

Supporting Information:
Pipecolic Acid-Catalyzed Asymmetric Mannich Reactions

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I. Experimental

General procedure for the pipecolic acid catalyzed asymmetric Mannich-type reaction between *N*-PMP protected α -imino ethyl glyoxylate and aldehyde donors:

N-PMP-protected α -imino ethyl glyoxylate (0.5 mmol) was dissolved in anhydrous DMSO (5 mL) and the corresponding aldehyde donor (1.0 mmol) was added, followed by L-pipecolic acid (0.15 mmol). After stirring for overnight (6-14 h) at room temperature, the mixture was worked up by addition of saturated ammonium chloride solution and extraction with ethyl acetate (three or four times). The combined organic layers were washed with brine, dried with MgSO₄, filtered, and concentrated, and purified by flash column chromatography (10-20% EtOAc/hexanes) to afford the corresponding Mannich addition product. The enantiomeric excesses of all products were determined by chiral-phase HPLC analyses.

Ethyl 3-formyl-2-(*p*-methoxyphenylamino)butanoate (1a + 2a): data were described previously.^{S1}

Ethyl 3-formyl-2-(*p*-methoxyphenylamino)-4-methyl-pentanoate (1b + 2b): ¹H NMR (500 MHz, CDCl₃): purified 1:1 mixture of diastereomers, * denotes *anti*-diastereomer (**2b**), δ = 1.03 (d, 3H x 1/2, *J* = 6.6 Hz, CHCH₃), 1.08 (d, 3H* x 1/2, *J* = 7

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[§] The Scripps Research Institute

(S1) Cordova, A.; Watanabe, S.; Tanaka, F.; Notz, W.; Barbas, C. F., III *J. Am. Chem. Soc.* **2002**, *124*, 1866.

Supporting Information

Hz, OCHCH₃), 1.12 (d, 3H* x 1/2, *J* = 7 Hz, CHCH₃), 1.16 (d, 3H x 1/2, *J* = 6.6 Hz, CHCH₃), 1.22 (t, 3H, OCH₂CH₃), 2.13 (m, 1H* x 1/2, CH(CH₃)₂), 2.34 (m, 1H x 1/2, CH(CH₃)₂), 2.54-2.61 (m, 1H, CHCHO), 3.74 (s, 3H, OCH₃), 3.93-3.87 (1H, NH), 4.17-4.12 (m, 2H, OCH₂CH₃), 4.35-4.31 (m, 1H, CHNHPMP), 6.64 (m, 2H, ArH), 6.78 (m, 2H, ArH), 9.75 (d, 1H* x 1/2, *J* = 3.5 Hz, CHCHO), 9.78 (d, 1H x 1/2, *J* = 3.0 Hz, CHCHO); ¹³C NMR (125 MHz, CDCl₃): mixture of diastereomers, δ = 203.6, 203.2, 172.8, 172.6, 153.3, 153.1, 140.4, 140.1, 115.9, 114.8, 114.7, 61.4, 59.6, 59.5, 57.2, 57.0, 55.6, 27.5, 26.3, 21.2, 20.9, 19.8, 19.2, 14.1; HPLC (Daicel Chiralcel AS-H, hexane /*i*-PrOH = 99:1, 1.0 mL/min, λ = 254 nm) t_R (*syn* major enantiomer, (2*S*,3*S*)-**1b**) = 30.3 min; t_R (*syn* minor enantiomer, (2*R*,3*R*) **1b**) = 57.1 min; t_R (*anti* major enantiomer, (2*S*,3*R*)-**2b**) = 23.1 min; t_R (*anti* minor enantiomer, (2*R*,3*S*)-**2b**) = 51.1 min. HRMS: calcd for C₁₆H₂₃NO₄ (MNa⁺) 316.1519, found: 316.1521.

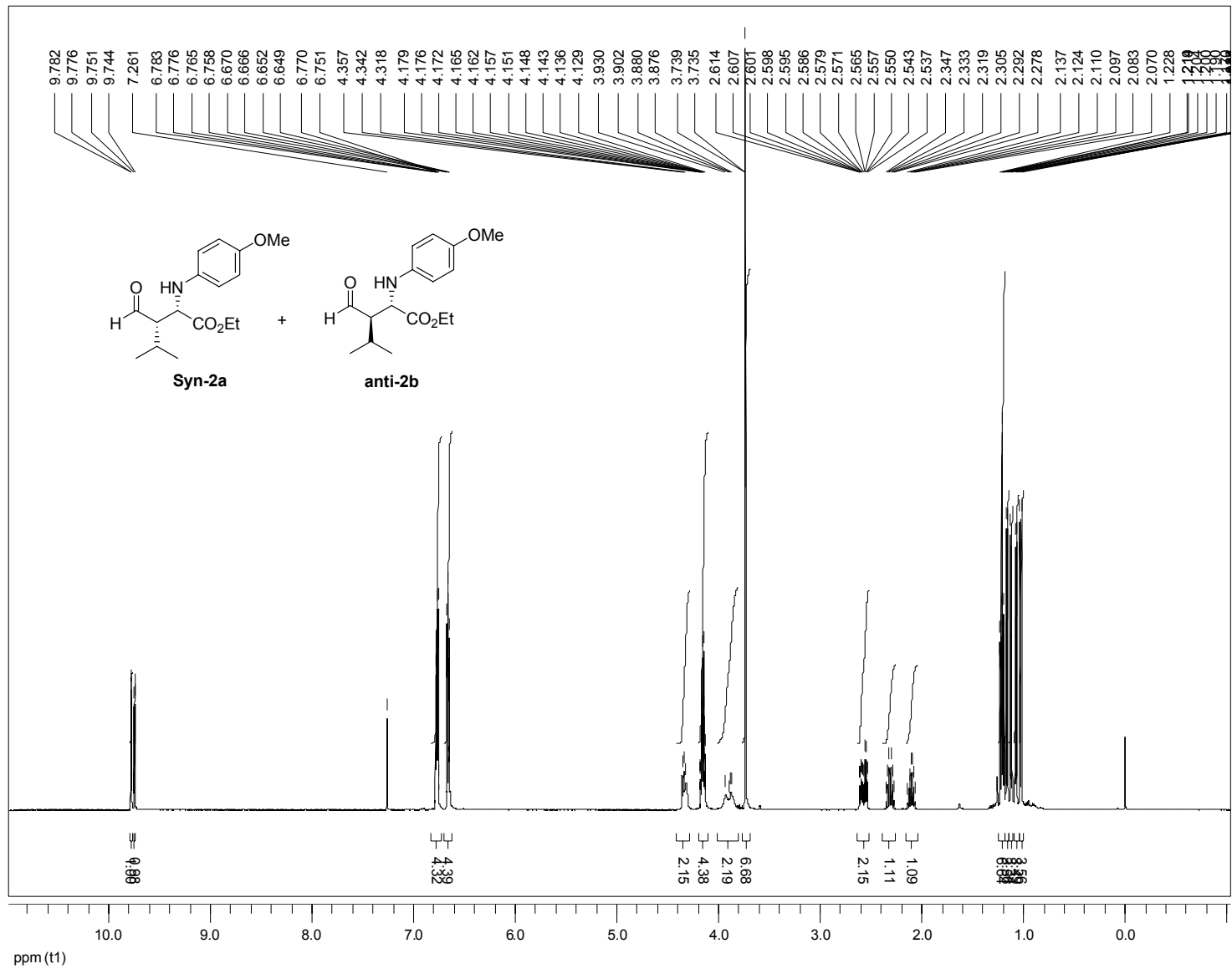
Ethyl 3-formyl-2-(*p*-methoxyphenylamino)heptanoate (1c + 2c): ¹H NMR (300 MHz, CDCl₃): purified 1.5:1 mixture of diastereomers, * denotes *anti*-diastereomer (**2c**), δ = 0.89-1.02 (m, 3H), 1.23 (t, 3H* x 2/5, *J* = 7.1 Hz), 1.24 (t, 3H x 3/5, *J* = 7.1 Hz), 1.28-1.90 (m, 6H), 2.68-2.78 (m, 1H), 3.73 (s, 3H), 3.89 (brd, 1H x 3/5, *J* = 10.2 Hz), 4.03 (brd, 1H* x 2/5, *J* = 10.2 Hz), 4.18 (m, 2H), 4.26 (m, 1H* x 2/5), 4.35 (dd, 1H x 3/5, *J* = 5.0 Hz, 10.2 Hz), 6.65 (d, 2H, *J* = 8.1 Hz), 6.77 (d, 2H, *J* = 8.1 Hz), 9.65 (d, 1H* x 2/5, *J* = 2.4 Hz), 9.71 (d, 1H x 3/5, *J* = 2.1 Hz); ¹³C NMR (75 MHz, CDCl₃): δ = 202.9, 202.8, 172.4, 172.2, 153.3, 153.1, 140.4, 140.3, 116.1, 115.7, 114.8, 114.8, 61.5, 61.5, 58.4, 58.1, 55.6, 53.9, 53.7, 29.6, 29.4, 25.4, 24.8, 22.6, 14.1, 13.8 (for ¹³C NMR hard copy, see ref S1); HPLC (Daicel Chiralpak AS-H, hexane/*i*-PrOH = 99:1, flow rate 1.0 mL/min, λ = 254 nm); t_R (*syn* major enantiomer, (2*S*,3*S*)-**1c**) = 35.3 min; t_R (*syn* minor enantiomer, (2*R*,3*R*)-**1c**) = 54.2 min; t_R (*anti* major enantiomer, (2*S*,3*R*)-**2c**) = 27.4 min; t_R (*anti* minor enantiomer, (2*R*,3*S*)-**2c**) = 32.8 min. HRMS: Calcd for C₁₇H₂₅NO₄ (MNa⁺): 307.1778, found: 307.1781.

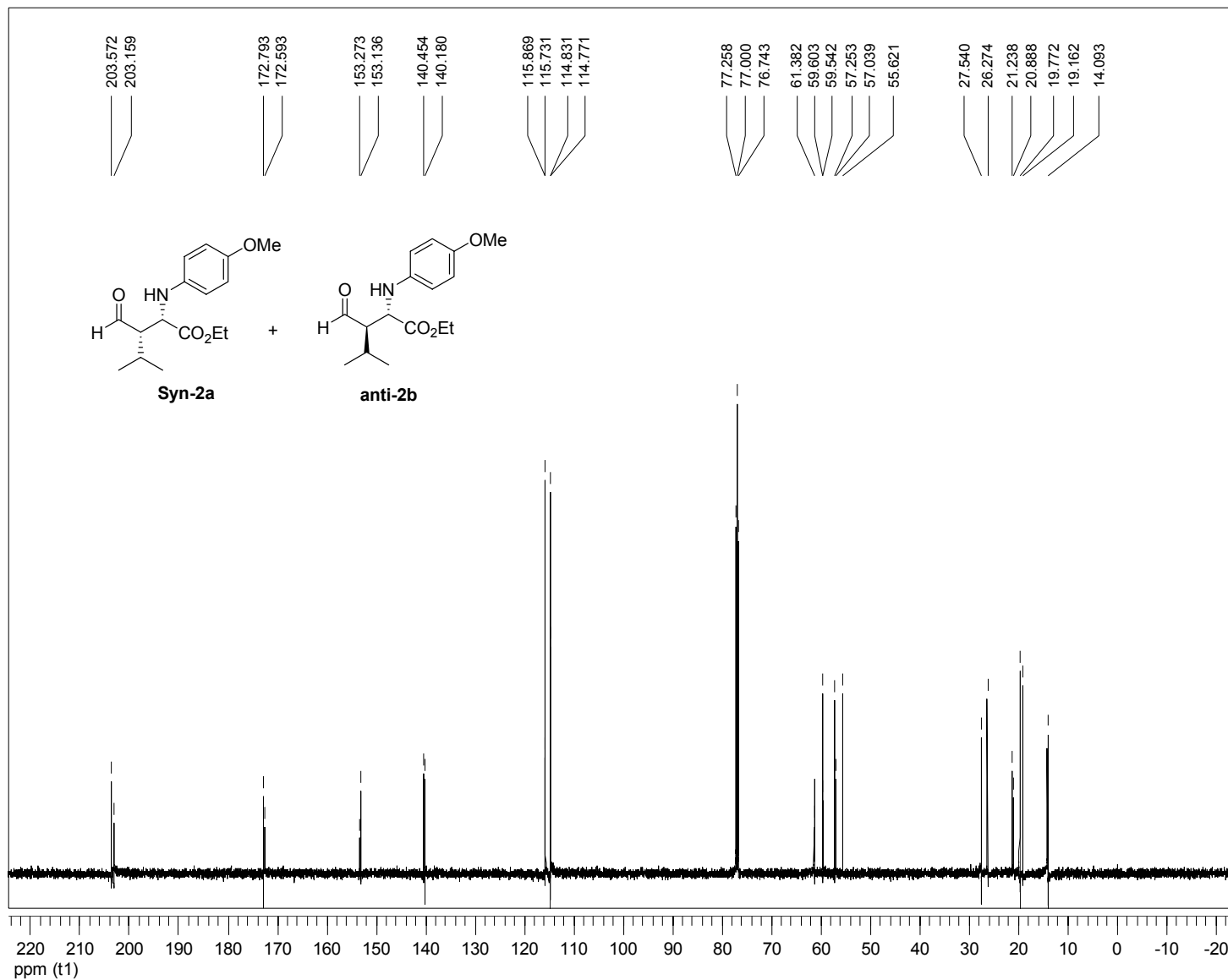
Ethyl 3-formyl-2-(*p*-methoxyphenylamino)octanoate (1d + 2d): ¹H NMR (500 MHz, CDCl₃): purified 1.5:1 mixture of diastereomers, * denotes *anti*-diastereomer (**2d**), δ = 0.89 (m, 3H), 1.24 (t, 3H, *J* = 7.1 Hz), 1.25-1.90 (m, 8H), 2.76 (m, 1H), 3.73 (s, 3H), 3.95-4.10 (1H), 4.14-4.20 (m, 2H), 4.26 (m, 1H* x 2/5), 4.37 (m, 1H x 3/5), 6.65 (m, 2H), 6.78 (m, 2H), 9.65 (d, 1H* x 2/5, *J* = 2.0 Hz), 9.71 (d, 1H x 3/5, *J* = 1.5 Hz); ¹³C

Supporting Information

NMR (120 MHz, CDCl₃): δ = 202.6, 202.2, 172.2, 153.3, 153.1, 140.5, 140.3, 116.0, 115.7, 114.8, 61.5, 58.4, 58.1, 57.2, 55.6, 53.9, 53.7, 31.6, 27.1 26.9, 25.6, 22.5, 22.3, 14.1, 13.9; HPLC (Daicel Chairalcel AS-H, hexane/*i*-PrOH =99:1, 1.0 mL/min, λ = 254 nm) t_R (*syn* major enantiomer, (2*S*,3*S*)-**1d**) = 24.9 min; t_R (*syn* minor enantiomer, (2*R*,3*R*)-**1d**) = 34.8 min; t_R (*anti* major enantiomer, (2*S*,3*R*)-**2d**) = 21.1 min; t_R (*anti* minor enantiomer (2*R*,3*S*)-**2d**) = 23.2 min. HRMS: Calcd for C₁₈H₂₇NO₄(MH⁺) 322.2013, found: 322.2021.

Ethyl 3-formyl-2-(*p*-methoxyphenylamino)hex-5-enoate (1e + 2e): ¹H NMR (400 MHz, CDCl₃): 1.6:1 mixture of diastereomers, * denotes *anti*-diastereomer (**2e**), δ = 1.23 (t, 3H* x 5/13, J = 7.2 Hz, OCHCH₃), 1.24 (t, 3H x 8/13, J = 7.2 Hz, OCHCH₃), 2.42-2.70 (m, 2H, CH₂CH=CH₂), 2.86-2.88 (m, 1H x 8/13, CHCHO), 2.96-2.97(m, 1H* x 5/13, CHCHO), 3.73 (s, 3H, OCH₃), 4.00 (d, 1H x 8/13, J = 9.6Hz, NH), 4.07 (d, 1H* x 5/13, J = 9.6Hz, NH), 4.15-4.20 (m, 2H, OCH₂CH₃), 4.26-4.30 (m, 1H* x 5/13, CHNHPMP), 4.36-4.39 (m, 1H x 8/13, CHNHPMP), 5.13-5.19 (m, 2H, CH=CH₂), 5.77-5.88 (m, 1H, CH=CH₂), 6.64-6.78 (m, 4H, ArH), 9.68 (d, 1H* x 5/13, J = 1.6 Hz, CHCHO), 9.72 (d, 1H x 8/13, J = 1.2 Hz, CHCHO); ¹³C NMR (100 MHz, CDCl₃): 201.9, 172.2, 172.2, 153.3, 153.1, 140.5, 140.3, 134.3, 118.2, 116.1, 115.8, 114.8, 61.6, 57.8, 57.7, 55.6, 53.1, 53.0, 30.0, 29.7, 14.1. HPLC (Daicel Chairalcel AS-H, hexane /*i*-PrOH =99:1, 1.0 mL/min, λ = 254 nm) t_R (*syn* major enantiomer, (2*S*,3*S*)-**1e**) = 45.5 min; t_R (*syn* minor enantiomer, (2*R*,3*R*)-**1e**) = 80.1 min; t_R (*anti* major enantiomer (2*S*,3*R*)-**2e**) = 33.9 min; t_R (*anti* minor enantiomer (2*R*,3*S*)-**2e**) = 42.7 min. HRMS: Calcd for C₁₆H₂₂NO₄(MH⁺) 292.1543, found: 292.1537.





