A Facile Domino Access to Chiral Bicyclo[3.2.1]octanes and Discovery of a New Catalytic Activation Mode

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X-ray crystallographic determination of **3f** (#CCDC 719547).

Theoretical Study of the Transition State Structures and Mechanism Considerations

Geometry optimizations were performed using the B3LYP-DFT procedure.¹ As for the basis set, 6-31G(d) basis² are used for all atoms except the protons in the amine groups, which uses 6-31G(d,p) basis.³ All transition state structures have been validated by vibrational analysis with the same level of theory/basis and have one imaginary vibrational frequency. All calculations have been done with Gaussian 03.⁴

(The following Figures are the Transition States using DFT calculation)

Table. Electronic and free energies of the transition states for the Michael addition catalyzed by catalyst **VI** by the DFT calculations

Transition state	Eelec (Hartree)	ΔE_{elec} (kcal/mol)	G (Hartree)	ΔG (Hartree)
TS-1 (S,S)	-3539.2775	8.53	-3538.5237	7.22
TS-2 (S,R)	-3539.2759	9.54	-3538.5181	10.7
TS-3 (R,S)	-3539.2742	10.6	-3538.5174	11.2
TS-4 (R,R)	-3539.2699	13.3	-3538.5130	13.9
TS-5 (R,R)	-3539.2771	8.79	-3538.5225	7.97
TS-6 (R,S)	-3539.2911	0.00	-3538.5352	0.00
TS-7 (S,R)	-3539.2820	5.71	-3538.5265	5.44
TS-8 (S,S)	-3539.2717	12.7	-3538.5169	11.5

Figure. Located transition state structures with distant parameters in angstroms using quinine amine catalyst VI (most H atoms are removed for clarity).

General Information: Analytical thin layer chromatography (TLC) was performed using Merck 60 F254 precoated silica gel plate (0.2 mm thickness). Subsequent to elution, plates were visualized using UV radiation (254 nm) on Spectroline Model ENF-24061/F 254 nm. Further visualization was possible by staining with basic solution of potassium permanganate or acidic solution of ceric molybdate.

Flash chromatography was performed using Merck silica gel 60 with freshly distilled solvents. Columns were typically packed as slurry and equilibrated with the appropriate solvent system prior to use.

Proton nuclear magnetic resonance spectra (^1H NMR) were recorded on Bruker AMX 400 spectrophotometer (CDCl_3 as solvent). Chemical shifts for ^1H NMR spectra are reported as δ in units of parts per million (ppm) downfield from SiMe_4 (δ 0.0) and relative to the signal of chloroform-d (δ 7.26, singlet). Multiplicities were given as: s (singlet), d (doublet), t (triplet), dd (double of doublet) or m (multiplets). The number of protons (n) for a given resonance is indicated by nH. Coupling constants are reported as a J value in Hz. Carbon nuclear magnetic resonance spectra (^{13}C NMR) are reported as δ in units of parts per million (ppm) downfield from SiMe_4 (δ 0.0) and relative to the signal of chloroform-d (δ 77.0, triplet).

Enantioselectivities were determined by High performance liquid chromatography (HPLC) analysis employing a Daicel Chiralpak AS-H column. Optical rotations were measured in CH_2Cl_2 on a *Schmidt + Haensdch* polarimeter (Polartronic MH8) with a 1 mL cell (c given in g/100 mL). Absolute configuration of the products was determined by X-ray.

High resolution mass spectrometry (HRMS) was recorded on Finnigan MAT 95 $\times$ P spectrometer.

Racemates were synthesized using Quinine and Quinidine thiourea derivatives (1:1 ratio)

Typical Procedure for Michael-Henry Reactions:

Catalyst **VI** (0.005 mmol, 0.05 eq) was added to a solution of methyl 2,5-dioxocyclohexanecarboxylate **1a** (0.2 mmol, 2 eq) and nitroolefins (0.1 mmol, 1eq) in benzonitrile (0.5 mL) at room temperature. The resulting mixture was stirred vigorously. After the reaction was complete (monitored by TLC and crude NMR), the products were afforded by flash chromatography over silica gel (EtOAc : Hexane = 1 : 4 to 1 : 2).

Characterization of the Michael-Henry Products

(1*R*,5*S*,6*R*,7*S*)-methyl 5-hydroxy-6-nitro-2-oxo-7-phenylbicyclo[3.2.1]

octane-1-carboxylate (**3a**)

The title compound was prepared according to the typical procedure, as described above in 93% yield.

¹H-NMR (400 MHz, CDCl₃) δ 7.36-7.29 (m, 3H), 7.21 (d, *J* = 7.6 Hz, 2H), 5.27 (d, *J* = 5.6 Hz, 1H), 4.88 (d, *J* = 5.6 Hz, 1H), 3.86 (s, 3H), 3.01 (dd, *J* = 3.6, 12.8 Hz, 1H), 2.64 (brs, 1H), 2.61-2.53 (m, 2H), 2.30-2.17 (m, 2H), 2.13-2.04 (m, 1H).

¹³C-NMR (100 MHz, CDCl₃) δ 203.4, 169.7, 135.7, 129.0, 127.8, 127.1, 98.6, 76.3, 64.9, 53.0, 52.3, 44.8, 37.0, 35.2.

HPLC: Chiralpak AD-H (hexane / *i*-PrOH = 85 / 15, flow rate 1 mL / min, λ = 210 nm), *t*_R

(major) = 9.0 min, t_R (minor) = 12.8 min; 94% ee.

$[\alpha]_D^{25} = -80.8$ ($c = 1.8$, CH_2Cl_2).

HRMS (ESI) calcd for $[\text{M}+\text{Na}] \text{C}_{16}\text{H}_{17}\text{NO}_6\text{Na}$, m/z 342.0954, found 342.0956.

(1*R*,5*S*,6*R*,7*S*)-methyl 5-hydroxy-7-(3-methoxyphenyl)-6-nitro-2-oxobicyclo[3.2.1]octane-1-carboxylate (**3b**)

The title compound was prepared according to the typical procedure, as described above in 84% yield.

^1H -NMR (400 MHz, CDCl_3) δ 7.26-7.22 (m, 1H), 6.83-6.77 (m, 3H), 5.27 (d, $J = 5.2$ Hz, 1H), 4.86 (d, $J = 5.6$ Hz, 1H), 3.85 (s, 3H), 3.77 (s, 3H), 3.00 (dd, $J = 3.6, 12.8$ Hz, 1H), 2.59-2.52 (m, 2H), 2.26-2.77 (m, 3H).

^{13}C -NMR (100 MHz, CDCl_3) δ 203.5, 169.8, 159.8, 137.3, 130.0, 119.2, 113.4, 113.0, 98.5, 76.2, 65.0, 55.2, 53.0, 52.2, 44.8, 37.0, 35.2.

HPLC: Chiralpak AD-H (hexane / *i*-PrOH = 85 / 15, flow rate 1 mL / min, $\lambda = 210$ nm), t_R (major) = 11.1 min, t_R (minor) = 16.8 min; 95% ee.

$[\alpha]_D^{25} = -88.3$ ($c = 1.0$, CH_2Cl_2).

HRMS (ESI) calcd for $[\text{M}+\text{Na}] \text{C}_{17}\text{H}_{19}\text{NO}_7\text{Na}$, m/z 370.1059, found 370.1054.

(1*R*,5*S*,6*R*,7*S*)-methyl 5-hydroxy-7-(4-methoxyphenyl)-6-nitro-2-oxobicyclo[3.2.1]octane-1-carboxylate (**3c**)

The title compound was prepared according to the typical procedure, as described above in 79% yield.

$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 7.13 (d, $J = 8.8$ Hz, 2H), 6.85 (d, $J = 8.4$ Hz, 2H), 5.23 (d, $J = 5.6$ Hz, 1H), 4.81 (d, $J = 5.6$ Hz, 1H), 3.84 (s, 3H), 3.78 (s, 3H), 2.98 (dd, $J = 3.6, 12.8$ Hz, 1H), 2.96 (brs, 1H), 2.58 (dd, $J = 6.8, 16.8$ Hz, 1H), 2.53 (d, $J = 12.4$ Hz, 1H), 2.26-2.07 (m, 3H).

$^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 203.7, 169.9, 158.9, 128.4, 127.4, 114.3, 98.7, 76.2, 65.2, 55.3, 53.0, 51.8, 44.6, 36.7, 35.2.

HPLC: Chiralpak AD-H (hexane / *i*-PrOH = 85 / 15, flow rate 1 mL / min, $\lambda = 210$ nm), t_R (major) = 13.9 min, t_R (minor) = 18.7 min; 90% ee.

$[\alpha]_D^{25} = -76.0$ ($c = 1.5$, CH_2Cl_2).

HRMS (ESI) calcd for $[\text{M}+\text{Na}]$ $\text{C}_{17}\text{H}_{19}\text{NO}_7\text{Na}$, m/z 370.1059, found 370.1055.

(1*R*,5*S*,6*R*,7*S*)-methyl 5-hydroxy-6-nitro-2-oxo-7-*p*-tolylbicyclo[3.2.1]octane-1-carboxylate (**3d**)

The title compound was prepared according to the typical procedure, as described above in

91% yield.

^1H -NMR (400 MHz, CDCl_3) δ 7.13 (d, $J = 8.4$ Hz, 2H), 7.08 (d, $J = 8.4$ Hz, 2H), 5.23 (dd, $J = 0.4, 5.6$ Hz, 1H), 4.81 (d, $J = 5.2$ Hz, 1H), 3.84 (s, 3H), 3.00 (dd, $J = 3.6, 12.4$ Hz, 1H), 2.91 (brs, 1H), 2.58-2.51 (m, 3H), 2.32 (s, 3H), 2.26-2.11 (m, 3H).

^{13}C -NMR (100 MHz, CDCl_3) δ 203.6, 169.8, 137.5, 132.6, 129.6, 127.0, 98.7, 76.2, 65.0, 53.0, 52.1, 44.7, 37.0, 35.2, 20.9.

HPLC: Chiralpak AD-H (hexane / *i*-PrOH = 85 / 15, flow rate 1 mL / min, $\lambda = 210$ nm), t_R (major) = 9.7 min, t_R (minor) = 12.4 min; 94% ee.

$[\alpha]_D^{25} = -94.4$ ($c = 0.9$, CH_2Cl_2).

HRMS (ESI) calcd for $[\text{M}+\text{Na}]$ $\text{C}_{17}\text{H}_{19}\text{NO}_6\text{Na}$, m/z 356.1110, found 356.1106.

(1*R*,5*S*,6*R*,7*S*)-methyl 7-(4-bromophenyl)-5-hydroxy-6-nitro-2-oxobicyclo[3.2.1]octane-1-carboxylate (**3e**)

The title compound was prepared according to the typical procedure, as described above in 81% yield.

^1H -NMR (400 MHz, CDCl_3) δ 7.46 (d, $J = 8.8$ Hz, 2H), 7.09 (d, $J = 8.0$ Hz, 2H), 5.20 (d, $J = 5.6$ Hz, 1H), 4.80 (d, $J = 5.2$ Hz, 1H), 3.85 (s, 3H), 2.99 (dd, $J = 3.6, 12.8$ Hz, 1H), 2.81 (brs, 1H), 2.63-2.53 (m, 2H), 2.31-2.10 (m, 2H), 2.07-2.00 (m, 1H).

^{13}C -NMR (100 MHz, CDCl_3) δ 203.2, 169.7, 134.7, 132.1, 129.0, 122.0, 98.7, 76.2, 65.0, 53.1, 51.8, 44.6, 36.9, 35.2.

HPLC: Chiralpak AD-H (hexane / *i*-PrOH = 85 / 15, flow rate 1 mL / min, λ = 210 nm), t_R (major) = 11.1 min, t_R (minor) = 14.6 min; 94% ee.

$[\alpha]_D^{25} = -70.3$ ($c = 1.2$, CH₂Cl₂).

HRMS (ESI) calcd for [M+Na] C₁₆H₁₆NO₆NaBr, m/z 420.0059, found 420.0046.

(1*R*,5*S*,6*R*,7*R*)-methyl 7-(2-chlorophenyl)-5-hydroxy-6-nitro-2-oxobicyclo[3.2.1]octane-1-carboxylate (**3f**)

The title compound was prepared according to the typical procedure, as described above in 86% yield.

¹H-NMR (400 MHz, CDCl₃) δ 7.43 (d, $J = 8.0$ Hz, 1H), 7.27-7.18 (m, 2H), 7.13 (d, $J = 8.0$ Hz, 1H), 5.14 (d, $J = 6.0$ Hz, 1H), 5.08 (d, $J = 6.0$ Hz, 1H), 3.76 (s, 3H), 3.00 (dd, $J = 3.2, 12.8$ Hz, 1H), 2.96 (brs, 1H), 2.81-2.76 (m, 1H), 2.60-2.49 (m, 2H), 2.35-2.25 (m, 2H).

