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Supplementary Information

The hexameric resorcinarene capsule as an artificial enzyme: ruling the regio and stereochemistry of a 1,3-dipolar cycloaddition between nitrones and unsaturated aldehydes

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1. General Methods

1.1. Experimental

All chemicals were reagent grade and were used without further purification. Reaction temperatures were measured externally. Reactions were monitored by TLC on Merck silica gel 60 F_{254} plates (0.25 mm) and visualized by UV light or $KMnO_4$ stain. Flash Chromatography was performed on Merck silica gel (60, 40–63 µm).

^{1}H NMR spectra were recorded on Bruker Avance-600 spectrometer [600.13 MHz (^{1}H)] and Bruker Avance-250 spectrometer [250.00 MHz (^{1}H)]. Chemical shifts are reported relative to the residual solvent peak ($CHCl_3$: δ 7.26). HPLC analysis was performed using a Jasco HPLC system equipped with PU-4180 HPLC pump, 20 µl loop injector (Rheodyne model 7725i) and MD-4015 Photodiode Array Detector at λ = 210 or 220 nm. As stationary phases, the following Chiralcel columns were used: OD-H (250 x 4.6 mm) and OD guard (50 mm), AD-H (250 x 4.6 mm) and AD guard (50 mm), AS-H (250 x 4.6 mm) and AS guard (50 mm).

Water saturated deuterated chloroform was prepared as reported in literature[1].

Resorcinarene **1**,[2] nitrones **3a**,[3] **3b**,[4] **3c**,[5] **3d**,[6] **3e**,[6] and **3**,**f**[5] catalyst **7d**,[7] and hexamethonium iodide **9**,[8] were synthesized according to literature procedures. Percentages of conversions, regioisomeric and diastereomeric ratios of the titles compounds **5a–i** and **6a–i** were determined by ^{1}H NMR analysis in comparison with literature data.[9]

2. Procedures

2.1. *General Remarks*

The progress of the cycloaddition reaction was controlled after 4 h, 16 h, 48 h and 72 h and was monitored following ^{1}H NMR signals associated with nitrones. The reaction was stopped after consumption of nitrone or when its conversion reached a plateau. The enantiomeric excess value was determined by HPLC analysis by converting the mixture of isoxazolidines to the corresponding alcohols.

2.2. Reaction monitoring

30 µL of the reaction solution in the vial was taken, diluted with 420 µL of $CDCl_3$ and the reaction progress was monitored by^{1}H NMR.

2.3. General procedure for 1,3 dipolar cycloaddition reaction without capsule

Catalyst **7** (32.5 µmol, 0.2 eq.) was weighed into 4 mL vial and water saturated chloroform-d (1.1

mL) was added. Next, aldehyde **4** (975.6 μmol, 6 eq.) was added, followed by nitrone **3** (162.6 μmol, 1 eq.). The vial was thermostatically controlled at 30 °C and maintained under vigorous stirring for an appropriate time. The progress of the reaction was monitored by ^{1}H-NMR analysis by periodically sampling from the reaction mixture at different times. The reaction mixture was concentrated under reduced pressure and purified by flash chromatography on silica gel (Hexane/Ethyl Acetate, from 90:10 to 80:20) to give the title compounds as a mixture of isoxazolidines **5** and **6**. Regioisomeric and diastereomeric ratios were determined by ^{1}H NMR analysis in comparison with literature data.[9] The determination of enantiomeric purity was performed by HPLC analysis after reduction of the formyl group with $NaBH_4$ and by comparison with literature.[9]

2.4. General procedure for 1,3 dipolar cycloaddition experiment with capsule

Resorcinarene **1** (281.6 mg, 254.7 μmol, 1.56 eq.) was weighed into a 4 mL vial. Then, 1.1 mL of water-saturated chloroform-d was added and the mixture was homogenized in an ultrasonic water bath at 40 °C for 10 min. To this clear reddish solution, catalyst **7** (32.6 μmol, 0.2 eq.) was added and the solution was stirred at 30 °C for 10 minutes. Later, the aldehyde **4** (975.6 μmol, 6 eq.) was added and the reaction mixture was stirred at 30 °C for other 10 minutes. Finally, nitrone **3** (162.6 μmol, 1 eq.) was introduced and the reaction system was kept at 30 °C under stirring at 1400 rpm for the appropriate time. The reaction was monitored by ^{1}H NMR analysis taking aliquots of the reaction mixture at various time intervals and diluting with water saturated chloroform. The reaction was stopped pouring the solution into a 50 mL Eppendorf conical tube and diluting with 0.13% (v/v) DMSO in *n*-hexane (35 mL). The tube was placed in a freezer at –20 °C for at least 3 h and successively centrifuged at 1750 rpm for 10 minutes. The diluted reaction mixture was subjected three times to this procedure. Finally, the clear solution was removed and concentrated under reduced pressure. The oily residue thus obtained was purified by flash chromatography on silica gel (Hexane/Ethyl Acetate, from 90:10 to 80:20) to afford the desired title compounds as an inseparable mixture of isoxazolidines **5** and **6**. Regioisomeric and diastereomeric ratios were determined by ^{1}H NMR analysis via integration of the aldehydic proton signal of the title compounds in comparison with literature data.[9]

2.5. General procedure for reduction of the mixture of isoxazolidine adducts

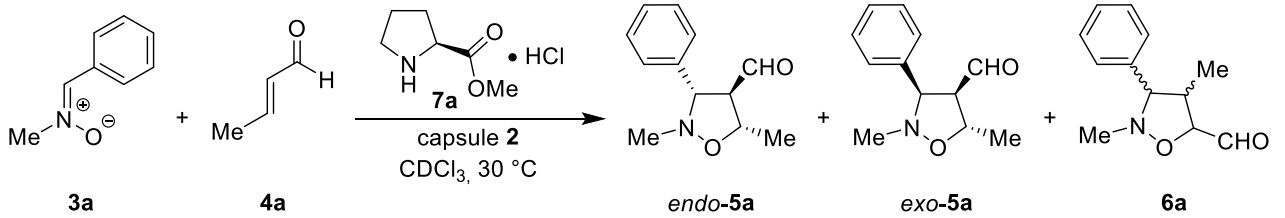
To a solution of compounds **5** and **6** (0.15 mmol) in EtOH (2 mL), $NaBH_4$ (0.45 mmol, 3 eq.) was added and the resulting mixture was stirred at 30 °C for 75 min. The reaction was quenched by the

addition of deionized H_2O (10 mL), then EtOH was removed under reduced pressure and the residue was extracted with EtOAc (3 × 15 mL). The combined organic phases were dried over Na_2SO_4, filtered and concentrated under reduced pressure. The colourless oil thus obtained was passed through a short plug of silica gel in CH_2Cl_2 to give the corresponding purified alcohols.

3. Control experiments with different aldehyde/nitrone ratios

A study to optimize the ratio aldehyde/nitrone was performed between aldehyde **4a** and nitrone **3a** in the presence of catalyst **7a**.

Table S1. Optimization of the aldehyde/nitrone ratio.[a]



3a **4a** *endo*-**5a** *exo*-**5a** **6a**

Run	**4a**/ **3a**	Capsule **2**	Yield (%)[b]	*endo*-**5a**/*exo*-**5a**/**6a**[c]	ee (%) *endo*-**5a**[d]	ee (%) *exo*-**5a**[d]	Δee (%) *endo*-**5a**	Δee (%) *exo*-**5a**
1	1/2.2	No	39	50:50:0	11(4S)	24 (3R)		
2	1/2.2	Yes	82	62:25:13	26 (4R)	-	37	24
3	1/1.2	No	45	64:36:0	15(4S)	20(3R)		
4	1/1.2	Yes	83	61:21:18	20(4R)	-	35	20
5	2/1	No	45	49:48:3	11(4S)	20(3R)		
6	2/1	Yes	83	64:28:8	46(4R)	-	57	20
7	4/1	No	44	50:50:0	10(4S)	8(3R)		
8	4/1	Yes	88	69:29:2	57 (4R)	8(3S)	67	16
9	6/1	No	42	24:67:9	14 (4S)	7(3R)		
10	6/1	Yes	88	85:1:14	43(4R)	-	57	7

[a] Reactions were performed on a 0.16 mmol scale using **7a** (0.2 equiv.) and capsule **2** (0.26 equiv.) in water saturated $CDCl_3$ (1.1 mL) under stirring for 4 h at 30°C. [b] Isolated yield. [c] Determined by ^{1}H NMR spectroscopy of the crude reaction mixture after removing resorcinarene. [d] Determined by HPLC analysis after borohydride reduction to the corresponding alcohol according to literature data.[9]

4. Control experiments on the role played by hexameric resorcinarene capsule 2

4.1. 1,3-dipolar cycloaddition reaction without catalyst 7

In a control experiment, the cycloaddition reaction between **4a** and **3a** was performed in the

absence of proline catalyst **7a** to assess the catalytic activity of the capsule alone.

Resorcinarene **1** (254.7 μmol, 1.56 eq.) was weighed into a 4 mL vial and water saturated deuterated chloroform (1.1 mL) was added. The mixture was homogenized in an ultrasonic water bath at 40 °C for 10 min before adding **4a** (975.6 μmol, 6 eq.). After another 10 minutes at 30 °C, **3a** (162.6 μmol, 1 eq.) was added. The reaction mixture was thermostatically controlled at 30 °C and stirred at 1400 rpm for the appropriate time (Table S2). The reaction was stopped by adding *n*-hexane (35mL) containing 0.13% (v/v) DMSO, centrifuged and decanted (need 3 cycles). The conversion, regio- and diastereoisomeric ratios were determined by ^{1}H-NMR analysis of the clear reaction solution.[9] The determination of enantiomeric purity was performed by HPLC analysis after reduction of the formyl group with $NaBH_4$ and by comparison with literature.[9]

Table S2. Control reactions with and without proline **7a**.

7a	**Time (h)**	**Yield (%)**[a]	*endo*-**5a**/*exo*-**5a**/**6a**[b]	ee (%) *endo*-**5a**[c]	ee (%) *exo*-**5a**[c]
No	24	23	14:86:0	0	0
Yes	4	88	85:1:14	43 (4R)	nd

[a] Isolated yield. [b] Determined by ^{1}H NMR spectroscopy of the crude reaction mixture after removing resorcinarene. [c] Determined by HPLC analysis after borohydride reduction to the corresponding alcohol according to literature data.[9]

This result proves that there is a capsule catalyzed background reaction but with low efficiency, also with prolonged reaction time. Furthermore, no enantioselectivity was found without **7a**.

4.2. Control experiment with increasing amount of capsule 2

In a control experiment, the cycloaddition reaction between **4a** and **3a** was performed in the presence of proline catalyst **7a** and an increased amount of capsule **2** (38 mol%) with respect to **7a**.

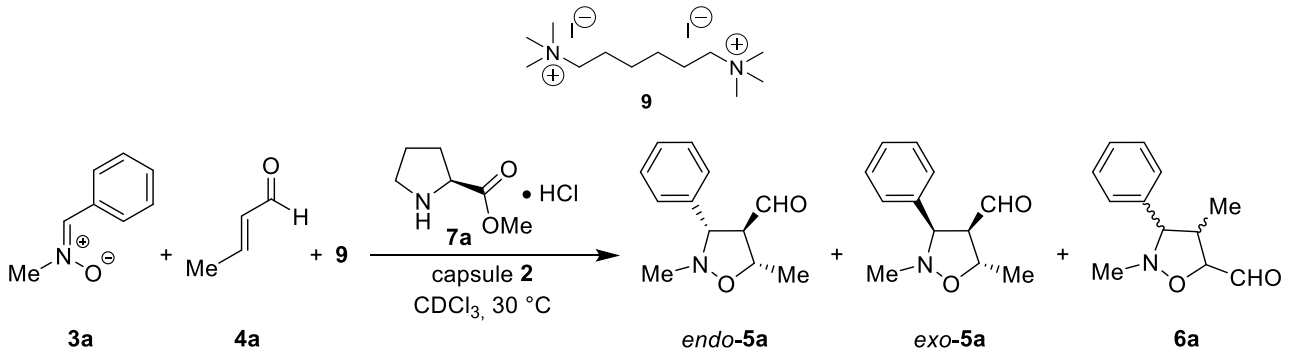
Table S3. Comparison between reaction performed with 26% and 38% amount of the capsule.

Capsule amount (mol%)	Time (h)	Yield (%)[b]	*endo*-**5a**/*exo*-**5a**/**6a**[c]	ee (%) *endo*-**5a**[d]	ee (%) *exo*-**5a**[d]
26%	4	88	85/1/14	43.2 (4R)	nd
38%	4[a]	51	52/40/8	53 (4R)	0

[a] After 22 h, no changes in conversion, regio- and diastereoselectivity were observed by ^{1}H NMR analysis. [b] Isolated yield. [c] Determined by ^{1}H NMR spectroscopy of the crude reaction mixture after removing resorcinarene. [d] Determined by HPLC analysis after borohydride reduction to the corresponding alcohol according to literature data.[9]

As can be seen in Table S3, increasing amount of capsule **2** leads to a remarkable lower yield, a slight decrease in diastereoselectivity and to a slight increase in enantioselectivity. This can be explained with a lower probability of **3a**, **7a** and **4a** to meet themselves and so to react inside the capsule.

4.3. Control experiment with hexamethonium iodide 9 as inhibitor of capsule 2



To provide further evidence that the reaction took place within **2**, a control experiment was performed in the presence of a large amount of competitive guest for the capsule as hexamethonium iodide (HMI) **9**. In fact, Tiefenbacher *et al*. have recently reported that a divalent ammonium salt competes very efficiently with iminium species for encapsulation inside **2**.[1]

To a solution of resorcinarene **1** (254.7 μmol, 1.56 eq.) in water saturated chloroform-d (1.1 mL), hexamethonium iodide **9** (763.8 μmol, 18 eq. respect to resorcinarene capsule) was added. Next, catalyst **7a** (32.6 μmol, 0.2 eq.) was introduced followed by aldehyde **4a** (975.6 μmol, 6 eq.) and, finally, nitrone **3a** (162.6 μmol, 1 eq.). The reaction system was kept at 30 °C under stirring at 1400 rpm for 4 h. The reaction was stopped as specified in paragraph 2.4.

Table S4. 1,3-cycloaddition reaction with inhibitor **9**.

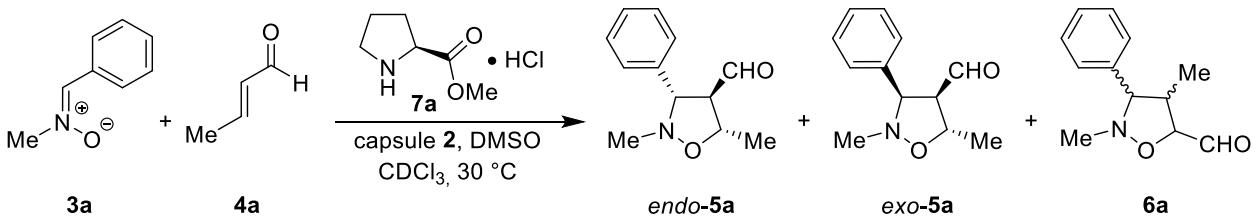
Run	Capsule	Yield(%)[a]	*endo*-**5a**/*exo*-**5a**/**6a**[b]	ee (%) *endo*-**5a**[c]	ee (%) *exo*-**5a**[c]
1	Yes	60	47/44/9	27.3 (4*R*)	12.6 (3*S*)
2	Yes[d]	88	86/1/13	43.2 (4*R*)	Not done
3	No	42	53/39/9	10.2 (4*S*)	8.3 (3*R*)

[a] Isolated yield. [b] Determined by ^{1}H NMR spectroscopy of the crude reaction mixture after removing resorcinarene. [c] Determined by HPLC analysis after borohydride reduction to the corresponding alcohol according to literature data.[9] [d] The reaction was performed without inhibitor **9**.

As reported in Table S4, the presence of **9** caused the reaction efficiency and selectivity to drop (cf. entry 1 and 2). This result can be attributed with the blocking of the cavity by **9** thus forcing the reaction outside the capsule.

4.4. 1,3-dipolar cycloaddition in the presence of DMSO

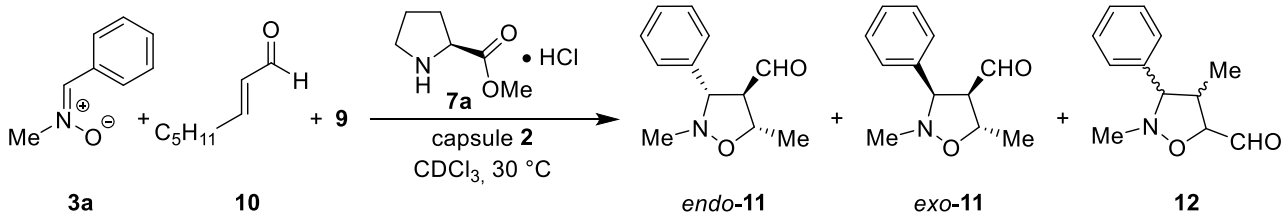
It is reported that DMSO can disrupt the hexameric structure of the capsule thanks to its ability to make hydrogen bonds.[1,10] So, as a further evidence that the reaction is catalyzed inside the capsule, a reaction in presence of DMSO (90 μL, 1.27 mmol) and the capsule (0.042 mmol) has been performed.



3a **4a** *endo*-**5a** *exo*-**5a** **6a**

Since catalyst **7e** did not work without the capsule, if catalysis of the reaction is due to the combination of capsule and proline, the reaction with the addition of DMSO should not proceed. In fact, with adding DMSO there was no conversion either with the capsule or without.

4.5. 1,3-dipolar cycloaddition with trans Oct-2-enal (10)



3a **10** *endo*-**11** *exo*-**11** **12**

To provide further evidence that the reaction occurs inside the cavity, we performed an additional experiment by using a more elongated aldehyde as **10** that could prove difficult to enter the host cavity.

When 1,3-dipolar cycloaddition was performed with proline methyl ester hydrochloride **7a** as catalyst (32.5 μmol), *trans* oct-2-enal (**10**, 975.6 μmol), nitrone **3a** (162.6 μmol) and capsule (26 mol%), no conversion was observed also after 40 h. When the same cycloaddition was performed without the capsule, 20% conversion was observed by ^{1}H NMR analysis.[9] Thus, unsaturated aldehyde **10** is too large to enter easily inside the capsule, so it is highly improbable the formation of iminium intermediate. Using catalyst **7e**, there was no conversion either with the capsule or without.

5. NMR experiments as proof of substrate encapsulation

5.1 Encapsulation of the catalyst

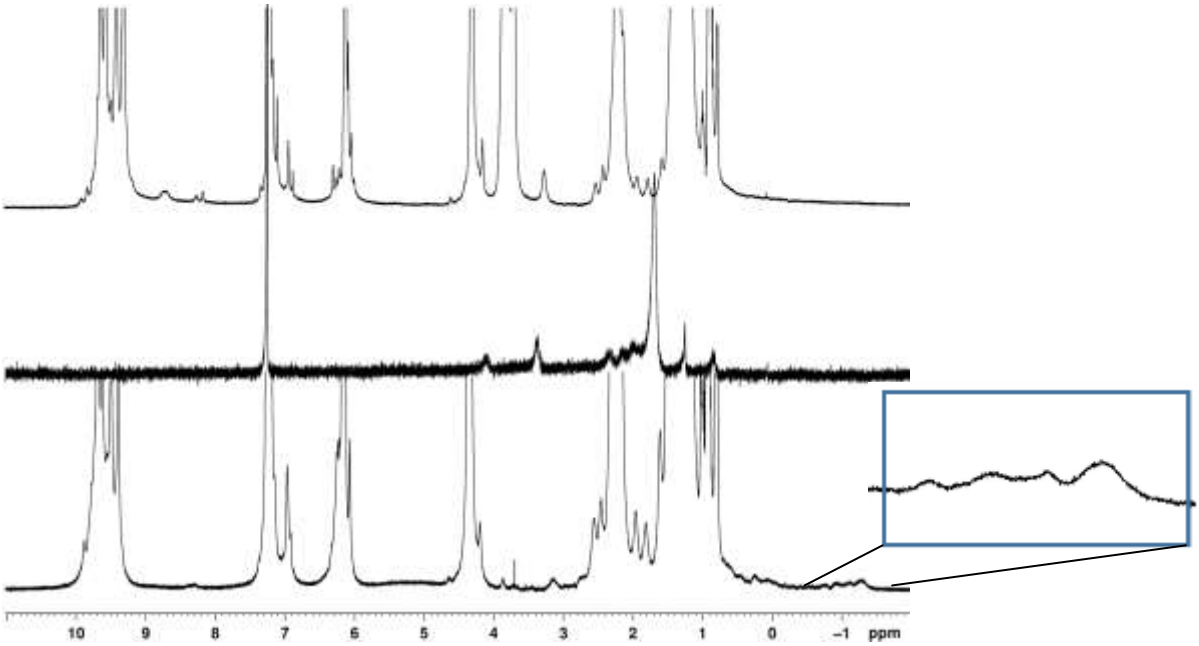


Figure S1. ^{1}H NMR spectra (600 MHz, 298 K, $CDCl_3$) of: (top) hexameric resorcinarene capsule **2**; (middle) L-proline **7e**; (bottom) mixture of L-proline **7e** and capsule. According to literature,[1] the presence of proton signals in the negative region of the spectrum (region delimited by blue rectangle) points out the encapsulation of **7e** inside the capsule.

