Supporting Information of Chiral Phosphoproline-Catalyzed Asymmetric Michael Addition of Ketones to Nitroolefins: an Experimental and Theoretical Study.

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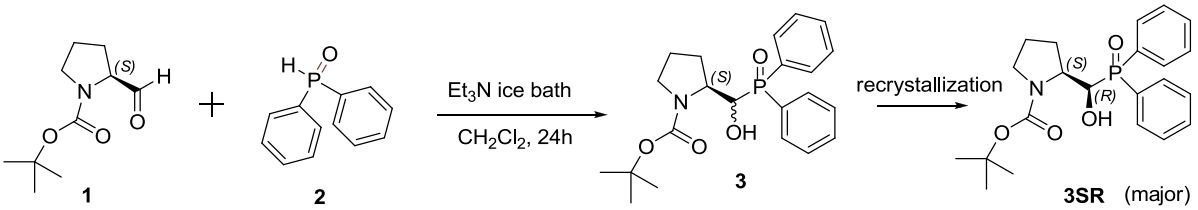
1 General Information:

- ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra were measured on Bruker 400M spectrometers with $CDCl_3$ as solvent and tetramethylsilane (TMS) as internal standard or 85% H_3PO_4 as external standard for ^{31}P NMR. Chemical shifts were reported in units (ppm) by assigning TMS resonance in the ^{1}H spectrum as 0.00 ppm and $CDCl_3$ resonance in the ^{13}C spectrum as 77.0 ppm. All coupling constants (*J* values) were reported in Hertz (Hz). Chemical shifts of common trace ^{1}H NMR impurities (ppm): H_2O: 1.56, $CHCl_3$: 7.26.
- Melting points were determined on a WRS-1B melting point apparatus and were uncorrected.
- Infrared spectra were measured with a Nicolet Avatar 330 FT-IR spectrometer.
- Optical rotations were measured in $CHCl_3$ with a Perkin-Elmer 341 automatic polarimeter. Absolute configuration of the products was determined by comparison with compounds previously published.
- Elemental analyses were performed by the Elemental Analysis Section of Xiamen University. HRMS spectra were recorded on a Bruker En Apex ultra 7.0 FT-MS apparatus. All new compounds were further characterized by elemental analysis or HRMS.
- Enantioselectivities were determined by High performance liquid chromatography (HPLC) analysis employing a Daicel Chirapak AS-H column.
- All the reagents were purchased from Alfa Aesar and J&K Chemical and used without further purification. Column chromatography was performed on silica gel 300- 400 mesh. Spectroscopy data of the known compounds matches with the data reported in the corresponding references. Nitroolefins were synthesized according to literature procedures[1]. the product from L-proline catalysed reaction gave very poor enantioselectivity[2]. Accordingly, These enantiomers were used as a reference to determine the ee values for our reaction.

2 Experimental section.

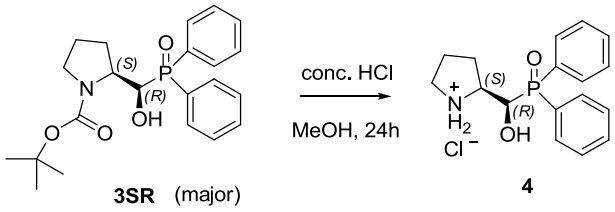
2.1 Synthesis of new catalyst 4:



***S*-2-(*R*-Diphenylphosphanyl-hydroxy-methyl)-pyrrolidine-1-carboxylic acid tert-butyl ester (3SR)**

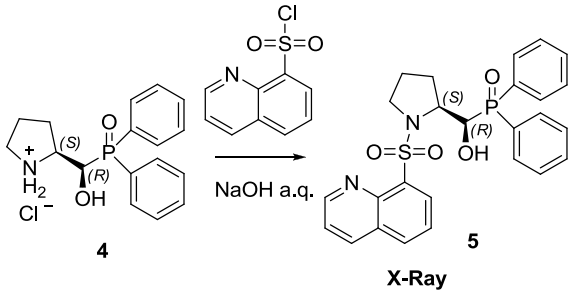
m.p. 162 °C (solvent: acetate); $[\alpha]_D^{25}$ = -5.40 (c = 1.0, $CHCl_3$), ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (m, 4H), 7.44 (m, 6H), 6.09 (d, *J* = 7.2 Hz, 1H), 4.79 (s, 1H), 4.41 - 4.20 (m, 1H), 3.56 - 3.42 (m, 1H), 3.33 (ddd, *J* = 10.6, 8.5, 6.7 Hz, 1H), 2.59 (m, 1H), 2.19 - 2.00 (m, 2H), 1.76 - 1.59 (m, 1H), 1.28 - 1.13 (m, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ157.2, 134.2 (d, *J* = 95.8 Hz), 132.2 (d, *J* = 8.3 Hz), 131.5 (d, *J* = 11.3 Hz), 130.9 (d, *J* = 8.7 Hz), 128.5 (d, *J* = 11.3 Hz), 128.0 (d, *J* = 11.3 Hz), 80.5, 73.9 (d, *J* = 83.2 Hz) 62.1, 48.2, 28.3, 24.6(2C); ^{31}P NMR (162 MHz, $CDCl_3$) δ 26.56; IR (KBr, film), υ_{max} (cm^{-1}): 3440, 3132, 2965, 2927, 2869, 1690, 1434,

1396, 1360, 1159, 1117, 1085, 752, 729, 695, 528; Anal. calcd. (%) for $C_{22}H_{28}NO_4P$: C, 65.82; H, 7.03; N, 3.49; Found: C, 65.90; H, 7.33; N, 3.46.



***S*-2-[*R*-(Diphenyl-phosphinoyl)-hydroxy-methyl]-pyrrolidinium chloride (4)**

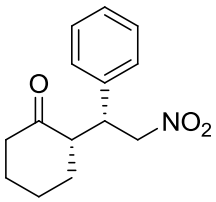
m.p. 130 °C (solvent: MeOH); $[\alpha]_D^{25}$ = -23.8 (c = 1.3, $CHCl_3$) ^{1}H NMR ($CDCl_3$, 400MHz): 1.47 - 1.55(m, 1H), 1.69 - 1.82 (m, 2H), 1.83 - 1.93 (m, 1H), 2.91 (s, 1H), 3.21 (s, 2H), 4.18 (s, 1H), 5.34 - 5.38 (m, 1H), 6.17 (dd, 1H, J= 6.3, 18.4 Hz), 7.38 - 7.43 (m, 2H), 7.44 - 7.51 (m, 3H), 7.54 - 7.61 (m, 1H), 7.82 - 7.87 (m, 2H), 7.91 - 7.96 (m, 2H), 9.32 (s, 1H), 9.73 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 132.6 (d, *J* = 8.6 Hz), 131.3 (d, *J* = 9.4 Hz), 129.1 (d, *J* = 227.8 Hz), 128.9 (d, *J* = 11.8 Hz), 128.5 (d, *J* = 11.6 Hz), 67.8 (d, *J* = 90.9 Hz), 61.1 (d, *J* = 9.1 Hz), 45.4, 24.6; ^{31}P NMR ($CDCl_3$, 160 MHz): 29.10; IR(KBr, film) υ_{max}(cm^{-1}): 3410, 3205, 3058, 2981, 2767, 2940, 1623, 1588, 1434, 1393, 1159, 1120, 1095, 1069, 1024, 995, 976, 749, 723, 694, 534; ESI-HRMS: calcd. for [$C_{17}H_{20}NO_2P$+H^+], 302.1304; found, 302.1303.



***R*-(Diphenyl-phosphinoyl)-[*S*-1-(quinoline-8-sulfonyl)-pyrrolidin-2-yl]-methanol (5)**

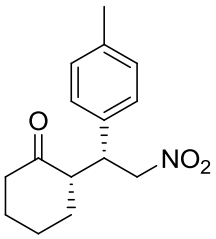
m.p. 168 °C (solvent: CH_2Cl_2:MeOH = 20 : 1); $[\alpha]_D^{25}$ = -73.3 (c = 1.2, $CHCl_3$); ^{1}H NMR ($CDCl_3$, 400 MHz): 1.42 - 1.53 (m, 1H), 1.78 - 1.88 (m, 2H), 2.20 - 2.29 (m, 2H), 3.06 - 3.12 (m, 1H), 3.50 (td, J = 4.28, 8.66 Hz, 1H), 4.76 (tt, J= 1.80, 7.25 Hz, 1H), 5.12 (dd, J = 5.20, 20.01 HZ, 1H), 5.30 (s, 1H), 5.64 (t, J = 5.54 Hz, 1H), 7.45 - 7.59 (m, 7H), 7.63 (t, J= 7.8 Hz, 1H), 7.98-8.04 (m, 4H), 8.06 (dd, J = 1.2, 8.2 Hz, 1H), 8.27 (dd, J = 1.7, 8.4 Hz, 1H), 8.54 (dd, J = 1.3, 7.4 Hz, 1H), 8.78 (dd, J = 1.7, 4.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): 25.4, 27.1, 48.9, 62.1 (d, J= 9.47 Hz), 71.0 (d, J= 85.73 Hz), 122.1, 125.6, 128.4 (d, J= 11.68 Hz), 128.7 (d, J = 11.40 Hz), 129.2, 131.2 (d, J = 9.03 Hz), 131.9 (d, J =8.85 Hz), 131.7 (d, J = 2.12 Hz), 131.3 (d, J =1.78 Hz), 134.1, 134.5, 137.2, 143.6, 151.2; ^{31}P NMR ($CDCl_3$, 160 MHz): 27.76; IR(KBr, film), υ_{max}(cm^{-1}): 3430, 3202, 3058, 2932, 2920, 2872, 2850, 1610, 1559, 1495, 1434, 1338, 1213, 1172, 1165, 1139, 1117, 1095, 1066, 1024, 1002, 823, 790, 743, 723, 695, 605, 573; Anal. calcd. (%) for $C_{26}H_{25}N_2O_4PS$: C, 63.40; H, 5.12; N, 5.69. Found: C, 63.38; H, 4.86; N, 5.55.

2.2 Characterization data of Michael products 3a-3m



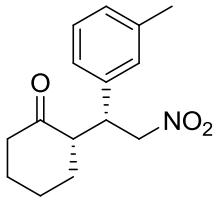
(*S*)-2-((*R*)-2-Nitro-1-phenylethyl)cyclohexanone

3a[3]**:** prepared according to the general procedure from (*E*)-(2-nitrovinyl)benzene (38 mg, 0.25 mmol) to provide the title compound as a white solid (51 mg, 82% yield) after silica gel chromatography (EtOAc : hexane = 1 : 9). white solid; m.p. 124.5 ℃ (solvent: EtOAc : hexane = 1 : 9); $[\alpha]_D^{20}$ = -20.4 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 - 7.23 (m, 3H), 7.17 (d, *J* = 7.7 Hz, 2H), 4.93 (dd, *J* = 12.5, 4.5 Hz, 1H), 4.64 (dd, *J* = 12.4, 9.9 Hz, 1H), 3.79 (td, *J* = 9.9, 4.5 Hz, 1H), 2.76 - 2.64 (m, 1H), 2.52 - 2.45 (m, 1H), 2.39 (td, *J* = 12.6, 5.9 Hz, 1H), 2.08 (dtd, *J* = 8.8, 5.9, 3.0 Hz, 1H), 1.86 - 1.57 (m, 4H), 1.34 - 1.16 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 211.8, 137.8, 129.0, 128.2, 127.8, 78.9, 52.6, 44.0, 42.7, 33.2, 28.5, 25.0; HPLC: Chiralpak AS-H (hexane/*i*-PrOH, 85/15, flow rate 1 mL/min, λ = 230 nm), *t*R (minor) = 17.9 min, *t*R (major) = 29.4 min; 96% ee.



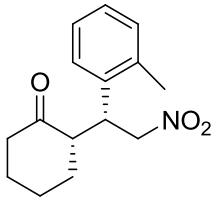
(*S*)-2-((*R*)-2-Nitro-1-*p*-tolylethyl)cyclohexanone

3b: prepared according to the general procedure from (*E*)-1-methyl-4-(2-nitrovinyl)benzene (41 mg, 0.25 mmol) to provide the title compound as a white solid (57 mg, 88% yield) after silica gel chromatography (EtOAc : hexane = 1 : 9). Crystals; m.p. 120.8 ℃ (solvent: EtOAc : hexane = 1 : 9); $[\alpha]_D^{20}$ = -26.2 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.12 (d, *J* = 8.0 Hz, 2H), 7.04 (d, *J* = 8.1 Hz, 2H), 4.91 (dd, *J* = 12.4, 4.6 Hz, 1H), 4.61 (dd, *J* = 12.4, 9.9 Hz, 1H), 3.72 (td, *J* = 9.9, 4.6 Hz, 1H), 2.70 - 2.63 (m, 1H), 2.51 - 2.33 (m, 2H), 2.31 (s, 1H), 2.11 - 2.02 (m, 1H), 1.85 - 1.50 (m, 4H), 1.32 - 1.23 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 211.9, 137.4, 134.6, 129.6, 128.0, 79.0, 52.6, 43.6, 42.7, 33.1, 28.5, 25.0, 21.0. HPLC analysis (Chiralpak AS-H column, hexane: 2-propanol = 85:15, flow rate = 1.0 mL/min, wavelength = 230 nm): Rt = 10.94 (minor) and 16.91 min (major); syn/anti = 92/8, 92% ee.



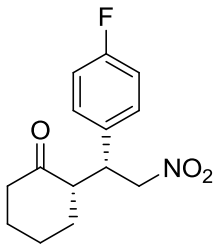
(*S*)-2-((*R*)-2-Nitro-1-*m*-tolylethyl)cyclohexanone

3c[4]**:** prepared according to the general procedure from (*E*)-1-methyl-3-(2-nitrovinyl)benzene (57 mg, 0.35 mmol) to provide the title compound as a white solid (74 mg, 91% yield) after silica gel chromatography (EtOAc : hexane = 1 : 9); pale yellow solid; m.p. 96.2 ℃ (solvent: EtOAc : hexane = 1 : 9); $[\alpha]_D^{20}$= -27.0 (c = 1.2, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 - 7.17 (m, 1H), 7.07 (d, *J* = 7.4 Hz, 1H), 6.95 (d, *J* = 6.1 Hz, 1H), 4.92 (dd, *J* = 12.5, 4.5 Hz, 1H), 4.62 (dd, *J* = 12.5, 9.9 Hz, 1H), 3.71 (td, *J* = 9.9, 4.5 Hz, 1H), 2.71 - 2.63 (m, 1H), 2.53 - 2.39 (m, 2H), 2.32 (s, 3H), 2.12 - 2.03 (m, 1H), 1.82 - 1.51 (m, 4H), 1.24 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 211.9, 138.6, 137.7, 129.0, 128.8, 128.5, 125.0, 78.9, 52.6, 43.9, 42.7, 33.2, 28.5, 25.0, 21.4; HPLC analysis (Chiralpak AS-H column, hexane: 2-propanol = 85:15, flow rate = 1.0 mL/min, wavelength = 230 nm): Rt = 10.94 (minor) and 16.20 min (major), syn/anti = 92/8, 96% ee.



(*S*)-2-((*R*)-2-Nitro-1-*o*-tolylethyl)cyclohexanone

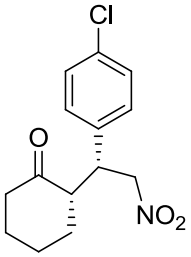
3d: prepared according to the general procedure from(*E*)-1-methyl-2-(2-nitrovinyl)benzene (53 mg, 0.33 mmol) to provide the title compound as a white solid (67 mg, 87% yield) after silica gel chromatography (EtOAc : hexane = 1 : 9); white liquid; $[\alpha]_D^{20}$ = -27.7 (c = 1.3, $CHCl_3$)**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 - 7.08 (m, 4H), 4.99 (dd, *J* = 12.6, 4.4 Hz, 1H), 4.61 (dd, *J* = 12.6, 10.1 Hz, 1H), 4.12 (td, *J* = 10.3, 4.4 Hz, 1H), 2.71 - 2.60 (m, 1H), 2.51 - 2.44 (m, 1H), 2.44 - 2.33 (m, 4H), 2.13 - 2.06 (m, 1H), 1.80 - 1.49 (m, 4H) , 1.29 - 1.22 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 212.2, 137.4, 136.4, 131.0, 127.3, 126.7, 125.7, 78.8, 53.5, 42.9, 38.3, 32.9, 28.7, 25.4, 19.9; HPLC analysis (Chiralpak AS-H column, hexane: 2-propanol = 85:15, flow rate = 1.0 mL/min, wavelength = 230 nm): Rt = 10.83 (minor) and 15.88 min (major) syn/anti = 93/7, 95% ee.



(*S*)-2-((*R*)-1-(4-Fluorophenyl)-2-nitroethyl)cyclohexanone

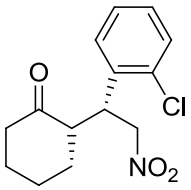
3e[5]**:** prepared according to the general procedure from (E)-1-fluoro-4-(2-nitrovinyl)benzene (42 mg, 0.25 mmol) to provide the title compound as a white solid (66 mg, 99% yield) after silica gel chromatography

(EtOAc : hexane = 1 : 9); pale yellow solid; m.p. 56.8 ℃ (solvent: EtOAc : hexane = 1 : 9); $[\alpha]_D^{20}$ = -16.4 (c = 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.22 - 7.09 (m, 2H), 7.07 - 6.94 (m, 2H), 4.92 (dd, *J* = 12.5, 4.6 Hz, 1H), 4.60 (dd, *J* = 12.5, 9.9 Hz, 1H), 3.77 (td, *J* = 9.8, 4.6 Hz, 1H), 2.73 - 2.61 (m, 1H), 2.52 - 2.44 (m, 1H), 2.42-2.34 (m, 1H), 2.15 - 2.03 (m, 1H), 1.85 - 1.51 (m, 4H), 1.26 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 211.5, 162.2 (d, *J* = 246.7 Hz), 133.5 (d, *J* = 3.4 Hz), 129.8 (d, *J* = 8.0 Hz), 115.9 (d, *J* = 21.5 Hz), 78.8, 52.6, 43.3, 42.7, 33.1, 28.4, 25.0; HPLC analysis (Chiralpak AS-H column, hexane: 2-propanol = 85:15, flow rate = 1.0 mL/min, wavelength = 230 nm): Rt = 15.93 (minor) and 24.71 min (major) syn/anti = 90/10, 94% ee.



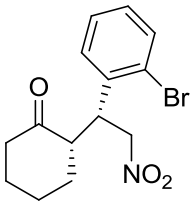
(*S*)-2-((*R*)-1-(4-Chlorophenyl)-2-nitroethyl)cyclohexanone

3f[6]**:** prepared according to the general procedure from (E)-1-chloro-4-(2-nitrovinyl)benzene (46 mg, 0.25 mmol) to provide the title compound as a white solid (61 mg, 87% yield) after silica gel chromatography (EtOAc : hexane = 1 : 9); pale yellow solid; m.p. 85.4 ℃ (solvent: EtOAc : hexane = 1 : 9); $[\alpha]_D^{20}$ = -27.8 (c = 1.1, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.30 (dt, *J* = 8.80, 2.24 Hz, 2H), 7.12 (dt, *J* = 8.76, 2.20 Hz, 2 H), 4.93 (dd, *J* = 12.6, 4.5 Hz, 1H), 4.61 (dd, *J* = 12.6, 10.0 Hz, 1H), 3.76 (td, *J* = 9.8, 4.5 Hz, 1H), 2.69 - 2.61 (m, 1H), 2.51 - 2.33 (m, 2H), 2.06 - 2.11 (m, 1H), 1.83 - 1.54 (m, 4H), 1.21 - 1.28 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 211.4, 136.3, 133.7, 129.1, 129.2, 78.6, 52.4, 43.4, 42.7, 33.1, 28.4, 25.1; HPLC analysis (Chiralpak AS-H column, hexane: 2-propanol = 85:15, flow rate = 1.0 mL/min, wavelength = 230 nm): Rt = 15.09 (minor) and 25.30 min (major), syn/anti = 92/8, 91% ee.



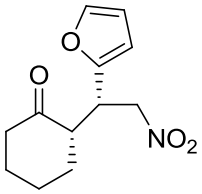
(*S*)-2-((*R*)-1-(2-Chlorophenyl)-2-nitroethyl)cyclohexanone

3g[6]**:** prepared according to the general procedure from (E)-1-chloro-4-(2-nitrovinyl)benzene (46 mg, 0.25 mmol) to provide the title compound as a white solid (66 mg, 94% yield) after silica gel chromatography (EtOAc : hexane = 1 : 9); white liquid; $[\alpha]_D^{20}$ = -48.9 (c = 0.9, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.39 - 7.36 (m, 1H), 7.28 - 7.17 (m, 3H), 4.94 - 4.85 (m, 1H), 4.26 - 4.32 (m, 1H), 2.92 (td, *J* = 12.0, 5.1 Hz, 1H), 2.52 - 2.44 (m, 1H), 2.35 - 2.43 (m, 1H), 2.07 - 2.13 (m,1H), 1.58 - 1.83 (m, 4H), 1.31 - 1.38 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 211.6, 135.5, 134.5, 130.4, 128.9, 127.4, 77.2, 51.7, 42.8, 33.1, 29.7, 28.5, 25.3; HPLC analysis (Chiralpak AS-H column, hexane: 2-propanol = 85:15, flow rate = 1.0 mL/min, wavelength = 230 nm): Rt = 14.01 (minor) and 19.31 min (major) syn/anti = 99/1, 96% ee.



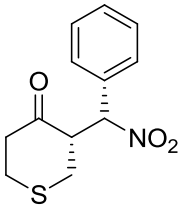
(*S*)-2-((*R*)-1-(2-Bromophenyl)-2-nitroethyl)cyclohexanone

3h[7]**:** prepared according to the general procedure from (E)-1-bromo-2-(2-nitrovinyl)benzene (57 mg, 0.25 mmol) to provide the title compound as a white solid (74 mg, 91% yield) after silica gel chromatography (EtOAc : hexane = 1 : 9); white solid; m.p. 80.3 ℃ (solvent: EtOAc : hexane = 1 : 9); $[\alpha]_D^{20}$ = -48.6 (c = 1.4, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.30 (td, *J* = 7.6, 1.2 Hz, 1H), 7.22 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.13 (td, *J* = 8.0, 1.8 Hz, 1H), 4.97 - 4.84 (m, 2H), 4.31 (m, 1H), 2.90 (br. s, 1H), 2.51 - 2.44 (m, 2H), 2.37 (tdd, *J* = 12.8, 5.9, 0.9 Hz, 1H), 2.10 (m, 1H), 1.86 - 1.53 (m, 4H), 1.40 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 211.5, 137.3, 133.7, 129.1, 128.0, 77.3, 52.1, 42.8, 33.0, 28.5, 25.3; HPLC analysis (Chiralpak AS-H column, hexane: 2-propanol = 85:15, flow rate = 1.0 mL/min, wavelength = 230 nm): Rt = 14.97 (minor) and 20.12 min (major) syn/anti = 99/1, 96% ee.



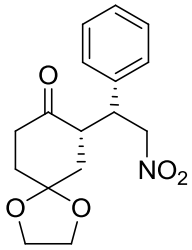
(*S*)-2-((*S*)-1-(Furan-2-yl)-2-nitroethyl)cyclohexanone

3i[8]**:** prepared according to the general procedure from (E)-2-(2-nitrovinyl)furan (35 mg, 0.25 mmol) to provide the title compound as a white solid (55 mg, 93% yield) after silica gel chromatography (EtOAc : hexane = 1 : 9); yellow liquid; $[\alpha]_D^{20}$ = -10.5 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (m, 1H), 6.29 (m, 1H), 6.21 - 6.10 (m, 1H), 5.07 - 4.53 (m, 2H), 3.97 (td, *J* = 9.1, 4.8 Hz, 1H), 2.86 - 2.71 (m, 1H), 2.51 - 2.30 (m, 2H), 2.20 - 2.04 (m, 1H), 1.96 - 1.58 (m, 5H), 1.36 - 1.24 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 210.9, 151.0, 142.3, 110.3, 109.0, 76.7, 51.1, 42.6, 37.6, 32.5, 28.2, 25.1; HPLC analysis (Chiralpak AS-H column, hexane: 2-propanol = 85:15, flow rate = 1.0 mL/min, wavelength = 254 nm): Rt = 12.75 (minor) and 15.28 min (major), syn/anti = 82/18, 91% ee.



(*S*)-3-((*R*)-Nitro(phenyl)methyl)dihydro-2*H*-thiopyran-4(3*H*)-one

3j[9]**:** To a solution of *trans*-nitrostyrene (38 mg, 0.25 mmol) and tetrahydrothiopyran-4-one **1b** (290 mg, 2.5 mmol) was added catalyst **4** (0.0125 mmol) in the presence of 10 mmol % 4-$NO_2C_6H_4COOH$ and 50 μL 1 mol/L KOH. The resulting mixture was stirred at room temperature (30℃). After the reaction was complete (monitored by TLC), the resulting residue was then purified by flash chromatography (hexane/EtOAc = 10/1) to give the product as white solid (84 mg, 87% yield). white solid; m.p. 121.3 ℃ (solvent: EtOAc : hexane = 1 : 10); $[\alpha]_D^{20}$ = -27.3 (c = 1.8, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 - 6.96 (m, 5H), 4.62 (ddd, *J* = 22.3, 12.6, 7.2 Hz, 2H), 3.91 (td, *J* = 10.2, 4.6 Hz, 1H), 3.21 - 2.64 (m, 5H), 2.59 - 2.51 (m, 1H), 2.39 (dd, *J* = 13.9, 9.3 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 209.5, 136.5, 129.3, 128.3, 128.2, 78.6, 55.0, 44.5, 43.5, 35.1, 31.6; HPLC analysis (Chiralpak AS-H column, hexane: 2-propanol = 85:15, flow rate = 1.0 mL/min, wavelength = 254 nm): Rt = 18.79(minor) and 24.78min (major), syn/anti = 95/5, 85% ee.

