Efficient Access to Functionalized Cyclopentenes Through a Tandem NHC-Catalyzed Dynamic Kinetic Resolution/Decarboxylation: Formal Synthesis of a Estrogen Receptor β-Agonist

Daniel T. Cohen,[a] Ryne C. Johnston,[b] Nick T. Rosson,[b] Paul Ha-Yeon Cheong,[b] and Karl A. Scheidt[a]*

[a]Department of Chemistry, Center for Molecular Innovation and Drug Discovery, Chemistry of Life Processes Institute
Northwestern University
2170 Campus Drive, Evanston, IL 60208 (USA)
[b]Department of Chemistry
Oregon State University
153 Gilbert Hall, Corvallis, Oregon 97331, (USA)

Supporting Information

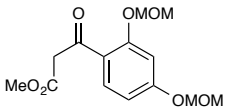
Table of Contents

General Information

All reactions were carried out under a nitrogen atmosphere in oven-dried glassware with magnetic stirring. THF, toluene, and DMF were purified by passage through a bed of activated alumina.[1] Reagents were purified prior to use unless otherwise stated following the guidelines of Perrin and Armarego.[2] 1,2-Dichloroethane (DCE) was distilled from CaH_2 and carefully degassed (3 freeze/pump thaw cycles). Purification of reaction products was carried out by flash chromatography using EM Reagent silica gel 60 (230-400 mesh). Analytical thin layer chromatography was performed on EM Reagent 0.25 mm silica gel 60-F plates. Visualization was accomplished with UV light and ceric ammonium nitrate stain or potassium permangenate stain followed by heating. Infrared spectra were recorded on a Bruker Tensor 37 FT-IR spectrometer. ^{1}H NMR spectra were recorded on AVANCE III 500 MHz w/ direct cryoprobe (500 MHz) spectrometer and are reported in ppm using solvent as an internal standard ($CDCl_3$ at 7.26 ppm). Data are reported as (ap = apparent, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, b = broad; coupling constant(s) in Hz; integration.) Proton-decoupled ^{13}C NMR spectra were recorded on an AVANCE III 500 MHz w/ direct cryoprobe (125 MHz) spectrometer and are reported in ppm using solvent as an internal standard ($CDCl_3$ at 77.0 ppm). Optical rotations were measured on a Perkin Elmer Model 341 Polarimeter with a sodium lamp. Mass spectra were obtained on a WATERS Acquity-H UPLC-MS with a single quad detector (ESI) .

Di-MOM protected ketone **4** has been previously reported in literature.[3]

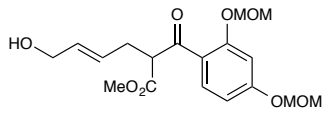
General Procedure for the formal Synthesis of the Cyclopentane Core



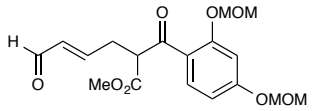
methyl 3-(2,4-bis(methoxymethoxy)phenyl)-3-oxopropanoate (5): Compound **5** was synthesized according to Lee *et al*.[4] using 1-(2,4-bis(methoxymethoxy)phenyl)ethanone (2.60 g, 10.82 mmol) and purified by flash chromatography using 30% EtOAc/hexanes to afford 2.44 g (76% yield) of 3-(2,4-bis(methoxymethoxy)phenyl)-3-oxopropanoate as a yellowish oil. Analytical data for **5**: ^{1}H NMR (500 MHz; $CDCl_3$): δ 7.91 (d, J = 8.9 Hz, 1H), 6.84 (d, J = 2.3 Hz, 1H), 6.75 (dd, J = 8.8, 2.3 Hz, 1H), 5.24 (s, 2H), 5.21 (s, 2H), 3.96 (s, 2H), 3.72 (s, 3H), 3.50 (s, 3H), 3.48 (s, 3H); ^{13}C NMR (125 MHz; $CDCl_3$): δ 191.3, 168.9, 162.8, 158.8, 133.1, 120.8,

[1] Pangborn, A. B.; Giardello, M. A.; Grubbs, R. H.; Rosen, R. K.; Timmers, F. J. *Organometallics* **1996**, *15*, 1518-1520.
[2] Perrin, D. D.; Armarego, W. L. *Purification of Laboratory Chemicals;* 3rd Ed., Pergamon Press, Oxford. 1988.
[3] Wang, H.; Yan, Z.; Lei, Y.; Sheng, K.; Yao, Q.; Lu, K.; Yu, P. *Tetrahedron Lett.* **2014**, *55*, 897-899.
[4] Chen, K.; Kuo, S. C.; Hsieh, M. C.; Mauger, A.; Lin, C. M.; Hamel, E.; Lee, K. H. *J. Med. Chem.* **1997**, *40*, 2266-2275.

109.4, 102.6, 94.6, 94.3, 56.7, 56.6, 52.3, 50.5; IR (film) 2993, 2953, 2829, 17.84, 1668, 1600, 1568, 1396, 1269, 1244, 1201, 1152, 1075, 996, 978, 962, 922 cm^{-1}; LRMS (ESI): Mass calcd for $C_{14}H_{19}O_7$ $[M+H]^+$: 299; found 299.

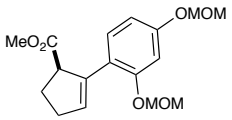


(*E*)-methyl 2-(2,4-bis(methoxymethoxy)benzoyl)-6-hydroxyhex-4-enoate: In a flame dried 50 mL round-bottomed flask was added $Pd(dba)_2$ (0.01 equiv) and triphenylphosphine (0.05 equiv). The flask was purged and diluted with THF (7 mL). In a flame dried 100 mL round-bottomed flask was added sodium hydride (60% in mineral oil) (1.2 equiv) and THF (20 mL) under nitrogen. Ketoester **5** (1.2 equiv) was slowly added to the NaH suspension at 23 °C causing a vigorous reaction. At the end of this addition, the solution becomes homogeneous and slightly yellow. At this time, THF (22 mL) and 4-hydroxybut-2-en-1-yl methyl carbonate (6.82 mmol) was added to the palladium catalyst and after 5 min of stirring; the catalyst solution was added to the sodium ketoester solution, which turns solution heterogeneous and yellow. The reaction mixture was stirred at 23 °C until completion (12 hours). The reaction mixture was quenched by the addition of saturated NH_4Cl (30 mL) and EtOAc (20 mL). The layers were separated and the aqueous layer was back extracted with EtOAc (40 mL). The combined organic was washed with brine, dried over $MgSO_4$, filtered, and concentrated *in-vacuo*. The material was purified by flash column chromatography EtOAc/hexanes (4:6) to afford 1.30 g (52% yield) of a mixture of *E* and *Z* isomers of methyl 2-(2,4-bis(methoxymethoxy)benzoyl)-6-hydroxyhex-4-enoate as a yellow oil. Analytical data: ^{1}H NMR (500 MHz; $CDCl_3$): δ 7.81 (d, *J* = 8.8 Hz, 1H), 6.85 (d, *J* = 2.3 Hz, 1H), 6.74 (dd, *J* = 8.8, 2.3 Hz, 1H), 5.82 – 5.59 (m, 2H), 5.26 – 5.19 (m, 4H), 4.39 (ap t, *J* = 7.0 Hz, 1H), 4.05 (m, 2H), 3.67 (s, 3H), 3.50 (s, 3H), 3.49 (s, 3H), 2.85 – 2.58 (m, 2H); ^{13}C NMR (125 MHz; $CDCl_3$): 194.1, 170.8, 162.5, 158.3, 133.2, 131.6, 129.4, 121.3, 109.5, 102.8, 94.7, 94.3, 63.6, 58.0, 56.8, 56.6, 52.3, 31.7; IR (film) 3480, 2998, 2917, 2849, 1748, 1668, 1574, 1435, 1247, 1220, 1151, 1076, 1010, 977, 970 cm^{-1}; LRMS (ESI): Mass calcd for $C_{18}H_{25}O_8$ $[M+H]^+$: 369; found 369.

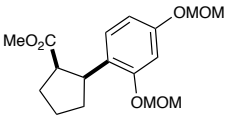


(*E*)-methyl 2-(2,4-bis(methoxymethoxy)benzoyl)-6-oxohex-4-enoate (7): In a flame dried 250 mL RBF with a stirbar was added PCC (1.5 equiv), Celite (~ 10 g), and CH_2Cl_2 (85 mL). To this RBF was added methyl-(2,4-bis(methoxymethoxy)benzoyl)-6-hydroxyhex-4-enoate (1.20 g, 3.26 mmol) dissolved in CH_2Cl_2 (9 mL). The resulting solution was stirred at 23 °C for 2 hrs. The reaction mixture was then filtered through a SiO_2 plug washed with Et2O and concentrated to afford 1.11 g (92% yield) of aldehyde **7** as a yellow oil. Analytical data for **7**: ^{1}H NMR (500 MHz; $CDCl_3$): δ 9.48 (d, *J* = 7.8 Hz, 1H), 7.85 (d, *J* = 8.8 Hz, 1H), 6.98 – 6.82 (m, 2H), 6.76 (dd, *J* = 8.8, 2.2 Hz, 1H), 6.12 (ap ddt, *J* = 15.6, 7.8, 1.5 Hz, 1H), 5.33 – 5.12 (m, 4H), 4.53 (ap t, *J* = 6.8 Hz, 1H), 3.68 (s, 3H), 3.50 (s, 3H), 3.48 (s, 3H), 3.03 (ap dtd, *J* = 15.5, 7.0, 1.5 Hz, 1H), 2.93 (ap dtd, *J* = 15.3, 6.7, 1.4 Hz, 1H); ^{13}C NMR (125 MHz; $CDCl_3$): 193.9, 192.8, 170.3, 162.9, 158.5, 154.9, 134.3, 133.4, 120.5, 109.7, 102.7, 94.7, 94.3, 56.8, 56.7, 56.6, 52.6, 31.8; IR (film)

2998, 2954, 2917, 2829, 1741, 1736, 1664, 1601, 1572, 1491, 1450, 1398, 1278, 1221, 1153, 1121, 1010, 979, 903, 844 cm^{-1}; LRMS (ESI): Mass calcd for $C_{18}H_{23}O_8$ $[M+H]^+$: 367; found 367.



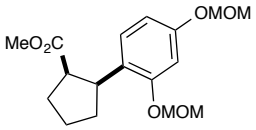
(anti)-methyl 2-(2,4-bis(methoxymethoxy)phenyl)cyclopent-2-enecarboxylate (9): In a nitrogen filled dry box a screw-capped vial equipped with a magnetic stirbar was charged with the corresponding enal **7** (146, mg, 0.400 mmol), azolium precatalyst **8** (0.07 equiv), and cesium carbonate (0.30 equiv). The vial was capped with a septum cap, removed from the drybox and put under positive N_2 pressure. The heterogeneous mixture was then diluted with degassed 1,2-dichloroethane (12 mL, 0.033 M) and stirred for 12 hours under static nitrogen pressure. After 12 hours the reaction mixture was diluted with dichloromethane (5 mL) washed with brine (10 mL) and separated. The aqueous phase was back extracted with dichloromethane (5 mL). The combined organic layers were filtered through a Biotage ISOLUTE® phase separator, and the organic filtrate was concentrated. The unpurified material was purified by flash chromatography using 20% EtOAc/hexanes to afford 110 mg (86% yield) of **9** as a yellow liquid. Analytical data of **9**: ^{1}H NMR (500 MHz; $CDCl_3$): δ 7.20 (d, J = 8.5 Hz, 1H), 6.80 (d, J = 2.4 Hz, 1H), 6.65 (dd, J = 8.6, 2.4 Hz, 1H), 6.26 (ap td, J = 2.6, 1.7 Hz, 1H), 5.33 – 4.92 (m, 4H), 4.10 (ap ddt, J = 9.2, 5.1, 1.9 Hz, 1H), 3.58 (s, 3H), 3.47 (s, 3H), 3.47 (s, 3H), 2.64 (ap dddt, J = 17.3, 8.7, 6.2, 2.5 Hz, 1H), 2.50 (ddddd, J = 16.8, 9.1, 4.7, 2.6, 1.5 Hz, 1H), 2.32 (ap dtd, J = 12.9, 9.0, 6.1 Hz, 1H), 2.15 (ap ddt, J = 12.9, 8.8, 5.0 Hz, 1H); ^{13}C NMR (125 MHz; $CDCl_3$): δ 176.0, 157.6, 155.7, 138.7, 132.2, 129.8, 120.0, 108.8, 103.8, 94.7, 94.6, 56.3, 56.2, 52.6, 51.8, 32.4, 29.3; IR (film) 2952, 2902, 2849, 2827, 1740, 1733, 1607, 1570, 1498, 1465, 1430, 1312, 1241, 1218, 1192, 1168, 1152, 1082, 1021, 1001, 923 cm^{-1}; LRMS (ESI): Mass calcd for $C_{17}H_{23}O_6$ $[M+H]^+$: 323; found 323. Enantiomeric ratio was measured by chiral phase HPLC (OJ, 5% *i*-PrOH/Hexanes, 1.0 mL/min, 210 nm), Rt_1 (major) = 9.4 min, Rt_2 (minor) = 11.9 min; ee = 92%.

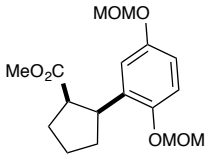


***cis*-(1*R*,2*S*)-methyl 2-(2,4-bis(methoxymethoxy)phenyl)cyclopentanecarboxylate (10):** A screw capped vial equipped with a stir bar and septum was charged with cyclopentene **9** (100 mg, 0.310 mmol) and 10% Pd/C (33 mg, 0.031 mmol). The vial was capped and diluted with MeOH (6.2 mL, 0.05M) under positive N_2 pressure. The solution was purged with H_2 for 5 minutes The reaction was then allowed to stir under H_2 atmosphere at 23 °C. After 12 hours the heterogeneous solution was filtered through a celite plug and washed with $CHCl_3$. The solution was concentrated and purified by flash column chromatography with 20% EtOAc in hexanes as an eluent to afford 48 mg (48%, 20:1 dr) of cyclopentane **10** as a light yellow oil. Analytical data of **10**: ^{1}H NMR (500 MHz; $CDCl_3$): d 7.06 (d, J = 8.5 Hz, 1H), 6.77 (d, J = 2.4 Hz, 1H), 6.61 (dd, J = 8.5, 2.4 Hz, 1H), 5.20 (s, 2H), 5.16 – 5.10 (m, 2H), 3.58 (ddd, J = 12.2, 9.0, 6.1 Hz, 1H), 3.51 (s, 3H), 3.46 (s, 3H), 3.29 (ap td, J = 8.6, 4.8 Hz, 1H), 3.18 (s, 3H), 2.20 – 1.94 (m, 4H), 1.84 (ap dt, J = 12.2, 6.4 Hz, 1H), 1.66 (dddd, J = 20.5, 10.5, 7.8, 5.1 Hz, 1H); ^{13}C NMR (125

MHz; $CDCl_3$): δ 176.1, 156.8, 156.3, 127.7, 123.5, 108.2, 103.0, 94.73, 94.71, 56.2, 56.1, 50.9, 47.4, 42.8, 29.8, 28.6, 24.9; IR (film) 2948, 2916, 2872, 2848, 2826, 1733, 1616, 1587, 1498, 1431, 1251, 1196, 1172, 1118, 1083, 1071, 1019, 1002, 924 cm^{-1}; LRMS (ESI): Mass calcd for $C_{17}H_{25}O_6$ $[M+H]^+$: 325; found 325.