5.2. Evidence for the encapsulation of the aldehyde

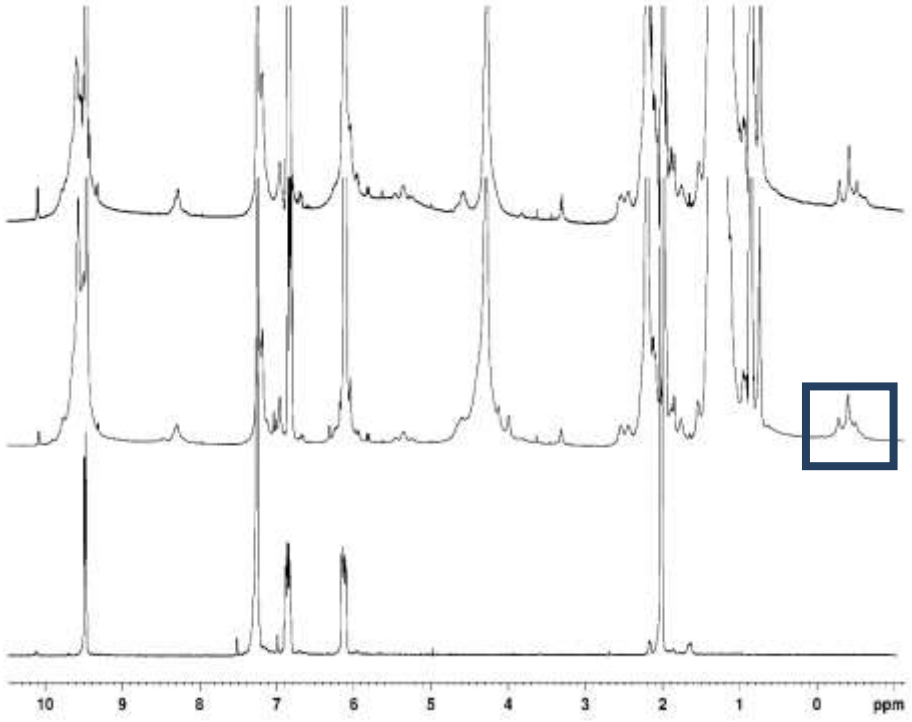


Figure S2. ^{1}H NMR (600 MHz, 298 K, $CDCl_3$) of: (bottom) aldehyde **4a**; (middle) capsule **2** with **4a**; (top) capsule **2** with **4a** after adding L-proline **7e**. The inclusion of **4a** is evidenced by the presence of high-field shifted signals (middle spectrum, blue rectangle).

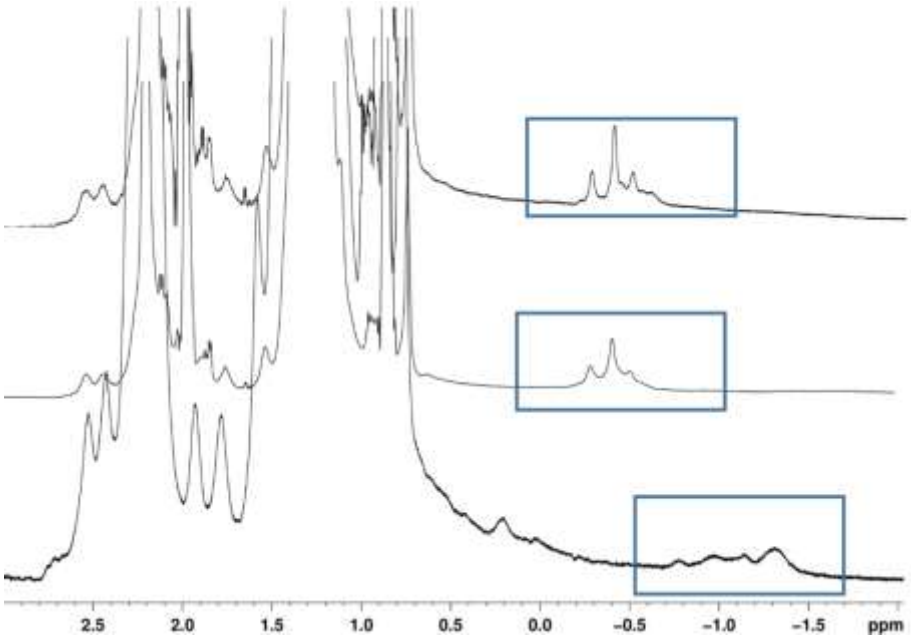


Figure S3. Relevant regions of ^{1}H NMR (600 MHz, 298 K, $CDCl_3$) representative of: (bottom) L-proline **7e** inside the capsule **2**; (middle) **4a** inside capsule; (top) mixture of **4a** and **7e** inside **2**. The presence of signals with different shift and shape with respect to the compounds alone (bottom and middle) is indicative of the formation of an iminium species inside **2**.

5.3. DOSY and NOESY NMR experiments

DOSY and NOESY experiments were performed to confirm that the high-field shifted signals correspond to encapsulated substrates **4a** and **7e**.

DOSY experiments were performed on a Bruker Avance-600 spectrometer equipped with 5 mm PABBO BB|19F-1H\D Z-GRD Z114607/0109. The standard Bruker pulse program, ledbpgp2s, employing a double stimulated echo sequence and LED, bipolar gradient pulses for diffusion, and two spoil gradients were utilized. Diffusion times were 150 ms, eddy current delay was 5 ms, gradient recovery delays was 0.2 ms and gradient pulse was 1400 ms. Individual rows of the quasi-2D diffusion databases were phased and baseline corrected. NOESY experiment in Figures S7 and S8 was performed on a Bruker Avance 400 spectrometer with a mixing time value of 150 ms.

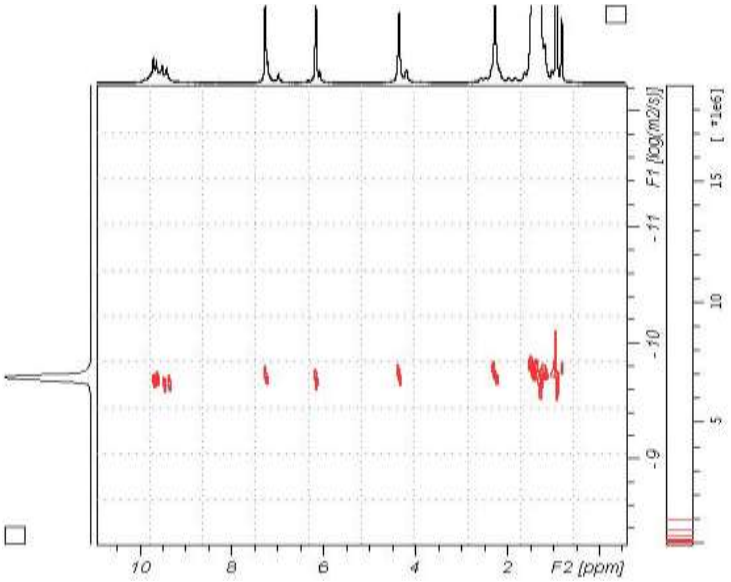


Figure S4. DOSY NMR (600 MHz, 298 K, $CDCl_3$) of capsule **2**.

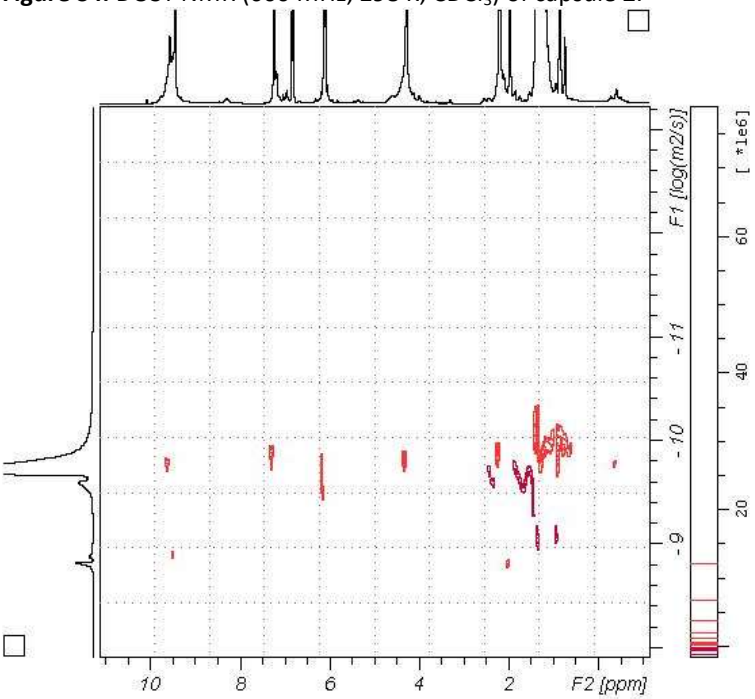


Figure S5. DOSY NMR (600 MHz, 298 K, $CDCl_3$) of capsule **2** (21 mM) with crotonaldehyde **4a**.

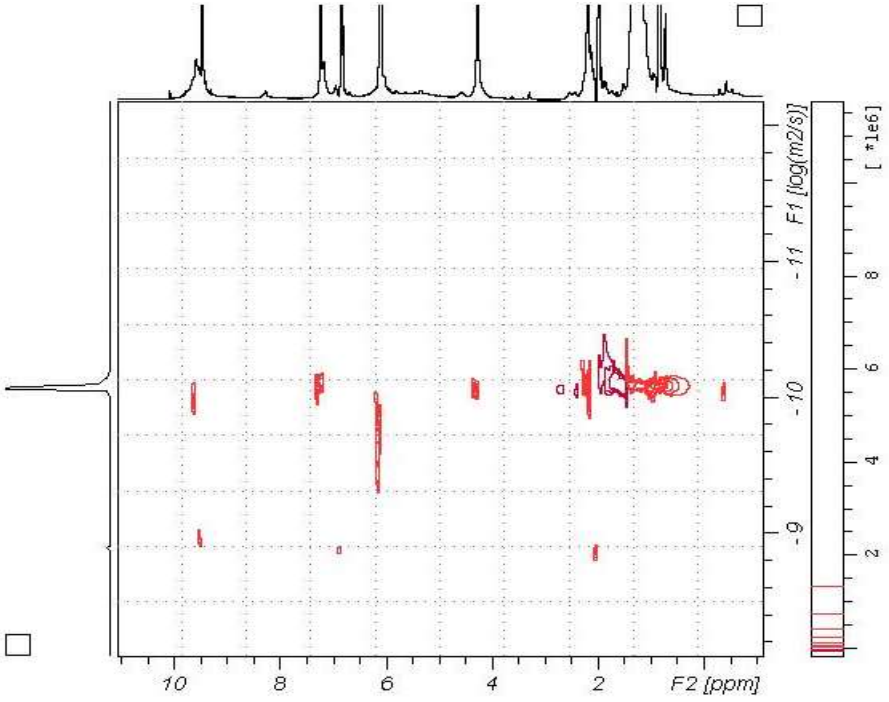


Figure S6. DOSY NMR (600 MHz, 298 K, $CDCl_3$) of capsule **2** (21 mM) and iminium species.

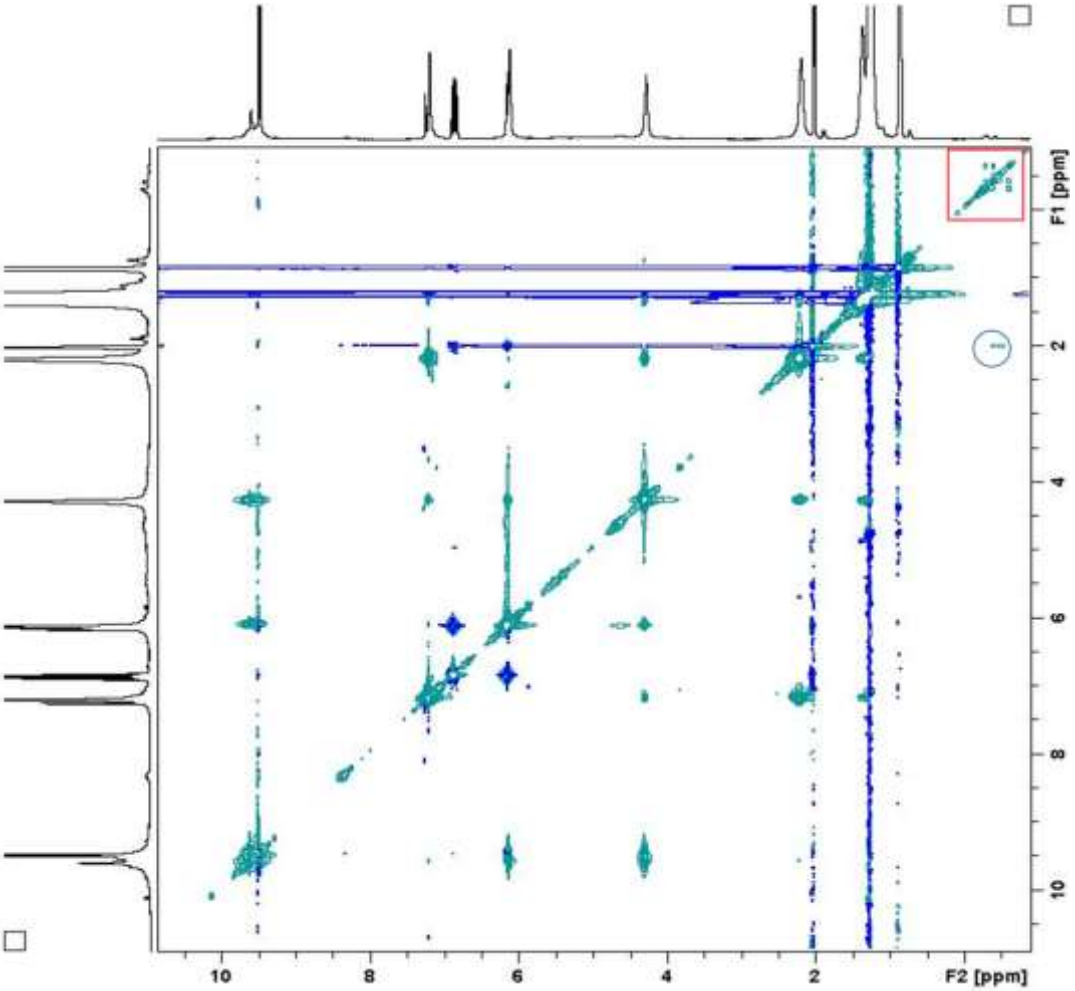


Figure S7. NOESY spectrum (400 MHz, 298 K, $CDCl_3$) of a mixture of **2, 4a** and **7e**.

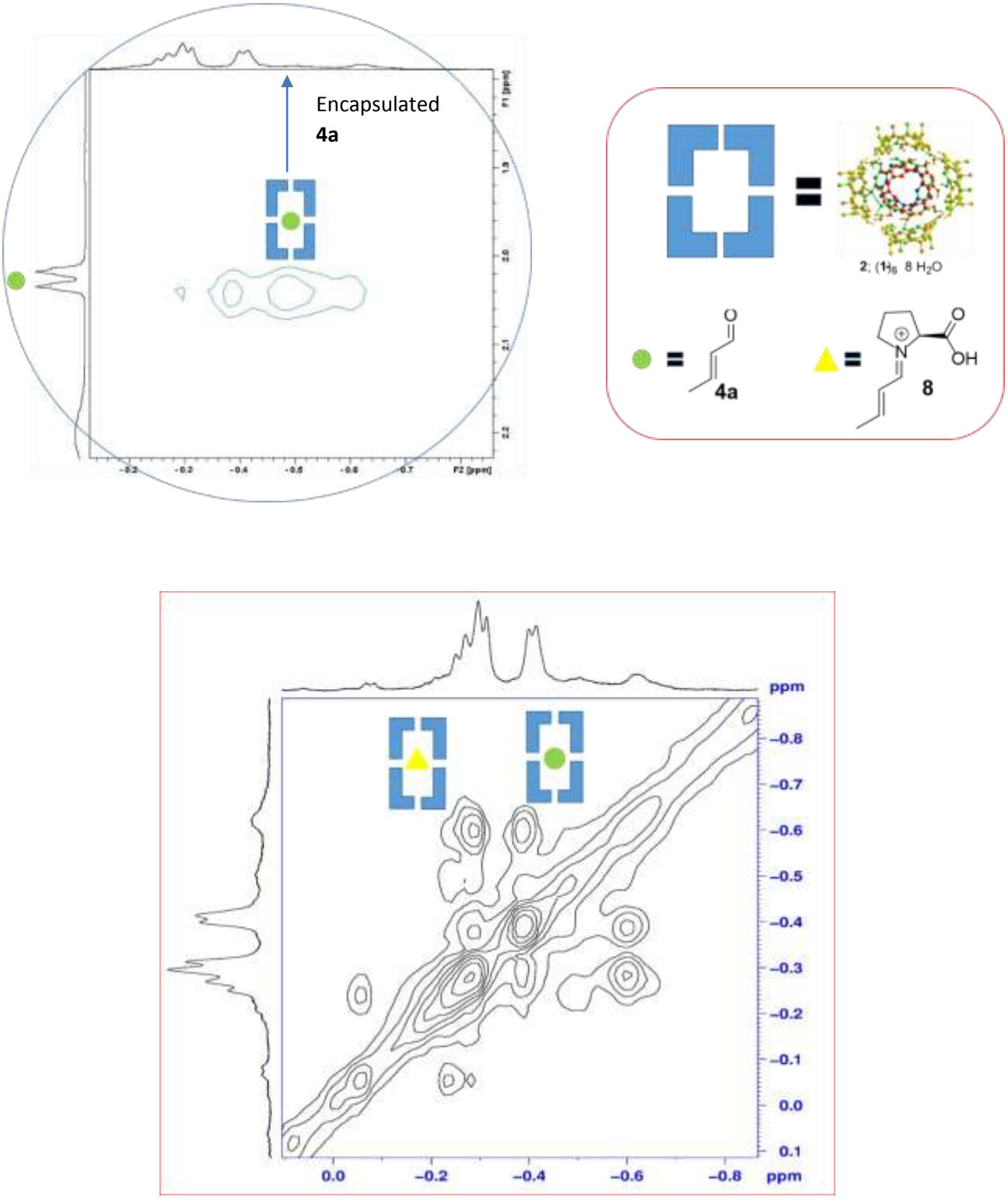
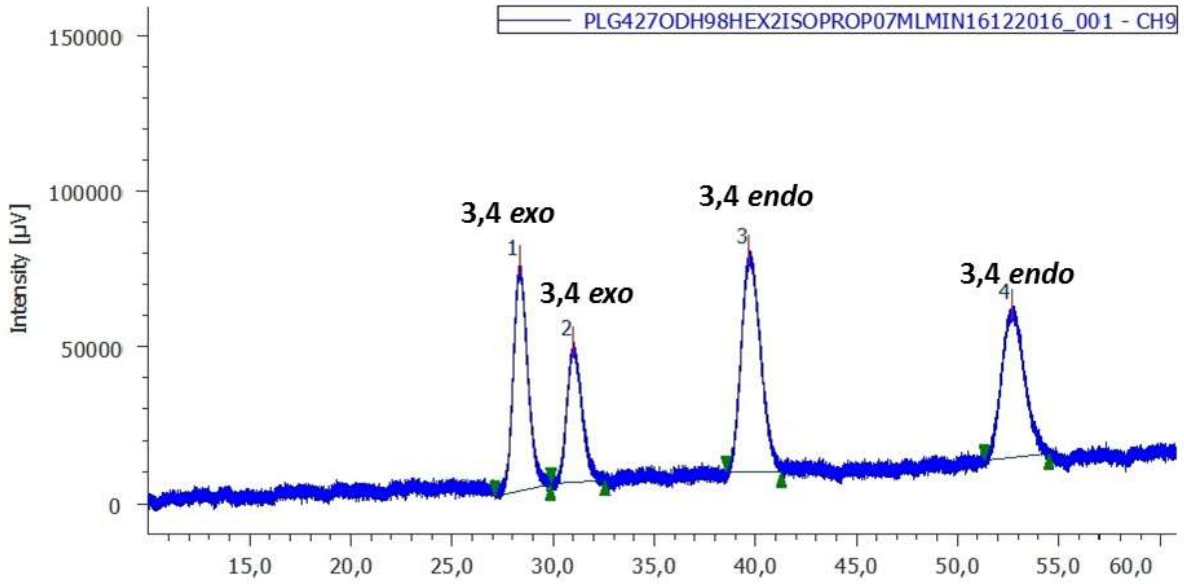


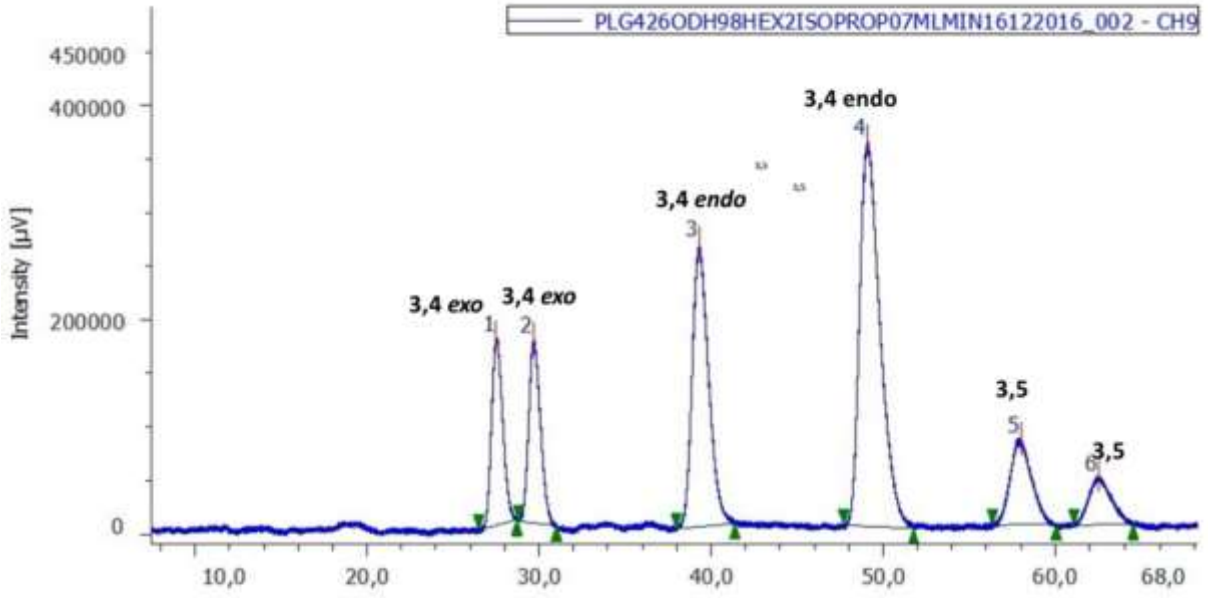
Figure S8. Selected expansions of NOESY NMR spectrum in Figure **S7**. Exchange peaks between aldehyde **4a** *outside* and *inside* the capsule **2** (top) and encapsulated aldehyde **4a** and iminium species **8** (bottom) indicatives of the formation of **8** by **4a** after reaction with L-proline inside the hexameric capsule.