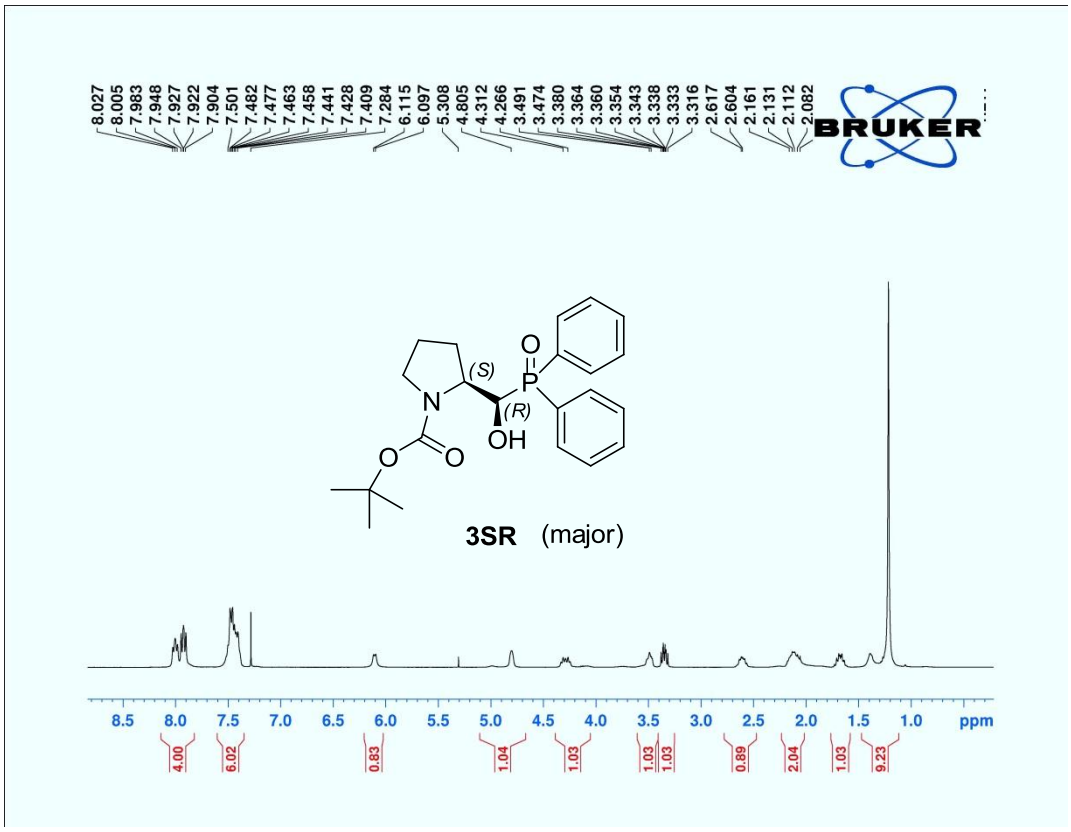


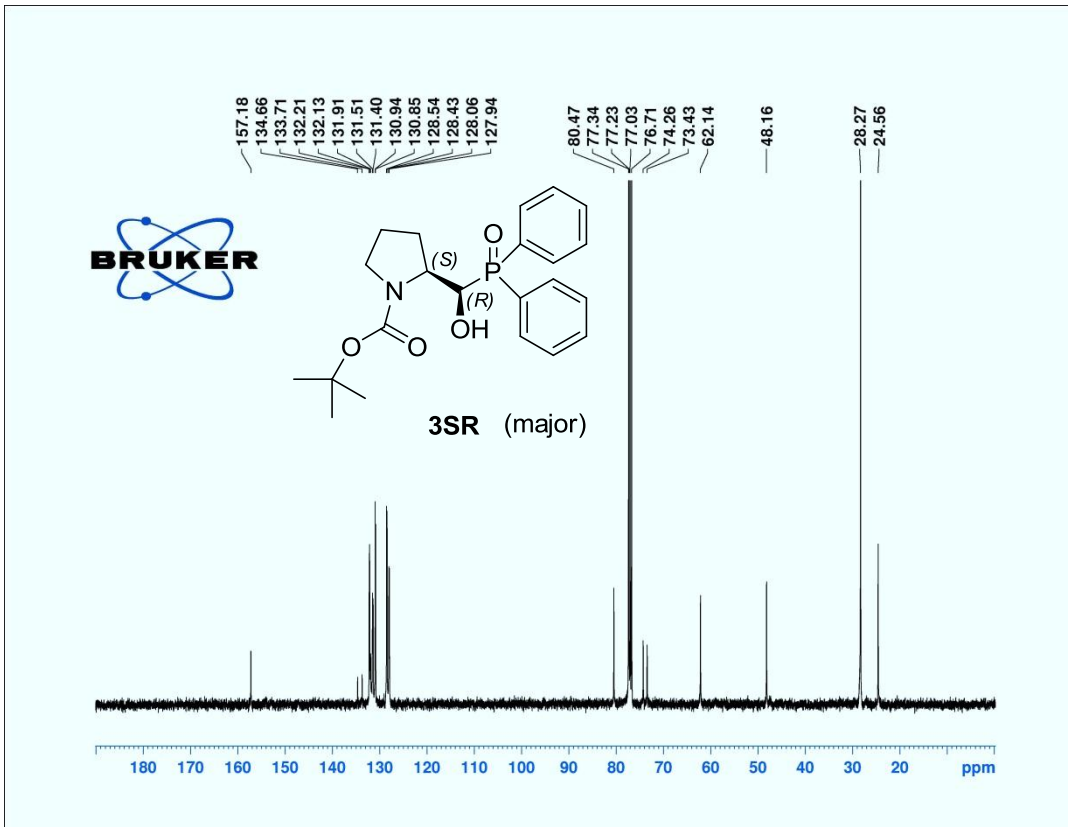
(*S*)-7-((*R*)-2-Nitro-1-phenylethyl)-1,4-dioxaspiro[4.5]decan-8-one

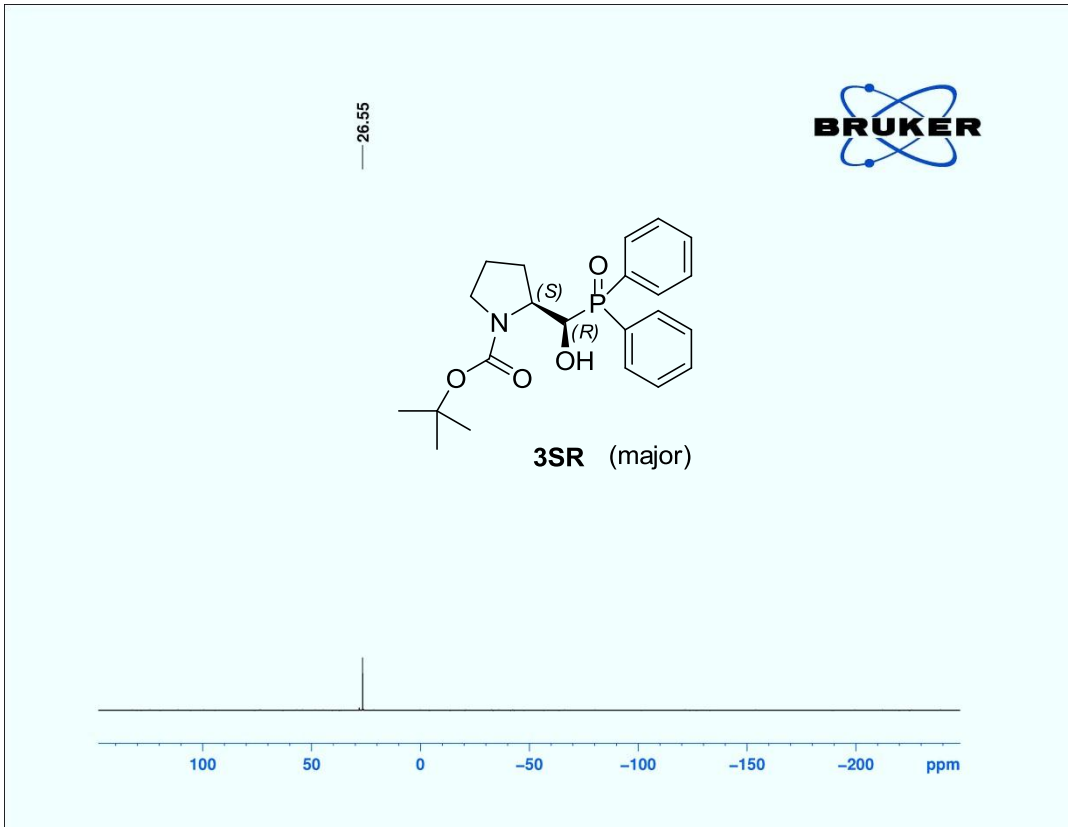
3k[10]**:** To a solution of *trans*-nitrostyrene (38 mg, 0.25 mmol) and tetrahydrothiopyran-4-one **1c** (390 mg, 2.5 mmol) was added catalyst **4** (0.0125 mmol) in the presence of 10 mmol % 4-$NO_2C_6H_4COOH$ and 50 μL 1 mol/L KOH. The resulting mixture was stirred at room 30 ℃. After the reaction was complete (monitored by TLC), the resulting residue was then purified by flash chromatography (hexane/EtOAc = 10/1) to give the product as white solid (70 mg, 90% yield). Crystals; m.p. 110 ℃ (solvent: EtOAc : hexane = 1 : 10); $[\alpha]_D^{20}$ = -9.8 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 - 7.14 (m, 3H), 7.09 (d, *J* = 7.0 Hz, 2H), 5.05 - 4.71 (m, 1H), 4.54 (dd, *J* = 12.4, 9.9 Hz, 1H), 4.03 - 3.55 (m, 5H), 2.99 (ddd, *J* = 12.8, 10.0, 5.5 Hz, 1H), 2.63 (td, *J* = 13.5, 6.5 Hz, 1H), 2.39 (ddd, *J* = 13.8, 5.0, 3.6 Hz, 1H), 2.04 - 1.80 (m, 2H), 1.61 (ddd, *J* = 13.3, 5.4, 3.4 Hz, 1H), 1.55 - 1.42 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 210.3, 137.3, 129.0, 128.2, 127.9, 107.0, 78.9, 64.8, 64.5, 48.2, 43.4, 39.4, 38.6, 35.1; HPLC analysis (Chiralpak AS-H column, hexane: 2-propanol = 85:15, flow rate = 1.0 mL/min, wavelength = 210 nm): Rt = 18.04 (minor) and 26.60 min (major), syn/anti = 90/10, 85% ee.

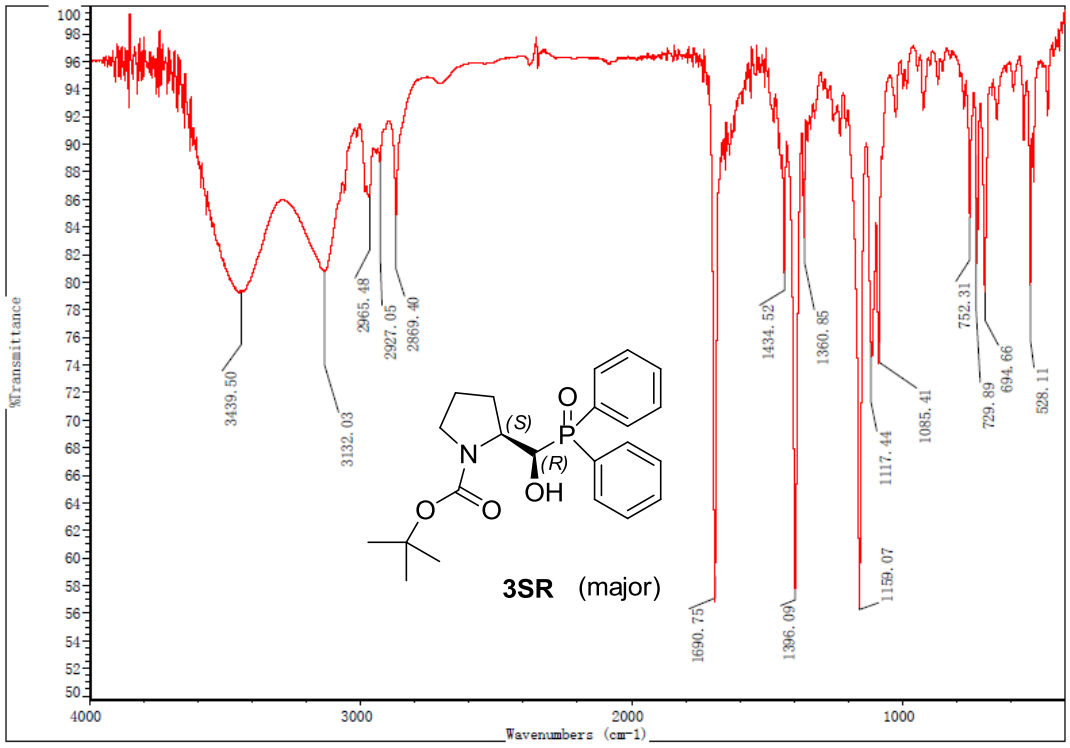
2.3 ^{1}H NMR and ^{13}C NMR Spectra of all compounds

2.3.1 The spectra of compound 3SR

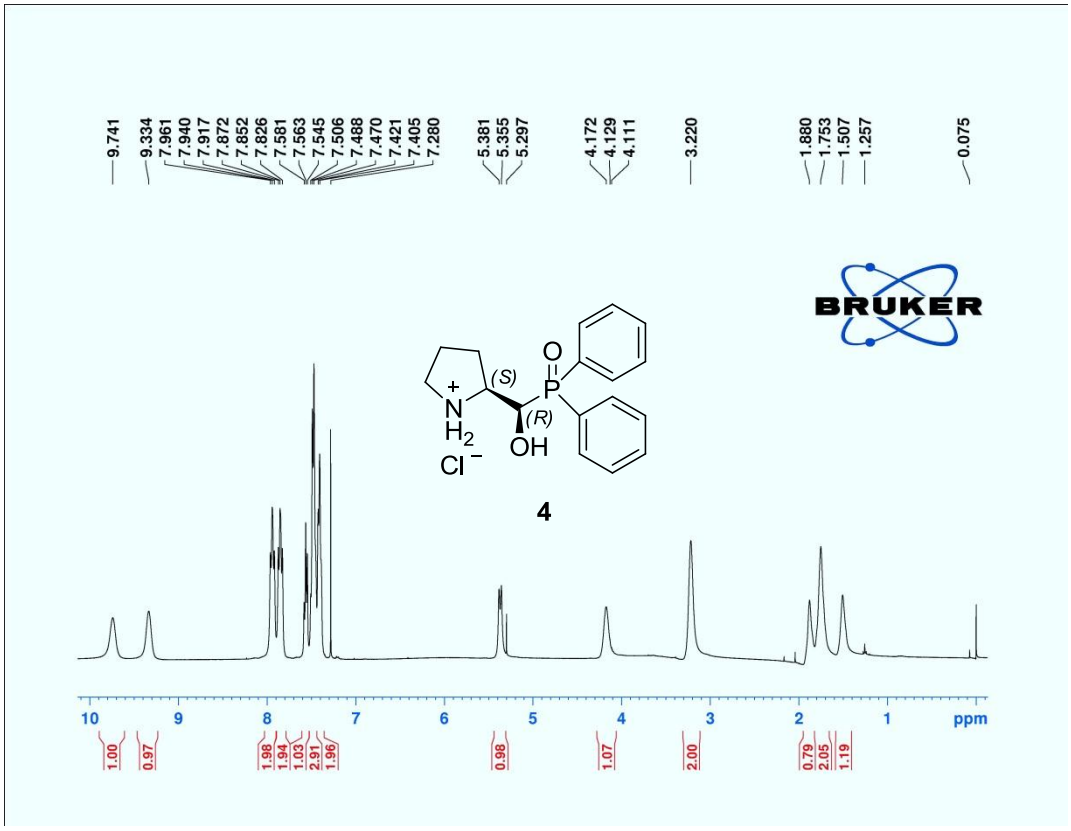


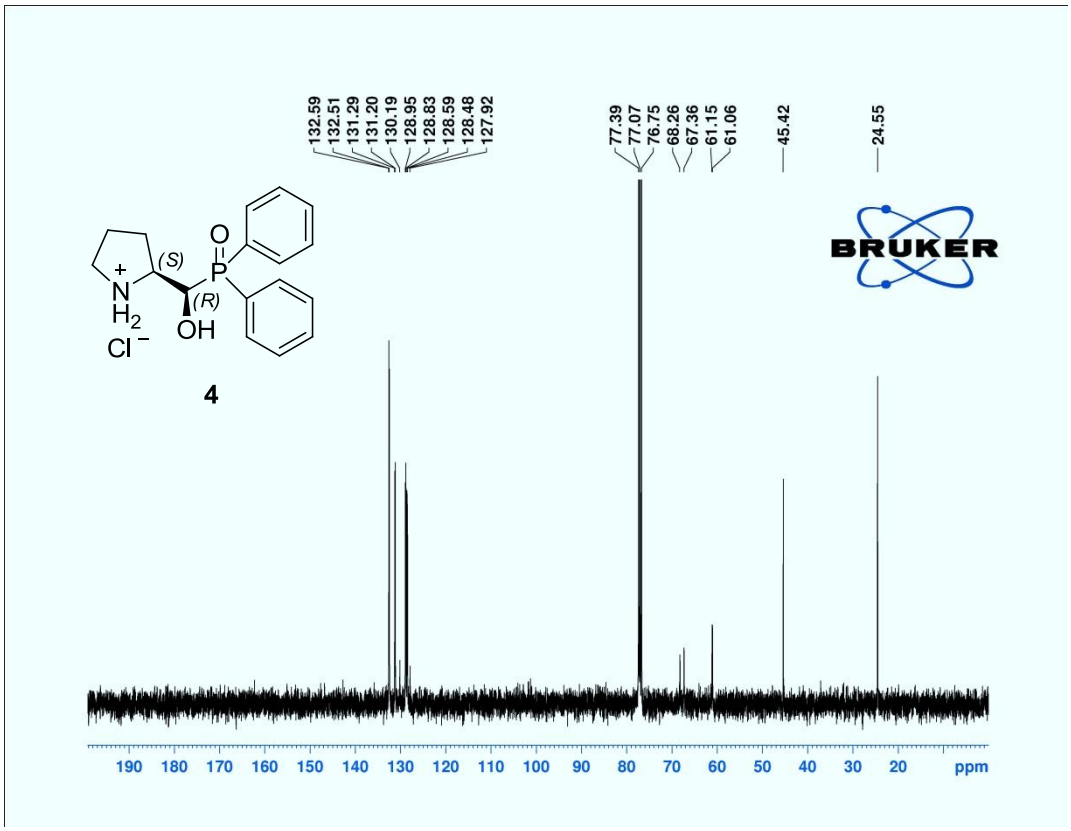


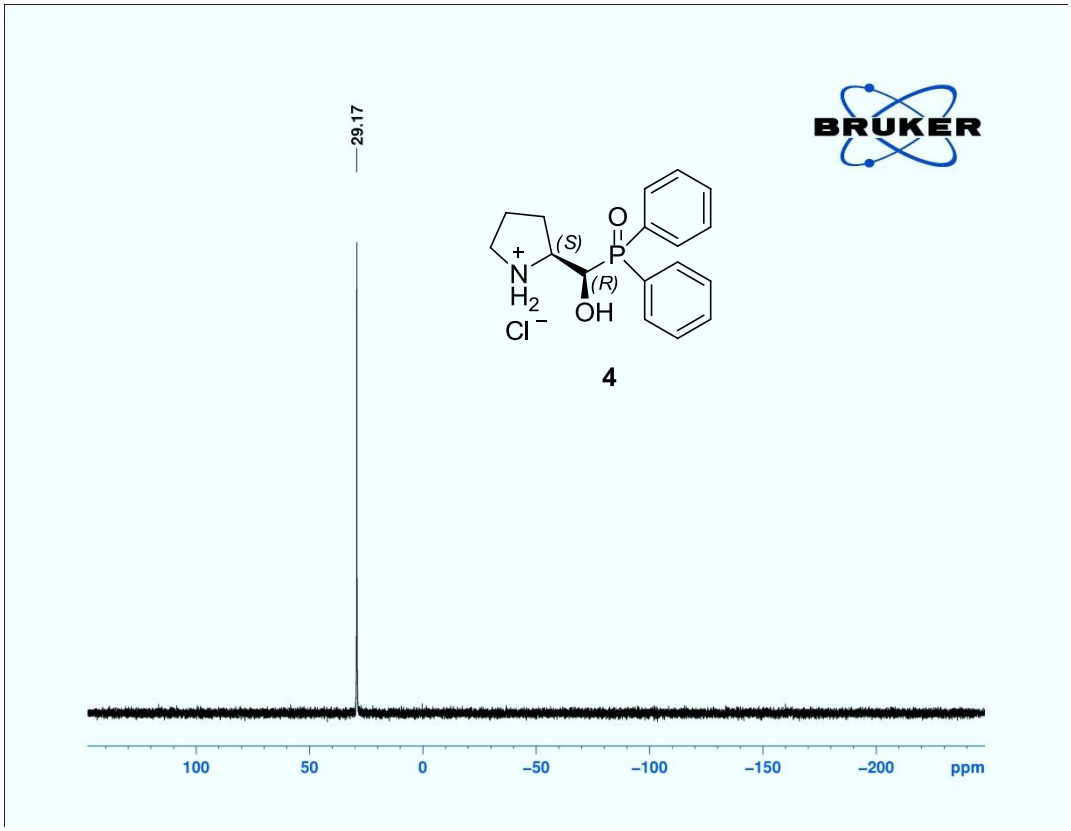

26.55
BRUKER
(S)
(R)
OH
3SR (major)
100
50
0
−50
−100
−150
−200
ppm

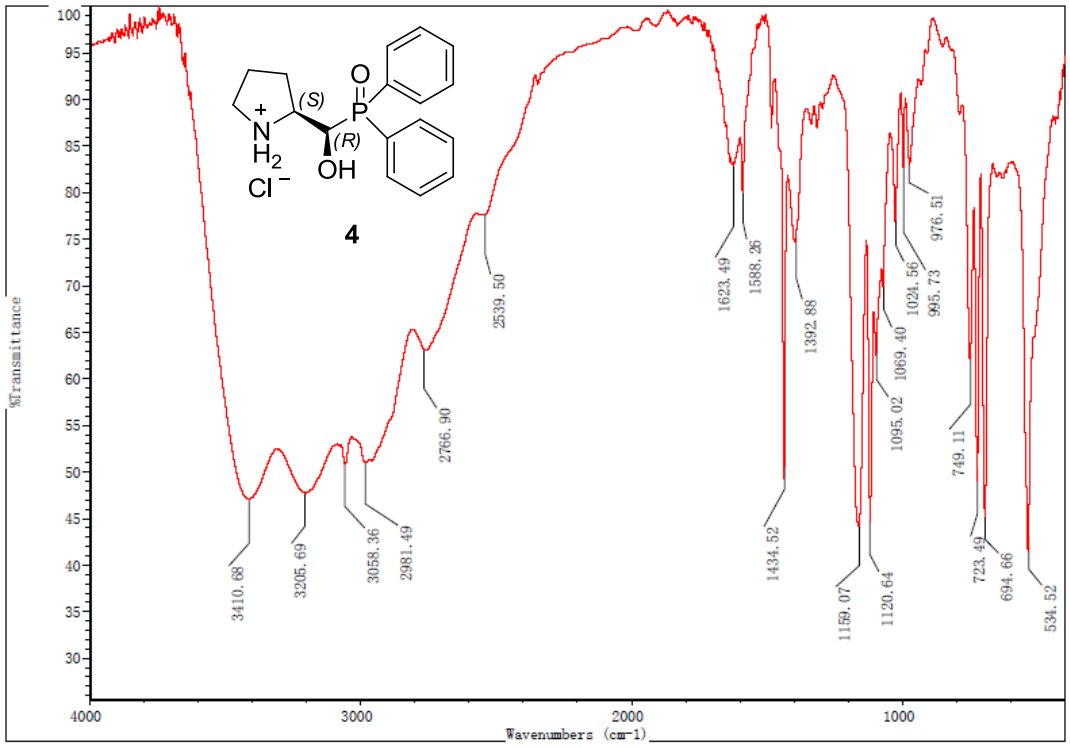

%Transmittance
3439.50
3132.03
2965.48
2927.05
2869.40
1690.75
1434.52
1396.09
1360.85
1159.07
1117.44
1085.41
752.31
729.89
694.66
528.11
(S)
(R)
OH
3SR (major)
4000
3000
2000
1000
Wavenumbers (cm-1)

