Supporting Information for

Tuning Through-Space Interactions via the Secondary Coordination Sphere of an Artificial Metalloenzyme leads to Enhanced Rh(III)-Catalysis

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1. General methods

Flash column chromatography was performed on SiliCycle Inc.® silica gel 60 (230-400 mesh). Thin Layer chromatography was performed on SiliCycle Inc.® 0.25 mm silica gel 60-F plates. Visualization was accomplished with UV light (254 nm) or $KMnO_4$ staining.

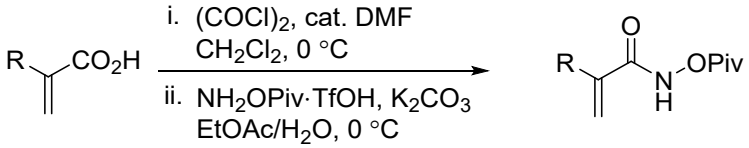
^{1}H-NMR and ^{13}C-NMR spectra were recorded on Bruker 300, 400 or 500 MHz spectrometers at ambient temperature. ^{1}H-NMR data are reported as the following: chemical shift in parts per million (δ, ppm) from chloroform ($CDCl_3$) taken as 7.26 ppm, integration, multiplicity (s=singlet, d=doublet, t=triplet, q=quartet, m=multiplet, dd=doublet of doublets) and coupling constant (*J* in Hz unit). ^{13}C-NMR is reported as the following: chemical shifts are reported in ppm from $CDCl_3$ taken as 77.0 ppm.

Low-resolution mass spectra (LSMS) were obtained on ACQUITY Waters UPLC/mass spectrometer equipped with electrospray ionization.

Infrared spectra (IR) were recorded on a Perkin Elmer Paragon 1000 FT-IR spectrometer.

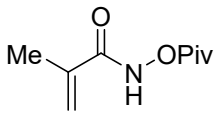
2. Preparation of starting materials

N-(pivaloyloxy) α-substituted acrylamides



To the solution of $NH_2OPiv·TfOH$ (1.1 equiv), K_2CO_3 (2.0 equiv) and $EtOAc/H_2O$ (2/1 by v/v, 0.1M) at 0 °C (ice bath), the crude acid chloride was added dropwise (while a small amount of EtOAc can be used as a solvent). The mixture was stirred at the same temperature for 0.75 - 1 h (prolonged reaction time led to the decomposition of the N-pivaloyloxy acrylamide). Upon the completion (monitored by TLC), saturated $NaHCO_3$ was added. The aqueous layer was extracted with EtOAc (×3), washed with brine, dried with $MgSO_4$, and filtered. The solvent was removed under reduced pressure to give a crude N-(pivaloyloxy) α-substituted acrylamide, which was purified by a flash column chromatography (10% EtOAc/hexane).

N-(Pivaloyloxy)methacrylamide (1)



2a

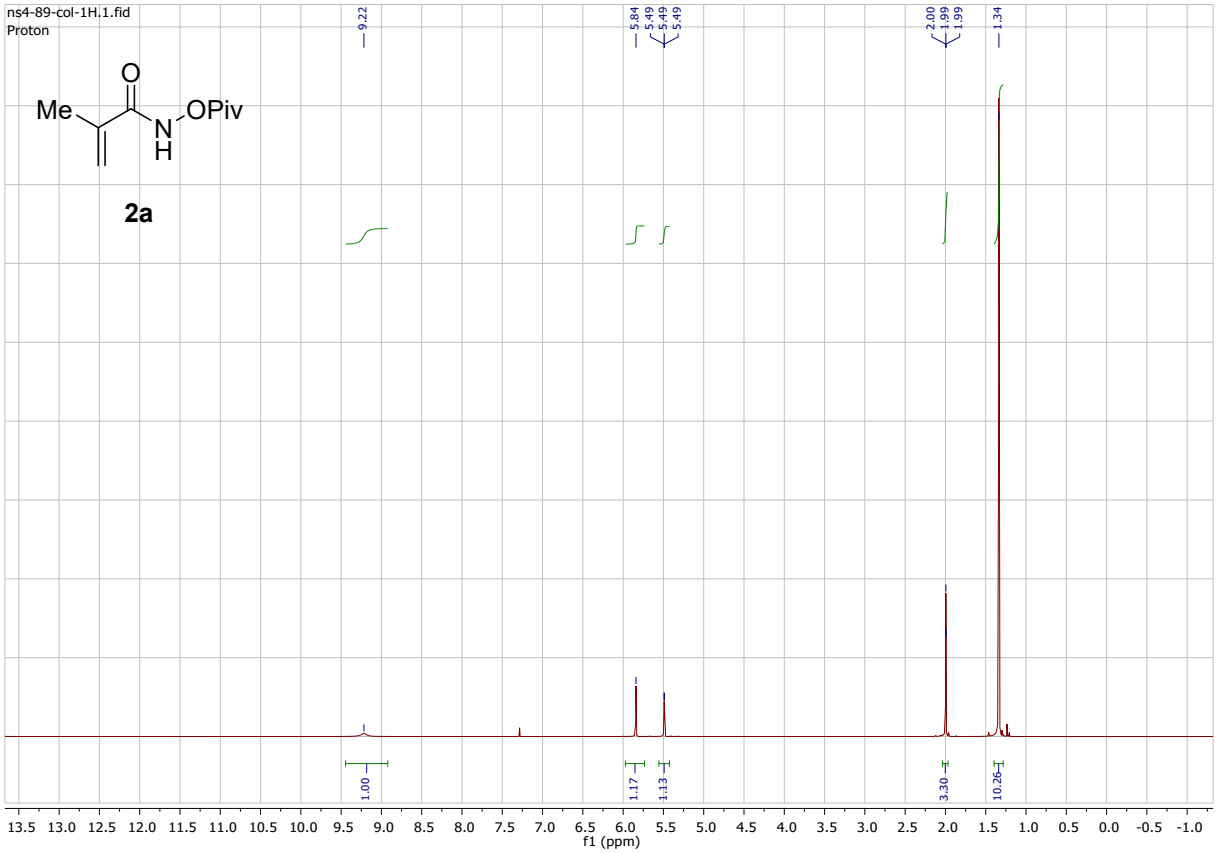
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.22 (s, NH), 5.84 (s, 1H), 5.50 – 5.47 (m, 1H), 1.99 (t, J = 1.3 Hz, 3H), 1.34 (s, 9H).

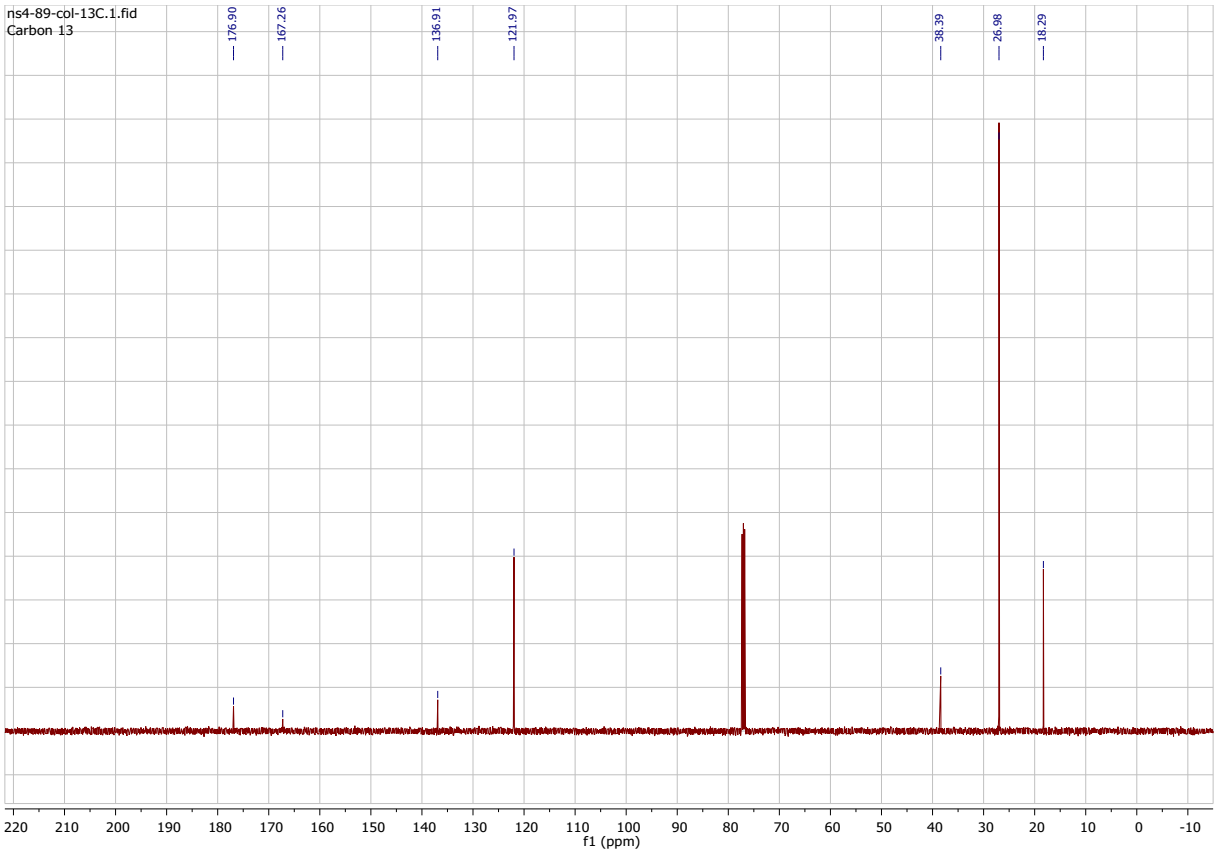
^{13}C NMR (126 MHz, $CDCl_3$) δ 176.90, 167.26, 136.91, 121.97, 38.39, 26.98, 18.29

IR (neat, cm^{-1}) 3225, 2977, 1782, 1671, 1629, 1481, 1055, 1033, 1015.

LRMS (ESI) m/z calcd for $C_9H_{15}NO_3$ $[M+H]^+$: 186.1, found: 186.2.

3. Copies of NMR spectra




ns4-89-col-13C.1.fid
Carbon 13
176.90
167.26
136.91
121.97
38.39
26.98
18.29
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

4. General procedures for asymmetric dihydropyridone synthesis

General procedure A for asymmetric dihydropyridone synthesis

To a 750 µL clear glass shell vial (8 x 30mm) equipped with a parylene coated stir bar (1.67 x 2.01 x 4.80mm) was added a solution of the acrylamide in MeOH (3.0 µL, 1.0 M, 0.0030 mmol). The alkene (0.0015 mmol) was added followed by 125 µL of acetate buffer (100 mM NaOAc, 100 mM NaCl, pH 7.4). 75 µL of the monomeric streptavidin wild-type metalloenzyme (600 µM, 3 mol%, 0.000045 mmol) in salt water (100 mM NaCl, pH 7.4) was added to the vial achieving the desired reaction mixture (225 µM enzyme, 62.5 mM NaOAc, 100 mM NaCl, pH 7.4). The vial was placed in a 24-well high-throughput experimentation block and the reaction mixture was allowed to stir at 200 rpm at 25 °C. After 72 h the reaction is diluted with ethyl acetate and filtered through a Celite plug into a 20 mL scintillation vial. The reaction vial was washed twice more with ethyl acetate and filtered through the Celite plug into the scintillation vial. The Celite plug was washed an additional three times with ethyl acetate, collecting the filtrate into the scintillation vial. The contents of the scintillation vial were carefully removed via concentration under vacuum. The crude residue of the scintillation vial was dissolved in 600 µL of MeOD. A trimethyl(phenyl)silane internal standard (0.258 µL, 0.0015 mmol) was added to the solution, and mixed thoroughly. The sample was then analyzed by NMR (400 MHz or 500 MHz, MeOD, minimum of 400 scans), and the yield was determined relative to the trimethyl(phenyl)silane internal standard. Enantioselectivity was determined by chiral HPLC.

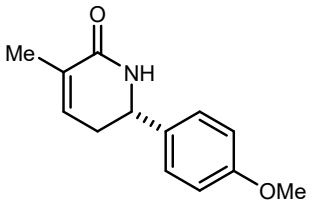
Chiral HPLC Analysis - The crude residue of the scintillation vial was rediluted with 120 µL of HPLC grade isopropanol and 300 µL of HPLC grade hexanes. 1.5 µL of a 1,3,5-trimethoxybenzene solution (1.0 M in MeOH) was added to the scintillation vial. The contents of the scintillation vial were thoroughly mixed via pipette to ensure uniformity of the solution. 180 µL of the uniform solution were incorporated into at 200 µL vial insert, and the sample was submitted for analysis. Enantioselectivity was also determined by chiral HPLC.

NMR Analysis - The crude residue of the scintillation vial was dissolved in 600 μL of MeOD. A trimethyl(phenyl)silane internal standard (0.258 μL, 0.0015 mmol) was added to the solution, and mixed thoroughly. The sample was then analyzed by NMR (400 MHz or 500 MHz, MeOD, minimum of 400 scans), and the yield was determined relative to the trimethyl(phenyl)silane internal standard. Enantioselectivity was determined by chiral HPLC.

5. **Extended mutant yield and enantioselectivity data**

Mutant	TON	ee (%)
G49A	97	91
WT	33	91
T111E	32	92
E113A	22	94
H87E	20	92
T32R	14	92
T111A	10	93

6. **Analytical data for enantioenriched dihydropyridones (NMR/HPLC)**

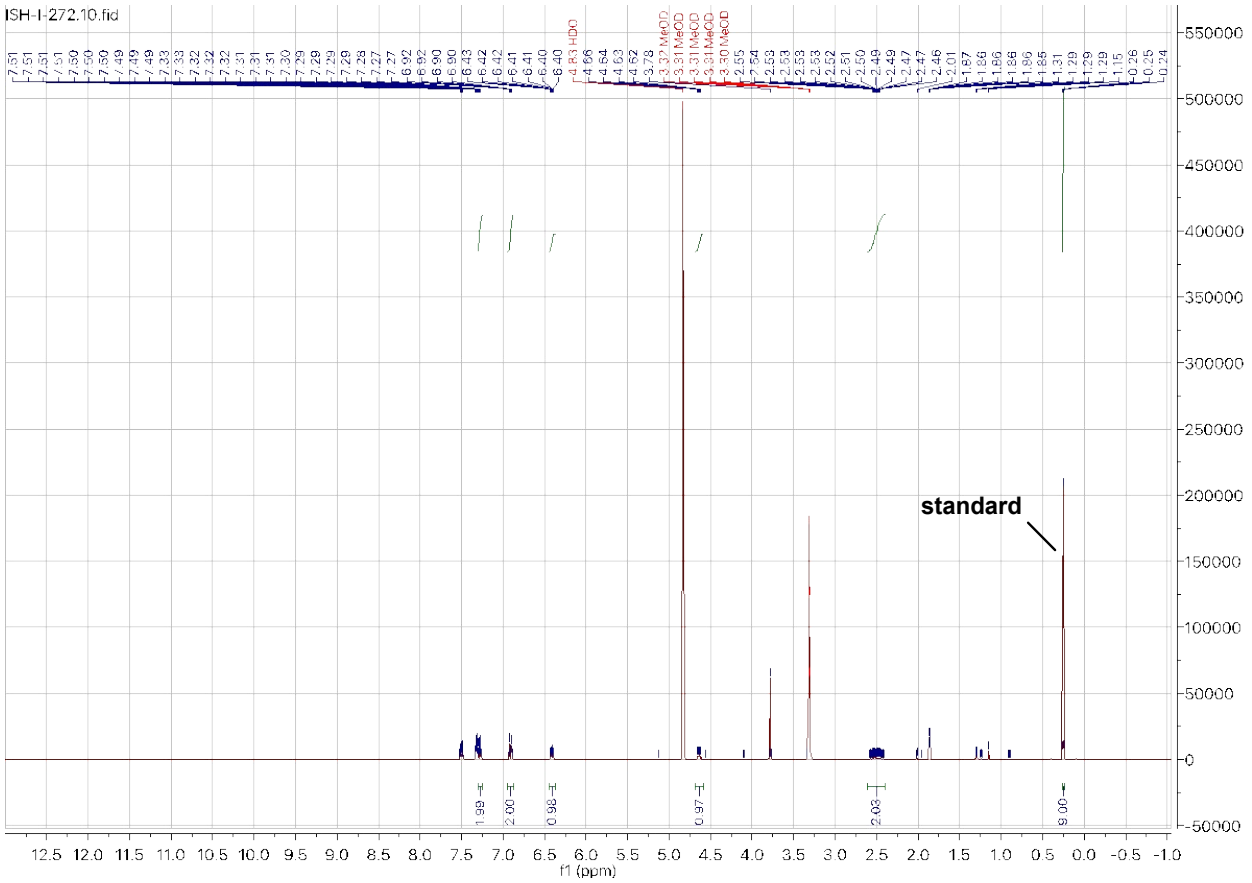


6-(4-Methoxyphenyl)-3-methyl-5,6-dihydropyridin-2(1H)-one (3)

Product synthesized according to general procedure A. Product yield was determined to be 99% by ^{1}H NMR analysis (400 MHz, MeOD) relative to a trimethyl(phenyl)silane internal standard. The product was determined to be 91% ee by chiral HPLC analysis. (Chiralpak IE, 20% ^{i}PrOH/hexanes, 1 mL/min, $t_r(e_1$, minor) = 30.8 min, $t_r(e_2$, major) = 34.1 min).

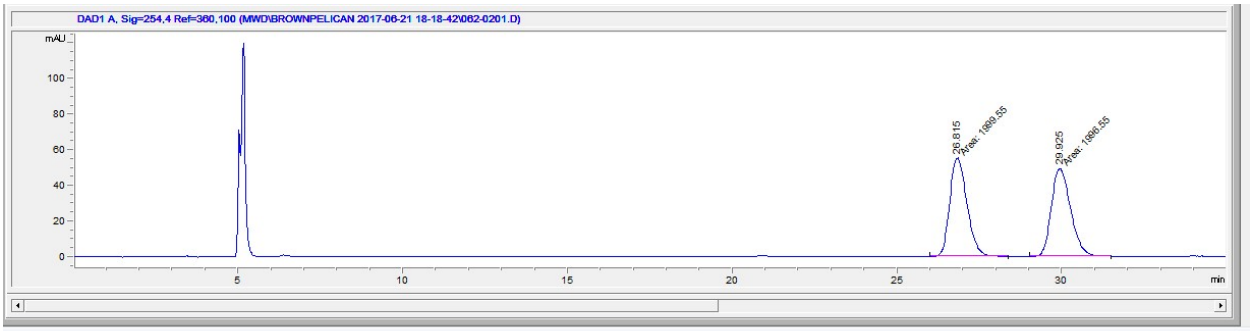
WT

NMR Yield Data



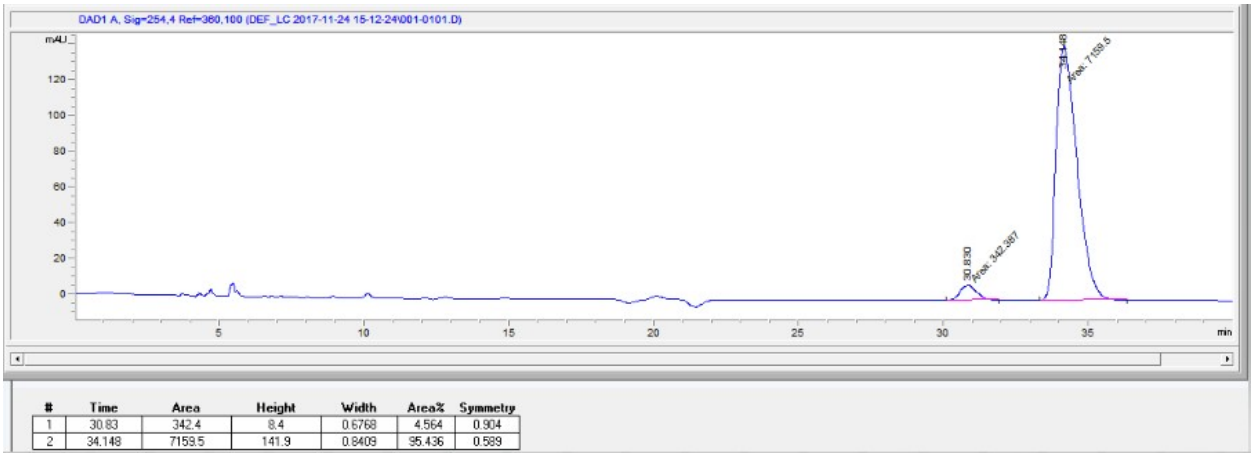
HPLC Racemic Assay (Full)

product



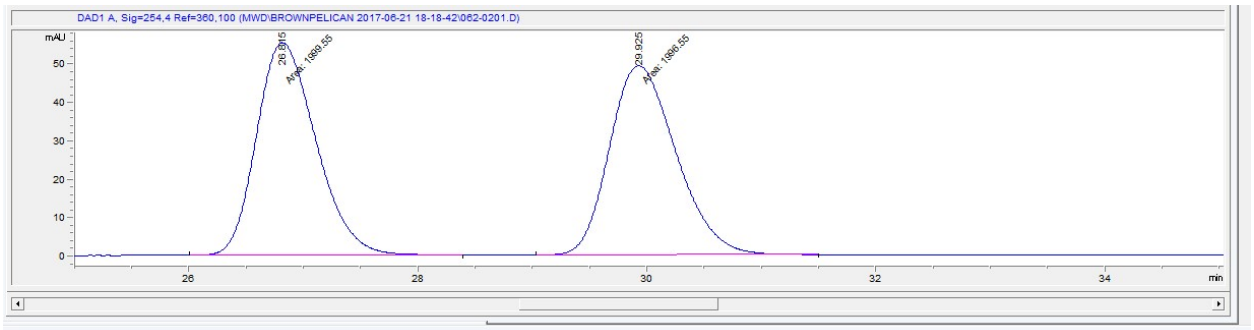
#	Time	Area	Height	Width	Area%	Symmetry
1	26.815	1999.6	55.4	0.6017	50.038	0.75
2	29.925	1996.6	49.3	0.6751	49.962	0.758

HPLC Enantioselective Assay (Full)



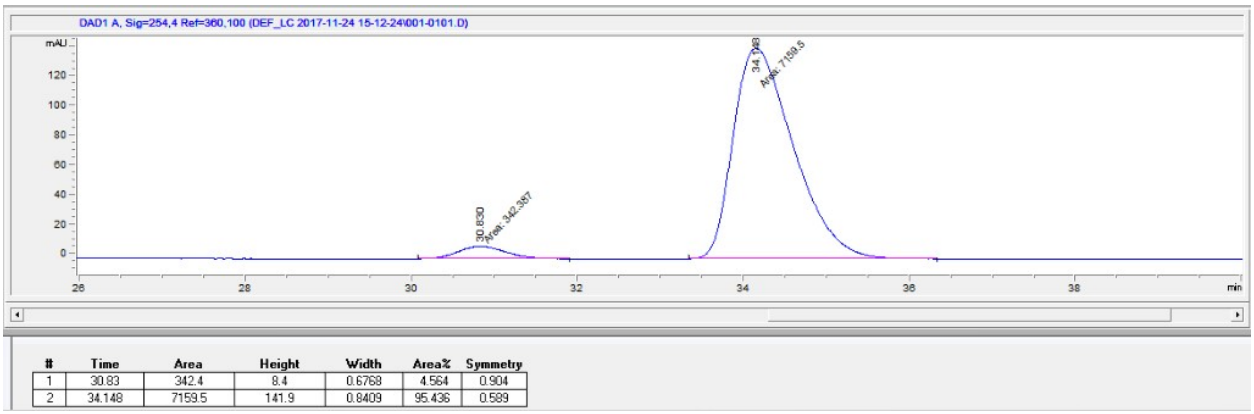
#	Time	Area	Height	Width	Area%	Symmetry
1	30.83	342.4	8.4	0.6768	4.564	0.904
2	34.148	7159.5	141.9	0.8409	95.436	0.589

HPLC Racemic Assay (Product)



#	Time	Area	Height	Width	Area%	Symmetry
1	26.815	1999.6	55.4	0.6017	50.038	0.75
2	29.925	1996.6	49.3	0.6751	49.962	0.758

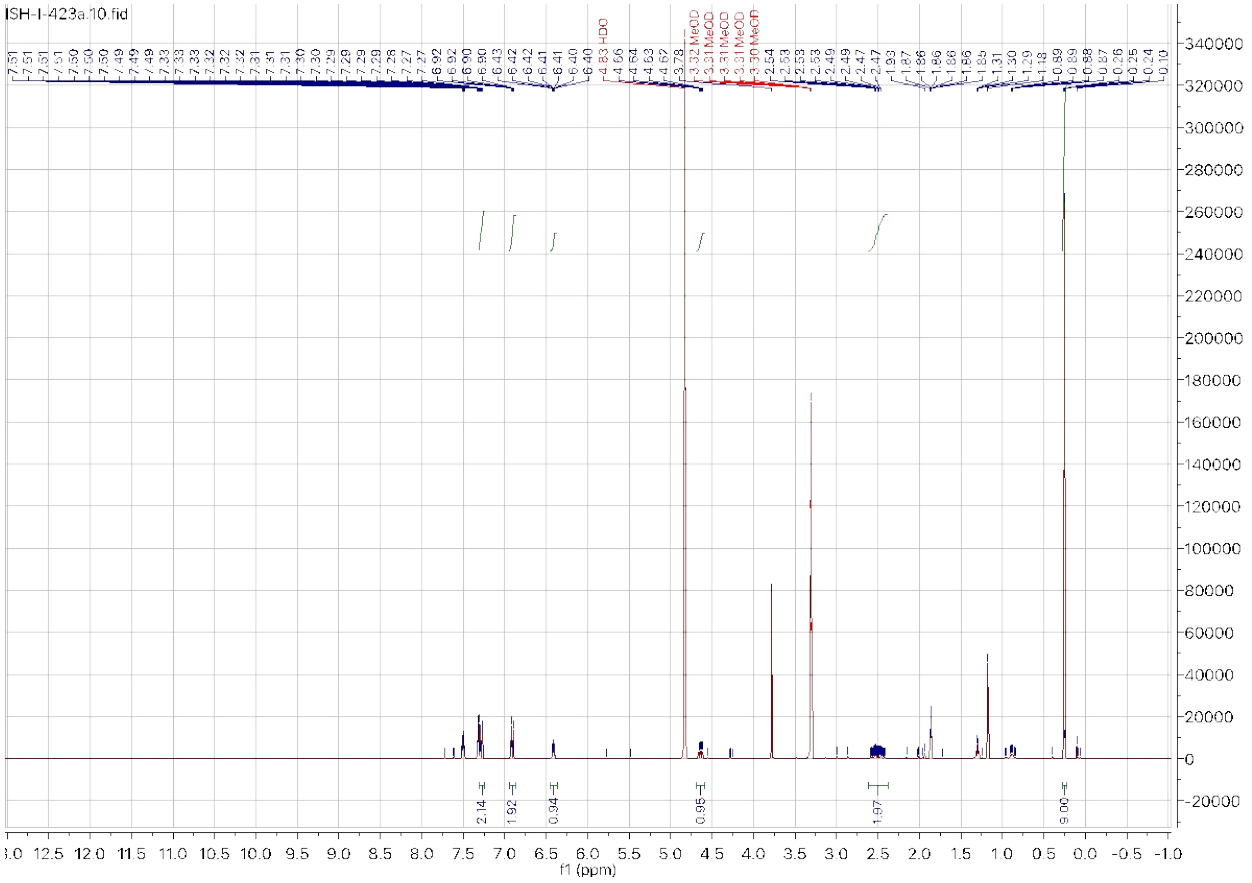
HPLC Enantioselective Assay (Product)



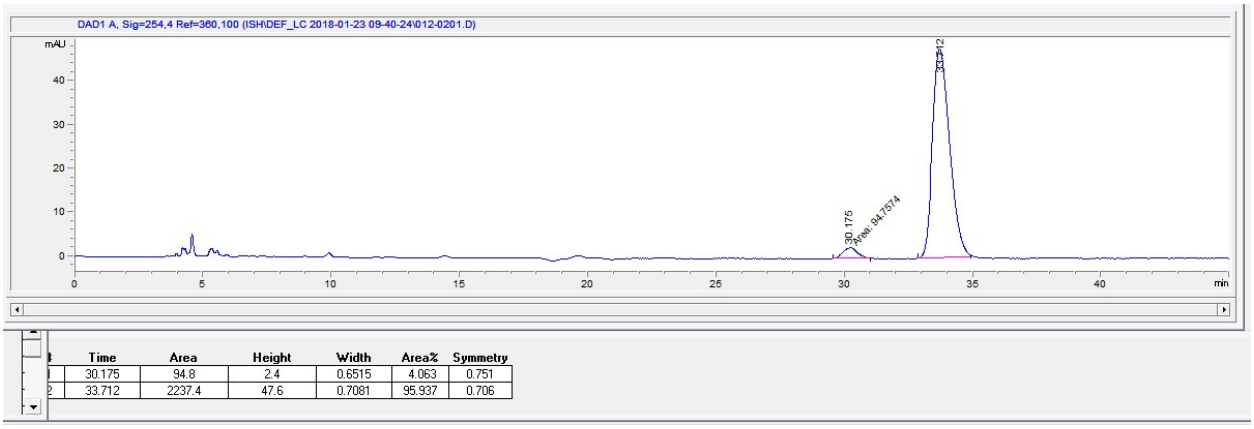
#	Time	Area	Height	Width	Area%	Symmetry
1	30.83	342.4	8.4	0.6768	4.564	0.904
2	34.148	7159.5	141.9	0.8409	95.436	0.589

T111E

NMR Yield Data

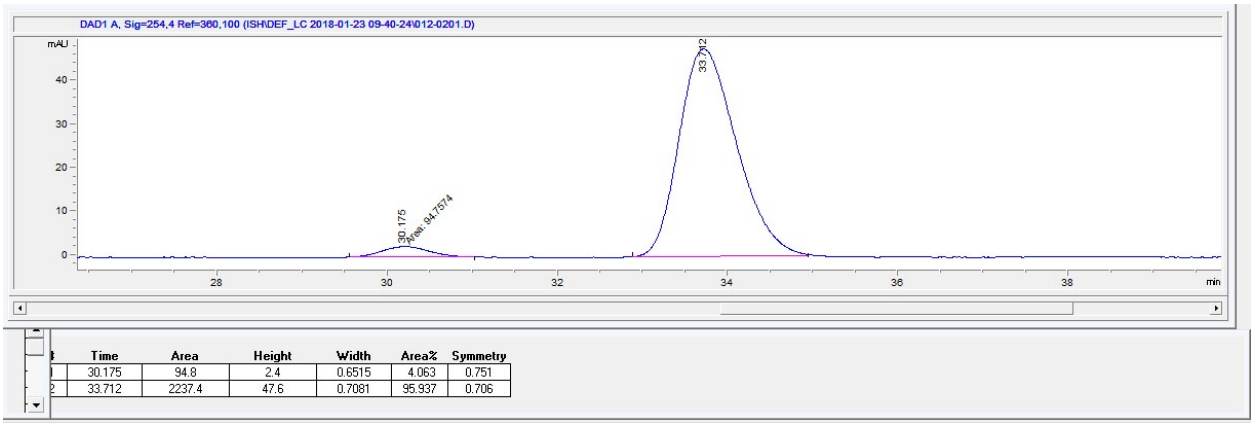


HPLC Enantioselective Assay (Full)



	Time	Area	Height	Width	Area%	Symmetry
1	30.175	94.8	2.4	0.6515	4.063	0.751
2	33.712	2237.4	47.6	0.7081	95.937	0.706

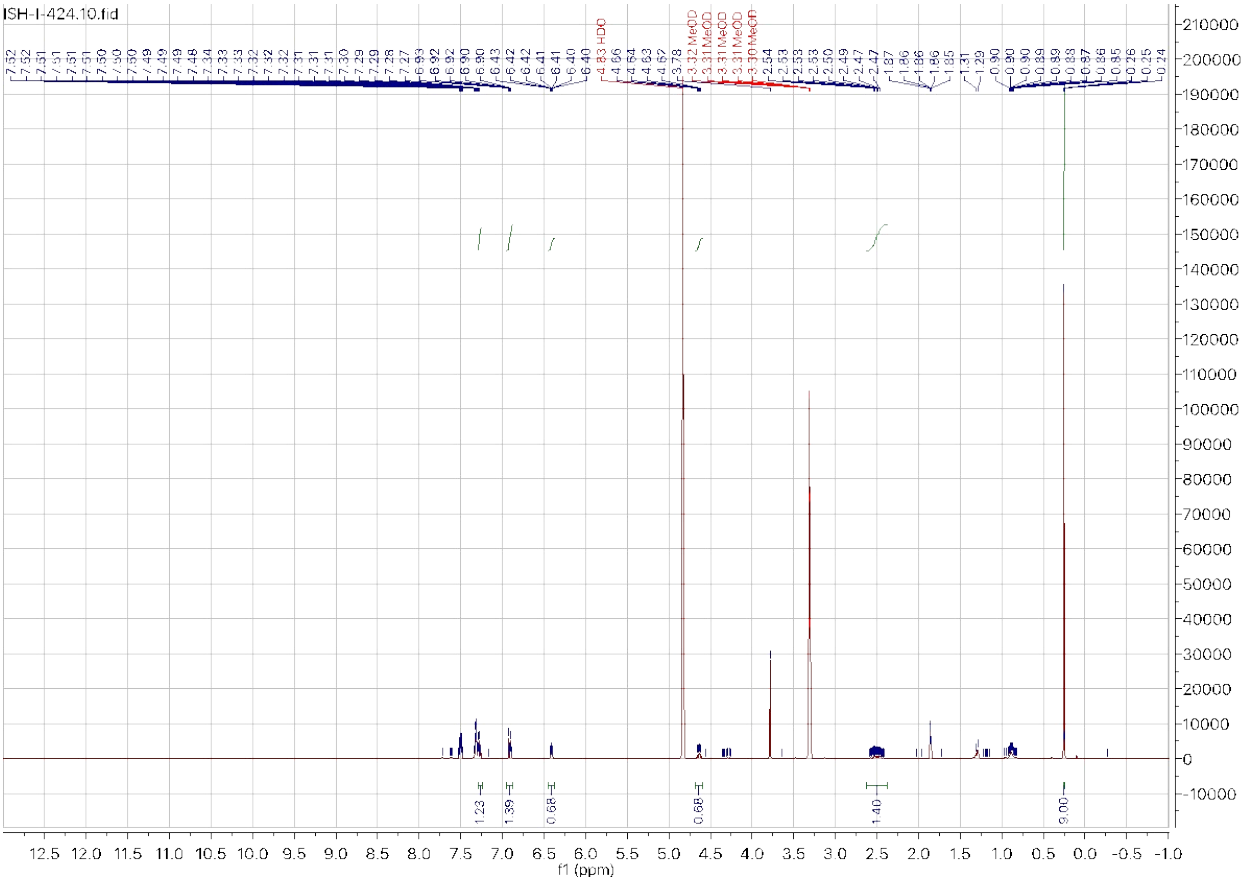
HPLC Enantioselective Assay (Product)