Date:

15 Aug 2005

Document's Title:

ZHL-1076forOL.mrc

Spectrum Title:

ZHL-1076sec_20Jun2005

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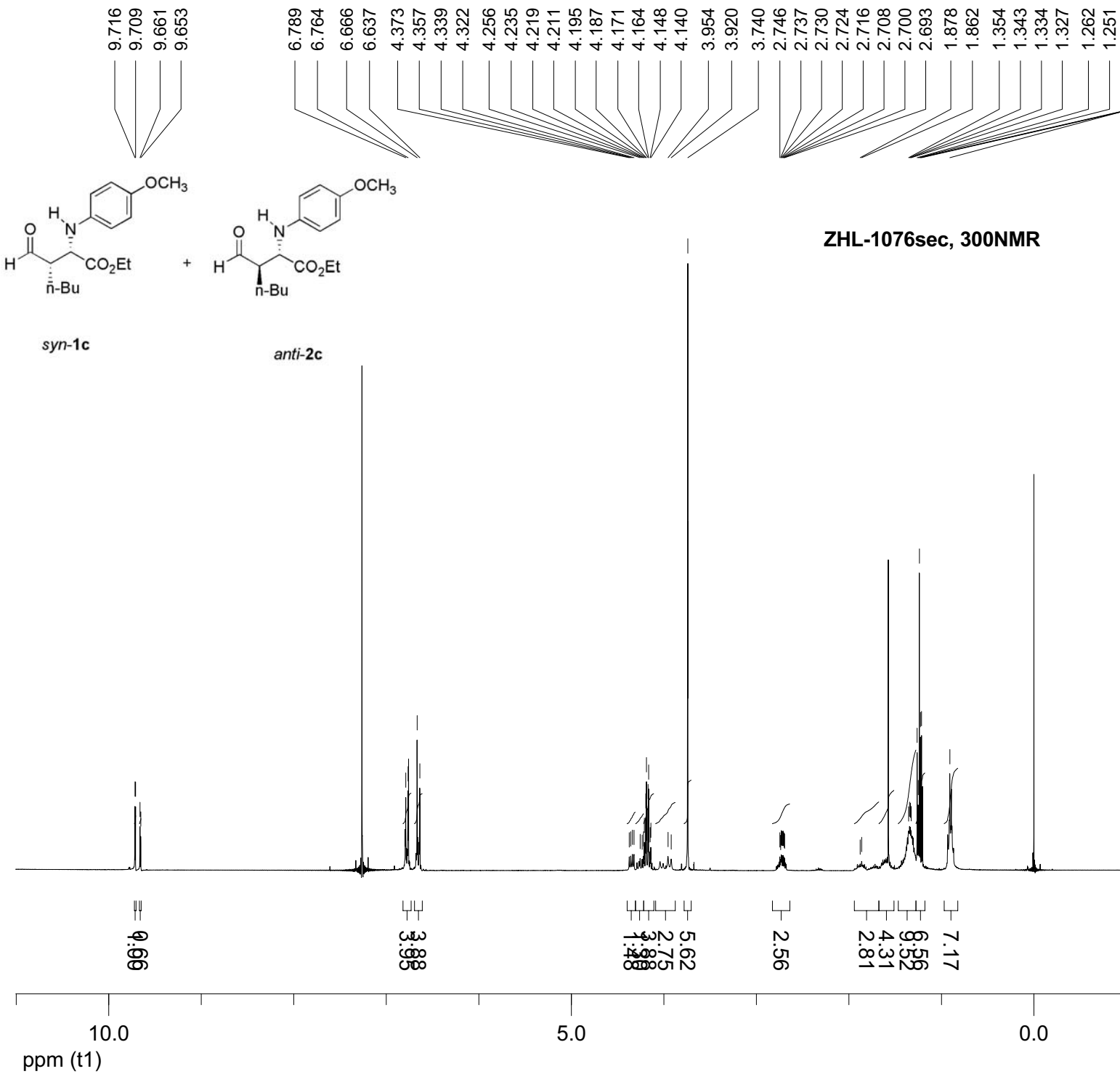
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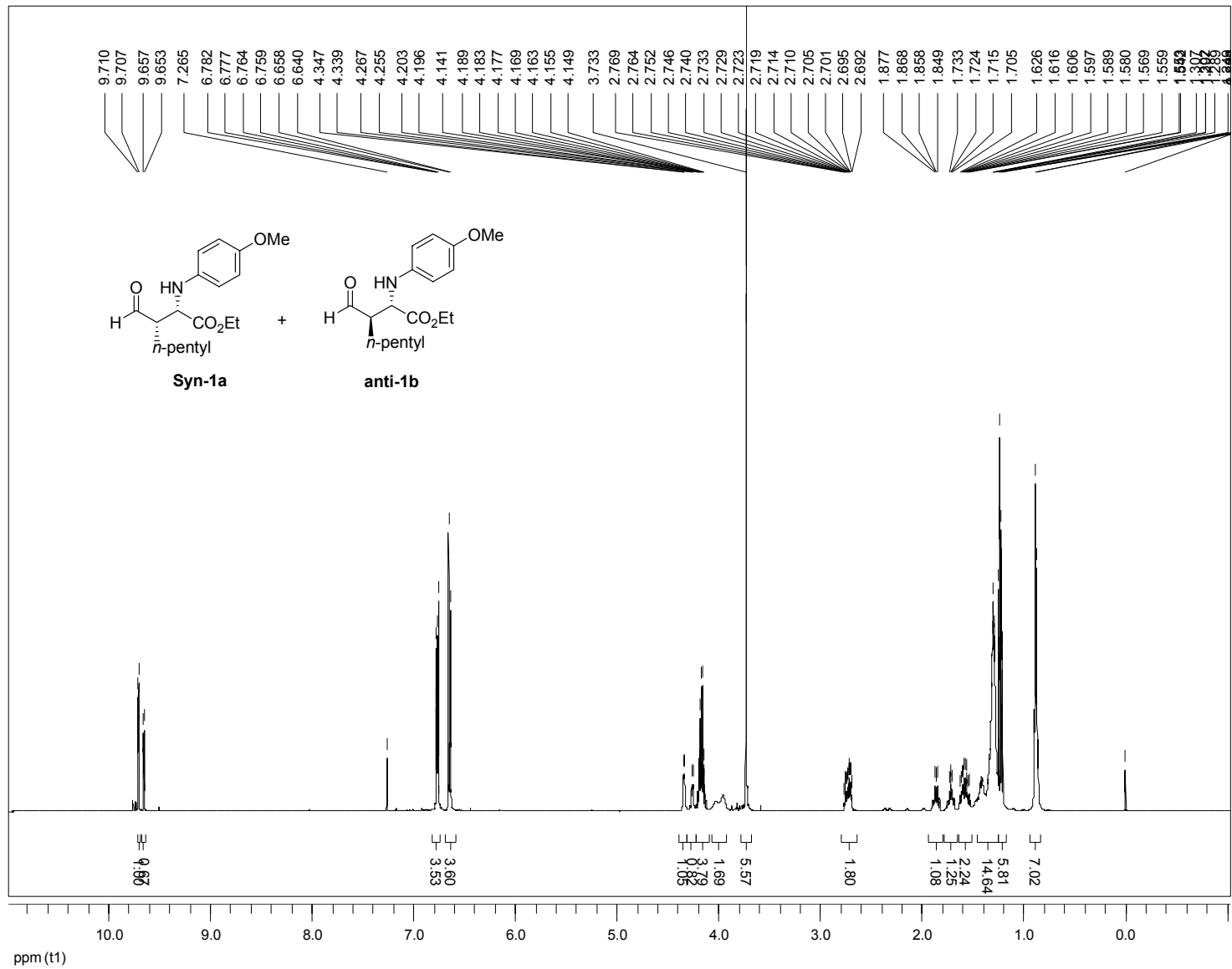
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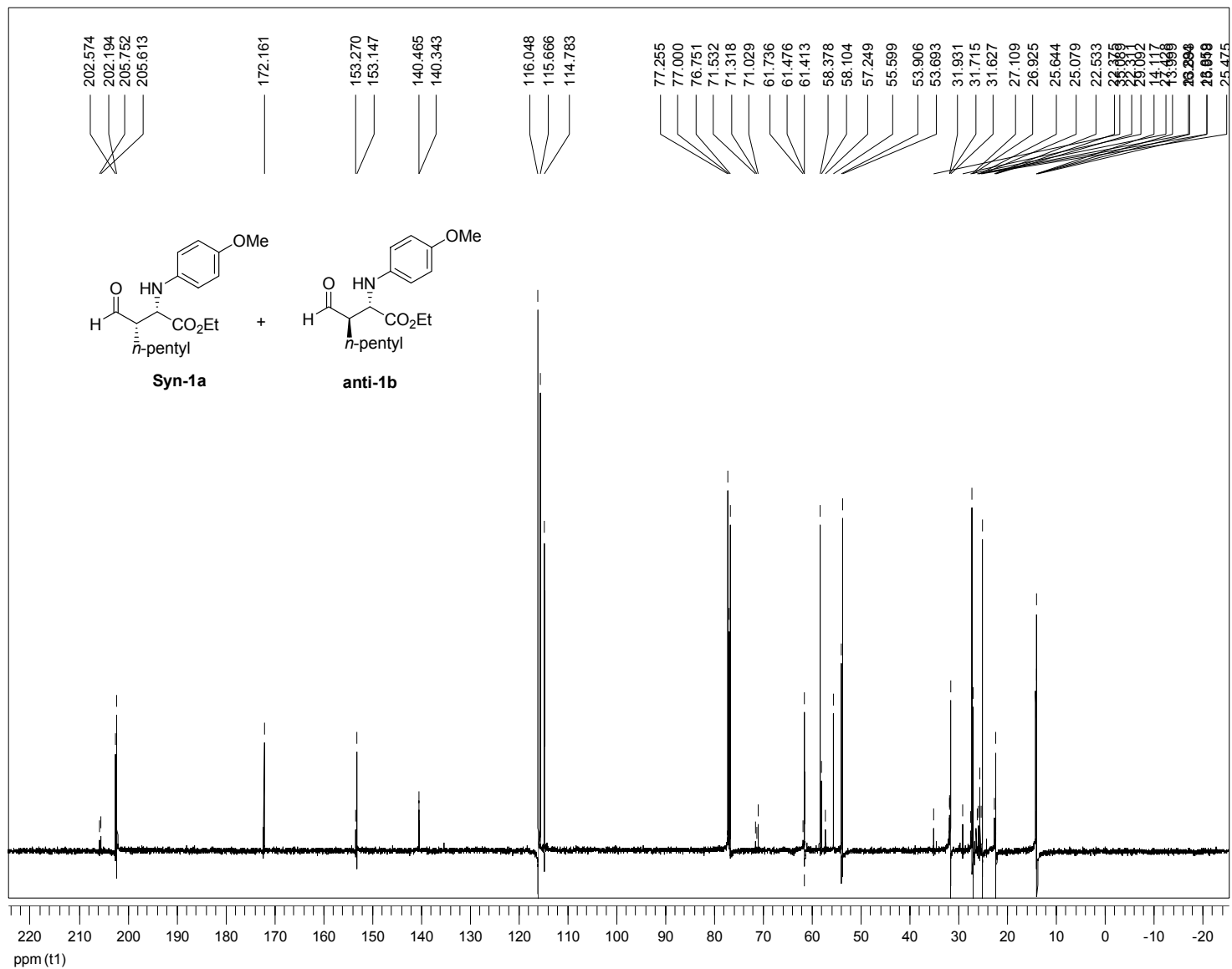
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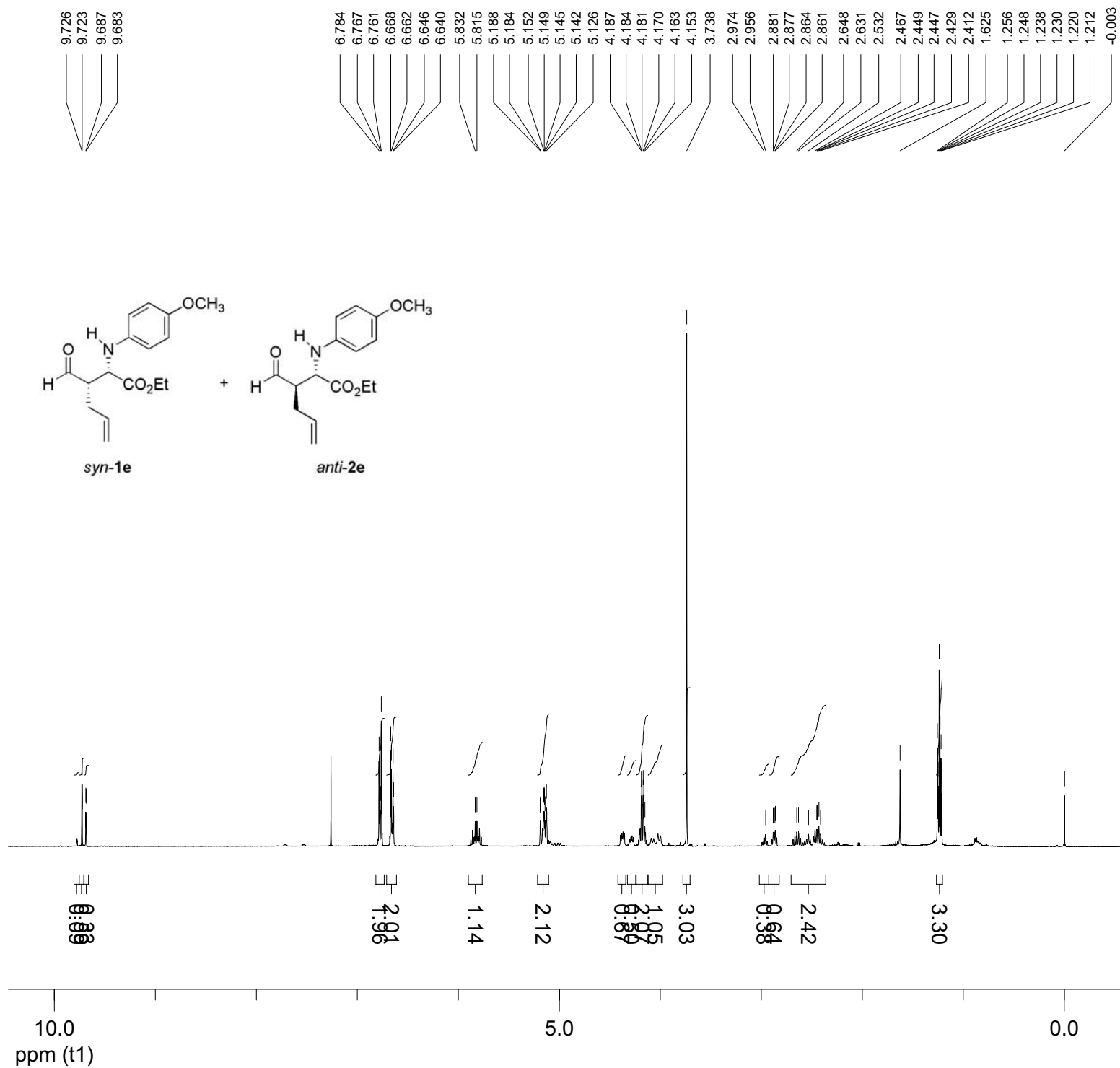
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**Date:**

15 Aug 2005

Document's Title:

ZHL-1121-b2-b3.mrc

Spectrum Title:

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Actual Points Count:

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Spectral Width (ppm):

(f1) 16.000

Pulse Program:

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Temperature:

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Number of Scans:

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Acq. Date:

Jul 15 2005

Date:
15 Aug 2005
Document's Title:
parameterZHL-1121-b4-b7car.mrc

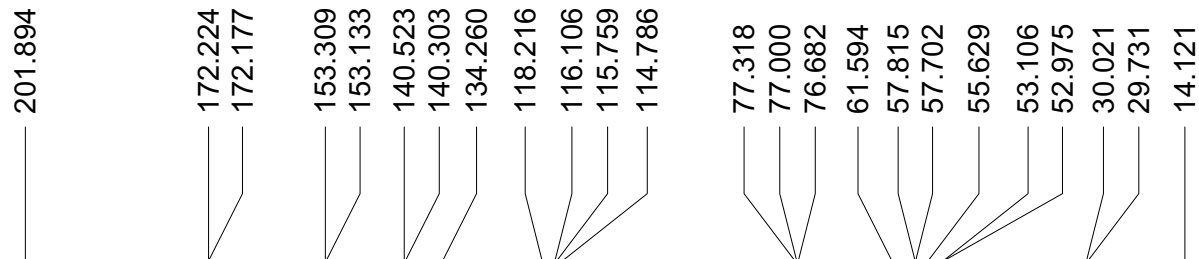
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Temperature:
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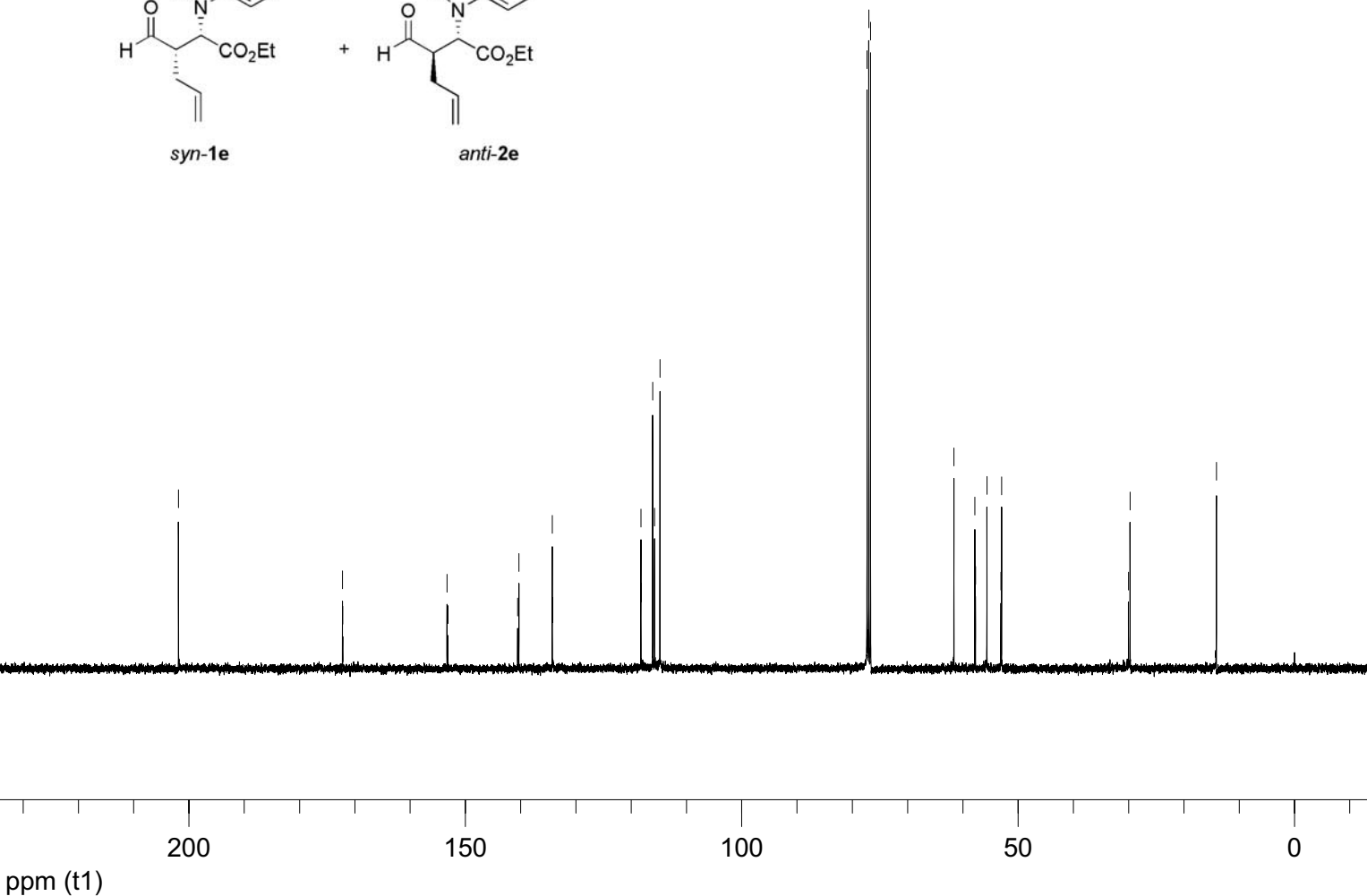
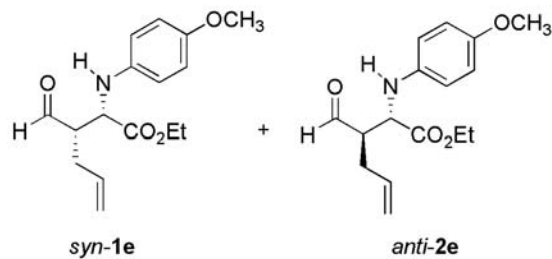
Number of Scans:
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Acq. Date:
Jul 16 2005

SI [10/37]



400 CNMR, ZHL-1121-b4-b7-car



II. Computational Supporting Information

A. Authors of Computational Packages

Authors of Q-Chem 3.1:

J. Kong, C. A. White, A. I. Krylov, C. D. Sherrill,
R. D. Adamson, T. R. Furlani, M. S. Lee, A. M. Lee,
S. R. Gwaltney, T. R. Adams, C. Ochsenfeld, A. T. B. Gilbert,
G. S. Kedziora, V. A. Rassolov, D. R. Maurice, N. Nair,
Y. Shao, N. A. Besley, P. E. Maslen, J. P. Dombroski,
H. Dachsel, W. M. Zhang, P. P. Korambath, J. Baker,
E. F. C. Byrd, T. Van Voorhis, M. Oumi, S. Hirata,
C. P. Hsu, N. Ishikawa, J. Florian, A. Warshel,
B. G. Johnson, P. M. W. Gill, M. Head-Gordon, J. A. Pople,
Q-Chem, Version 2.0, Q-Chem, Inc., Export, PA (2000).