¹³C-NMR (100 MHz, CDCl₃) δ 205.2, 169.0, 134.8, 133.6, 130.8, 129.3, 128.1, 127.0, 97.7, 76.2, 64.8, 52.9, 50.9, 44.0, 36.8, 35.6.

HPLC: Chiralpak AD-H (hexane / *i*-PrOH = 85 / 15, flow rate 1 mL / min, λ = 210 nm), t_R (major) = 11.5 min, t_R (minor) = 21.8 min; 96% ee.

$[\alpha]_D^{25} = -81.7$ ($c = 0.4$, CH₂Cl₂).

HRMS (ESI) calcd for [M+Na] C₁₆H₁₆NO₆NaCl, m/z 376.0564, found 376.0558.

(1*R*,5*S*,6*R*,7*S*)-methyl 7-(4-chlorophenyl)-5-hydroxy-6-nitro-2-oxobicyclo[3.2.1]octane-1-carboxylate (**3g**)

o[3.2.1]octane-1-carboxylate (**3g**)

The title compound was prepared according to the typical procedure, as described above in 93% yield.

$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 7.29 (d, $J = 8.8$ Hz, 2H), 7.16 (d, $J = 8.4$ Hz, 2H), 5.20 (d, $J = 5.6$ Hz, 1H), 4.82 (d, $J = 5.2$ Hz, 1H), 3.85 (s, 3H), 2.99 (dd, $J = 3.6, 12.8$ Hz, 1H), 2.76 (brs, 1H), 2.64-2.54 (m, 2H), 2.32-2.18 (m, 2H), 2.10-2.06 (m, 1H).

$^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 203.2, 169.7, 134.1, 133.9, 129.1, 128.6, 98.3, 76.2, 65.0, 53.1, 51.8, 44.6, 36.9, 35.1.

HPLC: Chiralpak AD-H (hexane / *i*-PrOH = 85 / 15, flow rate 1 mL / min, $\lambda = 210$ nm), t_R (major) = 10.0 min, t_R (minor) = 13.6 min; 95% ee.

$[\alpha]_D^{25} = -95.3$ ($c = 0.9$, CH_2Cl_2).

HRMS (ESI) calcd for $[\text{M}+\text{Na}] \text{C}_{16}\text{H}_{16}\text{NO}_6\text{NaCl}$, m/z 376.0564, found 376.0556.

(1*R*,5*S*,6*R*,7*S*)-methyl

7-(4-fluorophenyl)-5-hydroxy-6-nitro-2-oxobicycl

o[3.2.1]octane-1-carboxylate (**3h**)

The title compound was prepared according to the typical procedure, as described above in

88% yield.

^1H -NMR (400 MHz, CDCl_3) δ 7.21-7.18 (m, 2H), 7.05-7.00 (m, 2H), 5.22 (d, $J = 5.2$ Hz, 1H), 4.83 (d, $J = 5.6$ Hz, 1H), 3.85 (s, 3H), 2.99 (dd, $J = 3.6, 12.4$ Hz, 1H), 2.91 (brs, 1H), 2.64-2.57 (m, 1H), 2.55 (d, $J = 12.8$ Hz, 1H), 2.29-2.22 (m, 2H), 2.11-2.03 (m, 1H).

^{13}C -NMR (100 MHz, CDCl_3) δ 203.4, 169.87, 131.4, 129.0, 128.9, 116.0, 115.8, 98.5, 76.2, 65.2, 53.1, 51.7, 44.6, 36.9, 35.2.

HPLC: Chiralpak AD-H (hexane / *i*-PrOH = 85 / 15, flow rate 1 mL / min, $\lambda = 210$ nm), t_R (major) = 8.9 min, t_R (minor) = 13.3 min; 94% ee.

$[\alpha]_D^{25} = -105.3$ ($c = 1.0$, CH_2Cl_2).

HRMS (ESI) calcd for $[\text{M}+\text{Na}]$ $\text{C}_{16}\text{H}_{16}\text{NO}_6\text{NaF}$, m/z 360.0859, found 360.0848.

(1*R*,5*S*,6*R*,7*S*)-methyl

5-hydroxy-6-nitro-2-oxo-7-(thiophen-2-yl)bicycle

[3.2.1]octane-1-carboxylate (**3i**)

The title compound was prepared according to the typical procedure, as described above in 80% yield.

^1H -NMR (400 MHz, CDCl_3) δ 7.25 (d, $J = 5.2$ Hz, 1H), 7.04 (d, $J = 3.2$ Hz, 1H), 6.95 (dd, $J = 4.0, 5.2$ Hz, 1H), 5.38 (d, $J = 5.2$ Hz, 1H), 5.02 (d, $J = 5.2$ Hz, 1H), 3.87 (s, 3H), 2.96-2.93 (m, 2H), 2.91 (brs, 1H), 2.64-2.53 (m, 2H), 2.32-2.27 (m, 3H).

^{13}C -NMR (100 MHz, CDCl_3) δ 202.2, 169.5, 137.4, 127.3, 126.7, 125.6, 97.8, 76.4, 66.3, 53.0, 48.9, 44.1, 36.8, 35.0.

HPLC: Chiralpak AD-H (hexane / *i*-PrOH = 85 / 15, flow rate 1 mL / min, λ = 210 nm), t_R (major) = 10.3 min, t_R (minor) = 15.0 min; 92% ee.

$[\alpha]_D^{25} = -116.8$ ($c = 1.0$, CH₂Cl₂).

HRMS (ESI) calcd for [M+Na] C₁₄H₁₅NO₆NaS, m/z 348.0518, found 348.0523.

(1*R*,5*S*,6*R*,7*S*)-methyl

7-(furan-3-yl)-5-hydroxy-6-nitro-2-oxobicyclo

[3.2.1]octane-1-carboxylate (**3j**)

The title compound was prepared according to the typical procedure, as described above in 84% yield.

¹H-NMR (400 MHz, CDCl₃) δ 7.34 (s, 1H), 6.34-6.31 (m, 2H), 5.43 (d, $J = 5.6$ Hz, 1H), 4.80 (d, $J = 5.2$ Hz, 1H), 3.82 (s, 3H), 2.86 (d, $J = 12.8$ Hz, 1H), 2.80 (brs, 1H), 2.67-2.49 (m, 3H), 2.31-2.26 (m, 2H).

¹³C-NMR (100 MHz, CDCl₃) δ 202.6, 169.1, 146.8, 142.4, 111.1, 109.7, 94.4, 76.4, 64.8, 52.8, 47.4, 43.5, 36.7, 34.3.

HPLC: Chiralpak AD-H (hexane / *i*-PrOH = 85 / 15, flow rate 1 mL / min, λ = 210 nm), t_R (major) = 9.1 min, t_R (minor) = 12.3 min; 94% ee.

$[\alpha]_D^{25} = -85.9$ ($c = 1.5$, CH₂Cl₂).

HRMS (ESI) calcd for [M+Na] C₁₄H₁₅NO₇Na, m/z 332.0746, found 332.0753.

(1*R*,5*S*,6*R*,7*S*)-methyl

5-hydroxy-7-(naphthalen-3-yl)-6-nitro-2-oxobicyc

lo[3.2.1]octane-1-carboxylate (**3k**)

The title compound was prepared according to the typical procedure, as described above in 85% yield.

$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 7.82-7.78 (m, 3H), 7.67 (s, 1H), 7.49 (dd, $J = 3.2, 6.0$ Hz, 1H), 7.30-7.28 (m, 1H), 5.36 (d, $J = 5.6$ Hz, 1H), 5.04 (d, $J = 5.6$ Hz, 1H), 3.87 (s, 3H), 3.06 (dd, $J = 3.2, 12.4$ Hz, 1H), 2.90 (brs, 1H), 2.59-2.51 (m, 2H), 2.30-2.06 (m, 3H).

$^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 203.7, 169.9, 133.1, 133.0, 132.4, 128.8, 128.1, 127.5, 126.7, 126.6, 126.1, 124.9, 98.6, 76.3, 65.1, 53.1, 52.4, 44.8, 37.0, 35.3.

HPLC: Chiralpak AD-H (hexane / *i*-PrOH = 85 / 15, flow rate 1 mL / min, $\lambda = 254$ nm), t_R (major) = 11.2 min, t_R (minor) = 21.0 min; 94% ee.

$[\alpha]_D^{25} = -77.7$ ($c = 1.2$, CH_2Cl_2).

HRMS (ESI) calcd for $[\text{M}+\text{Na}]$ $\text{C}_{20}\text{H}_{19}\text{NO}_6\text{Na}$, m/z 392.1110, found 392.1107.

(1*R*,5*S*,6*R*,7*S*)-methyl

5-hydroxy-6-nitro-7-(4-nitrophenyl)-2-oxobicyclo

[3.2.1]octane-1-carboxylate (**3l**)

The title compound was prepared according to the typical procedure, as described above in

77% yield.

^1H -NMR (400 MHz, CDCl_3) δ 8.19 (d, J = 8.8 Hz, 2H), 7.41 (d, J = 9.2 Hz, 2H), 5.25 (d, J = 6.0 Hz, 1H), 4.93 (d, J = 5.6 Hz, 1H), 3.86 (s, 3H), 3.00 (dd, J = 3.6, 12.8 Hz, 1H), 2.96 (brs, 1H), 2.68-2.58 (m, 2H), 2.36-2.21 (m, 2H), 2.06-1.99 (m, 1H).

^{13}C -NMR (100 MHz, CDCl_3) δ 202.8, 169.5, 147.3, 143.0, 128.4, 124.0, 97.8, 76.3, 65.1, 53.3, 52.0, 44.3, 36.8, 35.1.

HPLC: Chiralpak AD-H (hexane / *i*-PrOH = 85 / 15, flow rate 1 mL / min, λ = 254 nm), t_R (major) = 20.2 min, t_R (minor) = 27.8 min; 94% ee.

$[\alpha]_D^{25}$ = -96.2 (c = 0.7, CH_2Cl_2).

HRMS (ESI) calcd for $[\text{M}+\text{Na}]$ $\text{C}_{16}\text{H}_{16}\text{N}_2\text{O}_8\text{Na}$, m/z 387.0804, found 387.0807.

(1*R*,5*S*,6*R*,7*S*)-methyl

5-hydroxy-6-nitro-2-oxo-7-styrylbicyclo[3.2.1]oct

ane-1-carboxylate (**3m**)

The title compound was prepared according to the typical procedure, as described above in 73% yield.

^1H -NMR (400 MHz, CDCl_3) δ 7.37-7.28 (m, 5H), 6.67 (d, J = 16.8 Hz, 1H), 6.30 (dd, J = 4.8, 12.0 Hz, 1H), 5.14 (d, J = 5.2 Hz, 1H), 4.26-4.22 (m, 1H), 3.85 (s, 3H), 2.89-2.86 (m, 1H), 2.79 (brs, 1H), 2.70-2.65 (m, 1H), 2.49 (d, J = 12.4 Hz, 1H), 2.39-2.24 (m, 3H).

^{13}C -NMR (100 MHz, CDCl_3) δ 202.5, 166.9, 149.9, 140.0, 129.6, 129.2, 128.5, 126.1, 121.1, 99.9, 78.1, 77.265.3, 49.1, 44.4, 34.2, 33.0.

HPLC: Chiralpak AD-H (hexane / *i*-PrOH = 85 / 15, flow rate 1 mL / min, λ = 254 nm), t_R (major) = 10.3 min, t_R (minor) = 14.2 min; 86% ee.

$[\alpha]_D^{25} = -37.6$ ($c = 1.5$, CH₂Cl₂).

HRMS (ESI) calcd for [M+Na] C₁₈H₁₉NO₆Na, m/z 368.1110, found 332.1113.

(1*R*,5*S*,6*R*,7*S*)-phenyl 5-hydroxy-6-nitro-2-oxo-7-phenylbicyclo[3.2.1]octane-1-carboxylate (**3n**)

Catalyst **VI** (0.005 mmol, 0.05 eq) was added to a solution of phenyl 2,5-dioxocyclohexanecarboxylate **1b** (0.2 mmol, 2 eq) and nitroolefin **2a** (0.1 mmol, 1eq) in diethyl ether (0.5 mL) at room temperature. The resulting mixture was stirred vigorously. After the reaction was complete (monitored by TLC and crude NMR), the products were afforded by flash chromatography over silica gel (EtOAc : Hexane = 1 : 4 to 1 : 2).