Although cyclopentane **10** has been reported in literature there were no reported spectra.[5] The relative configuration was assigned by analogy of the similar cyclopentane prepared by the same group.[6] The side-by-side comparison of the ^1H NMR's are shown below. The methine protons are fairly identical (boxed off).



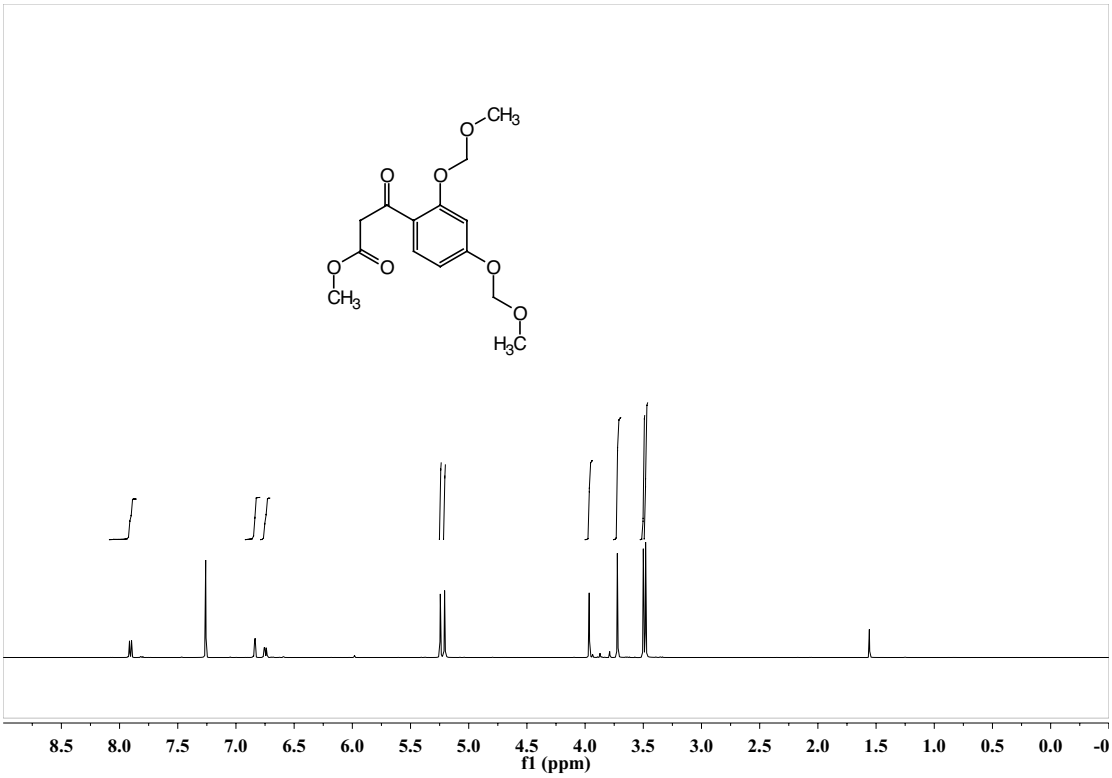


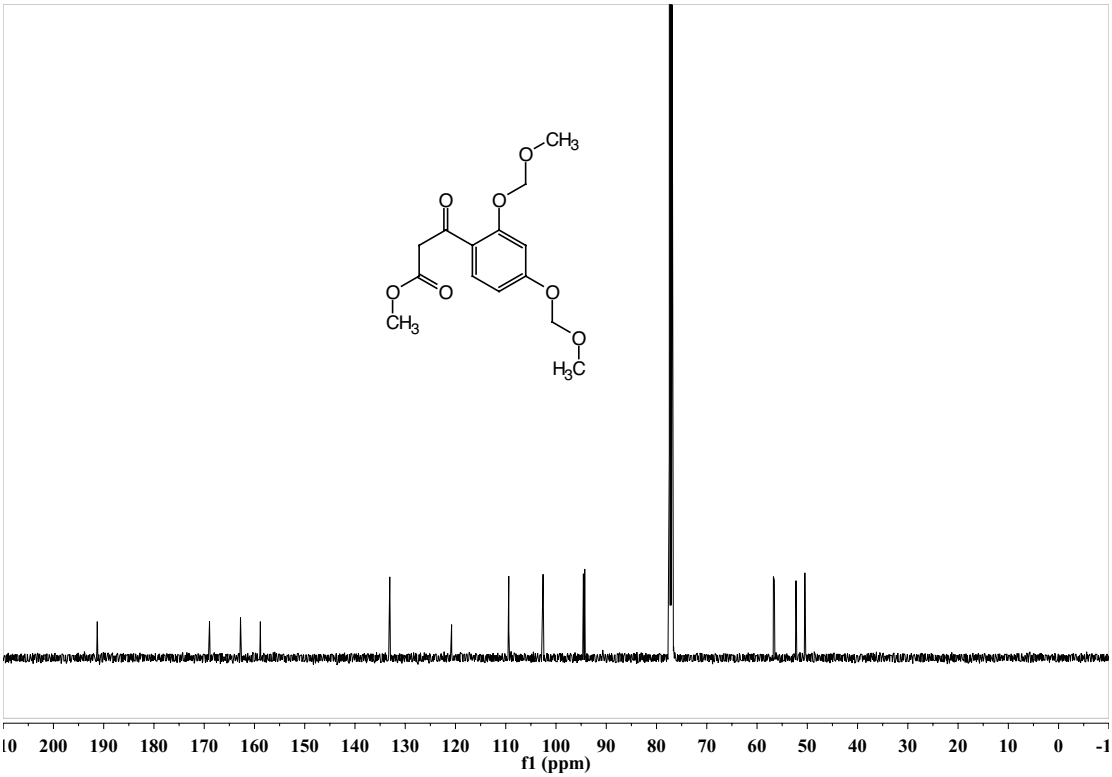
Cyclopentane **II-110**	reported in literature[105]
7.06 (d, *J* = 8.5 Hz, 1H),	6.98 (d, *J* = 8.6 Hz, 1H),
6.77 (d, *J* = 2.4 Hz, 1H),	6.86 (d, *J* = 3.1 Hz, 1H),
6.61 (dd, *J* = 8.5, 2.5 Hz, 1H),	6.81 (dd, *J* = 3.1, 9.0 Hz, 1H),
5.20 (s, 1H),	5.10 (s, 2H),
5.17 – 5.09 (m, 2H),	5.08 (s, 2H),
3.61-3.56 (ddd, *J* = 12.2, 9.0, 6.1 Hz, 1H),	3.64-3.59 (m, 1H),
3.51 (s, 3H),	3.50 (s, 3H),
3.46 (s, 3H),	3.45 (s, 3H),
3.32-3.27 (td, *J* = 8.6, 4.8 Hz, 1H),	3.39-3.30 (m, 1H),
3.18 (s, 3H),	3.19 (s, 3H),
2.22 – 1.92 (m, 4H),	2.12- 1.98 (m, 4H),
1.87-1.81 (dt, *J* = 12.2, 6.4 Hz, 1H),	1.93-1.82 (m, 1H),
1.71-1.60 (dddd, *J* = 20.2, 10.5, 7.8, 5.1 Hz, 1H)	1.72-1.63 (m, 1H)

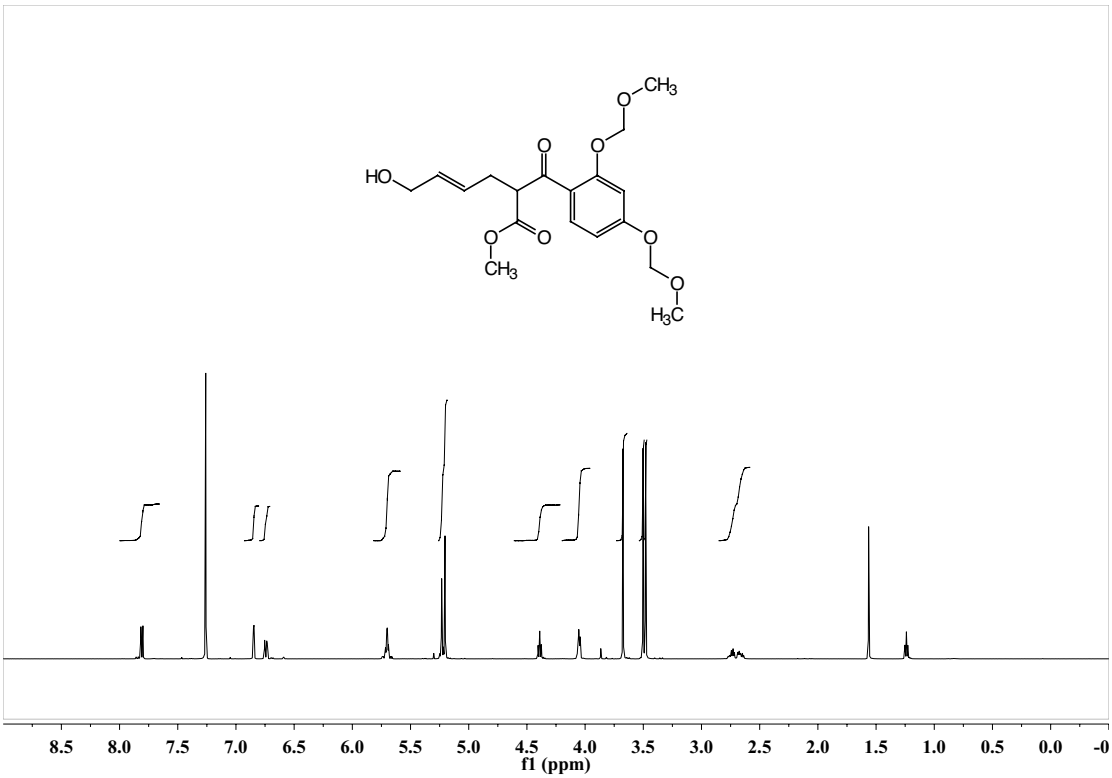
[5] Richardson, T. I.; Norman, B. H.; Lugar, C. W.; Jones, S. A.; Wang, Y.; Durbin, J. D.; Krishnan, V.; Dodge, J. A. *Bioorg. Med. Chem. Lett.* **2007**, *17*, 3570-3574.

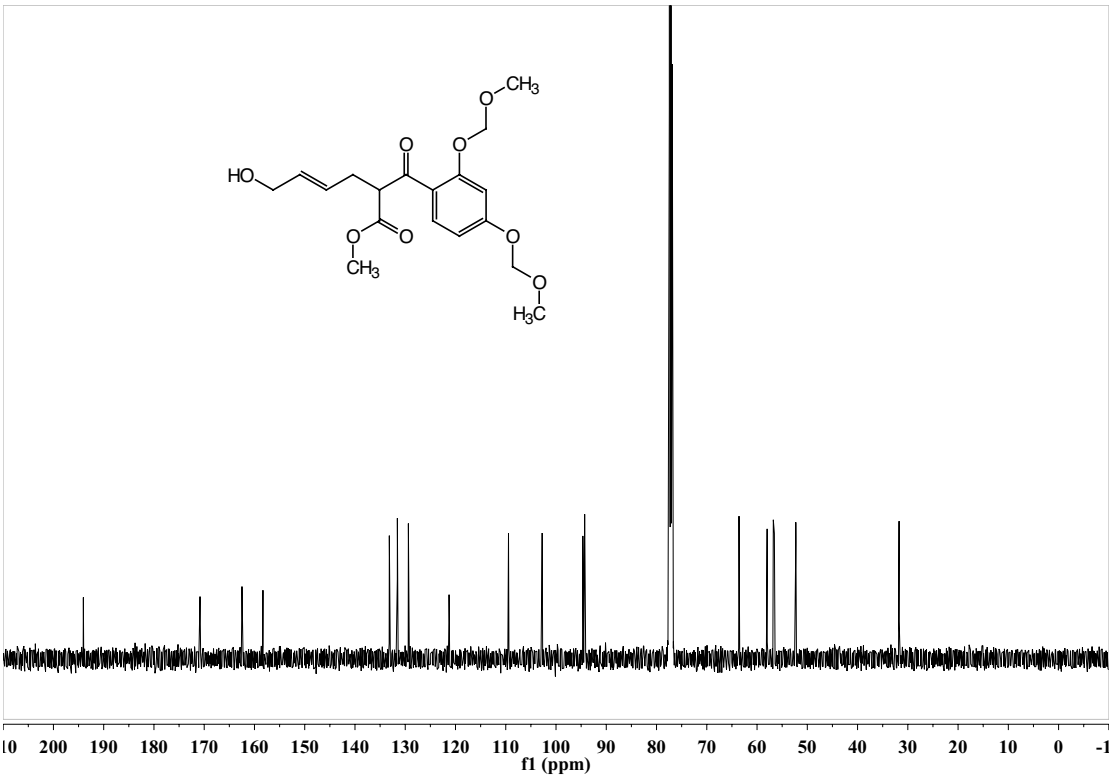
[6] Norman, B. H.; Dodge, J. A.; Richardson, T. I.; Borromeo, P. S.; Lugar, C. W.; Jones, S. A.; Chen, K.; Wang, Y.; Durst, G. L.; Barr, R. J.; Montrose-Rafizadeh, C.; Osborne, H. E.; Amos, R. M.; Guo, S.; Boodhoo, A.; Krishnan, V. *J. Med. Chem.* **2006**, *49*, 6155-6157.