Authors of Gaussian 03:

Gaussian 03, Revision C.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven,
K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi,
V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega,
G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota,
R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao,
H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross,
C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev,
A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala,
K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg,
V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain,
O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford,
J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz,
I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill,
B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople,
Gaussian, Inc., Wallingford CT, 2004.

B. Relevant geometries, energies, thermodynamic data, frequencies, and Gaussian route section of structures.

i. Proline

Supporting Information: s-Trans-Re-3D-(Methyl-Syn)-(Esther-Anti).output

Using Gaussian 03: Al64T-G03RevC.01 3-Apr-2004

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Item Max Val. Criteria Pass? RMS Val. Criteria Pass?
Force 0.00003 || 0.00045 [ YES ] 0.00000 || 0.00030 [ YES ]
Displ 0.00294 || 0.00180 [ NO ] 0.00294 || 0.00180 [ YES ]
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Supporting Information

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H	7.533940	-1.641407	0.262727
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Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

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Frequencies --  -318.6211           28.3273           29.6629
    
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Supporting Information: s-Trans-Re-3D-(Methyl-Syn)-(Esther-Syn).output

Using Gaussian 03: Al64T-G03RevC.01 3-Apr-2004

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```

-----
SCF Energy= -1178.73180651    Predicted Change= -2.397847D-08
    
```

```

=====
Optimization completed.            {Found        2        times}
Item    Max Val.    Criteria    Pass?    RMS Val.    Criteria    Pass?
    
```

Supporting Information

```

H      -3.876720    1.841079   -1.415817
H      -2.941161    2.350734   -2.823099
  
```

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

```

SCF Energy=      -1178.73180651      Predicted Change= -2.397847D-08
Zero-point correction (ZPE)=      -1178.2939      0.43783
Internal Energy (U)=      -1178.2705      0.46123
Enthalpy (H)=      -1178.2696      0.46217
Gibbs Free Energy (G)=      -1178.3476      0.38413
  
```

Frequencies -- -359.9596 30.2640 35.2485

Supporting Information: s-Trans-Re-3U-(Methyl-Anti)-(Esther-Anti).output

Using Gaussian 03: Al64T-G03RevC.01 3-Apr-2004

```

# opt=(calcf,ts,maxcycle=150,noeigentest) freq=noraman hf/6-31g(d)
geom=connectivity scf=(direct,tight,maxcycle=300)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
  
```

Pointgroup= C1 Stoichiometry= C18H24N2O5 C1[X(C18H24N2O5)] #Atoms= 49
Charge = 0 Multiplicity = 1

SCF Energy= -1178.72599682 Predicted Change= -8.664731D-08

```

Optimization completed.      {Found      1      times}
Item      Max Val.      Criteria      Pass?      RMS Val.      Criteria      Pass?
Force      0.00005 || 0.00045 [ YES ]      0.00000 || 0.00030 [ YES ]
Displ      0.00527 || 0.00180 [ NO ]      0.00527 || 0.00180 [ YES ]
  
```

Atomic Coordinates (Angstroms)
Type X Y Z

```

N      -2.478103    -0.998102    0.883540
C      -3.804374    -0.397913    0.744714
C      -4.663470    -1.559366    0.245728
C      -3.673706    -2.390693    -0.574753
C      -2.386873    -2.335612    0.243521
C      -1.435669    -0.406498    1.411720
C      -1.286653    0.924183    1.778154
C      -0.188141    1.553627    -0.180686
C      -0.231310    1.305129    2.797168
N      0.451964    0.617738    -0.817353
C      4.464231    -0.393147    -0.070679
C      4.088738    0.939452    -0.134435
C      2.763801    1.266230    -0.390053
C      1.812130    0.279106    -0.557104
C      2.190597    -1.062490    -0.513352
C      3.506162    -1.385305    -0.268886
O      5.717966    -0.822332    0.165838
C      6.748193    0.104609    0.356025
  
```

```

C      -1.456681    2.097034    -0.771332
O      -1.700151    3.299532    -0.288569
O      -2.107677    1.541682    -1.587273
C      -2.857970    3.965040    -0.775478
C      -1.072667    -2.423533    -0.573481
O      -0.978329    -1.608849    -1.508657
O      -0.244116    -3.222330    -0.163260
H      -3.777911    0.401884    0.016899
H      -4.133357    0.005044    1.695989
H      -5.038267    -2.134555    1.086984
H      -5.514552    -1.214489    -0.329308
H      -4.005105    -3.409456    -0.734532
H      -3.493291    -1.927092    -1.536328
H      -2.376142    -3.092828    1.018010
H      -0.571808    -1.045461    1.495850
H      -2.171964    1.539072    1.783691
H      0.371214    2.224234    0.435503
H      0.667586    0.706545    2.683160
H      0.052687    2.349682    2.699572
H      -0.583212    1.173718    3.817923
H      -0.098690    -0.076301    -1.335242
H      4.803379    1.729090    -0.010064
H      2.496077    2.304029    -0.480455
H      1.464845    -1.842414    -0.659165
H      3.812807    -2.413156    -0.224732
H      6.886007    0.729457    -0.520219
H      6.561467    0.733217    1.220618
H      7.645003    -0.471971    0.524548
H      -3.746594    3.408356    -0.515545
H      -2.863996    4.929219    -0.293906
H      -2.802780    4.075986    -1.847922
  
```

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

```

SCF Energy=      -1178.72599682      Predicted Change= -8.664731D-08
Zero-point correction (ZPE)=      -1178.2884      0.43757
Internal Energy (U)=      -1178.2648      0.46111
Enthalpy (H)=      -1178.2639      0.46205
Gibbs Free Energy (G)=      -1178.3429      0.38303
  
```

Frequencies -- -353.2953 25.0887 36.4296

Supporting Information: s-Trans-Re-3U-(Methyl-Anti)-(Esther-Syn).output

Using Gaussian 03: Al64T-G03RevC.01 3-Apr-2004

```

#hf/6-31g* scf=(direct,tight,maxcycle=300)
opt=(calcf,ts,maxcycle=150,noeigentest) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
  
```

Pointgroup= C1 Stoichiometry= C18H24N2O5 C1[X(C18H24N2O5)] #Atoms= 49
Charge = 0 Multiplicity = 1

Supporting Information

SCF Energy= -1178.72658857 Predicted Change= -7.524670D-09

```

Optimization completed.      {Found      2      times}
Item      Max Val.      Criteria      Pass?      RMS Val.      Criteria      Pass?
Force      0.00001 || 0.00045 [ YES ]      0.00000 || 0.00030 [ YES ]
Displ      0.00080 || 0.00180 [ YES ]      0.00080 || 0.00180 [ YES ]
    
```

Atomic Coordinates (Angstroms)

Atomic Type	X	Y	Z
N	-2.472152	-1.157933	0.899739
C	-3.744743	-0.592153	1.341800
C	-4.767041	-1.456311	0.606429
C	-4.063645	-1.765696	-0.718898
C	-2.603954	-1.987412	-0.319589
C	-1.284617	-0.846654	1.376889
C	-0.920336	0.194423	2.205319
C	-0.145608	1.491397	0.438044
C	0.338038	0.087723	3.040344
N	0.532980	0.859165	-0.478099
C	4.504006	-0.479687	-0.241888
C	4.170391	0.763139	0.272881
C	2.858957	1.213030	0.191530
C	1.879986	0.423694	-0.376865
C	2.215241	-0.821400	-0.907291
C	3.516735	-1.262693	-0.837641
O	5.741774	-1.008746	-0.220342
C	6.799885	-0.285063	0.340549
C	-1.442222	2.165565	0.010312
O	-1.341227	2.586955	-1.220499
O	-2.358395	2.366228	0.734685
C	-2.523001	3.076236	-1.842404
C	-1.552821	-1.509609	-1.348498
O	-1.628611	-0.299338	-1.648657
O	-0.704060	-2.321837	-1.681024
H	-3.825182	0.445861	1.051950
H	-3.822285	-0.654270	2.421213
H	-4.950935	-2.371700	1.160848
H	-5.714874	-0.946790	0.478279
H	-4.476577	-2.626953	-1.229659
H	-4.121926	-0.911761	-1.382556
H	-2.413479	-3.024575	-0.071185
H	-0.494214	-1.475972	1.000058
H	-1.697180	0.825746	2.596958
H	0.383657	1.969933	1.235610
H	1.100679	-0.506880	2.547906
H	0.766240	1.065379	3.249900
H	0.138367	-0.372079	4.005513
H	-0.039562	0.460655	-1.224120
H	4.909164	1.398213	0.720739
H	2.623797	2.194690	0.562262
H	1.453432	-1.431322	-1.362680

H	3.792032	-2.219679	-1.238926
H	6.963031	0.649822	-0.185269
H	6.627202	-0.081505	1.392262
H	7.676686	-0.906329	0.239316
H	-2.919672	3.914701	-1.289938
H	-2.222482	3.378625	-2.831743
H	-3.249072	2.280299	-1.897647

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1178.72658857 Predicted Change= -7.524670D-09
 Zero-point correction (ZPE)= -1178.2887 0.43786
 Internal Energy (U)= -1178.2652 0.46130
 Enthalpy (H)= -1178.2643 0.46224
 Gibbs Free Energy (G)= -1178.3430 0.38352

Frequencies -- -380.4655 28.2735 36.5807

Supporting Information: s-Trans-Re-3U-(Methyl-Syn)-(Esther-Anti).output

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

```

# opt=(calcf,ts,maxcycle=150,noeigentest) freq=normal hf/6-31g(d)
geom=connectivity scf=(direct,tight,maxcycle=300)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
    
```

Pointgroup= C1 Stoichiometry= C18H24N2O5 C1[X(C18H24N2O5)] #Atoms= 49
 Charge = 0 Multiplicity = 1

SCF Energy= -1178.72745322 Predicted Change= -4.261283D-09

```

Optimization completed.      {Found      2      times}
Item      Max Val.      Criteria      Pass?      RMS Val.      Criteria      Pass?
Force      0.00002 || 0.00045 [ YES ]      0.00000 || 0.00030 [ YES ]
Displ      0.00139 || 0.00180 [ YES ]      0.00139 || 0.00180 [ YES ]
    
```

Atomic Coordinates (Angstroms)

Atomic Type	X	Y	Z
N	-2.310596	-1.184266	0.869085
C	-3.700839	-0.755343	0.723134
C	-4.407564	-2.020930	0.239339
C	-3.322636	-2.728636	-0.576573
C	-2.049097	-2.500601	0.233982
C	-1.354071	-0.466598	1.403220
C	-1.377416	0.870759	1.775329
C	-0.363417	1.651389	-0.171175
C	-0.384703	1.378010	2.802388
N	0.385713	0.805880	-0.814996
C	4.472284	0.204999	-0.026393
C	3.943248	1.494762	-0.032232
C	2.608617	1.694155	-0.297404

Supporting Information

C	1.770195	0.608436	-0.539829
C	2.293258	-0.671618	-0.555502
C	3.643276	-0.871276	-0.296371
O	5.788219	0.113266	0.240571
C	6.409733	-1.142574	0.241979
C	-1.685779	2.042575	-0.764102
O	-2.078688	3.199380	-0.269368
O	-2.258811	1.420378	-1.590439
C	-3.307066	3.723042	-0.756836
C	-0.743448	-2.426905	-0.598146
O	-0.750957	-1.585330	-1.514161
O	0.169801	-3.146475	-0.223216
H	-3.772591	0.032496	-0.014757
H	-4.078766	-0.384840	1.669339
H	-4.704374	-2.629968	1.087882
H	-5.296790	-1.792689	-0.336092
H	-3.521624	-3.783052	-0.723965
H	-3.207487	-2.256516	-1.544089
H	-1.934772	-3.246497	1.011109
H	-0.416200	-0.990658	1.490247
H	-2.334474	1.366647	1.779888
H	0.107774	2.378806	0.454034
H	0.584289	0.900679	2.690613
H	-0.236521	2.450853	2.711744
H	-0.722092	1.196865	3.820418
H	-0.079107	0.060076	-1.342564
H	4.600080	2.323581	0.153655
H	2.228700	2.699460	-0.338938
H	1.663879	-1.519469	-0.755616
H	4.017907	-1.875631	-0.307177
H	5.984199	-1.793247	0.998037
H	6.335037	-1.621136	-0.728262
H	7.449120	-0.962709	0.471329
H	-4.121580	3.057776	-0.509651
H	-3.434614	4.673117	-0.264265
H	-3.259786	3.853121	-1.827491

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1178.72745322 Predicted Change= -4.261283D-09
 Zero-point correction (ZPE)= -1178.2898 0.43764
 Internal Energy (U)= -1178.2662 0.46120
 Enthalpy (H)= -1178.2653 0.46214
 Gibbs Free Energy (G)= -1178.3444 0.38301

Frequencies -- -357.7627 24.4570 34.6059

Supporting Information: s-Trans-Re-3U-(Methyl-Syn)-(Esther-Syn).output

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

opt=(calcf,ts,maxcycle=150,noeigentest) freq=norman hf/6-31g(d)

geom=connectivity scf=(direct,tight,maxcycle=300)
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq

Pointgroup= C1 Stoichiometry= C18H24N2O5 C1[X(C18H24N2O5)] #Atoms= 49
 Charge = 0 Multiplicity = 1

SCF Energy= -1178.72758451 Predicted Change= -3.552982D-08

Optimization completed. {Found 1 times}
 Item Max Val. Criteria Pass? RMS Val. Criteria Pass?
 Force 0.00002 || 0.00045 [YES] 0.00000 || 0.00030 [YES]
 Displ 0.00230 || 0.00180 [NO] 0.00230 || 0.00180 [YES]

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
N	-2.374516	-1.199598	0.930735
C	-3.708156	-0.712528	1.275539
C	-4.621040	-1.716670	0.575089
C	-3.835913	-2.066346	-0.693065
C	-2.381448	-2.127229	-0.222986
C	-1.240515	-0.754197	1.430719
C	-1.003362	0.370102	2.194565
C	-0.265282	1.610295	0.376990
C	0.219606	0.430673	3.085166
N	0.495283	0.978253	-0.472695
C	4.538383	-0.052332	-0.014036
C	4.084340	1.188819	0.430479
C	2.762700	1.539606	0.282129
C	1.863556	0.647222	-0.294651
C	2.310077	-0.579879	-0.748387
C	3.647180	-0.929958	-0.609575
O	5.848852	-0.296927	0.172906
C	6.398132	-1.509523	-0.263298
C	-1.594003	2.146467	-0.137790
O	-1.488499	2.472292	-1.396782
O	-2.545322	2.331624	0.544515
C	-2.682925	2.824045	-2.083759
C	-1.332769	-1.639479	-1.250046
O	-1.492710	-0.463689	-1.639621
O	-0.413334	-2.403821	-1.498281
H	-3.860968	0.288798	0.898306
H	-3.829181	-0.695304	2.352528
H	-4.752342	-2.598383	1.195146
H	-5.601444	-1.302908	0.370128
H	-4.151687	-2.997864	-1.146574
H	-3.936770	-1.275562	-1.426265
H	-2.114639	-3.121695	0.114031
H	-0.383679	-1.337487	1.133383
H	-1.848015	0.955583	2.509391
H	0.192812	2.181947	1.157146
H	1.052588	-0.124945	2.666749
H	0.552219	1.454079	3.242949

Supporting Information

H	0.015617	0.019946	4.071303
H	-0.015224	0.484864	-1.206926
H	4.789820	1.867144	0.872159
H	2.439428	2.515020	0.598896
H	1.617577	-1.268051	-1.202992
H	3.965083	-1.888792	-0.968746
H	5.941830	-2.354371	0.241106
H	6.290125	-1.629010	-1.335815
H	7.447525	-1.470962	-0.013495
H	-3.152444	3.673751	-1.611418
H	-2.375861	3.066285	-3.087494
H	-3.351018	1.976980	-2.090173

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

=====
 SCF Energy= -1178.72758451 Predicted Change= -3.552982D-08
 Zero-point correction (ZPE)= -1178.2896 0.43791
 Internal Energy (U)= -1178.2662 0.46135
 Enthalpy (H)= -1178.2652 0.46230
 Gibbs Free Energy (G)= -1178.3440 0.38350

Frequencies -- -385.7647 29.2599 33.2389

Supporting Information: s-Trans-Si-3D-(Methyl-Syn)-(Esther-Anti).output

Using Gaussian 03: Al64T-G03RevC.01 3-Apr-2004

=====
 # opt=(calcf,ts,maxcycle=150,noeigentest) freq=noraman hf/6-31g(d)
 geom=connectivity scf=(direct,tight,maxcycle=300)
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq

Pointgroup= C1 Stoichiometry= C18H24N2O5 C1[X(C18H24N2O5)] #Atoms= 49
 Charge = 0 Multiplicity = 1

=====
 SCF Energy= -1178.72819201 Predicted Change= -3.823938D-09

=====
 Optimization completed. {Found 2 times}
 Item Max Val. Criteria Pass? RMS Val. Criteria Pass?
 Force 0.00000 || 0.00045 [YES] 0.00000 || 0.00030 [YES]
 Displ 0.00092 || 0.00180 [YES] 0.00092 || 0.00180 [YES]

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
N	-1.238687	1.514613	0.987649
C	0.025475	1.719464	1.700296
C	0.499742	3.097618	1.224135
C	-0.788937	3.794038	0.776617
C	-1.567791	2.654781	0.114666
C	-2.075011	0.533543	1.237691
C	-1.804473	-0.661137	1.875576
C	-1.030797	-1.635952	-0.109801

C	-2.922865	-1.518880	2.425075
N	-0.117259	-0.887446	-0.636054
C	4.028933	-1.033717	0.044165
C	3.185230	-1.862937	0.778137
C	1.822570	-1.828540	0.580914
C	1.271248	-0.962392	-0.360329
C	2.109047	-0.130696	-1.085837
C	3.480723	-0.164798	-0.886979
O	5.342563	-1.145470	0.311976
C	6.264614	-0.353675	-0.385653
C	-2.383463	-1.694844	-0.760648
O	-2.927075	-2.873907	-0.542991
O	-2.867356	-0.824590	-1.398512
C	-4.202988	-3.110949	-1.128585
C	-1.139257	2.495564	-1.376301
O	-0.449818	1.497779	-1.678318
O	-1.500934	3.416669	-2.076185
H	0.741537	0.941336	1.481079
H	-0.171811	1.705878	2.768343
H	1.028851	3.630381	2.005378
H	1.169579	2.983292	0.380582
H	-1.332066	4.170375	1.639669
H	-0.625988	4.609237	0.088044
H	-2.636294	2.823104	0.132536
H	-3.051540	0.665334	0.805011
H	-0.851983	-0.758693	2.370378
H	-0.754048	-2.503500	0.450379
H	-3.852836	-1.351608	1.889893
H	-2.693492	-2.578117	2.355277
H	-3.112861	-1.303464	3.474001
H	-0.404918	-0.031660	-1.160737
H	3.618226	-2.527947	1.501440
H	1.207213	-2.480245	1.172622
H	1.681179	0.554667	-1.792607
H	4.098779	0.492310	-1.466427
H	6.228582	-0.551894	-1.451279
H	6.091879	0.702356	-0.208955
H	7.238591	-0.622819	-0.006495
H	-4.925892	-2.406343	-0.745535
H	-4.141366	-3.018041	-2.202199
H	-4.468727	-4.116916	-0.848150

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

=====
 SCF Energy= -1178.72819201 Predicted Change= -3.823938D-09
 Zero-point correction (ZPE)= -1178.2911 0.43706
 Internal Energy (U)= -1178.2676 0.46055
 Enthalpy (H)= -1178.2666 0.46149
 Gibbs Free Energy (G)= -1178.3458 0.38232

Frequencies -- -335.0995 23.8204 31.9805

Supporting Information

Supporting Information: s-Trans-Si-3D-(Methyl-Syn)-(Esther-Syn).output

Using Gaussian 03: Al64T-G03RevC.01 3-Apr-2004