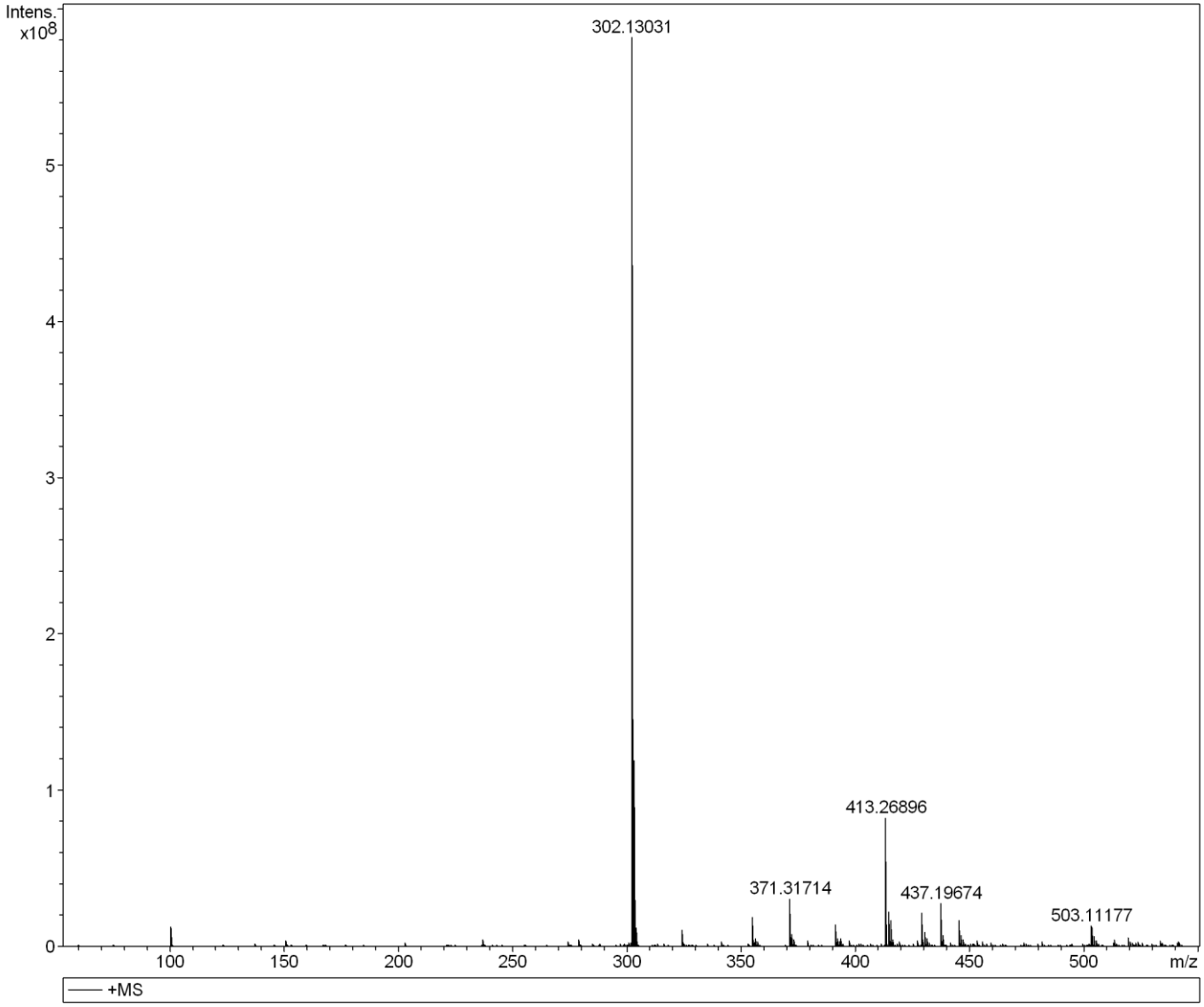
2.3.2 **The spectra of compound 4**



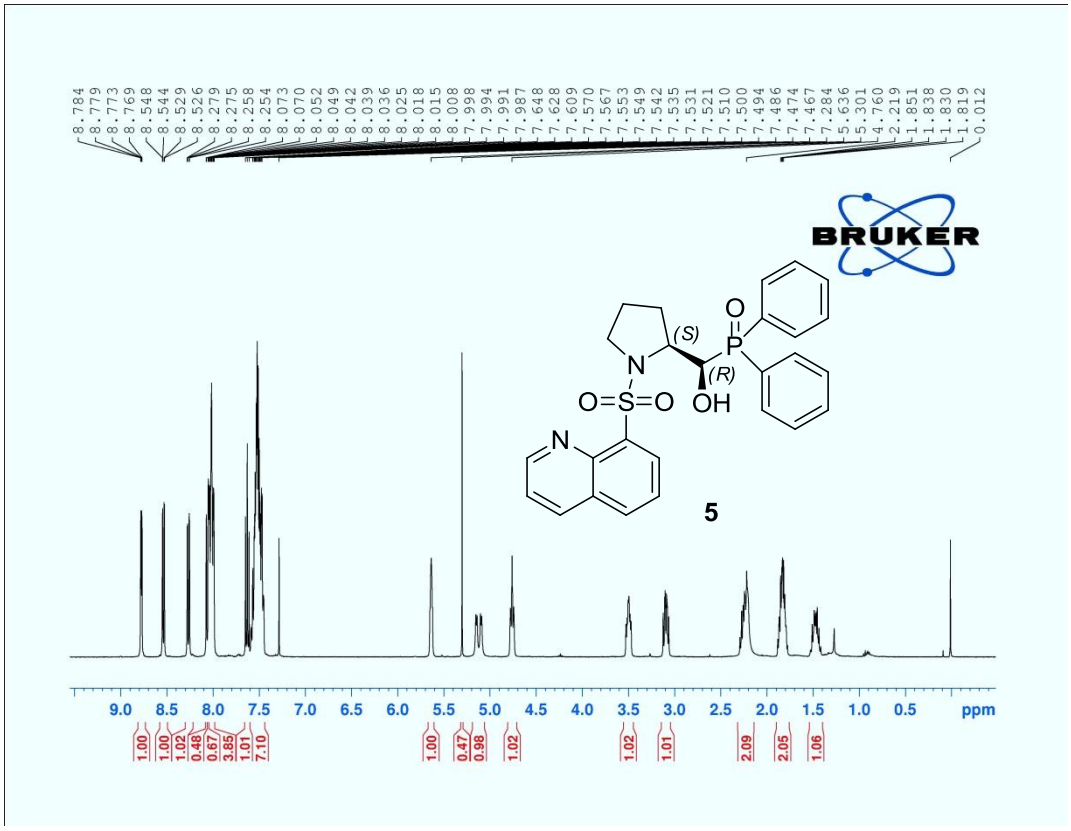


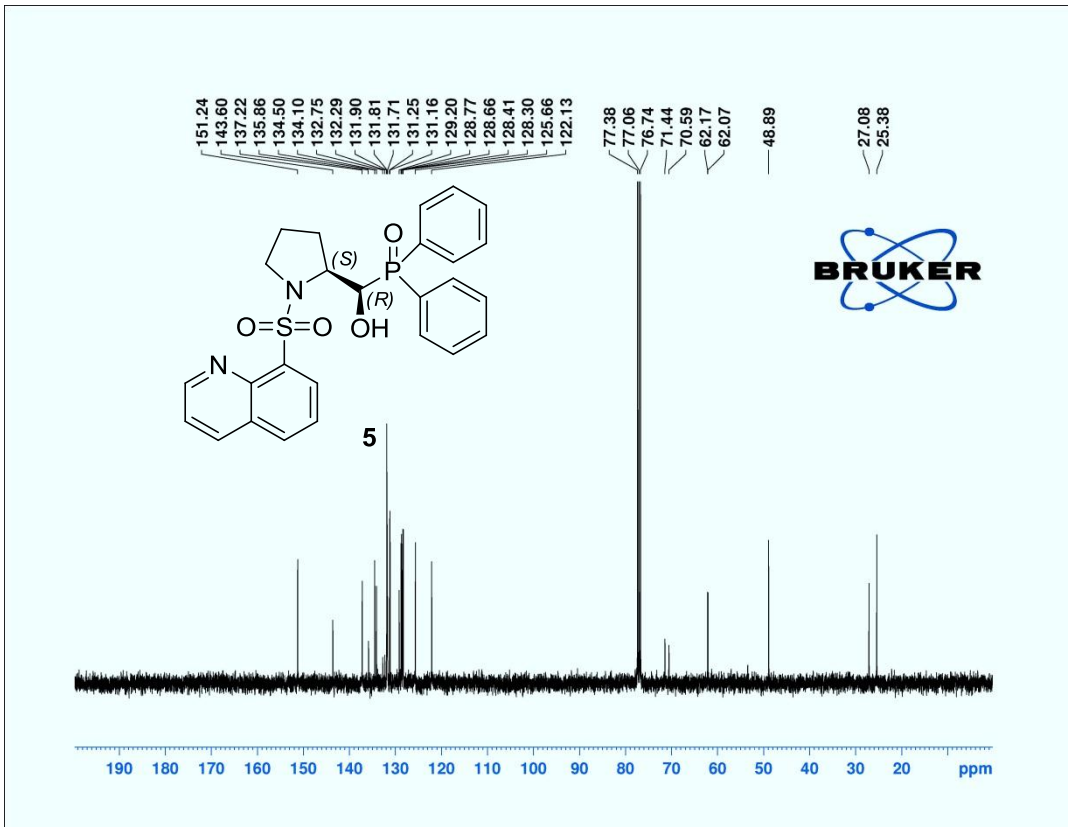


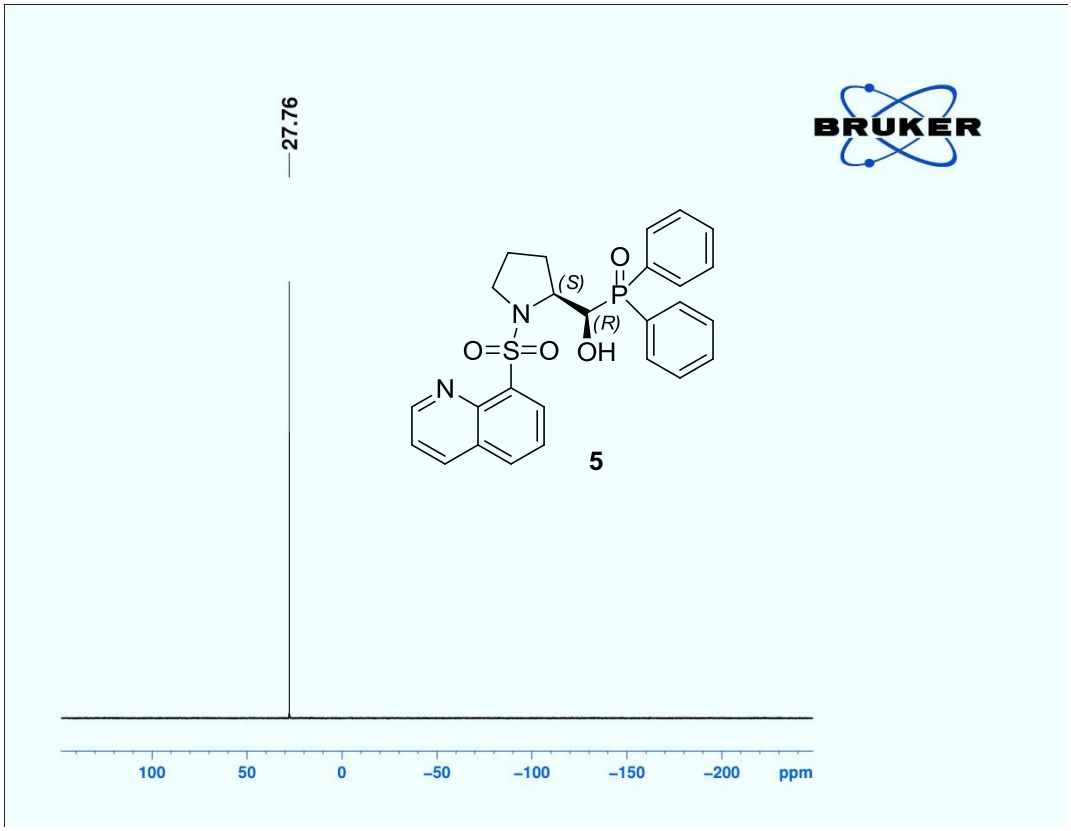


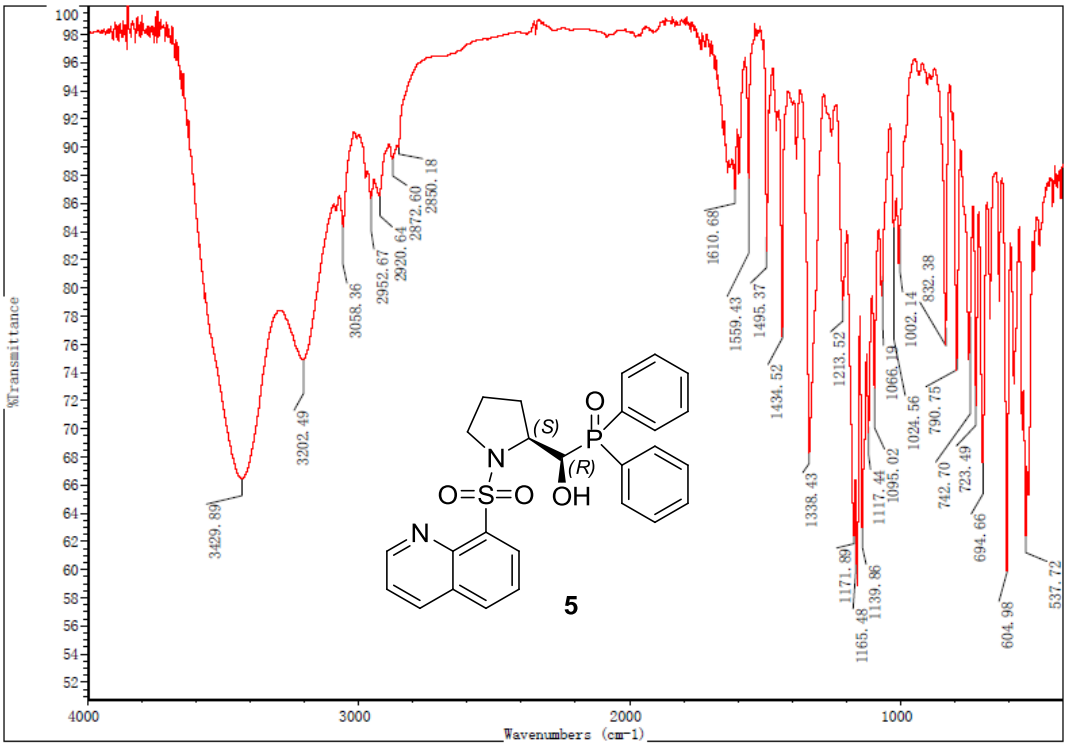


2.3.3 **The spectra of compound 5**

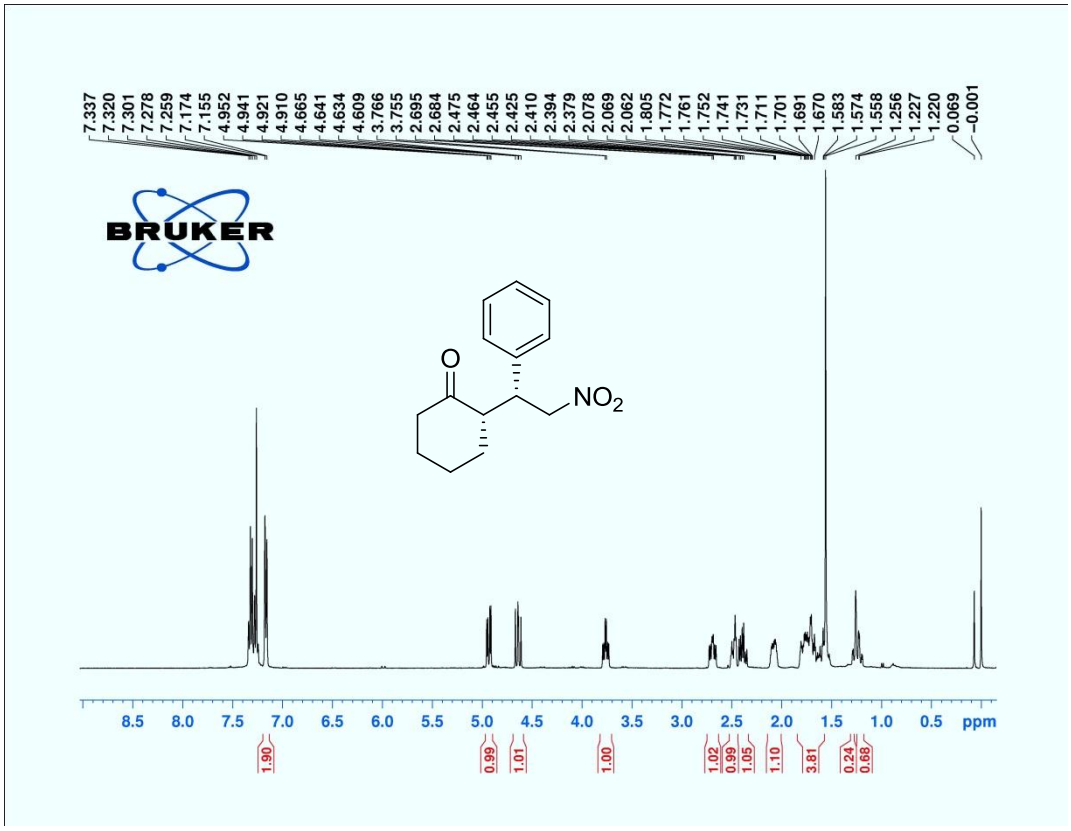


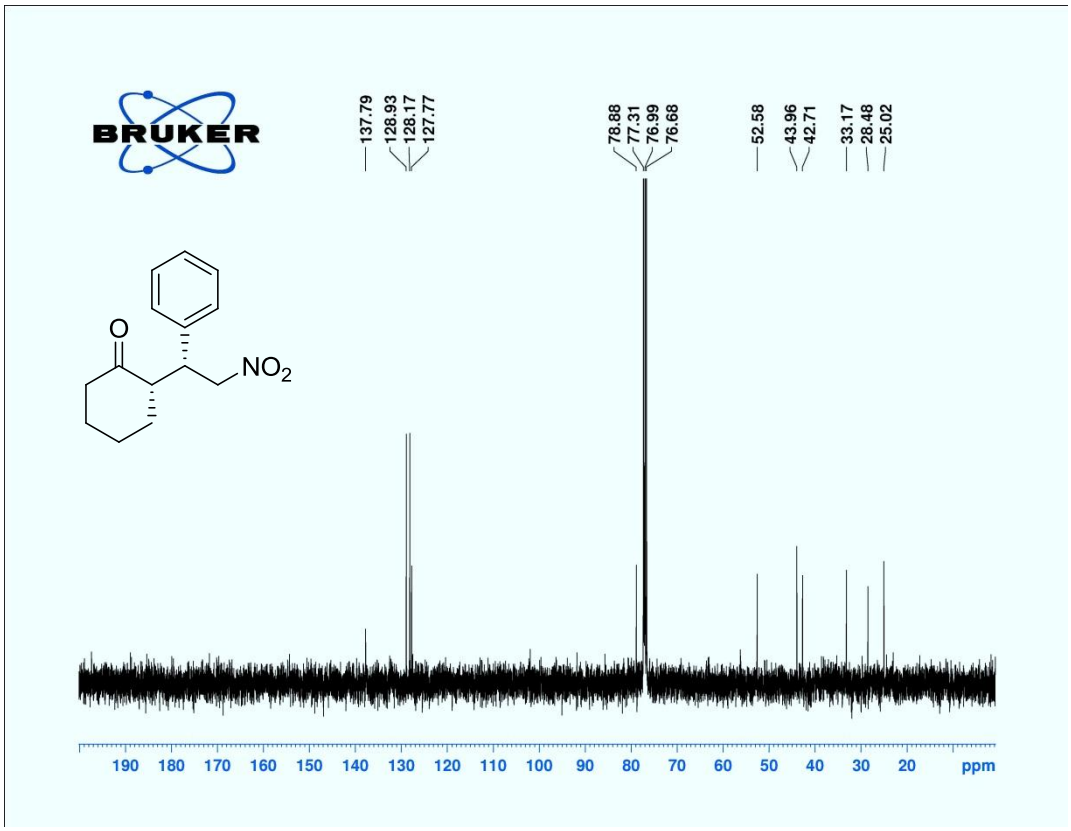



27.76
BRUKER
(S)
(R)
O=S=O
OH
5
100
50
0
−50
−100
−150
−200
ppm

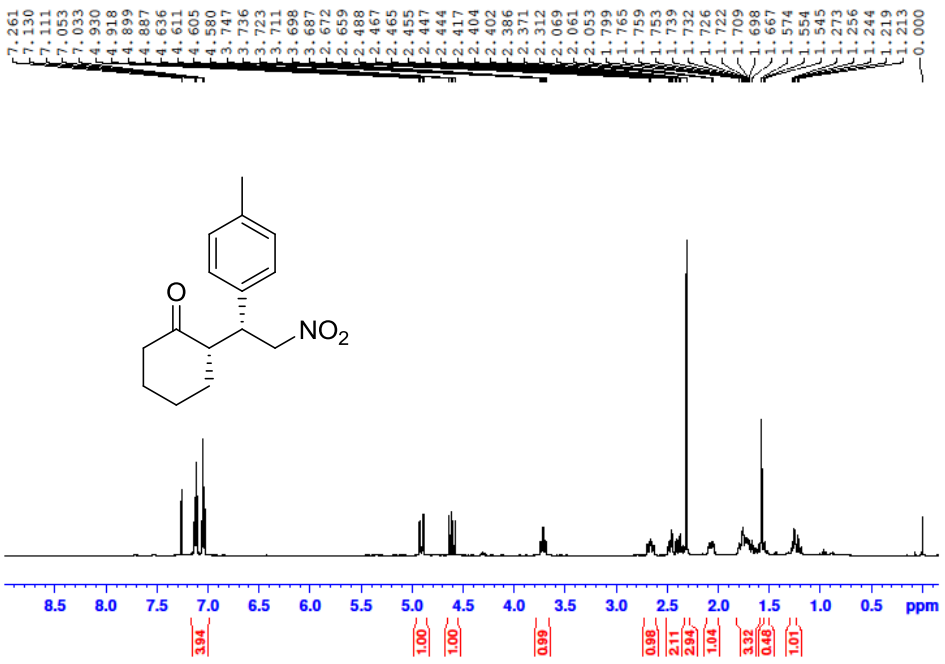

%Transmittance
3429.89
3202.49
3058.36
2952.67
2920.64
2872.60
2850.18
1610.68
1559.43
1495.37
1434.52
1338.43
1213.52
1171.89
1165.48
1139.86
1117.44
1095.02
1066.19
1024.56
1002.14
832.38
790.75
742.70
723.49
694.66
604.98
537.72
(S)
(R)
O=S=O
OH
5
4000
3000
2000
1000
Wavenumbers (cm-1)