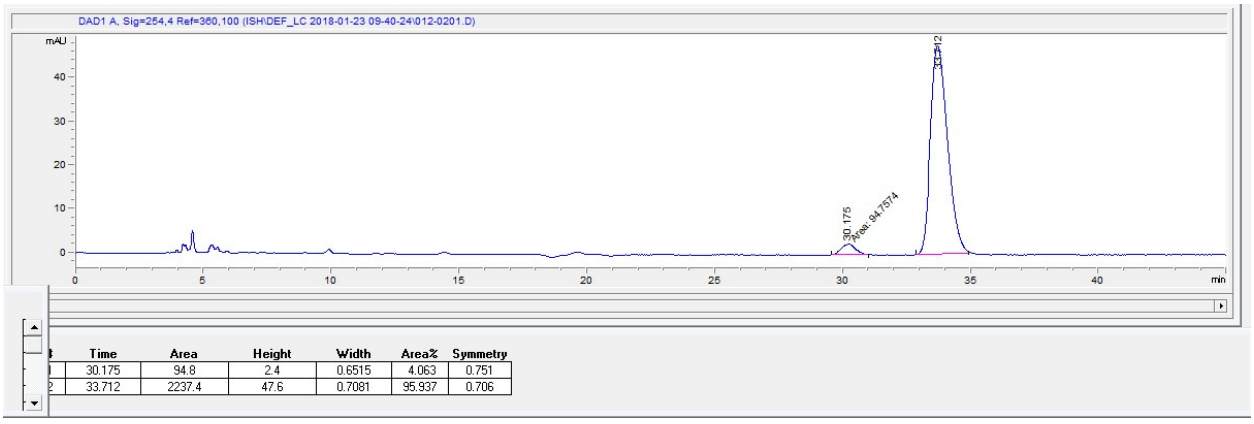
	Time	Area	Height	Width	Area%	Symmetry
1	30.175	94.8	2.4	0.6515	4.063	0.751
2	33.712	2237.4	47.6	0.7081	95.937	0.706

E113A

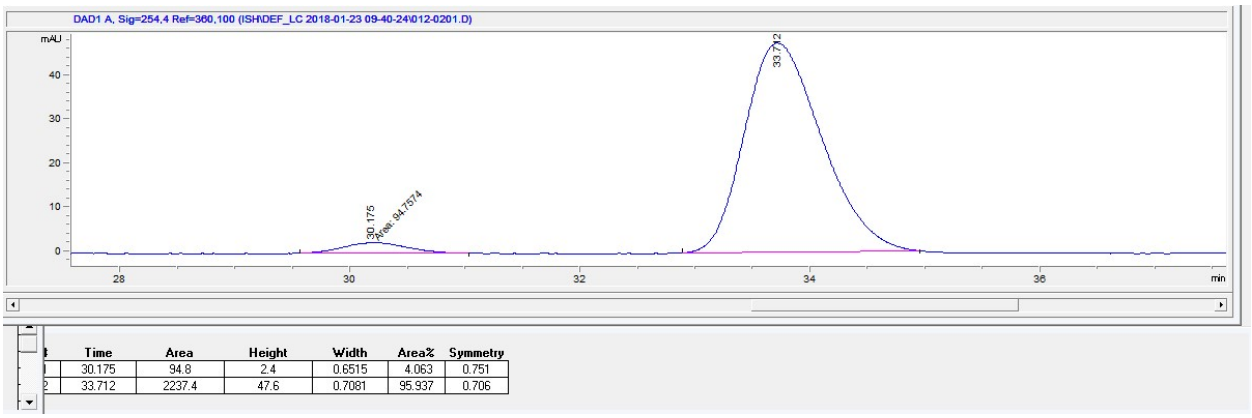
NMR Yield Data



HPLC Enantioselective Assay (Full)



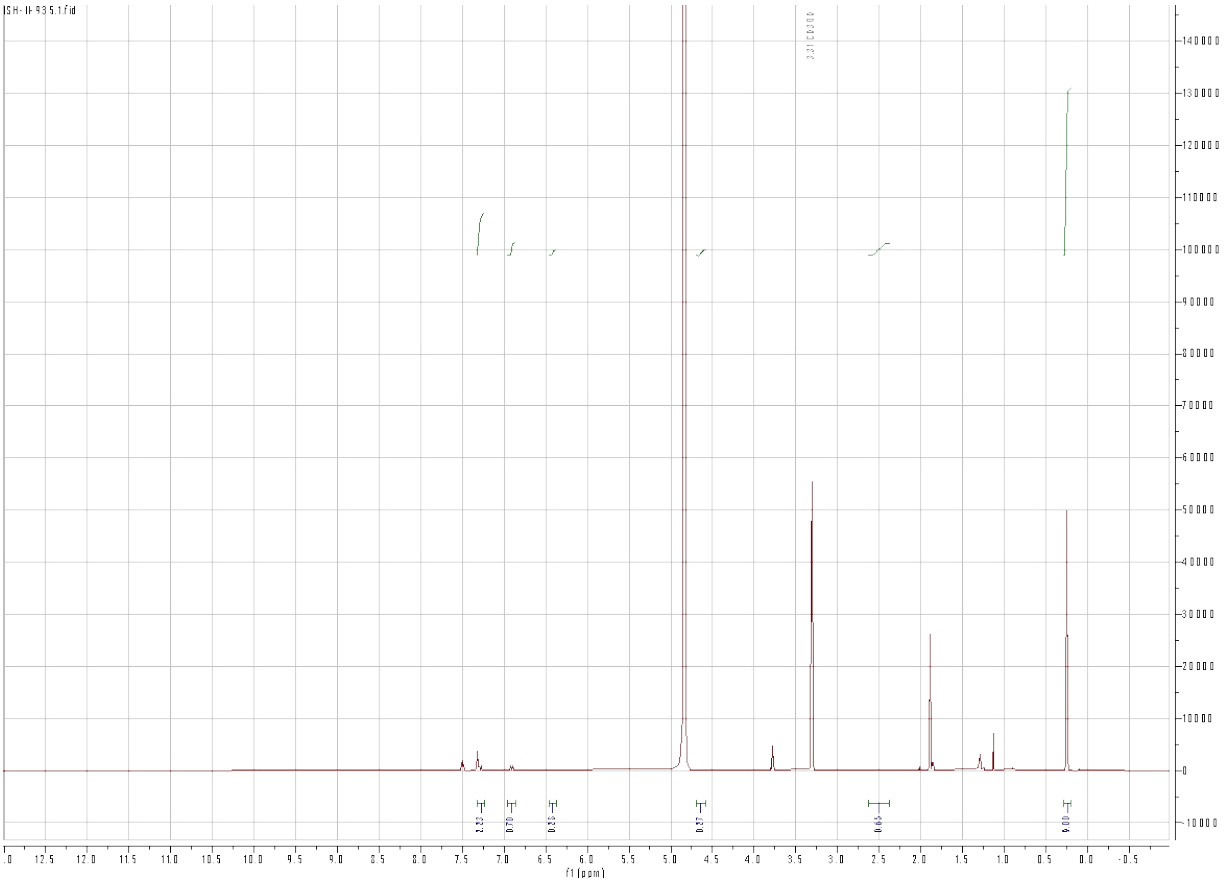
HPLC Enantioselective Assay (Product)



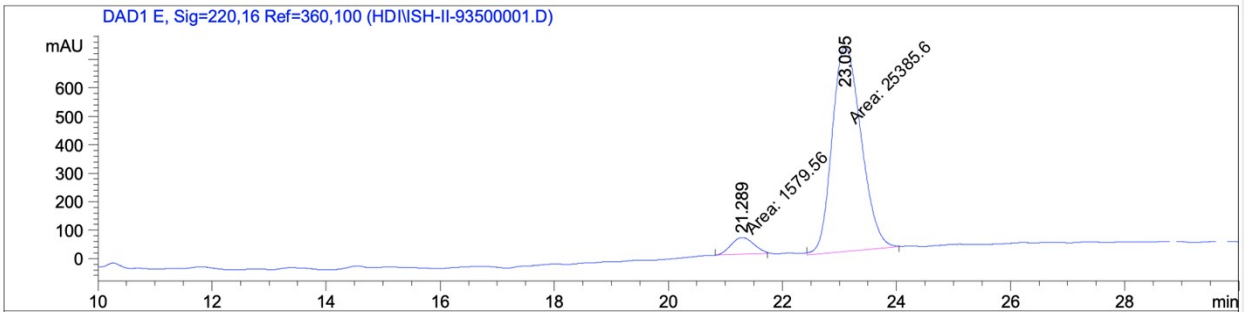
	Time	Area	Height	Width	Area%	Symmetry
1	30.175	94.8	2.4	0.6515	4.063	0.751
2	33.712	2237.4	47.6	0.7081	95.937	0.706

G49A

NMR Yield Data



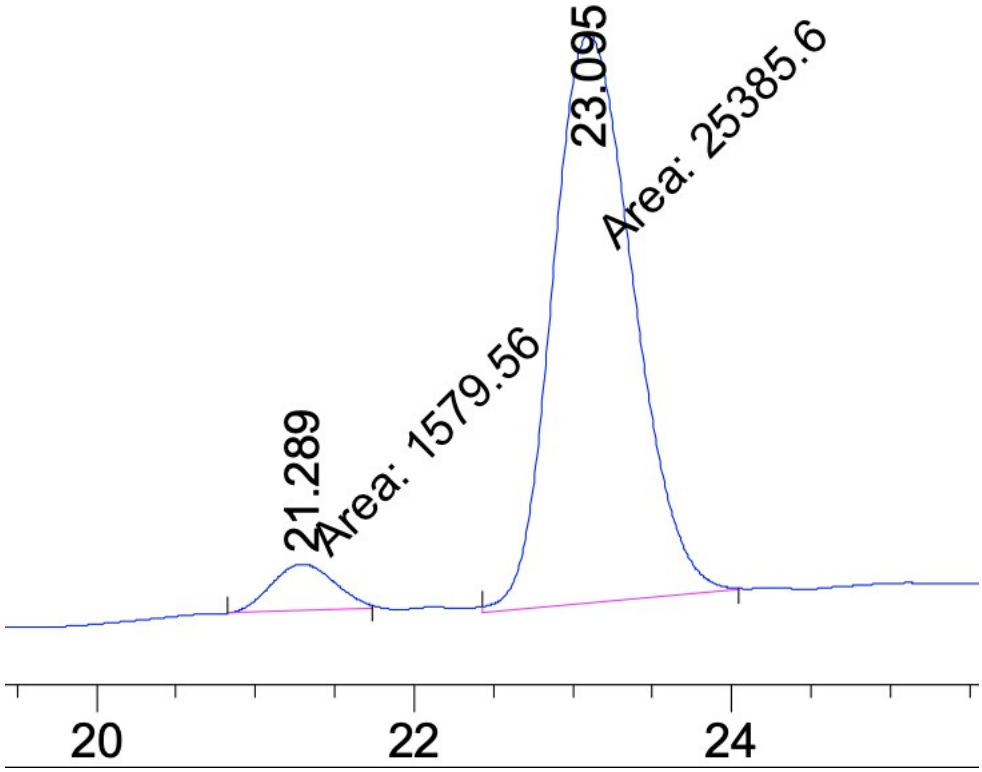
HPLC Enantioselective Assay (Full)



Signal 5: DAD1 E, Sig=220,16 Ref=360,100

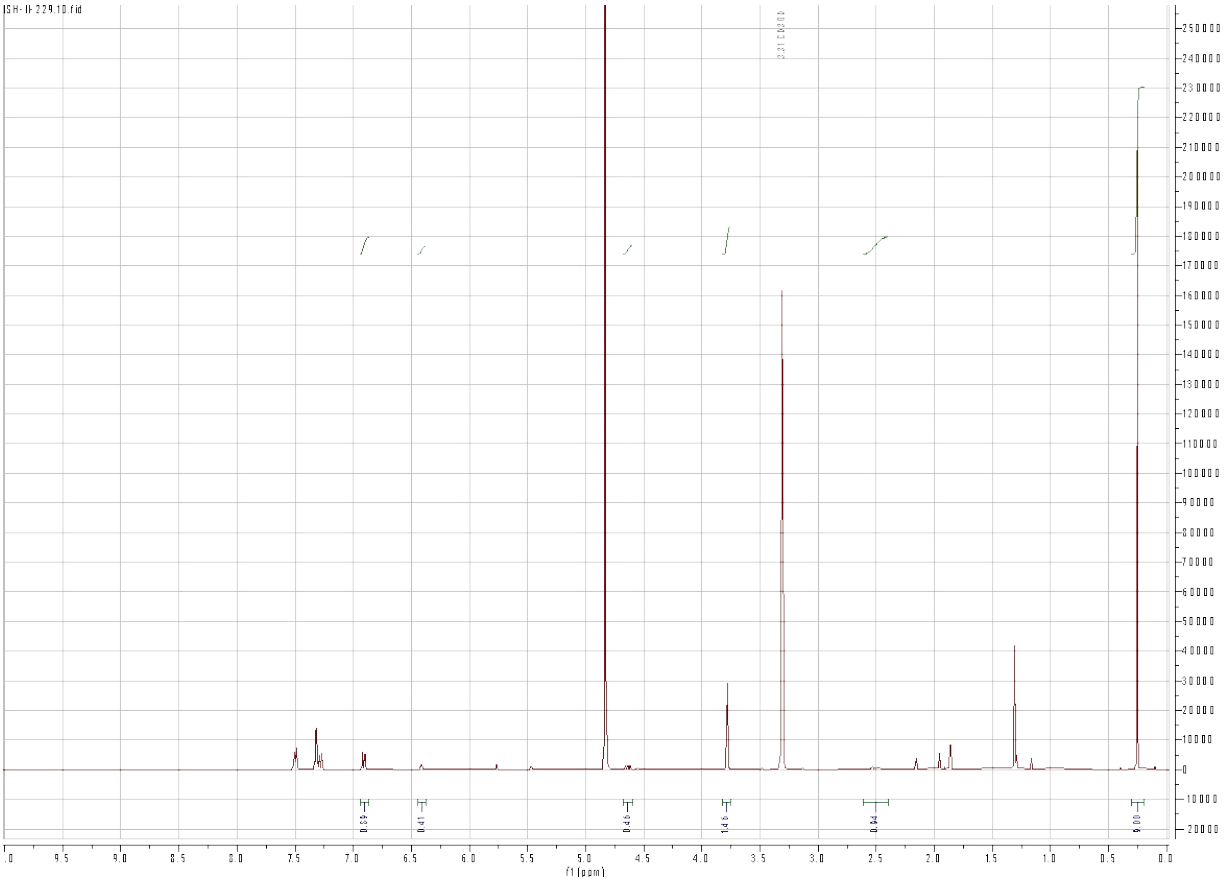
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.289	MM T	0.4537	1579.55676	58.01941	5.8578
2	23.095	MM T	0.5867	2.53856e4	721.11731	94.1422
Totals :				2.69651e4	779.13672	

HPLC Enantioselective Assay (Product)

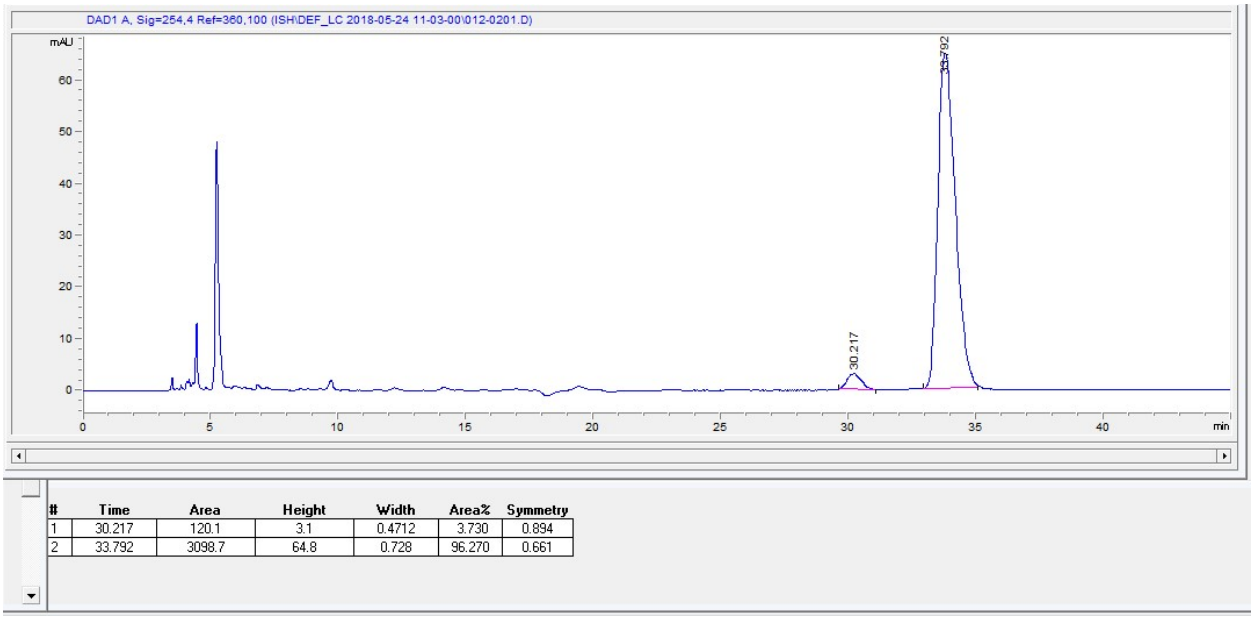


T32R

NMR Yield Data

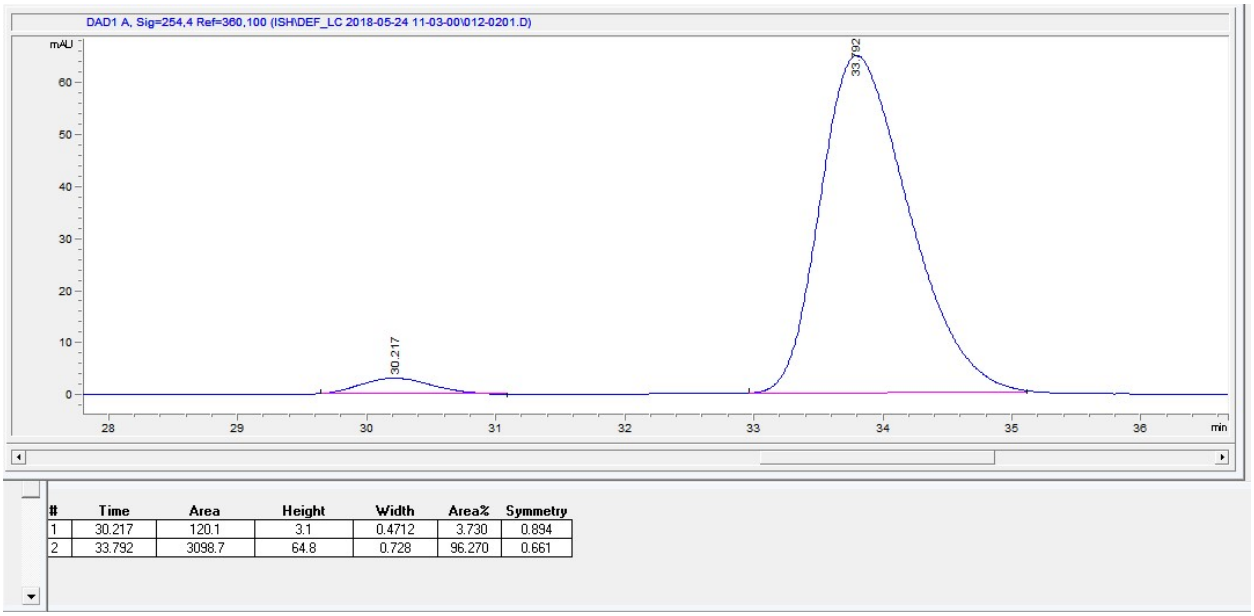


HPLC Enantioselective Assay (Full)



#	Time	Area	Height	Width	Area%	Symmetry
1	30.217	120.1	3.1	0.4712	3.730	0.894
2	33.792	3098.7	64.8	0.728	96.270	0.661

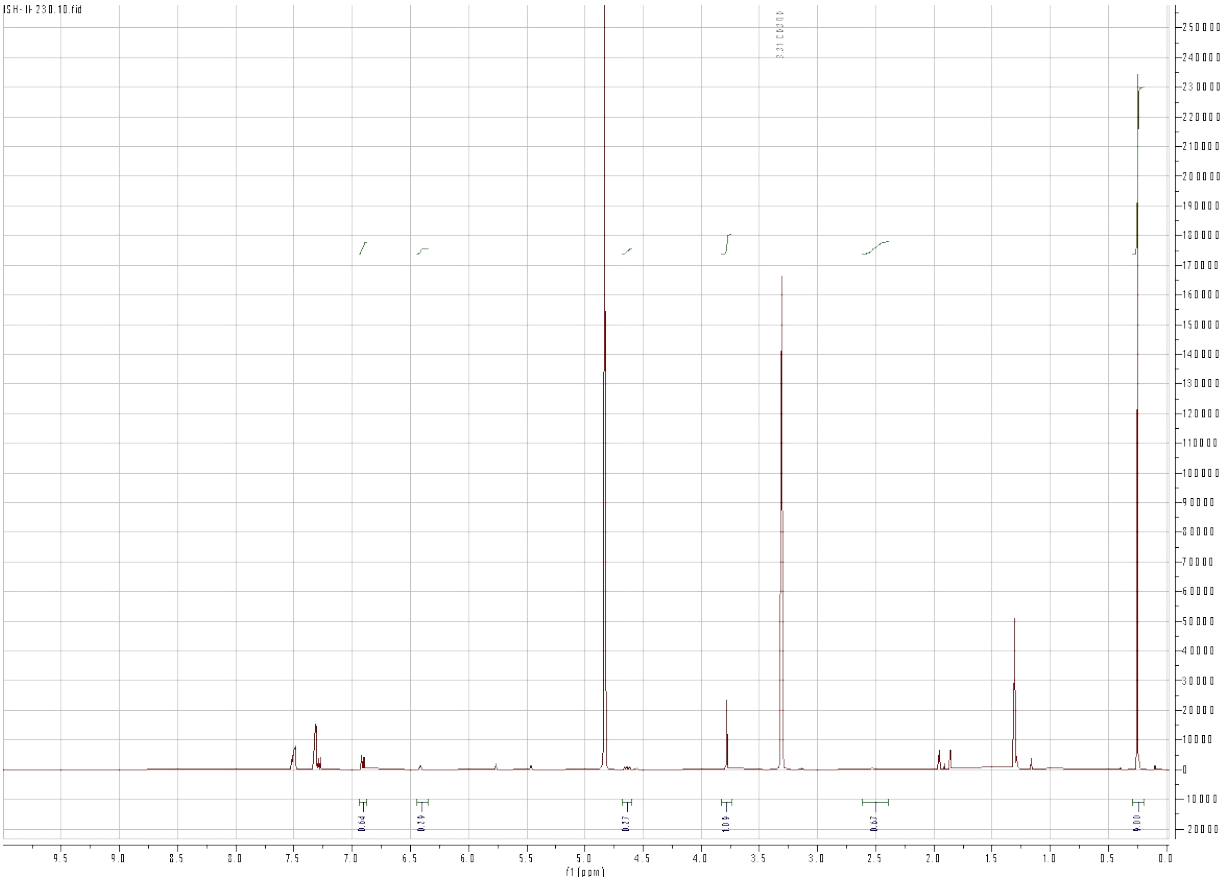
HPLC Enantioselective Assay (Product)



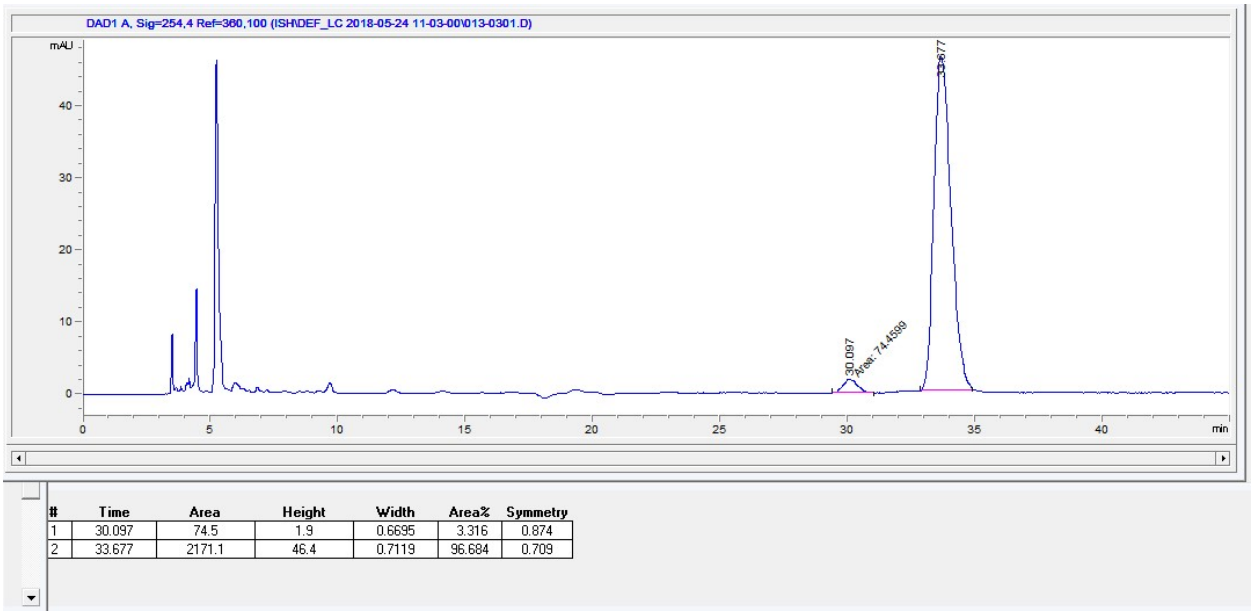
#	Time	Area	Height	Width	Area%	Symmetry
1	30.217	120.1	3.1	0.4712	3.730	0.894
2	33.792	3098.7	64.8	0.728	96.270	0.661

T111A

NMR Yield Data

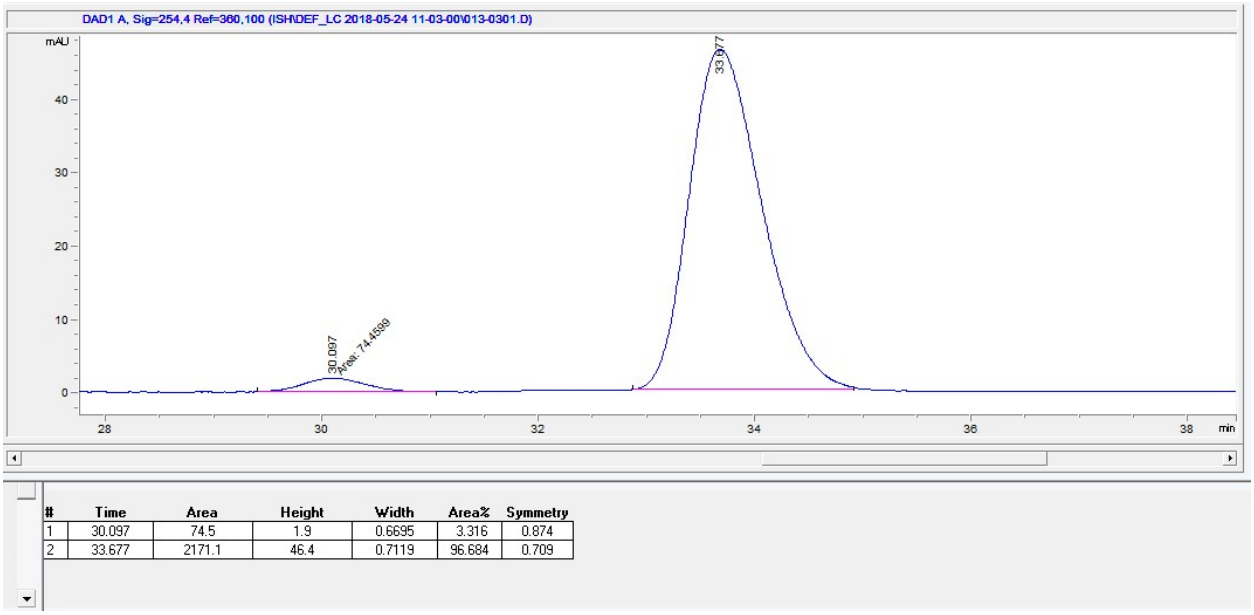


HPLC Enantioselective Assay (Full)



#	Time	Area	Height	Width	Area%	Symmetry
1	30.097	74.5	1.9	0.6695	3.316	0.874
2	33.677	2171.1	46.4	0.7119	96.684	0.709

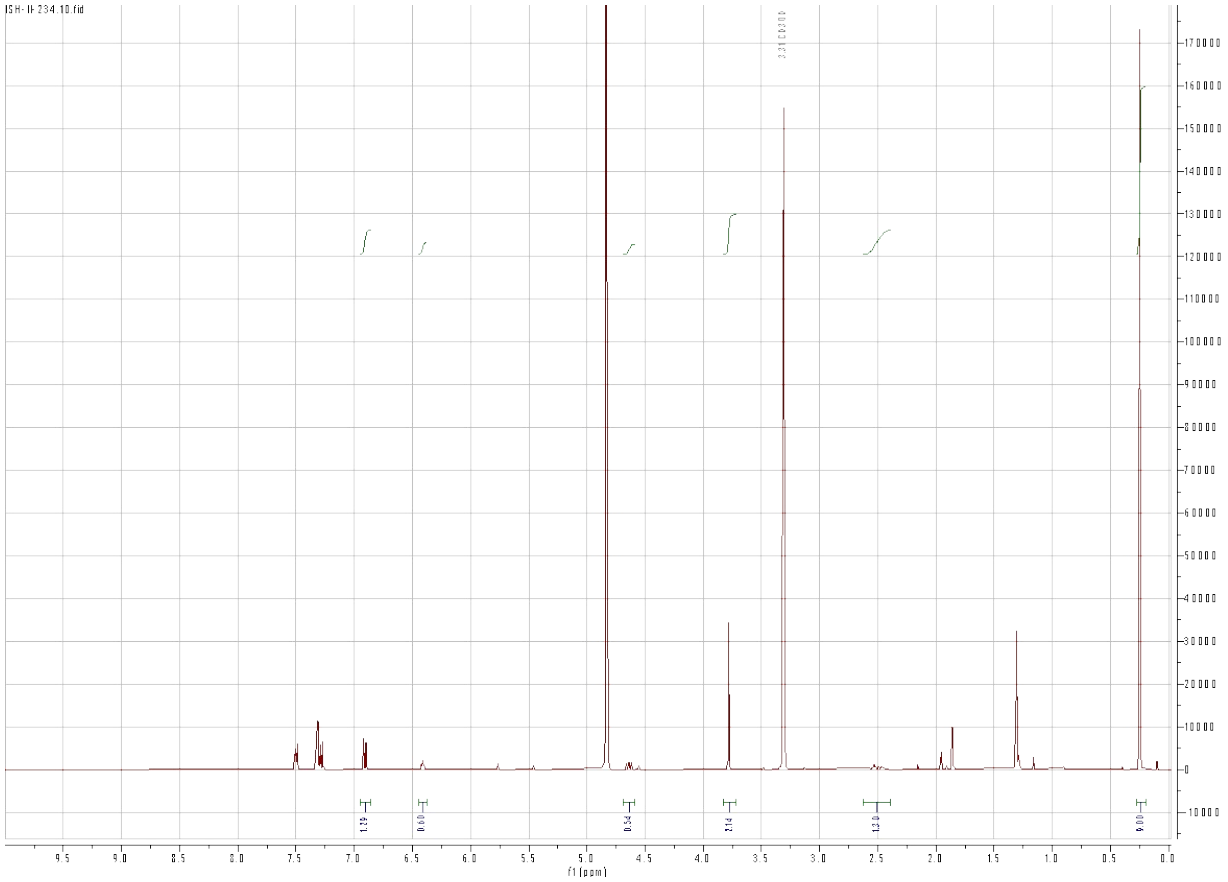
HPLC Enantioselective Assay (Product)



