Densely Substituted Unnatural L- and D-Prolines as Catalysts for Highly Enantioselective Stereodivergent (3+2) Cycloadditions and Aldol Reactions

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Supporting Information

List of Contest:

Computational studies about the copper(I)-assisted reaction between imine 6b and nitroalkene 5a employing L-3a and D-3b as chiral ligands. In order to understand the origins of this different behaviour for both catalysts, we performed ONIOM computational studies at the B3LYP/LANL2DZ:PM6 and M06/6-31++G**&LANL2DZ levels of theory for the geometry optimisation and for the evaluation of the energies, respectively.

In a previous work we demonstrated that the stereoselectivity obtained employing chiral ligand-metallated azomethine ylides in 1,3-dipolar cycloadditions is a consequence of the blockage of one of the ylide stereogenic faces by the chiral ligand.[20]

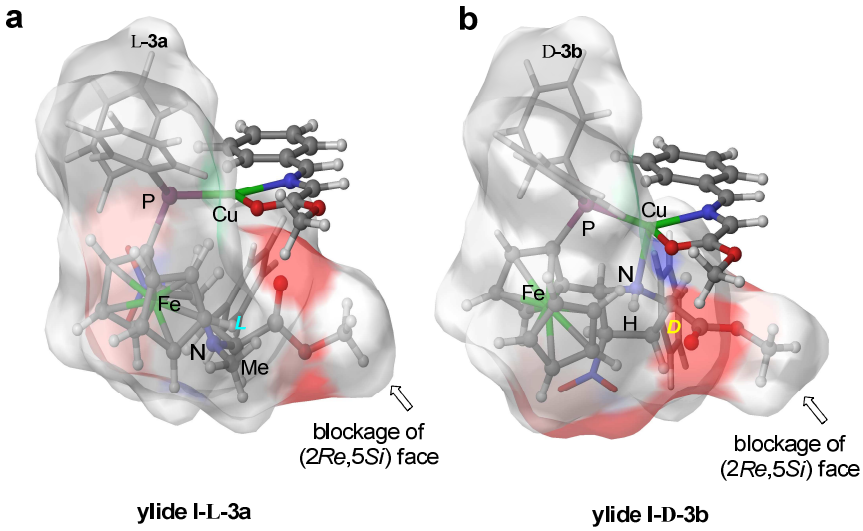


Figure S1. Main geometrical features of the most stable ylide copper (I) complexes computed considering a, L-**3a** or b, D-**3b** as chiral ligand.

As it is shown in Fig. S1 there is an effective blockage of the (2*Re*,5*Si*) prochiral face in both cases due to the proline derived catalyst.

We computed the transition structures corresponding to the possible approaches of the dipolarophile **5a** to the previously described ylide complex. The geometrical features and relative Gibbs free energies of these transition structures are gathered in Fig. S2.

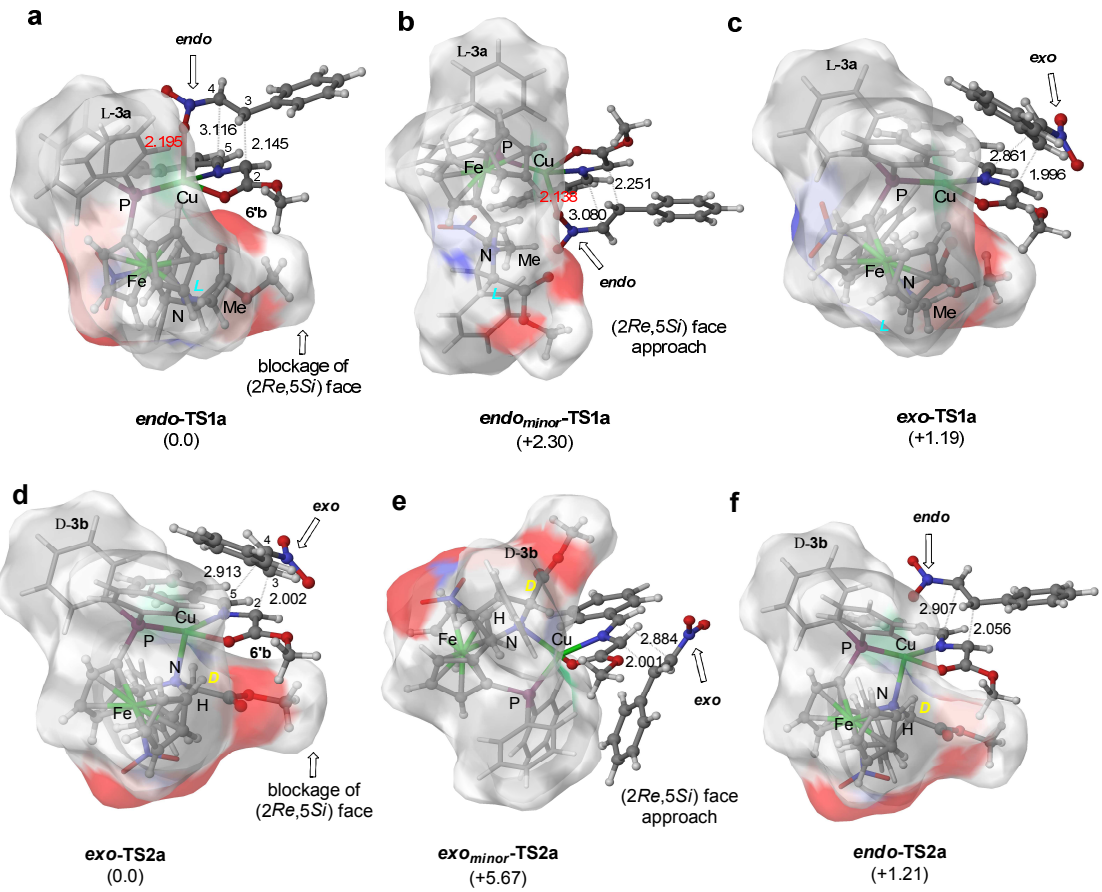


Figure S2. Main geometrical features and relative Gibbs free energies (in kcal mol^{-1}) of the computed transition structures associated to the (3+2) reaction of Cu(I)-azomethine ylide **6'b** derived from imine **6b** catalysed by L-**3a** (a-c) or D-**3b** (d-f).

Computational studies about the L-Pro and *exo*-L-2a catalysed aldol reaction of cyclohexanone and 10e. Since the electrophilic aldehyde and the enamine may adopt many arrangements about the forming carbon-carbon bond, there are 24 reasonable transition states for this reaction. However, it is known that the proton transfer from the carboxylic moiety is essential to facilitate the formation of the carbon-carbon bond.[27,28] Consequently, the number of possible transition structures is reduced to four, according to the Houk-List model.[27]

In Figure S3 were report the computed possible transition structures for the reaction between L-Pro or *exo*-L-**2a** catalysed aldol reaction of cyclohexanone and **10e.** We considered protonated species when *exo*-L-**2a** is the catalyst.

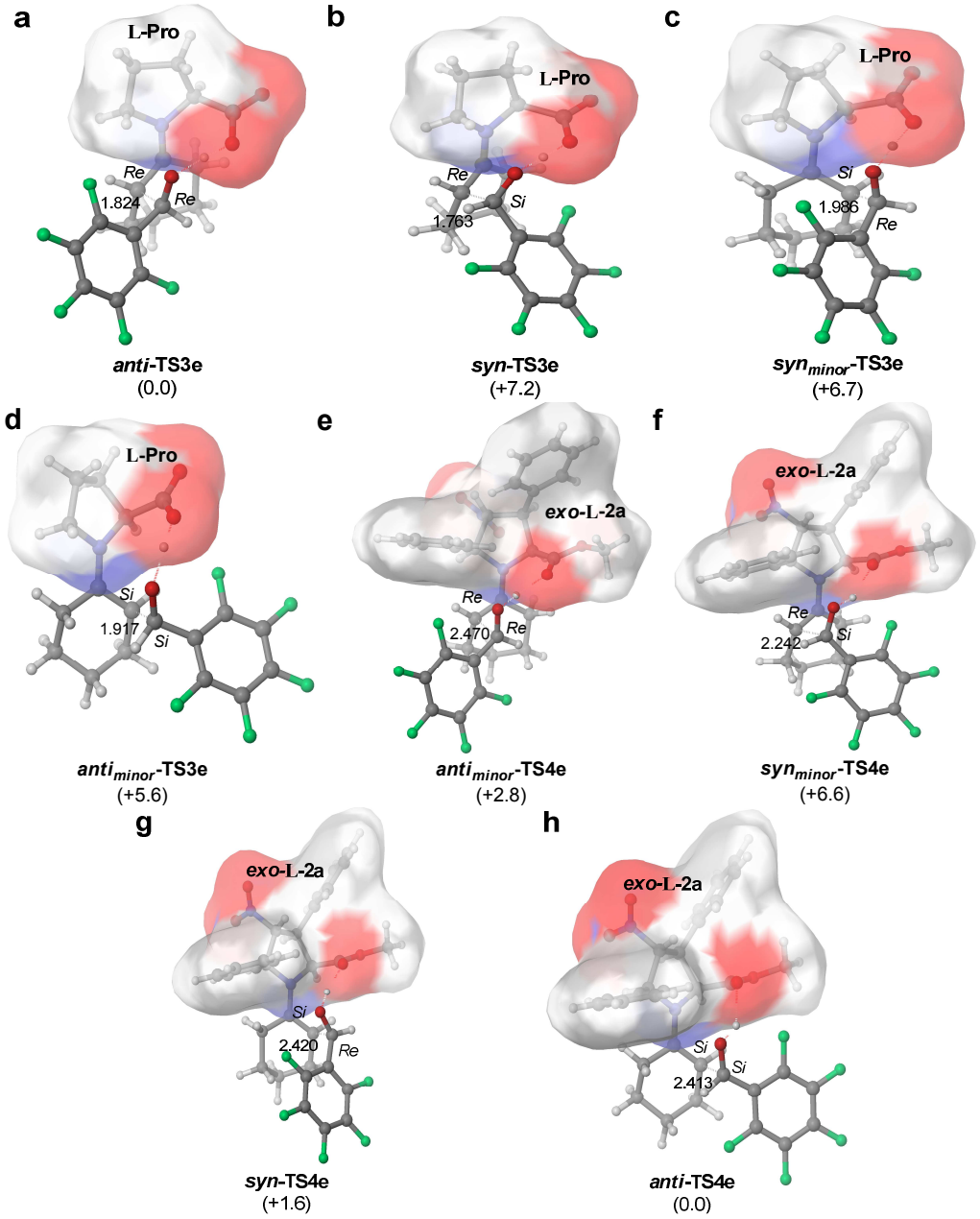


Figure S3. Main geometrical features and relative Gibbs free energies (in kcal mol^{-1}) of the possible TS's for the reaction of L-Pro (a-d) and *exo*-L-**2a** (e-h) catalysed aldol reaction between cyclohexanone and **10e.** The structures were computed at M06/6-31++G(d)//B3LYP/6-31G(d) level of theory.

Supplementary Materials and Methods

General experimental procedures. All reactions were carried out under an atmosphere of argon unless otherwise stated. All melting points are uncorrected. Flash column cromatographies were carried out with silica gel 60 (0.040-0.063mm) eluting with ethyl acetate/hexane. Infrared spectra were recorded on a FT-IR spectrometer. ^{1}H, ^{13}C and ^{31}P NMR spectra were recorded at 500 MHz, 125 MHz and 202 MHz respectively in $CDCl_3$ solvent with tetramethylsilane as internal reference. Optical rotations were measured at the wavelength of 589 nm (sodium D line). The absolute configurations of the known products were determined by comparing optical rotation values with the literature data. The HPLC chromatograms of the racemic and enantiomerically enriched products were performed using Daicel Chiralpak IA, IB, IC and AD-H columns.

All solvents were of p.a. quality and were dried by standard procedures prior to use if necessary. The commercially available reagents were used without further purification. Imines **6b-d**[23] and chiral aldehyde **4**[9] were prepared according to the previously published procedures.

Computational methods. DFT calculations were performed with the Gaussian 09 package.[29] ONIOM method was employed for the optimisation of the stationary points along the (3+2) cycloadditions at the B3LYP(LANL2DZ:PM6) level of theory. B3LYP/6-31G(d) level of theory was used for the reaction of cyclohexanone and perfluorobenzaldehyde. Single points calculations of the optimised geometries were performed using the M06 functional and the 6-31++G(d,p) basis set for C, N, P, F, H and O atoms and LANL2DZ effective core potentials for Cu and Fe atoms.

The geometries for all species described were optimised in the gas phase without symmetry restrictions. Frequency calculations were performed on the optimised structures at the same level of theory to characterise the stationary points.

Preparation of catalysts L-3a and D-3b

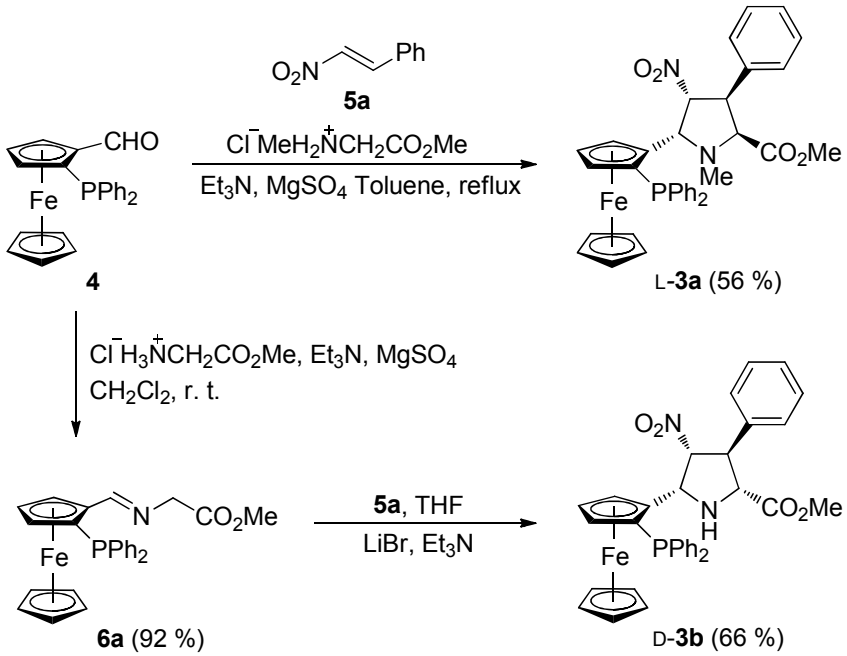


Figure S4. Preparation of catalysts L-**3a** and D-**3b**.

(S_p)-2-(Diphenylphosphino)-[(2-methoxy-2oxoethyl)-iminomethyl]ferrocene (6a). To a solution of glycine methyl ester hydrochloride (0.38 g, 3.0 mmol) in dry CH_2Cl_2 (10 ml), $MgSO_4$ and Et_3N (0.4 ml, 3.0 mmol) were added at room temperature. The resulting mixture was stirred at the same temperature for 1h. Then the aldehyde **4** (1.00 g, 2.5 mmol) was added, and the resulting mixture was stirred for 20 h. Then the $MgSO_4$ was filtered off and the organic layer washed three times with water, dried over anhydrous Na_2SO_4, and evaporated under reduced pressure to afford the pure product as an orange oil (1.08 g, 92% yield) which was used in the next step without further purification.^{31}P NMR (202 MHz, $CDCl_3$) δ = -22.26 (s). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.47 (d, *J*=2.4, 1H), 7.59 – 7.53 (m, 2H), 7.42-7.39 (m, 3H), 7.25 – 7.21 (m, 3H), 7.18-7.12 (m, 2H), 5.20 (dt, *J*=2.5, 1.3, 1H), 4.56 (t, *J*=2.6, 1H), 4.31 (d, *J*=15.8, 1H), 4.15 (s, 5H), 4.12 (d, *J*=15.9, 1H), 3.91 (dt, *J*=2.5, 1.2, 1H), 3.73 (s, 3H).

(2*R*,3*S*,4*R*,5*S*)-Methyl 5-((*Sp*)-2-(diphenylphosphino)ferrocenyl)-4-nitro-3-phenyl-pyrrolidine-2-carboxylate (D-3b). A mixture of imine **6a** (0.49g, 1.0 mmol), nitroalkene **5a** (0.18 g, 1.2 mmol), triethylamine (0.14 ml, 1.0 mmol) and LiBr (0.14 g, 1.6 mmol) in dry THF (10 ml) was stirred at room temperature for 2 hours and 45 minutes. The resulting reaction mixture was treated with aqueous saturated solution of NH_4Cl and ethyl acetate. After usual work-up the crude product was purified by flash chromatography on silica gel (Ethyl acetate:hexanes 1:4). The compound D-**3b** was obtained as a yellow solid (0.42 g, 66 %). M. p. 172-173ºC. IR (neat) 3311, 1738, 1544, 1364, 820, 742, 695 cm^{-1}. ^{31}P NMR (202 MHz, $CDCl_3$) δ = -23.09 (s). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.60 – 7.57 (m, 2H), 7.42 – 7.37 (m, 3H), 7.35 – 7.18 (m, 8H), 7.08 – 7.03 (m, 2H), 4.94 (dt, *J*=11.4, 5.6, 1H), 4.50 – 4.47 (m, 1H), 4.35 (t, *J*=2.6, 1H), 4.22 (dd, *J*=5.4, 1.2, 1H), 4.17 (s, 5H), 4.03 – 3.98 (m, 2H), 3.88 – 3.85 (m, 1H), 3.84 (s, 3H), 3.27 (dd, *J*=10.8, 8.1, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 172.5, 139.6, 138.5 (d, *J*=8.5), 136.5 (d, *J*=8.2), 134.8 (d, *J*=20.7), 133.4 (d, *J*=19.6), 129.4, 129.2, 128.7, 128.4 (d, *J*=6.4), 128.4 (d, *J*=7.9), 127.7, 127.2, 95.6, 86.2 (d, *J*=23.8), 72.1 (d, *J*=3.6), 70.4, 70.2, 68.2, 66.8 (d, *J*=2.9), 64.3 (d, *J*=16.4), 56.1, 52.7 (1C is missing). $[\alpha]_D^{25}$ =-73.2 (*c* 1.00, $CHCl_3$). Anal. Calcd. for $C_{34}H_{31}FeN_2O_4P$: C, 66.0; H, 5.1; N, 4.5; Found: C, 65.8; H, 4.8; N, 4.5.

(2*S*,3*S*,4*R*,5*S*)-Methyl 5-((*Sp*)-2-(diphenylphosphino)ferrocenyl)-1-methyl-4-nitro-3-phenylpyrrolidine-2-carboxylate (L-3a). A mixture of aldehyde **4** (0.52 g, 1.3 mmol), sarcosine methyl ester hydrochloride (0.24 g, 1.7 mmol), nitroalkene **5a** (0.25 g, 1.7 mmol), triethylamine (0.24 ml, 1.7 mmol) and $MgSO_4$ in toluene (20 ml) was refluxed for 7 hours. After usual work-up, the resulting oily residue was purified by flash chromatography on silica gel (Ethyl acetate:hexanes 1:4) to yield the title pure

product as an orange solid (0.46 g, 56 %). M.p. 81-83ºC. IR (neat) 1731, 1550, 1364, 819, 742, 696 cm^{-1}. ^{31}P NMR (202 MHz, $CDCl_3$) δ = -24.13 (s). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.75 – 7.68 (m, 2H), 7.43 – 7.34 (m, 5H), 7.26 – 7.19 (m, 6H), 7.08 – 7.04 (m, 2H), 5.42 (t, *J*=7.7, 1H), 5.20 (dd, *J*=8.0, 5.0, 1H), 4.48 (t, *J*=2.4, 1H), 4.46 (d, *J*=1.1, 1H), 4.40 (t, *J*=7.8, 1H), 4.35 (d, *J*=8.4, 1H), 4.33 – 4.29 (m, 1H), 3.84 (s, 5H), 3.33 (s, 3H), 2.92 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 171.3, 139.4 (d, *J*=8.2), 139.2 (d, *J*=7.2), 135.5 (d, *J*=22.7), 134.8, 133.0 (d, *J*=18.6), 129.4, 128.6, 128.2 (d, *J*=8.5), 127.9 (d, *J*=8.9), 127.9, 127.9, 127.8, 92.6, 91.5 (d, *J*=27.4), 75.3 (d, *J*=14.6), 72.1 (d, *J*=4.2), 71.7, 70.4, 70.1, 68.4 (d, *J*=4.4), 63.7 (d, *J*=13.8), 51.1, 49.6, 37.7. $[\alpha]_D^{25}$ =-253.5 (*c* 1.00, $CHCl_3$). Anal. Calcd. For $C_{35}H_{33}FeN_2O_4P$: C, 66.5; H, 5.3; N, 4.4; Found: C, 66.3; H, 5.0; N, 4.2.

General procedure for the (3+2) cycloadditions using catalyst L-3a or D-3b (See Fig. S5). A solution of chiral ligand L-**3a** or D-**3b** (0.015 mmol) and $Cu(CH_3CN)_4PF_6$ (5.2 mg, 0.014 mmol) in 1.0 ml of dry THF or dry CH_2Cl_2 (see Fig. S5) was stirred at the temperature indicated in each case for 15 minutes. Then, a solution of imine **6** (0.45 mmol) in 1.0 ml of solvent, triethylamine (3.2 µl 0.023 mmol) and the corresponding dipolarophile **5, 7, 8** or **9** (0.50 mmol) in 1.0 ml of solvent were successively added. The reaction was monitorized by TLC once the starting material was consumed the mixture was filtered through a pad of celite and the filtrate was concentrated under reduced pressure. The residue was purified by flash cromatography on silica gel (ethyl acetate:hexanes 1:2) to yield the corresponding cycloadduct *endo* or *exo*-L-**2a-l**. The enantiomeric excess was determined by comparison with the chromatogram recorded for the racemic mixture of the corresponding cycloadduct.

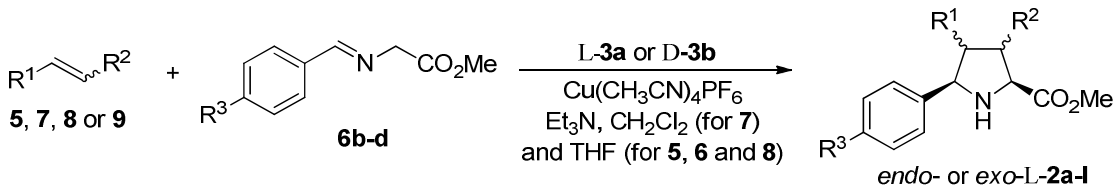
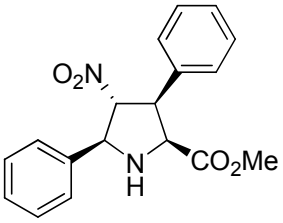
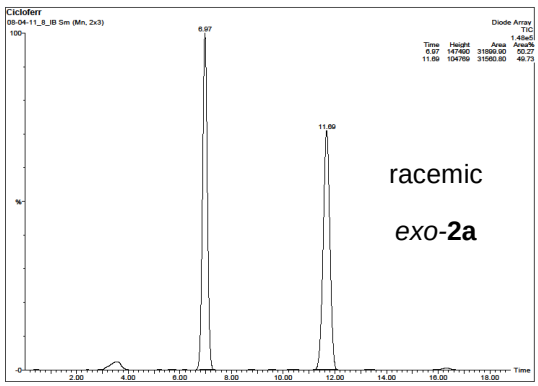


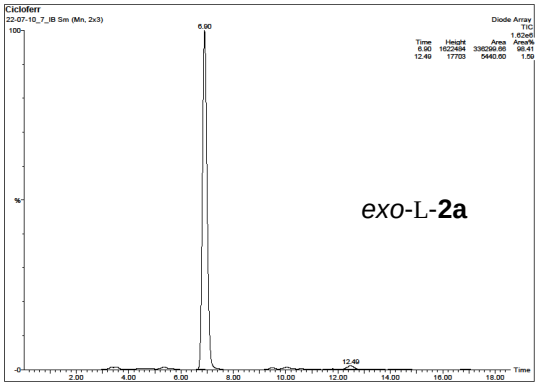
Figure S5. Enantioselective 1,3-dipolar cycloadditions of azomethine ylides **6'b-d** and dipolarophiles **5**, **7**, **8** and **9**.

(2*S*,3*S*,4*R*,5*S*)-Methyl 4-nitro-3,5-diphenylpirrolidine-2-carboxylate (*exo*-L-2a).[22]



Yield: 85%. White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.58 – 7.55 (m, 2H), 7.47 – 7.18 (m, 8H), 5.22 (t, *J*=8.1, 1H), 4.77 (d, *J*=8.2, 1H), 4.51 (d, *J*=9.1, 1H), 4.39 (t, *J*=8.5, 1H), 3.29 (s, 3H), 2.75 (bs, 1H). $[\alpha]_D^{25}$ =+125.2 (*c* 1.00, $CHCl_3$), 97% *ee*. Lit:[22] $[\alpha]_D^{20}$ =+118.2 (*c* 1.10, $CHCl_3$), 97% *ee*. HPLC: Daicel Chiralpak IB, *iso*-propanol/hexane 20/80, flow rate 1.0 ml/min, tr: 7.0 min (2*S*,3*S*,4*R*,5*S*)-isomer and 11.7 min (2*R*,3*R*,4*S*,5*R*)-isomer, 254 nm.





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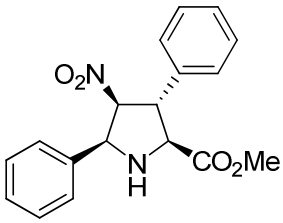
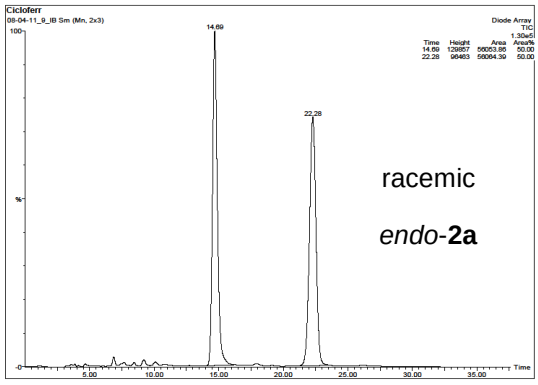
11.69	104769	31560.80	49.73

Time	Height	Area	Area%
6.90	1622484	336299.66	98.41
12.49	17703	5440.60	1.59

(2*S*,3*R*,4*S*,5*S*)-Methyl 4-nitro-3,5-diphenylpirrolidine-2-carboxylate (*endo*-L-2a).[22]



Yield: 81%. White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.46 – 7.27 (m, 10H), 5.28 (dd, *J*=6.4, 3.5, 1H), 4.91 (d, *J*=6.4, 1H), 4.22 (dd, *J*=7.2, 3.4, 1H), 4.15 (d, *J*=7.3, 1H), 3.81 (s, 3H), 2.90 (bs, 1H). $[\alpha]_D^{25}$ =-46.5 (*c* 1.00, $CHCl_3$), 92% *ee*. Lit:[22] $[\alpha]_D^{20}$ =-66.9 (*c* 0.92, $CHCl_3$), 97% *ee*. HPLC: Daicel Chiralpak IB, *iso*-propanol/hexane 15/85, flow rate 1.0 ml/min, tr: 14.7 min (2*S*,3*R*,4*S*,5*S*)-isomer and 22.3 min (2*R*,3*S*,4*R*,5*R*)-isomer, 254 nm.



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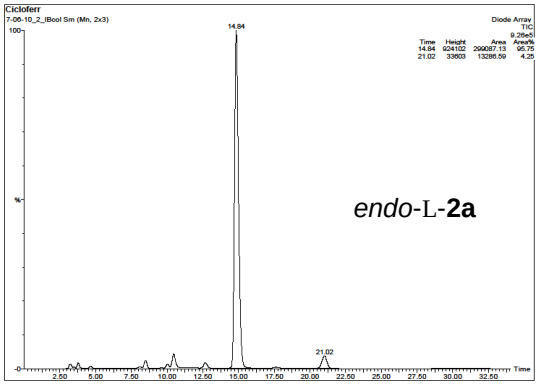
22.28	96463	56064.39	50.00



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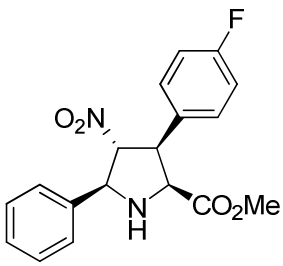
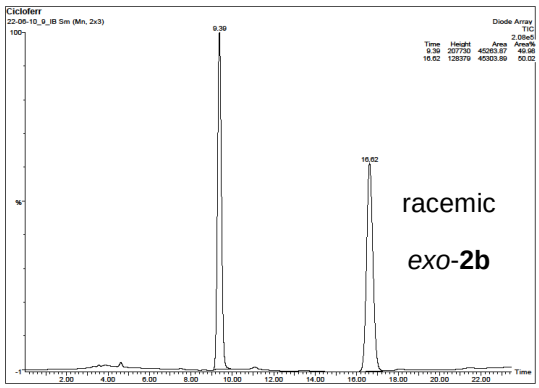
14.84	924102	299087.13	95.75
21.02	33603	13286.59	4.25

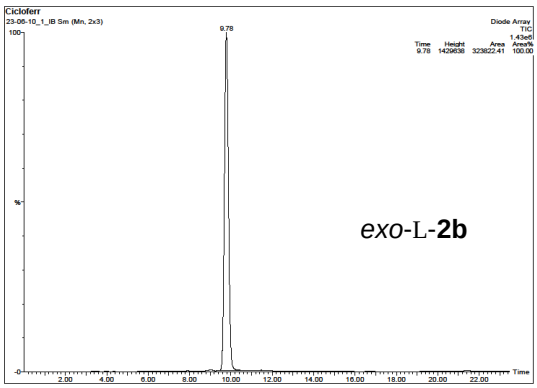
(2*S*,3*S*,4*R*,5*S*)-Methyl 3-(4-fluorophenyl)-4-nitro-5-phenylpyrrolidine-2-carboxylate (*exo*-L-2b).



Yield: 83%. White solid, m. p. 134-135ºC. IR (neat) 3367, 1735, 1546, 1366 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.55 (d, *J*=7.2, 2H), 7.44 – 7.36 (m, 3H), 7.25 (dd, *J*=5.5, 2.5, 2H), 7.01 (t, *J*=8.5, 2H), 5.13 (t, *J*=7.9, 1H), 4.76 (d, *J*=7.9, 1H), 4.49 (d, *J*=8.9, 1H), 4.35 (t, *J*=8.3, 1H), 3.34 (s, 3H), 2.70 (bs, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 171.8, 162.6 (d, *J*=247.6), 137.7, 132.0 (d, *J*=3.3), 129.7 (d, *J*=8.1), 129.2,

129.1, 126.9, 115.8 (d, *J*=21.6), 95.3, 67.4, 64.2, 52.9, 52.0. $[\alpha]_D^{25}$ =+104.8 (*c* 0.85, $CHCl_3$), >99% *ee*. HPLC: Daicel Chiralpak IB, *iso*-propanol/hexane 10/90, flow rate 1.0 ml/min, tr: 9.4 min (2*S*,3*S*,4*R*,5*S*)-isomer and 16.6 min (2*R*,3*R*,4*S*,5*R*)-isomer, 254 nm. Anal. Calcd. for $C_{18}H_{17}FN_2O_4$: C, 62.8; H, 5.0; N, 8.1; Found: C, 63.1; H, 4.8; N, 8.4.





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16.62	128379	45303.89	50.02

Time	Height	Area	Area%
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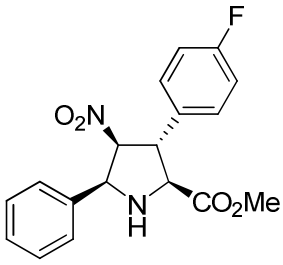
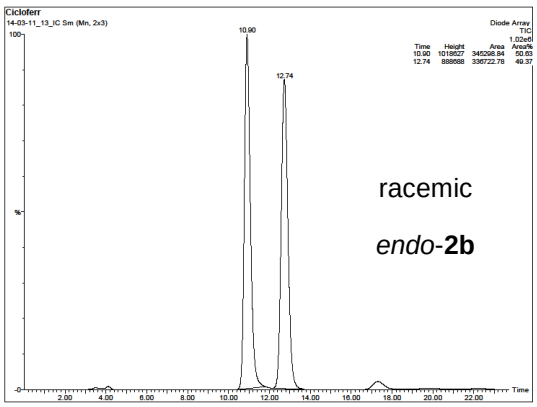
(2*S*,3*R*,4*S*,5*S*)-Methyl 3-(4-fluorophenyl)-4-nitro-5-phenylpyrrolidine-2-carboxylate (*endo*-L-2b).



Yield: 79%. Pale yellow oil. IR (neat) 3345, 1741, 1549, 1365 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$) δ = 7.37 – 7.32 (m, 5H), 7.27 (dd, *J*=7.9, 5.5, 2H), 7.09 (t, *J*=8.4, 2H), 5.24 (dd, *J*=6.3, 4.1, 1H), 4.89 (d, *J*=6.6, 1H), 4.21 (dd, *J*=7.3, 3.9, 1H), 4.09 (d, *J*=7.6, 1H), 3.80 (s, 3H), 3.20 (bs, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 171.6, 162.5 (d, *J*=247.6), 134.5, 134.3 (d, *J*=3.2), 129.3 (d, *J*=8.1), 128.9, 128.9, 126.6, 116.4 (d, *J*=21.6), 97.0, 67.6, 67.4, 54.5, 52.8. $[\alpha]_D^{26}$ =-42.8 (*c* 1.00, $CHCl_3$), 92% *ee*. HPLC: Daicel Chiralpak IC, *iso*-propanol/hexane 15/85, flow rate 1.0 ml/min, tr 10.9 min (2*S*,3*R*,4*S*,5*S*)-isomer and 12.7 min (2*R*,3*S*,4*R*,5*R*)-isomer, 254 nm.



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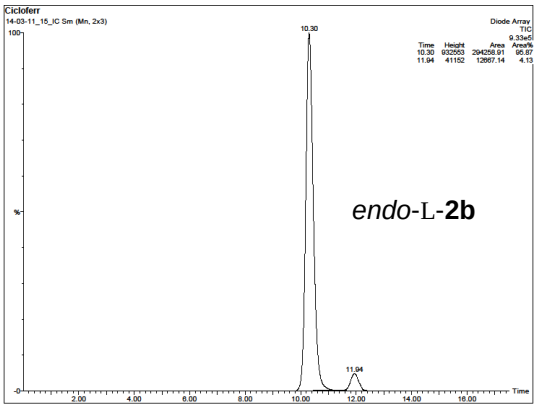

Time	Height	Area	Area%
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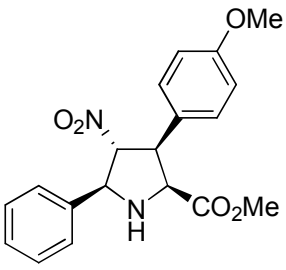
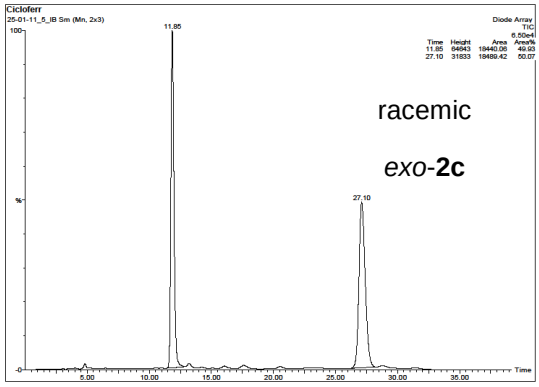
11.94	41152	12667.14	4.13

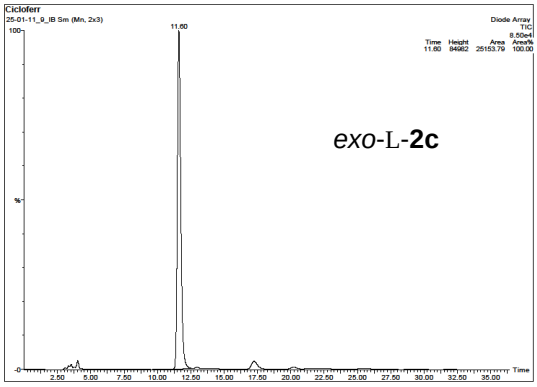
(2*S*,3*S*,4*R*,5*S*)-Methyl 3-(4-methoxyphenyl)-4-nitro-5-phenylpyrrolidine-2-carboxylate (*exo*-L-2c).[22]



Yield: 86%. White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.56 (d, *J*=7.1, 2H), 7.45 – 7.33 (m, 3H), 7.16 (d, *J*=8.5, 2H), 6.84 (d, *J*=8.5, 2H), 5.17 (t, *J*=8.1, 1H), 4.75 (d, *J*=8.2, 1H), 4.46 (d, *J*=9.0, 1H), 4.33 (t, *J*=8.5, 1H), 3.77 (s, 3H), 3.34 (s, 3H), 2.72 (bs, 1H). $[\alpha]_D^{22}$ =+137.1 (*c* 0.86, $CHCl_3$), >99% *ee*. Lit:[22] $[\alpha]_D^{20}$ =+126.5 (*c* 2.25, $CHCl_3$), 96% *ee*. HPLC: Daicel Chiralpak IB, *iso*-propanol/hexane 10/90, flow rate 1.0 ml/min, tr: 11.9 min (2*S*,3*S*,4*R*,5*S*)-isomer and 27.1 min (2*R*,3*R*,4*S*,5*R*)-isomer, 254 nm.