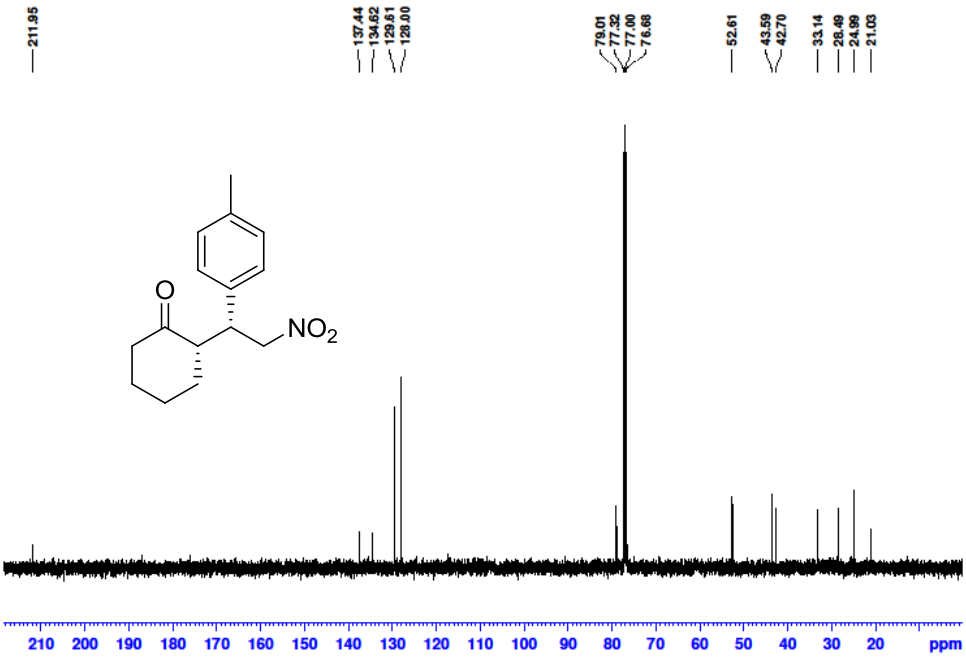
2.3.4 **The spectra of compound 3a**



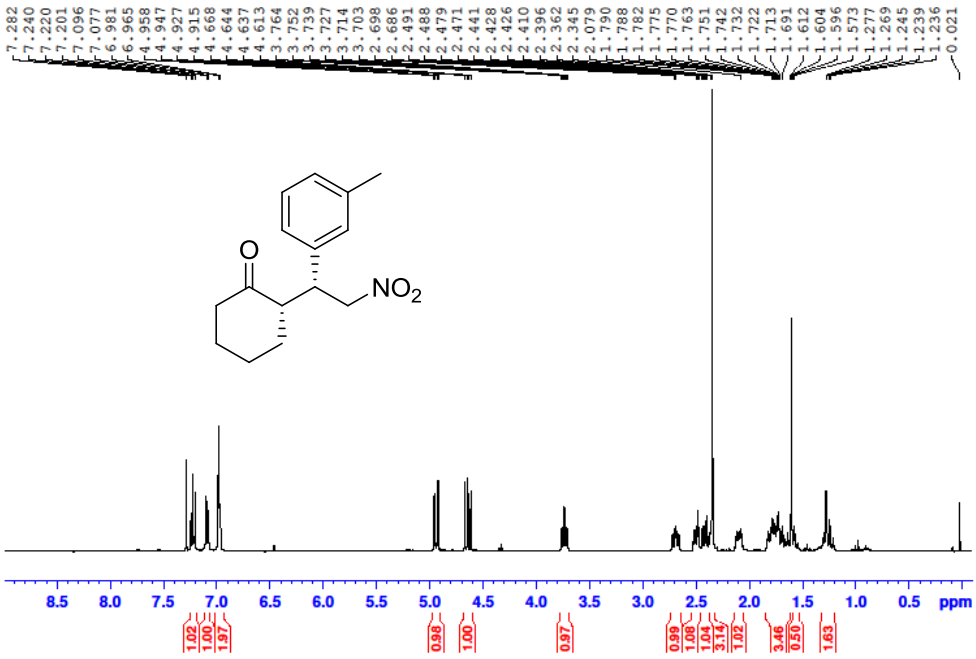


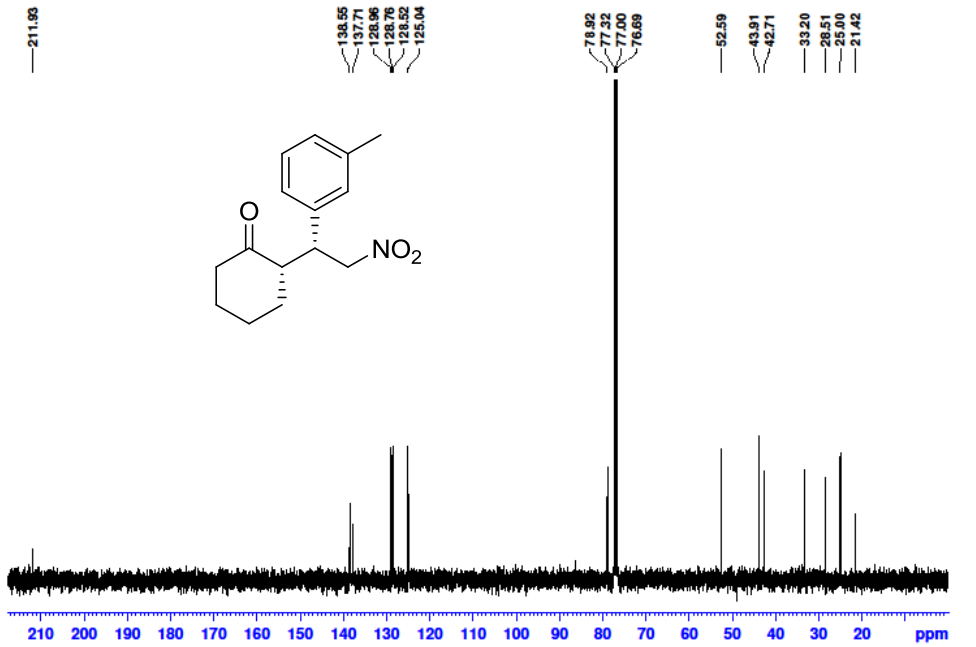
2.3.5 **The spectra of compound 3b**



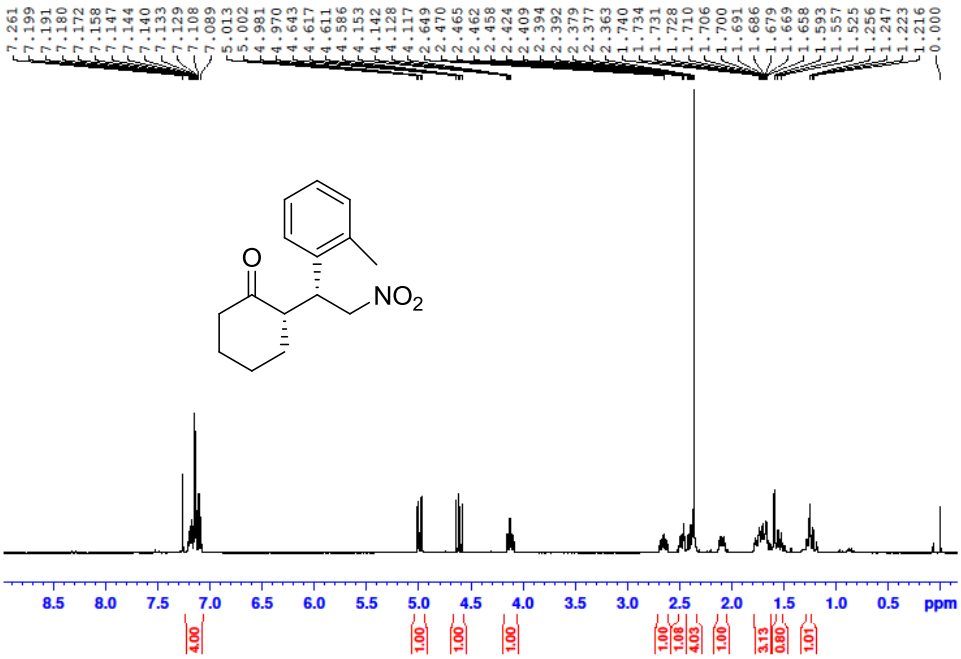


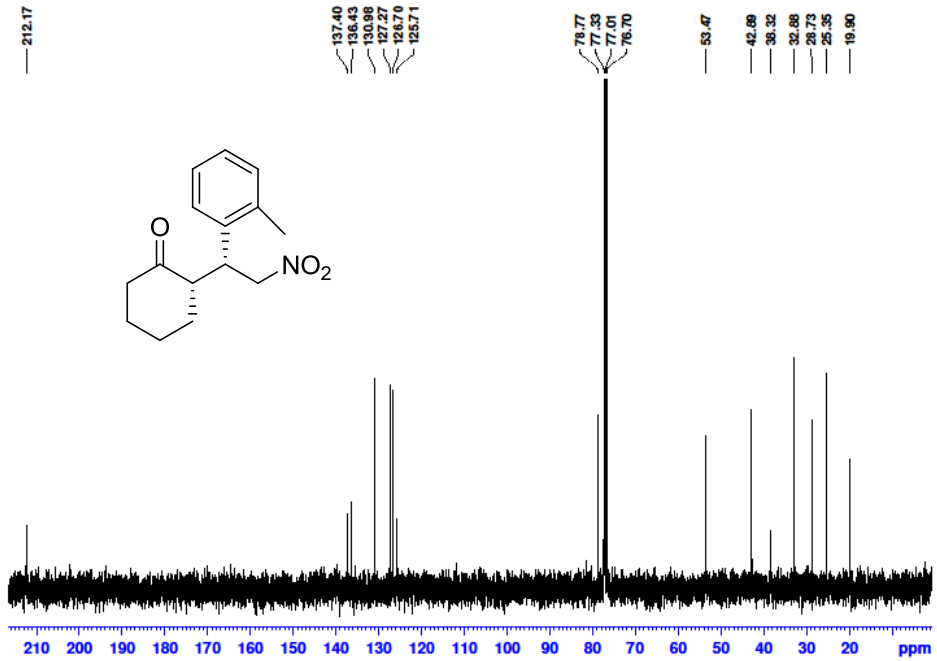
2.3.6 **The spectra of compound 3c**



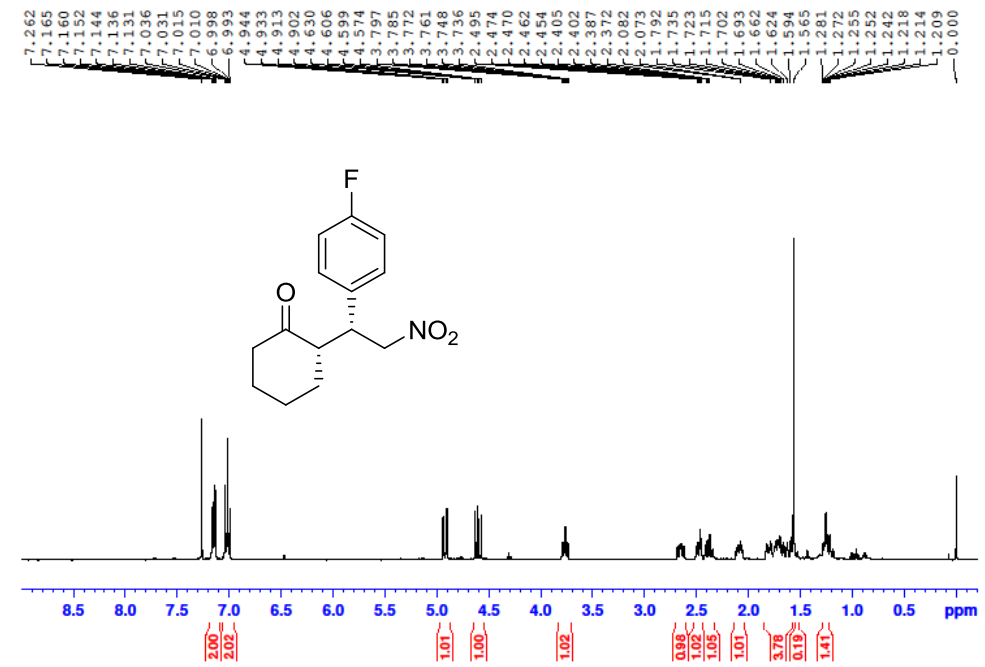


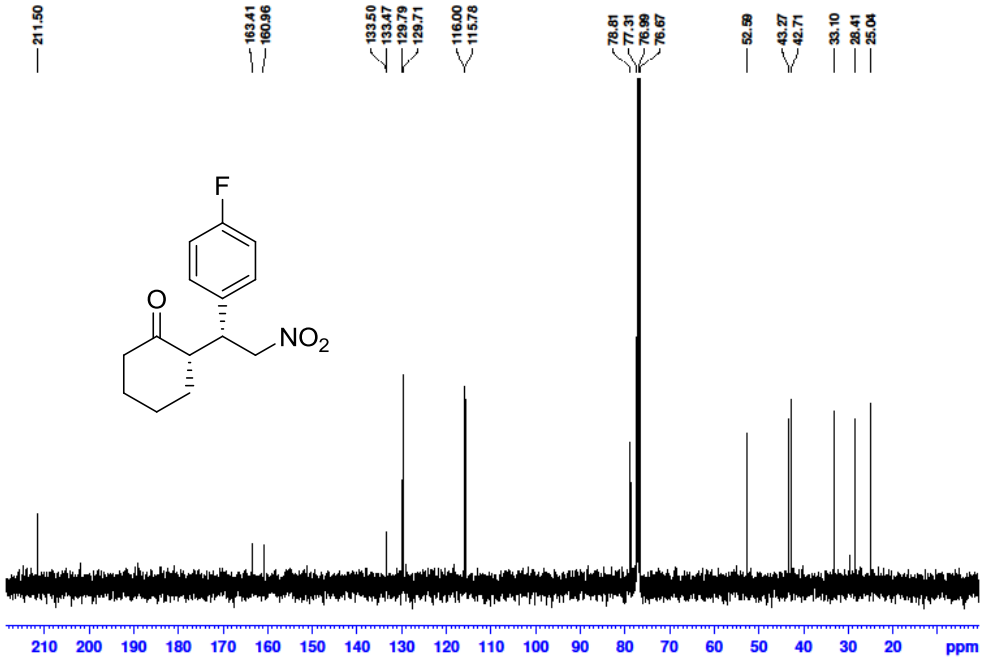
2.3.7 **The spectra of compound 3d**



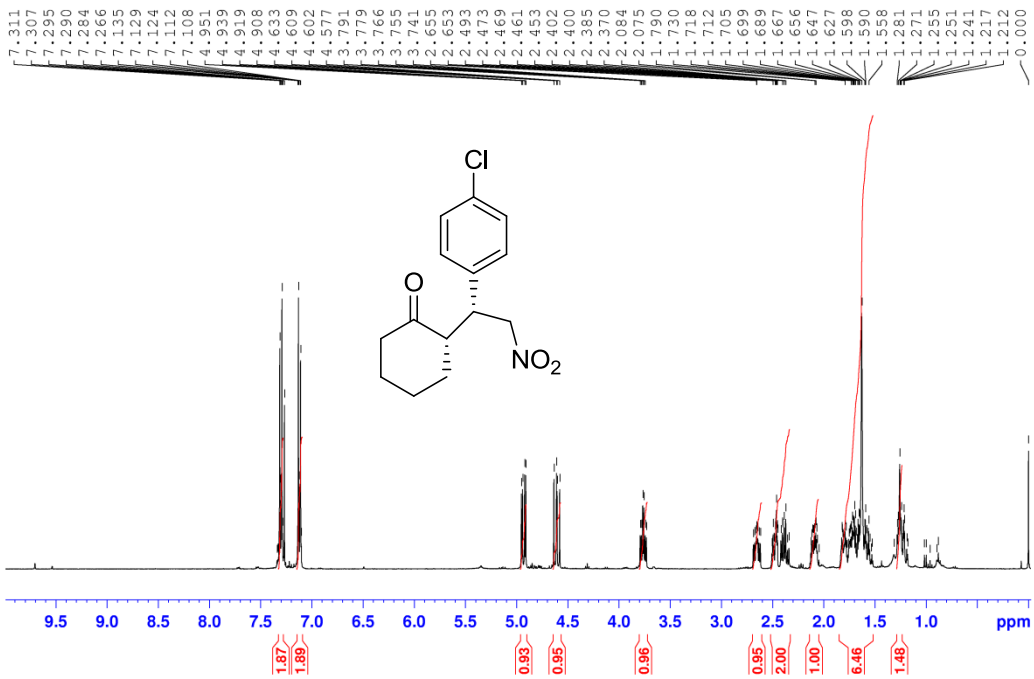


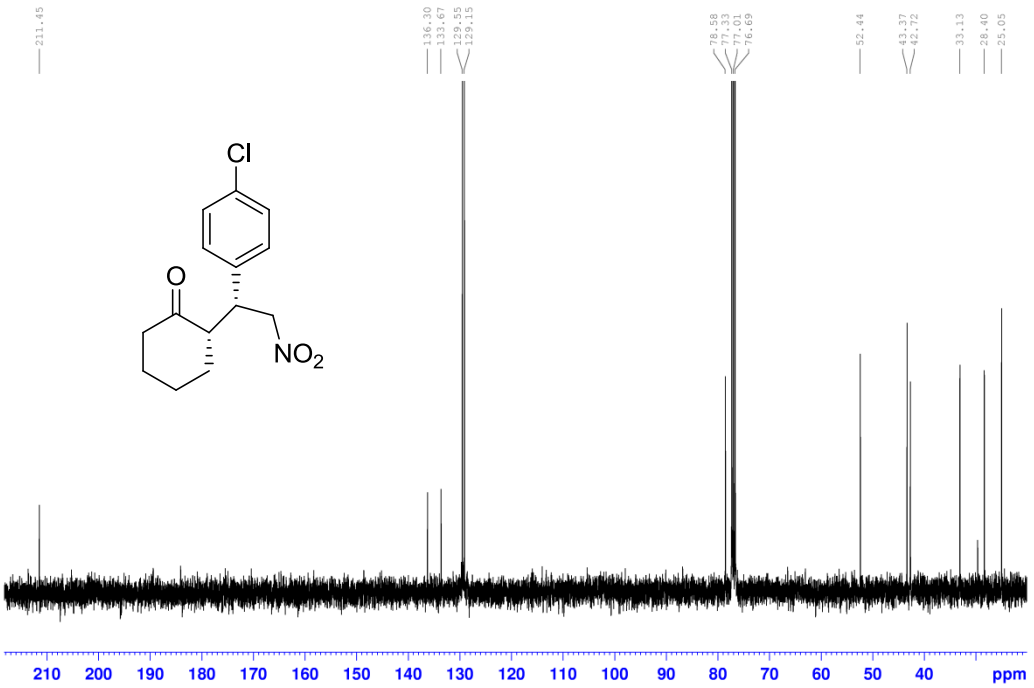
2.3.8 **The spectra of compound 3e**



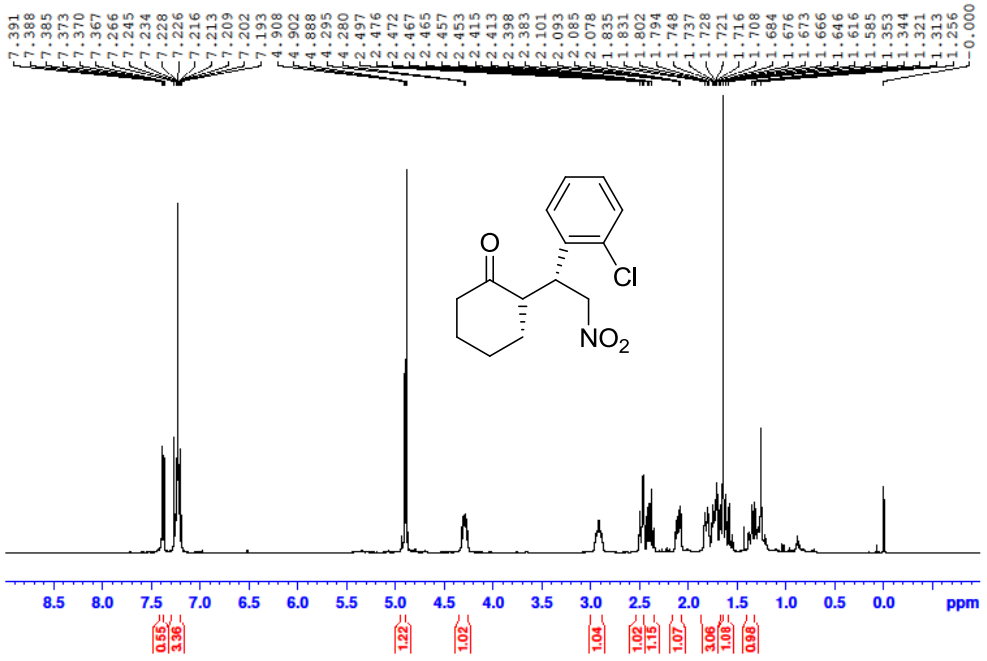


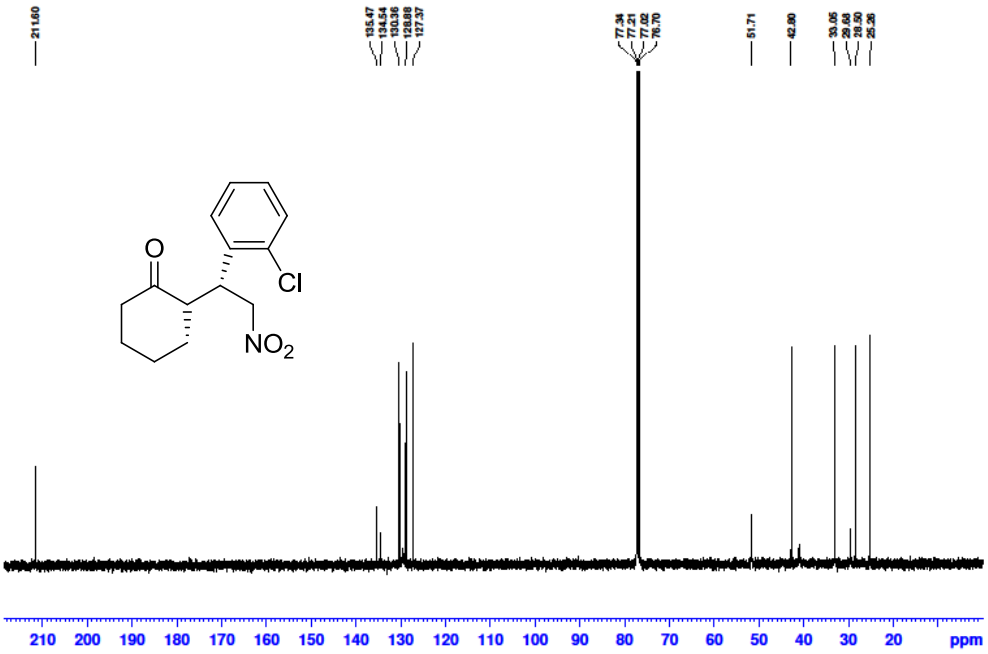
2.3.9 **The spectra of compound 3f**



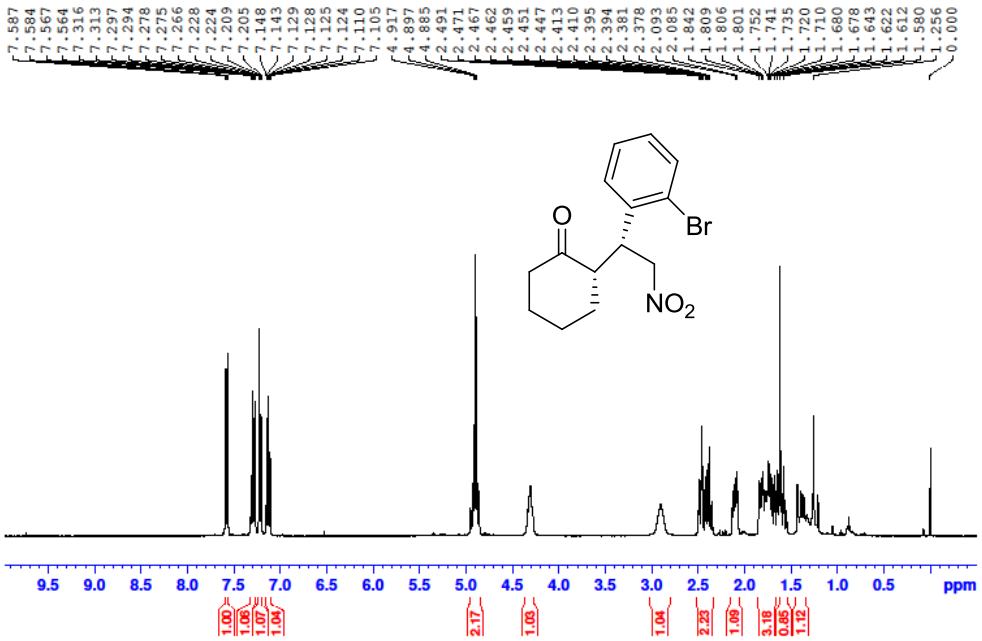


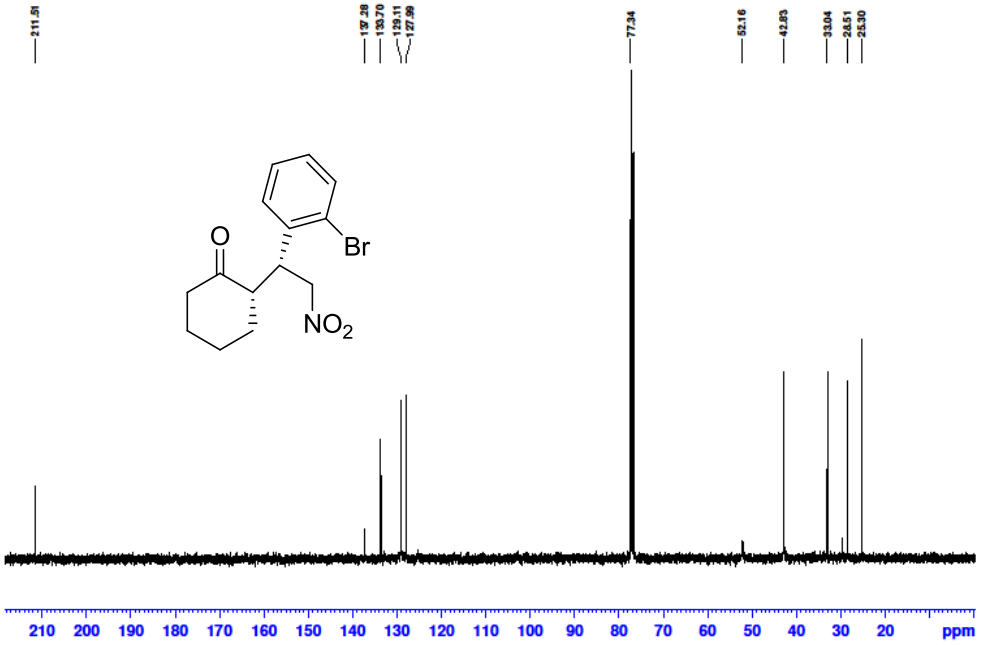
2.3.10 **The spectra of compound 3g**



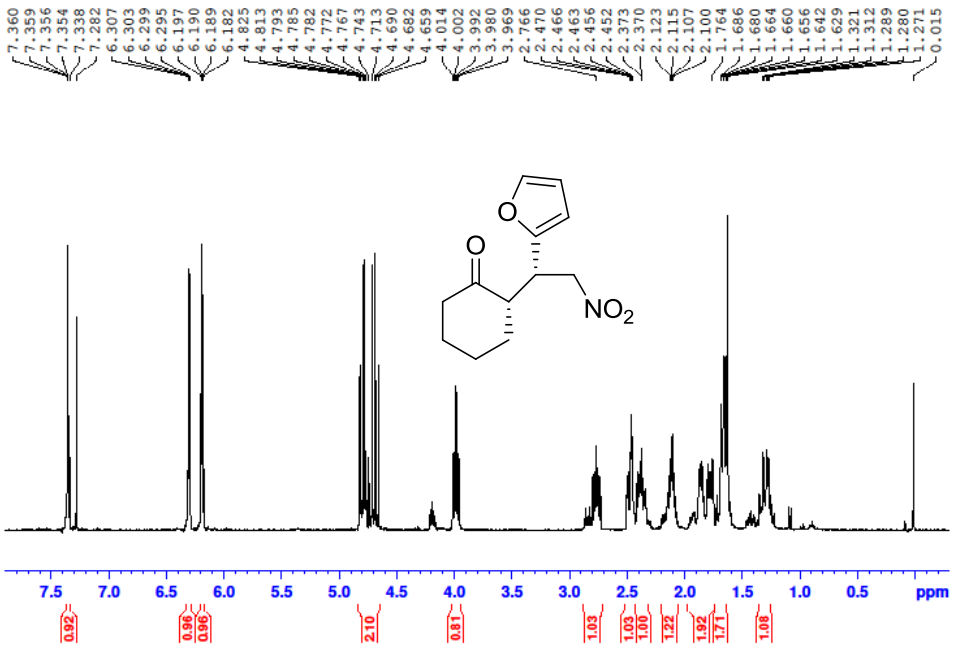


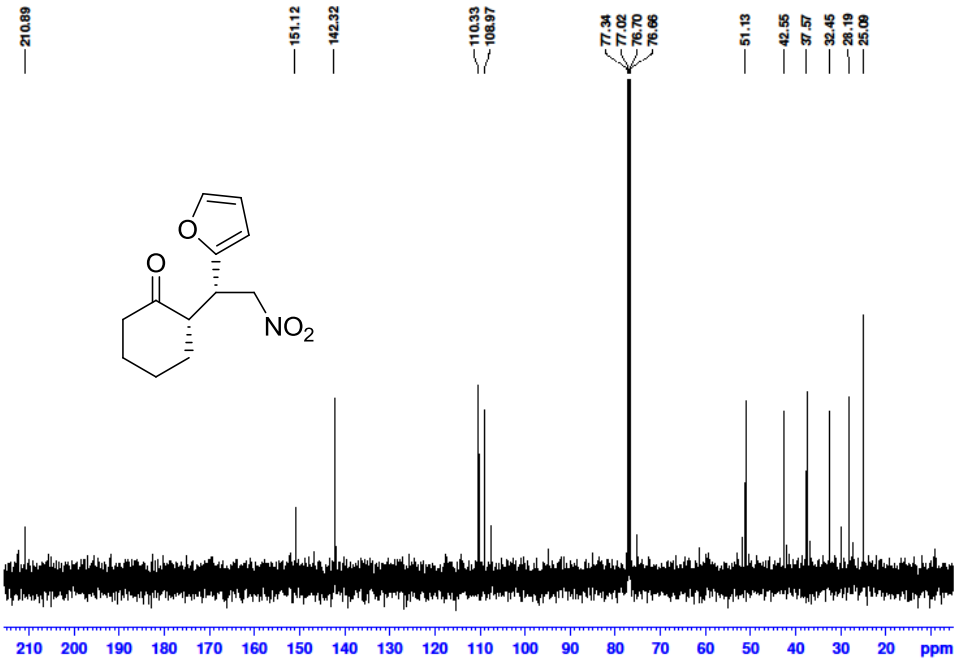
2.3.11 The spectra of compound 3h



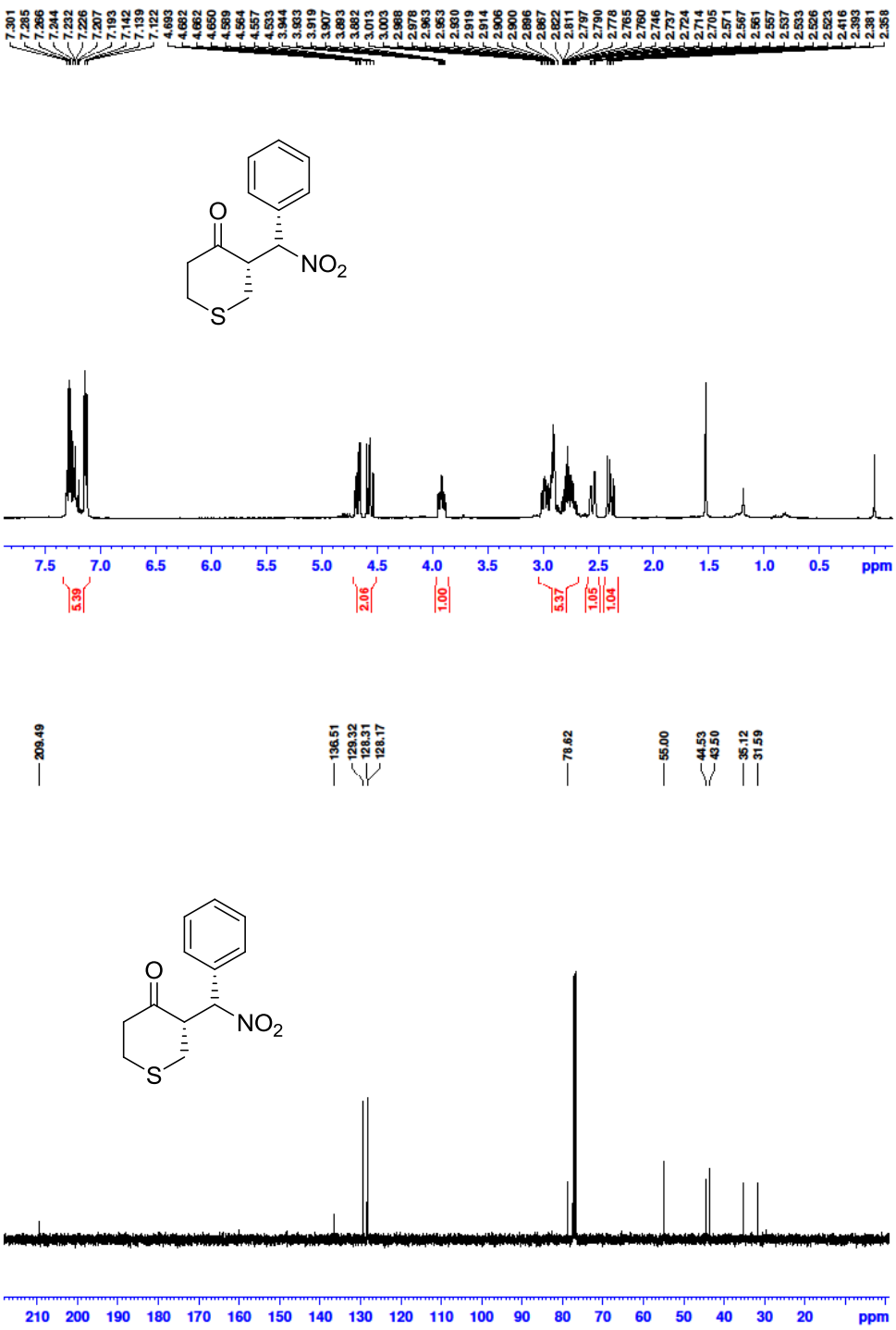


2.3.12 The spectra of compound 3i

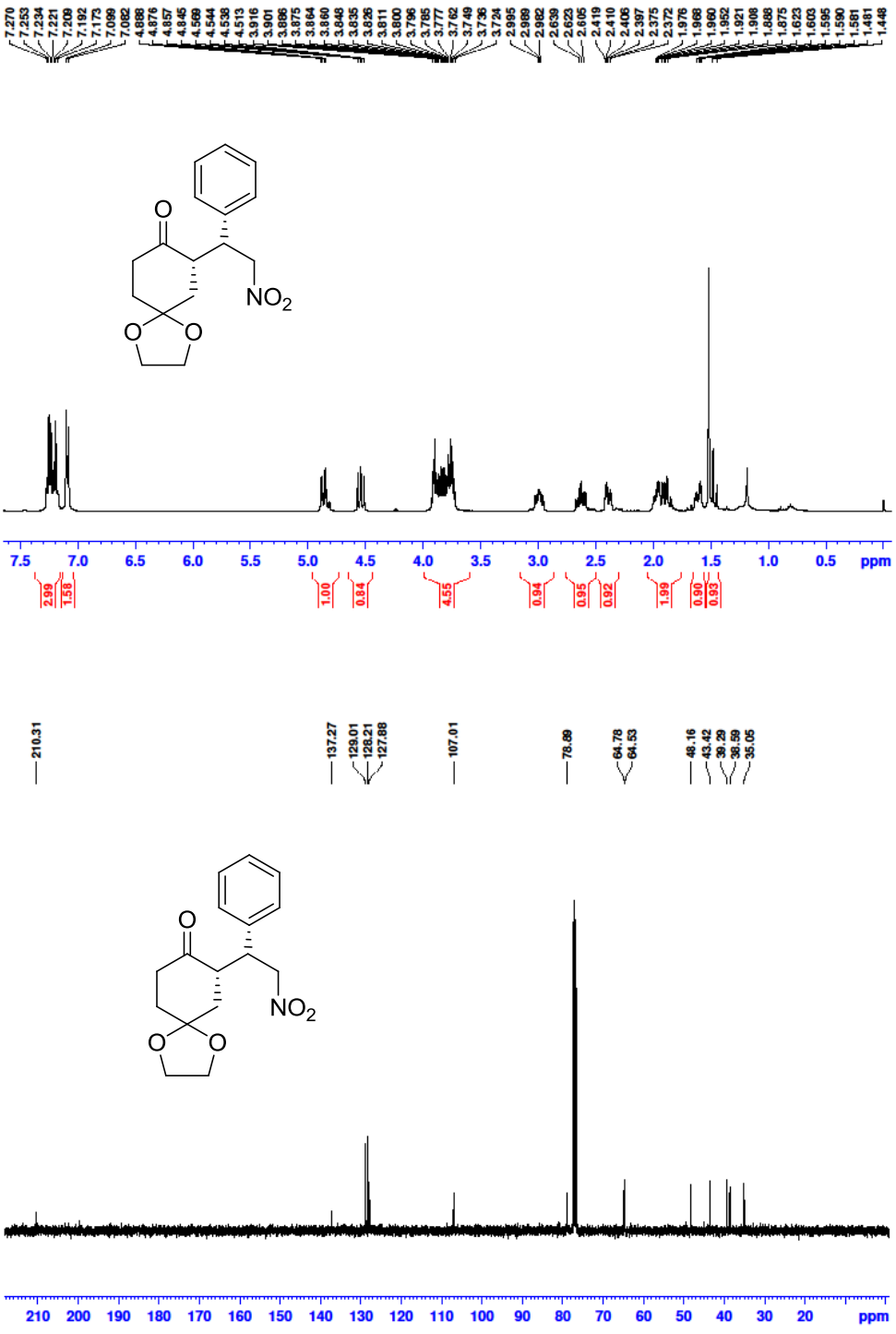




2.3.13 **The spectra of compound 3j**



2.3.14 **The spectra of compound 3k**



2.4 The X-ray data of compound 5

Table 1. Crystal data and structure refinement for 5.

Empirical formula	C26 H25 N2 O4 P S
Formula weight	492.13
Temperature	173(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, 2/mB
Unit cell dimensions	a = 8.494(2) A alpha = 90 deg. b = 11.250(3) A beta = 93.010(4) deg. c = 14.974(4) A gamma = 90 deg.
Volume	1429.0(6) A^3
Z, Calculated density	3, 1.504 Mg/m^3
Absorption coefficient	0.291 mm^-1
F(000)	675
Crystal size	0.90 x 0.33 x 0.09 mm
Theta range for data collection	1.36 to 28.34 deg.
Limiting indices	-11<=h<=10, -14<=k<=14, -19<=l<=19
Reflections collected / unique	12400 / 6483 [R(int) = 0.0350]
Completeness to theta = 25	95.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9743 and 0.7797
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6483 / 1 / 307
Goodness-of-fit on F^2	1.716
Final R indices [I>2sigma(I)]	R1 = 0.1423, wR2 = 0.3780
R indices (all data)	R1 = 0.1469, wR2 = 0.3844
Absolute structure parameter	0.1(2)
Largest diff. peak and hole	4.565 and -0.774 e.A^-3

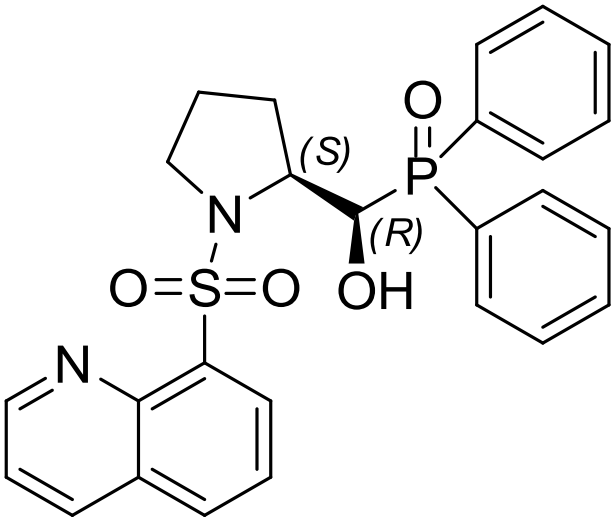


Table 2. Bond lengths [A] and angles [deg] for sad.

P(1)-O(6)	1.485(5)	C(8)-C(12)-P(1)	110.7(4)
P(1)-C(1)	1.783(6)	O(2)-C(12)-H(12A)	108.6
P(1)-C(9)	1.786(6)	C(8)-C(12)-H(12A)	108.6
P(1)-C(12)	1.812(6)	P(1)-C(12)-H(12A)	108.6
S(2)-O(4)	1.399(5)	C(31)-C(13)-C(1)	119.8(7)
S(2)-O(5)	1.425(6)	C(31)-C(13)-H(13A)	120.1
S(2)-N(3)	1.602(6)	C(1)-C(13)-H(13A)	120.1
S(2)-C(7)	1.747(8)	C(30)-C(14)-C(15)	117.3(13)
C(1)-C(13)	1.383(10)	C(30)-C(14)-C(25)	122.9(12)
C(1)-C(11)	1.401(10)	C(15)-C(14)-C(25)	119.4(10)
O(2)-C(12)	1.405(7)	N(16)-C(15)-C(14)	123.7(9)
O(2)-H(2A)	0.8200	N(16)-C(15)-C(7)	119.1(7)