6. HPLC chromatograms



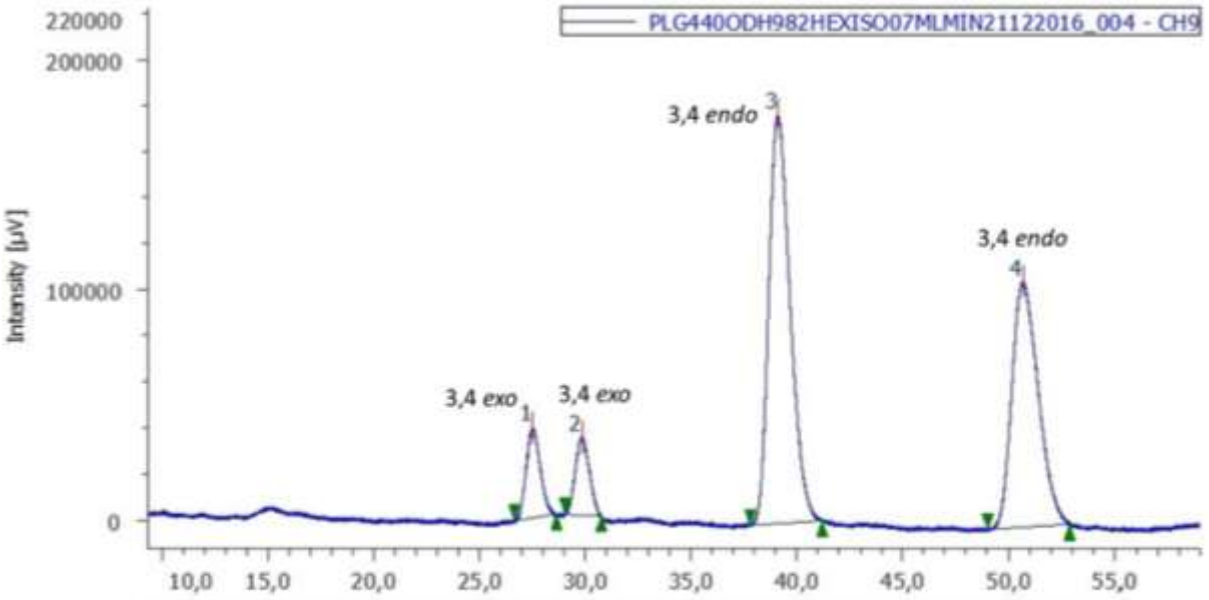
#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	28,342	3579498	73393	25,401	30,846	N/A	7889	1,993	1,052	
2	Unknown	9	31,004	2248196	44884	15,954	18,864	N/A	7814	5,475	1,236	
3	Unknown	9	39,680	4599523	70958	32,639	29,823	N/A	8000	6,602	1,320	
4	Unknown	9	52,661	3664746	48695	26,006	20,466	N/A	9435	N/A	1,174	

Figure S9. HPLC spectrum of Table S1, run 1. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 0.7 mL min^{-1} at λ = 210 nm.



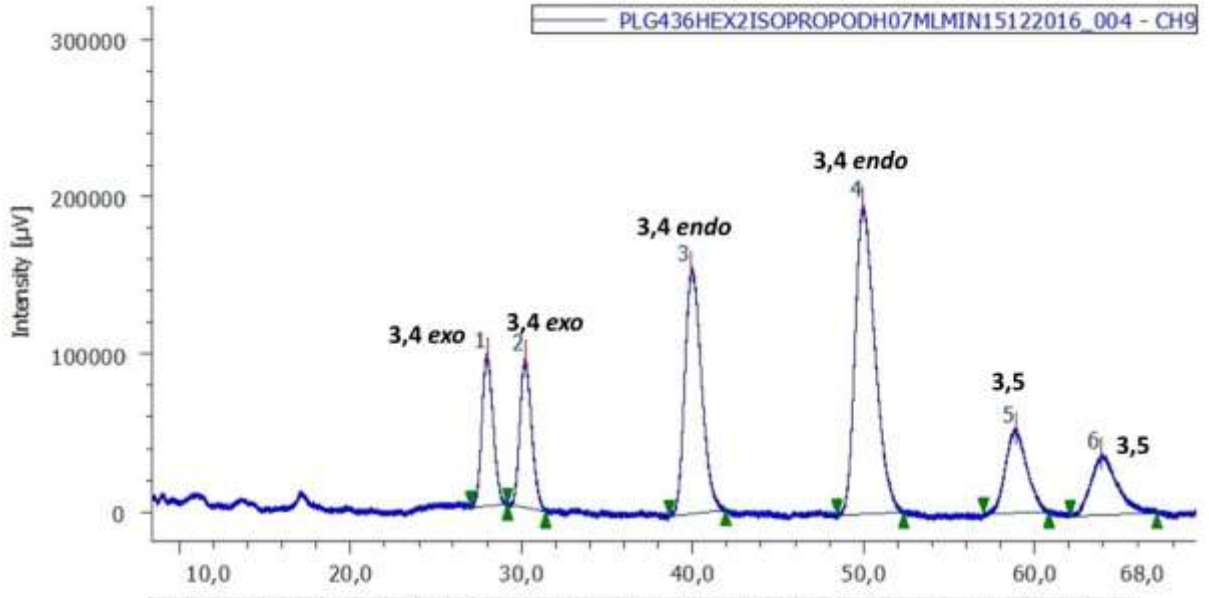
#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	27,508	7812916	175392	10,660	15,961	N/A	8394	1,770	1,255	
2	Unknown	9	29,672	8015737	172048	10,937	15,656	N/A	8991	6,533	1,250	
3	Unknown	9	39,310	17283324	265602	23,582	24,170	N/A	8489	5,065	1,285	
4	Unknown	9	49,070	29447133	359835	40,179	32,745	N/A	8279	3,926	1,502	
5	Unknown	9	57,996	6783017	80229	9,255	7,301	N/A	9326	1,801	1,135	
6	Unknown	9	62,475	3947059	45787	5,386	4,167	N/A	9359	N/A	1,218	

Figure S10. HPLC spectrum of Table S1, run 2. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 0.7 mL min^{-1} at λ = 210 nm.



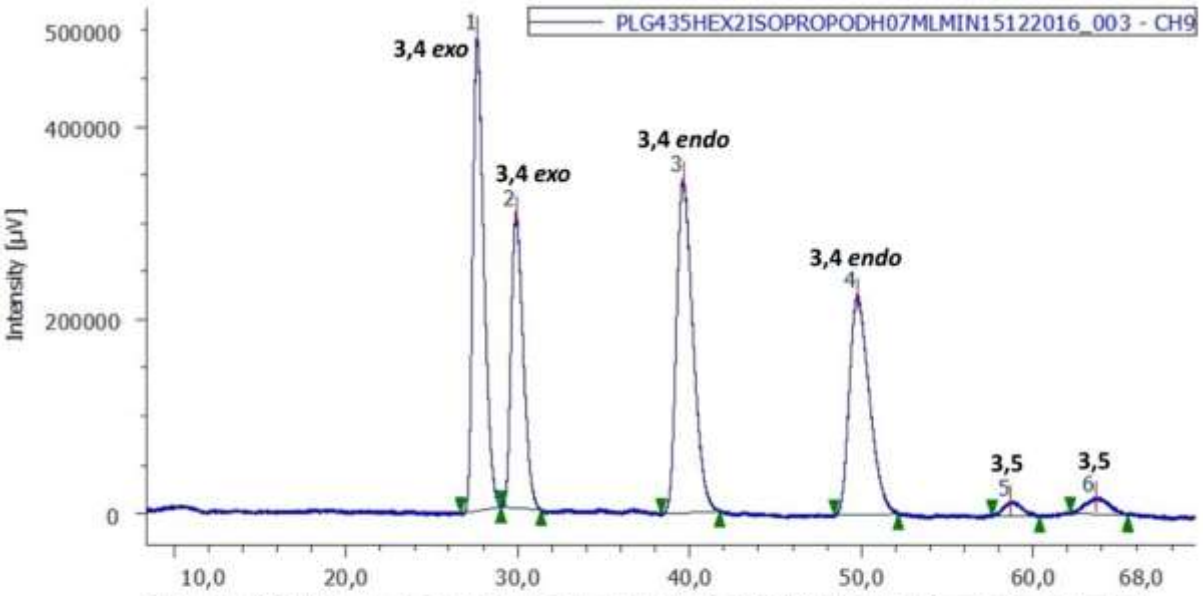
#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	27,514	1776078	38938	7,127	10,912	N/A	7670	1,879	1,164	
2	Unknown	9	29,875	1539954	33622	6,179	9,422	N/A	8943	5,965	1,018	
3	Unknown	9	39,109	12431955	177706	49,884	49,799	N/A	7225	5,614	1,287	
4	Unknown	9	50,709	9173786	106577	36,810	29,867	N/A	7756	N/A	1,275	

Figure S11. HPLC spectrum of Table S1, run 3. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 0.7 mL min^{-1} at λ = 210 nm.



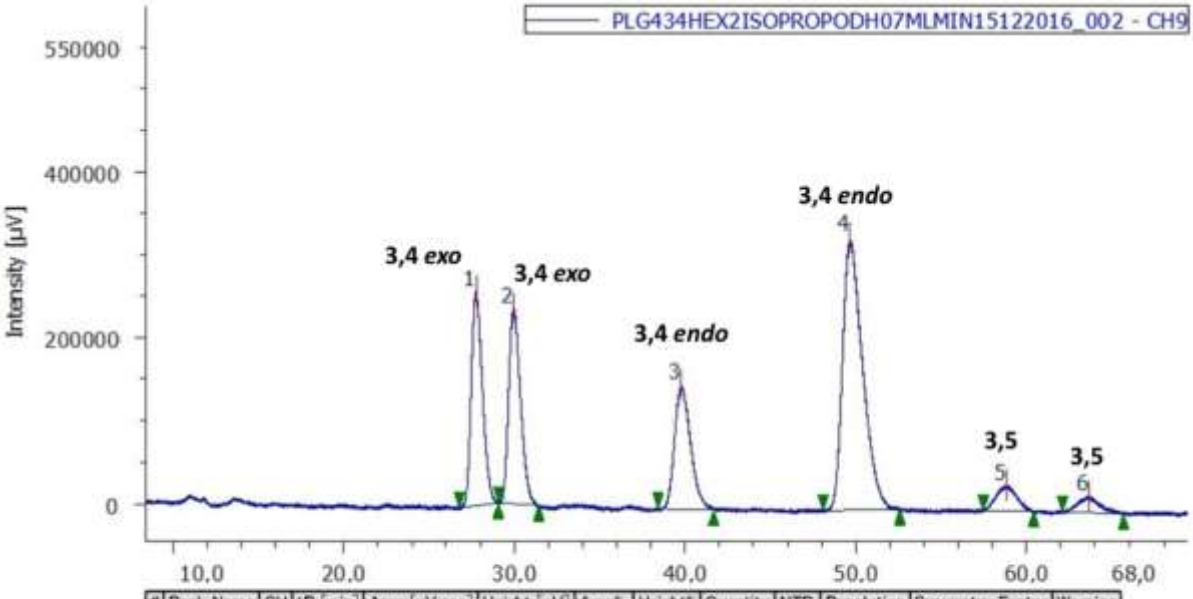
#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	28,020	4047994	96439	9,959	15,128	N/A	8541	1,780	1,072	
2	Unknown	9	30,230	4495740	95278	10,297	14,946	N/A	8962	6,339	1,214	
3	Unknown	9	39,910	10499571	156269	24,049	24,514	N/A	7999	5,159	1,360	
4	Unknown	9	49,952	15787723	197561	36,161	30,991	N/A	8895	4,028	1,397	
5	Unknown	9	58,878	4551441	53323	10,425	8,365	N/A	10255	2,008	1,055	
6	Unknown	9	63,899	3976762	38599	9,109	6,055	N/A	9038	N/A	1,347	

Figure S12. HPLC spectrum of Table S1, run 4. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 0.7 mL min^{-1} at λ = 210 nm.



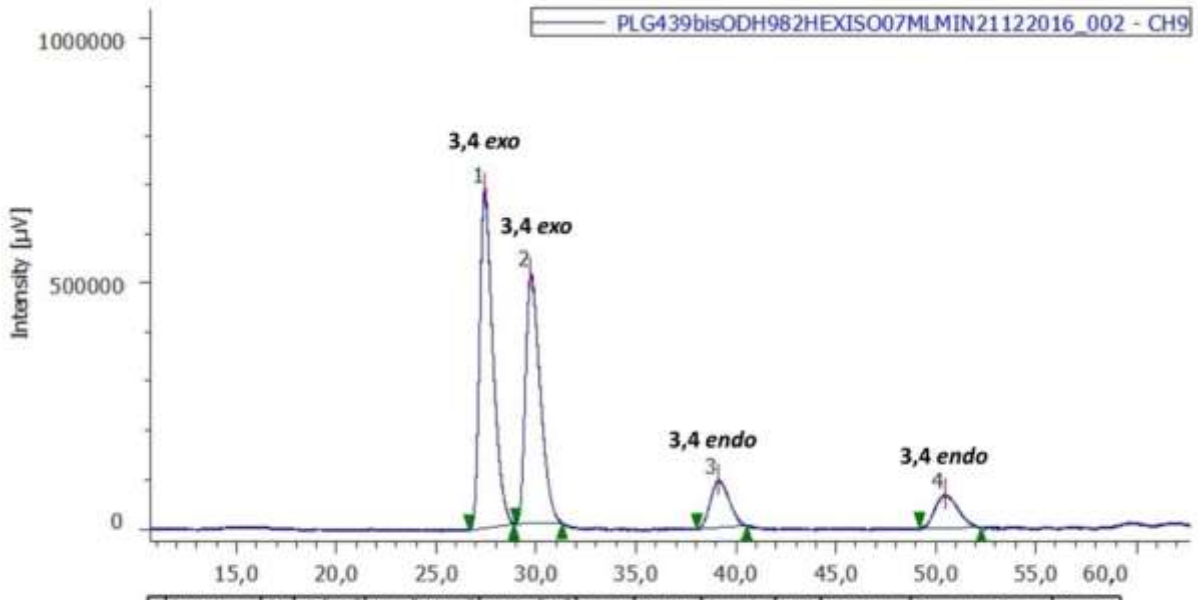
#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	27.647	21948831	494965	27.196	35.117	N/A	8973	1.852	1.431	
2	Unknown	9	29.907	14753721	306372	18.281	21.737	N/A	8742	6.440	1.392	
3	Unknown	9	39.637	22956571	346914	28.445	24.613	N/A	8203	5.201	1.354	
4	Unknown	9	49.742	18357150	228127	22.746	16.185	N/A	8601	4.062	1.429	
5	Unknown	9	58.689	1113724	15423	1.380	1.094	N/A	10682	1.894	1.270	
6	Unknown	9	63.661	1575771	17672	1.952	1.254	N/A	7242	N/A	1.087	

Figure S13. HPLC spectrum of Table S1, run 5. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 0.7 mL min^{-1} at λ = 210 nm.



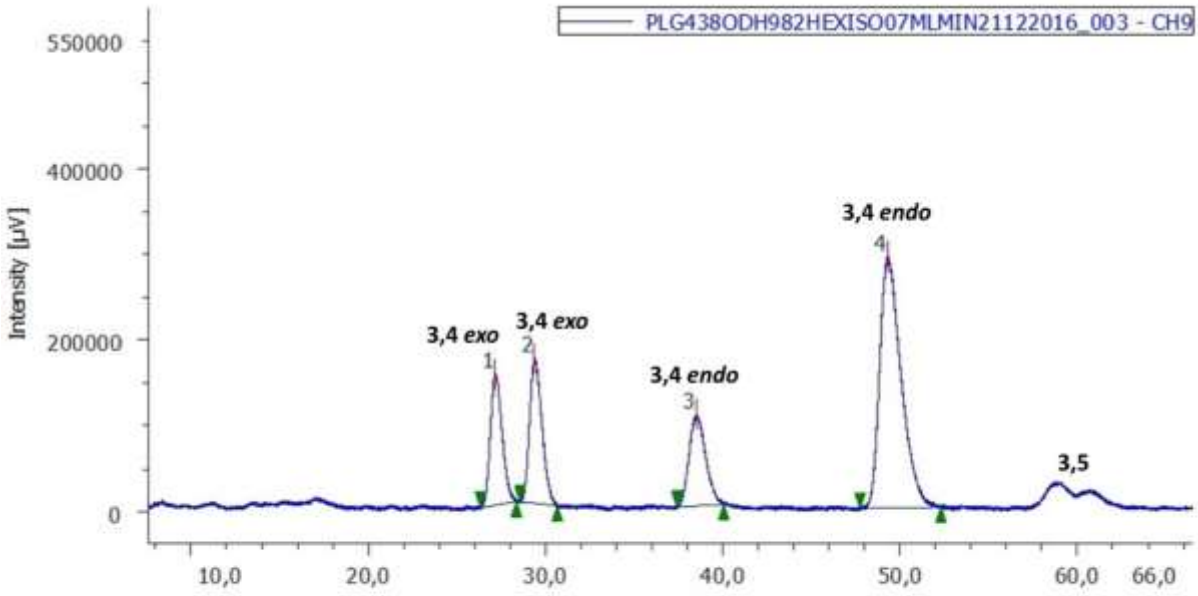
#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	27.762	11627923	257475	18.436	25.261	N/A	8487	1.772	1.306	
2	Unknown	9	29.956	11215760	234214	17.782	22.979	N/A	8802	6.572	1.333	
3	Unknown	9	39.774	9680205	148477	15.348	14.567	N/A	8570	5.152	1.357	
4	Unknown	9	49.650	26409863	327712	41.872	32.153	N/A	8732	4.109	1.503	
5	Unknown	9	58.865	2503712	31451	3.970	3.086	N/A	9854	1.935	1.006	
6	Unknown	9	63.079	1635007	19911	2.592	1.953	N/A	9469	N/A	1.144	

Figure S14. HPLC spectrum of Table S1, run 6. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 0.7 mL min^{-1} at λ = 210 nm.