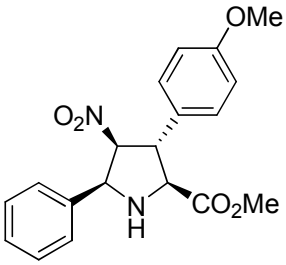


Time	Height	Area	Area%
11.85	64643	18440.06	49.93
27.10	31833	18489.42	50.07

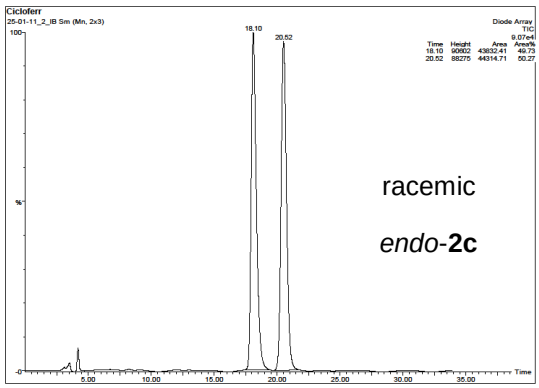


Time	Height	Area	Area%
11.60	84.982	25153.79	100.00

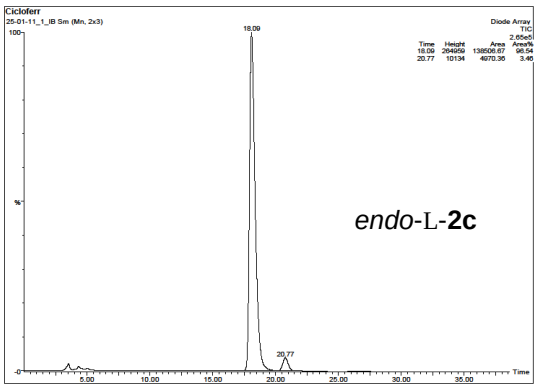
(2*S*,3*R*,4*S*,5*S*)-Methyl 3-(4-methoxyphenyl)-4-nitro-5-phenylpyrrolidine-2-carboxylate (*endo*-L-2c).[22]



Yield: 84%. White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.38 – 7.28 (m, 5H), 7.21 (d, *J*=8.6, 2H), 6.92 (d, *J*=8.6, 2H), 5.23 (dd, *J*=6.5, 3.7, 1H), 4.88 (d, *J*=6.6, 1H), 4.16 (dd, *J*=7.4, 3.7, 1H), 4.10 (d, *J*=7.5, 1H), 3.80 (s, 3H), 3.79 (s, 3H), 3.24 (bs, 1H). $[\alpha]_D^{24}$ =-45.4 (*c* 1.00, $CHCl_3$), 93% *ee*. Lit:[22] $[\alpha]_D^{20}$=-69.9 (*c* 0.50, $CHCl_3$), 95% *ee*. HPLC: Daicel Chiralpak IB, *iso*-propanol/hexane 30/70, flow rate 1.0 ml/min, tr: 18.1 min (2*S*,3*R*,4*S*,5*S*)-isomer and 20.5 min (2*R*,3*S*,4*R*,5*R*)-isomer, 254 nm.

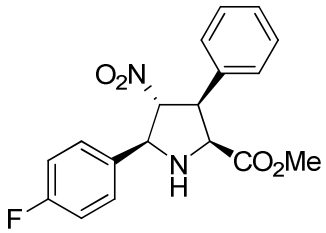


Time	Height	Area	Area%
18.10	90602	43832.41	49.73
20.52	88275	44314.71	50.27



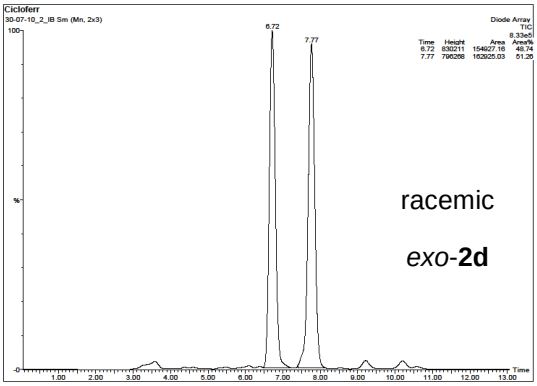
Time	Height	Area	Area%
18.09	264959	138506.67	96.54
20.77	10134	4970.36	3.46

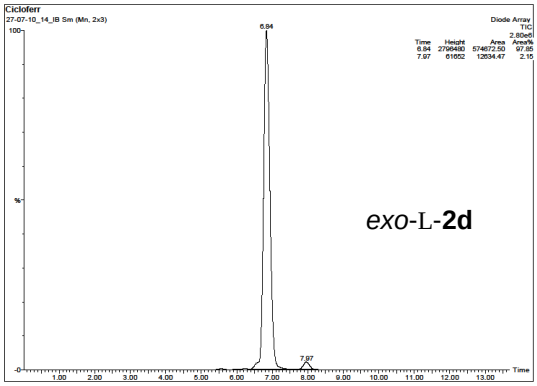
(2*S*,3*S*,4*R*,5*S*)-Methyl5-(4-fluorophenyl)-4-nitro-3-phenylpyrrolidine-2-carboxylate (*exo*-L-2d).



Yield: 86%. White solid, m. p. 106-108ºC. IR (neat) 3325, 1727, 1545, 1372 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.55 (dd, *J*=8.4, 5.4, 2H), 7.34 – 7.22 (m, 5H), 7.09 (t, *J*=8.6, 2H), 5.17 (t, *J*=8.2, 1H), 4.74 (d, *J*=8.2, 1H), 4.47 (d, *J*=9.1, 1H), 4.38 (t, *J*=8.6, 1H), 3.28 (s, 3H), 2.69 (bs, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ =

172.0, 163.1 (d, *J*=247.6), 135.8, 133.8 (d, *J*=3.6), 128.9, 128.8 (d, *J*=7.8), 128.3, 127.9, 116.1 (d, *J*=21.6), 95.0, 66.9, 64.2, 53.5, 51.9. $[\alpha]_D^{22}$ =+65.2 (*c* 1.00, $CHCl_3$), 96% *ee*. HPLC: Daicel Chiralpak IB, *iso*-propanol/hexane 20/80, flow rate 1.0 ml/min, tr: 6.7 min (2*S*,3*S*,4*R*,5*S*)-isomer and 7.8 min (2*R*,3*R*,4*S*,5*R*)-isomer, 254 nm. Anal. Calcd. for $C_{18}H_{17}FN_2O_4$: C, 62.8; H, 5.0; N, 8.1; Found: C, 63.0; H, 4.8; N, 8.1.

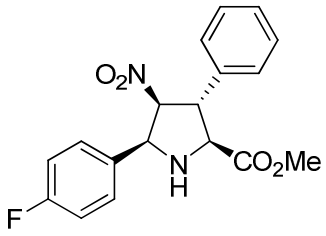




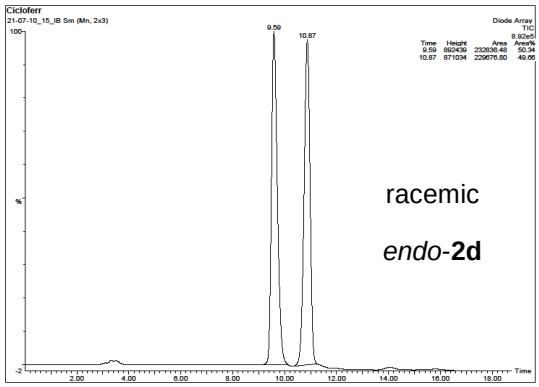
Time	Height	Area	Area%
6.72	830211	154927.16	48.74
7.77	796268	162925.03	51.26

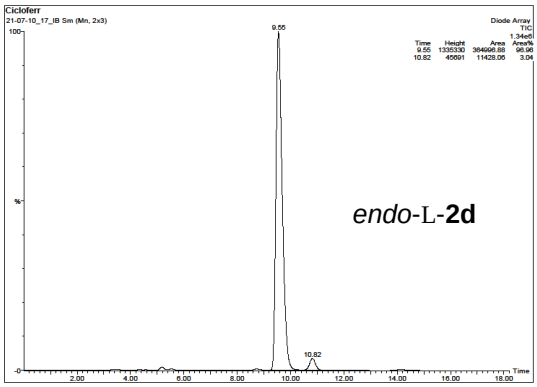
Time	Height	Area	Area%
6.84	2796480	574672.50	97.85
7.97	61652	12634.47	2.15

(2*S*,3*R*,4*S*,5*S*)-Methyl 5-(4-fluorophenyl)-4-nitro-3-phenylpyrrolidine-2-carboxylate (*endo*-L-2d).



Yield: 85%. Pale yellow oil. IR (neat) 3347, 1739, 1548, 1364 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$) δ = 7.44 – 7.27 (m, 7H), 7.05 (t, *J*=8.6, 2H), 5.25 (dd, *J*=6.6, 3.9, 1H), 4.90 (d, *J*=6.6, 1H), 4.23 (dd, *J*=7.4, 3.8, 1H), 4.15 (d, *J*=7.5, 1H), 3.80 (s, 3H), 2.94 (bs, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 171.8, 162.9 (d, *J*=247.8), 138.4, 130.6 (d, *J*=2.8), 129.4, 128.5 (d, *J*=8.3), 128.3, 127.6, 115.8 (d, *J*=21.7), 96.9, 67.2, 66.9, 55.0, 52.7. $[\alpha]_D^{28}$ =-37.2 (*c* 1.00, $CHCl_3$), 94% *ee*. HPLC: Daicel Chiralpak IB, *iso*-propanol/hexane 20/80, flow rate 1.0 ml/min, tr 9.6 min (2*S*,3*R*,4*S*,5*S*)-isomer and 10.9 min (2*R*,3*S*,4*R*,5*R*)-isomer, 254 nm.

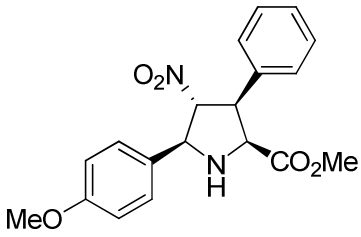




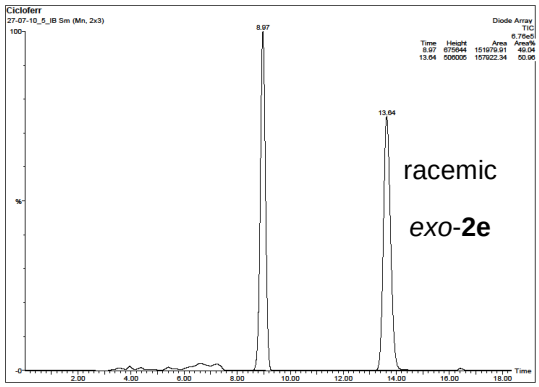
Time	Height	Area	Area%
9.59	892439	232836.48	50.34
10.87	871034	229676.80	49.66

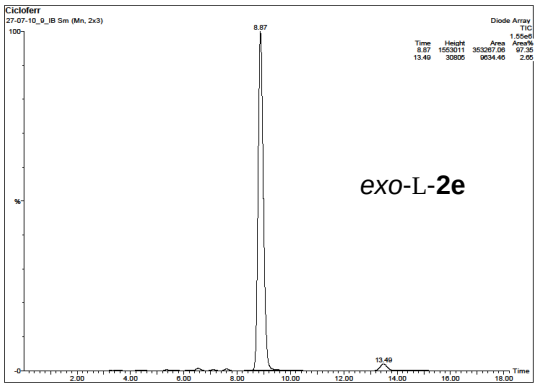
Time	Height	Area	Area%
9.55	1335330	364996.88	96.96
10.82	45691	11428.06	3.04

(2*S*,3*S*,4*R*,5*S*)-Methyl 5-(4-methoxyphenyl)-4-nitro-3-phenylpyrrolidine-2-carboxylate (*exo*-L-2e).[22]



Yield: 90%. Pale yellow solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.48 (d, *J*=8.5, 2H), 7.34 – 7.22 (m, 5H), 6.94 (d, *J*=8.5, 2H), 5.19 (t, *J*=8.2, 1H), 4.69 (d, *J*=8.3, 1H), 4.47 (d, *J*=9.1, 1H), 4.38 (t, *J*=8.6, 1H), 3.82 (s, 3H), 3.28 (s, 3H), 2.69 (bs, 1H). $[\alpha]_D^{24}$ =+72.4 (*c* 0.53, $CHCl_3$), 95% *ee*. Lit:[22] $[\alpha]_D^{20}$=+82.8 (*c* 1.68, $CHCl_3$), 97% *ee*. HPLC: Daicel Chiralpak IB, *iso*-propanol/hexane 20/80, flow rate 1.0 ml/min, tr: 9.0 min (2*S*,3*S*,4*R*,5*S*)-isomer and 13.6 min (2*R*,3*R*,4*S*,5*R*)-isomer, 254 nm.

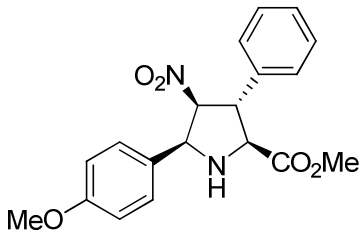




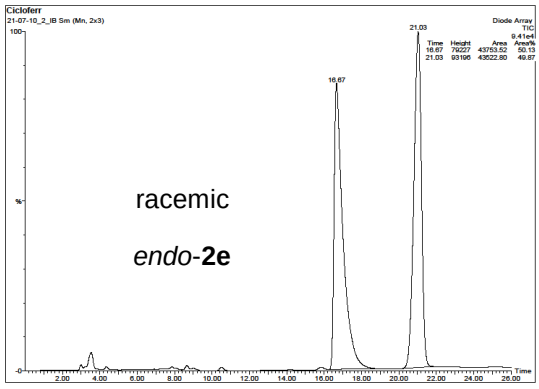
Time	Height	Area	Area%
8.97	675644	151979.91	49.04
13.64	506005	157922.34	50.96

Time	Height	Area	Area%
8.87	1553011	353267.06	97.35
13.49	30805	9634.46	2.65

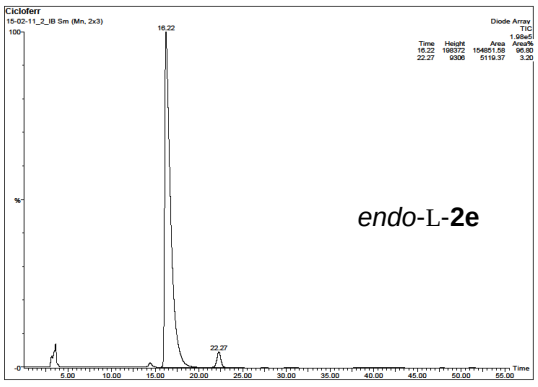
(2*S*,3*R*,4*S*,5*S*)-Methyl 5-(4-methoxyphenyl)-4-nitro-3-phenylpyrrolidine-2-carboxylate (*endo*-L-2e).[22]



Yield: 81%. Pale yellow solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.41 (t, *J*=7.4, 2H), 7.37 – 7.27 (m, 5H), 6.89 (d, *J*=8.6, 2H), 5.23 (dd, *J*=6.4, 3.6, 1H), 4.88 (d, *J*=6.5, 1H), 4.22 (dd, *J*=7.2, 3.5, 1H), 4.13 (d, *J*=7.4, 1H), 3.81 (s, 3H), 3.79 (s, 3H), 3.28 (bs, 1H). $[\alpha]_D^{25}$ =-41.1 (*c* 1.00, $CHCl_3$), 94% *ee*. Lit:[22] $[\alpha]_D^{20}$=-51.1 (*c* 1.15, $CHCl_3$), 95% *ee*. HPLC: Daicel Chiralpak IB, *iso*-propanol/hexane 20/80, flow rate 1.0 ml/min, tr: 16.7 min (2*S*,3*R*,4*S*,5*S*)-isomer and 21.0 min (2*R*,3*S*,4*R*,5*R*)-isomer, 254 nm.

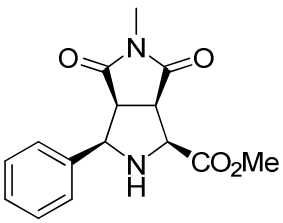


Time	Height	Area	Area%
16.67	79227	43753.52	50.13
21.03	93196	43522.80	49.87



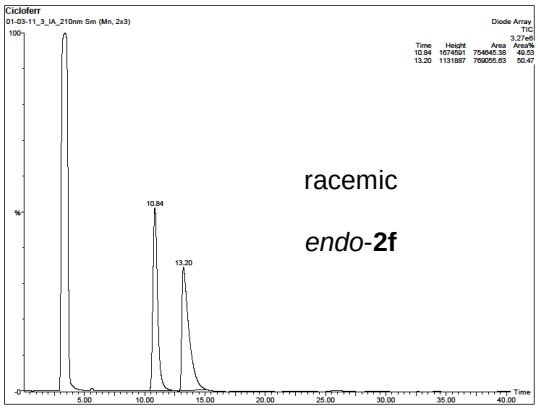
Time	Height	Area	Area%
16.22	198372	154851.58	96.80
22.27	9306	5119.37	3.20

(1*S*,3*R*,3a*S*,6a*R*)-Methyl 5-methyl-4,6-dioxo-3-phenyl-octahydropyrrolo[3,4-*c*]pyrrole-1-carboxylate (*endo*-L-2f)[23]:

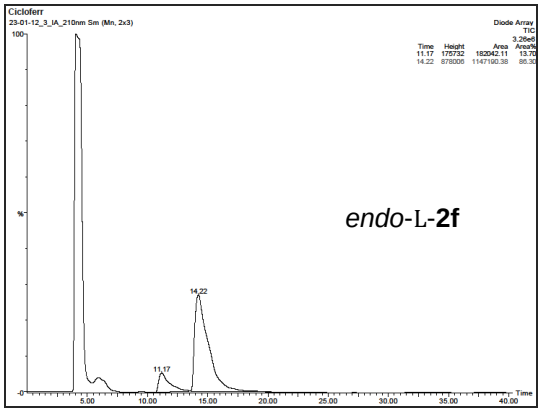


White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.38 – 7.29 (m, 5H), 4.50 (dd, *J*=8.5, 5.5, 1H), 4.09 – 4.03 (m, 1H), 3.88 (s, 3H), 3.56 (t, *J*=7.2, 1H), 3.43 (t, *J*=8.1, 1H), 2.87 (s, 3H), 2.41 (bs, 1H).

Using L-3a as chiral ligand: Yield: 90%. $[\alpha]_D^{22}$ =+63.2 (*c* 1.00, $CHCl_3$), 73% *ee*. Lit:[23] $[\alpha]_D^{20}$ =+51 (*c* 0.14, CH_2Cl_2), >99% *ee*. HPLC: Daicel Chiralpak IA, *iso*-propanol/hexane 30/70, flow rate 1.0 ml/min, tr: 11.2 min (1*R*,3*S*,3a*R*,6a*S*)-isomer and 14.2 min (1*S*,3*R*,3a*S*,6a*R*)-isomer, 210 nm.

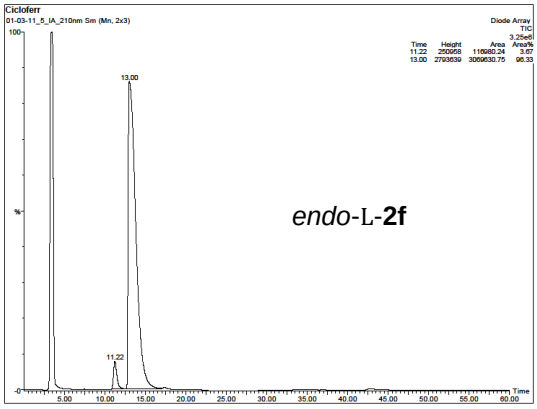


Time	Height	Area	Area%
10.84	1674591	754645.38	49.53
13.20	1131887	769055.63	50.47



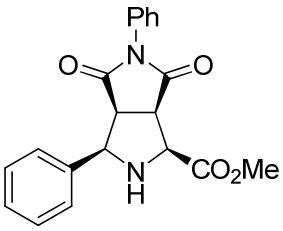
Time	Height	Area	Area%
11.17	175732	182042.11	13.70
14.22	878006	1147190.38	86.30

Using D-3b as chiral ligand: Yield: 95%. $[\alpha]_D^{22}$ =+80.3 (*c* 1.00, $CHCl_3$), 93% *ee*. Lit:[23] $[\alpha]_D^{20}$ =+51 (*c* 0.14, CH_2Cl_2), >99% *ee*. HPLC: Daicel Chiralpak IA, *iso*-propanol/hexane 30/70, flow rate 1.0 mL/min, tr: 11.2 min (1*R*,3*S*,3a*R*,6a*S*)-isomer and 13.0 min (1*S*,3*R*,3a*S*,6a*R*)-isomer, 210 nm.

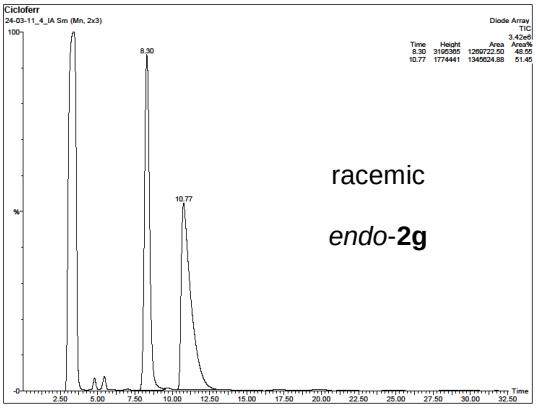


Time	Height	Area	Area%
11.22	250958	116980.24	3.67
13.00	2793639	3069630.75	96.33

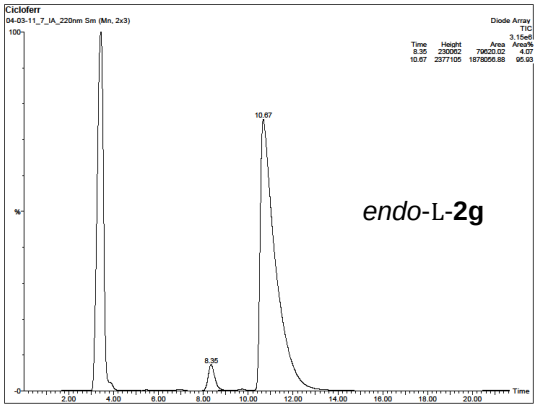
(1*S*,3*R*,3a*S*,6a*R*)-Methyl 4,6-dioxo-3,5-diphenyl-octahydropyrrolo[3,4-*c*]pyrrole-1-carboxylate (*endo*-L-2g)[23]:



Yield: 90%. White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.43 (d, *J*=7.3, 2H), 7.41 – 7.27 (m, 6H), 7.13 (d, *J*=7.5, 2H), 4.57 (d, *J*=8.8, 1H), 4.10 (d, *J*=6.6, 1H), 3.86 (s, 3H), 3.69 (t, *J*=7.2, 1H), 3.52 (t, *J*=8.3, 1H), 2.50 (bs, 1H). $[\alpha]_D^{29}$ =+109.3 (*c* 1.00, $CHCl_3$), 92% *ee*. Lit:[23] $[\alpha]_D^{20}$ =+114 (*c* 1.22, CH_2Cl_2), >99% *ee*. HPLC: Daicel Chiralpak IA, *iso*-propanol/hexane 70/30, flow rate 1.0 mL/min, tr: 8.3 min (1*R*,3*S*,3a*R*,6a*S*)-isomer and 10.8 min (1*S*,3*R*,3a*S*,6a*R*)-isomer, 220 nm.

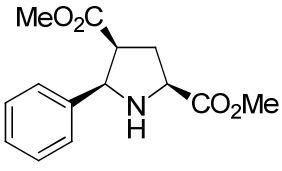


Time	Height	Area	Area%
8.30	3195365	1269722.50	48.55
10.77	1774441	1345624.88	51.45



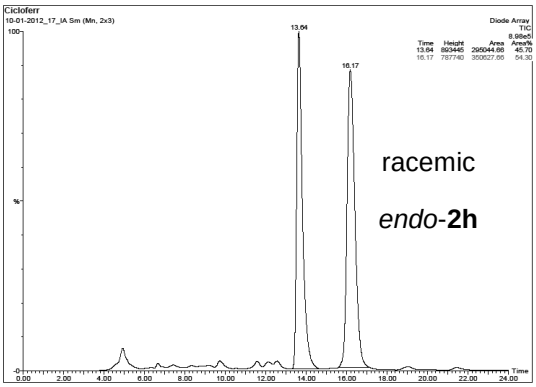
Time	Height	Area	Area%
8.35	230062	79620.02	4.07
10.67	2377105	1878056.88	95.93

(2*S*,4*S*,5*R*)-Dimethyl 5-phenylpyrrolidine-2,4-dicarboxylate (*endo*-L-2h).[23]

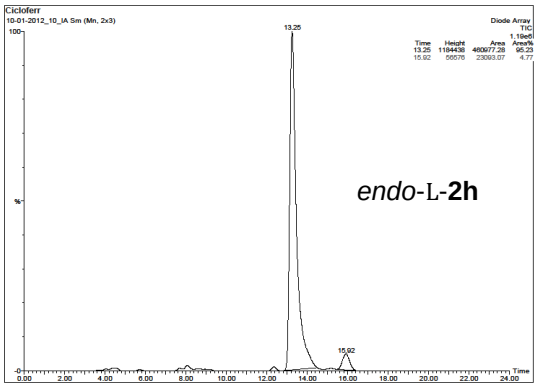


Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.36 – 7.19 (m, 5H), 4.54 (d, *J* = 7.8, 1H), 3.98 (t, *J* = 8.1, 1H), 3.82 (s, 3H), 3.31 (q, *J* = 7.2, 1H), 3.22 (s, 3H), 2.65 (bs, 1H), 2.42 (t, *J* = 7.5, 2H).

Using L-3a as a catalyst: Yield: 85%. $[\alpha]_D^{20}$ =+19.6 (*c* 1.00, $CHCl_3$), 90% *ee*. Lit:[23] $[\alpha]_D^{20}$ =+36 (*c* 0.08, CH_2Cl_2), 95% *ee*. HPLC: Daicel Chiralpak IA, *iso*-propanol/hexane 20/80, flow rate 1.0 ml/min, tr: 13.3 min (2*S*,4*S*,5*R*)-isomer and 15.9 min (2*R*,4*R*,5*S*)-isomer, 210 nm.

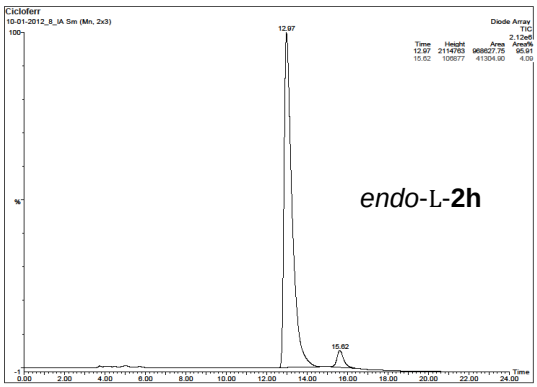


Time	Height	Area	Area%
13.64	893445	295044.66	45.70
16.17	787740	350627.66	54.30



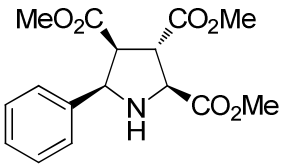
Time	Height	Area	Area%
13.25	1184438	460977.28	95.23
15.92	56576	23093.07	4.77

Using D-3b as a catalyst: Yield: 73%. $[\alpha]_D^{20}$ =+23.2 (*c* 1.00, $CHCl_3$), 92% *ee*. Lit:[23] $[\alpha]_D^{20}$ =+36 (*c* 0.08, CH_2Cl_2), 95% *ee*. HPLC: Daicel Chiralpak IA, *iso*-propanol/hexane 20/80, flow rate 1.0 ml/min, tr: 13.0 min (2*S*,4*S*,5*R*)-isomer and 15.6 min (2*R*,4*R*,5*S*)-isomer, 210 nm.



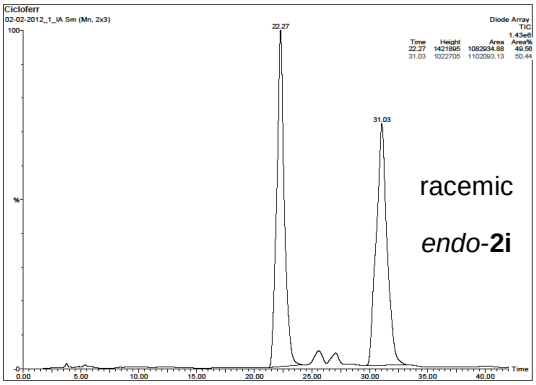
Time	Height	Area	Area%
12.97	2114763	968627.75	95.91
15.62	106877	41304.90	4.09

(2*S*,3*S*,4*S*,5*R*)-Trimethyl 5-phenylpyrrolidine-2,3,4-tricarboxylate (*endo*-L-2i).[23]

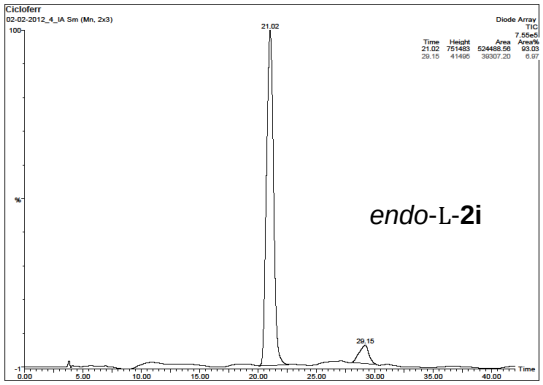


Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.35 – 7.20 (m, 5H), 4.66 (d, *J* = 8.0, 1H), 4.21 (d, *J* = 7.5, 1H), 3.84 (s, 3H), 3.77 (s, 3H), 3.67 (dd, *J* = 14.6, 8.6, 1H), 3.58 (dd, *J* = 7.2, 6.3, 1H), 3.21 (s, 3H), 2.84 (bs, 1H).

Using L-3a as a catalyst: Yield: 81%. $[\alpha]_D^{20}$ =+18.9 (*c* 1.00, $CHCl_3$), 86% *ee*. Lit:[23] $[\alpha]_D^{20}$ =+43 (*c* 0.10, CH_2Cl_2), >99% *ee*. HPLC: Daicel Chiralpak IA, *iso*-propanol/hexane 10/90, flow rate 1.0 ml/min, tr: 21.0 min (2*S*,3*S*,4*S*,5*R*)-isomer and 29.2 min (2*R*,3*R*,4*R*,5*S*)-isomer, 210 nm.

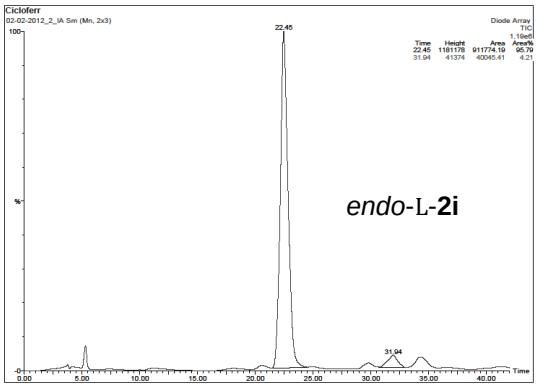


Time	Height	Area	Area%
22.27	1421895	1082934.88	49.56
31.03	1022705	1102093.13	50.44



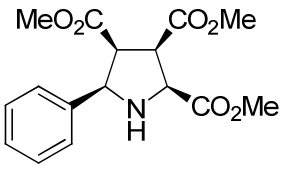
Time	Height	Area	Area%
21.02	751483	524488.56	93.03
29.15	41495	39307.20	6.97

Using D-3b as a catalyst: Yield: 74%. $[\alpha]_D^{20}$ =+22.2 (*c* 1.00, $CHCl_3$), 92% *ee*. Lit:[23] $[\alpha]_D^{20}$ =+43 (*c* 0.10, CH_2Cl_2), >99% *ee*. HPLC: Daicel Chiralpak IA, *iso*-propanol/hexane 10/90, flow rate 1.0 ml/min, tr: 22.5 min (2*S*,3*S*,4*S*,5*R*)-isomer and 31.9 min (2*R*,3*R*,4*R*,5*S*)-isomer, 210 nm.



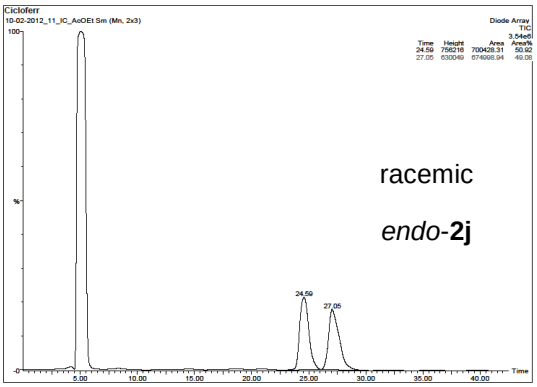
Time	Height	Area	Area%
22.45	1181178	911774.19	95.79
31.94	41374	40045.41	4.21

(2*S*,3*R*,4*S*,5*R*)-Trimethyl 5-phenylpyrrolidine-2,3,4-tricarboxylate (*endo*-L-2j).[23]

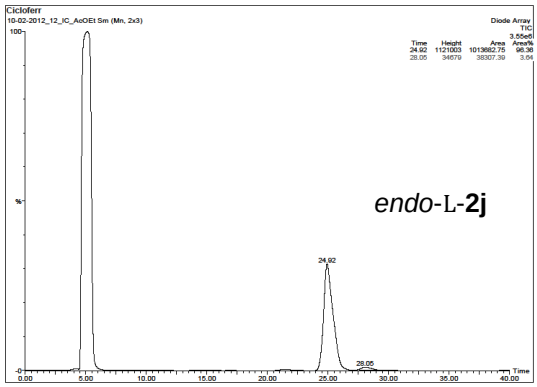


White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.36 – 7.23 (m, 5H), 4.48 (d, *J* = 6.9, 1H), 4.16 (d, *J* = 8.9, 1H), 3.81 (s, 3H), 3.74 – 3.70 (m, 1H), 3.70 (s, 3H), 3.57 (dd, *J* = 7.7, 7.2, 1H), 3.41 (bs, 1H), 3.22 (s, 3H).

Using L-3a as a catalyst: Yield: 87%. $[\alpha]_D^{23}$ =+65.5 (*c* 1.00, $CHCl_3$), 93% *ee*. Lit:[23] $[\alpha]_D^{20}$ =+100 (*c* 0.05, CH_2Cl_2), 94% *ee*. HPLC: Daicel Chiralpak IC, *iso*-propanol/hexane 30/70, flow rate 1.0 ml/min, tr: 24.9 min (2*S*,3*R*,4*S*,5*R*)-isomer and 28.1 min (2*R*,3*S*,4*R*,5*S*)-isomer, 210 nm.

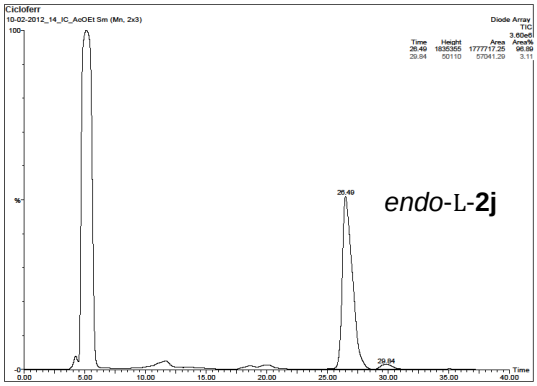


Time	Height	Area	Area%
24.59	756216	700428.31	50.92
27.05	630049	674998.94	49.08



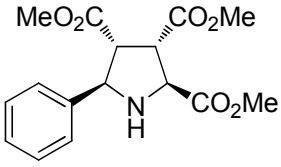
Time	Height	Area	Area%
24.92	1121003	1013682.75	96.36
28.05	34679	38307.39	3.64

Using D-3b as a catalyst: Yield: 41%. $[\alpha]_D^{23}$ =+65.7 (*c* 1.00, $CHCl_3$), 94% *ee*. Lit:[23] $[\alpha]_D^{20}$ =+100 (*c* 0.05, CH_2Cl_2), 94% *ee*. HPLC: Daicel Chiralpak IC, *iso*-propanol/hexane 30/70, flow rate 1.0 ml/min, tr: 26.5 min (2*S*,3*R*,4*S*,5*R*)-isomer and 29.8 min (2*R*,3*S*,4*R*,5*S*)-isomer, 210 nm.



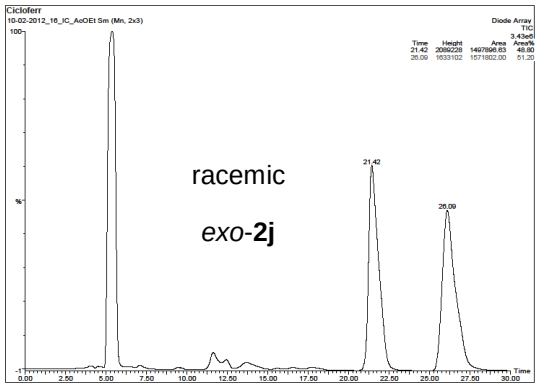
Time	Height	Area	Area%
26.49	1835355	1777717.25	96.89
29.84	50110	57041.29	3.11

(2*S*,3*S*,4*R*,5*R*)-Trimethyl 5-phenylpyrrolidine-2,3,4-tricarboxylate (*exo*-L-2j).[23]

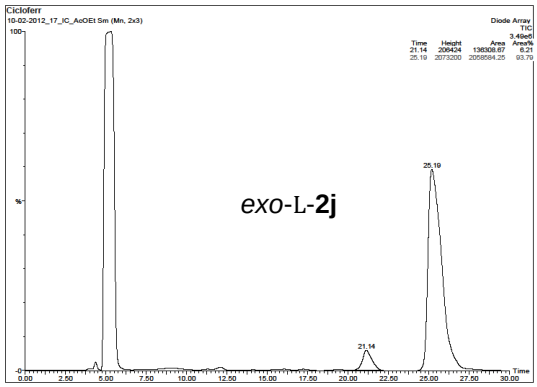


Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.45 (d, *J* = 7.4, 2H), 7.33 (t, *J* = 7.5, 2H), 7.29 – 7.24 (m, 1H), 4.67 (d, *J* = 7.8, 1H), 4.38 (d, *J* = 6.0, 1H), 3.80 (s, 3H), 3.72 (s, 3H), 3.65 (s, 3H), 3.63 (dd, *J* = 8.9, 6.2, 1H), 3.26 (t, *J* = 8.4, 1H), 2.62 (bs, 1H).