N(3)-C(26)	1.427(9)	C(14)-C(15)-C(7)	117.2(9)
N(3)-C(8)	1.487(9)	C(27)-N(16)-C(15)	119.1(11)
C(7)-C(19)	1.354(11)	C(18)-C(17)-C(9)	117.8(8)
C(7)-C(15)	1.447(10)	C(18)-C(17)-H(17A)	121.1
C(8)-C(10)	1.529(9)	C(9)-C(17)-H(17A)	121.1
C(8)-C(12)	1.531(8)	C(22)-C(18)-C(17)	124.3(10)
C(8)-H(8A)	0.9800	C(22)-C(18)-H(18A)	117.8
C(9)-C(20)	1.396(9)	C(17)-C(18)-H(18A)	117.8
C(9)-C(17)	1.399(10)	C(7)-C(19)-C(21)	120.4(10)
C(10)-C(29)	1.458(11)	C(7)-C(19)-H(19A)	119.8
C(10)-H(10A)	0.9700	C(21)-C(19)-H(19A)	119.8
C(10)-H(10B)	0.9700	C(33)-C(20)-C(9)	119.8(8)
C(11)-C(28)	1.374(11)	C(33)-C(20)-H(20A)	120.1
C(11)-H(11A)	0.9300	C(9)-C(20)-H(20A)	120.1
C(12)-H(12A)	0.9800	C(25)-C(21)-C(19)	123.8(11)
C(13)-C(31)	1.383(10)	C(25)-C(21)-H(21A)	118.1
C(13)-H(13A)	0.9300	C(19)-C(21)-H(21A)	118.1
C(14)-C(30)	1.373(18)	C(18)-C(22)-C(33)	118.6(8)
C(14)-C(15)	1.421(14)	C(18)-C(22)-H(22A)	120.7
C(14)-C(25)	1.467(18)	C(33)-C(22)-H(22A)	120.7
C(15)-N(16)	1.328(12)	C(31)-C(24)-C(28)	119.7(7)
N(16)-C(27)	1.264(12)	C(31)-C(24)-H(24A)	120.1
C(17)-C(18)	1.352(11)	C(28)-C(24)-H(24A)	120.1
C(17)-H(17A)	0.9300	C(21)-C(25)-C(14)	119.1(10)
C(18)-C(22)	1.330(14)	C(21)-C(25)-H(25A)	120.5
C(18)-H(18A)	0.9300	C(14)-C(25)-H(25A)	120.5
C(19)-C(21)	1.407(15)	N(3)-C(26)-C(29)	102.3(6)

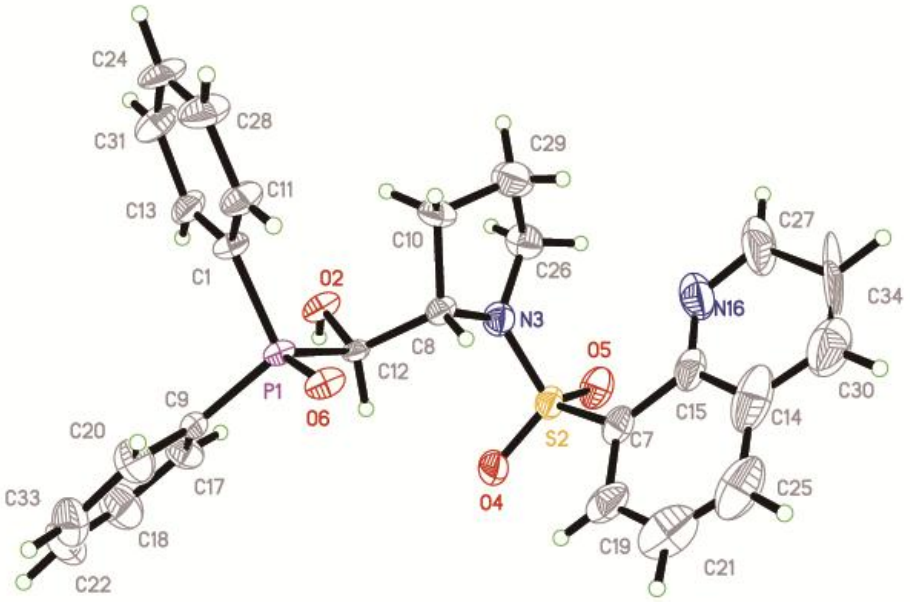


Figure. ORTEP drawing showing 50% probability displacement ellipsoids of compound 5

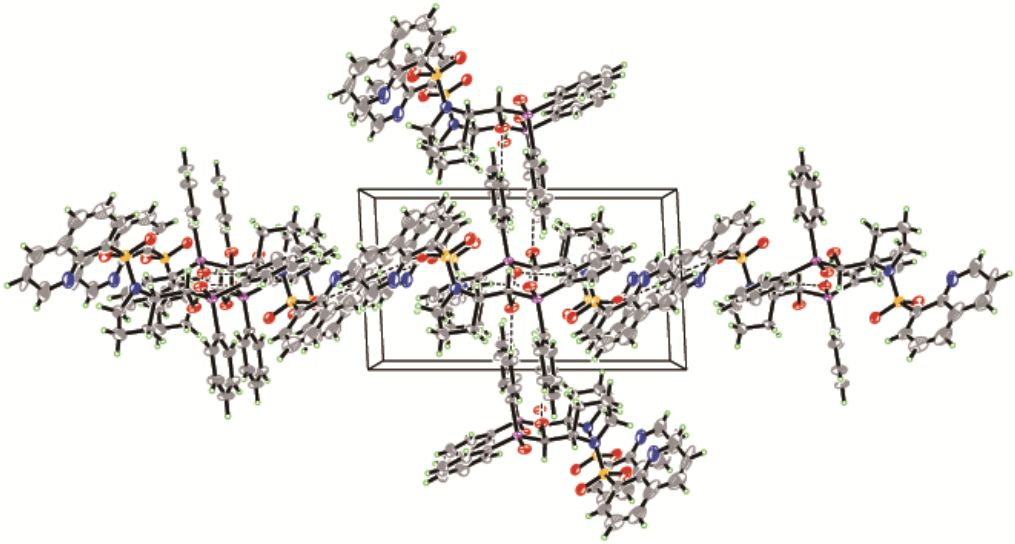
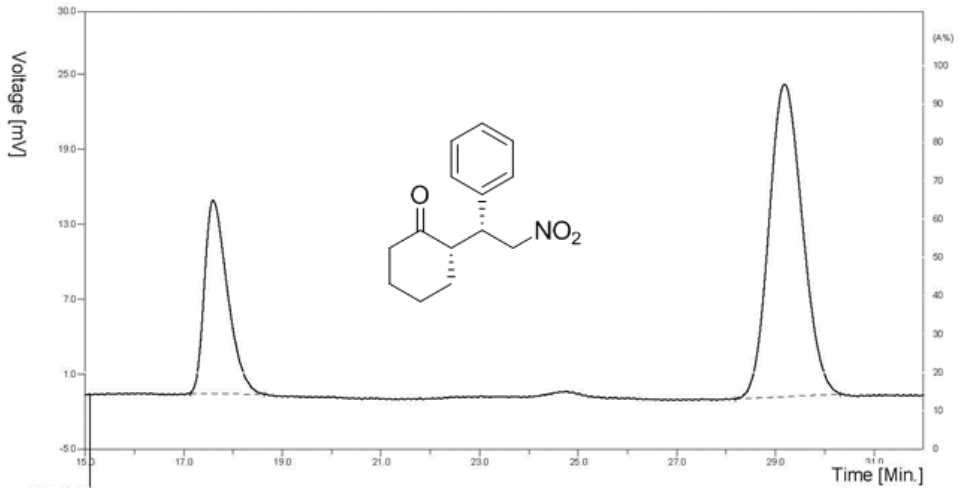


Figure. The cell crystal structure of compound 5

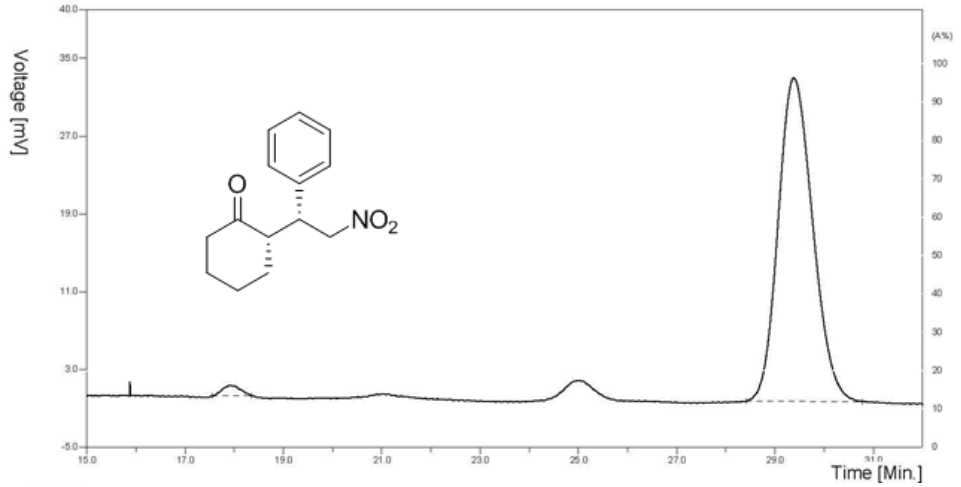
2.5 The HPLC Spectra of all compounds 3a~3k

2.5.1 The HPLC Spectra of compound 3a



Peak Table

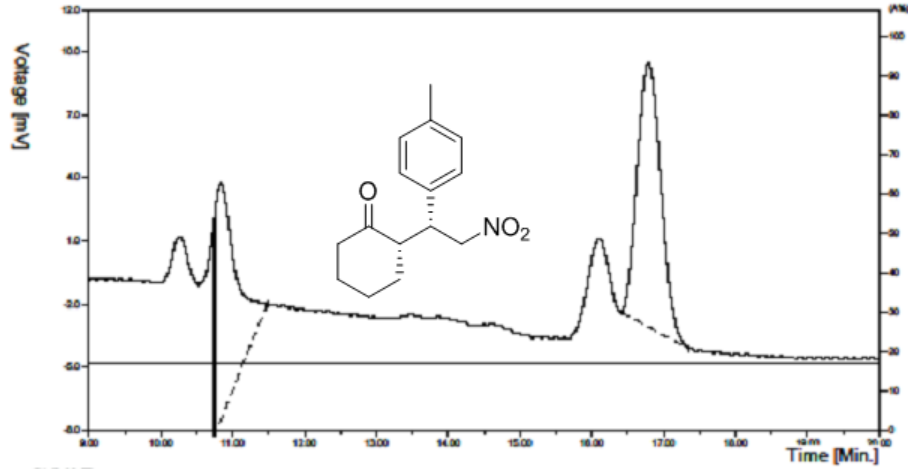
Peak#	Ret. Time(min)	Height(mV)	Area(mv.sec)	Area%
1	17.59	15.46	502.83	29.9459
2	29.18	24.98	1176.30	70.0541
Total		40.44	1679.13	100



Peak Table

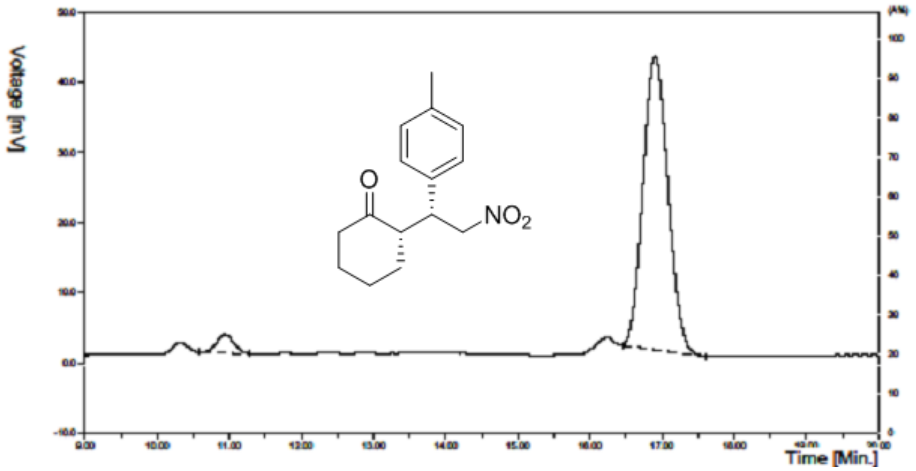
Peak#	Ret. Time(min)	Height(mV)	Area(mv.sec)	Area%
1	17.91	1.07	26.99	1.6381
2	29.38	33.26	1620.69	98.3619
Total		34.33	1647.68	100

2.5.2 **The HPLC Spectra of compound 3b**[11]



Peak Table

Peak#	Ret. Time(min)	Height(mV)	Area(mv.sec)	Area%
1	10.84	5.08	79.84	21.8054
2	16.79	12.54	286.30	78.1946
Total		17.63	366.14	100

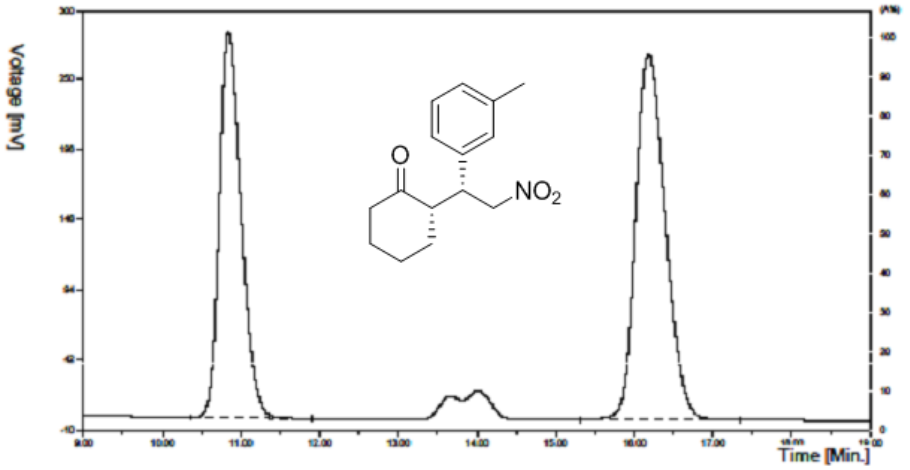


Peak Table

Peak#	Ret. Time(min)	Height(mV)	Area(mv.sec)	Area%
1	10.94	2.63	43.53	4.1444
2	16.91	41.85	1006.88	95.8556
Total		44.48	1050.41	100

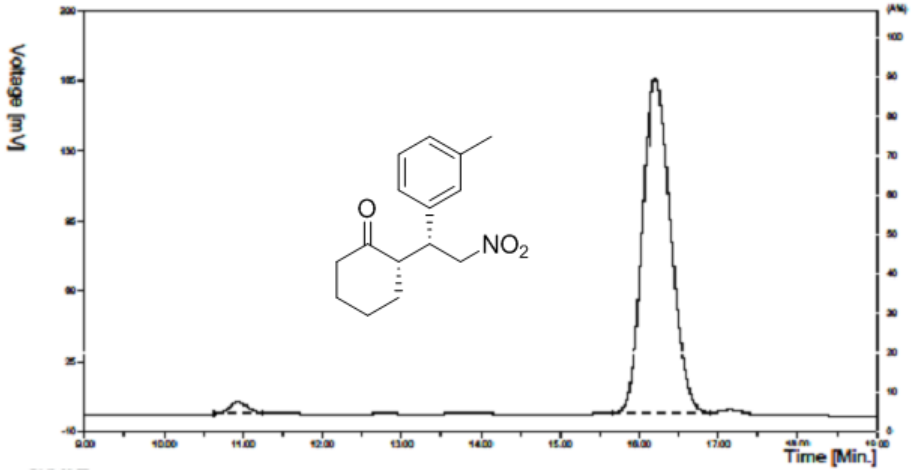
The affected result of this overlapping peaks at ESI 2.6.2 will underestimate the area of the main peak at 16.91 min in our calculation(see: the cut line is upon the base line in the picture), which will also result in a little underestimate of the ee value of this case. That means the real ee value will exceed 91.7% if the two peaks is separated well enough.