```
#hf/6-31G* opt=(gdiis,calcfc,ts,noeigentest,maxcycle=300)
scf=(maxcycle=300,direct) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
```

Pointgroup= C1 Stoichiometry= C18H24N2O5 C1[X(C18H24N2O5)] #Atoms= 49
Charge = 0 Multiplicity = 1

SCF Energy= -1178.72983665 Predicted Change= -1.400913D-09

```
Optimization completed.      {Found      2      times}
Item      Max Val.  Criteria  Pass?      RMS Val.  Criteria  Pass?
Force     0.00000 || 0.00045 [ YES ]    0.00000 || 0.00030 [ YES ]
Displ     0.00076 || 0.00180 [ YES ]    0.00076 || 0.00180 [ YES ]
```

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z

N	-1.272555	1.724564	0.944926
C	0.022169	2.183868	1.443783
C	0.343297	3.420498	0.587821
C	-0.998779	3.825181	-0.034437
C	-1.716285	2.496026	-0.226667
C	-1.955208	0.704095	1.442950
C	-1.465377	-0.288903	2.254240
C	-1.085285	-1.670768	0.361385
C	-2.348921	-1.123176	3.151531
N	-0.186812	-1.161155	-0.420757
C	3.971068	-0.882125	0.058785
C	3.249934	-1.792864	0.828363
C	1.885033	-1.901283	0.689256
C	1.210205	-1.091965	-0.220143
C	1.922415	-0.186305	-0.986952
C	3.299119	-0.080484	-0.850667
O	5.299322	-0.858025	0.269958
C	6.106063	0.015434	-0.471780
C	-2.480553	-1.861351	-0.223984
O	-2.381036	-2.267528	-1.460296
O	-3.486966	-1.746279	0.388300
C	-3.572810	-2.265246	-2.241625
C	-1.301630	1.693677	-1.487093
O	-1.870195	0.581613	-1.577440
O	-0.424424	2.149397	-2.200968
H	0.785887	1.422174	1.344647
H	-0.073203	2.422628	2.498527
H	0.788919	4.209695	1.182017
H	1.034704	3.156737	-0.199852
H	-1.563980	4.450415	0.651630
H	-0.875080	4.351230	-0.969146
H	-2.796183	2.584260	-0.205581

H	-2.978757	0.648225	1.121315
H	-0.434672	-0.211848	2.561568
H	-0.805107	-2.340072	1.147194
H	-3.379855	-1.104649	2.828659
H	-2.034521	-2.165440	3.178492
H	-2.305166	-0.761232	4.176330
H	-0.581577	-0.594667	-1.173298
H	3.782447	-2.413099	1.524419
H	1.361367	-2.627237	1.283597
H	1.404851	0.451883	-1.682425
H	3.820893	0.631738	-1.458751
H	6.043235	-0.195222	-1.533764
H	5.836332	1.050507	-0.292459
H	7.117700	-0.151725	-0.135020
H	-4.312533	-2.914576	-1.798426
H	-3.941817	-1.254432	-2.311594
H	-3.278615	-2.628440	-3.212283

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

```
SCF Energy= -1178.72983665 Predicted Change= -1.400913D-09
Zero-point correction (ZPE)= -1178.2919 0.43789
Internal Energy (U)= -1178.2685 0.46129
Enthalpy (H)= -1178.2675 0.46224
Gibbs Free Energy (G)= -1178.3460 0.38376
```

Frequencies -- -311.6497 26.8917 34.1086

Supporting Information: s-Trans-Si-3D-(Methyl-Syn)-(Esther-Syn)2.output

Using Gaussian 03: Al64T-G03RevC.01 3-Apr-2004

```
# opt=(calcfc,ts,maxcycle=150,noeigentest) freq=noraman hf/6-31g(d)
geom=connectivity scf=(direct,tight,maxcycle=300)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
```

Pointgroup= C1 Stoichiometry= C18H24N2O5 C1[X(C18H24N2O5)] #Atoms= 49
Charge = 0 Multiplicity = 1

SCF Energy= -1178.73475146 Predicted Change= -5.162964D-08

```
Optimization completed.      {Found      1      times}
Item      Max Val.  Criteria  Pass?      RMS Val.  Criteria  Pass?
Force     0.00002 || 0.00045 [ YES ]    0.00000 || 0.00030 [ YES ]
Displ     0.00344 || 0.00180 [ NO ]     0.00344 || 0.00180 [ YES ]
```

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z

N	-1.456171	1.108427	1.253720
C	-0.178308	1.575374	1.795414
C	-0.042847	3.004598	1.257239

Supporting Information

C	-1.480670	3.424357	0.933546
C	-2.131728	2.130110	0.435488
C	-1.995933	-0.063050	1.507587
C	-1.373534	-1.198854	1.984665
C	-0.701816	-1.842178	-0.130289
C	-2.173393	-2.345430	2.560352
N	0.076268	-0.938987	-0.647236
C	4.220322	-0.470723	-0.134880
C	3.564732	-1.516789	0.508670
C	2.206099	-1.689443	0.363601
C	1.470127	-0.815808	-0.433101
C	2.119828	0.229314	-1.069167
C	3.487687	0.403075	-0.923606
O	5.547384	-0.391920	0.072209
C	6.289818	0.620635	-0.549612
C	-2.071525	-2.066982	-0.710075
O	-2.511762	-1.016035	-1.337023
O	-2.623300	-3.112337	-0.595864
C	-3.766088	-1.070093	-2.018152
C	-1.908481	1.914176	-1.087218
O	-0.769600	1.512529	-1.413837
O	-2.862415	2.184450	-1.791647
H	0.643635	0.948064	1.484678
H	-0.231618	1.549794	2.880161
H	0.434322	3.658375	1.978008
H	0.547799	2.997201	0.352863
H	-1.986763	3.767294	1.831663
H	-1.535281	4.213819	0.195466
H	-3.194884	2.104396	0.632465
H	-3.031178	-0.142010	1.220233
H	-0.363690	-1.098170	2.347315
H	-0.283280	-2.712730	0.327873
H	-3.171946	-2.388371	2.140234
H	-1.702321	-3.303243	2.360570
H	-2.272004	-2.257285	3.639656
H	-0.357812	-0.121587	-1.104345
H	4.140152	-2.186479	1.119601
H	1.739320	-2.509141	0.876925
H	1.549137	0.913784	-1.668203
H	3.957855	1.222029	-1.431385
H	6.225977	0.550340	-1.630001
H	5.960622	1.604037	-0.231787
H	7.314147	0.472893	-0.243508
H	-3.714802	-1.800656	-2.811726
H	-4.548363	-1.340488	-1.324000
H	-3.907914	-0.075195	-2.401627

Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1178.73475146 Predicted Change= -5.162964D-08
 Zero-point correction (ZPE)= -1178.2970 0.43774
 Internal Energy (U)= -1178.2735 0.46117

Enthalpy (H)= -1178.2726 0.46212
 Gibbs Free Energy (G)= -1178.3508 0.38387

Frequencies -- -343.5980 29.4364 32.0136

Supporting Information: s-Trans-Si-3D-(Methyl-Syn)-EW.output

Using Gaussian 03: Al64T-G03RevC.01 3-Apr-2004

hf/6-31g(d) geom=connectivity scf=(direct,maxcycle=300,tight)
 opt=(maxcycle=250,ts,calcfc,noeigentest) freq=noraman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq

Pointgroup= C1 Stoichiometry= C18H24N2O5 C1[X(C18H24N2O5)] #Atoms= 49
 Charge = 0 Multiplicity = 1

SCF Energy= -1178.72418360 Predicted Change= -7.036011D-08

Optimization completed.		{Found		1		times}	
Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?	
Force	0.00004	0.00045	[YES]	0.00000	0.00030	[YES]	
Displ	0.00362	0.00180	[NO]	0.00362	0.00180	[YES]	

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z

N	-1.219070	1.661855	0.989019
C	0.077003	2.005934	1.571014
C	0.500824	3.282128	0.825556
C	-0.791598	3.816411	0.195984
C	-1.581071	2.554678	-0.124218
C	-1.956189	0.619138	1.335023
C	-1.544505	-0.488220	2.035739
C	-1.070717	-1.667309	0.050740
C	-2.507994	-1.383110	2.779850
N	-0.128551	-1.089082	-0.627244
C	4.007428	-0.955209	0.066484
C	3.231963	-1.911821	0.717645
C	1.873146	-1.974821	0.506106
C	1.258872	-1.072001	-0.356544
C	2.025467	-0.120535	-1.006220
C	3.395955	-0.061166	-0.798348
O	5.324698	-0.981683	0.340110
C	6.184298	-0.073221	-0.291641
C	-2.371981	-1.886811	-0.710212
O	-3.465550	-1.485916	-0.124467
O	-2.316821	-2.482099	-1.731284
C	-4.663930	-1.610498	-0.886945
C	-1.177463	1.825661	-1.433059
O	-1.806433	0.761422	-1.622096
O	-0.248773	2.279735	-2.081324
H	0.800938	1.211167	1.442543
H	-0.049995	2.171122	2.636545

Supporting Information

H	0.971811	3.994116	1.493156
H	1.202534	3.036404	0.041260
H	-1.341951	4.421759	0.911443
H	-0.603068	4.403820	-0.690062
H	-2.653902	2.708937	-0.121680
H	-2.963418	0.647911	0.967150
H	-0.532255	-0.491583	2.406913
H	-0.823424	-2.418065	0.771946
H	-3.525530	-1.249443	2.437998
H	-2.261454	-2.438317	2.665808
H	-2.485331	-1.175820	3.846973
H	-0.476671	-0.454842	-1.343719
H	3.717647	-2.604730	1.378544
H	1.308631	-2.739729	1.006676
H	1.553732	0.587124	-1.665860
H	3.960727	0.687737	-1.317508
H	6.164141	-0.194614	-1.369144
H	5.931732	0.950927	-0.039123
H	7.175663	-0.294805	0.072991
H	-4.573986	-1.029602	-1.791495
H	-4.850342	-2.646496	-1.125352
H	-5.446894	-1.219418	-0.257643

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

=====

SCF Energy=	-1178.72418360	Predicted Change=	-7.036011D-08
Zero-point correction (ZPE)=	-1178.2863		0.43782
Internal Energy (U)=		-1178.2628	0.46132
Enthalpy (H)=		-1178.2619	0.46227
Gibbs Free Energy (G)=		-1178.3409	0.38321

Frequencies --	-321.1312	27.3948	33.6774
----------------	-----------	---------	---------

Supporting Information: s-Trans-Si-3U-(Methyl-Anti)-(Esther-Anti).output

Using Gaussian 03: Al64T-G03RevC.01 3-Apr-2004

=====

```
# opt=(calcf,ts,maxcycle=150,noeigentest) freq=noraman hf/6-31g(d)
geom=connectivity scf=(direct,tight,maxcycle=300)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
```

```
Pointgroup= C1    Stoichiometry= C18H24N2O5    C1[X(C18H24N2O5)]    #Atoms= 49
Charge = 0        Multiplicity = 1
```

SCF Energy= -1178.72476431 Predicted Change= -5.196492D-08

Optimization completed.		{Found	1	times}		
Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00003	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00491	0.00180	[NO]	0.00491	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
N	-1.053632	1.566540	0.993135
C	0.191019	1.792266	1.726930
C	0.337277	3.311427	1.685811
C	-0.217988	3.667279	0.306670
C	-1.389930	2.693960	0.095542
C	-1.915106	0.609366	1.264036
C	-1.675439	-0.576538	1.928591
C	-0.971879	-1.618512	-0.041991
C	-2.815712	-1.387444	2.504750
N	-0.158353	-0.849454	-0.689622
C	4.029362	-0.669717	-0.371895
C	3.327557	-1.521582	0.462536
C	1.940572	-1.590196	0.379854
C	1.249331	-0.816844	-0.531812
C	1.959672	0.048274	-1.368403
C	3.329001	0.117201	-1.286426
O	5.367465	-0.526699	-0.374437
C	6.151474	-1.289314	0.498865
C	-2.366129	-1.819493	-0.569102
O	-2.748301	-3.055814	-0.321547
O	-3.005983	-1.007174	-1.140363
C	-4.036835	-3.435034	-0.794253
C	-1.523412	2.357167	-1.414847
O	-0.853704	1.388557	-1.840996
H	-2.207084	3.145502	-2.028291
O	1.024017	1.305504	1.234750
H	0.107099	1.397152	2.731028
H	-0.266780	3.759676	2.469096
H	1.363684	3.628689	1.828885
H	-0.539169	4.695893	0.219001
H	0.538063	3.488567	-0.450243
H	-2.321461	3.134512	0.427998
H	-2.884937	0.752723	0.818938
H	-0.722606	-0.693479	2.418752
H	-0.587877	-2.427316	0.542567
H	-3.739195	-1.216000	1.959804
H	-2.609540	-2.453264	2.476858
H	-3.004318	-1.128018	3.543887
H	-0.552745	-0.045208	-1.235148
H	3.830946	-2.137976	1.181173
H	1.431955	-2.260262	1.047605
H	1.418676	0.665111	-2.060887
H	3.883238	0.777794	-1.926175
H	5.913118	-1.074141	1.535299
H	6.030197	-2.351474	0.314096
H	7.175930	-1.010148	0.305641
H	-4.084872	-3.326423	-1.867065
H	-4.157979	-4.467525	-0.510265
H	-4.797703	-2.822571	-0.334231

Statistical Thermodynamic Analysis

Supporting Information

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

```

=====
SCF Energy=      -1178.72476431      Predicted Change= -5.196492D-08
Zero-point correction (ZPE)=      -1178.2880      0.43669
Internal Energy (U)=      -1178.2644      0.46030
Enthalpy (H)=      -1178.2635      0.46124
Gibbs Free Energy (G)=      -1178.3434      0.38133
=====
Frequencies --  -341.8275                      21.7791                      32.6269
    
```

Supporting Information: s-Trans-Si-3U-(Methyl-Anti)-(Esther-Syn).output

Using Gaussian 03: AL64T-G03RevC.01 3-Apr-2004

```

=====
# hf/6-31g(d) geom=connectivity scf=(direct,maxcycle=300,tight)
opt=(maxcycle=250,ts,calcf, noeigentest) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq

Pointgroup= C1    Stoichiometry= C18H24N2O5    C1[X(C18H24N2O5)]    #Atoms= 49
Charge = 0                      Multiplicity = 1

SCF Energy= -1178.7333904    Predicted Change= -1.065985D-07
    
```

```

=====
Optimization completed.                      {Found                      1                      times}
Item    Max Val.    Criteria    Pass?    RMS Val.    Criteria    Pass?
Force    0.00003 || 0.00045    [ YES ]    0.00000 || 0.00030    [ YES ]
Displ    0.00771 || 0.00180    [ NO ]    0.00771 || 0.00180    [ NO ]
    
```

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
N	-1.240376	1.354868	1.113335
C	0.025418	1.812392	1.681849
C	-0.048812	3.325820	1.493408
C	-0.801699	3.470346	0.168338
C	-1.842079	2.345479	0.188597
C	-1.876205	0.257247	1.466897
C	-1.348782	-0.857038	2.086961
C	-0.687569	-1.809885	0.076958
C	-2.238995	-1.861855	2.783575
N	0.009694	-0.969645	-0.628107
C	4.141980	-0.221357	-0.468988
C	3.607605	-1.224368	0.320595
C	2.241703	-1.484153	0.287356
C	1.404662	-0.747835	-0.527562
C	1.945014	0.267127	-1.320880
C	3.294428	0.522743	-1.289558
O	5.445400	0.110129	-0.512623
C	6.371371	-0.600187	0.260584
C	-2.062555	-2.211909	-0.382601
O	-2.614051	-1.290752	-1.109712
O	-2.515385	-3.272826	-0.098546
C	-3.901533	-1.505741	-1.687244

