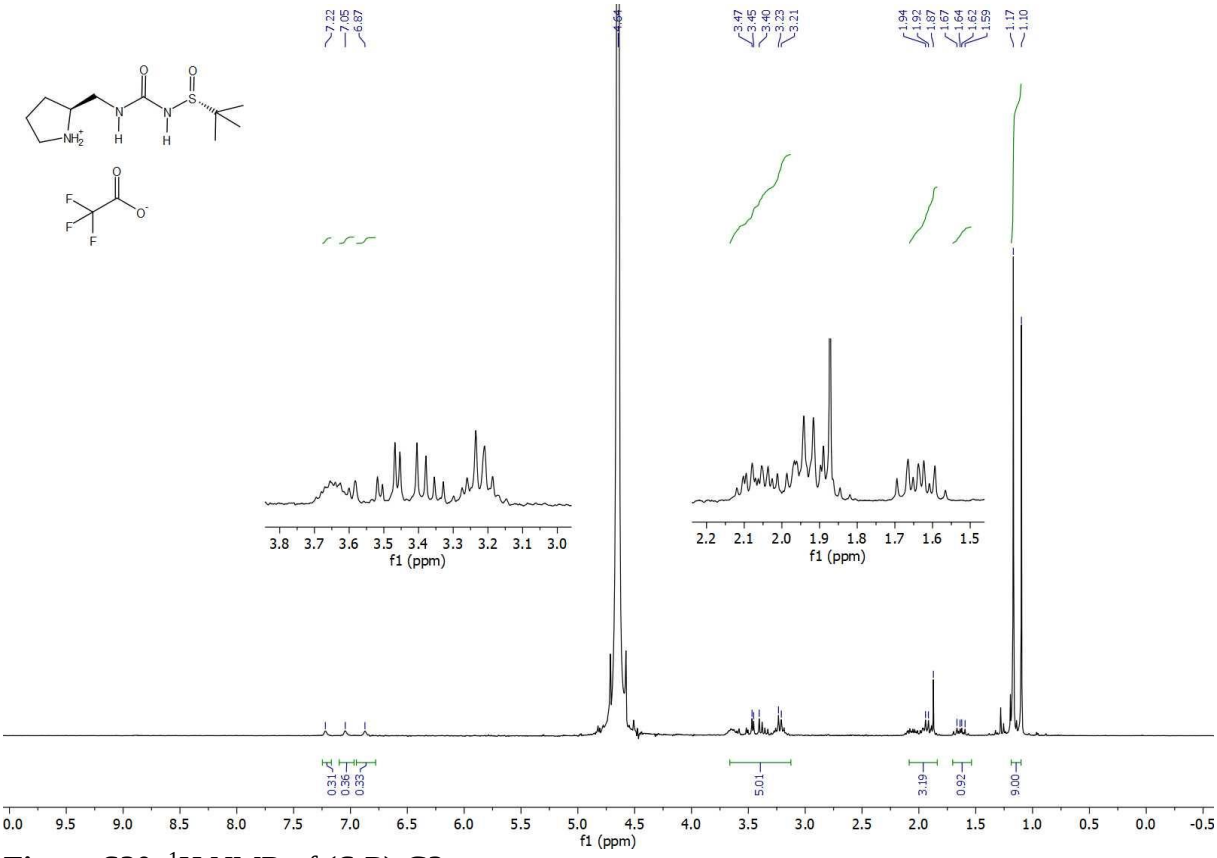



**Figure S20.** $^{1}$H NMR of **(*S*,*R*)-C2**

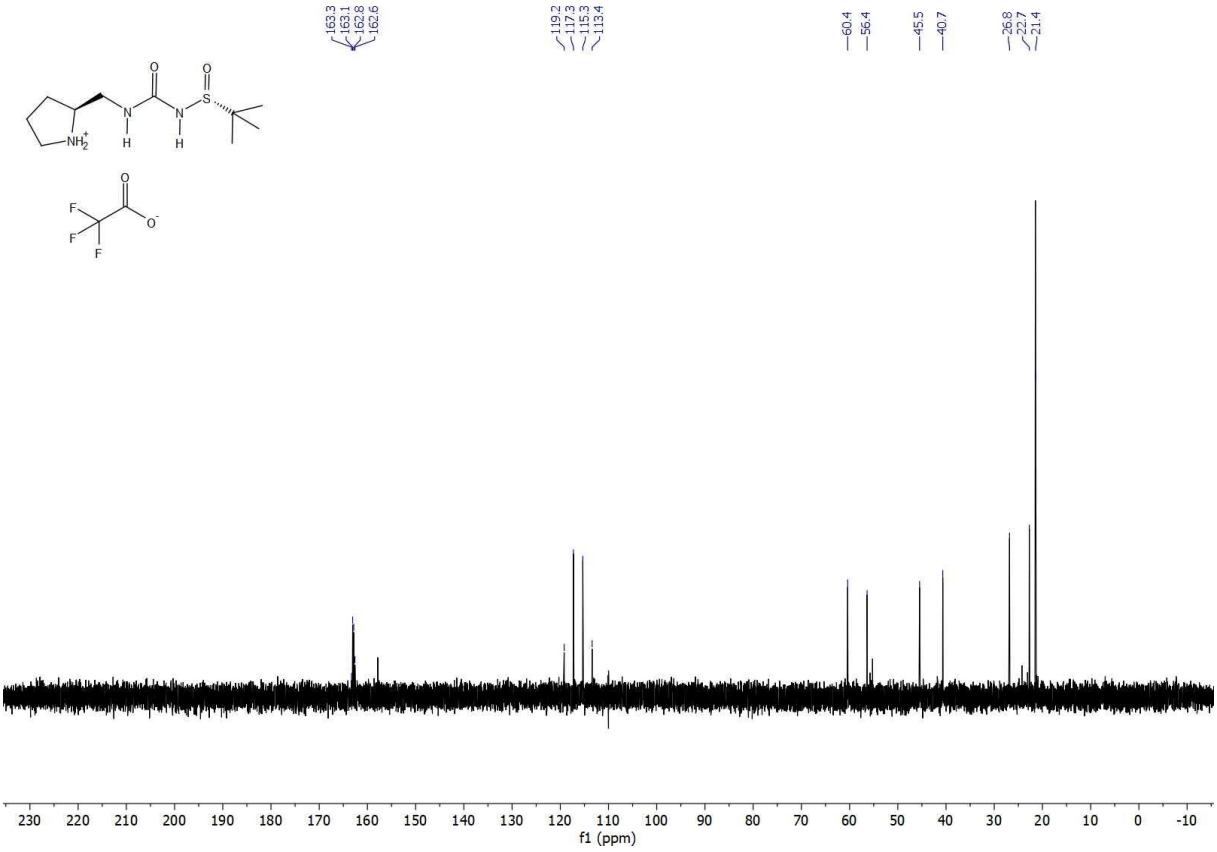



**Figure S21.** $^{13}$C NMR of **(*S*,*R*)-C2**

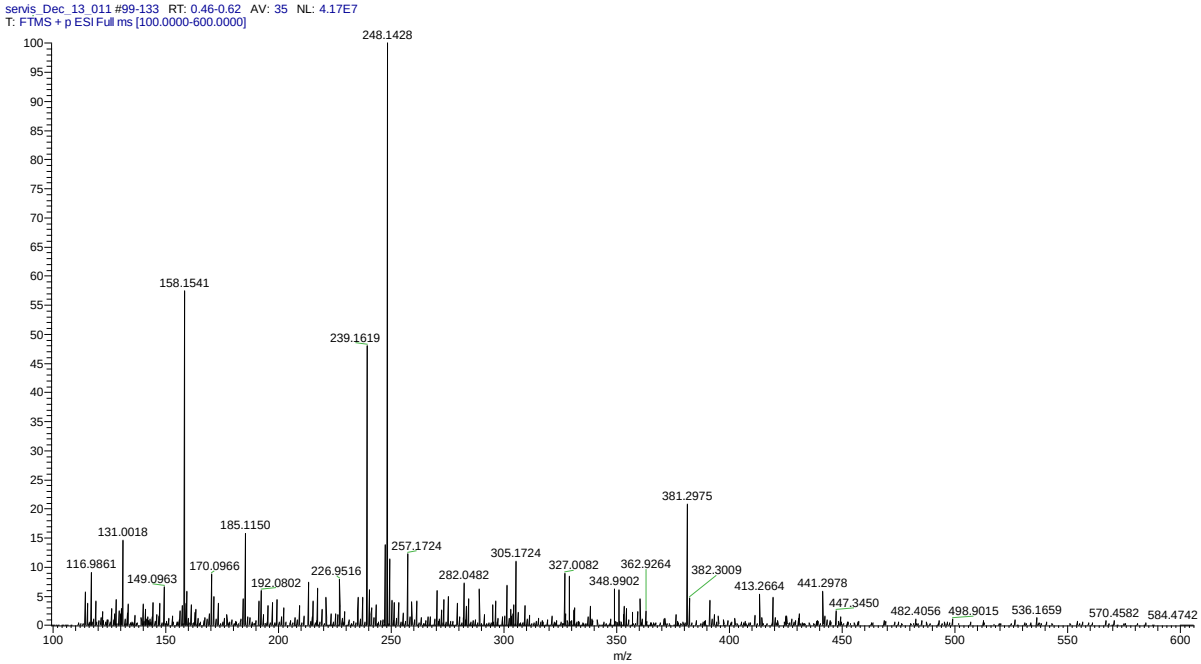



**Figure S22.** HRMS of **(*S*,*R*)-C2**

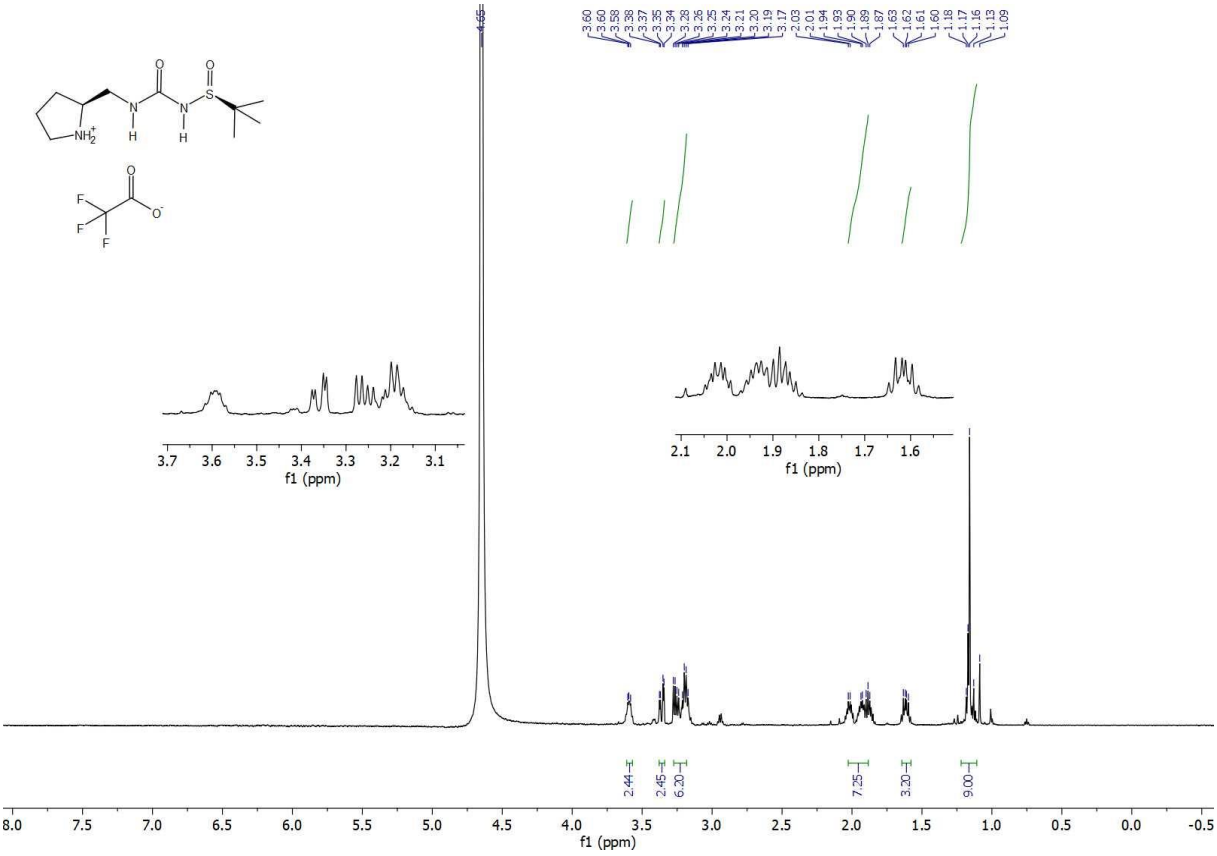



**Figure S23.** $^{1}$H NMR of **(*S*,*S*)-C2**

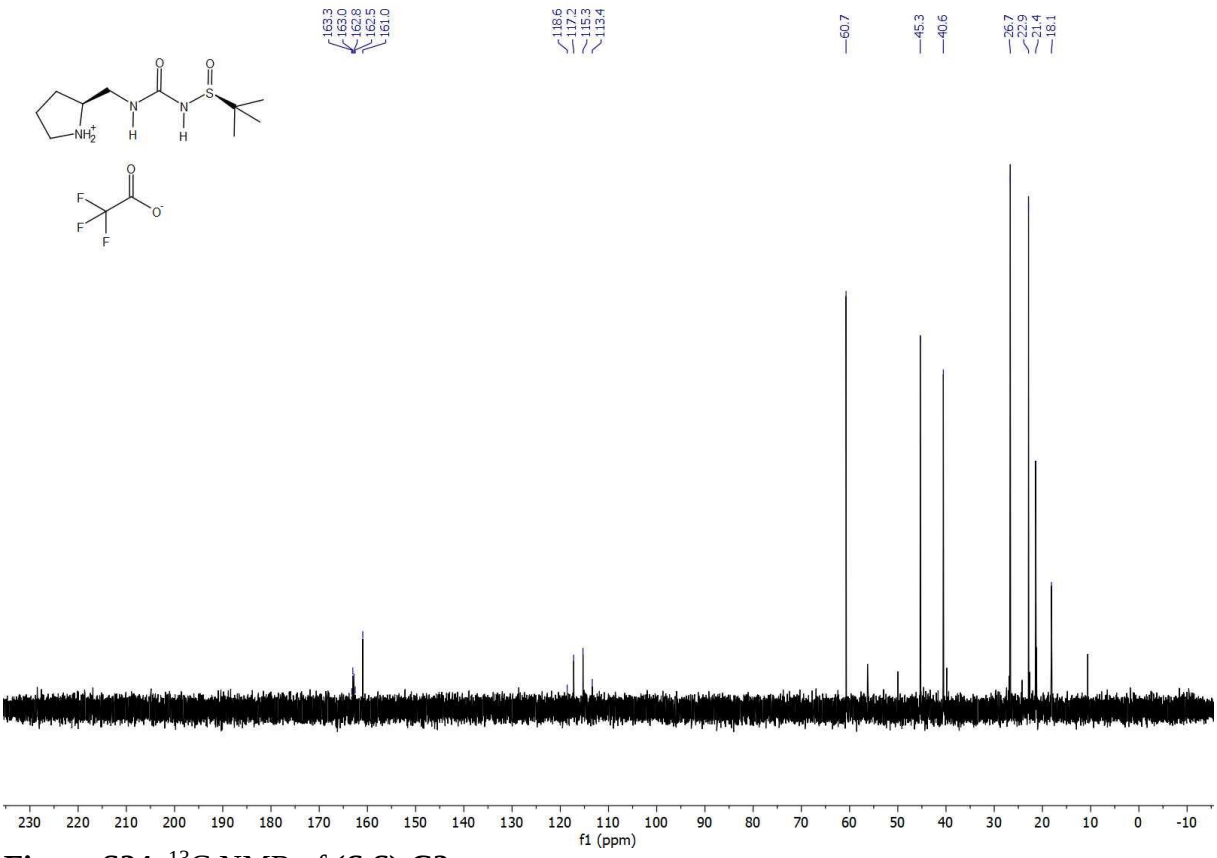



**Figure S24.** $^{13}$C NMR of **(*S*,*S*)-C2**

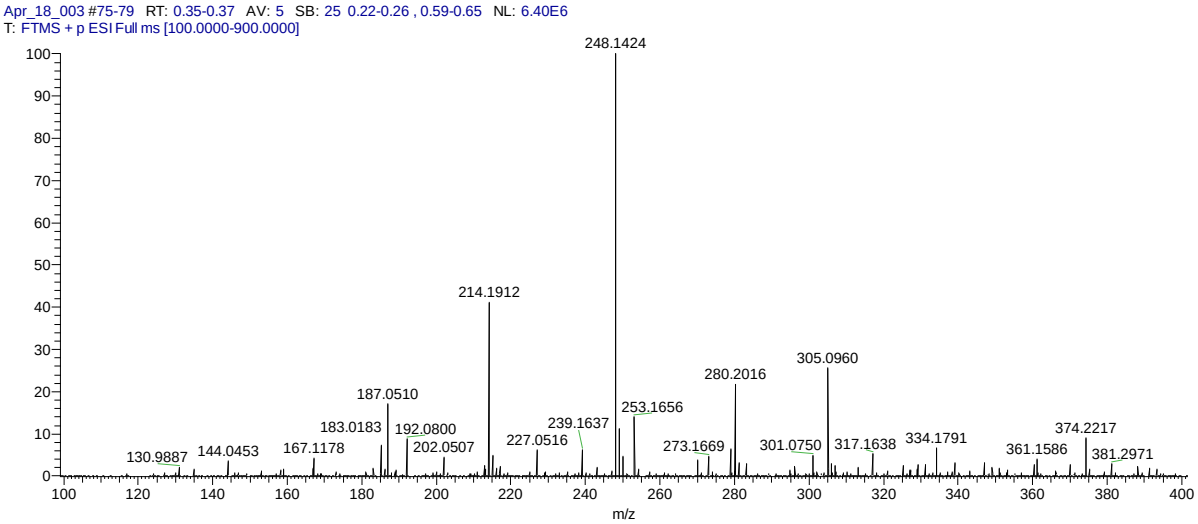



**Figure S25.** HRMS1 of **(*S*,*S*)-C2**

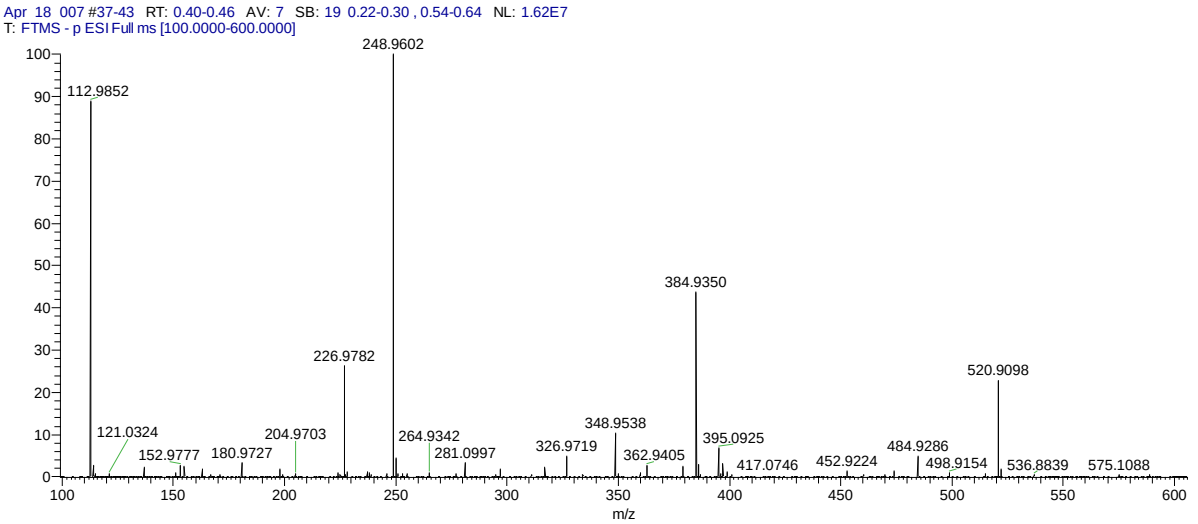



**Figure S26.** HRMS2 of **(*S*,*S*)-C2**

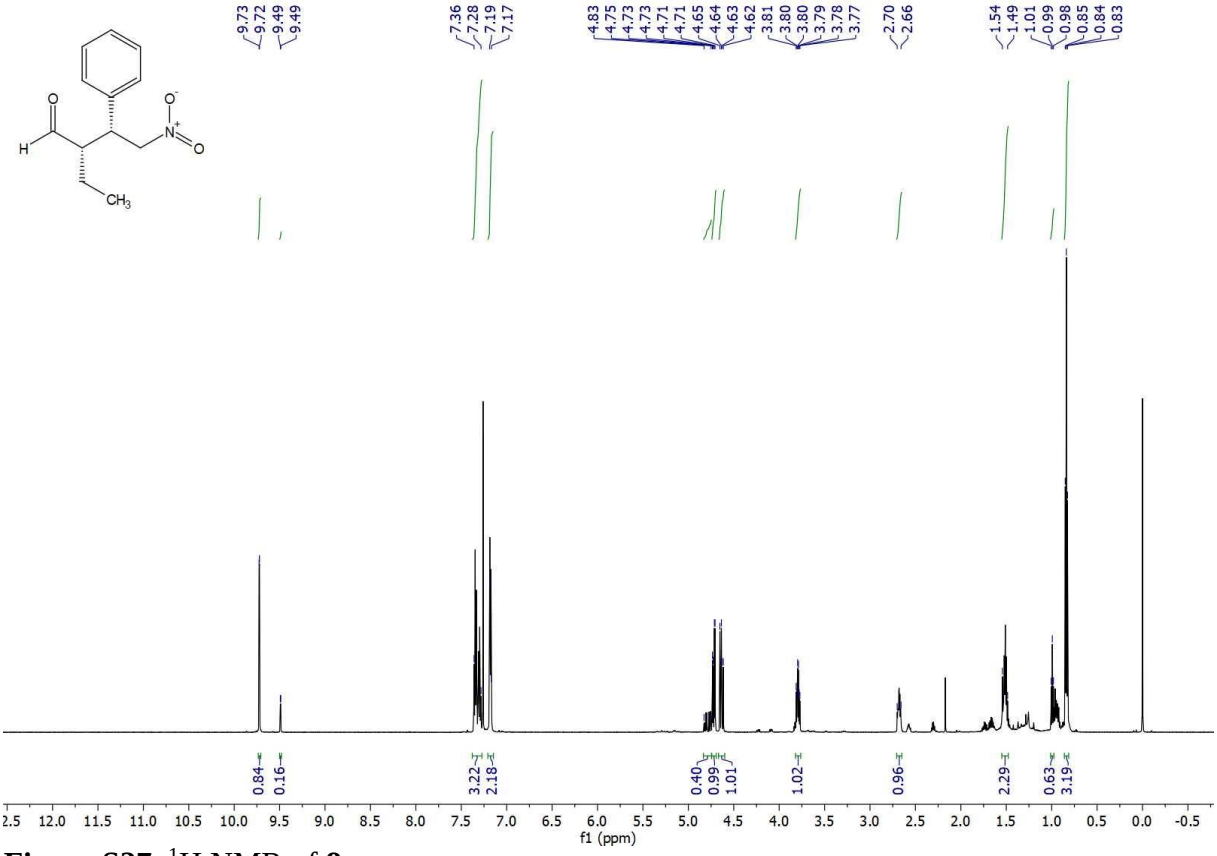



**Figure S27.** $^{1}$H NMR of **8a**

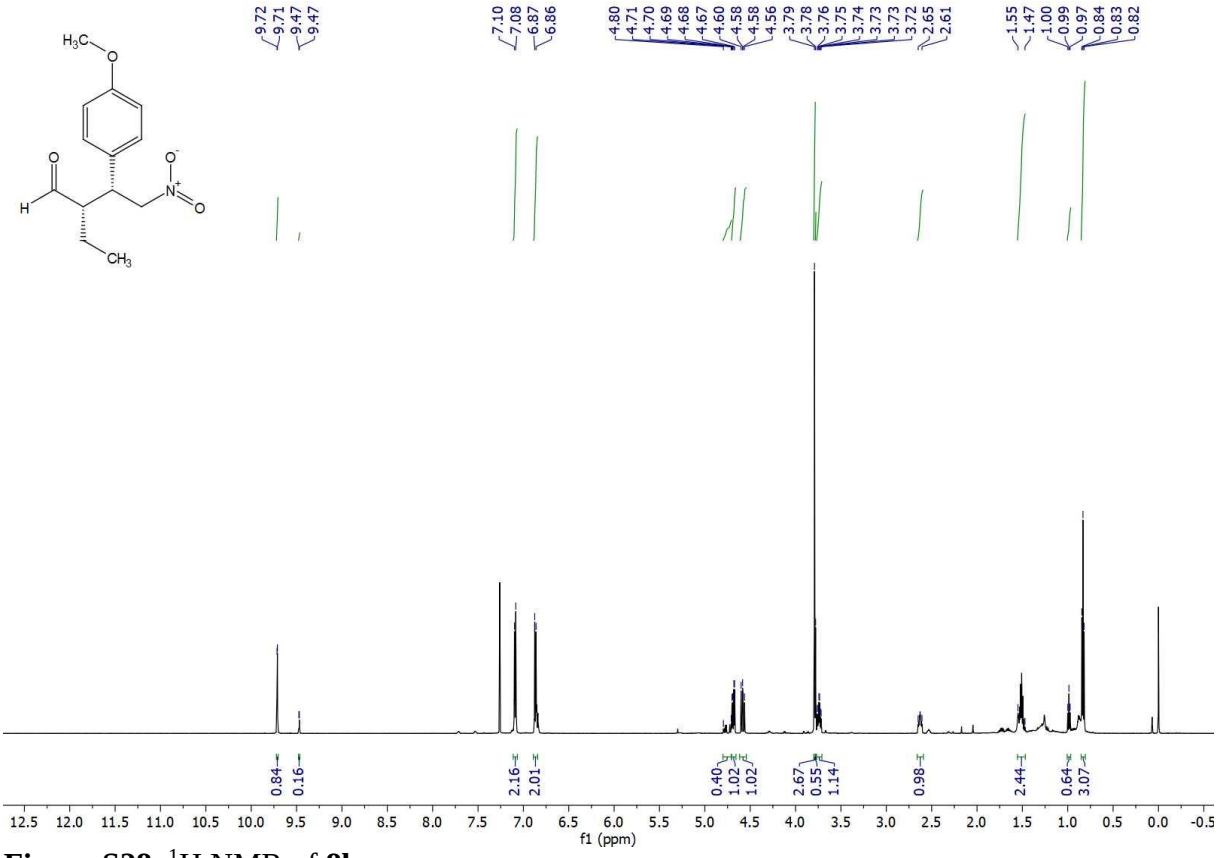



**Figure S28.** $^{1}$H NMR of **8b**

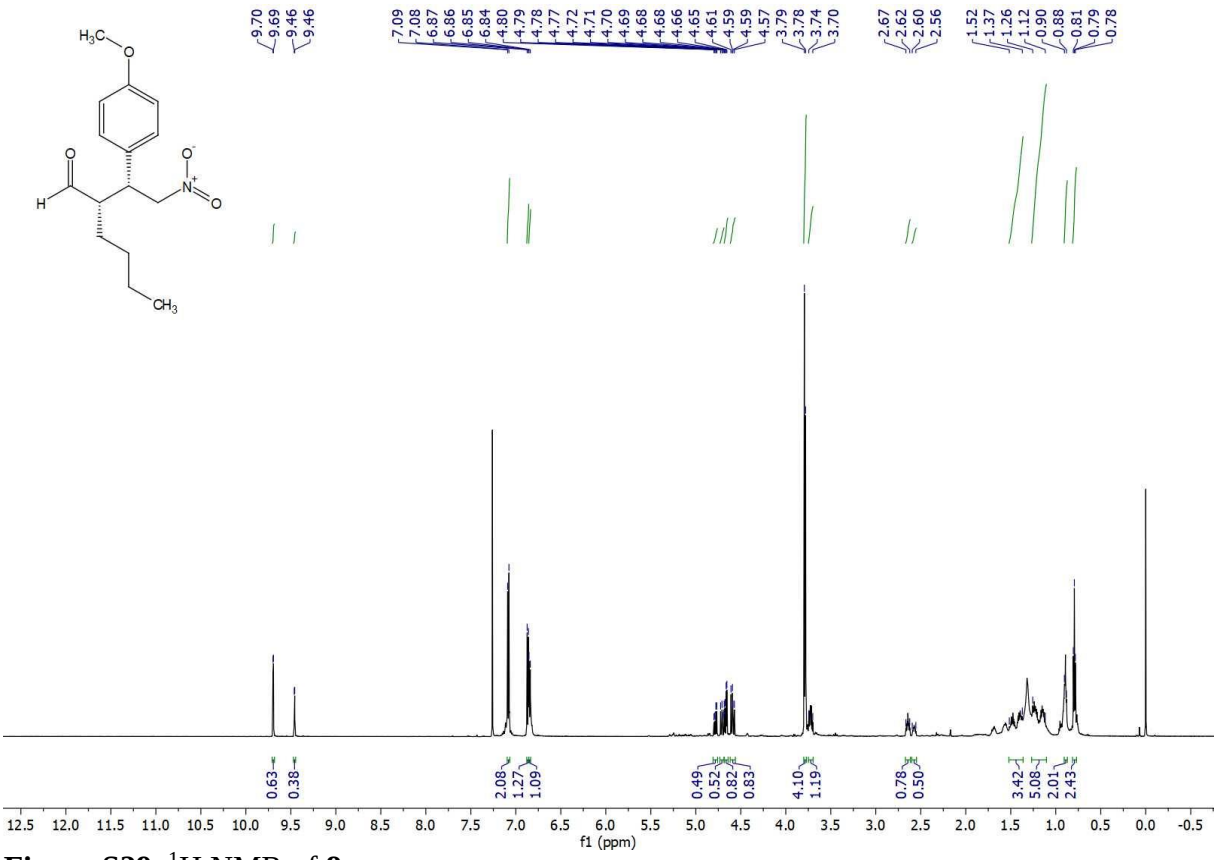



**Figure S29.** $^{1}$H NMR of **8c**

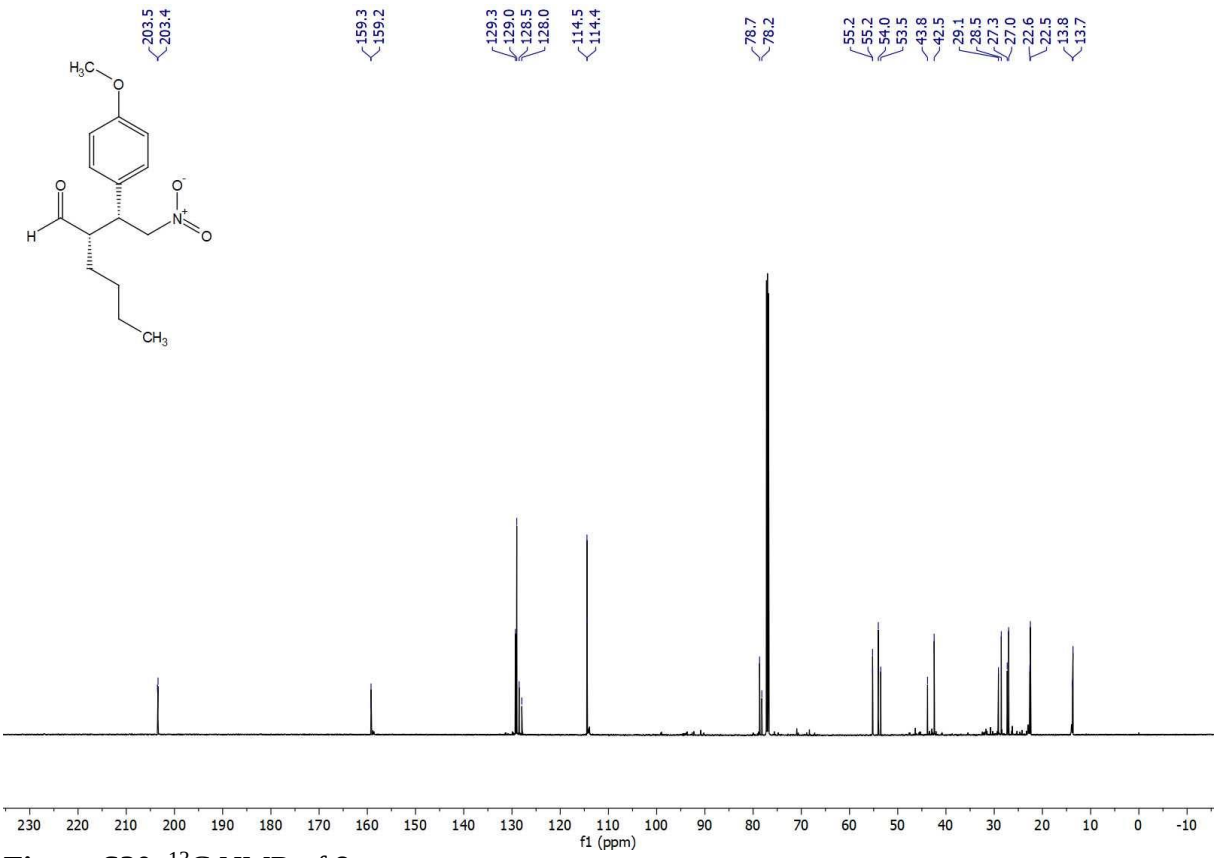



**Figure S30.** $^{13}$C NMR of **8c**

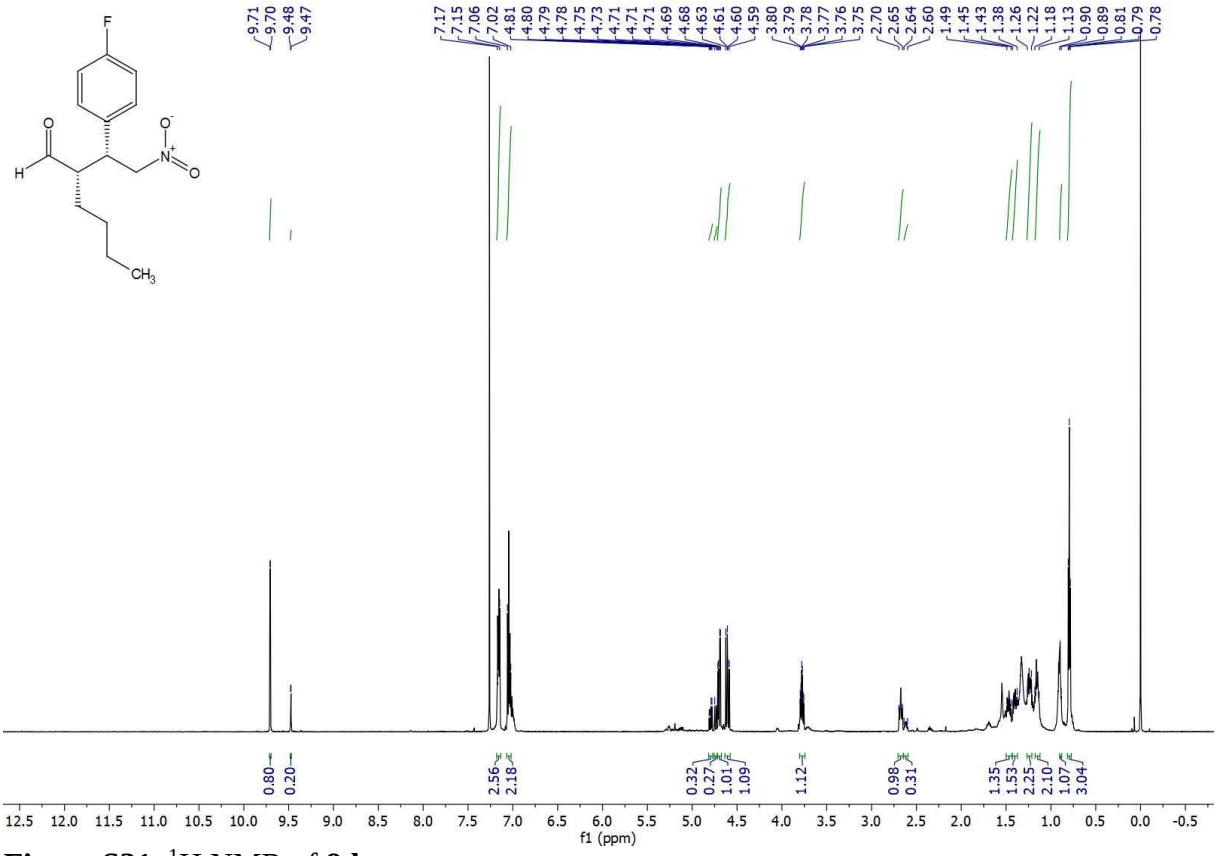



**Figure S31.** $^{1}$H NMR of **8d**

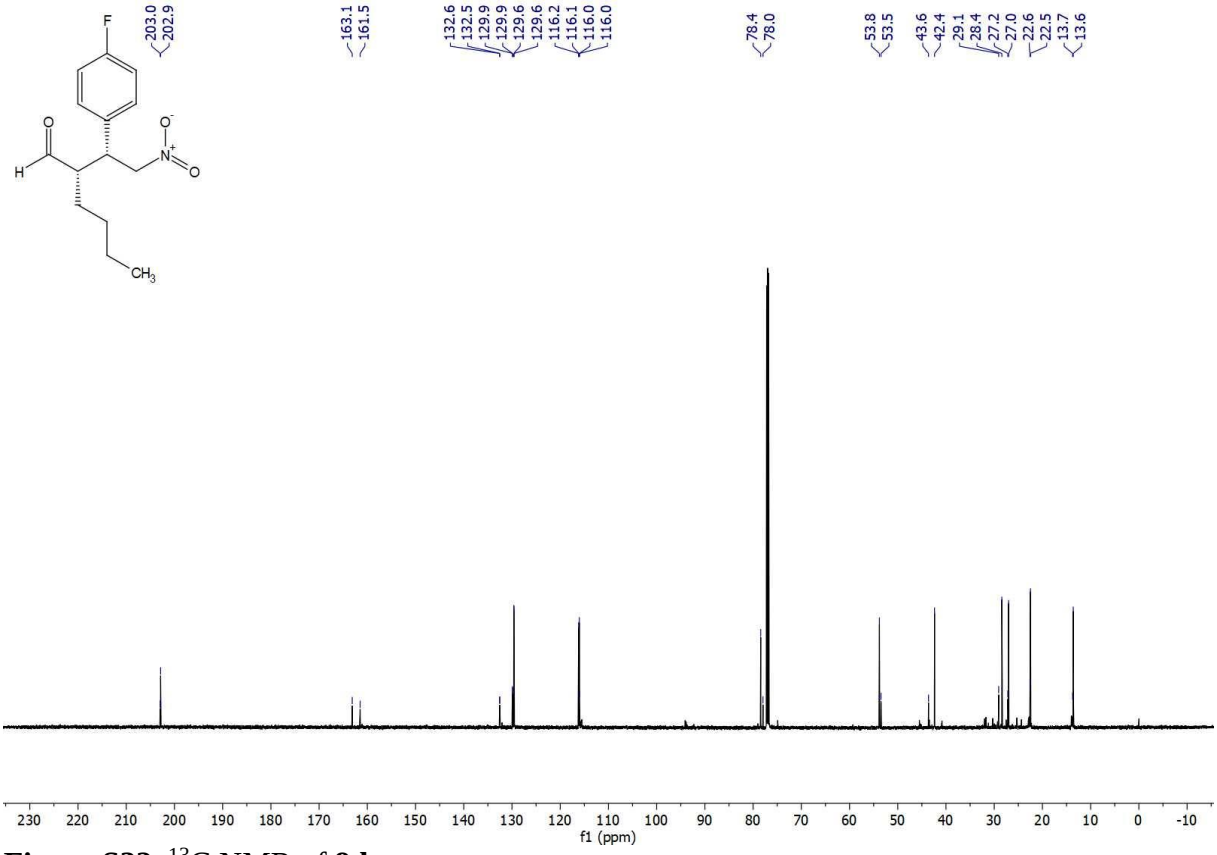



**Figure S32.** $^{13}$C NMR of **8d**

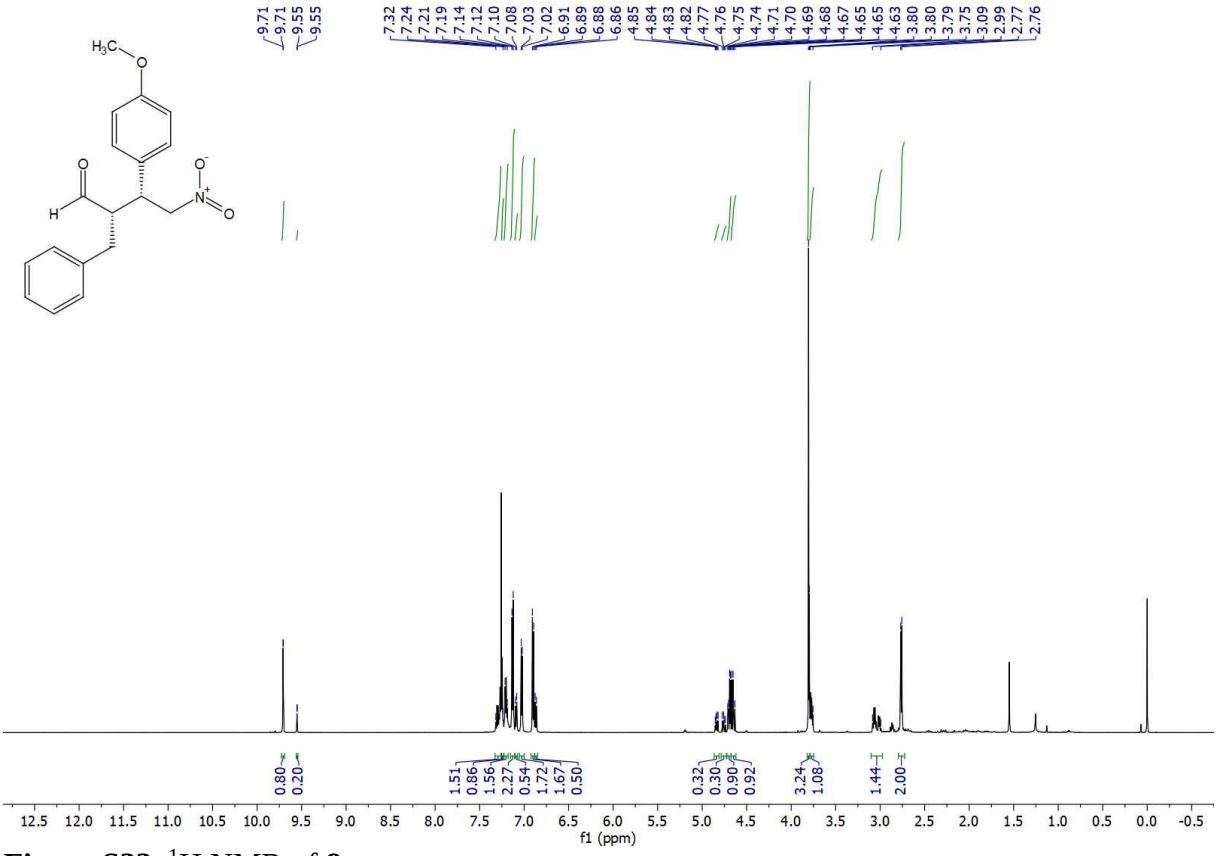



**Figure S33.** $^{1}$H NMR of **8e**

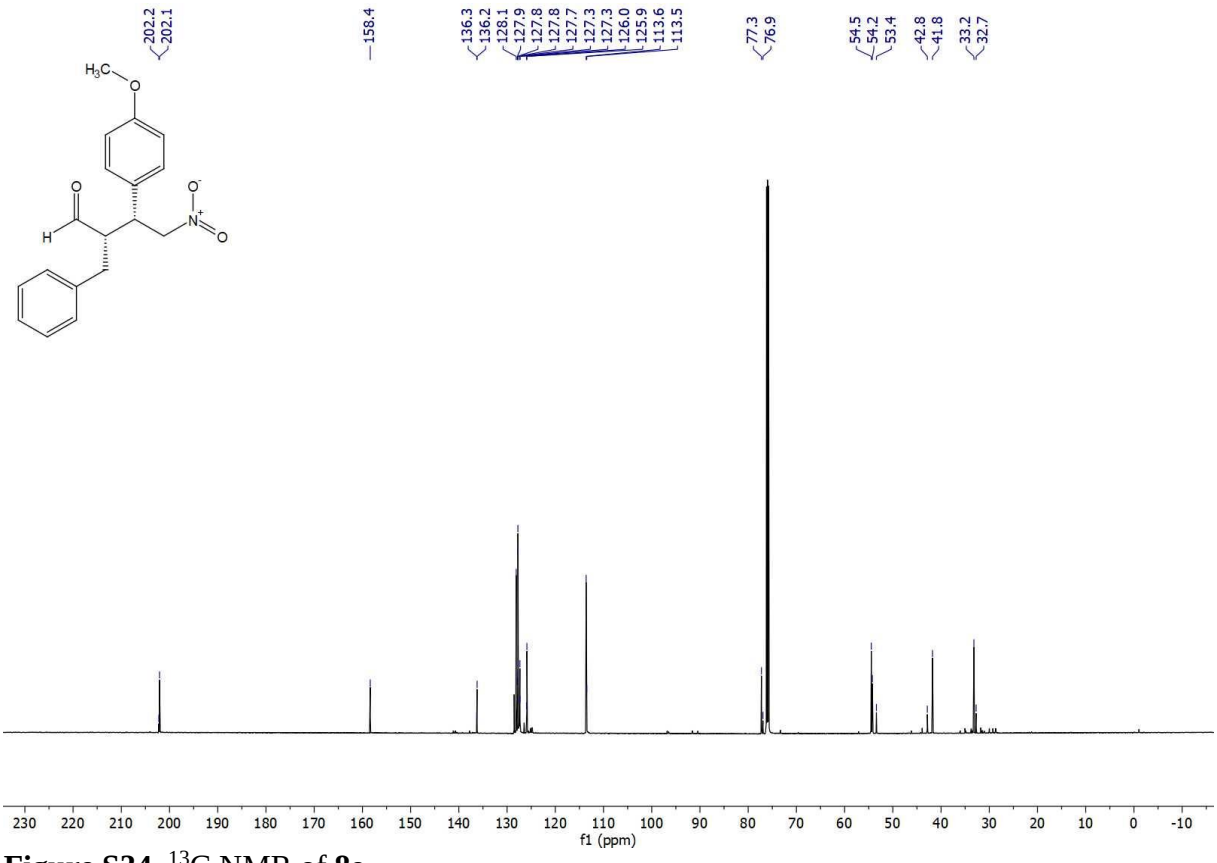



**Figure S34.** $^{13}$C NMR of **8e**

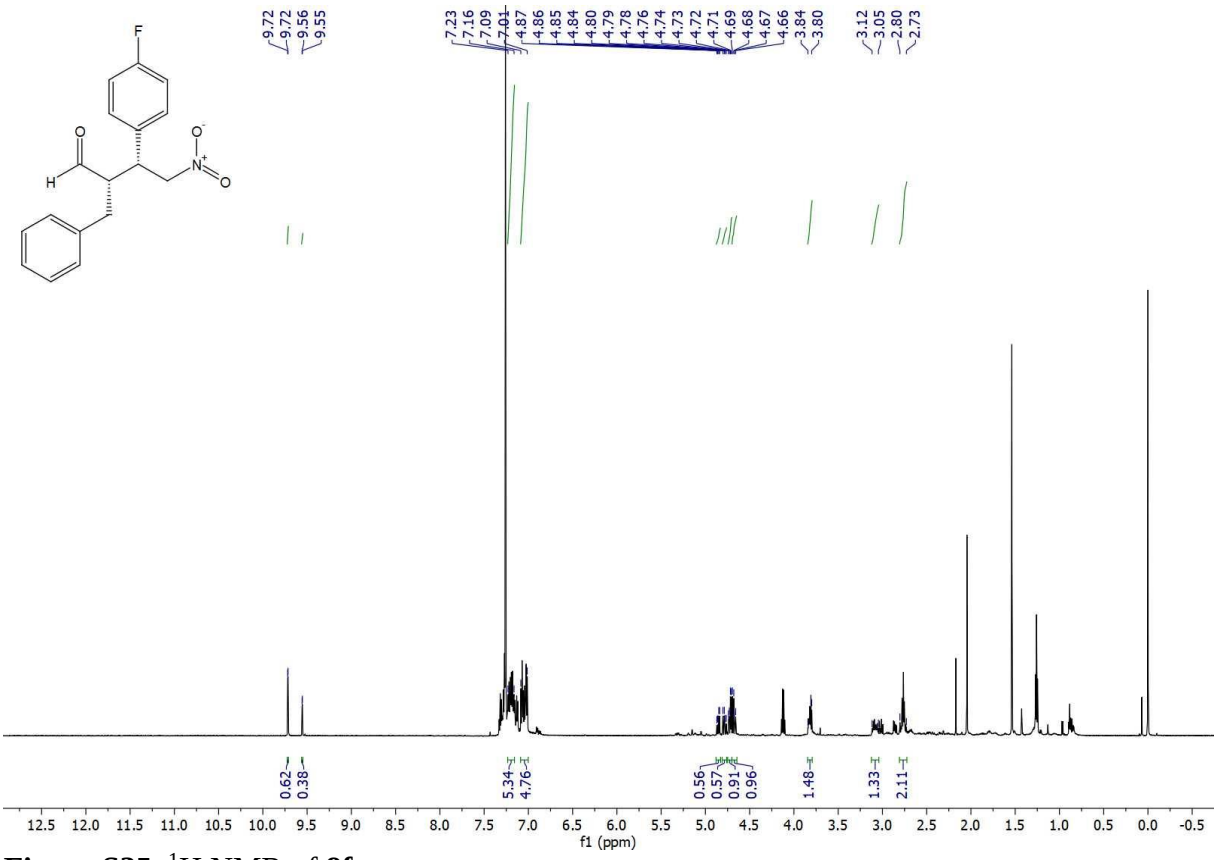



**Figure S35.** $^{1}$H NMR of **8f**

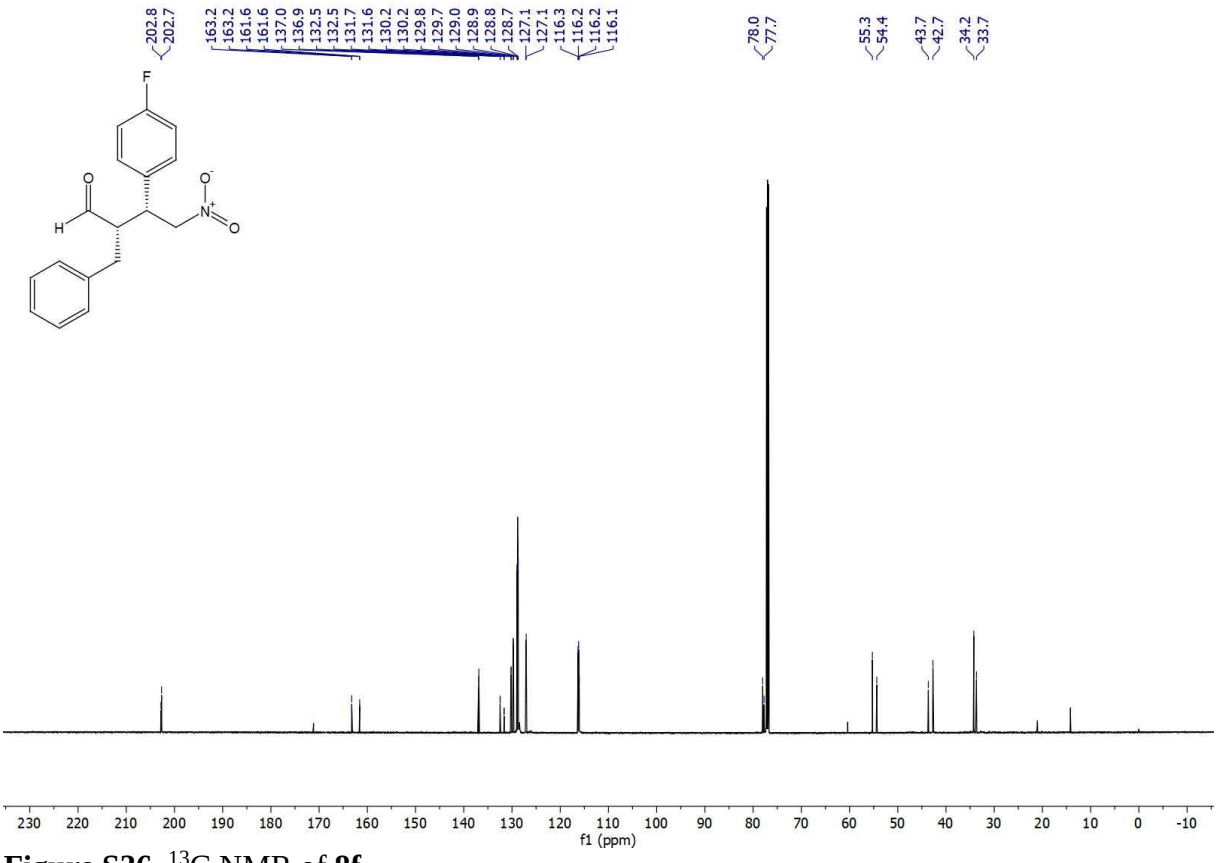