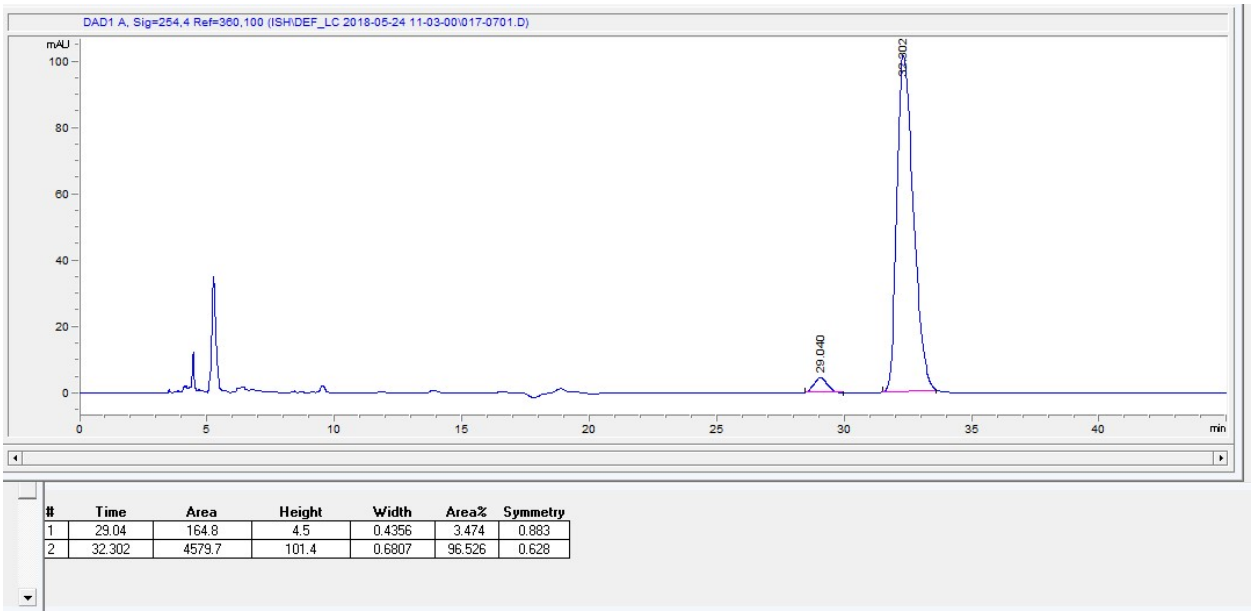
#	Time	Area	Height	Width	Area%	Symmetry
1	30.097	74.5	1.9	0.6695	3.316	0.874
2	33.677	2171.1	46.4	0.7119	96.684	0.709

H87E

NMR Yield Data

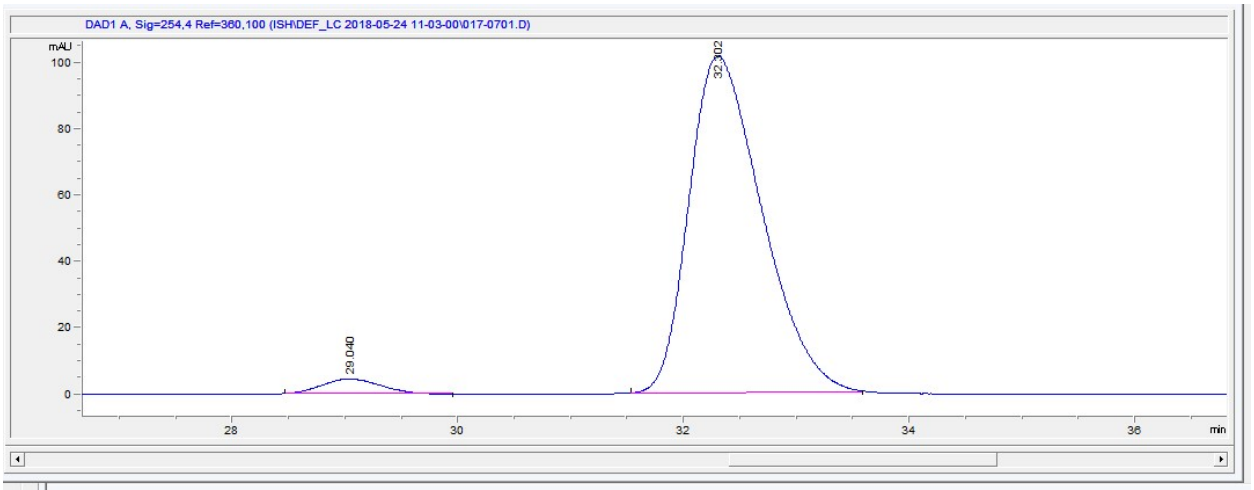


HPLC Enantioselective Assay (Full)



#	Time	Area	Height	Width	Area%	Symmetry
1	29.04	164.8	4.5	0.4356	3.474	0.883
2	32.302	4579.7	101.4	0.6807	96.526	0.628

HPLC Enantioselective Assay (Product)



#	Time	Area	Height	Width	Area%	Symmetry
1	29.04	164.8	4.5	0.4356	3.474	0.883
2	32.302	4579.7	101.4	0.6807	96.526	0.628

7. Preparation of artificial metalloenzyme

Protein production and purification:

MBP-mSav was expressed from plasmid pET-MBP-mSav purchased from addgene (plasmid #52319). Plasmid was transformed into BL21 (DE3) *E.coli* for protein production. An overnight culture was grown in LB containing kanamycin at 37 °C shaking at 200 RPM and used to inoculate 1 L (x8) of LB containing kanamycin at 37 °C shaking at 200 RPM for 3.5 hrs to an OD_{600} of 0.6-0.9. Culture was then induced with IPTG (final concentration of 1 mM) and brought to 20 °C shaking at 200 RPM overnight. Cells were harvested by centrifugation (5000 RPM for 10 min at 4 °C) and resuspended in acetate glycerol lysis buffer (10 mL, 25 mM sodium acetate, 100 mM sodium chloride, 10% glycerol, 0.2% Triton-X-100, pH 7.4) with a protease inhibitor tablet (1/2 tablet, Roche cOmplete ULTRA Tables, Mini, EDTA free, EASYpack). Cell suspension was subject to one freeze-thaw cycle at -20 °C followed by sonication (6 min cycle, 50% amplitude, over ice). Cell lysate was cleared by centrifugation (9500 RPM for 20 min at 4 °C) and the supernatant was incubated with Ni-NTA agarose resin (2 mL) rotating overnight at 4 °C. The resin was collected by centrifugation (4750 RPM for 10 min at 4 °C) and washed with acetate wash buffer (50 mL, 25 mM sodium acetate, 100 mM sodium chloride, 50 mM imidazole, pH 7.4). Protein was then eluted with acetate elution buffer (12 mL, 25 mM sodium acetate, 100 mM sodium chloride, 400 mM imidazole, pH 7.4) and dialyzed in acetate buffer (2 L, 25 mM sodium acetate, 100 mM sodium chloride, pH 7.4) overnight. Purified protein was then observed by SDS-PAGE.

Protein cleavage and re-purification:

Purified MBP-mSav was then subjected to a TEV protease cleavage. TEV protease was expressed from plasmid pRK793 purchased from addgene (plasmid #8827). An overnight culture was grown in LB containing chloramphenicol and carbenicillin at 37 °C shaking at 200 RPM and used to inoculate 1 L (x2) of LB containing chloramphenicol and carbenicillin at 37 °C shaking at 200 RPM for 3 hrs to an OD_{600} of ~0.5. Culture was then induced with IPTG (final concentration of 1 mM) and brought to 30 °C shaking at 200 RPM overnight. Cells were harvested by centrifugation (5000 RPM for 10 min at 4 °C) and resuspended in acetate glycerol lysis buffer (10 mL, 25 mM sodium acetate, 100 mM sodium chloride, 10% glycerol, 0.2% Triton-X-100, pH 7.4) with a protease inhibitor tablet (1/2 tablet, Roche cOmplete ULTRA Tables, Mini, EDTA free, EASYpack). Cell suspension was subject to one freeze-thaw cycle at -20 °C followed by sonication (2 min cycle, 50% amplitude, over ice). Cell lysate was cleared by centrifugation (9500 RPM for 20 min at 4 °C) and the supernatant was incubated with Ni-NTA agarose

resin (1 mL) rotating for 30 min at 4 °C. The resin was collected by centrifugation (4750 RPM for 10 min at 4 °C) and washed with acetate wash buffer (50 mL, 25 mM sodium acetate, 100 mM sodium chloride, 50 mM imidazole, pH 7.4). Protein was then eluted with acetate elution buffer (12 mL, 25 mM sodium acetate, 100 mM sodium chloride, 400 mM imidazole, pH 7.4) and dialyzed in acetate buffer (2 L, 25 mM sodium acetate, 100 mM sodium chloride, pH 7.4) overnight. Purified protein was then observed by SDS-PAGE.

Purified TEV protease was then added to purified MBP-mSav (100 mg protein to 1 mg protease) and rotated for 48 hrs at 4 °C. Ni-NTA resin was then added to cleavage mixture and rotated for ~12 hrs at 4 °C. Supernatant was separated from the resin. Cleaved and re-purified protein was observed by SDS-PAGE.

Metalloenzyme preparation:

The metalloenzyme was prepared by incubating purified mSav with Cp*biotinRh (30uM protein:60uM biotin) in acetate buffer at RT rotating overnight. Mixtures were then centrifuged to eliminate any precipitation (14000 RPM, 10 min) and transferred to a 10 kDa MWCO ultracentrifugal filter unit for several washes with acetate buffer. Protein solution will now have a yellowish tint due to binding of Rh.

8. Protein sequences

mSav –
GAEAGITGTWYNQHGSTFTVTAGADGNLTGQYENRAQGTGCQNSPYTLTGRYNGTKLEWRVE
WNNSTENCHSRTEWRGQYQGGAEARINTQWNLTYEGGSGPATEQGQDTFTKVKPSAASGSDY
KDDDDK

mSav T32R–

GAEAGITGTWYNQHGSTFTVRAGADGNLTGQYENRAQGTGCQNSPYTLTGRYNGTKLEWRVE
WNNSTENCHSRTEWRGQYQGGAEARINTQWNLTYEGGSGPATEQGQDTFTKVKPSAASGSDY
KDDDDK

mSav H87E –

GAEAGITGTWYNQHGSTFTVTAGADGNLTGQYENRAQGTGCQNSPYTLTGRYNGTKLEWRVE
WNNSTENCESRTEWRGQYQGGAEARINTQWNLTYEGGSGPATEQGQDTFTKVKPSAASGSDYK
DDDDK

mSav T111E –

GAEAGITGTWYNQHGSTFTVTAGADGNLTGQYENRAQGTGCQNSPYTLTGRYNGTKLEWRVE
WNNSTENCHSRTEWRGQYQGGAEARINTQWNLEYEGGSGPATEQGQDTFTKVKPSAASGSDY
KDDDDK

mSav T111A –

GAEAGITGTWYNQHGSTFTVTAGADGNLTGQYENRAQGTGCQNSPYTLTGRYNGTKLEWRVE
WNNSTENCHSRTEWRGQYQGGAEARINTQWNLEAYEGGSGPATEQGQDTFTKVKPSAASGSD
YKDDDDK

mSav E113A –

GAEAGITGTWYNQHGSTFTVTAGADGNLTGQYENRAQGTGCQNSPYTLTGRYNGTKLEWRVE
WNNSTENCHSRTEWRGQYQGGAEARINTQWNLTYAGGSGPATEQGQDTFTKVKPSAASGSDY
KDDDDK

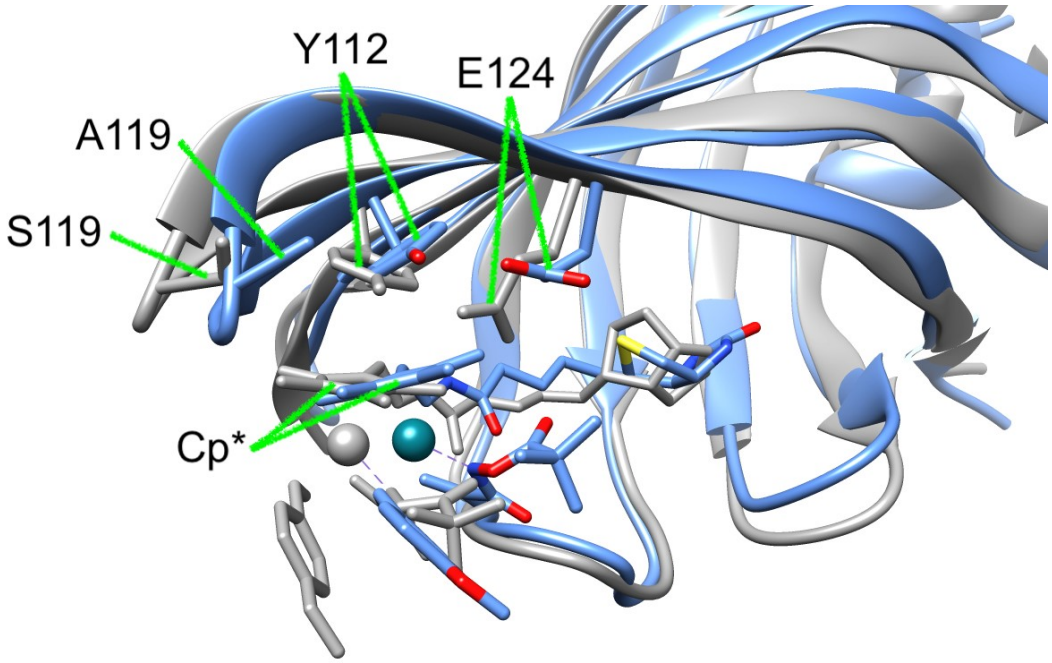
mSav G49A –

GAEAGITGTWYNQHGSTFTVTAGADGNLTGQYENRAQGTACQNSPYTLTGRYNGTKLEWRVE
WNNSTENCHSRTEWRGQYQGGAEARINTQWNLTYEGGSGPATEQGQDTFTKVKPSAASGSDY
KDDDDK

9. Protein data bank

mSav – 4JNJ

10. **Overlay of representative WT and T111E S119A structures**

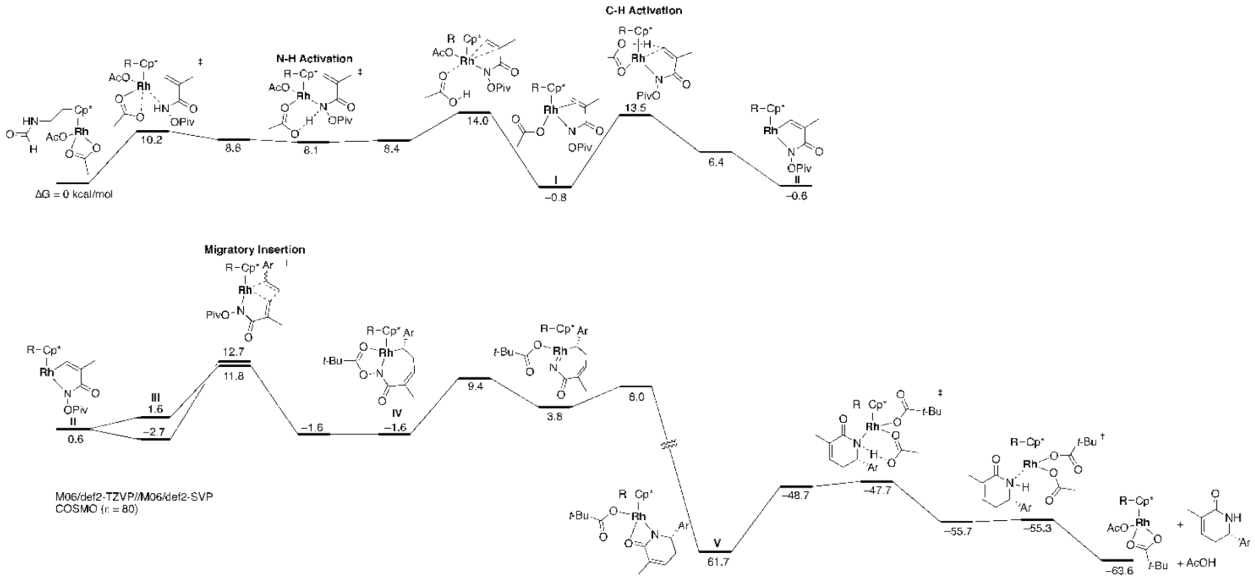


11. Computational methods

All quantum-mechanical calculations were performed in Turbomole (1-13) with the M06 density functional (14). Geometries were optimized with the def2-SVP basis set, and final electronic energies were calculated with the def2-TZVP basis set (15). The conductor-like screening model (COSMO) was used as an implicit solvent model with a dielectric of 80 to simulate water (16) for the mechanistic calculations. For the scan represented in Figure 5a of the text, the calculations were performed in vacuum with the following atoms frozen: the methyl group of acetate, the methyl group of 4-methylphenol, and the 11 atoms corresponding to the linker between Cp* and biotin.

Full enzymes were modeled with QM/DMD (17). QM/DMD is a hybrid quantum mechanics/molecular mechanics (QM/MM) method that simulates proteins piecewise. Discrete molecular dynamics (DMD) equilibrates the entire system except for the metal and part of the substrate (18). After a trajectory of ~0.5 ns, quantum mechanics (QM) is used to optimize the metal region plus sidechains and residues immediately surrounding it. This process is repeated, providing efficient sampling of the entire protein scaffold while treating the metal environment quantum-mechanically. For this study, the migratory insertion transition state was modeled in WT by freezing the coordinates of the rhodium atom and the two carbon atoms forming a bond. For each system, five replicate simulations were run for ~20 ns each. The QM region consisted of the side chains of C86, S88, Y112, and E113; the segment from the T48 carbonyl to the C50 sidechain; the segment from the G115 alpha-carbon to the S119 sidechain; and the Rh complex up to the amide of the linker, inclusive.

12. **Calculated free energy surface**



13. **M06/def2-TZVP//M06/def2-SVP COSMO(□ = 80)-solvated energies (Ha) and XYZ coordinates (Å)**

N-(Pivaloyloxy)Methacrylamide
Electronic Energy: -632.228828814
Free Energy Correction: 0.191609217

N	31.628965779	-15.411817810	-20.509552136
C	31.488722522	-15.456453766	-23.327741245
C	32.783078821	-15.626367942	-21.230350674
O	33.806685691	-16.029080785	-20.711063742
C	32.664181335	-15.355339699	-22.692941488
H	31.418305104	-15.274678032	-24.404930042
C	33.958892297	-15.040522549	-23.366041232
H	34.441068792	-14.158765942	-22.911541032
H	34.664897169	-15.877931740	-23.242519521
H	33.814102559	-14.851353285	-24.438707353
O	31.735873218	-15.563590929	-19.149959925
C	32.366534149	-14.524135954	-18.513231854
O	32.650257404	-13.509677687	-19.085305255
C	32.680269732	-14.882227171	-17.078040026
C	32.942642651	-13.601004407	-16.297431458
H	32.044190214	-12.963002812	-16.261212392
H	33.226411826	-13.852282227	-15.262599187
H	33.759083154	-13.015536694	-16.747119031
C	31.549625527	-15.676679359	-16.428663114
H	30.604697092	-15.108529412	-16.431979878
H	31.376634868	-16.638762529	-16.933549829
H	31.814198496	-15.886013646	-15.379198911
C	33.956936306	-15.731591183	-17.143243887
H	34.251483441	-16.028250178	-16.122867080
H	33.802724950	-16.639426308	-17.747495109
H	34.787388412	-15.160851890	-17.591306457
H	30.568385956	-15.744589586	-22.811046267
H	30.982184782	-14.673677957	-20.786958914

p-Methoxystyrene
Electronic Energy: -424.020085596
Free Energy Correction: 0.132211007

C	29.433871156	-16.596918597	-21.662090608
H	29.970178901	-17.406638165	-21.153970136
C	29.471035357	-16.432478912	-22.990626221
H	28.905906036	-15.597880155	-23.428523007
C	30.194457190	-17.253032466	-23.966403363
C	30.112408671	-16.937409707	-25.327557956
C	30.982490374	-18.362514169	-23.604240922
C	30.776890522	-17.680781788	-26.302757182
C	31.648912586	-19.111049932	-24.557898437
C	31.553551537	-18.778729052	-25.919791163
H	29.506960009	-16.078670901	-25.637994666
H	31.075921019	-18.646641069	-22.551156258

H	30.679987538	-17.392690377	-27.352042313
H	32.260468953	-19.973422898	-24.276368144
O	32.236118481	-19.565840066	-26.775061527
C	32.177139518	-19.277037456	-28.151123968
H	31.143575230	-19.335726343	-28.535573656
H	32.582773926	-18.274316759	-28.374353228
H	32.788988992	-20.029335458	-28.665027179
H	28.856493395	-15.918876308	-21.027201722

Acetic Acid
Electronic Energy: -229.068686332
Free Energy Correction: 0.035604647

H	16.340124022	-21.991925645	0.205261264
O	16.339578245	-22.471035309	1.053085568
O	16.339932502	-20.380087135	1.831091462
C	16.339764569	-21.570826920	2.039533100
C	16.339828020	-22.218711412	3.383474577
H	17.224261962	-22.865707906	3.484220094
H	16.339874627	-21.457361057	4.171854081
H	15.455542261	-22.865884522	3.484355785

Acetate
Electronic Energy: -228.600302349
Free Energy Correction: 0.022647115

O	16.339292155	-22.443641029	1.028748919
O	16.340164348	-20.371850229	1.871944869
C	16.339757834	-21.618776273	1.971827063
C	16.339849836	-22.217234868	3.383217152
H	17.222029874	-22.866510094	3.512412450
H	16.339676565	-21.444795664	4.167075368
H	15.457978754	-22.866937297	3.512352795

Pivalic Acid
Electronic Energy: -346.955994067
Free Energy Correction: 0.115082841

H	16.337871809	-21.976582986	0.197700340
O	16.336478016	-22.466117402	1.039497505
O	16.341954208	-20.386770217	1.836095369
C	16.339485813	-21.579433033	2.036487281
C	16.339835806	-22.244450394	3.402173970
C	17.593109514	-23.114648549	3.525120545
H	17.617336092	-23.583809707	4.522729376
H	17.607624689	-23.914769950	2.769338138
H	18.511375123	-22.514200049	3.411717563
C	16.339577728	-21.173575970	4.483042824
H	15.448294275	-20.530311643	4.410623351
H	16.341273124	-21.649236058	5.477680738
H	17.228854519	-20.527813581	4.408630756
C	15.087840413	-23.116264793	3.526121820

H	15.074283726	-23.917181377	2.771174994
H	15.064411659	-23.584512250	4.524180893
H	14.168719988	-22.517211826	3.412269602

Catalyst
Electronic Energy: -1165.500944705
Free Energy Correction: 0.322871834

N	0.107839724	-1.496735432	-4.757575786
C	2.072230979	2.583752877	-0.741879811
C	1.879757718	2.197250380	-2.116052349
C	1.748581741	0.766656136	-2.174243469
C	1.841783326	0.270782793	-0.826828541
C	2.062293643	1.382261379	0.058294866
C	1.610628652	-0.069030353	-3.406397732
C	0.174511327	-0.472459316	-3.741789984
C	0.314680642	-2.790294564	-4.450053198
C	1.674130106	-1.142057400	-0.406645949
C	1.772142998	3.104918330	-3.282362616
C	2.308288478	1.300180177	1.518502503
C	2.251331046	3.962597662	-0.224042404
O	0.555378694	-3.206125375	-3.327742512
Rh	0.195224542	1.624044642	-0.949923722
H	-0.404373280	0.404431449	-4.074026573
H	-0.320222689	-0.853072715	-2.832613515
H	2.206290948	-0.987576894	-3.268443012
H	2.057407875	0.461889236	-4.263876999
H	-0.049963732	-1.244834095	-5.728738012
H	3.323460411	4.198227182	-0.114008955
H	1.778661510	4.078239789	0.762781449
H	1.811475904	4.709770826	-0.900741004
H	2.754368455	3.206060247	-3.774887190
H	1.441043159	4.110560013	-2.985411054
H	1.062698083	2.711642780	-4.026291067
H	3.388892658	1.169096821	1.702508011
H	1.769762915	0.457927407	1.971919343
H	1.990865969	2.217862288	2.035235912
H	2.640840369	-1.558640966	-0.076365903
H	1.289082315	-1.772432513	-1.223501494
H	0.978167080	-1.205948544	0.445257357
H	0.236898016	-3.461128267	-5.337410918
O	-0.918813892	2.700175320	0.448736446
C	-1.152244057	2.134383751	1.584430535
O	-0.751859368	1.022856791	1.919226733
C	-2.008979239	2.970685437	2.508327475
H	-3.035096520	3.016893766	2.110053678
H	-1.635934608	4.004645153	2.554397548
H	-2.036450145	2.535570217	3.516389704
O	-1.594309604	0.322796139	-1.060601630
C	-2.140103906	1.108503270	-1.884566553

O	-1.491191994	2.118503024	-2.285396986
C	-3.497986414	0.815275400	-2.430214565
H	-4.091317301	0.229022393	-1.716039394
H	-3.377770907	0.212550159	-3.346253872
H	-4.023251094	1.740415257	-2.702873319

Substrate Association TS
Electronic Energy: -1797.742016249
Free Energy Correction: 0.542902304

N	-0.218084983	-3.043123270	-3.345724757
C	1.692276140	2.402533429	-1.560088528
C	1.186621069	1.584970722	-2.661954428
C	1.438325946	0.220559350	-2.345736634
C	2.056760220	0.176749870	-1.038319222
C	2.245216183	1.528780946	-0.572799031
C	1.145052578	-0.976275970	-3.189644146
C	-0.110497690	-1.730277755	-2.756063089
C	0.444796271	-4.094348475	-2.832153781
C	2.480843070	-1.049484912	-0.324232338
C	0.501929523	2.094481207	-3.873099770
C	2.842527334	1.906518451	0.730132014
C	1.569814229	3.874843798	-1.474505561
O	1.189211520	-4.040399481	-1.865211852
N	-0.464730925	-1.184151419	1.224263922
C	-2.397681521	-2.573058970	-0.316863836
Rh	0.163331430	1.149681977	-0.864224872
H	-1.012711549	-1.145916858	-2.986172756
H	-0.108779940	-1.849814293	-1.659671223
H	2.010304432	-1.658563305	-3.121155003
H	1.066235515	-0.678764186	-4.248173736
H	-0.804941372	-3.188746086	-4.161635969
H	2.363511155	4.359997852	-2.067903031
H	1.652875556	4.225016617	-0.436323423
H	0.599758842	4.206779338	-1.875488537
H	1.238984031	2.351959098	-4.652928432
H	-0.084192517	2.995981750	-3.643448986
H	-0.184877514	1.341169729	-4.288018037
H	3.939561768	1.983406166	0.651142431
H	2.611103574	1.142853939	1.488436090
H	2.454876636	2.870229800	1.090895800
H	3.576239722	-1.154467033	-0.420788465
H	2.012953636	-1.957885580	-0.732647881
H	2.245670122	-0.994988314	0.750456302
C	-0.393532477	-2.555150431	1.162200147
O	0.499499325	-3.173259732	1.717756313
C	-1.448951500	-3.241178024	0.354622402
H	-3.151370880	-3.125350286	-0.889352359
C	-1.340007688	-4.731077565	0.359121973
H	-0.361852272	-5.036332183	-0.047692770

H	-1.394730298	-5.135210068	1.383430157
H	-2.136769902	-5.187109425	-0.246289593
O	0.370696331	-0.606291578	2.156419125
C	-0.031962401	-0.762455499	3.451100495
O	-1.037119423	-1.344101642	3.750962554
C	0.942616111	-0.079196050	4.386527337
C	0.600003634	-0.465789670	5.818214818
H	0.708184857	-1.551182907	5.976951796
H	1.279995173	0.052200330	6.513691079
H	-0.434148051	-0.186724692	6.073401536
C	2.366476046	-0.524020212	4.051548690
H	2.448392840	-1.624061408	4.051602534
H	2.689286534	-0.165856181	3.062893970
H	3.065892501	-0.124507921	4.804093003
C	0.780007925	1.432413694	4.194708043
H	1.519814219	1.965128227	4.815025413
H	0.914980421	1.729945378	3.142383460
H	-0.225343772	1.758946277	4.512516278
H	0.241542379	-5.042652509	-3.382798653
H	-2.444464917	-1.478645883	-0.370539564
O	-0.494806342	2.056856882	0.872468047
C	-1.635477631	1.922356764	1.447792061
O	-2.274079390	0.867077708	1.536283529
C	-2.187040094	3.197456899	2.028106254
H	-2.550302447	3.814054539	1.189253580
H	-1.395496009	3.770492351	2.532500711
H	-3.019220111	2.999283420	2.716910869
H	-1.333474538	-0.620112845	1.140943127
O	-1.744396503	0.424320131	-1.337817055
C	-2.551549629	1.403930613	-1.534163031
O	-2.181227283	2.577784957	-1.629246172
C	-4.005426337	1.018409715	-1.588591970
H	-4.325064087	0.784079012	-0.559375689
H	-4.148883857	0.108804514	-2.190575112
H	-4.624595206	1.836909856	-1.979308183

N-H Activation Association Complex
Electronic Energy: -1797.745438401
Free Energy Correction: 0.543824034

N	0.039546499	-1.422541576	-5.013919893
C	2.100598759	1.860064194	-0.318627768
C	1.537126230	1.895780460	-1.656967074
C	1.656573165	0.571567106	-2.214561166
C	2.201460119	-0.286640946	-1.211953984
C	2.489480521	0.519607834	-0.039449661
C	1.348264872	0.147737980	-3.613519631
C	0.045800259	-0.636015783	-3.801868046
C	0.564655645	-2.658960142	-5.055628210
C	2.575309419	-1.713448414	-1.377222140

C	1.035745429	3.103796669	-2.353686250
C	3.125539799	0.005743381	1.198344933
C	2.182835886	3.019745348	0.599859989
O	1.078203276	-3.232803516	-4.106982102
N	-0.350732699	-0.847143740	1.165016172
C	-2.411653460	-2.560370127	0.144447684
Rh	0.372698526	0.604197383	-0.448234142
H	-0.801781987	0.062786037	-3.820179657
H	-0.115950556	-1.314724031	-2.948580963
H	2.186542532	-0.489233054	-3.948496713
H	1.349136767	1.030472100	-4.273768450
H	-0.339473410	-1.029606850	-5.870533038
H	3.075806810	3.625417524	0.370591219
H	2.247869692	2.698696170	1.649612038
H	1.295925071	3.661200888	0.496288699
H	1.863236687	3.629264054	-2.861400490
H	0.577234789	3.801294269	-1.636360998
H	0.263763557	2.836231803	-3.087429196
H	4.207566107	-0.130412335	1.029794460
H	2.702433466	-0.967540938	1.492981489
H	3.000951564	0.703584273	2.039323084
H	3.659898809	-1.779178183	-1.577412546
H	2.051336865	-2.194153615	-2.218303859
H	2.384955812	-2.293876728	-0.461158673
C	-0.107714711	-2.208108027	0.878463707
O	0.888385514	-2.762563753	1.293992360
C	-1.113919887	-2.862452601	0.005961198
H	-3.171718349	-3.089963220	-0.438720738
C	-0.589308178	-3.915805089	-0.914907099
H	0.013083035	-3.475817459	-1.730861320
H	0.066373770	-4.617687425	-0.375770397
H	-1.413086801	-4.480729198	-1.373685614
O	0.256227913	-0.404461880	2.336488420
C	-0.394723871	-0.799785136	3.471070226
O	-1.276752664	-1.612699149	3.446108703
C	0.144043367	-0.049432965	4.669204841
C	-0.630698638	-0.484679999	5.904616696
H	-0.521001216	-1.565640449	6.086741291
H	-0.249441723	0.054405721	6.786377881
H	-1.705326235	-0.264394332	5.803028389
C	1.630914301	-0.367393736	4.837009039
H	1.794793741	-1.447554251	4.986869003
H	2.216640445	-0.047491387	3.962258258
H	2.019272796	0.161829929	5.722393054
C	-0.061650288	1.446912874	4.410976173
H	0.229046661	2.020307049	5.306238612
H	0.542326387	1.798796421	3.557857180
H	-1.121056139	1.664357621	4.188569182
H	0.478761669	-3.128316589	-6.063508070

H	-2.769352741	-1.802627081	0.848951804
O	-0.763339321	2.044520836	0.629025367
C	-1.853953433	1.893812594	1.272421025
O	-2.360866503	0.811943920	1.618397050
C	-2.549237122	3.187096642	1.617766929
H	-2.860416478	3.685777956	0.685761038
H	-1.849289020	3.868142051	2.125533324
H	-3.429065577	3.010336923	2.250876157
H	-1.331731911	-0.461453429	1.166126069
O	-1.496131322	0.048414218	-1.182900009
C	-2.242936983	0.824403545	-1.882127396
O	-1.862064670	1.783704535	-2.550758524
C	-3.702666869	0.434009798	-1.820550261
H	-4.026986210	0.433174651	-0.766720552
H	-3.828550946	-0.594467629	-2.194899374
H	-4.326294867	1.119898299	-2.409885182

N-H Activation TS
Electronic Energy: -1797.740372434
Free Energy Correction: 0.537924205