2.5.3 **The HPLC Spectra of compound 3c**



Peak Table

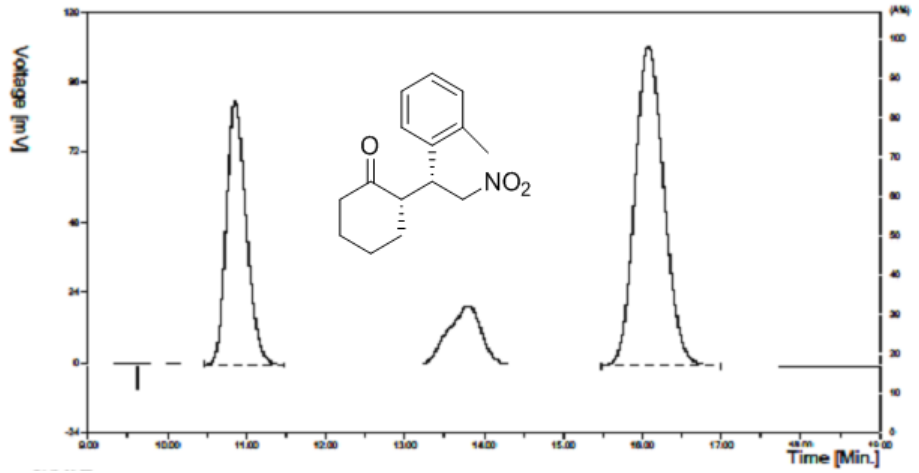
Peak#	Ret. Time(min)	Height(mV)	Area(mv.sec)	Area%
1	10.84	284.97	5494.66	43.5255
2	16.18	270.05	7129.35	56.4745
Total		555.02	12624.01	100



Peak Table

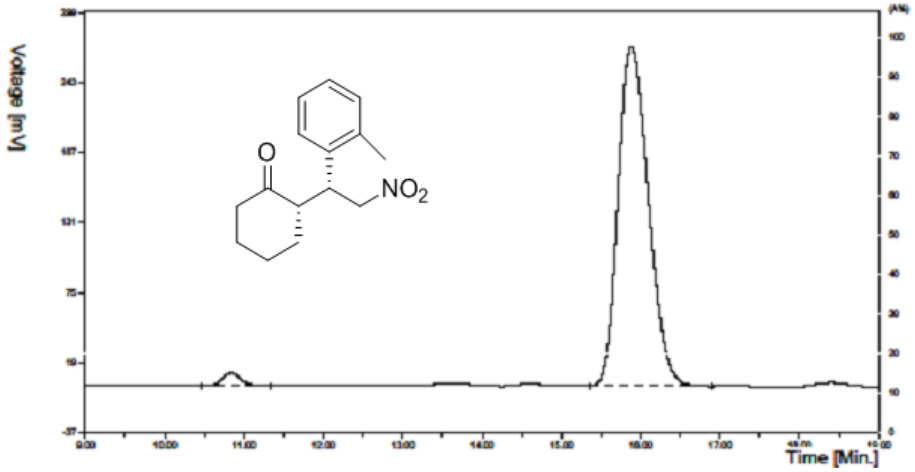
Peak#	Ret. Time(min)	Height(mV)	Area(mv.sec)	Area%
1	10.94	5.56	88.50	2.0994
2	16.20	167.00	4126.83	97.9006
Total		172.56	4215.33	100

2.5.4 **The HPLC Spectra of compound 3d**



Peak Table

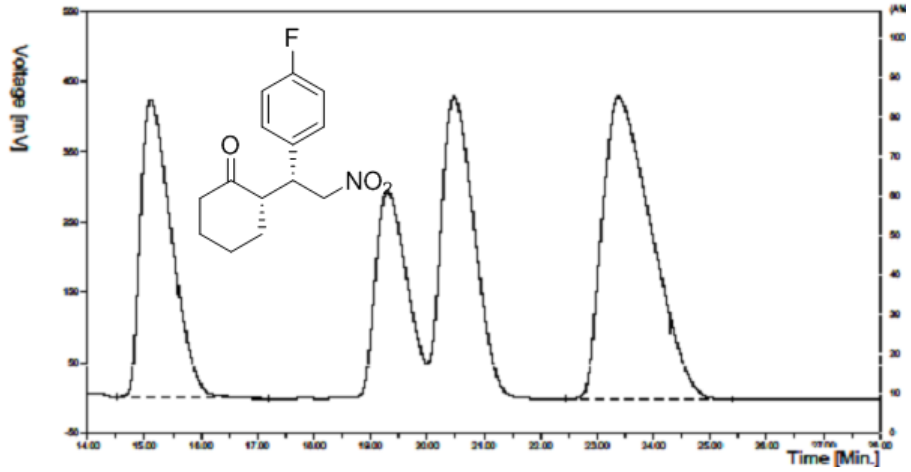
Peak#	Ret. Time(min)	Height(mV)	Area(mv.sec)	Area%
1	10.85	90.48	1611.47	36.6909
2	16.08	109.18	2780.54	63.3091
Total		199.66	4392.01	100



Peak Table

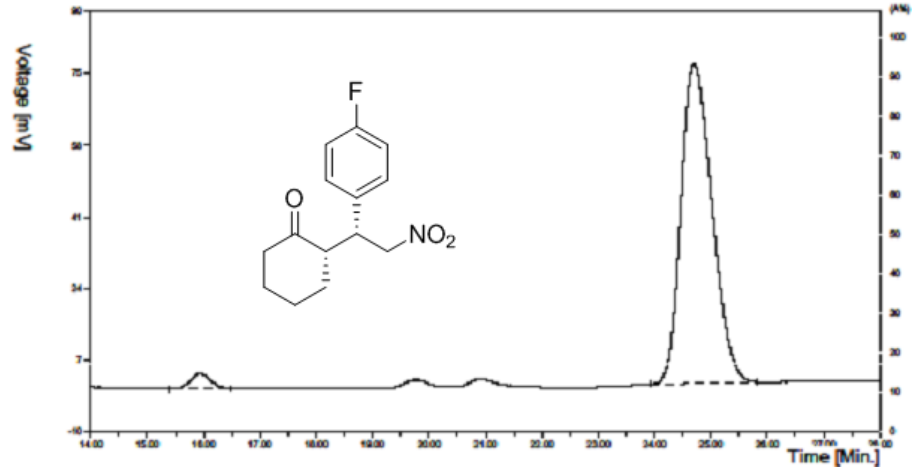
Peak#	Ret. Time(min)	Height(mV)	Area(mv.sec)	Area%
1	10.83	10.61	181.01	2.4496
2	15.88	271.83	7208.23	97.5504
Total		282.44	7389.24	100

2.5.5 **The HPLC Spectra of compound 3e**



Peak Table

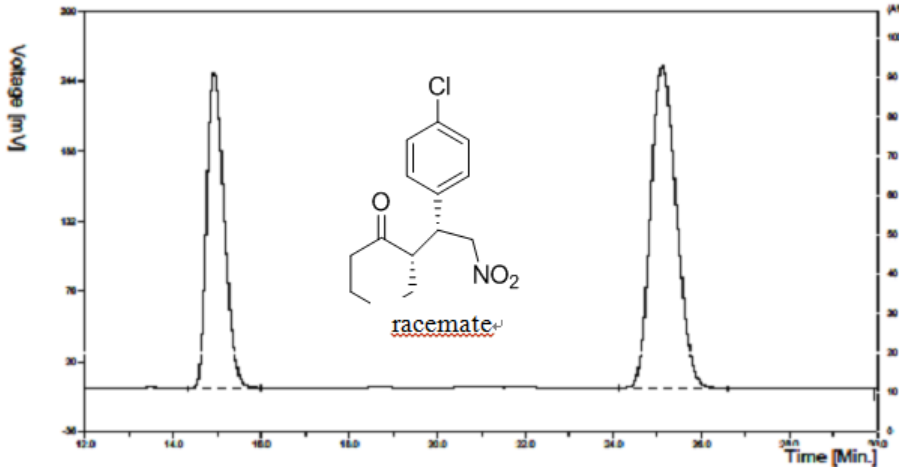
Peak#	Ret. Time(min)	Height(mV)	Area(mv.sec)	Area%
1	15.12	422.36	16180.57	38.3357
2	23.39	429.11	26027.04	61.6643
Total		851.47	42207.61	100



Peak Table

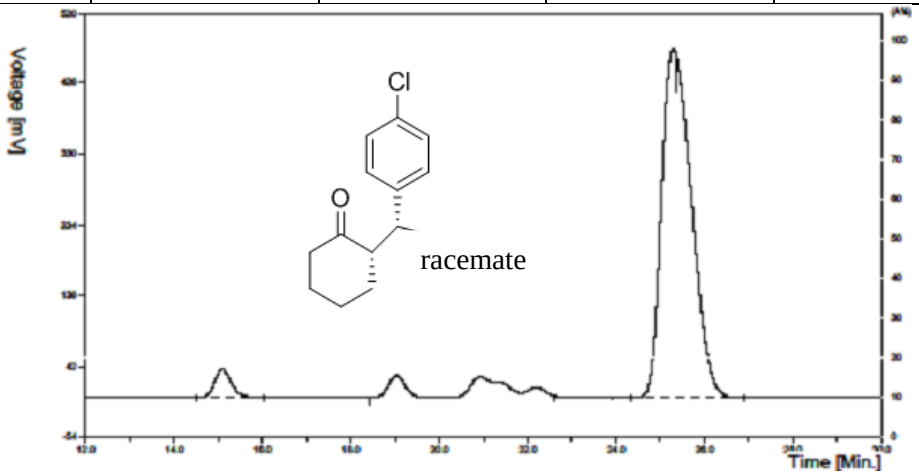
Peak#	Ret. Time(min)	Height(mV)	Area(mv.sec)	Area%
1	15.93	3.60	87.53	2.9281
2	24.71	75.82	2901.66	97.0719
Total		79.42	2989.19	100

2.5.6 **The HPLC Spectra of compound 3f**



Peak Table

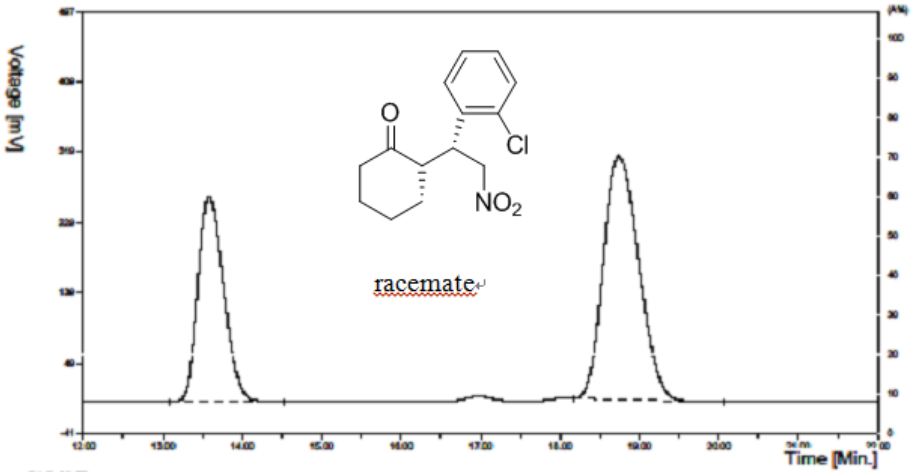
Peak#	Ret. Time(min)	Height(mV)	Area(mv.sec)	Area%
1	14.92	251.87	6996.93	39.9799
2	25.11	257.49	10504.20	60.0201
Total		509.36	17501.13	100



Peak Table

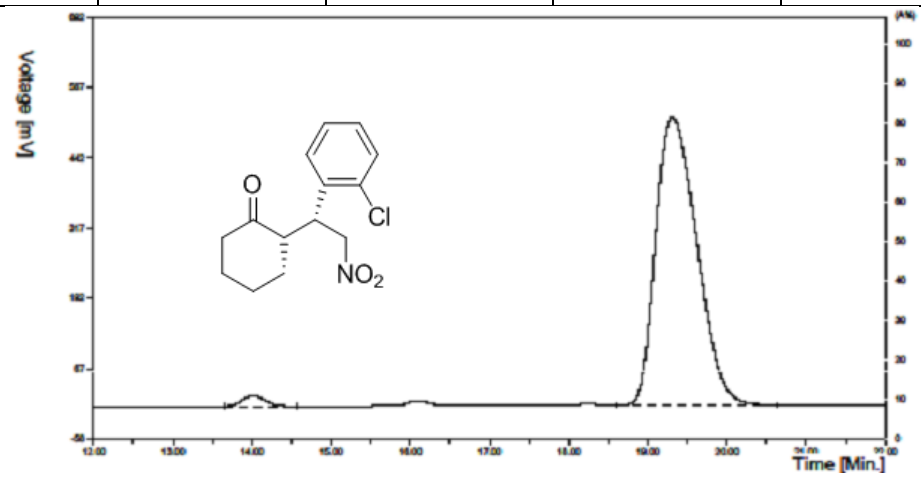
Peak#	Ret. Time(min)	Height(mV)	Area(mv.sec)	Area%
1	15.09	38.34	1029.76	4.4421
2	25.30	474.06	22152.25	95.5579
Total		512.40	23182.01	100

2.5.7 **The HPLC Spectra of compound 3g**



Peak Table

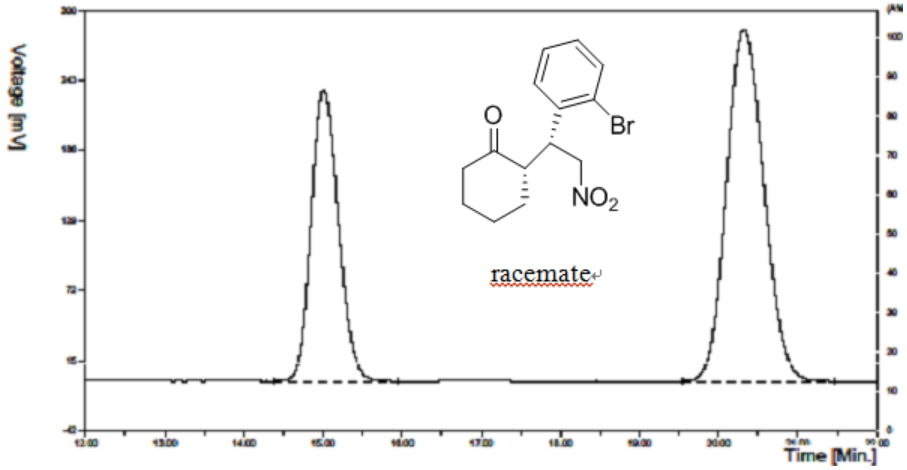
Peak#	Ret. Time(min)	Height(mV)	Area(mv.sec)	Area%
1	13.58	261.99	5925.75	38.0151
2	18.74	310.75	9662.13	61.9849
Total		572.74	15587.88	100



Peak Table

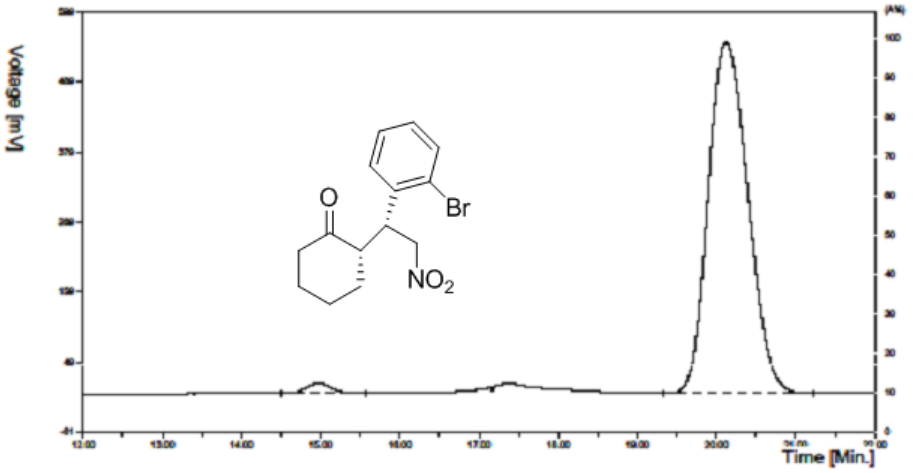
Peak#	Ret. Time(min)	Height(mV)	Area(mv.sec)	Area%
1	14.01	19.92	414.42	2.1977
2	19.31	511.41	18442.32	97.8023
Total		531.33	18856.74	100

2.5.8 **The HPLC Spectra of compound 3h**



Peak Table

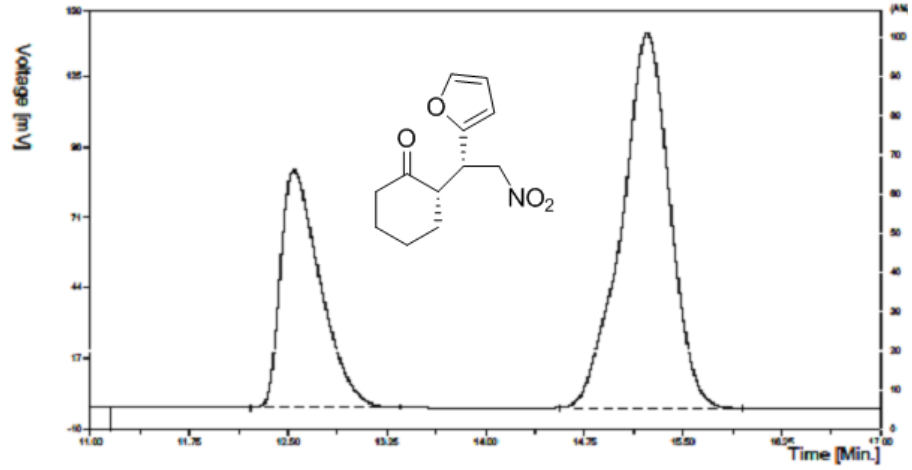
Peak#	Ret. Time(min)	Height(mV)	Area(mv.sec)	Area%
1	15.01	237.06	5673.47	37.6128
2	20.32	286.17	9410.41	62.3872
Total		523.23	15083.88	100



Peak Table

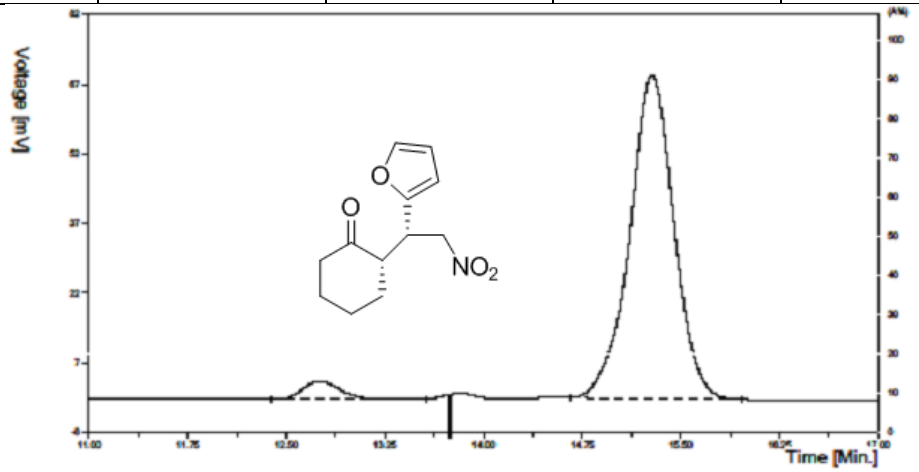
Peak#	Ret. Time(min)	Height(mV)	Area(mv.sec)	Area%
1	14.97	16.61	366.50	1.8713
2	20.12	551.21	19218.53	98.1287
Total		567.82	19585.03	100

2.5.9 **The HPLC Spectra of compound 3i**



Peak Table

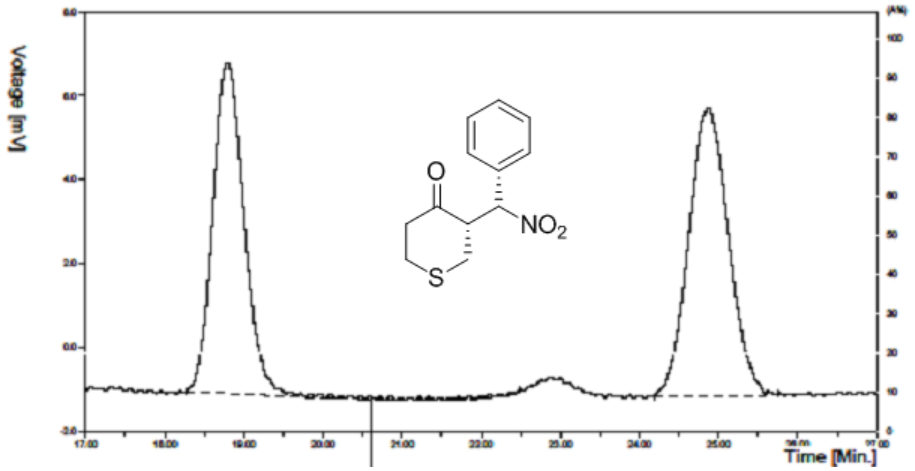
Peak#	Ret. Time(min)	Height(mV)	Area(mv.sec)	Area%
1	12.55	90.54	1886.80	34.0903
2	15.23	143.14	3647.91	65.9097
Total		233.68	5534.71	100



Peak Table

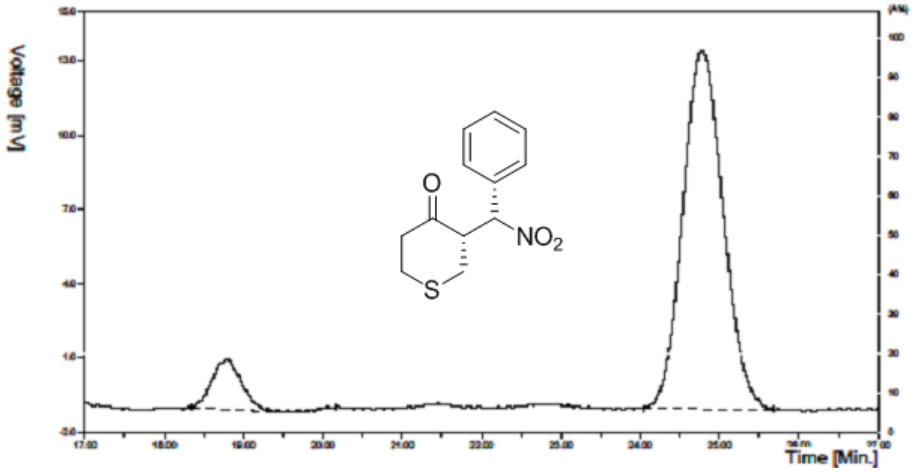
Peak#	Ret. Time(min)	Height(mV)	Area(mv.sec)	Area%
1	12.75	3.88	71.96	4.2260
2	15.28	69.76	1630.89	95.7740
Total		73.64	1702.85	100

2.5.10 **The HPLC Spectra of compound 3j**



Peak Table

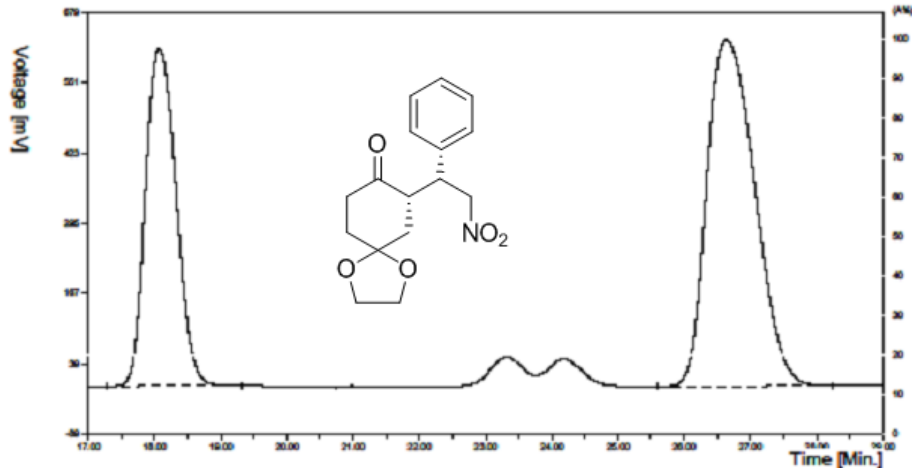
Peak#	Ret. Time(min)	Height(mV)	Area(mv.sec)	Area%
1	18.79	7.82	182.97	43.4258
2	24.87	6.84	238.37	56.5742
Total		14.66	421.34	100