**Figure S36.** $^{13}$C NMR of **8f**

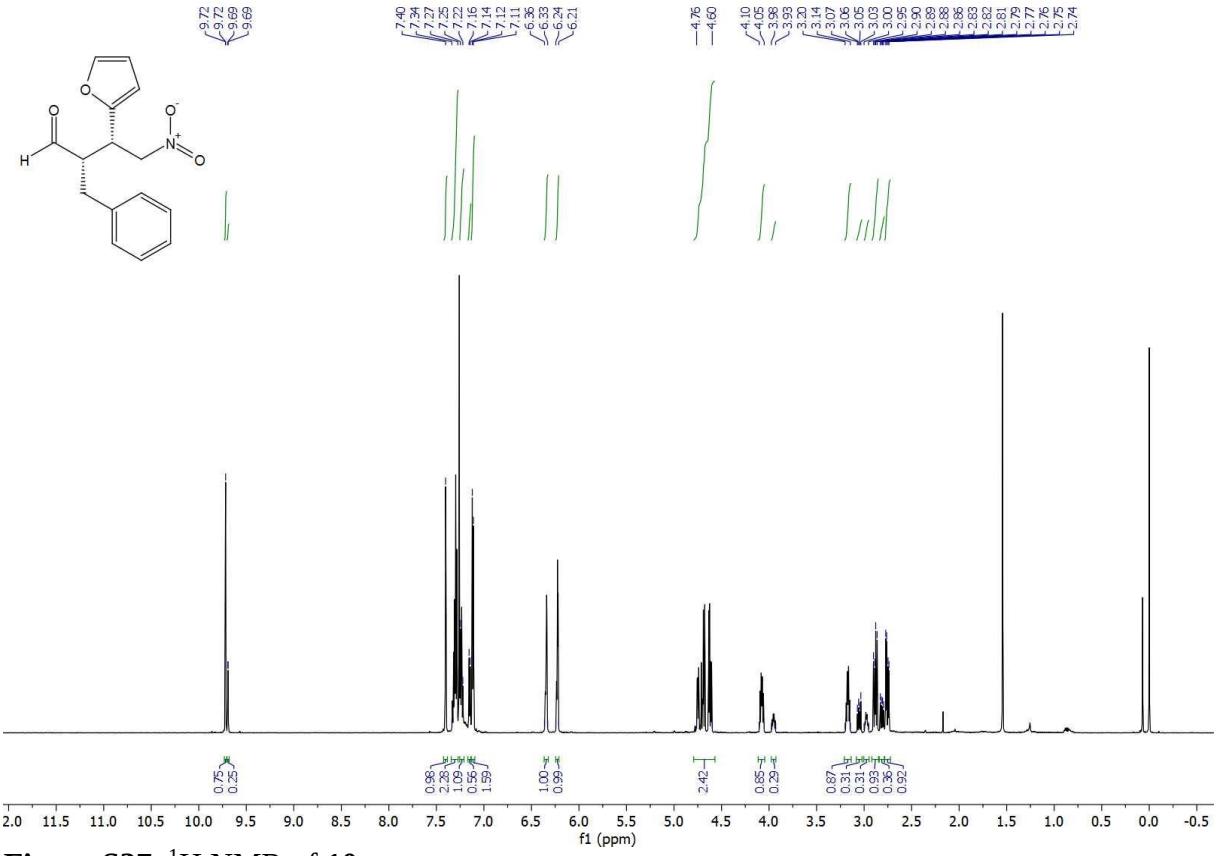



**Figure S37.** $^{1}$H NMR of **10a**

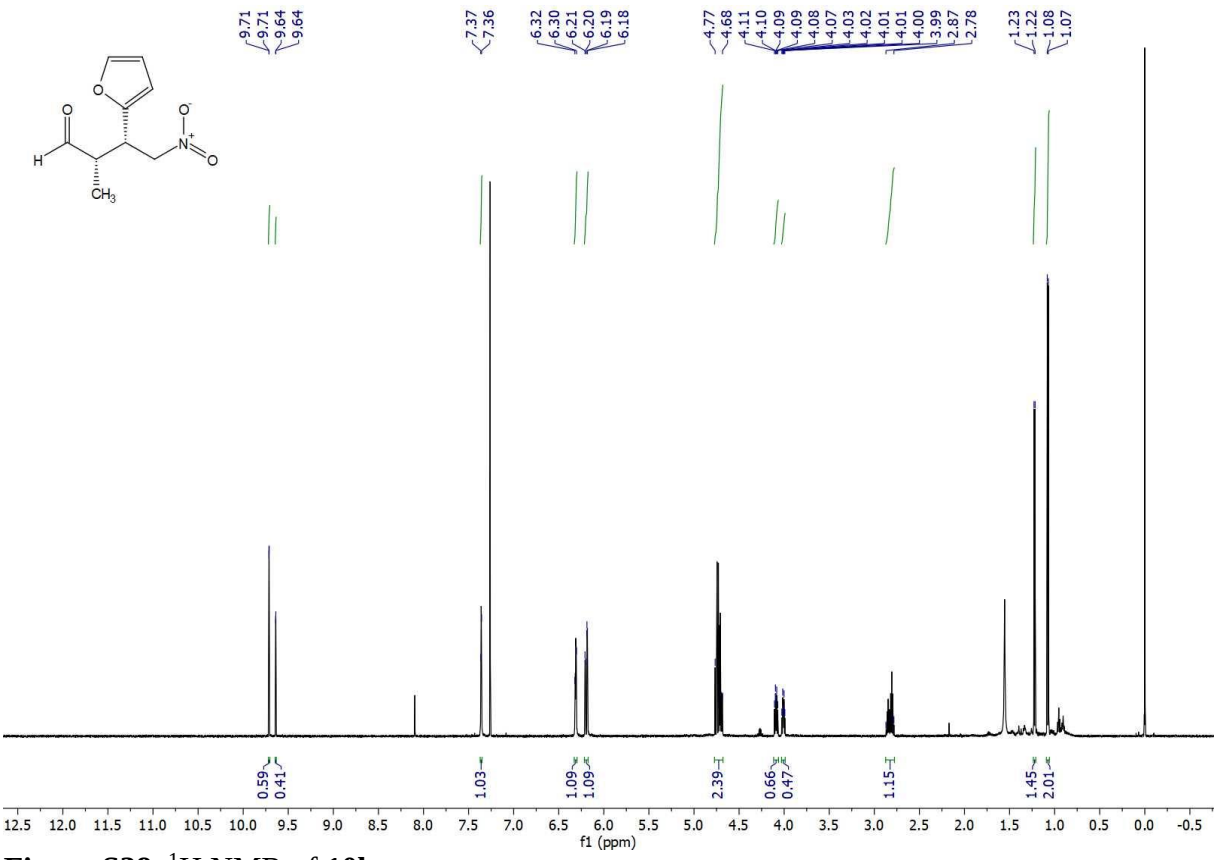



**Figure S38.** $^{1}$H NMR of **10b**

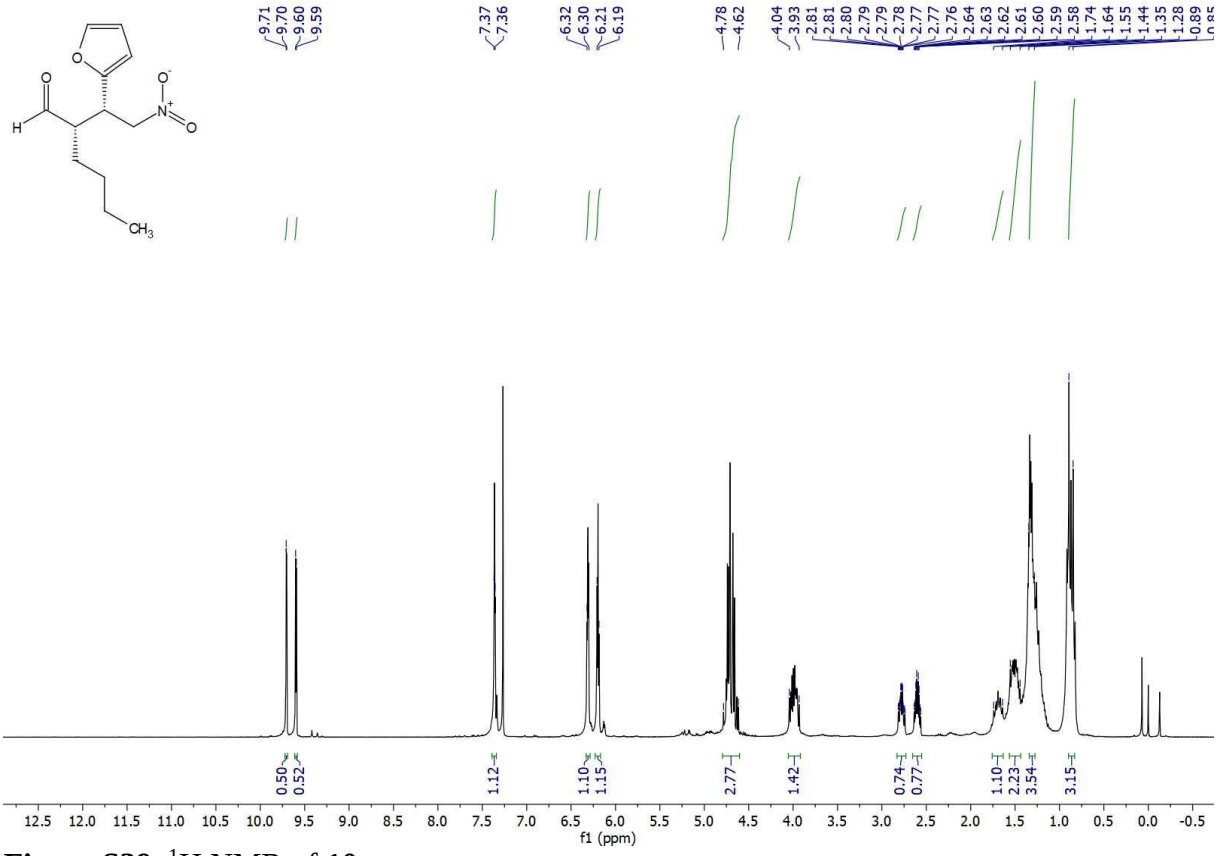



**Figure S39.** $^{1}$H NMR of **10c**

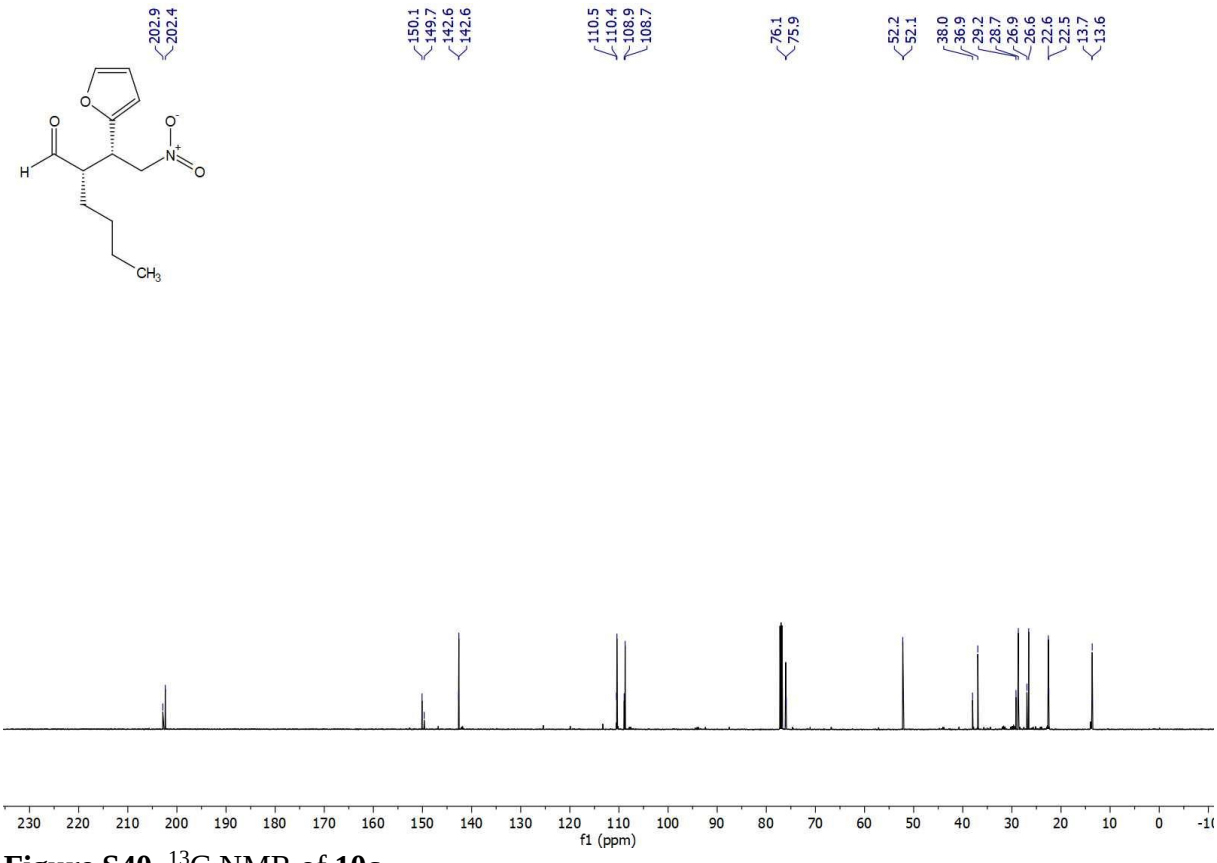



**Figure S40.** $^{13}$C NMR of **10c**

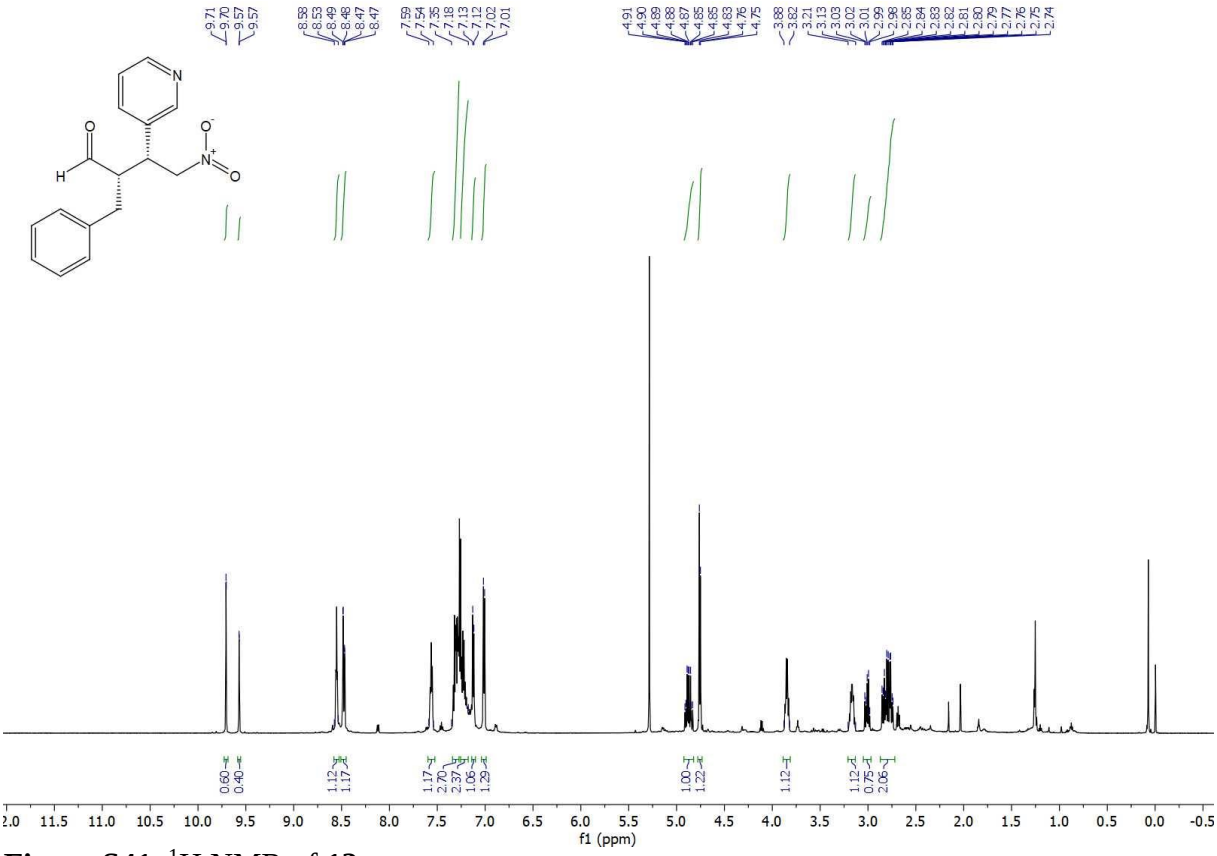



**Figure S41.** $^{1}$H NMR of **12**

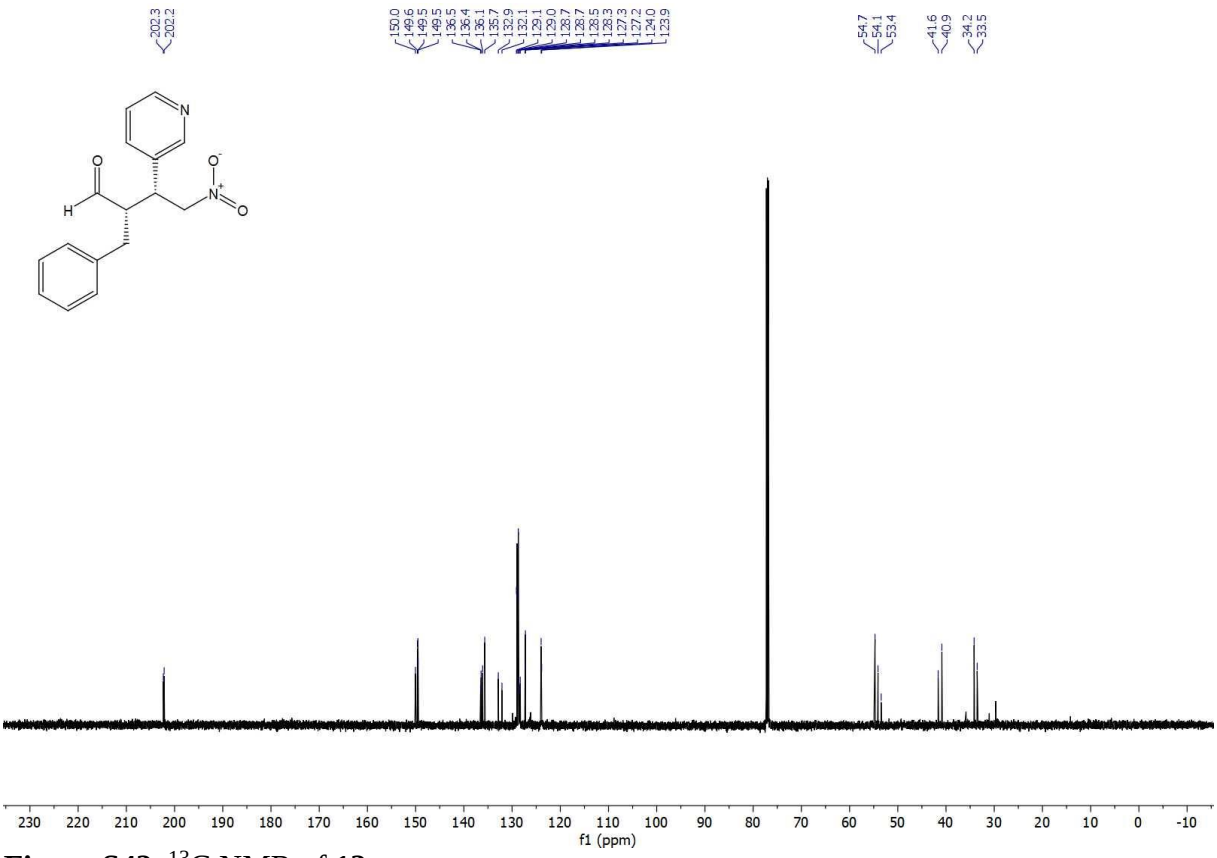
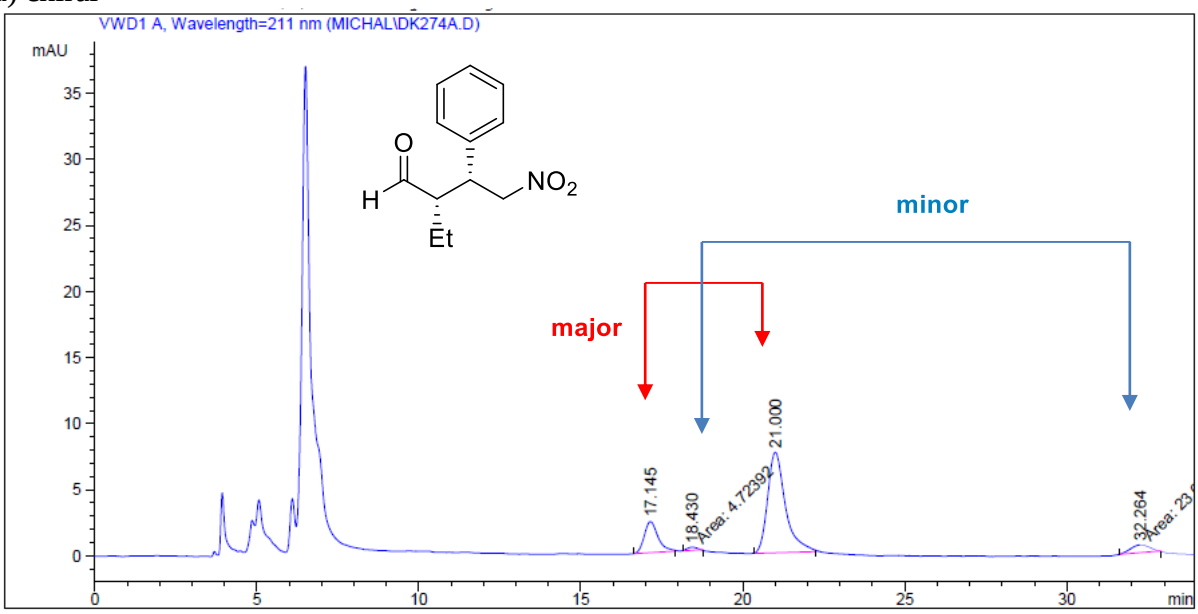



**Figure S42.** $^{13}$C NMR of **12**

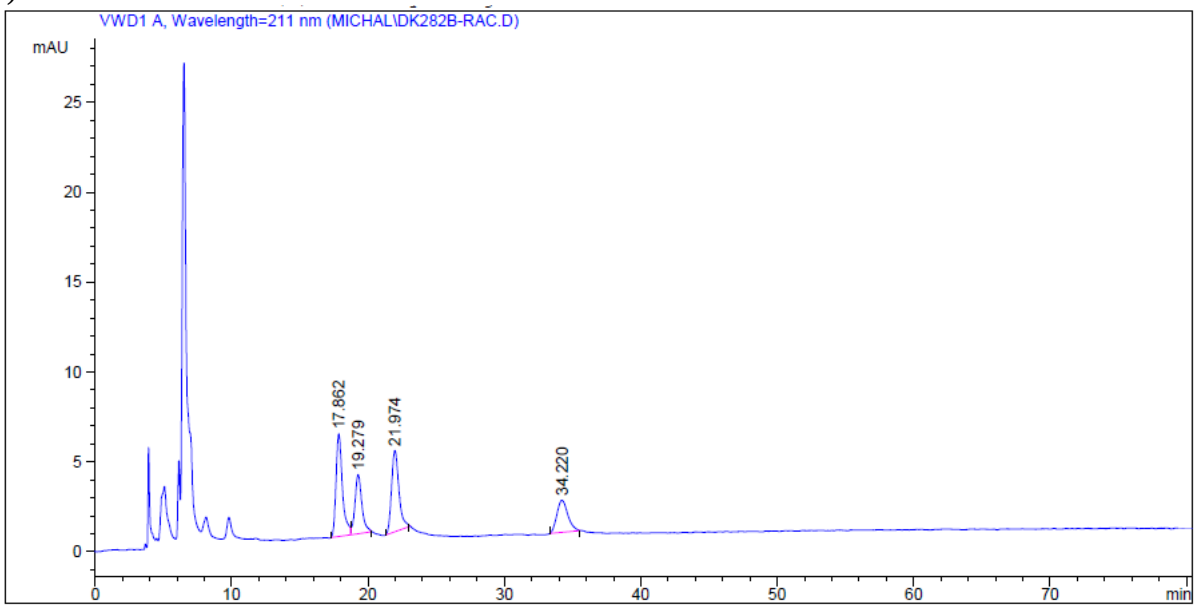
# 4. Copies of HPLC records

a) chiral



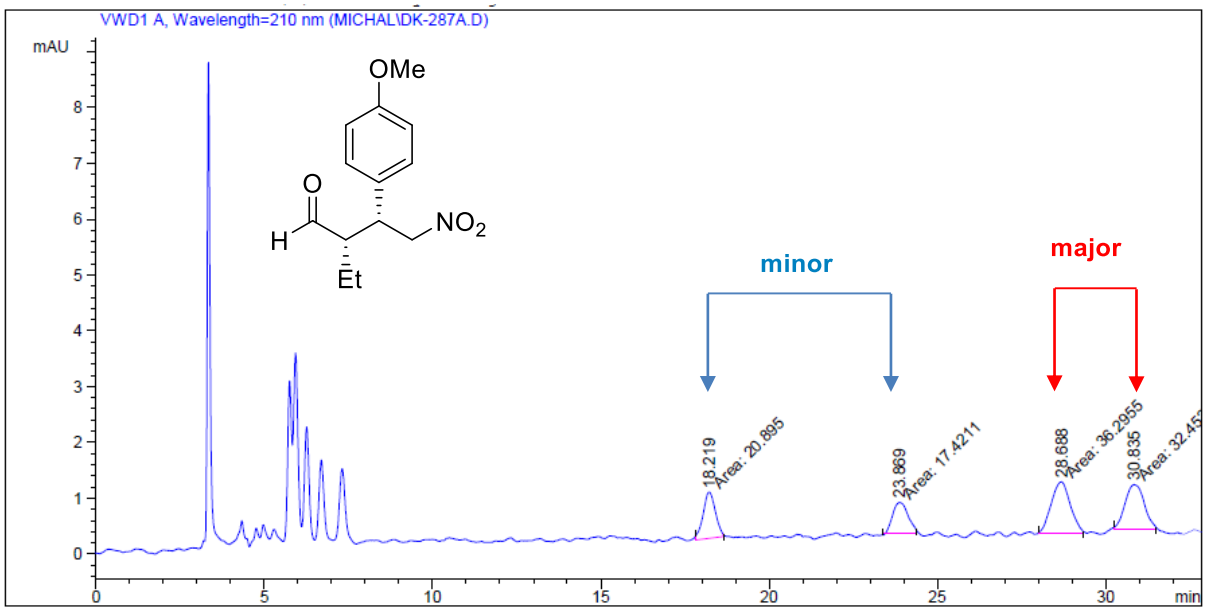

| Peak # | RetTime [min] | Type | Width [min] | Area mAU *s | Height [mAU ] | Area % |
|---|---|---|---|---|---|---|
| 1 | 17.145 | BB | 0.4454 | 69.50437 | 2.36074 | 17.8788 |
| 2 | 18.430 | MM | 0.3304 | 4.72392 | 2.38321e-1 | 1.2151 |
| 3 | 21.000 | BB | 0.5710 | 290.85626 | 7.61127 | 74.8177 |
| 4 | 32.264 | MM | 0.6692 | 23.66880 | 5.89492e-1 | 6.0884 |

b) racemic




| Peak # | RetTime [min] | Type | Width [min] | Area mAU *s | Height [mAU ] | Area % |
|---|---|---|---|---|---|---|
| 1 | 17.862 | BB | 0.4909 | 186.76668 | 5.70906 | 32.6174 |
| 2 | 19.279 | BB | 0.5238 | 115.60297 | 3.28738 | 20.1892 |
| 3 | 21.974 | BB | 0.5755 | 170.00082 | 4.52189 | 29.6894 |