N	-0.297912031	-0.878260974	-5.097150230
C	2.289416354	1.527576993	-0.133764153
C	1.747243776	1.792459617	-1.456348789
C	1.617899654	0.531010718	-2.132681506
C	1.987283605	-0.506374675	-1.216955513
C	2.435256121	0.119564114	0.012201437
C	1.248892087	0.300961429	-3.562072277
C	-0.169625550	-0.216562543	-3.818596282
C	-0.006625339	-2.181503632	-5.250606553
C	2.081781563	-1.958146925	-1.510547600
C	1.476860771	3.135370523	-2.022802090
C	2.994340116	-0.621853576	1.168594338
C	2.581869745	2.564346137	0.884206591
O	0.381994876	-2.920500626	-4.358794978
N	-0.579567408	-0.731754299	1.200789750
C	-2.896791849	-1.994023438	0.057719877
Rh	0.361846169	0.624516591	-0.346479010
H	-0.876723845	0.622879977	-3.776749307
H	-0.464122324	-0.926828371	-3.029537975
H	1.963368250	-0.443457498	-3.958322065
H	1.416733302	1.225926021	-4.137332985
H	-0.590081594	-0.349477456	-5.913745681
H	3.559212455	3.033834516	0.681266394
H	2.611407191	2.138517046	1.897843043
H	1.814607207	3.352720373	0.870255345
H	2.399772019	3.572926699	-2.441743252
H	1.102235752	3.814566173	-1.241428881
H	0.706170001	3.083003118	-2.803333814
H	4.013975528	-0.965266640	0.922411358

H	2.384932650	-1.508026273	1.407367760
H	3.057136444	0.006010902	2.068712272
H	3.142818091	-2.228284034	-1.658533889
H	1.533112114	-2.241371848	-2.422685946
H	1.712141673	-2.567832307	-0.670218294
C	-0.571664912	-2.075152710	0.811893581
O	0.282452499	-2.854865113	1.199423270
C	-1.661442862	-2.479349568	-0.116679992
H	-3.727391406	-2.348938388	-0.562012019
C	-1.307385135	-3.519855622	-1.128736999
H	-0.658011490	-3.108518473	-1.923704518
H	-0.753077705	-4.348947268	-0.660607785
H	-2.208771723	-3.921737731	-1.613120164
O	0.188847342	-0.526621677	2.360007033
C	-0.412658661	-0.966348238	3.493816237
O	-1.477826209	-1.523601832	3.487351796
C	0.462532829	-0.706448292	4.703071638
C	-0.391679401	-0.840847378	5.956628119
H	-0.854169551	-1.837599974	6.019628844
H	0.236074060	-0.692056346	6.850042115
H	-1.198705525	-0.089834867	5.974041255
C	1.548947095	-1.788216052	4.689762385
H	1.103371611	-2.797199751	4.698627525
H	2.190613644	-1.705223412	3.798491906
H	2.184510220	-1.684029065	5.584630925
C	1.092577439	0.683350655	4.636814880
H	1.671897942	0.868200845	5.556229638
H	1.774815682	0.783616988	3.778469747
H	0.324963274	1.471239632	4.552846180
H	-0.164112450	-2.536397503	-6.296013451
H	-3.128510149	-1.250130024	0.825072364
O	-0.562141282	2.172341490	0.840719539
C	-1.658304210	2.086697536	1.452580014
O	-2.253200786	1.004897762	1.725962550
C	-2.315665077	3.372903897	1.854684311
H	-2.820439246	3.789708943	0.967051296
H	-1.564306518	4.106725175	2.177041107
H	-3.064799272	3.209707998	2.640056146
H	-1.526560618	-0.006888392	1.352861253
O	-1.563502861	0.467996006	-1.119886315
C	-2.147870775	1.402072655	-1.778263756
O	-1.600056014	2.363627478	-2.315244702
C	-3.645571552	1.204155235	-1.855982326
H	-4.058201119	1.143183857	-0.835675091
H	-3.866307108	0.241769600	-2.344714924
H	-4.128394181	2.021005663	-2.409394196

N-H Activation Product
Electronic Energy: -1797.744192824

Free Energy Correction: 0.542296705

N	0.287006879	-0.945317166	-5.052829232
C	1.063584482	2.542176172	-0.125325106
C	0.481929043	2.483046821	-1.455082812
C	1.048319407	1.346840632	-2.118982571
C	1.931958931	0.680970358	-1.198099829
C	1.958693067	1.445546235	0.028233548
C	0.854364318	0.937025457	-3.541886391
C	0.033873153	-0.337407644	-3.766502424
C	1.327590165	-1.771191654	-5.255186907
C	2.837845268	-0.458237640	-1.486577249
C	-0.448324376	3.488285176	-2.024008368
C	2.832614869	1.140992250	1.187559690
C	0.744008163	3.561681996	0.901035313
O	2.147378944	-2.082588739	-4.404568771
N	-0.044148922	-0.941639746	1.102060530
C	-1.168572002	-3.141959373	-0.328400270
Rh	-0.042026629	0.721271180	-0.339570113
H	-1.033360185	-0.091591433	-3.698460475
H	0.246521351	-1.080667684	-2.979137119
H	1.862593066	0.780289778	-3.966589880
H	0.404373211	1.769548433	-4.106995478
H	-0.324307084	-0.738324683	-5.837129438
H	1.441032886	4.412955723	0.817384286
H	0.835776138	3.148925930	1.916698665
H	-0.277545155	3.946832094	0.777110613
H	0.102593288	4.397976364	-2.319445747
H	-1.207045509	3.777862930	-1.280022869
H	-0.985064876	3.086246745	-2.891807236
H	3.873668695	1.416267811	0.945027180
H	2.808232641	0.067141085	1.432957966
H	2.534148654	1.706031974	2.082828537
H	3.869095191	-0.071724986	-1.573348157
H	2.594310947	-0.974810713	-2.427308255
H	2.846374726	-1.191156389	-0.662394227
C	0.736544057	-2.024538355	0.750499112
O	1.818452072	-2.287658252	1.267189265
C	0.149986535	-2.909529308	-0.302976401
H	-1.596923204	-3.856534930	-1.040617760
C	1.117725857	-3.614530644	-1.200901175
H	1.518531119	-2.943406041	-1.981945136
H	1.979552312	-3.988252262	-0.625951093
H	0.636798431	-4.461004955	-1.712849924
O	0.454570101	-0.366976760	2.303865115
C	0.145070323	-1.059598368	3.415666920
O	-0.486150033	-2.086000551	3.402444866
C	0.734204222	-0.394890436	4.647300113
C	0.096929489	-1.009214992	5.886261113
H	0.266677377	-2.096268892	5.926623971

H	0.532705654	-0.556442980	6.791887842
H	-0.991680732	-0.836030574	5.905429611
C	2.236748647	-0.692894223	4.631790152
H	2.422193161	-1.779529518	4.592026085
H	2.731524632	-0.231883309	3.762861077
H	2.703513962	-0.297450724	5.549444433
C	0.487703269	1.112314465	4.623599715
H	0.881430975	1.566438006	5.547878251
H	0.984816681	1.596215936	3.768110373
H	-0.589833446	1.343770648	4.567152890
H	1.370534653	-2.160576303	-6.299023739
H	-1.858430619	-2.649948664	0.360219890
O	-1.678322043	1.554091756	0.915373027
C	-2.565663458	0.932099671	1.503518172
O	-2.530729484	-0.349509103	1.722802222
C	-3.792040399	1.615300978	1.998128735
H	-3.639041718	2.699706165	2.044965933
H	-4.093054635	1.215194755	2.975966424
H	-4.610747118	1.404043103	1.290704361
H	-1.651629984	-0.737732491	1.370780544
O	-1.649916792	-0.365098004	-1.104374820
C	-2.580847753	0.139811790	-1.829123285
O	-2.554482118	1.236834580	-2.384382067
C	-3.766304008	-0.789674109	-1.973953450
H	-4.104935207	-1.122384226	-0.979426656
H	-3.449726505	-1.695023124	-2.517457355
H	-4.590798340	-0.306942366	-2.515710791

Acetic Acid Dissociation TS
Electronic Energy: -1797.737242545
Free Energy Correction: 0.544281089

N	0.233104528	-0.949826041	-5.038832707
C	0.344143274	2.638825629	-0.212486158
C	-0.277973207	2.496558694	-1.520525153
C	0.550321455	1.630859181	-2.287014903
C	1.706160067	1.269947382	-1.471583561
C	1.583916746	1.909233250	-0.206972664
C	0.332863344	1.123061279	-3.671493988
C	0.020503381	-0.379251035	-3.730005708
C	1.438392630	-1.405651109	-5.423792062
C	2.881473227	0.473604730	-1.893744535
C	-1.535805619	3.163752945	-1.932497699
C	2.594029574	1.837322745	0.879471387
C	-0.197066644	3.425666890	0.913727297
O	2.447042085	-1.377589841	-4.735856434
N	0.303310328	-0.890599679	0.958481101
C	-0.322957081	-3.000322664	-0.822762808
Rh	-0.099657178	0.587586634	-0.528563320
H	-1.024711626	-0.532772402	-3.423534321

H	0.651186589	-0.934018442	-3.014105877
H	1.255910087	1.319040197	-4.247529613
H	-0.478457357	1.687297441	-4.157930687
H	-0.538384472	-1.006427714	-5.697025830
H	0.225347495	4.445731600	0.883821946
H	0.070050780	2.970440190	1.879170403
H	-1.291506812	3.496174161	0.868742914
H	-1.344687784	4.229078918	-2.146656180
H	-2.286291756	3.116244620	-1.126463284
H	-1.972010132	2.687522352	-2.819360767
H	3.516140979	2.351471960	0.560332208
H	2.851146223	0.792533868	1.120442638
H	2.238592078	2.323271231	1.798718652
H	3.706666086	1.172392477	-2.121399448
H	2.701472641	-0.130300811	-2.796786753
H	3.236706843	-0.177731704	-1.078597752
C	1.299297602	-1.756033311	0.569871419
O	2.398047508	-1.842932978	1.109987467
C	0.943466317	-2.618192278	-0.606284381
H	-0.569514125	-3.666641309	-1.657301663
C	2.093936748	-3.098401446	-1.431381316
H	2.590079299	-2.267156850	-1.960834534
H	2.859792351	-3.565849405	-0.792351676
H	1.763467484	-3.824862306	-2.188345485
O	0.681853949	-0.212239001	2.144574922
C	0.575159149	-0.948032617	3.265738056
O	0.259015878	-2.109726984	3.275701544
C	0.959091537	-0.138679066	4.492794809
C	0.299941392	-0.775834807	5.709534826
H	0.596037050	-1.830054293	5.819491375
H	0.594078074	-0.232752609	6.622389567
H	-0.800084268	-0.740436943	5.628566050
C	2.484192574	-0.239333380	4.602501380
H	2.806631712	-1.292318086	4.663537848
H	2.975892719	0.219524597	3.729053229
H	2.830093122	0.282171290	5.510712219
C	0.535530857	1.322198078	4.375002586
H	0.755962922	1.848340348	5.318342515
H	1.077011374	1.837543050	3.567402871
H	-0.544578315	1.420930570	4.170248617
H	1.428156787	-1.828208673	-6.455401210
H	-1.142152154	-2.656818023	-0.187465283
O	-2.266722653	1.356474270	1.824044607
C	-2.768113647	0.378609565	2.338596655
O	-2.348070735	-0.860298057	2.122755453
C	-3.925566762	0.422914698	3.284043216
H	-4.200196839	1.460884760	3.506098667
H	-3.677936514	-0.112952654	4.212865513
H	-4.784497098	-0.100759989	2.834915673

H	-1.618851191	-0.849987204	1.453546302
O	-1.900008505	-0.351060143	-0.649157987
C	-2.907604293	-0.039821783	-1.402492982
O	-2.827350754	0.452366750	-2.521880594
C	-4.237202285	-0.326398230	-0.751941385
H	-4.399724158	0.429611461	0.035349082
H	-4.229374820	-1.310147725	-0.259574756
H	-5.059948459	-0.262891108	-1.476404834

Intermediate I
Electronic Energy: -1568.662002778
Free Energy Correction: 0.478472672

N	29.641434519	-12.735117717	-26.208954231
C	30.172479933	-12.835472703	-20.116537198
C	29.276475722	-13.015067370	-21.225954805
C	29.930716711	-12.554049231	-22.420884377
C	31.216313369	-12.035066478	-22.031786092
C	31.382088451	-12.224067630	-20.622262600
C	29.320033217	-12.424877498	-23.777139726
C	30.056894937	-13.164425962	-24.892214127
C	30.139899478	-11.623791465	-26.777266930
C	32.173033303	-11.305651279	-22.904743149
C	27.908353152	-13.578034703	-21.141222922
C	32.544653712	-11.777631004	-19.813837741
C	29.892507569	-13.208368841	-18.706494987
O	30.985426891	-10.901125253	-26.271631792
N	32.259821263	-15.336844406	-20.227170421
C	32.436479364	-15.315084502	-23.062010004
Rh	31.082824400	-14.179758936	-21.502015173
H	29.876544654	-14.242127387	-24.773687801
H	31.143742546	-12.993818324	-24.812627710
H	29.284565614	-11.347125489	-24.025523203
H	28.274453969	-12.771738738	-23.747443761
H	28.916988822	-13.246985364	-26.703706180
H	29.172662521	-12.508205002	-18.250531848
H	30.811507023	-13.192425248	-18.102017028
H	29.455379344	-14.219504111	-18.649883731
H	27.184329227	-12.759531807	-20.987754524
H	27.808594450	-14.272849509	-20.294499463
H	27.637952040	-14.107182802	-22.066298059
H	32.289911724	-10.855883830	-19.262975619
H	33.411286796	-11.549386731	-20.451816597
H	32.845161874	-12.543393419	-19.081789111
H	32.265463949	-10.269625452	-22.536286823
H	31.842035049	-11.256929755	-23.952140493
H	33.185649527	-11.736106594	-22.872192893
C	33.414984894	-15.662971435	-20.793070842
O	34.349400033	-16.344135071	-20.385543317
C	33.381400510	-14.953036915	-22.134914507

H	32.450679973	-14.858631646	-24.057876269
C	34.490015708	-13.998284214	-22.393131662
H	34.602850572	-13.262379849	-21.579483675
H	35.430333382	-14.576352431	-22.408128842
H	34.388582313	-13.485405698	-23.360503433
O	31.914803991	-15.959616757	-19.039522556
C	32.442858614	-15.423946583	-17.918124199
O	33.146753451	-14.446667776	-17.912484074
C	32.073084428	-16.250227970	-16.699373926
C	32.283399657	-15.400613902	-15.452612466
H	31.626714356	-14.514195247	-15.458835622
H	32.046728286	-15.992751024	-14.553644398
H	33.323503390	-15.049630223	-15.373729920
C	30.627944786	-16.738107579	-16.764091943
H	29.920034875	-15.893115620	-16.808254685
H	30.447868818	-17.380123428	-17.638929083
H	30.398574421	-17.318882600	-15.855256029
C	33.036438203	-17.443393331	-16.696402461
H	32.846755070	-18.072324553	-15.810634113
H	32.907782965	-18.062724130	-17.598959294
H	34.085038279	-17.103295551	-16.659106167
H	29.703696902	-11.422138181	-27.783675449
H	31.845231719	-16.225560926	-22.933293155
O	29.971066352	-15.990348405	-21.506511029
C	29.127857937	-16.318352335	-22.417408696
O	28.943958004	-15.730338946	-23.483665386
C	28.284344930	-17.521030778	-22.054219684
H	27.449082085	-17.176841293	-21.421279275
H	28.856500661	-18.255411371	-21.470211668
H	27.863141844	-17.987488585	-22.955768871

C-H Activation TS
Electronic Energy: -1568.642131565
Free Energy Correction: 0.481504475

N	0.140089464	-2.403241224	-4.338427536
C	-2.215234535	1.263610264	-0.184029097
C	-2.344575387	0.065010623	-0.947849530
C	-1.537044862	0.192735063	-2.140675369
C	-0.929295870	1.489775870	-2.118206251
C	-1.302320180	2.143162872	-0.891619409
C	-1.412976078	-0.793939412	-3.258813770
C	-0.251158222	-1.778728634	-3.096149122
C	0.950143955	-1.769453788	-5.205988590
C	-0.072684581	2.051313648	-3.192222639
C	-3.148172783	-1.130574399	-0.592740359
C	-0.918720009	3.513207614	-0.464093144
C	-2.881123589	1.585997902	1.105277538
O	1.423011242	-0.657449891	-5.029694491
N	0.622528441	0.917263779	1.403329283

C	1.841419739	0.802961849	-0.890553337
Rh	-0.255022037	0.357888694	-0.387080671
H	-0.503740380	-2.563798012	-2.365824389
H	0.623195907	-1.240155216	-2.693514518
H	-1.263573242	-0.235657103	-4.198716667
H	-2.360029701	-1.347554244	-3.378388659
H	-0.225331264	-3.316564480	-4.590718498
H	-3.610700329	2.401489221	0.965934684
H	-2.151734059	1.915396749	1.862950529
H	-3.424456924	0.719657260	1.509771918
H	-4.170508970	-1.037517080	-0.997526562
H	-3.227251007	-1.260635308	0.496813461
H	-2.706957186	-2.047696188	-1.010013297
H	-1.665177421	4.252020806	-0.803088546
H	0.054015583	3.807293485	-0.886138267
H	-0.851876416	3.586458817	0.632127286
H	-0.707002806	2.586600038	-3.920032253
H	0.467394148	1.262442932	-3.741973843
H	0.659500012	2.773478810	-2.800554455
C	1.830673943	1.505271980	1.450844031
O	2.444412795	1.885215847	2.447139813
C	2.346284782	1.649124897	0.044401425
H	2.177077172	0.921674115	-1.933502762
C	3.364223810	2.706445555	-0.181434987
H	2.953162448	3.699937700	0.074446496
H	4.224932274	2.558803910	0.492452410
H	3.715576471	2.724603386	-1.223038842
O	0.020010575	0.613155187	2.617057061
C	0.450171309	-0.520789301	3.220158608
O	1.455124143	-1.101798424	2.907109492
C	-0.549887410	-0.968417744	4.270668187
C	0.050905810	-2.118249296	5.065450175
H	0.966225057	-1.806784131	5.594639903
H	-0.675318972	-2.474169856	5.814362970
H	0.311932012	-2.962419235	4.407553932
C	-0.926453465	0.184778156	5.198648831
H	-0.042549851	0.585847924	5.721724549
H	-1.406750463	1.009287532	4.649078601
H	-1.636374800	-0.175535638	5.961837267
C	-1.787295181	-1.451481827	3.505051803
H	-2.525091930	-1.865962390	4.212019771
H	-2.258529057	-0.624389023	2.950591870
H	-1.524933912	-2.237094456	2.775370528
H	1.158833567	-2.373611107	-6.119695633
H	1.827822993	-0.458797695	-0.535824171
O	-0.046351624	-1.652851170	0.341232986
C	1.080055338	-2.214831574	0.338215024
O	2.118281917	-1.703961545	-0.162763948
C	1.172536909	-3.593180162	0.918221959

H	0.870950776	-4.322832000	0.149334021
H	0.485718292	-3.696316817	1.770161201
H	2.201147830	-3.819229987	1.227709802

Intermediate II (Acetic Acid Associated)
Electronic Energy: -1568.657342496
Free Energy Correction: 0.485286612

N	29.614869160	-13.253550462	-25.710579858
C	30.277163454	-12.597832475	-19.745397118
C	29.422752903	-12.769396277	-20.850938933
C	30.127432164	-12.333209279	-22.054701659
C	31.409204340	-11.851852903	-21.666495156
C	31.555256570	-12.099350668	-20.249433191
C	29.557256182	-12.264443728	-23.437409754
C	29.865352242	-13.485572757	-24.306169147
C	30.509705729	-12.607493908	-26.479871149
C	32.413699302	-11.216107606	-22.558464490
C	28.050786878	-13.337886177	-20.865301308
C	32.725951864	-11.734400490	-19.408980355
C	29.998643769	-12.899820494	-18.316096604
O	31.584666526	-12.180391121	-26.089122953
N	32.328790135	-15.240942742	-19.933144545
C	33.064421575	-14.345048330	-22.178714498
Rh	31.306618324	-13.962550152	-21.192687695
H	29.277517365	-14.356083709	-23.977139221
H	30.927976240	-13.756734698	-24.185444778
H	29.964214447	-11.372203601	-23.943044194
H	28.464493878	-12.115396947	-23.384314230
H	28.735459205	-13.543489774	-26.127621446
H	29.919413890	-11.969337397	-17.727925894
H	30.803055165	-13.506698939	-17.870456888
H	29.056965840	-13.454647190	-18.193563518
H	27.304766223	-12.557781798	-21.095182886
H	27.780533406	-13.788011628	-19.899397525
H	27.957534928	-14.118184919	-21.637908785
H	32.618074874	-10.713687825	-19.002193763
H	33.660202089	-11.767073826	-19.990223939
H	32.835454702	-12.423547474	-18.557700176
H	32.326801292	-10.117258594	-22.502337560
H	32.271110382	-11.509462856	-23.611087450
H	33.441759051	-11.479384413	-22.265689700
C	33.560296066	-15.700148415	-20.243215909
O	34.230210692	-16.500593119	-19.587921578
C	33.989516898	-15.098616708	-21.546643782
H	33.309363808	-13.864922622	-23.142563778
C	35.374660623	-15.404890589	-22.009814421
H	36.121903068	-15.049389884	-21.278924651
H	35.530959439	-16.493798903	-22.099183672
H	35.587760503	-14.936947891	-22.982511175

O	31.793548269	-15.766277706	-18.759004451
C	31.354429967	-17.040430921	-18.827030219
O	31.318122861	-17.686391260	-19.842957425
C	30.977588491	-17.550724042	-17.447050822
C	32.296841362	-17.823146301	-16.716276837
H	32.881275442	-16.898621592	-16.590030756
H	32.089886423	-18.251203162	-15.721032190
H	32.917383210	-18.539411396	-17.280282681
C	30.151065397	-16.518747077	-16.683199177
H	30.712914381	-15.587440420	-16.512305988
H	29.224994230	-16.265159059	-17.226995345
H	29.864124771	-16.931228077	-15.701760447
C	30.189288499	-18.844336164	-17.599556007
H	29.928018711	-19.240888580	-16.604882836
H	29.254876984	-18.680832258	-18.161566928
H	30.774623149	-19.608401819	-18.133846763
H	30.170197660	-12.504122963	-27.537429637
H	32.313174202	-16.157951756	-22.630126071
O	30.160223943	-15.738039895	-21.877801063
C	30.549983023	-16.788670377	-22.377891309
O	31.766358561	-16.959262630	-22.834556977
C	29.668850766	-17.975173146	-22.519409264
H	29.888261649	-18.524362682	-23.444737184
H	28.614894156	-17.676011035	-22.477887344
H	29.884584074	-18.636582697	-21.665576368

Intermediate II
Electronic Energy: -1339.575801430
Free Energy Correction: 0.425667492

N	32.614063053	-11.263209481	-24.733429855
C	28.602225340	-13.536734605	-20.926702542
C	28.803136801	-12.939074100	-22.214987200
C	30.009814056	-12.183704573	-22.125729702
C	30.489469846	-12.211174173	-20.739474591
C	29.615614691	-13.022176612	-20.002263784
C	30.659448604	-11.402497902	-23.220042302
C	31.825421290	-12.132334541	-23.891258437
C	33.554427280	-10.451703629	-24.215926525
C	31.707173047	-11.517489690	-20.243103638
C	27.954052593	-13.106636797	-23.424659139
C	29.686940908	-13.348762525	-18.555259154
C	27.511027986	-14.460212450	-20.536134736
O	33.835575484	-10.381619753	-23.030114605
N	31.948019254	-15.458723920	-21.160663833
C	30.434010179	-15.586430398	-23.222067817
Rh	30.462417072	-14.233406358	-21.679771168
H	31.455962762	-12.976714268	-24.494458481
H	32.488014160	-12.562332334	-23.120029969
H	31.039392856	-10.458164894	-22.792251555

H	29.911203290	-11.122610786	-23.980035734
H	32.434050963	-11.223971513	-25.732286450
H	26.700620910	-13.903096327	-20.033390581
H	27.874827251	-15.222053838	-19.829006443
H	27.078934640	-14.972222420	-21.407986894
H	27.203287350	-12.301554233	-23.494000679
H	27.411243012	-14.064096931	-23.407243741
H	28.554440787	-13.082751597	-24.347520544
H	28.950223170	-12.756161231	-17.986018755
H	30.681446492	-13.124013482	-18.139825254
H	29.472472044	-14.412861279	-18.369943431
H	31.444298274	-10.546822741	-19.787939109
H	32.424744413	-11.311166136	-21.053220769
H	32.222466018	-12.113611378	-19.473019128
C	32.028647667	-16.679310191	-21.793098258
O	32.630369240	-17.652538976	-21.365887526
C	31.242863242	-16.652055759	-23.072159708
H	29.794350319	-15.501111490	-24.116148799
C	31.431521837	-17.803759152	-24.001939007
H	32.475339590	-17.866408274	-24.357487071
H	31.225803799	-18.760811373	-23.492154969
H	30.771718877	-17.722233937	-24.878479643
O	32.559756091	-15.450530795	-19.904092005
C	31.840888829	-16.019545157	-18.911813366
O	30.724812853	-16.448127878	-19.062829803
C	32.647048138	-16.090634551	-17.627693314
C	33.574691199	-17.301377822	-17.789471424
H	34.257094184	-17.168095182	-18.643779503
H	34.175880448	-17.434432080	-16.874612429
H	32.993071735	-18.223101120	-17.959564748
C	33.471409281	-14.825749298	-17.403362257
H	34.200873663	-14.660653839	-18.209960992
H	32.829510873	-13.931022815	-17.332079271
H	34.025070716	-14.914592875	-16.454038577
C	31.694333090	-16.312557820	-16.460684499
H	32.268157583	-16.409751878	-15.524706519
H	30.996291269	-15.465545773	-16.347182583
H	31.096679112	-17.226517405	-16.598546195
H	34.068506428	-9.840073444	-24.993901186

Intermediate III (Major Stereoisomer)
Electronic Energy: -1763.621753239
Free Energy Correction: 0.587362407

N	31.262758492	-11.343202456	-25.662394248
C	28.913559538	-13.619751722	-20.472938491
C	28.780220222	-13.287282990	-21.879468625
C	29.951310231	-12.578415293	-22.282124087
C	30.880984384	-12.615210542	-21.190345273
C	30.198572499	-13.214677895	-20.053447940

C	30.106008496	-11.757303586	-23.524726652
C	30.961595038	-12.328767063	-24.648485137
C	32.269565735	-10.464286756	-25.508338369
C	32.228462655	-11.982217454	-21.154900403
C	27.548953890	-13.466851446	-22.694576123
C	30.721699119	-13.321560703	-18.666157751
C	27.856358134	-14.195705188	-19.599928982
O	33.013823473	-10.419615213	-24.541711545
N	32.234827510	-15.484676091	-20.867045469
C	31.708551771	-15.135245612	-23.302971423
Rh	30.499452697	-14.712036757	-21.696937839
H	30.452855029	-13.180536916	-25.126567501
H	31.914056980	-12.705468033	-24.241551608
H	30.551069759	-10.793571560	-23.218531150
H	29.106257037	-11.513398777	-23.923111310
H	30.681283874	-11.273760463	-26.492227179
H	27.321751394	-13.391415572	-19.064509347
H	28.275486749	-14.870809481	-18.836017215
H	27.099608424	-14.752997183	-20.173651601
H	26.865800875	-12.609037382	-22.567064263
H	26.990048551	-14.368599116	-22.397740843
H	27.780485051	-13.550922514	-23.768550862
H	30.192146852	-12.616181697	-18.003109334
H	31.795173351	-13.088371451	-18.615718609
H	30.573090657	-14.334380719	-18.255940296
H	32.224539004	-11.090978605	-20.503128607
H	32.552541523	-11.660202166	-22.157272149
H	32.975126979	-12.685949861	-20.751347126
C	33.226945196	-15.973427434	-21.648897399
O	34.228459180	-16.571176601	-21.253046347
C	32.910415227	-15.685315528	-23.070818518
H	31.355042289	-14.970624330	-24.329511959
C	33.917820949	-16.092306543	-24.095110037
H	34.884140420	-15.583644010	-23.932427981
H	34.127705723	-17.174575622	-24.027563934
H	33.573196234	-15.866370210	-25.115561887
O	32.350931622	-15.860998041	-19.532154652
C	33.344245826	-15.271949727	-18.839899620
O	33.971189797	-14.316524886	-19.225442003
C	33.583220160	-15.999744891	-17.524926759
C	34.535104722	-15.174718308	-16.671084940
H	34.101825266	-14.190528406	-16.425857940
H	34.741461638	-15.703734786	-15.725779873
H	35.492522418	-15.001796895	-17.187165459
C	32.273259252	-16.226084747	-16.773057964
H	31.794441785	-15.269880801	-16.501273433
H	31.561951677	-16.818289982	-17.368346395
H	32.479288667	-16.772791432	-15.837419319
C	34.220923270	-17.346604208	-17.879533427

H	34.429063596	-17.915312210	-16.956900312
H	33.549951593	-17.937166509	-18.521439578
H	35.167664277	-17.203520132	-18.426189801
C	29.440184463	-16.383348145	-22.683140260
H	30.081531330	-16.958849280	-23.356887513
C	29.409653603	-16.683654241	-21.322051478
H	28.535619617	-16.348617602	-20.749731347
C	30.187265152	-17.721040798	-20.640987247
C	31.251661838	-18.403076784	-21.242093173
C	29.865714686	-18.047541465	-19.314048513
C	31.993070836	-19.351179521	-20.547154523
C	30.578871371	-19.007266901	-18.614150575
C	31.663697949	-19.655270522	-19.219920778
H	31.534289849	-18.177034182	-22.275775883
H	29.036328140	-17.524990021	-18.822184526
H	32.836931521	-19.831792371	-21.047105733
H	30.333069980	-19.260209002	-17.578383907
O	32.334929400	-20.542214847	-18.455343245
C	33.469624371	-21.177548555	-18.991093793
H	33.216869238	-21.791493004	-19.873557581
H	34.247033943	-20.447081100	-19.279285171
H	33.872430351	-21.832479437	-18.207915866
H	28.570102975	-15.921221479	-23.161373283
H	32.365362638	-9.767346663	-26.374272980

Intermediate III (Minor Stereoisomer)
Electronic Energy: -1763.625386457
Free Energy Correction: 0.584102076

N	30.684196642	-11.335925907	-25.647799137
C	29.344397628	-13.754823520	-20.162704454
C	28.833845414	-13.493353240	-21.488747183
C	29.830561649	-12.719243580	-22.193739494
C	30.960609472	-12.581136256	-21.322442566
C	30.655536472	-13.227936118	-20.066433747
C	29.657513536	-12.040341211	-23.515421011
C	30.768023492	-12.262134524	-24.540656492
C	31.201746942	-10.097106033	-25.565695439
C	32.180713097	-11.755068566	-21.563798792
C	27.466356614	-13.857638224	-21.949224076
C	31.522973379	-13.273031835	-18.857432077
C	28.594677217	-14.402956308	-19.058874297
O	31.798987046	-9.655999085	-24.596351839
Rh	30.585072795	-14.747329630	-21.777395622
H	30.739369024	-13.286344781	-24.939702063
H	31.757033818	-12.131346816	-24.074291892
H	29.585143592	-10.952226593	-23.324742297
H	28.691332257	-12.329853020	-23.962218635
H	30.173170489	-11.594281938	-26.486809050
H	28.116405719	-13.629854159	-18.432747986

H	29.262172370	-14.983098485	-18.401530778
H	27.810550076	-15.075843331	-19.430850616
H	26.704232660	-13.188383884	-21.514089638
H	27.223555410	-14.889238165	-21.646052115
H	27.377756490	-13.805612266	-23.044292296
H	31.215560860	-12.519308421	-18.111580347
H	32.578728998	-13.078981241	-19.100577494
H	31.470926307	-14.259316091	-18.364164755
H	32.454888815	-11.210536221	-20.646614718
H	32.019170844	-11.008466243	-22.356611377
H	33.064151569	-12.352275610	-21.851866868
H	31.036295917	-9.500475581	-26.492981796
N	30.012667476	-16.660343787	-21.271368956
C	29.915850687	-15.583852042	-23.535209830
C	29.669635360	-17.569709882	-22.211886110
O	29.462946209	-18.768584280	-22.023005522
C	29.555013701	-16.876340250	-23.523859643
H	29.869929374	-14.993783402	-24.462935706
C	29.053860621	-17.676695964	-24.680079401
H	28.042636535	-18.073794481	-24.482922102
H	29.697518884	-18.556266748	-24.856106111
H	29.018532668	-17.078862263	-25.603474583
O	30.171410536	-17.174019614	-19.990946461
C	29.040565120	-17.589828970	-19.385936481
O	27.933374995	-17.438581153	-19.836611502
C	29.369229394	-18.311340840	-18.087781452
C	28.084871920	-18.499359603	-17.293613854
H	27.632189846	-17.528187266	-17.030552299
H	28.299688532	-19.042366617	-16.358440217
H	27.339761802	-19.073461488	-17.865794327
C	30.388160641	-17.530565676	-17.260099880
H	29.998212536	-16.541021813	-16.964464876
H	31.329763806	-17.385442100	-17.810919989
H	30.612342177	-18.087248217	-16.334437298
C	29.954210725	-19.670844915	-18.483531481
H	30.192013827	-20.254356540	-17.577682353
H	30.873168495	-19.540566852	-19.075243007
H	29.239118801	-20.246621092	-19.094212365
C	32.497622754	-15.073553976	-22.802078125
H	32.447356744	-15.878985208	-23.541078774
C	32.767310381	-15.361690120	-21.463346032
H	33.129970616	-14.540327093	-20.830771033
C	33.006399492	-16.687226225	-20.890138407
C	32.789321370	-17.877526346	-21.594646431
C	33.465665093	-16.784826812	-19.566894343
C	32.985967790	-19.119615976	-21.003662555
C	33.689525958	-18.014783177	-18.969239511
C	33.433767000	-19.196156373	-19.678553924
H	32.433845036	-17.847422879	-22.629607370