Using D-3b as a catalyst: Yield: 43%. $[\alpha]_D^{23}$ =-14.7 (*c* 1.00, $CHCl_3$), 88% *ee*. HPLC: Daicel Chiralpak IC, *iso*-propanol/hexane 50/50, flow rate 1.0 ml/min, tr: 21.1 min (2*R*,3*R*,4*S*,5*S*)-isomer and 25.2 min (2*S*,3*S*,4*R*,5*R*)-isomer, 210 nm.

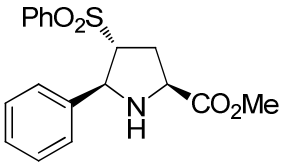


Time	Height	Area	Area%
21.42	2089228	1497896.63	48.80
26.09	1633102	1571802.00	51.20

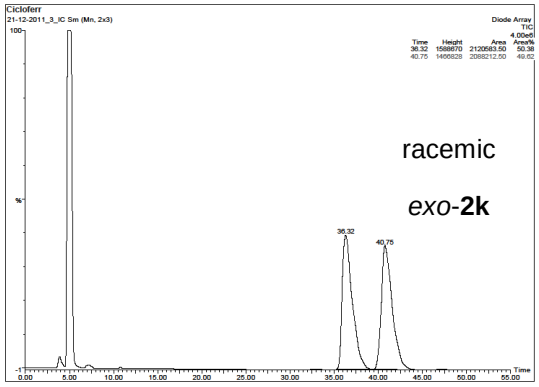


Time	Height	Area	Area%
21.14	206424	136308.67	6.21
25.19	2073200	2058584.25	93.79

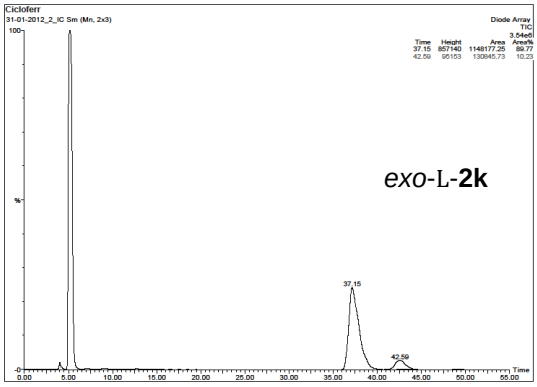
(2*S*,4*R*,5*S*)-Methyl 5-phenyl-4-phenylsulfonylpyrrolidine-2-carboxylate (*exo*-L-2k).[30]



Yield: 91%. White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.81 (d, *J* = 8.0, 2H), 7.59 (t, *J* = 7.5, 1H), 7.47 (t, *J* = 7.7, 2H), 7.21 (s, 5H), 4.73 (d, *J* = 5.7, 1H), 4.17 (t, *J* = 7.9, 1H), 3.76 (s, 3H), 3.66 (dt, *J* = 9.6, 5.0, 1H), 2.70 (ddd, *J* = 13.5, 7.3, 4.4, 1H), 2.51 (bs, 1H), 2.36 (dt, *J* = 14.0, 8.8, 1H). $[\alpha]_D^{22}$ =+19.8 (*c* 1.00, $CHCl_3$), 80% *ee*. Literature data for (2*R*,4*S*,5*R*)-isomer:[30] $[\alpha]_D^{20}$ =-21 (*c* 0.50, $CHCl_3$), 99% *ee*. HPLC: Daicel Chiralpak IC, *iso*-propanol/hexane 40/60, flow rate 1.0 mL/min, tr: 37.2 min (2*S*,4*R*,5*S*)-isomer and 42.6 min (2*R*,4*S*,5*R*)-isomer, 210 nm.

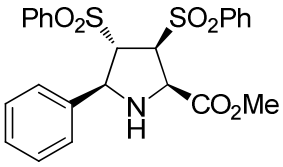


Time	Height	Area	Area%
36.32	1588670	2120583.50	50.38
40.75	1466828	2088212.50	49.62



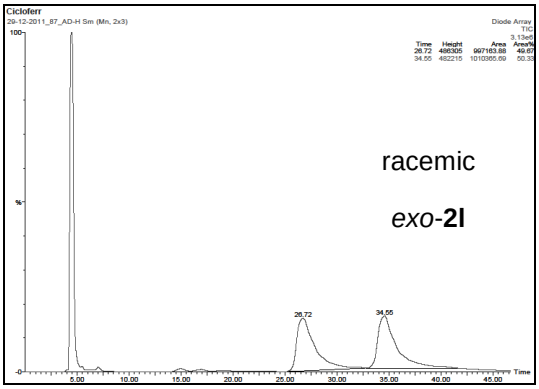
Time	Height	Area	Area%
37.15	857140	1148177.25	89.77
42.59	95153	130845.73	10.23

(2*R*,3*S*,4*S*,5*S*)-Methyl 5-phenyl-3,4-bis(phenylsulfonyl)pyrrolidine-2-carboxylate (*exo*-L-2l).[31]

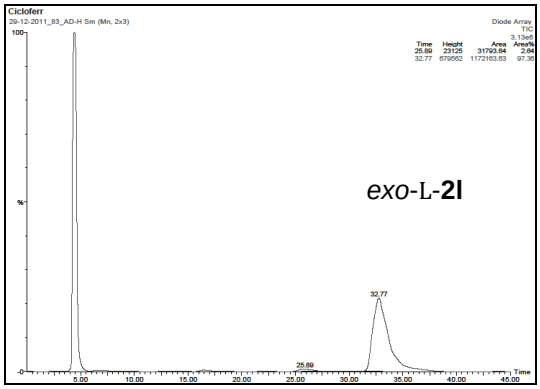


White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.71 – 7.62 (m, 5H), 7.57 (t, *J* = 7.5, 1H), 7.51 (t, *J* = 7.6, 2H), 7.41 (t, *J* = 7.5, 2H), 7.33 – 7.28 (m, 2H), 7.28 – 7.22 (m, 3H), 4.63 (d, *J* = 6.4, 1H), 4.44 (dd, *J* = 6.1, 1.8, 1H), 4.39 (dd, *J* = 6.6, 2.3, 1H), 4.32 (d, *J* = 5.9, 1H), 3.66 (s, 3H), 2.83 (bs, 1H).

Using L-3a as a catalyst: Yield: 82%. $[\alpha]_D^{23}$ =-2.5 (*c* 1.00, $CHCl_3$), 95% *ee*. Lit:[31] $[\alpha]_D^{20}$ =-2.4 (*c* 1.00, $CHCl_3$), >99% *ee*. HPLC: Daicel Chiralpak AD-H, *iso*-propanol/hexane 50/50, flow rate 1.0 ml/min, tr: 26.0 min (2*S*,3*R*,4*R*,5*R*)-isomer and 32.8 min (2*R*,3*S*,4*S*,5*S*)-isomer, 210 nm.

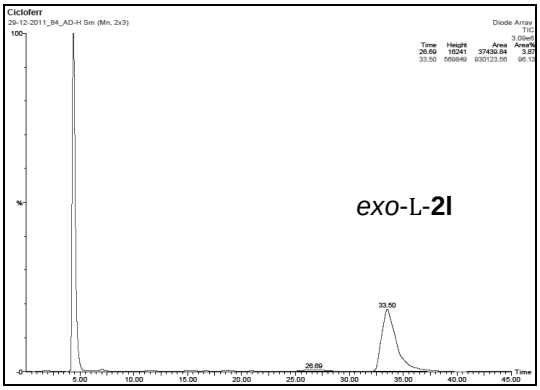


Time	Height	Area	Area%
26.72	486305	997163.88	49.67
34.55	482215	1010365.69	50.33



Time	Height	Area	Area%
25.99	23125	31793.64	2.64
32.77	679562	1172163.63	97.36

Using D-3b as a catalyst: Yield: 89%. $[\alpha]_D^{23}$ =-2.4 (*c* 1.00, $CHCl_3$), 92% *ee*. Lit:[31] $[\alpha]_D^{20}$ =-2.4 (*c* 1.00, $CHCl_3$), >99% *ee*. HPLC: Daicel Chiralpak AD-H, *iso*-propanol/hexane 50/50, flow rate 1.0 ml/min, tr: 26.7 min (2*S*,3*R*,4*R*,5*R*)-isomer and 33.5 min (2*R*,3*S*,4*S*,5*S*)-isomer, 210 nm.

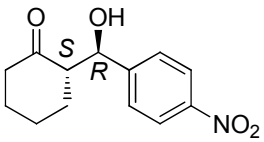


Time	Height	Area	Area%
26.69	16241	37439.84	3.87
33.50	569849	930123.56	96.13

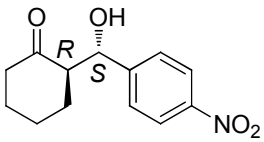
General procedure for the synthesis of compounds (2*S*,1'*R*)-11a, (2*S*,1'*R*)-11b, (2*S*,1'*R*)-11c, (2*S*,1'*R*)-11d, (2*S*,1'*R*)-11e using L-Pro as a catalyst. The corresponding aldehydes **10** (6.62 mmol) and cyclohexanone (0.649 g, 0.69 ml, 6.62 mmol, 5 equiv) were dissolved in dichloroethane/ethanol (99:1, 0.70 ml), the resulting mixtures cooled to 4 ºC and L-Pro (0.396 mmol, 46mg, 0.3 equiv) was added. The resulting mixture was stirred at 4 ºC for 36h, washed with a 10% aqueous solution of potassium carbonate, dried onto sodium sulfate, filtered and concentrated under reduced pressure to furnish colourless, waxy solids. Purification by flash chromatography eluting with ethyl acetate:hexanes 1:2, gave the corresponding *anti*-aldol products. The enantiomeric excesses were determined by chiral HPLC analysis of the purified *anti*-products (the HPLC spectra of the corresponding racemic mixtures are also given for comparison).

General procedure for the synthesis of compounds (2*R*,1'*S*)-11a, (2*R*,1'*S*)-11b, (2*R*,1'*S*)-11c, (2*R*,1'*S*)-11d, (2*R*,1'*S*)-11e using *exo*-L-2a or *exo*-L-2c as a catalyst.[24] The corresponding aldehydes **10** (0.25 mmol) were dissolved in neat cyclohexanone (1.5ml, 15.3 mmol, 61.2 equiv), the resulting mixtures cooled to -15 ºC and either *exo*-L-**2a** or *exo*-L-**2c** (0.075 mmol, 27 mg, 0.3 equiv) were added, followed by trifluoroacetic acid (75.0 µmol, 6.0 µL, 0.3 equiv). The resulting mixtures were stirred at -15 ºC for 20h, then warmed to RT, diluted with ethyl acetate, washed with 0.1 M (pH 7) phosphate buffer solution, dried onto sodium sulfate, filtered and concentrated under reduced pressure to furnish colourless, waxy solids. Purification by Biotage Isolera Four apparatus, eluting with ethyl acetate:hexanes 1:2, gave the corresponding *anti*-aldol products. The enantiomeric excesses were determined by chiral HPLC analysis of the purified *anti*-products (the HPLC spectra of the corresponding racemic mixtures are also given for comparison).

2-[Hydroxy-(4-nitro-phenyl)-methyl]-cyclohexan-1-one [(2*S*,1'*R*)-11a; (2*R*,1'*S*)-11a]



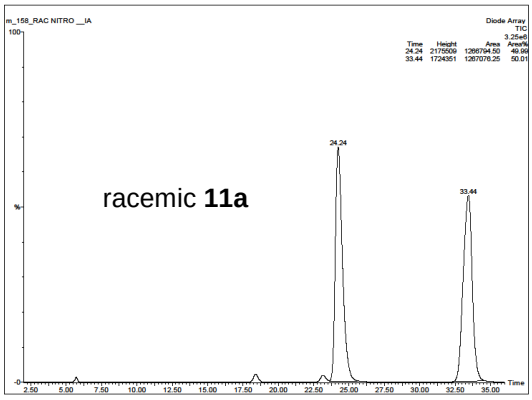
(2*S*,1'*R*)-**11a**

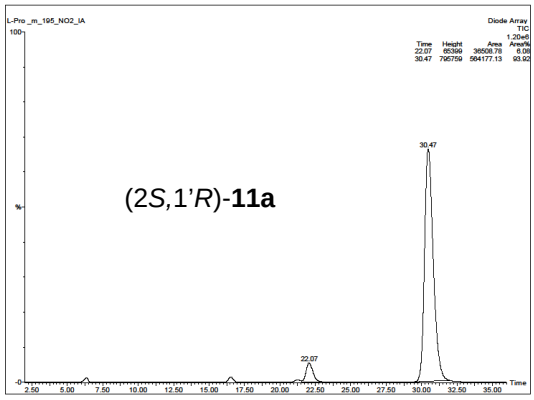


(2*R*,1'*S*)-**11a**

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.21 (d, *J* = 8.7, 2H), 7.51 (d, *J* = 8.6, 2H), 4.90 (dd, *J* = 8.3, 3.0, 1H), 4.07 (d, *J* = 3.2, 1H), 2.68 – 2.55 (m, 1H), 2.54 – 2.44 (m, 1H), 2.43 – 2.29 (m, 1H), 2.11 (dtd, *J* = 8.9, 5.9, 2.9, 1H), 1.93 – 1.77 (m, 1H), 1.73 – 1.56 (m, 3H), 1.45 – 1.31 (m, 1H). These data are in good agreement with the literature values.[32]

(2*S*,1'*R*)-11a (using L-Pro as a catalyst): Yield 70%; HPLC analysis: 88% *ee* [Daicel Chiralpak IA, *iso*-propanol/hexane 10/90, flow rate 1.0 ml/min, 254 nm; t_r (2*R*,1'*S*)-**11a** = 22.07 min (minor), t_r (2*S*,1'*R*)-**11a** = 30.47min (major)]; $[\alpha]_D^{27}$= +7.3 (*c* 0.5, $CHCl_3$); Lit.[32] $[\alpha]_D^{23}$= +10.9 (*c* 0.5, $CHCl_3$).

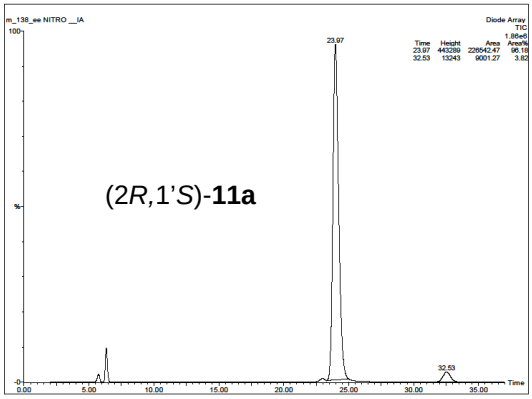




Time	Height	Area	Area%
24.24	2175509	1266794.5	49.99
33.44	1724351	1267076.2	50.01

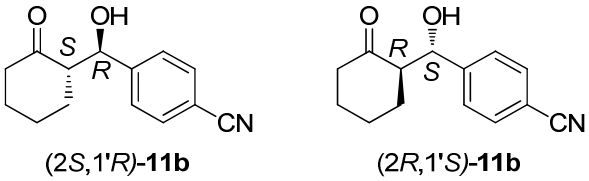
Time	Height	Area	Area%
22.07	65399	36508.78	6.08
30.47	795759	584177.13	93.92

(2*R*,1'*S*)-11a (using *exo*-L-2c as a catalyst): Yield 83%; HPLC analysis: 92% *ee* [Daicel Chiralpak IA, *iso*-propanol/hexane 10/90, flow rate 1.0 ml/min, 254 nm; t_r (2*R*,1'*S*)-**11a** = 23.97 min (major), t_r (2*S*,1'*R*)-**11a** = 32.53 min (minor)]; $[\alpha]_D^{26}$= -5.0 (*c* 1.1, $CHCl_3$).



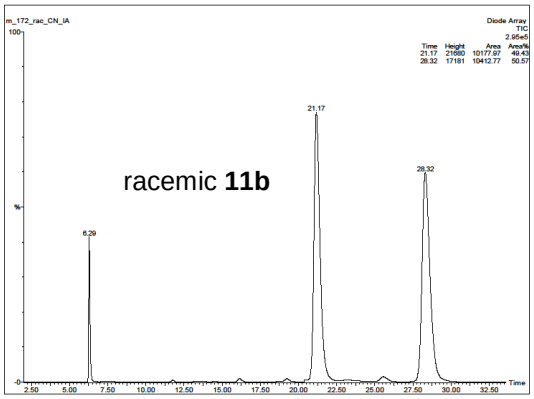
Time	Height	Area	Area%
23.97	443289	226542.47	96.18
32.53	13243	9001.27	3.82

2-[Hydroxy-(4-cyano-phenyl)-methyl]-cyclohexan-1-one [(2*S*,1'*R*)-11b; (2*R*,1'*S*)-11b]

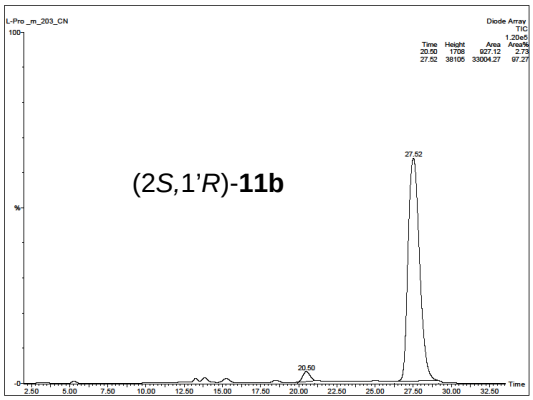


^{1}H NMR (500 MHz, $CDCl_3$): δ 7.64 (d, *J* = 8.3 Hz, 2H), 7.44 (d, *J* = 8.2 Hz, 2H), 4.84 (dd, *J* = 8.4, 3.0 Hz, 1H), 4.03 (d, *J* = 3.1 Hz, 1H), 2.57 (ddd, *J* = 12.2, 7.3, 5.2 Hz, 1H), 2.53 – 2.47 (m, 1H), 2.36 (td, *J* = 13.5, 6.2 Hz, 1H), 2.11 (dtd, *J* = 8.8, 5.8, 2.8 Hz, 1H), 1.88 – 1.79 (m, 1H), 1.73 – 1.64 (m, 1H), 1.55 – 1.53 (m, 1H), 1.40 – 1.27 (m, 1H). These data are in good agreement with the literature values.[32]

(2*S*,1'*R*)-11b (using L-Pro as a catalyst): Yield 47%; HPLC analysis: 95% *ee* [Daicel Chiralpak IA, *iso*-propanol/hexane 10/90, flow rate 1.0 ml/min, 254 nm; t_r (2*R*,1'*S*)-**11b** = 20.50 min (minor), t_r (2*S*,1'*R*)-**11b** = 27.52min (major)]; $[\alpha]_D^{27}$= +21.0 (*c* 1.0, $CHCl_3$; Lit.[32] $[\alpha]_D^{23}$= +21.4 (*c* 0.6, $CHCl_3$).

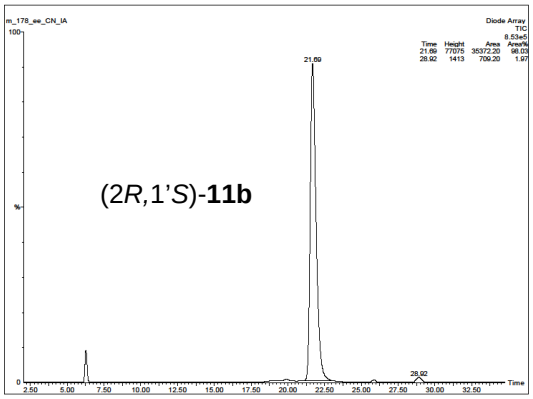


Time	Height	Area	Area%
21.17	21080	10177.97	49.43
28.32	17181	10412.77	50.57



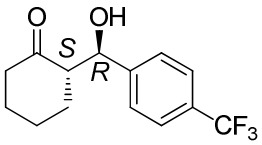
Time	Height	Area	Area%
20.50	1078	927.12	2.73
27.52	38105	33004.27	97.27

(2*R*,1'*S*)-11b (using *exo*-L-2c as a catalyst): Yield 67%; HPLC analysis: 96% *ee* [Daicel Chiralpak IA, *iso*-propoanol/hexane 10/90, flow rate 1.0 ml/min, 254 nm; t_r (2*R*,1'*S*)-**11b** = 21.69 min (major), t_r (2*S*,1'*R*)-**11b** = 28.92 min (minor)]; $[\alpha]_D^{26}$ = -11.7 (*c* 0.5, $CHCl_3$).

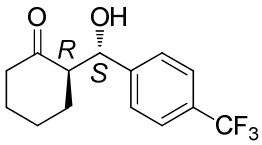


Time	Height	Area	Area%
21.69	77075	35372.20	98.03
28.92	1413	709.20	1.97

2-[Hydroxy-(4- trifluoromethyl -phenyl)-methyl]-cyclohexan-1-one [(2*S*,1'*R*)-11c; (2*R*,1'*S*)-11c]



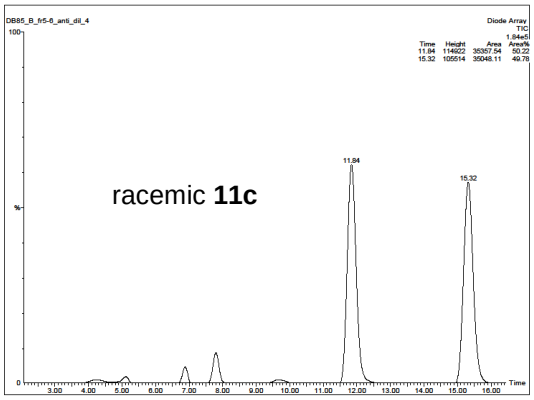
(2*S*,1'*R*)-**11c**



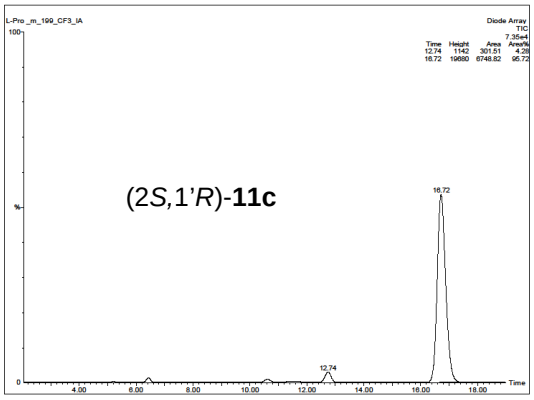
(2*R*,1'*S*)-**11c**

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.61 (d, *J* = 8.1, 2H), 7.45 (d, *J* = 8.1, 2H), 4.85 (dd, *J* = 8.5, 1.5, 1H), 4.02 (d, *J* = 2.6, 1H), 2.63 – 2.53 (m, 1H), 2.53 – 2.44 (m, 1H), 2.40 – 2.31 (m, 1H), 2.10 (dtd, *J* = 8.9, 5.9, 2.9, 1H), 1.86 – 1.76 (m, 1H), 1.73 – 1.61 (m, 1H), 1.61 – 1.53 (m, 2H), 1.42 – 1.29 (m, 1H). These data are in good agreement with the literature values.[32]

(2*S*,1'*R*)-11c (using L-Pro as a catalyst): Yield 60%; HPLC analysis: 91% *ee* [Daicel Chiralpak IA, *iso*-propanol/hexane 10/90, flow rate 1.0 ml/min, 254 nm; t_r (2*R*,1'*S*)-**11c** = 12.74 min (minor), t_r (2*S*,1'*R*)-**11c** = 16.72 min (major)]; $[\alpha]_D^{27}$= +33.0 (*c* 1.0, $CHCl_3$; Lit.[32] $[\alpha]_D^{23}$= +20.0 (*c* 1.0, $CHCl_3$).

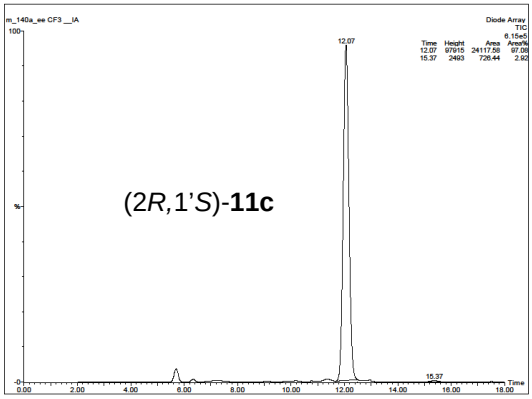


Time	Height	Area	Area%
11.84	114922	35357.54	50.22
15.32	105514	35048.11	49.78



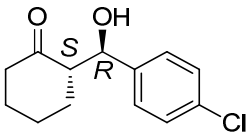
Time	Height	Area	Area%
12.74	1142	301.51	4.28
16.72	19680	6748.82	95.72

(2*R*,1'*S*)-11c (using *exo*-L-2c as a catalyst): Yield 82%; HPLC analysis: 94% *ee* [Daicel Chiralpak IA, *iso*-propanol/hexane 10/90, flow rate 1.0 ml/min, 254 nm; t_r (2*R*,1'*S*)-**11c** = 12.07 min (major), t_r (2*S*,1'*R*)-**11c** = 15.37 min (minor)]; $[\alpha]_D^{26}$= -4.28 (*c* 0.8, $CHCl_3$).

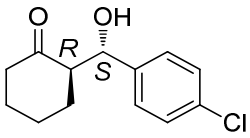


Time	Height	Area	Area%
12.07	97915	24117.58	97.08
15.37	2493	726.44	2.92

2-[Hydroxy-(4-chloro-phenyl)-methyl]-cyclohexan-1-one [(2*S*,1'*R*)-11d; (2*R*,1'*S*)-11d]



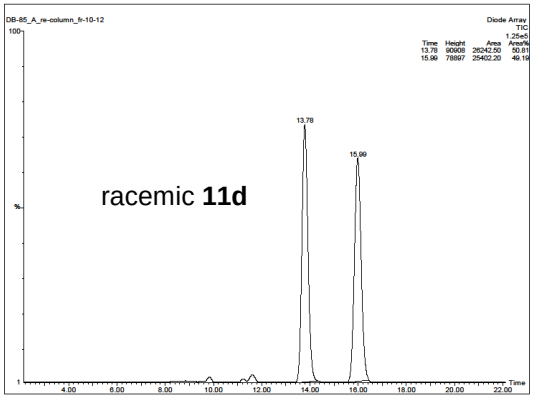
(2*S*,1'*R*)-**11d**

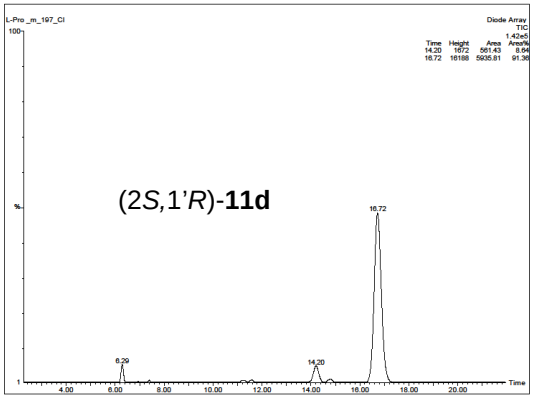


(2*R*,1'*S*)-**11d**

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.34 – 7.30 (m, 1H), 7.27 – 7.24 (m, 1H), 4.76 (dd, *J* = 8.7, 2.6 Hz, 1H), 3.97 (d, *J* = 2.8 Hz, 1H), 2.60 – 2.52 (m, 1H), 2.51 – 2.45 (m, 1H), 2.40 – 2.31 (m, 1H), 2.10 (ddt, *J* = 12.6, 5.9, 3.0 Hz, 1H), 1.84 – 1.77 (m, 1H), 1.72 – 1.49 (m, 3H), 1.35 – 1.24 (m, 1H). These data are in good agreement with the literature values.[32]

(2*S*,1'*R*)-11d (using L-Pro as a catalyst): Yield 80%; HPLC analysis: 83% *ee* [Daicel Chiralpak IA, *iso*-propanol/hexane 10/90, flow rate 1.0 ml/min, 254 nm; t_r (2*R*,1'*S*)-**11d** = 14.20 min (minor), t_r (2*S*,1'*R*)-**11d** = 16.72 min (major)]; $[\alpha]_D^{27}$= +27.0 (*c* 1.0, $CHCl_3$; Lit.[32] $[\alpha]_D^{23}$= +22.5 (*c* 0.7, $CHCl_3$).



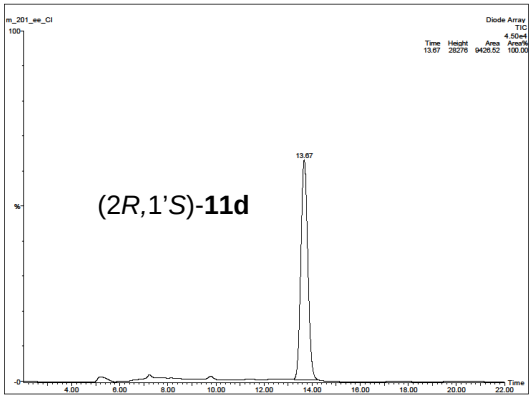


Time	Height	Area	Area%
13.78	90908	26242.50	50.81
15.99	78897	25402.20	49.19

Time	Height	Area	Area%
14.20	1672	581.43	8.64
16.72	16188	5935.81	91.36

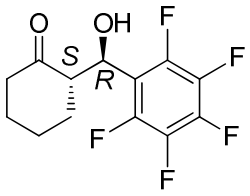
Although these compounds have been previously described, it was found that 2-[hydroxy-(4-chloro-phenyl)-methyl]-cyclohexan-1-one is particularly prone to decomposition *via* retroaldolic reaction (as suggested by the formation of the *syn*-aldol isomers in pure *anti*-aldol samples). Thus, for compound (2*R*,1'*S*)-**11d**, the enantiomeric excess was estimated by chiral HPLC analysis immediately after the chromatographic purification, while pure samples (>99% optical purity) of the corresponding compound were obtained by crystallisation in ethyl acetate/hexane to further improve the chemical purity and therefore perform accurate optical rotation measurements.

(2*R*,1'*S*)-11d (using *exo*-L-2c as a catalyst): Yield 93%; HPLC analysis: 96% *ee* (before crystallisation), [Daicel Chiralpak IA, *iso*-propanol/hexane 10/90, flow rate 1.0 ml/min, 254 nm; t_r (2*R*,1'*S*)-**11d** = 13.57 min (major), 100% *ee* after crystallisation]; $[\alpha]_D^{26}$= -12.3 (*c* 0.5, $CHCl_3$).

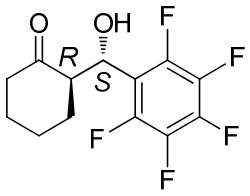


Time	Height	Area	Area%
13.57	28276	9426.52	100
-	-	-	-

2-[Hydroxy-(4-pentafluorophenyl-methyl]-cyclohexan-1-one [(2*S*,1'*R*)-11e; (2*R*,1'*S*)-11e]



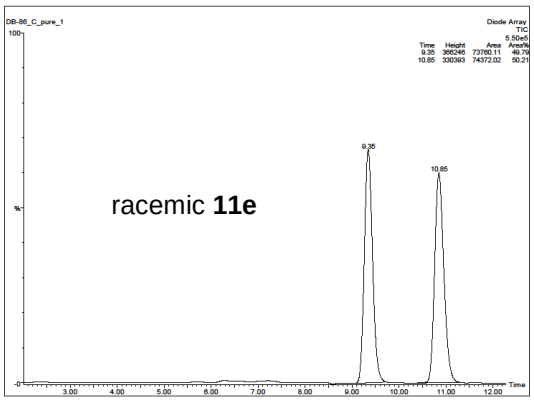
(2*S*,1'*R*)-**11e**

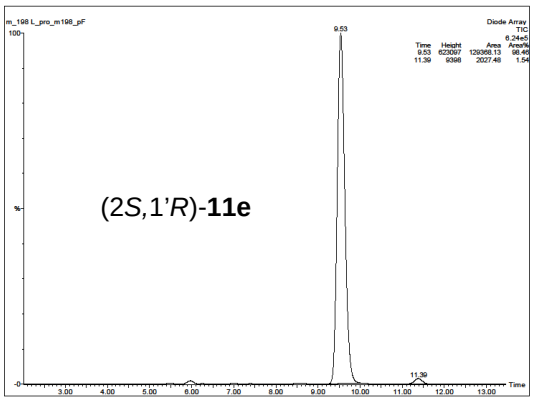


(2*R*,1'*S*)-**11e**

^{1}H NMR (500 MHz, $CDCl_3$): δ 5.39 – 5.30 (m, 1H), 3.92 (d, *J* = 3.3 Hz, 1H), 3.09 – 2.99 (m, 1H), 2.60 – 2.48 (m, 1H), 2.43 (td, *J* = 12.9, 6.3 Hz, 1H), 2.22 – 2.11 (m, 1H), 1.95 – 1.85 (m, 1H), 1.76 – 1.61 (m, 3H), 1.41 – 1.26 (m, 1H). This data are in good agreement with the literature data.[33]

(2*S*,1'*R*)-11e (using L-Pro as a catalyst): Yield 77%; HPLC analysis: 97% *ee* [Daicel Chiralpak IA, *iso*-propanol/hexane 10/90, flow rate 1.0 ml/min, 254 nm; t_r (2*S*,1'*R*)-**11e** = 9.53 min (major), t_r (2*R*,1'*S*)-**11e** = 11.39 min (minor)]; $[\alpha]_D^{27}$ = -8.0 (*c* 1.0, $CHCl_3$; Lit.[33] $[\alpha]_D^{25}$ = -15.0 (*c* 1.8, $CHCl_3$).

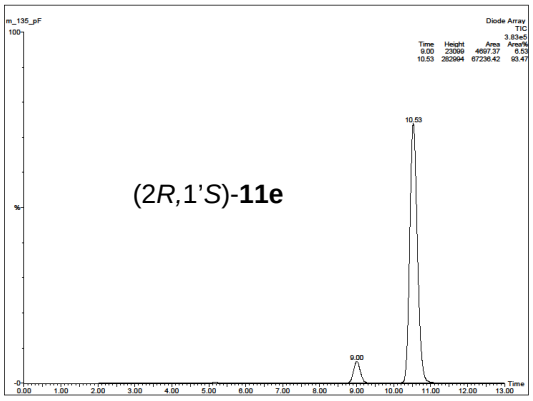




Time	Height	Area	Area%
9.35	366248	73760.11	49.79
10.85	330393	74372.02	50.21

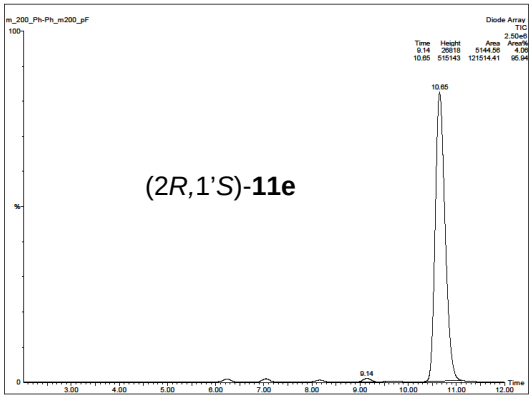
Time	Height	Area	Area%
9.53	623097	129368.13	98.46
11.39	9398	2027.48	1.54

(2*R*,1'*S*)-11e (using *exo*-L-2c as a catalyst): Yield 81%; HPLC analysis: 87% *ee*, [Daicel Chiralpak IA, *iso*-propanol/hexane 10/90, flow rate 1.0 ml/min, 254 nm; t_r (2*S*,1'*R*)-**11e** = 9.00 min (minor), t_r (2*R*,1'*S*)-**11e** = 10.53 min (major)]; $[\alpha]_D^{27}$ = +15.5 (*c* 1.4, $CHCl_3$).



Time	Height	Area	Area%
9.00	23099	4697.37	6.53
10.53	282994	67236.42	93.47

(2*R*,1'*S*)-11e (using catalyst *exo*-L-2a): Yield: 70%, HPLC analysis: 92%, [Daicel Chiralpak IA, *iso*-propanol/hexane 10/90, flow rate 1.0 ml/min, 254 nm; t_r (2*S*,1'*R*)-**11e** = 9.14 min (minor), t_r (2*R*,1'*S*)-**11e** = 10.65 min (major)]; $[\alpha]_D^{27}$ = +14.0 (*c* 1.0, $CHCl_3$).