```

C    -2.102563      1.707451      -1.204796
O    -1.086166      1.244595      -1.766532
O    -3.260560      1.706004      -1.579017
H    0.867976      1.392899      1.146606
H    0.094021      1.511964      2.720045
H    -0.615340      3.770310      2.306127
H    0.932953      3.784381      1.478466
H    -1.267101      4.440806      0.049192
H    -0.128193      3.310346      -0.663513
H    -2.784693      2.680436      0.603959
H    -2.901845      0.222877      1.139141
H    -0.338763      -0.786198      2.457776
H    -0.194537      -2.558200      0.659493
H    -3.240243      -1.866344      2.367067
H    -1.852891      -2.872416      2.697082
H    -2.326746      -1.639963      3.844489
H    -0.498358      -0.274388      -1.196674
H    4.227674      -1.817378      0.963658
H    1.866791      -2.275616      0.908888
H    1.289988      0.850074      -1.940810
H    3.719044      1.299776      -1.896845
H    6.160006      -0.502213      1.320271
H    6.387500      -1.651026      -0.008375
H    7.336215      -0.164931      0.049983
H    -4.614304      -1.746475      -0.912182
H    -4.139847      -0.570986      -2.161868
H    -3.846783      -2.317153      -2.398064
    
```

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

```

=====
SCF Energy=      -1178.7333904      Predicted Change= -1.065985D-07
Zero-point correction (ZPE)=      -1178.2956      0.43767
Internal Energy (U)=      -1178.2722      0.46113
Enthalpy (H)=      -1178.2712      0.46208
Gibbs Free Energy (G)=      -1178.3499      0.38336
=====
Frequencies --  -334.0180                      22.0279                      31.1287

Supporting Information: s-Trans-Si-3U-(Methyl-Anti)-EW.output

-----

Using Gaussian 03: AL64T-G03RevC.01 3-Apr-2004

=====
#hf/6-31G* opt=(gdiis,ts, noeigentest, calcf, maxcycle=300)
scf=(maxcycle=300) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq

Pointgroup= C1    Stoichiometry= C18H24N2O5    C1[X(C18H24N2O5)]    #Atoms= 49
Charge = 0                      Multiplicity = 1

SCF Energy= -1178.72709534    Predicted Change= -8.164340D-11

Optimization completed.                      {Found                      2                      times}
    
```

Supporting Information

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00024	0.00180	[YES]	0.00024	0.00180	[YES]

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
N	-1.273567	1.511027	0.982120
C	-0.032406	2.220329	1.274101
C	-0.300009	3.623350	0.728732
C	-1.216815	3.358096	-0.466186
C	-2.122864	2.215087	0.010208
C	-1.706101	0.443141	1.646196
C	-0.953874	-0.428034	2.383847
C	-0.616911	-1.709468	0.371751
C	-1.555920	-1.392088	3.377517
N	0.063898	-0.981025	-0.447805
C	4.177009	-0.154030	-0.553139
C	3.669913	-0.921570	0.481298
C	2.309339	-1.202262	0.540418
C	1.451450	-0.725813	-0.430430
C	1.965103	0.049753	-1.469978
C	3.307706	0.332117	-1.530008
O	5.471585	0.176343	-0.702053
C	6.419333	-0.277406	0.224396
C	-2.030853	-2.114219	-0.040101
O	-2.001092	-2.554135	-1.266988
O	-2.963756	-2.127271	0.687307
C	-3.256237	-2.710450	-1.931886
C	-2.623163	1.363648	-1.181179
O	-2.006755	0.296427	-1.423074
O	-3.556625	1.846205	-1.783237
H	0.815826	1.763997	0.775062
H	0.162587	2.207707	2.340282
H	-0.818288	4.216526	1.476056
H	0.613638	4.142743	0.463329
H	-1.792143	4.218727	-0.777302
H	-0.628791	3.027004	-1.317363
H	-2.995423	2.615991	0.514837
H	-2.752062	0.230520	1.518250
H	0.089735	-0.194013	2.523991
H	-0.120253	-2.366996	1.055543
H	-2.605959	-1.558989	3.181804
H	-1.061372	-2.361804	3.353152
H	-1.453498	-1.018261	4.393903
H	-0.533274	-0.402402	-1.056416
H	4.308139	-1.308097	1.251202
H	1.948732	-1.793624	1.361016
H	1.301067	0.422333	-2.229237
H	3.710725	0.926078	-2.328309
H	6.210719	0.100026	1.219781
H	6.459358	-1.361099	0.249387
H	7.371667	0.105794	-0.108117

H	-3.711349	-1.738181	-2.032914
H	-3.015956	-3.120719	-2.898836
H	-3.891208	-3.384902	-1.378294

Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1178.72709534 Predicted Change= -8.164340D-11
 Zero-point correction (ZPE)= -1178.2901 0.43691
 Internal Energy (U)= -1178.2665 0.46053
 Enthalpy (H)= -1178.2656 0.46147
 Gibbs Free Energy (G)= -1178.3452 0.38182

Frequencies -- -276.6720 18.4877 32.1715

Supporting Information: s-Cis-Re-3D-(Methyl-Syn)-(Esther-Syn).output

Using Gaussian 03: AL64T-G03RevC.01 3-Apr-2004

#hf/6-31g* scf=(direct,tight,maxcycle=300)
 opt=(calcfc,maxcycle=150,ts,noeigentest) freq=norman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq

Pointgroup= C1 Stoichiometry= C18H24N2O5 C1[X[C18H24N2O5]] #Atoms= 49
 Charge = 0 Multiplicity = 1

SCF Energy= -1178.72895441 Predicted Change= -2.836096D-09

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00120	0.00180	[YES]	0.00120	0.00180	[YES]

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
N	2.714871	0.883153	0.825957
C	4.033226	1.002841	0.199134
C	4.010507	2.388185	-0.454022
C	2.964928	3.153133	0.362591
C	1.901163	2.084866	0.637226
C	2.322905	-0.221808	1.423506
C	1.069496	-0.575945	1.885179
C	0.176022	-1.778746	0.077240
C	0.957407	-1.610367	2.988490
N	-0.514991	-0.989911	-0.683005
C	-4.544687	-0.006426	-0.015932
C	-3.641304	0.966380	-0.412756
C	-2.308934	0.640853	-0.629637
C	-1.879650	-0.660448	-0.445845
C	-2.791353	-1.645221	-0.073450
C	-4.108782	-1.320248	0.149838
O	-5.850882	0.210760	0.222075

Supporting Information

C	-6.380158	1.499206	0.069046
C	0.901244	1.979928	-0.538136
O	0.026304	2.833120	-0.534737
O	1.093885	1.056031	-1.349762
C	1.458368	-2.405897	-0.396099
O	1.895597	-1.893608	-1.511458
O	1.950470	-3.314760	0.192017
C	3.072393	-2.450053	-2.080015
H	4.185257	0.213553	-0.525705
H	4.807679	0.927866	0.957659
H	4.988052	2.855653	-0.444828
H	3.681402	2.300437	-1.481294
H	3.394721	3.501851	1.297460
H	2.545952	4.002623	-0.158204
H	1.343599	2.292610	1.540619
H	3.108473	-0.952756	1.544788
H	-0.041514	-2.034262	3.035517
H	1.653789	-2.428989	2.838208
H	1.155396	-1.181165	3.968125
H	0.018784	-0.349638	-1.278659
H	-3.944165	1.985144	-0.552411
H	-1.616573	1.412183	-0.916507
H	-2.481534	-2.671030	0.018560
H	-4.822988	-2.069623	0.434677
H	-5.907377	2.203238	0.744894
H	-6.273003	1.851453	-0.950992
H	-7.429367	1.423062	0.310994
H	-0.329125	-2.349850	0.826742
H	0.293086	0.169935	1.849799
H	3.270082	-1.862722	-2.960751
H	3.894625	-2.380733	-1.383454
H	2.905863	-3.485284	-2.339135

Charge = 0 Multiplicity = 1

 SCF Energy= -1178.73093062 Predicted Change= -1.241419D-07

Optimization completed. {Found 1 times}
 Item Max Val. Criteria Pass? RMS Val. Criteria Pass?
 Force 0.00002 || 0.00045 [YES] 0.00000 || 0.00030 [YES]
 Displ 0.00674 || 0.00180 [NO] 0.00674 || 0.00180 [YES]

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
N	-2.862789	-1.000658	0.819330
C	-4.295994	-0.742111	0.742320
C	-4.816827	-1.972870	0.010347
C	-3.695560	-2.261022	-0.992460
C	-2.398956	-1.899483	-0.244519
C	-2.079701	-0.417537	1.709531
C	-0.706589	-0.435770	1.791984
C	-0.114845	1.434711	0.476094
C	-0.041121	-0.083359	3.107035
N	0.657270	0.988461	-0.464449
C	4.674845	-0.132327	-0.002119
C	3.785546	-0.965788	-0.662432
C	2.455524	-0.593552	-0.806474
C	2.017946	0.612947	-0.295338
C	2.913395	1.461720	0.347785
C	4.228218	1.087907	0.503073
O	5.978191	-0.403666	0.194136
C	6.520538	-1.600768	-0.290870
C	-1.369513	-1.230237	-1.175272
O	-1.628042	-0.058241	-1.510246
O	-0.389980	-1.900115	-1.476076
C	-1.422811	2.110606	0.090570
O	-1.295923	2.709362	-1.063188
O	-2.356897	2.199124	0.814782
C	-2.480924	3.225771	-1.654617
H	-4.484139	0.162921	0.174682
H	-4.713502	-0.617984	1.734426
H	-4.928341	-2.797368	0.708136
H	-5.775932	-1.799798	-0.463766
H	-3.684198	-3.286546	-1.338836
H	-3.800770	-1.614021	-1.855222
H	-1.943438	-2.772753	0.206547
H	-2.613331	0.164700	2.439191
H	0.975970	0.269912	2.960266
H	-0.587882	0.695957	3.632643
H	0.026328	-0.939125	3.775213
H	0.159835	0.663710	-1.286288
H	4.100866	-1.908458	-1.064174
H	1.752640	-1.242650	-1.296957
H	2.589590	2.422388	0.707101
H	4.933062	1.731674	0.994528

 Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

 SCF Energy= -1178.72895441 Predicted Change= -2.836096D-09
 Zero-point correction (ZPE)= -1178.2915 0.43737
 Internal Energy (U)= -1178.2679 0.46102
 Enthalpy (H)= -1178.2669 0.46196
 Gibbs Free Energy (G)= -1178.3466 0.38234

Frequencies -- -343.3812 26.7189 28.3309

Supporting Information: s-Cis-Re-3U-(Methyl-Syn)-(Esther-Syn).output

Using Gaussian 03: AL64T-G03RevC.01 3-Apr-2004

 # opt=(calcf,c,ts,maxcycle=150,noeigentest) freq=norman hf/6-31g(d)
 geom=connectivity scf=(direct,tight,maxcycle=300)
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq

Pointgroup= C1 Stoichiometry= C18H24N2O5 C1[X(C18H24N2O5)] #Atoms= 49

Supporting Information

```

H      6.042768   -2.462982   0.161438
H      6.433658   -1.665256  -1.370004
H      7.564881   -1.589285  -0.018229
H      0.328095   1.770882   1.390413
H     -0.169016  -1.114958   1.154224
H     -2.168268   3.671439  -2.584655
H     -3.165843   2.412462  -1.837167
H     -2.932211   3.965759  -1.010794
  
```

```

C      1.997534   0.183733  -1.447687
C      1.343665  -0.755571  -0.645055
C      2.075332  -1.483520   0.272967
C      3.448356  -1.296707   0.395317
O      5.414296  -0.114779  -0.370564
C      6.239909  -0.823430   0.510349
C     -1.883412   1.953570  -1.189348
O     -2.838660   2.441810  -1.750126
O     -0.850875   1.436193  -1.672974
C     -2.213924  -1.937349  -0.690568
O     -2.716638  -3.037115  -0.166047
O     -2.755541  -1.239732  -1.473939
C     -4.039853  -3.382943  -0.561899
H      1.127362   2.095895   0.633255
H      0.585748   2.479375   2.262122
H      0.035468   4.587499   1.325619
H      0.012137   3.929468  -0.299464
H     -2.185054   3.683192   1.787134
H     -2.367275   4.183591   0.107312
H     -2.884916   1.635864   0.703630
H      0.061529   0.185170   2.358329
H     -2.027980  -2.725411   2.440610
H     -0.695828  -1.888662   3.215622
H     -2.347837  -1.524719   3.665961
H     -0.495132  -0.125890  -1.362749
H      3.864584   1.086741  -1.939907
H      1.423550   0.769260  -2.140243
H      1.610029  -2.210977   0.911566
H      3.985065  -1.881184   1.116460
H      5.958326  -0.648791   1.543496
H      6.215458  -1.888321   0.304746
H      7.240641  -0.453357   0.348374
H     -0.399826  -2.495214   0.413435
H     -2.712394  -0.493349   1.322589
H     -4.270606  -4.295805  -0.037502
H     -4.728697  -2.599397  -0.283647
H     -4.080267  -3.536348  -1.629633
  
```

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

```

=====
SCF Energy=      -1178.73093062      Predicted Change= -1.241419D-07
Zero-point correction (ZPE)=      -1178.2929      0.43801
Internal Energy (U)=                -1178.2695      0.46140
Enthalpy (H)=                       -1178.2685      0.46234
Gibbs Free Energy (G)=              -1178.3467      0.38416
  
```

```

-----
Frequencies --  -358.0984           32.3287           36.4093
  
```

Supporting Information: s-Cis-Si-3D-(Methyl-Anti)-(Esther-Anti).output

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

```

=====
# opt=(calcf,ts,maxcycle=150,noeigentest) freq=norman hf/6-31g(d)
geom=connectivity scf=(direct,tight,maxcycle=300)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
  
```

```

-----
Pointgroup= C1    Stoichiometry= C18H24N2O5    C1[X(C18H24N2O5)]    #Atoms= 49
Charge = 0        Multiplicity = 1
  
```

```

-----
SCF Energy= -1178.72183168    Predicted Change= -2.098532D-09
  
```

```

=====
Optimization completed.            {Found            2            times}
Item    Max Val.    Criteria    Pass?    RMS Val.    Criteria    Pass?
Force   0.00000 || 0.00045    [ YES ]    0.00000 || 0.00030    [ YES ]
Displ   0.00132 || 0.00180    [ YES ]    0.00132 || 0.00180    [ YES ]
  
```

```

-----
Atomic                    Coordinates (Angstroms)
Type                    X                    Y                    Z
-----
N       -0.827746       1.464654       1.096756
C       0.280846       2.420756       1.222439
C       -0.299737       3.752485       0.721824
C       -1.816300       3.538802       0.774861
C       -1.954117       2.068442       0.366995
C       -0.829885       0.334977       1.769494
C       -1.746943       -0.694201       1.753878
C       -0.815872       -1.716303       -0.188721
C       -1.702172       -1.763470       2.823571
N       -0.048086       -0.912157       -0.843256
C       4.094683       -0.372352       -0.406395
C       3.352905       0.368559       -1.327426
  
```

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

```

=====
SCF Energy=      -1178.72183168      Predicted Change= -2.098532D-09
Zero-point correction (ZPE)=      -1178.2851      0.43667
Internal Energy (U)=                -1178.2615      0.46032
Enthalpy (H)=                       -1178.2605      0.46126
Gibbs Free Energy (G)=              -1178.3402      0.38155
  
```

```

-----
Frequencies --  -321.3832           26.6393           29.8186
  
```

Supporting Information: s-Cis-Si-3D-(Methyl-Anti)-(Esther-Syn).output

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

Supporting Information

```
# opt=(calcf,ts,maxcycle=150,noeigentest) freq=noraman hf/6-31g(d)
geom=connectivity scf=(direct,tight,maxcycle=300)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
```

```
Pointgroup= C1 Stoichiometry= C18H24N2O5 C1[X(C18H24N2O5)] #Atoms= 49
Charge = 0 Multiplicity = 1
```

```
SCF Energy= -1178.73150774 Predicted Change= -7.686978D-08
```

```
Optimization completed. {Found 1 times}
Item Max Val. Criteria Pass? RMS Val. Criteria Pass?
Force 0.00001 || 0.00045 [ YES ] 0.00000 || 0.00030 [ YES ]
Displ 0.01922 || 0.00180 [ NO ] 0.01922 || 0.00180 [ NO ]
```

```
Atomic Coordinates (Angstroms)
Type X Y Z
```

N	-0.937990	1.412953	1.173257
C	0.069980	2.479889	1.192878
C	-0.589875	3.636126	0.435523
C	-2.087360	3.353071	0.582215
C	-2.159688	1.824810	0.466739
C	-0.780352	0.307344	1.871587
C	-1.589481	-0.805865	1.925397
C	-0.610584	-1.878224	0.056773
C	-1.412644	-1.833170	3.021815
N	0.055247	-1.072407	-0.708472
C	4.128594	-0.064399	-0.483715
C	3.239360	0.661768	-1.275839
C	1.908746	0.323066	-1.328819
C	1.430610	-0.759305	-0.586279
C	2.311083	-1.483170	0.194132
C	3.656577	-1.137845	0.252046
O	5.407591	0.351194	-0.501196
C	6.374892	-0.336090	0.242272
C	-2.228622	1.411884	-1.031214
O	-3.352761	1.435635	-1.497048
O	-1.142121	1.156174	-1.591582
C	-1.985736	-2.343076	-0.339082
O	-2.547356	-1.525696	-1.172970
O	-2.428691	-3.361539	0.083955
C	-3.876125	-1.775278	-1.630859
H	0.987085	2.147312	0.725403
H	0.287687	2.751121	2.221894
H	-0.295615	4.598665	0.836969
H	-0.309779	3.598693	-0.608380
H	-2.438706	3.668832	1.560844
H	-2.694829	3.836357	-0.170142
H	-3.025495	1.424734	0.974120
H	0.148529	0.270477	2.419382
H	-1.691106	-2.824764	2.680055
H	-0.381474	-1.874062	3.364625
H	-2.032336	-1.612551	3.887877

H	-0.488594	-0.398140	-1.267713
H	3.616793	1.491268	-1.843605
H	1.220815	0.892857	-1.924354
H	1.982724	-2.335759	0.761276
H	4.311699	-1.723513	0.866399
H	6.153396	-0.305242	1.303915
H	6.459991	-1.368697	-0.078924
H	7.310133	0.170708	0.060393
H	-0.097087	-2.545194	0.714753
H	-2.581741	-0.715798	1.518162
H	-4.153175	-0.878540	-2.154786
H	-3.877315	-2.640372	-2.277849
H	-4.526480	-1.947571	-0.786512

```
Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
```

```
SCF Energy= -1178.73150774 Predicted Change= -7.686978D-08
Zero-point correction (ZPE)= -1178.2940 0.43745
Internal Energy (U)= -1178.2705 0.46099
Enthalpy (H)= -1178.2695 0.46194
Gibbs Free Energy (G)= -1178.3491 0.38240
```