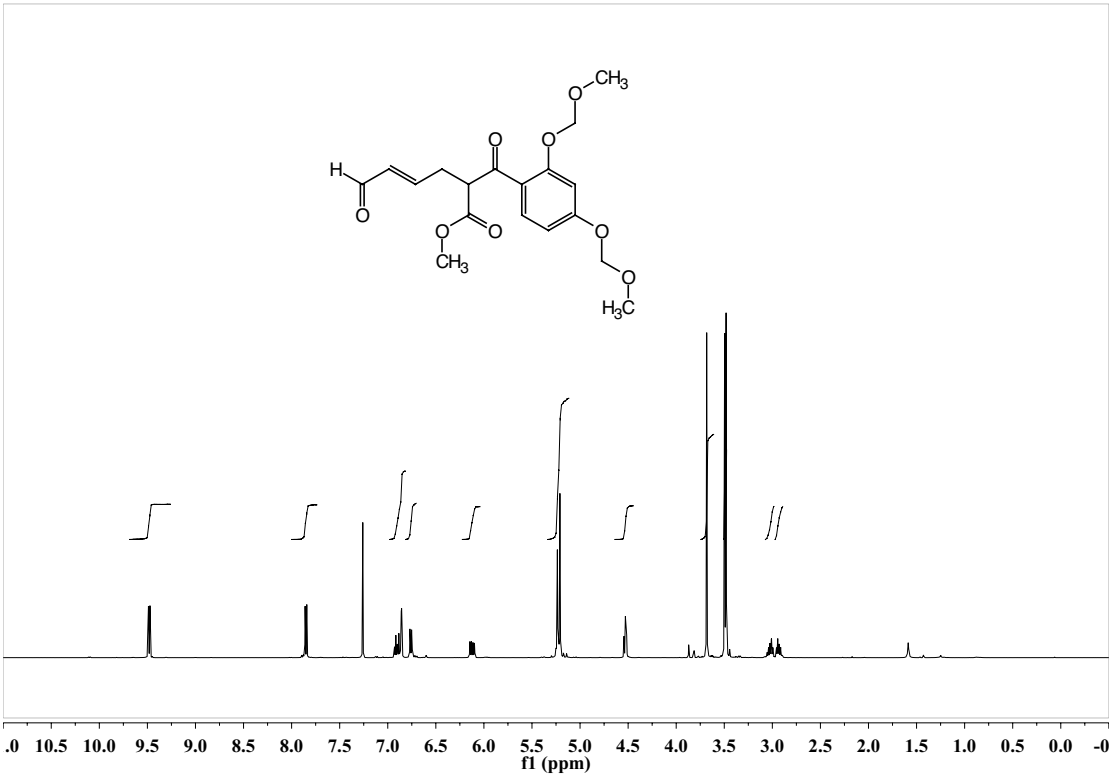
Selected NMR Spectra

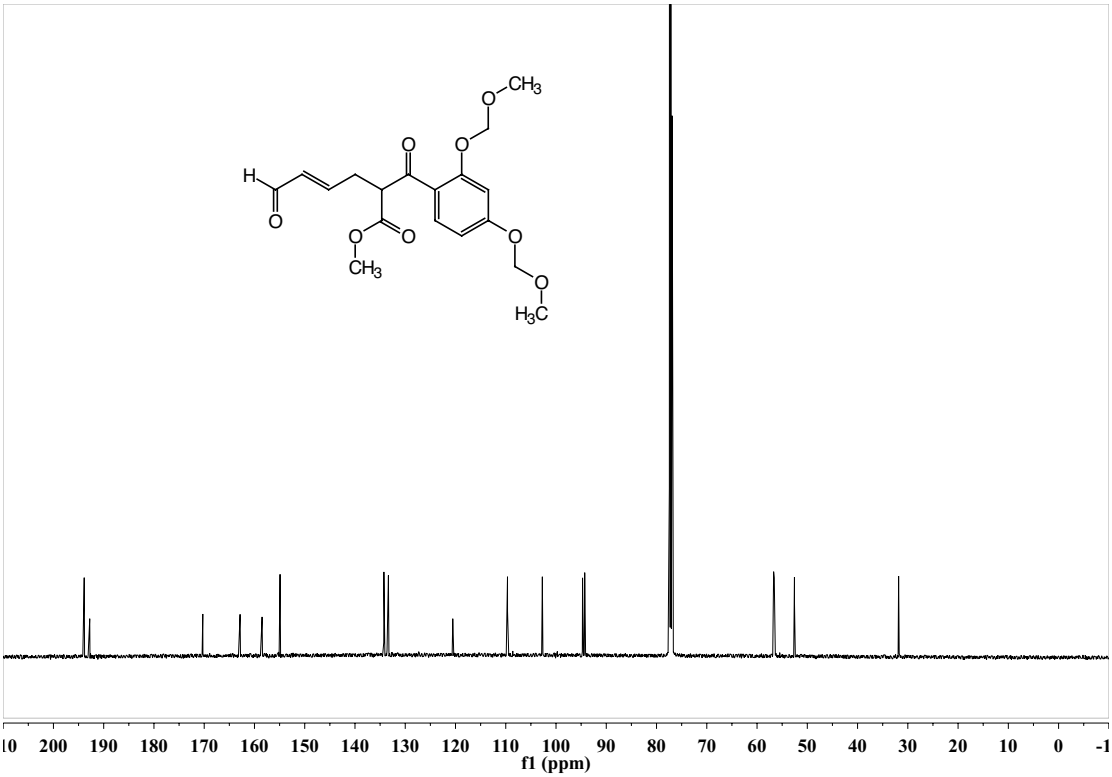


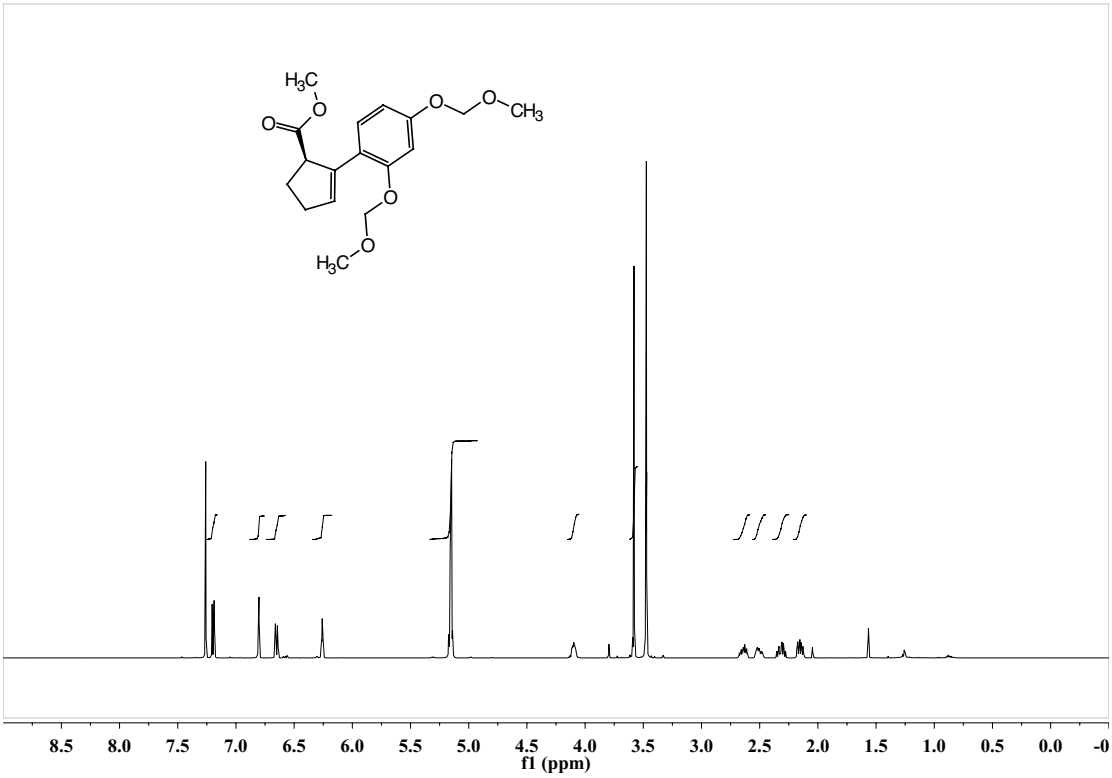


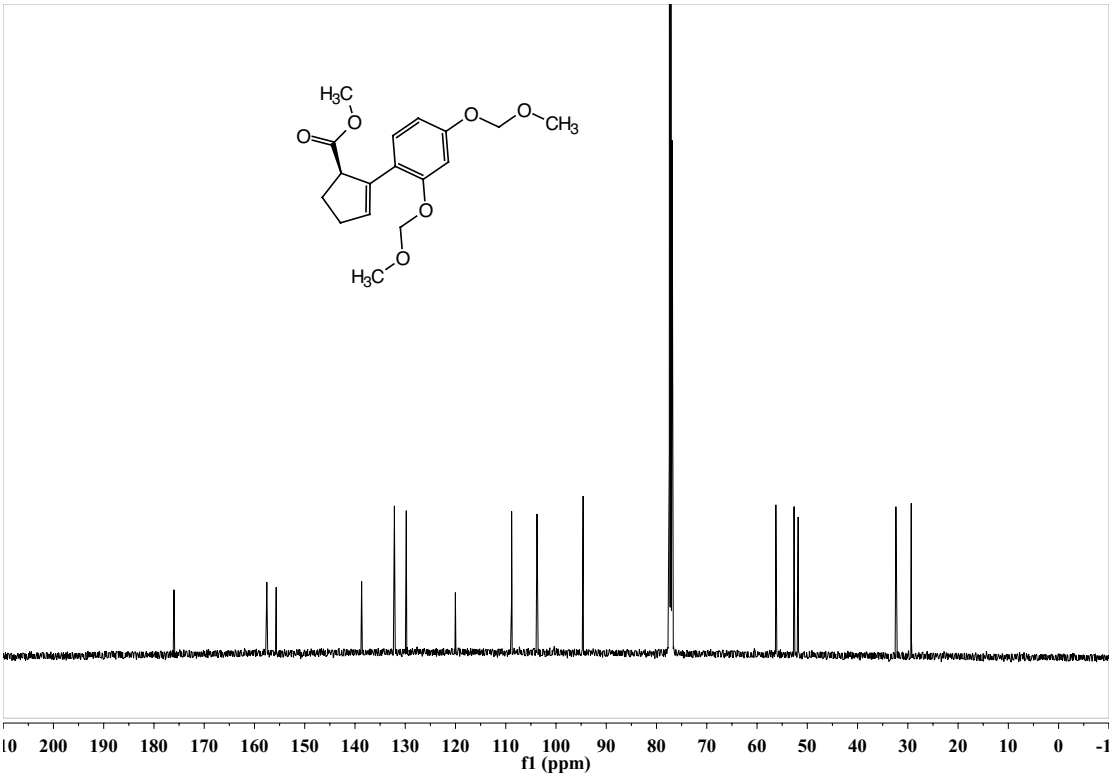

HO
O
O
O
O
O
O
O
O
O
CH3
CH3
H3C
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)

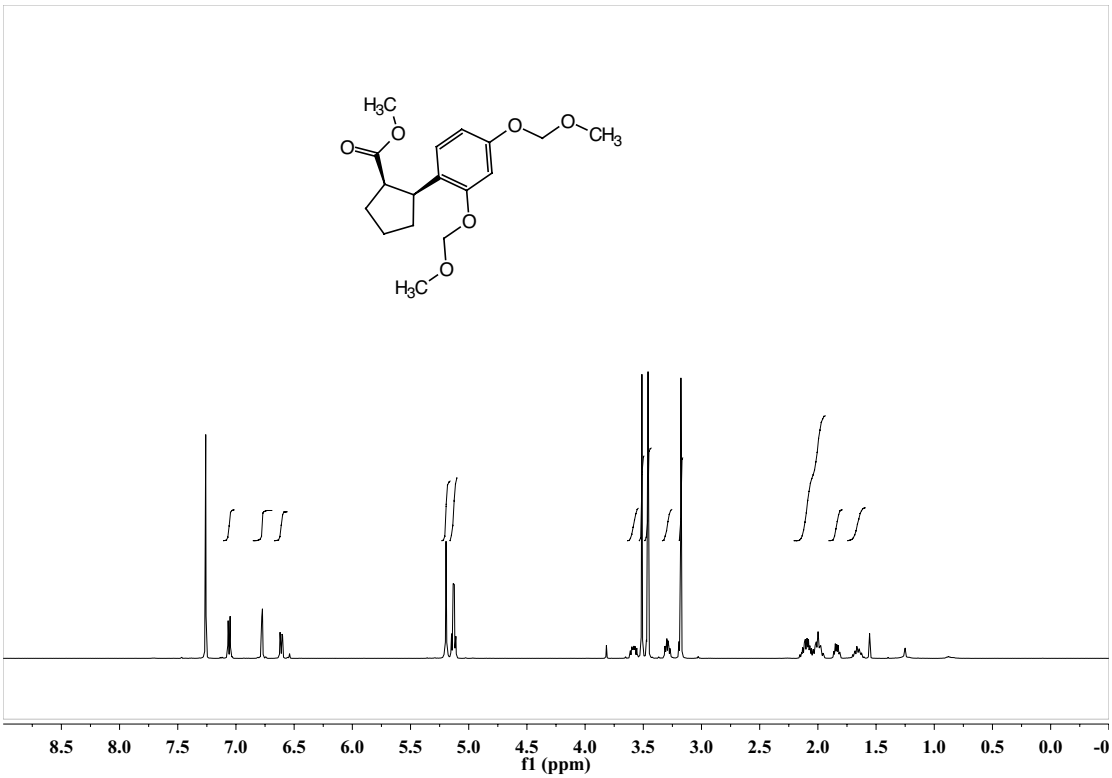

HO
O
O
O
O
O
O
O
O
O
CH3
CH3
H3C
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

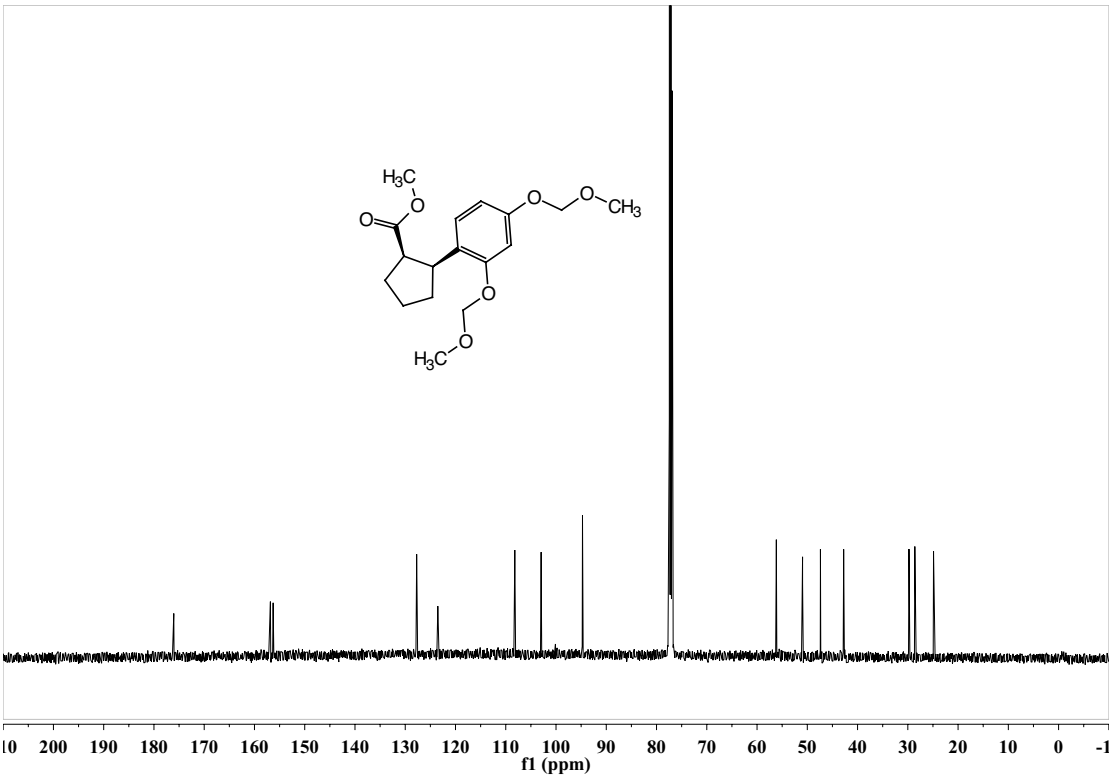

O
CH3
O
O
H
O
O
O
CH3
O
O
H3C
.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)