H	33.640311925	-15.865793020	-18.994909517
H	32.770546669	-20.020858821	-21.582195014
H	34.043364675	-18.092571569	-17.936850953
O	33.635259775	-20.351978178	-19.010919147
C	33.370796378	-21.569575777	-19.663603760
H	34.005745851	-21.701008605	-20.557585328
H	32.311579188	-21.648616303	-19.968433752
H	33.592746797	-22.372697673	-18.949285029
H	32.766094366	-14.093919767	-23.212309340

Migratory Insertion TS (Major Stereoisomer)
Electronic Energy: -1763.603513857
Free Energy Correction: 0.585244715

N	1.194077404	5.574984609	-1.017636534
C	-2.235570661	1.248351633	1.665157594
C	-2.213801564	2.403117163	0.802878024
C	-0.883543428	2.972671786	0.852488375
C	-0.066596031	2.103912261	1.610861973
C	-0.897051027	1.005522845	2.093137651
C	-0.464971323	4.299487326	0.300160905
C	0.602280854	4.274571435	-0.793525205
C	2.183188733	6.046423346	-0.238492565
C	1.370855727	2.286270534	1.952857935
C	-3.384434207	3.011405718	0.112199925
C	-0.416770259	-0.087068680	2.982444103
C	-3.440485125	0.472458067	2.058228371
O	2.685674672	5.439849383	0.694603529
N	0.751734081	-0.301917644	-0.481232032
C	-0.381757753	1.393012509	-2.076010478
Rh	-0.910613683	0.876161113	-0.071388282
H	0.177158217	3.920349287	-1.742771968
H	1.406862125	3.568105807	-0.527355829
H	-0.067883823	4.893611028	1.144253730
H	-1.347646178	4.850469306	-0.064582137
H	0.828966140	6.176207124	-1.750356217
H	-3.186306879	-0.556902183	2.354135735
H	-4.192711273	0.427801681	1.254534329
H	-3.928840536	0.948434057	2.926047962
H	-3.834210071	3.824397164	0.708385544
H	-4.173782716	2.266798251	-0.075325335
H	-3.093252724	3.439761574	-0.861579201
H	-0.514984441	0.188400984	4.047338848
H	0.648621735	-0.301130086	2.797327077
H	-0.977892652	-1.021205384	2.822081123
H	1.513667716	2.215713127	3.044853233
H	1.754101055	3.265244391	1.625268146
H	1.992861868	1.499030896	1.493454353
C	1.416045709	-0.178182489	-1.649456239
O	2.337911966	-0.896640940	-2.048082183

C	0.866888951	0.980458425	-2.403166975
H	-0.818596333	2.257965397	-2.593869765
C	1.728701965	1.597681437	-3.449069880
H	2.669993460	1.982184692	-3.015802218
H	2.025352123	0.845935736	-4.201664417
H	1.218335484	2.426259226	-3.963746742
O	1.064351846	-1.470406238	0.211331024
C	2.235872206	-1.481134238	0.866113744
O	2.942727000	-0.515135978	1.017026622
C	2.567126550	-2.886880049	1.341748280
C	3.691448734	-2.810370583	2.364604910
H	3.382308754	-2.236269248	3.254396723
H	3.968067711	-3.826112804	2.692010946
H	4.585441044	-2.324801650	1.943864886
C	1.347956723	-3.574264522	1.949687817
H	0.977108857	-3.027683246	2.833778002
H	0.522759570	-3.654771805	1.226562198
H	1.623743139	-4.592380419	2.274611493
C	3.033354607	-3.652013211	0.098355145
H	3.323041566	-4.678921785	0.380605279
H	2.230357064	-3.699626061	-0.655342697
H	3.904979411	-3.160921298	-0.366177297
C	-1.861951990	0.208496547	-2.047882981
H	-1.464498056	-0.305732528	-2.929200632
C	-2.173651367	-0.636788467	-0.920374893
H	-3.125819836	-0.419558946	-0.418338915
C	-1.794454982	-2.053557473	-0.829667318
C	-0.886751803	-2.682407578	-1.690632020
C	-2.375460549	-2.842788570	0.179739185
C	-0.542031739	-4.023429977	-1.541123677
C	-2.047275424	-4.178907344	0.340735266
C	-1.109317959	-4.779234554	-0.508942313
H	-0.405601570	-2.118801632	-2.496874549
H	-3.106075243	-2.386609179	0.857528530
H	0.181806013	-4.463653389	-2.231892240
H	-2.493899841	-4.783677482	1.135574520
O	-0.808532964	-6.071944415	-0.254081566
C	0.220550525	-6.683068899	-0.991050230
H	-0.022541355	-6.747173933	-2.066462139
H	1.176814006	-6.140157476	-0.878103766
H	0.341699192	-7.700113253	-0.596314184
H	-2.639542384	0.933976148	-2.315526436
H	2.514973955	7.067994618	-0.538915350

Migratory Insertion TS (Minor Stereoisomer)
Electronic Energy: -1763.602096630
Free Energy Correction: 0.585378023

N	-1.249327192	5.762721731	-1.083570983
C	1.539898533	1.417635333	1.984479209

C	1.376212924	2.634790998	1.232946918
C	-0.030976942	2.961659232	1.219887606
C	-0.738831661	1.885317131	1.801478893
C	0.240608495	0.913071713	2.280843924
C	-0.612145391	4.264625326	0.770971439
C	-0.843599604	4.422271498	-0.726736406
C	-0.348500061	6.749813784	-1.241017152
C	-2.214773655	1.770461498	1.941099013
C	2.473626833	3.523849760	0.756642141
C	-0.063497754	-0.316565560	3.062177086
C	2.830761480	0.819767089	2.414644997
O	0.859510944	6.613521768	-1.132704538
N	-0.894179289	-0.559513648	-0.383837352
C	-0.220355844	1.456961414	-1.871095278
Rh	0.417377383	0.978660535	0.124124256
H	0.088104921	4.194268344	-1.270883566
H	-1.606860297	3.709613518	-1.078541533
H	-1.565604244	4.436710076	1.299162803
H	0.067783648	5.072391995	1.096740334
H	-2.236394421	5.989030969	-1.161867483
H	2.753166826	-0.271088403	2.544394456
H	3.647820206	1.026441356	1.705411903
H	3.139067710	1.241848949	3.386894028
H	2.912922526	4.093801423	1.594439111
H	3.294386166	2.951060029	0.294105825
H	2.115047385	4.257285078	0.016576611
H	0.057049509	-0.136116136	4.144413236
H	-1.098697902	-0.651640682	2.895501316
H	0.607587853	-1.144843636	2.781539813
H	-2.539143521	1.976407913	2.976367949
H	-2.730117033	2.482387600	1.277347888
H	-2.557429485	0.758441039	1.671189458
C	-1.567682029	-0.538512723	-1.553202135
O	-2.286132582	-1.439085755	-1.998135445
C	-1.320163047	0.754800856	-2.238124966
H	-0.028014523	2.419248682	-2.359932385
C	-2.288862618	1.176204523	-3.288265360
H	-3.317635396	1.220849452	-2.889839076
H	-2.314341286	0.439179529	-4.111005278
H	-2.032298705	2.160107943	-3.709416445
O	-0.907379650	-1.815928251	0.223039761
C	-2.052313209	-2.164152740	0.832782612
O	-2.961432207	-1.403926753	1.060969447
C	-2.061072516	-3.649596199	1.158929220
C	-3.204173610	-3.935052398	2.122611645
H	-3.075326754	-3.384471232	3.069641366
H	-3.235823220	-5.012505667	2.354340492
H	-4.175333789	-3.644533417	1.693024039
C	-0.736542876	-4.097996940	1.770909850

H	-0.543828445	-3.591170815	2.732265329
H	0.112097687	-3.897935779	1.099826882
H	-0.772635975	-5.183673694	1.965665414
C	-2.295533890	-4.379016287	-0.168091319
H	-2.377284431	-5.464078079	0.015569957
H	-1.464942763	-4.195754351	-0.868773581
H	-3.224497597	-4.034601830	-0.652153367
C	1.534665276	0.751037474	-1.863582468
H	1.321469657	0.254905841	-2.816704621
C	2.022076368	-0.100354480	-0.805133591
H	2.880835856	0.288246011	-0.241764376
C	1.977437827	-1.567564636	-0.855402102
C	1.264380091	-2.292721845	-1.817416574
C	2.673982867	-2.303658864	0.119992751
C	1.210188542	-3.683748134	-1.797384121
C	2.633503731	-3.687720802	0.153339224
C	1.880609877	-4.392817119	-0.794669067
H	0.707111782	-1.771137238	-2.602669307
H	3.258493371	-1.767261838	0.876488603
H	0.627179333	-4.201121160	-2.563491208
H	3.165102431	-4.254796626	0.923491464
O	1.847012887	-5.736831331	-0.655910211
C	1.010016179	-6.480646225	-1.505421142
H	1.331085088	-6.417153504	-2.560562546
H	-0.040098605	-6.143065301	-1.435799892
H	1.067067148	-7.527911880	-1.181820296
H	2.099565676	1.679304156	-2.011222187
H	-0.824664236	7.726353528	-1.494201473

Intermediate IV
Electronic Energy: -1763.628721931
Free Energy Correction: 0.589144925

N	31.049492974	-11.277571939	-25.854014999
C	29.076453766	-13.998482776	-20.870677565
C	29.007606433	-13.574686680	-22.233763327
C	29.986403446	-12.520554432	-22.412372458
C	30.746515122	-12.393266973	-21.230047017
C	30.204949435	-13.344437488	-20.272549723
C	30.072333937	-11.635192101	-23.611210550
C	30.697818524	-12.258888431	-24.852810698
C	32.143284063	-10.505755568	-25.712333214
C	31.908479026	-11.488934967	-21.004103425
C	27.939158088	-13.939221037	-23.206113483
C	30.655174177	-13.511911131	-18.863564584
C	28.073562813	-14.843897298	-20.173768814
O	32.924261164	-10.572745793	-24.776692034
N	32.775182892	-15.123281344	-21.037455469
C	31.789252898	-15.643886418	-23.792064584
Rh	30.956246069	-14.577202044	-21.876969171

H	30.035129981	-13.008742547	-25.312736398
H	31.615034688	-12.776826031	-24.547222013
H	30.664149229	-10.744086083	-23.347377636
H	29.055503345	-11.273235436	-23.851861963
H	30.436674293	-11.113161105	-26.646990893
H	27.167924981	-14.245098614	-19.971250821
H	28.443018841	-15.211022430	-19.205374224
H	27.751224403	-15.707433805	-20.777691867
H	27.047380692	-13.297859592	-23.083208482
H	27.610398140	-14.982333034	-23.075856615
H	28.279070537	-13.829288470	-24.247593736
H	29.963976708	-13.007908500	-18.166275499
H	31.656327054	-13.080509357	-18.712306937
H	30.702157497	-14.578076817	-18.580222798
H	31.654044982	-10.644211727	-20.339986271
H	32.273351353	-11.071384950	-21.957117434
H	32.746727234	-12.037447357	-20.541080858
C	33.596674929	-15.493297486	-22.007479606
O	34.698620860	-16.034585043	-21.973979815
C	32.895387617	-15.010124663	-23.267239455
H	31.410239034	-15.250080462	-24.745124621
C	33.647403204	-13.919701635	-23.958300928
H	33.636137762	-12.976724010	-23.385237781
H	34.701998003	-14.235110835	-24.032485013
H	33.280517086	-13.721655521	-24.975214789
O	33.106460461	-15.516363182	-19.748272694
C	33.979756542	-14.715487565	-19.106991522
O	34.362210582	-13.655708389	-19.534457828
C	34.446730386	-15.378884046	-17.823200757
C	35.260459662	-14.379678473	-17.014116140
H	34.656635271	-13.499776114	-16.736706837
H	35.617936587	-14.857017741	-16.087214007
H	36.136084233	-14.024202760	-17.579436462
C	33.259707717	-15.883596177	-17.004402701
H	32.621636998	-15.048053241	-16.668723807
H	32.635765668	-16.586053275	-17.578285397
H	33.629125115	-16.404124982	-16.104219414
C	35.331603884	-16.554479893	-18.255055455
H	35.773174012	-17.036325078	-17.366046754
H	34.745342017	-17.301086454	-18.814264617
H	36.154183004	-16.213437860	-18.906780034
C	31.219363341	-16.957495920	-23.305495774
H	32.006794835	-17.731139323	-23.264320727
C	30.558793693	-16.695069844	-21.964488862
H	29.459748879	-16.688698615	-22.048321751
C	30.981638004	-17.499872112	-20.795369628
C	32.213408117	-18.162626189	-20.705912817
C	30.125014845	-17.624065915	-19.683965401
C	32.595328336	-18.877309432	-19.570528061

C	30.490685593	-18.317283386	-18.541914476
C	31.743018195	-18.940713113	-18.465849327
H	32.935306925	-18.104015186	-21.526491247
H	29.135409678	-17.161673020	-19.725147398
H	33.574043379	-19.364335868	-19.557562750
H	29.816256138	-18.393363782	-17.683292851
O	32.036718296	-19.566249639	-17.301718152
C	33.315495517	-20.125324097	-17.144259695
H	33.505785488	-20.935653193	-17.870601559
H	34.108246868	-19.362567142	-17.253027523
H	33.364823331	-20.543114306	-16.130192736
H	30.481204184	-17.316617475	-24.040149475
H	32.271834064	-9.787079559	-26.556103754

Intermediate IV (Conformation 2)
Electronic Energy: -1763.627452235
Free Energy Correction: 0.587922301

N	31.044876972	-12.298579081	-25.202683165
C	28.890762291	-13.775863353	-19.668115725
C	28.642683424	-13.864172391	-21.068286038
C	29.677497211	-13.113798830	-21.733815193
C	30.460598734	-12.417523527	-20.710094147
C	29.981849965	-12.821961262	-19.457220567
C	29.688930591	-12.759314977	-23.185680101
C	31.011498194	-12.961074889	-23.916555398
C	31.316203411	-10.986621666	-25.317607006
C	31.591238104	-11.479920917	-20.969726134
C	27.506691717	-14.570717874	-21.716783956
C	30.494995374	-12.431088725	-18.118474549
C	28.116474548	-14.412937195	-18.569709432
O	31.577016980	-10.243677367	-24.384376626
N	32.623095798	-15.075020077	-21.070527841
C	31.459038901	-16.422478784	-23.586877079
Rh	30.598192159	-14.687759223	-20.579120109
H	31.196557731	-14.033072570	-24.064923090
H	31.852827740	-12.582594349	-23.313670577
H	29.412398391	-11.688967750	-23.255086672
H	28.894842793	-13.311230854	-23.716590702
H	30.806173201	-12.815776451	-26.043676409
H	27.404638657	-13.698313507	-18.120026804
H	28.784244263	-14.760766388	-17.764825377
H	27.538830891	-15.278743496	-18.926981072
H	26.658066447	-13.879591900	-21.857725127
H	27.143050802	-15.409886677	-21.104090940
H	27.772666222	-14.965756519	-22.709112941
H	29.719544135	-11.900867489	-17.539414757
H	31.373402359	-11.772887646	-18.191789954
H	30.783885923	-13.317141825	-17.527160496
H	31.724318467	-10.775423308	-20.135392703

H	31.431079243	-10.894633106	-21.890562827
H	32.544298828	-12.023372379	-21.098367718
C	33.328311595	-15.777014513	-21.977890417
O	34.461911139	-16.234767873	-21.811049747
C	32.683201769	-15.936610697	-23.321922868
H	31.248279709	-16.539628550	-24.662188367
C	33.622735655	-15.583678583	-24.438493643
H	33.911655147	-14.517338414	-24.382308194
H	34.556664606	-16.163009166	-24.364428450
H	33.167251435	-15.760447955	-25.424762029
O	33.403986996	-15.047827354	-19.860893535
C	32.751726822	-15.359194936	-18.769185735
O	31.529724744	-15.466613438	-18.734969398
C	33.648999437	-15.528242774	-17.562291082
C	32.820860622	-16.006230361	-16.378265502
H	32.337769003	-16.972836802	-16.597476115
H	33.476753676	-16.134335996	-15.502117264
H	32.030784150	-15.283478884	-16.117510627
C	34.734103187	-16.554096552	-17.896784771
H	34.285128266	-17.540064232	-18.109376131
H	35.317616642	-16.253578850	-18.780302039
H	35.416653150	-16.663138594	-17.037682652
C	34.275386387	-14.163921105	-17.259382910
H	34.886562475	-14.235527183	-16.344870240
H	34.922200341	-13.823915852	-18.082892897
H	33.499018864	-13.398320624	-17.087837828
C	30.268887513	-16.822058727	-22.773706110
H	30.051581397	-17.882460937	-23.037862402
C	30.147351235	-16.660920586	-21.269220070
H	29.068843936	-16.694723016	-21.032598587
C	30.819488771	-17.670999900	-20.415961463
C	32.013656715	-18.314986265	-20.758682302
C	30.277911686	-17.974462651	-19.150943456
C	32.684259112	-19.159909611	-19.869860606
C	30.919747637	-18.816766758	-18.260471242
C	32.149822957	-19.398008238	-18.601630158
H	32.465041712	-18.144376726	-21.740549376
H	29.341051714	-17.488307571	-18.851397952
H	33.629988355	-19.610735315	-20.180839814
H	30.500527138	-19.027363691	-17.271392386
O	32.743731287	-20.153428299	-17.645302185
C	33.980756502	-20.751952137	-17.935583043
H	33.907236683	-21.458984455	-18.781580415
H	34.754322869	-19.999016967	-18.173868367
H	34.293093985	-21.304120050	-17.039493374
H	29.423024094	-16.274043621	-23.235155307
H	31.287101931	-10.634747266	-26.375804435

N-O Bond Cleavage TS

Electronic Energy: -1763.607785808
Free Energy Correction: 0.585827461

N	0.139944636	5.014184812	-2.098825707
C	-1.529091652	1.159360566	2.329349415
C	-2.009691134	1.990879305	1.278156102
C	-0.898056562	2.776087993	0.804808539
C	0.235891828	2.531761836	1.682545824
C	-0.140564162	1.529229946	2.596257554
C	-0.968901729	3.891211963	-0.189494918
C	-0.004649193	3.774444669	-1.367660707
C	0.958172528	5.996775698	-1.683418324
C	1.574448610	3.181627033	1.589838151
C	-3.406610758	2.066082758	0.775733726
C	0.714479851	0.913115294	3.644747788
C	-2.288719249	0.150783053	3.116794239
O	1.664138450	5.945408891	-0.688651437
N	1.132904630	0.493736355	-0.674158236
C	-0.618605503	0.750687326	-3.051331804
Rh	-0.394524213	0.656059508	0.538063561
H	-0.348457496	2.998117761	-2.066370748
H	0.991676763	3.451491768	-1.019318080
H	-0.745019539	4.830623158	0.351036379
H	-1.999275679	3.997430701	-0.568355283
H	-0.427277083	5.179610100	-2.925153359
H	-2.519457824	0.527445740	4.128350211
H	-1.702524423	-0.776346830	3.235738800
H	-3.241796377	-0.112421700	2.634085948
H	-3.937029599	2.908296167	1.251973083
H	-3.976893095	1.153164885	1.004259324
H	-3.450791637	2.229502596	-0.312598468
H	0.447877278	1.289512336	4.647434514
H	1.780845118	1.125213286	3.474596064
H	0.587584112	-0.181885884	3.667846712
H	1.988527776	3.375912562	2.591378321
H	1.532984208	4.138229378	1.045938883
H	2.294346037	2.535530562	1.056057756
C	1.378199046	-0.195042394	-1.790509828
O	2.089193503	-1.155726314	-2.039659726
C	0.706042009	0.589407868	-2.903803517
H	-0.920314506	1.271850617	-3.972719741
C	1.703228116	1.144423944	-3.871182871
H	2.349649915	1.888696439	-3.370730595
H	2.367186674	0.352057622	-4.253252353
H	1.205839765	1.638065959	-4.719836210
O	2.273623870	-0.602044754	0.584252934
C	1.488343412	-1.393575403	1.158751195
O	0.240579552	-1.227559544	1.246401459
C	2.070835895	-2.681765429	1.744669989
C	1.092344705	-3.328917496	2.714678438

H	0.144618085	-3.582173852	2.214390032
H	1.532759652	-4.254492559	3.122732209
H	0.860247741	-2.659376409	3.560868849
C	2.299297651	-3.598884513	0.539006803
H	1.349333587	-3.792625413	0.011020232
H	2.992326564	-3.136944261	-0.181574008
H	2.718008697	-4.563028540	0.875743898
C	3.392514219	-2.384509180	2.443826137
H	3.823535235	-3.319074953	2.840864731
H	4.119388473	-1.933578265	1.751229269
H	3.250402859	-1.691204698	3.291041695
C	-1.786362793	0.413406211	-2.184718876
H	-2.519487556	-0.109994139	-2.837349284
C	-1.676734171	-0.347683553	-0.879276913
H	-2.625492091	-0.199379335	-0.336554131
C	-1.446303480	-1.811939921	-0.965132760
C	-0.793434556	-2.446499990	-2.027730744
C	-1.926876281	-2.643831283	0.066483830
C	-0.585889312	-3.828279301	-2.055281484
C	-1.740526423	-4.013799422	0.054021244
C	-1.045129503	-4.620710713	-1.002796545
H	-0.418893524	-1.858046640	-2.868911966
H	-2.451013486	-2.184070886	0.912267972
H	-0.054816888	-4.265882880	-2.904195066
H	-2.111263367	-4.647131907	0.866317799
O	-0.864423760	-5.959507418	-0.913672576
C	-0.066887747	-6.593719687	-1.880316072
H	-0.505548603	-6.521220486	-2.891760969
H	0.952553078	-6.166856516	-1.908583282
H	-0.000019296	-7.653556272	-1.601711392
H	-2.282085592	1.385171021	-1.980880983
H	0.934670362	6.885152815	-2.357675865

Nitrene Intermediate
Electronic Energy: -1763.615138347
Free Energy Correction: 0.584182061

N	30.783796096	-12.087959030	-25.112017135
C	28.853636941	-13.926670440	-19.635341240
C	28.599325967	-13.914571132	-21.034949203
C	29.460917508	-12.918727946	-21.639724109
C	30.188143869	-12.263945378	-20.595197725
C	29.844944750	-12.909306090	-19.367578222
C	29.443297760	-12.505967767	-23.075944142
C	30.736468851	-12.780052203	-23.844695011
C	31.144633074	-10.794628597	-25.191779901
C	31.148977307	-11.137509535	-20.736206363
C	27.554977277	-14.689551622	-21.753727034
C	30.316702043	-12.526564368	-18.013973803
C	28.196669575	-14.751432957	-18.584951260

O	31.471908429	-10.103825907	-24.239714638
N	32.319070675	-14.489830260	-21.651546314
C	31.805906320	-16.654777715	-23.498684142
Rh	30.743220178	-14.499000590	-20.676423483
H	30.859867988	-13.859417068	-24.024799148
H	31.605893947	-12.470423699	-23.241715703
H	29.250654607	-11.417957227	-23.107354015
H	28.596131612	-12.982038497	-23.596863991
H	30.497343367	-12.565132978	-25.961646324
H	27.547756949	-14.132336543	-17.942145883
H	28.948424734	-15.229210474	-17.932458071
H	27.568884402	-15.546485359	-19.015527642
H	26.686475239	-14.039516634	-21.956333390
H	27.188384575	-15.541309632	-21.162565154
H	27.904377369	-15.072158171	-22.725639305
H	29.577454382	-11.857395655	-17.538946479
H	31.286772835	-12.013679273	-18.049354361
H	30.420868364	-13.407944672	-17.361860359
H	30.829822207	-10.280624100	-20.119354510
H	31.238027289	-10.792555455	-21.777831076
H	32.149272509	-11.437133532	-20.382611051
C	33.239937604	-15.449539166	-21.811630604
O	34.235229331	-15.673866011	-21.130328620
C	32.990368978	-16.132304004	-23.131558301
H	31.784143570	-17.115307194	-24.496876458
C	34.197181063	-16.170048388	-24.014310481
H	34.534699636	-15.149046980	-24.264955263
H	35.037260755	-16.657647301	-23.493499949
H	33.993658127	-16.707357033	-24.952548496
O	33.090020672	-13.658207081	-18.863465834
C	32.638308755	-14.733324656	-18.484906737
O	31.658794639	-15.376121213	-19.027856768
C	33.263583833	-15.467375145	-17.283386642
C	32.209615318	-16.203269336	-16.465602544
H	31.685250438	-16.955732978	-17.073838500
H	32.687159207	-16.715134879	-15.611389522
H	31.452833509	-15.507925458	-16.059551020
C	34.256669187	-16.472366112	-17.868665614
H	33.734641893	-17.210730233	-18.499677538
H	35.004365781	-15.965502482	-18.501041662
H	34.780653688	-17.008851160	-17.056920305
C	33.993899999	-14.463632431	-16.402170666
H	34.464289171	-14.980105179	-15.547771905
H	34.777457434	-13.933602153	-16.964889973
H	33.299839822	-13.704238565	-16.000578428
C	30.474489708	-16.701952318	-22.819404341
H	30.019178549	-17.677230523	-23.091912690
C	30.253615651	-16.544177769	-21.331497554
H	29.169039660	-16.474132564	-21.172478986

C	30.779686452	-17.568820315	-20.414516894
C	31.990461089	-18.252136695	-20.591128230
C	30.010913828	-17.911680588	-19.284346948
C	32.432005361	-19.211185434	-19.681280713
C	30.430082491	-18.863648377	-18.375266010
C	31.663714104	-19.507743832	-18.552161388
H	32.621582547	-18.035588544	-21.456000342
H	29.055029164	-17.401731472	-19.120789860
H	33.389154678	-19.707326494	-19.859408227
H	29.830578274	-19.117414702	-17.495953574
O	32.027499553	-20.382358471	-17.591412428
C	33.319934886	-20.935238903	-17.640032227
H	33.462531240	-21.572542670	-18.530534743
H	34.094379799	-20.146748199	-17.640661696
H	33.441184985	-21.554085840	-16.741802112
H	29.826948668	-15.974339394	-23.353164455
H	31.122022392	-10.406182252	-26.236751423

Reductive Elimination TS
Electronic Energy: -1763.607729221
Free Energy Correction: 0.583462198

N	-0.922325572	5.291752437	-1.441366653
C	-0.543939535	0.844393436	2.717864455
C	-1.368582146	1.787518248	2.021303542
C	-0.516552432	2.741713385	1.361135236
C	0.843196760	2.383603435	1.655557411
C	0.820155042	1.203668517	2.475586377
C	-0.951883718	3.988615135	0.658547436
C	-0.751645328	3.980970551	-0.854859247
C	0.070819905	6.198426131	-1.434593972
C	2.069746428	3.089333094	1.202514531
C	-2.853509041	1.847762409	2.036836419
C	1.991645521	0.515915492	3.075113902
C	-0.964839048	-0.240657814	3.645354891
O	1.181791742	6.012243297	-0.963171472
N	-0.049619428	0.974964306	-1.321813234
C	-2.011143822	-0.292108230	-2.994796112
Rh	-0.094479749	0.743995574	0.523216928
H	-1.444590802	3.274210192	-1.336453678
H	0.260159542	3.617096243	-1.095702252
H	-0.373775858	4.832031162	1.077921594
H	-2.009530664	4.201514899	0.887920291
H	-1.820066725	5.559893654	-1.833451929
H	-0.698358777	0.019961126	4.684491780
H	-0.462612842	-1.194660780	3.411138225
H	-2.051618157	-0.411491278	3.625130197
H	-3.193101967	2.604296856	2.765055864
H	-3.309126833	0.889965512	2.331661136
H	-3.263040596	2.137284531	1.055139899

H	2.118486059	0.837826452	4.124114980
H	2.913537942	0.726281031	2.519400070
H	1.849664996	-0.576415137	3.082186224
H	2.593401471	3.539436827	2.063732404
H	1.845856847	3.891677402	0.482422323
H	2.756338705	2.365883732	0.732805134
C	0.346245818	0.349718557	-2.425970674
O	1.532887591	0.352371040	-2.798624492
C	-0.716161468	-0.190774222	-3.337494852
H	-2.694367174	-0.685497883	-3.759354692
C	-0.216372515	-0.628700991	-4.676459250
H	0.326906470	0.183314860	-5.187157768
H	0.507831708	-1.454864282	-4.570129427
H	-1.042129934	-0.967143708	-5.320352329
O	2.891692213	-0.063485228	0.196391848
C	2.169326852	-1.048277021	0.062030545
O	0.888710364	-1.069523487	0.194828328
C	2.761575845	-2.424224309	-0.297042756
C	2.267452518	-3.466708227	0.703455681
H	1.170622308	-3.551644960	0.678716611
H	2.703836562	-4.455300389	0.472800804
H	2.563161378	-3.201289672	1.734365015
C	2.286165044	-2.782783951	-1.704280749
H	1.187343249	-2.855676721	-1.737356444
H	2.587457381	-2.009253553	-2.430877874
H	2.710786328	-3.753410983	-2.018073131
C	4.281109225	-2.360290913	-0.266401367
H	4.709418892	-3.343533495	-0.528244875
H	4.663250424	-1.613841788	-0.980687089
H	4.649178079	-2.080508464	0.734627010
C	-2.651257048	0.064599829	-1.687157416
H	-3.700084583	-0.294977174	-1.710939370
C	-2.089307182	-0.477363583	-0.402961067
H	-2.580991616	-0.013714064	0.457842506
C	-1.809176187	-1.874383171	-0.183072950
C	-1.450047016	-2.793579334	-1.187382745
C	-1.925548252	-2.378841192	1.133973811
C	-1.194775668	-4.127091167	-0.900200266
C	-1.674679572	-3.697558293	1.437343963
C	-1.274625659	-4.585292295	0.421285945
H	-1.353374591	-2.459857155	-2.221668294
H	-2.231793100	-1.695907131	1.931082109
H	-0.905786920	-4.796750702	-1.713133688
H	-1.760873117	-4.077168397	2.459374589
O	-0.980073739	-5.833771393	0.805724575
C	-0.456852722	-6.737360615	-0.143155074
H	-1.186297173	-6.956888652	-0.941055524
H	0.468156161	-6.342965717	-0.600691221
H	-0.223359895	-7.665193655	0.393247799

H	-2.732462624	1.164374402	-1.593043104
H	-0.222556987	7.159346372	-1.919283429

Intermediate V
Electronic Energy: -1763.722758437
Free Energy Correction: 0.587438583

N	-1.338726275	5.075912518	-1.479672001
C	-0.090452254	1.022015586	2.821024657
C	-1.048034358	1.900316148	2.201479217
C	-0.328414819	2.915129056	1.482909268
C	1.082852304	2.662690402	1.672895386
C	1.233504314	1.515261710	2.511000959
C	-0.916973303	4.075991251	0.746281253
C	-1.041761309	3.857499055	-0.761115047
C	-0.371821228	5.963341193	-1.773542382
C	2.191525373	3.422160364	1.039525069
C	-2.525884751	1.786279792	2.272358111
C	2.504554081	0.944741887	3.024694891
C	-0.369767222	-0.171663341	3.660961558
O	0.807044438	5.829164560	-1.485524859
N	-1.144351382	0.402222508	-0.848847537
C	-1.569562139	-0.496622768	-3.461628319
Rh	0.178525377	0.973759849	0.712112011
H	-1.822842162	3.111499494	-0.978665557
H	-0.096065078	3.443258625	-1.150613645
H	-0.279185001	4.960403484	0.918477158
H	-1.905159175	4.322387473	1.170484514
H	-2.296539843	5.299654815	-1.732527078
H	-0.087505321	0.019404285	4.710196605
H	0.211155936	-1.041331036	3.309962771
H	-1.434230436	-0.447684923	3.638352082
H	-2.912439934	2.400697132	3.103819573
H	-2.847526118	0.747045891	2.440246817
H	-3.002276395	2.138993400	1.344283996
H	2.696124037	1.316499639	4.046649909
H	3.356892550	1.217432294	2.388263125
H	2.464123850	-0.154043967	3.067834156
H	2.718763909	4.035849941	1.789545622
H	1.829305283	4.091627168	0.242984807
H	2.925503624	2.726660690	0.601502997
C	-0.264908954	0.632302213	-1.793024415
O	0.835890433	1.154577926	-1.404787195
C	-0.529790856	0.318680765	-3.212352065
H	-1.782922800	-0.805705000	-4.492486829
C	0.394653242	0.878558738	-4.238154120
H	0.422611523	1.980878705	-4.193280389
H	1.428327184	0.537786774	-4.058145737
H	0.097100994	0.576982868	-5.253312535
O	2.991317658	-0.463945544	0.301128206