```
Frequencies -- -322.0500 10.6624 32.0141
```

```
Supporting Information: s-Cis-Si-3D-(Methyl-Syn)-(Esther-Anti).output
```

```
Using Gaussian 03: A164T-G03RevC.01 3-Apr-2004
```

```
# hf/6-31g(d) geom=connectivity scf=(direct,maxcycle=300,tight)
opt=(maxcycle=250,ts,calcf,noeigentest) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
```

```
Pointgroup= C1 Stoichiometry= C18H24N2O5 C1[X(C18H24N2O5)] #Atoms= 49
Charge = 0 Multiplicity = 1
```

```
SCF Energy= -1178.72252053 Predicted Change= -1.336334D-08
```

```
Optimization completed. {Found 1 times}
Item Max Val. Criteria Pass? RMS Val. Criteria Pass?
Force 0.00001 || 0.00045 [ YES ] 0.00000 || 0.00030 [ YES ]
Displ 0.00287 || 0.00180 [ NO ] 0.00287 || 0.00180 [ YES ]
```

```
Atomic Coordinates (Angstroms)
Type X Y Z
```

N	-0.760318	1.505950	1.089275
C	0.431348	2.342236	1.283959
C	0.030892	3.719469	0.731431
C	-1.499408	3.663405	0.666819
C	-1.756956	2.207647	0.265140
C	-0.929615	0.394466	1.769865
C	-1.946411	-0.534353	1.696102

Supporting Information

C	-0.989220	-1.691767	-0.146907
C	-2.094401	-1.578725	2.781246
N	-0.091419	-0.993992	-0.758063
C	4.044604	-0.892593	-0.026824
C	3.461317	-0.078173	-0.986247
C	2.092453	-0.124545	-1.199920
C	1.291958	-0.983061	-0.462897
C	1.878796	-1.796171	0.503735
C	3.238758	-1.749490	0.717569
O	5.358750	-0.924724	0.258263
C	6.246550	-0.109044	-0.456181
C	-1.573819	2.055129	-1.278918
O	-2.423080	2.630451	-1.922010
O	-0.567092	1.421872	-1.669263
C	-2.360479	-1.774781	-0.753407
O	-3.019399	-2.799978	-0.251706
O	-2.760718	-1.043174	-1.589273
C	-4.338323	-3.011041	-0.744615
H	1.276609	1.920184	0.757812
H	0.669118	2.384877	2.341657
H	0.402567	4.524402	1.354477
H	0.437048	3.849549	-0.263472
H	-1.928433	3.863922	1.645154
H	-1.926916	4.348694	-0.049113
H	-2.751324	1.879382	0.530172
H	-0.104136	0.162779	2.424735
H	-2.495639	-2.507787	2.388996
H	-1.137967	-1.803437	3.246788
H	-2.767853	-1.253267	3.571197
H	-0.411589	-0.180054	-1.322118
H	4.050010	0.597205	-1.575212
H	1.636749	0.521299	-1.926009
H	1.294391	-2.474158	1.097230
H	3.699370	-2.374604	1.459174
H	6.230460	-0.341194	-1.515401
H	6.019603	0.941885	-0.313406
H	7.229107	-0.317119	-0.061180
H	-0.706590	-2.495224	0.498603
H	-2.851288	-0.240909	1.192499
H	-4.707050	-3.880019	-0.224559
H	-4.956491	-2.150949	-0.534860
H	-4.313554	-3.186401	-1.809445

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1178.72252053 Predicted Change= -1.336334D-08
 Zero-point correction (ZPE)= -1178.2857 0.43678
 Internal Energy (U)= -1178.2620 0.46044
 Enthalpy (H)= -1178.2611 0.46139
 Gibbs Free Energy (G)= -1178.3409 0.38161

Frequencies -- -323.4870 27.5171 28.9670

Supporting Information: s-Cis-Si-3D-(Methyl-Syn)-(Esther-Anti)2.output

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

opt=(calcfc,ts,maxcycle=150,noeigentest) freq=noraman hf/6-31g(d)
 geom=check guess=read scf=(direct,tight,maxcycle=300)
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq

Pointgroup= C1 Stoichiometry= C18H24N2O5 C1[X(C18H24N2O5)] #Atoms= 49
 Charge = 0 Multiplicity = 1

SCF Energy= -1178.71969856 Predicted Change= -5.136462D-09

Optimization completed. {Found 2 times}
 Item Max Val. Criteria Pass? RMS Val. Criteria Pass?
 Force 0.00004 || 0.00045 [YES] 0.00000 || 0.00030 [YES]
 Displ 0.00103 || 0.00180 [YES] 0.00103 || 0.00180 [YES]

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
N	-0.415185	1.761291	0.873615
C	0.848190	2.366391	1.311578
C	0.723406	3.853669	0.921575
C	-0.582184	3.952254	0.105978
C	-0.906629	2.512997	-0.297585
C	-1.066485	0.889708	1.613629
C	-2.281344	0.268212	1.404787
C	-1.511528	-1.473371	-0.007249
C	-2.961769	-0.400221	2.583307
N	-0.485318	-1.112265	-0.702653
C	3.582505	-1.592960	0.238575
C	3.180964	-0.815300	-0.836602
C	1.833364	-0.666358	-1.125774
C	0.874722	-1.288821	-0.342182
C	1.278735	-2.073348	0.735408
C	2.617448	-2.220888	1.021854
O	4.861124	-1.799561	0.602674
C	5.896966	-1.209536	-0.134643
C	-0.113989	2.032341	-1.551020
O	0.957716	2.579954	-1.751184
O	-0.631146	1.088764	-2.177801
C	-2.853078	-1.490763	-0.686929
O	-3.685490	-2.269390	-0.024164
O	-3.098865	-0.928255	-1.695308
C	-4.994126	-2.410189	-0.565081
H	1.671482	1.896484	0.793129
H	0.972007	2.213100	2.376075
H	0.686207	4.483993	1.803192
H	1.570501	4.150007	0.323330
H	-1.385765	4.342053	0.724300
H	-0.474505	4.590801	-0.758851

Supporting Information

H	-1.960280	2.327396	-0.436954	C	-0.274398	3.609730	0.524854
H	-0.523072	0.600348	2.498767	C	-1.797973	3.462553	0.567976
H	-3.564582	-1.247420	2.277941	C	-1.999304	1.949430	0.415339
H	-2.232447	-0.762256	3.303623	C	-0.864575	0.295764	1.884598
H	-3.621486	0.284857	3.111931	C	-1.776216	-0.737377	1.869110
H	-0.653017	-0.432061	-1.464387	C	-0.790109	-1.883133	0.059164
H	3.893238	-0.310358	-1.458370	C	-1.768603	-1.784405	2.961360
H	1.530382	-0.043951	-1.946438	N	0.002817	-1.145974	-0.653687
H	0.567077	-2.585621	1.355767	C	4.134854	-0.562468	-0.156706
H	2.938578	-2.825961	1.848752	C	3.385408	0.265385	-0.978288
H	5.893501	-1.551971	-1.163599	C	2.020694	0.058550	-1.116785
H	5.829335	-0.127434	-0.114607	C	1.391947	-0.974328	-0.441337
H	6.816066	-1.517828	0.339925	C	2.147806	-1.809943	0.377782
H	-1.398280	-2.127543	0.829604	C	3.501118	-1.601294	0.520653
H	-2.924886	0.682492	0.647822	O	5.459089	-0.447803	0.049047
H	-5.513973	-3.078573	0.101683	C	6.184178	0.547840	-0.619145
H	-5.487597	-1.450431	-0.601853	C	-1.994259	1.566169	-1.092289
H	-4.942665	-2.828298	-1.559011	O	-3.071942	1.708568	-1.639724

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1178.71969856 Predicted Change= -5.136462D-09
 Zero-point correction (ZPE)= -1178.2823 0.43730
 Internal Energy (U)= -1178.2587 0.46099
 Enthalpy (H)= -1178.2577 0.46193
 Gibbs Free Energy (G)= -1178.3378 0.38186

Frequencies -- -339.4115 22.9344 27.9273

Supporting Information: s-Cis-Si-3D-(Methyl-Syn)-(Esther-Syn).output

Using Gaussian 03: AL64T-G03RevC.01 3-Apr-2004

#hf/6-31G* scf=(direct,tight,maxcycle=300)
 opt=(gdiis,calcf,maxcycle=150,ts,noeigentest) freq=norman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq

Pointgroup= C1 Stoichiometry= C18H24N2O5 C1[X(C18H24N2O5)] #Atoms= 49
 Charge = 0 Multiplicity = 1

SCF Energy= -1178.73199827 Predicted Change= -2.461299D-09

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00336	0.00180	[NO]	0.00336	0.00180	[YES]

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
N	-0.873577	1.418583	1.197189
C	0.228745	2.382598	1.292159

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1178.73199827 Predicted Change= -2.461299D-09
 Zero-point correction (ZPE)= -1178.2944 0.43753

Supporting Information

```
Internal Energy (U)=      -1178.2709      0.46107
Enthalpy (H)=            -1178.2699      0.46201
Gibbs Free Energy (G)=   -1178.3492      0.38279
```

```
-----
Frequencies --  -327.8982          15.3882          31.0796
```

Supporting Information: s-Cis-Si-3D-(Methyl-Syn)-(Esther-Syn)2.output

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

```
=====
# hf/6-31g(d) scf=(direct,maxcycle=300,tight)
opt=(gdiis,maxcycle=250,calcfc,ts,noeigentest) freq=noraman
geom=connectivity
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq

Pointgroup= C1  Stoichiometry= C18H24N2O5  C1[X(C18H24N2O5)]  #Atoms= 49
Charge = 0      Multiplicity = 1

-----
SCF Energy= -1178.72425683  Predicted Change= -7.558432D-09
```

```
-----
Optimization completed.      {Found      1      times}
Item  Max Val.  Criteria  Pass?      RMS Val.  Criteria  Pass?
Force  0.00000  || 0.00045  [ YES ]    0.00000  || 0.00030  [ YES ]
Displ  0.00182  || 0.00180  [ NO ]     0.00182  || 0.00180  [ YES ]
```

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
N	-0.600339	1.741333	0.940976
C	0.646564	2.438473	1.272898
C	0.458802	3.869713	0.729934
C	-0.921399	3.866832	0.046413
C	-1.226078	2.393611	-0.224349
C	-1.124759	0.826682	1.732786
C	-2.272841	0.079004	1.589078
C	-1.337815	-1.693108	0.302900
C	-2.866052	-0.599644	2.807081
N	-0.413965	-1.283613	-0.504055
C	3.740404	-1.271731	0.136353
C	3.169587	-0.512996	-0.873201
C	1.795740	-0.525134	-1.064882
C	0.981765	-1.290538	-0.246631
C	1.556946	-2.064214	0.759032
C	2.919710	-2.049178	0.950558
O	5.057209	-1.327497	0.405124
C	5.957603	-0.590926	-0.376787
C	-0.550420	1.839284	-1.510278
O	0.479704	2.393241	-1.861833
O	-1.093833	0.831317	-2.000529
C	-2.719288	-1.995324	-0.205869
O	-2.990150	-1.397471	-1.328703
O	-3.426834	-2.752352	0.376555
C	-4.258740	-1.631232	-1.925685

```
H      1.480498      1.944618      0.792974
H      0.798670      2.409529      2.344955
H      0.504996      4.599483      1.530435
H      1.232768      4.096004      0.013904
H     -1.675826      4.271199      0.715292
H     -0.924832      4.447431     -0.865082
H     -2.281965      2.170561     -0.239204
H     -0.523605      0.629043      2.606119
H     -3.394524     -1.508671      2.545647
H     -2.093351     -0.861299      3.525908
H     -3.576264      0.045160      3.320487
H     -0.716922     -0.683912     -1.285285
H      3.767075      0.099408     -1.518922
H      1.366447      0.085025     -1.837192
H      0.960467     -2.697949      1.388689
H      3.372671     -2.644348      1.720930
H      5.919586     -0.897327     -1.416334
H      5.762070      0.473474     -0.307298
H      6.939427     -0.799216      0.020159
H     -1.081907     -2.233653      1.188209
H     -2.960086      0.371656      0.813805
H     -4.266287     -1.029910     -2.818711
H     -4.368957     -2.678383     -2.165866
H     -5.047171     -1.327313     -1.253086
```

```
-----
Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin  Pressure= 1.00000 Atm
-----
SCF Energy=      -1178.72425683      Predicted Change= -7.558432D-09
Zero-point correction (ZPE)=      -1178.2868      0.43744
Internal Energy (U)=      -1178.2630      0.46118
Enthalpy (H)=      -1178.2621      0.46213
Gibbs Free Energy (G)=      -1178.3423      0.38188

-----
Frequencies --  -318.9165          19.6659          24.3034
```

Supporting Information: s-Cis-Si-3U-(Methyl-Anti)-(Esther-Anti).output

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004

```
=====
# opt=(calcfc,ts,maxcycle=150,noeigentest) freq=noraman hf/6-31g(d)
geom=connectivity scf=(direct,tight,maxcycle=300)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq

Pointgroup= C1  Stoichiometry= C18H24N2O5  C1[X(C18H24N2O5)]  #Atoms= 49
Charge = 0      Multiplicity = 1

-----
SCF Energy= -1178.72375123  Predicted Change= -4.159150D-08
```

```
-----
Optimization completed.      {Found      1      times}
Item  Max Val.  Criteria  Pass?      RMS Val.  Criteria  Pass?
Force  0.00001  || 0.00045  [ YES ]    0.00000  || 0.00030  [ YES ]
Displ  0.00334  || 0.00180  [ NO ]     0.00334  || 0.00180  [ YES ]
```

Supporting Information

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
N	-0.563982	1.815911	0.874958
C	0.562483	2.737417	0.770694
C	-0.117457	4.069163	0.476614
C	-1.281731	3.653310	-0.427854
C	-1.735366	2.287104	0.109161
C	-0.552713	0.749973	1.656782
C	-1.527091	-0.211548	1.797449
C	-0.928231	-1.653041	0.038021
C	-1.480975	-1.143516	2.989315
N	-0.088610	-1.120728	-0.797097
C	4.042925	-0.531241	-0.372893
C	3.301950	0.160387	-1.331793
C	1.947835	-0.038529	-1.446782
C	1.295883	-0.943445	-0.606054
C	2.028233	-1.630322	0.341897
C	3.398476	-1.424918	0.464532
O	5.360883	-0.261267	-0.340791
C	6.188576	-0.936086	0.564553
C	-2.095107	1.270960	-1.004790
O	-3.169148	0.696327	-0.879213
O	-1.212903	1.100616	-1.865318
C	-2.293672	-2.000113	-0.537761
O	-3.224175	-2.129839	0.369383
O	-2.400050	-2.243592	-1.688776
C	-4.553706	-2.294512	-0.121794
H	1.212395	2.442665	-0.046285
H	1.140281	2.735648	1.687156
H	-0.483091	4.507213	1.400588
H	0.551864	4.780680	0.007308
H	-2.093916	4.369859	-0.426141
H	-0.936144	3.530579	-1.445539
H	-2.572749	2.375543	0.790390
H	0.363665	0.629485	2.212025
H	-1.908832	-2.113358	2.755346
H	-0.461607	-1.302936	3.335083
H	-2.047527	-0.751783	3.830967
H	-0.506874	-0.544293	-1.527809
H	3.812655	0.851472	-1.975612
H	1.373794	0.509319	-2.171082
H	1.564005	-2.348693	0.991731
H	3.936969	-1.978018	1.208738
H	5.905386	-0.727471	1.590975
H	6.168525	-2.007409	0.395424
H	7.187986	-0.567678	0.390921
H	-0.569455	-2.276527	0.828902
H	-2.491581	-0.011415	1.373247
H	-5.181998	-2.315467	0.753984
H	-4.798637	-1.456345	-0.753967
H	-4.635692	-3.221582	-0.669433

Statistical Thermodynamic Analysis						
Temperature= 298.150 Kelvin		Pressure= 1.00000 Atm				
SCF Energy=	-1178.72375123	Predicted Change= -4.1591500-08				
Zero-point correction (ZPE)=	-1178.2861	0.43764				
Internal Energy (U)=		-1178.2626	0.46112			
Enthalpy (H)=		-1178.2616	0.46206			
Gibbs Free Energy (G)=		-1178.3403	0.38340			

Frequencies --	-383.9040	22.1556	39.3927			
Supporting Information: s-Cis-Si-3U-(Methyl-Anti)-(Esther-Syn).output						

Using Gaussian 03: IA32L-G03RevC.02 12-Jun-2004						

# opt=(calcfrc,ts,maxcycle=150,noeigentest) freq=noraman hf/6-31g(d)						
geom=check guess=read scf=(direct,tight,maxcycle=300)						
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq						

Pointgroup=	C1	Stoichiometry=	C18H24N2O5	C1[X(C18H24N2O5)]	#Atoms= 49	
Charge =	0	Multiplicity =	1			

SCF Energy=	-1178.72974093	Predicted Change= -8.129503D-10				

Optimization completed. {Found 2 times}						
Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00062	0.00180	[YES]	0.00062	0.00180	[YES]

Atomic Type	Coordinates (Angstroms)					
	X	Y	Z			
N	-0.765186	1.676164	0.950532			
C	0.327781	2.644136	0.946109			
C	-0.392696	3.965609	0.708298			
C	-1.495002	3.564823	-0.275656			
C	-1.911414	2.141214	0.145721			
C	-0.790413	0.638361	1.763068			
C	-1.738800	-0.356546	1.854297			
C	-0.722568	-1.813612	0.293745			
C	-1.805071	-1.216131	3.099246			
N	-0.009536	-1.197124	-0.597906			
C	4.088700	-0.288669	-0.451904			
C	3.217355	0.413099	-1.284847			
C	1.876569	0.112885	-1.310610			
C	1.371725	-0.906377	-0.500634			
C	2.235423	-1.612906	0.313185			
C	3.590238	-1.302794	0.347919			
O	5.379457	0.088010	-0.498824			
C	6.330776	-0.584172	0.278136			
C	-2.214863	1.268966	-1.099639			
O	-3.395994	1.059827	-1.310197			

Supporting Information

O	-1.213900	0.912845	-1.756289
C	-2.088844	-2.337909	-0.068787
O	-2.532730	-1.794150	-1.155181
O	-2.616580	-3.176317	0.588484
C	-3.874642	-2.036542	-1.573707
H	1.014504	2.423546	0.136915
H	0.874282	2.604293	1.880372
H	-0.818602	4.325588	1.640096
H	0.266206	4.732796	0.318720
H	-2.339837	4.241106	-0.268726
H	-1.095328	3.534898	-1.281865
H	-2.786650	2.157607	0.782492
H	0.076690	0.558751	2.399277
H	-2.183172	-2.206965	2.878203
H	-0.824392	-1.324069	3.557517
H	-2.463852	-0.783403	3.848611
H	-0.527957	-0.634124	-1.283254
H	3.616897	1.193574	-1.904775
H	1.199715	0.664057	-1.936213
H	1.887978	-2.429717	0.918416
H	4.232464	-1.872826	0.989999
H	6.116637	-0.487156	1.337330
H	6.384083	-1.635325	0.015592
H	7.279289	-0.116064	0.063968
H	-0.247150	-2.333684	1.097261
H	-2.662783	-0.206152	1.320633
H	-4.079586	-1.266196	-2.293601
H	-3.942703	-3.026061	-2.002576
H	-4.541230	-1.950080	-0.730346

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1178.72974093 Predicted Change= -8.129503D-10
 Zero-point correction (ZPE)= -1178.2922 0.43753
 Internal Energy (U)= -1178.2686 0.46113
 Enthalpy (H)= -1178.2676 0.46207
 Gibbs Free Energy (G)= -1178.3471 0.38262

Frequencies -- -331.5534 20.1899 30.4895

Supporting Information: s-Cis-Si-3U-(Methyl-Syn)-(Esther-Anti).output

Using Gaussian 03: Al64T-G03RevC.01 3-Apr-2004

hf/6-31g(d) geom=connectivity scf=(direct,maxcycle=300,tight)
 opt=(maxcycle=250,ts,calcfc,noeigentest) freq=norman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq

Pointgroup= C1 Stoichiometry= C18H24N2O5 C1[X(C18H24N2O5)] #Atoms= 49
 Charge = 0 Multiplicity = 1

SCF Energy= -1178.72410708 Predicted Change= -1.670266D-08