| 4 | 34.220 | BB | 0.7422 | 100.22718 | 1.78969 | 17.5039 |

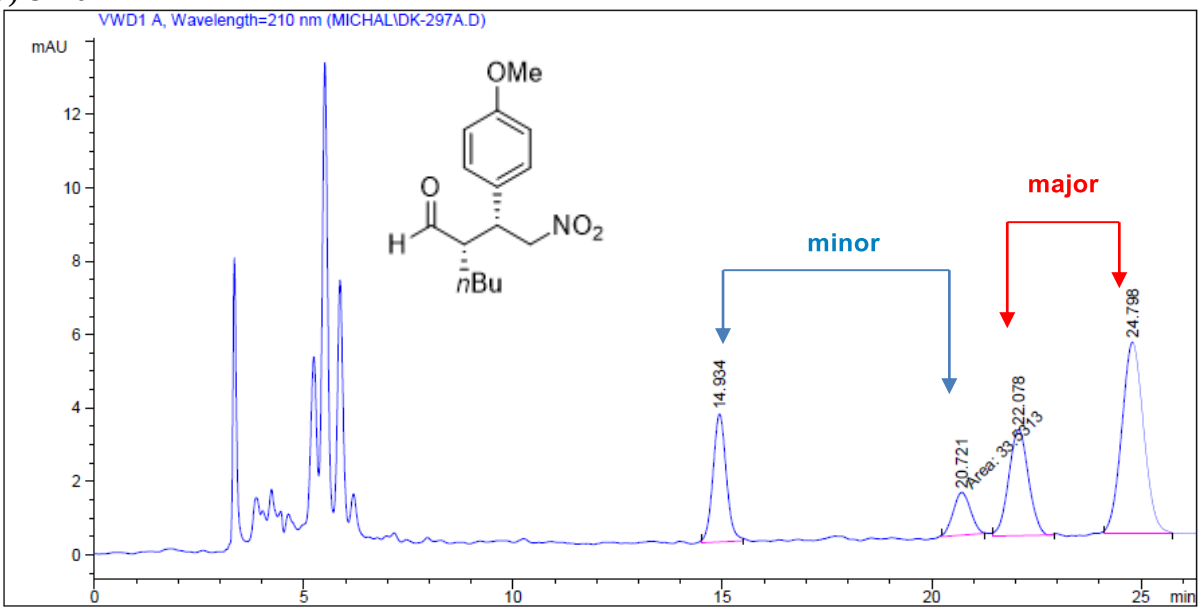
**Figure S43.** HPLC trace of **8a**




| Peak # | RetTime [min] | Type | Width [min] | Area mAU *s | Height [mAU ] | Area % |
|---|---|---|---|---|---|---|
| 1 | 18.219 | MM | 0.4205 | 20.89495 | 8.28197e-1 | 19.5162 |
| 2 | 23.869 | MM | 0.5247 | 17.42112 | 5.53404e-1 | 16.2716 |
| 3 | 28.688 | MM | 0.6567 | 36.29554 | 9.21120e-1 | 33.9006 |
| 4 | 30.835 | MM | 0.6661 | 32.45287 | 8.11955e-1 | 30.3115 |

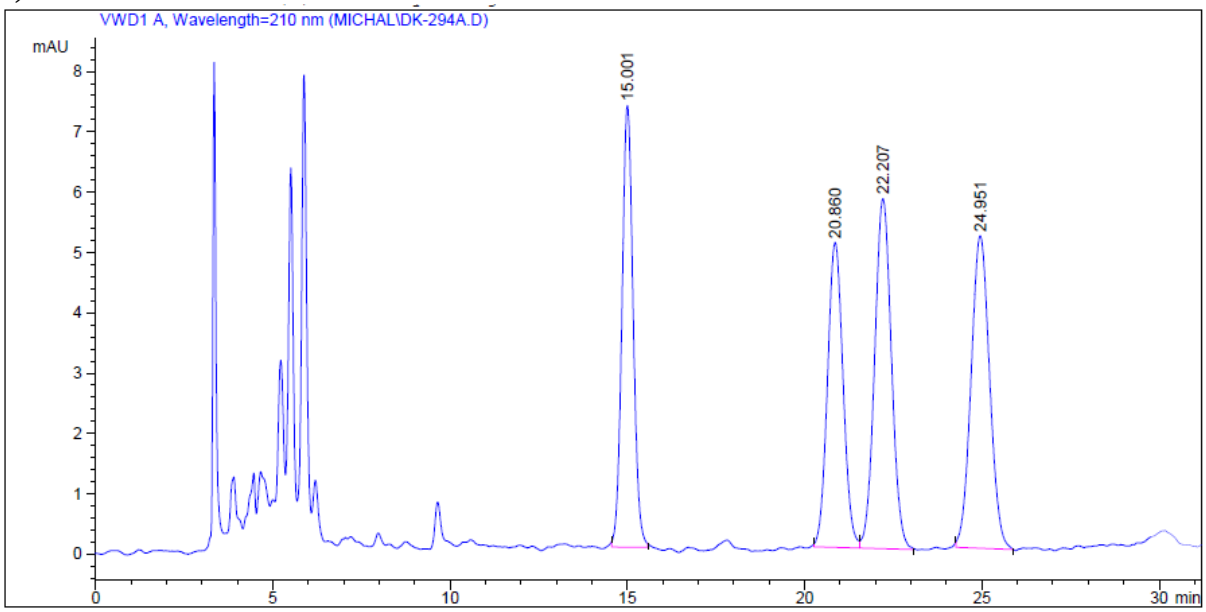
**Figure S44.** HPLC trace of **8b** (racemic)

a) chiral




| Peak # | RetTime [min] | Type | Width [min] | Area mAU *s | Height [mAU ] | Area % |
|---|---|---|---|---|---|---|
| 1 | 14.934 | BB | 0.3376 | 77.00037 | 3.48780 | 19.5584 |
| 2 | 20.721 | MM | 0.4785 | 33.53126 | 1.16787 | 8.5171 |
| 3 | 22.078 | BB | 0.5113 | 94.90208 | 2.88984 | 24.1055 |
| 4 | 24.798 | BB | 0.5562 | 188.26102 | 5.20222 | 47.8190 |

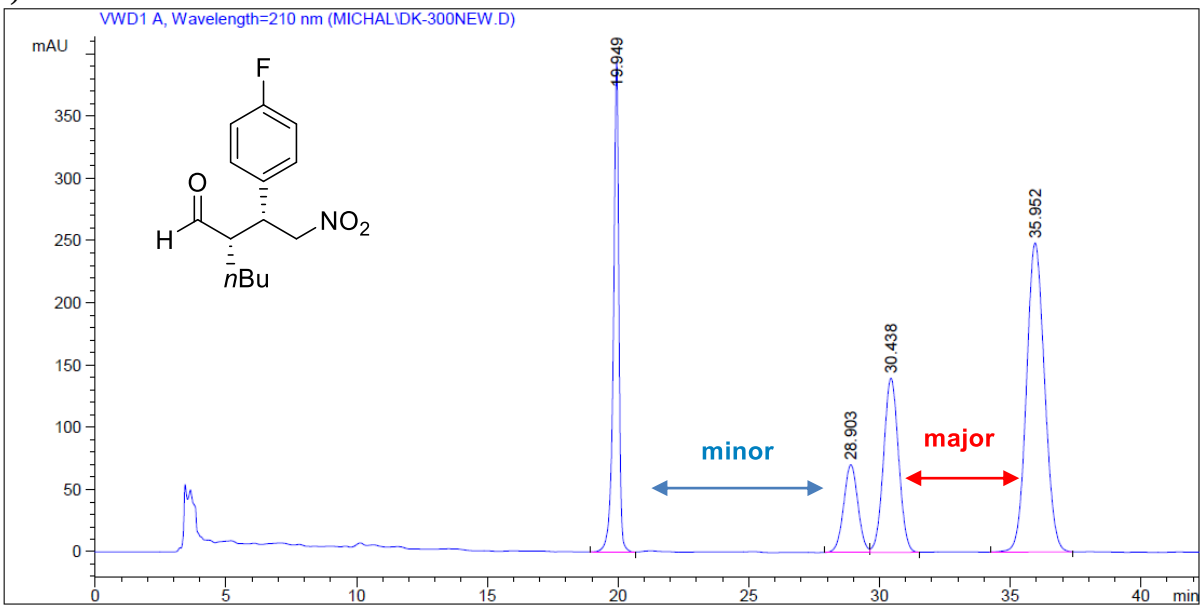
b) racemic




| Peak # | RetTime [min] | Type | Width [min] | Area mAU *s | Height [mAU ] | Area % |
|---|---|---|---|---|---|---|
| 1 | 15.001 | BB | 0.3380 | 160.01204 | 7.32058 | 23.0781 |
| 2 | 20.860 | BV | 0.4789 | 154.47105 | 5.05434 | 22.2789 |
| 3 | 22.207 | VB | 0.5132 | 190.72850 | 5.80097 | 27.5082 |
| 4 | 24.951 | BB | 0.5563 | 188.13889 | 5.17905 | 27.1347 |