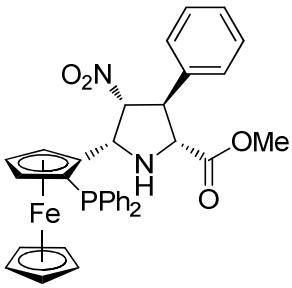
(2*R*,1'*S*)-**11e**

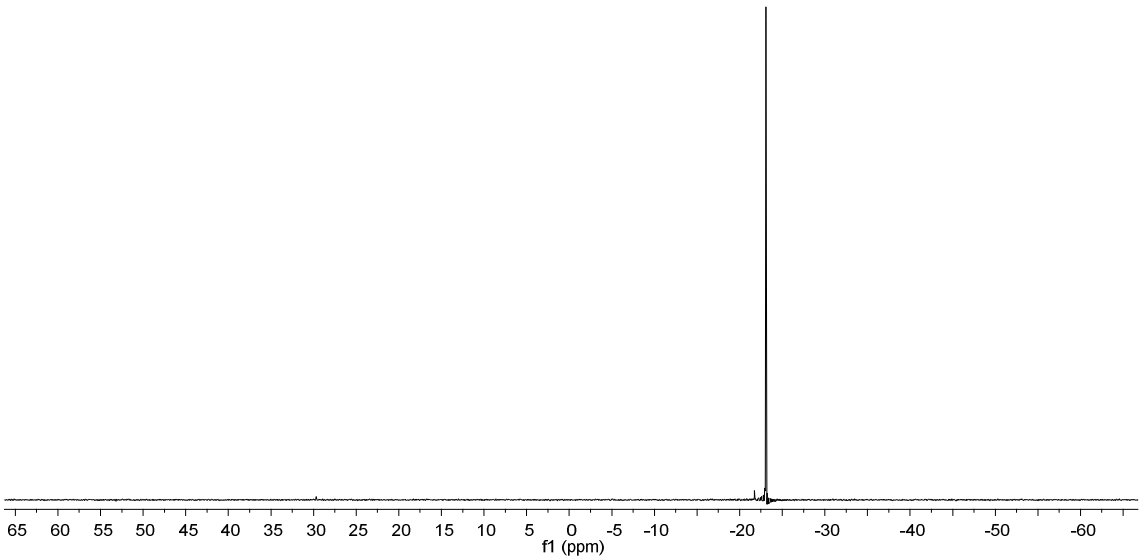
Time	Height	Area	Area%
9.14	26818	5144.56	4.06
10.65	515143	121514.41	95.94

Supplementary Data: Copies of NMR spectra

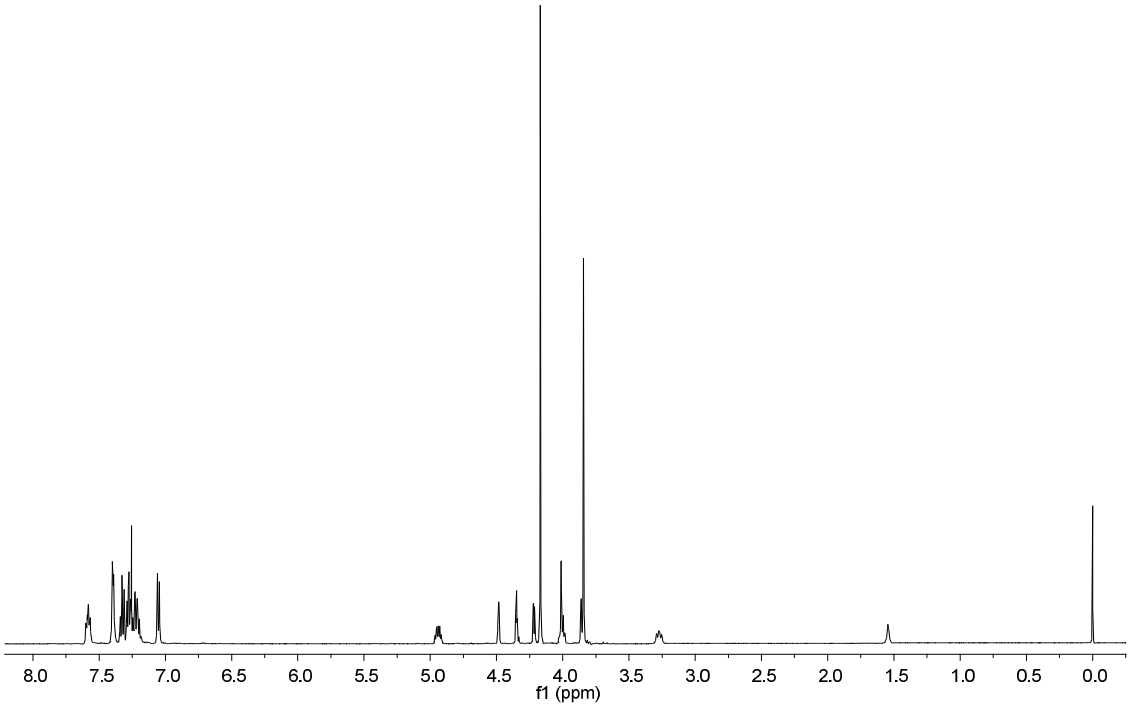
Compound D-3b

^{31}P-NMR ($CDCl_3$)



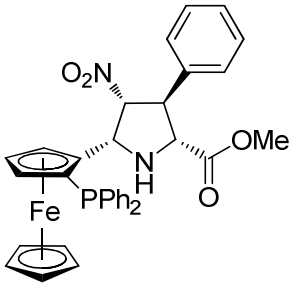


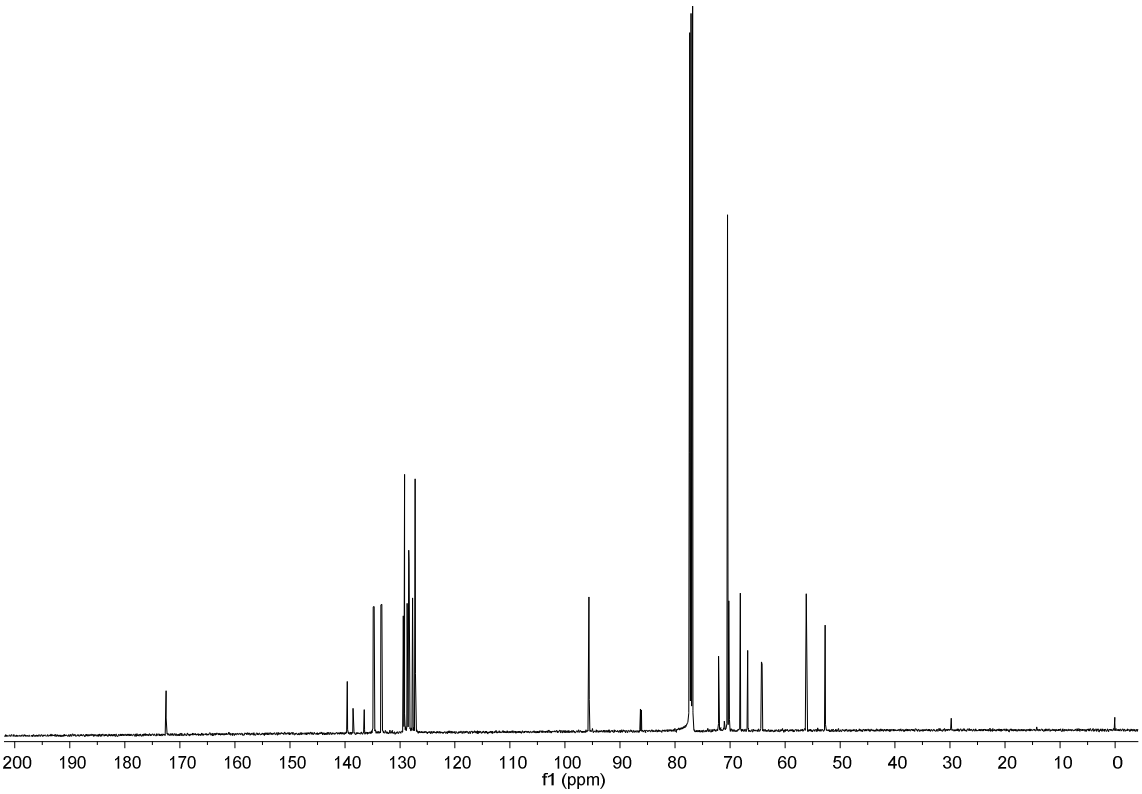
^{1}H-NMR ($CDCl_3$)

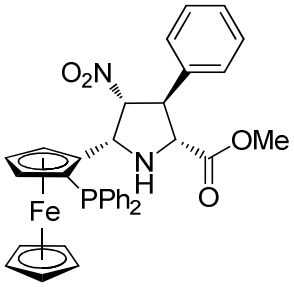


Compound D-3b

^{13}C-NMR ($CDCl_3$)

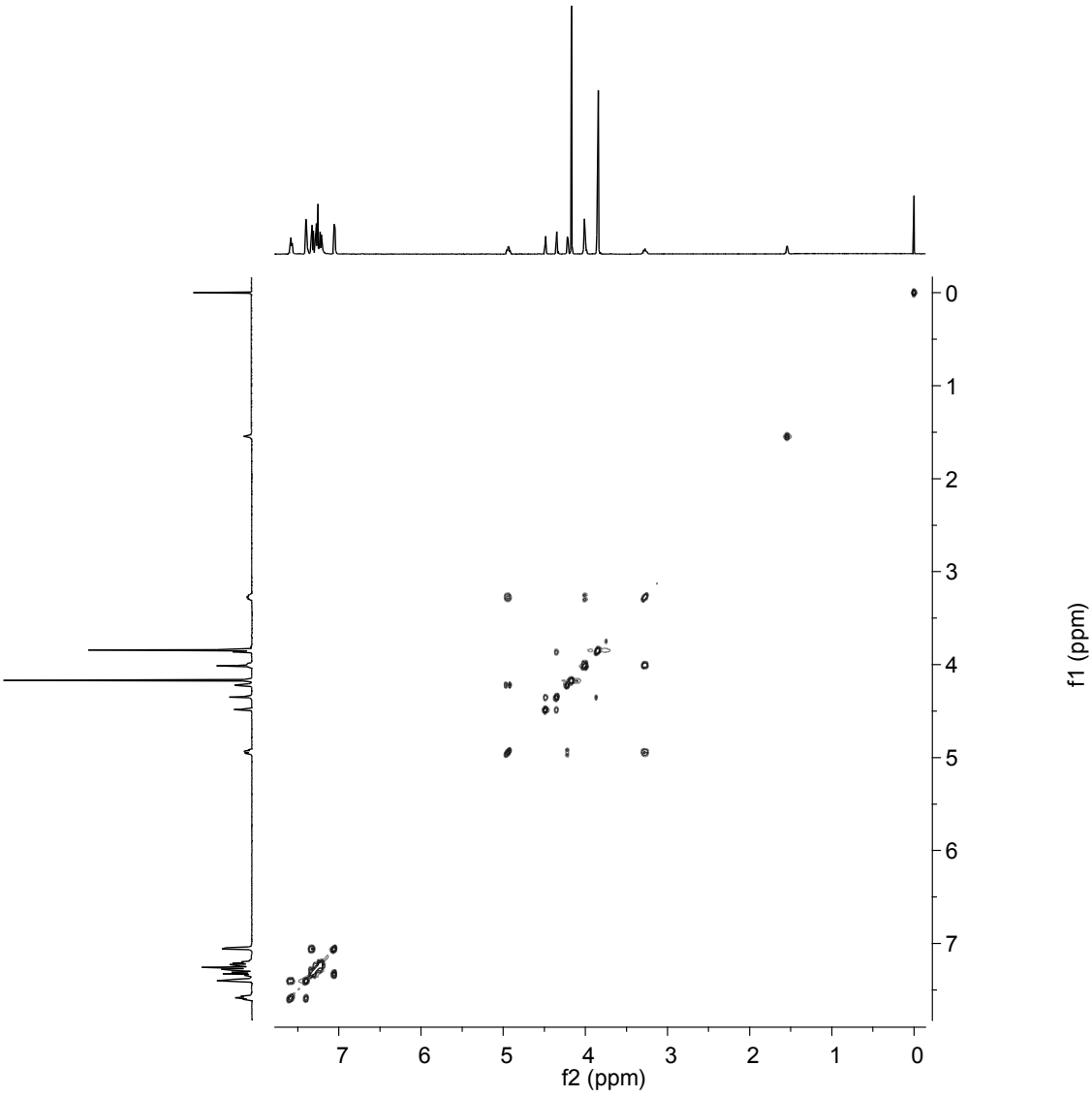






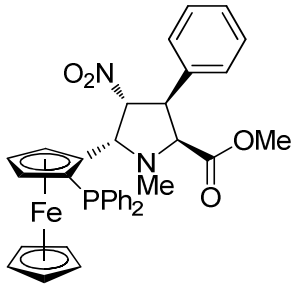
COSY spectrum

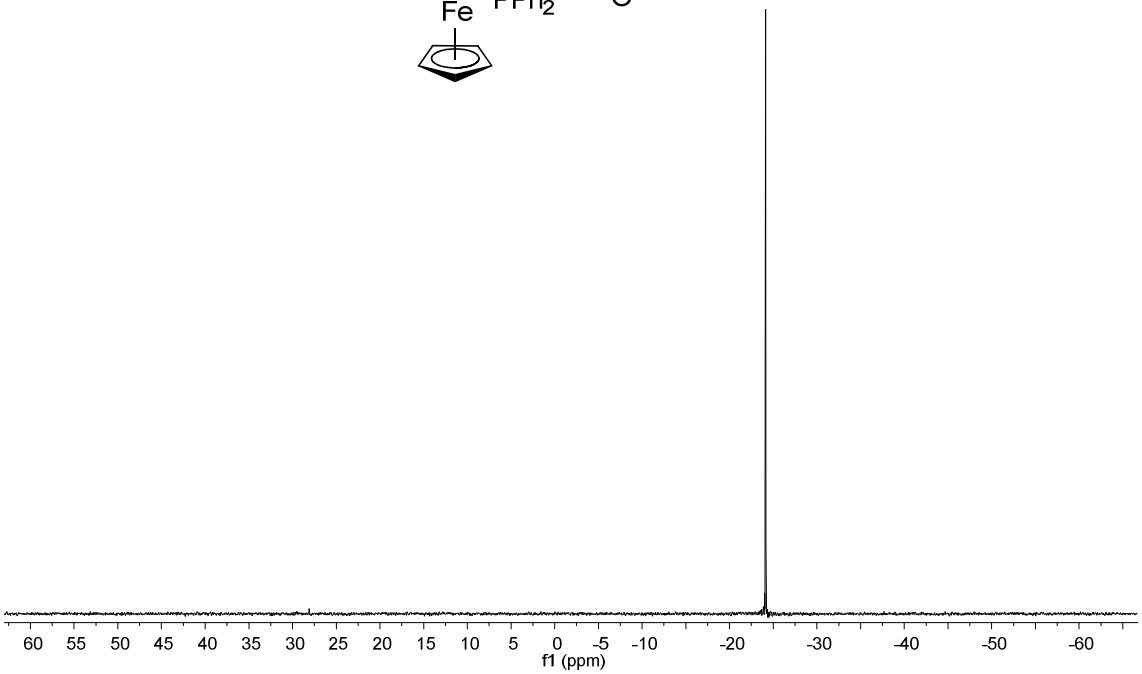
Compound D-3b



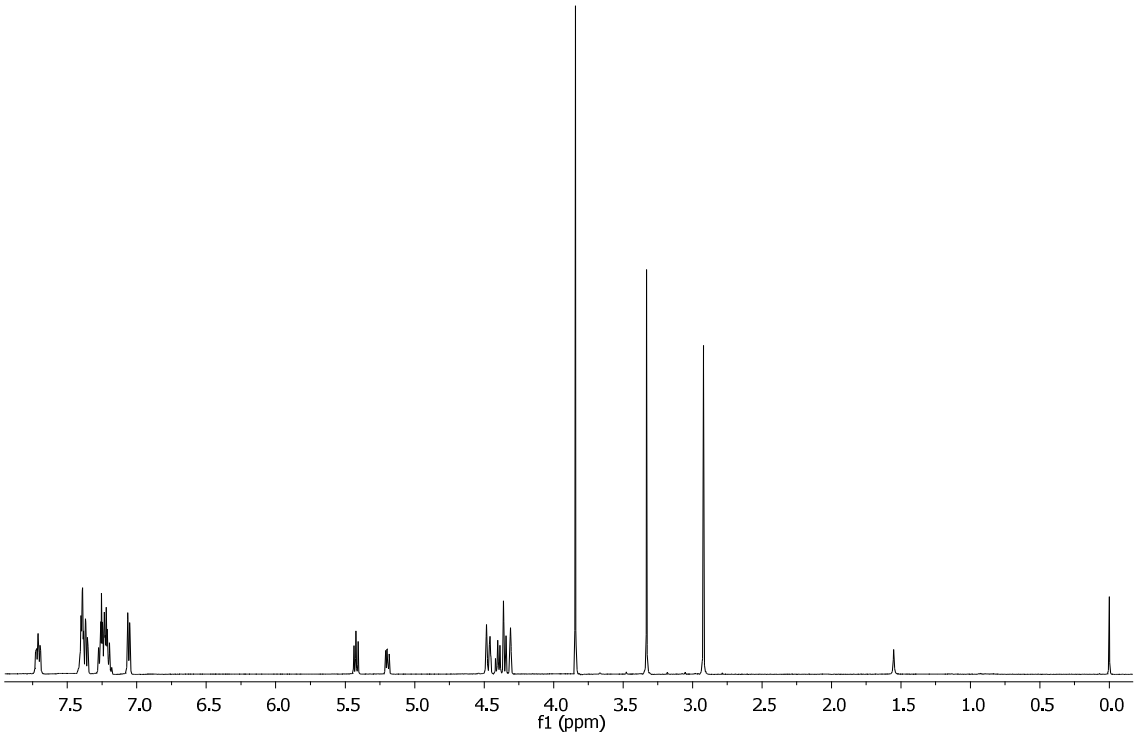
Compound L-3a

^{31}P-NMR ($CDCl_3$)



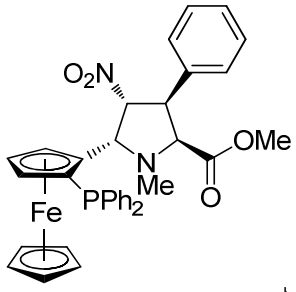


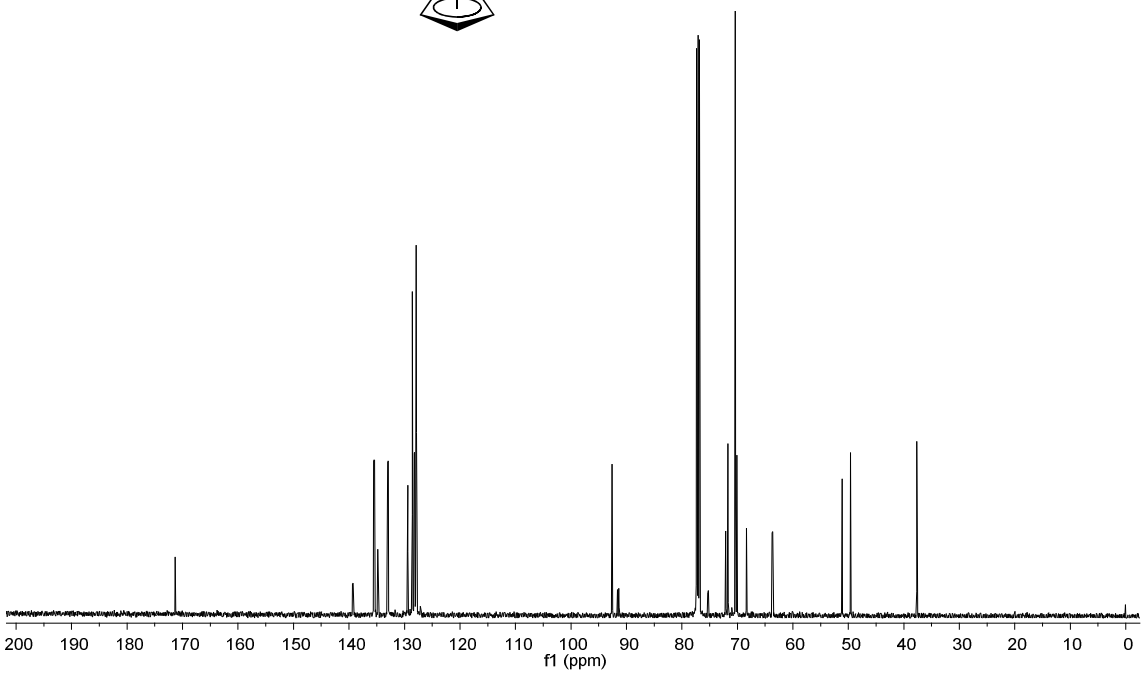
^{1}H-NMR($CDCl_3$)

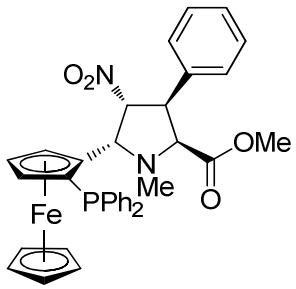


Compound L-3a

^{13}C-NMR ($CDCl_3$)

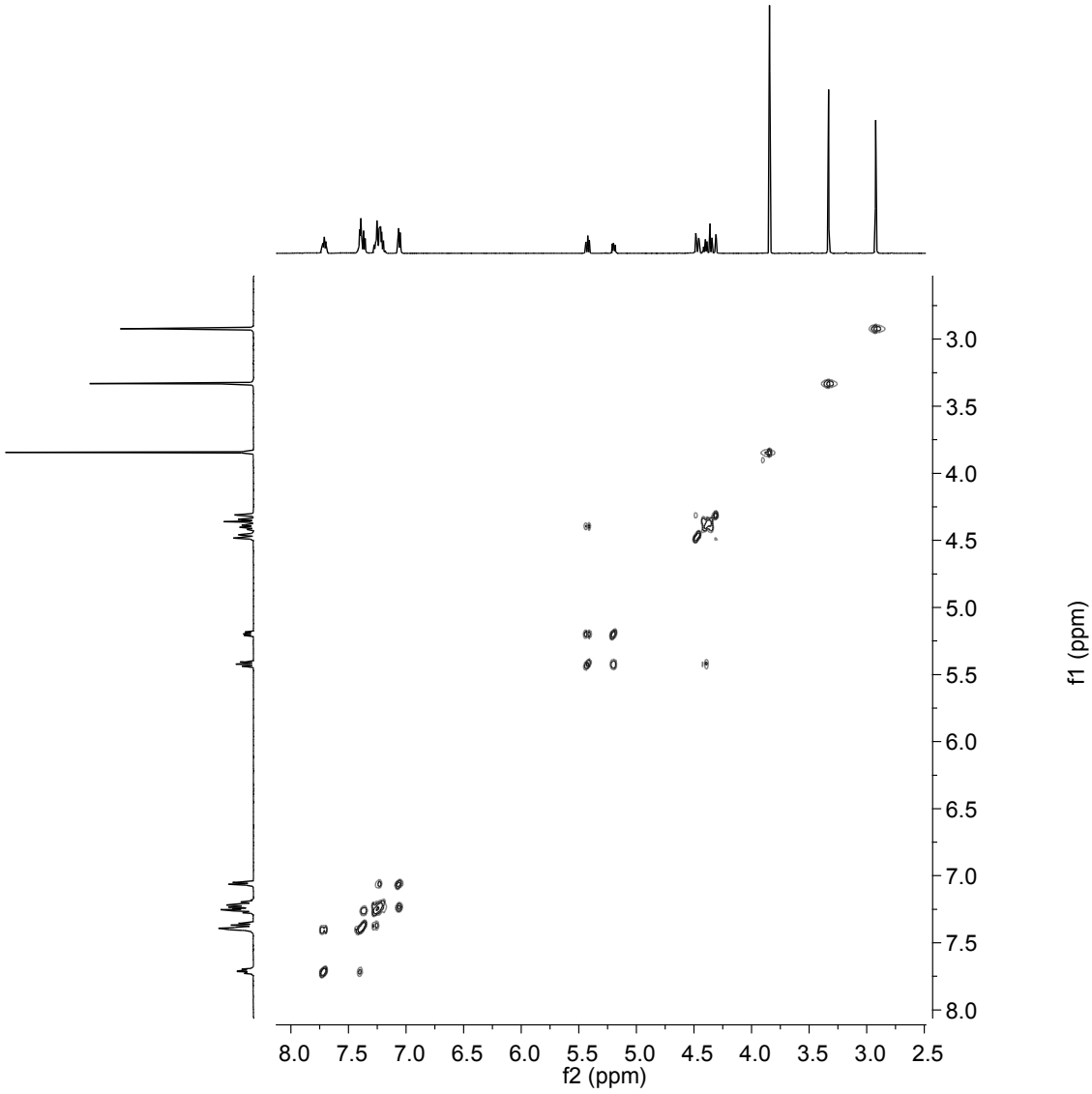






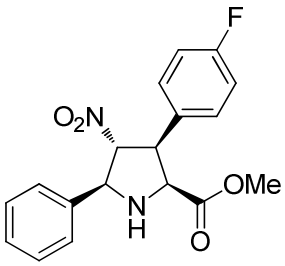
COSY spectrum

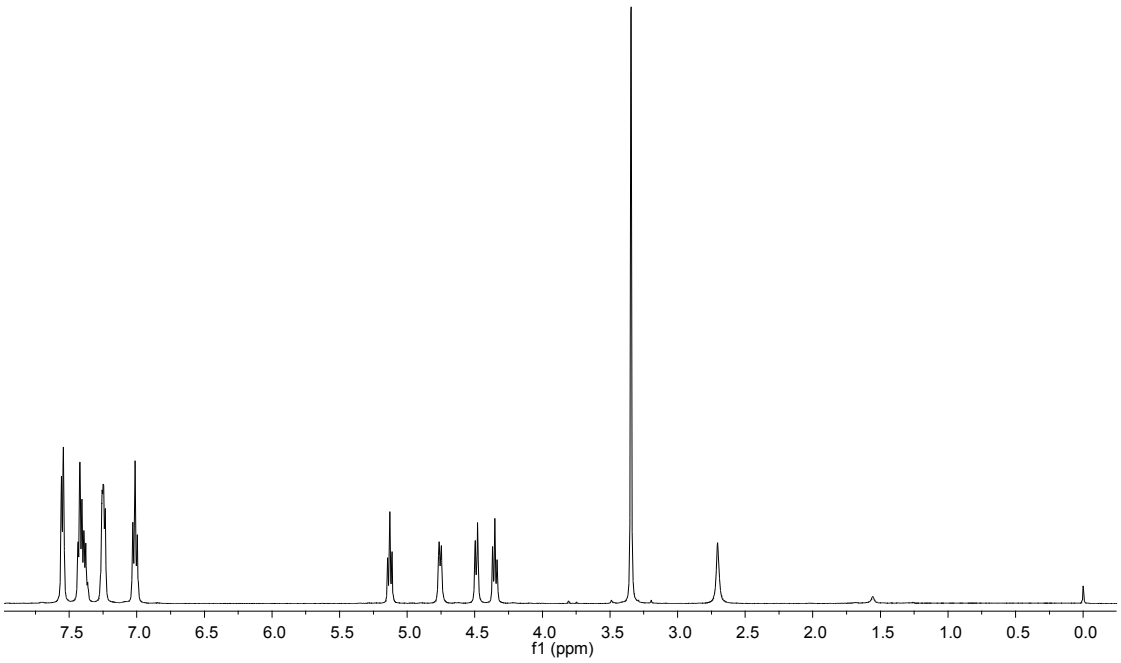
Compound L-3a



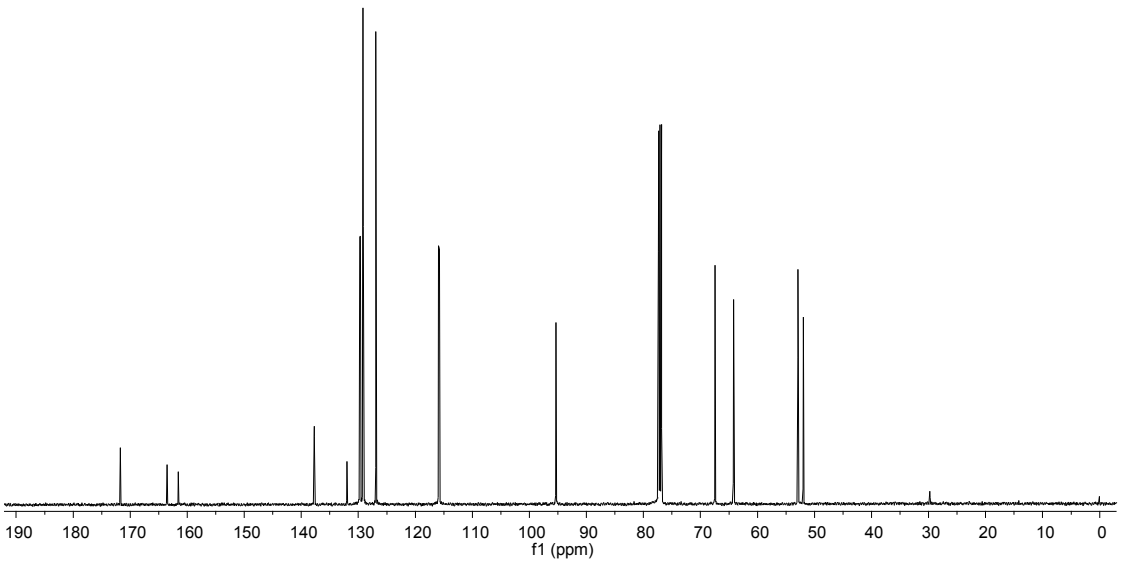
Compound *exo*-L-2b

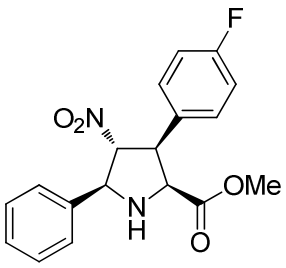
^{1}H-NMR ($CDCl_3$)





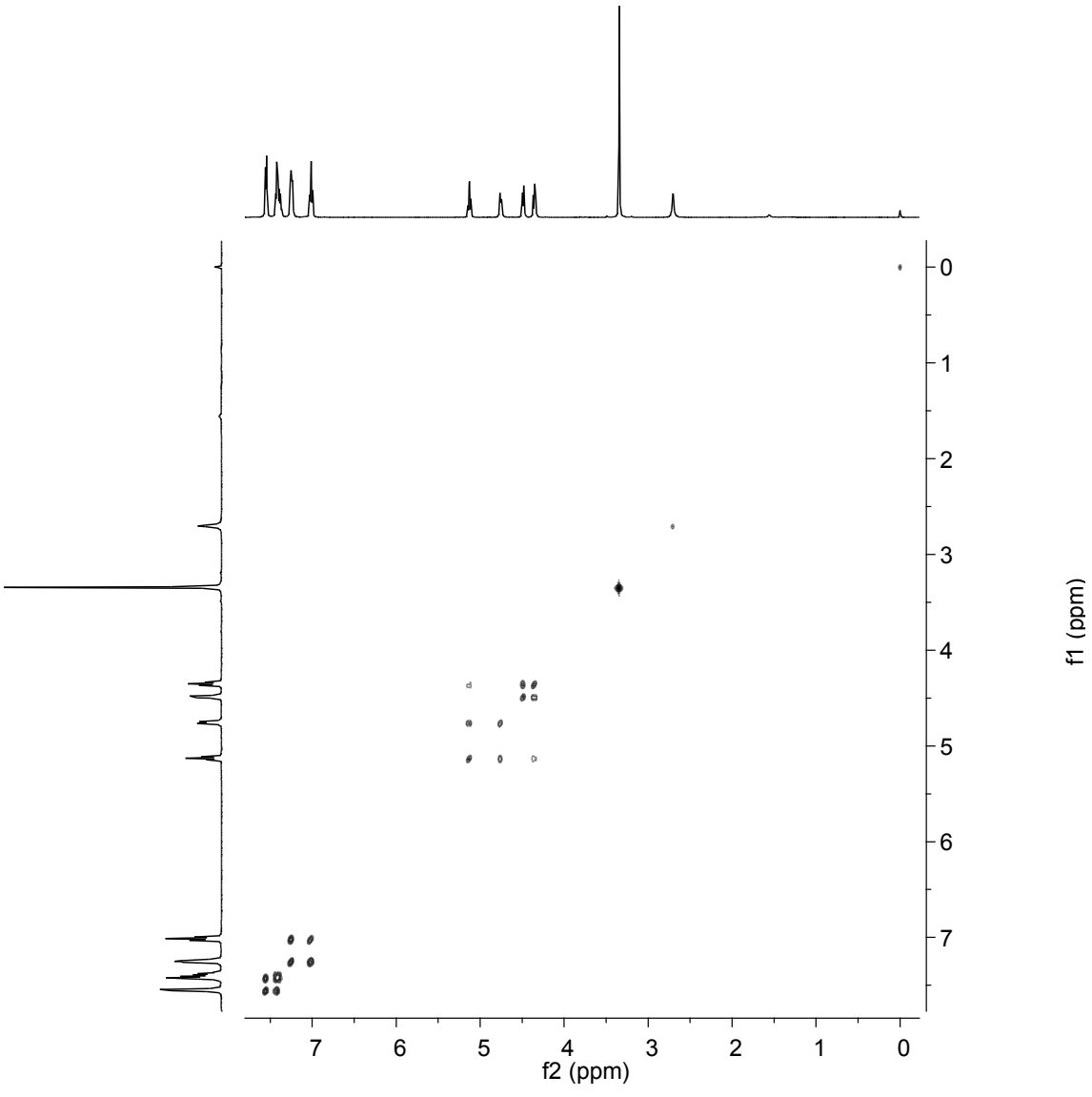
^{13}C-NMR ($CDCl_3$)





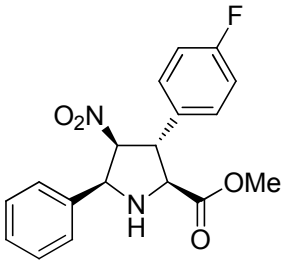
COSY spectrum

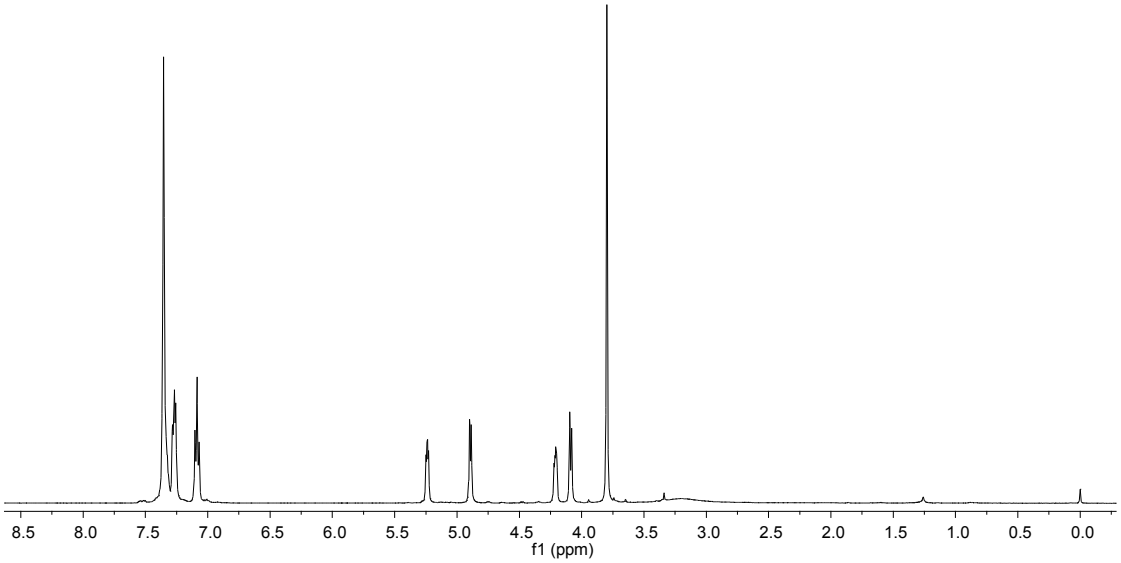
Compound *exo*-L-2b



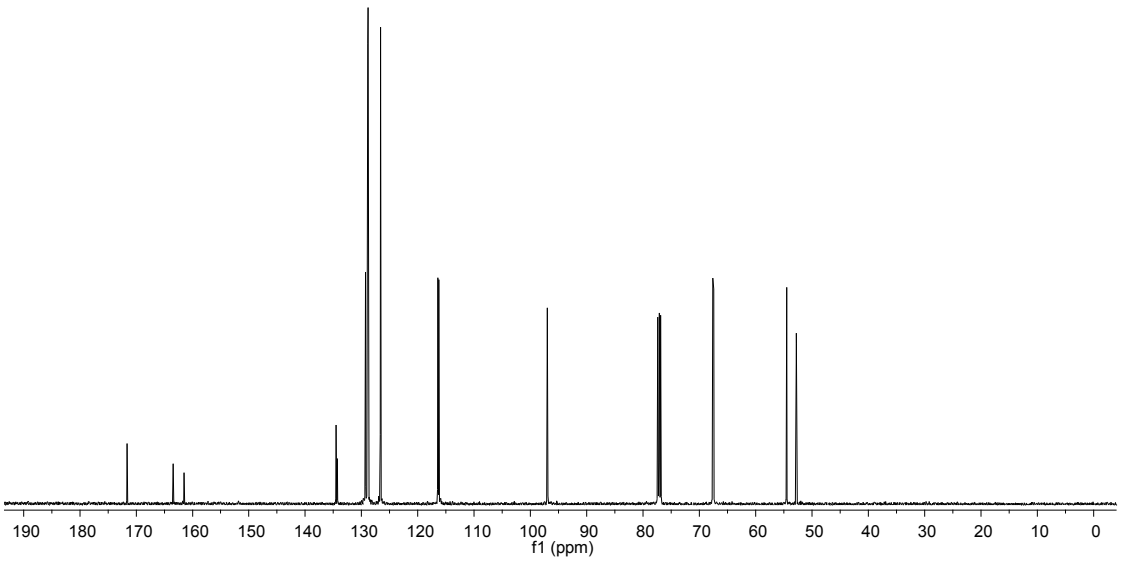
Compound *endo*-L-2b

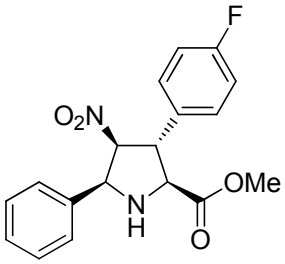
^{1}H-NMR ($CDCl_3$)