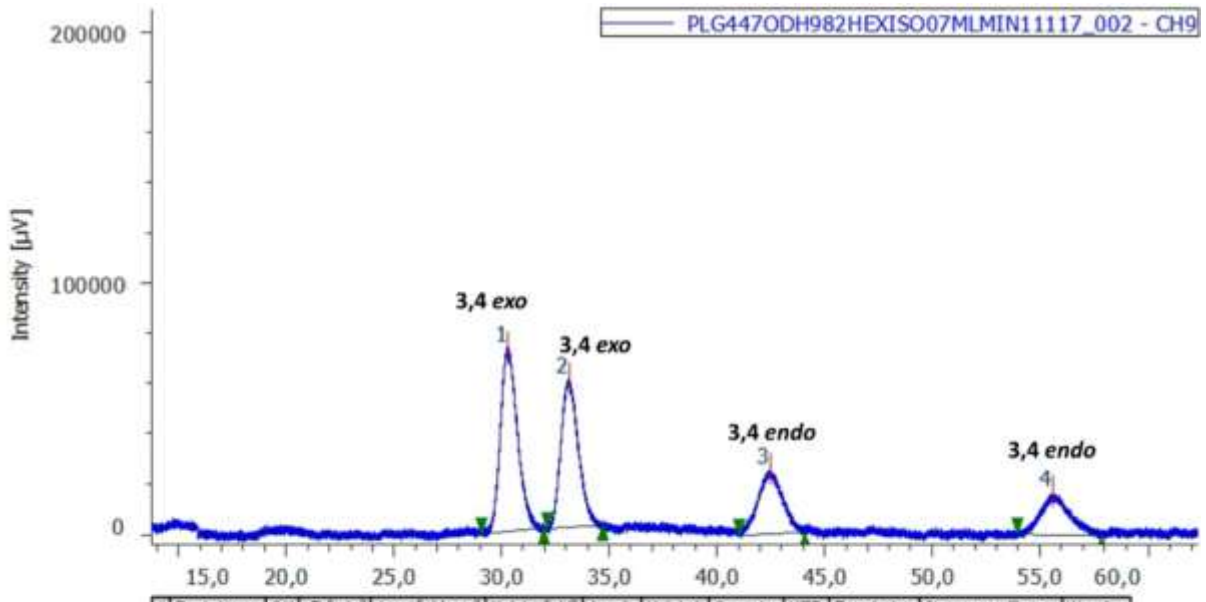
#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	27,435	31711457	691938	45,905	50,587	N/A	8528	1,818	1,492	
2	Unknown	9	29,731	25871860	510012	37,452	37,286	N/A	7836	6,071	1,563	
3	Unknown	9	39,114	6230445	98115	9,019	7,173	N/A	7937	5,735	1,169	
4	Unknown	9	50,463	5266431	67758	7,624	4,954	N/A	8326	N/A	1,220	

Figure S15. HPLC spectrum of Table S1, run 7. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 0.7 mL min^{-1} at λ = 210 nm.



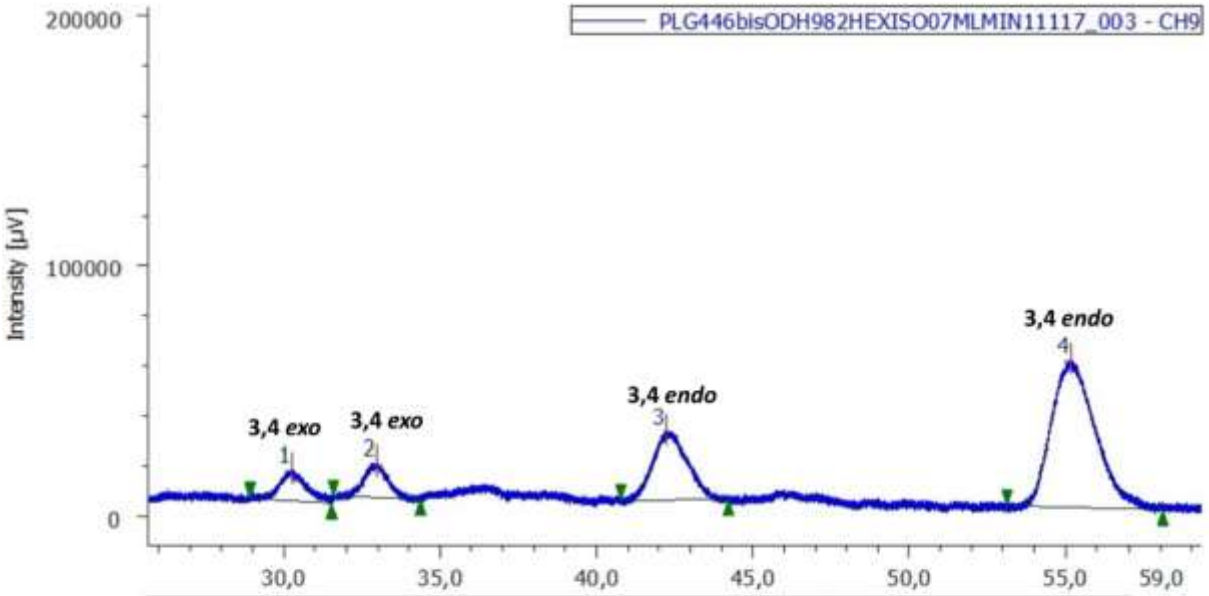
#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	27,161	6970335	151822	14,941	21,139	N/A	7672	1,757	1,313	
2	Unknown	9	29,384	8117747	167739	17,400	23,355	N/A	8207	6,011	1,327	
3	Unknown	9	38,526	6831122	105882	14,642	14,743	N/A	7732	5,452	1,207	
4	Unknown	9	49,301	24733853	292768	53,017	40,763	N/A	7955	N/A	1,523	

Figure S16. HPLC spectrum of Table S1, run 8. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 0.7 mL min^{-1} at λ = 210 nm.



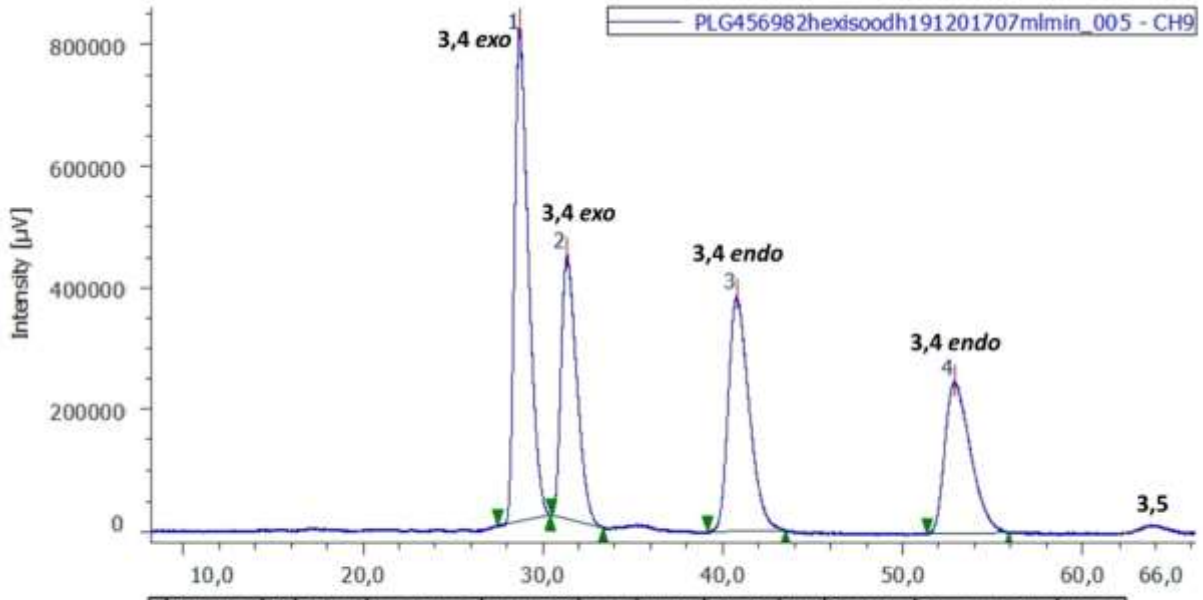
#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	30.304	4003198	73137	37.483	41.811	N/A	7068	1.946	1.251	
2	Unknown	9	33.142	3248399	58840	30.416	33.638	N/A	7994	5.119	1.213	
3	Unknown	9	42.480	1957078	25677	18.325	14.679	N/A	6102	5.535	1.054	
4	Unknown	9	55.579	1471326	17267	13.776	9.872	N/A	7481	N/A	1.198	

Figure S17. HPLC spectrum of Table S1, run 9. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 0.7 mL min^{-1} at λ = 210 nm.



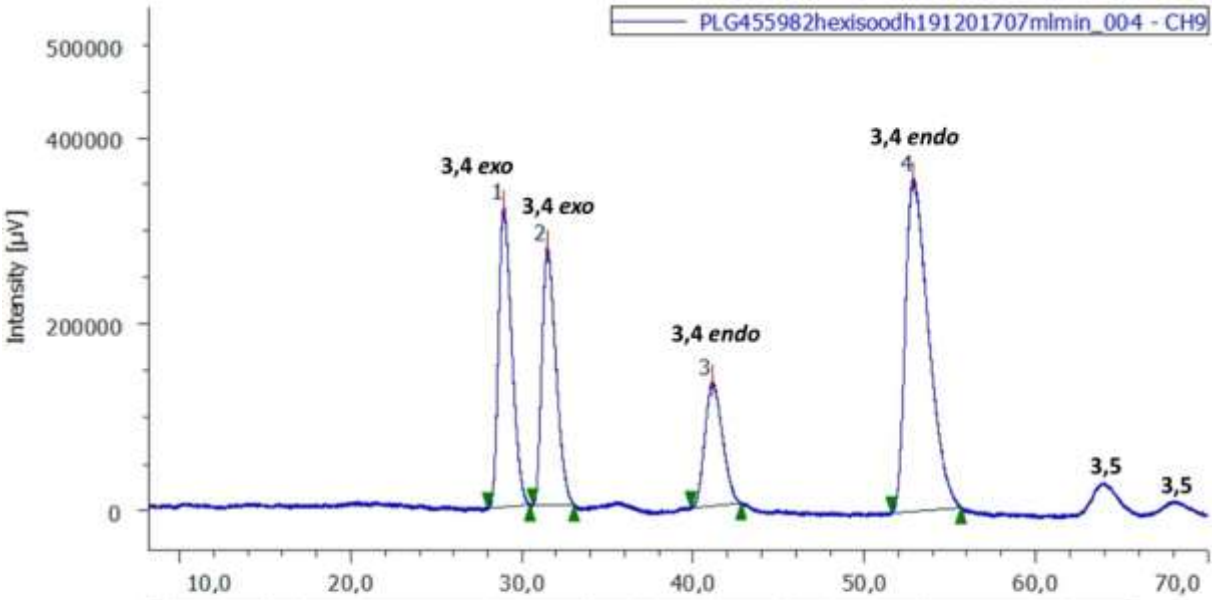
#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	30.268	699857	12874	7.759	11.388	N/A	5641	1.765	0.967	
2	Unknown	9	32.960	682766	14022	7.569	12.403	N/A	8297	5.125	1.008	
3	Unknown	9	42.237	2046386	27522	22.687	24.344	N/A	5990	5.407	1.265	
4	Unknown	9	55.170	5591081	58634	61.985	51.865	N/A	7128	N/A	1.498	

Figure S18. HPLC spectrum of Table S1, run 10. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 0.7 mL min^{-1} at λ = 210 nm.



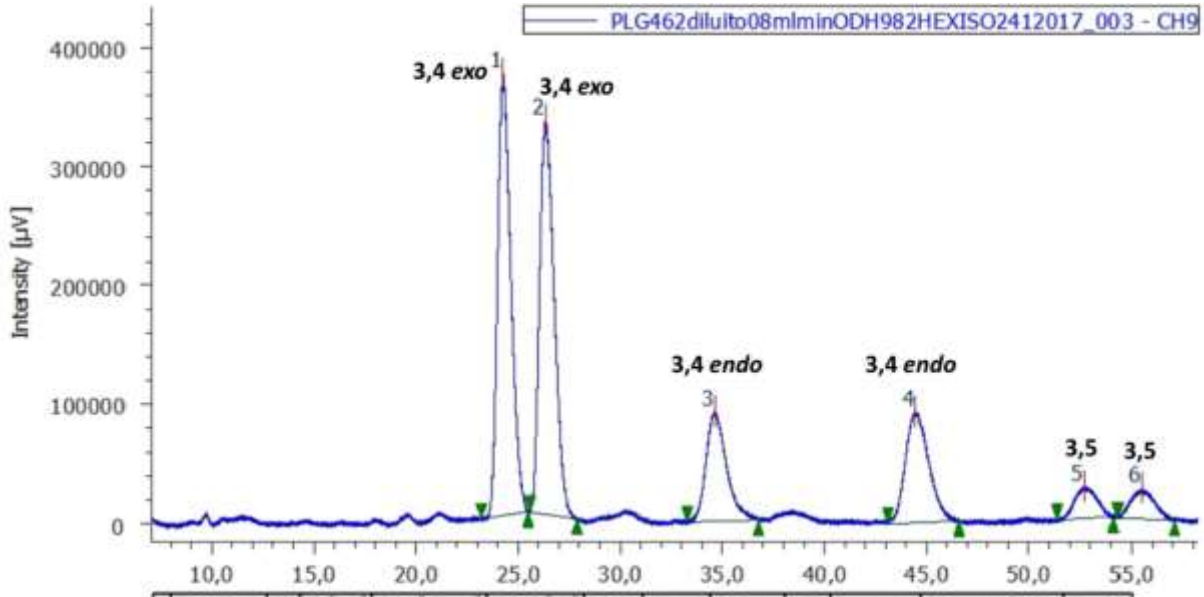
#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	28,730	43363533	816181	34,722	43,314	N/A	6774	1,733	1,502	
2	Unknown	9	31,323	26118225	433312	20,913	22,996	N/A	6095	5,148	1,539	
3	Unknown	9	40,801	30829459	386630	24,685	20,518	N/A	6114	5,128	1,355	
4	Unknown	9	52,899	24578013	248211	19,680	13,172	N/A	6407	N/A	1,491	

Figure S19. HPLC spectrum of Table 1, entry 2 (in the manuscript), for reaction without the capsule. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 0.7 mL min^{-1} at λ = 210 nm.



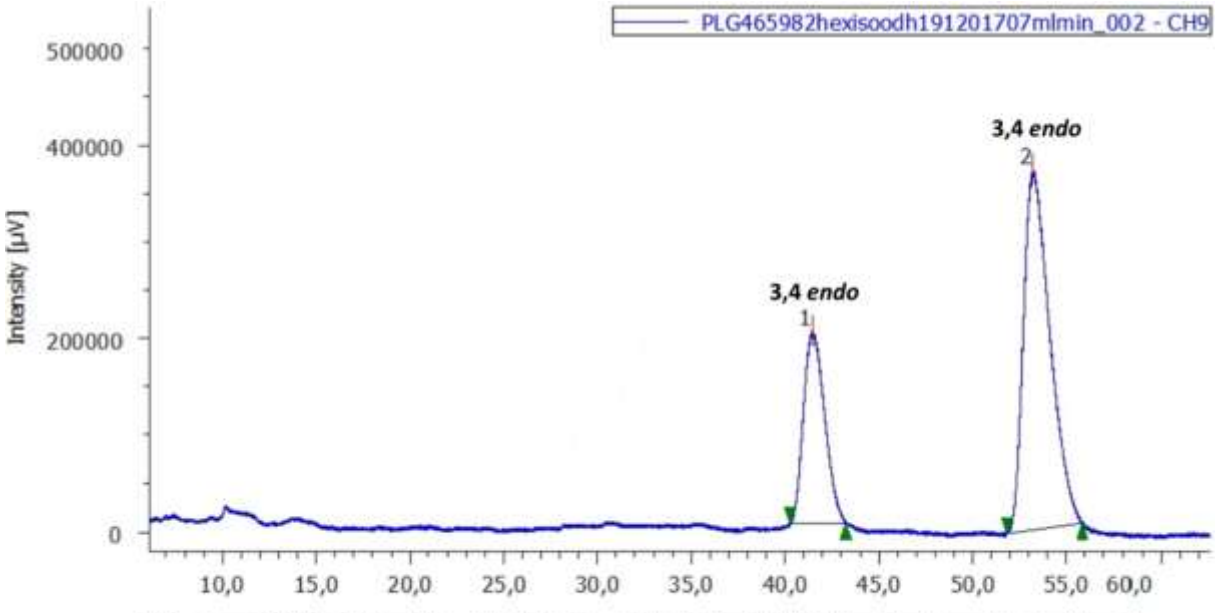
#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	28,952	17255623	322969	22,635	29,573	N/A	6656	1,740	1,368	
2	Unknown	9	31,500	15686985	276948	20,578	25,359	N/A	6905	5,655	1,409	
3	Unknown	9	41,125	9449245	133926	12,395	12,263	N/A	7519	5,341	1,192	
4	Unknown	9	52,885	33840911	358253	44,392	32,804	N/A	7057	N/A	1,603	

Figure S20. HPLC spectrum of Table 1, entry 2 (in the manuscript), for reaction with the capsule. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 0.7 mL min^{-1} at λ = 210 nm.



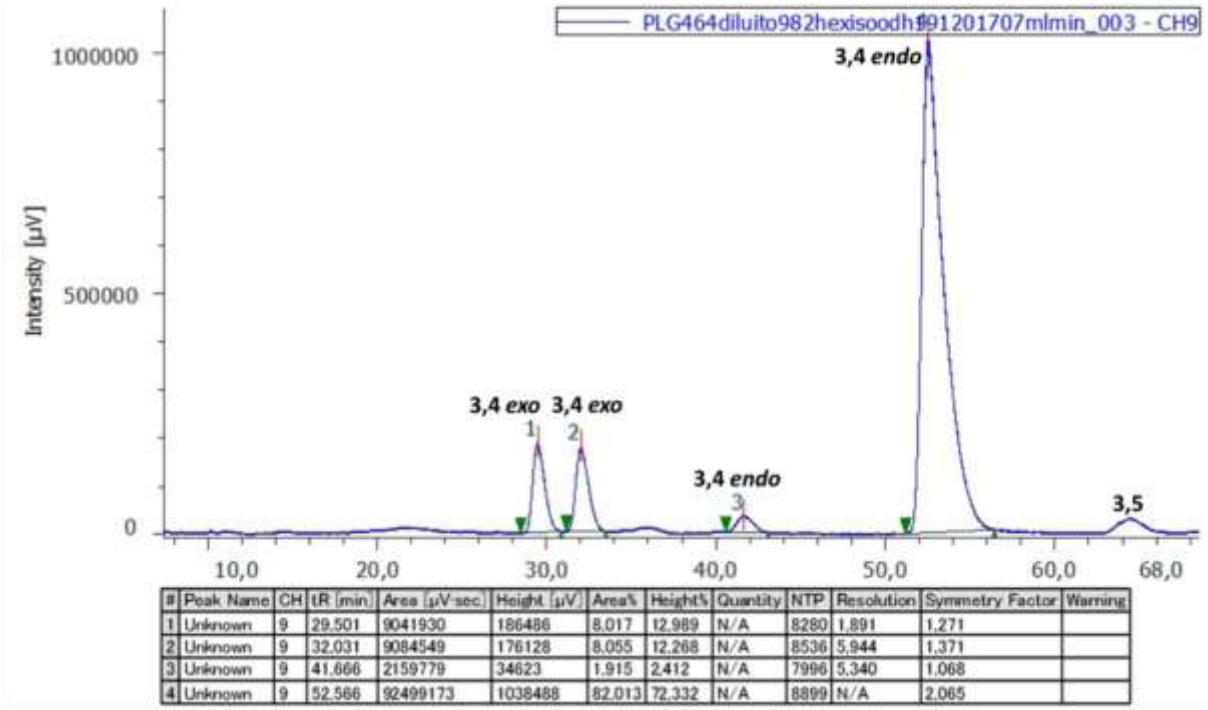
#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	24,265	16716756	371607	32,944	39,545	N/A	6617	1,638	1,329	
2	Unknown	9	26,338	16434628	330991	32,388	35,222	N/A	6137	5,323	1,352	
3	Unknown	9	34,660	6332439	91422	12,479	9,729	N/A	5996	5,001	1,369	
4	Unknown	9	44,435	7337676	92737	14,460	9,869	N/A	6967	3,798	1,221	
5	Unknown	9	52,699	1942514	27012	3,828	2,874	N/A	8906	1,220	1,068	
6	Unknown	9	55,486	1978895	25949	3,900	2,761	N/A	8946	N/A	1,178	

Figure S21. HPLC spectrum of Table 1, entry 3 (in the manuscript), for reaction with the capsule. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 0.8 mL min^{-1} at λ = 210 nm.