O
CH3
O
O
H
O
O
O
CH3
O
O
H3C
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)


H3C
O
O
O
O
CH3
O
H3C
O
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)

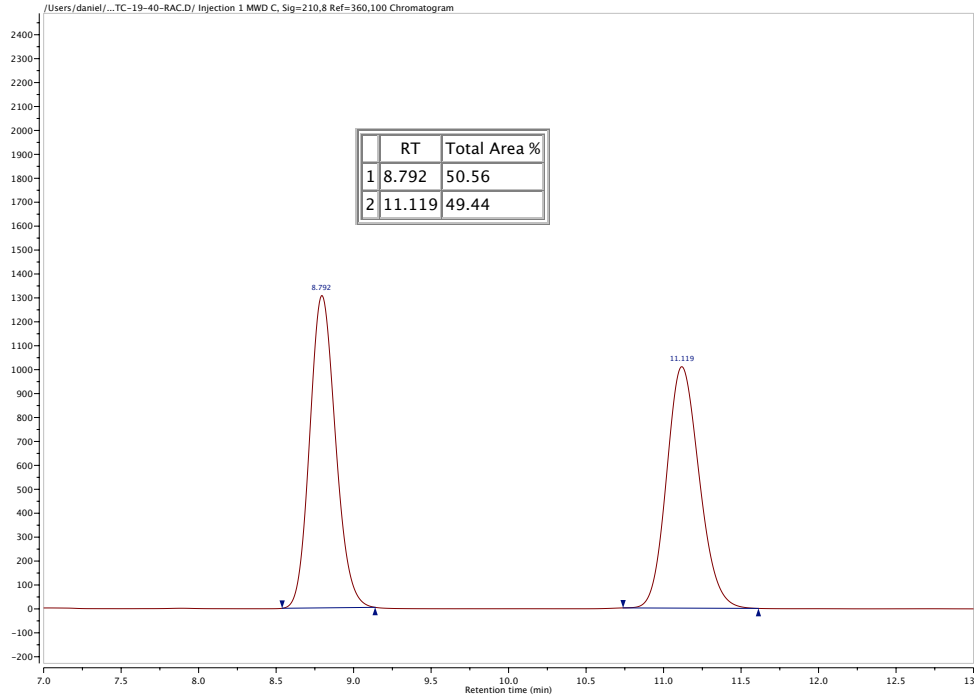

H3C
O
O
O
O
CH3
O
H3C
O
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)


H3C
O
O
O
O
CH3
O
H3C
O
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)

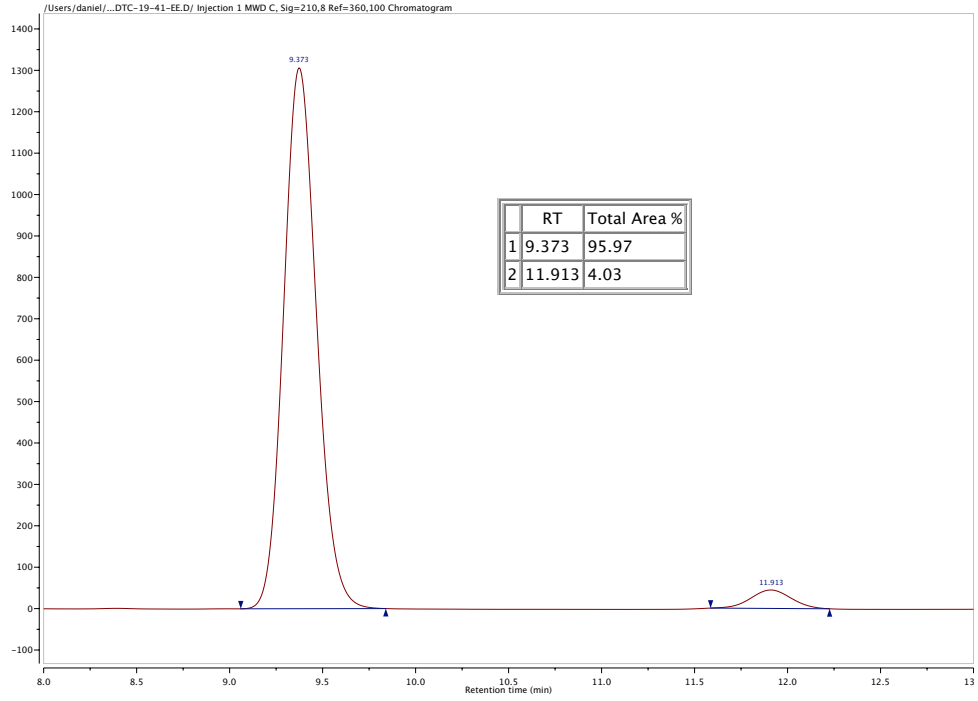

H3C
O
O
O
O
CH3
O
H3C
O
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

HPLC Traces of Racemic and Enantioenriched Cyclopentene 9

Racemic



Enantioenriched

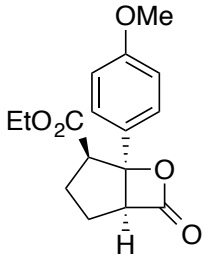


Computational Methods

Gas phase molecular geometries were obtained with B3LYP[7]/6-31G*[8] in Gaussian 09,[9] with SCS-MP2[10]/def2-TZVP[11] and /def2-QZVP extrapolated to an infinite basis set [12] (hereafter referred to as def2-∞ZVP) single point energy refinements computed in Turbomole 6.4. Energies of solvation were computed with B3LYP/6-31+G(d,p) using PCM[13] with UFF radii in dichloroethane.

[7] A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648.
[8] P. C. Hariharan and J. A. Pople, *Theoretica chimica acta*, 1973, **28**, 213.
[9] Gaussian 09, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.
[10] M. Gerenkamp and S. Grimme, *Chem. Phys. Lett.*, 2004, **392**, 229.
[11] a) A. Schäfer, C. Huber and R. Ahlrichs, *J. Chem. Phys.*, 1994, **100**, 5829; b) S. Zhong, E. C. Barnes and G. A. Petersson, *J. Chem. Phys.*, 2008, **129**, 184116.
[12] S. Zhong, E. C. Barnes and G. A. Petersson, *J. Chem. Phys.*, 2008, **129**, 184116.
[13] S. Miertuš, E. Scrocco and J. Tomasi, *Chem. Phys.*, 1981, **55**, 117.

Molecular Geometries and Energies of Compounds Reported



***(syn)*-2a**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.899665	-0.576294	-0.047802
C	0.593395	-0.417915	0.057276
C	-1.663699	0.403040	-0.982804
H	-1.023674	0.566008	-1.858909
C	-2.951822	-0.341509	-1.385121
H	-3.370908	0.036858	-2.321860
H	-3.709949	-0.186876	-0.611256
C	-2.537372	-1.822708	-1.466006
H	-2.060327	-2.042692	-2.429297
H	-3.381741	-2.509962	-1.352578
C	-1.501843	-1.985901	-0.343409
H	-0.801034	-2.813607	-0.471592
C	-2.064943	-1.855682	1.069965
O	-2.732963	-2.504861	1.818691
O	-1.545925	-0.597351	1.286731
C	-1.933446	1.760768	-0.348881
O	-3.031469	2.204357	-0.096760
O	-0.783013	2.421714	-0.108440
C	-0.928468	3.704504	0.525351
H	-1.432682	3.599103	1.489262
H	-1.508563	4.380882	-0.108115
H	0.086499	4.078734	0.660211
C	2.793201	-0.520314	-0.988084
H	3.389463	-0.716398	-1.871766
C	3.391509	-0.139309	0.219222
C	2.586642	0.097403	1.342417
H	3.066451	0.388204	2.271706
C	1.207205	-0.041340	1.260199
H	0.593259	0.139114	2.135671
O	4.733283	0.024345	0.403840
C	5.597042	-0.204481	-0.698125
H	5.381816	0.480039	-1.529422
H	6.607380	-0.017210	-0.330130
H	5.528726	-1.240059	-1.056970
C	1.405161	-0.655403	-1.055304
H	0.958605	-0.956930	-2.000813

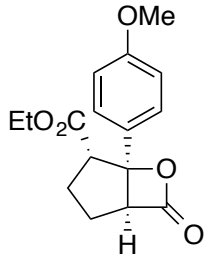
SCF Energy= -957.342074647 Predicted Change= -8.564827D-09

Zero-point correction (ZPE)=	-957.0519	0.29013
Internal Energy (U)=	-957.0336	0.30839
Enthalpy (H)=	-957.0327	0.30933
Gibbs Free Energy (G)=	-957.1003	0.24169

Frequencies -- 21.3288 30.3948 39.8145

E_{solv} = -0.014900792

$E_{SCS\text{-}MP2/\infty}$ = -956.059353



***(anti)*-2a**

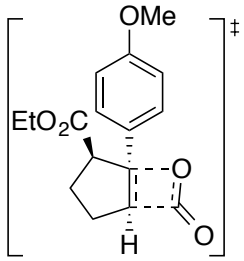
Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.125563	-0.571296	-0.184794
C	0.366731	-0.519853	0.010878
C	-1.839582	0.701232	-0.732796
H	-1.717434	0.732463	-1.818345
C	-3.315947	0.521001	-0.294775
H	-3.830869	-0.098230	-1.037151
H	-3.848627	1.473891	-0.232549
C	-3.250495	-0.203979	1.065709
H	-4.171882	-0.745508	1.302742
H	-3.056935	0.517772	1.863463
C	-2.044300	-1.148193	0.934490
H	-1.580087	-1.444180	1.877140
C	-2.261670	-2.284755	-0.059593
O	-2.860753	-3.318586	-0.107412
O	-1.505265	-1.711903	-1.058729
C	-1.238943	1.966552	-0.144531
O	-1.434314	2.371713	0.984823
O	-0.444684	2.592611	-1.032505
C	0.226258	3.767944	-0.543162
H	0.791436	4.154221	-1.391454
H	0.897091	3.504226	0.278387
H	-0.499528	4.505932	-0.192688
C	0.923803	0.057681	1.164803
C	2.300228	0.121454	1.336372
H	2.735247	0.560746	2.228615
C	3.159319	-0.399488	0.356872
C	2.617537	-0.983097	-0.793893
H	3.256670	-1.400928	-1.563160
C	1.231350	-1.037750	-0.955959
H	0.818290	-1.507242	-1.842757
H	0.275648	0.468715	1.933344
O	4.492906	-0.293711	0.621794
C	5.410106	-0.819608	-0.325293
H	5.320907	-0.315463	-1.296616
H	6.403772	-0.634995	0.086728
H	5.270197	-1.899488	-0.465422

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -957.343130117 Predicted Change= -3.410116D-09

Zero-point correction (ZPE)=	-957.0524	0.29068
Internal Energy (U)=	-957.0343	0.30875
Enthalpy (H)=	-957.0334	0.30970
Gibbs Free Energy (G)=	-957.0998	0.24325

Frequencies -- 28.5676 37.7136 52.7896
E_{solv} = -0.012402154
$E_{SCS\text{-}MP2/\infty}$ = -956.0617947



***(syn)*-TS3a**

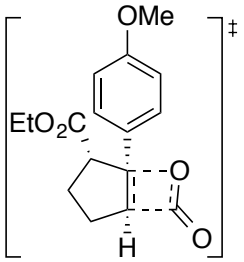
Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.731230	-0.541743	-0.573881
C	0.671848	-0.284050	-0.428886
C	-1.759785	0.445614	-1.100623
H	-1.346517	0.924799	-1.999936
C	-3.014918	-0.402670	-1.439974
H	-3.436597	-0.124386	-2.409792
H	-3.778709	-0.205092	-0.685179
C	-2.554041	-1.873159	-1.383220
H	-2.237086	-2.232878	-2.370643
H	-3.332472	-2.545619	-1.011020
C	-1.367054	-1.839997	-0.416755
H	-0.714432	-2.712758	-0.454565
C	-1.898776	-1.668391	1.155274
O	-2.611766	-2.570081	1.563351
O	-1.469212	-0.603954	1.667499
C	-2.099424	1.587825	-0.120414
O	-3.221592	1.861386	0.230943
O	-1.007335	2.280044	0.242485
C	-1.228931	3.289499	1.245784
H	-1.616986	2.825102	2.154998
H	-1.938257	4.038790	0.885689
H	-0.251399	3.736735	1.427389
C	1.293274	0.873082	-0.966088
H	0.694122	1.625702	-1.462091
C	2.657446	1.060412	-0.879233
H	3.135511	1.935842	-1.306164
C	3.462416	0.112654	-0.219065
C	2.870686	-1.033228	0.343541
H	3.467275	-1.766555	0.872792
C	1.504361	-1.223276	0.225887
H	1.059724	-2.096872	0.688344
O	4.781317	0.392676	-0.177411
C	5.662824	-0.516277	0.479560
H	5.643273	-1.502849	0.001789
H	6.658479	-0.082766	0.380240
H	5.410594	-0.615517	1.541785

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -957.296640488 Predicted Change= -2.905245D-09
Zero-point correction (ZPE)= -957.0093 0.28725
Internal Energy (U)= -956.9907 0.30589
Enthalpy (H)= -956.9897 0.30684
Gibbs Free Energy (G)= -957.0577 0.23884

Frequencies -- -549.4244 31.2267 42.4267

E_{solv} = -0.025875457
$E_{SCS\text{-}MP2/\infty}$ = -955.9993388



***(anti)*-TS3a**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.830381	-0.504426	0.069497
C	0.574812	-0.238102	0.003389
C	-1.890739	0.413474	-0.521523
H	-1.720364	0.596993	-1.583508
C	-3.232748	-0.328049	-0.246903
H	-3.459131	-0.951471	-1.115373
H	-4.065015	0.365332	-0.095832
C	-2.938988	-1.202219	0.986854
H	-3.583299	-2.084142	1.046275
H	-3.053819	-0.621597	1.908450
C	-1.470508	-1.601188	0.777203
H	-0.959561	-2.011454	1.647314
C	-1.414635	-2.722988	-0.462438
O	-1.049448	-2.189796	-1.540151
O	-1.757813	-3.853025	-0.158558
C	-1.883657	1.748759	0.223141
O	-1.991799	1.878561	1.422947
O	-1.773455	2.786330	-0.635796
C	-1.805429	4.092881	-0.029356
H	-2.744513	4.239007	0.509817
H	-1.721321	4.798325	-0.856023
H	-0.971617	4.210782	0.667342
C	1.504537	-1.078820	0.659191
H	1.150222	-1.947060	1.203319
C	2.867059	-0.836322	0.612990
H	3.546301	-1.507377	1.124806
C	3.349863	0.274435	-0.103103
C	2.445159	1.124588	-0.768836
H	2.842428	1.970272	-1.320294
C	1.090882	0.868516	-0.721250
H	0.414881	1.532490	-1.248378
O	4.651741	0.607641	-0.212535
C	5.633737	-0.212056	0.419355
H	5.612650	-1.233239	0.021505
H	6.594002	0.249905	0.188017
H	5.490555	-0.235361	1.506043