C	2.062766819	-1.267189526	0.284944331
O	0.827039406	-0.999351043	0.504744928
C	2.285568793	-2.756811546	-0.033073446
C	1.702109761	-3.598527789	1.100807235
H	0.616645340	-3.435945157	1.201706674
H	1.877311064	-4.673019540	0.915395732
H	2.172488678	-3.342257297	2.067371284
C	1.550353728	-3.058020074	-1.339598439
H	0.473042312	-2.842534618	-1.244240641
H	1.942826991	-2.437766019	-2.165383951
H	1.674977057	-4.118096223	-1.622718472
C	3.768791630	-3.052524872	-0.189719875
H	3.924016543	-4.119316897	-0.427939936
H	4.211171109	-2.449635407	-0.998808476
H	4.321243956	-2.820944370	0.735829099
C	-2.395978688	-1.065450737	-2.352007430
H	-1.957548883	-2.037368840	-2.039832140
C	-2.456886120	-0.136401399	-1.136999808
H	-3.135376681	0.709807398	-1.396537606
C	-3.047752297	-0.842551842	0.054852258
C	-2.262841797	-1.688212908	0.840576767
C	-4.400599980	-0.698596019	0.380894346
C	-2.799564132	-2.360878325	1.938237648
C	-4.950367894	-1.362437481	1.470210124
C	-4.149764962	-2.193008524	2.265316701
H	-1.195129829	-1.796922724	0.610306349
H	-5.034515348	-0.037379218	-0.221970926
H	-2.147204321	-3.003377848	2.536209576
H	-6.004660417	-1.244045744	1.738046275
O	-4.758708190	-2.784827705	3.318110043
C	-3.981595892	-3.551383582	4.204149609
H	-3.530619470	-4.427445754	3.705163576
H	-3.173803321	-2.950338402	4.659688970
H	-4.651195289	-3.904984935	4.998855098
H	-3.420587208	-1.296593875	-2.688453952
H	-0.758716255	6.853384941	-2.323566717

Intermediate V (Acetic Acid Associated)
Electronic Energy: -1992.789857375
Free Energy Correction: 0.642163397

N	-2.798457800	-3.375284271	-1.915723327
C	1.582428960	-2.277920686	2.142972250
C	1.245802650	-3.018964767	0.971061492
C	-0.192199485	-2.983972455	0.817292440
C	-0.744240038	-2.322103424	1.976819539
C	0.339761470	-1.835363447	2.758372726
C	-1.002158089	-3.676990154	-0.226792031
C	-1.807504825	-2.714626723	-1.097313978
C	-4.047394723	-3.601810196	-1.472841901

C	-2.168724120	-2.333863424	2.382806596
C	2.198440913	-3.706841340	0.067495349
C	0.206072069	-1.064854074	4.020466592
C	2.955610390	-1.995574246	2.630187676
O	-4.471093287	-3.279980803	-0.373048711
N	-0.740554739	0.550735791	-0.060486400
C	-2.279465864	0.819629988	-2.435908800
Rh	0.574815466	-0.990420671	0.787995288
H	-1.109018152	-2.151625570	-1.732714906
H	-2.342028794	-1.995033033	-0.458807749
H	-1.698149543	-4.368333302	0.284718188
H	-0.346592252	-4.292596335	-0.864538113
H	-2.549621546	-3.709966820	-2.841829506
H	3.327182992	-2.818588123	3.263871468
H	2.987478648	-1.069832057	3.222322277
H	3.652540790	-1.873637686	1.786401744
H	2.293909543	-4.761732771	0.377433872
H	3.200312150	-3.255453111	0.113734297
H	1.848941395	-3.679907811	-0.973914988
H	-0.060191864	-1.739899522	4.851956421
H	-0.588452203	-0.306986335	3.940459377
H	1.142601557	-0.558892911	4.295148971
H	-2.324829672	-3.248070337	2.986078228
H	-2.861591318	-2.374387236	1.530797014
H	-2.432304493	-1.468381475	3.003320592
C	-2.097592799	0.383934501	-0.023887952
O	-2.682312549	0.073838432	1.017085083
C	-2.901064986	0.560384965	-1.274186385
H	-2.866327949	0.872069604	-3.362261306
C	-4.373122494	0.355716514	-1.143185138
H	-4.597148311	-0.652141871	-0.752024293
H	-4.811229441	1.066977783	-0.422075957
H	-4.880684204	0.482000037	-2.111517858
O	-0.181313971	1.926231359	2.109281824
C	1.103115934	1.748251900	2.192786534
O	1.688706120	0.824740135	1.619367977
C	-0.804534390	0.995055804	-2.514920556
H	-0.536614520	1.763117118	-3.262736841
C	-0.191850768	1.358089197	-1.163700797
H	0.875774716	1.113815016	-1.223003649
C	-0.234705599	2.843735609	-0.850583735
C	-1.393886133	3.537348974	-0.492637504
C	0.965855647	3.567400529	-0.868007675
C	-1.369541446	4.893573659	-0.167111128
C	1.013030335	4.917992585	-0.548535328
C	-0.159105537	5.594703233	-0.191459819
H	-2.356285125	3.017023740	-0.447599588
H	1.897230158	3.047928414	-1.124630442
H	-2.303138947	5.389116554	0.110153987

H	1.955677752	5.473293285	-0.557545443
O	-0.030147050	6.905068231	0.114838514
C	-1.174643321	7.623788345	0.503283619
H	-1.931176423	7.655175146	-0.301041211
H	-1.639169908	7.193376773	1.408393216
H	-0.852382204	8.649231785	0.725023544
H	-0.353833830	0.049355751	-2.883097008
H	-4.681458182	-4.120945539	-2.230073239
C	1.822569625	2.729646218	3.051131694
H	2.908015128	2.596119726	2.976314373
H	1.535536542	3.752710841	2.765871067
H	1.506091215	2.585664309	4.096758582
H	-0.514365965	1.331441511	1.322416906
O	1.936062849	-0.642672526	-0.790213589
C	1.889293505	-1.171393044	-1.954757866
O	1.024593275	-1.951416256	-2.360594519
C	3.062502146	-0.756971139	-2.865127587
C	4.321906684	-1.431965337	-2.321672300
H	4.529293087	-1.108904475	-1.288267473
H	4.216041655	-2.531329414	-2.324343454
H	5.195431601	-1.176930988	-2.946834699
C	2.805505869	-1.211738950	-4.293479646
H	3.653356384	-0.928071760	-4.940699422
H	2.675403613	-2.303856020	-4.347934717
H	1.891891981	-0.747360818	-4.701852531
C	3.235171442	0.759648992	-2.827765461
H	3.434715643	1.111213941	-1.803567625
H	4.076553096	1.066289779	-3.473608161
H	2.329840643	1.277024081	-3.196224039

Protodemetallation TS
Electronic Energy: -1992.789790150
Free Energy Correction: 0.643633594

N	-2.803874381	-3.370792561	-1.919115325
C	1.582262293	-2.287323136	2.138804969
C	1.242428996	-3.025717317	0.965719502
C	-0.195399490	-2.986624424	0.813259102
C	-0.744515897	-2.324574719	1.974241476
C	0.341337220	-1.842763749	2.756281313
C	-1.006319686	-3.676117173	-0.232372845
C	-1.813965208	-2.711646983	-1.098317496
C	-4.049311831	-3.609514853	-1.472776184
C	-2.168893974	-2.331059731	2.380756627
C	2.192166300	-3.712405815	0.058177226
C	0.210755914	-1.073479982	4.019360640
C	2.956165800	-2.008911958	2.625896496
O	-4.469362506	-3.300538378	-0.367949597
N	-0.738781000	0.559740530	-0.048421188
C	-2.273694679	0.811193224	-2.429131363

Rh	0.577237748	-0.995244967	0.787216071
H	-1.116381373	-2.145698549	-1.732123303
H	-2.349543323	-1.994735717	-0.457289585
H	-1.700565345	-4.370733489	0.277125640
H	-0.350978037	-4.288150918	-0.873709589
H	-2.556499764	-3.695874602	-2.849022853
H	3.322437447	-2.829898753	3.265282431
H	2.991538134	-1.079583059	3.212174662
H	3.654902513	-1.895719577	1.782502664
H	2.285570785	-4.768728825	0.363798354
H	3.195106699	-3.263502742	0.104156070
H	1.841060319	-3.680725935	-0.982641730
H	-0.059248161	-1.748242486	4.849844797
H	-0.579986320	-0.311538238	3.939662762
H	1.149756239	-0.572560042	4.294869168
H	-2.328601539	-3.245404138	2.982800860
H	-2.862354976	-2.368358300	1.529092610
H	-2.428627792	-1.465422941	3.002699451
C	-2.097673380	0.387878786	-0.015373304
O	-2.682021827	0.085946744	1.027154128
C	-2.897247936	0.550723825	-1.268665657
H	-2.858227098	0.856617291	-3.357270554
C	-4.367702913	0.332722623	-1.141609589
H	-4.583129843	-0.676475573	-0.748669429
H	-4.814807826	1.041278998	-0.423533224
H	-4.873332815	0.451665668	-2.111820578
O	-0.179432819	1.915149168	2.096353105
C	1.101044214	1.736836924	2.192045631
O	1.693899621	0.815550551	1.618602481
C	-0.799982656	0.995279412	-2.505852683
H	-0.535896181	1.763813710	-3.254496686
C	-0.188851674	1.363575828	-1.155140349
H	0.879003586	1.118670139	-1.211791907
C	-0.233082429	2.849984595	-0.848300385
C	-1.395111153	3.544882700	-0.502652065
C	0.967643598	3.573214995	-0.860994113
C	-1.373313447	4.902952845	-0.184776361
C	1.012132306	4.925636948	-0.549351641
C	-0.162767004	5.604066490	-0.204850104
H	-2.357627473	3.024266983	-0.462254912
H	1.900731808	3.052180150	-1.108088831
H	-2.308921583	5.400116408	0.082721095
H	1.954601297	5.481264097	-0.555093889
O	-0.036270627	6.916376034	0.094034892
C	-1.183084052	7.636872388	0.472228597
H	-1.935180757	7.663924855	-0.336387431
H	-1.652474908	7.211056538	1.376984967
H	-0.862213735	8.663521298	0.690425071
H	-0.345095352	0.051481949	-2.873213680

H	-4.683889234	-4.124980322	-2.232038917
C	1.817531860	2.711499001	3.061962244
H	2.903501163	2.579114683	2.991027784
H	1.531589490	3.737073787	2.784479644
H	1.496964856	2.558645201	4.105094798
H	-0.507090652	1.317616962	1.289048327
O	1.941843671	-0.649845863	-0.788188872
C	1.887359639	-1.168019335	-1.957092180
O	1.015449851	-1.938187271	-2.366521532
C	3.061105226	-0.754282691	-2.866830730
C	4.319952261	-1.431447395	-2.324883373
H	4.526987025	-1.111513849	-1.290489291
H	4.213542221	-2.530768031	-2.330822534
H	5.193793455	-1.175167181	-2.949092297
C	2.803574711	-1.205861339	-4.296073730
H	3.652432932	-0.923113807	-4.942342734
H	2.670979977	-2.297615332	-4.352552901
H	1.891303474	-0.738672178	-4.704128147
C	3.234724765	0.762248131	-2.826117632
H	3.440969773	1.110931180	-1.802204039
H	4.071760116	1.070527578	-3.476794780
H	2.327291779	1.281085317	-3.187191909

Intermediate V (Protonated)
Electronic Energy: -1992.805570582
Free Energy Correction: 0.646726338

N	-2.933828136	-3.099028027	-2.039603159
C	1.464894973	-2.515403617	2.105358699
C	1.079461327	-3.168547104	0.881795194
C	-0.342594194	-3.038311874	0.734189778
C	-0.847055431	-2.375344384	1.916440221
C	0.256207112	-2.032352125	2.749114148
C	-1.187694043	-3.624733399	-0.348309567
C	-1.886508550	-2.567622740	-1.198237936
C	-4.170238462	-3.329000286	-1.565496068
C	-2.271612882	-2.197094299	2.284013774
C	1.996560312	-3.851939623	-0.059816889
C	0.152865425	-1.343026438	4.059928301
C	2.853348305	-2.373786615	2.606355575
O	-4.527495800	-3.108595808	-0.417704738
N	-0.711040924	0.763417038	0.151063939
C	-2.011314553	0.938954846	-2.334355048
Rh	0.589792262	-1.083161582	0.850142421
H	-1.131138274	-2.061150333	-1.817077821
H	-2.343620671	-1.815503483	-0.536180573
H	-1.949777325	-4.270521238	0.125459298
H	-0.574107374	-4.273568026	-0.994673459
H	-2.736494941	-3.334363075	-3.007596788
H	3.167122982	-3.281621349	3.148860317

H	2.949912477	-1.516056842	3.287180307
H	3.554396394	-2.217361746	1.771338861
H	2.073240559	-4.917908862	0.215655035
H	3.009132959	-3.423911145	-0.020870496
H	1.631135039	-3.776293668	-1.092755366
H	-0.256972049	-2.028782034	4.820987889
H	-0.513508752	-0.469435098	3.991513833
H	1.132023293	-0.992270346	4.416238052
H	-2.527081430	-2.967680841	3.033841164
H	-2.955953630	-2.320389953	1.430978326
H	-2.456732330	-1.212506479	2.735306247
C	-2.106831814	0.623726648	0.081938969
O	-2.753032305	0.473759129	1.104861557
C	-2.750952966	0.654548686	-1.248309794
H	-2.492514505	0.940922647	-3.320377278
C	-4.217603916	0.382191377	-1.270849315
H	-4.453271097	-0.576892358	-0.777557058
H	-4.771075665	1.157244108	-0.713952137
H	-4.598443343	0.354649450	-2.302122626
O	0.150067190	1.704713767	2.622033790
C	1.347209677	1.427738801	2.445098645
O	1.782361386	0.514142148	1.665870874
C	-0.551657573	1.210740966	-2.276267674
H	-0.278438690	2.004443772	-2.993572460
C	-0.040831458	1.586203576	-0.887947042
H	1.021759459	1.308645629	-0.839579160
C	-0.120319489	3.054900200	-0.539277007
C	-1.312298820	3.783534268	-0.527988299
C	1.052204698	3.720353236	-0.156723017
C	-1.346477731	5.126789184	-0.153608889
C	1.039422911	5.055351274	0.219745748
C	-0.164012438	5.772292948	0.226196244
H	-2.254292858	3.304402377	-0.815652046
H	1.999907937	3.167671322	-0.147160364
H	-2.302693710	5.655027668	-0.159964809
H	1.956642452	5.571078742	0.519521845
O	-0.090679665	7.064198746	0.608696137
C	-1.267073055	7.835949341	0.624263780
H	-1.726517750	7.899611572	-0.377935192
H	-2.012401480	7.429864255	1.331040021
H	-0.985339955	8.845868567	0.948592655
H	-0.032211548	0.298884047	-2.634471542
H	-4.859169704	-3.741006720	-2.339664521
C	2.418041148	2.188777167	3.187569241
H	3.228455534	2.480505819	2.503162627
H	1.999361047	3.077247838	3.679123195
H	2.864162563	1.530402954	3.951444411
H	-0.502327376	1.141975570	1.103488459
O	1.888832210	-0.676541638	-0.753364244

C	1.842126614	-1.152982626	-1.939340709
O	0.980018189	-1.916197802	-2.381841943
C	3.022728944	-0.706099342	-2.824102742
C	4.220095792	-1.566531083	-2.415981578
H	4.472956226	-1.412559813	-1.353342505
H	4.009635674	-2.639524295	-2.571542974
H	5.105344552	-1.305231593	-3.021552742
C	2.693012716	-0.938858068	-4.291397399
H	3.546255165	-0.644259819	-4.926511218
H	2.462109207	-1.997912515	-4.482993659
H	1.815777139	-0.345277867	-4.603259741
C	3.345883898	0.766948596	-2.587015003
H	3.593215309	0.956310101	-1.530719193
H	4.205061040	1.073008553	-3.209448989
H	2.494473163	1.417266652	-2.855815525

Product Dissociation TS
Electronic Energy: -1992.804144486
Free Energy Correction: 0.645880785

N	-3.348126789	-2.232363579	-2.052467800
C	1.311247768	-3.131982523	1.603376069
C	0.565779336	-3.575107544	0.434284703
C	-0.779672707	-3.138510832	0.587558108
C	-0.886993358	-2.456090201	1.863362331
C	0.389606122	-2.468210089	2.499578429
C	-1.902452845	-3.353122723	-0.373131926
C	-2.105205846	-2.169901119	-1.320104576
C	-4.519844264	-1.963521632	-1.447832236
C	-2.124406165	-1.854631672	2.405949085
C	1.106562448	-4.333127674	-0.717780743
C	0.696785668	-1.923919424	3.845780765
C	2.762914580	-3.335461309	1.808885743
O	-4.638023432	-1.677050087	-0.266524570
N	-1.054051703	0.980726229	0.389720739
C	-2.708241436	1.497239157	-1.783654847
Rh	0.566060014	-1.453923145	0.608722661
H	-1.265782520	-2.100281605	-2.031392295
H	-2.095295151	-1.233723873	-0.735356151
H	-2.829613127	-3.508145223	0.202711201
H	-1.729696812	-4.275058557	-0.952548541
H	-3.352620016	-2.489558081	-3.034753618
H	2.971091340	-4.393088600	2.045229269
H	3.146527687	-2.716994369	2.632749233
H	3.305338863	-3.067914684	0.888476931
H	0.947874773	-5.413298215	-0.555914823
H	2.179405082	-4.145549863	-0.851148942
H	0.596889199	-4.053222711	-1.652232724
H	0.481302795	-2.681559655	4.618375471
H	0.095974492	-1.028932470	4.059175243

H	1.756833081	-1.645846186	3.939521280
H	-2.502569892	-2.480908665	3.232913735
H	-2.913678067	-1.775388302	1.640660716
H	-1.943140748	-0.843113132	2.800539706
C	-2.400874653	1.139687393	0.615382999
O	-2.872077290	1.044062365	1.743393811
C	-3.266264445	1.401235322	-0.564372275
H	-3.355157188	1.654929829	-2.656263692
C	-4.724486422	1.549532864	-0.293553350
H	-5.122614617	0.637993328	0.179460332
H	-4.913399618	2.384913834	0.401719472
H	-5.281337268	1.735472279	-1.224293471
O	0.703479254	1.053731434	2.649761912
C	1.785277285	0.836294033	2.088930674
O	1.948751033	0.050414176	1.089416205
C	-1.243521415	1.368599927	-2.017072010
H	-0.916726663	2.048656428	-2.823005743
C	-0.401108606	1.608202474	-0.771355442
H	0.545342815	1.066598188	-0.913749865
C	-0.032801267	3.047274596	-0.487881003
C	-0.939742707	4.107794172	-0.547136390
C	1.282965338	3.335688524	-0.098259473
C	-0.562638372	5.411908176	-0.224826682
C	1.676776901	4.625016038	0.229640372
C	0.752956530	5.677016867	0.172544959
H	-1.975457954	3.925794853	-0.852948656
H	2.010458258	2.514861753	-0.053488703
H	-1.305978398	6.210147933	-0.287663805
H	2.703956705	4.847981387	0.534907130
O	1.215036148	6.899862921	0.510230956
C	0.330770270	7.993134022	0.473317767
H	-0.066435131	8.163191792	-0.543051616
H	-0.518104401	7.855652499	1.166609954
H	0.900038732	8.878952791	0.783087909
H	-1.031029714	0.345929487	-2.388798368
H	-5.389648622	-2.029388595	-2.142535688
C	3.044759065	1.504959148	2.577145740
H	3.724434597	1.732964724	1.743524666
H	2.810212929	2.414924339	3.146560998
H	3.574237491	0.803919099	3.244582704
H	-0.514643625	1.026832681	1.271745166
O	1.015850923	-1.002406356	-1.370391038
C	2.187447849	-1.279671520	-1.830170851
O	3.056954775	-1.898592175	-1.222085841
C	2.436101496	-0.746069423	-3.250393519
C	2.539626467	0.777637558	-3.162155269
H	1.588908259	1.231932374	-2.838788028
H	3.322297302	1.081521678	-2.444920781
H	2.798585094	1.201826659	-4.147778371

C	3.736377725	-1.315505607	-3.799235309
H	3.924075268	-0.923989122	-4.813668062
H	4.591462662	-1.046331622	-3.159542407
H	3.697388371	-2.415806138	-3.856599727
C	1.273909544	-1.140523059	-4.158644275
H	0.328643995	-0.688612926	-3.819669468
H	1.463953005	-0.805308058	-5.192956186
H	1.137285224	-2.236793966	-4.178612169

Product (Dissociated from Catalyst with Acetate Dissociated)
Electronic Energy: -709.403313992
Free Energy Correction: 0.217013902

N	-0.514177177	0.420823821	1.804173957
C	-1.958874407	-1.617987257	2.984685674
C	-1.807022891	0.677311996	2.143427652
O	-2.356049526	1.734102404	1.846806887
C	-2.530252997	-0.407224356	2.865758548
H	-2.520811073	-2.433338676	3.456840524
C	-3.900312081	-0.073006840	3.348752307
H	-3.879112707	0.766350938	4.063780526
H	-4.540092609	0.254288243	2.512591192
H	-4.371347821	-0.938634328	3.837025316
C	-0.603811898	-1.916031693	2.438052553
H	-0.705425852	-2.344559681	1.419209161
C	0.265675410	-0.666453215	2.377061989
H	0.553847736	-0.405087452	3.418501296
C	1.527644497	-0.912417958	1.593200978
C	2.700060178	-1.282796092	2.250085088
C	1.540343077	-0.863181893	0.192161479
C	3.862755725	-1.604173761	1.547955651
C	2.689817219	-1.168824403	-0.521349681
C	3.861351202	-1.547958781	0.150106202
H	2.712201206	-1.325545829	3.345205664
H	0.630537421	-0.579218964	-0.347512416
H	4.759553603	-1.890373657	2.102258840
H	2.708620950	-1.126197401	-1.614248736
O	4.928414746	-1.835494017	-0.624403382
C	6.118907666	-2.252559564	-0.001563905
H	6.524856337	-1.473058832	0.667033356
H	5.969967624	-3.178143835	0.582345416
H	6.847947266	-2.450022755	-0.797612304
H	-0.089204174	-2.686055128	3.036095323
H	-0.008465825	1.223285141	1.432380317

Intermediate with 4-Methylphenol and Acetate
Electronic Energy: -2338.934331686
Free Energy Correction: 0.753605028

N	30.575528094	-11.083172302	-24.975060610
C	29.531293876	-13.950722181	-19.647966954

C	28.971275725	-13.595924793	-20.930308156
C	29.940815650	-12.769212320	-21.613038937
C	31.101874883	-12.692480253	-20.775040593
C	30.848073359	-13.443726977	-19.568821344
C	29.705497774	-12.000617098	-22.871215512
C	30.767509144	-12.098418296	-23.961225312
C	30.960526761	-9.810692539	-24.769897422
C	32.305777731	-11.831867206	-20.963852903
C	27.587075400	-13.925736727	-21.364848788
C	31.760235084	-13.586722921	-18.403170686
C	28.819809301	-14.637049415	-18.544121500
O	31.540485510	-9.411129120	-23.772692597
Rh	30.703340926	-14.816772498	-21.390537900
H	30.759511721	-13.084222376	-24.448747589
H	31.774658759	-11.963916566	-23.535884684
H	29.623445952	-10.937070327	-22.583950042
H	28.724280202	-12.272876267	-23.298597360
H	30.065411186	-11.305349117	-25.824803731
H	28.442777843	-13.866132672	-17.847373767
H	29.495909667	-15.290714134	-17.968936606
H	27.973815899	-15.242201081	-18.895903261
H	26.846353095	-13.285452879	-20.854356933
H	27.350700624	-14.975759586	-21.129023979
H	27.457732197	-13.793166065	-22.449071092
H	31.526274573	-12.837503574	-17.628209321
H	32.811514701	-13.418401088	-18.683945337
H	31.681079053	-14.592564054	-17.957034267
H	32.512010514	-11.313732711	-20.009825902
H	32.145061518	-11.068686974	-21.741201989
H	33.213272478	-12.404600796	-21.229426105
H	30.700047083	-9.141288653	-25.623709884
N	30.105799313	-16.753332863	-21.017854523
C	29.955151987	-15.495080247	-23.185815339
C	29.685779060	-17.571094378	-22.009434905
O	29.439959820	-18.773690473	-21.905757470
C	29.548791867	-16.772557203	-23.258555479
H	29.895145551	-14.836661511	-24.065707338
C	28.979655546	-17.466155931	-24.452196070
H	27.964531209	-17.848787055	-24.246425965
H	29.587177574	-18.347656464	-24.723201355
H	28.928418398	-16.797166303	-25.324919235
O	30.316878881	-17.377400176	-19.794879527
C	29.210868949	-17.808368812	-19.160181803
O	28.083858306	-17.592856846	-19.529285221
C	29.587633580	-18.640320745	-17.943953747
C	28.351385109	-18.820413755	-17.074531362
H	27.973715161	-17.848529698	-16.713340245
H	28.598928807	-19.439685826	-16.196759818
H	27.537075714	-19.311853247	-17.629150709

C	30.702264869	-17.978464274	-17.136920599
H	30.398492276	-16.983325181	-16.766688378
H	31.619391572	-17.862505491	-17.733903201
H	30.938021099	-18.600755947	-16.257124864
C	30.066300066	-19.994736249	-18.477986613
H	30.309889687	-20.664034493	-17.635027957
H	30.962052297	-19.872211779	-19.107273914
H	29.287071488	-20.475440110	-19.092363892
C	32.575935386	-15.011741079	-22.510356477
H	32.493305343	-15.709778638	-23.349557406
C	32.881196647	-15.478724899	-21.229443366
H	33.285398169	-14.754022759	-20.509318926
C	33.110018165	-16.875893574	-20.852383306
C	32.802595572	-17.952783662	-21.692565937
C	33.640951910	-17.169017349	-19.586250421
C	32.966542772	-19.270101531	-21.281380031
C	33.835306512	-18.476782977	-19.169004787
C	33.476348829	-19.541819489	-20.005745188
H	32.393800171	-17.768449885	-22.691018014
H	33.898268405	-16.345197423	-18.910486999
H	32.672483839	-20.075088193	-21.958790463
H	34.242516505	-18.705262191	-18.179438406
O	33.646835591	-20.784773518	-19.503485266
C	33.248197617	-21.888214204	-20.278469338
H	33.823451208	-21.958552937	-21.218661790
H	32.171974714	-21.845016205	-20.526373825
H	33.437033167	-22.788696684	-19.679777406
H	32.845763803	-13.988613378	-22.792429709
H	27.696389513	-7.680624940	-23.078084317
C	27.353537837	-8.712207227	-22.897279055
C	27.869347689	-9.253824173	-21.598664150
C	27.114964540	-10.137827622	-20.818439195
C	29.168837537	-8.964247784	-21.165319548
C	27.636974107	-10.726194206	-19.668926256
C	29.709179994	-9.550451019	-20.025419766
C	28.949982565	-10.452703533	-19.261769326
O	29.434709999	-11.058511475	-18.173630508
H	30.409988173	-10.808873926	-18.038536582
H	27.710892858	-9.319494212	-23.751470686
H	26.252866723	-8.720159089	-22.938766844
H	26.091993463	-10.385610934	-21.127973806
H	29.796220264	-8.294312247	-21.765981162
H	27.041594292	-11.425218783	-19.070729516
H	30.738371899	-9.341165820	-19.718074977
O	31.926369888	-10.430120510	-17.878503696
O	33.363320554	-8.998670614	-16.955174583
C	32.215302615	-9.397463164	-17.191374319
C	31.028311145	-8.607783339	-16.656077649
H	30.320054278	-9.273143209	-16.136899575

H	31.350247217	-7.804609247	-15.977974921
H	30.475007080	-8.161431599	-17.500636847

Migratory Insertion TS with 4-Methylphenol and Acetate
Electronic Energy: -2338.912525491
Free Energy Correction: 0.749316321

N	1.277848121	3.110900776	-4.402585917
C	-1.711691672	1.017513472	0.534462029
C	-1.829839192	1.615414448	-0.769681374
C	-0.497072491	1.927909181	-1.240757031
C	0.427113844	1.419102059	-0.300453590
C	-0.325108921	0.813468805	0.790743400
C	-0.157714524	2.754146486	-2.437780267
C	0.733566389	2.117216662	-3.499359954
C	2.274424259	3.934223532	-4.034464720
C	1.911453305	1.527061345	-0.338612029
C	-3.094516973	2.011508964	-1.446178030
C	0.284829989	0.215088023	2.007463765
C	-2.824656676	0.707592133	1.467705638
O	2.839456737	3.908493150	-2.951561917
N	0.646529775	-1.779908941	-1.059744660
C	-0.711104197	-0.857880505	-3.066477929
Rh	-0.824162607	-0.305840829	-1.001275777
H	0.178943829	1.380037699	-4.095388005
H	1.566800061	1.569198972	-3.025530591
H	0.374894538	3.642152958	-2.056139127
H	-1.079842378	3.133687891	-2.911363462
H	0.861565152	3.239540288	-5.319958786
H	-2.602905006	-0.175645825	2.087581506
H	-3.780539145	0.535443147	0.948348866
H	-2.959241429	1.561480507	2.154723064
H	-3.333816492	3.071687585	-1.245032024
H	-3.947420645	1.407087124	-1.099872316
H	-3.022224906	1.891265848	-2.540235721
H	0.430058613	0.970839893	2.802699384
H	1.273371445	-0.215516773	1.775613001
H	-0.343255167	-0.594166656	2.415557421
H	2.290943228	1.837923668	0.649744884
H	2.247501215	2.271187155	-1.078214573
H	2.379014922	0.554323032	-0.569437334
C	1.044136722	-2.312484385	-2.233391236
O	1.815635662	-3.266475802	-2.383972581
C	0.411616516	-1.562409763	-3.351133844
H	-1.193954463	-0.270598862	-3.860539120
C	1.060456868	-1.642037392	-4.689415600
H	2.091123046	-1.244275213	-4.660129295
H	1.149736228	-2.693552027	-5.015244044
H	0.494440074	-1.085852808	-5.452480592
O	1.036841223	-2.531437613	0.047934581

C	2.314538845	-2.404297850	0.435560027
O	3.091575727	-1.601517908	-0.019599284
C	2.652590342	-3.446260621	1.491440064
C	3.978700883	-3.079061206	2.141396837
H	3.915415536	-2.103751603	2.652955684
H	4.251102263	-3.841844450	2.889433230
H	4.788049553	-3.017688665	1.397286204
C	1.557066048	-3.541542347	2.550296221
H	1.437680718	-2.588448900	3.093293411
H	0.585342620	-3.807791429	2.108291306
H	1.825972261	-4.317548146	3.287711634
C	2.777036658	-4.780895805	0.749612086
H	3.030987901	-5.582630012	1.464705042
H	1.831362331	-5.034254443	0.243708874
H	3.569120520	-4.737253123	-0.016822282
C	-2.213752751	-1.652728785	-2.232458343
H	-2.049453264	-2.570112341	-2.808051625
C	-2.325666417	-1.824102755	-0.802309315
H	-3.135372367	-1.257975182	-0.322835145
C	-2.014086768	-3.077328397	-0.100753569
C	-1.346145007	-4.161970621	-0.682132813
C	-2.402903227	-3.210338255	1.244742610
C	-1.047874374	-5.314486353	0.041529049
C	-2.116823417	-4.349714438	1.978826696
C	-1.417551334	-5.409396734	1.387579922
H	-1.018349874	-4.115282682	-1.725993662
H	-2.943007875	-2.386534888	1.725978110
H	-0.511996055	-6.126599758	-0.456336545
H	-2.411757287	-4.439995239	3.028723864
O	-1.137411319	-6.464444366	2.186169855
C	-0.344834014	-7.505016910	1.673297707
H	-0.832612692	-8.016454205	0.824220652
H	0.642992474	-7.136295179	1.342458422
H	-0.198738503	-8.230548672	2.483846199
H	-2.989546977	-1.024346710	-2.686349656
H	2.548302544	4.659457424	-4.836910931
H	0.127931028	7.339433679	-1.357637053
C	0.170979411	6.250654872	-1.538775482
C	-0.250573100	5.459093645	-0.335703517
C	-1.603585020	5.260896901	-0.030776925
C	0.689508966	4.881590852	0.524119460
C	-2.002919005	4.536696237	1.088083023
C	0.308715811	4.150870737	1.647152746
C	-1.050144905	3.976097189	1.951872602
O	-1.466042520	3.286460983	3.018775226
H	-0.675491847	2.980711669	3.582713777
H	1.205373869	6.008861019	-1.832717229
H	-0.481685635	6.047597923	-2.405320471
H	-2.368343435	5.681401575	-0.696175415

H	1.757626520	4.992762255	0.298516066
H	-3.064811189	4.383943981	1.312083756
H	1.054797688	3.685406601	2.300441918
O	0.528602006	2.512976483	4.432767075
O	2.018976757	3.035730721	6.002301973
C	1.060886642	3.312166196	5.269238703
C	0.455246107	4.707448234	5.322738061
H	-0.642057312	4.652253102	5.404505091
H	0.863564743	5.293292291	6.158290814
H	0.673425854	5.237698498	4.378628477

Intermediate with 4-Methylphenol, Acetate, and Methanol
Electronic Energy: -2454.652711206
Free Energy Correction: 0.799683870

N	30.446786730	-11.072027234	-24.865351030
C	29.459649847	-14.046293815	-19.581802789
C	28.892526368	-13.679720112	-20.858898128
C	29.843667458	-12.821759100	-21.528154711
C	31.003707858	-12.736661443	-20.691564473
C	30.762599879	-13.504345465	-19.492701622
C	29.594683136	-12.031043123	-22.770875040
C	30.647968104	-12.105216039	-23.872233560
C	30.891723435	-9.816568251	-24.671595998
C	32.191150888	-11.852919301	-20.879602791
C	27.509585479	-14.017676455	-21.288764576
C	31.669889442	-13.615644978	-18.319753415
C	28.764770795	-14.793992609	-18.506610262
O	31.543299557	-9.448462240	-23.707748452
Rh	30.648633818	-14.858265439	-21.337741960
H	30.638860177	-13.082024860	-24.377108882
H	31.658006982	-11.974522132	-23.453678721
H	29.508637884	-10.971378917	-22.466509617
H	28.610519870	-12.299360480	-23.194359496
H	29.878885114	-11.263274703	-25.685591513
H	28.338658044	-14.077466964	-17.780991042
H	29.462772977	-15.442576868	-17.951624656
H	27.953027230	-15.422477705	-18.896263599
H	26.769102136	-13.391249739	-20.760076348
H	27.285063358	-15.073442773	-21.065559958
H	27.369067427	-13.869307029	-22.369547532
H	31.399668419	-12.873694049	-17.548074327
H	32.717667991	-13.412050384	-18.590771932
H	31.622847513	-14.620438063	-17.867878946
H	32.395153723	-11.326005741	-19.930016838
H	32.014849335	-11.091622030	-21.655018290
H	33.107052308	-12.409564168	-21.150015690
H	30.609289723	-9.129986581	-25.504721582
N	30.100469757	-16.818965296	-21.010782961
C	29.915252247	-15.514395929	-23.147581500