¹H-NMR (400 MHz, CDCl₃) δ 7.44-7.38 (m, 5H), 7.22-7.13 (m, 3H), 6.327 (d, $J = 7.6$ Hz, 2H), 5.34 (d, $J = 6.8$ Hz, 1H), 4.58 (d, $J = 6.8$ Hz, 1H), 3.26 (dd, $J = 3.6, 13.6$ Hz, 1H), 3.14 (brs, 1H), 3.11-3.02 (m, 1H), 2.68 (dd, $J = 8.0, 16.8$ Hz, 1H), 2.55 (d, $J = 13.2$ Hz, 1H), 2.30-2.14 (m, 2H).

¹³C-NMR (100 MHz, CDCl₃) δ 202.5, 169.5, 135.6, 134.0, 128.7, 128.4, 126.6, 123.1, 95.0, 76.6, 65.0, 52.8, 50.4, 43.1, 36.8, 34.7.

HPLC: Chiralpak AD-H (hexane / *i*-PrOH = 85 / 15, flow rate 1 mL / min, λ = 210 nm), t_R (major) = 12.4 min, t_R (minor) = 19.7 min; 85% ee.

$[\alpha]_D^{25} = -79.5$ ($c = 1.4$, CH₂Cl₂).

HRMS (ESI) calcd for [M+Na] C₂₁H₁₉NO₆Na, m/z 404.1110, found 404.1104.

General procedure for the preparation of (1a) and (1b)

NaHMDS (20 mmol, 2 M in THF) was slowly added to solution of cyclohexane-1,4-dione (20 mmol) in dry THF (30 mL) at -78 °C. After 30 min stirring at the same temperature, a solution of methyl or phenyl chloroformate (20 mmol) was added, and the resulting mixture was stirred for 1 h at -78 °C, and then allowed to warm to room temperature. The reaction was then quenched by addition of sat. NH₄Cl (aq.), and the product extracted with Et₂O (3 x 30 mL). The combined organic phases were then dried over Na₂SO₄, filtered and evaporated under reduced pressure. Purification of the crude mixture by FC (ethyl acetate in *n*-hexane 1:8), gave the corresponding β-ketoesters **1a** or **1b**.

Methyl 2,5-dioxocyclohexanecarboxylate (**1a**)

The title compound was obtained according to the general procedure as colorless oil (15%

yield).

^1H -NMR (400 MHz, CDCl_3) δ 12.21 (s, 1H), 3.79 (s, 3H), 3.10 (s, 2H), 2.71 (t, $J = 6.8$ Hz, 2H), 2.59 (t, $J = 6.8$ Hz, 2H). (**Almost 100% enol form**)

^{13}C -NMR (100 MHz, CDCl_3) δ 207.5, 171.7, 170.7, 94.5, 51.8, 37.2, 36.6, 28.3.

HRMS (ESI) calcd for $[\text{M}+\text{Na}] \text{C}_8\text{H}_{10}\text{O}_4\text{Na}$, m/z 193.0477, found 193.0477.

Phenyl 2,5-dioxocyclohexanecarboxylate (**1b**)

The title compound was obtained according to the general procedure as colorless oil (20% yield).

^1H -NMR (400 MHz, CDCl_3) δ 12.06 (s, 1H), 7.43 (t, $J = 8.0$ Hz, 2H), 7.31-7.27 (m, 1H), 7.13 (d, $J = 8.0$ Hz, 2H), 3.34 (s, 2H), 2.79 (t, $J = 6.8$ Hz, 2H), 2.66 (t, $J = 6.8$ Hz, 2H).

(**Almost 100% enol form**)

^{13}C -NMR (100 MHz, CDCl_3) δ 207.0, 172.9, 170.0, 150.0, 129.6, 126.2, 121.6, 94.2, 37.1, 36.7, 28.6.

HRMS (ESI) calcd for $[\text{M}+\text{H}] \text{C}_{13}\text{H}_{14}\text{O}_4$, m/z 233.0814, found 233.0812.

DFT calculation

TSI-1(S,S)

C	0.86070	2.80113	1.22678
C	1.01950	2.96015	3.73649
C	0.22158	3.40800	2.49451
H	1.65216	3.46183	0.86992
H	0.22873	4.49962	2.39968
H	-0.82899	3.10714	2.56674
C	2.89612	2.03066	2.35261
H	3.37577	1.13749	2.75352
H	3.53432	2.43010	1.56176
C	2.52792	3.07782	3.42991
H	3.11981	2.89753	4.33344
H	2.76599	4.09088	3.08613
H	0.75534	3.57162	4.60429
C	0.71925	1.46491	4.02972
H	1.48612	1.09895	4.72459
C	0.84715	0.70908	2.68223
H	1.39373	-0.22919	2.76523
H	-0.12400	0.50408	2.23936
N	1.62223	1.55349	1.68716
C	-0.62672	1.22159	4.66235

H	-1.49987	1.50593	4.07407
C	-0.80264	0.68597	5.87088
H	-1.79410	0.53514	6.28825
H	0.03771	0.37544	6.48905
C	-0.14131	2.63285	0.04409
N	-0.94431	1.43805	0.15849
H	-0.45995	0.53221	0.08438
C	-2.31313	1.40815	0.05569
S	-3.27947	2.76515	0.31265
N	-2.73954	0.14693	-0.27091
H	-2.00486	-0.47102	-0.63506
C	-4.01612	-0.43459	-0.30678
C	-4.10628	-1.67005	-0.97426
C	-5.16226	0.09389	0.30324
C	-5.31774	-2.35063	-1.03743
H	-3.22127	-2.08936	-1.44335
C	-6.36889	-0.60493	0.22461
H	-5.11207	1.03744	0.82695
C	-6.46592	-1.82414	-0.44236
H	-7.40951	-2.35268	-0.49653
C	-7.60025	0.01109	0.83763
C	-5.37605	-3.70169	-1.69969
C	-8.17632	0.90841	0.00651

C	-7.31604	0.66582	1.98498
C	-8.53900	-0.91916	1.12469
C	-4.45599	-3.82555	-2.68038
C	-5.14278	-4.69935	-0.81414
C	-6.58891	-3.94067	-2.24587
H	-0.84596	3.46697	0.15939
C	0.52402	2.78299	-1.32964
C	1.08804	4.04456	-1.72640
C	0.56836	1.75054	-2.23915
C	1.72374	4.10924	-3.01193
C	1.03351	5.22388	-0.94432
C	1.20168	1.93693	-3.49456
H	0.11718	0.78702	-2.02851
C	2.30434	5.33252	-3.42949
C	1.60148	6.40903	-1.38590
H	0.51281	5.25353	0.00639
H	1.22361	1.10972	-4.20374
C	2.25589	6.46179	-2.64266
H	2.78100	5.34863	-4.40451
H	2.70484	7.38311	-2.99541
N	1.78151	3.05384	-3.87589
O	1.48236	7.47722	-0.54580
C	1.97619	8.73937	-0.96938

H	1.48727	9.07606	-1.89248
H	1.73969	9.43609	-0.16319
H	3.06346	8.72030	-1.12121
O	-0.60962	-1.50184	-1.56904
O	0.33031	-1.01455	0.36382
N	0.29873	-1.72105	-0.70274
C	1.19990	-2.71322	-0.90127
H	1.03513	-3.28187	-1.80392
C	2.18006	-2.98950	0.08844
H	1.99051	-2.45065	1.00960
C	2.66817	-4.37489	0.27255
C	2.99408	-4.80339	1.57282
C	2.77774	-5.30040	-0.78092
C	3.40549	-6.11233	1.81504
H	2.89835	-4.10382	2.39918
C	3.19833	-6.60649	-0.53993
H	2.54841	-5.00136	-1.79842
C	3.51095	-7.01873	0.75777
H	3.63878	-6.42616	2.82888
H	3.28296	-7.30285	-1.36909
H	3.83381	-8.03942	0.94306
H	1.93084	0.94363	0.89732
O	3.01436	0.30807	-0.32372

C	3.61211	-0.64342	-0.83797
C	4.00060	-0.52546	-2.30948
C	4.02531	-1.87906	-0.14448
C	3.91059	-1.84579	-3.08048
H	3.37925	0.25356	-2.75758
C	5.01626	-2.74821	-0.92061
C	4.67629	-2.96569	-2.39190
H	2.86144	-2.16246	-3.15518
H	6.01848	-2.28656	-0.90344
C	4.31115	-1.72114	1.29864
O	3.64717	-1.08848	2.11308
O	5.41905	-2.41065	1.67704
C	5.74662	-2.35182	3.07032
H	4.92019	-2.72567	3.68109
H	6.62663	-2.98466	3.18990
H	5.97186	-1.32483	3.37227
H	5.03753	-0.15508	-2.33620
H	4.27746	-1.74807	-4.10746
H	5.14113	-3.72681	-0.45510
O	5.01714	-3.97123	-2.98453

TSI-2 (R,S)

C	1.47694	2.47999	1.29665
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C	1.71582	2.17316	3.78639
C	0.94623	2.92143	2.67952
H	2.33599	3.09811	1.03079
H	1.08033	4.00435	2.77635
H	-0.12964	2.73147	2.75085
C	3.42607	1.28841	2.17193
H	3.80434	0.29039	2.38972
H	4.09171	1.75187	1.43934
C	3.21899	2.16228	3.43320
H	3.80604	1.75265	4.26183
H	3.57489	3.18436	3.26052
H	1.55460	2.65088	4.75709
C	1.23260	0.69808	3.83401
H	1.96408	0.12699	4.42069
C	1.23174	0.18518	2.37350
H	1.66103	-0.80955	2.26812
H	0.23291	0.16790	1.94346
N	2.08635	1.09147	1.50096
C	-0.11679	0.51459	4.48057
H	-0.97331	0.93148	3.95064
C	-0.31140	-0.12075	5.63639
H	-1.30242	-0.22334	6.06874
H	0.51005	-0.57109	6.19087

C	0.43427	2.64049	0.14014
N	-0.41420	1.47965	-0.03427
H	0.00288	0.65685	-0.46345
C	-1.79015	1.51875	0.08805
S	-2.60901	2.87498	0.67382
N	-2.37017	0.34508	-0.27692
H	-1.74391	-0.46803	-0.39645
C	-3.73765	-0.00554	-0.21196
C	-4.05151	-1.27925	0.27981
C	-4.75750	0.83060	-0.68086
C	-5.37934	-1.70599	0.30299
H	-3.25476	-1.90630	0.66660
C	-6.08098	0.39191	-0.63657
H	-4.52080	1.81376	-1.06355
C	-6.40430	-0.87460	-0.14820
H	-7.43644	-1.20125	-0.10747
C	-7.16901	1.27201	-1.19329
C	-5.70474	-3.09675	0.77951
C	-7.36468	1.04375	-2.51453
C	-6.87824	2.58285	-1.06226
C	-8.35472	1.05333	-0.58132
C	-5.67112	-3.98983	-0.23795
C	-4.83162	-3.53174	1.71184

C	-6.94365	-3.16632	1.31787
H	-0.25359	3.42125	0.49336
C	1.05319	3.15969	-1.16239
C	1.70088	4.44390	-1.20326
C	0.96518	2.46344	-2.34573
C	2.29197	4.84778	-2.44838
C	1.76413	5.34132	-0.10993
C	1.56568	2.96879	-3.52562
H	0.43729	1.52046	-2.39166
C	2.95690	6.09731	-2.51928
C	2.41009	6.56365	-0.21482
H	1.27222	5.12561	0.83100
H	1.49434	2.39349	-4.44853
C	3.02694	6.94207	-1.43417
H	3.39911	6.37054	-3.47206
H	3.53732	7.89393	-1.52504
N	2.22988	4.10105	-3.58926
O	2.40164	7.34074	0.90565
C	2.98193	8.63583	0.84475
H	2.49199	9.26305	0.08923
H	2.82857	9.07603	1.83157
H	4.05849	8.58849	0.63458
O	-0.58013	-1.86997	-0.71752

O	-0.92634	-1.84571	1.46215
N	-0.25136	-2.24320	0.46952
C	0.81303	-3.05763	0.66825
H	0.97948	-3.29583	1.70650
C	1.55395	-3.64591	-0.39951
H	0.99756	-3.71105	-1.33220
C	2.27007	-4.91297	-0.05361
C	2.24331	-5.99434	-0.94957
C	2.93788	-5.07815	1.17334
C	2.85111	-7.20791	-0.62320
H	1.75436	-5.88136	-1.91259
C	3.54575	-6.28910	1.49708
H	2.97973	-4.25353	1.87894
C	3.50211	-7.36099	0.60113
H	2.81354	-8.03222	-1.32988
H	4.05050	-6.39917	2.45337
H	3.97294	-8.30632	0.85667
H	2.22620	0.57569	0.60303
O	1.98521	-0.26596	-0.89852
C	2.18631	-1.27126	-1.59977
C	1.49882	-1.33509	-2.96224
C	2.98407	-2.43882	-1.16570
C	2.27430	-2.06512	-4.07390