```
=====
Optimization completed.      {Found      1      times}
Item      Max Val.      Criteria      Pass?      RMS Val.      Criteria      Pass?
Force      0.00001 || 0.00045 [ YES ]      0.00000 || 0.00030 [ YES ]
Displ      0.00316 || 0.00180 [ NO ]      0.00316 || 0.00180 [ YES ]
=====
```

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
N	-0.477105	1.820875	0.875739
C	0.733591	2.632570	0.830975
C	0.199946	4.012793	0.467040
C	-0.934000	3.682423	-0.508774
C	-1.542184	2.371397	0.014006
C	-0.615380	0.775537	1.672503
C	-1.678471	-0.094926	1.755937
C	-1.078747	-1.625300	0.081929
C	-1.802884	-0.995997	2.966014
N	-0.136666	-1.193018	-0.700854
C	3.990653	-0.961424	0.015476
C	3.396266	-0.232599	-1.003658
C	2.027729	-0.317533	-1.210428
C	1.241018	-1.131602	-0.412876
C	1.840208	-1.865301	0.607698
C	3.198128	-1.775802	0.819957
O	5.305172	-0.949258	0.303963
C	6.182982	-0.190016	-0.480570
C	-1.899958	1.363380	-1.108117
O	-3.026137	0.885258	-1.059563
O	-0.970541	1.098978	-1.891829
C	-2.423160	-1.869305	-0.588873
O	-3.426589	-1.894308	0.246686
O	-2.465160	-2.132753	-1.739703
C	-4.724914	-1.959893	-0.341347
H	1.404766	2.259324	0.064539
H	1.247885	2.600356	1.783950
H	-0.185296	4.503656	1.355769
H	0.961487	4.650130	0.032853
H	-1.677584	4.467400	-0.571672
H	-0.533696	3.510611	-1.498902
H	-2.418451	2.544812	0.626345
H	0.244612	0.588282	2.295400
H	-2.299429	-1.929295	2.719819
H	-0.829729	-1.236844	3.388997
H	-2.390153	-0.533232	3.755770
H	-0.447642	-0.603178	-1.472460
H	3.975079	0.404689	-1.642881
H	1.562557	0.262952	-1.985646
H	1.264969	-2.522370	1.233104
H	3.669700	-2.341379	1.601408
H	6.165972	-0.511819	-1.516157
H	5.947169	0.867493	-0.427370
H	7.168725	-0.354395	-0.073090

Supporting Information

```

H      -0.834645   -2.257695   0.908676
H      -2.587947   0.178871   1.257802
H      -5.416270   -1.903606   0.483902
H      -4.849151   -1.121984   -1.008198
H      -4.845412   -2.891518   -0.873922
  
```

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

```

=====
SCF Energy=      -1178.72410708      Predicted Change= -1.670266D-08
Zero-point correction (ZPE)=      -1178.2864      0.43768
Internal Energy (U)=      -1178.2629      0.46116
Enthalpy (H)=      -1178.2619      0.46210
Gibbs Free Energy (G)=      -1178.3406      0.38345
  
```

```

-----
Frequencies --  -388.5692           25.0763           34.1499
  
```

Supporting Information: s-Cis-Si-3U-(Methyl-Syn)-(Esther-Syn).output

Using Gaussian 03: Al64T-G03RevC.01 3-Apr-2004

```

=====
#hf/6-31G* scf=(direct,tight,maxcycle=300)
opt=(gdiis,calcfc,maxcycle=150,ts,noeigentest) freq=norman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
  
```

```

-----
Pointgroup= C1    Stoichiometry= C18H24N2O5    C1[X(C18H24N2O5)]    #Atoms= 49
Charge = 0        Multiplicity = 1
  
```

```

=====
SCF Energy= -1178.73011743    Predicted Change= -6.412429D-09
  
```

```

-----
Optimization completed.            {Found        2        times}
Item    Max Val.    Criteria    Pass?    RMS Val.    Criteria    Pass?
Force   0.00001 || 0.00045 [ YES ]    0.00000 || 0.00030 [ YES ]
Displ   0.00149 || 0.00180 [ YES ]    0.00149 || 0.00180 [ YES ]
  
```

```

-----
Atomic            Coordinates (Angstroms)
Type            X            Y            Z
-----
N            -0.657293    1.668072    0.979086
C            0.530103    2.513319    1.046117
C            -0.033086    3.905240    0.786970
C            -1.112224    3.631565    -0.264367
C            -1.691471    2.249077    0.101635
C            -0.840858    0.636515    1.778262
C            -1.888746    -0.258164    1.797020
C            -0.922070    -1.802918    0.301168
C            -2.126282    -1.107827    3.027862
N            -0.087620    -1.262293    -0.533212
C            4.062539    -0.780027    -0.097729
C            3.341873    -0.010700    -0.998199
C            1.969384    -0.176965    -1.113524
C            1.305494    -1.112488    -0.338166
C            2.032863    -1.894502    0.555802
  
```

```

C            3.393342    -1.722657    0.678907
O            5.391493    -0.695763    0.095145
C            6.151775    0.194226    -0.674688
C            -1.980615    1.425818    -1.180087
O            -3.155193    1.350526    -1.492382
O            -0.971642    0.969708    -1.757802
C            -2.305692    -2.180859    -0.162673
O            -2.615485    -1.583021    -1.267445
O            -2.961384    -2.966227    0.442768
C            -3.941048    -1.687017    -1.783779
H            1.231476    2.225656    0.270986
H            1.017944    2.408365    2.007347
H            -0.472161    4.299583    1.698469
H            0.723525    4.602755    0.446862
H            -1.884820    4.388886    -0.289144
H            -0.660879    3.579048    -1.247518
H            -2.606210    2.341936    0.672630
H            -0.030106    0.467251    2.468887
H            -2.588745    -2.053947    2.773621
H            -1.194827    -1.317336    3.549157
H            -2.785617    -0.610533    3.735469
H            -0.495076    -0.648267    -1.248148
H            3.824654    0.721004    -1.615796
H            1.404146    0.431369    -1.794516
H            1.556987    -2.655157    1.146518
H            3.962715    -2.323313    1.362928
H            6.076003    -0.034249    -1.732176
H            5.849207    1.222010    -0.504965
H            7.175143    0.068519    -0.355872
H            -0.561116    -2.375439    1.128221
H            -2.755089    -0.012764    1.205034
H            -4.016588    -0.893253    -2.503518
H            -4.075143    -2.660712    -2.232811
H            -4.655036    -1.543470    -0.988246
  
```

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

```

=====
SCF Energy=      -1178.73011743      Predicted Change= -6.412429D-09
Zero-point correction (ZPE)=      -1178.2925      0.43757
Internal Energy (U)=      -1178.2689      0.46117
Enthalpy (H)=      -1178.2679      0.46211
Gibbs Free Energy (G)=      -1178.3474      0.38266
  
```

```

-----
Frequencies --  -336.4616           22.4299           29.0862
  
```

ii. Pipecolinic Acid Transition Structures.

Supporting Information: Pipecolinic-Acid-TS-s-Trans-Re.output

Using Gaussian 03: Al64T-G03RevC.01 3-Apr-2004

Supporting Information

```

=====
# opt=(calcf, gdiis, ts, noeigentest, maxcycle=250) hf/6-31G* freq=norman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
-----
Pointgroup= C1 Stoichiometry= C19H26N2O5 C1[X(C19H26N2O5)] #Atoms= 52
Charge = 0 Multiplicity = 1
-----
SCF Energy= -1217.76421776 Predicted Change= -5.366109D-09
=====
Optimization completed. {Found 1 times}
Item Max Val. Criteria Pass? RMS Val. Criteria Pass?
Force 0.00001 || 0.00045 [ YES ] 0.00000 || 0.00030 [ YES ]
Displ 0.00228 || 0.00180 [ NO ] 0.00228 || 0.00180 [ YES ]
-----
Atomic Coordinates (Angstroms)
Type X Y Z
-----
C 3.290076 3.253638 0.125697
C 1.908400 3.395331 0.761495
C 1.058345 2.142795 0.540460
C 3.127047 0.754525 0.444911
C 3.980912 2.002099 0.663841
H 0.170076 2.22538 1.155163
H 2.021592 3.567182 1.830126
H 1.368845 4.233194 0.343104
H 3.191514 3.186052 -0.954599
H 3.891518 4.133187 0.334862
H 3.587720 -0.088086 0.938738
H 3.035644 0.534709 -0.609531
H 4.175251 2.120774 1.727305
H 4.940738 1.848573 0.178313
N 1.780467 0.937469 0.986092
C 0.540311 2.036420 -0.928239
O -0.113260 2.996087 -1.292482
O 0.802043 0.986690 -1.548831
C 1.130006 -0.017489 1.618269
C 1.460731 -1.344573 1.826875
H 2.457907 -1.671036 1.592851
C 0.780930 -2.128060 2.930166
H 0.758849 -3.189913 2.700143
H 1.299341 -2.027933 3.881069
H -0.243223 -1.798333 3.084073
H 0.157801 0.289626 1.967102
C 0.294692 -2.154085 -0.067351
H -0.184376 -2.833115 0.602495
C 1.572439 -2.689682 -0.646258
N -0.411601 -1.281513 -0.716571
H 0.097508 -0.599861 -1.289419
C -1.746614 -0.902683 -0.411500
C -2.567218 -1.640865 0.439994
C -2.248514 0.237864 -1.015040
C -3.855099 -1.227648 0.690085
H -2.223573 -2.544222 0.908131

```

```

C -3.547425 0.654419 -0.762183
H -1.628657 0.818493 -1.671077
C -4.358193 -0.072519 0.093525
H -4.494538 -1.789998 1.344089
H -3.894631 1.549960 -1.237757
O -5.626111 0.245613 0.407616
C -6.210408 1.394789 -0.143625
H -6.256417 1.333404 -1.225316
H -7.212985 1.440908 0.253325
H -5.669352 2.289207 0.144382
O 2.008243 -3.737445 -0.296449
O 2.076508 -1.915344 -1.566201
C 3.263563 -2.345540 -2.220566
H 3.490889 -1.573338 -2.935838
H 4.064748 -2.451853 -1.504126
H 3.092478 -3.289038 -2.716810

```

```

-----
Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
-----
SCF Energy= -1217.76421776 Predicted Change= -5.366109D-09
Zero-point correction (ZPE)= -1217.2950 0.46913
Internal Energy (U)= -1217.2706 0.49360
Enthalpy (H)= -1217.2696 0.49454
Gibbs Free Energy (G)= -1217.3512 0.41295
-----
Frequencies -- -330.0387 16.0619 32.0403

```

```

Supporting Information: Pipecolonic-Acid-TS-s-Trans-Re2.output
-----
Using Gaussian 03: A164T-G03RevC.01 3-Apr-2004
-----
# opt=(calcf, ts, maxcycle=150, noeigentest) freq=norman hf/6-31g(d)
geom=connectivity scf=(direct, tight, maxcycle=300)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
-----
Pointgroup= C1 Stoichiometry= C19H26N2O5 C1[X(C19H26N2O5)] #Atoms= 52
Charge = 0 Multiplicity = 1
-----
SCF Energy= -1217.76278775 Predicted Change= -9.060687D-09
=====
Optimization completed. {Found 2 times}
Item Max Val. Criteria Pass? RMS Val. Criteria Pass?
Force 0.00004 || 0.00045 [ YES ] 0.00000 || 0.00030 [ YES ]
Displ 0.00179 || 0.00180 [ YES ] 0.00179 || 0.00180 [ YES ]

```

```

Atomic Coordinates (Angstroms)
Type X Y Z
-----
C 2.876590 3.665036 0.044365
C 1.542891 3.615919 0.787931
C 0.807927 2.297852 0.534357
C 2.989663 1.147100 0.178232

```

Supporting Information

C	3.730906	2.458646	0.430023
H	-0.035167	2.242116	1.211958
H	1.723128	3.725120	1.855819
H	0.890343	4.418556	0.474751
H	2.698559	3.662963	-1.027656
H	3.401741	4.586647	0.277123
H	3.571431	0.322256	0.560155
H	2.826475	0.992919	-0.878154
H	4.001065	2.523270	1.481892
H	4.656511	2.441363	-0.138494
N	1.682352	1.151102	0.841202
C	0.194001	2.238209	-0.900401
O	-0.574940	3.148880	-1.143884
O	0.511394	1.268970	-1.617991
C	1.208738	0.121533	1.508673
C	1.704266	-1.162322	1.656269
H	2.717607	-1.359434	1.355252
C	1.185527	-2.048654	2.768371
H	1.235354	-3.099243	2.492390
H	1.763813	-1.941448	3.683685
H	0.151455	-1.820275	3.012364
H	0.241144	0.307157	1.945168
C	0.523907	-2.004492	-0.248400
H	0.142846	-2.768002	0.393159
C	1.840177	-2.290995	-0.908479
N	-0.284139	-1.167008	-0.809395
H	0.128142	-0.407737	-1.368351
C	-1.639568	-0.947751	-0.442798
C	-2.313428	-1.741378	0.484217
C	-2.312384	0.094815	-1.057860
C	-3.630486	-1.484945	0.787323
H	-1.831259	-2.564236	0.977706
C	-3.639255	0.354671	-0.749869
H	-1.798779	0.723551	-1.759345
C	-4.307218	-0.431829	0.174196
H	-4.157526	-2.090368	1.500445
H	-4.120600	1.180032	-1.235269
O	-5.588342	-0.263080	0.544355
C	-6.337846	0.786148	-0.006934
H	-6.432107	0.680544	-1.082048
H	-7.316480	0.724087	0.443955
H	-5.896808	1.749275	0.223988
O	2.333321	-1.609939	-1.739429
O	2.327252	-3.431337	-0.464567
C	3.570080	-3.854485	-1.012314
H	3.792071	-4.795654	-0.536636
H	3.483174	-3.979585	-2.081060
H	4.339966	-3.128953	-0.794732

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1217.7627875 Predicted Change= -9.060687D-09

Zero-point correction (ZPE)= -1217.2938 0.46893
 Internal Energy (U)= -1217.2694 0.49337
 Enthalpy (H)= -1217.2684 0.49431
 Gibbs Free Energy (G)= -1217.3498 0.41290

Frequencies -- -306.4482 16.8712 31.1788

Supporting Information: Pipecolinic-Acid-TS-s-Trans-Si.output

Using Gaussian 03: A164T-G03RevC.01 3-Apr-2004

opt=(gdiis,maxcycle=300,ts,calcf, noigentest) hf/6-31G* freq=norman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq

Pointgroup= C1 Stoichiometry= C19H26N2O5 C1[X(C19H26N2O5)] #Atoms= 52
 Charge = 0 Multiplicity = 1

SCF Energy= -1217.76570246 Predicted Change= -5.088931D-08

Optimization completed. {Found 1 times}
 Item Max Val. Criteria Pass? RMS Val. Criteria Pass?
 Force 0.00001 || 0.00045 [YES] 0.00000 || 0.00030 [YES]
 Displ 0.00571 || 0.00180 [NO] 0.00571 || 0.00180 [YES]

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	-0.923314	4.061285	0.873216
C	-2.207963	3.497875	0.263936
C	-1.978660	2.108946	-0.335473
C	-0.131343	1.696027	1.250200
C	-0.323516	3.076616	1.879352
H	-2.930748	1.678285	-0.621470
H	-2.974581	3.426974	1.034731
H	-2.573362	4.147505	-0.517236
H	-0.211607	4.254428	0.076490
H	-1.123728	5.012295	1.357892
H	0.226856	0.990675	1.983154
H	0.596494	1.745610	0.452418
H	-0.977427	2.984216	2.743957
H	0.638099	3.431172	2.240743
N	-1.394700	1.220652	0.686282
C	-1.132832	2.143372	-1.654192
O	-1.285435	3.135259	-2.333480
O	-0.420677	1.142604	-1.887829
C	-2.057090	0.170349	1.128512
C	-1.607590	-0.916344	1.852156
H	-0.630627	-0.872188	2.301135
C	-2.589529	-1.850756	2.523468
H	-2.235307	-2.877598	2.519918
H	-2.758951	-1.576844	3.562373
H	-3.554961	-1.840000	2.026498
H	-3.069164	0.119378	0.767265

Supporting Information

C	-0.743390	-1.926404	-0.087822
H	-0.385301	-2.730669	0.519009
C	-2.080364	-2.148187	-0.732363
N	0.090539	-1.107448	-0.636465
H	-0.272467	-0.322079	-1.224454
C	1.472679	-1.017244	-0.329134
C	2.072670	-1.717200	0.714867
C	2.250419	-0.194230	-1.127064
C	3.425961	-1.600366	0.940843
H	1.501178	-2.351843	1.366184
C	3.612793	-0.074644	-0.898390
H	1.782076	0.367888	-1.912626
C	4.210704	-0.779830	0.134734
H	3.896798	-2.135925	1.743586
H	4.183938	0.572204	-1.534648
O	5.520212	-0.735403	0.439221
C	6.383967	0.066264	-0.319294
H	6.104442	1.112526	-0.261520
H	7.366455	-0.063497	0.108167
H	6.401988	-0.245685	-1.357805
O	-2.621645	-1.378167	-1.449505
O	-2.538669	-3.338274	-0.406820
C	-3.790551	-3.720840	-0.965879
H	-3.983156	-4.713855	-0.594367
H	-4.565368	-3.039637	-0.647200
H	-3.731021	-3.722047	-2.043653

Force 0.00003 || 0.00045 [YES] 0.00000 || 0.00030 [YES]
 Displ 0.00386 || 0.00180 [NO] 0.00386 || 0.00180 [YES]

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	-1.342410	3.802555	0.608515
C	-2.664163	3.081224	0.352181
C	-2.452217	1.597858	0.032187
C	-0.342093	1.629896	1.407058
C	-0.589158	3.100591	1.736509
H	-3.412533	1.102813	0.078860
H	-3.292916	3.167527	1.236232
H	-3.201521	3.522415	-0.477300
H	-0.738388	3.800796	-0.294131
H	-1.527962	4.840203	0.869523
H	0.077924	1.129738	2.267513
H	0.353735	1.552531	0.586468
H	-1.160832	3.174279	2.658955
H	0.372178	3.573755	1.916353
N	-1.591691	0.955827	1.046282
C	-1.942917	1.404263	-1.428865
O	-2.801538	1.579523	-2.273019
O	-0.737893	1.109807	-1.580043
C	-1.910028	-0.250661	1.483743
C	-1.122337	-1.220812	2.067205
H	-0.116672	-0.965663	2.353938
C	-1.749607	-2.374439	2.817202
H	-1.156894	-3.280258	2.726738
H	-1.838990	-2.158732	3.879389
H	-2.740934	-2.604433	2.442822
H	-2.930390	-0.526779	1.276334
C	-0.395572	-2.066837	0.018806
H	0.084970	-2.835825	0.584824
C	-1.743554	-2.464123	-0.516276
N	0.308137	-1.166585	-0.592308
H	-0.190546	-0.443420	-1.135011
C	1.680908	-0.890279	-0.379977
C	2.477445	-1.597960	0.517064
C	2.243631	0.132333	-1.124927
C	3.810501	-1.283778	0.654658
H	2.077376	-2.395182	1.115129
C	3.586694	0.449223	-0.986443
H	1.624953	0.689432	-1.803334
C	4.379759	-0.258224	-0.096633
H	4.433122	-1.823936	1.342664
H	3.989511	1.246967	-1.578724
O	5.689004	-0.033205	0.113643
C	6.346931	0.972857	-0.606532
H	5.919505	1.948561	-0.402455
H	7.373396	0.957827	-0.273569
H	6.314311	0.780267	-1.673321
O	-2.219383	-3.520447	-0.256789

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1217.76570246 Predicted Change= -5.088931D-08
 Zero-point correction (ZPE)= -1217.2969 0.46872
 Internal Energy (U)= -1217.2727 0.49294
 Enthalpy (H)= -1217.2718 0.49388
 Gibbs Free Energy (G)= -1217.3519 0.41374

Frequencies -- -317.0773 28.8534 32.5125

Supporting Information: Pipecolinic-Acid-TS-s-Trans-Si2.output

Using Gaussian 03: Al64T-G03RevC.01 3-Apr-2004

opt=(calcf,ts,maxcycle=150,noeigentest) freq=noraman hf/6-31g(d)
 geom=connectivity scf=(direct,tight,maxcycle=300)
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq

Pointgroup= C1 Stoichiometry= C19H26N2O5 C1[X(C19H26N2O5)] #Atoms= 52
 Charge = 0 Multiplicity = 1

SCF Energy= -1217.76997963 Predicted Change= -5.192499D-08

Optimization completed. {Found 1 times}
 Item Max Val. Criteria Pass? RMS Val. Criteria Pass?

Supporting Information