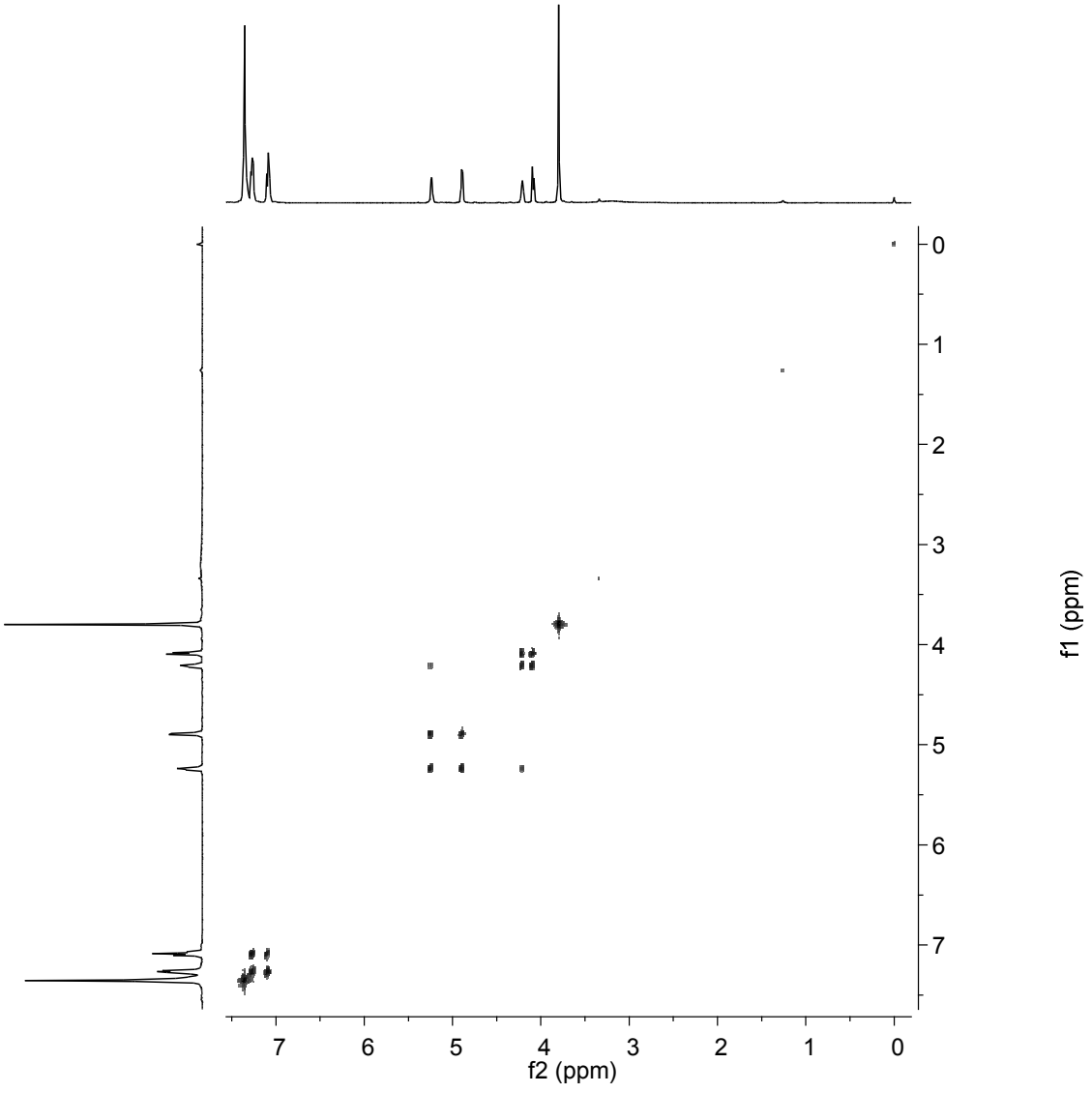
^{13}C-NMR ($CDCl_3$)





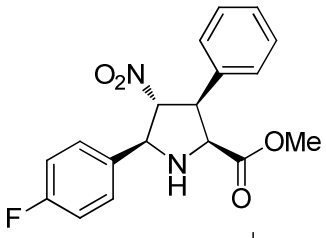
COSY spectrum

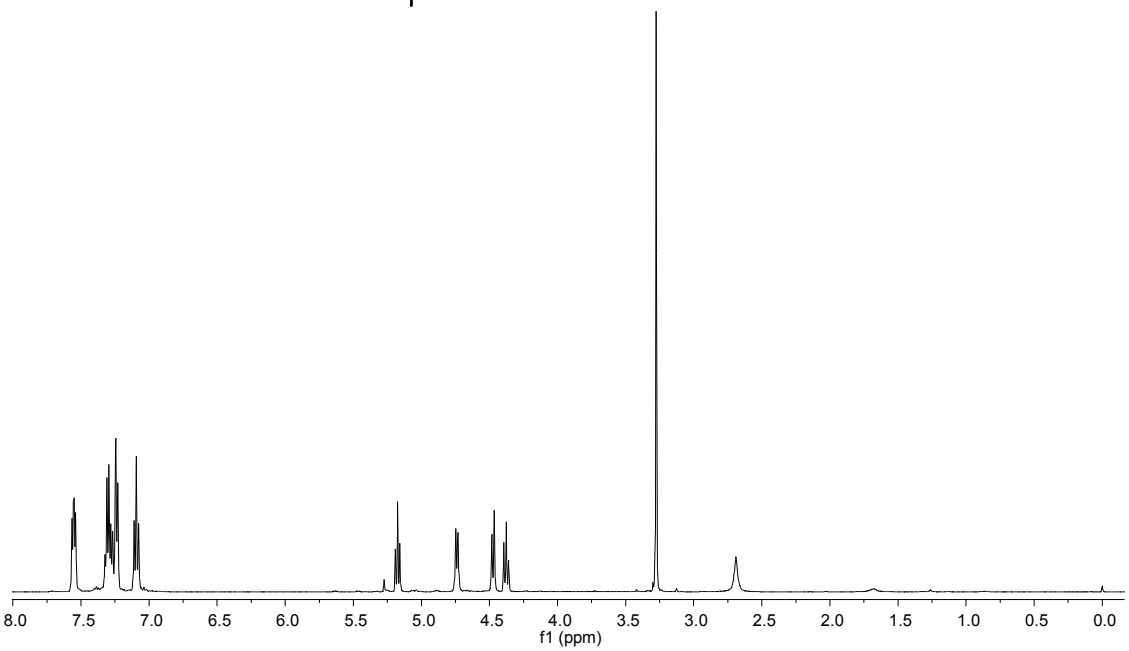
Compound *endo*-L-2b



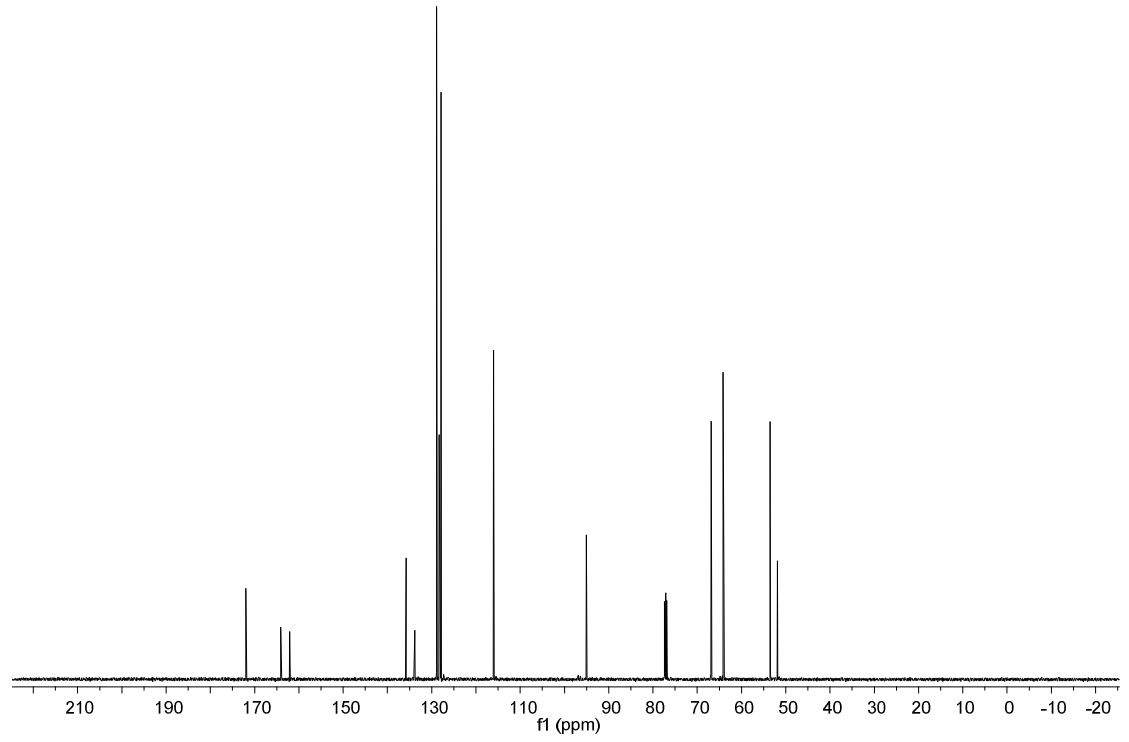
Compound *exo*-L-2d

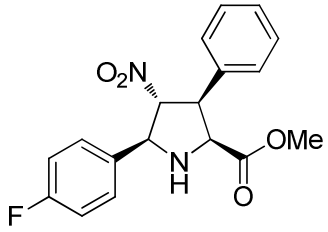
^{1}H-NMR ($CDCl_3$)





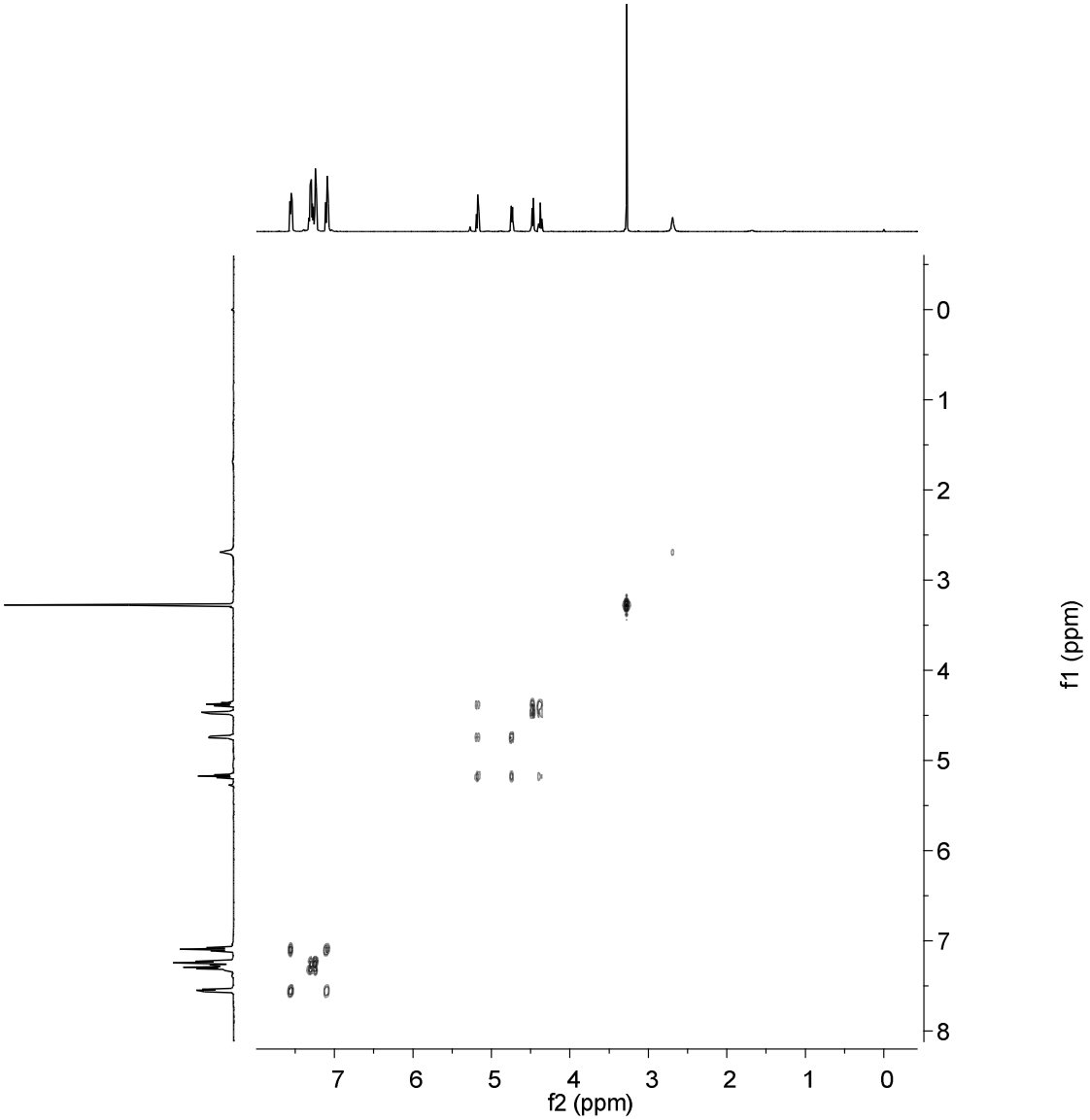
^{13}C-NMR ($CDCl_3$)





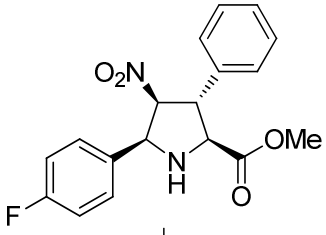
COSY spectrum

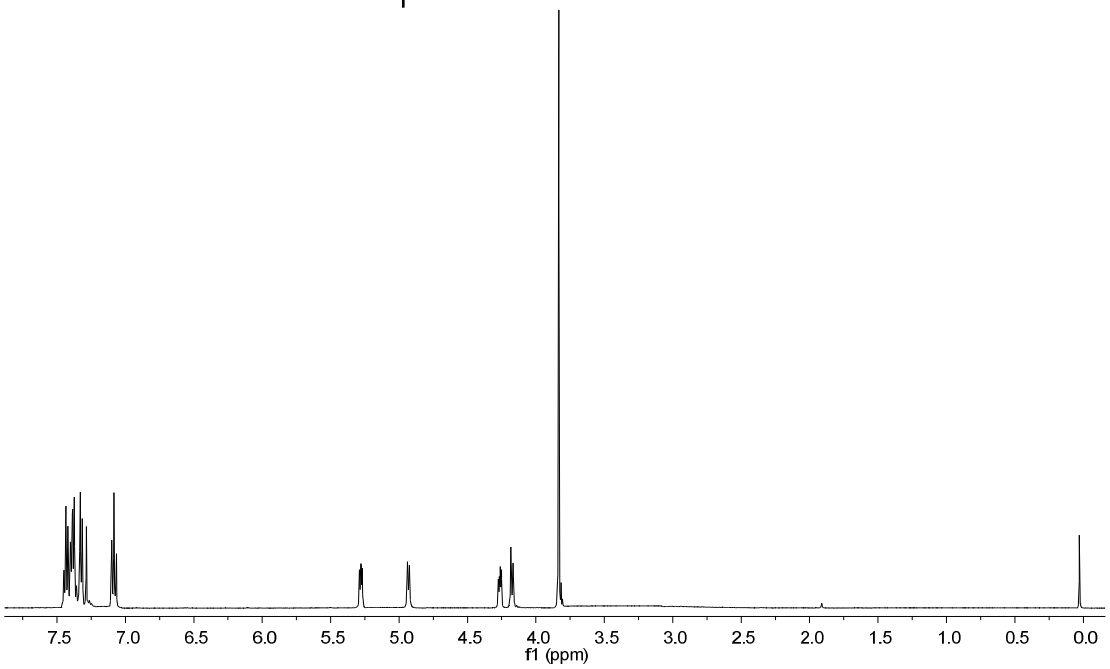
Compound *exo*-L-2d



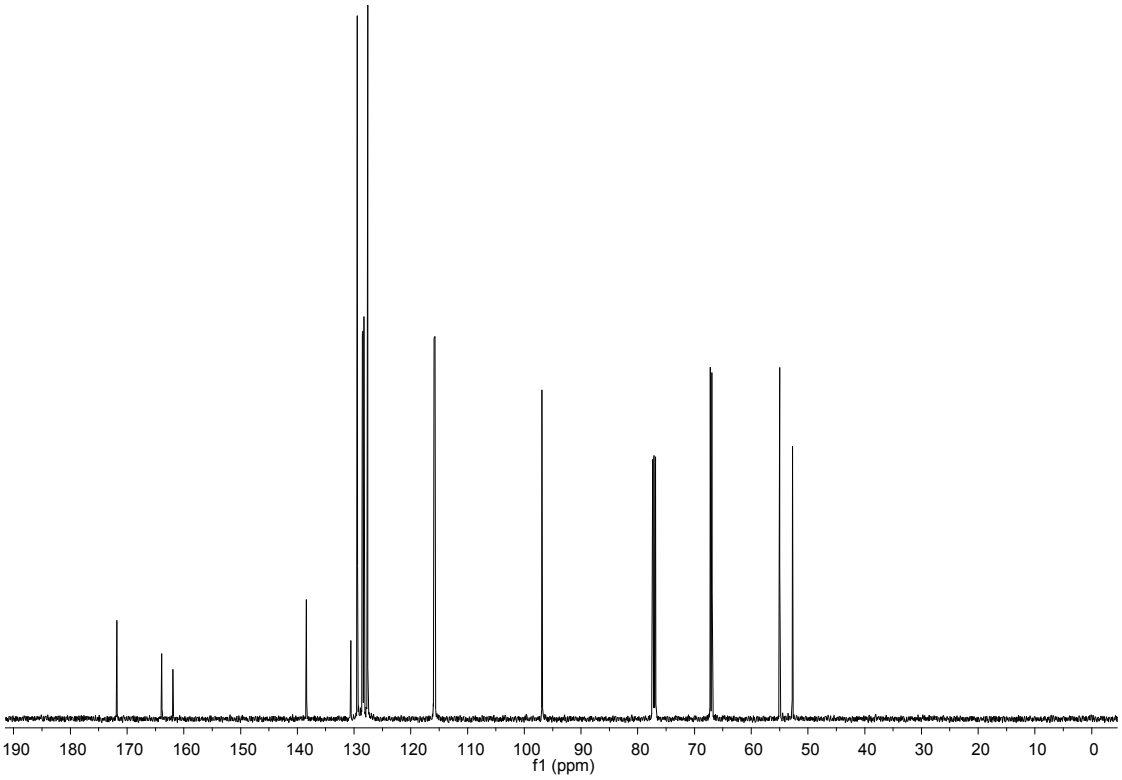
Compound *endo*-L-2d

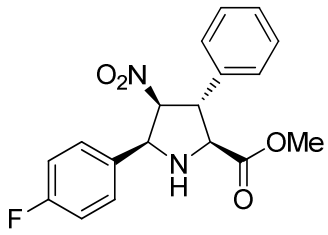
^{1}H-NMR ($CDCl_3$)





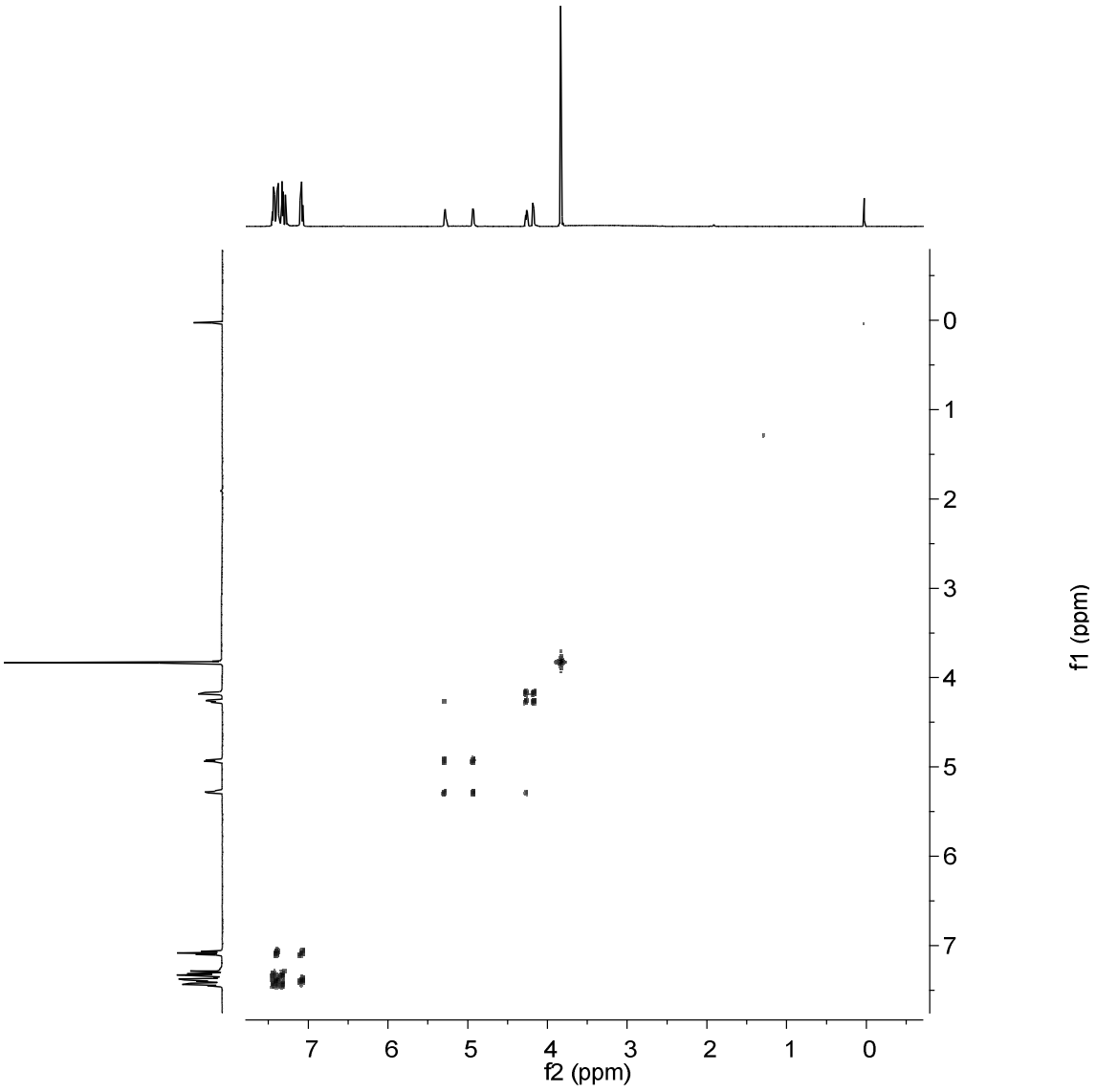
^{13}C-NMR ($CDCl_3$)





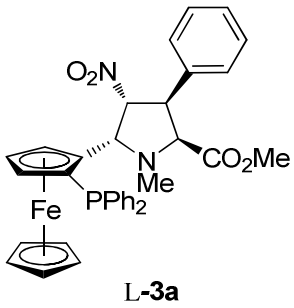
COSY spectrum

Compound *endo*-L-2d

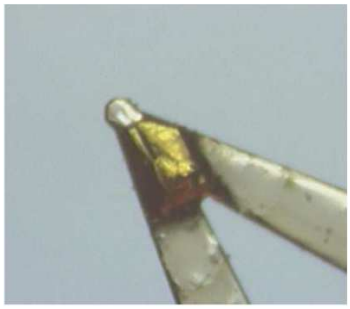


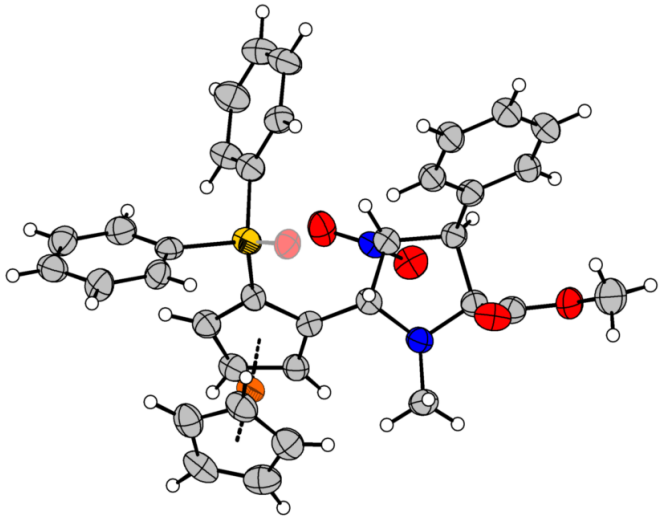
Supplementary Data: Ortep diagrams of compounds L-3a and D-3b

ORTEP diagram of compound L-**3a**



L-**3a**





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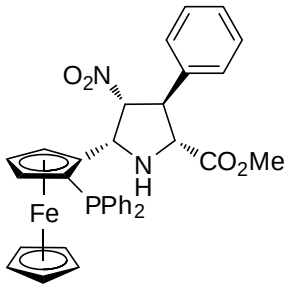
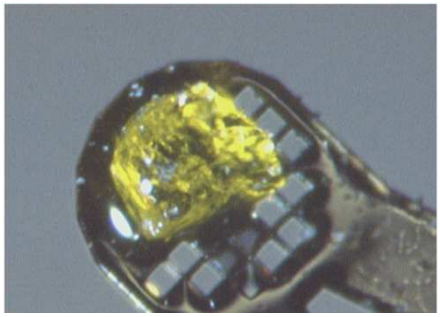
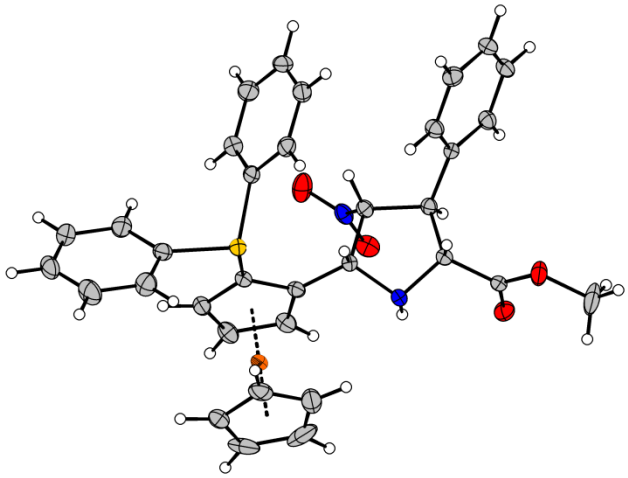
The crystallization of compound L-**3a** was carried out heating in hexane. Due to that crystallization process the phosphine moiety was oxidized partially due to the heat and air effects. We also demonstrate that fact by heating a pure sample of L-**3a,** the phosphine group was oxidized to phosphine oxide and we obtain an approximately equimolar mixture of phosphine and phosphine oxide.

ORTEP diagram of compound D-**3b**



D-**3b**





CCDC 8300112

Supplementary Data: Total electronic and thermal free energies, number of imaginary frequencies and Cartesian coordinates of all the stationary points calculated.

Supplementary Table S1. Total electronic energies of single points[a] (E, in a.u.), thermal corrections to Gibbs free energies[b] (TCGE, in a.u.) and number of imaginary frequencies[c] (NIMAG) of all stationary points discussed in the main text and in the Section 2 of the supporting information.

Structure	E	TCGE	NIMAG (ν)
Nitrostyrene **5a**	-513.829907	0.101455	0
Ylide I L-**3a**	-2976.398711	0.650888	0
Ylide I minor L-**3a**	-2976.382270	0.649863	0
Ylide I minor' L-**3a**	-2976.383050	0.644904	0
Ylide I D-**3b**	-3015.650748	0.675539	0
Ylide I minor D-**3b**	-3015.649219	0.674755	0
Ylide I minor' D **-3b**	-3015.645892	0.679174	0
endo-**TS1a**	-3529.493960	0.799232	1 (-286.67)
endo-minor-**TS1a**	-3529.494215	0.803151	1 (-241.45)
exo-**TS1a**	-3529.493711	0.800875	1 (-307.84)
exo-minor-**TS1a**	-3529.486209	0.801661	1 (-292.22)
exo-**TS2a**	-3490.237331	0.775766	1 (-307.81)
exo-minor-**TS2a**	-3490.229424	0.776899	1 (-305.11)
endo-**TS2a**	-3490.235307	0.775679	1 (-308.16)
endo-minor-**TS2a**	-3490.225632	0.776780	1 (-308.05)

[a]Computed at the M06/6-31++G**&LANL2DZ//ONIOM(B3LYP/6-31G*& LANL2DZ:PM6) and M06/6-31++G** (for **5a)** levels of theory. [b]Computed at 298 K at ONIOM(B3LYP/6-31G*& LANL2DZ:PM6) level of theory. [c]If NIMAG=1, the imaginary frequency ν (in parentheses) is given in cm^{-1}.

Supplementary Table S2. Total electronic energies[a] (E, in a.u.), thermal corrections to Gibbs free energies[b] (TCGE, in a.u.) and number of imaginary frequencies[c] (NIMAG) of all stationary points discussed in the main text for the reaction of cyclohexanone and **10e** catalysed by L-**Pro** and *exo*-L-**2a**.

Structure	E	TCGE	NIMAG(ν)
10e	-841.388289	0.032021	0
L-**Pro-imine**(*Re*)	-634.222172	0.418312	0
L-**Pro-imine**(*Si*)	-634.225382	0.233607	0
exo-L-**2a-imine**(*Re*)	-1340.029643	0.418312	0
exo-L-**2a-imine**(*Si*)	-1340.028956	0.416710	0
anti-**TS3e**	- 1475.620065	0.288714	1 (-323.641)
anti-minor**TS3e**	-1475.611695	0.289245	1 (-247.336)
syn-**TS3e**	-1475.608260	0.288398	1 (-632.755)
syn-minor-**TS3e**	-1475.607682	0.287107	1 (-614.866)
anti-**TS4e**	-2181.4564659	0.477069	1 (-257.508)
anti-minor**TS4e**	-2181.451642	0.476490	1 (-50.676)
syn-**TS4e**	-2181.452659	0.475531	1 (-104.770)
syn-minor-**TS4e**	-2181.446390	0.477330	1 (-184.680)

[a]Computed at M06/6-31++G**//B3LYP/6-31G* level of theory.[b]Computed at 298 K at B3LYP/6-31G* level of theory. [c]If NIMAG=1, the imaginary frequency ν (in parentheses) is given in cm^{-1}.

Cartesian coordinates of all the computed stationary points.

Nitrostyrene **5a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.110562	1.075576	0.000158
2	6	0	-1.720845	1.276671	0.000123
3	6	0	-0.827120	0.175446	-0.000076
4	6	0	-1.365458	-1.138723	-0.000175
5	6	0	-2.752656	-1.338021	-0.000115
6	6	0	-3.630740	-0.232756	0.000043
7	1	0	-3.782604	1.929546	0.000292
8	1	0	-1.319661	2.288210	0.000221
9	1	0	-0.704100	-2.001283	-0.000273
10	1	0	-3.154361	-2.347972	-0.000182
11	1	0	-4.706026	-0.392332	0.000096
12	6	0	0.610914	0.453136	-0.000114
13	6	0	1.610648	-0.460704	0.000106
14	1	0	0.913321	1.500080	-0.000385
15	1	0	1.515855	-1.537898	0.000347
16	7	0	3.000735	-0.035938	0.000018
17	8	0	3.881201	-0.971526	0.000245
18	8	0	3.287217	1.215210	-0.000238

Ylide I-L-3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.113024	0.385384	-1.232516
2	6	0	4.090462	-1.014429	-1.306420
3	6	0	5.223109	-1.698894	-1.777650
4	6	0	6.361565	-0.988810	-2.166793
5	6	0	6.381223	0.407551	-2.087064
6	6	0	5.256594	1.091428	-1.616762
7	6	0	2.877413	-1.814866	-0.911540
8	6	0	2.142400	-1.247747	0.385991
9	7	0	0.739370	-0.933969	-0.005996
10	6	0	0.729423	-0.709296	-1.481755
11	6	0	1.772535	-1.757115	-2.051920
12	6	0	-0.657861	-0.655059	-2.080571
13	6	0	-1.764136	0.188547	-1.622580
14	6	0	-2.879976	-0.024987	-2.511183
15	6	0	-2.485232	-0.974135	-3.514944
16	6	0	-1.124411	-1.352296	-3.258540
17	15	0	-1.723461	1.356928	-0.176136
18	29	0	-0.135094	0.612893	1.258895
19	7	0	1.169098	1.013805	2.807645
20	6	0	2.282567	1.735037	2.818877
21	6	0	2.780683	2.570174	1.728183
22	6	0	2.033315	2.897098	0.562338
23	6	0	2.577136	3.710321	-0.443673
24	6	0	3.885370	4.225196	-0.324954
25	6	0	4.637384	3.920667	0.828812
26	6	0	4.093505	3.110932	1.837652
27	26	0	-2.325747	-1.833336	-1.567509
28	6	0	-3.874245	-2.390091	-0.238590
29	6	0	-3.853689	-3.278469	-1.376960
30	6	0	-2.567458	-3.932779	-1.403986
31	6	0	-1.803554	-3.458904	-0.276315
32	6	0	-2.608790	-2.504599	0.446591
33	6	0	2.119633	-2.258437	1.526153
34	8	0	3.282915	-2.227895	2.245627
35	6	0	3.363271	-3.122292	3.421234
36	7	0	1.205306	-3.135995	-2.298779
37	8	0	0.991018	-3.421311	-3.466896
38	6	0	-3.483857	1.386303	0.391476
39	6	0	-3.811409	0.683418	1.553070
40	6	0	-5.140777	0.671193	1.998548
41	6	0	-6.125492	1.363499	1.290448
42	6	0	-5.786478	2.074926	0.133262
43	6	0	-4.463314	2.087933	-0.318937
44	6	0	-1.593280	3.034177	-0.974800
45	6	0	-1.443875	3.186426	-2.353402
46	6	0	-1.334918	4.471976	-2.899738

47	6	0	-1.374271	5.594166	-2.067840
48	6	0	-1.520867	5.433955	-0.685756
49	6	0	-1.627936	4.152058	-0.135057
50	8	0	-1.143263	-0.627749	2.760703
51	6	0	-0.383705	-0.524066	3.808514
52	6	0	0.776991	0.267558	3.902478
53	8	0	-0.687601	-1.242548	4.963980
54	6	0	-1.849884	-2.132287	4.900875
55	8	0	1.172782	-3.025245	1.770242
56	8	0	1.052352	-3.886650	-1.356525
57	1	0	1.212050	0.268674	-1.652906
58	1	0	3.173895	-2.866654	-0.725635
59	1	0	2.201352	-1.385766	-3.012636
60	1	0	2.647056	-0.347404	0.750384
61	1	0	-3.850783	0.445179	-2.416888
62	1	0	-3.106479	-1.354181	-4.314351
63	1	0	-0.552640	-2.044721	-3.868054
64	1	0	-0.809508	-3.792384	0.002309
65	1	0	-2.303771	-1.967495	1.335521
66	1	0	-4.693811	-1.744459	0.050991
67	1	0	-4.651051	-3.413420	-2.095163
68	1	0	-2.234605	-4.659053	-2.135107
69	1	0	0.123190	-1.719596	0.243206
70	1	0	-2.765770	-1.563728	4.705855
71	1	0	-1.894286	-2.606059	5.884562
72	1	0	-1.719561	-2.884863	4.114902
73	1	0	1.342733	0.294117	4.830702
74	1	0	2.907799	1.711532	3.719247
75	1	0	4.684392	2.885102	2.724482
76	1	0	5.643685	4.319028	0.942394
77	1	0	4.299851	4.863558	-1.101585
78	1	0	1.972552	3.961079	-1.314875
79	1	0	1.008323	2.542311	0.473129
80	1	0	4.364865	-2.963257	3.822099
81	1	0	2.594152	-2.838252	4.145416
82	1	0	3.218287	-4.163262	3.114828
83	1	0	5.223176	-2.786398	-1.837347
84	1	0	7.237055	-1.525854	-2.529531
85	1	0	7.271065	0.958940	-2.385651
86	1	0	5.266262	2.180148	-1.537411
87	1	0	3.249883	0.940112	-0.856656
88	1	0	-4.222988	2.659959	-1.218111
89	1	0	-6.553274	2.620513	-0.412926
90	1	0	-7.157246	1.354469	1.639882
91	1	0	-5.400862	0.123274	2.902914
92	1	0	-3.055292	0.137102	2.143861
93	1	0	-1.737558	4.058801	0.948653
94	1	0	-1.546843	6.307542	-0.035615
95	1	0	-1.288882	6.593126	-2.493920
96	1	0	-1.219208	4.595095	-3.975228
97	1	0	-1.409301	2.328144	-3.029102

Ylide I minor L-**3a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.355352	3.709656	1.180787
2	7	0	-0.594613	3.353756	0.078719
3	6	0	-0.156303	4.264619	-0.778099
4	6	0	0.597237	3.997922	-2.000297
5	6	0	0.728293	2.708350	-2.584333
6	6	0	1.449088	2.522198	-3.774292
7	6	0	2.063643	3.615355	-4.419647
8	6	0	1.934820	4.903992	-3.860142
9	6	0	1.209030	5.092357	-2.673963
10	6	0	-1.783898	2.711969	2.067851
11	8	0	-2.516113	3.192308	3.159122
12	6	0	-2.965381	2.222846	4.155695
13	8	0	-1.559492	1.433958	1.944142
14	29	0	-0.047263	1.386075	0.269934
15	7	0	-1.071209	-0.354736	-0.538495
16	6	0	-1.265910	-1.352186	0.558047
17	6	0	-2.515549	-2.211926	0.100005
18	6	0	-3.426757	-1.153464	-0.652773
19	6	0	-2.427204	0.033229	-1.024351
20	6	0	-0.010370	-2.087314	0.959262
21	6	0	1.321483	-1.525221	1.188953
22	6	0	2.172465	-2.593170	1.657603
23	6	0	1.395773	-3.799255	1.729348
24	6	0	0.060326	-3.488823	1.305283
25	15	0	1.807853	0.268683	1.016194