H	0.53869	-1.83551	-2.78295
C	3.63868	-3.25865	-2.29301
C	2.78264	-3.38810	-3.54233
H	1.64386	-2.23549	-4.95064
H	4.57522	-2.76660	-2.59583
C	3.86883	-2.20447	0.00507
O	3.58856	-1.56054	1.00815
O	5.05976	-2.83837	-0.12105
C	5.95269	-2.72995	0.99372
H	5.49971	-3.15432	1.89370
H	6.83997	-3.29750	0.71188
H	6.21221	-1.68429	1.18232
H	1.26811	-0.31014	-3.26088
H	3.13752	-1.45928	-4.38467
H	3.91092	-4.25481	-1.94382
O	2.52811	-4.45953	-4.05968

TSI-3 (S,R)

C	0.36723	2.98946	1.15203
C	0.82490	3.21297	3.62152
C	-0.19815	3.48829	2.50085
H	0.97881	3.77629	0.70763

H	-0.40307	4.56109	2.41565
H	-1.15671	3.00151	2.71073
C	2.63468	2.59720	1.99777
H	3.30083	1.80601	2.34010
H	3.09293	3.07982	1.13195
C	2.23191	3.59048	3.11140
H	2.96276	3.53975	3.92528
H	2.23598	4.62118	2.73879
H	0.57500	3.78434	4.52031
C	0.83590	1.69323	3.94065
H	1.74907	1.47386	4.50846
C	0.89010	0.95103	2.58238
H	1.57872	0.10913	2.57800
H	-0.09190	0.60311	2.27060
N	1.38582	1.89712	1.49858
C	-0.33929	1.23080	4.76295
H	-1.32620	1.35611	4.31593
C	-0.23956	0.68466	5.97547
H	-1.11770	0.37129	6.53286
H	0.72391	0.52694	6.45653
C	-0.73464	2.63744	0.10491
N	-1.20383	1.27654	0.22035
H	-0.52888	0.51335	0.08352

C	-2.53168	0.91838	0.19429
S	-3.77310	1.99010	0.57883
N	-2.66435	-0.39348	-0.17677
H	-1.82568	-0.80007	-0.60668
C	-3.76404	-1.26474	-0.17927
C	-3.59398	-2.45955	-0.90360
C	-4.96561	-1.05150	0.50980
C	-4.60867	-3.40933	-0.94378
H	-2.66320	-2.63402	-1.43485
C	-5.97261	-2.01790	0.45297
H	-5.11195	-0.14396	1.07729
C	-5.81328	-3.19803	-0.26917
H	-6.60479	-3.93637	-0.30588
C	-7.27858	-1.74143	1.15285
C	-4.39014	-4.70962	-1.67103
C	-8.09803	-0.97736	0.39622
C	-7.09431	-1.08377	2.31851
C	-7.95021	-2.88133	1.43283
C	-3.45967	-4.59972	-2.64323
C	-3.96894	-5.68393	-0.83039
C	-5.52882	-5.15716	-2.24562
H	-1.59610	3.25975	0.37985
C	-0.34154	3.02606	-1.32574

C	-0.16703	4.40911	-1.67903
C	-0.19370	2.08858	-2.32229
C	0.21345	4.70230	-3.03159
C	-0.36456	5.49103	-0.78753
C	0.15528	2.49836	-3.63513
H	-0.34246	1.03147	-2.12836
C	0.41327	6.05276	-3.41085
C	-0.16870	6.80302	-1.19094
H	-0.70963	5.33589	0.22813
H	0.25783	1.74512	-4.41590
C	0.23530	7.08776	-2.51976
H	0.70329	6.24237	-4.43946
H	0.39171	8.11009	-2.84398
N	0.37415	3.74451	-3.99129
O	-0.38857	7.75803	-0.24214
C	-0.26608	9.12519	-0.60639
H	-0.96603	9.39461	-1.40761
H	-0.51186	9.69462	0.29169
H	0.75681	9.37118	-0.92055
O	-0.25455	-1.38534	-1.64591
O	0.55173	-0.91422	0.35011
N	0.65780	-1.52937	-0.76355
C	1.69911	-2.36209	-1.00954

H	1.64182	-2.85881	-1.96584
C	2.71494	-2.57265	-0.04367
H	2.48027	-2.15379	0.92910
C	3.40671	-3.88000	-0.02561
C	3.72307	-4.46172	1.21569
C	3.70837	-4.59971	-1.19582
C	4.32149	-5.71868	1.28614
H	3.47521	-3.92657	2.12951
C	4.31962	-5.84946	-1.12538
H	3.47052	-4.17836	-2.16808
C	4.62840	-6.41391	0.11426
H	4.54543	-6.15652	2.25512
H	4.55600	-6.38415	-2.04075
H	5.10233	-7.38988	0.16640
H	1.68520	1.32737	0.68112
O	2.83248	0.72972	-0.65639
C	3.57370	-0.16540	-1.05628
C	4.35179	-1.13563	-0.26005
C	5.52108	-1.77410	-1.01484
H	6.15606	-0.98282	-1.44982
C	4.60710	-0.76728	1.14387
O	3.75120	-0.29503	1.89950
C	6.02266	-0.99660	1.67131

O	3.74732	-0.38335	-2.37919
C	2.95468	0.41157	-3.27387
H	3.06233	1.47542	-3.05394
H	3.32989	0.18428	-4.27243
H	1.90294	0.12832	-3.18874
C	6.59418	-2.36587	1.28365
C	6.47828	-2.64890	-0.20836
H	5.18219	-2.35914	-1.87165
H	6.66208	-0.20361	1.25284
H	6.00475	-0.85802	2.75597
H	7.64488	-2.46858	1.57510
H	6.04918	-3.16481	1.80174
O	7.15387	-3.50201	-0.74903

TSI-4 (R,R)

C	1.28888	-2.65415	1.26956
C	0.69622	-2.80912	3.70991
C	1.82076	-2.47450	2.70801
H	1.40371	-3.70212	0.98441
H	2.67847	-3.14173	2.84305
H	2.18791	-1.45336	2.85535
C	-0.80662	-3.74052	1.92021

H	-1.87083	-3.55643	2.05986
H	-0.69315	-4.51419	1.15661
C	-0.04930	-4.07380	3.22875
H	-0.76537	-4.40731	3.98696
H	0.65803	-4.89595	3.07124
H	1.10577	-2.96439	4.71205
C	-0.32866	-1.64249	3.72704
H	-1.24411	-2.01015	4.20883
C	-0.62851	-1.29793	2.24943
H	-1.68502	-1.13193	2.05179
H	-0.07806	-0.42388	1.90921
N	-0.22900	-2.46232	1.35136
C	0.13294	-0.42705	4.49032
H	0.96769	0.13008	4.06525
C	-0.41934	-0.00683	5.62865
H	-0.04958	0.87140	6.14968
H	-1.26857	-0.51803	6.07864
C	2.03829	-1.81921	0.18118
N	1.45721	-0.51311	-0.05789
H	0.55707	-0.47065	-0.53155
C	2.16648	0.66251	0.08761
S	3.74826	0.71086	0.67265
N	1.43142	1.75609	-0.26230

H	0.40538	1.65394	-0.30955
C	1.84482	3.10887	-0.21013
C	0.98057	4.03228	0.38853
C	3.03534	3.54781	-0.80108
C	1.31468	5.38796	0.39739
H	0.07062	3.67543	0.85988
C	3.35855	4.90339	-0.77223
H	3.70324	2.83710	-1.26869
C	2.50439	5.83345	-0.17591
H	2.76922	6.88355	-0.14838
C	4.60797	5.38338	-1.46211
C	0.35416	6.37939	0.99894
C	4.35797	5.74147	-2.74522
C	5.56485	4.43320	-1.50060
C	5.13376	6.46929	-0.85191
C	-0.59091	6.75948	0.10679
C	-0.29764	5.86785	2.06452
C	0.98165	7.50531	1.40765
H	3.01894	-1.58923	0.61273
C	2.28475	-2.66227	-1.07299
C	3.30562	-3.67552	-1.05738
C	1.54886	-2.51937	-2.22603
C	3.46309	-4.47211	-2.24211

C	4.15747	-3.93043	0.04357
C	1.79602	-3.35887	-3.34174
H	0.75873	-1.78372	-2.28679
C	4.45485	-5.48393	-2.26110
C	5.11768	-4.92943	-0.00570
H	4.11253	-3.33593	0.94825
H	1.19964	-3.23422	-4.24558
C	5.26656	-5.71952	-1.17394
H	4.55241	-6.06747	-3.17102
H	6.01697	-6.50016	-1.22158
N	2.70652	-4.30621	-3.36644
O	5.87574	-5.08317	1.11646
C	6.92496	-6.04044	1.11030
H	7.66427	-5.82479	0.32844
H	7.40324	-5.96171	2.08810
H	6.54252	-7.06097	0.97720
O	-1.44279	1.66762	-0.58126
O	-1.17492	1.65925	1.60685
N	-1.88602	1.41081	0.59231
C	-3.12480	0.87301	0.76002
H	-3.39139	0.73074	1.79509
C	-4.01331	0.64210	-0.32285
H	-3.79476	1.22804	-1.21293

C	-5.46145	0.60074	0.03675
C	-6.40095	1.23980	-0.78746
C	-5.91954	-0.01871	1.21455
C	-7.75585	1.25897	-0.45215
H	-6.06599	1.73508	-1.69475
C	-7.27131	0.00435	1.55217
H	-5.21539	-0.53360	1.86115
C	-8.19628	0.64207	0.71879
H	-8.46415	1.75686	-1.10796
H	-7.60515	-0.47678	2.46778
H	-9.24994	0.65811	0.98298
H	-0.66863	-2.26705	0.43173
O	-1.22777	-1.23763	-1.13224
C	-2.24232	-0.85486	-1.72654
C	-3.65403	-1.10103	-1.34211
C	-4.60766	-1.08901	-2.54556
H	-4.17530	-1.68095	-3.36787
C	-3.85428	-2.17393	-0.35179
O	-3.12774	-2.31651	0.63759
O	-2.18260	-0.15817	-2.87413
C	-0.90542	0.27462	-3.35890
H	-1.12753	0.94813	-4.18716
H	-0.36142	0.80653	-2.57800

H	-0.32341	-0.57617	-3.72344
H	-4.70962	-0.08361	-2.96382
C	-4.99267	-3.16464	-0.58644
H	-4.59656	-3.92261	-1.28147
H	-5.18610	-3.68018	0.35896
C	-6.27485	-2.56372	-1.17444
C	-6.01741	-1.64986	-2.36067
O	-6.88633	-1.39752	-3.17251
H	-6.97858	-3.34184	-1.48834
H	-6.79277	-1.96348	-0.41671

TSI-5 (R,R)

C	3.60608	-0.79981	1.17144
C	3.79758	-0.52762	3.67055
C	4.13035	0.11415	2.30603
H	4.38612	-1.51794	0.90885
H	5.21272	0.23391	2.19089
H	3.68899	1.11261	2.22537
C	3.14973	-2.71776	2.62595
H	2.33442	-3.25117	3.11946
H	3.64790	-3.41657	1.94938
C	4.12629	-2.03646	3.61614

H	4.02504	-2.48978	4.60776
H	5.16451	-2.18615	3.29864
H	4.36527	-0.04204	4.46970
C	2.27390	-0.39285	3.94297
H	2.02049	-1.07570	4.76470
C	1.55602	-0.85073	2.64930
H	0.69352	-1.49134	2.82655
H	1.21681	-0.00622	2.05524
N	2.50438	-1.65345	1.78189
C	1.83646	0.99252	4.34481
H	1.94636	1.77500	3.59302
C	1.32487	1.29936	5.53781
H	1.02759	2.31439	5.78540
H	1.18317	0.54838	6.31316
C	3.20464	-0.06202	-0.16153
N	1.78789	0.23627	-0.26324
H	1.16014	-0.55098	-0.42098
C	1.26404	1.50333	-0.19739
S	2.20562	2.86784	0.14637
N	-0.08366	1.52677	-0.38737
H	-0.59574	0.63807	-0.42731
C	-0.93581	2.65460	-0.37479
C	-2.14654	2.54223	0.31635