```

O      -2.256758   -1.545166   -1.282048
C      -3.497611   -1.793406   -1.945015
H      -3.712023   -0.879571   -2.470904
H      -3.384668   -2.625227   -2.624144
H      -4.263504   -2.018545   -1.217368
    
```

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

```

=====
SCF Energy=      -1217.76997963      Predicted Change= -5.192499D-08
Zero-point correction (ZPE)=      -1217.3006      0.46928
Internal Energy (U)=      -1217.2764      0.49356
Enthalpy (H)=      -1217.2754      0.49450
Gibbs Free Energy (G)=      -1217.3553      0.41465
    
```

```

-----
Frequencies --  -320.7281           31.3717           32.6586
    
```

Supporting Information: Pipecolinic-Acid-TS-s-Cis-Re.output

Using Gaussian 03: AL64T-G03RevC.01 3-Apr-2004

```

=====
# opt=(gdiis,maxcycle=300,ts,calcfc,noeigentest) hf/6-31G* freq=norman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
    
```

```

-----
Pointgroup= C1    Stoichiometry= C19H26N2O5    C1[X(C19H26N2O5)]    #Atoms= 52
Charge = 0        Multiplicity = 1
    
```

```

-----
SCF Energy= -1217.76593061    Predicted Change= -2.071789D-08
    
```

```

=====
Optimization completed.            {Found    1            times}
Item    Max Val.    Criteria    Pass?    RMS Val.    Criteria    Pass?
Force    0.00004 || 0.00045    [ YES ]    0.00000 || 0.00030    [ YES ]
Displ    0.00267 || 0.00180    [ NO ]     0.00267 || 0.00180    [ YES ]
    
```

```

-----
Atomic                    Coordinates (Angstroms)
Type                    X                    Y                    Z
-----
C                    -4.077379           -2.674330           -0.553438
C                    -2.716247           -3.018787           0.046028
C                    -1.839777           -1.779771           0.263327
C                    -3.916122           -0.403054           0.495073
C                    -4.778873           -1.648113           0.333957
H                    -1.018468           -2.082111           0.897784
H                    -2.868498           -3.512869           1.003116
H                    -2.164377           -3.697497           -0.590383
H                    -3.951554           -2.269217           -1.554596
H                    -4.681854           -3.571633           -0.647386
H                    -4.367273           0.281984           1.202082
H                    -3.825658           0.107152           -0.455787
H                    -4.978565           -2.083087           1.310606
H                    -5.735058           -1.353851           -0.089796
N                    -2.571728           -0.732038           0.976490
C                    -1.188745           -1.271638           -1.047132
    
```

```

O       -0.408649       -2.057526       -1.568385
O       -1.459831       -0.108650       -1.402829
C       -1.935582       0.157357       1.727581
C       -0.591427       0.301522       1.993703
H       0.092658       -0.460505       1.665854
C       -0.171921       1.076138       3.227332
H       -0.190039       0.462807       4.125487
H       0.844248       1.452692       3.137424
H       -0.824212       1.927921       3.399515
H       -2.587444       0.887658       2.170426
C       0.093211       1.775168       0.275777
H       0.575544       2.248291       1.104464
C       -1.183275       2.440632       -0.214287
N       0.806066       1.104867       -0.573213
H       0.265231       0.684462       -1.322346
C       2.129582       0.637103       -0.356293
C       3.091653       1.449089       0.236716
C       2.464155       -0.637425       -0.772893
C       4.366897       0.974059       0.435611
H       2.854904       2.458324       0.522743
C       3.754631       -1.113391       -0.582541
H       1.718567       -1.263879       -1.231676
C       4.708989       -0.314690       0.027485
H       5.121740       1.588497       0.888792
H       3.987698       -2.106668       -0.911695
O       5.981286       -0.682833       0.261378
C       6.421148       -1.954679       -0.129348
H       6.336887       -2.089129       -1.202142
H       7.460355       -2.013351       0.156191
H       5.866644       -2.737101       0.377081
O       -2.081042       2.743231       0.498103
O       -1.076282       2.748348       -1.477865
C       -2.243072       3.231333       -2.132016
H       -1.940586       3.435489       -3.145682
H       -3.003420       2.466209       -2.113171
H       -2.598769       4.129920       -1.650906
    
```

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

```

=====
SCF Energy=      -1217.76593061      Predicted Change= -2.071789D-08
Zero-point correction (ZPE)=      -1217.2964      0.46945
Internal Energy (U)=      -1217.2721      0.49375
Enthalpy (H)=      -1217.2712      0.49470
Gibbs Free Energy (G)=      -1217.3521      0.41381
    
```

```

-----
Frequencies --  -345.0952           20.5232           30.2146
    
```

Supporting Information: Pipecolinic-Acid-TS-s-Cis-Re2-R.output

Using Gaussian 03: AL64T-G03RevC.01 3-Apr-2004

```

=====
# fopt=(calcfc,ts,maxcycle=150,noeigentest,gdiis) freq=norman hf/6-31g(d)
    
```

Supporting Information

```
scf=(direct,tight,maxcycle=300)
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
-----
Pointgroup= C1  Stoichiometry= C19H26N2O5  C1[X(C19H26N2O5)]  #Atoms= 52
Charge = 0      Multiplicity = 1
-----
```

```
SCF Energy= -1217.76351487  Predicted Change= -9.678852D-09
=====
```

```
Optimization completed.      {Found      2      times}
Item  Max Val.  Criteria  Pass?  RMS Val.  Criteria  Pass?
Force  0.00004 || 0.00045  [ YES ]  0.00000 || 0.00030  [ YES ]
Displ  0.00139 || 0.00180  [ YES ]  0.00139 || 0.00180  [ YES ]
-----
```

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	-3.463297	-3.409885	-0.097639
C	-2.313512	-3.208810	0.887710
C	-1.542488	-1.911910	0.615527
C	-3.613867	-0.913541	-0.337895
C	-4.392048	-2.196630	-0.068250
H	-0.874384	-1.749062	1.449438
H	-2.711177	-3.178888	1.900292
H	-1.605077	-4.022958	0.830820
H	-3.066668	-3.545586	-1.100441
H	-4.014619	-4.312191	0.149744
H	-4.252773	-0.047878	-0.212012
H	-3.230548	-0.902087	-1.349279
H	-4.876538	-2.129277	0.903583
H	-5.176750	-2.289102	-0.813916
N	-2.471799	-0.776790	0.572622
C	-0.633556	-2.018246	-0.641288
O	0.139615	-2.962634	-0.623224
O	-0.743572	-1.118577	-1.493800
C	-2.214760	0.390818	1.126637
C	-1.058794	0.884986	1.706047
H	-0.222804	0.219279	1.831531
C	-1.161414	2.003314	2.723476
H	-1.319607	1.618931	3.728683
H	-0.254299	2.600657	2.760754
H	-1.982176	2.676469	2.498618
H	-3.048967	1.073774	1.086695
C	-0.036266	1.910035	-0.152849
H	0.438955	2.537272	0.570446
C	-1.296283	2.440135	-0.774875
N	0.668177	1.048607	-0.810182
H	0.150389	0.382469	-1.394355
C	2.008017	0.692441	-0.490950
C	2.909051	1.638881	-0.007745
C	2.430164	-0.606958	-0.707214
C	4.200835	1.276046	0.292309
H	2.617249	2.666716	0.112542
C	3.736366	-0.970981	-0.409824

H	1.753392	-1.348700	-1.087999
C	4.625366	-0.037654	0.097506
H	4.905239	1.996860	0.662507
H	4.028742	-1.988594	-0.576723
O	5.906024	-0.292732	0.419624
C	6.421820	-1.584322	0.244982
H	6.384595	-1.886565	-0.795769
H	7.451207	-1.542009	0.566970
H	5.886921	-2.308030	0.849890
O	-1.831345	1.962865	-1.714311
O	-1.678601	3.540847	-0.157724
C	-2.831645	4.196030	-0.671100
H	-2.972610	5.065918	-0.050702
H	-2.670113	4.484297	-1.698917
H	-3.691330	3.544935	-0.611400

```
-----
Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin  Pressure= 1.00000 Atm
-----
SCF Energy= -1217.76351487  Predicted Change= -9.678852D-09
Zero-point correction (ZPE)= -1217.2946  0.46885
Internal Energy (U)= -1217.2702  0.49326
Enthalpy (H)= -1217.2693  0.49420
Gibbs Free Energy (G)= -1217.3504  0.41306
-----
Frequencies -- -319.4486  20.5595  31.1478
-----
```

```
Supporting Information: Pipecolinic-Acid-TS-s-Cis-Si.output
-----
Using Gaussian 03: AL64T-G03RevC.01 3-Apr-2004
-----
```

```
# opt=(gdiis,maxcycle=300,ts,calcfc,noeigentest) hf/6-31G* freq=norman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq
-----
Pointgroup= C1  Stoichiometry= C19H26N2O5  C1[X(C19H26N2O5)]  #Atoms= 52
Charge = 0      Multiplicity = 1
-----
```

```
SCF Energy= -1217.76936200  Predicted Change= -8.067874D-09
=====
```

```
Optimization completed.      {Found      2      times}
Item  Max Val.  Criteria  Pass?  RMS Val.  Criteria  Pass?
Force  0.00001 || 0.00045  [ YES ]  0.00000 || 0.00030  [ YES ]
Displ  0.00179 || 0.00180  [ YES ]  0.00179 || 0.00180  [ YES ]
-----
```

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	-1.793376	3.868424	0.350005
C	-2.808213	2.732285	0.474883
C	-2.190003	1.366961	0.142864
C	0.024240	2.216570	0.870339
C	-0.566740	3.580636	1.216576
H	-2.906906	0.608810	0.412837

Supporting Information

H	-3.191659	2.705568	1.493279
H	-3.644074	2.884230	-0.192915
H	-1.491134	3.974364	-0.688692
H	-2.248972	4.809315	0.643815
H	0.843406	1.969879	1.533494
H	0.398900	2.217748	-0.143358
H	-0.844759	3.598786	2.268336
H	0.197108	4.339833	1.072207
N	-0.987326	1.161142	0.967024
C	-1.958828	1.188479	-1.393850
O	-2.963615	1.361967	-2.057181
O	-0.812897	0.868300	-1.772010
C	-0.817423	0.146538	1.794594
C	-1.558226	-1.005328	1.950601
H	-2.556551	-1.032121	1.553964
C	-1.307458	-1.928036	3.122490
H	-1.947003	-1.694861	3.970779
H	-1.507623	-2.961607	2.854832
H	-0.278193	-1.867006	3.467247
H	0.095334	0.207501	2.363773
C	-0.498355	-2.104471	0.121037
H	-0.030814	-2.780852	0.803557
C	-1.855535	-2.547789	-0.348135
N	0.216859	-1.303680	-0.600473
H	-0.273012	-0.638491	-1.222243
C	1.581268	-0.990884	-0.387812
C	2.344699	-1.540992	0.638802
C	2.171536	-0.095837	-1.264916
C	3.672836	-1.201428	0.772256
H	1.923477	-2.235334	1.341385
C	3.508086	0.246049	-1.131717
H	1.577733	0.345938	-2.042561
C	4.269006	-0.306662	-0.112318
H	4.270032	-1.621994	1.559212
H	3.932438	0.941679	-1.828503
O	5.569563	-0.043025	0.105339
C	6.255696	0.832021	-0.747707
H	5.825489	1.827304	-0.721741
H	7.270046	0.873768	-0.381680
H	6.258726	0.466283	-1.768653
O	-2.325605	-3.572043	0.026356
O	-2.378297	-1.705838	-1.188939
C	-3.659372	-1.977450	-1.757709
H	-3.897676	-1.093836	-2.323036
H	-3.596874	-2.850859	-2.389826
H	-4.380373	-2.145679	-0.971574

Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1217.76936200 Predicted Change= -8.067874D-09
 Zero-point correction (ZPE)= -1217.3003 0.46904
 Internal Energy (U)= -1217.2760 0.49331

Enthalpy (H)= -1217.2750 0.49426
 Gibbs Free Energy (G)= -1217.3550 0.41431

Frequencies -- -309.8659 29.9834 33.3325

Supporting Information: Pipecolinic-Acid-TS-s-Cis-Si2.output

Using Gaussian 03: Al64T-G03RevC.01 3-Apr-2004

opt=(calcfc,ts,maxcycle=150,noeigentest) freq=noraman hf/6-31g(d)
 geom=connectivity scf=(direct,tight,maxcycle=300)
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RHF/6-31G(d) Freq

Pointgroup= C1 Stoichiometry= C19H26N2O5 C1[X(C19H26N2O5)] #Atoms= 52
 Charge = 0 Multiplicity = 1

SCF Energy= -1217.76366569 Predicted Change= -8.569846D-09

Optimization completed.		{Found		2		times}	
Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?	
Force	0.00005	0.00045	[YES]	0.00000	0.00030	[YES]	
Displ	0.00139	0.00180	[YES]	0.00139	0.00180	[YES]	

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	-1.568110	4.045689	0.612430
C	-2.602163	2.931572	0.431951
C	-1.960071	1.652616	-0.115874
C	0.185591	2.262310	0.917761
C	-0.386661	3.570351	1.463240
H	-2.692841	0.860180	-0.129213
H	-3.071324	2.706784	1.389113
H	-3.372773	3.245243	-0.256511
H	-1.216592	4.354345	-0.366024
H	-2.030484	4.913176	1.074224
H	0.965843	1.875290	1.560408
H	0.610158	2.407904	-0.066251
H	-0.707240	3.413928	2.491625
H	0.399702	4.320002	1.483528
N	-0.869839	1.254511	0.796305
C	-1.477937	1.797496	-1.602256
O	-2.094731	2.600147	-2.266505
O	-0.532733	1.054863	-1.948984
C	-0.910681	0.237832	1.630679
C	-1.790872	-0.825420	1.689782
H	-2.753778	-0.710777	1.225531
C	-1.745976	-1.778210	2.864470
H	-2.433322	-1.485291	3.655067
H	-2.021283	-2.785614	2.566336
H	-0.752057	-1.825333	3.301731
H	-0.059942	0.191185	2.290285
C	-0.736145	-1.942865	-0.097320

Supporting Information

H	-0.371780	-2.693804	0.570364
C	-2.090052	-2.193878	-0.692948
N	0.090221	-1.182045	-0.736610
H	-0.290897	-0.430200	-1.355867
C	1.462199	-1.025616	-0.424535
C	2.082992	-1.657144	0.650151
C	2.213998	-0.202853	-1.249371
C	3.429391	-1.473704	0.881210
H	1.535523	-2.294844	1.318778
C	3.567160	-0.017563	-1.017329
H	1.730643	0.307526	-2.060319
C	4.185702	-0.654739	0.048849
H	3.915555	-1.959066	1.706487
H	4.117064	0.625629	-1.675725
O	5.489924	-0.541913	0.359768
C	6.328699	0.251811	-0.434051
H	6.012549	1.289283	-0.428575
H	7.312942	0.178091	0.002593
H	6.363105	-0.109512	-1.456017
O	-2.587705	-1.523484	-1.530262
O	-2.619029	-3.282075	-0.171483
C	-3.906978	-3.658123	-0.646619
H	-4.160276	-4.560977	-0.115451
H	-4.624448	-2.879171	-0.435308
H	-3.873033	-3.838911	-1.710256

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy=	-1217.76366569	Predicted Change=	-8.569846D-09
Zero-point correction (ZPE)=	-1217.2951		0.46853
Internal Energy (U)=		-1217.2708	0.49277
Enthalpy (H)=		-1217.2699	0.49371
Gibbs Free Energy (G)=		-1217.3500	0.41362

Frequencies -- -341.0823 30.0428 36.1660