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

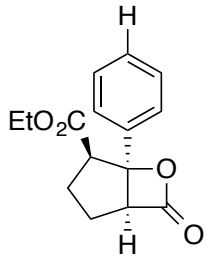
SCF Energy= -957.298763099 Predicted Change= -4.597832D-09

Zero-point correction (ZPE)=	-957.0110	0.28767
Internal Energy (U)=	-956.9924	0.30630
Enthalpy (H)=	-956.9915	0.30724
Gibbs Free Energy (G)=	-957.0597	0.23897

Frequencies -- -592.0414 27.2230 35.3647

E_{solv} = -0.024944837

$E_{SCS\text{-}MP2/\infty}$ = -956.0019535



***(syn)*-2b**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.284516	-0.568349	-0.066455
C	1.219854	-0.491644	-0.070018
C	-1.058301	0.461092	-0.934944
H	-0.474163	0.605606	-1.852588
C	-2.407529	-0.211864	-1.256366
H	-2.867866	0.200235	-2.158731
H	-3.104121	-0.029819	-0.432176
C	-2.075480	-1.710411	-1.381235
H	-1.675981	-1.939936	-2.376953
H	-2.943904	-2.356441	-1.218194
C	-0.975905	-1.942108	-0.333855
H	-0.329400	-2.802515	-0.519268
C	-1.433199	-1.802921	1.116463
O	-2.080527	-2.426997	1.903336
O	-0.836156	-0.574881	1.309060
C	-1.213248	1.822776	-0.271008
O	-2.269703	2.335074	0.024160
O	-0.013107	2.400340	-0.062728
C	-0.048750	3.684007	0.585196
H	-0.521956	3.603053	1.567023
H	-0.606067	4.403007	-0.021084
H	0.993252	3.988822	0.683366
C	1.924167	-0.725689	-1.259484
H	1.384232	-0.957085	-2.175444
C	3.316782	-0.672242	-1.281434
H	3.848534	-0.859111	-2.210544
C	4.024791	-0.384371	-0.112448
H	5.110491	-0.343598	-0.128028
C	3.329478	-0.153325	1.074511
H	3.872171	0.069001	1.989447
C	1.934735	-0.207782	1.097989
H	1.393464	-0.032517	2.021072

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

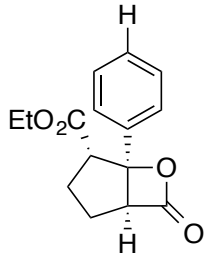
SCF Energy= -842.819466143 Predicted Change= -1.618595D-08

Zero-point correction (ZPE)=	-842.5619	0.25749
Internal Energy (U)=	-842.5463	0.27311
Enthalpy (H)=	-842.5454	0.27405
Gibbs Free Energy (G)=	-842.6068	0.21258

Frequencies -- 23.7926 31.8948 49.7944

E_{solv} = -0.013076256

$E_{SCS\text{-}MP2/\infty}$ = -841.6686078



***(anti)*-2b**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.747820	-0.343477	-0.180216
C	0.597921	-0.992003	0.022018
C	-0.773451	1.115284	-0.726332
H	-0.641334	1.087570	-1.810726
C	-2.165194	1.650138	-0.300488
H	-2.904024	1.348738	-1.050775
H	-2.186954	2.741409	-0.235528
C	-2.462172	0.976525	1.055708
H	-3.532507	0.928840	1.280196
H	-1.962820	1.522018	1.860726
C	-1.838284	-0.423302	0.929561
H	-1.575964	-0.902683	1.874581
C	-2.554742	-1.325050	-0.071208
O	-1.607985	-1.173525	-1.061549
O	-3.568386	-1.956299	-0.128493
C	0.346054	1.949507	-0.126262
O	0.358348	2.388624	1.007082
O	1.342277	2.140927	-1.010169
C	2.482036	2.865637	-0.513270
H	2.183513	3.857222	-0.164018
H	3.167215	2.943346	-1.357406
H	2.946583	2.318427	0.310895
C	1.332821	-0.759353	1.193444
H	0.927115	-0.116683	1.969409
C	2.590005	-1.340606	1.363798
H	3.147261	-1.156358	2.278402
C	3.124029	-2.163162	0.370404
H	4.100759	-2.619599	0.506541
C	2.393751	-2.402555	-0.794752
H	2.799241	-3.047253	-1.569866
C	1.137608	-1.821322	-0.969072
H	0.562512	-2.020371	-1.867401

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

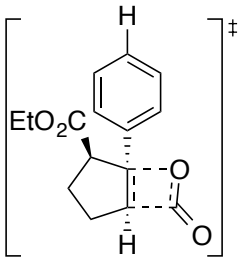
SCF Energy= -842.820071910 Predicted Change= -1.289883D-07

Zero-point correction (ZPE)=	-842.5620	0.25804
Internal Energy (U)=	-842.5466	0.27346
Enthalpy (H)=	-842.5456	0.27440
Gibbs Free Energy (G)=	-842.6057	0.21433

Frequencies -- 35.8631 49.5705 54.5701

E_{solv} = -0.01087943

$E_{SCS\text{-}MP2/\infty}$ = -841.6705523



***(syn)*-TS3b**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.122112	-0.555630	0.536604
C	-1.302079	-0.421720	0.310999
C	1.034349	0.520156	1.097204
H	0.550683	0.927192	1.997914
C	2.357556	-0.205287	1.456395
H	2.759343	0.140259	2.412695
H	3.098597	0.030177	0.689617
C	2.018610	-1.708726	1.448941
H	1.708290	-2.056744	2.442628
H	2.856807	-2.329378	1.119296
C	0.853235	-1.801491	0.461493
H	0.270743	-2.722094	0.488690
C	1.425026	-1.599256	-1.116884
O	2.208134	-2.451046	-1.489265
O	0.935670	-0.567327	-1.638846
C	1.277065	1.717361	0.157081
O	2.374502	2.107000	-0.161416
O	0.129616	2.306193	-0.214329
C	0.269826	3.375736	-1.169682
H	0.737963	2.998550	-2.081509
H	0.878227	4.182631	-0.753692
H	-0.745143	3.719079	-1.370139
C	-2.048670	0.624078	0.895593
H	-1.546487	1.392378	1.469863
C	-3.431312	0.674233	0.752663
H	-3.991782	1.476498	1.223673
C	-4.094641	-0.296828	-0.000339
H	-5.173599	-0.249332	-0.119243
C	-3.368398	-1.327719	-0.606979
H	-3.879175	-2.074478	-1.207575
C	-1.991996	-1.396974	-0.446186
H	-1.431937	-2.180911	-0.942798

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

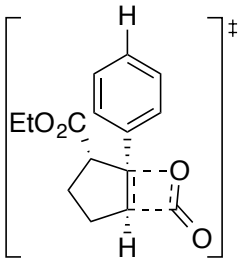
SCF Energy= -842.768810382 Predicted Change= -9.121044D-09

Zero-point correction (ZPE)=	-842.5146	0.25411
Internal Energy (U)=	-842.4985	0.27022
Enthalpy (H)=	-842.4976	0.27116
Gibbs Free Energy (G)=	-842.5598	0.20900

Frequencies -- -637.2643 35.2215 42.0718

E_{solv} = -0.021359966

$E_{SCS\text{-}MP2/\infty}$ = -841.6046034



***(anti)*-TS3b**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.343571	-0.405414	0.083301
C	0.798866	0.966160	0.072688
C	-0.955719	-0.862753	-0.560269
H	-1.010284	-0.583526	-1.613409
C	-0.965656	-2.405180	-0.341374
H	-0.503756	-2.875349	-1.213279
H	-1.979812	-2.801179	-0.237540
C	-0.099382	-2.616706	0.914779
H	0.365213	-3.606314	0.948616
H	-0.692996	-2.477128	1.824404
C	0.956951	-1.510559	0.785758
H	1.549582	-1.295146	1.672985
C	2.007173	-1.948971	-0.466951
O	1.749107	-1.302152	-1.511869
O	2.805931	-2.821110	-0.185854
C	-2.135972	-0.237496	0.186339
O	-2.309411	-0.294650	1.384089
O	-2.989876	0.363694	-0.669137
C	-4.163436	0.940852	-0.062844
H	-4.742756	0.170758	0.452117
H	-4.735099	1.367353	-0.886979
H	-3.879875	1.714779	0.654700
C	1.961909	1.345903	0.781257
H	2.534019	0.598207	1.318912
C	2.392710	2.665271	0.782017
H	3.290691	2.939506	1.327490
C	1.674014	3.637959	0.078797
H	2.013304	4.670114	0.080693
C	0.523314	3.282414	-0.629646
H	-0.032264	4.035537	-1.180582
C	0.091297	1.961444	-0.638576
H	-0.799814	1.698589	-1.197630

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

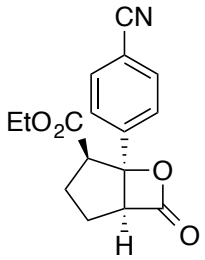
SCF Energy= -842.770601903 Predicted Change= -1.100520D-08

Zero-point correction (ZPE)=	-842.5160	0.25460
Internal Energy (U)=	-842.4999	0.27066
Enthalpy (H)=	-842.4989	0.27160
Gibbs Free Energy (G)=	-842.5614	0.20914

Frequencies -- -668.3250 27.0736 37.7094

E_{solv} = -0.020522123

$E_{SCS\text{-}MP2/\infty}$ = -841.6067542



***(syn)*-2c**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.790511	-0.569240	-0.064040
C	0.710339	-0.445777	-0.053113
C	-1.583713	0.432847	-0.944703
H	-0.999285	0.590113	-1.860444
C	-2.909984	-0.281268	-1.273765
H	-3.374726	0.114879	-2.180592
H	-3.618507	-0.117761	-0.455885
C	-2.532106	-1.769447	-1.391243
H	-2.117619	-1.990802	-2.382552
H	-3.381548	-2.441032	-1.232665
C	-1.435324	-1.966091	-0.333092
H	-0.762964	-2.808431	-0.509971
C	-1.909439	-1.836049	1.113019
O	-2.543613	-2.474504	1.897111
O	-1.349677	-0.587161	1.304844
C	-1.782750	1.795038	-0.291549
O	-2.857592	2.301315	-0.062655
O	-0.599249	2.377442	-0.014814
C	-0.677037	3.668482	0.618126
H	-1.205754	3.593707	1.571526
H	-1.201192	4.378066	-0.027105
H	0.356338	3.978761	0.772699
C	2.821405	-0.549535	-1.248961
H	3.376616	-0.709760	-2.167409
C	3.510444	-0.243978	-0.063070
C	2.790554	-0.044680	1.125263
H	3.322389	0.189186	2.041858
C	1.402639	-0.147448	1.125940
H	0.846219	0.004398	2.043490
C	1.435374	-0.648302	-1.236774
H	0.915854	-0.890659	-2.160557
C	4.940391	-0.138524	-0.068831
N	6.100503	-0.051937	-0.075361

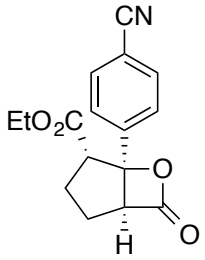
Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -935.062014156 Predicted Change= -1.485578D-08
Zero-point correction (ZPE)= -934.8060 0.25599
Internal Energy (U)= -934.7885 0.27343
Enthalpy (H)= -934.7876 0.27438
Gibbs Free Energy (G)= -934.8533 0.20866

Frequencies -- 27.7741 34.9776 39.6901

E_{solv} = -0.017854208

$E_{SCS\text{-}MP2/\infty}$ = -933.7957567



***(anti)*-2c**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.040313	-0.553747	-0.190801
C	0.462053	-0.600601	-0.069394
C	-1.686421	0.777391	-0.676814
H	-1.614102	0.828570	-1.765878
C	-3.151700	0.680684	-0.173452
H	-3.737815	0.112702	-0.903663
H	-3.618469	1.663921	-0.069440
C	-3.071922	-0.076490	1.168165
H	-4.014675	-0.563140	1.437146
H	-2.795105	0.611920	1.970679
C	-1.938284	-1.095012	0.962450
H	-1.452105	-1.440952	1.876684
C	-2.276025	-2.193873	-0.041289
O	-2.941712	-3.184383	-0.082628
O	-1.528051	-1.645287	-1.065473
C	-0.983636	1.989371	-0.086875
O	-1.052244	2.334018	1.077057
O	-0.262525	2.640377	-1.016045
C	0.471630	3.786877	-0.544207
H	0.970093	4.193837	-1.423673
H	1.203490	3.483385	0.208423
H	-0.208669	4.522338	-0.108192
C	1.103657	-0.084004	1.066507
C	2.490726	-0.110539	1.169368
H	2.982668	0.286649	2.051305
C	3.260395	-0.661950	0.131976
C	2.622514	-1.187418	-1.003283
H	3.216899	-1.619803	-1.801583
C	1.234950	-1.156159	-1.097679
H	0.741692	-1.578299	-1.966297
H	0.517940	0.350593	1.870153
C	4.690573	-0.689902	0.234571
N	5.850748	-0.708183	0.317941

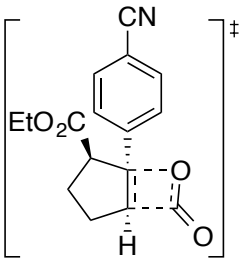
Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy=	-935.062366287	Predicted Change= -2.217380D-08
Zero-point correction (ZPE)=	-934.8059	0.25642
Internal Energy (U)=	-934.7886	0.27375
Enthalpy (H)=	-934.7876	0.27469
Gibbs Free Energy (G)=	-934.8528	0.20951

Frequencies -- 21.7873 41.4729 53.4631

E_{solv} = -0.015335828

$E_{SCS\text{-}MP2/\infty}$ = -933.7973863



***(syn)*-TS3c**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.668371	-0.547238	0.542673
C	-0.763357	-0.387738	0.339990
C	1.611050	0.522482	1.058335
H	1.162719	0.934306	1.975701
C	2.936294	-0.216781	1.375425
H	3.394382	0.154484	2.295799
H	3.640386	-0.025102	0.562608
C	2.566018	-1.711200	1.440664
H	2.286766	-2.014037	2.457895
H	3.377427	-2.362836	1.104308
C	1.360668	-1.812475	0.504301
H	0.758037	-2.717864	0.572278
C	1.880417	-1.659758	-1.111759
O	2.643354	-2.525085	-1.483947
O	1.374346	-0.638058	-1.638079
C	1.827854	1.715143	0.106997
O	2.913393	2.075944	-0.277206
O	0.673670	2.330342	-0.194737
C	0.782216	3.413499	-1.141323
H	1.192824	3.043527	-2.083188
H	1.428132	4.200925	-0.745601
H	-0.235151	3.779022	-1.279856
C	-1.481282	0.652360	0.965396
H	-0.958737	1.400542	1.547276
C	-2.862947	0.731095	0.855481
H	-3.407747	1.526251	1.353228
C	-3.560406	-0.216591	0.089274
C	-2.855920	-1.247124	-0.560720
H	-3.394934	-1.967681	-1.166460
C	-1.480209	-1.333190	-0.427158
H	-0.942549	-2.110107	-0.957274
C	-4.985581	-0.130454	-0.033455
N	-6.142683	-0.059822	-0.129954