C	-0.64656	3.83136	-1.07738
C	-3.06095	3.59644	0.30224
H	-2.34844	1.63846	0.87850
C	-1.56162	4.88313	-1.06449
H	0.28446	3.92514	-1.61885
C	-2.77488	4.77688	-0.38063
H	-3.47522	5.60368	-0.37069
C	-1.27800	6.13287	-1.85699
C	-4.38425	3.42945	0.99672
C	-1.87561	6.09478	-3.07182
C	0.04050	6.31309	-2.07085
C	-1.74644	7.23546	-1.22922
C	-5.30131	2.83599	0.18488
C	-4.28685	2.64990	2.09621
C	-4.91412	4.61009	1.37640
H	3.68284	0.92174	-0.11128
C	3.76223	-0.78740	-1.38934
C	5.17733	-0.75504	-1.64488
C	2.97219	-1.47999	-2.27865
C	5.66143	-1.48298	-2.78360
C	6.11178	-0.04538	-0.85334
C	3.55981	-2.15616	-3.37844
H	1.90065	-1.54962	-2.14464

C	7.05139	-1.48076	-3.05826
C	7.46589	-0.06027	-1.15019
H	5.79947	0.55880	-0.00996
H	2.91837	-2.70768	-4.06500
C	7.94376	-0.79345	-2.26572
H	7.38711	-2.04066	-3.92538
H	9.00066	-0.81077	-2.50557
N	4.84901	-2.17787	-3.63255
O	8.26798	0.65987	-0.31430
C	9.65534	0.74617	-0.60378
H	9.83548	1.19210	-1.59031
H	10.07925	1.39363	0.16585
H	10.14234	-0.23676	-0.55584
H	1.91186	-2.12993	1.02035
O	-2.00532	-0.44182	-1.22325
C	-3.14209	-0.82104	-0.90598
C	-4.26863	-0.62642	-1.91979
C	-3.44092	-1.52014	0.34857
C	-5.64777	-0.41172	-1.27706
H	-3.98447	0.21663	-2.55626
C	-4.89114	-1.84637	0.71100
C	-5.94988	-1.57085	-0.35158
H	-5.63299	0.51698	-0.68941

H	-5.01950	-2.88071	1.04282
C	-2.56524	-1.22076	1.50333
O	-1.52386	-0.57667	1.50031
O	-3.06356	-1.77266	2.64335
C	-2.26746	-1.61693	3.82246
H	-1.97465	-0.57361	3.96433
H	-2.89600	-1.95522	4.64781
H	-1.37295	-2.24214	3.74741
H	-4.30182	-1.51555	-2.56459
H	-6.44050	-0.32935	-2.02569
H	-5.18763	-1.23402	1.57646
O	-6.97380	-2.22391	-0.41018
O	0.99365	-2.60771	-0.16085
N	-0.14291	-3.03530	0.32028
O	-0.21907	-3.34931	1.53656
C	-1.16446	-3.15449	-0.55565
H	-0.89654	-2.90220	-1.56820
C	-2.47563	-3.45556	-0.13147
H	-2.55876	-3.76648	0.90540
C	-3.42536	-4.11531	-1.05127
C	-3.34306	-3.98880	-2.45274
C	-4.42611	-4.94894	-0.51966
C	-4.24012	-4.65663	-3.28230

H	-2.57385	-3.36536	-2.89814
C	-5.32637	-5.61415	-1.35085
H	-4.48621	-5.08780	0.55628
C	-5.23898	-5.46795	-2.73514
H	-4.15900	-4.54547	-4.36015
H	-6.09397	-6.24693	-0.91502
H	-5.93956	-5.98437	-3.38514

TSI-6(S,R)

C	2.30548	-2.65842	0.99550
C	3.74462	-3.85890	2.69503
C	3.63132	-3.43591	1.21821
H	1.54968	-3.28510	0.52132
H	3.65720	-4.31714	0.56976
H	4.48770	-2.81590	0.93244
C	1.26529	-3.66680	2.98627
H	0.86418	-3.39972	3.96692
H	0.44062	-4.03590	2.37540
C	2.46849	-4.63187	3.07726
H	2.55204	-5.03689	4.09144
H	2.33079	-5.48314	2.40113
H	4.62938	-4.48703	2.83684

C	3.84990	-2.60953	3.61833
H	3.73192	-2.96329	4.65059
C	2.66241	-1.66258	3.27040
H	2.09385	-1.37129	4.15700
H	2.98034	-0.74208	2.77480
N	1.70459	-2.36838	2.35330
C	5.17436	-1.89459	3.53165
H	5.40001	-1.39490	2.58916
C	6.06124	-1.83341	4.52565
H	7.00626	-1.30937	4.41499
H	5.87463	-2.30060	5.49087
C	2.52638	-1.38474	0.13639
N	1.36738	-0.50355	0.07690
H	0.57227	-0.80639	-0.49247
C	1.38232	0.81066	0.46588
S	2.66899	1.50225	1.32962
N	0.24237	1.47464	0.10954
H	-0.51537	0.89357	-0.25732
C	-0.08801	2.84206	0.22971
C	-1.45289	3.15505	0.29596
C	0.85089	3.88379	0.19531
C	-1.86735	4.48589	0.33189
H	-2.18813	2.35862	0.30102

C	0.41582	5.20790	0.25427
H	1.90554	3.66591	0.11898
C	-0.94088	5.52698	0.32154
H	-1.26541	6.55968	0.35544
C	1.43644	6.31501	0.29020
C	-3.34270	4.78078	0.31766
C	0.96579	7.44936	-0.27837
C	2.57342	5.98013	-0.35733
C	1.78405	6.63118	1.55889
C	-3.86112	4.66023	-0.93410
C	-4.04071	3.93233	1.10331
C	-3.61831	6.03649	0.73110
H	3.31230	-0.79645	0.60763
C	2.98187	-1.79643	-1.27032
C	4.12503	-1.19802	-1.90166
C	2.28772	-2.75597	-1.97981
C	4.47324	-1.67891	-3.21331
C	4.92034	-0.18226	-1.32025
C	2.71124	-3.13862	-3.27588
H	1.40649	-3.23443	-1.56344
C	5.60801	-1.13431	-3.86400
C	6.02275	0.32976	-1.98714
H	4.66749	0.26161	-0.36354

H	2.15177	-3.89910	-3.82017
C	6.37439	-0.15568	-3.27347
H	5.84786	-1.51832	-4.85034
H	7.23625	0.24140	-3.79743
N	3.76666	-2.63751	-3.87880
O	6.71648	1.30123	-1.33180
C	7.81526	1.92064	-1.98265
H	7.50957	2.40946	-2.91673
H	8.18361	2.67604	-1.28649
H	8.61915	1.20320	-2.19479
H	0.78413	-1.81628	2.23838
O	-1.21144	-0.68356	-1.21218
C	-2.06408	-1.47344	-1.65197
C	-1.55704	-2.73981	-2.35028
C	-3.50256	-1.30471	-1.45219
C	-2.51805	-3.37179	-3.37424
H	-0.59920	-2.48734	-2.81476
C	-4.45775	-2.10665	-2.33976
C	-3.89603	-3.45516	-2.75144
H	-2.57081	-2.73843	-4.27053
H	-5.42066	-2.25452	-1.84698
C	-3.96683	0.05430	-1.08466
O	-3.40866	0.81951	-0.31503

O	-5.14779	0.36633	-1.67364
C	-5.68748	1.65327	-1.33034
H	-4.98628	2.45175	-1.58124
H	-6.60494	1.74520	-1.91270
H	-5.90693	1.70395	-0.26068
H	-1.34482	-3.45919	-1.54905
H	-2.18407	-4.36884	-3.67453
H	-4.66506	-1.53832	-3.25958
O	-4.48227	-4.50612	-2.56395
C	-2.73773	-1.55967	1.38424
C	-3.64161	-2.21312	0.51717
C	-5.09459	-2.13854	0.80178
C	-5.91555	-3.22898	0.46016
C	-5.68415	-1.03211	1.44339
C	-7.27768	-3.22095	0.76251
H	-5.48453	-4.08157	-0.05746
C	-7.04438	-1.02634	1.74126
H	-5.07881	-0.16942	1.70131
C	-7.84653	-2.12162	1.40641
H	-7.89186	-4.07551	0.49232
H	-7.48031	-0.16509	2.24050
H	-8.90674	-2.11483	1.64441
H	-3.30491	-3.18318	0.16437

H	-2.97974	-0.69656	1.98144
N	-1.45341	-1.96302	1.51249
O	-0.98161	-2.95638	0.87458
O	-0.71062	-1.32352	2.35059

TSI-7 (R,S)

C	3.58390	-1.18114	0.93844
C	3.80522	-1.94578	3.32541
C	4.03065	-0.76304	2.35760
H	4.42356	-1.66878	0.43839
H	5.08867	-0.48274	2.32569
H	3.47877	0.12386	2.68684
C	3.31873	-3.55721	1.45718
H	2.56699	-4.31484	1.68994
H	3.85192	-3.87298	0.55719
C	4.26663	-3.25532	2.64558
H	4.24215	-4.08693	3.35732
H	5.30168	-3.15919	2.29900
H	4.35181	-1.78816	4.25976
C	2.28569	-2.08536	3.61211
H	2.11909	-3.07317	4.06162
C	1.57425	-2.01767	2.23847

H	0.78321	-2.75809	2.12160
H	1.13661	-1.04133	2.04115
N	2.56404	-2.29922	1.12315
C	1.73337	-1.05332	4.56109
H	1.78082	-0.01434	4.23354
C	1.19204	-1.33818	5.74645
H	0.80855	-0.55928	6.39925
H	1.11084	-2.36093	6.11001
C	3.13800	-0.00626	0.00355
N	1.71586	0.27410	0.06572
H	1.09512	-0.42132	-0.34459
C	1.20476	1.52414	0.33182
S	2.16581	2.80155	0.87581
N	-0.14790	1.58516	0.14956
H	-0.66513	0.69760	0.11994
C	-0.97186	2.72369	0.27835
C	-2.21190	2.56767	0.90712
C	-0.62307	3.97088	-0.25605
C	-3.08663	3.64945	1.00935
H	-2.48056	1.60301	1.31869
C	-1.50138	5.04599	-0.13197
H	0.32706	4.10124	-0.75448
C	-2.73686	4.89932	0.50103

H	-3.40721	5.74456	0.60368
C	-1.15161	6.37342	-0.75221
C	-4.44236	3.45316	1.62875
C	-1.71638	6.51056	-1.97604
C	0.17782	6.52921	-0.91160
C	-1.59829	7.40687	-0.00246
C	-5.37563	3.12958	0.69475
C	-4.44805	2.45689	2.54126
C	-4.88648	4.57068	2.24233
H	3.60615	0.89429	0.41732
C	3.67957	-0.18100	-1.42033
C	5.09088	-0.04244	-1.66304
C	2.87479	-0.46004	-2.50115
C	5.55596	-0.25593	-3.00422
C	6.03918	0.30011	-0.66944
C	3.44362	-0.63950	-3.78815
H	1.80494	-0.57666	-2.38859
C	6.94169	-0.13989	-3.27616
C	7.38860	0.40997	-0.96807
H	5.74099	0.52386	0.34799
H	2.79034	-0.87144	-4.62860
C	7.84780	0.18015	-2.28957
H	7.26272	-0.30779	-4.29930

H	8.90085	0.26366	-2.53221
N	4.72913	-0.55725	-4.04790
O	8.20484	0.74425	0.07258
C	9.58794	0.94407	-0.17971
H	9.75409	1.74532	-0.91106
H	10.02493	1.23515	0.77716
H	10.07354	0.02470	-0.53259
H	1.97906	-2.45065	0.23928
O	-2.81163	0.09574	-1.09223
C	-3.65298	-0.63341	-0.58206
C	-3.40378	-1.73326	0.36194
C	-4.60010	-2.51327	0.88929
H	-5.32053	-2.73114	0.09962
C	-2.26797	-1.60311	1.25436
O	-1.25308	-0.91601	1.02918
O	0.96865	-2.38265	-0.99712
N	-0.16403	-2.95454	-0.71422
O	-0.23019	-3.77803	0.23300
C	-1.22272	-2.64902	-1.50850
H	-1.00113	-1.92584	-2.27592
C	-2.48804	-3.17916	-1.24908
H	-2.51207	-3.98969	-0.53070
C	-3.55602	-3.19727	-2.25830

C	-3.56428	-2.33626	-3.37425
C	-4.59280	-4.14244	-2.13218
C	-4.57063	-2.42766	-4.33141
H	-2.79031	-1.58448	-3.48624
C	-5.59818	-4.23056	-3.09354
H	-4.61128	-4.80630	-1.27226
C	-5.58978	-3.37600	-4.19725
H	-4.55918	-1.75883	-5.18779
H	-6.38699	-4.96870	-2.97908
H	-6.37136	-3.44592	-4.94886
C	-2.38687	-2.35383	2.58309
O	-4.97975	-0.49894	-0.85001
C	-5.33294	0.58252	-1.72350
H	-4.77612	0.52246	-2.66129
H	-6.40273	0.46982	-1.90565
H	-5.13044	1.54139	-1.24038
H	-5.14882	-1.92221	1.64516
C	-4.19263	-3.82280	1.55223
C	-2.93905	-3.77476	2.41945
H	-1.41092	-2.35322	3.07444
H	-3.06317	-1.76944	3.22628
H	-2.18746	-4.41263	1.93719
O	-4.81278	-4.85792	1.38584