C	29.704086767	-17.624297394	-22.021973379
O	29.491959201	-18.835416596	-21.947919297
C	29.543554098	-16.800073572	-23.251015690
H	29.834016279	-14.837334645	-24.011044219
C	28.989402308	-17.478419738	-24.460366922
H	27.985926320	-17.893982953	-24.261378833
H	29.619924278	-18.335600135	-24.755979630
H	28.916348066	-16.788870766	-25.315415833
O	30.318599705	-17.465029985	-19.800569219
C	29.219029251	-17.938180793	-19.185205336
O	28.089899329	-17.746593482	-19.561243495
C	29.606274119	-18.784642161	-17.982523009
C	28.371169662	-19.000308822	-17.119522359
H	27.978945372	-18.041774811	-16.738652378
H	28.626372189	-19.634159188	-16.254422790
H	27.565286947	-19.491926932	-17.686058560
C	30.709612305	-18.121398498	-17.161521013
H	30.395041486	-17.133442608	-16.781712986
H	31.628132343	-17.989614611	-17.752716452
H	30.947278073	-18.752197863	-16.288307838
C	30.105743811	-20.121230187	-18.541890599
H	30.358034753	-20.804172668	-17.712505606
H	31.000664918	-19.971964432	-19.166807565
H	29.334694876	-20.601043170	-19.167453676
C	32.528750630	-15.001931395	-22.455326190
H	32.461339000	-15.693858597	-23.300914142
C	32.842692548	-15.475808359	-21.179384680
H	33.228211051	-14.751263941	-20.449007866
C	33.101250242	-16.872418346	-20.819929674
C	32.825368265	-17.944012627	-21.677665461
C	33.632643310	-17.170868329	-19.555333893
C	33.022174925	-19.262629565	-21.285935174
C	33.859342501	-18.479508141	-19.157082381
C	33.532614409	-19.540526854	-20.011942848
H	32.416885022	-17.755889191	-22.675396692
H	33.864502894	-16.350665951	-18.865715325
H	32.753003606	-20.064217163	-21.977468676
H	34.267175447	-18.712587219	-18.168877804
O	33.733930674	-20.786317391	-19.528519658
C	33.380063441	-21.887724859	-20.327681197
H	33.968862938	-21.923035915	-21.261452503
H	32.306342185	-21.874366290	-20.588899792
H	33.590230166	-22.792430358	-19.742664840
H	32.776987548	-13.970955580	-22.727833588
H	27.511656389	-7.627497035	-23.022760995
C	27.260483050	-8.686971539	-22.853306816
C	27.847407823	-9.204111596	-21.575260379
C	27.186216889	-10.165226988	-20.801124331
C	29.123209525	-8.806132859	-21.158978095

C	27.779682429	-10.727068629	-19.674438114
C	29.734852249	-9.360429799	-20.038517556
C	29.070231543	-10.339910660	-19.287480913
O	29.630971131	-10.923568500	-18.219539136
H	30.627666463	-10.651486516	-18.090700231
H	27.648568819	-9.249625420	-23.723695166
H	26.164014775	-8.787672557	-22.872151513
H	26.183915581	-10.496989820	-21.098978335
H	29.670933092	-8.064040981	-21.751587567
H	27.268815074	-11.491965744	-19.077465300
H	30.746706004	-9.064725398	-19.741435148
O	32.046276889	-10.325758038	-17.926803140
O	33.517811476	-9.033923000	-16.869746201
C	32.362114830	-9.401385962	-17.103440152
C	31.197542358	-8.727381611	-16.395338120
H	30.557472531	-9.480285984	-15.908030258
H	31.547551697	-8.001550803	-15.648265450
H	30.562038952	-8.207090945	-17.132504427
C	27.146009014	-11.065556776	-16.113249599
H	26.273418780	-11.400576541	-15.529491124
H	27.791723738	-10.480231850	-15.429608819
H	26.772468043	-10.371257749	-16.893348496
O	27.791423148	-12.182541956	-16.651354070
H	28.539730814	-11.851259080	-17.189749808

Migratory Insertion TS with 4-Methylphenol, Acetate, and Methanol
Electronic Energy: -2454.632298212
Free Energy Correction: 0.799082080

N	0.491806590	2.239486497	-5.086297963
C	-1.459602382	0.986599335	0.598189314
C	-1.827115862	1.427239816	-0.721854564
C	-0.613978594	1.591031163	-1.493729425
C	0.466446668	1.137249428	-0.703733355
C	-0.059929912	0.719966988	0.589796427
C	-0.501674589	2.243775050	-2.833403137
C	0.094789143	1.412305498	-3.965305309
C	1.604755971	2.992181788	-5.053881660
C	1.912396075	1.139457005	-1.058031158
C	-3.195380036	1.807382989	-1.167779780
C	0.775305425	0.215190776	1.712444188
C	-2.372442980	0.872839773	1.763593491
O	2.396216658	3.029948776	-4.123676548
N	0.399120116	-2.131822532	-1.076586272
C	-1.338095442	-1.378595668	-2.846012354
Rh	-0.970176039	-0.574522060	-0.897099504
H	-0.622287526	0.663838248	-4.329575300
H	0.976038520	0.851927506	-3.606624542
H	0.151620067	3.122976266	-2.694822765
H	-1.483267737	2.640794970	-3.146210659

H	-0.110814615	2.306746004	-5.900969686
H	-1.972140998	0.191102742	2.530397990
H	-3.380338164	0.527784120	1.482477368
H	-2.487155877	1.862864494	2.235759173
H	-3.371063310	2.891804878	-1.051941647
H	-3.969117155	1.284448419	-0.583119756
H	-3.355034132	1.559707518	-2.230562275
H	1.163154228	1.039205211	2.339271198
H	1.642672897	-0.345634820	1.325605594
H	0.203798802	-0.468437271	2.361282919
H	2.496283586	1.588368686	-0.236142495
H	2.110305081	1.724390477	-1.970222761
H	2.292135846	0.113252616	-1.199645978
C	0.509735812	-2.826175347	-2.228079047
O	1.195823837	-3.837389847	-2.413178234
C	-0.329748712	-2.179296755	-3.271681338
H	-1.964500597	-0.861666268	-3.586781581
C	0.002973905	-2.460320666	-4.695951172
H	1.022605526	-2.115081791	-4.946576010
H	-0.004646072	-3.547842172	-4.888495926
H	-0.706433872	-1.977366442	-5.385346537
O	0.993418827	-2.766641508	0.012526240
C	2.328340386	-2.682744786	0.104538780
O	3.022388065	-1.993365482	-0.602126616
C	2.844385776	-3.619041066	1.187565775
C	4.287642207	-3.258482589	1.508114003
H	4.363880147	-2.231188307	1.902672446
H	4.683660640	-3.948303582	2.271712050
H	4.927696145	-3.324472436	0.614807201
C	1.990935369	-3.538762662	2.450461672
H	2.022267635	-2.529478724	2.895535191
H	0.939576025	-3.791637447	2.248621645
H	2.379354506	-4.248570471	3.201185132
C	2.768479905	-5.030515162	0.596146959
H	3.148729862	-5.762795845	1.329114393
H	1.729342615	-5.287093880	0.334309699
H	3.376543754	-5.108556826	-0.320474855
C	-2.641468736	-1.971950052	-1.611444068
H	-2.640564048	-2.962629895	-2.078733891
C	-2.440089480	-1.960592317	-0.180413088
H	-3.100922858	-1.288318875	0.383108438
C	-2.033156644	-3.139403066	0.597461087
C	-1.551357294	-4.327645861	0.034973812
C	-2.128733733	-3.086281469	2.000222275
C	-1.149875979	-5.404070189	0.823115113
C	-1.738806895	-4.148416812	2.799133594
C	-1.225619702	-5.314575053	2.217167173
H	-1.456887615	-4.427370524	-1.051372399
H	-2.519126581	-2.177402567	2.472263003

H	-0.767812376	-6.303763707	0.334247731
H	-1.804847704	-4.095125374	3.890048006
O	-0.822604491	-6.283975800	3.069857979
C	-0.188463244	-7.422717099	2.545624768
H	-0.860403271	-8.007227203	1.892018386
H	0.716208750	-7.154109752	1.969925537
H	0.107452640	-8.049648161	3.396826059
H	-3.478574260	-1.358973043	-1.967188658
H	1.744147731	3.590952578	-5.984886863
H	0.460139133	6.893189030	-2.425790172
C	0.335718452	5.797330109	-2.484823777
C	0.145596411	5.176126014	-1.132687377
C	-1.114783837	5.123792930	-0.523419757
C	1.220173892	4.620668553	-0.431108970
C	-1.297021261	4.555192800	0.733063068
C	1.057576816	4.041320381	0.825252346
C	-0.208476818	4.006373831	1.425937987
O	-0.412776506	3.451920729	2.631082513
H	0.478464597	3.177380520	3.090914437
H	1.231255413	5.394082989	-2.984535094
H	-0.531350666	5.610369026	-3.141095244
H	-1.981929164	5.537875685	-1.053190416
H	2.216440894	4.621617021	-0.891229990
H	-2.285507729	4.522017600	1.206048171
H	1.904740598	3.593364894	1.355711194
O	1.737028474	2.770796668	3.723619359
O	3.518658381	3.412785729	4.890582973
C	2.443391159	3.646014947	4.329268042
C	1.889855636	5.061743413	4.317115174
H	0.839494903	5.068721039	4.649995921
H	2.485761317	5.731189952	4.952783539
H	1.893400851	5.451053354	3.284212051
C	-2.463692233	5.636922010	3.956865686
H	-3.388269492	6.201271387	4.160506451
H	-1.810981788	5.746924380	4.845875067
H	-1.951464359	6.138959753	3.110362955
O	-2.789937016	4.306564060	3.678759464
H	-1.960515567	3.871198152	3.397060418

Intermediate with 3-Methylindole and Acetate
Electronic Energy: -2395.238646352
Free Energy Correction: 0.778708817

N	30.451278752	-11.095431044	-24.900356636
C	29.554865012	-13.980811519	-19.550578003
C	28.962185270	-13.621766284	-20.817912031
C	29.913102161	-12.793105397	-21.522383974
C	31.098213369	-12.719151941	-20.718984115
C	30.867560935	-13.455988752	-19.498343319
C	29.638356531	-12.010018215	-22.765400470

C	30.641821131	-12.132518433	-23.909067413
C	30.964562303	-9.861989183	-24.740247602
C	32.311075503	-11.886788501	-20.968229829
C	27.569441497	-13.949933741	-21.223063531
C	31.789429048	-13.567948141	-18.337152598
C	28.887278204	-14.717630701	-18.449756984
O	31.673173079	-9.514044310	-23.809298382
Rh	30.687656381	-14.845484906	-21.311401681
H	30.566825147	-13.109026920	-24.408810325
H	31.673154164	-12.048687134	-23.532820598
H	29.600754196	-10.946490817	-22.464305493
H	28.628522303	-12.251680214	-23.140914955
H	29.837335615	-11.262472313	-25.692178825
H	28.488608036	-13.998183995	-17.712508602
H	29.595355687	-15.369892303	-17.913648383
H	28.055595319	-15.337546341	-18.809376299
H	26.849783790	-13.267147102	-20.738096612
H	27.318973060	-14.982753499	-20.930022381
H	27.433823539	-13.873372509	-22.312084322
H	31.516453380	-12.833635044	-17.559563010
H	32.831707329	-13.348732854	-18.614672177
H	31.752176009	-14.574705026	-17.887517946
H	32.555925753	-11.329964877	-20.046801118
H	32.146844760	-11.155768516	-21.774220572
H	33.201045070	-12.486503763	-21.230993242
H	30.678435159	-9.171015741	-25.568765111
N	30.118205675	-16.791853006	-20.928393339
C	29.907748512	-15.531248911	-23.087321277
C	29.691386572	-17.613419042	-21.913902475
O	29.467855506	-18.820338216	-21.810086369
C	29.514569990	-16.812778715	-23.156025130
H	29.818927951	-14.868757862	-23.961178968
C	28.923814551	-17.506822363	-24.338755492
H	27.918636660	-17.902257825	-24.109791403
H	29.534494347	-18.379771959	-24.629569743
H	28.842977554	-16.834029927	-25.206326401
O	30.358645770	-17.417597680	-19.711405381
C	29.268711803	-17.868927129	-19.062539566
O	28.133284902	-17.669165105	-19.414598144
C	29.676486632	-18.698288511	-17.854575434
C	28.458192590	-18.895148413	-16.963743694
H	28.077670986	-17.929072356	-16.590043043
H	28.728025253	-19.516610816	-16.094082437
H	27.638954711	-19.391736096	-17.506402687
C	30.797901315	-18.025068032	-17.066622579
H	30.490554870	-17.034225347	-16.688543751
H	31.702212853	-17.897508400	-17.680285713
H	31.056981138	-18.646593137	-16.192832340
C	30.161282599	-20.045499472	-18.400934533

H	30.433450246	-20.712804694	-17.565092508
H	31.040397260	-19.908394990	-19.050153435
H	29.375293427	-20.535968147	-18.998843274
C	32.539468154	-15.048179566	-22.469836530
H	32.442614611	-15.760367596	-23.295199222
C	32.877817669	-15.493871404	-21.190527865
H	33.288210942	-14.757459334	-20.485771227
C	33.129503529	-16.883105434	-20.799901388
C	32.819798455	-17.975295574	-21.619352657
C	33.692728186	-17.151708374	-19.542278448
C	33.016246314	-19.284310083	-21.196526858
C	33.918724516	-18.450790657	-19.113808255
C	33.560449071	-19.531814801	-19.930158615
H	32.385745924	-17.811084529	-22.610659187
H	33.952543519	-16.315470730	-18.882970277
H	32.720682613	-20.102371555	-21.857440751
H	34.352425488	-18.660394273	-18.131344675
O	33.765244125	-20.765408763	-19.418683766
C	33.388402486	-21.885297714	-20.181001948
H	33.950834982	-21.943506794	-21.129806781
H	32.307696835	-21.877026013	-20.412112198
H	33.614396696	-22.775813019	-19.580406651
H	32.793364879	-14.027821117	-22.775568323
O	32.271446167	-10.351184171	-18.088943626
O	33.537647884	-10.192637257	-16.259630742
C	32.441605832	-10.220071277	-16.840765223
C	31.166729783	-10.114863947	-16.009456074
H	30.643867408	-11.087782723	-16.013436156
H	31.379302186	-9.841566452	-14.965451346
H	30.472898444	-9.379292007	-16.449861648
C	26.600747394	-10.111238932	-20.577197979
C	27.960750541	-9.771200562	-20.482536385
C	28.734421193	-10.297299498	-19.409727572
C	28.173016652	-11.134371876	-18.439155364
C	26.823549917	-11.445261394	-18.550425069
C	26.043102402	-10.938859507	-19.610761769
C	28.846058876	-8.967790269	-21.279242971
C	30.076424834	-9.051558706	-20.665560872
N	30.015798653	-9.841397680	-19.544932826
H	25.987954220	-9.724360868	-21.399853218
H	28.787515669	-11.523104555	-17.618730185
H	26.358326884	-12.098943391	-17.805015058
H	24.983750031	-11.208662720	-19.671607733
H	31.023474111	-8.609372700	-20.981741882
H	30.827096312	-10.071146292	-18.924070181
C	28.515302617	-8.273482915	-22.554042257
H	29.416059345	-7.825535817	-23.003430343
H	28.094574735	-8.978524852	-23.296125836
H	27.764503937	-7.474441571	-22.422988827

Migratory Insertion TS with 3-Methylindole and Acetate
Electronic Energy: -2395.216082255
Free Energy Correction: 0.775897924

N	-0.133457839	2.981193380	-4.684436986
C	-0.871918764	1.088729542	1.104892322
C	-1.454623266	1.756128806	-0.028551998
C	-0.419663430	1.918185391	-1.027702332
C	0.734940810	1.237469095	-0.577582117
C	0.444126197	0.686197203	0.740642661
C	-0.521571268	2.760230138	-2.258517877
C	-0.358628285	2.049270212	-3.599708861
C	1.075404096	3.520617838	-4.914931664
C	2.051257815	1.138768774	-1.264809550
C	-2.827529663	2.323664038	-0.121234736
C	1.392378352	-0.058444550	1.615496617
C	-1.481199317	0.880520363	2.443078060
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N	0.197031980	-1.921198193	-1.257456409
C	-1.742768948	-0.778610517	-2.552268840
Rh	-0.916676884	-0.272178691	-0.641754000
H	-1.249377134	1.452058299	-3.839536530
H	0.489075777	1.344385442	-3.562126016
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H	-1.475898119	3.314268423	-2.251241585
H	-0.916935344	3.296133149	-5.248899129
H	-1.236508409	-0.113385908	2.851442236
H	-2.575729171	1.000815425	2.436709381
H	-1.046141852	1.610698986	3.148941809
H	-2.830519306	3.400274295	0.125046371
H	-3.520425906	1.821398768	0.572469380
H	-3.236137723	2.213373776	-1.140212053
H	1.664786080	0.548338039	2.498694727
H	2.307670913	-0.343201536	1.070702706
H	0.930783207	-0.987334766	1.992805353
H	2.855280564	1.493057356	-0.595221823
H	2.087688240	1.753185106	-2.177810357
H	2.285605695	0.093194269	-1.527670881
C	0.008345300	-2.463405902	-2.477743778
O	0.530988908	-3.497941082	-2.907925647
C	-0.932895903	-1.610975686	-3.252637243
H	-2.430982030	-0.118192139	-3.098223961
C	-0.902588701	-1.725275513	-4.737680722
H	0.090145372	-1.452822399	-5.139830759
H	-1.081894924	-2.768552155	-5.052621325
H	-1.657397420	-1.080015382	-5.212917243
O	0.902888381	-2.756436720	-0.391850881
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O	2.859655143	-2.086816431	-1.294260247

C	2.817841586	-3.979468663	0.217287915
C	4.332841207	-3.838588388	0.250473155
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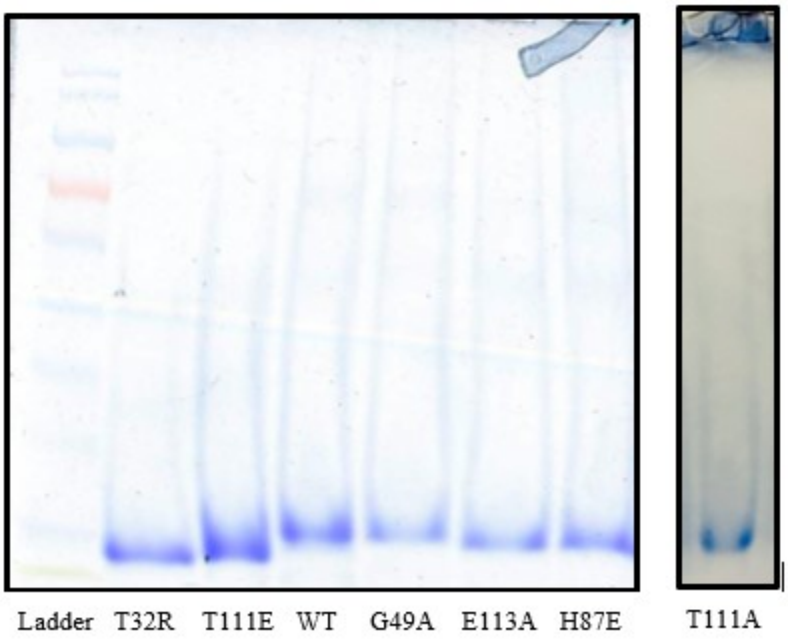
H	4.774694160	-4.688143935	0.796771776
H	4.757088771	-3.820185382	-0.765408216
C	2.263413501	-4.032357470	1.638071719
H	2.545970994	-3.133789041	2.213113547
H	1.166177956	-4.114766859	1.646025548
H	2.680565522	-4.909670283	2.162374900
C	2.422437812	-5.248058464	-0.546852822
H	2.868829996	-6.131841825	-0.058804083
H	1.327128113	-5.364161915	-0.571975181
H	2.777743622	-5.208041291	-1.590324552
C	-2.866813245	-1.359755893	-1.146411056
H	-3.106640890	-2.262378937	-1.719259354
C	-2.391734847	-1.583775529	0.200168050
H	-2.830722758	-0.936494836	0.971840409
C	-1.999995099	-2.904545130	0.710674974
C	-1.800065648	-4.028728502	-0.100691955
C	-1.805774271	-3.070018533	2.094442058
C	-1.390921577	-5.251615121	0.425169352
C	-1.399520533	-4.279611438	2.634773911
C	-1.167468827	-5.379998777	1.800423122
H	-1.940861246	-3.960052364	-1.184294480
H	-1.977721710	-2.218049750	2.762631292
H	-1.238299439	-6.094936162	-0.253379715
H	-1.237235202	-4.396905116	3.710417654
O	-0.725795860	-6.508032850	2.402079251
C	-0.355814248	-7.599167979	1.598296662
H	-1.213691882	-8.009417708	1.036219272
H	0.436071427	-7.321578932	0.878507084
H	0.032227565	-8.378265223	2.267252304
H	-3.656099081	-0.604586535	-1.241393605
H	1.067577572	4.244211765	-5.763775827
O	1.150165912	1.998997206	4.226370555
O	1.020578880	1.586076522	6.413719971
C	0.788278643	2.276120648	5.408161948
C	-0.036834405	3.548093198	5.571184214
H	-1.084069772	3.332210367	5.292858894
H	-0.035241617	3.902130415	6.612663129
H	0.318897345	4.348861329	4.902528285
C	-0.375765720	5.849039600	-0.381355173
C	0.485856241	5.001016798	0.334648013
C	0.042042769	4.435853073	1.564466269
C	-1.228798570	4.716337717	2.083024537
C	-2.053309040	5.569950507	1.361005946
C	-1.634251927	6.127981573	0.135587321
C	1.823021907	4.525912387	0.112583213
C	2.108904037	3.716166351	1.189224223

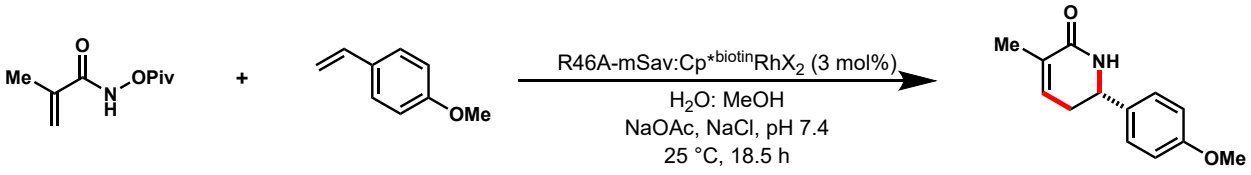
N	1.051899563	3.659744288	2.063884190
H	-0.055516777	6.283555785	-1.335787558
H	-1.560709189	4.276000183	3.029585848
H	-3.050379938	5.805769629	1.746758860
H	-2.313005855	6.790008327	-0.411552102
H	3.026482372	3.161337785	1.398981632
H	1.023771156	3.065536913	2.926921019
C	2.708520414	4.847432449	-1.041698822
H	2.823189917	5.936832427	-1.181680810
H	3.714816864	4.423170772	-0.897891432
H	2.324880505	4.444144177	-1.997804090

14. **Protein Gel**



15. **Biochemical and technical replicate data**

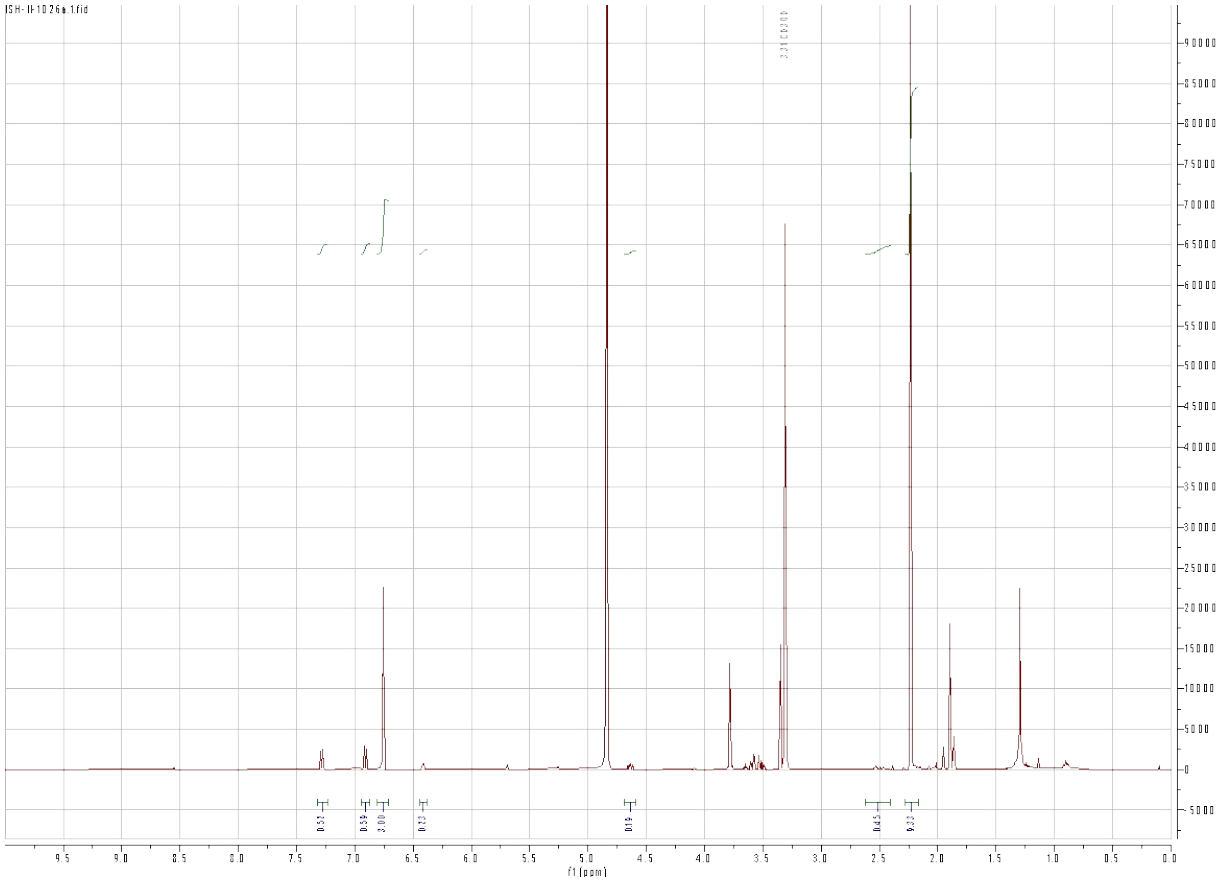
Mutant R46A was used to assess quality of data via biochemical and technical replicates. To assess technical replicates the following reaction was repeated in triplicate:

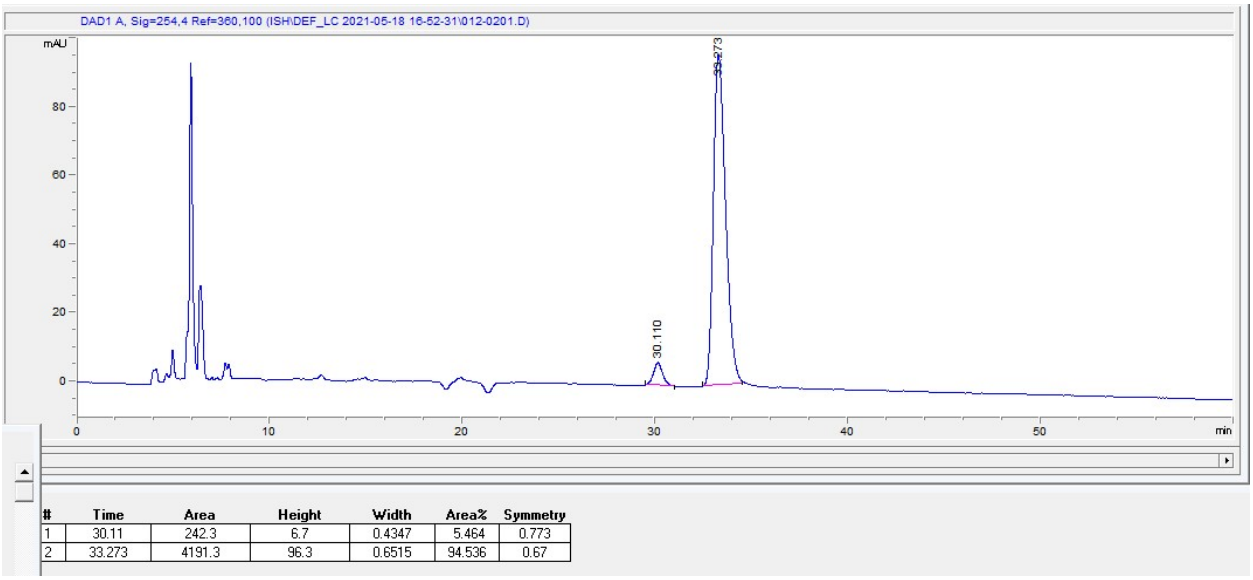


	A	B	C	D	E
1	**Technical Replicate Analysis**				
2					
3	**Trial**	**Yield**	**ee**		
4	1	23	89.072		
5	2	26	88.502		
6	3	24	88.794		
7					
8	**Yield Analysis**				
9	Mean			24.3	
10	Sample Standard Deviation			1.5275252	
11	Sample Size			3	
12	Standard Uncertainty			0.8819171	
13	Degrees of freedom			2	
14	t-value			4.3026527	
15	95% Confidence deviation			3.794583	
16				**Maximum**	**Minimum**
17	95% Confidence interval			28.1	20.5
18					
19	**ee Analysis**				
20	Mean			88.8	
21	Sample Standard Deviation			0.2850287	
22	Sample Size			3	
23	Standard Uncertainty			0.1645614	
24	Degrees of freedom			2	
25	t-value			4.3026527	
26	95% Confidence deviation			0.7080504	
27				**Maximum**	**Minimum**
28	95% Confidence interval			89.5	88.1