26	26	0	1.423597	-3.043663	-0.262306
27	6	0	3.091046	-3.364044	-1.524211
28	6	0	2.285757	-4.561107	-1.454212
29	6	0	0.970732	-4.240178	-1.952123
30	6	0	0.964376	-2.850605	-2.342429
31	6	0	2.274398	-2.309575	-2.073321
32	1	0	-1.616690	-0.773592	1.426365
33	1	0	-3.829461	-1.593129	-1.587304
34	1	0	-3.037803	-2.632780	0.991164
35	1	0	-2.746804	0.957569	-0.532061
36	1	0	3.220058	-2.487309	1.911201
37	1	0	1.754662	-4.774569	2.028242
38	1	0	-0.755824	-4.201926	1.255352
39	1	0	0.131944	-2.327537	-2.799077
40	1	0	2.598181	-1.292894	-2.255319
41	1	0	4.124082	-3.268921	-1.218515
42	1	0	2.605975	-5.523858	-1.080276
43	1	0	0.131226	-4.921356	-2.033758
44	1	0	-0.529275	-0.764549	-1.310173
45	1	0	-3.879542	1.710877	3.814616
46	1	0	-3.181502	2.811291	5.051489
47	1	0	-2.188470	1.477993	4.357008
48	1	0	-1.611014	4.749310	1.369809
49	1	0	-0.368424	5.319841	-0.569090
50	1	0	1.114038	6.092016	-2.251687
51	1	0	2.397234	5.758239	-4.351115
52	1	0	2.618169	3.469359	-5.343927
53	1	0	1.512821	1.526526	-4.209623
54	1	0	0.234410	1.858398	-2.122221
55	6	0	2.430894	0.673311	2.718619
56	6	0	3.421017	0.211969	0.092712
57	7	0	-2.182330	-3.356487	-0.829244
58	6	0	-4.563735	-0.701165	0.222797
59	6	0	-2.361815	0.282976	-2.523570
60	6	0	3.437682	1.631226	2.870549
61	6	0	3.885959	1.965897	4.153429
62	6	0	3.325106	1.349370	5.276615
63	6	0	2.311711	0.399815	5.117948
64	6	0	1.857744	0.062925	3.836576
65	1	0	3.892264	2.132343	2.012507
66	1	0	4.669099	2.712098	4.276240
67	1	0	3.674194	1.613171	6.273957
68	1	0	1.868783	-0.075259	5.991386
69	1	0	1.056093	-0.674232	3.742351
70	6	0	3.533605	0.932005	-1.098345
71	6	0	4.739689	0.909958	-1.811585
72	6	0	5.824844	0.172139	-1.332089
73	6	0	5.709478	-0.539801	-0.133202
74	6	0	4.507955	-0.517632	0.583689
75	1	0	2.708649	1.529058	-1.502345
76	1	0	4.827549	1.474027	-2.739795
77	1	0	6.761221	0.153943	-1.888669
78	1	0	6.556929	-1.108722	0.244643
79	1	0	4.451677	-1.070217	1.525592
80	8	0	-2.184935	-4.472271	-0.335594
81	8	0	-1.999964	-3.116668	-2.008490
82	6	0	-5.875648	-1.069453	-0.116887
83	6	0	-6.945769	-0.672400	0.689219
84	6	0	-6.715947	0.094537	1.836488
85	6	0	-5.410494	0.462726	2.172892
86	6	0	-4.336283	0.065911	1.373334
87	1	0	-6.067745	-1.660124	-1.011266
88	1	0	-7.961489	-0.958351	0.420356
89	1	0	-7.551189	0.407231	2.460502
90	1	0	-5.215603	1.074418	3.060486
91	1	0	-3.314101	0.379309	1.645769
92	8	0	-3.486183	0.912390	-2.978888
93	8	0	-1.408245	-0.044672	-3.254051
94	6	0	-3.543529	1.230765	-4.423157
95	1	0	-4.512895	1.710369	-4.561160
96	1	0	-2.724476	1.906789	-4.684532
97	1	0	-3.466347	0.311639	-5.012948

Ylide I minor' L-**3a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.193197	3.719481	-1.010483
2	6	0	-1.683517	2.502110	-1.477568
3	6	0	-0.921784	2.452619	-2.644344

4	6	0	-0.664544	3.634396	-3.353242
5	6	0	-1.171756	4.852084	-2.895497
6	6	0	-1.937767	4.894143	-1.724031
7	15	0	-2.028091	0.979865	-0.483107
8	6	0	-3.874485	0.936534	-0.519118
9	6	0	-4.559572	0.451247	0.596977
10	6	0	-5.960556	0.395039	0.574858
11	6	0	-6.664047	0.827412	-0.551249
12	6	0	-5.970632	1.322043	-1.662460
13	6	0	-4.573792	1.377352	-1.648408
14	6	0	-1.550571	-0.441558	-1.578678
15	6	0	-0.291794	-1.177866	-1.545940
16	6	0	-0.381938	-2.213687	-2.552682
17	6	0	-1.652632	-2.104399	-3.214590
18	6	0	-2.375137	-1.011769	-2.619655
19	6	0	0.897734	-0.914512	-0.668018
20	7	0	1.443801	-2.119468	-0.041695
21	6	0	2.862203	-1.912327	0.246655
22	6	0	3.419431	-1.079140	-0.985962
23	6	0	2.171475	-0.213354	-1.423416
24	6	0	4.631562	-0.256664	-0.654650
25	6	0	4.592650	0.734806	0.336898
26	6	0	5.741666	1.473807	0.630944
27	6	0	6.932135	1.232746	-0.061849
28	6	0	6.971796	0.248145	-1.053948
29	6	0	5.826634	-0.495516	-1.351158
30	7	0	2.012781	-0.191671	-2.915845
31	26	0	-1.939325	-2.445031	-1.133778
32	6	0	-2.770402	-2.630318	0.822588
33	6	0	-3.741094	-3.011626	-0.175947
34	6	0	-3.203183	-4.122790	-0.924539
35	6	0	-1.895967	-4.425560	-0.390154
36	6	0	-1.631454	-3.503587	0.687669
37	29	0	-1.164725	0.935975	1.595124
38	8	0	-2.381814	-0.209673	2.943583
39	6	0	-1.752460	-0.119101	4.083231
40	8	0	-2.261049	-0.754738	5.208592
41	6	0	-3.498302	-1.522337	5.041052
42	7	0	0.005693	1.266794	3.219681
43	6	0	-0.558844	0.591370	4.289275
44	6	0	1.132595	1.952780	3.354588
45	6	0	1.812261	2.749647	2.335325
46	6	0	1.304853	3.005442	1.032140
47	6	0	2.018330	3.793610	0.117529
48	6	0	3.261467	4.359415	0.472749
49	6	0	3.776169	4.126003	1.763699
50	6	0	3.064763	3.332481	2.677660
51	1	0	0.614730	-0.195646	0.118807
52	1	0	3.646806	-1.806700	-1.796875
53	1	0	2.261627	0.838921	-1.065964
54	1	0	-3.368258	-0.675757	-2.891723
55	1	0	-2.009028	-2.738402	-4.014928
56	1	0	0.399337	-2.921616	-2.801571
57	1	0	-0.723546	-3.445355	1.269279
58	1	0	-2.856218	-1.826115	1.542051
59	1	0	-4.701092	-2.538650	-0.341422
60	1	0	-3.686389	-4.631242	-1.748186
61	1	0	-1.232760	-5.204944	-0.740105
62	1	0	-4.306765	-0.880968	4.674230
63	1	0	-3.728475	-1.901864	6.039079
64	1	0	-3.349770	-2.350705	4.339377
65	1	0	-0.100008	0.619271	5.273102
66	1	0	1.614618	1.947684	4.338396
67	1	0	3.470267	3.163536	3.673994
68	1	0	4.725450	4.568238	2.057986
69	1	0	3.808874	4.975162	-0.237181
70	1	0	1.598620	3.980950	-0.871008
71	1	0	0.331370	2.609335	0.749597
72	1	0	5.867514	-1.259786	-2.126375
73	1	0	7.896291	0.059354	-1.597558
74	1	0	7.825040	1.810345	0.169892
75	1	0	5.702980	2.242374	1.403404
76	1	0	3.671024	0.941165	0.884654
77	1	0	-4.056975	1.777725	-2.524678
78	1	0	-6.519932	1.666055	-2.536902
79	1	0	-7.752699	0.784178	-0.565079
80	1	0	-6.497945	0.016377	1.443161
81	1	0	-4.040323	0.113648	1.509375
82	1	0	-2.793026	3.783728	-0.099407
83	1	0	-2.331601	5.844062	-1.365701
84	1	0	-0.970927	5.770059	-3.446999
85	1	0	-0.062497	3.595050	-4.261257
86	1	0	-0.504129	1.515082	-3.032393
87	8	0	2.360430	-1.166734	-3.558274
88	8	0	1.531472	0.822358	-3.396228
89	1	0	1.236590	-3.005085	-0.503766
90	1	0	3.001484	-1.336393	1.171474

91	6	0	3.568084	-3.246528	0.396194
92	8	0	3.178126	-4.309842	-0.119969
93	8	0	4.706905	-3.141801	1.151151
94	6	0	5.512019	-4.368850	1.325940
95	1	0	6.368529	-4.054349	1.923642
96	1	0	4.923884	-5.130920	1.846174
97	1	0	5.829252	-4.753716	0.351534

Ylide I D-3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.702959	3.846316	-0.499596
2	6	0	-0.953797	2.696308	-1.257133
3	6	0	-0.757767	2.701087	-2.637896
4	6	0	-0.304906	3.868124	-3.269286
5	6	0	-0.055044	5.019680	-2.520110
6	6	0	-0.254758	5.008780	-1.134609
7	15	0	-1.589516	1.205856	-0.358550
8	6	0	-3.369963	1.700627	-0.183603
9	6	0	-4.051165	1.379958	0.992540
10	6	0	-5.395637	1.750375	1.136745
11	6	0	-6.048124	2.442321	0.114138
12	6	0	-5.356854	2.770938	-1.057596
13	6	0	-4.016061	2.402546	-1.207177
14	6	0	-1.648269	-0.179750	-1.598843
15	6	0	-0.710534	-1.295760	-1.717569
16	6	0	-1.189900	-2.141147	-2.780402
17	6	0	-2.372308	-1.552381	-3.346312
18	6	0	-2.651088	-0.335154	-2.630626
19	6	0	0.607991	-1.445940	-1.002002
20	7	0	1.131457	-2.837192	-0.946201
21	6	0	2.589879	-2.783207	-0.715196
22	6	0	3.035041	-1.661346	-1.702498
23	6	0	1.811218	-0.656635	-1.711684
24	6	0	4.360224	-1.019993	-1.390565
25	6	0	4.509954	-0.087828	-0.354191
26	6	0	5.757393	0.490857	-0.105463
27	6	0	6.864121	0.140947	-0.884330
28	6	0	6.720064	-0.791767	-1.916691
29	6	0	5.473893	-1.369450	-2.171838
30	6	0	2.944869	-2.481853	0.749571
31	8	0	3.780973	-3.434022	1.282738
32	6	0	4.204034	-3.240474	2.687156
33	6	0	0.399836	-3.829505	-0.148627
34	7	0	1.487436	-0.246233	-3.128009
35	26	0	-2.727385	-1.939159	-1.289323
36	6	0	-3.674274	-1.906067	0.633560
37	6	0	-4.656248	-1.851490	-0.421113
38	6	0	-4.522175	-3.045914	-1.221906
39	6	0	-3.450422	-3.835946	-0.664040
40	6	0	-2.933263	-3.129751	0.483006
41	29	0	-0.648133	0.732373	1.636739
42	8	0	-2.054159	-0.319796	2.885112
43	6	0	-1.441726	-0.398722	4.036204
44	8	0	-2.061989	-1.039039	5.106532
45	6	0	-3.402783	-1.579327	4.873214
46	7	0	0.511799	0.784433	3.299895
47	6	0	-0.168276	0.118312	4.309413
48	6	0	1.715769	1.293038	3.505988
49	6	0	2.537725	2.046087	2.562396
50	6	0	2.140350	2.409268	1.248007
51	6	0	2.986229	3.153651	0.413578
52	6	0	4.262486	3.558255	0.859949
53	6	0	4.675375	3.206882	2.160815
54	6	0	3.826532	2.464210	2.996577
55	8	0	2.508292	-1.515504	1.404712
56	1	0	0.523228	-1.017592	0.016034
57	1	0	3.080307	-2.156529	-2.696297
58	1	0	2.028540	0.264915	-1.125623
59	1	0	-3.479878	0.338382	-2.811188
60	1	0	-2.955497	-1.953158	-4.164219
61	1	0	-0.695067	-3.043677	-3.111146
62	1	0	-2.135001	-3.452279	1.132455
63	1	0	-3.487584	-1.172405	1.406439
64	1	0	-5.362048	-1.047012	-0.588553
65	1	0	-5.110445	-3.299007	-2.093728
66	1	0	-3.111013	-4.792139	-1.037995
67	1	0	-4.105643	-0.779717	4.613613
68	1	0	-3.685601	-2.045574	5.819914
69	1	0	-3.392448	-2.320632	4.066332

70	1	0	0.268056	0.009058	5.297971
71	1	0	2.162122	1.152096	4.497095
72	1	0	4.153955	2.205276	4.002585
73	1	0	5.652357	3.518654	2.524325
74	1	0	4.913710	4.139792	0.211249
75	1	0	2.648107	3.428142	-0.586066
76	1	0	1.154013	2.122174	0.889149
77	1	0	5.371829	-2.090325	-2.982034
78	1	0	7.579646	-1.067341	-2.525542
79	1	0	7.834601	0.593235	-0.689170
80	1	0	5.857866	1.221117	0.699532
81	1	0	3.657328	0.188623	0.277335
82	1	0	-3.497592	2.688463	-2.125843
83	1	0	-5.861635	3.318652	-1.851084
84	1	0	-7.092098	2.731109	0.229336
85	1	0	-5.927821	1.499875	2.053209
86	1	0	-3.570154	0.839911	1.826471
87	1	0	-0.846879	3.872950	0.583625
88	1	0	-0.056693	5.905021	-0.548723
89	1	0	0.298956	5.925260	-3.011382
90	1	0	-0.137431	3.866680	-4.345625
91	1	0	-0.926144	1.808811	-3.252235
92	1	0	3.048445	-3.743978	-0.973679
93	1	0	0.924963	-4.790999	-0.209733
94	1	0	0.304266	-3.549328	0.918585
95	1	0	-0.603203	-3.960137	-0.559450
96	1	0	3.329298	-3.223973	3.344277
97	1	0	4.848709	-4.093381	2.904164
98	1	0	4.749844	-2.296467	2.784393
99	8	0	1.674078	-1.037192	-4.033243
100	8	0	1.062482	0.888922	-3.273986

Ylide I minor D-**3b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.066901	0.818628	3.839069
2	6	0	1.508760	-0.193570	3.048867
3	6	0	0.949797	-1.326009	3.641043
4	6	0	0.957629	-1.453716	5.036927
5	6	0	1.519354	-0.451648	5.830612
6	6	0	2.073812	0.685371	5.230748
7	15	0	1.498158	0.032688	1.209898
8	6	0	3.272863	0.519439	0.967228
9	6	0	3.568390	1.684265	0.254985
10	6	0	4.903797	2.070341	0.078949
11	6	0	5.935134	1.296486	0.617241
12	6	0	5.633269	0.137292	1.339734
13	6	0	4.300768	-0.250887	1.520139
14	6	0	1.385738	-1.701700	0.532556
15	6	0	0.355532	-2.226053	-0.359879
16	6	0	0.662667	-3.612504	-0.596638
17	6	0	1.822508	-3.970186	0.174004
18	6	0	2.265982	-2.796534	0.879894
19	6	0	-0.897009	-1.514287	-0.799384
20	7	0	-1.490727	-2.003644	-2.071477
21	6	0	-2.894382	-1.566916	-2.120732
22	6	0	-3.396597	-1.890829	-0.673441
23	6	0	-2.115732	-1.668591	0.234383
24	6	0	-4.612693	-1.111352	-0.253095
25	6	0	-4.528103	0.234996	0.125753
26	6	0	-5.681028	0.938648	0.483979
27	6	0	-6.925525	0.302313	0.468259
28	6	0	-7.013790	-1.043403	0.096024
29	6	0	-5.863352	-1.750169	-0.263203
30	6	0	-3.058309	-0.083393	-2.501228
31	8	0	-4.202700	0.130652	-3.229841
32	6	0	-4.516839	1.531704	-3.586691
33	6	0	-0.732804	-1.850989	-3.318096
34	7	0	-1.929694	-2.841912	1.167581
35	26	0	2.358672	-2.430550	-1.175598
36	6	0	3.632514	-0.944880	-2.035620
37	6	0	4.407118	-2.074083	-1.586919
38	6	0	3.952128	-3.240109	-2.305776
39	6	0	2.893196	-2.828906	-3.193907
40	6	0	2.698937	-1.407892	-3.028399
41	29	0	-0.089146	1.520674	0.596626
42	8	0	-1.975367	1.360328	1.584352
43	6	0	-2.392260	2.592859	1.681249
44	8	0	-3.505011	2.886336	2.463241
45	6	0	-3.987865	1.824290	3.353624

46	7	0	-0.717588	3.432710	0.212114
47	6	0	-1.811143	3.685600	1.017940
48	6	0	-0.078549	4.375991	-0.460445
49	6	0	1.004025	4.117477	-1.407594
50	6	0	1.155521	2.870249	-2.075277
51	6	0	2.214163	2.664927	-2.975949
52	6	0	3.137603	3.695296	-3.247372
53	6	0	2.980153	4.946673	-2.615852
54	6	0	1.925079	5.155901	-1.714132
55	8	0	-2.258710	0.827670	-2.209491
56	1	0	-0.692108	-0.428310	-0.860884
57	1	0	-3.630774	-2.977205	-0.687686
58	1	0	-2.187425	-0.741765	0.849394
59	1	0	3.110768	-2.733183	1.555196
60	1	0	2.285226	-4.946948	0.214226
61	1	0	0.070863	-4.271367	-1.217079
62	1	0	1.987076	-0.795579	-3.559635
63	1	0	3.740986	0.075142	-1.688721
64	1	0	5.187889	-2.047157	-0.838062
65	1	0	4.329667	-4.246889	-2.190976
66	1	0	2.352491	-3.475000	-3.871095
67	1	0	-4.221611	0.913152	2.792293
68	1	0	-4.884567	2.235805	3.822020
69	1	0	-3.231671	1.588493	4.113325
70	1	0	-2.216864	4.686950	1.131300
71	1	0	-0.372492	5.422335	-0.320951
72	1	0	1.812211	6.124009	-1.227925
73	1	0	3.676894	5.754709	-2.829635
74	1	0	3.950171	3.533270	-3.951996
75	1	0	2.305830	1.711562	-3.493142
76	1	0	0.406202	2.096704	-1.927556
77	1	0	-5.943077	-2.797495	-0.550446
78	1	0	-7.981043	-1.542713	0.085679
79	1	0	-7.823148	0.851361	0.745851
80	1	0	-5.599201	1.986506	0.780127
81	1	0	-3.553775	0.743978	0.153131
82	1	0	4.094893	-1.150167	2.107475
83	1	0	6.435619	-0.460424	1.768383
84	1	0	6.973018	1.597530	0.478435
85	1	0	5.132028	2.978228	-0.479596
86	1	0	2.790595	2.321204	-0.182792
87	1	0	2.503087	1.719254	3.400890
88	1	0	2.505866	1.470163	5.848910
89	1	0	1.522270	-0.550561	6.915202
90	1	0	0.514252	-2.335349	5.498126
91	1	0	0.488519	-2.126078	3.047947
92	1	0	-3.455091	-2.151418	-2.859952
93	1	0	-1.317774	-2.279944	-4.142460
94	1	0	-0.502513	-0.797081	-3.565678
95	1	0	0.205493	-2.404074	-3.245802
96	1	0	-3.727337	1.943513	-4.222548
97	1	0	-5.467323	1.476185	-4.119362
98	1	0	-4.606153	2.135645	-2.678261
99	8	0	-2.343073	-3.937632	0.831848
100	8	0	-1.374969	-2.611535	2.229925

Ylide I minor' D-**3b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.013487	-0.820958	-1.368670
2	6	0	4.702691	-1.503321	-0.183401
3	6	0	5.739113	-2.064309	0.580826
4	6	0	7.066505	-1.944797	0.161322
5	6	0	7.370729	-1.268034	-1.024001
6	6	0	6.341983	-0.705806	-1.785968
7	6	0	3.285992	-1.666888	0.296642
8	6	0	2.616437	-0.355264	0.888638
9	7	0	1.140309	-0.521505	0.629488
10	6	0	1.088757	-1.100440	-0.760509
11	6	0	2.283104	-2.157659	-0.834673
12	6	0	-0.253140	-1.490728	-1.335620
13	6	0	-1.562108	-0.880076	-1.124923
14	6	0	-2.464395	-1.416473	-2.118135
15	6	0	-1.735272	-2.334617	-2.950007
16	6	0	-0.385758	-2.389752	-2.462080
17	15	0	-1.963251	0.505528	0.071035
18	29	0	-0.007733	1.405374	0.865213
19	7	0	0.574660	3.370031	1.092720
20	6	0	0.624789	4.358740	0.208972

21	6	0	0.438834	4.255936	-1.236406
22	6	0	0.409616	3.032674	-1.958998
23	6	0	0.219113	3.019495	-3.348735
24	6	0	0.060298	4.223449	-4.065573
25	6	0	0.101284	5.448020	-3.367477
26	6	0	0.290963	5.462909	-1.977239
27	26	0	-1.724453	-3.000848	-0.946325
28	6	0	-3.384822	-3.997732	-0.085123
29	6	0	-2.710113	-4.870099	-1.016805
30	6	0	-1.355170	-5.049155	-0.555817
31	6	0	-1.197554	-4.300204	0.666309
32	6	0	-2.448680	-3.646603	0.954828
33	7	0	1.886214	-3.595358	-0.604270
34	8	0	1.756717	-4.288485	-1.597273
35	6	0	-3.091621	-0.251450	1.332073
36	6	0	-2.709960	-0.191044	2.674887
37	6	0	-3.539946	-0.756381	3.652204
38	6	0	-4.739799	-1.371570	3.285350
39	6	0	-5.118578	-1.420971	1.939383
40	6	0	-4.293920	-0.859262	0.957664
41	6	0	-3.151190	1.534935	-0.909890
42	6	0	-2.893775	1.785601	-2.260824
43	6	0	-3.763454	2.602156	-2.993229
44	6	0	-4.878816	3.173643	-2.373492
45	6	0	-5.122672	2.932506	-1.018081
46	6	0	-4.255735	2.116750	-0.281340
47	8	0	0.249802	1.347061	3.054815
48	6	0	0.590924	2.564976	3.356897
49	6	0	0.764654	3.614970	2.443307
50	8	0	0.809097	2.914692	4.692309
51	6	0	0.617663	1.863324	5.690674
52	8	0	1.782242	-3.997112	0.543830
53	1	0	1.450811	-0.281497	-1.398149
54	1	0	3.269524	-2.408397	1.124449
55	1	0	2.747929	-2.098972	-1.845806
56	1	0	-3.506872	-1.145058	-2.221423
57	1	0	-2.136141	-2.906577	-3.775275
58	1	0	0.404936	-3.006466	-2.874379
59	1	0	-0.295000	-4.261979	1.264950
60	1	0	-2.661998	-3.009272	1.805021
61	1	0	-4.412460	-3.669157	-0.148559
62	1	0	-3.137870	-5.296613	-1.913406
63	1	0	-0.585587	-5.642884	-1.035479
64	1	0	-0.398376	1.455894	5.641116
65	1	0	0.789459	2.353724	6.652012
66	1	0	1.335736	1.047870	5.543343
67	1	0	1.004570	4.612954	2.801594
68	1	0	0.774982	5.376924	0.588846
69	1	0	0.315325	6.414068	-1.446507
70	1	0	-0.014898	6.386099	-3.906681
71	1	0	-0.081242	4.208720	-5.143754
72	1	0	0.214255	2.070206	-3.880631
73	1	0	0.569597	2.100113	-1.428447
74	1	0	5.515266	-2.595082	1.505610
75	1	0	7.865134	-2.380921	0.760064
76	1	0	8.405255	-1.177486	-1.351055
77	1	0	6.573990	-0.171756	-2.707032
78	1	0	4.221543	-0.352288	-1.960590
79	1	0	-4.616340	-0.902882	-0.085318
80	1	0	-6.055998	-1.895129	1.656139
81	1	0	-5.383097	-1.810089	4.047569
82	1	0	-3.248203	-0.710380	4.700208
83	1	0	-1.775251	0.295255	3.001671
84	1	0	-4.467950	1.958178	0.779221
85	1	0	-5.983927	3.386186	-0.530613
86	1	0	-5.551773	3.812675	-2.943604
87	1	0	-3.560804	2.802526	-4.044216
88	1	0	-2.021046	1.366969	-2.769457
89	1	0	2.775229	-0.281487	1.966562
90	6	0	0.543128	-1.374765	1.707760
91	1	0	-0.494185	-1.607914	1.458026
92	1	0	1.078381	-2.331777	1.838505
93	1	0	0.562632	-0.799714	2.635413
94	6	0	3.139035	0.939308	0.270231
95	8	0	3.011027	1.267408	-0.927678
96	8	0	3.793298	1.696484	1.195864
97	6	0	4.303012	3.014829	0.756009
98	1	0	3.459460	3.647407	0.467812
99	1	0	4.819626	3.414874	1.629020
100	1	0	4.984645	2.888659	-0.091282

endo-**TS1a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.353499	-1.248031	3.703829
2	6	0	-1.363937	-1.387995	2.744838
3	6	0	-2.705772	-1.235851	3.093683
4	6	0	-3.044508	-0.931339	4.418532
5	6	0	-2.043346	-0.789744	5.383335
6	6	0	-0.700314	-0.948545	5.025879
7	15	0	-0.829014	-1.838556	1.032192
8	6	0	-0.448162	-3.627143	1.361269
9	6	0	0.839351	-4.103290	1.105794
10	6	0	1.151603	-5.442305	1.382199
11	6	0	0.185392	-6.292477	1.923399
12	6	0	-1.094940	-5.802418	2.205483
13	6	0	-1.409184	-4.467121	1.934226
14	6	0	-2.345015	-1.863746	-0.051416
15	6	0	-2.695169	-0.863248	-1.062200
16	6	0	-3.860657	-1.347501	-1.756547
17	6	0	-4.267583	-2.593489	-1.169762
18	6	0	-3.347126	-2.906599	-0.108021
19	6	0	-2.099753	0.513728	-1.232355
20	7	0	-2.299210	1.098317	-2.587740
21	6	0	-2.289963	2.571330	-2.499247
22	6	0	-3.128545	2.831537	-1.211324
23	6	0	-2.769016	1.611359	-0.272168
24	6	0	-2.918931	4.180300	-0.576258
25	6	0	-1.789242	4.463724	0.205009
26	6	0	-1.638166	5.723409	0.790066
27	6	0	-2.608077	6.711248	0.594541
28	6	0	-3.733165	6.434783	-0.188852
29	6	0	-3.891300	5.174296	-0.770851
30	6	0	-0.873964	3.164830	-2.428724
31	8	0	-0.667700	4.104702	-3.413824
32	6	0	0.652693	4.767190	-3.443394
33	6	0	-1.527196	0.522544	-3.697010
34	7	0	-4.010110	1.115355	0.429895
35	26	0	-2.288814	-2.805629	-1.910512
36	6	0	-0.403908	-3.773977	-2.149522
37	6	0	-1.472878	-4.741280	-2.178452
38	6	0	-2.340400	-4.412295	-3.284397
39	6	0	-1.807215	-3.238281	-3.933160
40	6	0	-0.607522	-2.847149	-3.230888
41	29	0	0.948120	-0.628657	0.308128
42	8	0	1.862837	-1.134632	-1.721257
43	6	0	2.850083	-0.343479	-1.804428
44	8	0	3.752332	-0.423492	-2.844798
45	6	0	3.525144	-1.469307	-3.856603
46	7	0	2.160684	1.015155	0.069631
47	6	0	3.200107	0.668978	-0.819551
48	6	0	2.310808	2.100032	0.796765
49	6	0	1.391593	2.616405	1.812088
50	6	0	0.323345	1.868467	2.363302
51	6	0	-0.521714	2.430059	3.330838
52	6	0	-0.317181	3.753029	3.773699
53	6	0	0.750693	4.506082	3.244836
54	6	0	1.597232	3.940955	2.278433
55	8	0	0.007211	2.831268	-1.613916
56	1	0	-1.025725	0.488515	-0.968043
57	1	0	-4.188286	2.722409	-1.527723
58	1	0	-2.024589	1.896782	0.504411
59	1	0	-3.380810	-3.785451	0.524454
60	1	0	-5.114025	-3.195379	-1.471456
61	1	0	-4.354557	-0.814454	-2.556635
62	1	0	0.038359	-2.010786	-3.445406
63	1	0	0.411251	-3.737958	-1.440762
64	1	0	-1.605753	-5.560729	-1.483484
65	1	0	-3.238315	-4.943373	-3.569704
66	1	0	-2.233103	-2.751154	-4.799287
67	1	0	3.425758	-2.450013	-3.381359
68	1	0	4.404269	-1.429275	-4.501707
69	1	0	2.616272	-1.251457	-4.427242
70	1	0	2.424333	4.524489	1.876793
71	1	0	0.925580	5.521159	3.593361
72	1	0	-0.970353	4.184078	4.529235
73	1	0	-1.328139	1.829097	3.752353
74	1	0	0.177990	0.836381	2.057423
75	1	0	-4.775574	4.967281	-1.372522
76	1	0	-4.490968	7.201390	-0.343394
77	1	0	-2.489551	7.691658	1.052107
78	1	0	-0.760531	5.928033	1.404069
79	1	0	-1.012900	3.705057	0.356459
80	1	0	-2.406426	-4.104282	2.196130

81	1	0	-1.842255	-6.457533	2.647976
82	1	0	0.429835	-7.331676	2.137741
83	1	0	2.156492	-5.811779	1.184645
84	1	0	1.640754	-3.456346	0.719572
85	1	0	0.719392	-1.360206	3.465235
86	1	0	0.085064	-0.836481	5.773279
87	1	0	-2.307860	-0.554683	6.413025
88	1	0	-4.089833	-0.799259	4.690605
89	1	0	-3.510447	-1.327568	2.356652
90	1	0	-2.776658	3.003571	-3.380941
91	1	0	-1.782596	1.051399	-4.624210
92	1	0	-0.432230	0.584880	-3.543357
93	1	0	-1.794593	-0.528585	-3.816994
94	1	0	1.441876	4.026692	-3.606831
95	1	0	0.593391	5.471670	-4.274292
96	1	0	0.831514	5.287935	-2.496891
97	8	0	-5.081837	1.192995	-0.141847
98	8	0	-3.851621	0.677255	1.556772
99	1	0	3.864458	1.458548	-1.169757
100	1	0	3.181904	2.738297	0.602477
101	6	0	4.669320	-0.327983	0.383926
102	1	0	4.404547	-1.306960	-0.009366
103	6	0	4.291300	-0.114128	1.738322
104	1	0	4.787913	0.559519	2.422341
105	7	0	3.229656	-0.798709	2.281037
106	8	0	2.513606	-1.615262	1.489481
107	8	0	2.887657	-0.643664	3.528023
108	6	0	5.954595	0.232319	-0.114060
109	6	0	6.663270	-0.449110	-1.131763
110	6	0	6.500175	1.439873	0.389915
111	6	0	7.883239	0.047418	-1.621635
112	1	0	6.255319	-1.372919	-1.534564
113	6	0	7.717764	1.939100	-0.100552
114	1	0	5.975268	1.991303	1.166829
115	6	0	8.417217	1.244945	-1.108371
116	1	0	8.415840	-0.496709	-2.398217
117	1	0	8.123589	2.864675	0.301822
118	1	0	9.361538	1.631091	-1.485121

endo-minor-**TS1a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.157255	-0.355059	3.658909
2	6	0	-2.564221	0.284258	2.482982
3	6	0	-3.295734	1.471640	2.539239
4	6	0	-3.636837	2.016404	3.784217
5	6	0	-3.243639	1.376939	4.962506
6	6	0	-2.502063	0.192325	4.899503
7	15	0	-2.124037	-0.530064	0.870743
8	6	0	-3.380544	-1.909533	0.931665
9	6	0	-3.052156	-3.157810	0.400113
10	6	0	-3.987019	-4.201667	0.445098
11	6	0	-5.239408	-3.999197	1.028725
12	6	0	-5.558885	-2.751116	1.574598
13	6	0	-4.629660	-1.706673	1.529226
14	6	0	-2.817118	0.594530	-0.447280
15	6	0	-2.123767	1.503595	-1.368244
16	6	0	-3.135880	2.107474	-2.194876
17	6	0	-4.429065	1.626660	-1.795076
18	6	0	-4.240241	0.708325	-0.707617
19	6	0	-0.641634	1.820659	-1.488487
20	7	0	-0.349842	2.612658	-2.724624
21	6	0	0.655793	3.653391	-2.483429
22	6	0	0.335578	4.096760	-1.021718
23	6	0	-0.026262	2.731819	-0.326472
24	6	0	1.436419	4.867128	-0.343919
25	6	0	2.524970	4.219082	0.256961
26	6	0	3.527793	4.965586	0.880146
27	6	0	3.454797	6.361854	0.902877
28	6	0	2.372745	7.011562	0.300219
29	6	0	1.364793	6.268976	-0.320415
30	6	0	2.111011	3.185534	-2.665429
31	8	0	2.927116	4.239736	-3.025156
32	6	0	4.368613	3.947322	-3.152573
33	6	0	-0.250602	1.886845	-3.997309
34	7	0	-0.935616	2.985479	0.844825
35	26	0	-3.233070	-0.035147	-2.380691
36	6	0	-2.481351	-2.016252	-2.659473
37	6	0	-3.924719	-2.012516	-2.698498
38	6	0	-4.341159	-1.160436	-3.786666