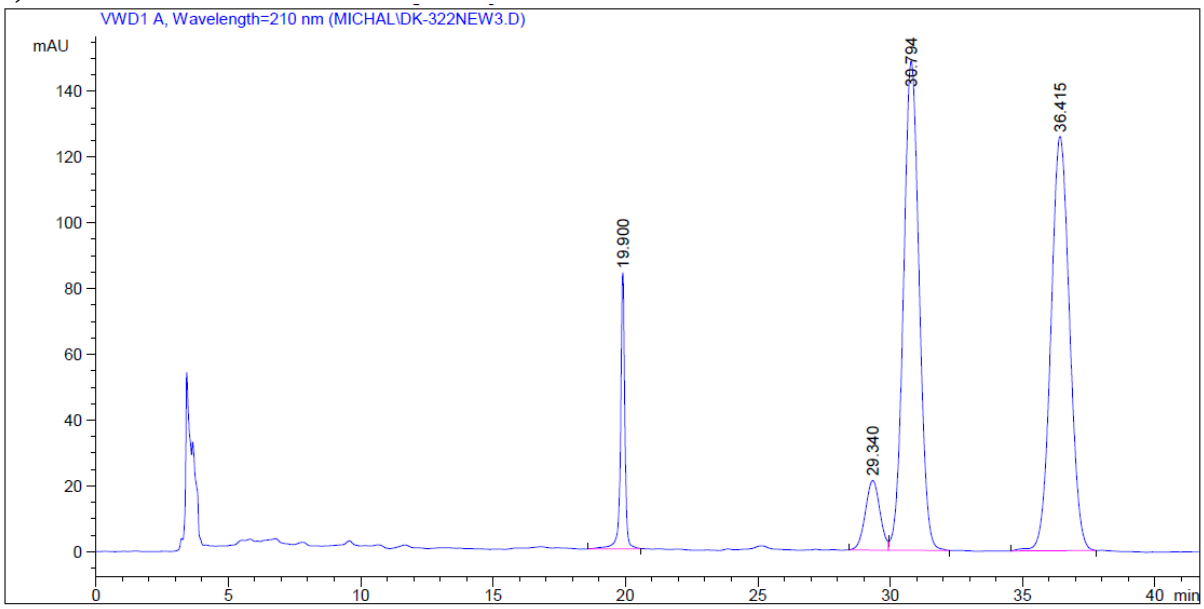
**Figure S45.** HPLC trace of **8c**

a) chiral




| Peak # | RetTime [min] | Type | Width [min] | Area mAU *s | Height [mAU ] | Area % |
|---|---|---|---|---|---|---|
| 1 | 19.949 | BB | 0.2138 | 5705.87549 | 394.69928 | 21.9846 |
| 2 | 28.903 | BV | 0.5981 | 2681.69531 | 70.50391 | 10.3325 |
| 3 | 30.438 | VB | 0.6243 | 5602.06152 | 139.92654 | 21.5846 |
| 4 | 35.952 | BB | 0.7472 | 1.19643e4 | 248.24681 | 46.0983 |

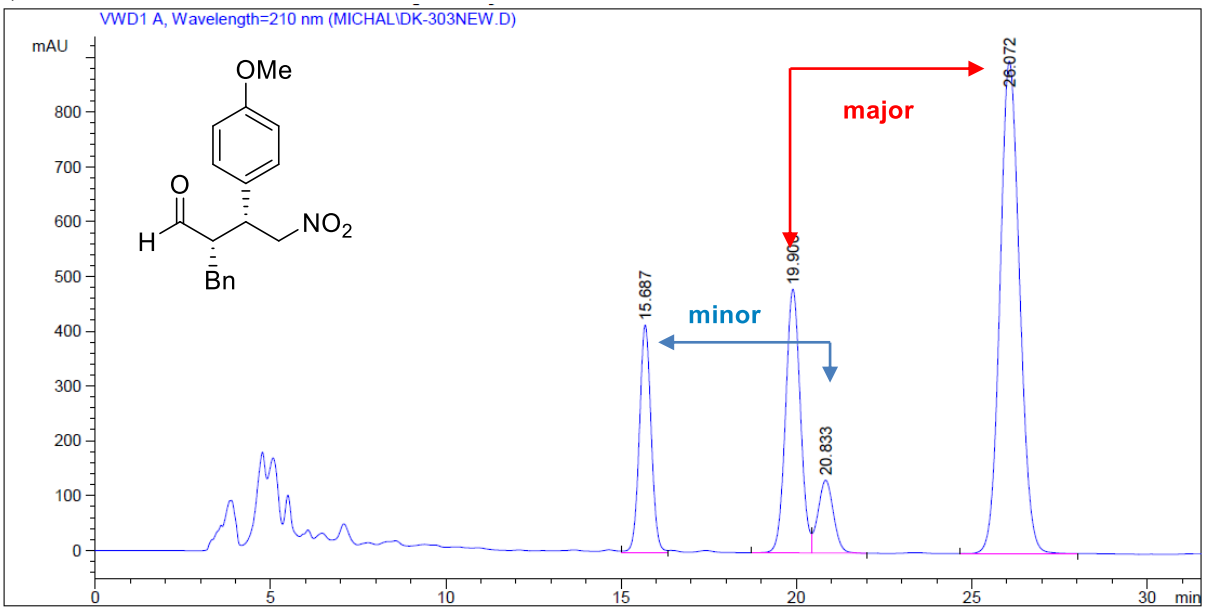
b) racemic




| Peak # | RetTime [min] | Type | Width [min] | Area mAU *s | Height [mAU ] | Area % |
|---|---|---|---|---|---|---|
| 1 | 19.900 | BB | 0.1624 | 939.63080 | 84.08176 | 6.7002 |
| 2 | 29.340 | BV | 0.5993 | 810.74005 | 21.18549 | 5.7811 |
| 3 | 30.794 | VB | 0.6385 | 6102.23535 | 148.84152 | 43.5129 |
| 4 | 36.415 | BB | 0.7605 | 6171.35889 | 126.03487 | 44.0058 |

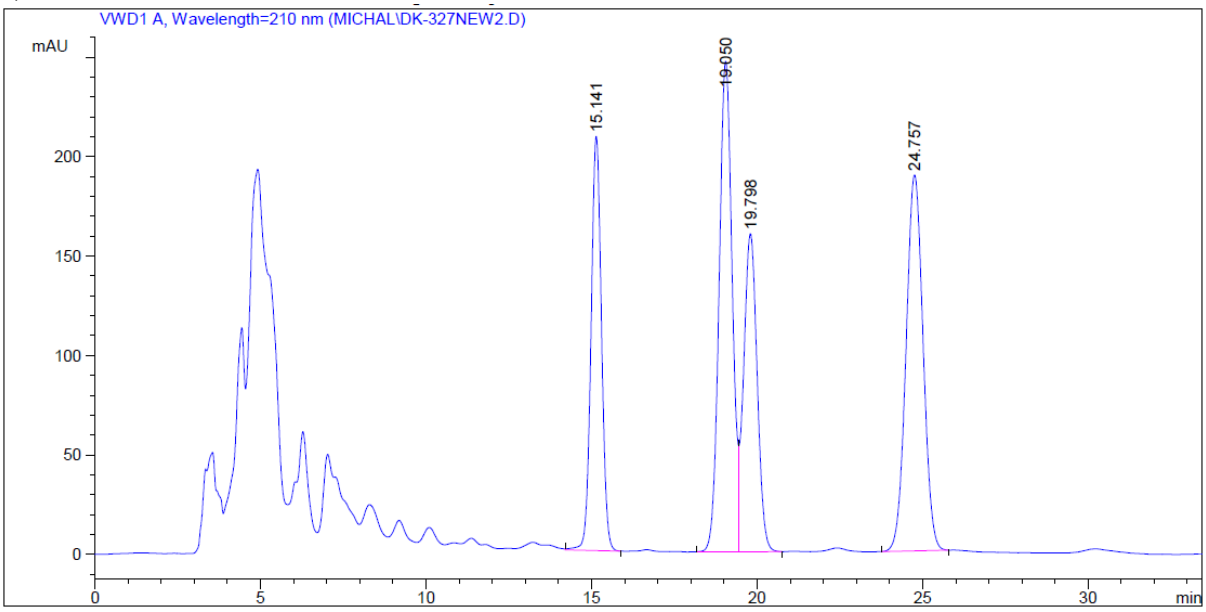
**Figure S46.** HPLC trace of **8d**

a) chiral




| Peak # | RetTime [min] | Type | Width [min] | Area mAU *s | Height [mAU ] | Area % |
|---|---|---|---|---|---|---|
| 1 | 15.687 | VV | 0.3600 | 9647.27539 | 414.96320 | 15.3298 |
| 2 | 19.900 | VV | 0.4557 | 1.41142e4 | 481.31055 | 22.4278 |
| 3 | 20.833 | VB | 0.4741 | 4068.56299 | 132.73634 | 6.4651 |
| 4 | 26.072 | BB | 0.6058 | 3.51016e4 | 898.48590 | 55.7774 |

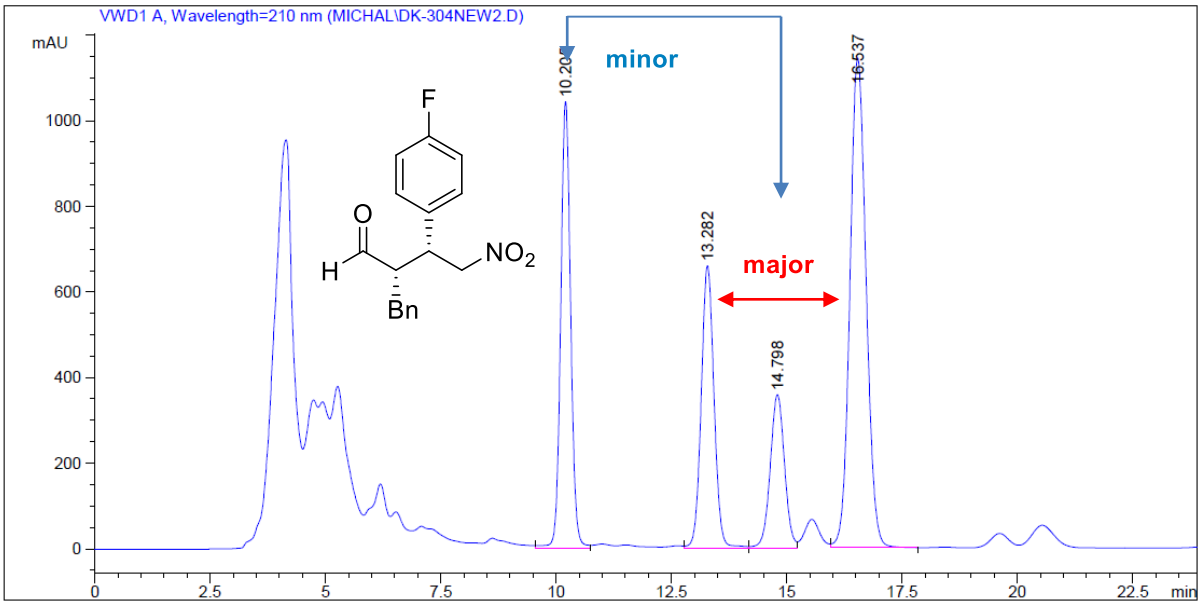
b) racemic




| Peak # | RetTime [min] | Type | Width [min] | Area mAU *s | Height [mAU ] | Area % |
|---|---|---|---|---|---|---|
| 1 | 15.141 | VB | 0.3383 | 4558.43652 | 208.27930 | 20.1474 |
| 2 | 19.050 | BV | 0.4237 | 6773.48535 | 246.68860 | 29.9375 |
| 3 | 19.798 | VB | 0.4376 | 4542.65479 | 159.97713 | 20.0776 |
| 4 | 24.757 | BB | 0.5564 | 6750.88086 | 189.05197 | 29.8375 |

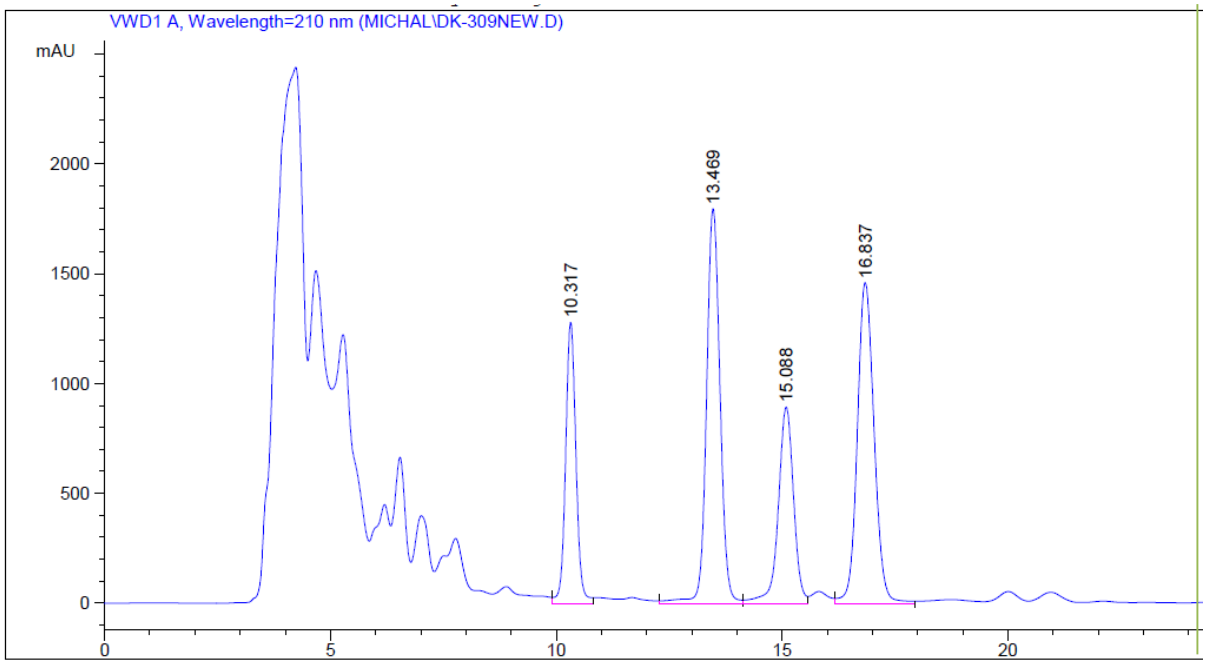
**Figure S47.** HPLC trace of **8e**

a) chiral




| Peak # | RetTime [min] | Type | Width [min] | Area mAU *s | Height [mAU ] | Area % |
|---|---|---|---|---|---|---|
| 1 | 10.205 | BV | 0.2317 | 1.56443e4 | 1043.22705 | 24.4991 |
| 2 | 13.282 | VV | 0.2988 | 1.26890e4 | 659.22009 | 19.8710 |
| 3 | 14.798 | VV | 0.3326 | 7696.46533 | 357.67654 | 12.0527 |
| 4 | 16.537 | VB | 0.3770 | 2.78270e4 | 1143.98840 | 43.5772 |

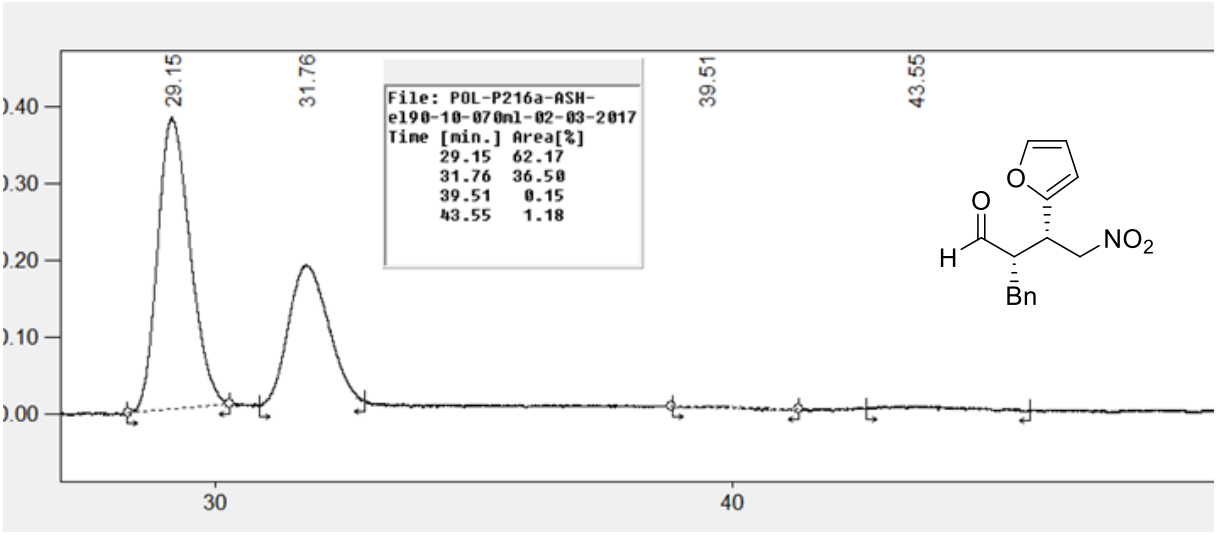
b) racemic




| Peak # | RetTime [min] | Type | Width [min] | Area mAU *s | Height [mAU ] | Area % |
|---|---|---|---|---|---|---|
| 1 | 10.317 | VV | 0.2451 | 2.03233e4 | 1278.85144 | 17.4373 |
| 2 | 13.469 | VV | 0.3228 | 3.73880e4 | 1796.75903 | 32.0787 |
| 3 | 15.088 | VV | 0.3612 | 2.10825e4 | 893.53259 | 18.0886 |
| 4 | 16.837 | VB | 0.4007 | 3.77572e4 | 1460.09802 | 32.3954 |

**Figure S48.** HPLC trace of **8f**

a) chiral




b) racemic

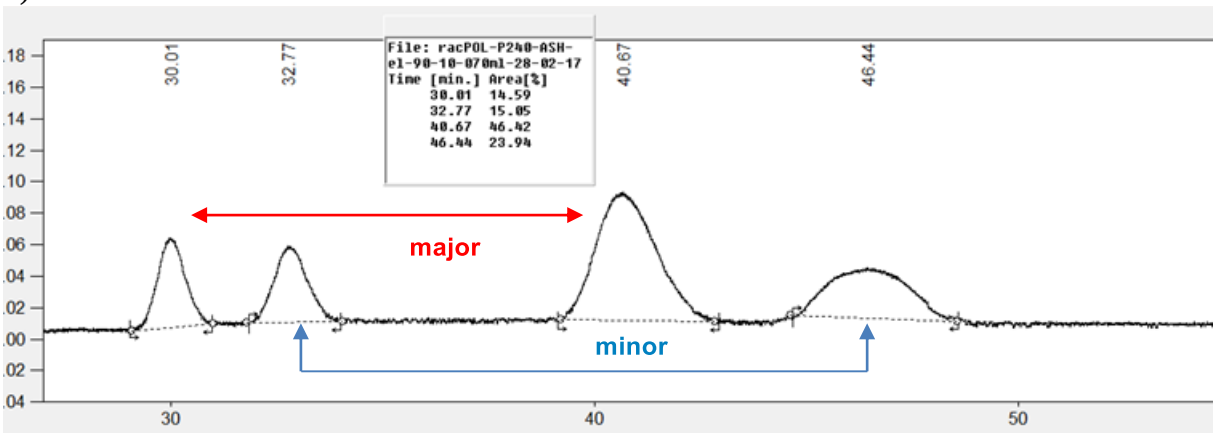
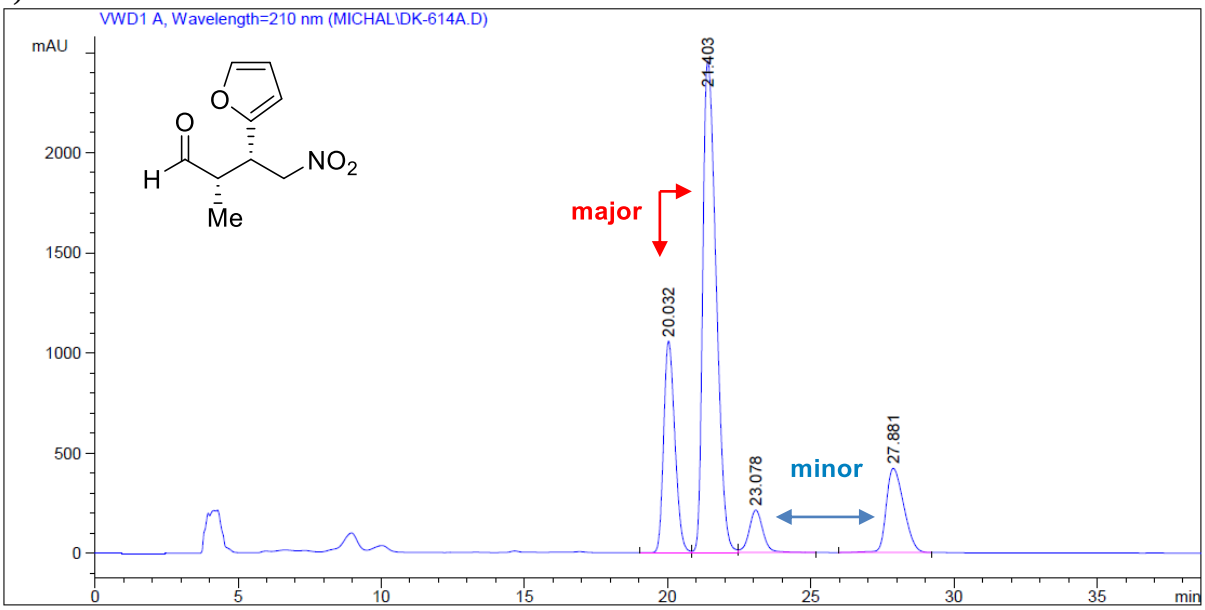


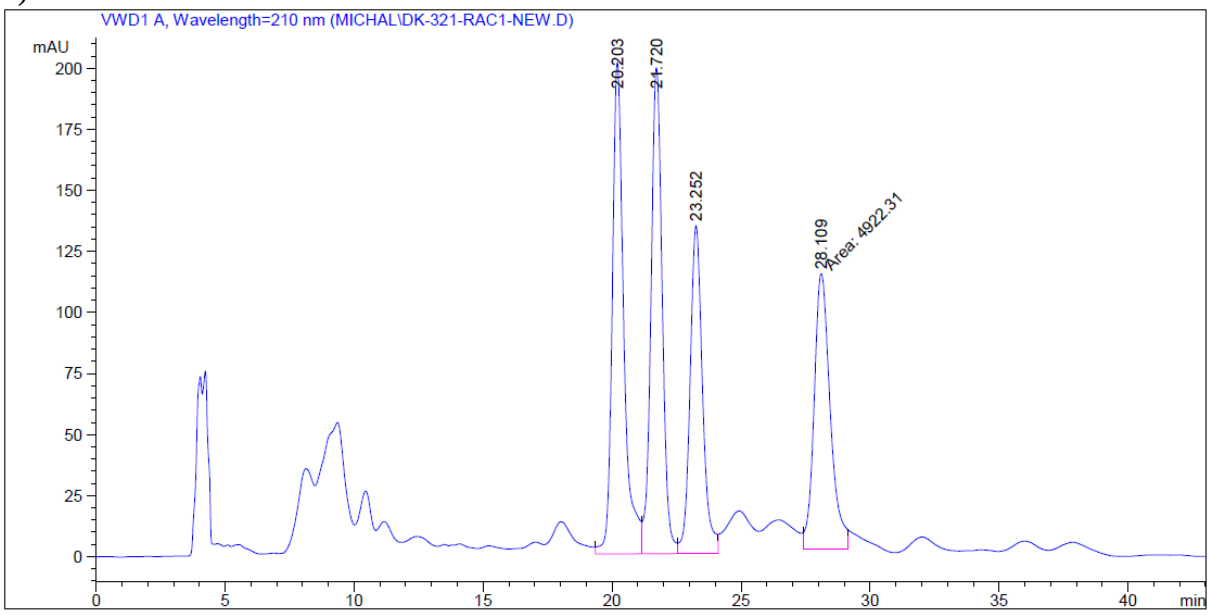

**Figure S49.** HPLC trace of **10a**

a) chiral




| Peak # | RetTime [min] | Type | Width [min] | Area mAU *s | Height [mAU ] | Area % |
|---|---|---|---|---|---|---|
| 1 | 20.032 | VV | 0.4230 | 2.86672e4 | 1056.00574 | 21.5231 |
| 2 | 21.403 | VV | 0.5112 | 7.96291e4 | 2453.29492 | 59.7849 |
| 3 | 23.078 | VB | 0.5133 | 7095.70605 | 211.73839 | 5.3274 |
| 4 | 27.881 | BB | 0.6683 | 1.78006e4 | 419.53726 | 13.3646 |

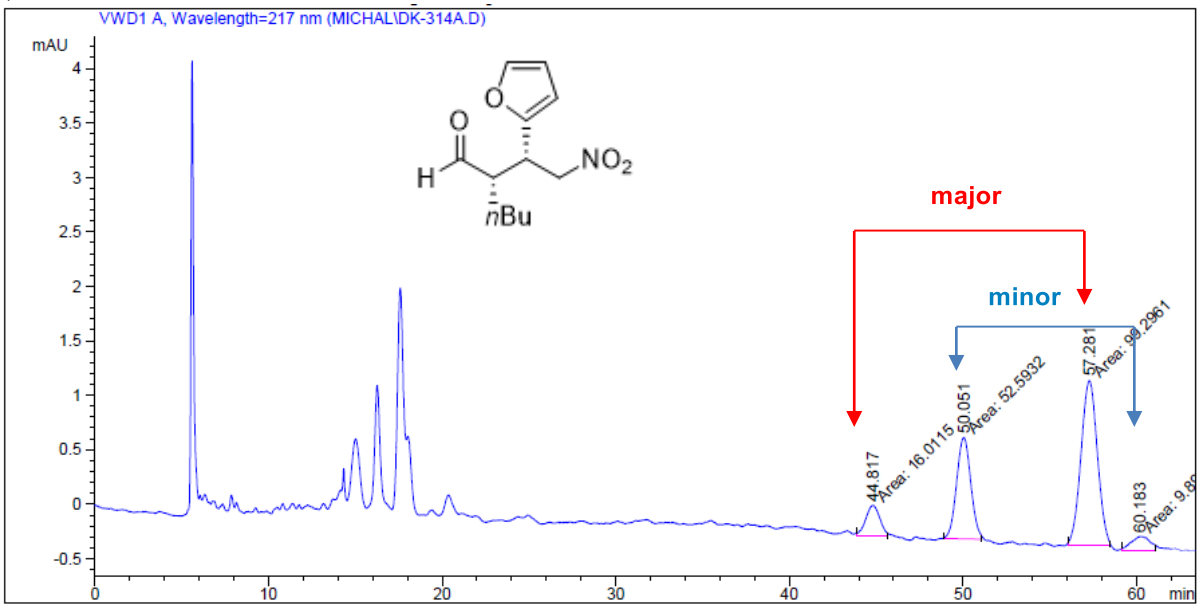
b) racemic




| Peak # | RetTime [min] | Type | Width [min] | Area mAU *s | Height [mAU ] | Area % |
|---|---|---|---|---|---|---|
| 1 | 20.203 | BV | 0.4680 | 6264.87842 | 201.23669 | 28.8620 |
| 2 | 21.720 | VV | 0.4655 | 6027.56592 | 198.98976 | 27.7688 |
| 3 | 23.252 | VB | 0.5099 | 4491.53027 | 134.17992 | 20.6923 |
| 4 | 28.109 | MM | 0.7259 | 4922.31250 | 113.01044 | 22.6769 |

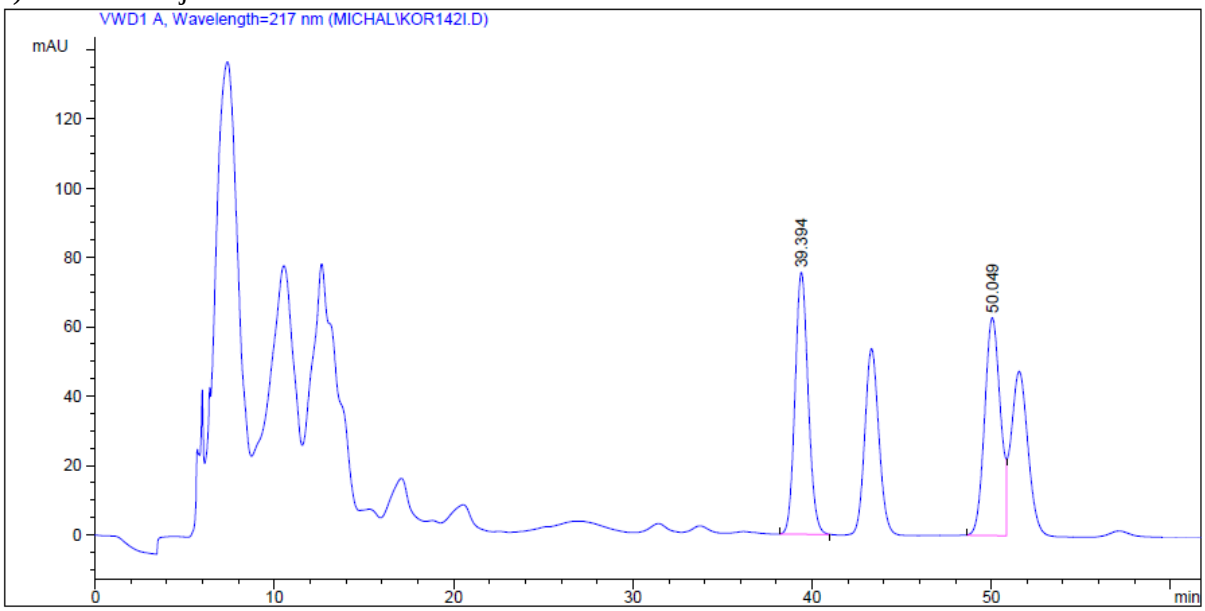
**Figure S50.** HPLC trace of **10b**

a) chiral



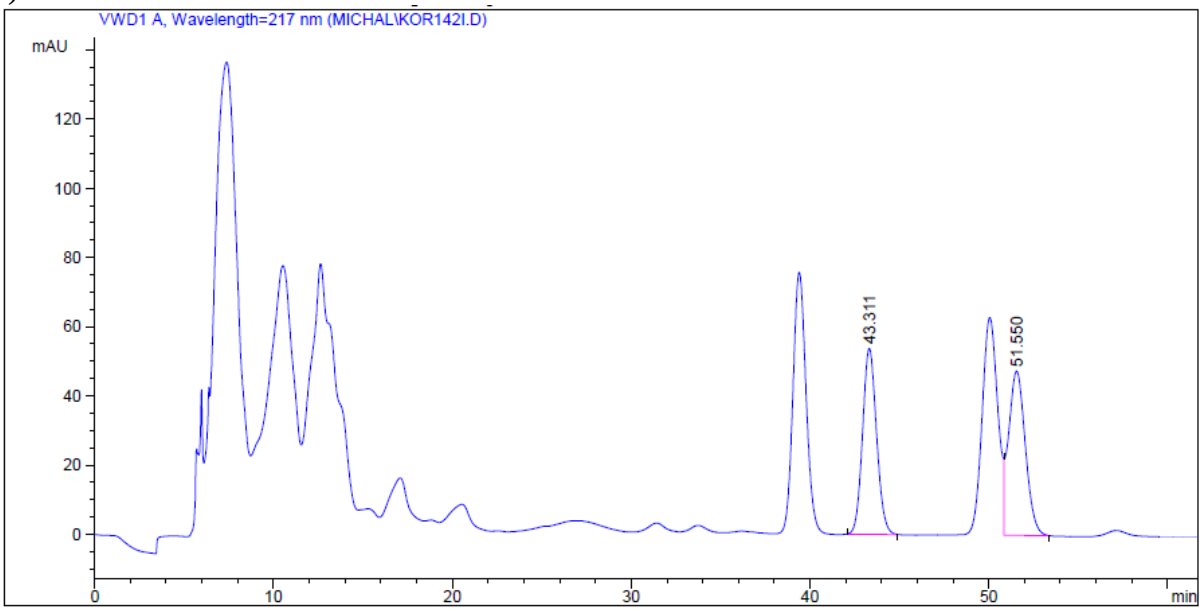

| Peak # | RetTime [min] | Type | Width [min] | Area mAU *s | Height [mAU ] | Area % |
|---|---|---|---|---|---|---|
| 1 | 44.817 | MM | 0.9445 | 16.01153 | 2.82544e-1 | 9.0053 |
| 2 | 50.051 | MM | 0.9422 | 52.59317 | 9.30323e-1 | 29.5799 |
| 3 | 57.281 | MM | 1.0923 | 99.29606 | 1.51508 | 55.8469 |
| 4 | 60.183 | MM | 1.2547 | 9.89963 | 1.31496e-1 | 5.5678 |

b) racemic major




| Peak # | RetTime [min] | Type | Width [min] | Area mAU *s | Height [mAU ] | Area % |
|---|---|---|---|---|---|---|
| 1 | 39.394 | BB | 0.7836 | 3840.16113 | 75.56295 | 50.0046 |
| 2 | 50.049 | BV | 0.9312 | 3839.45044 | 62.84376 | 49.9954 |