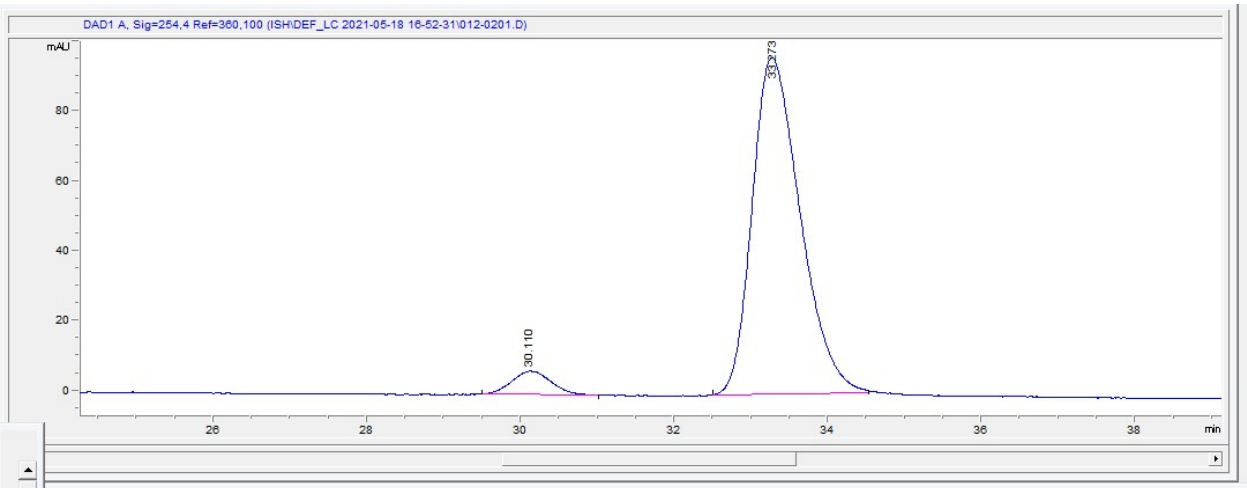
NMR and HPLC data

Trial 1



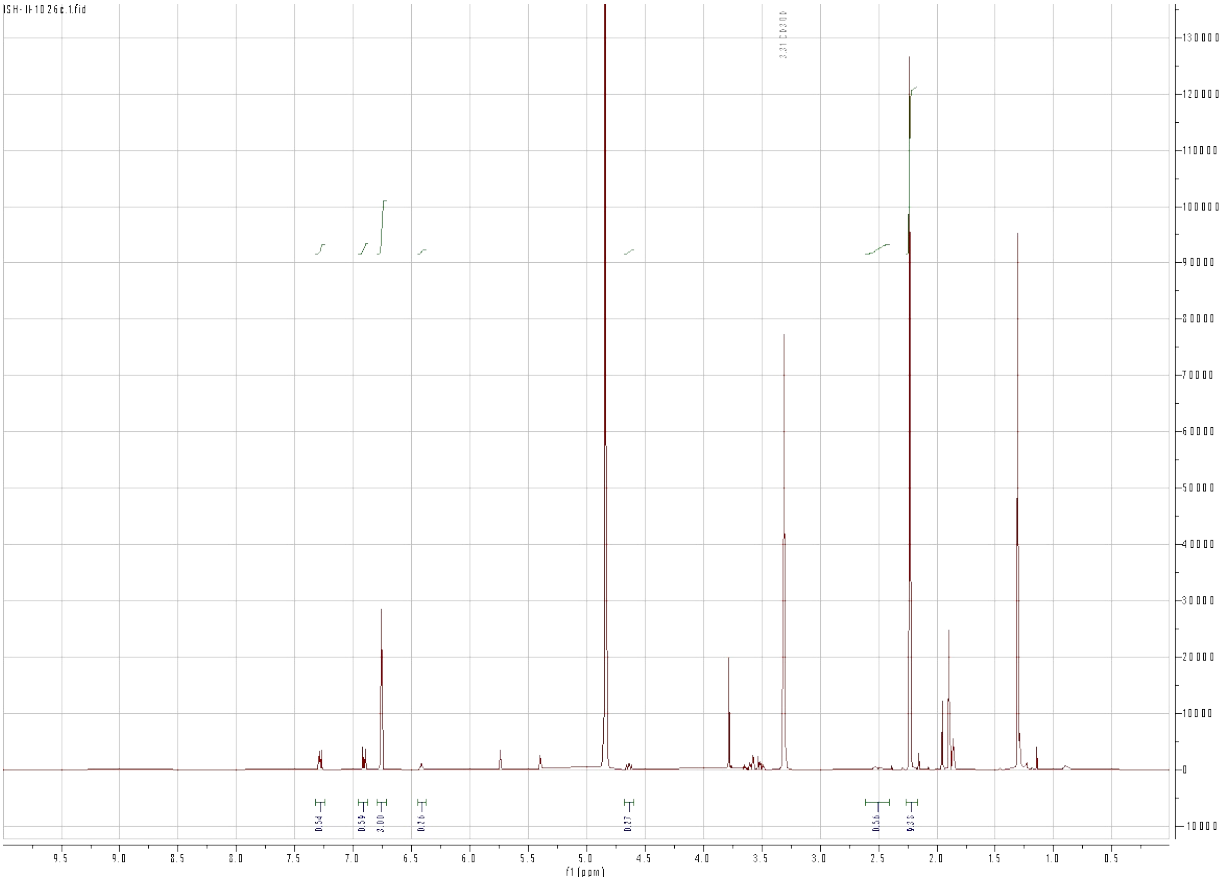


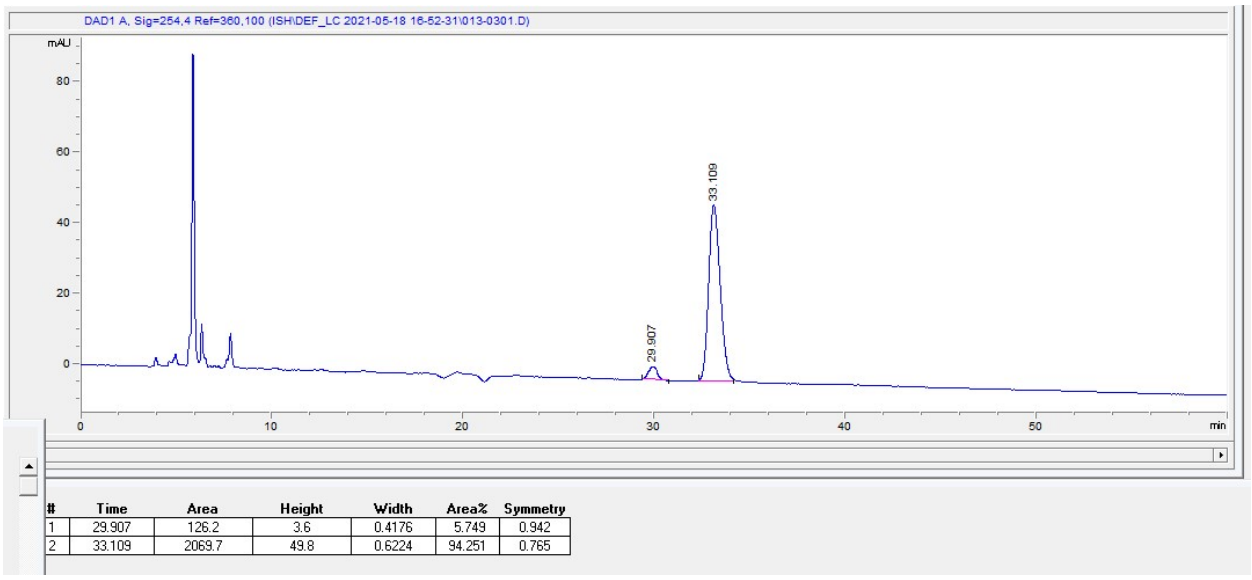
#	Time	Area	Height	Width	Area%	Symmetry
1	30.11	242.3	6.7	0.4347	5.464	0.773
2	33.273	4191.3	96.3	0.6515	94.536	0.67



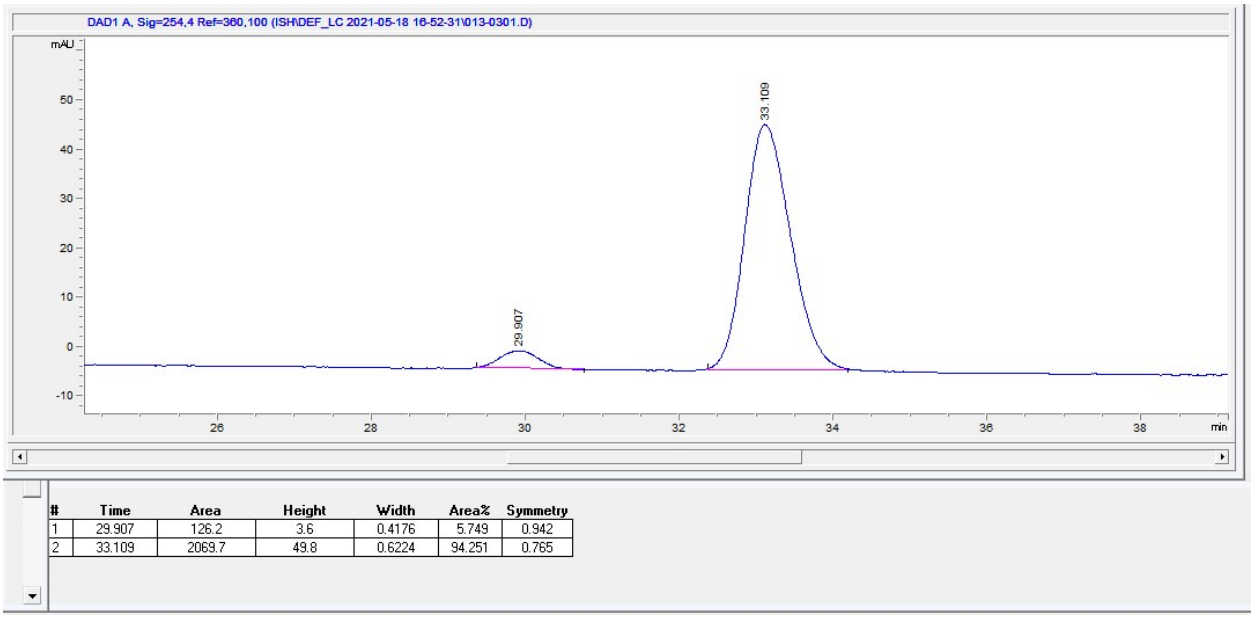
#	Time	Area	Height	Width	Area%	Symmetry
1	30.11	242.3	6.7	0.4347	5.464	0.773
2	33.273	4191.3	96.3	0.6515	94.536	0.67

Trial 2



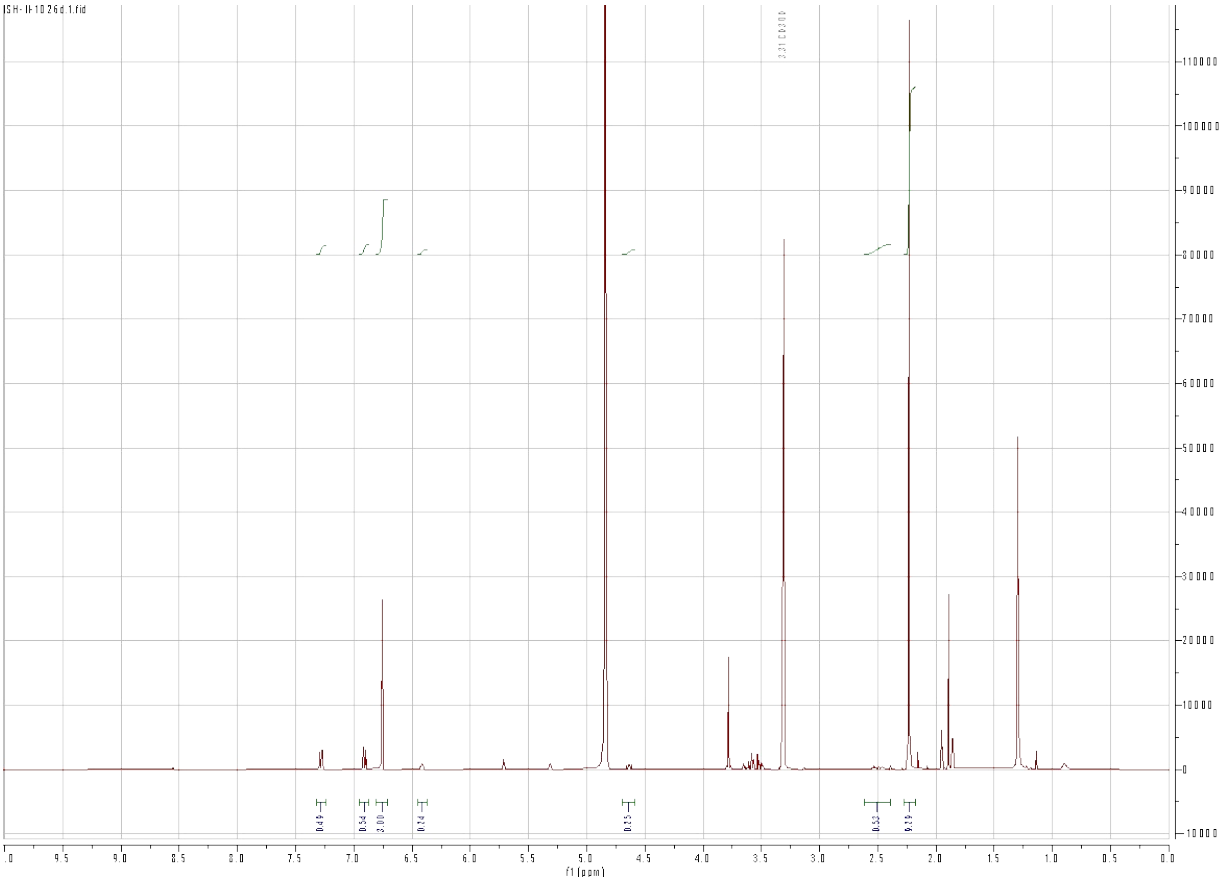


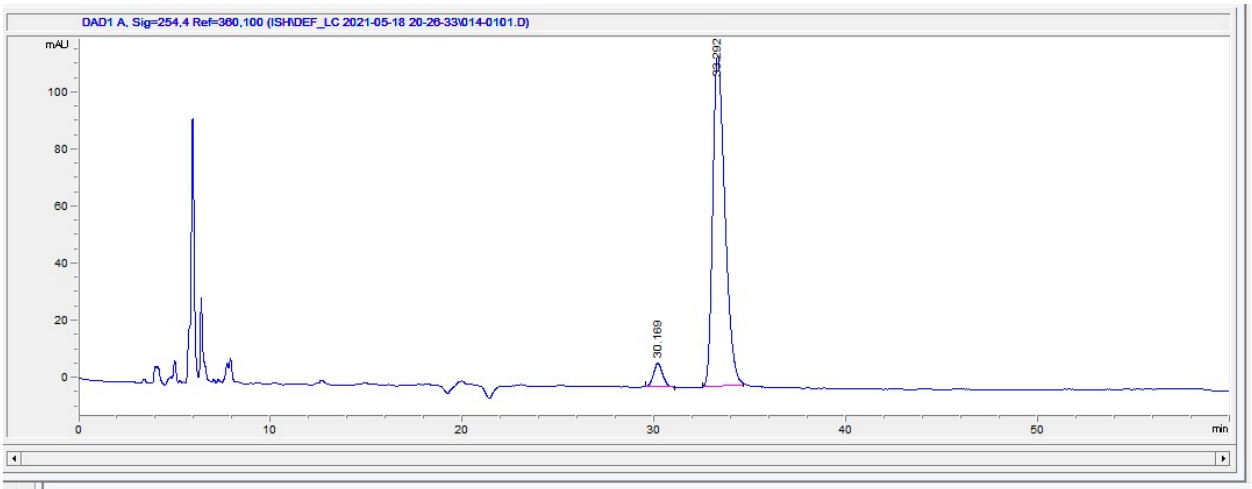
#	Time	Area	Height	Width	Area%	Symmetry
1	29.907	126.2	3.6	0.4176	5.749	0.942
2	33.109	2069.7	49.8	0.6224	94.251	0.765



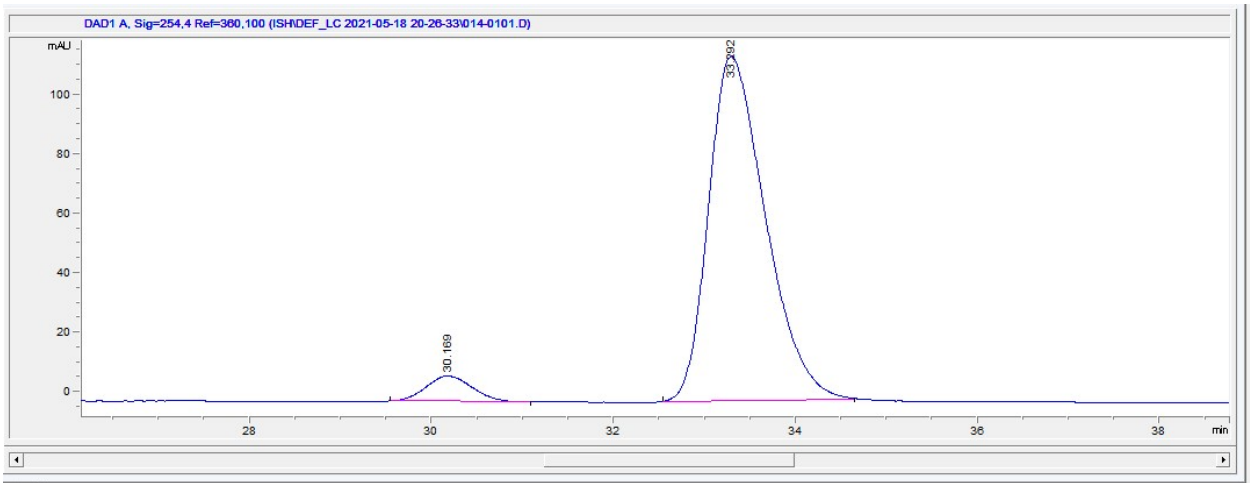
#	Time	Area	Height	Width	Area%	Symmetry
1	29.907	126.2	3.6	0.4176	5.749	0.942
2	33.109	2069.7	49.8	0.6224	94.251	0.765

Trial 3



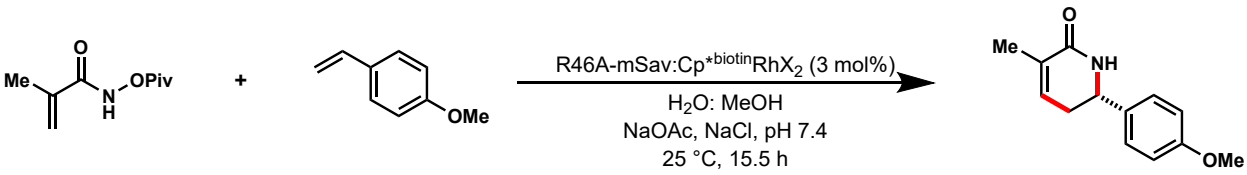


#	Time	Area	Height	Width	Area%	Symmetry
1	30.169	300.9	8.5	0.4577	5.603	0.827
2	33.292	5068.8	116	0.6596	94.397	0.637



#	Time	Area	Height	Width	Area%	Symmetry
1	30.169	300.9	8.5	0.4577	5.603	0.827
2	33.292	5068.8	116	0.6596	94.397	0.637

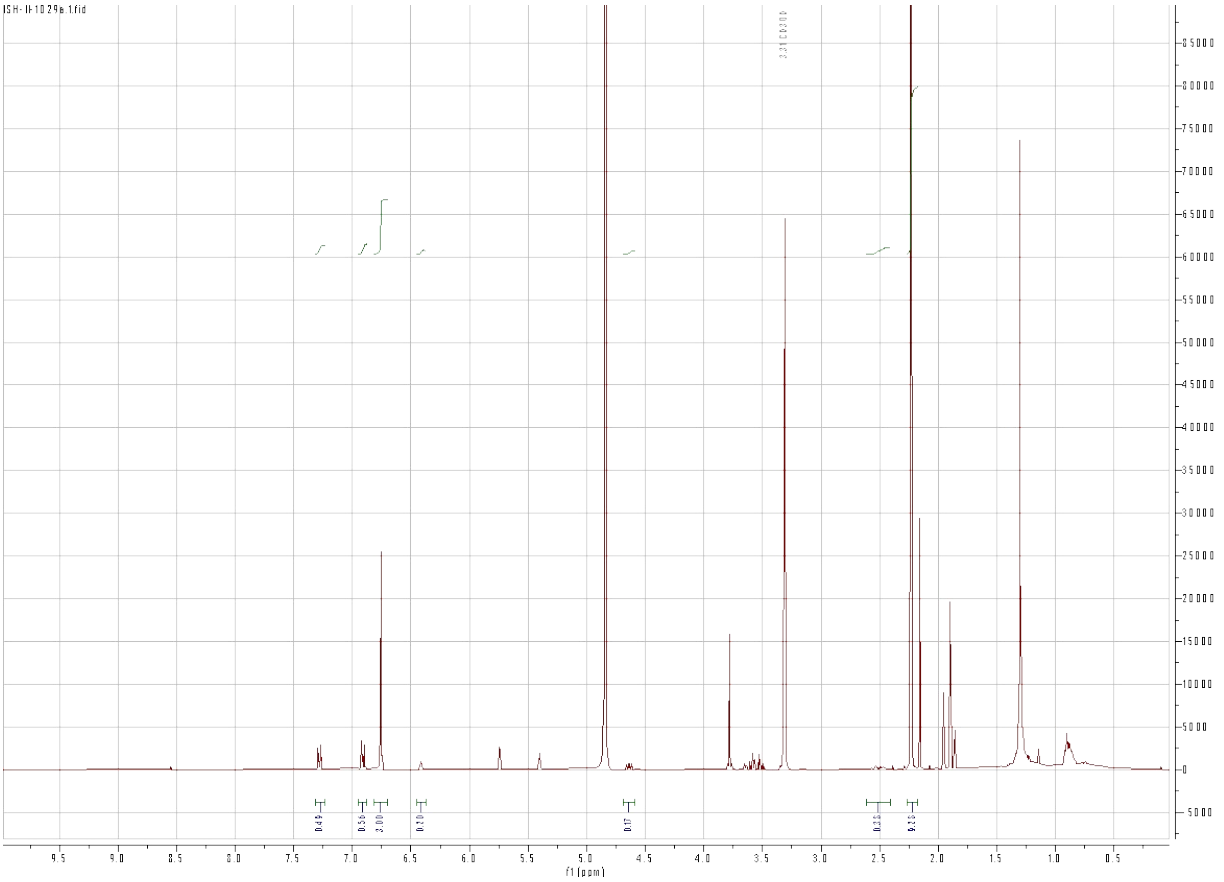
To assess biochemical replicates the following reaction was setup in duplicate using different batches of protein:

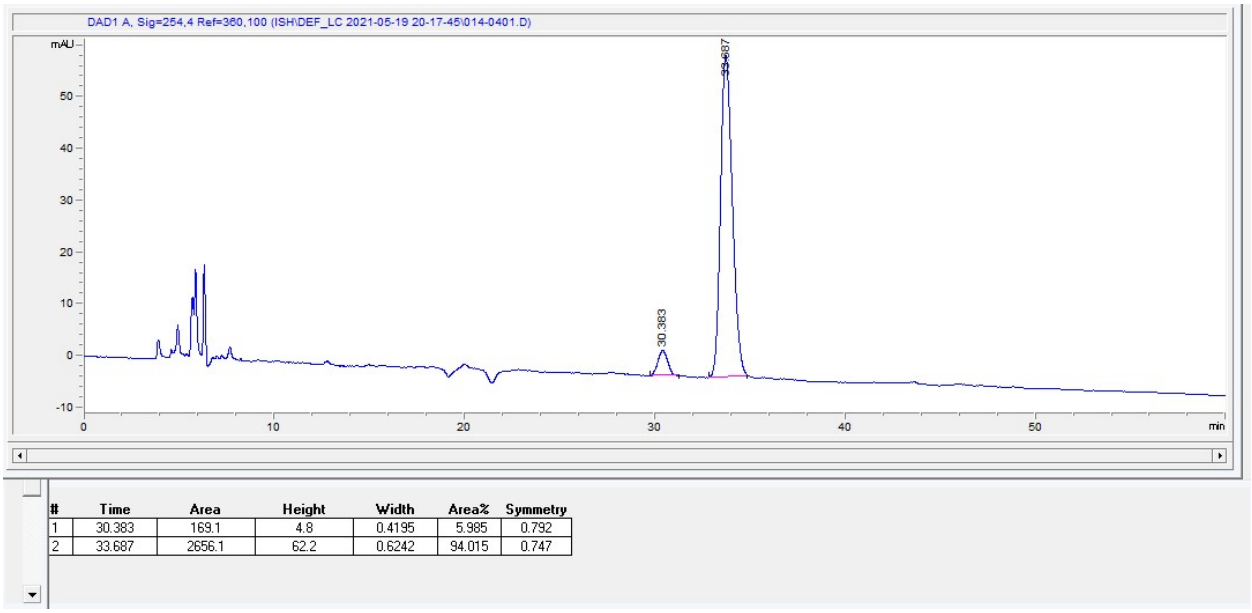


	A	B	C	D	E
1	**Biochemical Replicate Analysis**				
2					
3	**Trial**	**Yield**	**ee**		
4	1	19.0	88.03		
5	2	21.0	88.07		
6					
7					
8	**Yield Analysis**				
9	Mean			20.0	
10	Sample Standard Deviation			1.4142136	
11	Sample Size			2	
12	Standard Uncertainty			1	
13	Degrees of freedom			1	
14	t-value			12.706205	
15	95% Confidence deviation			12.706205	
16				**Maximum**	**Minimum**
17	95% Confidence interval			32.7	7.3
18					
19	**ee Analysis**				
20	Mean			88.0	
21	Sample Standard Deviation			0.0268701	
22	Sample Size			2	
23	Standard Uncertainty			0.019	
24	Degrees of freedom			1	
25	t-value			12.706205	
26	95% Confidence deviation			0.2414179	
27				**Maximum**	**Minimum**
28	95% Confidence interval			88.3	87.8

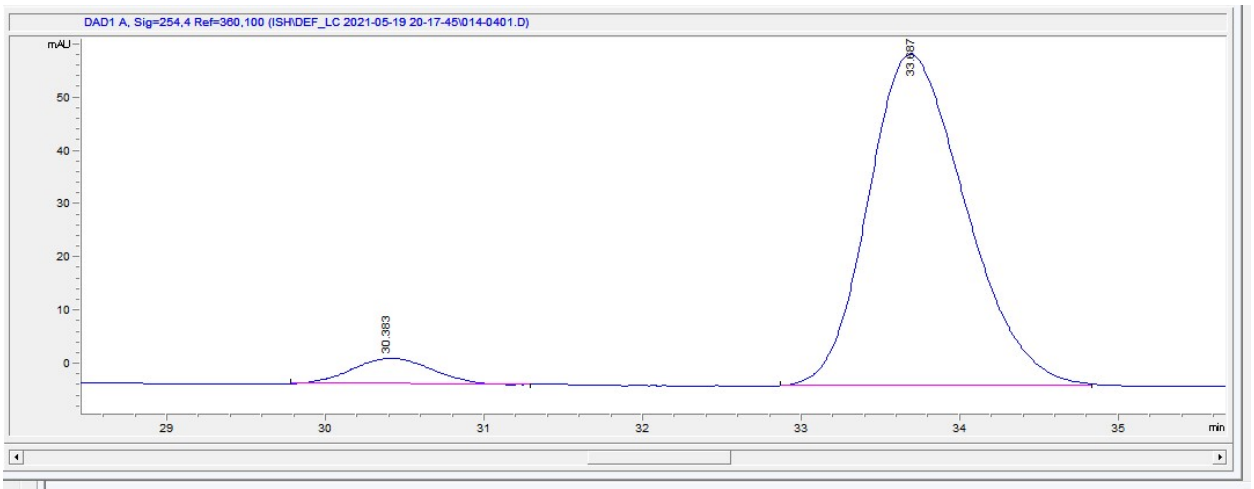
NMR and HPLC data

Trial 1



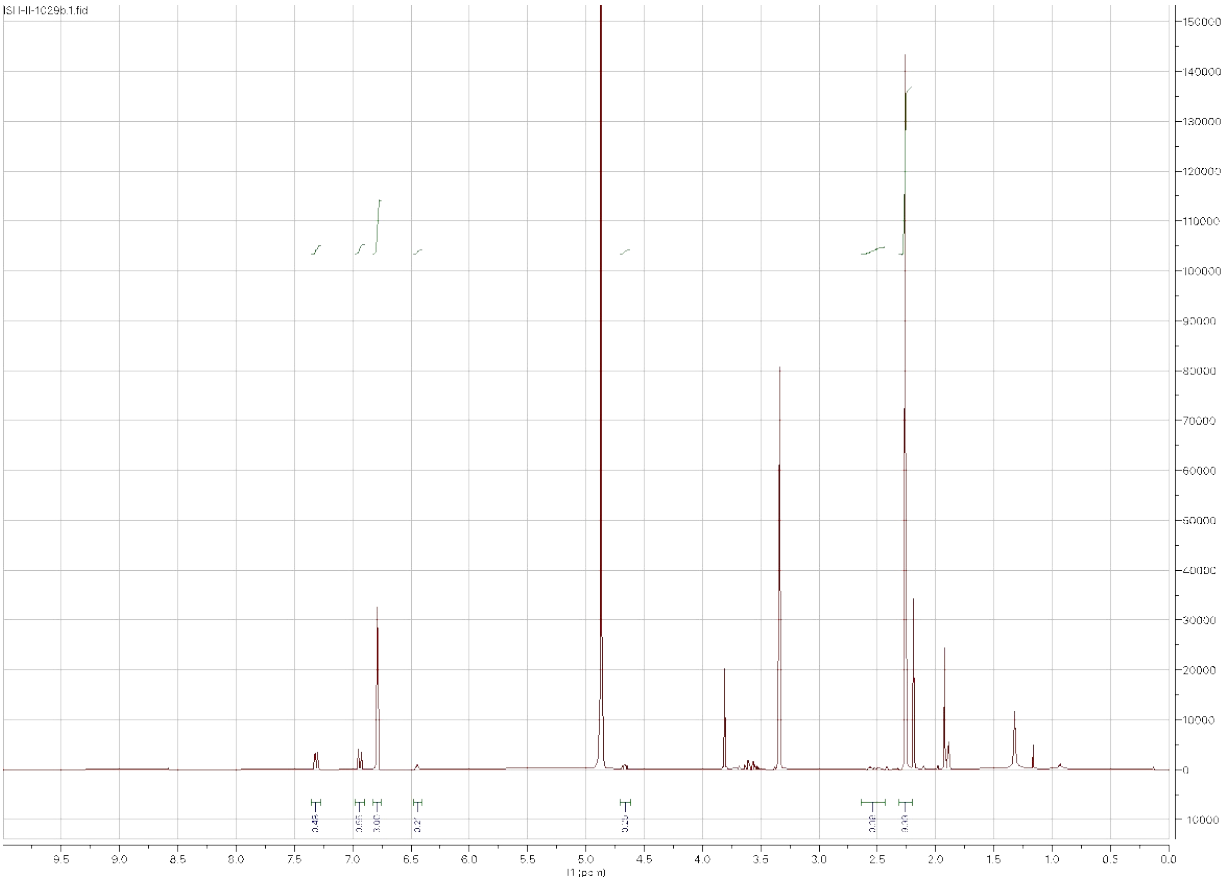


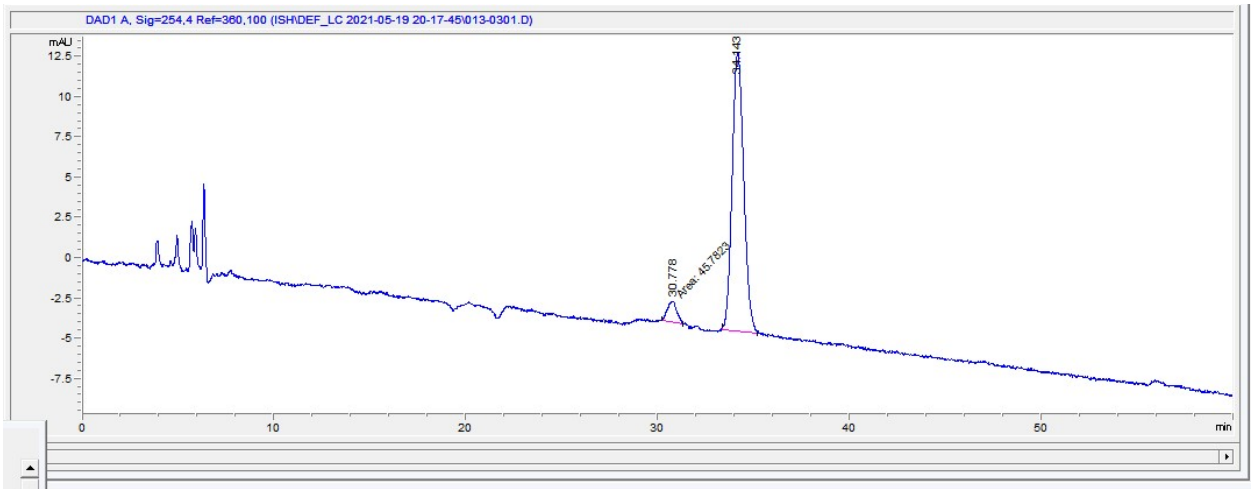
#	Time	Area	Height	Width	Area%	Symmetry
1	30.383	169.1	4.8	0.4195	5.985	0.792
2	33.687	2656.1	62.2	0.6242	94.015	0.747



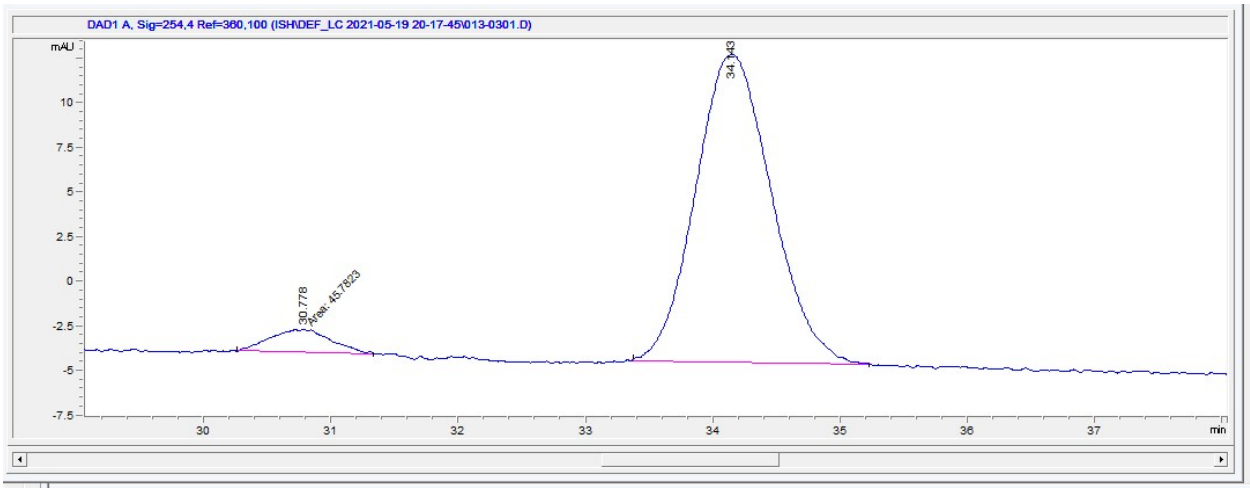
#	Time	Area	Height	Width	Area%	Symmetry
1	30.383	169.1	4.8	0.4195	5.985	0.792
2	33.687	2656.1	62.2	0.6242	94.015	0.747

Trial 2





#	Time	Area	Height	Width	Area%	Symmetry
1	30.778	45.8	1.3	0.5736	5.966	1.083
2	34.143	721.6	17.3	0.5285	94.034	0.885



#	Time	Area	Height	Width	Area%	Symmetry
1	30.778	45.8	1.3	0.5736	5.966	1.083
2	34.143	721.6	17.3	0.5285	94.034	0.885

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