#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	41,455	15478191	198192	29,941	34,724	N/A	5991	4,985	1,268	
2	Unknown	9	53,219	36218273	372568	70,059	65,276	N/A	6755	N/A	1,558	

Figure S22. HPLC spectrum of Table 1, entry 4 (in the manuscript), for reaction with the capsule. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 0.7 mL min^{-1} at λ = 210 nm.



#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	29.501	9041930	186486	8.017	12.989	N/A	8280	1.891	1.271	
2	Unknown	9	32.031	9084549	176128	8.055	12.268	N/A	8536	5.944	1.371	
3	Unknown	9	41.666	2159779	34623	1.915	2.412	N/A	7996	5.340	1.068	
4	Unknown	9	52.566	92499173	1038488	82.013	72.332	N/A	8899	N/A	2.065	

Figure S23. HPLC spectrum of Table 1, entry 5 (in the manuscript), for reaction *with the* capsule. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 0.7 mL min^{-1} at λ = 210 nm.

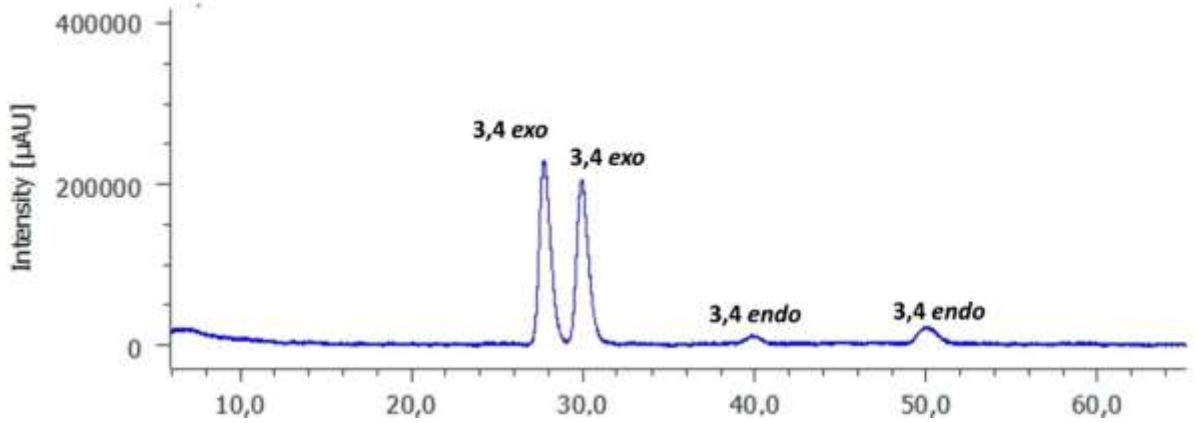
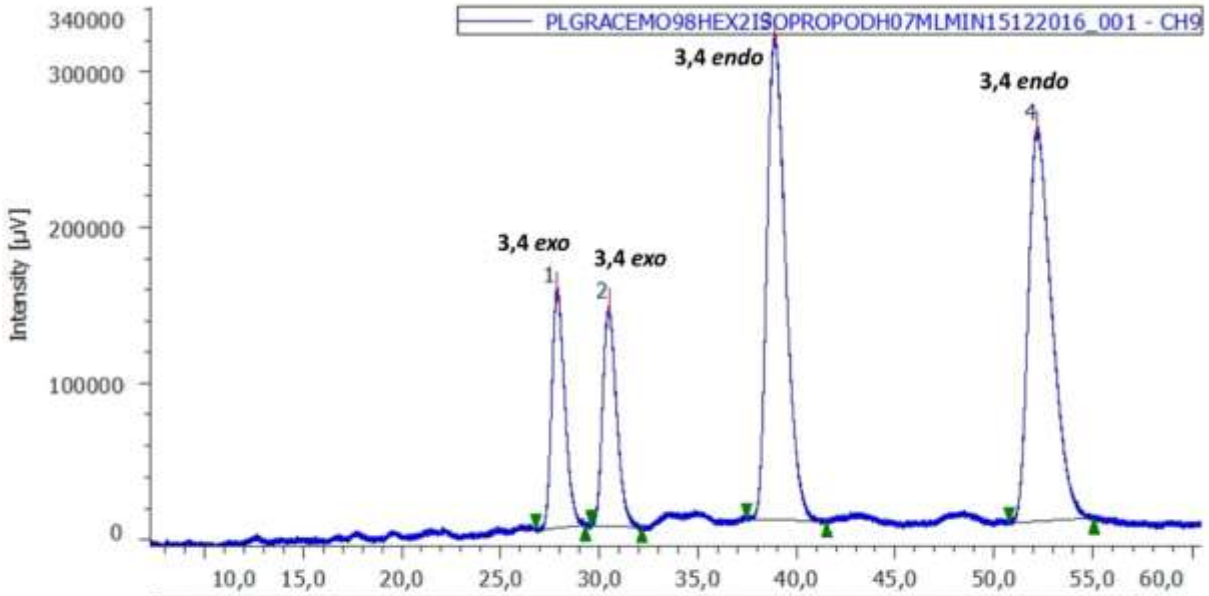


Figure S24. HPLC spectrum of the reduced 3,4 *exo* adduct for the 1,3 dipolar cycloaddition between crotonaldehyde **4a** and nitrone **3a**. Traces of enantiomers of the reduced 3,4-*endo* adduct are present. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 0.7 mL min^{-1} at λ = 210 nm.



#	Peak Name	CH	tR [min]	Area [µV sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	27,866	6967044	153473	12,657	17,838	N/A	8710	2,135	1,349	
2	Unknown	9	30,491	6857691	142127	12,459	16,519	N/A	9210	5,611	1,309	
3	Unknown	9	38,876	20442856	311870	37,139	36,248	N/A	8120	6,863	1,407	
4	Unknown	9	52,226	20775909	252914	37,745	29,395	N/A	9224	N/A	1,459	

Figure S25. HPLC spectrum of the racemic mixture of alcohols for the 1,3-dipolar cycloaddition between crotonaldehyde **4a** and nitrone **3a**. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 0.7 mL min^{-1} at λ = 210 nm.

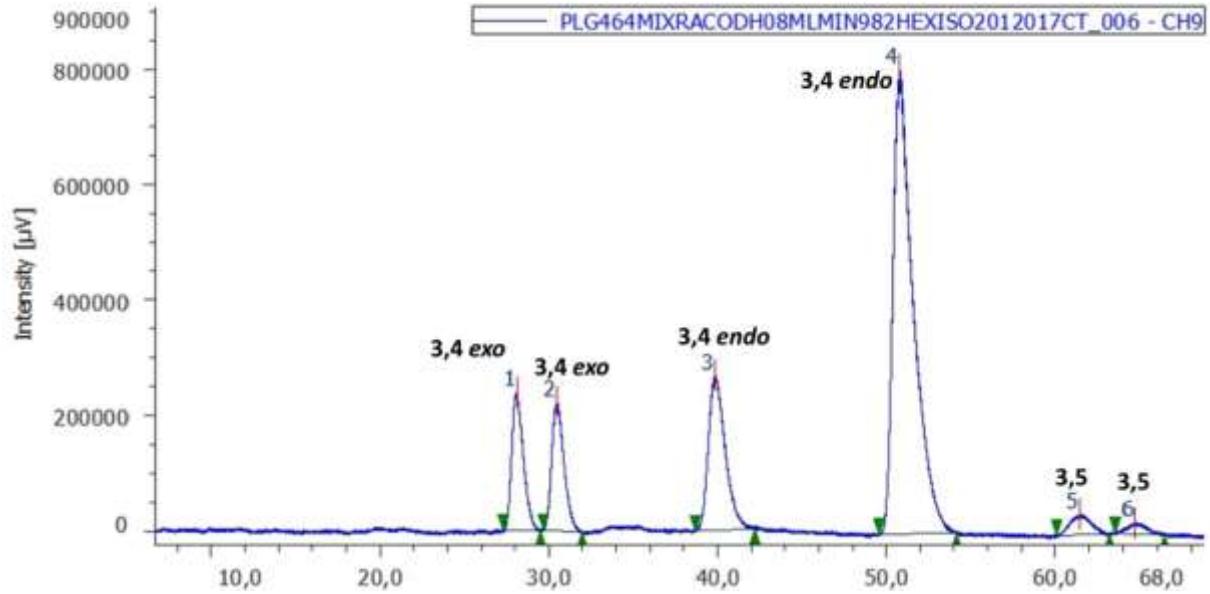
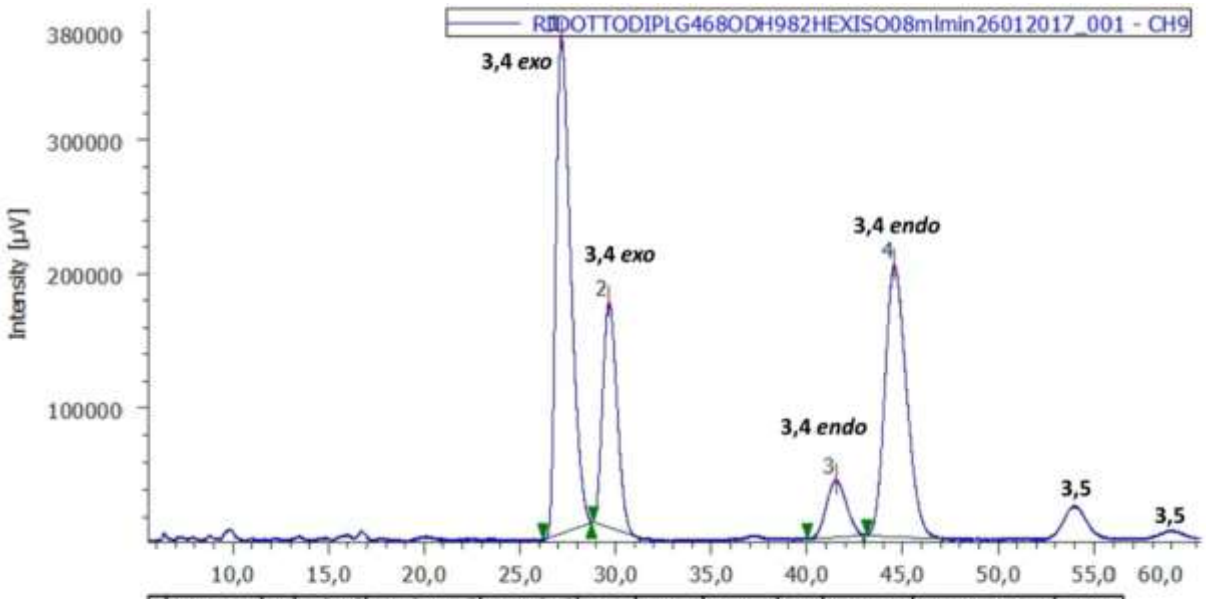
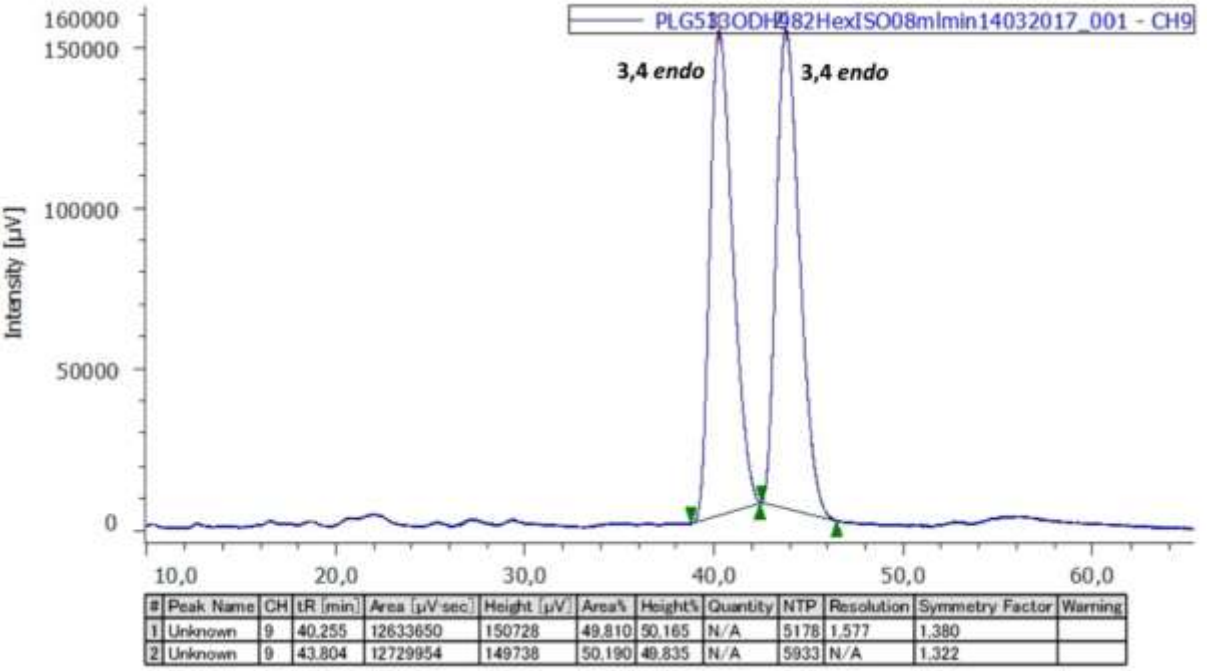


Figure S26. HPLC spectrum of the mixture of racemic (Figure S24) + chiral (Figure S22) for 1,3-dipolar cycloaddition between **4a** and **3a**. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 0.7 mL min^{-1} at λ = 210 nm.



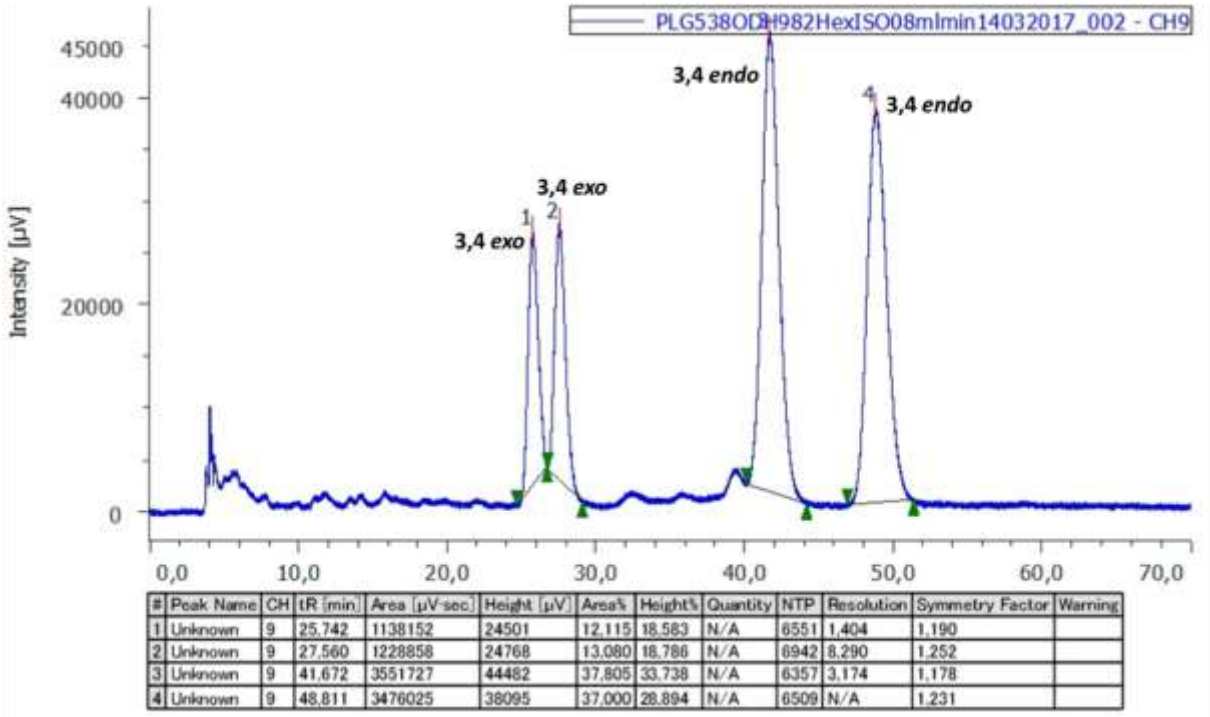
#	Peak Name	CH	tR [min]	Area [µV sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	27,169	20061048	370956	41,884	47,303	N/A	5748	1,763	1,546	
2	Unknown	9	29,660	8739838	167801	18,247	21,397	N/A	7176	7,018	1,201	
3	Unknown	9	41,524	3133155	43169	6,541	5,505	N/A	6971	1,507	1,042	
4	Unknown	9	44,586	15962764	202283	33,327	25,795	N/A	7312	N/A	1,190	

Figure S27. HPLC spectrum of Table 2, entry 2 (in the manuscript), for the reaction between **4a** and **3b** with the capsule. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 0.8 mL min^{-1} at λ = 220 nm.



#	Peak Name	CH	tR [min]	Area [µV sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	40,255	12633650	150728	49,810	50,165	N/A	5178	1,577	1,380	
2	Unknown	9	43,804	12729954	149738	50,190	49,835	N/A	5933	N/A	1,322	

Figure S28. HPLC spectrum of the racemic mixture of 3,4 *endo* diastereomer for the 1,3-dipolar cycloaddition between crotonaldehyde **4a** and nitrone **3b**. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 0.8 mL min^{-1} at λ = 220 nm.



#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	25,742	1138152	24501	12,115	18,583	N/A	6551	1,404	1,190	
2	Unknown	9	27,560	1228858	24768	13,080	18,786	N/A	6942	8,290	1,252	
3	Unknown	9	41,672	3551727	44482	37,805	33,738	N/A	6357	3,174	1,178	
4	Unknown	9	48,811	3476025	38095	37,000	28,894	N/A	6509	N/A	1,231	

Figure S29. HPLC spectrum of the racemic mixture of 3,4-*endo* and 3,4-*exo* diastereomers for the 1,3 dipolar cycloaddition between crotonaldehyde **4a** and nitrone **3b**. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 0.8 mL min^{-1} at λ = 220 nm.