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

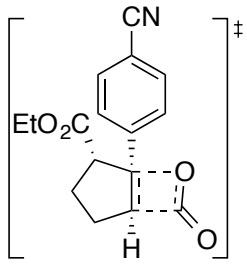
SCF Energy= -935.008185308 Predicted Change= -1.447063D-10

Zero-point correction (ZPE)=	-934.7558	0.25236
Internal Energy (U)=	-934.7378	0.27034
Enthalpy (H)=	-934.7368	0.27129
Gibbs Free Energy (G)=	-934.8036	0.20456

Frequencies -- -690.8340 33.8678 41.2570

E_{solv} = -0.023688736

$E_{SCS\text{-}MP2/\infty}$ = -933.730019



***(anti)*-TS3c**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.762869	-0.488657	0.081247
C	0.682543	-0.363401	0.058313
C	-1.701068	0.520348	-0.559078
H	-1.474803	0.679807	-1.614453
C	-3.118811	-0.082519	-0.326159
H	-3.374531	-0.697208	-1.193498
H	-3.883980	0.691429	-0.221195
C	-2.960303	-0.955907	0.933369
H	-3.679502	-1.778887	0.972137
H	-3.067279	-0.353922	1.841694
C	-1.524942	-1.478804	0.800510
H	-1.083212	-1.943577	1.680164
C	-1.505041	-2.619306	-0.467573
O	-0.964573	-2.132648	-1.490866
O	-2.029558	-3.680738	-0.204862
C	-1.585579	1.853652	0.186066
O	-1.702763	1.988827	1.384119
O	-1.365088	2.871562	-0.670542
C	-1.291158	4.180495	-0.067666
H	-2.227037	4.414612	0.444953
H	-1.120223	4.869853	-0.894130
H	-0.468656	4.222135	0.650454
C	1.497633	-1.281939	0.756488
H	1.045698	-2.107528	1.293932
C	2.877133	-1.157398	0.753796
H	3.494706	-1.869650	1.290294
C	3.483629	-0.101123	0.049188
C	2.688961	0.819344	-0.654626
H	3.160867	1.628633	-1.201483
C	1.308354	0.684128	-0.651799
H	0.711463	1.401556	-1.203107
C	4.909968	0.036965	0.049469
N	6.067379	0.153064	0.051740

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

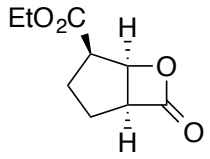
SCF Energy= -935.009456865 Predicted Change= -1.148036D-09

Zero-point correction (ZPE)=	-934.7565	0.25286
Internal Energy (U)=	-934.7386	0.27081
Enthalpy (H)=	-934.7376	0.27175
Gibbs Free Energy (G)=	-934.8048	0.20464

Frequencies -- -717.6194 25.3047 36.6871

E_{solv} = -0.02264074

$E_{SCS\text{-}MP2/\infty}$ = -933.7315975



***(syn)*-2d**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.527658	-0.313113	-0.963550
C	0.337244	0.848158	-0.453900
H	0.608335	1.444573	-1.337262
C	-0.597953	1.656757	0.466314
H	-0.264723	2.689910	0.594742
H	-0.610046	1.198562	1.460357
C	-1.979352	1.549613	-0.212393
H	-2.069784	2.284552	-1.021535
H	-2.811108	1.716134	0.478973
C	-2.001896	0.132737	-0.818933
H	-2.676174	0.006410	-1.668905
C	-2.061933	-1.001162	0.208761
O	-2.871587	-1.496831	0.933922
O	-0.733884	-1.346892	0.066822
C	1.631366	0.400465	0.205297
O	1.975284	0.675429	1.331996
O	2.364470	-0.348133	-0.647394
C	3.602566	-0.853842	-0.116248
H	3.413122	-1.483540	0.756514
H	4.259817	-0.029654	0.173111
H	4.049076	-1.437004	-0.921909
H	-0.187077	-0.776206	-1.888939

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

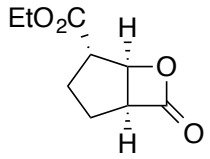
SCF Energy= -611.766157398 Predicted Change= -1.318925D-06

Zero-point correction (ZPE)=	-611.5889	0.17716
Internal Energy (U)=	-611.5781	0.18799
Enthalpy (H)=	-611.5772	0.18894
Gibbs Free Energy (G)=	-611.6267	0.13941

Frequencies -- 38.4476 62.1701 112.8694

E_{solv} = -0.012654385

$E_{SCS\text{-}MP2/\infty}$ = -611.3703829



***(anti)*-2d**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.519774	-0.800470	-0.153132
C	-0.342738	0.061773	0.783821
H	-0.464115	-0.453713	1.743135
C	0.434586	1.390834	0.899189
H	1.204064	1.290947	1.672278
H	-0.218390	2.221718	1.174271
C	1.082235	1.588156	-0.488863
H	1.964158	2.235379	-0.461864
H	0.356472	2.032405	-1.177668
C	1.423266	0.162217	-0.961627
H	1.486724	0.038520	-2.045053
C	2.549538	-0.518667	-0.180453
O	3.740806	-0.459294	-0.107341
O	1.702934	-1.334023	0.543048
C	-1.734715	0.262038	0.192070
O	-2.193975	1.313400	-0.198393
O	-2.408377	-0.907675	0.151511
C	-3.740319	-0.838541	-0.389930
H	-4.124740	-1.857704	-0.348768
H	-3.716842	-0.475606	-1.420684
H	-4.360971	-0.167707	0.209467
H	-0.007239	-1.607543	-0.662158

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

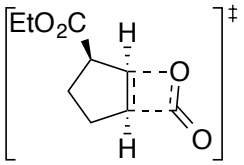
SCF Energy= -611.766435478 Predicted Change= -1.467407D-08

Zero-point correction (ZPE)=	-611.5892	0.17723
Internal Energy (U)=	-611.5783	0.18804
Enthalpy (H)=	-611.5774	0.18898
Gibbs Free Energy (G)=	-611.6269	0.13945

Frequencies -- 34.1564 72.9554 100.7333

E_{solv} = -0.011271013

$E_{SCS\text{-}MP2/\infty}$ = -611.370721



***(syn)*-TS3d**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.504556	0.020062	1.184839
C	-0.300769	1.009526	0.406653
H	-0.637459	1.745249	1.160406
C	0.710826	1.650813	-0.572015
H	0.479043	2.698999	-0.775157
H	0.658526	1.114375	-1.523486
C	2.087063	1.446424	0.104753
H	2.336337	2.289024	0.763319
H	2.899781	1.339200	-0.619834
C	1.886189	0.168608	0.922110
H	2.621073	-0.126150	1.668714
C	1.765678	-1.218913	-0.202482
O	2.782389	-1.456086	-0.794777
O	0.594624	-1.665431	-0.152989
C	-1.565463	0.445866	-0.238373
O	-1.856567	0.578285	-1.402496
O	-2.321859	-0.187677	0.676266
C	-3.517753	-0.807956	0.164151
H	-3.258295	-1.565358	-0.579048
H	-4.169172	-0.059137	-0.293200
H	-4.000933	-1.264510	1.027881
H	0.060448	-0.610987	1.944564

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

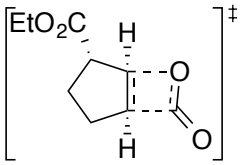
SCF Energy= -611.706032962 Predicted Change= -6.202190D-10

Zero-point correction (ZPE)=	-611.5333	0.17268
Internal Energy (U)=	-611.5219	0.18411
Enthalpy (H)=	-611.5209	0.18506
Gibbs Free Energy (G)=	-611.5718	0.13418

Frequencies -- -793.3788 49.3912 52.7238

E_{solv} = -0.01570163

$E_{SCS\text{-}MP2/\infty}$ = -611.2997325



***(anti)*-TS3d**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.379662	-0.719376	0.325348
C	0.345423	0.098211	-0.701156
H	0.383731	-0.423008	-1.665329
C	-0.426425	1.437793	-0.737219
H	-1.177045	1.392273	-1.531945
H	0.243495	2.274694	-0.941835
C	-1.114877	1.532675	0.645885
H	-2.062918	2.077095	0.607331
H	-0.467567	2.037045	1.374568
C	-1.321735	0.065870	1.030393
H	-1.604176	-0.200936	2.047210
C	-2.598774	-0.624013	-0.015670
O	-2.072375	-1.476747	-0.769230
O	-3.687537	-0.150621	0.165072
C	1.812683	0.272501	-0.256082
O	2.398870	1.326323	-0.194882
O	2.366029	-0.922430	0.029490
C	3.757521	-0.889609	0.407937
H	4.362169	-0.489195	-0.409289
H	4.025889	-1.925391	0.614254
H	3.895285	-0.267833	1.295730
H	-0.083693	-1.731267	0.569102

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

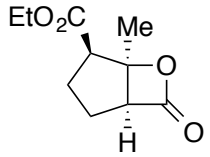
SCF Energy= -611.704906181 Predicted Change= -1.438706D-08

Zero-point correction (ZPE)=	-611.5320	0.17290
Internal Energy (U)=	-611.5205	0.18437
Enthalpy (H)=	-611.5195	0.18532
Gibbs Free Energy (G)=	-611.5711	0.13380

Frequencies -- -810.5918 30.5916 53.5322

E_{solv} = -0.015481563

$E_{SCS\text{-}MP2/\infty}$ = -611.298722



***(syn)*-2e**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.550774	-0.658112	-0.535872
C	-0.155083	-1.930890	-1.251173
C	0.345525	0.588784	-0.745154
H	0.644977	0.588333	-1.801852
C	-0.567344	1.795409	-0.447194
H	-0.212380	2.710955	-0.928802
H	-0.569728	1.982283	0.631136
C	-1.960884	1.358547	-0.937343
H	-2.056018	1.503468	-2.020635
H	-2.775063	1.911195	-0.458176
C	-2.015099	-0.145037	-0.624232
H	-2.718798	-0.718115	-1.233443
C	-2.050998	-0.489738	0.864867
O	-2.840958	-0.445384	1.761675
O	-0.742524	-0.911214	0.917891
C	1.615255	0.583113	0.093514
O	1.862605	1.355113	0.991465
O	2.457452	-0.399542	-0.300437
C	3.677275	-0.502846	0.457145
H	3.457219	-0.705252	1.508245
H	4.250941	0.424616	0.384624
H	4.227958	-1.331760	0.011878
H	-0.135628	-1.766708	-2.334639
H	0.839423	-2.257848	-0.937021
H	-0.872738	-2.728329	-1.033409

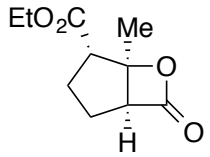
Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy=	-651.086734965	Predicted Change= -1.340264D-08
Zero-point correction (ZPE)=	-650.8819	0.20475
Internal Energy (U)=	-650.8696	0.21711
Enthalpy (H)=	-650.8686	0.21806
Gibbs Free Energy (G)=	-650.9211	0.16563

Frequencies -- 36.3778 59.0412 109.3810

E_{solv} = -0.012646663

$E_{SCS\text{-}MP2/\infty}$ = -650.6610849



***(anti)*-2e**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.596170	-0.688377	0.096712
C	-0.003816	-1.905160	0.775193
C	0.357003	0.210733	-0.734369
H	0.504711	-0.237565	-1.720154
C	-0.374142	1.577311	-0.798640
H	-1.086403	1.555660	-1.630536
H	0.313222	2.409250	-0.974755
C	-1.116150	1.702371	0.548722
H	-1.970331	2.385221	0.501026
H	-0.428619	2.058666	1.320326
C	-1.542557	0.263045	0.880635
H	-1.708148	0.065922	1.942436
C	-2.612965	-0.300575	-0.051312
O	-3.789857	-0.176660	-0.226846
O	-1.738908	-1.088409	-0.766771
C	1.710048	0.338984	-0.055119
O	1.941503	1.016272	0.926086
O	2.641935	-0.419229	-0.670525
C	3.955889	-0.382830	-0.084016
H	4.569420	-1.036863	-0.703690
H	3.925811	-0.744540	0.947134
H	4.349010	0.636876	-0.091339
H	0.492706	-2.554943	0.046942
H	0.729841	-1.604546	1.530602
H	-0.791441	-2.481933	1.269618

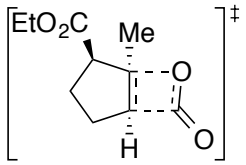
Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy=	-651.086446805	Predicted Change= -1.710189D-08
Zero-point correction (ZPE)=	-650.8813	0.20507
Internal Energy (U)=	-650.8690	0.21738
Enthalpy (H)=	-650.8681	0.21832
Gibbs Free Energy (G)=	-650.9206	0.16583

Frequencies -- 27.7645 67.5595 99.2661

E_{solv} = -0.010970117

$E_{SCS\text{-}MP2/\infty}$ = -650.6616946



***(syn)*-TS3e**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.756844	1.061852	0.205284
C	-0.603269	2.369139	-0.474208
C	0.335403	0.410495	1.022009
H	0.518956	1.125122	1.844039
C	-0.301763	-0.884531	1.579903
H	0.095181	-1.143939	2.564858
H	-0.077203	-1.712400	0.903817
C	-1.818171	-0.591448	1.585697
H	-2.127983	-0.101412	2.518543
H	-2.422614	-1.494940	1.463999
C	-1.980508	0.354860	0.395432
H	-2.919184	0.892307	0.263286
C	-1.724503	-0.574059	-1.068036
O	-2.579235	-1.398577	-1.281951
O	-0.653061	-0.214373	-1.611249
C	1.667242	0.314657	0.276140
O	2.264851	1.282740	-0.144155
O	2.096740	-0.947250	0.163282
C	3.312809	-1.121777	-0.589859
H	4.127593	-0.553056	-0.135338
H	3.164389	-0.786061	-1.618633
H	3.520124	-2.191119	-0.559050
H	0.366271	2.452898	-0.967825
H	-1.416552	2.546164	-1.180838
H	-0.645721	3.150990	0.301565

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

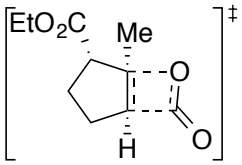
SCF Energy= -651.032937939 Predicted Change= -5.390633D-09

Zero-point correction (ZPE)=	-650.8320	0.20091
Internal Energy (U)=	-650.8191	0.21380
Enthalpy (H)=	-650.8181	0.21474
Gibbs Free Energy (G)=	-650.8719	0.16095