H	-3.17002	-4.23993	3.38521
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TSI-8 (S,S)

C	3.10447	-1.30197	1.32181
C	2.99543	-1.04559	3.82519
C	3.62875	-0.49131	2.53083
H	3.75933	-2.16121	1.16016
H	4.72034	-0.57756	2.56443
H	3.40057	0.57162	2.40583
C	2.08948	-3.07787	2.66804
H	1.12822	-3.42856	3.05032
H	2.52027	-3.87239	2.05448
C	3.03952	-2.58901	3.78759
H	2.72479	-3.00901	4.74860
H	4.06322	-2.93505	3.60477
H	3.52776	-0.66905	4.70359
C	1.50175	-0.62086	3.88690
H	1.00941	-1.23274	4.65399
C	0.88725	-0.94622	2.50070
H	-0.10222	-1.40188	2.55620
H	0.80299	-0.05607	1.88297
N	1.78264	-1.91857	1.75539
C	1.29097	0.82668	4.25079

H	1.69171	1.56683	3.55708
C	0.64886	1.23879	5.34450
H	0.52438	2.29462	5.56753
H	0.21857	0.53715	6.05668
C	3.05241	-0.51778	-0.03716
N	1.79251	0.17248	-0.25311
H	0.97996	-0.38966	-0.53565
C	1.64644	1.52696	-0.14696
S	2.92274	2.58074	0.19650
N	0.34240	1.93102	-0.29882
H	-0.39460	1.22843	-0.20537
C	-0.13727	3.26121	-0.32210
C	-1.31625	3.54726	0.37227
C	0.48346	4.27056	-1.07304
C	-1.87278	4.82715	0.30964
H	-1.80156	2.76528	0.94431
C	-0.06889	5.54875	-1.09976
H	1.38996	4.05903	-1.62248
C	-1.25175	5.84055	-0.41389
H	-1.67373	6.83798	-0.44185
C	0.56711	6.62569	-1.94008
C	-3.18838	5.06766	0.99720
C	-0.06589	6.76087	-3.13029

C	1.86238	6.36821	-2.20747
C	0.50477	7.83052	-1.32973
C	-4.21552	4.52527	0.28925
C	-3.22869	4.50155	2.22259
C	-3.46177	6.37976	1.14288
H	3.79112	0.28451	0.06275
C	3.48179	-1.39536	-1.21367
C	4.86682	-1.76103	-1.34492
C	2.60525	-1.86200	-2.16693
C	5.22407	-2.61057	-2.44553
C	5.89122	-1.33035	-0.46754
C	3.07473	-2.69009	-3.21869
H	1.54818	-1.62849	-2.12622
C	6.57829	-2.99608	-2.60253
C	7.20796	-1.72432	-0.64920
H	5.68910	-0.65646	0.35693
H	2.36520	-3.05584	-3.96012
C	7.55637	-2.57319	-1.72999
H	6.81715	-3.63822	-3.44439
H	8.58344	-2.88522	-1.88030
N	4.32510	-3.06706	-3.36592
O	8.10497	-1.24682	0.26138
C	9.47896	-1.56497	0.09907

H	9.86943	-1.19706	-0.85850
H	9.99877	-1.06103	0.91589
H	9.65676	-2.64610	0.17120
H	1.24411	-2.32756	0.92281
O	-2.24343	0.51270	0.33101
C	-3.17716	-0.11826	-0.14651
C	-3.79780	-1.35844	0.37637
C	-5.31924	-1.39167	0.24340
H	-5.64274	-1.31031	-0.79575
C	-3.22253	-1.92296	1.59848
O	-2.01040	-1.95828	1.82619
C	-1.75133	-3.32283	-0.66330
C	-2.90976	-2.72895	-1.20226
C	-4.19663	-2.54400	2.60131
O	-3.82428	0.30227	-1.26954
C	-3.39934	1.55192	-1.83108
H	-2.33370	1.52890	-2.07278
H	-3.98879	1.67534	-2.74067
H	-3.59978	2.37510	-1.14081
H	-5.75400	-0.50824	0.74495
C	-6.04085	-2.59154	0.85479
C	-5.30242	-3.37078	1.93388
H	-3.61447	-3.14410	3.30664

H	-4.65083	-1.72264	3.17705
H	-4.86819	-4.25465	1.44729
O	-7.17126	-2.88012	0.51409
H	-6.03656	-3.74389	2.65554
C	-4.04377	-3.55361	-1.65792
C	-4.91350	-3.02673	-2.63172
C	-4.28015	-4.86372	-1.19815
C	-5.98640	-3.77178	-3.11700
H	-4.73679	-2.02173	-3.00552
C	-5.35196	-5.60797	-1.68380
H	-3.62013	-5.30917	-0.45953
C	-6.21233	-5.06431	-2.64180
H	-6.64600	-3.34234	-3.86574
H	-5.51734	-6.61631	-1.31441
H	-7.05072	-5.64564	-3.01461
H	-2.72549	-1.85234	-1.81004
H	-1.70501	-4.30277	-0.21501
N	-0.58444	-2.64721	-0.59309
O	-0.47151	-1.46484	-1.04537
O	0.43386	-3.23814	-0.07351

TSII-1 (S,S)

C	2.46414	1.25087	0.28308
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C	2.90235	3.43116	1.46632
C	3.51274	2.35182	0.54849
H	2.55613	0.45973	1.03113
H	4.39476	1.90403	1.01642
H	3.83041	2.78634	-0.40363
C	0.95744	1.96564	2.08324
H	0.00623	2.46304	2.26926
H	0.87372	0.94646	2.46061
C	2.18053	2.73418	2.63809
H	1.84937	3.46971	3.37938
H	2.86992	2.05179	3.14861
H	3.68297	4.10061	1.84076
C	1.83970	4.25144	0.68246
H	1.25724	4.82519	1.41535
C	0.91670	3.22930	-0.02934
H	-0.14367	3.46796	0.06258
H	1.16332	3.13343	-1.08339
N	1.09651	1.86177	0.58540
C	2.42724	5.22575	-0.30580
H	2.96318	4.78955	-1.14929
C	2.31944	6.55181	-0.21263
H	2.76602	7.21395	-0.94924
H	1.77800	7.02801	0.60284

C	2.55663	0.54858	-1.10288
C	3.87209	-0.21967	-1.13115
C	3.99741	-1.50480	-0.50044
C	4.98967	0.29829	-1.75196
C	5.27972	-2.14799	-0.56608
C	2.93573	-2.16704	0.16359
C	6.20793	-0.42582	-1.75294
H	4.94551	1.26507	-2.24276
C	5.43759	-3.42101	0.03506
C	3.12600	-3.41405	0.73669
H	1.94687	-1.72646	0.23690
H	7.08171	-0.00072	-2.24664
C	4.39218	-4.04948	0.67444
H	6.41622	-3.88584	-0.03087
H	4.54473	-5.02566	1.12014
N	6.36751	-1.60122	-1.18555
O	2.03336	-3.96838	1.34530
C	2.15269	-5.26050	1.91977
H	2.89245	-5.27776	2.73091
H	1.16847	-5.49643	2.32862
H	2.42128	-6.01512	1.16911
N	2.44113	1.50203	-2.21394
H	2.86984	1.08144	-3.03553

H	1.44098	1.52355	-2.43431
H	1.74009	-0.18073	-1.15226
O	0.01073	-0.48641	-2.93875
N	-0.78751	0.08361	-2.14880
O	-0.45262	1.20203	-1.60020
C	-2.00860	-0.46038	-1.90640
H	-2.20068	-1.36119	-2.46992
C	-2.91766	0.16860	-1.00183
H	-2.55442	1.15855	-0.74352
C	-4.37799	0.14197	-1.30712
C	-5.00170	-0.91658	-1.98833
C	-5.16792	1.24179	-0.92956
C	-6.36519	-0.87874	-2.27485
H	-4.42267	-1.78070	-2.29789
C	-6.53050	1.28573	-1.22215
H	-4.69938	2.07797	-0.41665
C	-7.13576	0.22230	-1.89450
H	-6.82602	-1.71291	-2.79644
H	-7.11782	2.15214	-0.92918
H	-8.19785	0.25145	-2.12225
H	0.34345	1.24834	0.20870
O	-0.38876	-0.53243	0.88779
C	-1.45427	-1.14345	0.96470

C	-1.42366	-2.66196	1.11208
C	-2.80048	-0.50723	0.90217
H	-1.61708	-2.89227	2.17182
C	-2.47857	-3.35743	0.24371
C	-3.95594	-1.46925	1.21209
H	-2.47150	-4.44453	0.37307
H	-4.92275	-1.02781	0.96853
C	-3.87691	-2.83715	0.54096
O	-4.87353	-3.48970	0.29771
H	-2.26652	-3.16631	-0.81706
H	-0.41154	-3.00930	0.89089
H	-3.99249	-1.67083	2.29575
C	-2.88205	0.79745	1.61526
O	-2.07189	1.71233	1.56218
O	-4.02988	0.91326	2.33704
C	-4.21879	2.16660	3.00359
H	-4.20128	2.99426	2.28886
H	-5.19518	2.09729	3.48476
H	-3.43655	2.33097	3.75053

TSII-2 (R,S)

C	2.31198	1.45695	0.48257
C	2.22254	3.76677	1.49531

C	3.08540	2.77813	0.69114
H	2.63618	0.70654	1.20810
H	4.02174	2.57416	1.22033
H	3.33749	3.19951	-0.28505
C	0.80854	1.88729	2.38242
H	-0.24026	2.04588	2.63291
H	1.11633	0.93822	2.82756
C	1.72847	3.06718	2.77761
H	1.18014	3.77084	3.41358
H	2.58541	2.70839	3.35868
H	2.80866	4.65473	1.75227
C	0.98266	4.19946	0.66193
H	0.33402	4.78375	1.32779
C	0.23302	2.90896	0.22726
H	-0.81084	2.90300	0.54435
H	0.24894	2.74443	-0.84964
N	0.85711	1.70486	0.88644
C	1.32553	5.06138	-0.52779
H	1.81963	4.55417	-1.35603
C	1.04799	6.36309	-0.61312
H	1.31787	6.94713	-1.48867
H	0.53518	6.89614	0.18596
C	2.49927	0.80521	-0.92779

C	3.90503	0.20636	-0.93472
C	4.17721	-1.07418	-0.34131
C	4.96804	0.89119	-1.48646
C	5.53503	-1.54151	-0.37630
C	3.19089	-1.89078	0.26399
C	6.27039	0.33223	-1.46362
H	4.81969	1.86566	-1.93993
C	5.83838	-2.80315	0.19236
C	3.52464	-3.11999	0.81109
H	2.15015	-1.58743	0.30769
H	7.09749	0.88800	-1.90502
C	4.86472	-3.58301	0.77610
H	6.87137	-3.13366	0.14931
H	5.13076	-4.54462	1.19998
N	6.56263	-0.83490	-0.93355
O	2.49505	-3.82769	1.36641
C	2.76926	-5.09983	1.93202
H	3.47843	-5.02912	2.76737
H	1.81341	-5.47218	2.30535
H	3.16143	-5.80160	1.18424
N	2.31093	1.76582	-2.02057
H	2.87510	1.47245	-2.81358
H	1.34026	1.70042	-2.34916

H	1.77617	-0.01549	-0.99635
C	-2.35192	0.89614	-1.56250
C	-3.18793	-0.18328	-1.17626
H	0.28569	0.84989	0.66211
O	-0.06449	-0.74217	0.32407
C	-1.00352	-1.50464	0.03812
C	-0.66742	-2.86221	-0.56509
C	-2.41969	-1.23502	0.36502
H	-0.45528	-3.53707	0.27930
C	-1.76885	-3.44392	-1.45463
C	-3.27567	-2.50540	0.42548
H	-1.55523	-4.47644	-1.75174
H	-4.33097	-2.27273	0.57100
C	-3.14193	-3.40013	-0.80318
O	-4.08381	-4.04246	-1.23099
H	-1.82144	-2.85500	-2.37933
H	0.26724	-2.75477	-1.11879
H	-2.97979	-3.11961	1.29249
C	-2.60965	-0.27368	1.47834
O	-2.01462	0.78763	1.62314
O	-3.57318	-0.67476	2.34455
C	-3.88336	0.23707	3.40418
H	-4.27780	1.17362	3.00094