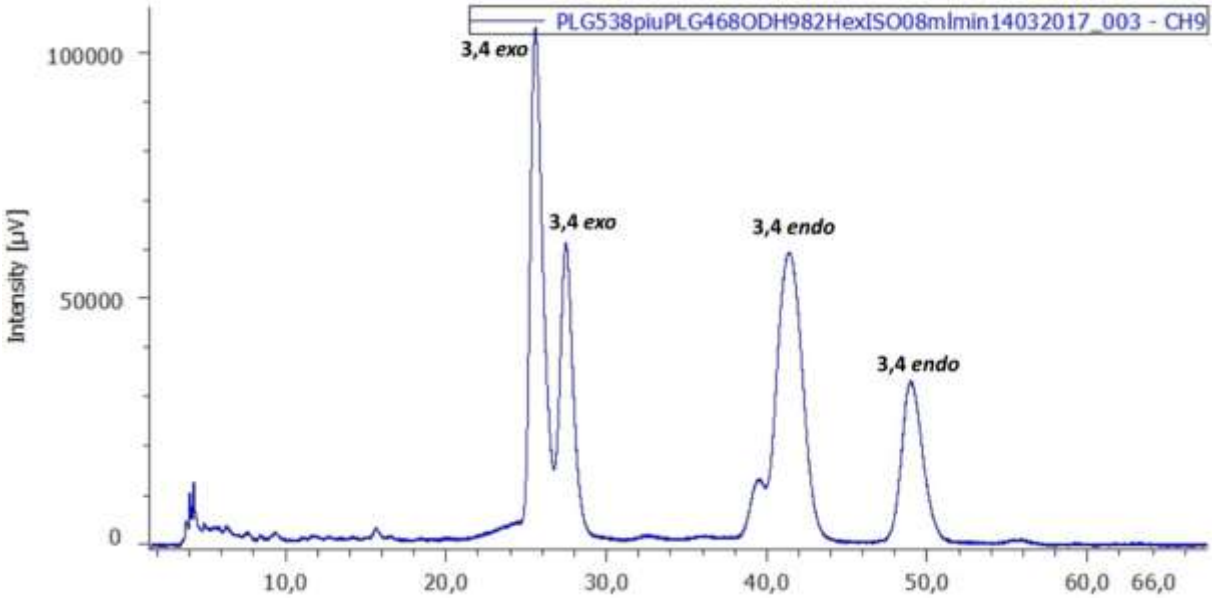
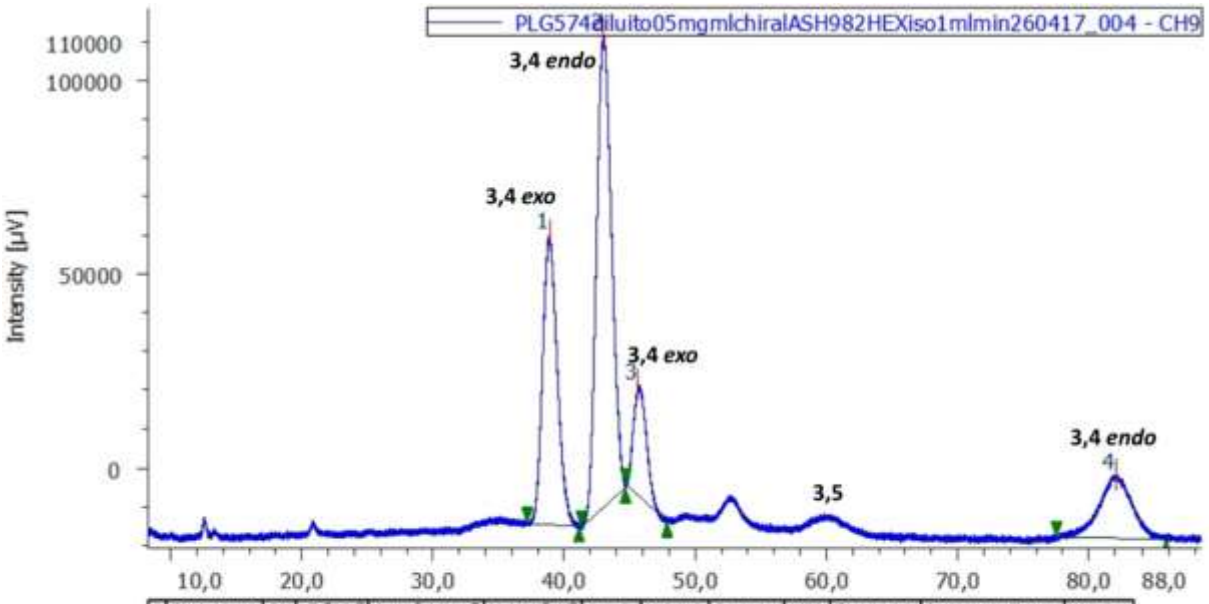
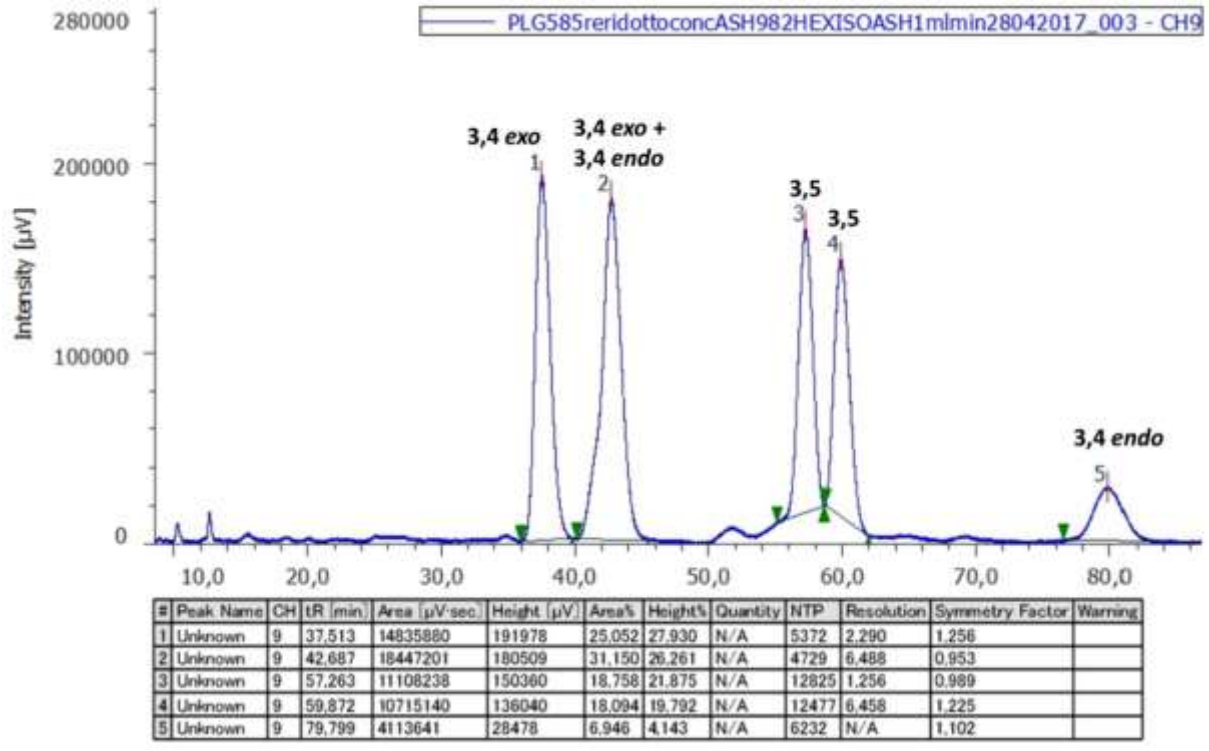


Figure S30. HPLC spectrum of the mixture of racemic (Figure S28) + chiral (Figure S26) for the 1,3-dipolar cycloaddition between crotonaldehyde **4a** and nitrone **3b**. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 0.8 mL min^{-1} at λ = 220 nm.



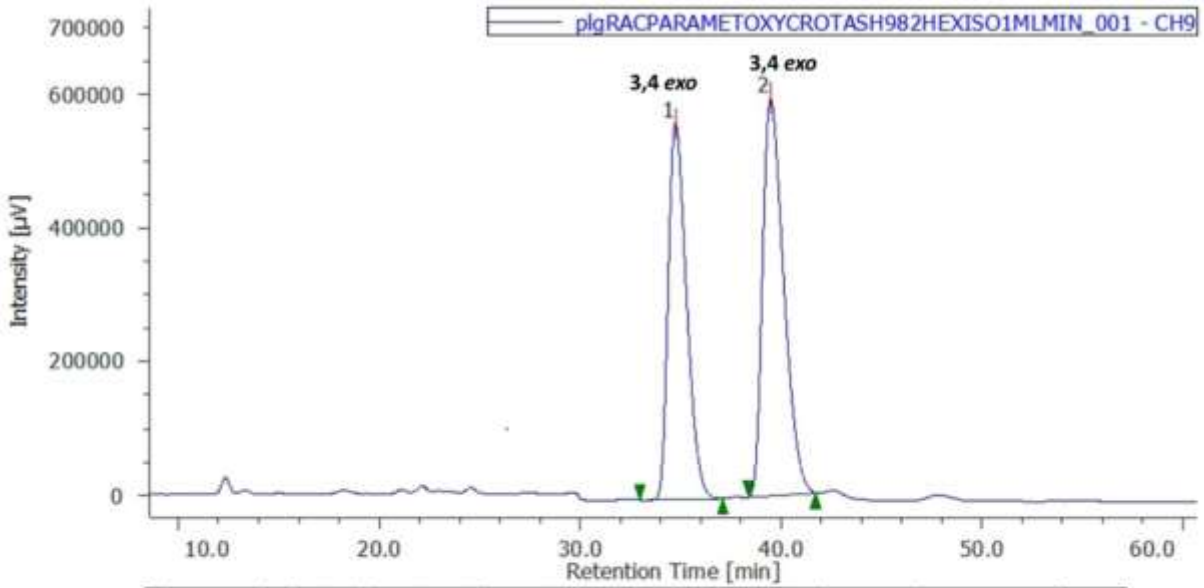
#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	38,891	5752197	74606	28,609	30,903	N/A	5782	1,961	1,160	
2	Unknown	9	43,005	9705885	122160	48,273	50,601	N/A	6333	1,293	1,112	
3	Unknown	9	45,628	1929208	28204	9,595	11,683	N/A	9156	11,439	1,342	
4	Unknown	9	82,070	2718774	16448	13,522	6,813	N/A	5367	N/A	0,909	

Figure S31. HPLC spectrum of Table 2, entry 3 (in the manuscript), for the reaction between aldehyde **4a** and nitrone **3c** with the capsule. The analysis was performed with Chiralcel AS-H as column, 98:2 Hexane/Isopropanol as eluent phase, 1.0 mL min^{-1} at λ = 210 nm.



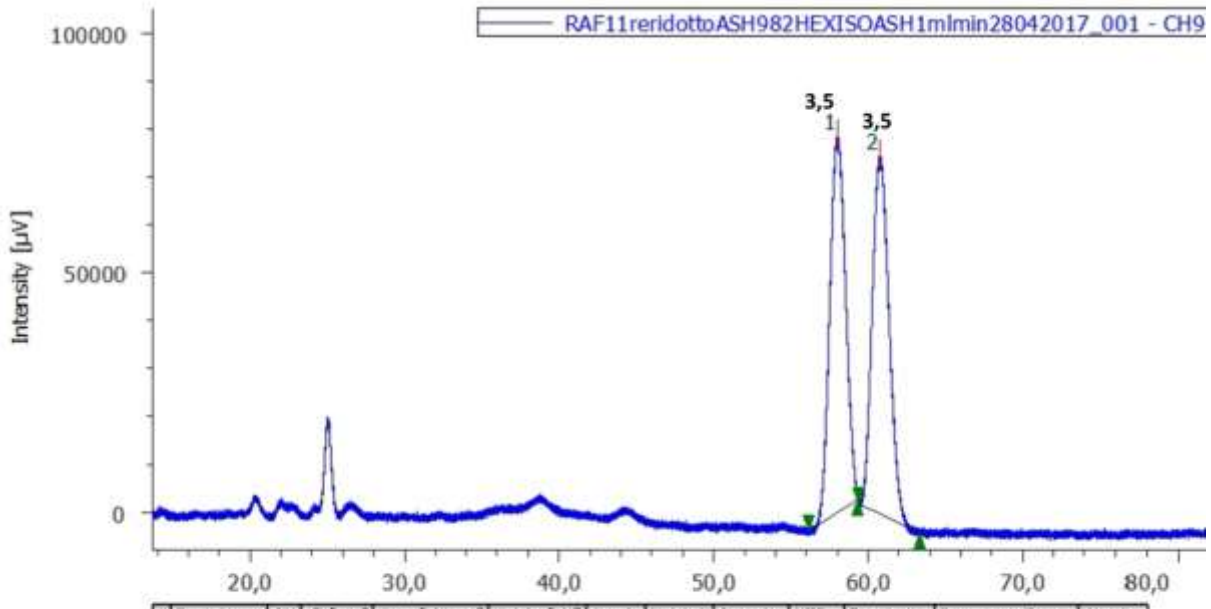
#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	37,513	14835880	191978	25,052	27,930	N/A	5372	2,290	1,256	
2	Unknown	9	42,687	18447201	180509	31,150	26,261	N/A	4729	6,488	0,953	
3	Unknown	9	57,263	11108238	150360	18,758	21,875	N/A	12825	1,256	0,989	
4	Unknown	9	59,872	10715140	136040	18,094	19,792	N/A	12477	6,458	1,225	
5	Unknown	9	79,799	4113641	28478	6,946	4,143	N/A	6232	N/A	1,102	

Figure S32. HPLC spectrum of the racemic mixture of alcohols (3,4-*endo,* 3,4-*exo,* and 3,5) for the 1,3-dipolar cycloaddition between crotonaldehyde **4a** and nitrone **3c**. The analysis was performed with Chiralcel AS-H as column, 98:2 Hexane/Isopropanol as eluent phase, 1.0 mL min^{-1} at λ = 210 nm.



#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	34.740	35473179	562061	45.038	48.584	N/A	6910	2.638	1.405	
2	Unknown	9	39.483	43289370	594819	54.962	51.416	N/A	8673	N/A	1.492	

Figure S33. HPLC spectrum of the racemic mixture of alcohols (3,4-*exo*, with traces of 3,4-*endo*) for the 1,3-dipolar cycloaddition between crotonaldehyde **4a** and nitrone **3c**. The analysis was performed with Chiralcel AS-H as column, 98:2 Hexane/Isopropanol as eluent phase, 1.0 mL min^{-1} at λ = 210 nm.



#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	58.016	5552375	78668	49.597	51.258	N/A	14505	1.390	1.043	
2	Unknown	9	60.769	5642689	74805	50.403	48.742	N/A	14114	N/A	1.150	

Figure S34. HPLC spectrum of the racemic mixture of the reduced 3,5-adduct for the 1,3-dipolar cycloaddition between crotonaldehyde **4a** and nitrone **3c**. The analysis was performed with Chiralcel AS-H as column, 98:2 Hexane/Isopropanol as eluent phase, 1.0 mL min^{-1} at λ = 210 nm.

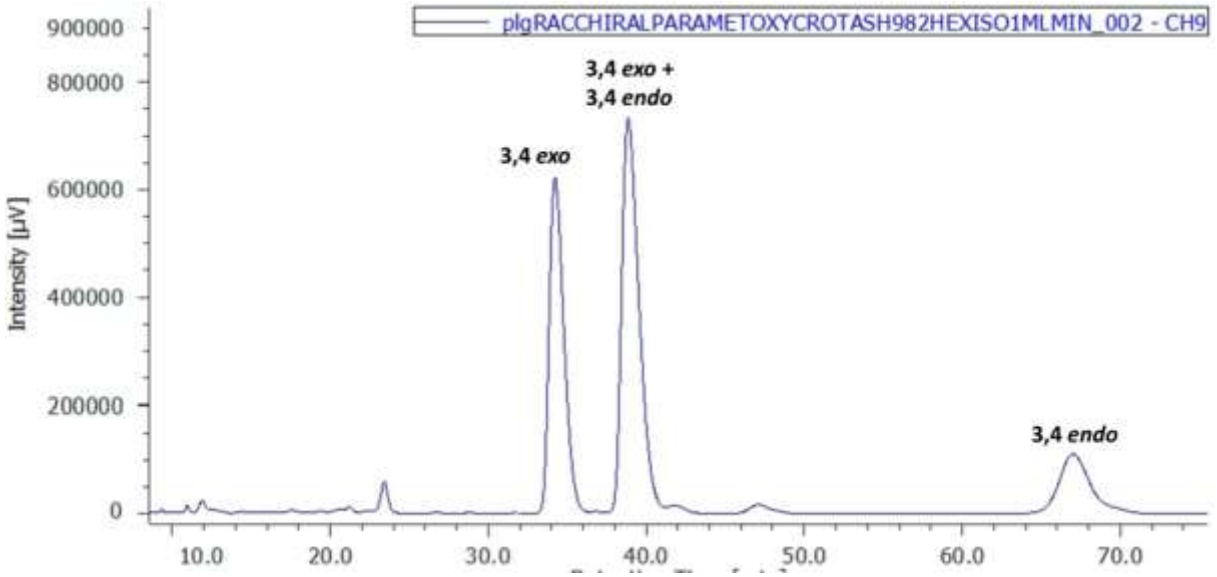
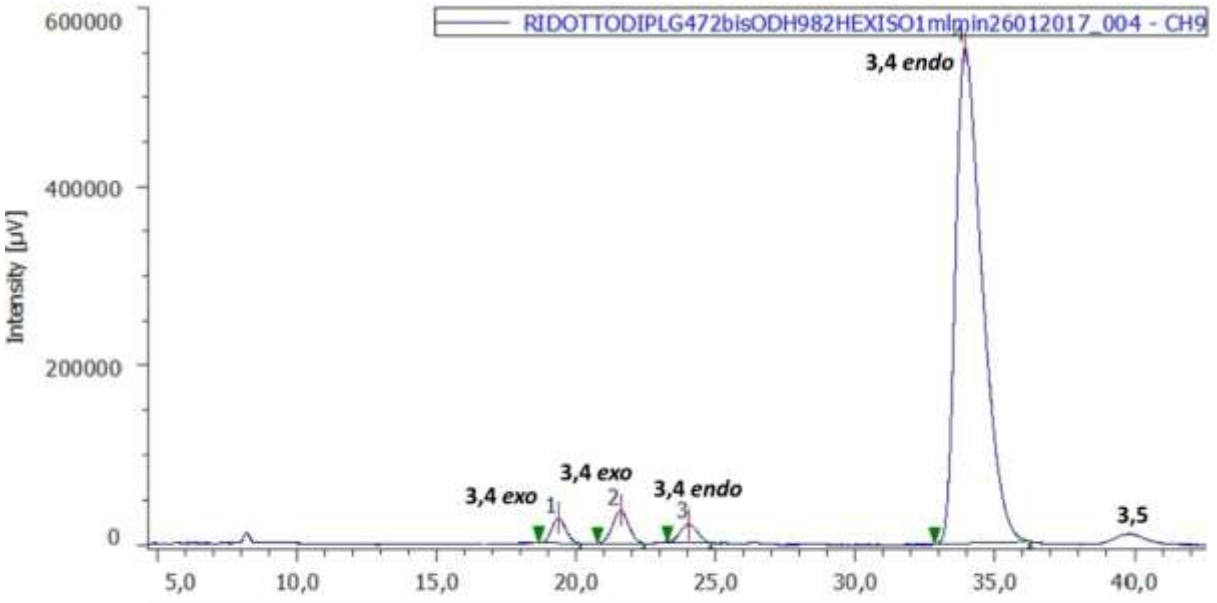
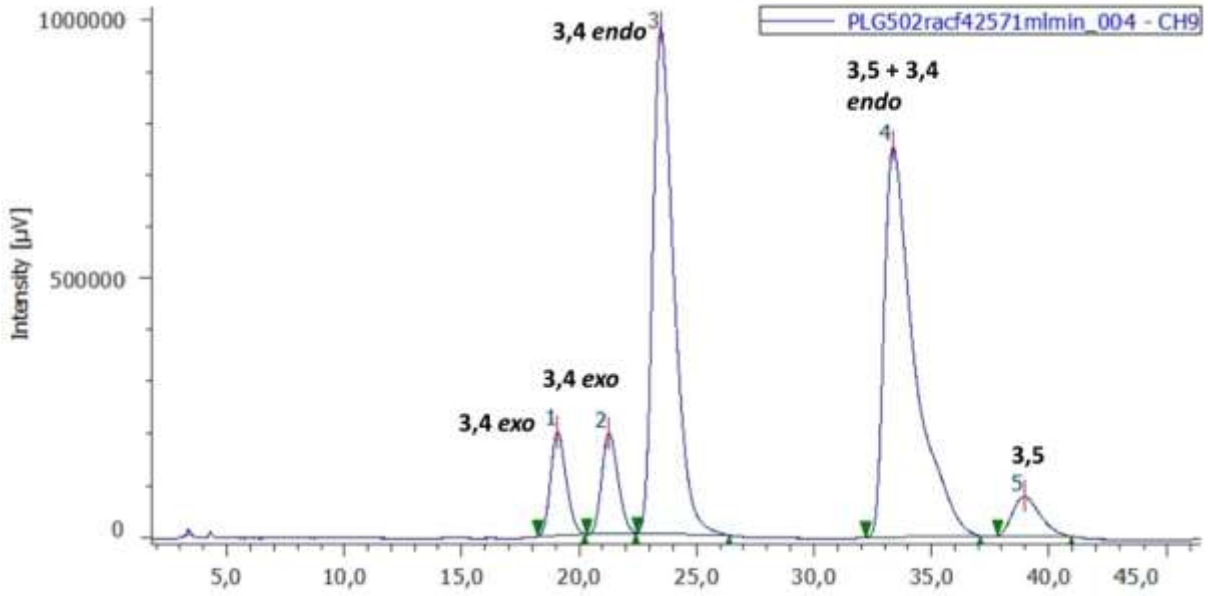


Figure S35. HPLC spectrum of the mixture of racemic + chiral (Figure S30) for the 1,3-dipolar cycloaddition between crotonaldehyde **4a** and nitrone **3c**. The analysis was performed with Chiralcel AS-H as column, 98:2 Hexane/Isopropanol as eluent phase, 1.0 mL min^{-1} at λ = 210 nm.



#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	19,379	975575	27854	2,443	4,357	N/A	6677	2,190	1,052	
2	Unknown	9	21,591	1511661	37216	3,785	5,822	N/A	6428	2,197	1,003	
3	Unknown	9	24,053	858079	20233	2,149	3,165	N/A	6761	6,834	1,023	
4	Unknown	9	33,966	36590367	553961	91,623	86,656	N/A	6107	N/A	1,559	

Figure S36. HPLC spectrum of Table 2, entry 4 (in the manuscript) for the 1,3-dipolar cycloaddition between crotonaldehyde **4a** and nitrone **3d**. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 1.0 mL min^{-1} at λ = 210 nm.