39	6	0	-3.154389	-0.631878	-4.415612
40	6	0	-2.007651	-1.164549	-3.718670
41	29	0	0.002131	-1.323727	0.710431
42	8	0	-0.054593	-3.233692	-0.608299
43	6	0	0.990412	-3.865909	-0.255212
44	8	0	1.337554	-5.064676	-0.844510
45	6	0	0.438139	-5.588572	-1.885455
46	7	0	1.536394	-2.395766	1.591924
47	6	0	1.963589	-3.402968	0.711630
48	6	0	2.313218	-2.067406	2.605351
49	6	0	2.071813	-0.990508	3.568843
50	6	0	1.195491	0.097333	3.328014
51	6	0	1.011804	1.096144	4.295680
52	6	0	1.704654	1.037342	5.521383
53	6	0	2.596573	-0.027150	5.766648
54	6	0	2.782171	-1.024928	4.797956
55	8	0	2.525047	2.021437	-2.541248
56	1	0	-0.052653	0.891181	-1.474743
57	1	0	-0.585962	4.713967	-1.086299
58	1	0	0.893265	2.219319	0.044586
59	1	0	-5.020075	0.171903	-0.180278
60	1	0	-5.377988	1.902306	-2.234279
61	1	0	-2.920963	2.825373	-2.971278
62	1	0	-0.971141	-0.961734	-3.940630
63	1	0	-1.853113	-2.547210	-1.956705
64	1	0	-4.578594	-2.545343	-2.018078
65	1	0	-5.361801	-0.943736	-4.071670
66	1	0	-3.134525	0.039269	-5.262990
67	1	0	-0.535419	-5.838223	-1.451593
68	1	0	0.936895	-6.484073	-2.259643
69	1	0	0.299155	-4.851239	-2.682494
70	1	0	2.700661	-4.129057	1.052506
71	1	0	3.205143	-2.676778	2.799725
72	1	0	3.471831	-1.844591	4.991969
73	1	0	3.142841	-0.074206	6.705304
74	1	0	1.562425	1.815102	6.267883
75	1	0	0.337570	1.926091	4.078383
76	1	0	0.678125	0.187281	2.376156
77	1	0	0.524926	6.783694	-0.783627
78	1	0	2.312893	8.098091	0.315991
79	1	0	4.236099	6.941299	1.390128
80	1	0	4.364675	4.451534	1.352269
81	1	0	2.596923	3.120437	0.246764
82	1	0	-4.904148	-0.749458	1.981260
83	1	0	-6.529817	-2.593589	2.040273
84	1	0	-5.963927	-4.811343	1.065056
85	1	0	-3.730018	-5.173456	0.027757
86	1	0	-2.071243	-3.362647	-0.057476
87	1	0	-1.567365	-1.274983	3.646701
88	1	0	-2.182275	-0.300230	5.816147
89	1	0	-3.505854	1.804178	5.929153
90	1	0	-4.196816	2.949131	3.828627
91	1	0	-3.594437	2.014549	1.636312
92	1	0	0.513252	4.496714	-3.173095
93	1	0	-0.040997	2.604026	-4.803007
94	1	0	0.547289	1.123086	-3.996906
95	1	0	-1.203662	1.400762	-4.223084
96	1	0	4.538173	3.221939	-3.954761
97	1	0	4.828661	4.909139	-3.386263
98	1	0	4.753258	3.544146	-2.210274
99	8	0	-1.916722	3.693104	0.694642
100	8	0	-0.610861	2.470033	1.902341
101	6	0	3.366662	-2.297813	-0.659005
102	6	0	3.636465	-1.079180	0.005479
103	6	0	4.444536	-3.287596	-0.885727
104	6	0	4.366366	-4.155623	-2.001712
105	6	0	5.561289	-3.406871	-0.019227
106	6	0	5.374383	-5.100436	-2.255247
107	1	0	3.514624	-4.081344	-2.673540
108	6	0	6.566990	-4.353639	-0.269465
109	1	0	5.644148	-2.763810	0.854103
110	6	0	6.480365	-5.204835	-1.389956
111	1	0	5.298999	-5.752165	-3.122437
112	1	0	7.417073	-4.430156	0.404742
113	1	0	7.261338	-5.936431	-1.583323
114	1	0	2.589770	-2.248550	-1.417418
115	7	0	2.694262	-0.079166	0.051303
116	8	0	2.966749	1.074647	0.594209
117	8	0	1.476509	-0.302545	-0.454945
118	1	0	4.571532	-0.830320	0.486933

exo-**TS1a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.913433	-0.034605	3.660016
2	6	0	0.720234	-1.196595	2.903119
3	6	0	0.160985	-2.335112	3.482488
4	6	0	-0.211002	-2.312370	4.834324
5	6	0	-0.018849	-1.158066	5.595785
6	6	0	0.544279	-0.018585	5.008237
7	15	0	1.278346	-1.166432	1.140438
8	6	0	3.096270	-1.404167	1.401107
9	6	0	3.997800	-0.647051	0.649839
10	6	0	5.375545	-0.810469	0.851816
11	6	0	5.843786	-1.721116	1.801406
12	6	0	4.935086	-2.468342	2.559623
13	6	0	3.559801	-2.307990	2.363555
14	6	0	0.713580	-2.757014	0.359485
15	6	0	-0.423068	-2.935734	-0.544904
16	6	0	-0.437418	-4.321542	-0.936578
17	6	0	0.631832	-5.007474	-0.265170
18	6	0	1.336028	-4.050179	0.547387
19	6	0	-1.496381	-1.925336	-0.869826
20	7	0	-2.229809	-2.185467	-2.137581
21	6	0	-3.551007	-1.528530	-2.071436
22	6	0	-4.021038	-1.882281	-0.626870
23	6	0	-2.680217	-1.887332	0.213478
24	6	0	-5.097286	-0.991992	-0.066701
25	6	0	-4.828004	0.310450	0.377315
26	6	0	-5.855879	1.102573	0.895404
27	6	0	-7.159409	0.603099	0.971335
28	6	0	-7.432949	-0.694699	0.527491
29	6	0	-6.407390	-1.491445	0.011942
30	6	0	-3.478828	-0.013945	-2.328324
31	8	0	-4.378424	0.391104	-3.280999
32	6	0	-4.428178	1.839220	-3.589732
33	6	0	-1.508549	-2.023718	-3.406457
34	7	0	-2.657496	-3.069436	1.151839
35	26	0	1.463347	-3.459793	-1.454765
36	6	0	2.963501	-2.131533	-2.197839
37	6	0	3.535716	-3.419668	-1.895574
38	6	0	2.871897	-4.406605	-2.713926
39	6	0	1.885308	-3.726567	-3.518021
40	6	0	1.946680	-2.320141	-3.198207
41	29	0	0.800944	0.713921	0.009076
42	8	0	2.218470	0.981041	-1.693151
43	6	0	1.927527	2.123876	-2.179049
44	8	0	2.608932	2.635279	-3.252932
45	6	0	3.691089	1.816931	-3.827284
46	7	0	0.104070	2.466240	-0.626943
47	6	0	0.933605	3.033796	-1.630431
48	6	0	-0.934349	3.194121	-0.252691
49	6	0	-1.815881	2.964657	0.895189
50	6	0	-1.733032	1.851626	1.768379
51	6	0	-2.602351	1.731430	2.861651
52	6	0	-3.575092	2.723510	3.110169
53	6	0	-3.663694	3.839111	2.254674
54	6	0	-2.794275	3.959155	1.158242
55	8	0	-2.682693	0.763224	-1.764588
56	1	0	-1.055942	-0.908590	-0.875562
57	1	0	-4.390409	-2.927973	-0.691892
58	1	0	-2.574685	-0.961586	0.822914
59	1	0	2.198751	-4.252053	1.169571
60	1	0	0.871899	-6.057968	-0.355783
61	1	0	-1.172264	-4.757683	-1.598753
62	1	0	1.342184	-1.533566	-3.621421
63	1	0	3.225309	-1.178735	-1.761472
64	1	0	4.317346	-3.612554	-1.171543
65	1	0	3.069493	-5.469925	-2.716083
66	1	0	1.228339	-4.194545	-4.237915
67	1	0	4.471498	1.645679	-3.079593
68	1	0	4.069774	2.405700	-4.663953
69	1	0	3.298200	0.854859	-4.171061
70	1	0	0.466473	3.724333	-2.336698
71	1	0	-1.212896	4.045168	-0.874380
72	1	0	-2.842789	4.838307	0.519117
73	1	0	-4.395177	4.619215	2.450156
74	1	0	-4.244180	2.630693	3.962715
75	1	0	-2.521444	0.870531	3.525026
76	1	0	-0.979506	1.085621	1.595406
77	1	0	-6.631531	-2.502419	-0.326540
78	1	0	-8.447289	-1.087315	0.584569
79	1	0	-7.959218	1.222207	1.374408
80	1	0	-5.632577	2.113270	1.241485

81	1	0	-3.815679	0.724057	0.313907
82	1	0	2.874214	-2.889104	2.985699
83	1	0	5.299370	-3.170791	3.307433
84	1	0	6.914932	-1.846904	1.956833
85	1	0	6.078767	-0.217964	0.267847
86	1	0	3.670497	0.086991	-0.102510
87	1	0	1.349582	0.872164	3.233463
88	1	0	0.690764	0.883178	5.601397
89	1	0	-0.310113	-1.140723	6.645827
90	1	0	-0.662234	-3.196963	5.282925
91	1	0	-0.022070	-3.250586	2.907754
92	1	0	-4.224643	-1.957188	-2.821510
93	1	0	-2.193686	-2.243169	-4.234885
94	1	0	-1.101829	-1.003505	-3.550130
95	1	0	-0.681108	-2.733989	-3.451493
96	1	0	-3.453821	2.180099	-3.951899
97	1	0	-5.193726	1.932992	-4.360787
98	1	0	-4.700723	2.401359	-2.691042
99	8	0	-3.207893	-4.101604	0.820257
100	8	0	-2.081590	-2.897282	2.214717
101	6	0	1.966913	4.499944	-0.754202
102	6	0	1.004896	5.292023	-0.056421
103	1	0	0.931434	5.364906	1.019011
104	1	0	2.291213	4.899879	-1.715481
105	7	0	0.080974	6.055255	-0.754512
106	8	0	-0.777353	6.791967	-0.097291
107	8	0	0.037118	5.958775	-2.070617
108	6	0	3.049387	3.856751	0.051814
109	6	0	4.357316	3.766132	-0.479155
110	6	0	2.806101	3.310321	1.336052
111	6	0	5.395778	3.161033	0.250892
112	1	0	4.561608	4.192298	-1.459269
113	6	0	3.842913	2.702675	2.065567
114	1	0	1.809570	3.367601	1.766747
115	6	0	5.143245	2.624768	1.528358
116	1	0	6.398390	3.119334	-0.168877
117	1	0	3.640859	2.295152	3.054929
118	1	0	5.944349	2.159412	2.098696

exo-minor-**TS1a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.249630	-1.400250	3.652197
2	6	0	-1.679609	-0.256975	2.967818
3	6	0	-1.999559	0.906849	3.666699
4	6	0	-1.905168	0.923644	5.065341
5	6	0	-1.490739	-0.217383	5.755048
6	6	0	-1.161099	-1.379318	5.047254
7	15	0	-1.797032	-0.362490	1.125699
8	6	0	-3.168183	-1.608292	1.004098
9	6	0	-3.028052	-2.706170	0.151367
10	6	0	-4.048650	-3.663060	0.078306
11	6	0	-5.199714	-3.523145	0.858723
12	6	0	-5.329010	-2.429174	1.720232
13	6	0	-4.310536	-1.472152	1.798357
14	6	0	-2.561573	1.244789	0.571587
15	6	0	-1.909441	2.284911	-0.221929
16	6	0	-2.862887	3.350279	-0.392527
17	6	0	-4.064619	3.018345	0.321978
18	6	0	-3.880649	1.724526	0.926215
19	6	0	-0.452057	2.352814	-0.609837
20	7	0	-0.169717	3.173072	-1.817414
21	6	0	1.224385	3.660906	-1.756113
22	6	0	1.354280	4.091016	-0.262829
23	6	0	0.467807	3.036086	0.514570
24	6	0	2.766893	4.214266	0.242119
25	6	0	3.565134	3.090024	0.496065
26	6	0	4.881814	3.247691	0.936598
27	6	0	5.407103	4.527225	1.140055
28	6	0	4.610393	5.651468	0.900206
29	6	0	3.295836	5.498116	0.452173
30	6	0	2.247203	2.590490	-2.172484
31	8	0	3.085215	3.033821	-3.162475
32	6	0	4.131172	2.094995	-3.633488
33	6	0	-0.593812	2.637195	-3.118756
34	7	0	-0.337058	3.725875	1.590709
35	26	0	-3.723275	1.536540	-1.148397
36	6	0	-4.183164	-0.313902	-2.093757
37	6	0	-5.395069	0.369022	-1.719253
38	6	0	-5.421919	1.635903	-2.408877

39	6	0	-4.225134	1.733750	-3.206011
40	6	0	-3.458040	0.526104	-3.013702
41	29	0	0.174983	-0.902783	0.169022
42	8	0	1.793543	-0.099474	1.421675
43	6	0	2.864374	-0.593916	0.941525
44	8	0	4.075920	-0.394355	1.557100
45	6	0	4.066250	0.337817	2.837085
46	7	0	1.704851	-1.588823	-0.928418
47	6	0	2.929012	-1.438842	-0.235693
48	6	0	1.779098	-2.165325	-2.115664
49	6	0	0.670105	-2.608469	-2.966565
50	6	0	-0.685999	-2.237595	-2.787731
51	6	0	-1.678210	-2.727257	-3.652068
52	6	0	-1.338015	-3.596654	-4.709036
53	6	0	0.006969	-3.971254	-4.897326
54	6	0	1.003299	-3.478189	-4.040033
55	8	0	2.300729	1.438947	-1.695853
56	1	0	-0.058664	1.324138	-0.738783
57	1	0	0.845734	5.077694	-0.203332
58	1	0	1.078054	2.238510	0.995133
59	1	0	-4.603553	1.193802	1.532611
60	1	0	-4.956637	3.626430	0.386563
61	1	0	-2.663366	4.262859	-0.936833
62	1	0	-2.519581	0.280579	-3.486303
63	1	0	-3.881509	-1.291255	-1.738899
64	1	0	-6.145366	-0.001649	-1.033526
65	1	0	-6.196273	2.386403	-2.330515
66	1	0	-3.960277	2.565720	-3.842899
67	1	0	3.691340	1.356843	2.693112
68	1	0	5.107463	0.344654	3.161954
69	1	0	3.428664	-0.180217	3.561065
70	1	0	3.843235	-1.381523	-0.827848
71	1	0	2.766969	-2.311718	-2.551555
72	1	0	2.039189	-3.787338	-4.169848
73	1	0	0.277342	-4.646149	-5.705711
74	1	0	-2.110128	-3.971513	-5.376837
75	1	0	-2.715483	-2.431251	-3.516279
76	1	0	-0.953030	-1.556597	-1.981685
77	1	0	2.684523	6.381077	0.267974
78	1	0	5.014948	6.649899	1.060751
79	1	0	6.433668	4.648484	1.481995
80	1	0	5.500441	2.366582	1.112245
81	1	0	3.167206	2.081425	0.336860
82	1	0	-4.429316	-0.641138	2.499141
83	1	0	-6.220541	-2.324723	2.337152
84	1	0	-5.992781	-4.268646	0.800198
85	1	0	-3.940563	-4.520265	-0.586152
86	1	0	-2.140689	-2.857052	-0.470499
87	1	0	-0.967774	-2.318590	3.129777
88	1	0	-0.825069	-2.265834	5.581979
89	1	0	-1.415961	-0.202266	6.841647
90	1	0	-2.144131	1.836630	5.609222
91	1	0	-2.303450	1.828899	3.157297
92	1	0	1.353945	4.516914	-2.427594
93	1	0	-0.312764	3.346446	-3.907087
94	1	0	-0.140231	1.654501	-3.354260
95	1	0	-1.679009	2.526819	-3.130761
96	1	0	3.667964	1.196531	-4.051538
97	1	0	4.679360	2.650007	-4.395584
98	1	0	4.783918	1.814851	-2.800961
99	8	0	-0.647798	4.893639	1.437319
100	8	0	-0.622626	3.056979	2.569795
101	6	0	3.445793	-3.312195	0.425677
102	6	0	3.337882	-4.156315	-0.714745
103	6	0	2.589022	-3.624950	1.606212
104	6	0	3.099975	-3.434607	2.911874
105	6	0	1.267402	-4.116869	1.466579
106	6	0	2.326453	-3.745828	4.044310
107	1	0	4.115177	-3.062771	3.034170
108	6	0	0.494230	-4.429923	2.597714
109	1	0	0.848484	-4.263177	0.474490
110	6	0	1.019593	-4.248659	3.892998
111	1	0	2.743891	-3.606203	5.039260
112	1	0	-0.512932	-4.823322	2.470013
113	1	0	0.423718	-4.501025	4.767219
114	7	0	4.220838	-4.031792	-1.778568
115	8	0	4.104169	-4.832893	-2.807588
116	8	0	5.108054	-3.056919	-1.764943
117	1	0	2.595674	-4.931612	-0.837714
118	1	0	4.448590	-2.958526	0.662649

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exo-**TS2a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.333386	-1.035546	1.367316
2	6	0	-4.547501	-1.683867	0.141699
3	6	0	-5.847083	-2.079227	-0.212363
4	6	0	-6.917499	-1.825199	0.649729
5	6	0	-6.700681	-1.173403	1.867654
6	6	0	-5.407504	-0.777104	2.222742
7	6	0	-3.415284	-1.974728	-0.807047
8	6	0	-2.447419	-0.722600	-1.010395
9	7	0	-1.072892	-1.161021	-0.635403
10	6	0	-1.234495	-2.293022	0.326702
11	6	0	-2.468087	-3.112432	-0.232455
12	6	0	0.046046	-3.028732	0.641312
13	6	0	1.306437	-2.427868	1.081433
14	6	0	2.237198	-3.497384	1.346141
15	6	0	1.576873	-4.747034	1.088784
16	6	0	0.234615	-4.462587	0.667742
17	15	0	1.630958	-0.609931	1.300119
18	29	0	0.202400	0.526565	-0.036197
19	7	0	-0.769710	2.240453	-0.552401
20	6	0	-1.804007	2.850765	0.004400
21	6	0	-2.379696	2.544720	1.318874
22	6	0	-1.819758	1.621359	2.240172
23	6	0	-2.428757	1.388491	3.482209
24	6	0	-3.610145	2.073955	3.836680
25	6	0	-4.167634	3.005559	2.938419
26	6	0	-3.558487	3.240919	1.695258
27	26	0	1.608527	-3.543403	-0.672523
28	6	0	3.272158	-3.077087	-1.893072
29	6	0	2.926838	-4.471659	-2.037360
30	6	0	1.576479	-4.544062	-2.540790
31	6	0	1.095085	-3.196335	-2.718856
32	6	0	2.141839	-2.287211	-2.319346
33	6	0	-2.440728	-0.210163	-2.444242
34	8	0	-3.548785	0.546129	-2.701876
35	6	0	-3.666675	1.149440	-4.049890
36	7	0	-2.109582	-4.093794	-1.325321
37	8	0	-1.918661	-3.670814	-2.448485
38	6	0	3.447568	-0.462616	1.008717
39	6	0	3.880627	0.083811	-0.201409
40	6	0	5.255482	0.185441	-0.458260
41	6	0	6.181529	-0.248624	0.492402
42	6	0	5.738885	-0.783250	1.708496
43	6	0	4.369647	-0.890843	1.969774
44	6	0	1.552873	-0.361065	3.140836
45	6	0	1.266434	-1.407486	4.017804
46	6	0	1.214469	-1.159927	5.395850
47	6	0	1.447555	0.127257	5.887589
48	6	0	1.731474	1.172548	5.001916
49	6	0	1.782500	0.930932	3.624809
50	8	0	1.246835	0.923954	-1.986194
51	6	0	0.688555	1.962292	-2.463185
52	6	0	-0.276299	2.797339	-1.758049
53	8	0	1.005183	2.438004	-3.710307
54	6	0	1.967443	1.658577	-4.507457
55	8	0	-1.546825	-0.446456	-3.275836
56	8	0	-2.089442	-5.269697	-1.001606
57	1	0	-1.609878	-1.849595	1.266159
58	1	0	-3.822532	-2.280546	-1.790842
59	1	0	-2.963855	-3.677365	0.591383
60	1	0	-2.765734	0.105704	-0.368944
61	1	0	3.262719	-3.366904	1.667558
62	1	0	2.015945	-5.731135	1.177649
63	1	0	-0.506150	-5.214836	0.417696
64	1	0	0.127697	-2.919800	-3.125379
65	1	0	2.077990	-1.208161	-2.332421
66	1	0	4.212685	-2.688841	-1.524118
67	1	0	3.558888	-5.313972	-1.791329
68	1	0	1.021508	-5.448816	-2.756135
69	1	0	-0.560497	-1.468838	-1.473862
70	1	0	2.925119	1.588003	-3.982934
71	1	0	2.070078	2.214081	-5.441014
72	1	0	1.572046	0.654338	-4.691668
73	1	0	-0.989794	3.340405	-2.384028
74	1	0	-2.340300	3.608187	-0.568995
75	1	0	-3.979676	3.976477	1.013311
76	1	0	-5.066363	3.553647	3.210430
77	1	0	-4.075839	1.899062	4.803503
78	1	0	-1.975491	0.688995	4.182954
79	1	0	-0.889435	1.113827	1.990512
80	1	0	-4.622442	1.673022	-4.034354

81	1	0	-2.839931	1.846159	-4.214346
82	1	0	-3.651889	0.365469	-4.813563
83	1	0	-6.031357	-2.578965	-1.162784
84	1	0	-7.924431	-2.131957	0.367671
85	1	0	-7.537188	-0.969662	2.534654
86	1	0	-5.233161	-0.254734	3.164171
87	1	0	-3.333056	-0.709949	1.656961
88	1	0	4.050872	-1.300258	2.931315
89	1	0	6.462286	-1.112799	2.452014
90	1	0	7.249426	-0.168141	0.291244
91	1	0	5.596989	0.612446	-1.400144
92	1	0	3.177881	0.451915	-0.965432
93	1	0	2.004386	1.768295	2.957157
94	1	0	1.909032	2.177481	5.384303
95	1	0	1.407194	0.318221	6.959837
96	1	0	0.992378	-1.973936	6.084390
97	1	0	1.079516	-2.424330	3.663351
98	6	0	0.680239	4.498135	-1.310155
99	6	0	-0.203398	5.238416	-0.468986
100	7	0	-1.379648	5.768240	-0.979028
101	8	0	-1.725320	5.476017	-2.221085
102	8	0	-2.156697	6.482025	-0.208151
103	1	0	-0.029574	5.446746	0.576703
104	1	0	0.682140	4.800787	-2.357732
105	6	0	2.026406	4.141803	-0.767803
106	6	0	3.151847	4.175535	-1.624144
107	6	0	2.220201	3.767842	0.583697
108	6	0	4.436050	3.861356	-1.145310
109	1	0	3.017939	4.469391	-2.663127
110	6	0	3.503223	3.455226	1.064089
111	1	0	1.367838	3.722391	1.256456
112	6	0	4.618436	3.500695	0.203572
113	1	0	5.290426	3.909004	-1.816856
114	1	0	3.638842	3.178161	2.108342
115	1	0	5.610638	3.259849	0.579738

exo-minor-**TS2a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.357456	3.885904	-1.891191
2	6	0	2.279608	4.150735	-0.867499
3	6	0	2.934907	5.392053	-0.829782
4	6	0	2.676941	6.352831	-1.811036
5	6	0	1.768625	6.080419	-2.838616
6	6	0	1.110702	4.847031	-2.875013
7	6	0	2.615107	3.124661	0.183023
8	6	0	1.326788	2.391302	0.767016
9	7	0	1.453850	0.941322	0.441059
10	6	0	2.395417	0.829920	-0.715477
11	6	0	3.476919	1.953029	-0.451229
12	6	0	2.867325	-0.579339	-0.982342
13	6	0	2.008346	-1.747180	-1.158731
14	6	0	2.851550	-2.870727	-1.484125
15	6	0	4.216094	-2.415957	-1.524745
16	6	0	4.225570	-1.011734	-1.224838
17	15	0	0.145977	-1.677975	-1.167817
18	29	0	-0.540074	0.076827	0.131379
19	7	0	-2.046049	0.923780	1.206533
20	6	0	-2.456285	0.764374	2.455309
21	6	0	-2.007702	-0.240979	3.423439
22	6	0	-0.850752	-1.045127	3.276762
23	6	0	-0.504980	-1.978959	4.265721
24	6	0	-1.312268	-2.137764	5.410838
25	6	0	-2.469663	-1.349252	5.563598
26	6	0	-2.811343	-0.403392	4.584438
27	26	0	3.388019	-2.091708	0.402220
28	6	0	3.533415	-3.732372	1.726016
29	6	0	4.747755	-2.953586	1.776924
30	6	0	4.404345	-1.623493	2.213325
31	6	0	2.980800	-1.578899	2.443558
32	6	0	2.442785	-2.882459	2.132880
33	6	0	1.184657	2.543169	2.276081
34	8	0	0.820927	3.814833	2.618268
35	6	0	0.612321	4.095846	4.058017
36	7	0	4.576629	1.533422	0.497215
37	8	0	4.339654	1.488739	1.688405
38	6	0	-0.356358	-3.432127	-0.851182
39	6	0	-0.834800	-3.745664	0.424840
40	6	0	-1.227679	-5.058058	0.716526
41	6	0	-1.146760	-6.048879	-0.265844

42	6	0	-0.675590	-5.727396	-1.542737
43	6	0	-0.280638	-4.417378	-1.838401
44	6	0	-0.198622	-1.464407	-2.981291
45	6	0	0.640349	-2.008622	-3.960077
46	6	0	0.350921	-1.812564	-5.313714
47	6	0	-0.771953	-1.066250	-5.690553
48	6	0	-1.595340	-0.508397	-4.711479
49	6	0	-1.305558	-0.699394	-3.352432
50	8	0	-1.181868	1.703187	-1.360328
51	6	0	-2.234567	2.208216	-0.848009
52	6	0	-2.815550	1.837821	0.432168
53	8	0	-2.975079	3.151337	-1.521937
54	6	0	-2.503332	3.565235	-2.851639
55	8	0	1.368393	1.626103	3.095380
56	8	0	5.662543	1.307351	-0.011849
57	1	0	1.841894	1.180729	-1.604186
58	1	0	3.167816	3.607141	1.012066
59	1	0	3.949906	2.269567	-1.410608
60	1	0	0.422665	2.798041	0.302362
61	1	0	2.506355	-3.882643	-1.653334
62	1	0	5.086686	-3.024988	-1.725780
63	1	0	5.116065	-0.392491	-1.194266
64	1	0	2.437169	-0.734595	2.847071
65	1	0	1.404944	-3.177477	2.186427
66	1	0	3.452784	-4.767423	1.423951
67	1	0	5.738778	-3.301675	1.519354
68	1	0	5.091781	-0.796990	2.361355
69	1	0	1.838423	0.437764	1.251078
70	1	0	-1.552252	4.102507	-2.762692
71	1	0	-3.284257	4.226428	-3.230762
72	1	0	-2.372853	2.692766	-3.498926
73	1	0	-3.317037	2.645300	0.974209
74	1	0	-3.194015	1.465368	2.845614
75	1	0	-3.715519	0.193701	4.692272
76	1	0	-3.100890	-1.469828	6.440700
77	1	0	-1.036606	-2.860003	6.176052
78	1	0	0.402007	-2.569874	4.165897
79	1	0	-0.212587	-0.907340	2.407197
80	1	0	0.330354	5.148080	4.095300
81	1	0	-0.185696	3.457086	4.446444
82	1	0	1.537830	3.910197	4.612242
83	1	0	3.644489	5.616214	-0.033842
84	1	0	3.185201	7.315962	-1.773679
85	1	0	1.572031	6.828059	-3.605702
86	1	0	0.403534	4.632252	-3.675399
87	1	0	0.812286	2.934382	-1.919683
88	1	0	0.068398	-4.199421	-2.849890
89	1	0	-0.619473	-6.497176	-2.311110
90	1	0	-1.454851	-7.069455	-0.038445
91	1	0	-1.602538	-5.303199	1.710318
92	1	0	-0.924521	-2.995387	1.216806
93	1	0	-1.963000	-0.222098	-2.612820
94	1	0	-2.468132	0.077298	-4.996409
95	1	0	-0.997680	-0.918159	-6.745924
96	1	0	1.001948	-2.236466	-6.075891
97	1	0	1.534757	-2.579638	-3.701598
98	6	0	-5.079843	0.495658	1.288448
99	6	0	-4.591608	0.983125	0.038863
100	1	0	-5.189487	-0.550063	1.536743
101	1	0	-5.003703	1.939632	-0.282458
102	7	0	-5.473005	1.372332	2.287149
103	8	0	-5.939933	0.899245	3.415380
104	8	0	-5.290728	2.667721	2.108964
105	6	0	-4.434760	-0.022927	-1.055641
106	6	0	-4.850600	0.302658	-2.367808
107	6	0	-3.928311	-1.323326	-0.813008
108	6	0	-4.794861	-0.649576	-3.401722
109	1	0	-5.251170	1.294585	-2.565479
110	6	0	-3.868531	-2.274674	-1.845645
111	1	0	-3.586321	-1.590366	0.183540
112	6	0	-4.308118	-1.945958	-3.144319
113	1	0	-5.144425	-0.387727	-4.397855
114	1	0	-3.482444	-3.272722	-1.638504
115	1	0	-4.269878	-2.686953	-3.940129

endo-**TS2a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.456267	5.586869	-0.774972
2	6	0	-2.051548	4.321479	-0.320573
3	6	0	-1.647789	4.163945	1.013504
4	6	0	-1.643558	5.260546	1.879658
5	6	0	-2.049130	6.518926	1.424795
6	6	0	-2.455337	6.679381	0.096392
7	6	0	-2.076726	3.163704	-1.282721
8	6	0	-0.749344	2.274481	-1.214541
9	7	0	-1.161178	0.889453	-0.868457
10	6	0	-2.474300	0.984907	-0.169457
11	6	0	-3.242708	2.148816	-0.924452
12	6	0	-3.175761	-0.338930	0.026070
13	6	0	-2.603130	-1.538676	0.637967
14	6	0	-3.635587	-2.543939	0.682092
15	6	0	-4.837828	-1.988800	0.123301
16	6	0	-4.560707	-0.636610	-0.269966
17	15	0	-0.861189	-1.709061	1.277214
18	29	0	0.499973	-0.225931	0.221059
19	7	0	2.180322	0.958727	0.045251
20	6	0	2.632314	1.905093	0.843985
21	6	0	1.907609	2.465943	1.990639
22	6	0	0.925168	1.738437	2.708005
23	6	0	0.267747	2.319036	3.803562
24	6	0	0.579621	3.632054	4.209477
25	6	0	1.571385	4.358021	3.517981
26	6	0	2.233634	3.776219	2.425672
27	26	0	-3.264714	-1.956995	-1.315946
28	6	0	-2.368665	-3.580386	-2.335441
29	6	0	-3.724429	-3.393857	-2.795302
30	6	0	-3.823589	-2.068196	-3.357317
31	6	0	-2.527743	-1.443689	-3.256230
32	6	0	-1.626073	-2.376695	-2.623872
33	6	0	0.007627	2.271474	-2.534410
34	8	0	0.718338	3.431717	-2.702153
35	6	0	1.507210	3.561755	-3.946871
36	7	0	-3.948975	1.710283	-2.186897
37	8	0	-5.163005	1.614391	-2.116002
38	6	0	-0.523989	-3.510974	1.045526
39	6	0	-1.093122	-4.466660	1.892823
40	6	0	-0.826530	-5.823231	1.680461
41	6	0	0.010459	-6.217827	0.630274
42	6	0	0.588151	-5.256558	-0.202343
43	6	0	0.328032	-3.894841	0.007375
44	6	0	-1.041535	-1.611397	3.115932
45	6	0	-2.285092	-1.515016	3.744737
46	6	0	-2.347578	-1.446994	5.140887
47	6	0	-1.171257	-1.474105	5.899066
48	6	0	0.068390	-1.566800	5.261579
49	6	0	0.138381	-1.635264	3.864512
50	8	0	1.380357	-1.110072	-1.701856
51	6	0	2.414908	-0.414262	-1.927203
52	6	0	3.055946	0.462652	-0.946702
53	8	0	3.071750	-0.460794	-3.132410
54	6	0	2.461427	-1.283557	-4.194440
55	8	0	-0.007951	1.349243	-3.368093
56	8	0	-3.290680	1.539989	-3.194854
57	1	0	-2.265525	1.407698	0.829887
58	1	0	-2.205735	3.542950	-2.316032
59	1	0	-3.997827	2.615751	-0.249198
60	1	0	-0.072026	2.670944	-0.450115
61	1	0	-3.508893	-3.550555	1.059997
62	1	0	-5.782331	-2.501324	0.002041
63	1	0	-5.288048	0.038455	-0.708486
64	1	0	-2.271120	-0.455900	-3.624667
65	1	0	-0.583418	-2.196001	-2.403546
66	1	0	-1.975581	-4.465259	-1.851281
67	1	0	-4.529936	-4.110632	-2.711826
68	1	0	-4.711546	-1.619914	-3.785432
69	1	0	-1.229719	0.306887	-1.712724
70	1	0	2.367095	-2.323740	-3.867986
71	1	0	3.146131	-1.198690	-5.039791
72	1	0	1.473292	-0.882482	-4.441718
73	1	0	3.791090	1.155135	-1.361363
74	1	0	3.591601	2.383370	0.613080
75	1	0	3.004408	4.337464	1.898969
76	1	0	1.831412	5.365048	3.836108
77	1	0	0.078937	4.072663	5.068581
78	1	0	-0.461316	1.733976	4.361922
79	1	0	0.728162	0.702870	2.444106
80	1	0	1.963401	4.550068	-3.883263

81	1	0	2.266335	2.774906	-3.986972
82	1	0	0.849728	3.484373	-4.818813
83	1	0	-1.320305	3.190942	1.385397
84	1	0	-1.313986	5.129888	2.911582
85	1	0	-2.045730	7.371740	2.101761
86	1	0	-2.770031	7.658678	-0.262583
87	1	0	-2.769175	5.726159	-1.809017
88	1	0	0.818146	-3.160379	-0.647360
89	1	0	1.251700	-5.561271	-1.009189
90	1	0	0.217977	-7.274688	0.468983
91	1	0	-1.262775	-6.572010	2.338225
92	1	0	-1.731611	-4.183201	2.732982
93	1	0	1.140654	-1.699305	3.390272
94	1	0	0.991106	-1.578881	5.843407
95	1	0	-1.223055	-1.421322	6.985446
96	1	0	-3.312100	-1.373287	5.637829
97	1	0	-3.217962	-1.488137	3.178739
98	6	0	7.726420	0.547759	-1.314182
99	6	0	6.542805	0.461139	-0.562721
100	6	0	5.647571	-0.622285	-0.739168
101	6	0	5.970655	-1.607157	-1.700730
102	6	0	7.156360	-1.525373	-2.451615
103	6	0	8.041009	-0.446664	-2.262429
104	6	0	4.385638	-0.748724	0.049698
105	6	0	4.384822	-0.342560	1.415946
106	7	0	3.380238	-0.777347	2.263320
107	8	0	2.374751	-1.487933	1.767022
108	8	0	3.408569	-0.472118	3.533067
109	1	0	3.820622	-1.663536	-0.127078
110	1	0	5.161360	0.235271	1.896714
111	1	0	5.293658	-2.445488	-1.851587
112	1	0	6.316714	1.237369	0.165434
113	1	0	7.390435	-2.299718	-3.178864
114	1	0	8.404030	1.385029	-1.160990
115	1	0	8.959231	-0.380986	-2.841754

endo-minor-**TS2a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.046992	4.513620	0.629812
2	6	0	-1.363457	4.380118	0.171795
3	6	0	-2.368320	5.187655	0.735534
4	6	0	-2.061498	6.083198	1.761359
5	6	0	-0.747471	6.194484	2.229779
6	6	0	0.257772	5.412164	1.656679
7	6	0	-1.727175	3.444621	-0.958796
8	6	0	-0.608123	2.376433	-1.300094
9	7	0	-1.082022	1.034019	-0.799231
10	6	0	-2.314067	1.273962	0.033652
11	6	0	-2.984529	2.559873	-0.583772
12	6	0	-3.185977	0.056252	0.243645
13	6	0	-2.757184	-1.230151	0.788358
14	6	0	-3.917330	-2.078785	0.898699
15	6	0	-5.062346	-1.338010	0.445083
16	6	0	-4.618402	-0.029541	0.053793
17	15	0	-1.017782	-1.638049	1.291186
18	29	0	0.407408	-0.278923	0.007845
19	7	0	2.422094	-0.477761	0.450362
20	6	0	3.062180	-0.094088	1.534511
21	6	0	2.507970	0.740093	2.604831
22	6	0	1.381592	1.581192	2.422809
23	6	0	0.903198	2.368339	3.481040
24	6	0	1.536585	2.333516	4.740086
25	6	0	2.668306	1.514318	4.929046
26	6	0	3.153066	0.732960	3.868655
27	26	0	-3.618916	-1.496529	-1.113782
28	6	0	-3.051671	-3.195108	-2.238527
29	6	0	-4.401857	-2.807241	-2.572434
30	6	0	-4.358508	-1.464550	-3.100864
31	6	0	-2.983940	-1.030865	-3.106669
32	6	0	-2.173682	-2.098452	-2.572852
33	6	0	-0.318951	2.261612	-2.794145
34	8	0	0.133261	3.446112	-3.300403
35	6	0	0.661640	3.421944	-4.677257
36	7	0	-3.842526	2.308287	-1.804263
37	8	0	-3.311481	2.078728	-2.870665
38	6	0	-0.990290	-3.487849	1.125659
39	6	0	-0.413028	-4.031825	-0.023984
40	6	0	-0.392394	-5.422650	-0.194505
41	6	0	-0.938972	-6.257527	0.783507

42	6	0	-1.507705	-5.705032	1.936454
43	6	0	-1.535349	-4.316924	2.110009
44	6	0	-1.045957	-1.466146	3.146732
45	6	0	-2.228162	-1.248977	3.856224
46	6	0	-2.185535	-1.124589	5.250521
47	6	0	-0.965203	-1.213661	5.926744
48	6	0	0.216467	-1.423507	5.209092
49	6	0	0.179031	-1.547308	3.815066
50	8	0	1.065016	-1.642948	-1.683049
51	6	0	2.325959	-1.717962	-1.616571
52	6	0	3.161304	-1.153080	-0.552174
53	8	0	3.054485	-2.357312	-2.595704
54	6	0	2.296852	-2.911945	-3.733469
55	8	0	-0.477634	1.228908	-3.468097
56	8	0	-5.047932	2.409692	-1.627781
57	1	0	-1.959633	1.611223	1.024155
58	1	0	-1.922285	4.062920	-1.856420
59	1	0	-3.630566	3.046781	0.185799
60	1	0	0.351798	2.651064	-0.846012
61	1	0	-3.909305	-3.103091	1.250134
62	1	0	-6.078683	-1.703228	0.387668
63	1	0	-5.271228	0.754905	-0.314313
64	1	0	-2.613373	-0.081224	-3.475666
65	1	0	-1.100666	-2.070308	-2.444980
66	1	0	-2.750471	-4.141172	-1.807123
67	1	0	-5.290874	-3.407332	-2.432979
68	1	0	-5.207378	-0.883606	-3.439582
69	1	0	-1.325669	0.459389	-1.620374
70	1	0	1.644173	-3.722528	-3.393475
71	1	0	3.057761	-3.288088	-4.419521
72	1	0	1.692579	-2.128589	-4.200924
73	1	0	3.981230	-1.797392	-0.229671
74	1	0	4.089846	-0.442886	1.695170
75	1	0	4.032048	0.106834	4.014580
76	1	0	3.168925	1.491749	5.894052
77	1	0	1.161196	2.944318	5.557853
78	1	0	0.048216	3.023635	3.322418
79	1	0	0.916459	1.642774	1.444291
80	1	0	0.973145	4.448686	-4.873792
81	1	0	1.510895	2.734408	-4.720949
82	1	0	-0.116681	3.102039	-5.378823
83	1	0	-3.391541	5.130878	0.368036
84	1	0	-2.846496	6.702245	2.192501
85	1	0	-0.509311	6.894597	3.027733
86	1	0	1.290129	5.501170	1.998514
87	1	0	0.773684	3.927435	0.173744
88	1	0	-1.979085	-3.913233	3.023309
89	1	0	-1.927762	-6.356078	2.700779
90	1	0	-0.920168	-7.338535	0.650715
91	1	0	0.054208	-5.851388	-1.089827
92	1	0	0.033062	-3.399859	-0.805776
93	1	0	1.121728	-1.695641	3.281661
94	1	0	1.169824	-1.480015	5.732137
95	1	0	-0.933990	-1.114490	7.010878
96	1	0	-3.105141	-0.954257	5.807449
97	1	0	-3.195639	-1.166859	3.355151
98	6	0	4.487648	0.218276	-1.408612
99	6	0	4.190552	1.470565	-0.798452
100	1	0	4.056239	0.068653	-2.394788
101	6	0	5.838296	-0.387473	-1.219683
102	6	0	6.302293	-1.339268	-2.160043
103	6	0	6.677781	-0.065939	-0.123781
104	6	0	7.565197	-1.939593	-2.021055
105	1	0	5.659378	-1.610339	-2.993389
106	6	0	7.940872	-0.666270	0.016851
107	1	0	6.354859	0.659726	0.618326
108	6	0	8.392811	-1.605283	-0.931107
109	1	0	7.903437	-2.664010	-2.758658
110	1	0	8.573589	-0.400087	0.860839
111	1	0	9.371679	-2.066881	-0.822518
112	1	0	4.788805	1.975497	-0.055180
113	7	0	2.987781	2.067425	-1.079868
114	8	0	2.606891	3.154609	-0.433571
115	8	0	2.181605	1.498722	-1.959751