Frequencies -- -705.9702 34.4721 61.6065

E_{solv} = -0.016714969

$E_{SCS\text{-}MP2/\infty}$ = -650.5950795



***(anti)*-TS3e**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.596755	0.777852	0.179344
C	0.518085	2.255737	0.232505
C	-0.412310	-0.075986	-0.556679
H	-0.461015	0.175087	-1.619704
C	0.073644	-1.539570	-0.307319
H	0.728026	-1.831660	-1.133486
H	-0.756488	-2.249546	-0.272283
C	0.874663	-1.454853	1.010590
H	1.657165	-2.216465	1.075077
H	0.217528	-1.564384	1.882521
C	1.466350	-0.045727	0.951384
H	1.936654	0.375796	1.839137
C	2.677412	-0.032776	-0.312112
O	2.269544	0.659846	-1.274857
O	3.653084	-0.699733	-0.067956
C	-1.800097	0.130637	0.049642
O	-2.032711	0.628522	1.131923
O	-2.745315	-0.359010	-0.771978
C	-4.097427	-0.282493	-0.279177
H	-4.197196	-0.848114	0.650538
H	-4.715703	-0.717741	-1.063977
H	-4.378132	0.757856	-0.097724
H	1.455122	2.693936	0.581506
H	0.252401	2.684913	-0.737241
H	-0.277618	2.506405	0.949512

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

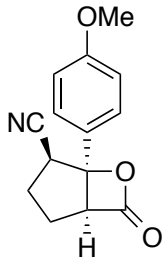
SCF Energy= -651.031310175 Predicted Change= -1.820783D-09

Zero-point correction (ZPE)=	-650.8303	0.20091
Internal Energy (U)=	-650.8173	0.21393
Enthalpy (H)=	-650.8164	0.21487
Gibbs Free Energy (G)=	-650.8708	0.16050

Frequencies -- -728.3993 35.2388 52.0656

E_{solv} = -0.015665419

$E_{SCS\text{-}MP2/\infty}$ = -650.593945



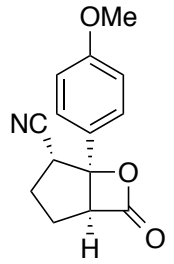
Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.175451	-0.066535	0.053038
C	-0.325675	0.050372	0.079366
C	1.770257	-1.440257	0.434832
H	1.165846	-2.185841	-0.102629
C	3.181959	-1.430892	-0.193093
H	3.579579	-2.441252	-0.333689
H	3.878545	-0.897817	0.466348
C	3.011665	-0.665774	-1.521140
H	2.606107	-1.327501	-2.296591
H	3.946887	-0.244381	-1.903558
C	1.975753	0.424028	-1.193224
H	1.414125	0.808387	-2.047266
C	2.489450	1.495492	-0.236210
O	3.227419	2.436581	-0.276618
O	1.812921	1.012172	0.858774
C	-2.499017	-0.601858	-0.815641
H	-3.067439	-1.178639	-1.536140
C	-3.139324	0.220774	0.119467
C	-2.369068	0.957384	1.029773
H	-2.880178	1.593055	1.746081
C	-0.982374	0.872712	1.007159
H	-0.395052	1.453291	1.710201
O	-4.491330	0.373717	0.222964
C	-5.320625	-0.346959	-0.674360
H	-5.188838	-1.431607	-0.563835
H	-6.346402	-0.080581	-0.413330
H	-5.128158	-0.065270	-1.718198
C	-1.104984	-0.678644	-0.824655
H	-0.625213	-1.319572	-1.561325
C	1.722347	-1.751198	1.930834
H	0.691271	-1.753236	2.301231
H	2.155909	-2.736472	2.136008
H	2.286042	-1.004189	2.498859

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -768.787817231 Predicted Change= -3.454760D-08
Zero-point correction (ZPE)= -768.5122 0.27560
Internal Energy (U)= -768.4971 0.29065
Enthalpy (H)= -768.4962 0.29159
Gibbs Free Energy (G)= -768.5549 0.23283

Frequencies -- 28.6658 50.9944 69.2970

E_{solv} = -0.015515356
$E_{SCS\text{-}MP2/\infty}$ = -821.1142395



Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.201714	0.012560	-0.201981
C	-0.290999	0.001417	-0.010224
C	1.854762	-1.176477	-0.952286
H	1.736696	-1.007732	-2.029410
C	3.345991	-1.090003	-0.534273
H	3.867150	-0.351738	-1.153866
H	3.867409	-2.044536	-0.660057
C	3.322691	-0.617952	0.935633
H	4.261069	-0.149574	1.249434
H	3.132466	-1.457626	1.614367
C	2.140890	0.364867	0.992198
H	1.699894	0.512696	1.979971
C	2.391995	1.647903	0.204378
O	3.027011	2.653977	0.337724
O	1.622776	1.281926	-0.871211
C	-0.881142	-0.604038	1.110538
C	-2.260981	-0.639705	1.264732
H	-2.718940	-1.103431	2.132750
C	-3.093110	-0.061007	0.295327
C	-2.520526	0.552580	-0.825091
H	-3.138450	1.016904	-1.585126
C	-1.131572	0.577504	-0.966793
H	-0.695258	1.072855	-1.828561
H	-0.255224	-1.053689	1.877368
O	-4.432844	-0.143146	0.538089
C	-5.322876	0.432529	-0.405740
H	-5.226158	-0.040316	-1.391981
H	-6.327058	0.253813	-0.017259
H	-5.160105	1.513620	-0.506806
C	1.237326	-2.537753	-0.601422
H	0.176770	-2.579871	-0.865194
H	1.757202	-3.330920	-1.150053
H	1.322013	-2.767057	0.467646

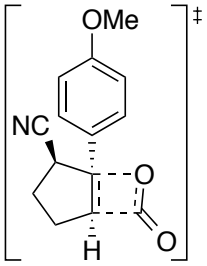
Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -768.783907129 Predicted Change= -7.189245D-09
Zero-point correction (ZPE)= -768.5081 0.27577
Internal Energy (U)= -768.4931 0.29073
Enthalpy (H)= -768.4922 0.29167
Gibbs Free Energy (G)= -768.5505 0.23331

Frequencies -- 34.0681 52.6720 77.6812

E_{solv} = -0.012842371

$E_{SCS\text{-}MP2/\infty}$ = -821.1150703



***(syn)*-TS3d**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.036407	0.044206	-0.472554
C	0.382876	0.114537	-0.320245
C	-1.960461	1.255114	-0.566320
H	-1.699839	1.738794	-1.524145
C	-3.391688	0.660717	-0.703780
H	-4.046155	1.326965	-1.271293
H	-3.815383	0.524553	0.293780
C	-3.142165	-0.698073	-1.379973
H	-3.053274	-0.585229	-2.468891
H	-3.935760	-1.423136	-1.179472
C	-1.810212	-1.150325	-0.763703
H	-1.302061	-1.967046	-1.274362
C	-2.115094	-1.601247	0.829572
O	-2.647013	-2.688660	0.961918
O	-1.757734	-0.696497	1.620961
C	1.077407	1.351262	-0.241001
H	0.530243	2.286508	-0.259188
C	2.451684	1.393638	-0.139317
H	2.984469	2.337018	-0.085834
C	3.195906	0.198550	-0.085166
C	2.531747	-1.041862	-0.141576
H	3.083500	-1.972426	-0.085456
C	1.153908	-1.072450	-0.261481
H	0.655554	-2.035256	-0.281443
O	4.529474	0.346409	0.023363
C	5.355571	-0.814775	0.110104
H	5.266151	-1.432111	-0.791334
H	6.376202	-0.441399	0.197014
H	5.106240	-1.411624	0.994830
C	-1.835706	2.275114	0.476735
N	-1.755986	3.125422	1.262582

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

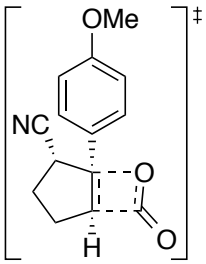
SCF Energy= -821.660325603 Predicted Change= -1.618803D-10

Zero-point correction (ZPE)=	-821.4175	0.24278
Internal Energy (U)=	-821.4016	0.25864
Enthalpy (H)=	-821.4007	0.25959
Gibbs Free Energy (G)=	-821.4618	0.19849

Frequencies -- -618.0876 39.4848 46.5785

E_{solv} = -0.017766138

$E_{SCS\text{-}MP2/\infty}$ = -821.0519291



***(anti)*-TS3d**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.077609	0.125524	-0.094822
C	-0.346906	0.147507	-0.023253
C	1.977257	1.204396	0.519753
H	1.782380	1.320225	1.590573
C	3.428009	0.710803	0.232967
H	3.752039	0.110049	1.085537
H	4.123564	1.543708	0.106937
C	3.279334	-0.166499	-1.023216
H	4.068177	-0.918764	-1.110087
H	3.291369	0.446327	-1.933645
C	1.904169	-0.823608	-0.823519
H	1.472779	-1.300998	-1.702228
C	2.055604	-1.956277	0.399453
O	1.635820	-1.492854	1.490190
O	2.562943	-3.015000	0.074341
C	-1.118219	-0.853030	-0.663898
H	-0.619123	-1.651382	-1.201746
C	-2.500244	-0.857603	-0.602844
H	-3.054165	-1.645343	-1.098870
C	-3.166702	0.158201	0.109483
C	-2.422095	1.165339	0.756858
H	-2.958716	1.936115	1.299515
C	-1.046047	1.153729	0.696909
H	-0.496801	1.938800	1.203983
O	-4.502878	0.253982	0.231946
C	-5.334117	-0.731350	-0.382530
H	-5.129584	-1.728785	0.022927
H	-6.357084	-0.441508	-0.141538
H	-5.200768	-0.737653	-1.470402
C	1.720546	2.491236	-0.147891
N	1.529952	3.507139	-0.677640

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

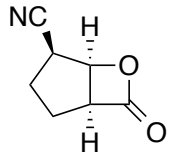
SCF Energy= -821.662031198 Predicted Change= -6.133344D-09

Zero-point correction (ZPE)=	-821.4190	0.24296
Internal Energy (U)=	-821.4032	0.25883
Enthalpy (H)=	-821.4022	0.25977
Gibbs Free Energy (G)=	-821.4636	0.19839

Frequencies -- -599.1291 32.2311 49.7146

E_{solv} = -0.014264308

$E_{SCS\text{-}MP2/\infty}$ = -821.0539874



***(syn)*-2d**

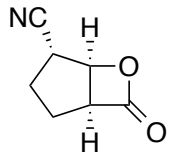
Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.036644	-0.269081	1.008732
C	-1.200217	0.511023	0.371330
H	-1.578167	1.197951	1.142395
C	-0.528098	1.345752	-0.753694
H	-1.144338	2.195974	-1.056373
H	-0.376204	0.715042	-1.635596
C	0.821440	1.759916	-0.133030
H	0.692228	2.631169	0.520019
H	1.572106	2.018175	-0.885757
C	1.245802	0.545858	0.716086
H	1.924143	0.774220	1.540586
C	1.628808	-0.691402	-0.102607
O	2.546692	-1.059862	-0.770128
O	0.447611	-1.359260	0.156026
H	-0.230250	-0.637472	2.016796
C	-2.318134	-0.323822	-0.069335
N	-3.213097	-0.973079	-0.422021

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -476.128578212 Predicted Change= -1.729369D-08
Zero-point correction (ZPE)= -475.9958 0.13277
Internal Energy (U)= -475.9877 0.14080
Enthalpy (H)= -475.9868 0.14174
Gibbs Free Energy (G)= -476.0290 0.09952

Frequencies -- 79.4877 132.3824 153.6379

E_{solv} = -0.016765537
$E_{SCS\text{-}MP2/\infty}$ = -475.8020758



***(anti)*-2d**

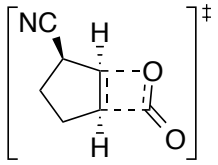
Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.012381	-0.904209	-0.299692
C	-1.082355	-0.352740	0.665875
H	-1.151724	-0.978791	1.562374
C	-0.582877	1.087344	0.986035
H	0.169910	1.020709	1.778521
H	-1.385826	1.736917	1.342310
C	0.054085	1.573263	-0.331943
H	0.776925	2.380240	-0.179985
H	-0.718820	1.939376	-1.016955
C	0.705051	0.312816	-0.931759
H	0.842667	0.337036	-2.014459
C	1.909321	-0.214287	-0.145690
O	3.054955	0.073854	0.022936
O	1.210957	-1.263752	0.425251
H	-0.339192	-1.729581	-0.932620
C	-2.391637	-0.335808	0.002521
N	-3.416640	-0.312142	-0.542395

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -476.130057133 Predicted Change= -1.720813D-07
Zero-point correction (ZPE)= -475.9973 0.13273
Internal Energy (U)= -475.9892 0.14077
Enthalpy (H)= -475.9883 0.14172
Gibbs Free Energy (G)= -476.0305 0.09946

Frequencies -- 82.0971 109.2521 163.8843

E_{solv} = -0.014381199
$E_{SCS\text{-}MP2/\infty}$ = -475.8042826



***(syn)*-TS3d**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.099193	0.029770	1.162964
C	-1.205760	0.615442	0.327317
H	-1.651460	1.386269	0.983852
C	-0.455695	1.335946	-0.832651
H	-1.026965	2.184375	-1.215748
H	-0.309606	0.626731	-1.652582
C	0.897411	1.728843	-0.198294
H	0.832869	2.705589	0.299415
H	1.701877	1.784902	-0.937542
C	1.138591	0.613853	0.820683
H	1.934487	0.697849	1.556816
C	1.479851	-0.917705	-0.102593
O	2.528235	-0.912073	-0.678174
O	0.488373	-1.667960	0.050992
H	-0.299254	-0.590008	2.028586
C	-2.283709	-0.291565	-0.067920
N	-3.163398	-0.977564	-0.386052

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

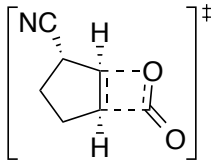
SCF Energy= -476.064168003 Predicted Change= -7.058537D-09

Zero-point correction (ZPE)=	-475.9359	0.12818
Internal Energy (U)=	-475.9273	0.13685
Enthalpy (H)=	-475.9263	0.13779
Gibbs Free Energy (G)=	-475.9702	0.09390

Frequencies -- -843.7129 59.6547 93.4813

E_{solv} = -0.027249056

$E_{SCS\text{-}MP2/\infty}$ = -475.7281364



***(anti)*-TS3d**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.174944	-0.748287	-0.585769
C	-1.084953	-0.389294	0.571061
H	-1.047782	-1.137282	1.369602
C	-0.572244	1.017199	1.014758
H	0.164741	0.870311	1.809817
H	-1.377179	1.640392	1.409785
C	0.102073	1.604570	-0.246679
H	0.923199	2.283134	0.002397
H	-0.617520	2.159913	-0.861230
C	0.595780	0.361733	-0.987357
H	0.965885	0.436579	-2.007172
C	1.950397	-0.371052	-0.027051
O	1.529465	-1.450767	0.453081
O	2.946600	0.291150	-0.008226
H	-0.271981	-1.688326	-1.115351
C	-2.455872	-0.342439	0.036358
N	-3.529900	-0.297482	-0.402659