#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	19,088	9201445	199140	6,021	9,051	N/A	3889	1,733	1,171	
2	Unknown	9	21,264	9327758	192747	6,104	8,761	N/A	4320	1,551	1,173	
3	Unknown	9	23,488	60321266	978111	39,475	44,457	N/A	3527	5,341	1,479	
4	Unknown	9	33,353	67781757	754340	44,357	34,286	N/A	3953	2,621	2,307	
5	Unknown	9	38,966	6178088	75770	4,043	3,444	N/A	5147	N/A	1,322	

Figure S37. HPLC spectrum of the racemic mixture of alcohols (3,4-*endo*, 3,4-*exo*, and *3,5*) for the 1,3-dipolar cycloaddition between crotonaldehyde **4a** and nitrone **3d**. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 1.0 mL min^{-1} at λ = 210 nm.

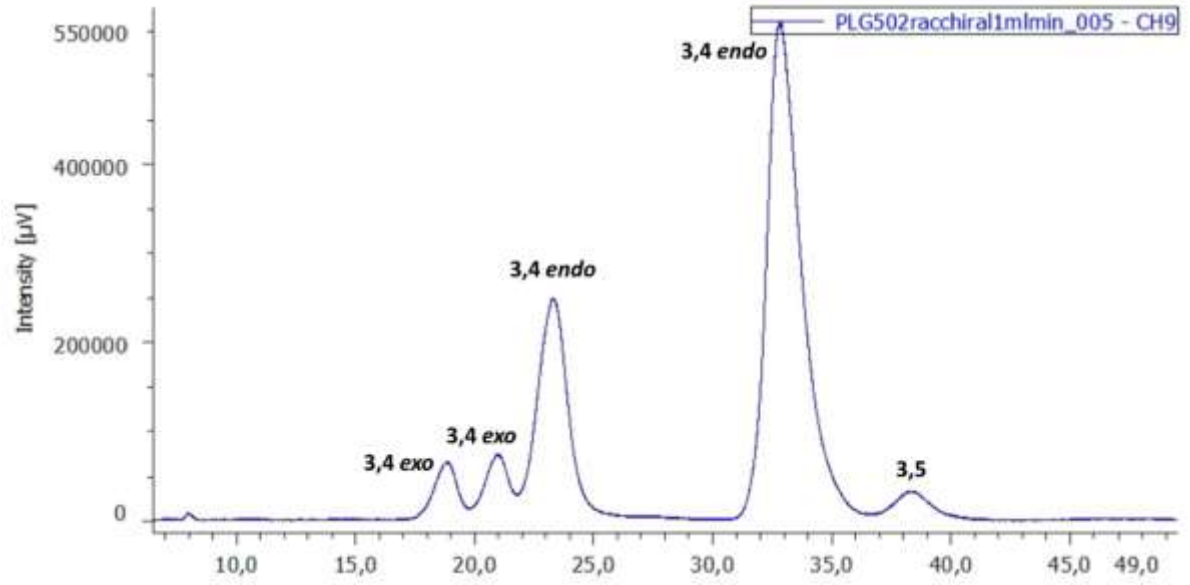
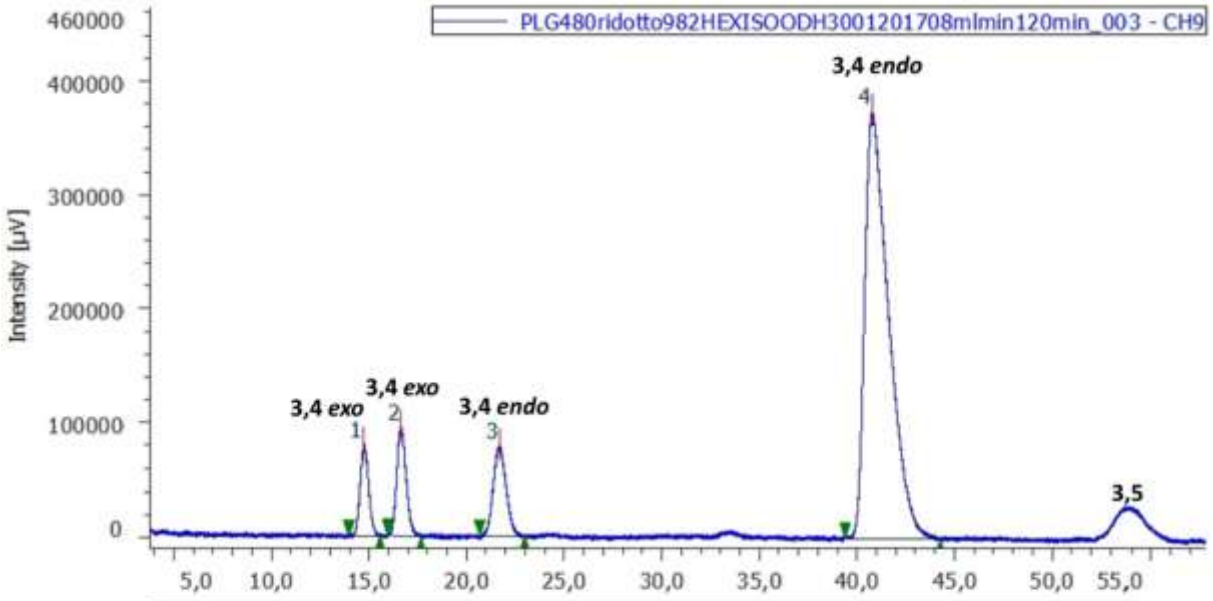
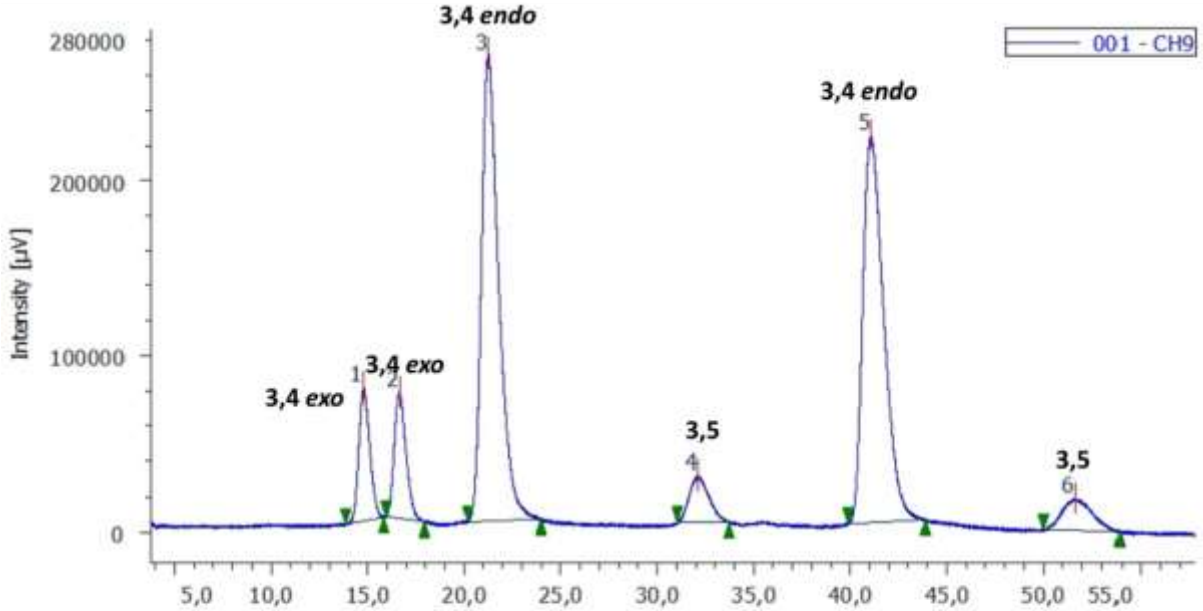


Figure 38. HPLC spectrum of the mixture of racemic + chiral (Figure S35) for the 1,3-dipolar cycloaddition between crotonaldehyde **4a** and nitrone **3d**. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 1.0 mL min^{-1} at λ = 210 nm.



#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	14,713	2442513	80349	5,963	12,757	N/A	5353	2,279	1,178	
2	Unknown	9	16,630	3190970	95676	7,790	15,190	N/A	5690	4,799	1,249	
3	Unknown	9	21,681	3579766	79136	8,739	12,564	N/A	4980	11,126	1,081	
4	Unknown	9	40,772	31747545	374692	77,507	59,489	N/A	5436	N/A	1,876	

Figure S39. HPLC spectrum of Table 2, entry 5 (in the manuscript) for the 1,3-dipolar cycloaddition between crotonaldehyde **4a** and nitrone **3e**. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 1.0 mL min^{-1} at λ = 210 nm.



#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	14,787	2973134	75420	6,943	11,102	N/A	3288	1,744	1,188	
2	Unknown	9	16,650	2995590	71331	6,996	10,500	N/A	3599	3,451	1,250	
3	Unknown	9	21,251	16454000	266842	38,425	39,279	N/A	2957	6,146	1,468	
4	Unknown	9	32,108	1867110	26598	4,360	3,915	N/A	4210	4,533	1,296	
5	Unknown	9	41,074	16591212	220586	38,746	32,471	N/A	6837	4,268	1,457	
6	Unknown	9	51,651	1939926	18567	4,530	2,733	N/A	4800	N/A	1,117	

Figure S40. HPLC spectrum of the racemic mixture of alcohols (3,4-*endo*, 3,4-*exo*, and *3,5*) for the 1,3-dipolar cycloaddition between crotonaldehyde **4a** and nitrone **3e**. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 1.0 mL min^{-1} at λ = 210 nm.

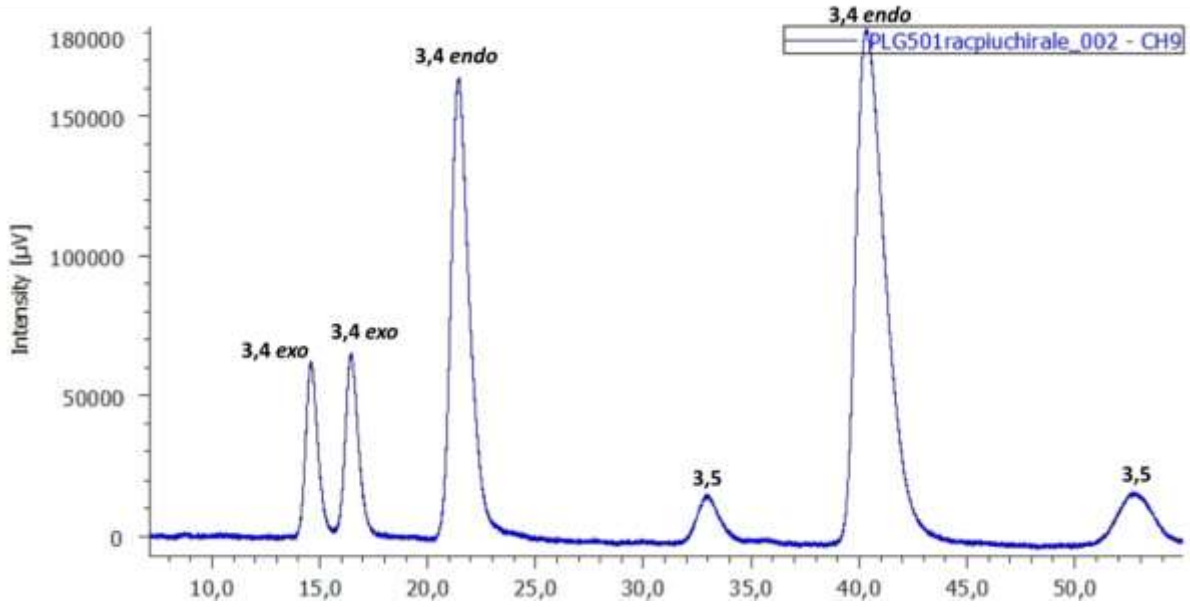
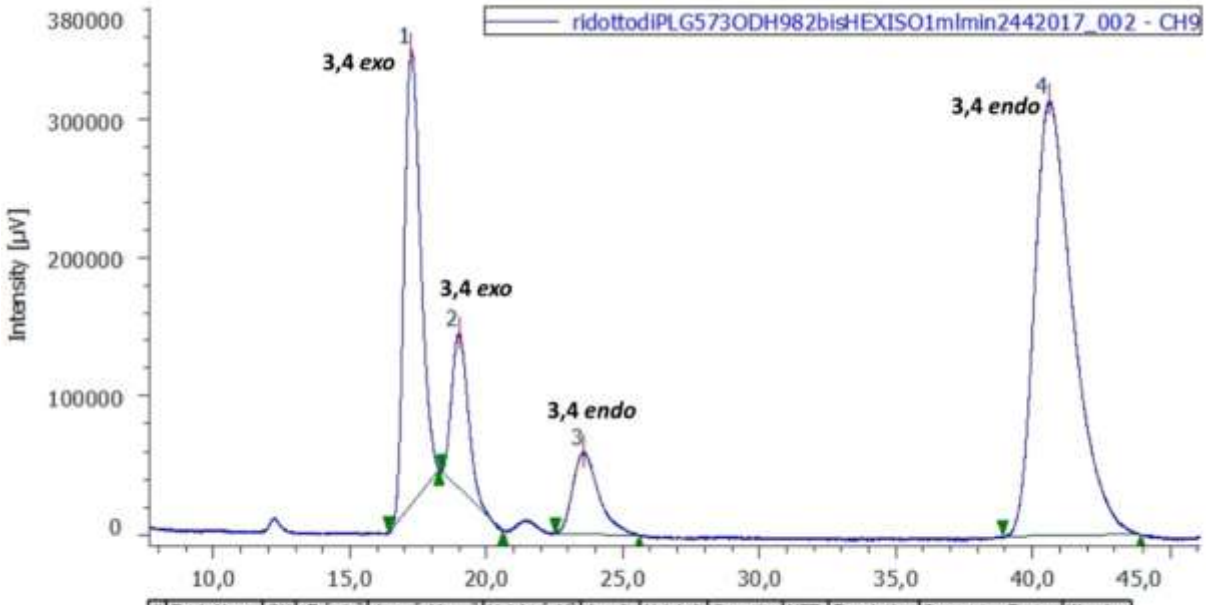
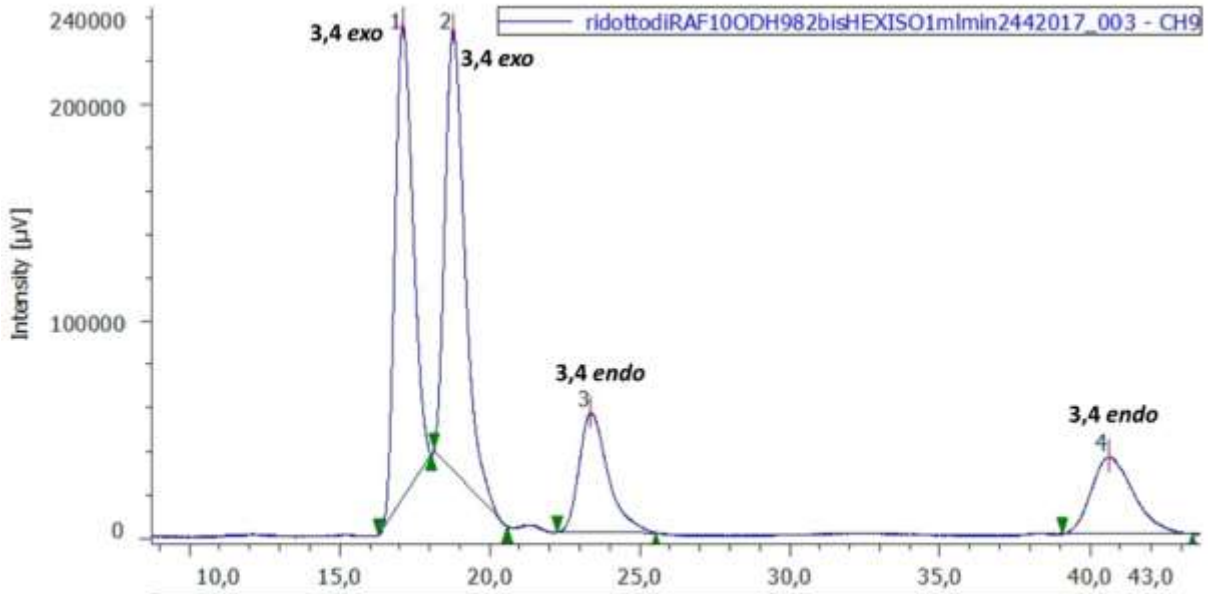


Figure S41. HPLC spectrum of the mixture of racemic + chiral (Figure S38) for the 1,3-dipolar cycloaddition between crotonaldehyde **4a** and nitrone **3d**. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 1.0 mL min^{-1} at λ = 210 nm.



#	Peak Name	CH	tR (min)	Area (µV·sec)	Height (µV)	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	17,244	13867490	329392	26,027	40,317	N/A	3772	1,574	1,293	
2	Unknown	9	19,003	4656114	112029	8,739	13,712	N/A	4620	3,272	1,256	
3	Unknown	9	23,572	3938100	60132	7,391	7,360	N/A	3144	8,166	1,466	
4	Unknown	9	40,616	30819890	315460	57,843	38,611	N/A	4210	N/A	1,491	

Figure S42. HPLC spectrum of Table 2, entry 6 (in the manuscript) for the 1,3-dipolar cycloaddition between crotonaldehyde **4a** and nitrone **3f**. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 1.0 mL min^{-1} at λ = 210 nm.



#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	17,109	9010449	218521	35,506	42,636	N/A	3806	1,466	1,236	
2	Unknown	9	18,781	9309543	203212	36,685	39,649	N/A	4066	3,214	1,529	
3	Unknown	9	23,367	3678239	55006	14,494	10,732	N/A	3084	8,309	1,485	
4	Unknown	9	40,614	3378747	35785	13,314	6,982	N/A	4293	N/A	1,302	

Figure S43. HPLC spectrum of the racemic mixture of alcohols (3,4-*endo*, 3,4-*exo*) for the 1,3-dipolar cycloaddition between crotonaldehyde **4a** and nitrone **3f**. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 1.0 mL min^{-1} at λ = 210 nm.