Peak Table

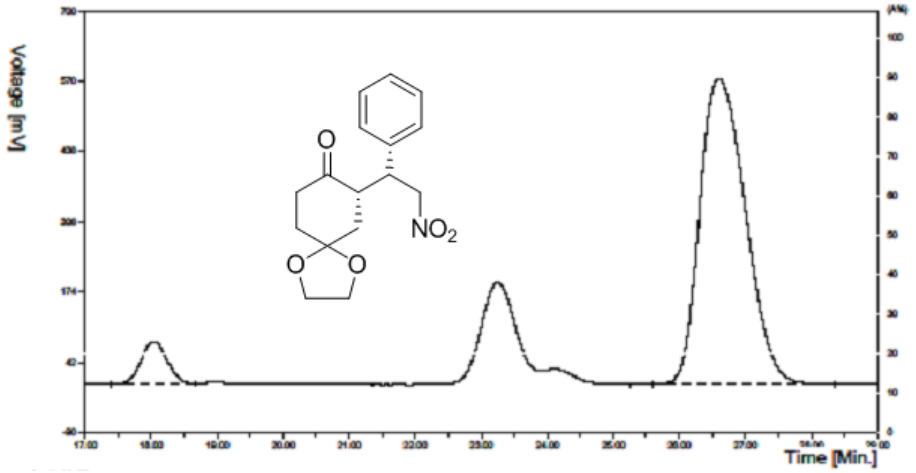
Peak#	Ret. Time(min)	Height(mV)	Area(mv.sec)	Area%
1	18.79	1.93	41.73	7.5451
2	24.76	14.45	511.32	92.4549
Total		16.38	553.05	100

2.5.11 The HPLC Spectra of compound 3k



Peak Table

Peak#	Ret. Time(min)	Height(mV)	Area(mv.sec)	Area%
1	18.07	614.76	19776.47	38.3977
2	26.64	631.06	31727.81	61.6023
Total		1245.82	51504.28	100



Peak Table

Peak#	Ret. Time(min)	Height(mV)	Area(mv.sec)	Area%
1	18.04	80.01	2181.56	7.3417
2	26.60	573.06	27533.14	92.6583
Total		653.07	29714.7	100

3 Cartesian Coordinates of Intermediates and Transition States

Table S1. Total energies using the B3LYP/6-31G(d) and imaginary frequencies using the DFTB-D method for all structures of the reaction pathways.

name	Total energy[a] (hartree)	imaginary freq [cm-1]	⊿H (kcal.mol^{-1})
4	-1206.070129		
cyclohexanone	-309.739549		
H_2O	-76.387785		
anti-enamine	-1439.391577		19.0
anti-SRts	-1953.398429	-290.24	4.9
anti-SR	-1953.410084		-7.3
anti-SSts	-1953.39171	-299.42	9.1
anti-SS	-1953.396587		-3.1
syn-enamine	-1439.394387		17.3
syn-RRts	-1953.393229	-313.23	10.0
syn-RR	-1953.381791		7.2
syn-RSts	-1953.38038	-255.53	18.0
syn-RS	-1953.366831		8.5

a Sum of electronic and zero-point Energies

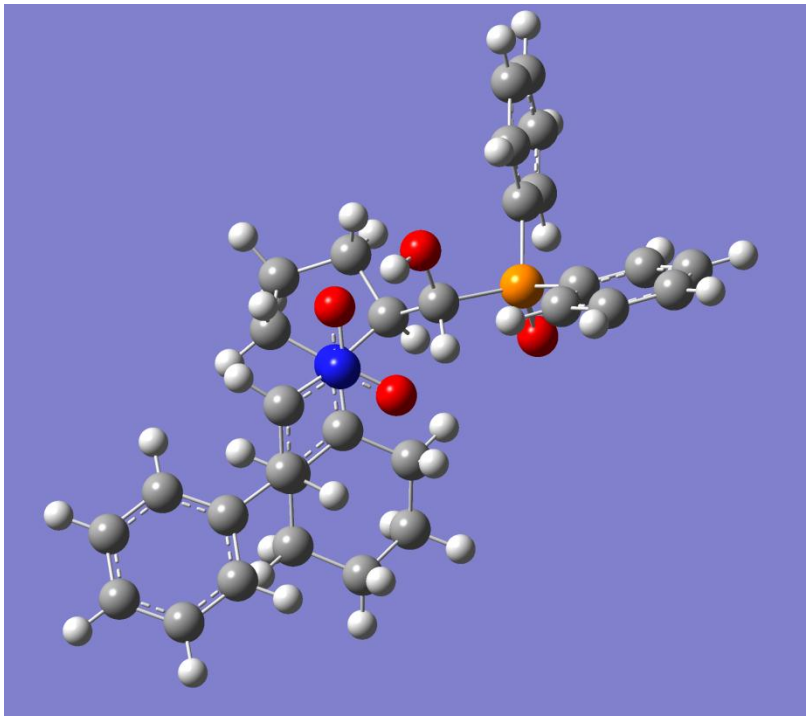


Figure S1 the transiton structure of anti-SRts

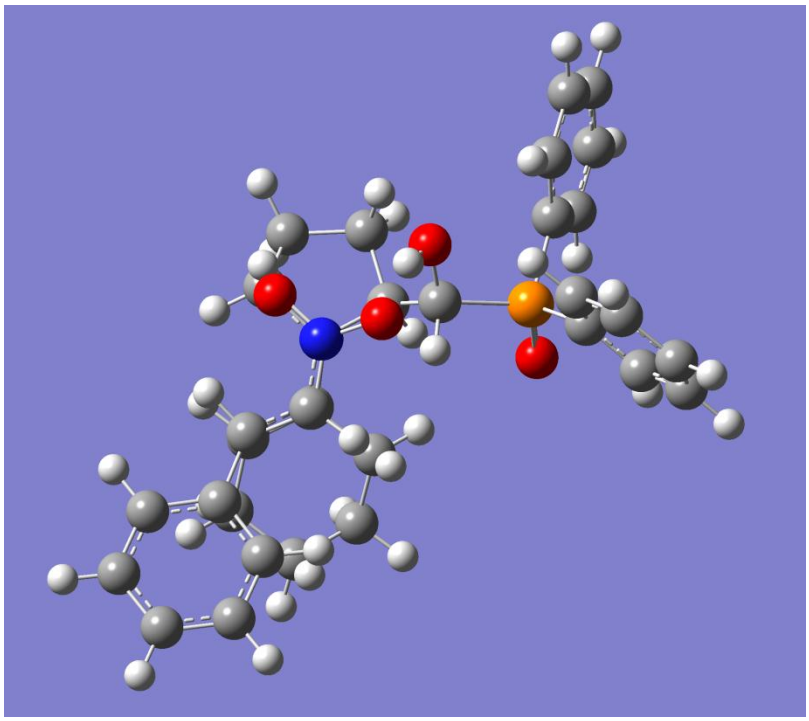


Figure S2 the transiton structure of anti-SSts

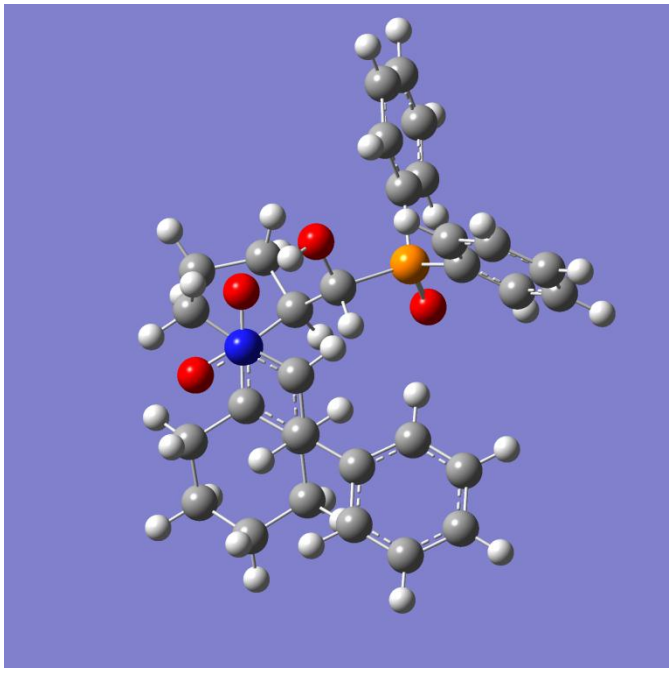


Figure S3 the transiton structure of Syn-RRts

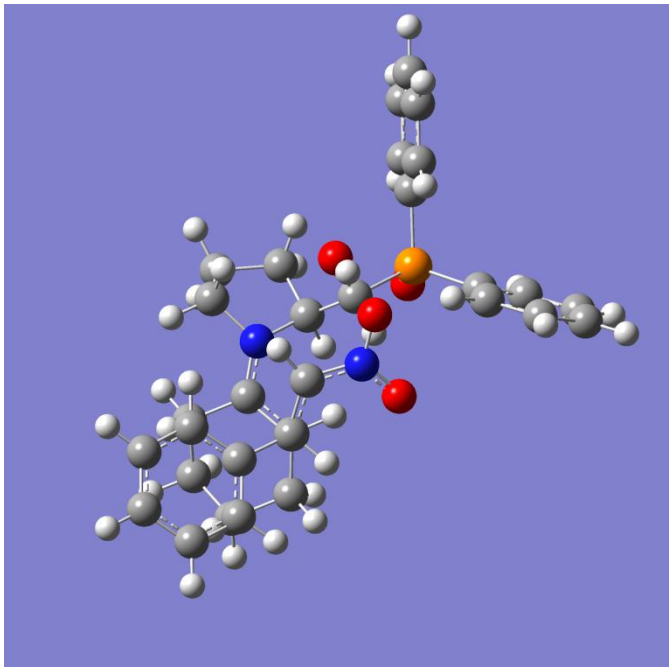


Figure S4 the transiton structure of Syn-RSts

Table S2. Cartesian coordinates in [Å] for the Optimized structures using the B3LYP/6-31G(d).

Cartesian coordinates of compound 4

Charge = 0 Multiplicity = 1

P,0,-0.0420130186,-0.0192336881,0.0569066365
C,0,0.0729128502,0.0519297117,1.8839703438
O,0,2.6754514174,0.1438948274,0.008466003
N,0,3.2584245033,-2.2804699444,-1.0105887056
O,0,-1.1446315823,-0.9384500149,-0.4015864326
C,0,1.8496793856,-2.0601810621,-0.5933582998
C,0,-0.2737788965,1.6999417296,-0.526108676
C,0,1.7915477238,-2.7306006854,0.7867200401
C,0,-0.9223283271,-0.6364738616,2.5924810087
C,0,1.6096226287,-0.5335844499,-0.6342488056
C,0,1.0492179691,0.7744718014,2.5878162154
C,0,0.7651117519,2.6404473394,-0.60669999

C,0,0.4982938869,3.9353115418,-1.053371504
C,0,-1.5720056724,2.0670134363,-0.9082494538
C,0,-0.7990316659,4.2997947287,-1.4207943153
C,0,0.0347946706,0.1084113179,4.6834698079
C,0,3.8090072204,-3.4671210649,-0.3048516526
C,0,-0.9404930474,-0.6073997338,3.9877614521
C,0,2.6647645325,-3.9787067019,0.5912166657
C,0,1.0282753529,0.7967744195,3.9822655168
C,0,-1.8327843692,3.3639899579,-1.3512323448
H,0,3.4513166039,-0.4139880081,-0.2342736595
H,0,1.1271286289,-2.5416882966,-1.2661527267
H,0,2.2304205827,-2.0666674433,1.5397738662
H,0,0.7656323688,-2.9572739073,1.0864735227
H,0,-1.6742679298,-1.1883886705,2.0360566481
H,0,1.5516804736,-0.2368460766,-1.6974356138
H,0,1.8296549878,1.3011396872,2.0509164128
H,0,1.7788940593,2.3549397491,-0.3421397275
H,0,1.306108176,4.6596576348,-1.1186169826
H,0,-2.3634847744,1.3242858686,-0.8690411035
H,0,-1.0019193605,5.3098660677,-1.767446784
H,0,0.0216202212,0.1322224274,5.770168614
H,0,4.6760400087,-3.1657860724,0.2968621719
H,0,4.1557443979,-4.2282213748,-1.0138576529
H,0,-1.7159575278,-1.1423403141,4.5297966296
H,0,2.0927864859,-4.7564747732,0.0703389513
H,0,3.0257015458,-4.4067673541,1.5317413279
H,0,1.7889150606,1.3539123945,4.5230620829
H,0,-2.8410471174,3.6419634935,-1.6467801697
H,0,3.3348114279,-2.3720227737,-2.0193105908

Cartesian coordinates of anti-enamine

Charge = 0 Multiplicity = 1

P,0,0.0990305924,0.1513855227,0.0345213114
C,0,-0.0498226715,0.0031651967,1.8541396267
O,0,2.7879386299,0.0056255588,0.4070416265
N,0,3.2571508637,-2.3698277216,-1.0024079756
O,0,-0.9974315865,-0.5910704753,-0.6840841903
C,0,1.8631736214,-1.9782061935,-0.6896897832
C,0,0.1047092278,1.9406689211,-0.349128634
C,0,1.5422734314,-2.7748979885,0.590222714
C,0,-1.176083734,-0.6847016945,2.327905018
C,0,1.7882216273,-0.4422093545,-0.497994442
C,0,0.8549205405,0.5632759964,2.7695176953
C,0,1.2234914903,2.7693927983,-0.1716881418
C,0,1.1395410932,4.1281129301,-0.4784239218
C,0,-1.0885116435,2.4844265975,-0.8457113156
C,0,-0.0549841547,4.6673811595,-0.9613812757
C,0,-0.4878353068,-0.2636255667,4.6067324728
C,0,3.700956001,-3.4922157094,-0.1528634019
C,0,-1.3933853715,-0.8166433202,3.7003005193
C,0,2.4103740448,-4.0302479686,0.473308272
C,0,0.6349548833,0.4247656364,4.1397168234
C,0,-1.1671619345,3.8441788466,-1.1477926488
H,0,3.5788432191,-0.5172574456,0.1656671664
H,0,1.1632102687,-2.2563599311,-1.4864659672
H,0,1.8414083302,-2.1945008933,1.4692563521
H,0,0.472540768,-2.9827233629,0.668505805
H,0,-1.8719815018,-1.1083949917,1.609736124
H,0,1.9262090469,0.0371228861,-1.4787492538
H,0,1.7332489753,1.0902694425,2.4149599512
H,0,2.159024739,2.3500550618,0.1866651075
H,0,2.0095043441,4.7656612279,-0.3438490601
H,0,-1.9407320833,1.8303298475,-1.0052901695
H,0,-0.1161916655,5.7264094076,-1.1983417386
H,0,-0.6560200448,-0.3660692619,5.6757487701
H,0,4.4102942184,-3.1588163012,0.6197914822
H,0,4.2157549723,-4.2373289597,-0.7689288016
H,0,-2.2692889316,-1.3500373514,4.0601675636
H,0,1.9444917864,-4.7564002442,-0.2039830411
H,0,2.5802886778,-4.5274202643,1.433707972
H,0,1.3407967532,0.856335282,4.8445946818
H,0,-2.0945414899,4.2594407268,-1.533366352
C,0,3.8823038671,-2.1687013796,-2.2550247791
C,0,3.045827984,-1.5947754035,-3.3890798168
C,0,5.1807699284,-2.4894149164,-2.4462139685
C,0,3.6781934253,-1.8445279455,-4.766382301

H,0,2.9131699713,-0.5117531223,-3.2524862456
H,0,2.0378516082,-2.0248607485,-3.3702512096
C,0,5.9218491494,-2.3350111072,-3.751951446
H,0,5.7589627505,-2.8859731693,-1.6149867081
C,0,5.1615094443,-1.4672813486,-4.7622789779
H,0,3.129017335,-1.2747891998,-5.5258683284
H,0,3.5734705278,-2.9065536648,-5.0281615917
H,0,6.9153054763,-1.9040472936,-3.5621806682
H,0,6.1163495129,-3.3266570405,-4.1941315648
H,0,5.5945495807,-1.5778960746,-5.7639986072
H,0,5.2618587789,-0.4078749453,-4.4872444224

Cartesian coordinates of syn-enamine

Charge = 0 Multiplicity = 1
P,0,0.1271428135,0.094127592,-0.011988123
C,0,-0.0593904358,-0.0118356579,1.8072727243
O,0,2.820009973,-0.0103212346,0.3743870515
N,0,3.2907433387,-2.4290167078,-0.9315521227
O,0,-0.9589276088,-0.6611807495,-0.7333851522
C,0,1.9005009563,-2.0655195417,-0.567956329
C,0,0.145773207,1.8737845501,-0.4390855669
C,0,1.6811374092,-2.7962389077,0.7648144126
C,0,-1.2087978059,-0.6663562551,2.272966595
C,0,1.8164925756,-0.5253981033,-0.4932527467
C,0,0.8408191956,0.5457444098,2.7286608461
C,0,1.2597687774,2.7073326598,-0.2542944052
C,0,1.1835583072,4.0577446514,-0.5975750318
C,0,-1.0343244468,2.4043772625,-0.9795261247
C,0,0.0018964401,4.5842302945,-1.1241900977
C,0,-0.5540431899,-0.2151439711,4.5558790642
C,0,3.7053075987,-3.6638990007,-0.2095885755
C,0,-1.4543591966,-0.7666591479,3.6432794065
C,0,2.457153412,-4.1027012988,0.5712463907
C,0,0.5922387919,0.4391233762,4.0969904234
C,0,-1.1052135302,3.755974287,-1.317994593
H,0,3.5989763866,-0.5714453142,0.1798946276
H,0,1.1675620452,-2.4238663823,-1.3028900691
H,0,2.1094924075,-2.2093012478,1.5843491123
H,0,0.6194969795,-2.9483389172,0.9732418429
H,0,-1.899764306,-1.0897299591,1.5497801903
H,0,1.9616468127,-0.1315886194,-1.5109607134
H,0,1.7376006047,1.045027529,2.3799318831
H,0,2.1861674162,2.296603624,0.1354639567
H,0,2.0501195483,4.6988224081,-0.4575596995
H,0,-1.8821053038,1.7458431242,-1.1443756097
H,0,-0.0530314727,5.6369197998,-1.3894562925
H,0,-0.7445562533,-0.2924951611,5.623282238
H,0,4.5443681266,-3.4514658963,0.4662437119
H,0,4.0337252052,-4.4380181134,-0.9119651431
H,0,-2.3482001527,-1.2740549723,3.9967008684
H,0,1.8669229493,-4.8032466606,-0.0314975997
H,0,2.7069853518,-4.6024896201,1.5124888788
H,0,1.2942456373,0.8688426214,4.8068687934
H,0,-2.022381948,4.1607790903,-1.7376886952
C,0,3.7585946507,-2.2439130369,-2.2595211012
C,0,2.9666807358,-1.9235639958,-3.3005265216
C,0,5.2683631658,-2.3270988498,-2.4060436736
C,0,3.4775172604,-1.5955694584,-4.6836582645
H,0,1.8887687663,-1.8804257013,-3.1710429303
C,0,5.7237584233,-2.3835537723,-3.8708198405
H,0,5.7152675514,-1.4538384661,-1.9051763846
H,0,5.6544675688,-3.2011797663,-1.8669083607
C,0,4.9891682166,-1.3326475562,-4.707764714
H,0,2.9379919436,-0.7238414898,-5.0798446991
H,0,3.2355207383,-2.42340778,-5.3701484519
H,0,6.8098466352,-2.2401441783,-3.9242705544
H,0,5.5160078331,-3.3821674326,-4.2799363838
H,0,5.3583061318,-1.3287529544,-5.7405853135
H,0,5.193805587,-0.335472155,-4.2931808747

Cartesian coordinates of anti-SRts

Charge = 0 Multiplicity = 1
P,0,2.8530089712,0.1356441389,0.7363712867
C,0,4.1796048808,-0.8845175721,-0.0018564316
O,0,1.5643999934,0.0037059607,-1.6211890422
N,0,-0.8461608281,-1.4917261131,0.0558566465

O,0,2.6272030569,-0.2111509987,2.1908739773
C,0,0.6567021874,-1.4994517963,0.1576187675
C,0,3.3313149253,1.8729380208,0.420897929
C,0,1.0995579452,-2.674513575,-0.7395794383
C,0,4.7971813385,-1.833688527,0.8246921813
C,0,1.2954290823,-0.139566926,-0.2441997332
C,0,4.5913114151,-0.7523451275,-1.3378203707
C,0,2.5019941077,2.7929733826,-0.2382134123
C,0,2.908165463,4.1216695339,-0.379899759
C,0,4.5656749286,2.3054696493,0.9333976785
C,0,4.1355332046,4.5431518403,0.1317361315
C,0,6.2205155124,-2.5124585087,-1.0079463557
C,0,-1.2604086409,-2.4272675975,-1.0124163797
C,0,5.81688516,-2.6441182312,0.3216991068
C,0,-0.1707488125,-3.4990825936,-0.9797238229
C,0,5.6065355113,-1.5683707994,-1.835865208
C,0,4.9649711012,3.6325609646,0.790896017
H,0,0.7749181448,0.4119133804,-2.0592936076
H,0,0.9133401712,-1.697846597,1.2006200082
H,0,1.4748948714,-2.2704689719,-1.6830675849
H,0,1.9031221424,-3.2475775004,-0.2704210452
H,0,4.4722869643,-1.920048666,1.8576947022
H,0,0.6215262437,0.6543060582,0.0926019423
H,0,4.1088513961,-0.0250325062,-1.9818088196
H,0,1.545445018,2.4894062929,-0.6500935412
H,0,2.2603235423,4.8261017038,-0.8945056113
H,0,5.2145384275,1.6012842011,1.4476426763
H,0,4.4468058956,5.5783143809,0.0173906822
H,0,7.0145343229,-3.1430607983,-1.3999853395
H,0,-1.2600636413,-1.8971396692,-1.9715931628
H,0,-2.2600981216,-2.8182603031,-0.822388314
H,0,6.2963113536,-3.3750683982,0.9677518927
H,0,-0.3582395381,-4.1935941812,-0.1518681829
H,0,-0.1350995164,-4.0777275195,-1.9077161507
H,0,5.9212229919,-1.4661677826,-2.871140507
H,0,5.9219819019,3.9556651123,1.1919067686
C,0,-1.6715010971,-0.8948225938,0.9345714087
C,0,-1.0726080776,-0.0839465846,2.0749393072
C,0,-3.0865534946,-0.9357946884,0.8029426817
C,0,-1.9036084705,-0.1665920156,3.365053572
H,0,-1.0393247426,0.96034309,1.7389723504
H,0,-0.0390460512,-0.3651834818,2.2842557546
C,0,-3.9463350603,-0.790401698,2.0525992786
H,0,-3.4813179655,-1.6715479441,0.1095255245
C,0,-3.3691092549,0.1733285686,3.0935817705
H,0,-1.4683185253,0.5144138132,4.1051741036
H,0,-1.8321988428,-1.17849504,3.7878709133
H,0,-4.9598987546,-0.4874025716,1.768815382
H,0,-4.0548600676,-1.7845500999,2.5158447689
H,0,-3.9598342069,0.1210627637,4.0161770381
H,0,-3.4412477583,1.2087025633,2.7313623346
C,0,-2.8299086358,0.5724943281,-1.6974997771
C,0,-5.0775044374,0.4735317622,-0.6384316304
C,0,-5.9435709573,1.3164073119,0.078015348
C,0,-5.6436760697,-0.5249132894,-1.4509514262
C,0,-7.328063388,1.1794358416,-0.0252681568
H,0,-5.5238640964,2.0961936714,0.7086576933
C,0,-7.025468467,-0.6656194957,-1.5510317236
H,0,-4.9971753476,-1.1999979898,-2.0054457415
C,0,-7.8743249359,0.1875801216,-0.8402167598
H,0,-7.9782438482,1.8486887187,0.5315992119
H,0,-7.4424618733,-1.4434216721,-2.1851215326
H,0,-8.9521481117,0.0768130632,-0.9202094361
C,0,-3.6133505944,0.6793641834,-0.5369496225
H,0,-3.3012742611,1.4548073253,0.1549558804
H,0,-3.1195023307,0.039363887,-2.5904320105
N,0,-1.5470622814,1.0403385392,-1.7172196603
O,0,-0.821807246,0.7725147803,-2.7313490393
O,0,-1.0937184019,1.7107930711,-0.7447291797

Cartesian coordinates of anti-SR

Charge = 0 Multiplicity = 1

P,0,-1.286327432,0.6335114529,-0.7171337385
C,0,-2.6865881178,-0.5130110797,-0.977098662
O,0,-0.5853986253,-0.7838971542,1.5036564999
N,0,2.1701057725,-1.3862788527,0.1412655239