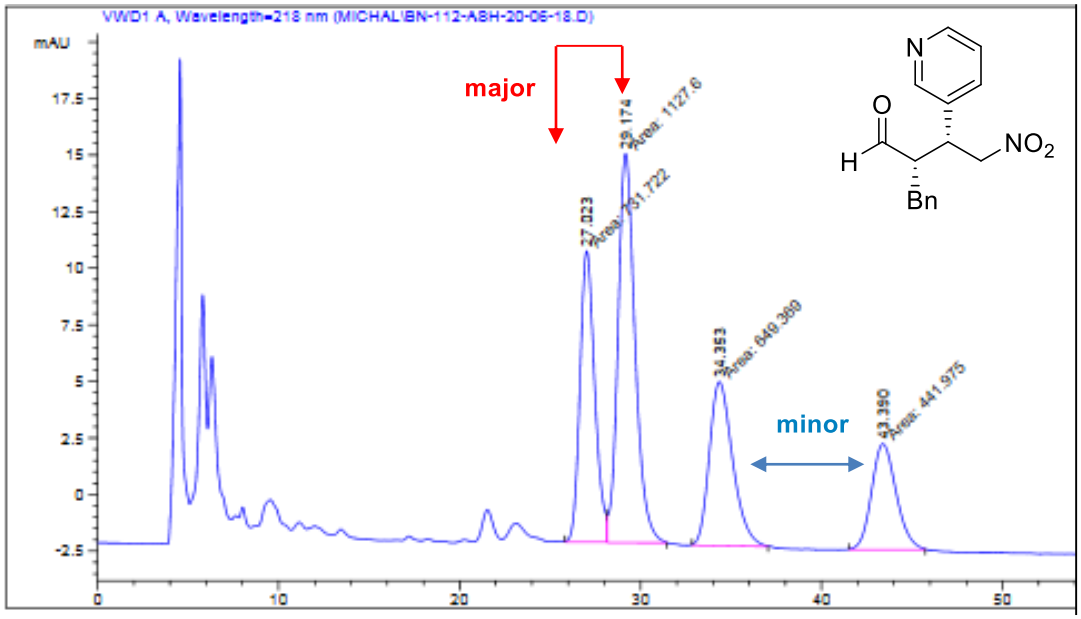
c) racemic minor




| Peak # | RetTime [min] | Type | Width [min] | Area mAU *s | Height [mAU ] | Area % |
|---|---|---|---|---|---|---|
| 1 | 43.311 | BB | 0.8358 | 2924.79077 | 53.74328 | 48.5121 |
| 2 | 51.550 | VB | 0.9870 | 3104.19531 | 47.47612 | 51.4879 |

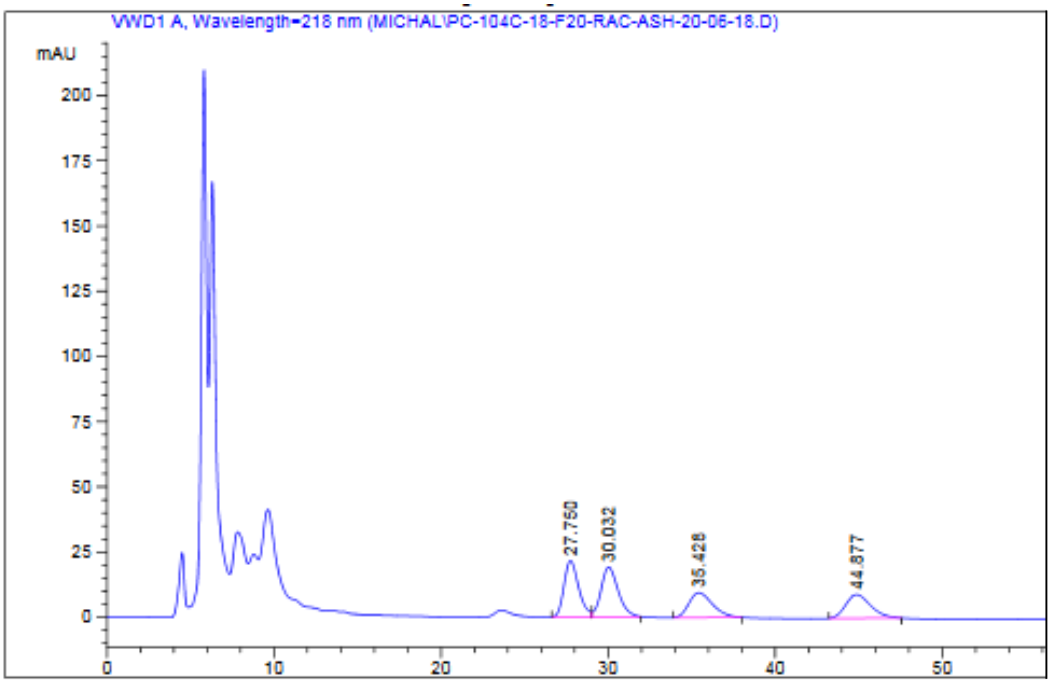
**Figure S51.** HPLC trace of **10c**

a) chiral




| Peak # | RetTime [min] | Type | Width [min] | Area mAU *s | Height [mAU ] | Area % |
|---|---|---|---|---|---|---|
| 1 | 27.023 | MM | 0.9480 | 731.72192 | 12.86442 | 24.7985 |
| 2 | 29.174 | MM | 1.0935 | 1127.60132 | 17.18574 | 38.2151 |
| 3 | 34.353 | MM | 1.4947 | 649.36920 | 7.24085 | 22.0075 |
| 4 | 43.390 | MM | 1.5756 | 441.97504 | 4.67526 | 14.9788 |

b) racemic



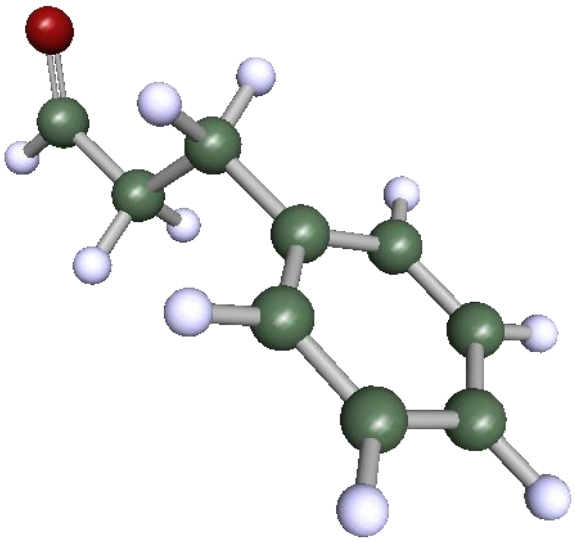

| Peak # | RetTime [min] | Type | Width [min] | Area mAU *s | Height [mAU ] | Area % |
|---|---|---|---|---|---|---|
| 1 | 27.750 | BV | 0.9236 | 1311.46362 | 21.60843 | 28.8472 |
| 2 | 30.032 | VB | 1.0615 | 1350.06152 | 19.04457 | 29.6962 |
| 3 | 35.428 | BB | 1.3847 | 942.12134 | 9.54311 | 20.7231 |
| 4 | 44.877 | BB | 1.4174 | 942.60071 | 9.05108 | 20.7336 |

**Figure S52.** HPLC trace of **12**

# 5. Computational details

All calculations were realized using Turbomole program package [7,8]. Geometric optimizations were performed using PBEh-3c functional [9]. Geometrical optimizations were performed with def2-SV(P) basis set [10]. Energies were refined at M06-2X/def2-TZVP level [11,12].

**3-phenylpropanal**



*Geometry optimization, frequency calculation: PBEh-3c/def2-SV(P)*

| | |
|---|---|
| SFC energy | -422.9562016 Hartree |
| Chemical potential | 0.134904 Hartree |
| Entropy | 0.000152 Hartree/K |
| Inner energy | 0.179399 Hartree |
| In(Qtrans) | 17.9533 |
| In(Qrot) | 13.4997 |
| In(Qvib) | 6.1921 |
| ZPE | 0.170448 Hartree |
| Enthalpy | 0.180343 Hartree |

*Single point energy: M06-2X/def2-TZVP*

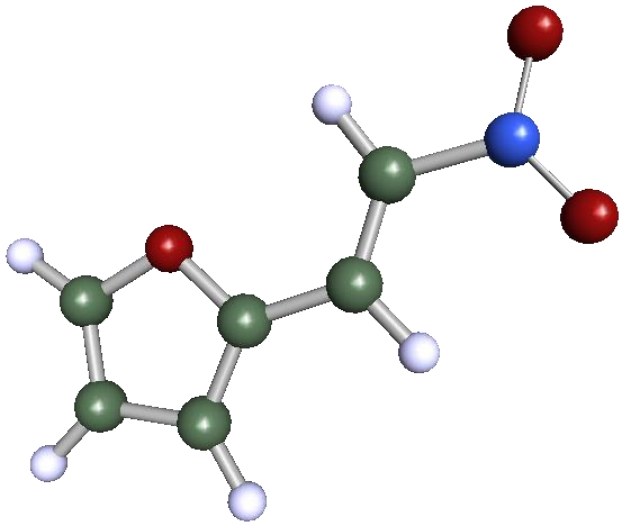
| | |
|---|---|
| SCF energy | -424.16538665 Hartree |

*Cartesian coordinates*

| | | | |
|---|---|---|---|
| C | 0.696695 | -2.582738 | -2.245463 |
| H | 1.641752 | -2.766935 | -2.818430 |
| O | -0.237057 | -3.317467 | -2.361399 |
| C | 0.739445 | -1.368415 | -1.361337 |
| C | -0.540423 | -1.102125 | -0.576966 |
| C | -0.423104 | 0.124684 | 0.286059 |
| C | -0.120195 | 2.422613 | 1.864623 |
| C | 0.069559 | 0.038291 | 1.587888 |
| C | -0.763408 | 1.382895 | -0.209735 |

| | | | |
|---|---|---|---|
| C | -0.614458 | 2.522815 | 0.570018 |
| C | 0.220718 | 1.174893 | 2.371955 |
| H | 1.004899 | -0.504923 | -1.997132 |
| H | 1.605573 | -1.481905 | -0.685066 |
| H | -0.777793 | -1.979030 | 0.042751 |
| H | 0.333289 | -0.938408 | 1.999165 |
| H | 0.603090 | 1.084380 | 3.389299 |
| H | -0.005839 | 3.315665 | 2.479603 |
| H | -0.891476 | 3.496574 | 0.164514 |
| H | -1.159758 | 1.471953 | -1.223441 |
| H | -1.381509 | -0.992817 | -1.277006 |

**Fur-nitroalkene**



*Geometry optimization, frequency calculation: PBEh-3c/def2-SV(P)*

| | |
|---|---|
| SFC energy | -510.4688093 Hartree |
| Chemical potential | 0.076329 Hartree |
| Entropy | 0.000145 Hartree/K |
| Inner energy | 0.000145 Hartree |
| In(Qtrans) | 18.0075 |
| In(Qrot) | 13.4168 |
| In(Qvib) | 4.8266 |
| ZPE | 0.110557 Hartree |
| Enthalpy | 0.119502 Hartree |

*Single point energy: M06-2X/def2-TZVP*

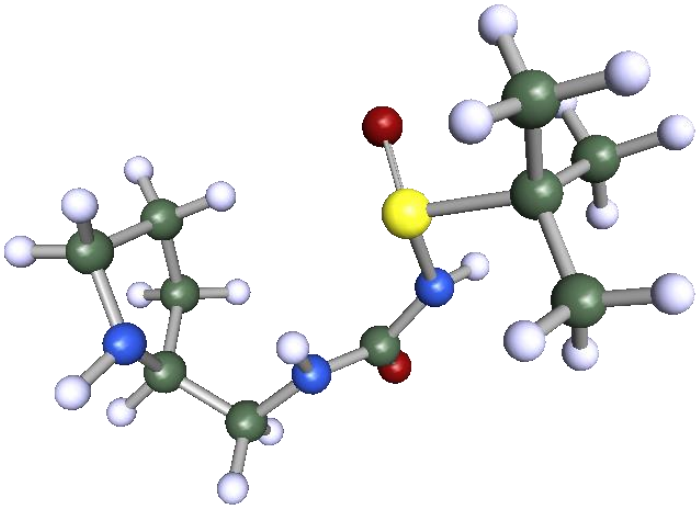
| | |
|---|---|
| SCF energy | -511.93038572 Hartree |

*Cartesian coordinates*

| | | | |
|---|---|---|---|
| C | 0.024362 | -0.000521 | 2.529793 |
| C | 1.379421 | 0.000113 | 2.402070 |
| C | 1.629610 | 0.000559 | 1.005012 |
| C | 0.403233 | 0.000177 | 0.396201 |
| O | -0.562521 | -0.000397 | 1.333051 |
| C | 0.050339 | 0.000040 | -0.991377 |
| C | -1.200050 | 0.000236 | -1.466395 |

| | | | |
|---|---|---|---|
| N | -1.450095 | -0.000149 | -2.889652 |
| O | -2.605807 | 0.001863 | -3.220584 |
| O | -0.516213 | -0.002513 | -3.646148 |
| H | 0.885046 | -0.000423 | -1.694537 |
| H | -2.106685 | 0.000843 | -0.865422 |
| H | 2.592721 | 0.001087 | 0.502814 |
| H | 2.107136 | 0.000253 | 3.207557 |
| H | -0.630497 | -0.001166 | 3.397518 |

**SR-cat (*S,R*)-C2**



*Geometry optimization, frequency calculation: PBEh-3c/def2-SV(P)*

| | |
|---|---|
| SFC energy | -1104.1083831 Hartree |
| Chemical potential | 0.282091 Hartree |
| Entropy | 0.000218 Hartree/K |
| Inner energy | 0.346062 Hartree |
| In(Qtrans) | 18.8708 |
| In(Qrot) | 15.1125 |
| In(Qvib) | 15.2198 |
| ZPE | 0.328548 Hartree |
| Enthalpy | 0.347007 Hartree |

*Single point energy: M06-2X/def2-TZVP*

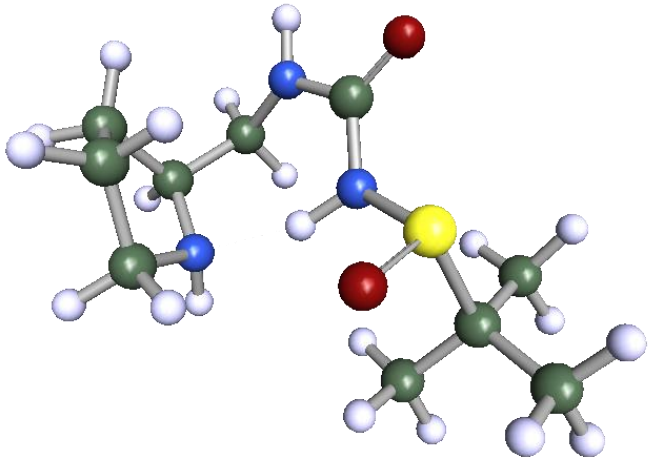
| | |
|---|---|
| SCF energy | -1106.5700552 Hartree |

*Cartesian coordinates*

| | | | |
|---|---|---|---|
| N | 0.397207 | -1.097265 | -3.018100 |
| C | -0.664397 | -2.073872 | -2.890237 |
| C | -1.801576 | -1.246193 | -2.309859 |
| C | -1.659285 | 0.085458 | -3.050828 |
| C | -0.158704 | 0.195739 | -3.403136 |
| C | 0.569894 | 1.316904 | -2.661873 |
| N | 0.551866 | 1.079299 | -1.243943 |
| C | -0.080197 | 1.885573 | -0.362784 |
| O | -0.531517 | 2.973878 | -0.615312 |
| N | -0.167448 | 1.384791 | 0.948673 |

| | | | |
|---|---|---|---|
| S | -0.042596 | -0.252676 | 1.339535 |
| O | -1.390247 | -0.835674 | 1.542468 |
| C | 0.713068 | -0.075989 | 3.024073 |
| C | -0.213641 | 0.714098 | 3.935688 |
| C | 0.856879 | -1.514708 | 3.518277 |
| C | 2.074556 | 0.583033 | 2.855930 |
| H | -1.666187 | -1.117033 | -1.226420 |
| H | -2.784995 | -1.713654 | -2.453999 |
| H | -0.363488 | -2.904857 | -2.234339 |
| H | -0.970463 | -2.519620 | -3.859950 |
| H | -2.255480 | 0.073039 | -3.974450 |
| H | -2.018011 | 0.940956 | -2.461446 |
| H | 1.170487 | -1.397962 | -3.596733 |
| H | 0.107462 | 2.289362 | -2.873226 |
| H | 1.612828 | 1.377408 | -3.018126 |
| H | -0.751650 | 1.964868 | 1.545220 |
| H | -0.045773 | 0.393015 | -4.486691 |
| H | 0.834441 | 0.143889 | -0.977403 |
| H | 1.339497 | -1.516204 | 4.506684 |
| H | 2.708317 | 0.034800 | 2.142572 |
| H | 2.601954 | 0.591137 | 3.821551 |
| H | 1.484818 | -2.118404 | 2.845448 |
| H | 1.992790 | 1.621398 | 2.509101 |
| H | -1.232936 | 0.303696 | 3.927847 |
| H | -0.258063 | 1.779910 | 3.669058 |
| H | 0.157214 | 0.664674 | 4.970423 |
| H | -0.116624 | -2.012817 | 3.616406 |

**SS-cat (*S*,*S*)-C2**



*Geometry optimization, frequency calculation: PBEh-3c/Def2-SV(P)*

| | |
|---|---|
| SFC energy | -1104.1113906 Hartree |
| Chemical potential | 0.283467 Hartree |
| Entropy | 0.000213 Hartree/K |
| Inner energy | 0.346045 Hartree |
| In(Qtrans) | 18.8708 |
| In(Qrot) | 14.9653 |
| In(Qvib) | 14.2446 |

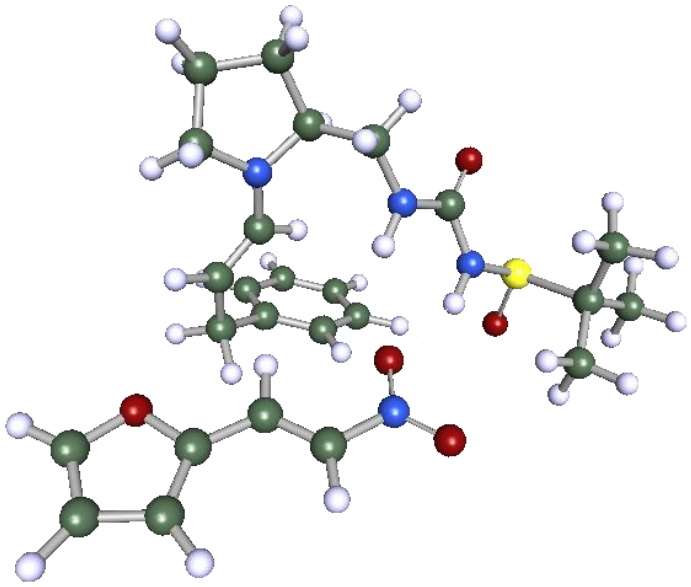
| | |
|---|---|
| ZPE | 0.328864 Hartree |
| Enthalpy | 0.346989 Hartree |

*Single point energy: M06-2X/Def2-TZVP*
SCF energy -1106.57049853 Hartree

*Cartesian coordinates*

| | | | |
|---|---|---|---|
| N | -0.929029 | -1.612729 | -0.631846 |
| C | -2.275210 | -1.113070 | -0.886722 |
| C | -2.151326 | -0.523752 | -2.282934 |
| C | -1.231136 | -1.518255 | -2.989492 |
| C | -0.286365 | -2.024812 | -1.884607 |
| C | 1.149108 | -1.488920 | -1.987478 |
| N | 1.290783 | -0.084827 | -2.290894 |
| C | 1.185304 | 0.988399 | -1.442085 |
| O | 1.565297 | 2.089288 | -1.750518 |
| N | 0.612989 | 0.687259 | -0.217974 |
| S | 0.079664 | 1.968359 | 0.752927 |
| O | -1.404385 | 1.886619 | 0.823968 |
| C | 0.700296 | 1.335397 | 2.384737 |
| C | 2.219752 | 1.291091 | 2.309201 |
| C | 0.233007 | 2.382783 | 3.393905 |
| C | 0.093556 | -0.022379 | 2.697320 |
| H | -1.694357 | 0.474730 | -2.227267 |
| H | -3.122898 | -0.407990 | -2.781043 |
| H | -2.561365 | -0.362495 | -0.135991 |
| H | -3.032086 | -1.920720 | -0.871074 |
| H | -1.819028 | -2.357107 | -3.390480 |
| H | -0.692083 | -1.071770 | -3.836054 |
| H | -0.888681 | -2.317826 | 0.092809 |
| H | 1.657079 | -2.036153 | -2.794147 |
| H | 1.693550 | -1.750213 | -1.062203 |
| H | 0.039410 | -0.187425 | -0.163925 |
| H | -0.202906 | -3.125292 | -1.933247 |
| H | 1.739897 | 0.155474 | -3.161524 |
| H | 0.588017 | 2.114468 | 4.400269 |
| H | -1.003224 | 0.006350 | 2.634989 |
| H | 0.362889 | -0.324797 | 3.721050 |
| H | -0.862337 | 2.453548 | 3.429094 |
| H | 0.463383 | -0.804580 | 2.019454 |
| H | 2.641206 | 2.257118 | 1.992628 |
| H | 2.573077 | 0.523638 | 1.607863 |
| H | 2.636384 | 1.058766 | 3.301246 |
| H | 0.631866 | 3.381725 | 3.159950 |

**SR-cat starting materials complex**



*Geometry optimization, frequency calculation: PBEh-3c/def2-SV(P)*

| | |
|---|---|
| SFC energy | -1961.3374171 Hartree |
| Chemical potential | 0.508668 Hartree |
| Entropy | 0.000381 Hartree/K |
| Inner energy | 0.621195 Hartree |
| In(Qtrans) | 19.9343 |
| In(Qrot) | 17.4328 |
| In(Qvib) | 43.5825 |
| ZPE | 0.585100 Hartree |
| Enthalpy | 0.622139 Hartree |

*Single point energy: M06-2X/def2-TZVP*

| | |
|---|---|
| SCF energy | -1966.24678927 Hartree |

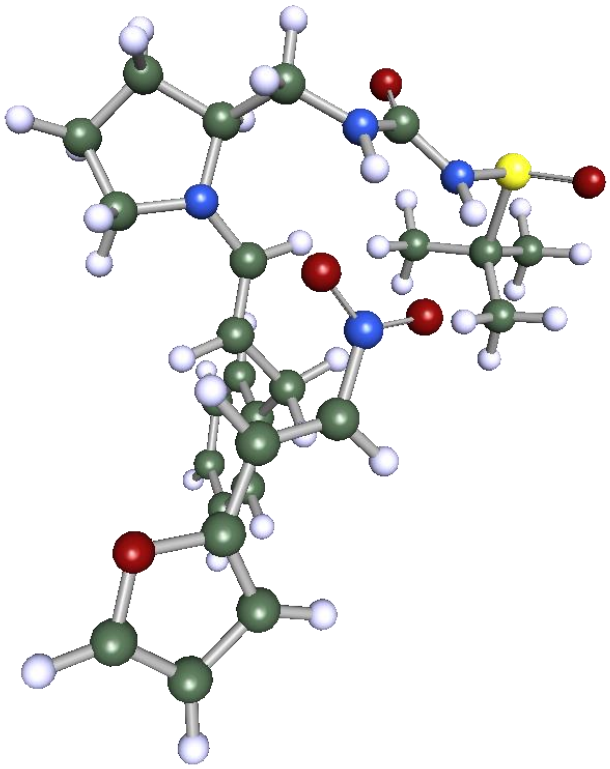
*Cartesian coordinates*

| | | | |
|---|---|---|---|
| N | -2.251282 | -0.138096 | -1.989899 |
| C | -3.508409 | 0.440351 | -2.386599 |
| C | -3.617368 | 0.052240 | -3.858006 |
| C | -2.167941 | 0.082962 | -4.334947 |
| C | -1.332732 | -0.301025 | -3.101868 |
| C | -0.088315 | 0.586793 | -2.994418 |
| N | 0.725108 | 0.354998 | -1.834499 |
| C | 1.873764 | -0.375020 | -1.873546 |
| O | 2.285254 | -0.936779 | -2.858377 |
| N | 2.562396 | -0.384174 | -0.670493 |
| S | 3.941911 | -1.342092 | -0.459882 |
| O | 3.844625 | -1.956362 | 0.890197 |
| C | 5.216832 | -0.000187 | -0.291850 |
| C | 4.926497 | 0.848112 | 0.935260 |
| C | 6.534391 | -0.757250 | -0.135256 |
| C | 5.204080 | 0.811201 | -1.579862 |
| C | -2.037359 | -0.722819 | -0.775470 |
| C | -2.761934 | -0.564310 | 0.348002 |

| | | | |
|---|---|---|---|
| C | -2.540020 | -1.345142 | 1.619783 |
| C | -4.954182 | 2.619513 | 3.171729 |
| C | -4.539144 | 3.651447 | 3.961058 |
| C | -3.140537 | 3.741262 | 3.764821 |
| C | -2.811383 | 2.755342 | 2.868914 |
| O | -3.928253 | 2.085784 | 2.520239 |
| C | -1.579454 | 2.326242 | 2.277386 |
| C | -0.392552 | 2.892628 | 2.540717 |
| N | 0.810249 | 2.419039 | 1.922089 |
| O | 1.820662 | 3.013888 | 2.173433 |
| O | 0.750331 | 1.457826 | 1.189000 |
| H | -0.223975 | 3.731325 | 3.212563 |
| H | -1.636917 | 1.488869 | 1.571174 |
| H | -2.457562 | 4.446808 | 4.229088 |
| H | -5.932589 | 2.180241 | 2.993999 |
| H | -5.159660 | 4.268270 | 4.603664 |
| H | 4.863593 | 0.233573 | 1.843472 |
| H | 5.737643 | 1.578277 | 1.080056 |
| H | 6.537015 | -1.387933 | 0.763988 |
| H | 7.365658 | -0.041763 | -0.046765 |
| H | 6.068680 | 1.492319 | -1.596378 |
| H | 6.743400 | -1.398552 | -1.005275 |
| H | 5.267983 | 0.171505 | -2.472908 |
| H | -3.508798 | -1.739887 | 1.967400 |
| H | -3.594867 | 0.144412 | 0.365720 |
| H | -4.327921 | 0.026353 | -1.778606 |
| H | -4.028443 | -0.965302 | -3.938895 |
| H | -4.274826 | 0.717078 | -4.434801 |
| H | -1.979301 | -0.585371 | -5.184977 |
| H | -0.997454 | -1.352294 | -3.158634 |
| H | -0.409136 | 1.641971 | -2.990931 |
| H | -1.901299 | 1.099111 | -4.668640 |
| H | -3.536911 | 1.539619 | -2.252393 |
| H | -2.205111 | -0.672513 | 2.430491 |
| H | -1.186528 | -1.410392 | -0.766616 |
| H | 2.215681 | 0.124507 | 0.139395 |
| H | 4.298624 | 1.425995 | -1.670081 |
| H | 0.530024 | 0.440637 | -3.890743 |
| H | 3.994219 | 1.423328 | 0.843929 |
| H | 0.417268 | 0.749746 | -0.958221 |
| C | -1.563926 | -2.481114 | 1.482753 |
| C | 0.257002 | -4.571664 | 1.083431 |
| C | -0.191288 | -2.266098 | 1.599531 |
| C | -2.009360 | -3.764008 | 1.167166 |
| C | -1.108736 | -4.803658 | 0.974311 |
| C | 0.717451 | -3.298158 | 1.395766 |
| H | 0.178986 | -1.267804 | 1.841698 |
| H | -3.080656 | -3.950212 | 1.066885 |
| H | -1.477012 | -5.801584 | 0.732369 |
| H | 0.967096 | -5.383659 | 0.923568 |

| | | | |
|---|---|---|---|
| H | 1.786818 | -3.098350 | 1.464888 |

**SS-cat starting materials complex**



*Geometry optimization, frequency calculation: PBEh-3c/Def2-SV(P)*

| | |
|---|---|
| SFC energy | -1961.3371845 Hartree |
| Chemical potential | 0.509657 Hartree |
| Entropy | 0.000374 Hartree/K |
| Inner energy | 0.620248 Hartree |
| In(Qtrans) | 19.9343 |
| In(Qrot) | 17.4656 |
| In(Qvib) | 42.4366 |
| ZPE | 0.585038 Hartree |
| Enthalpy | 0.621192 Hartree |