H	-4.64224	-0.26380	4.00651
H	-2.99580	0.45010	4.00671
C	-4.58819	0.15300	-0.77490
C	-4.90343	1.32210	-0.05874
C	-5.64048	-0.69672	-1.15507
C	-6.22524	1.63171	0.25662
H	-4.10801	1.98879	0.25871
C	-6.96408	-0.38627	-0.83844
H	-5.42136	-1.60977	-1.70185
C	-7.26239	0.77963	-0.13288
H	-6.44745	2.54469	0.80345
H	-7.76043	-1.05780	-1.14762
H	-8.29268	1.02450	0.11105
H	-3.13459	-1.02742	-1.85772
H	-2.53806	1.93224	-1.33213
N	-1.22105	0.66761	-2.28456
O	-0.87920	-0.51305	-2.58356
O	-0.52165	1.67209	-2.65013

TSII-3 (S,R)

C	2.40552	1.27478	0.32592
C	2.66208	3.41274	1.62817
C	3.34581	2.46166	0.62418

H	2.59509	0.46725	1.03662
H	4.28538	2.08011	1.03533
H	3.58311	2.98113	-0.30893
C	0.87999	1.73649	2.18979
H	-0.10247	2.14625	2.41991
H	0.88707	0.69312	2.50716
C	2.04762	2.57134	2.76623
H	1.67547	3.21849	3.56793
H	2.81270	1.92182	3.20742
H	3.38429	4.13082	2.02877
C	1.50058	4.17174	0.92644
H	0.87913	4.62627	1.70905
C	0.67077	3.11172	0.15713
H	-0.40586	3.23658	0.27316
H	0.91225	3.10571	-0.90264
N	0.99233	1.73192	0.68436
C	1.95822	5.27107	0.00328
H	2.52459	4.95712	-0.87380
C	1.70474	6.56703	0.19038
H	2.06117	7.32438	-0.50233
H	1.12795	6.92152	1.04272
C	2.54104	0.64577	-1.09070
C	3.93830	0.04197	-1.17824

C	4.25222	-1.21056	-0.54745
C	4.95508	0.68894	-1.84908
C	5.60259	-1.68572	-0.65975
C	3.31336	-1.99294	0.16858
C	6.25295	0.12208	-1.90177
H	4.77044	1.64045	-2.33642
C	5.94858	-2.91462	-0.04549
C	3.68815	-3.18881	0.75994
H	2.27809	-1.68514	0.26682
H	7.04345	0.64690	-2.43799
C	5.02248	-3.65658	0.65344
H	6.97554	-3.25084	-0.14752
H	5.31981	-4.59303	1.11134
N	6.58459	-1.01602	-1.33281
O	2.70365	-3.86219	1.42972
C	3.01640	-5.10651	2.03708
H	3.78413	-4.99653	2.81405
H	2.08948	-5.45435	2.49657
H	3.35256	-5.84553	1.29820
N	2.29210	1.62531	-2.15442
H	2.70500	1.26709	-3.01309
H	1.28151	1.57884	-2.32065
H	1.81080	-0.17160	-1.15367

O	-0.00615	-0.61998	-2.85141
N	-0.85341	-0.00882	-2.14099
O	-0.53866	1.10777	-1.58325
C	-2.10441	-0.51534	-1.98981
H	-2.27764	-1.42555	-2.54354
C	-3.02811	0.07118	-1.07419
H	-2.71987	1.06841	-0.77522
C	-4.47888	-0.04534	-1.38992
C	-5.04852	-1.20405	-1.94555
C	-5.31268	1.06613	-1.17750
C	-6.40552	-1.25386	-2.25868
H	-4.42712	-2.07506	-2.13192
C	-6.66890	1.02171	-1.50110
H	-4.88288	1.97980	-0.77271
C	-7.22206	-0.14271	-2.03671
H	-6.82709	-2.16364	-2.67707
H	-7.29183	1.89735	-1.33800
H	-8.27955	-0.18372	-2.28236
H	0.28717	1.07614	0.29255
O	-0.37723	-0.80333	0.76531
C	-1.47598	-1.32728	0.61527
C	-2.81332	-0.70234	0.81173
C	-3.91121	-1.72887	1.12625

H	-3.57708	-2.38585	1.94772
C	-2.81541	0.51203	1.66655
O	-2.03490	1.45296	1.51215
O	-1.59776	-2.59748	0.18012
C	-0.38886	-3.24575	-0.25791
H	0.05018	-2.68864	-1.09044
H	0.33137	-3.32921	0.55850
H	-0.70380	-4.23657	-0.58887
H	-4.08985	-2.39947	0.28474
C	-3.87249	0.58254	2.76716
H	-3.55489	-0.09311	3.57684
H	-3.87030	1.59807	3.17314
C	-5.26253	-1.18769	1.58526
C	-5.26704	0.16826	2.27968
H	-5.99492	0.13659	3.09735
H	-5.64659	0.89753	1.55283
O	-6.28000	-1.83875	1.45155

TSII-4 (R,R)

C	2.33803	1.32085	0.61509
C	2.22210	3.47289	1.92689
C	3.09579	2.61060	0.99940
H	2.66481	0.48912	1.24412

H	4.03372	2.34657	1.49829
H	3.34595	3.16010	0.08880
C	0.81789	1.47805	2.54078
H	-0.23366	1.59509	2.80052
H	1.13198	0.47958	2.85455
C	1.72645	2.60006	3.09776
H	1.16814	3.20584	3.81982
H	2.58320	2.17273	3.63114
H	2.80026	4.32107	2.30661
C	0.98411	4.00523	1.15156
H	0.32630	4.48991	1.88492
C	0.24703	2.78298	0.53895
H	-0.79740	2.72316	0.84395
H	0.27086	2.76873	-0.55001
N	0.87695	1.50022	1.03161
C	1.33005	5.02354	0.09312
H	1.83242	4.63745	-0.79350
C	1.04605	6.32339	0.18481
H	1.31858	7.02323	-0.60034
H	0.52456	6.73926	1.04547
C	2.55151	0.85408	-0.86185
C	3.98259	0.32041	-0.93027
C	4.31922	-0.99244	-0.45355

C	5.00869	1.09840	-1.42542
C	5.69597	-1.39291	-0.53593
C	3.37697	-1.90356	0.08177
C	6.33529	0.60005	-1.45793
H	4.81151	2.10117	-1.78891
C	6.06112	-2.68428	-0.08169
C	3.76971	-3.16049	0.51391
H	2.32494	-1.65128	0.15650
H	7.13208	1.23000	-1.85282
C	5.12861	-3.55715	0.43349
H	7.10775	-2.96152	-0.15776
H	5.44013	-4.53961	0.76894
N	6.68548	-0.59408	-1.03378
O	2.77471	-3.96314	0.99977
C	3.10293	-5.27430	1.43500
H	3.80851	-5.25710	2.27582
H	2.16344	-5.72145	1.76457
H	3.52433	-5.87847	0.62114
N	2.33495	1.93162	-1.83005
H	2.87416	1.72781	-2.66756
H	1.35535	1.91544	-2.14173
H	1.86149	0.01775	-1.03259
C	-2.29567	1.01073	-1.54390

C	-3.12198	-0.11832	-1.30025
H	0.30633	0.69068	0.69388
O	-0.12247	-0.94116	0.17162
C	-1.15152	-1.54880	-0.13390
C	-2.54399	-1.22251	0.27919
C	-3.45117	-2.46181	0.30526
H	-2.92010	-3.30132	0.78122
C	-2.64249	-0.30924	1.43323
O	-1.94090	0.70179	1.54635
C	-4.56921	0.18625	-1.07831
C	-4.99018	1.29873	-0.32621
C	-5.55134	-0.62189	-1.67193
C	-6.34532	1.58815	-0.17650
H	-4.25111	1.93227	0.15435
C	-6.90919	-0.33606	-1.51836
H	-5.24802	-1.47892	-2.26711
C	-7.31208	0.77026	-0.77041
H	-6.64871	2.45441	0.40590
H	-7.64954	-0.98017	-1.98438
H	-8.36820	0.99613	-0.65140
H	-2.95009	-0.94167	-1.99146
H	-2.54721	2.01777	-1.25434
N	-1.13191	0.91537	-2.24907

O	-0.71625	-0.19199	-2.68441
O	-0.48328	1.99593	-2.47081
H	-3.66463	-2.81841	-0.70659
O	-1.12126	-2.65846	-0.88817
C	0.13779	-3.01954	-1.48047
H	-0.09274	-3.85190	-2.14703
H	0.53010	-2.17317	-2.04677
H	0.84543	-3.33696	-0.71091
C	-4.78271	-2.37360	1.04824
C	-3.63838	-0.65109	2.54015
H	-3.12540	-1.37073	3.19876
H	-3.80026	0.25327	3.13442
C	-4.96390	-1.25950	2.06577
H	-5.55126	-1.65307	2.90231
H	-5.58186	-0.49042	1.58691
O	-5.64890	-3.20512	0.85391

TSII-5 (R,R)

C	-2.30355	1.10727	-0.42401
C	-2.57246	3.23972	-1.73164
C	-3.25429	2.28386	-0.72768
H	-2.46852	0.30130	-1.14113
H	-4.18813	1.89176	-1.14141

H	-3.50994	2.81057	0.19699
C	-0.74018	1.60467	-2.25020
H	0.23605	2.04965	-2.45053
H	-0.71250	0.56133	-2.56616
C	-1.91677	2.40757	-2.85493
H	-1.54774	3.06117	-3.65283
H	-2.65491	1.73491	-3.30649
H	-3.30215	3.93967	-2.15045
C	-1.43684	4.02266	-1.01544
H	-0.80105	4.47276	-1.78923
C	-0.61541	2.98012	-0.21277
H	0.46066	3.12633	-0.28982
H	-0.90557	2.97408	0.83563
N	-0.89468	1.59657	-0.74974
C	-1.92567	5.13171	-0.12126
H	-2.53471	4.83034	0.73151
C	-1.65584	6.42493	-0.30519
H	-2.03809	7.18959	0.36543
H	-1.04112	6.76975	-1.13466
C	-2.42504	0.44036	0.97808
C	-3.87525	0.00407	1.14996
C	-4.37941	-1.18391	0.51659
C	-4.76057	0.76628	1.88459

C	-5.78351	-1.45694	0.66668
C	-3.58108	-2.08401	-0.23127
C	-6.12151	0.38499	1.98329
H	-4.42530	1.67304	2.37736
C	-6.32740	-2.60265	0.03687
C	-4.15158	-3.19558	-0.83443
H	-2.50389	-1.97014	-0.30957
H	-6.80772	0.99811	2.56777
C	-5.54032	-3.45500	-0.70464
H	-7.38987	-2.78511	0.16400
H	-5.98641	-4.32449	-1.17387
N	-6.63366	-0.67286	1.39420
O	-3.30108	-3.99552	-1.53888
C	-3.80111	-5.18914	-2.11573
H	-4.56340	-4.98620	-2.88061
H	-2.94317	-5.67291	-2.58641
H	-4.22280	-5.86246	-1.35749
N	-2.00214	1.34787	2.05982
H	-2.37099	0.99024	2.93809
H	-0.98653	1.28319	2.14135
H	-1.79641	-0.45725	0.94393
H	-0.20795	0.90286	-0.38057
O	-0.34907	-2.44761	0.79246

N	0.46564	-1.73717	0.14719
O	0.02743	-0.87874	-0.70732
C	1.80245	-1.90631	0.32964
H	2.04775	-2.71367	1.00320
C	2.74191	-1.05204	-0.32742
H	2.23314	-0.45417	-1.07745
C	4.03245	-1.62347	-0.81234
C	4.68729	-2.69087	-0.17580
C	4.60828	-1.09694	-1.98173
C	5.87627	-3.20829	-0.68742
H	4.27081	-3.12421	0.72778
C	5.79325	-1.61796	-2.49979
H	4.10599	-0.28290	-2.49856
C	6.43416	-2.67556	-1.85170
H	6.36733	-4.02996	-0.17364
H	6.21293	-1.20155	-3.41189
H	7.35903	-3.08289	-2.25101
O	1.03402	1.07476	1.38772
C	2.16288	0.70921	1.71134
C	2.43768	0.37428	3.17497
C	3.29701	0.55065	0.75966
C	3.35234	-0.84117	3.36166
H	2.90776	1.26133	3.62762