O,0,-0.6480299682,1.0504406267,-2.0242132687
C,0,0.8092148494,-1.2039305997,-0.4945970925
C,0,-1.946789159,1.990711463,0.3155611244
C,0,0.2062276542,-2.627009703,-0.5435252527
C,0,-3.0270289645,-0.8354589478,-2.2980994102
C,0,-0.0212763561,-0.2043612982,0.3534297348
C,0,-3.414198061,-1.0730732974,0.0858892704
C,0,-1.2819498348,2.4719265809,1.4552012487
C,0,-1.8038162616,3.5613142701,2.1561013336
C,0,-3.1323637583,2.6164874186,-0.1042719309
C,0,-2.979968663,4.1792272507,1.730631023
C,0,-4.8058371329,-2.2640336174,-1.4975995605
C,0,2.1264100202,-2.6655282897,0.9017377005
C,0,-4.0869776384,-1.7070413902,-2.5564794171
C,0,1.3034360197,-3.5678365394,-0.0144318512
C,0,-4.4670152924,-1.9486547099,-0.1785130417
C,0,-3.6445061325,3.7061640092,0.5968666118
H,0,-0.0155829164,-0.5381629485,2.2927005549
H,0,0.9521260936,-0.7914000286,-1.4932220611
H,0,-0.6636376638,-2.658963593,0.1145165483
H,0,-0.1141432306,-2.8853606772,-1.5556312405
H,0,-2.4573160158,-0.3922268529,-3.1099963264
H,0,0.6565431323,0.6066125247,0.6411218099
H,0,-3.1444761714,-0.8335866213,1.1090980701
H,0,-0.366340012,2.0121314613,1.8152313414
H,0,-1.2861717113,3.9225581097,3.0404346413
H,0,-3.6571218748,2.2487820899,-0.982132616
H,0,-3.380415993,5.0261624059,2.2819527852
H,0,-5.6311395818,-2.9426005022,-1.6980865527
H,0,1.6050407552,-2.4609727847,1.8425227765
H,0,3.1249486889,-3.0385148939,1.1171310382
H,0,-4.3514166894,-1.948959746,-3.5826575744
H,0,1.933833042,-3.944726712,-0.82860461
H,0,0.8996746844,-4.4284090333,0.5260844325
H,0,-5.0267444257,-2.3831455986,0.6456288132
H,0,-4.5619781112,4.1825732668,0.2616068712
C,0,3.155874191,-0.5280238217,0.0743029457
C,0,3.0491004011,0.7291498414,-0.7589095997
C,0,4.4726146737,-0.7811920125,0.774600817
C,0,4.2527697397,0.919253297,-1.7025431685
H,0,3.0340924042,1.5500379977,-0.0332513938
H,0,2.1100950516,0.7890836934,-1.3096449274
C,0,5.6649392747,-0.4749290827,-0.1734963955
H,0,4.5448325337,-1.8396837286,1.0289439789
C,0,5.5633887939,0.8588266067,-0.9171034517
H,0,4.137177864,1.8814015666,-2.2134934152
H,0,4.2485998067,0.1453302731,-2.4827457319
H,0,6.5870114227,-0.5289373143,0.4124598933
H,0,5.7221224321,-1.2833286773,-0.9165642444
H,0,6.4226940705,0.9698560055,-1.5893884449
H,0,5.6080417457,1.6965998374,-0.2082904055
C,0,3.4214254551,-0.4268615015,3.0776524712
C,0,5.8967490656,-0.3107015258,2.8578219702
C,0,6.7975984518,0.7336901466,3.1032481886
C,0,6.2588485984,-1.6058288819,3.2591123227
C,0,8.0220584877,0.4962139798,3.7305465571
H,0,6.5316705308,1.7459743585,2.8080226918
C,0,7.4815579017,-1.8480439395,3.8850414582
H,0,5.5758192727,-2.4358247682,3.091916735
C,0,8.3693631066,-0.7967251748,4.1226588885
H,0,8.702383616,1.323767226,3.9136948938
H,0,7.7392609444,-2.8586683339,4.1910488224
H,0,9.321599629,-0.984404531,4.6111981088
C,0,4.5575221595,-0.0249549382,2.1946646583
H,0,4.482130166,1.047930951,1.9928343525
H,0,3.483091374,-1.21625173,3.8124593044
N,0,2.2231575427,0.1017121756,2.8802893082
O,0,1.1800026738,-0.355905163,3.4941890423
O,0,2.0873974115,1.0650099295,2.0240762027

Cartesian coordinates of anti-SSts

Charge = 0 Multiplicity = 1

P,0,-2.6968089421,0.3204601388,-0.8205647802
C,0,-4.2171212819,-0.5351391156,-0.2684400851
O,0,-1.6183723337,-0.2558061365,1.6106657022
N,0,0.6569809795,-1.9110518309,-0.0489974244

O,0,-2.4077477117,0.0636825371,-2.2827464597
C,0,-0.8109306332,-1.6696902945,-0.2700664346
C,0,-2.8880458622,2.0988513139,-0.4468331703
C,0,-1.5103557876,-2.8411720408,0.4547767173
C,0,-4.9223884128,-1.2485258072,-1.2487713279
C,0,-1.2761451661,-0.2731705657,0.2472898924
C,0,-4.7046145797,-0.4984173982,1.047879307
C,0,-2.7663426171,2.6498466611,0.8385091654
C,0,-2.9311621761,4.0227404473,1.0247420001
C,0,-3.166137633,2.9369322512,-1.5374006138
C,0,-3.2209269044,4.8510639567,-0.0615161074
C,0,-6.5824035336,-1.8793086653,0.3913480772
C,0,0.8260076498,-2.9513217339,0.9857389827
C,0,-6.1021633147,-1.9173648646,-0.9184605664
C,0,-0.3963126927,-3.8446631744,0.7839333303
C,0,-5.8820455179,-1.1718178555,1.37204702
C,0,-3.3356996517,4.3077022288,-1.3425378994
H,0,-0.8834394213,0.2215326474,2.0959886852
H,0,-0.9933964207,-1.7121651349,-1.3455777465
H,0,-1.9598505702,-2.4625434941,1.3749518752
H,0,-2.3021115812,-3.2696757794,-0.1646081558
H,0,-4.5364324871,-1.2664035771,-2.2637916936
H,0,-0.481813955,0.457079327,0.0520707587
H,0,-4.1593716766,0.0374074396,1.8164032353
H,0,-2.5217951419,2.014311094,1.6819380192
H,0,-2.8265597727,4.4449281172,2.0204650553
H,0,-3.2327138393,2.5057486806,-2.5318822506
H,0,-3.350305025,5.9196772312,0.0896335728
H,0,-7.5015420256,-2.3990862688,0.6494209076
H,0,0.834894413,-2.4452100497,1.9605082308
H,0,1.7715928801,-3.4772083771,0.8528307384
H,0,-6.6455868321,-2.4653963905,-1.6837595479
H,0,-0.2217865577,-4.5338974952,-0.0512483138
H,0,-0.615510828,-4.4412650916,1.6740764592
H,0,-6.2540340074,-1.1435733444,2.3927831306
H,0,-3.5520537666,4.9513273324,-2.1911954747
C,0,1.6418065362,-1.3409076965,-0.7343176685
C,0,1.311431956,-0.3249397585,-1.8033137821
C,0,3.0331955811,-1.5308393732,-0.4131775027
C,0,2.2187541125,-0.4640696155,-3.038396155
H,0,1.4762205242,0.6650672406,-1.3450424054
H,0,0.2627751814,-0.3514443743,-2.1031843788
C,0,4.0116202735,-1.4842362664,-1.5910301174
H,0,3.2286163794,-2.3965244999,0.2142031612
C,0,3.6937213259,-0.4149341557,-2.6414218042
H,0,1.9729985321,0.3355933645,-3.7462491513
H,0,1.994870388,-1.4123360445,-3.5462427329
H,0,5.0301867315,-1.3516402441,-1.2136858125
H,0,3.9977866316,-2.4726763412,-2.0775557116
H,0,4.3345136657,-0.560505519,-3.519583099
H,0,3.9307693686,0.5780819446,-2.2417883774
C,0,2.426725428,0.7417470053,1.3432250078
C,0,3.4797770549,-0.1679207693,1.0341537343
C,0,4.8156857357,0.3827666965,0.6664091126
C,0,5.9702594213,-0.3292493726,1.0336348914
C,0,4.9832400097,1.6148268375,0.0107710043
C,0,7.2444813321,0.1664608512,0.7578933077
H,0,5.863480448,-1.2783575195,1.5541293111
C,0,6.255097346,2.1114528391,-0.2685197019
H,0,4.1134901749,2.2002200777,-0.2720611329
C,0,7.3920137276,1.3895539759,0.1023924655
H,0,8.1207047337,-0.4005728468,1.0607659345
H,0,6.3585902744,3.0693490358,-0.7712868907
H,0,8.3827412949,1.7805452296,-0.1122511958
N,0,1.4518938413,0.3851554279,2.220425578
O,0,1.5148066498,-0.6897664654,2.8845362359
O,0,0.4519402703,1.1829266552,2.3690578454
H,0,3.5446664612,-0.9409661437,1.794571256
H,0,2.2718353667,1.7060462261,0.8830546437

Cartesian coordinates of anti-SS

Charge = 0 Multiplicity = 1

P,0,2.7374662675,0.1617155666,0.6287662655
C,0,4.1088282127,-1.0210620066,0.3794103791
O,0,1.4781526478,-1.0829029785,-1.4561212566
N,0,-0.9260154056,-1.6746867804,0.4676975045

O,0,2.4737391653,0.4251628325,2.0946774216
C,0,0.5440042495,-1.5520642559,0.7862550877
C,0,3.1397923496,1.6795787937,-0.3047521978
C,0,1.0921601265,-2.9880642349,0.6546451893
C,0,4.7538490646,-1.4937227159,1.531416373
C,0,1.2089325192,-0.5398864176,-0.192743216
C,0,4.5409396602,-1.4504483386,-0.8855957951
C,0,2.8601719745,1.8550048381,-1.6689072857
C,0,3.2017285205,3.0530047648,-2.2986862444
C,0,3.7504694047,2.7161574435,0.4183765994
C,0,3.8234358508,4.0751837303,-1.5793296523
C,0,6.2446259253,-2.8151920462,0.1622624174
C,0,-1.1707599441,-3.0213553958,-0.1296905219
C,0,5.8198359014,-2.3881604999,1.421304825
C,0,-0.1491422286,-3.890190248,0.6001564402
C,0,5.6038861916,-2.3473217577,-0.9882841228
C,0,4.0946872804,3.9072082435,-0.2194789098
H,0,0.778478307,-0.7073437714,-2.089145329
H,0,0.6478360435,-1.1811677823,1.8063690872
H,0,1.6505225941,-3.0646697962,-0.2809202986
H,0,1.763642892,-3.2308109562,1.4815878177
H,0,4.4125033805,-1.1489002252,2.503239255
H,0,0.5448567163,0.3296130932,-0.290346129
H,0,4.0390239899,-1.0986303309,-1.7799309129
H,0,2.3600248395,1.0740140712,-2.2305052122
H,0,2.9740498396,3.1867715105,-3.3526272563
H,0,3.9341371287,2.5872686576,1.4811104828
H,0,4.0887042164,5.0051809891,-2.075600641
H,0,7.0753830699,-3.510859433,0.075592597
H,0,-0.9800266333,-2.9400298648,-1.2013701681
H,0,-2.2042415457,-3.3242115248,0.0295506451
H,0,6.3186360187,-2.7486432555,2.3171969769
H,0,-0.5076717928,-4.1369410459,1.6072485362
H,0,0.0306452324,-4.8277937037,0.0665956397
H,0,5.9338230499,-2.6806521158,-1.968611537
H,0,4.5677850405,4.7059095095,0.3457625566
C,0,-1.8062536529,-0.7392772891,0.6892473236
C,0,-1.5108377792,0.4137213477,1.6112501396
C,0,-3.2415104571,-0.8422220022,0.2165705776
C,0,-2.3829164909,0.2189471881,2.8820799164
H,0,-1.812129369,1.3410804983,1.1190029966
H,0,-0.4570859373,0.5088531772,1.8737729913
C,0,-4.1818849955,-0.8719173299,1.4519156996
H,0,-3.3599096901,-1.7802377587,-0.3195125433
C,0,-3.873456535,0.1853661153,2.5242374937
H,0,-2.1657173024,1.0385968273,3.5759780409
H,0,-2.0852290685,-0.7098531579,3.3883715974
H,0,-5.2187330247,-0.7770887895,1.1126246488
H,0,-4.0960073632,-1.8699435825,1.9066356212
H,0,-4.4685354046,-0.0263768078,3.4211072429
H,0,-4.1786738154,1.1751350753,2.1706813891
C,0,-2.2080394212,0.7295616142,-1.5309848875
C,0,-3.506898284,0.2752137986,-0.923007311
C,0,-4.42012344,1.4283208902,-0.5283320151
C,0,-5.8099900263,1.2486761669,-0.6216049648
C,0,-3.9558172405,2.6840255961,-0.1050728742
C,0,-6.7022993532,2.2655057769,-0.2816946743
H,0,-6.1968255076,0.2985915458,-0.9835537425
C,0,-4.8437796074,3.7068498851,0.2340179398
H,0,-2.8900011723,2.8823228355,-0.0481994434
C,0,-6.2212889139,3.5011319231,0.1531958887
H,0,-7.7721954704,2.0950382367,-0.3686509874
H,0,-4.4542365455,4.6696379719,0.5544243021
H,0,-6.9114648796,4.2989013599,0.4136956068
N,0,-1.4846032798,-0.1335181008,-2.2400304286
O,0,-1.8742136365,-1.3413738031,-2.3906255028
O,0,-0.3443292191,0.2451188221,-2.7439694438
H,0,-4.0465440566,-0.298707322,-1.6871137502
H,0,-1.853024181,1.7481497283,-1.5373442573

Cartesian coordinates of syn-RRts

Charge = 0 Multiplicity = 1

P,0,-2.1426228729,0.4719031389,-0.7267028873
C,0,-3.8387944442,-0.1140735197,-0.3725473745
O,0,-1.3949926906,-0.5982176245,1.6390902424
N,0,0.7069223266,-2.4594927955,0.1234738364

O,0,-1.8005863925,0.3672780577,-2.1927473379
C,0,-0.5650400629,-1.8278805064,-0.3685806157
C,0,-2.0026638251,2.1915483136,-0.1128665142
C,0,-1.6470168897,-2.9134597856,-0.1128546485
C,0,-4.6112033599,-0.4736642052,-1.4868705493
C,0,-0.9186184836,-0.4863191936,0.3163464215
C,0,-4.3972720957,-0.1947218185,0.91343199
C,0,-1.9432371371,2.5434576172,1.2457880831
C,0,-1.8252792446,3.8845212248,1.6133033999
C,0,-1.9365219171,3.1950872464,-1.0911594365
C,0,-1.7699511014,4.8805299595,0.6353732029
C,0,-6.4780661857,-0.9864838816,-0.0391277999
C,0,0.3569541429,-3.5560151321,1.045119443
C,0,-5.9270948893,-0.9073040469,-1.3187776674
C,0,-0.8988480333,-4.1523987855,0.4132883688
C,0,-5.7115123011,-0.6326849276,1.0743625976
C,0,-1.8235516778,4.5347156666,-0.7163272915
H,0,-0.6283440686,-0.697583955,2.2674094059
H,0,-0.4346857032,-1.6245023929,-1.4345433058
H,0,-2.3380108067,-2.5486403101,0.6495658114
H,0,-2.2186571225,-3.1179750819,-1.0215775126
H,0,-4.168475267,-0.4075770143,-2.4763020772
H,0,-0.0269517352,0.1474976026,0.2778511222
H,0,-3.8030123186,0.0614513558,1.7827935448
H,0,-1.96807475,1.7714183465,2.0077771582
H,0,-1.7742296233,4.1510244755,2.6656054854
H,0,-1.963948243,2.9107222676,-2.1389222686
H,0,-1.681221309,5.9237471603,0.9272604276
H,0,-7.502993303,-1.3237153993,0.0923698385
H,0,0.1615300179,-3.1037508834,2.0278329135
H,0,1.1789856413,-4.2552443615,1.1704020103
H,0,-6.5204792618,-1.1822447053,-2.1868316347
H,0,-0.6165503751,-4.8220313476,-0.4081829744
H,0,-1.4920651945,-4.7282341906,1.1295392168
H,0,-6.1380988963,-0.6976271775,2.0717948311
H,0,-1.776924252,5.3071465243,-1.4795940736
C,0,1.9292576831,-2.2361490066,-0.382965064
C,0,2.268687904,-0.9758102426,-0.9596160166
C,0,3.0065153149,-3.3066985807,-0.2893321296
C,0,3.3469512008,-0.9259964709,-2.0372703229
H,0,1.4280902191,-0.3243445675,-1.1856488336
C,0,3.9289877498,-3.3114366568,-1.5212457823
H,0,3.593963154,-3.1316788214,0.6186138689
H,0,2.5513103784,-4.2946555923,-0.1829207666
C,0,4.490176939,-1.9174572698,-1.8024932703
H,0,3.7319343731,0.0948991097,-2.1232846049
H,0,2.8728355706,-1.1488413585,-3.0055088462
H,0,4.7359622424,-4.0345127297,-1.3527627346
H,0,3.368927449,-3.6630785053,-2.3991342845
H,0,5.1517016592,-1.9368903634,-2.6769535201
H,0,5.1057796796,-1.5934313265,-0.9518573684
C,0,1.9752410596,0.0906784384,1.6883686266
C,0,2.9534250054,0.0776916258,0.6618821586
C,0,3.326855069,1.3917042118,0.0659873566
C,0,4.682320529,1.7040574048,-0.1270870035
C,0,2.3651060211,2.3508178606,-0.295502458
C,0,5.0674090605,2.9386289873,-0.6503478614
H,0,5.4408159388,0.9760929258,0.1504378952
C,0,2.74833627,3.5822692825,-0.8222129146
H,0,1.3070582848,2.1385866851,-0.1695706512
C,0,4.1011351419,3.8824330391,-1.0007165477
H,0,6.1227379871,3.1614938401,-0.7830542043
H,0,1.9853064025,4.3066014567,-1.0935765533
H,0,4.3985296987,4.8433242663,-1.4116732942
H,0,3.7988498357,-0.5742791307,0.864212154
H,0,1.2875675023,0.9053044939,1.8588148093
N,0,1.7837143288,-0.994808657,2.4947156347
O,0,2.5861643799,-1.9633851586,2.4699747255
O,0,0.7591899138,-1.0185135047,3.266966682

Cartesian coordinates of syn-RR

Charge = 0 Multiplicity = 1

P,0,-2.3608730857,0.445823725,-0.8870080203
C,0,-3.857900953,-0.2278282552,-0.0774303985
O,0,-0.9100409329,-0.7971697932,1.0785466379
N,0,0.5352999741,-2.5697499186,-0.5264623566

O,0,-2.4611864053,0.4065010284,-2.3918957414
C,0,-0.574259787,-1.7431564402,-1.1498807408
C,0,-2.0995250505,2.1325276093,-0.2356190704
C,0,-1.7636552072,-2.7209290506,-1.2129670769
C,0,-4.9544531701,-0.4685175887,-0.919111481
C,0,-0.8500902296,-0.4858647824,-0.2881081376
C,0,-3.9755006062,-0.4696643369,1.3013179727
C,0,-1.7072166727,2.4025575946,1.0859420305
C,0,-1.5212755556,3.7218805025,1.4992516711
C,0,-2.2991627623,3.1919366591,-1.1323907115
C,0,-1.7296416249,4.7747362477,0.6048070372
C,0,-6.2681928759,-1.182767247,0.9802417736
C,0,0.0062185804,-3.9195810911,-0.1744001874
C,0,-6.1554766324,-0.9426889432,-0.3900731612
C,0,-1.1421863474,-4.1155422621,-1.1584411767
C,0,-5.1776677702,-0.9491375683,1.8218829698
C,0,-2.1172781167,4.5095309899,-0.70975545
H,0,0.0326534749,-0.600585788,1.4113335751
H,0,-0.2610796129,-1.4477995843,-2.1546543001
H,0,-2.3980974694,-2.5716516353,-0.3346515582
H,0,-2.3656230004,-2.5338870116,-2.103952858
H,0,-4.8507273943,-0.2820629929,-1.9839996534
H,0,-0.0450128789,0.2369321383,-0.466827504
H,0,-3.1272736706,-0.3095689407,1.9564282521
H,0,-1.5277449093,1.5900991125,1.7826948273
H,0,-1.2086195449,3.9253186011,2.5195693524
H,0,-2.5865964783,2.9699691579,-2.155936185
H,0,-1.5848458632,5.8008536126,0.9323987226
H,0,-7.2035351946,-1.5517098256,1.3931405204
H,0,-0.3487644436,-3.8866432601,0.8615524209
H,0,0.7889472524,-4.6705743087,-0.2681723949
H,0,-7.0014252185,-1.1240135255,-1.0478678328
H,0,-0.7511603401,-4.4194512294,-2.1367797626
H,0,-1.8404801125,-4.8850502657,-0.8181484909
H,0,-5.2622997831,-1.1393288172,2.8884812542
H,0,-2.275229438,5.3273835753,-1.4078843783
C,0,1.7523419564,-2.1789758933,-0.2575885592
C,0,2.3572059888,-0.9041618683,-0.8036515323
C,0,2.7060354125,-3.0505689822,0.5000593977
C,0,3.5396088294,-1.3181751141,-1.7302689953
H,0,1.6273997593,-0.3805626668,-1.4235103037
C,0,3.9166779839,-3.4358498204,-0.3903672735
H,0,3.0413285274,-2.4499979124,1.3655472789
H,0,2.2301670234,-3.941781178,0.908861655
C,0,4.5750952444,-2.2052937915,-1.0259357635
H,0,4.0029918887,-0.398874903,-2.1044534033
H,0,3.139158712,-1.8488785184,-2.6059473566
H,0,4.6347851196,-3.9881468237,0.2252373409
H,0,3.5801667609,-4.1239502011,-1.1794405723
H,0,5.3375256553,-2.5227821795,-1.7475281472
H,0,5.0992305605,-1.6317918749,-0.2530931154
C,0,1.7474304366,0.1429325895,1.4799307254
C,0,2.7952332129,0.0447429635,0.3696852451
C,0,3.2249649084,1.402607609,-0.1727152008
C,0,4.537445164,1.8542374272,0.0299059824
C,0,2.3377416456,2.2490038176,-0.8569828919
C,0,4.9513401529,3.1053826812,-0.4305873598
H,0,5.2396426367,1.2219448783,0.5682950902
C,0,2.7466014398,3.4994757632,-1.3200340974
H,0,1.3069040185,1.9444605587,-1.0209085332
C,0,4.0572979473,3.9328246349,-1.1104969202
H,0,5.9731814442,3.432319256,-0.2555874387
H,0,2.036366026,4.1367759045,-1.8402919285
H,0,4.376400309,4.907279627,-1.4705093962
H,0,3.6709102825,-0.4040621253,0.8447748328
H,0,1.2385248268,1.0987024671,1.5803685464
N,0,2.1545951772,-0.2878686289,2.7506849163
O,0,3.1178613167,-1.1083998041,2.8679535829
O,0,1.5157154894,0.0978290165,3.7515468058

Cartesian coordinates of syn-RSts

Charge = 0 Multiplicity = 1

P,0,-2.7873161462,-0.2068909781,-0.7130971583
C,0,-4.0095010864,-0.7598052857,0.5344139076
O,0,-1.1305230563,-0.3535646052,1.511151131
N,0,1.0727324946,-1.7222433924,0.0670069061

O,0,-2.8587884004,-1.036964848,-1.9739705673
C,0,-0.3325356392,-1.5121602981,-0.4672661376
C,0,-3.1358158013,1.5610318915,-1.0146919146
C,0,-1.0506819102,-2.8507373329,-0.1184740646
C,0,-4.8081687048,-1.8602612254,0.1945034653
C,0,-1.0689716291,-0.2884366769,0.1033009011
C,0,-4.2026292065,-0.1199593431,1.7677522837
C,0,-2.6242148275,2.610397221,-0.2370955427
C,0,-2.9759424397,3.9282092943,-0.5377537586
C,0,-3.986494061,1.8456452688,-2.0953552218
C,0,-3.8331765603,4.2061963738,-1.6027418827
C,0,-5.9658992228,-1.6867659899,2.3093158798
C,0,1.0165410341,-2.8249288599,1.0483504003
C,0,-5.783611136,-2.3219495871,1.0803014994
C,0,0.0254780372,-3.8029221331,0.4265532325
C,0,-5.1757474188,-0.5856179172,2.6506679446
C,0,-4.33569433,3.1632448559,-2.3850447103
H,0,-0.7873687603,0.5086336068,1.8594061107
H,0,-0.2445730554,-1.3885769511,-1.5480120897
H,0,-1.792468571,-2.6635988646,0.6623118306
H,0,-1.5758941942,-3.2324388055,-0.994789883
H,0,-4.6596614966,-2.3377969745,-0.7696868735
H,0,-0.5635987788,0.6206991732,-0.2320853574
H,0,-3.5967282202,0.7378827397,2.0389561039
H,0,-1.9254709018,2.4324869331,0.575341472
H,0,-2.5632191421,4.7367641531,0.0589865711
H,0,-4.35313272,1.0295126385,-2.711203537
H,0,-4.1012381694,5.2347534158,-1.8311397377
H,0,-6.7256604901,-2.0442351406,2.9997995926
H,0,0.6052400757,-2.3958937395,1.9689971528
H,0,2.0068158389,-3.2241736724,1.2631203097
H,0,-6.4022944532,-3.1733553736,0.8084115513
H,0,0.5107242767,-4.3674094967,-0.379516208
H,0,-0.3718234335,-4.5189957339,1.1518362568
H,0,-5.3194547263,-0.0873428186,3.6057699327
H,0,-4.9930167548,3.376735112,-3.2240244049
C,0,2.1904002673,-1.3582107041,-0.5768597167
C,0,2.3080702716,-0.0590112697,-1.1664997272
C,0,3.3850889791,-2.2900420791,-0.632405557
C,0,3.2005998072,0.1029572508,-2.3992319128
H,0,1.3646194024,0.4730960383,-1.2832302601
C,0,4.0217281427,-2.2575743307,-2.0393091348
H,0,4.1395193275,-1.9956349806,0.107683525
H,0,3.0848322959,-3.3147555948,-0.3998920304
C,0,4.4158736285,-0.8346681611,-2.4376517929
H,0,3.521248977,1.1486706757,-2.4836296338
H,0,2.5750895787,-0.0843994388,-3.2842577902
H,0,4.8952585985,-2.9200802639,-2.0443949878
H,0,3.3083947232,-2.6687635326,-2.7668671742
H,0,4.8492731651,-0.8294019701,-3.4450921828
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Cartesian coordinates of syn-RS

Charge = 0 Multiplicity = 1

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C,0,-0.8529139405,-0.4336229036,-0.2411746877
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C,0,-1.6640756651,2.6560095,0.8073252906
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H,0,1.8774397781,-0.5107096385,2.804541439

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