*Single point energy: M06-2X/Def2-TZVP*

| | |
|---|---|
| SCF energy | -1966.24915538 Hartree |

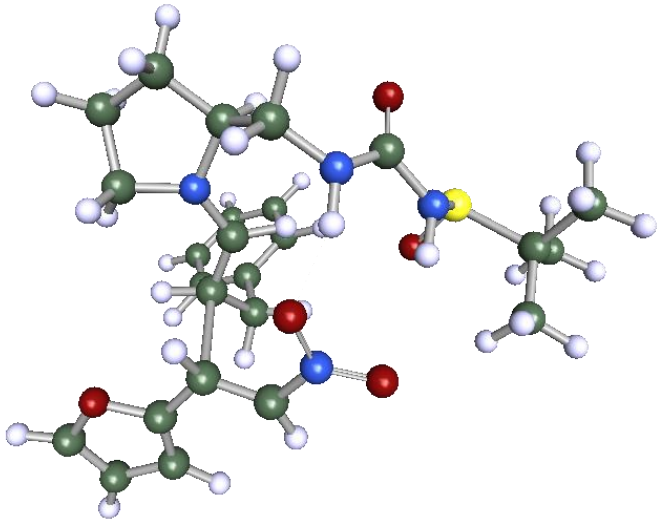
*Cartesian coordinates*

| | | | |
|---|---|---|---|
| N | -1.281975 | 0.925343 | -2.140187 |
| C | -2.695916 | 1.190042 | -2.237611 |
| C | -2.984592 | 1.032066 | -3.726369 |
| C | -1.693672 | 1.508721 | -4.381173 |
| C | -0.584088 | 1.093273 | -3.406192 |
| C | 0.530030 | 2.146321 | -3.379450 |
| N | 1.592849 | 1.887065 | -2.447181 |
| C | 2.500983 | 0.897999 | -2.651072 |
| O | 2.599907 | 0.274662 | -3.680523 |

| | | | |
|---|---|---|---|
| N | 3.290262 | 0.628464 | -1.543881 |
| S | 4.641211 | -0.397072 | -1.659741 |
| O | 5.748295 | 0.273920 | -0.938430 |
| C | 4.060051 | -1.764299 | -0.539656 |
| C | 2.824626 | -2.386121 | -1.175066 |
| C | 5.223300 | -2.753824 | -0.525773 |
| C | 3.788890 | -1.223279 | 0.853917 |
| C | -0.726400 | 0.303789 | -1.064571 |
| C | -1.279075 | 0.073537 | 0.142241 |
| C | -0.586877 | -0.727094 | 1.204101 |
| C | -4.167139 | 2.896394 | 4.518361 |
| C | -3.304793 | 2.301267 | 5.391032 |
| C | -2.072536 | 2.202362 | 4.701087 |
| C | -2.281507 | 2.747514 | 3.459659 |
| O | -3.560249 | 3.162763 | 3.367080 |
| C | -1.451455 | 2.934285 | 2.307869 |
| C | -0.162616 | 2.577208 | 2.244349 |
| N | 0.579452 | 2.721991 | 1.028532 |
| O | 1.662194 | 2.186873 | 0.998631 |
| O | 0.109723 | 3.346892 | 0.115395 |
| H | 0.405342 | 2.104399 | 3.042221 |
| H | -1.921438 | 3.379498 | 1.428162 |
| H | -1.143922 | 1.779213 | 5.073295 |
| H | -5.214734 | 3.175475 | 4.599050 |
| H | -3.526904 | 1.973559 | 6.401854 |
| H | 3.005015 | -2.688195 | -2.217273 |
| H | 2.527893 | -3.284340 | -0.612363 |
| H | 5.460330 | -3.120746 | -1.536311 |
| H | 4.959332 | -3.628695 | 0.087145 |
| H | 3.566428 | -2.055471 | 1.539459 |
| H | 6.132770 | -2.306818 | -0.102524 |
| H | 4.659341 | -0.683917 | 1.252499 |
| H | -0.553197 | -0.167394 | 2.153833 |
| H | -2.290142 | 0.420617 | 0.371951 |
| H | -3.265966 | 0.474138 | -1.624674 |
| H | -3.164429 | -0.028564 | -3.957937 |
| H | -3.869583 | 1.592805 | -4.056655 |
| H | -1.536078 | 1.094234 | -5.385542 |
| H | -0.137919 | 0.132594 | -3.719661 |
| H | 0.096515 | 3.120562 | -3.111801 |
| H | -1.708324 | 2.605748 | -4.488915 |
| H | -2.958456 | 2.202098 | -1.874021 |
| H | 0.465711 | -0.886930 | 0.915163 |
| H | 0.292460 | -0.055960 | -1.236745 |
| H | 3.213571 | 1.186955 | -0.698012 |
| H | 2.921062 | -0.548713 | 0.876213 |
| H | 0.939860 | 2.240952 | -4.396711 |
| H | 1.967134 | -1.699694 | -1.170340 |
| H | 1.534586 | 2.340524 | -1.547924 |
| C | -1.233711 | -2.066955 | 1.472940 |

| | | | |
|---|---|---|---|
| C | -2.425616 | -4.560065 | 1.952540 |
| C | -1.333836 | -3.018727 | 0.457300 |
| C | -1.746035 | -2.384683 | 2.727651 |
| C | -2.339440 | -3.619552 | 2.969067 |
| C | -1.917986 | -4.254428 | 0.693452 |
| H | -0.950759 | -2.781035 | -0.537197 |
| H | -1.681557 | -1.650682 | 3.534093 |
| H | -2.736811 | -3.846213 | 3.959284 |
| H | -2.888663 | -5.529807 | 2.137789 |
| H | -1.981126 | -4.986848 | -0.112436 |

**TS-major-si-SR-cat**



*Geometry optimization, frequency calculation: PBEh-3c/def2-SV(P)*

| | |
|---|---|
| SFC energy | -1961.3235111 Hartree |
| Chemical potential | 0.519363 Hartree |
| Entropy | 0.000345 Hartree |
| Inner energy | 0.621267 Hartree |
| In(Qtrans) | 19.9343 |
| In(Qrot) | 17.2619 |
| In(Qvib) | 35.1157 |
| ZPE | 0.587639 Hartree |
| Enthalpy | 0.622211 |

*Single point energy: M06-2X/def2-TZVP*

| | |
|---|---|
| SCF energy | -1966.23666674 Hartree |

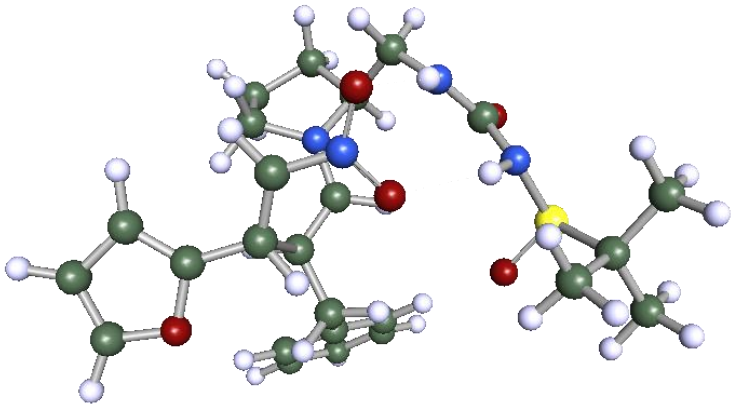
*Cartesian coordinates*

| | | | |
|---|---|---|---|
| N | -1.730925 | 0.372242 | -1.807458 |
| C | -3.172149 | 0.462988 | -1.969327 |
| C | -3.410901 | -0.154080 | -3.338959 |
| C | -2.182951 | 0.281988 | -4.127499 |
| C | -1.039242 | 0.295853 | -3.107363 |
| C | -0.060560 | 1.441623 | -3.396835 |
| N | 1.044079 | 1.551134 | -2.491153 |
| C | 2.006608 | 0.601407 | -2.437081 |

| | | | |
|---|---|---|---|
| O | 2.124226 | -0.299206 | -3.232270 |
| N | 2.861524 | 0.736484 | -1.336834 |
| S | 3.506767 | -0.699019 | -0.711554 |
| O | 2.644301 | -1.130998 | 0.424659 |
| C | 5.047242 | 0.003871 | 0.042019 |
| C | 4.717124 | 1.075905 | 1.068939 |
| C | 5.704571 | -1.202288 | 0.712189 |
| C | 5.908286 | 0.529444 | -1.098539 |
| C | -1.128985 | 0.153482 | -0.649545 |
| C | -1.710979 | 0.075594 | 0.621630 |
| C | -0.959488 | -0.735596 | 1.653651 |
| C | -4.804379 | 1.560181 | 3.155680 |
| C | -4.040142 | 1.450306 | 4.273501 |
| C | -2.695628 | 1.617529 | 3.837952 |
| C | -2.750888 | 1.819363 | 2.487509 |
| O | -4.035911 | 1.779971 | 2.084391 |
| C | -1.736892 | 2.019942 | 1.466500 |
| C | -0.437157 | 2.346012 | 1.869008 |
| N | 0.484224 | 2.666581 | 0.916476 |
| O | 1.664729 | 2.790318 | 1.205005 |
| O | 0.089510 | 2.795449 | -0.252524 |
| H | -0.039248 | 2.184180 | 2.866656 |
| H | -2.103205 | 2.475783 | 0.546547 |
| H | -1.800413 | 1.603193 | 4.451752 |
| H | -5.877399 | 1.512459 | 2.989504 |
| H | -4.391155 | 1.277183 | 5.286174 |
| H | 3.967575 | 0.729871 | 1.793491 |
| H | 5.627858 | 1.337976 | 1.628995 |
| H | 5.081344 | -1.610894 | 1.518775 |
| H | 6.666700 | -0.897884 | 1.149901 |
| H | 6.894186 | 0.825409 | -0.709415 |
| H | 5.910912 | -2.010503 | -0.006088 |
| H | 6.075115 | -0.234437 | -1.872955 |
| H | -1.260148 | -0.416657 | 2.664311 |
| H | -2.798389 | -0.038984 | 0.645729 |
| H | -3.689418 | -0.072407 | -1.162462 |
| H | -3.449216 | -1.250160 | -3.251584 |
| H | -4.356038 | 0.172767 | -3.791561 |
| H | -1.958762 | -0.372963 | -4.978885 |
| H | -0.480470 | -0.651894 | -3.142808 |
| H | -0.602779 | 2.397924 | -3.373463 |
| H | -2.335867 | 1.294660 | -4.534980 |
| H | -3.503456 | 1.514629 | -1.928659 |
| H | 0.120261 | -0.543684 | 1.567027 |
| H | -0.054440 | -0.031879 | -0.717595 |
| H | 2.651516 | 1.460233 | -0.647852 |
| H | 5.459917 | 1.407735 | -1.580825 |
| H | 0.299324 | 1.301780 | -4.428117 |
| H | 4.347140 | 2.003429 | 0.611956 |
| H | 0.901839 | 2.168161 | -1.688118 |

| | | | |
|---|---|---|---|
| C | -1.232044 | -2.211893 | 1.500424 |
| C | -1.808324 | -4.928276 | 1.133981 |
| C | -0.317731 | -3.050739 | 0.864110 |
| C | -2.433795 | -2.754737 | 1.956992 |
| C | -2.722437 | -4.100893 | 1.776264 |
| C | -0.605993 | -4.398668 | 0.682474 |
| H | 0.637508 | -2.646464 | 0.522621 |
| H | -3.154181 | -2.112543 | 2.469977 |
| H | -3.664666 | -4.508707 | 2.144911 |
| H | -2.030663 | -5.986578 | 0.992934 |
| H | 0.122733 | -5.042203 | 0.187999 |

**TS-major-re-SR-cat**



*Geometry optimization, frequency calculation: PBEh-3c/def2-SV(P)*

| | |
|---|---|
| SFC energy | -1961.3240405 Hartree |
| Chemical potential | 0.520006 Hartree |
| Entropy | 0.000343 Hartree/K |
| Inner energy | 0.621207 Hartree |
| In(Qtrans) | 19.9343 |
| In(Qrot) | 17.2407 |
| In(Qvib) | 34.5162 |
| ZPE | 0.587696 Hartree |
| Enthalpy | 0.622151 Hartree |

*Single point energy: M06-2X/def2-TZVP*

| | |
|---|---|
| SCF energy | -1966.24273958 Hartree |

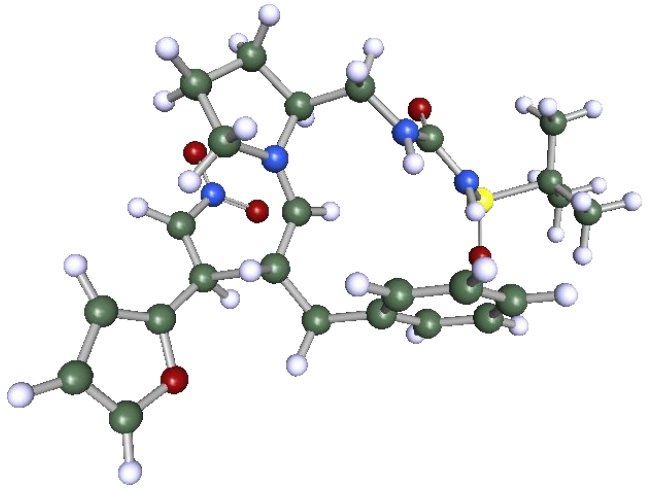
*Cartesian coordinates*

| | | | |
|---|---|---|---|
| N | -1.168501 | 0.274731 | -1.815880 |
| C | -2.557560 | 0.542212 | -2.162412 |
| C | -2.756166 | -0.288261 | -3.421153 |
| C | -1.430316 | -0.097391 | -4.154169 |
| C | -0.375831 | 0.100752 | -3.049147 |
| C | 0.551895 | 1.275762 | -3.374320 |
| N | 1.529517 | 1.551753 | -2.364847 |
| C | 2.444116 | 0.623495 | -1.994583 |
| O | 2.697176 | -0.367617 | -2.637649 |

| | | | |
|---|---|---|---|
| N | 3.046879 | 0.895026 | -0.766560 |
| S | 3.798506 | -0.425253 | -0.015040 |
| O | 2.784053 | -1.149225 | 0.800638 |
| C | 4.826890 | 0.544145 | 1.187525 |
| C | 3.950967 | 1.383478 | 2.105854 |
| C | 5.559539 | -0.534045 | 1.986025 |
| C | 5.810001 | 1.384960 | 0.384074 |
| C | -0.762446 | -0.187897 | -0.642847 |
| C | -1.539295 | -0.323602 | 0.508931 |
| C | -0.932716 | -1.087179 | 1.665313 |
| C | -4.935464 | 0.874468 | 2.848518 |
| C | -5.517418 | 1.559823 | 1.830304 |
| C | -4.446567 | 2.006628 | 1.005415 |
| C | -3.296358 | 1.559589 | 1.593124 |
| O | -3.606072 | 0.871934 | 2.706759 |
| C | -1.890785 | 1.647073 | 1.225614 |
| C | -1.521660 | 2.623461 | 0.295415 |
| N | -0.201594 | 2.800272 | 0.009052 |
| O | 0.144088 | 3.636489 | -0.824683 |
| O | 0.622290 | 2.075966 | 0.575503 |
| H | -2.213376 | 3.225554 | -0.286329 |
| H | -4.521963 | 2.595223 | 0.096007 |
| H | -5.337586 | 0.361905 | 3.718329 |
| H | -6.579853 | 1.732254 | 1.687617 |
| H | 3.162173 | 0.779279 | 2.574453 |
| H | 4.568267 | 1.810381 | 2.911000 |
| H | 4.862773 | -1.169842 | 2.548556 |
| H | 6.239978 | -0.058069 | 2.707695 |
| H | 6.535208 | 1.856030 | 1.064821 |
| H | 6.168508 | -1.182555 | 1.337703 |
| H | 6.380375 | 0.774035 | -0.331782 |
| H | -1.423715 | -0.785305 | 2.602660 |
| H | -2.606160 | -0.500655 | 0.349346 |
| H | -3.237650 | 0.286635 | -1.341564 |
| H | -2.909975 | -1.343562 | -3.149757 |
| H | -3.625616 | 0.030865 | -4.010828 |
| H | -1.177019 | -0.940398 | -4.808997 |
| H | 0.236711 | -0.802939 | -2.932215 |
| H | -0.042658 | 2.190741 | -3.508135 |
| H | -1.478651 | 0.797248 | -4.794864 |
| H | -2.689303 | 1.615466 | -2.371436 |
| H | 0.129398 | -0.819031 | 1.762376 |
| H | 0.294995 | -0.462682 | -0.589743 |
| H | 2.514432 | 1.511949 | -0.147721 |
| H | 5.308028 | 2.183317 | -0.177487 |
| H | 1.025866 | 1.056088 | -4.345207 |
| H | 3.475260 | 2.228835 | 1.589619 |
| H | 1.383281 | 2.388348 | -1.807948 |
| C | -1.077910 | -2.577755 | 1.484093 |
| C | -1.400069 | -5.325246 | 1.047942 |

| | | | |
|---|---|---|---|
| C | -0.023459 | -3.345155 | 0.989716 |
| C | -2.291549 | -3.207186 | 1.762562 |
| C | -2.454607 | -4.569009 | 1.546429 |
| C | -0.185650 | -4.708834 | 0.773697 |
| H | 0.938900 | -2.871752 | 0.783898 |
| H | -3.122469 | -2.620762 | 2.162290 |
| H | -3.409352 | -5.044891 | 1.774554 |
| H | -1.523752 | -6.395744 | 0.880252 |
| H | 0.650844 | -5.295458 | 0.391982 |
| H | -1.181669 | 1.431993 | 2.027114 |

**TS-minor-SR-cat**



*Geometry optimization, frequency calculation: PBEh-3c/Def2-SV(P)*

| | |
|---|---|
| SFC energy | -1961.3152305 Hartree |
| Chemical potential | 0.517947 Hartree |
| Entropy | 0.000348 Hartree/K |
| Inner energy | 0.620700 Hartree |
| In(Qtrans) | 19.9343 |
| In(Qrot) | 17.2754 |
| In(Qvib) | 35.8387 |
| ZPE | 0.586918 Hartree |
| Enthalpy | 0.621644 Hartree |

*Single point energy: M06-2X/Def2-TZVP*

| | |
|---|---|
| SCF energy | -1966.23002198 Hartree |

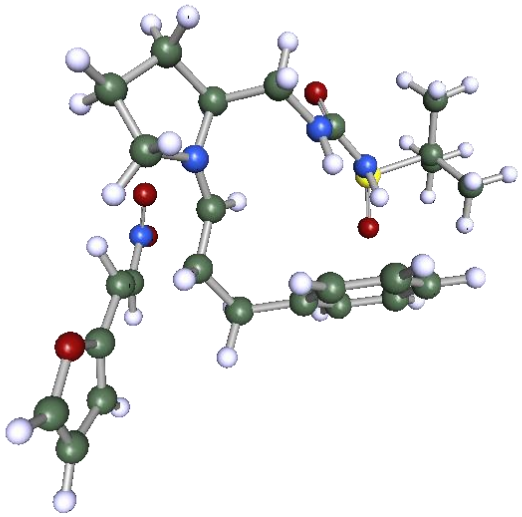
Cartesian coordinates

| | | | |
|---|---|---|---|
| N | -1.787421 | 1.016079 | -1.084338 |
| C | -2.960392 | 1.857950 | -0.914104 |
| C | -3.267344 | 2.298688 | -2.338472 |
| C | -1.891694 | 2.393516 | -3.011039 |
| C | -0.947081 | 1.518515 | -2.169580 |
| C | 0.231061 | 2.337732 | -1.615697 |
| N | 1.119482 | 1.617073 | -0.745779 |
| C | 2.112831 | 0.829200 | -1.256596 |

| | | | |
|---|---|---|---|
| O | 2.353378 | 0.750722 | -2.434625 |
| N | 2.843994 | 0.142018 | -0.306444 |
| S | 3.813055 | -1.185683 | -0.779840 |
| O | 3.597040 | -2.236461 | 0.245568 |
| C | 5.493132 | -0.477592 | -0.432746 |
| C | 5.625685 | -0.135523 | 1.041058 |
| C | 6.452474 | -1.599664 | -0.826724 |
| C | 5.675695 | 0.737169 | -1.331689 |
| C | -1.422421 | 0.010976 | -0.325402 |
| C | -2.185838 | -0.534083 | 0.721788 |
| C | -1.416623 | -1.445787 | 1.655639 |
| C | -5.711073 | -2.214039 | 2.519000 |
| C | -6.531438 | -1.320418 | 1.910599 |
| C | -5.860201 | -0.932448 | 0.714476 |
| C | -4.685326 | -1.626480 | 0.690556 |
| O | -4.602656 | -2.396025 | 1.790280 |
| C | -3.551764 | -1.648186 | -0.239237 |
| C | -3.815984 | -1.191476 | -1.546266 |
| N | -2.854015 | -1.308120 | -2.514221 |
| O | -3.062354 | -0.879575 | -3.641215 |
| O | -1.777206 | -1.819866 | -2.196609 |
| H | -4.728886 | -0.685234 | -1.846426 |
| H | -2.926987 | -2.542895 | -0.161810 |
| H | -6.216170 | -0.235805 | -0.038560 |
| H | -5.792774 | -2.785590 | 3.439515 |
| H | -7.501361 | -0.983868 | 2.264167 |
| H | 5.442359 | -1.011682 | 1.677578 |
| H | 6.646890 | 0.219309 | 1.248727 |
| H | 6.299887 | -2.501201 | -0.217981 |
| H | 7.491167 | -1.267504 | -0.681676 |
| H | 6.721390 | 1.076863 | -1.282066 |
| H | 6.342491 | -1.877855 | -1.885956 |
| H | 5.448620 | 0.511240 | -2.383856 |
| H | -1.094350 | -2.346005 | 1.109042 |
| H | -2.876539 | 0.156191 | 1.214502 |
| H | -3.780963 | 1.312408 | -0.438284 |
| H | -3.875716 | 1.534455 | -2.838626 |
| H | -3.823820 | 3.244362 | -2.367907 |
| H | -1.928338 | 2.047936 | -4.050100 |
| H | -0.566430 | 0.657884 | -2.739070 |
| H | -0.157690 | 3.207914 | -1.063480 |
| H | -1.530939 | 3.433528 | -3.029406 |
| H | -2.708570 | 2.719347 | -0.265920 |
| H | -2.084096 | -1.805197 | 2.452997 |
| H | -0.480360 | -0.464305 | -0.596950 |
| H | 2.599816 | 0.170571 | 0.681446 |
| H | 5.039782 | 1.577940 | -1.024591 |
| H | 0.799603 | 2.732987 | -2.468953 |
| H | 4.936991 | 0.667644 | 1.341397 |
| H | 0.915058 | 1.591961 | 0.243665 |

| | | | |
|---|---|---|---|
| C | -0.198875 | -0.791734 | 2.270008 |
| C | 2.075692 | 0.419821 | 3.392902 |
| C | -0.250243 | 0.515374 | 2.767096 |
| C | 1.014009 | -1.473279 | 2.341188 |
| C | 2.139525 | -0.879636 | 2.906496 |
| C | 0.872767 | 1.117853 | 3.318851 |
| H | -1.186541 | 1.074398 | 2.725499 |
| H | 1.098741 | -2.480146 | 1.931080 |
| H | 3.073432 | -1.439451 | 2.939147 |
| H | 2.957537 | 0.887497 | 3.832367 |
| H | 0.806791 | 2.135789 | 3.705407 |

**TS-minor-re-SR-cat**



*Geometry optimization, frequency calculation: PBEh-3c/def2-SV(P)*

| | |
|---|---|
| SFC energy | -1961.310462744 Hartree |
| Chemical potential | 0.517148 Hartree |
| Entropy | 0.000349 Hartree/K |
| Inner energy | 0.620277 Hartree |
| In(Qtrans) | 19.9343 |
| In(Qrot) | 17.2885 |
| In(Qvib) | 36.0136 |
| ZPE | 0.586297 Hartree |
| Enthalpy | 0.621221 Hartree |

*Single point energy: M06-2X/def2-TZVP*

| | |
|---|---|
| SCF energy | -1966.223109725 Hartree |

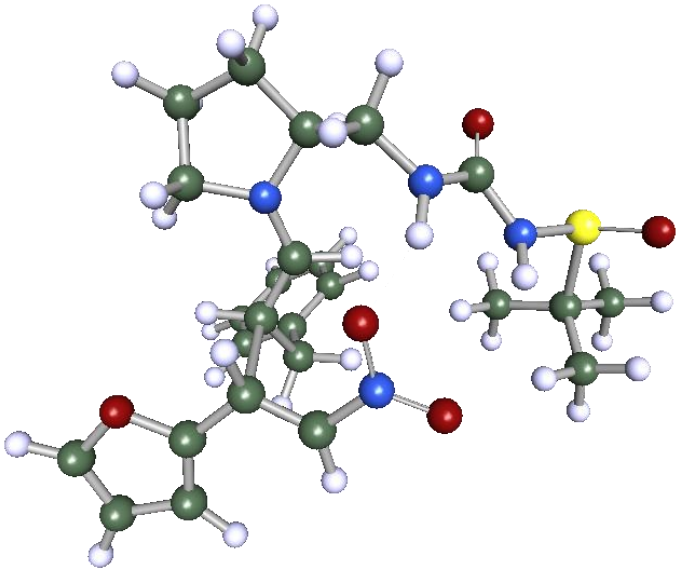
*Cartesian coordinates*

| | | | |
|---|---|---|---|
| N | -1.948672 | 1.211631 | -1.117280 |
| C | -3.253957 | 1.840942 | -1.051595 |
| C | -3.455479 | 2.308215 | -2.486823 |
| C | -2.055244 | 2.757037 | -2.905045 |
| C | -1.093637 | 1.860861 | -2.108080 |

| | | | |
|---|---|---|---|
| C | 0.018194 | 2.674710 | -1.431473 |
| N | 0.918008 | 1.903672 | -0.619026 |
| C | 1.977708 | 1.245769 | -1.176758 |
| O | 2.245622 | 1.301075 | -2.351019 |
| N | 2.740700 | 0.529244 | -0.276609 |
| S | 3.830376 | -0.664569 | -0.833508 |
| O | 3.688813 | -1.810770 | 0.098276 |
| C | 5.435037 | 0.155105 | -0.386045 |
| C | 5.504892 | 0.387814 | 1.113220 |
| C | 6.497746 | -0.844401 | -0.839743 |
| C | 5.529243 | 1.450028 | -1.181061 |
| C | -1.590516 | 0.105269 | -0.503729 |
| C | -2.306648 | -0.581336 | 0.496079 |
| C | -1.465036 | -1.478898 | 1.373237 |
| C | -6.129512 | -1.750862 | 1.973588 |
| C | -5.712759 | -3.004312 | 2.284467 |
| C | -4.636146 | -3.286322 | 1.393709 |
| C | -4.488516 | -2.181195 | 0.608170 |
| O | -5.395602 | -1.253055 | 0.969628 |
| C | -3.561447 | -1.822082 | -0.465818 |
| C | -2.866599 | -2.867086 | -1.095984 |
| N | -2.102801 | -2.588604 | -2.202715 |
| O | -1.513415 | -3.480384 | -2.779243 |
| O | -2.024995 | -1.405153 | -2.562058 |
| H | -2.802878 | -3.885612 | -0.723782 |
| H | -3.948595 | -1.044140 | -1.128480 |
| H | -4.052986 | -4.200075 | 1.335971 |
| H | -6.917903 | -1.115608 | 2.368396 |
| H | -6.124565 | -3.653849 | 3.051010 |
| H | 5.371873 | -0.546992 | 1.674322 |
| H | 6.490867 | 0.798783 | 1.379303 |
| H | 6.413795 | -1.801076 | -0.306756 |
| H | 7.499561 | -0.435132 | -0.642088 |
| H | 6.539238 | 1.874442 | -1.073878 |
| H | 6.433700 | -1.046469 | -1.919840 |
| H | 5.347131 | 1.290995 | -2.253915 |
| H | -1.082984 | -2.319061 | 0.769364 |
| H | -3.055138 | 0.018789 | 1.022341 |
| H | -4.022068 | 1.138655 | -0.708116 |
| H | -3.786769 | 1.458318 | -3.100644 |
| H | -4.209279 | 3.101560 | -2.574867 |
| H | -1.887841 | 2.672005 | -3.985614 |
| H | -0.643107 | 1.084018 | -2.744178 |
| H | -0.436742 | 3.451454 | -0.796854 |
| H | -1.897823 | 3.815357 | -2.641094 |
| H | -3.244183 | 2.691464 | -0.345273 |
| H | -2.109924 | -1.937671 | 2.140350 |
| H | -0.611997 | -0.278399 | -0.796851 |
| H | 2.481806 | 0.457082 | 0.705179 |
| H | 4.814465 | 2.205053 | -0.827915 |

| | | | |
|---|---|---|---|
| H | 0.588989 | 3.195328 | -2.213265 |
| H | 4.750317 | 1.112364 | 1.452453 |
| H | 0.689308 | 1.758676 | 0.355185 |
| C | -0.300854 | -0.789447 | 2.047508 |
| C | 1.871047 | 0.470256 | 3.314037 |
| C | -0.428278 | 0.494606 | 2.588799 |
| C | 0.937267 | -1.421449 | 2.145583 |
| C | 2.011035 | -0.805573 | 2.782012 |
| C | 0.644184 | 1.121171 | 3.211456 |
| H | -1.385725 | 1.014782 | 2.528248 |
| H | 1.081140 | -2.407266 | 1.701674 |
| H | 2.966991 | -1.325463 | 2.832217 |
| H | 2.712570 | 0.956042 | 3.809266 |
| H | 0.518701 | 2.120041 | 3.631776 |

**TS-major-si-SS-cat**



*Geometry optimization, frequency calculation: PBEh-3c/def2-SV(P)*

| | |
|---|---|
| SFC energy | -1961.3180557 Hartree |
| Chemical potential | 0.515745 Hartree |
| Entropy | 0.000355 Hartree/K |
| Inner energy | 0.620712 Hartree |
| In(Qtrans) | 19.9343 |
| In(Qrot) | 17.3117 |
| In(Qvib) | 38.0181 |
| ZPE | 0.586809 Hartree |
| Enthalpy | 0.621656 Hartree |