C	4.65119	0.31004	1.44030
C	4.65022	-0.70487	2.57863
H	3.59325	-1.01665	4.41510
H	5.41338	0.00974	0.72053
O	5.64275	-1.34533	2.86605
H	2.84130	-1.74407	3.00283
H	1.47391	0.23494	3.67190
H	5.01897	1.25216	1.87992
C	3.32801	1.58175	-0.31536
O	2.37937	1.97098	-0.98388
O	4.58462	2.05006	-0.53661
C	4.71272	3.00747	-1.59458
H	4.12273	3.90314	-1.38026
H	5.77467	3.25179	-1.63984
H	4.37668	2.58350	-2.54516

TSII-6 (R,S)

C	-2.15852	1.16578	-0.54819
C	-2.33084	3.17721	-2.05308
C	-3.09442	2.28336	-1.05019
H	-2.20569	0.30430	-1.21444
H	-3.96634	1.82618	-1.52725
H	-3.46595	2.87818	-0.21008

C	-0.39761	1.57957	-2.21597
H	0.57879	2.04845	-2.34137
H	-0.31265	0.51182	-2.42338
C	-1.52265	2.27881	-3.01412
H	-1.08563	2.87605	-3.82188
H	-2.18214	1.53912	-3.48178
H	-3.02863	3.80874	-2.61151
C	-1.31355	4.06514	-1.28313
H	-0.60026	4.46985	-2.01298
C	-0.57015	3.12760	-0.29856
H	0.50289	3.31418	-0.25604
H	-0.99160	3.18803	0.70408
N	-0.72966	1.68916	-0.74498
C	-1.93616	5.22856	-0.55654
H	-2.64869	4.98087	0.23091
C	-1.66640	6.50964	-0.81153
H	-2.14754	7.31489	-0.26328
H	-0.95324	6.80346	-1.57948
C	-2.42555	0.59892	0.87665
C	-3.89120	0.17989	0.96949
C	-4.36064	-1.08922	0.48263
C	-4.81891	1.03543	1.53077
C	-5.76929	-1.35650	0.61938

C	-3.53012	-2.07590	-0.10226
C	-6.18258	0.66356	1.61247
H	-4.51066	2.00324	1.91241
C	-6.27852	-2.59480	0.15921
C	-4.06865	-3.27771	-0.54097
H	-2.46038	-1.93512	-0.23419
H	-6.89992	1.35318	2.05772
C	-5.45667	-3.54057	-0.41068
H	-7.34346	-2.76984	0.27536
H	-5.87640	-4.48009	-0.75192
N	-6.65797	-0.48168	1.17655
O	-3.18782	-4.16131	-1.08900
C	-3.66417	-5.41548	-1.54305
H	-4.40077	-5.30560	-2.35082
H	-2.78908	-5.94289	-1.92727
H	-4.10915	-6.00308	-0.72849
N	-2.09453	1.58043	1.92711
H	-2.58004	1.31579	2.78071
H	-1.09948	1.48257	2.12680
H	-1.79745	-0.29714	0.95989
H	-0.03993	1.14158	-0.19846
C	1.70199	-1.30763	-0.88657
C	2.83906	-1.40221	-0.02605

O	0.77996	0.83359	1.49883
C	1.79390	0.21612	1.81746
C	3.09039	0.18480	1.07338
C	4.28917	-0.12293	1.99557
H	4.07716	0.26320	3.00312
C	3.23696	1.27975	0.07730
O	2.29551	1.65034	-0.62869
C	5.54452	1.89579	1.04992
C	5.62932	0.49271	1.61838
C	4.61329	1.89789	-0.17030
O	6.68168	-0.08211	1.81519
O	1.85213	-0.52178	2.94025
C	0.61441	-0.72593	3.63925
H	0.22426	0.22290	4.01939
H	-0.10615	-1.19519	2.96677
H	0.86055	-1.38871	4.46960
H	4.43574	-1.19822	2.12501
H	6.54850	2.24777	0.79778
H	5.13581	2.55866	1.82722
H	4.44607	2.91073	-0.55044
H	5.08500	1.33027	-0.98338
C	4.14479	-1.67233	-0.71377
C	5.03450	-2.61499	-0.17556

C	4.49451	-1.05191	-1.92729
C	6.23683	-2.92043	-0.81512
H	4.77485	-3.12612	0.74757
C	5.69412	-1.35724	-2.56864
H	3.82182	-0.32509	-2.37359
C	6.57278	-2.29137	-2.01342
H	6.90859	-3.65165	-0.37431
H	5.94164	-0.86721	-3.50684
H	7.50813	-2.52752	-2.51326
H	2.66930	-2.06096	0.82455
H	1.75381	-1.01120	-1.92133
N	0.44508	-1.57436	-0.44401
O	0.23762	-1.99209	0.73356
O	-0.53106	-1.39706	-1.25201

TSII-7 (S,S)

C	-2.15852	1.16578	-0.54819
C	-2.33084	3.17721	-2.05308
C	-3.09442	2.28336	-1.05019
H	-2.20569	0.30430	-1.21444
H	-3.96634	1.82618	-1.52725
H	-3.46595	2.87818	-0.21008
C	-0.39761	1.57957	-2.21597

H	0.57879	2.04845	-2.34137
H	-0.31265	0.51182	-2.42338
C	-1.52265	2.27881	-3.01412
H	-1.08563	2.87605	-3.82188
H	-2.18214	1.53912	-3.48178
H	-3.02863	3.80874	-2.61151
C	-1.31355	4.06514	-1.28313
H	-0.60026	4.46985	-2.01298
C	-0.57015	3.12760	-0.29856
H	0.50289	3.31418	-0.25604
H	-0.99160	3.18803	0.70408
N	-0.72966	1.68916	-0.74498
C	-1.93616	5.22856	-0.55654
H	-2.64869	4.98087	0.23091
C	-1.66640	6.50964	-0.81153
H	-2.14754	7.31489	-0.26328
H	-0.95324	6.80346	-1.57948
C	-2.42555	0.59892	0.87665
C	-3.89120	0.17989	0.96949
C	-4.36064	-1.08922	0.48263
C	-4.81891	1.03543	1.53077
C	-5.76929	-1.35650	0.61938
C	-3.53012	-2.07590	-0.10226

C	-6.18258	0.66356	1.61247
H	-4.51066	2.00324	1.91241
C	-6.27852	-2.59480	0.15921
C	-4.06865	-3.27771	-0.54097
H	-2.46038	-1.93512	-0.23419
H	-6.89992	1.35318	2.05772
C	-5.45667	-3.54057	-0.41068
H	-7.34346	-2.76984	0.27536
H	-5.87640	-4.48009	-0.75192
N	-6.65797	-0.48168	1.17655
O	-3.18782	-4.16131	-1.08900
C	-3.66417	-5.41548	-1.54305
H	-4.40077	-5.30560	-2.35082
H	-2.78908	-5.94289	-1.92727
H	-4.10915	-6.00308	-0.72849
N	-2.09453	1.58043	1.92711
H	-2.58004	1.31579	2.78071
H	-1.09948	1.48257	2.12680
H	-1.79745	-0.29714	0.95989
H	-0.03993	1.14158	-0.19846
C	1.70199	-1.30763	-0.88657
C	2.83906	-1.40221	-0.02605
O	0.77996	0.83359	1.49883

C	1.79390	0.21612	1.81746
C	3.09039	0.18480	1.07338
C	4.28917	-0.12293	1.99557
H	4.07716	0.26320	3.00312
C	3.23696	1.27975	0.07730
O	2.29551	1.65034	-0.62869
C	5.54452	1.89579	1.04992
C	5.62932	0.49271	1.61838
C	4.61329	1.89789	-0.17030
O	6.68168	-0.08211	1.81519
O	1.85213	-0.52178	2.94025
C	0.61441	-0.72593	3.63925
H	0.22426	0.22290	4.01939
H	-0.10615	-1.19519	2.96677
H	0.86055	-1.38871	4.46960
H	4.43574	-1.19822	2.12501
H	6.54850	2.24777	0.79778
H	5.13581	2.55866	1.82722
H	4.44607	2.91073	-0.55044
H	5.08500	1.33027	-0.98338
C	4.14479	-1.67233	-0.71377
C	5.03450	-2.61499	-0.17556
C	4.49451	-1.05191	-1.92729

C	6.23683	-2.92043	-0.81512
H	4.77485	-3.12612	0.74757
C	5.69412	-1.35724	-2.56864
H	3.82182	-0.32509	-2.37359
C	6.57278	-2.29137	-2.01342
H	6.90859	-3.65165	-0.37431
H	5.94164	-0.86721	-3.50684
H	7.50813	-2.52752	-2.51326
H	2.66930	-2.06096	0.82455
H	1.75381	-1.01120	-1.92133
N	0.44508	-1.57436	-0.44401
O	0.23762	-1.99209	0.73356
O	-0.53106	-1.39706	-1.25201

TSII-8 (S,R)

C	-2.13791	1.23990	-0.40293
C	-2.27730	3.43133	-1.63483
C	-3.06046	2.42157	-0.76493
H	-2.18932	0.47293	-1.17607
H	-3.93032	2.03911	-1.30715
H	-3.43746	2.90654	0.14077
C	-0.35736	1.84542	-1.98430
H	0.62876	2.30990	-2.04014

H	-0.28853	0.81315	-2.32965
C	-1.46290	2.66155	-2.69741
H	-1.00805	3.35758	-3.41045
H	-2.12151	1.99875	-3.26990
H	-2.96303	4.13646	-2.11452
C	-1.26109	4.20204	-0.74535
H	-0.53802	4.69318	-1.40956
C	-0.53519	3.13619	0.11228
H	0.53997	3.30186	0.18985
H	-0.96613	3.06768	1.11034
N	-0.70512	1.77048	-0.51839
C	-1.88383	5.26531	0.12115
H	-2.59924	4.92150	0.86920
C	-1.61241	6.56803	0.03069
H	-2.09472	7.29809	0.67477
H	-0.89670	6.95598	-0.69174
C	-2.41682	0.49317	0.93492
C	-3.88566	0.07904	0.96534
C	-4.36074	-1.11313	0.31724
C	-4.81064	0.86393	1.62548
C	-5.77272	-1.38162	0.40541
C	-3.53166	-2.02660	-0.37873
C	-6.17826	0.49817	1.64654

H	-4.49638	1.77045	2.13231
C	-6.28728	-2.54679	-0.21283
C	-4.07519	-3.15855	-0.97018
H	-2.45882	-1.88136	-0.47870
H	-6.89406	1.13157	2.17072
C	-5.46695	-3.42164	-0.88823
H	-7.35482	-2.72492	-0.13014
H	-5.89051	-4.30697	-1.34856
N	-6.65940	-0.57615	1.06145
O	-3.19597	-3.97558	-1.61579
C	-3.67701	-5.16374	-2.21891
H	-4.40372	-4.95306	-3.01554
H	-2.80180	-5.65031	-2.65341
H	-4.13552	-5.83841	-1.48327
N	-2.07891	1.32180	2.10644
H	-2.56522	0.94670	2.91729
H	-1.08337	1.18390	2.28573
H	-1.79686	-0.41197	0.90129
H	-0.03138	1.15025	-0.02244
C	1.76520	-1.10735	-1.10853
C	2.94204	-1.31757	-0.34707
O	0.75678	0.64129	1.47660
C	1.72508	-0.04179	1.84909

C	1.59407	-0.87351	3.11946
C	3.04758	-0.01553	1.19357
C	2.42657	-2.15844	3.10028
H	1.91172	-0.23174	3.95745
C	4.17690	-0.55144	2.08074
C	3.87289	-1.91471	2.69475
H	2.41620	-2.66992	4.06896
H	5.12076	-0.61746	1.53855
O	4.73857	-2.75646	2.85054
H	1.98910	-2.85244	2.37129
H	0.53397	-1.09171	3.26635
H	4.35743	0.13949	2.92128
C	3.32865	1.24926	0.46706
O	2.55734	1.84154	-0.27666
O	4.59113	1.69462	0.68975
C	4.97138	2.87495	-0.02684
H	4.29825	3.70483	0.20596
H	5.98624	3.10148	0.30233
H	4.95476	2.69173	-1.10466
C	4.25413	-1.21029	-1.05373
C	5.29698	-2.08626	-0.70846
C	4.47867	-0.28338	-2.08781
C	6.52015	-2.04591	-1.37971

H	5.15080	-2.80268	0.09525
C	5.70029	-0.24375	-2.75756
H	3.69624	0.41694	-2.36203
C	6.72627	-1.12615	-2.40822
H	7.30977	-2.73661	-1.09662
H	5.85079	0.47533	-3.55893
H	7.67680	-1.09566	-2.93409
N	0.55605	-1.51951	-0.63586
O	0.47584	-2.15054	0.45764
O	-0.48956	-1.24306	-1.31442
H	1.72944	-0.57446	-2.04428
H	2.88036	-2.18675	0.30080

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