10e

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.224465	1.020150	0.000020
2	6	0	-0.131330	1.324624	-0.000008
3	6	0	-1.121876	0.330394	-0.000063
4	6	0	-0.691575	-1.007741	-0.000019

5	6	0	0.662302	-1.331591	0.000009
6	6	0	1.618854	-0.316780	0.000055
7	9	0	-0.481285	2.618780	-0.000097
8	6	0	-2.558052	0.719260	0.000040
9	8	0	-3.485489	-0.062645	0.000160
10	9	0	-1.564111	-2.011204	-0.000119
11	9	0	1.053973	-2.608351	-0.000019
12	9	0	2.913391	-0.625787	0.000067
13	9	0	2.144201	1.988723	0.000006
14	1	0	-2.728336	1.811813	-0.000012

L-**Pro-imine***(Re)*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.189118	1.584684	1.701749
2	6	0	-1.136384	-0.575518	1.281513
3	1	0	-1.293489	-1.147603	2.196400
4	1	0	2.610248	-2.556182	0.868294
5	6	0	3.309612	0.270570	-0.287406
6	1	0	3.039835	1.322392	-0.325564
7	7	0	0.956896	-0.289610	0.013562
8	6	0	2.681909	-2.148738	-0.151298
9	6	0	2.360493	-0.665994	-0.136370
10	1	0	0.471289	-2.058757	1.144933
11	6	0	0.014510	-1.311725	0.492586
12	6	0	0.687913	1.028373	0.659745
13	6	0	-0.539467	-2.000499	-0.732825
14	8	0	-1.191062	-3.089208	-0.619853
15	8	0	-0.340114	-1.446424	-1.869501
16	1	0	1.580671	1.285319	1.242016
17	6	0	-0.478634	0.763433	1.651607
18	1	0	1.947786	-2.705987	-0.752349
19	6	0	0.420714	2.182057	-0.306320
20	6	0	0.646261	2.079537	-1.683686
21	6	0	0.000319	3.414458	0.218250
22	6	0	0.419320	3.171154	-2.526896
23	1	0	1.049660	1.164273	-2.109389
24	6	0	-0.222838	4.503684	-0.621920
25	1	0	-0.139060	3.530940	1.290573
26	6	0	-0.023243	4.382919	-1.999445
27	1	0	0.601225	3.072562	-3.593066
28	1	0	-0.549228	5.448791	-0.198396
29	1	0	-0.198243	5.231974	-2.653161
30	6	0	-2.480841	-0.454948	0.574771
31	6	0	-2.697801	0.408688	-0.510650
32	6	0	-3.546869	-1.244427	1.032450
33	6	0	-3.951677	0.475970	-1.121431
34	1	0	-1.900413	1.050143	-0.875041
35	6	0	-4.799221	-1.176600	0.421373
36	1	0	-3.399652	-1.908744	1.880731
37	6	0	-5.003991	-0.316294	-0.659075
38	1	0	-4.106290	1.157804	-1.952526
39	1	0	-5.615282	-1.786785	0.797067
40	7	0	0.137156	0.687943	3.041404
41	8	0	0.583814	-0.398253	3.406502
42	8	0	0.193460	1.737457	3.665042
43	1	0	-5.980383	-0.255320	-1.130501
44	6	0	4.780213	-0.033569	-0.432203
45	6	0	4.084695	-2.431627	-0.714985
46	6	0	5.121366	-1.490296	-0.097191
47	1	0	5.349942	0.650427	0.209639
48	1	0	5.092130	0.203320	-1.460984
49	1	0	6.125616	-1.735709	-0.457910
50	1	0	5.133138	-1.625841	0.992401
51	1	0	4.070049	-2.296580	-1.804634
52	1	0	4.341551	-3.479391	-0.526274
53	6	0	-1.815590	-3.698747	-1.807140
54	1	0	-2.234446	-4.632185	-1.440265
55	1	0	-2.591663	-3.023523	-2.168109
56	1	0	-1.050543	-3.870072	-2.564600
57	1	0	0.222887	-0.628024	-1.614043

L-**Pro-imine***(Si)*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.650013	-0.582526	0.252543
2	6	0	-2.729092	-1.420888	-0.642128
3	6	0	-1.293369	-0.954607	-0.590468
4	6	0	-0.904383	0.236920	-0.094914
5	6	0	-1.906132	1.241755	0.444275
6	6	0	-3.354725	0.906334	0.058765
7	7	0	0.461925	0.596361	0.064200
8	6	0	0.872681	2.015702	0.104026
9	6	0	2.399531	1.934479	0.091263
10	6	0	2.657588	0.785042	-0.892300
11	6	0	1.499705	-0.206040	-0.611785
12	6	0	1.973180	-1.380769	0.267712
13	8	0	2.680704	-2.263480	-0.156100
14	8	0	1.576248	-1.312759	1.550905
15	1	0	0.993121	-0.519754	1.595550
16	1	0	0.509775	2.568344	-0.777993
17	1	0	2.772567	1.679741	1.090470
18	1	0	-0.556029	-1.665150	-0.952042
19	1	0	1.135064	-0.637814	-1.550045
20	1	0	2.579577	1.148543	-1.922973
21	1	0	-3.518579	1.172040	-0.994741
22	1	0	-4.040032	1.525246	0.650296
23	1	0	-1.809883	1.289229	1.540562
24	1	0	-1.666541	2.248745	0.081822
25	1	0	-2.777444	-2.477736	-0.346195
26	1	0	-3.096038	-1.391477	-1.681178
27	1	0	-4.701431	-0.801439	0.030700
28	1	0	-3.482966	-0.851956	1.304801
29	1	0	3.635060	0.309594	-0.781691
30	1	0	2.864692	2.876237	-0.213877
31	1	0	0.480174	2.510584	0.996754

exo-L-**2a-imine***(Re)*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.189118	1.584684	1.701749
2	6	0	-1.136384	-0.575518	1.281513
3	1	0	-1.293489	-1.147603	2.196400
4	1	0	2.610248	-2.556182	0.868294
5	6	0	3.309612	0.270570	-0.287406
6	1	0	3.039835	1.322392	-0.325564
7	7	0	0.956896	-0.289610	0.013562
8	6	0	2.681909	-2.148738	-0.151298
9	6	0	2.360493	-0.665994	-0.136370
10	1	0	0.471289	-2.058757	1.144933
11	6	0	0.014510	-1.311725	0.492586
12	6	0	0.687913	1.028373	0.659745
13	6	0	-0.539467	-2.000499	-0.732825
14	8	0	-1.191062	-3.089208	-0.619853
15	8	0	-0.340114	-1.446424	-1.869501
16	1	0	1.580671	1.285319	1.242016
17	6	0	-0.478634	0.763433	1.651607
18	1	0	1.947786	-2.705987	-0.752349
19	6	0	0.420714	2.182057	-0.306320
20	6	0	0.646261	2.079537	-1.683686
21	6	0	0.000319	3.414458	0.218250
22	6	0	0.419320	3.171154	-2.526896
23	1	0	1.049660	1.164273	-2.109389
24	6	0	-0.222838	4.503684	-0.621920
25	1	0	-0.139060	3.530940	1.290573
26	6	0	-0.023243	4.382919	-1.999445
27	1	0	0.601225	3.072562	-3.593066
28	1	0	-0.549228	5.448791	-0.198396
29	1	0	-0.198243	5.231974	-2.653161
30	6	0	-2.480841	-0.454948	0.574771
31	6	0	-2.697801	0.408688	-0.510650
32	6	0	-3.546869	-1.244427	1.032450
33	6	0	-3.951677	0.475970	-1.121431
34	1	0	-1.900413	1.050143	-0.875041
35	6	0	-4.799221	-1.176600	0.421373
36	1	0	-3.399652	-1.908744	1.880731
37	6	0	-5.003991	-0.316294	-0.659075
38	1	0	-4.106290	1.157804	-1.952526
39	1	0	-5.615282	-1.786785	0.797067

40	7	0	0.137156	0.687943	3.041404
41	8	0	0.583814	-0.398253	3.406502
42	8	0	0.193460	1.737457	3.665042
43	1	0	-5.980383	-0.255320	-1.130501
44	6	0	4.780213	-0.033569	-0.432203
45	6	0	4.084695	-2.431627	-0.714985
46	6	0	5.121366	-1.490296	-0.097191
47	1	0	5.349942	0.650427	0.209639
48	1	0	5.092130	0.203320	-1.460984
49	1	0	6.125616	-1.735709	-0.457910
50	1	0	5.133138	-1.625841	0.992401
51	1	0	4.070049	-2.296580	-1.804634
52	1	0	4.341551	-3.479391	-0.526274
53	6	0	-1.815590	-3.698747	-1.807140
54	1	0	-2.234446	-4.632185	-1.440265
55	1	0	-2.591663	-3.023523	-2.168109
56	1	0	-1.050543	-3.870072	-2.564600
57	1	0	0.222887	-0.628024	-1.614043

exo-L-**2a-imine***(Si)*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.585491	2.896340	-0.556458
2	6	0	2.646913	3.950830	-0.764341
3	6	0	4.062770	3.413961	-0.526482
4	6	0	4.221895	2.048328	-1.196621
5	6	0	3.238109	1.019468	-0.615193
6	6	0	1.837880	1.578182	-0.476056
7	7	0	0.773639	0.627816	-0.152200
8	6	0	0.925153	-0.818730	-0.537521
9	6	0	-0.520458	-1.338724	-0.412357
10	6	0	-1.415003	-0.196076	-0.905507
11	6	0	-0.596709	1.078167	-0.469183
12	6	0	1.899180	-1.625459	0.299496
13	6	0	2.752044	-2.530499	-0.343692
14	6	0	3.606741	-3.348310	0.396584
15	6	0	3.621151	-3.266096	1.789039
16	6	0	2.769682	-2.370487	2.440017
17	6	0	1.909524	-1.560970	1.699133
18	7	0	-0.712812	-2.573875	-1.269825
19	8	0	-0.492852	-2.449500	-2.472483
20	6	0	-2.875846	-0.250891	-0.500814
21	6	0	-3.856906	0.067596	-1.447935
22	6	0	-5.210432	0.039668	-1.108766
23	6	0	-5.600614	-0.309203	0.184448
24	6	0	-4.631424	-0.632737	1.137000
25	6	0	-3.278075	-0.602544	0.797808
26	6	0	-1.104980	1.717635	0.805457
27	8	0	-0.446295	1.468500	1.873320
28	8	0	-2.136942	2.463343	0.790936
29	6	0	-2.670086	3.016184	2.047130
30	8	0	-1.068217	-3.592043	-0.697822
31	1	0	1.204908	-0.884496	-1.595070
32	1	0	-0.744272	-1.666902	0.601423
33	1	0	0.573569	3.284763	-0.462331
34	1	0	-0.631016	1.823928	-1.268548
35	1	0	-1.352601	-0.207822	-1.997782
36	1	0	-3.562559	0.328864	-2.461575
37	1	0	-2.545539	-0.882684	1.552251
38	1	0	-5.957834	0.280213	-1.858802
39	1	0	-4.928530	-0.927726	2.139298
40	1	0	2.746769	-2.599955	-1.429010
41	1	0	1.242262	-0.884376	2.229715
42	1	0	4.261128	-4.046384	-0.116586
43	1	0	2.771186	-2.306069	3.524064
44	1	0	4.289058	-3.898398	2.366120
45	1	0	-6.653835	-0.342420	0.446501
46	1	0	4.045856	2.148963	-2.275703
47	1	0	5.241688	1.667900	-1.077027
48	1	0	3.589575	0.668513	0.364633
49	1	0	3.231671	0.133915	-1.258371
50	1	0	2.440085	4.799485	-0.099338
51	1	0	2.559264	4.349929	-1.786183
52	1	0	4.802953	4.123497	-0.910677
53	1	0	4.244336	3.317263	0.552413
54	1	0	-1.858524	3.466993	2.618093
55	1	0	-3.400341	3.755085	1.727226
56	1	0	-3.143146	2.200819	2.595021
57	1	0	0.366547	0.943316	1.471708

anti-**TS3e**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.114840	0.319105	0.562951
2	1	0	-3.212052	-3.725399	-1.007843
3	6	0	-4.144660	-2.099926	0.150920
4	1	0	-5.220733	-2.283850	0.148334
5	1	0	-3.526550	1.956331	-1.202839
6	6	0	-0.501126	0.603180	-1.130394
7	1	0	-0.183406	-0.326502	-1.595497
8	7	0	-2.561654	-0.492063	-0.625675
9	1	0	0.005236	1.332874	0.981913
10	6	0	-2.622051	1.947793	-0.577052
11	6	0	-1.913575	0.638960	-0.844491
12	8	0	-0.532256	-0.642604	1.175155
13	1	0	-4.619798	-0.037169	-0.408410
14	6	0	-3.838149	-0.585459	0.125531
15	6	0	-2.118807	-1.835486	-1.102289
16	6	0	-3.802354	-0.015418	1.572498
17	6	0	1.595532	0.026188	0.347562
18	8	0	-4.880250	0.273138	2.060854
19	8	0	-2.651669	0.078719	2.186940
20	1	0	-1.729107	-0.265256	1.695203
21	1	0	-1.688299	-1.738253	-2.102306
22	6	0	-3.412281	-2.652542	-1.076656
23	6	0	4.353630	-0.577218	0.163686
24	6	0	2.578103	0.940444	0.731059
25	6	0	2.048457	-1.203243	-0.140913
26	6	0	3.401602	-1.510299	-0.242753
27	6	0	3.940481	0.660624	0.645232
28	1	0	-2.977344	1.978930	0.458622
29	6	0	0.146682	1.844336	-1.764911
30	6	0	-1.767074	3.191435	-0.876817
31	6	0	-0.860524	2.957029	-2.086013
32	1	0	0.686745	1.548588	-2.671324
33	1	0	0.902140	2.251906	-1.080395
34	1	0	-0.327667	3.876364	-2.354012
35	1	0	-1.470551	2.677523	-2.957277
36	1	0	-1.148061	3.435567	-0.003980
37	1	0	-2.433266	4.046363	-1.034645
38	1	0	-1.360652	-2.222518	-0.421742
39	1	0	-3.995038	-2.473844	-1.988295
40	1	0	-3.730687	-2.540633	1.064721
41	9	0	2.225249	2.158607	1.186658
42	9	0	4.847207	1.568889	1.024297
43	9	0	5.655149	-0.863845	0.071490
44	9	0	3.794556	-2.694042	-0.728897
45	9	0	1.175807	-2.127122	-0.583213

anti-minor-**TS3e**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.236337	3.478656	1.024752
2	6	0	-0.016530	2.075160	1.605793
3	6	0	-0.720162	0.975375	0.812098
4	6	0	-2.016139	1.238313	0.276515
5	6	0	-2.304316	2.641534	-0.205651
6	6	0	-1.719749	3.716032	0.731137
7	7	0	-2.861230	0.253184	-0.018777
8	6	0	-4.071662	0.427949	-0.869391
9	6	0	-4.919771	-0.827645	-0.609036
10	6	0	-4.428903	-1.298851	0.766512
11	6	0	-2.909231	-1.078616	0.647951
12	6	0	-2.308854	-2.321653	-0.092779
13	8	0	-2.568009	-3.402034	0.402844
14	8	0	-1.640050	-2.174845	-1.208685
15	6	0	0.168125	0.712460	-0.865592
16	6	0	1.524407	0.155505	-0.429957
17	6	0	1.705961	-1.125354	0.097959
18	6	0	2.965021	-1.637466	0.397261
19	6	0	4.098211	-0.863078	0.156240
20	6	0	3.957454	0.421554	-0.359381
21	6	0	2.683045	0.908178	-0.640715
22	9	0	3.095762	-2.860935	0.920931
23	9	0	5.311511	-1.345225	0.438072
24	9	0	0.643699	-1.893234	0.393012
25	9	0	2.596493	2.161734	-1.129681
26	9	0	5.040068	1.177071	-0.581894

27	8	0	-0.556228	0.028559	-1.681581
28	1	0	-1.212180	-1.239912	-1.367527
29	1	0	-4.613224	1.326005	-0.560416
30	1	0	-4.715525	-1.594338	-1.363144
31	1	0	-0.599344	-0.012392	1.251181
32	1	0	-2.419417	-1.008351	1.620634
33	1	0	-4.839410	-0.667823	1.564300
34	1	0	0.293029	1.773873	-1.124953
35	1	0	-2.284928	3.711025	1.673355
36	1	0	-1.875455	4.701822	0.277893
37	1	0	-1.867656	2.736055	-1.212411
38	1	0	-3.377030	2.808599	-0.324987
39	1	0	1.055373	1.850195	1.654060
40	1	0	-0.374447	2.051962	2.645782
41	1	0	0.134358	4.233361	1.728354
42	1	0	0.348723	3.599632	0.104779
43	1	0	-4.650125	-2.342866	0.985808
44	1	0	-5.989463	-0.603371	-0.637096
45	1	0	-3.761600	0.547787	-1.911048

syn-**TS3e**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.096532	-1.078033	-0.877507
2	1	0	5.133745	-1.690953	-2.025840
3	6	0	4.722977	0.259508	-1.085597
4	1	0	5.683998	0.704922	-0.821478
5	1	0	1.527920	1.331313	1.571878
6	6	0	0.723388	-1.678747	0.569840
7	1	0	1.178771	-2.564082	0.126700
8	7	0	2.784167	-0.582193	0.041851
9	6	0	-1.445894	-0.422192	-0.535853
10	6	0	1.618897	0.317748	1.976091
11	6	0	1.753414	-0.683465	0.854018
12	8	0	0.706140	-0.383756	-1.676227
13	1	0	4.065623	0.856274	0.922619
14	6	0	3.631823	0.632184	-0.054849
15	6	0	3.254862	-1.625679	-0.914630
16	6	0	2.861888	1.907978	-0.523887
17	1	0	-0.352201	-2.052426	-1.313632
18	8	0	3.410669	2.968524	-0.270415
19	8	0	1.761778	1.757348	-1.195164
20	1	0	1.267638	0.742564	-1.349812
21	1	0	3.094883	-2.616701	-0.483757
22	6	0	4.731672	-1.273640	-1.098336
23	6	0	-3.999971	0.776272	-0.226788
24	6	0	-1.600622	0.881333	-0.060579
25	6	0	-2.630702	-1.100342	-0.844073
26	6	0	-3.892205	-0.527782	-0.698198
27	6	0	-2.845854	1.481655	0.104043
28	1	0	2.571897	0.300290	2.524698
29	6	0	0.461055	0.016118	2.944456
30	6	0	-0.196804	-2.087042	1.739681
31	6	0	0.235193	-1.490779	3.087200
32	1	0	0.686219	0.475937	3.912760
33	1	0	-0.456265	0.490061	2.579431
34	1	0	-0.231125	-3.180066	1.805427
35	1	0	-1.223241	-1.763775	1.532753
36	1	0	-0.530717	-1.694364	3.844342
37	1	0	1.160127	-1.972923	3.436712
38	1	0	5.324045	-1.668146	-0.263977
39	1	0	4.438594	0.641046	-2.072044
40	1	0	2.675688	-1.531608	-1.835105
41	9	0	-2.587746	-2.368731	-1.296799
42	9	0	-4.994311	-1.221400	-1.008778
43	9	0	-2.940607	2.726933	0.583819
44	9	0	-0.527006	1.599808	0.309505
45	9	0	-5.200660	1.341222	-0.074455

syn-minor-**TS3e**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.777772	-1.454882	-1.871285
2	1	0	-1.798346	-0.819238	-1.726190
3	8	0	-4.909807	-1.764491	-1.273496

4	6	0	-0.011143	-0.923948	-0.708905
5	8	0	-0.742677	-0.244609	-1.559045
6	1	0	-2.942547	2.585126	1.000861
7	6	0	-2.936825	1.993871	0.077676
8	6	0	3.099768	1.341619	-0.756792
9	6	0	-3.712652	-0.337703	0.157334
10	1	0	-4.305061	1.710658	-1.585572
11	6	0	-3.810369	-1.247879	-1.126720
12	6	0	3.790206	-0.911454	-0.279875
13	6	0	-1.441532	0.287341	1.041929
14	6	0	-0.896354	-1.035834	0.963484
15	6	0	-4.902039	0.637782	0.204274
16	7	0	-2.552436	0.591748	0.386663
17	1	0	-1.624712	-1.772560	0.629542
18	1	0	-3.729558	-1.038078	0.996938
19	6	0	-4.349023	1.879148	-0.504028
20	1	0	-5.161944	0.876554	1.243271
21	6	0	1.403639	-0.410180	-0.559807
22	1	0	0.006575	-2.015486	-0.837593
23	6	0	-0.665875	1.392378	1.721576
24	6	0	4.115562	0.422050	-0.506807
25	6	0	2.455031	-1.302641	-0.322104
26	6	0	1.771699	0.922400	-0.793429
27	1	0	-0.310560	2.109535	0.973390
28	1	0	-1.375423	1.944000	2.354243
29	6	0	-0.030818	-1.537598	2.126974
30	6	0	0.502008	0.883935	2.591645
31	6	0	0.173106	-0.473840	3.217562
32	1	0	-0.506428	-2.424015	2.563164
33	1	0	0.941376	-1.879329	1.758045
34	1	0	-0.741109	-0.383541	3.821807
35	1	0	0.971478	-0.785406	3.900499
36	1	0	0.714928	1.631689	3.363670
37	1	0	1.411428	0.792836	1.988623
38	1	0	-4.935683	2.784344	-0.325016
39	1	0	-2.199615	2.420004	-0.607733
40	1	0	-5.767072	0.188297	-0.282095
41	9	0	2.191004	-2.607438	-0.112313
42	9	0	4.754086	-1.806578	-0.039218
43	9	0	5.388719	0.820989	-0.469617
44	9	0	3.405361	2.627001	-0.967931
45	9	0	0.853612	1.873531	-1.029791

anti-**TS4e**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.597363	-0.665087	0.077115
2	6	0	-3.382707	-0.167928	-0.424644
3	6	0	-3.396043	1.150820	-0.897653
4	6	0	-4.533513	1.943918	-0.874908
5	6	0	-5.722796	1.416175	-0.364464
6	6	0	-5.755129	0.105394	0.113940
7	6	0	-2.200034	-1.044320	-0.480165
8	6	0	-1.220045	-0.635577	1.446633
9	6	0	-2.169637	-1.105931	2.538834
10	6	0	-2.238088	-2.631598	2.680478
11	6	0	-0.833486	-3.235358	2.697308
12	6	0	-0.031570	-2.861368	1.433317
13	6	0	-0.016616	-1.367930	1.201284
14	7	0	1.088798	-0.777369	0.738901
15	6	0	2.341451	-1.522320	0.345316
16	6	0	3.318914	-0.378929	0.025751
17	6	0	2.902095	0.775629	0.944818
18	6	0	1.339450	0.678492	0.880438
19	6	0	2.210375	-2.538425	-0.771007
20	6	0	2.763120	-3.812644	-0.586229
21	6	0	2.744111	-4.747934	-1.621517
22	6	0	2.168141	-4.416755	-2.848400
23	6	0	1.619894	-3.146024	-3.039297
24	6	0	1.645398	-2.206354	-2.009694
25	7	0	4.742702	-0.803834	0.321422
26	8	0	4.957533	-1.291819	1.429684
27	6	0	3.526739	2.129316	0.667698
28	6	0	3.918416	2.924968	1.751894
29	6	0	4.498210	4.176690	1.545317
30	6	0	4.699044	4.647157	0.247156
31	6	0	4.318326	3.859530	-0.841114
32	6	0	3.735497	2.608827	-0.634248
33	6	0	0.758166	1.528025	-0.252366
34	8	0	0.588644	1.147672	-1.397956

35	9	0	-2.258701	1.679753	-1.396300
36	9	0	-4.494960	3.193055	-1.331030
37	9	0	-6.816337	2.162222	-0.332288
38	9	0	-6.885855	-0.401190	0.594013
39	9	0	-4.661720	-1.926625	0.525110
40	8	0	0.507757	2.749725	0.197703
41	6	0	0.150908	3.765863	-0.776777
42	8	0	5.568453	-0.608661	-0.555847
43	8	0	-1.280852	-0.927151	-1.442541
44	1	0	-1.029693	-0.001252	-1.638973
45	1	0	2.722971	-2.015868	1.245130
46	1	0	3.309672	-0.118340	-1.030372
47	1	0	-1.155492	0.446648	1.351614
48	1	0	0.912330	1.033820	1.819750
49	1	0	3.173752	0.472250	1.962280
50	1	0	-2.412351	-2.088842	-0.282267
51	1	0	3.778811	2.559127	2.766645
52	1	0	3.458678	2.011037	-1.498298
53	1	0	4.802039	4.776854	2.397825
54	1	0	4.487884	4.211124	-1.854717
55	1	0	3.223738	-4.072319	0.364661
56	1	0	1.227678	-1.217990	-2.166700
57	1	0	3.180760	-5.730267	-1.468438
58	1	0	1.177849	-2.882365	-3.995670
59	1	0	2.151488	-5.143340	-3.655385
60	1	0	5.160503	5.616433	0.083210
61	1	0	-0.288451	-2.885896	3.584052
62	1	0	-0.877695	-4.327036	2.767495
63	1	0	-0.470778	-3.344284	0.548586
64	1	0	0.981772	-3.254898	1.509098
65	1	0	-3.165815	-0.683703	2.366181
66	1	0	-1.830829	-0.667568	3.489718
67	1	0	-2.773089	-2.888716	3.600778
68	1	0	-2.818671	-3.062426	1.856123
69	1	0	-0.807140	3.522365	-1.235092
70	1	0	0.087177	4.690275	-0.205594
71	1	0	0.930922	3.832598	-1.536688

anti-minor**TS4e**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.862145	-0.585474	-1.052834
2	1	0	-3.399468	1.264289	1.852876
3	6	0	-3.513397	-0.575353	0.610125
4	1	0	-4.134612	-1.331176	1.092766
5	1	0	-0.739541	-3.398686	1.364108
6	6	0	1.238914	-0.884559	1.318450
7	1	0	1.235401	0.196409	1.434166
8	7	0	-1.065362	-0.754413	0.644928
9	1	0	1.733923	-1.647344	-1.237999
10	6	0	0.024639	-2.995707	0.683250
11	6	0	0.071624	-1.493674	0.891484
12	8	0	0.954653	0.238156	-1.476535
13	1	0	-2.364897	-2.394960	0.410622
14	6	0	-2.260769	-1.366909	0.057154
15	6	0	-1.377340	0.425995	1.496803
16	6	0	-2.159705	-1.459235	-1.464736
17	6	0	3.206441	-0.106596	-0.835299
18	8	0	-3.124705	-2.205176	-1.962208
19	8	0	-1.273460	-0.958782	-2.153019
20	1	0	0.082081	-0.222868	-1.685727
21	1	0	-0.871568	0.257786	2.452564
22	6	0	-2.911348	0.300840	1.730123
23	6	0	5.881915	0.719308	-0.541842
24	6	0	4.272391	-1.029094	-0.875974
25	6	0	3.530731	1.251203	-0.624838
26	6	0	4.849535	1.661314	-0.480729
27	6	0	5.595125	-0.634055	-0.738053
28	1	0	-0.319297	-3.235103	-0.332170
29	6	0	-0.939072	1.803008	1.015335
30	6	0	-0.974113	2.212675	-0.322482
31	6	0	-0.518665	2.718820	1.991699
32	6	0	-0.594228	3.508481	-0.676260
33	1	0	-1.294437	1.524904	-1.096487
34	6	0	-0.144972	4.015448	1.639841
35	1	0	-0.486475	2.417671	3.036802
36	6	0	-0.180455	4.413145	0.302247
37	1	0	-0.621233	3.808355	-1.719848
38	1	0	0.177805	4.710382	2.409402
39	1	0	0.115093	5.420469	0.024312

40	6	0	-4.422452	0.143924	-0.381324
41	6	0	-4.264003	1.483468	-0.759362
42	6	0	-5.512080	-0.571677	-0.904278
43	6	0	-5.156984	2.083310	-1.650862
44	1	0	-3.455633	2.080993	-0.353266
45	6	0	-6.401870	0.024147	-1.795922
46	1	0	-5.668216	-1.604822	-0.604338
47	6	0	-6.224595	1.356416	-2.175379
48	1	0	-5.019495	3.125624	-1.923723
49	1	0	-7.242305	-0.546776	-2.180066
50	7	0	-3.085148	-0.401193	3.067919
51	8	0	-2.809783	-1.602674	3.105587
52	8	0	-3.431822	0.283980	4.017342
53	1	0	-6.922222	1.827046	-2.861877
54	6	0	2.342632	-1.640645	2.024872
55	6	0	1.367436	-3.693747	0.955929
56	6	0	2.020160	-3.129648	2.219318
57	1	0	2.517737	-1.159587	2.996129
58	1	0	3.291939	-1.531108	1.480767
59	1	0	2.932396	-3.682379	2.465228
60	1	0	1.336000	-3.253572	3.068929
61	1	0	2.048402	-3.564882	0.104789
62	1	0	1.189298	-4.769882	1.048489
63	6	0	-3.184507	-2.351269	-3.406474
64	1	0	-4.041022	-2.997354	-3.588022
65	1	0	-3.327313	-1.372995	-3.867854
66	1	0	-2.263277	-2.808710	-3.771225
67	9	0	2.570353	2.165624	-0.530789
68	9	0	5.137468	2.942719	-0.277493
69	9	0	7.136975	1.111905	-0.403690
70	9	0	6.579429	-1.525126	-0.793439
71	9	0	4.009849	-2.327307	-1.078865

syn-**TS4e**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.165682	-1.322738	-1.668763
2	1	0	0.215147	-0.395918	-1.599087
3	8	0	-2.211142	-2.948060	-0.521900
4	6	0	1.838847	-0.965524	-0.806409
5	8	0	1.138142	-0.053503	-1.428391
6	1	0	-1.759453	1.922165	1.699430
7	6	0	-1.682677	1.521732	0.683155
8	6	0	5.258043	0.637615	-0.572691
9	6	0	-1.892804	-0.937993	0.643799
10	1	0	-3.240871	1.185369	-0.824423
11	6	0	-1.710199	-1.735821	-0.647449
12	6	0	5.454915	-1.759667	-0.252312
13	6	0	0.257367	0.045943	1.352713
14	6	0	0.896221	-1.192388	1.411017
15	6	0	-3.319340	-0.302434	0.799112
16	7	0	-0.964832	0.200877	0.761021
17	1	0	0.347106	-2.066783	1.072048
18	1	0	-1.733081	-1.637900	1.468186
19	6	0	-3.102518	1.112785	0.252156
20	1	0	-3.464990	-0.192684	1.879047
21	6	0	3.250773	-0.748751	-0.599654
22	1	0	1.507347	-1.995876	-0.874992
23	6	0	0.930627	1.280438	1.905865
24	6	0	6.046181	-0.498739	-0.359919
25	6	0	4.076301	-1.868539	-0.368064
26	6	0	3.880203	0.511094	-0.687840
27	1	0	1.080220	1.998676	1.092370
28	1	0	0.227244	1.760118	2.600602
29	7	0	-4.126372	2.066977	0.837440
30	8	0	-4.100486	2.230204	2.055711
31	8	0	-4.906306	2.585759	0.054413
32	6	0	-4.501250	-1.063253	0.230790
33	6	0	-5.338881	-1.767120	1.104540
34	6	0	-4.791624	-1.077114	-1.142091
35	6	0	-6.439251	-2.476059	0.621304
36	1	0	-5.135525	-1.753908	2.172794
37	6	0	-5.892322	-1.784128	-1.626094
38	1	0	-4.170247	-0.528857	-1.846319
39	6	0	-6.718036	-2.486559	-0.745455
40	1	0	-7.082086	-3.010345	1.314537
41	1	0	-6.112957	-1.773575	-2.689621
42	6	0	-1.085626	2.584375	-0.223353
43	6	0	-0.797680	3.848462	0.306214
44	6	0	-0.913200	2.368726	-1.597945
45	6	0	-0.330091	4.874231	-0.517043

46	1	0	-0.948132	4.037453	1.366717
47	6	0	-0.441271	3.390330	-2.419532
48	1	0	-1.160886	1.405026	-2.034509
49	6	0	-0.146576	4.645209	-1.880509
50	1	0	-0.115757	5.850287	-0.092186
51	1	0	-0.312819	3.210370	-3.482823
52	1	0	0.215343	5.442110	-2.523309
53	1	0	-7.579807	-3.029202	-1.122541
54	6	0	1.991663	-1.479265	2.421689
55	6	0	2.260321	1.005581	2.630036
56	6	0	2.213543	-0.315663	3.397561
57	1	0	1.723216	-2.390339	2.970464
58	1	0	2.938423	-1.715832	1.916393
59	1	0	1.396626	-0.286944	4.130925
60	1	0	3.139205	-0.471067	3.961290
61	1	0	2.472309	1.844790	3.300206
62	1	0	3.080822	0.978049	1.903849
63	6	0	-2.228042	-3.799411	-1.698351
64	1	0	-1.224648	-3.878430	-2.119762
65	1	0	-2.583710	-4.764165	-1.342226
66	1	0	-2.915354	-3.379642	-2.434635
67	9	0	3.157069	1.616642	-0.856769
68	9	0	5.833873	1.832679	-0.653450
69	9	0	7.357757	-0.374215	-0.246613
70	9	0	6.206328	-2.835713	-0.043929
71	9	0	3.518065	-3.081591	-0.273867

syn-minor-**TS4e**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.068003	1.042307	-0.791032
2	1	0	-3.287460	0.907330	-0.807586
3	6	0	-3.035674	-0.471649	0.887628
4	1	0	-3.170032	-0.322461	1.964396
5	1	0	0.963729	-1.628266	1.499599
6	6	0	1.231730	1.616121	1.208540
7	1	0	0.773850	2.480092	0.740311
8	7	0	-0.782639	0.379991	0.739956
9	6	0	3.187202	0.112081	-0.599251
10	6	0	0.946293	-0.726339	2.121987
11	6	0	0.435949	0.466418	1.327823
12	8	0	1.023843	0.777590	-1.546724
13	1	0	-1.273824	-1.519346	1.566195
14	6	0	-1.538384	-0.887532	0.719722
15	6	0	-1.701074	1.580083	0.550008
16	6	0	-1.222018	-1.698321	-0.543359
17	1	0	2.365113	2.080506	-0.891628
18	8	0	-1.520094	-2.972799	-0.359626
19	8	0	-0.744887	-1.236466	-1.568804
20	1	0	0.655561	-0.138144	-1.522602
21	1	0	-1.764257	2.050466	1.536178
22	6	0	-3.064362	0.924504	0.256489
23	6	0	5.445113	-1.568244	-0.337814
24	6	0	3.086221	-1.282780	-0.704511
25	6	0	4.474631	0.632764	-0.375528
26	6	0	5.591369	-0.183891	-0.233339
27	6	0	4.183204	-2.121770	-0.573685
28	1	0	0.202858	-0.919498	2.909287
29	6	0	-1.373344	2.657135	-0.469871
30	6	0	-1.224617	3.976722	-0.019690
31	6	0	-1.354178	2.404360	-1.849131
32	6	0	-1.039663	5.022428	-0.926336
33	1	0	-1.270125	4.192711	1.045667
34	6	0	-1.166292	3.446895	-2.753404
35	1	0	-1.469335	1.390023	-2.218261
36	6	0	-1.008188	4.757908	-2.295104
37	1	0	-0.933580	6.039710	-0.561626
38	1	0	-1.150198	3.237204	-3.818848
39	1	0	-0.870930	5.569095	-3.004009
40	6	0	-4.097431	-1.437786	0.399894
41	6	0	-4.828412	-2.174792	1.339014
42	6	0	-4.382359	-1.607902	-0.963467
43	6	0	-5.819347	-3.067959	0.929522
44	1	0	-4.628561	-2.043848	2.399969
45	6	0	-5.373326	-2.498919	-1.373981
46	1	0	-3.838840	-1.043374	-1.717850
47	6	0	-6.093660	-3.232030	-0.428111
48	1	0	-6.381134	-3.626515	1.672270
49	1	0	-5.590921	-2.611271	-2.432212
50	7	0	-4.178651	1.754410	0.869022
51	8	0	-4.105885	1.974505	2.076587

52	8	0	-5.065954	2.126740	0.118147
53	1	0	-6.870681	-3.919605	-0.748716
54	6	0	2.317145	-0.514371	2.789304
55	6	0	2.357483	1.919108	2.183284
56	6	0	2.445613	0.907652	3.333403
57	1	0	2.426679	-1.254855	3.588403
58	1	0	3.124644	-0.708562	2.075129
59	1	0	2.195702	2.928271	2.581719
60	1	0	3.317805	1.969444	1.658273
61	1	0	3.390559	1.033836	3.871291
62	1	0	1.642440	1.097196	4.058157
63	6	0	-1.337584	-3.863982	-1.490332
64	1	0	-0.312263	-3.793049	-1.857151
65	1	0	-1.551031	-4.858581	-1.103473
66	1	0	-2.040154	-3.596620	-2.281552
67	9	0	4.649483	1.959468	-0.306761
68	9	0	6.790799	0.345895	-0.021624
69	9	0	6.498355	-2.359330	-0.207879
70	9	0	4.039630	-3.440532	-0.672094
71	9	0	1.879177	-1.845344	-0.917513

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