*Single point energy: M06-2X/def2-TZVP*

| | |
|---|---|
| SCF energy | -1966.22974711 Hartree |

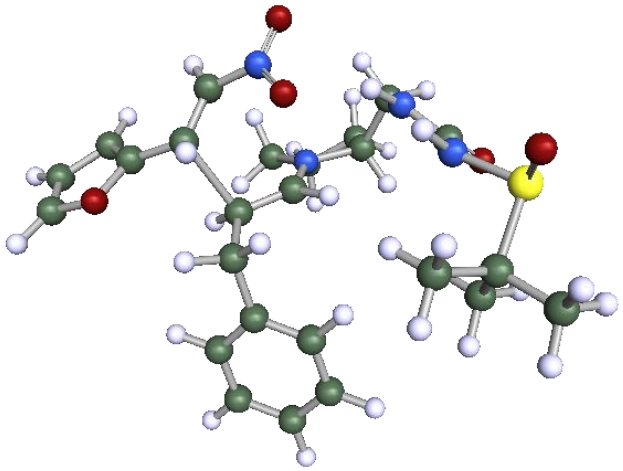
*Cartesian coordinates*

| | | | |
|---|---|---|---|
| N | -1.238731 | 1.112187 | -1.877240 |
| C | -2.609441 | 1.494461 | -2.179333 |

| | | | |
|---|---|---|---|
| C | -2.732922 | 1.216065 | -3.669917 |
| C | -1.343480 | 1.550260 | -4.195660 |
| C | -0.385520 | 1.121573 | -3.081281 |
| C | 0.831475 | 2.050443 | -3.009143 |
| N | 1.814162 | 1.717537 | -2.023425 |
| C | 2.640903 | 0.652384 | -2.166505 |
| O | 2.676157 | -0.050308 | -3.148230 |
| N | 3.425178 | 0.415240 | -1.042446 |
| S | 4.661867 | -0.748489 | -1.111721 |
| O | 5.970795 | -0.067084 | -1.005436 |
| C | 4.361517 | -1.536366 | 0.547672 |
| C | 2.947803 | -2.098582 | 0.549919 |
| C | 5.394247 | -2.661246 | 0.603782 |
| C | 4.592694 | -0.534187 | 1.667059 |
| C | -0.843970 | 0.631650 | -0.714819 |
| C | -1.602721 | 0.485931 | 0.458827 |
| C | -1.152870 | -0.599912 | 1.410729 |
| C | -4.723351 | 2.181298 | 2.799065 |
| C | -4.167915 | 1.784984 | 3.973397 |
| C | -2.764980 | 1.730680 | 3.736269 |
| C | -2.580136 | 2.102681 | 2.434820 |
| O | -3.775693 | 2.370709 | 1.874931 |
| C | -1.402592 | 2.218845 | 1.586045 |
| C | -0.143345 | 2.215881 | 2.205661 |
| N | 0.964796 | 2.456086 | 1.448395 |
| O | 2.084173 | 2.311562 | 1.911955 |
| O | 0.792572 | 2.796004 | 0.266939 |
| H | 0.048399 | 1.862936 | 3.214973 |
| H | -1.530398 | 2.881141 | 0.728594 |
| H | -1.989423 | 1.466991 | 4.448859 |
| H | -5.749801 | 2.371224 | 2.496579 |
| H | -4.691664 | 1.566143 | 4.898899 |
| H | 2.753261 | -2.726298 | -0.333545 |
| H | 2.793943 | -2.727507 | 1.439708 |
| H | 5.262707 | -3.380285 | -0.219347 |
| H | 5.287293 | -3.216219 | 1.547576 |
| H | 4.560364 | -1.051823 | 2.638218 |
| H | 6.420299 | -2.272351 | 0.556645 |
| H | 5.576931 | -0.054665 | 1.577359 |
| H | -1.523652 | -0.379340 | 2.423733 |
| H | -2.686998 | 0.555943 | 0.333274 |
| H | -3.317774 | 0.913245 | -1.573921 |
| H | -2.966540 | 0.153472 | -3.833742 |
| H | -3.529875 | 1.803585 | -4.143696 |
| H | -1.106424 | 1.054925 | -5.145702 |
| H | -0.026451 | 0.094925 | -3.256683 |
| H | 0.490769 | 3.076127 | -2.805280 |
| H | -1.255303 | 2.635113 | -4.369680 |
| H | -2.774711 | 2.559180 | -1.943977 |
| H | -0.053966 | -0.599696 | 1.478499 |

| | | | |
|---|---|---|---|
| H | 0.190772 | 0.282608 | -0.699877 |
| H | 3.474139 | 1.117540 | -0.306574 |
| H | 3.822750 | 0.250266 | 1.704600 |
| H | 1.284975 | 2.055722 | -4.012508 |
| H | 2.193998 | -1.299580 | 0.576211 |
| H | 1.728234 | 2.195242 | -1.124303 |
| C | -1.646632 | -1.961322 | 0.989632 |
| C | -2.627364 | -4.445003 | 0.137898 |
| C | -0.902749 | -2.763969 | 0.125111 |
| C | -2.888688 | -2.424430 | 1.421674 |
| C | -3.377296 | -3.654942 | 1.000110 |
| C | -1.386340 | -3.995438 | -0.297431 |
| H | 0.076425 | -2.425855 | -0.220568 |
| H | -3.481864 | -1.812079 | 2.104709 |
| H | -4.349168 | -4.001814 | 1.353004 |
| H | -3.006728 | -5.412884 | -0.190701 |
| H | -0.785920 | -4.610713 | -0.968437 |

**TS-major-re-SS-cat**



*Geometry optimization, frequency calculation: PBEh-3c/def2-SV(P)*

| | |
|---|---|
| SFC energy | -1961.3162281 Hartree |
| Chemical potential | 0.51645 Hartree |
| Entropy | 0.000352 Hartree/K |
| Inner energy | 0.620591 Hartree |
| In(Qtrans) | 19.9343 |
| In(Qrot) | 17.3228 |
| In(Qvib) | 37.1549 |
| ZPE | 0.586710 Hartree |
| Enthalpy | 0.621535 Hartree |

*Single point energy: M06-2X/def2-TZVP*

| | |
|---|---|
| SCF energy | -1966.23161921 Hartree |

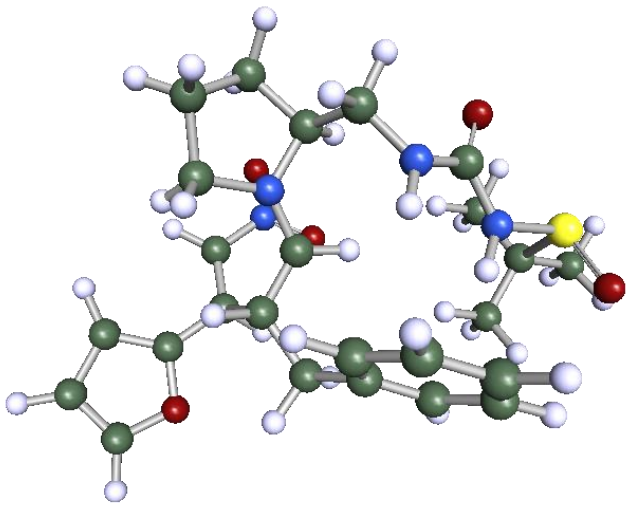
*Cartesian coordinates*

| | | | |
|---|---|---|---|
| N | -0.889895 | 0.977455 | -1.722546 |
| C | -2.198286 | 1.180730 | -2.339368 |

| | | | |
|---|---|---|---|
| C | -1.988610 | 0.701798 | -3.767195 |
| C | -0.572921 | 1.177728 | -4.063787 |
| C | 0.183356 | 1.005889 | -2.743352 |
| C | 1.231471 | 2.103329 | -2.550174 |
| N | 2.043702 | 1.961036 | -1.377562 |
| C | 3.021396 | 1.026546 | -1.303509 |
| O | 3.381791 | 0.343612 | -2.235004 |
| N | 3.558128 | 0.872962 | -0.034999 |
| S | 5.050566 | 0.069297 | 0.190997 |
| O | 5.760957 | 0.841131 | 1.237680 |
| C | 4.436981 | -1.471953 | 1.027892 |
| C | 3.632920 | -1.110552 | 2.264493 |
| C | 3.623473 | -2.251466 | 0.004627 |
| C | 5.710419 | -2.227876 | 1.400604 |
| C | -0.699670 | 0.490731 | -0.511185 |
| C | -1.683311 | 0.269569 | 0.462502 |
| C | -1.276924 | -0.557615 | 1.663734 |
| C | -5.361838 | 1.157932 | 2.521401 |
| C | -5.872281 | 1.810932 | 1.445711 |
| C | -4.748628 | 2.324063 | 0.737026 |
| C | -3.642906 | 1.945173 | 1.443658 |
| O | -4.026216 | 1.234804 | 2.519722 |
| C | -2.209976 | 2.120335 | 1.222210 |
| C | -1.825778 | 3.182756 | 0.392324 |
| N | -0.502375 | 3.470221 | 0.233849 |
| O | -0.152002 | 4.392239 | -0.486775 |
| O | 0.321765 | 2.744427 | 0.813893 |
| H | -2.509748 | 3.786511 | -0.197048 |
| H | -4.762842 | 2.907927 | -0.178413 |
| H | -5.821881 | 0.620941 | 3.346590 |
| H | -6.922104 | 1.921196 | 1.191393 |
| H | 2.691276 | -0.603261 | 2.009116 |
| H | 3.370386 | -2.023052 | 2.821783 |
| H | 2.704139 | -1.726285 | -0.286051 |
| H | 3.330554 | -3.224190 | 0.429159 |
| H | 5.447546 | -3.193846 | 1.857349 |
| H | 4.194947 | -2.446088 | -0.914389 |
| H | 6.333008 | -2.442481 | 0.518225 |
| H | -1.966891 | -0.360623 | 2.496643 |
| H | -2.686458 | 0.058077 | 0.082249 |
| H | -2.979796 | 0.631161 | -1.799227 |
| H | -2.052310 | -0.396162 | -3.812732 |
| H | -2.737798 | 1.105074 | -4.460848 |
| H | -0.087497 | 0.628368 | -4.880213 |
| H | 0.693012 | 0.029906 | -2.724197 |
| H | 0.739891 | 3.084068 | -2.501269 |
| H | -0.585380 | 2.240812 | -4.353658 |
| H | -2.467518 | 2.246537 | -2.314646 |
| H | -0.283419 | -0.229206 | 2.006112 |
| H | 0.342356 | 0.273477 | -0.265742 |

| | | | |
|---|---|---|---|
| H | 3.291515 | 1.495861 | 0.722788 |
| H | 6.320995 | -1.667896 | 2.121217 |
| H | 1.865763 | 2.101894 | -3.449360 |
| H | 4.205104 | -0.460382 | 2.940984 |
| H | 1.741617 | 2.461953 | -0.545759 |
| C | -1.263367 | -2.035811 | 1.369358 |
| C | -1.261595 | -4.764843 | 0.726183 |
| C | -0.072488 | -2.703606 | 1.091693 |
| C | -2.454956 | -2.760398 | 1.327137 |
| C | -2.456259 | -4.111680 | 1.008213 |
| C | -0.068469 | -4.055746 | 0.771105 |
| H | 0.872882 | -2.159824 | 1.135020 |
| H | -3.398455 | -2.258508 | 1.553366 |
| H | -3.397620 | -4.661975 | 0.984895 |
| H | -1.261312 | -5.826399 | 0.477844 |
| H | 0.876268 | -4.557996 | 0.559125 |
| H | -1.581824 | 1.930265 | 2.096011 |

**TS-minor-si-SS-cat**



*Geometry optimization, frequency calculation: PBEh-3c/Def2-SV(P)*

| | |
|---|---|
| SFC energy | -1961.3162133 Hartree |
| Chemical potential | 0.519481 Hartree |
| Entropy | 0.000343 Hartree/K |
| Inner energy | 0.620676 Hartree |
| In(Qtrans) | 19.9343 |
| In(Qrot) | 17.1698 |
| In(Qvib) | 34.3804 |
| ZPE | 0.586976 Hartree |
| Enthalpy | 0.621620 Hartree |

*Single point energy: M06-2X/Def2-TZVP*

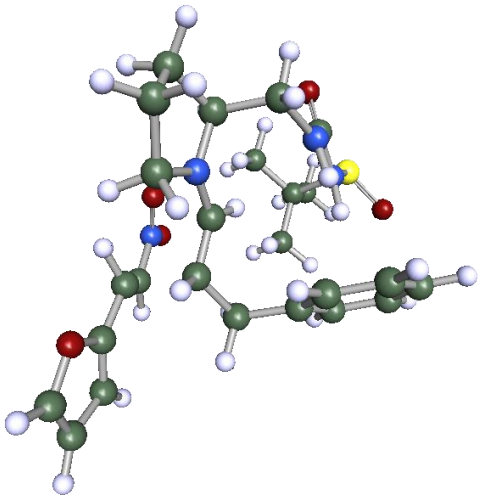
| | |
|---|---|
| SCF energy | -1966.23102434 Hartree |

Cartesian coordinates

| | | | |
|---|---|---|---|
| N | -1.295277 | 1.548393 | -0.673200 |
| C | -2.520487 | 2.303809 | -0.404787 |
| C | -2.477012 | 3.466275 | -1.398005 |
| C | -1.511283 | 2.994673 | -2.484103 |
| C | -0.482811 | 2.169407 | -1.720369 |
| C | 0.653664 | 3.013595 | -1.115610 |
| N | 1.586340 | 2.237313 | -0.345023 |
| C | 2.535525 | 1.478656 | -0.979996 |
| O | 2.879038 | 1.673110 | -2.119056 |
| N | 3.038960 | 0.445204 | -0.223368 |
| S | 4.459954 | -0.387774 | -0.691019 |
| O | 5.109403 | -0.768656 | 0.589096 |
| C | 3.726678 | -1.950004 | -1.380585 |
| C | 4.953559 | -2.790190 | -1.734246 |
| C | 2.871112 | -2.639605 | -0.333897 |
| C | 2.930461 | -1.595965 | -2.628979 |
| C | -0.891683 | 0.519619 | 0.031259 |
| C | -1.677246 | -0.142344 | 0.993734 |
| C | -0.904358 | -1.018151 | 1.962301 |
| C | -5.136245 | -2.251854 | 2.406520 |
| C | -6.002155 | -1.433325 | 1.756949 |
| C | -5.282460 | -0.918689 | 0.639434 |
| C | -4.036264 | -1.470906 | 0.697924 |
| O | -3.956016 | -2.272955 | 1.774725 |
| C | -2.832661 | -1.328814 | -0.126974 |
| C | -3.028559 | -0.845624 | -1.438917 |
| N | -1.981920 | -0.831780 | -2.317516 |
| O | -2.127875 | -0.380277 | -3.444094 |
| O | -0.889226 | -1.256374 | -1.919284 |
| H | -3.954274 | -0.410571 | -1.804599 |
| H | -2.131425 | -2.163473 | -0.031866 |
| H | -5.652514 | -0.235004 | -0.118525 |
| H | -5.228034 | -2.868379 | 3.296591 |
| H | -7.031769 | -1.226847 | 2.033122 |
| H | 5.550938 | -3.042730 | -0.847835 |
| H | 4.628909 | -3.730615 | -2.203500 |
| H | 3.416943 | -2.779683 | 0.609656 |
| H | 2.571378 | -3.633318 | -0.699705 |
| H | 2.646176 | -2.522940 | -3.149445 |
| H | 1.945076 | -2.081093 | -0.137210 |
| H | 1.995846 | -1.067285 | -2.401397 |
| H | -0.566193 | -1.932985 | 1.449543 |
| H | -2.469841 | 0.459556 | 1.447699 |
| H | -3.398127 | 1.664291 | -0.551761 |
| H | -3.473487 | 3.703944 | -1.790947 |
| H | -2.105328 | 4.378415 | -0.908945 |
| H | -2.022602 | 2.345550 | -3.208585 |
| H | -0.049247 | 1.380014 | -2.352603 |
| H | 0.246376 | 3.807930 | -0.471738 |
| H | -1.053647 | 3.820816 | -3.044600 |

| | | | |
|---|---|---|---|
| H | -2.534800 | 2.643376 | 0.644045 |
| H | -1.577475 | -1.361826 | 2.761530 |
| H | 0.093717 | 0.127645 | -0.213387 |
| H | 2.723016 | 0.257904 | 0.726011 |
| H | 3.510682 | -0.982313 | -3.332523 |
| H | 1.187762 | 3.510818 | -1.936188 |
| H | 5.607735 | -2.275923 | -2.455193 |
| H | 1.387471 | 2.071461 | 0.632250 |
| C | 0.303835 | -0.333650 | 2.563728 |
| C | 2.595058 | 0.952036 | 3.567830 |
| C | 0.255195 | 0.999024 | 2.983705 |
| C | 1.517163 | -1.010739 | 2.680495 |
| C | 2.655754 | -0.378127 | 3.172363 |
| C | 1.385925 | 1.635044 | 3.482795 |
| H | -0.682189 | 1.554395 | 2.917950 |
| H | 1.582411 | -2.051906 | 2.361458 |
| H | 3.601341 | -0.918344 | 3.211345 |
| H | 3.488075 | 1.454220 | 3.939508 |
| H | 1.323111 | 2.674845 | 3.806416 |

**TS-minor-si-SS-cat**



*Geometry optimization, frequency calculation: PBEh-3c/Def2-SV(P)*

| | |
|---|---|
| SFC energy | -1961.3167839 Hartree |
| Chemical potential | 0.51997 Hartree |
| Entropy | 0.00034 Hartree/K |
| Inner energy | 0.620485 Hartree |
| In(Qtrans) | 19.9343 |
| In(Qrot) | 17.1456 |
| In(Qvib) | 33.7004 |
| ZPE | 0.5868 Hartree |
| Enthalpy | 0.621429 Hartree |

*Single point energy: M06-2X/Def2-TZVP*

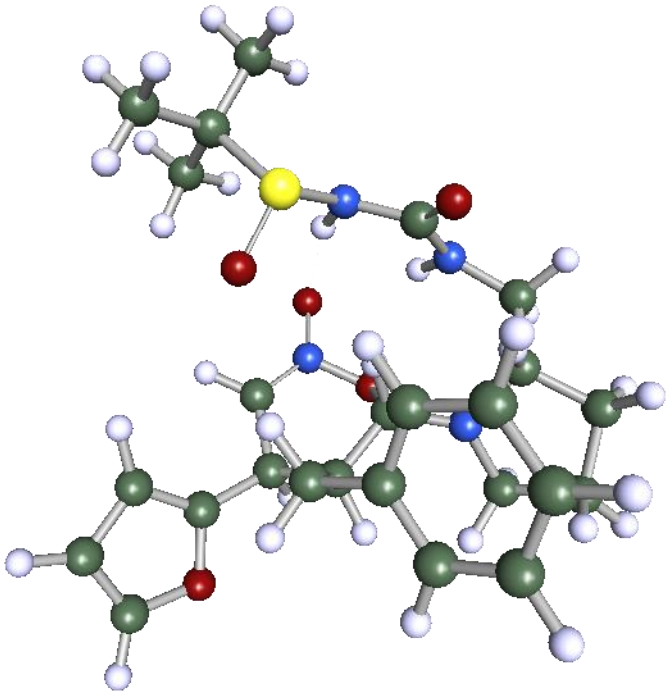
| | |
|---|---|
| SCF energy | -1966.229824173 Hartree |

*Cartesian coordinates*

| | | | |
|---|---|---|---|
| N | -1.334573 | 1.788056 | -0.793096 |
| C | -2.622127 | 2.448197 | -0.626418 |
| C | -2.491644 | 3.736198 | -1.435874 |
| C | -1.421342 | 3.404234 | -2.474530 |
| C | -0.453440 | 2.498640 | -1.719113 |
| C | 0.637237 | 3.279391 | -0.962535 |
| N | 1.504313 | 2.431241 | -0.193908 |
| C | 2.480187 | 1.699664 | -0.822656 |
| O | 2.887134 | 1.962898 | -1.927048 |
| N | 2.922099 | 0.613718 | -0.106265 |
| S | 4.329360 | -0.255849 | -0.553206 |
| O | 4.902971 | -0.719893 | 0.735694 |
| C | 3.558457 | -1.749151 | -1.345994 |
| C | 4.759770 | -2.624481 | -1.701566 |
| C | 2.640269 | -2.452299 | -0.364109 |
| C | 2.826001 | -1.296355 | -2.600674 |
| C | -0.991825 | 0.672243 | -0.188325 |
| C | -1.783831 | -0.056432 | 0.719469 |
| C | -1.022819 | -0.907248 | 1.710896 |
| C | -5.733439 | -1.411474 | 1.541475 |
| C | -5.305884 | -2.633184 | 1.949357 |
| C | -4.082461 | -2.865854 | 1.256197 |
| C | -3.867368 | -1.766112 | 0.478059 |
| O | -4.871357 | -0.887305 | 0.660682 |
| C | -2.794266 | -1.372612 | -0.434587 |
| C | -1.942038 | -2.387626 | -0.901856 |
| N | -1.017959 | -2.101728 | -1.874121 |
| O | -0.273821 | -2.977290 | -2.280879 |
| O | -0.957068 | -0.939632 | -2.294934 |
| H | -1.884750 | -3.387808 | -0.482313 |
| H | -3.098153 | -0.625407 | -1.171200 |
| H | -3.449601 | -3.745558 | 1.318806 |
| H | -6.610818 | -0.817661 | 1.783493 |
| H | -5.803329 | -3.293559 | 2.653217 |
| H | 5.323595 | -2.934400 | -0.811234 |
| H | 4.407813 | -3.532169 | -2.213174 |
| H | 3.162781 | -2.708012 | 0.568478 |
| H | 2.258022 | -3.379277 | -0.814722 |
| H | 2.500959 | -2.179503 | -3.168777 |
| H | 1.759460 | -1.839696 | -0.125782 |
| H | 1.911968 | -0.732451 | -2.377551 |
| H | -0.590348 | -1.776530 | 1.186171 |
| H | -2.638625 | 0.488137 | 1.130850 |
| H | -3.429687 | 1.803104 | -1.005904 |
| H | -3.446391 | 4.039264 | -1.883767 |
| H | -2.167153 | 4.566194 | -0.790989 |
| H | -1.859879 | 2.854841 | -3.320191 |
| H | 0.030781 | 1.771171 | -2.387213 |

| | | | |
|---|---|---|---|
| H | 0.181511 | 4.016972 | -0.284679 |
| H | -0.927784 | 4.294134 | -2.887918 |
| H | -2.835584 | 2.632782 | 0.438627 |
| H | -1.733630 | -1.327518 | 2.440515 |
| H | 0.010980 | 0.310149 | -0.414196 |
| H | 2.550997 | 0.382683 | 0.812953 |
| H | 3.463304 | -0.681607 | -3.252365 |
| H | 1.232313 | 3.841715 | -1.695051 |
| H | 5.451720 | -2.110870 | -2.386899 |
| H | 1.239610 | 2.202269 | 0.754849 |
| C | 0.086375 | -0.179728 | 2.437181 |
| C | 2.202327 | 1.179278 | 3.698577 |
| C | -0.064050 | 1.139962 | 2.872895 |
| C | 1.310926 | -0.806983 | 2.668276 |
| C | 2.363288 | -0.137456 | 3.286084 |
| C | 0.979653 | 1.811863 | 3.499695 |
| H | -1.013790 | 1.655922 | 2.719805 |
| H | 1.456776 | -1.836453 | 2.338408 |
| H | 3.322316 | -0.639880 | 3.410268 |
| H | 3.027906 | 1.710912 | 4.171471 |
| H | 0.837656 | 2.840920 | 3.832669 |

**H-bonded product-major-SR-cat**



*Geometry optimization, frequency calculation: PBEh-3c/Def2-SV(P)*

| | |
|---|---|
| SFC energy | -1961.3706396 Hartree |
| Chemical potential | 0.525118 Hartree |
| Entropy | 0.000337 Hartree/K |
| Inner energy | 0.624621 Hartree |
| In(Qtrans) | 19.9343 |
| In(Qrot) | 17.0800 |

| | |
|---|---|
| In(Qvib) | 33.8792 |
| ZPE | 0.592055 Hartree |
| Enthalpy | 0.625565 Hartree |

*Single point energy: M06-2X/Def2-TZVP*

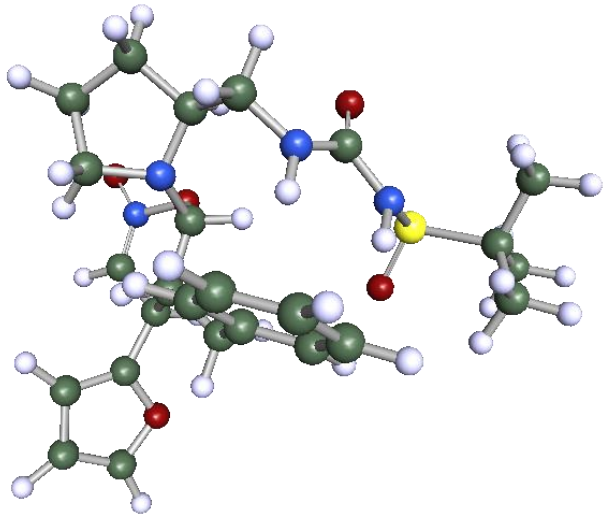
| | |
|---|---|
| SCF energy | -1966.28312483 Hartree |

*Cartesian coordinates*

| | | | |
|---|---|---|---|
| N | 1.774257 | -0.135299 | -1.773382 |
| C | 3.149547 | -0.359044 | -2.149974 |
| C | 3.452717 | 0.846539 | -3.028643 |
| C | 2.136551 | 1.072576 | -3.765176 |
| C | 1.041509 | 0.619404 | -2.786067 |
| C | -0.060032 | -0.137758 | -3.545197 |
| N | -1.140752 | -0.643827 | -2.735490 |
| C | -1.955641 | 0.178874 | -2.030409 |
| O | -2.028993 | 1.371779 | -2.193521 |
| N | -2.704106 | -0.487391 | -1.050301 |
| S | -3.154048 | 0.436050 | 0.291390 |
| O | -2.115458 | 0.251732 | 1.349433 |
| C | -4.616183 | -0.568452 | 0.828589 |
| C | -4.199124 | -1.980772 | 1.207342 |
| C | -5.141292 | 0.183444 | 2.051874 |
| C | -5.635093 | -0.540999 | -0.302413 |
| C | 1.153537 | -0.664220 | -0.658427 |
| C | 1.905807 | -0.618716 | 0.683752 |
| C | 1.537205 | 0.661063 | 1.449244 |
| C | 2.996678 | -1.628887 | 4.752723 |
| C | 1.722543 | -1.418938 | 5.164608 |
| C | 0.914729 | -1.506659 | 3.989258 |
| C | 1.769256 | -1.766143 | 2.964587 |
| O | 3.027685 | -1.838927 | 3.427668 |
| C | 1.584065 | -1.916884 | 1.494865 |
| C | 0.217266 | -2.434924 | 1.184077 |
| N | -0.126069 | -2.545344 | -0.053532 |
| O | -1.167251 | -3.001958 | -0.537102 |
| O | 0.784785 | -2.081587 | -0.946933 |
| H | -0.505850 | -2.765604 | 1.925062 |
| H | 2.305967 | -2.681371 | 1.151869 |
| H | -0.159579 | -1.364044 | 3.914391 |
| H | 3.947708 | -1.664243 | 5.277084 |
| H | 1.392104 | -1.224623 | 6.180462 |
| H | -3.387601 | -1.974249 | 1.947723 |
| H | -5.055614 | -2.507440 | 1.655196 |
| H | -4.400512 | 0.213668 | 2.862362 |
| H | -6.040666 | -0.320198 | 2.435672 |
| H | -6.581295 | -0.984149 | 0.043110 |
| H | -5.422626 | 1.218714 | 1.806524 |
| H | -5.854115 | 0.486268 | -0.630964 |
| H | 2.140153 | 0.709370 | 2.367174 |

| | | | |
|---|---|---|---|
| H | 2.990588 | -0.621642 | 0.509272 |
| H | 3.811414 | -0.407492 | -1.273656 |
| H | 3.688510 | 1.712339 | -2.393630 |
| H | 4.302003 | 0.682156 | -3.705732 |
| H | 1.996020 | 2.115048 | -4.078956 |
| H | 0.578843 | 1.495460 | -2.305584 |
| H | 0.376307 | -0.999735 | -4.070088 |
| H | 2.105598 | 0.457367 | -4.679132 |
| H | 3.291099 | -1.306095 | -2.706678 |
| H | 0.485863 | 0.602379 | 1.768715 |
| H | 0.193481 | -0.143168 | -0.509945 |
| H | -2.430805 | -1.454050 | -0.841662 |
| H | -5.295100 | -1.109339 | -1.177563 |
| H | -0.455911 | 0.539052 | -4.318873 |
| H | -3.871448 | -2.577151 | 0.344967 |
| H | -1.093729 | -1.617953 | -2.471095 |
| C | 1.750772 | 1.923960 | 0.658333 |
| C | 2.150825 | 4.254785 | -0.845708 |
| C | 0.668684 | 2.625706 | 0.130391 |
| C | 3.036973 | 2.418476 | 0.436172 |
| C | 3.238030 | 3.573066 | -0.307514 |
| C | 0.865948 | 3.779227 | -0.620798 |
| H | -0.344584 | 2.263138 | 0.309555 |
| H | 3.897771 | 1.895256 | 0.859559 |
| H | 4.250356 | 3.947465 | -0.465682 |
| H | 2.307082 | 5.161563 | -1.430897 |
| H | 0.003241 | 4.303252 | -1.032881 |

**H-bonded product-minor-SR-cat**



*Geometry optimization, frequency calculation: PBEh-3c/Def2-SV(P)*

| | |
|---|---|
| SFC energy | -1961.3593467 Hartree |
| Chemical potential | 0.523767 Hartree |
| Entropy | 0.00034 Hartree |
| Inner energy | 0.624072 Hartree |
| ln(Qtrans) | 19.9343 |

| | |
|---|---|
| In(Qrot) | 17.2079 |
| In(Qvib) | 34.2804 |
| ZPE | 0.591203 Hartree |
| Enthalpy | 0.625017 Hartree |