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

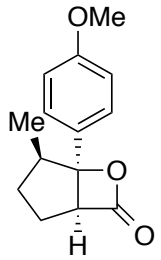
SCF Energy= -476.065091637 Predicted Change= -6.191872D-09

Zero-point correction (ZPE)=	-475.9366	0.12844
Internal Energy (U)=	-475.9279	0.13715
Enthalpy (H)=	-475.9269	0.13810
Gibbs Free Energy (G)=	-475.9710	0.09402

Frequencies -- -846.7863 60.3044 85.5107

E_{solv} = -0.024887874

$E_{SCS\text{-}MP2/\infty}$ = -475.7292272



***(syn)*-2d**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.175451	-0.066535	0.053038
C	-0.325675	0.050372	0.079366
C	1.770257	-1.440257	0.434832
H	1.165846	-2.185841	-0.102629
C	3.181959	-1.430892	-0.193093
H	3.579579	-2.441252	-0.333689
H	3.878545	-0.897817	0.466348
C	3.011665	-0.665774	-1.521140
H	2.606107	-1.327501	-2.296591
H	3.946887	-0.244381	-1.903558
C	1.975753	0.424028	-1.193224
H	1.414125	0.808387	-2.047266
C	2.489450	1.495492	-0.236210
O	3.227419	2.436581	-0.276618
O	1.812921	1.012172	0.858774
C	-2.499017	-0.601858	-0.815641
H	-3.067439	-1.178639	-1.536140
C	-3.139324	0.220774	0.119467
C	-2.369068	0.957384	1.029773
H	-2.880178	1.593055	1.746081
C	-0.982374	0.872712	1.007159
H	-0.395052	1.453291	1.710201
O	-4.491330	0.373717	0.222964
C	-5.320625	-0.346959	-0.674360
H	-5.188838	-1.431607	-0.563835
H	-6.346402	-0.080581	-0.413330
H	-5.128158	-0.065270	-1.718198
C	-1.104984	-0.678644	-0.824655
H	-0.625213	-1.319572	-1.561325
C	1.722347	-1.751198	1.930834
H	0.691271	-1.753236	2.301231
H	2.155909	-2.736472	2.136008
H	2.286042	-1.004189	2.498859

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

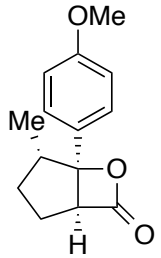
SCF Energy= -768.787817231 Predicted Change= -3.454760D-08

Zero-point correction (ZPE)=	-768.5122	0.27560
Internal Energy (U)=	-768.4971	0.29065
Enthalpy (H)=	-768.4962	0.29159
Gibbs Free Energy (G)=	-768.5549	0.23283

Frequencies -- 28.6658 50.9944 69.2970

E_{solv} = -0.010359111

$E_{SCS\text{-}MP2/\infty}$ = -768.2309019



***(anti)*-2d**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.201714	0.012560	-0.201981
C	-0.290999	0.001417	-0.010224
C	1.854762	-1.176477	-0.952286
H	1.736696	-1.007732	-2.029410
C	3.345991	-1.090003	-0.534273
H	3.867150	-0.351738	-1.153866
H	3.867409	-2.044536	-0.660057
C	3.322691	-0.617952	0.935633
H	4.261069	-0.149574	1.249434
H	3.132466	-1.457626	1.614367
C	2.140890	0.364867	0.992198
H	1.699894	0.512696	1.979971
C	2.391995	1.647903	0.204378
O	3.027011	2.653977	0.337724
O	1.622776	1.281926	-0.871211
C	-0.881142	-0.604038	1.110538
C	-2.260981	-0.639705	1.264732
H	-2.718940	-1.103431	2.132750
C	-3.093110	-0.061007	0.295327
C	-2.520526	0.552580	-0.825091
H	-3.138450	1.016904	-1.585126
C	-1.131572	0.577504	-0.966793
H	-0.695258	1.072855	-1.828561
H	-0.255224	-1.053689	1.877368
O	-4.432844	-0.143146	0.538089
C	-5.322876	0.432529	-0.405740
H	-5.226158	-0.040316	-1.391981
H	-6.327058	0.253813	-0.017259
H	-5.160105	1.513620	-0.506806
C	1.237326	-2.537753	-0.601422
H	0.176770	-2.579871	-0.865194
H	1.757202	-3.330920	-1.150053
H	1.322013	-2.767057	0.467646

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

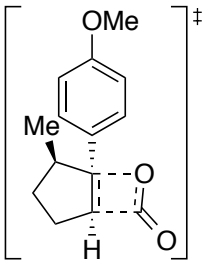
SCF Energy= -768.783907129 Predicted Change= -7.189245D-09

Zero-point correction (ZPE)=	-768.5081	0.27577
Internal Energy (U)=	-768.4931	0.29073
Enthalpy (H)=	-768.4922	0.29167
Gibbs Free Energy (G)=	-768.5505	0.23331

Frequencies -- 34.0681 52.6720 77.6812

E_{solv} = -0.010632435

$E_{SCS\text{-}MP2/\infty}$ = -768.2285162



***(syn)*-TS3d**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.080735	0.293877	-0.343191
C	0.351603	0.275493	-0.226008
C	-1.943052	1.517784	-0.111734
H	-1.594960	2.261416	-0.850518
C	-3.372470	1.063897	-0.510467
H	-3.946173	1.876710	-0.966417
H	-3.909168	0.746398	0.390646
C	-3.163359	-0.140693	-1.444770
H	-3.003147	0.183767	-2.481739
H	-3.997134	-0.848412	-1.431444
C	-1.896242	-0.790234	-0.871507
H	-1.397278	-1.514825	-1.516779
C	-2.282117	-1.542877	0.562969
O	-3.099563	-2.444975	0.476840
O	-1.667765	-1.024394	1.530159
C	1.110264	1.470116	-0.141197
H	0.608309	2.430945	-0.157014
C	2.489507	1.442894	-0.081586
H	3.072033	2.357138	-0.036695
C	3.171554	0.211807	-0.072727
C	2.442750	-0.989238	-0.141997
H	2.946330	-1.948287	-0.120134
C	1.060508	-0.947498	-0.227472
H	0.508174	-1.879961	-0.244605
O	4.517322	0.289523	0.004419
C	5.279449	-0.915385	0.029823
H	5.130681	-1.498818	-0.886518
H	6.321844	-0.602035	0.096996
H	5.024143	-1.527994	0.902476
C	-1.866730	2.139108	1.293105
H	-2.155721	1.385413	2.029643
H	-0.862109	2.490722	1.544453
H	-2.551350	2.992302	1.356878

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

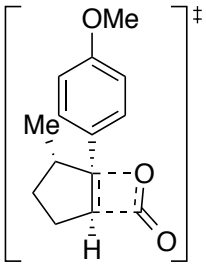
SCF Energy= -768.743835760 Predicted Change= -4.631974D-09

Zero-point correction (ZPE)=	-768.4711	0.27266
Internal Energy (U)=	-768.4557	0.28808
Enthalpy (H)=	-768.4548	0.28903
Gibbs Free Energy (G)=	-768.5141	0.22969

Frequencies -- -526.9860 45.9245 54.8248

E_{solv} = -0.022030259

$E_{SCS\text{-}MP2/\infty}$ = -768.1709828



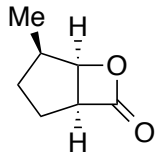
***(anti)*-TS3d**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.130725	0.289910	-0.137412
C	-0.303386	0.249715	-0.047723
C	1.976031	1.456011	0.331261
H	1.768424	1.705493	1.376607
C	3.433084	0.970079	0.126615
H	3.774848	0.456898	1.029642
H	4.116508	1.802206	-0.070533
C	3.337229	-0.029843	-1.043122
H	4.141142	-0.771265	-1.043531
H	3.357789	0.486292	-2.012321
C	1.973920	-0.694675	-0.799371
H	1.556499	-1.262946	-1.629871
C	2.148294	-1.728290	0.510328
O	1.661878	-1.224137	1.552573
O	2.736692	-2.769621	0.273249
C	-1.055911	-0.710272	-0.760039
H	-0.546076	-1.437606	-1.381866
C	-2.440036	-0.755638	-0.688403
H	-2.978819	-1.507775	-1.252094
C	-3.123158	0.170536	0.118615
C	-2.395873	1.131971	0.847326
H	-2.943622	1.826952	1.475136
C	-1.019604	1.166234	0.764649
H	-0.477171	1.897165	1.353872
O	-4.464177	0.220308	0.263355
C	-5.270399	-0.736074	-0.421155
H	-5.030563	-1.757501	-0.103254
H	-6.299765	-0.501559	-0.147936
H	-5.151631	-0.650401	-1.507895
C	1.675900	2.697041	-0.549928
H	1.882039	2.496043	-1.607028
H	0.634323	3.020898	-0.468165
H	2.320040	3.524479	-0.234034

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -768.741636490 Predicted Change= -3.424605D-08
Zero-point correction (ZPE)= -768.4688 0.27283
Internal Energy (U)= -768.4533 0.28829
Enthalpy (H)= -768.4524 0.28923
Gibbs Free Energy (G)= -768.5122 0.22943

Frequencies -- -581.8261 32.3986 52.4538
E_{solv} = -0.023065949
$E_{SCS\text{-}MP2/\infty}$ = -768.1704906



***(syn)*-2d**

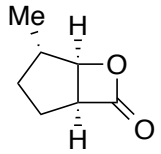
Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.231770	-0.458354	0.923166
C	-1.495273	0.092625	0.259589
H	-2.045232	0.615566	1.057983
C	-0.953998	1.159296	-0.721671
H	-1.716657	1.892908	-1.001490
H	-0.616555	0.673542	-1.646078
C	0.243456	1.793592	0.016466
H	-0.103129	2.551999	0.729100
H	0.962368	2.274976	-0.653992
C	0.870294	0.619717	0.794961
H	1.440932	0.905533	1.681491
C	1.554543	-0.429464	-0.084868
O	2.569765	-0.534862	-0.708403
O	0.539271	-1.351728	0.028809
H	-0.383077	-0.955253	1.883786
C	-2.404118	-0.968517	-0.362304
H	-2.774807	-1.669593	0.394593
H	-3.273329	-0.505055	-0.842404
H	-1.861609	-1.545267	-1.118272

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -423.210405045 Predicted Change= -3.369239D-08

Zero-point correction (ZPE)=	-423.0480	0.16236
Internal Energy (U)=	-423.0402	0.17011
Enthalpy (H)=	-423.0393	0.17105
Gibbs Free Energy (G)=	-423.0803	0.13010

Frequencies -- 100.6444 156.0922 228.1187E_{solv} =
E_{solv} = -0.008377591
$E_{SCS\text{-}MP2/\infty}$ = -422.9192498



***(anti)*-2d**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.183552	-0.901218	0.385480
C	1.349948	-0.431346	-0.485780
H	1.449446	-1.089686	-1.356739
C	0.926249	0.999297	-0.909834
H	0.250791	0.944370	-1.771181
H	1.780363	1.616521	-1.207221
C	0.173092	1.573694	0.311586
H	-0.522183	2.376392	0.046491
H	0.875076	1.979071	1.049365
C	-0.552294	0.355296	0.914435
H	-0.775824	0.431632	1.980880
C	-1.707768	-0.176054	0.062558
O	-2.831947	0.138768	-0.197775
O	-1.007494	-1.261193	-0.412173
H	0.414338	-1.711803	1.080399
C	2.664614	-0.452055	0.308936
H	2.918472	-1.469257	0.629373
H	3.491210	-0.077313	-0.304200
H	2.609487	0.173787	1.208125

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

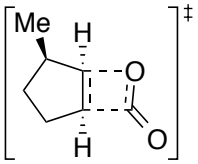
SCF Energy= -423.208799237 Predicted Change= -1.728368D-07

Zero-point correction (ZPE)=	-423.0465	0.16228
Internal Energy (U)=	-423.0387	0.17006
Enthalpy (H)=	-423.0377	0.17101
Gibbs Free Energy (G)=	-423.0788	0.12994

Frequencies -- 98.3277 142.9239 209.1589

E_{solv} = -0.008509072

$E_{SCS\text{-}MP2/\infty}$ = -422.9184377



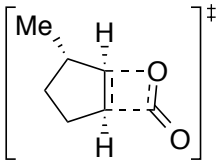
***(anti)*-TS3d**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.384767	-0.199142	1.108738
C	-1.531796	0.146035	0.219627
H	-2.204227	0.703503	0.903770
C	-0.918384	1.157029	-0.785279
H	-1.650985	1.892351	-1.130064
H	-0.562459	0.607331	-1.664671
C	0.276127	1.787393	-0.033118
H	-0.039170	2.664510	0.548054
H	1.083246	2.101495	-0.701541
C	0.722803	0.655868	0.896297
H	1.428703	0.854347	1.700882
C	1.475778	-0.619463	-0.098547
O	2.483739	-0.269152	-0.652390
O	0.763986	-1.649588	-0.040607
H	-0.468767	-0.926960	1.908548
C	-2.313955	-1.025635	-0.379460
H	-2.717055	-1.678179	0.402844
H	-3.152732	-0.657991	-0.979929
H	-1.653188	-1.622996	-1.013469

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -423.151954418 Predicted Change= -1.914241D-09
Zero-point correction (ZPE)= -422.9941 0.15785
Internal Energy (U)= -422.9857 0.16621
Enthalpy (H)= -422.9847 0.16715
Gibbs Free Energy (G)= -423.0273 0.12456

Frequencies -- -759.2363 59.5962 132.2421
E_{solv} = -0.012615218
$E_{SCS\text{-}MP2/\infty}$ = -422.8501678



***(anti)*-TS3d**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.361312	-0.774603	0.625955
C	1.353196	-0.452232	-0.445220
H	1.340952	-1.206882	-1.238213
C	0.905182	0.951169	-0.936874
H	0.222227	0.835792	-1.784996
H	1.750787	1.558229	-1.274489
C	0.151379	1.575524	0.263043
H	-0.636883	2.267316	-0.048561
H	0.832926	2.126444	0.924520
C	-0.423696	0.350075	0.975484
H	-0.840217	0.442772	1.976898
C	-1.742546	-0.320469	-0.028345
O	-1.389439	-1.447621	-0.446415
O	-2.688901	0.411870	-0.139900
H	0.377904	-1.716276	1.163414
C	2.763548	-0.445694	0.199496
H	3.023707	-1.427186	0.610758
H	3.505643	-0.190916	-0.564321
H	2.839418	0.294089	1.004279

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -423.148965457 Predicted Change= -7.821573D-08

Zero-point correction (ZPE)=	-422.9908	0.15814
Internal Energy (U)=	-422.9824	0.16655
Enthalpy (H)=	-422.9814	0.16750
Gibbs Free Energy (G)=	-423.0242	0.12470

Frequencies -- -788.3104 59.5144 119.8466

E_{solv} = -0.012677933

$E_{SCS\text{-}MP2/\infty}$ = -422.8478843