*Single point energy: M06-2X/Def2-TZVP*

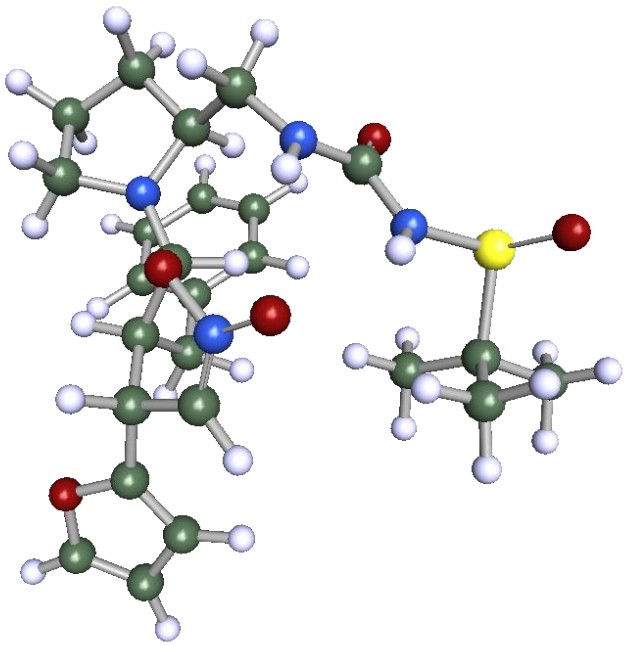
| | |
|---|---|
| SCF energy | -1966.27014037 Hartree |

*Cartesian coordinates*

| | | | |
|---|---|---|---|
| N | -1.616065 | 1.457813 | -1.067225 |
| C | -2.947891 | 2.049544 | -0.990728 |
| C | -3.162404 | 2.711351 | -2.346808 |
| C | -1.768672 | 3.227443 | -2.678564 |
| C | -0.813476 | 2.198592 | -2.049833 |
| C | 0.392350 | 2.894999 | -1.416514 |
| N | 1.288159 | 2.016402 | -0.710578 |
| C | 2.100672 | 1.152231 | -1.368911 |
| O | 2.241416 | 1.119880 | -2.563832 |
| N | 2.789531 | 0.279321 | -0.520028 |
| S | 3.096256 | -1.295577 | -1.068644 |
| O | 2.259456 | -2.214960 | -0.249042 |
| C | 4.830300 | -1.477819 | -0.439588 |
| C | 4.877594 | -1.286016 | 1.067503 |
| C | 5.217437 | -2.906253 | -0.818309 |
| C | 5.684686 | -0.461553 | -1.184469 |
| C | -1.433657 | 0.061073 | -1.000985 |
| C | -2.037956 | -0.604612 | 0.255964 |
| C | -0.972868 | -0.958174 | 1.294163 |
| C | -4.092551 | -3.825407 | 2.565547 |
| C | -5.075146 | -2.892503 | 2.620429 |
| C | -4.782678 | -1.962692 | 1.576727 |
| C | -3.646490 | -2.410731 | 0.976743 |
| O | -3.233195 | -3.536833 | 1.578344 |
| C | -2.828602 | -1.874042 | -0.150590 |
| C | -3.700771 | -1.550594 | -1.320118 |
| N | -3.187214 | -0.918146 | -2.329683 |
| O | -3.705003 | -0.584941 | -3.373715 |
| O | -1.846672 | -0.645370 | -2.212836 |
| H | -4.755649 | -1.805622 | -1.390516 |
| H | -2.098881 | -2.654470 | -0.436802 |
| H | -5.349864 | -1.076218 | 1.305887 |
| H | -3.889477 | -4.721266 | 3.145823 |
| H | -5.910172 | -2.868306 | 3.314111 |
| H | 4.176929 | -1.958038 | 1.582711 |
| H | 5.888391 | -1.514952 | 1.438359 |
| H | 4.581452 | -3.648342 | -0.317425 |
| H | 6.259197 | -3.098082 | -0.521609 |
| H | 6.746818 | -0.625198 | -0.946899 |
| H | 5.149737 | -3.073727 | -1.903943 |
| H | 5.571941 | -0.553160 | -2.275121 |

| | | | |
|---|---|---|---|
| H | -0.261370 | -1.671662 | 0.848455 |
| H | -2.769610 | 0.078050 | 0.712587 |
| H | -3.725792 | 1.310938 | -0.757529 |
| H | -3.484438 | 1.960730 | -3.080760 |
| H | -3.923167 | 3.503931 | -2.320432 |
| H | -1.596117 | 3.341115 | -3.756709 |
| H | -0.449989 | 1.510905 | -2.828785 |
| H | 0.041883 | 3.646583 | -0.693508 |
| H | -1.611847 | 4.220450 | -2.224801 |
| H | -2.986247 | 2.805961 | -0.183322 |
| H | -1.464912 | -1.503717 | 2.116457 |
| H | -0.357327 | -0.153091 | -1.030359 |
| H | 2.618953 | 0.351262 | 0.480903 |
| H | 5.431974 | 0.570402 | -0.907417 |
| H | 0.945501 | 3.435618 | -2.199104 |
| H | 4.658187 | -0.249151 | 1.361262 |
| H | 1.085196 | 1.858948 | 0.266345 |
| C | -0.193452 | 0.173587 | 1.912943 |
| C | 1.320582 | 2.189300 | 3.163698 |
| C | -0.721221 | 1.450377 | 2.107926 |
| C | 1.102449 | -0.077470 | 2.374569 |
| C | 1.852624 | 0.915586 | 2.994798 |
| C | 0.028688 | 2.448177 | 2.722958 |
| H | -1.728990 | 1.686476 | 1.769334 |
| H | 1.528959 | -1.072343 | 2.232771 |
| H | 2.859951 | 0.691001 | 3.349025 |
| H | 1.906929 | 2.973350 | 3.642965 |
| H | -0.404264 | 3.440142 | 2.856533 |

**H-bonded-product-major-SS-cat**



*Geometry optimization, frequency calculation: PBEh-3c/Def2-SV(P)*
SFC energy -1961.3635364 Hartree

| | |
|---|---|
| Chemical potential | 0.526896 Hartree |
| Entropy | 0.000326 Hartree/K |
| Inner energy | 0.623136 Hartree |
| In(Qtrans) | 19.9343 |
| In(Qrot) | 17.1413 |
| In(Qvib) | 31.0628 |
| ZPE | 0.591231 Hartree |
| Enthalpy | 0.624080 Hartree |

*Single point energy: M06-2X/Def2-TZVP*

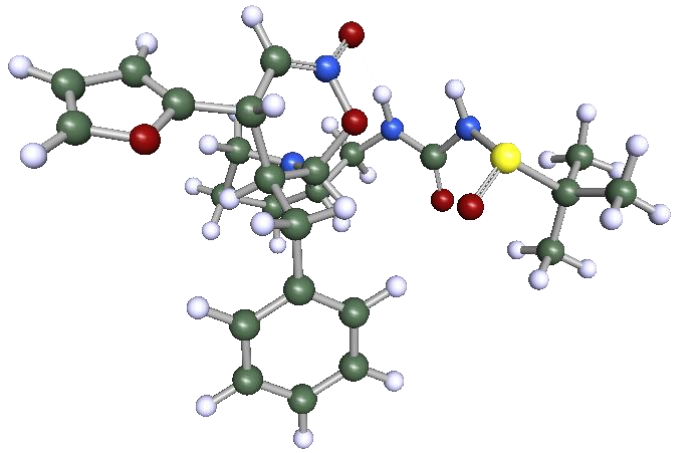
| | |
|---|---|
| SCF energy | -1966.27427535 Hartree |

*Cartesian coordinates*

| | | | |
|---|---|---|---|
| N | -1.295175 | 1.029443 | -1.846941 |
| C | -2.566786 | 1.573847 | -2.263723 |
| C | -2.906233 | 0.724989 | -3.480299 |
| C | -1.544986 | 0.507768 | -4.130046 |
| C | -0.550430 | 0.448706 | -2.961923 |
| C | 0.760447 | 1.148797 | -3.342713 |
| N | 1.791224 | 1.134502 | -2.336819 |
| C | 2.418810 | -0.007129 | -1.956587 |
| O | 2.288071 | -1.070910 | -2.511994 |
| N | 3.204920 | 0.149971 | -0.819200 |
| S | 4.283238 | -1.073079 | -0.353763 |
| O | 5.668064 | -0.570951 | -0.495999 |
| C | 3.921339 | -1.041069 | 1.473128 |
| C | 2.455635 | -1.399785 | 1.667576 |
| C | 4.827899 | -2.130874 | 2.043227 |
| C | 4.273776 | 0.315269 | 2.063127 |
| C | -0.750089 | 1.138371 | -0.584851 |
| C | -1.680296 | 0.911987 | 0.621262 |
| C | -1.608668 | -0.556902 | 1.062325 |
| C | -3.326664 | 1.130972 | 4.579155 |
| C | -2.174215 | 0.710429 | 5.154291 |
| C | -1.149972 | 0.942996 | 4.184952 |
| C | -1.768945 | 1.488071 | 3.104199 |
| O | -3.085098 | 1.600308 | 3.345074 |
| C | -1.302272 | 1.914300 | 1.756068 |
| C | 0.163786 | 2.201741 | 1.756890 |
| N | 0.721426 | 2.520469 | 0.632983 |
| O | 1.879656 | 2.854971 | 0.407559 |
| O | -0.106247 | 2.477490 | -0.444777 |
| H | 0.797042 | 2.227143 | 2.640489 |
| H | -1.823787 | 2.860101 | 1.515080 |
| H | -0.092239 | 0.719094 | 4.286092 |
| H | -4.356897 | 1.162898 | 4.922894 |
| H | -2.060086 | 0.288423 | 6.148127 |
| H | 2.187752 | -2.332477 | 1.147422 |
| H | 2.244477 | -1.551037 | 2.737416 |
| H | 4.613895 | -3.115340 | 1.599472 |

| | | | |
|---|---|---|---|
| H | 4.669068 | -2.216991 | 3.128586 |
| H | 4.216685 | 0.268047 | 3.161773 |
| H | 5.889354 | -1.904757 | 1.874952 |
| H | 5.297313 | 0.612495 | 1.796658 |
| H | -2.308390 | -0.717134 | 1.894946 |
| H | -2.719763 | 1.133603 | 0.343433 |
| H | -3.329941 | 1.486974 | -1.477099 |
| H | -3.331411 | -0.234196 | -3.150788 |
| H | -3.632857 | 1.205313 | -4.149571 |
| H | -1.501405 | -0.397793 | -4.748703 |
| H | -0.313704 | -0.600130 | -2.721985 |
| H | 0.560276 | 2.202348 | -3.585866 |
| H | -1.303001 | 1.357209 | -4.789868 |
| H | -2.504327 | 2.646946 | -2.529357 |
| H | -0.605337 | -0.771120 | 1.463980 |
| H | 0.086517 | 0.422166 | -0.508063 |
| H | 3.335679 | 1.078465 | -0.424321 |
| H | 3.585490 | 1.110577 | 1.740875 |
| H | 1.133856 | 0.674014 | -4.263585 |
| H | 1.789730 | -0.604861 | 1.304808 |
| H | 1.922834 | 1.975277 | -1.792690 |
| C | -1.933072 | -1.526136 | -0.043747 |
| C | -2.559438 | -3.277239 | -2.141578 |
| C | -0.932935 | -2.238291 | -0.702107 |
| C | -3.256473 | -1.716845 | -0.444662 |
| C | -3.569349 | -2.583114 | -1.482643 |
| C | -1.240327 | -3.104087 | -1.745870 |
| H | 0.111222 | -2.113302 | -0.409186 |
| H | -4.058830 | -1.183229 | 0.070176 |
| H | -4.610115 | -2.721919 | -1.777820 |
| H | -2.803471 | -3.957966 | -2.957604 |
| H | -0.436150 | -3.638227 | -2.252344 |

**H-bonded-product-major2-SS-cat**



*Geometry optimization, frequency calculation: PBEh-3c/def2-SV(P)*

| | |
|---|---|
| SFC energy | -1961.3558144 Hartree |
| Chemical potential | 0.524979 Hartree |
| Entropy | 0.000338 Hartree/K |
| Inner energy | 0.624800 Hartree |
| In(Qtrans) | 19.9343 |
| In(Qrot) | 17.1777 |
| In(Qvib) | 34.0836 |
| ZPE | 0.592201 Hartree |
| Enthalpy | 0.625744 Hartree |

*Single point energy: M06-2X/def2-TZVP*

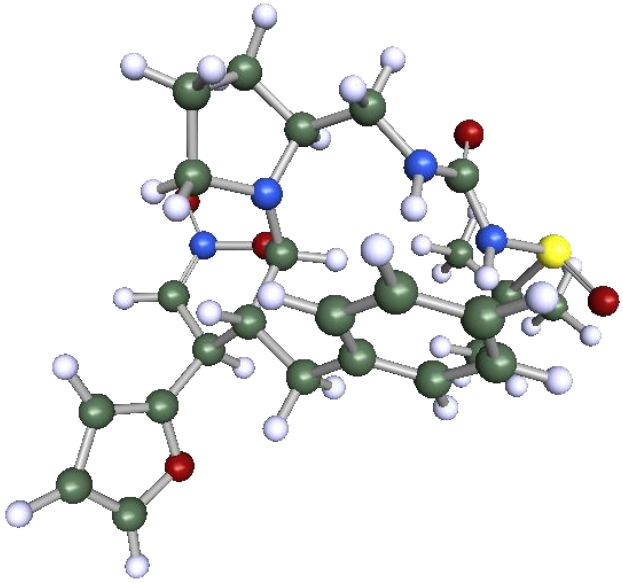
| | |
|---|---|
| SCF energy | -1966.26861183 Hartree |

*Cartesian coordinates*

| | | | |
|---|---|---|---|
| N | -1.325373 | 0.678216 | -1.142194 |
| C | -2.706558 | 1.042156 | -1.369006 |
| C | -3.198974 | -0.045460 | -2.318269 |
| C | -1.984543 | -0.291519 | -3.215604 |
| C | -0.761699 | 0.122511 | -2.366185 |
| C | 0.128899 | 1.115661 | -3.127857 |
| N | 1.168595 | 1.694651 | -2.320180 |
| C | 2.205441 | 0.936784 | -1.880865 |
| O | 2.477222 | -0.150121 | -2.327175 |
| N | 2.952718 | 1.543796 | -0.866643 |
| S | 3.643997 | 0.700408 | 0.442181 |
| O | 2.779492 | -0.427676 | 0.872882 |
| C | 5.197647 | -0.049224 | -0.271885 |
| C | 5.782564 | 0.886203 | -1.318045 |
| C | 6.106257 | -0.113182 | 0.960667 |
| C | 4.946027 | -1.447127 | -0.810906 |
| C | -0.722310 | 0.432640 | 0.094951 |
| C | -1.649678 | 0.185415 | 1.288578 |
| C | -1.020154 | -0.830618 | 2.255474 |
| C | -5.207011 | 1.019547 | 3.438744 |
| C | -5.615421 | 1.992420 | 2.589616 |
| C | -4.445194 | 2.401412 | 1.876682 |
| C | -3.423804 | 1.642505 | 2.357924 |
| O | -3.888405 | 0.807927 | 3.301461 |
| C | -1.975142 | 1.530841 | 2.018732 |
| C | -1.525193 | 2.741084 | 1.262971 |
| N | -0.433629 | 2.708191 | 0.571774 |
| O | 0.122619 | 3.617616 | -0.035429 |
| O | 0.193808 | 1.508782 | 0.515233 |
| H | -2.029814 | 3.703030 | 1.313698 |
| H | -4.382344 | 3.161690 | 1.104080 |
| H | -5.726074 | 0.414433 | 4.176986 |
| H | -6.624140 | 2.379205 | 2.480992 |
| H | 5.857864 | 1.922782 | -0.956602 |
| H | 6.801301 | 0.553329 | -1.569977 |
| H | 6.334343 | 0.885614 | 1.361170 |

| | | | |
|---|---|---|---|
| H | 7.059847 | -0.590650 | 0.690868 |
| H | 5.910764 | -1.888578 | -1.107136 |
| H | 5.657011 | -0.711167 | 1.767482 |
| H | 4.498505 | -2.099095 | -0.049836 |
| H | -1.606696 | -0.835025 | 3.186186 |
| H | -2.587705 | -0.253563 | 0.921206 |
| H | -3.287099 | 1.094490 | -0.439887 |
| H | -3.442684 | -0.949974 | -1.739727 |
| H | -4.099637 | 0.239889 | -2.879289 |
| H | -1.914220 | -1.333709 | -3.552437 |
| H | -0.147581 | -0.754758 | -2.107913 |
| H | -0.485659 | 1.944621 | -3.510271 |
| H | -2.047034 | 0.327649 | -4.124229 |
| H | -2.789643 | 2.040248 | -1.838780 |
| H | -0.003335 | -0.501041 | 2.518935 |
| H | -0.003773 | -0.392034 | -0.009721 |
| H | 2.589262 | 2.429557 | -0.529175 |
| H | 4.283982 | -1.437637 | -1.682132 |
| H | 0.563259 | 0.611899 | -4.003902 |
| H | 5.189935 | 0.886911 | -2.240861 |
| H | 0.895517 | 2.500402 | -1.770070 |
| C | -0.986809 | -2.220996 | 1.678801 |
| C | -0.990566 | -4.776416 | 0.530097 |
| C | 0.183417 | -2.761944 | 1.147071 |
| C | -2.156783 | -2.982363 | 1.630822 |
| C | -2.161648 | -4.248820 | 1.063459 |
| C | 0.178982 | -4.029936 | 0.574675 |
| H | 1.110862 | -2.186632 | 1.175359 |
| H | -3.079721 | -2.577698 | 2.053204 |
| H | -3.084051 | -4.830466 | 1.041319 |
| H | -0.990940 | -5.771470 | 0.083900 |
| H | 1.103594 | -4.433725 | 0.161016 |
| H | -1.412787 | 1.518004 | 2.972792 |

**H-bonded-product-minor-SS-cat**



*Geometry optimization, frequency calculation: PBEh-3c/def2-SV(P)*

| | |
|---|---|
| SFC energy | -1961.3594854 Hartree |
| Chemical potential | 0.522772 Hartree |
| Entropy | 0.000342 Hartree/K |
| Inner energy | 0.623820 Hartree |
| In(Qtrans) | 19.9343 |
| In(Qrot) | 17.1991 |
| In(Qvib) | 34.9254 |
| ZPE | 0.590809 Hartree |
| Enthalpy | 0.624764 Hartree |

*Single point energy: M06-2X/def2-TZVP*

| | |
|---|---|
| SCF energy | -1966.26982049 Hartree |

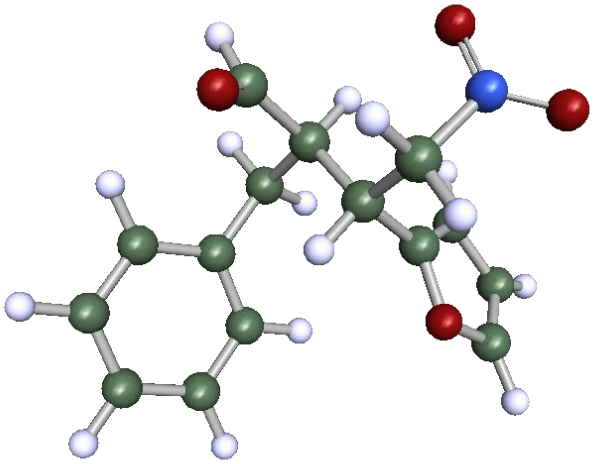
*Cartesian coordinates*

| | | | |
|---|---|---|---|
| N | -1.113229 | 1.713613 | -0.718225 |
| C | -2.354919 | 2.448083 | -0.487571 |
| C | -2.111188 | 3.805131 | -1.136518 |
| C | -1.206529 | 3.453548 | -2.310349 |
| C | -0.280011 | 2.393064 | -1.719530 |
| C | 0.975406 | 3.005315 | -1.090943 |
| N | 1.786343 | 2.036940 | -0.401791 |
| C | 2.672458 | 1.248161 | -1.068418 |
| O | 3.052814 | 1.452164 | -2.195043 |
| N | 3.086276 | 0.143102 | -0.343645 |
| S | 4.481382 | -0.733764 | -0.771215 |
| O | 5.118326 | -1.093888 | 0.522080 |
| C | 3.687986 | -2.292292 | -1.398653 |
| C | 4.871822 | -3.186504 | -1.762540 |
| C | 2.839776 | -2.921258 | -0.307727 |
| C | 2.871109 | -1.935692 | -2.632720 |
| C | -1.039486 | 0.308942 | -0.645229 |
| C | -1.819190 | -0.310499 | 0.536498 |

| | | | |
|---|---|---|---|
| C | -0.898914 | -0.929828 | 1.588841 |
| C | -4.693381 | -3.081791 | 2.523420 |
| C | -5.458140 | -1.962405 | 2.548415 |
| C | -4.890803 | -1.085289 | 1.574414 |
| C | -3.830074 | -1.748280 | 1.039439 |
| O | -3.713857 | -2.954498 | 1.616711 |
| C | -2.824445 | -1.366966 | 0.004801 |
| C | -3.497044 | -0.835351 | -1.220673 |
| N | -2.763230 | -0.306612 | -2.150709 |
| O | -3.081955 | 0.195976 | -3.205150 |
| O | -1.412478 | -0.358361 | -1.886852 |
| H | -4.572641 | -0.833751 | -1.381562 |
| H | -2.254922 | -2.278425 | -0.256806 |
| H | -5.232468 | -0.089615 | 1.305161 |
| H | -4.732430 | -4.017203 | 3.074841 |
| H | -6.323500 | -1.780994 | 3.178668 |
| H | 5.489928 | -3.424792 | -0.886339 |
| H | 4.504837 | -4.133466 | -2.185374 |
| H | 3.413193 | -3.065911 | 0.618528 |
| H | 2.479706 | -3.907813 | -0.637285 |
| H | 2.523720 | -2.858370 | -3.122154 |
| H | 1.952315 | -2.311398 | -0.083658 |
| H | 1.981110 | -1.340723 | -2.387419 |
| H | -0.385232 | -1.798672 | 1.146924 |
| H | -2.424338 | 0.469218 | 1.018626 |
| H | -3.234401 | 1.973360 | -0.953363 |
| H | -3.047853 | 4.293178 | -1.436346 |
| H | -1.602901 | 4.486361 | -0.436584 |
| H | -1.799594 | 3.010734 | -3.123869 |
| H | 0.038383 | 1.686458 | -2.500808 |
| H | 0.698051 | 3.788317 | -0.369256 |
| H | -0.664002 | 4.315193 | -2.724542 |
| H | -2.579665 | 2.551322 | 0.587441 |
| H | -1.525274 | -1.340017 | 2.398520 |
| H | 0.017157 | 0.008324 | -0.591449 |
| H | 2.781774 | 0.005587 | 0.617140 |
| H | 3.458135 | -1.368254 | -3.369050 |
| H | 1.579144 | 3.485727 | -1.872857 |
| H | 5.517863 | -2.718796 | -2.521298 |
| H | 1.497073 | 1.783467 | 0.532362 |
| C | 0.131712 | -0.016419 | 2.201473 |
| C | 2.088687 | 1.619786 | 3.386802 |
| C | -0.142821 | 1.315481 | 2.517213 |
| C | 1.400581 | -0.513303 | 2.509227 |
| C | 2.373844 | 0.291988 | 3.092512 |
| C | 0.824559 | 2.124280 | 3.103863 |
| H | -1.123079 | 1.740693 | 2.301736 |
| H | 1.637949 | -1.554922 | 2.283869 |
| H | 3.363360 | -0.119354 | 3.294235 |
| H | 2.849610 | 2.259269 | 3.833821 |

| | | | |
|---|---|---|---|
| H | 0.587907 | 3.163096 | 3.335939 |

**Isolated RR-product**



*Geometry optimization, frequency calculation: PBEh-3c/def2-SV(P)*

| | |
|---|---|
| SFC energy | -933.4607713 Hartree |
| Chemical potential | 0.237089 Hartree |
| Entropy | 0.000226 Hartree/K |
| Inner energy | 0.303608 Hartree |
| In(Qtrans) | 19.0204 |
| In(Qrot) | 15.4418 |
| In(Qvib) | 17.7625 |
| ZPE | 0.286399 Hartree |
| Enthalpy | 0.304552 Hartree |

*Single point energy: M06-2X/def2-TZVP*

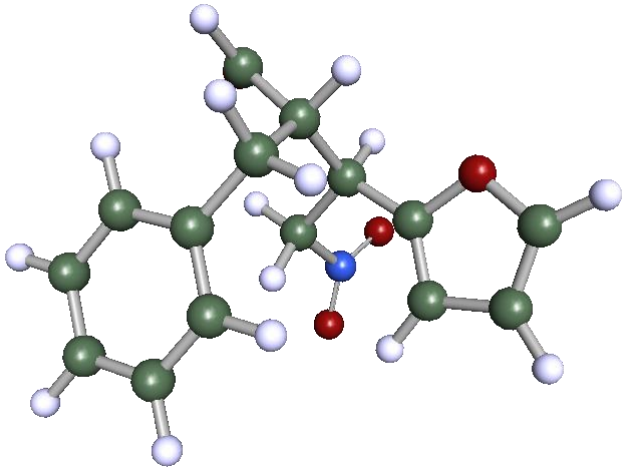
| | |
|---|---|
| SCF energy | -936.12893716 Hartree |

*Cartesian coordinates*

| | | | |
|---|---|---|---|
| C | 2.344567 | 0.868390 | -0.980698 |
| C | 0.909937 | 0.435612 | -1.154957 |
| C | 0.009146 | 1.606079 | -0.674345 |
| C | -2.659302 | -2.389883 | -0.243311 |
| C | -2.882729 | -1.836520 | -1.460375 |
| C | -1.685564 | -1.129666 | -1.788678 |
| C | -0.839356 | -1.307264 | -0.738596 |
| O | -1.431206 | -2.074838 | 0.191674 |
| C | 0.577036 | -0.903517 | -0.484469 |
| C | 1.513526 | -2.079569 | -0.818845 |
| N | 1.443003 | -2.456420 | -2.258362 |
| O | 0.929736 | -3.496941 | -2.544207 |
| O | 1.899902 | -1.670347 | -3.045962 |
| H | 1.217422 | -2.962361 | -0.242198 |
| H | 0.701851 | -0.769683 | 0.602784 |
| H | -1.486436 | -0.568057 | -2.696955 |
| H | -3.266757 | -3.010407 | 0.409835 |

| | | | |
|---|---|---|---|
| H | -3.784761 | -1.921796 | -2.058531 |
| H | -0.996430 | 1.463228 | -1.089495 |
| H | 0.388664 | 2.535837 | -1.128736 |
| H | 2.624006 | 1.735898 | -1.631038 |
| C | -0.081132 | 1.762869 | 0.819401 |
| C | -0.244033 | 1.999267 | 3.608114 |
| C | 0.924794 | 2.404811 | 1.542491 |
| C | -1.176789 | 1.254262 | 1.517519 |
| C | -1.258314 | 1.368567 | 2.899614 |
| C | 0.846824 | 2.520989 | 2.923933 |
| H | 1.783651 | 2.833071 | 1.023027 |
| H | -1.985483 | 0.767383 | 0.969560 |
| H | -2.124159 | 0.964447 | 3.424923 |
| H | -0.306135 | 2.090623 | 4.692806 |
| H | 1.643962 | 3.027280 | 3.468997 |
| O | 3.135758 | 0.406128 | -0.215197 |
| H | 2.558899 | -1.838480 | -0.595842 |
| H | 0.755902 | 0.371109 | -2.243983 |

**Isolated SR-product**



*Geometry optimization, frequency calculation: PBEh-3c/def2-SV(P)*

| | |
|---|---|
| SFC energy | -933.4598453 Hartree |
| Chemical potential | 0.239000 Hartree |
| Entropy | 0.000220 Hartree/K |
| Inner energy | 0.303533 Hartree |
| In(Qtrans) | 19.0204 |
| In(Qrot) | 15.4157 |
| In(Qvib) | 15.7766 |
| ZPE | 0.286411 Hartree |
| Enthalpy | 0.304478 Hartree |

*Single point energy: M06-2X/def2-TZVP*

| | |
|---|---|
| SCF energy | -936.12811706 Hartree |

*Cartesian coordinates*

| | | | |
|---|---|---|---|
| C | 1.666760 | -0.329502 | -2.389405 |
| C | 1.600217 | 0.019887 | -0.922565 |
| C | 0.943087 | 1.393067 | -0.689739 |
| C | 2.493459 | -0.224820 | 3.155223 |
| C | 1.209930 | -0.252945 | 3.586807 |
| C | 0.424772 | -0.619810 | 2.449376 |
| C | 1.302026 | -0.788576 | 1.423192 |
| O | 2.551538 | -0.546335 | 1.853489 |
| C | 1.144484 | -1.147109 | -0.019155 |
| C | -0.267290 | -1.651880 | -0.292341 |
| N | -0.552078 | -2.928157 | 0.445873 |
| O | -1.648649 | -3.048960 | 0.913500 |
| O | 0.311844 | -3.754735 | 0.487317 |
| H | -0.396957 | -1.899185 | -1.353868 |
| H | 1.827073 | -1.982842 | -0.241264 |
| H | -0.652493 | -0.752091 | 2.419096 |
| H | 3.436539 | -0.007263 | 3.649111 |
| H | 0.857219 | -0.046166 | 4.592638 |
| H | 1.426151 | 2.115047 | -1.369910 |
| H | 2.668747 | 0.183027 | -0.680017 |
| H | 1.202228 | 1.730459 | 0.322812 |
| H | 2.005144 | 0.525213 | -3.031539 |
| C | -0.550733 | 1.453435 | -0.866977 |
| C | -3.340035 | 1.495778 | -1.157348 |
| C | -1.380951 | 1.687900 | 0.228739 |
| C | -1.142848 | 1.263845 | -2.116392 |
| C | -2.523925 | 1.280007 | -2.261247 |
| C | -2.763204 | 1.707324 | 0.088170 |
| H | -0.935497 | 1.846643 | 1.212241 |
| H | -0.524314 | 1.106630 | -3.002086 |
| H | -2.965632 | 1.125043 | -3.245964 |
| H | -4.424314 | 1.505034 | -1.269850 |
| H | -3.393359 | 1.886956 | 0.959608 |
| O | 1.443630 | -1.397311 | -2.873360 |
| H | -1.052667 | -0.947411 | -0.004465 |

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