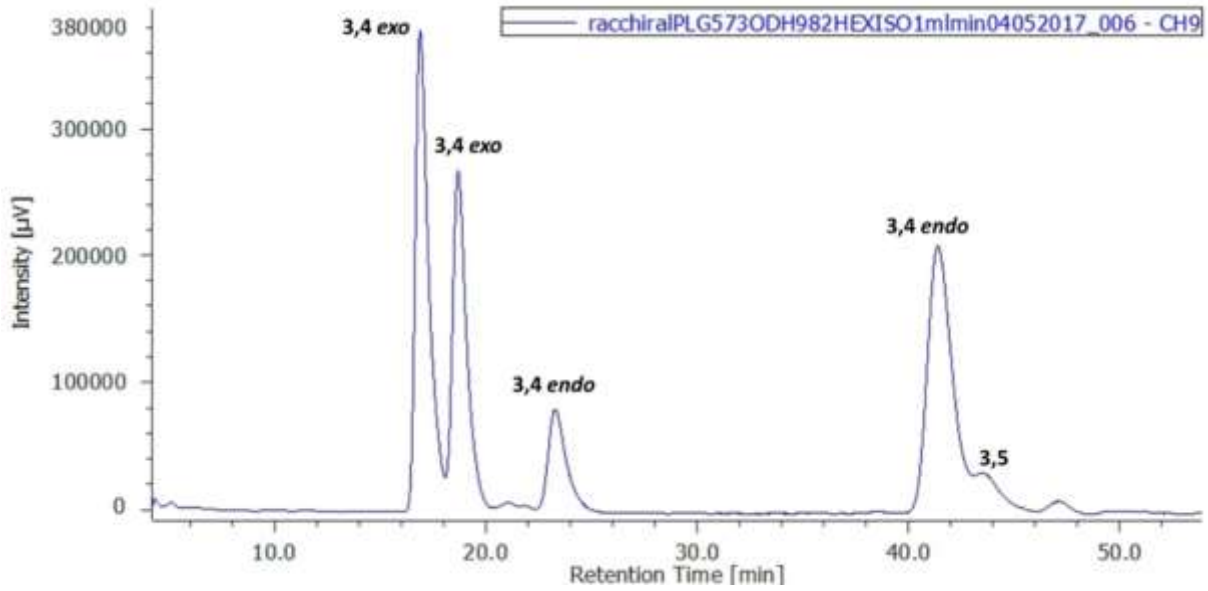
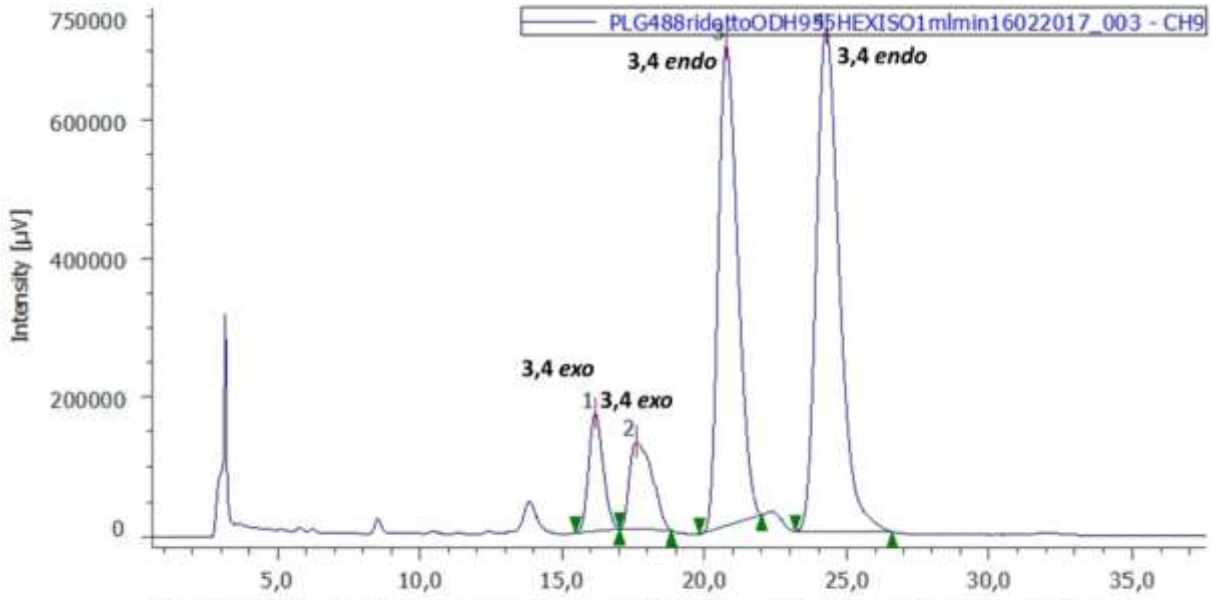
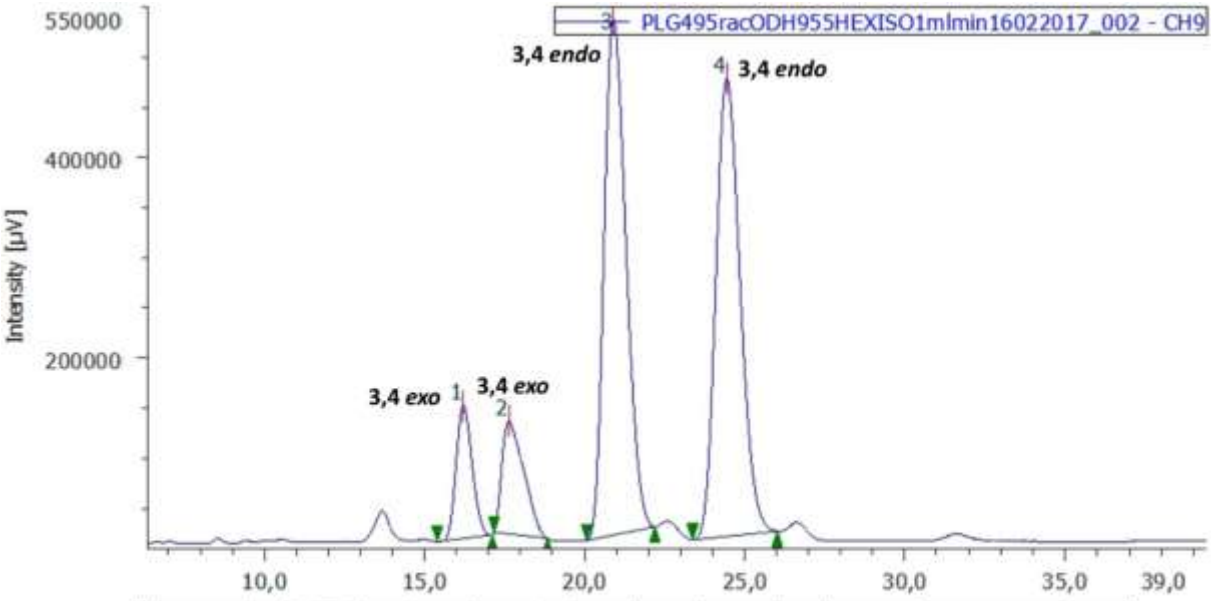


Figure S44. HPLC spectrum of the mixture of racemic + chiral (Figure 41) for the 1,3-dipolar cycloaddition between crotonaldehyde **4a** and nitrone **3f**. The analysis was performed with Chiralcel OD-H as column, 98:2 Hexane/Isopropanol as eluent phase, 1.0 mL min^{-1} at λ = 210 nm.



#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	16,157	5968593	168106	6,916	9,850	N/A	4659	1,121	1,186	
2	Unknown	9	17,600	7076959	124351	8,200	7,286	N/A	1853	2,184	1,661	
3	Unknown	9	20,763	32712420	691112	37,904	40,494	N/A	4283	2,598	1,307	
4	Unknown	9	24,277	40545439	723137	46,980	42,370	N/A	4528	N/A	1,334	

Figure S45. HPLC spectrum of Table 2, entry 8 (in the manuscript) for the 1,3-dipolar cycloaddition between acrolein **4c** and nitrone **3b** in the presence of the capsule. The analysis was performed with Chiralcel OD-H as column, 95:5 Hexane/Isopropanol as eluent phase, 1.0 mL min^{-1} at λ = 220 nm.



#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	16,217	4583133	131753	7,845	10,844	N/A	4857	1,249	1,169	
2	Unknown	9	17,633	5308081	111725	9,086	9,196	N/A	2756	2,501	1,708	
3	Unknown	9	20,900	24470554	514771	41,886	42,369	N/A	4295	2,656	1,274	
4	Unknown	9	24,437	24060360	456724	41,184	37,591	N/A	4909	N/A	1,209	

Figure S46. HPLC spectrum of the racemic mixture of alcohols (3,4-*endo*, 3,4-*exo*) for the 1,3-dipolar cycloaddition between acrolein **4c** and nitrone **3b**. The analysis was performed with Chiralcel OD-H as column, 95:5 Hexane/Isopropanol as eluent phase, 1.0 mL min^{-1} at λ = 220 nm.

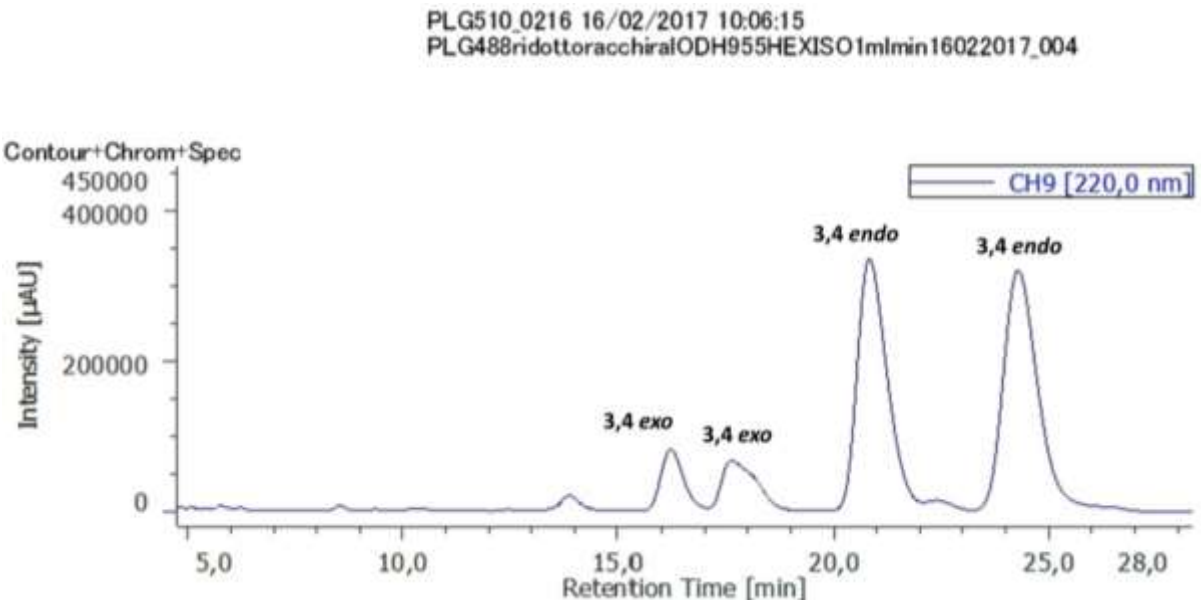
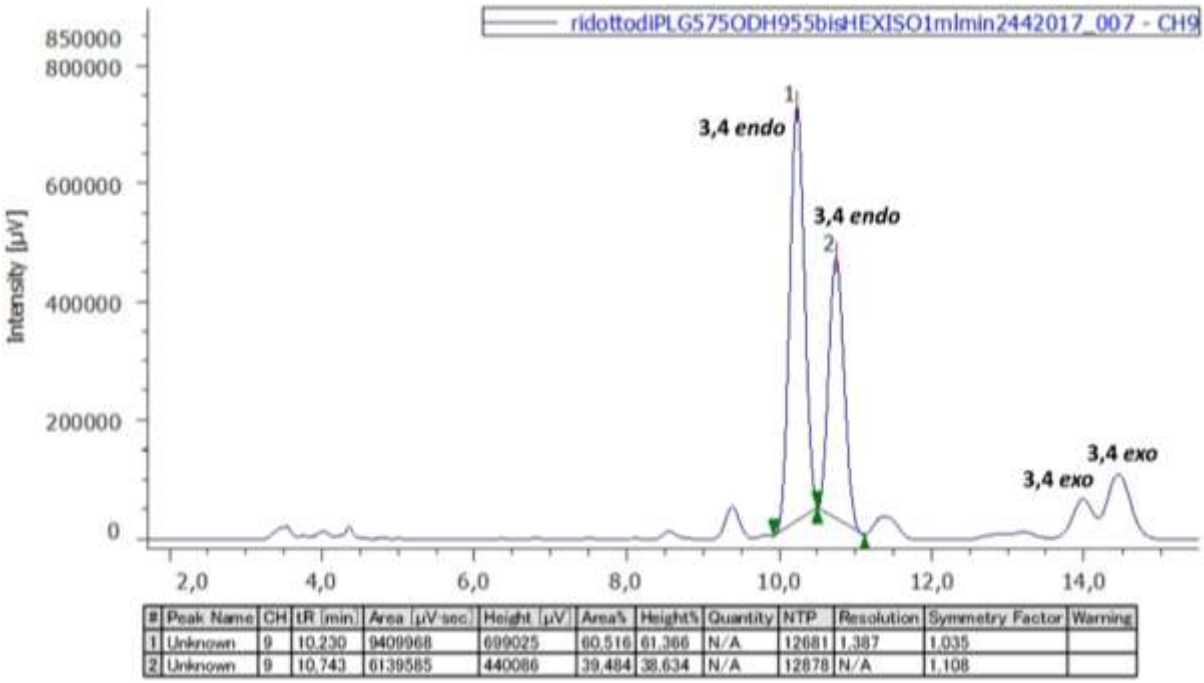
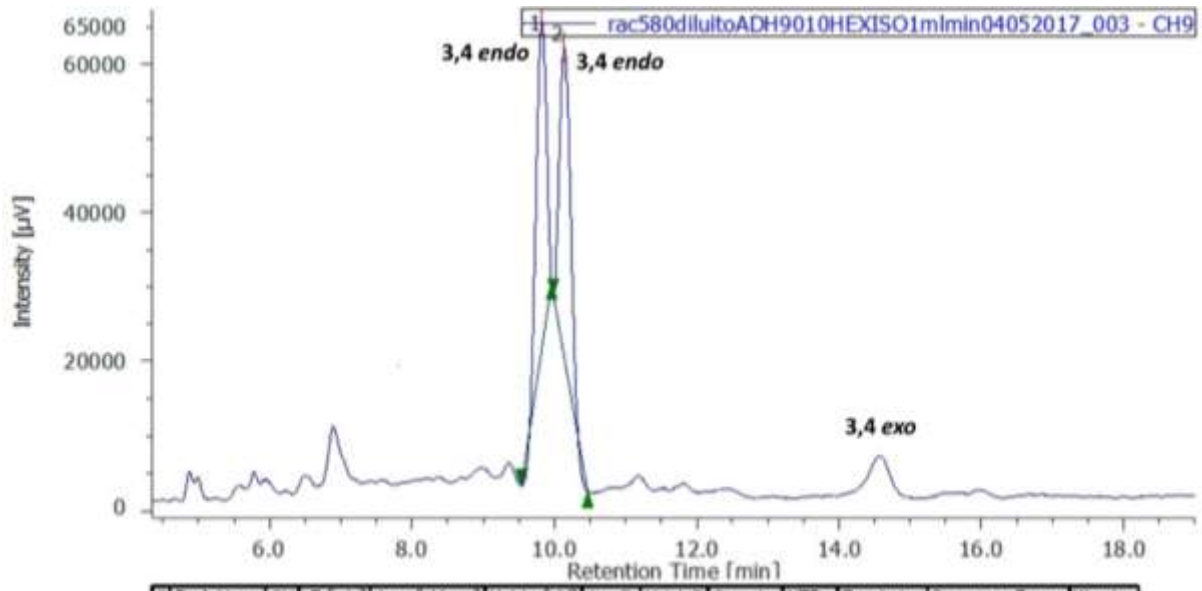


Figure S47. HPLC spectrum of the mixture of racemic + chiral (Figure S44) for the 1,3-dipolar cycloaddition between acrolein **4c** and nitrone **3b**. The analysis was performed with Chiralcel OD-H as column, 95:5 Hexane/Isopropanol as eluent phase, 1.0 mL min^{-1} at λ = 220 nm.



#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	10,230	9409968	699025	60,516	61,366	N/A	12681	1,387	1,035	
2	Unknown	9	10,743	6139585	440086	39,484	38,634	N/A	12878	N/A	1,108	

Figure S48. HPLC spectrum of Table 2, entry 9 (in the manuscript) for the 1,3-dipolar cycloaddition between acrolein **4c** and nitrone **3f** with the capsule. The analysis was performed with Chiralcel AD-H as column, 90:10 Hexane/Isopropanol as eluent phase, 1.0 mL min^{-1} at λ = 210 nm.



#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	9.823	439747	43897	49.408	51.277	N/A	19289	1.074	0.898	
2	Unknown	9	10.137	450293	41702	50.592	48.723	N/A	18041	N/A	1.154	

Figure S49. HPLC spectrum of the racemic mixture of alcohols (3,4-*endo*, 3,4-*exo*) for the 1,3-dipolar cycloaddition between acrolein **4c** and nitrone **3f**. 3,4 *exo* enantiomers are overlapped. The analysis was performed with Chiralcel AD-H as column, 90:10 Hexane/Isopropanol as eluent phase, 1.0 mL min^{-1} at λ = 210 nm.

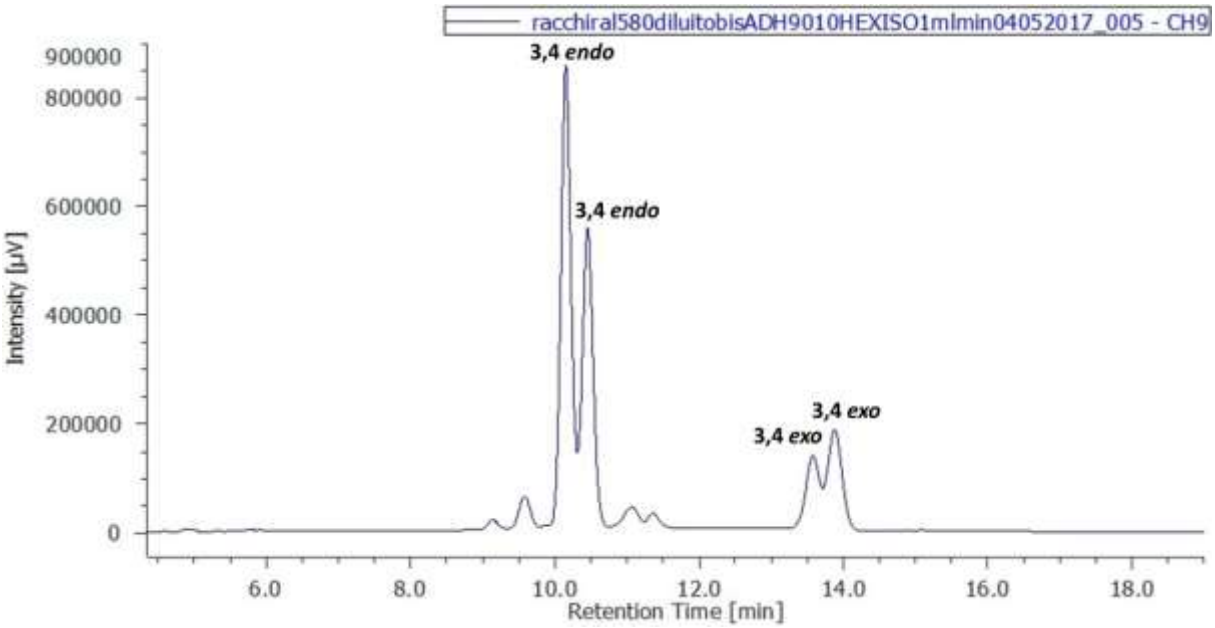
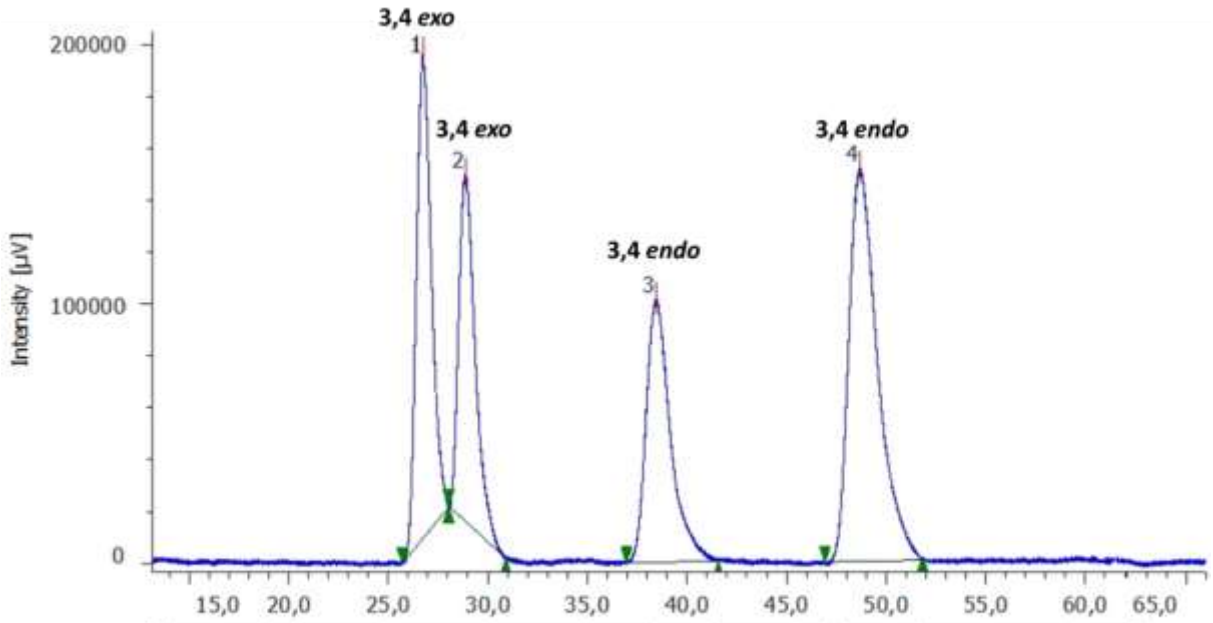


Figure S50. HPLC spectrum of the mixture of racemic + chiral (Figure S47) for the 1,3-dipolar cycloaddition between acrolein **4c** and nitrone **3f**. The analysis was performed with a Chiralcel AD-H column, 90:10 Hexane:Isopropanol as eluent phase, 1.0 mL min^{-1} at λ = 210 nm.



#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	26,751	9909178	187061	24,046	32,595	N/A	5809	1,489	1,257	
2	Unknown	9	28,886	7684243	133807	18,647	23,315	N/A	6165	5,367	1,519	
3	Unknown	9	38,441	8582220	101455	20,826	17,678	N/A	5369	4,412	1,561	
4	Unknown	9	48,654	15032880	151580	36,480	26,412	N/A	5854	N/A	1,578	

Figure S51. HPLC spectrum of a mixture of alcohols for the control experiment performed with hexamethonium iodide **9**, proline **7a**, aldehyde **4a**, nitrone **3a**, and resorcinarene hexameric capsule **2**. The analysis was performed with a Chiralcel OD-H column, 98:2 Hexane:Isopropanol as eluent phase, 0.7 mL min^{-1} at λ = 210 nm.

7. ^{1}H NMR Spectra of reaction mixtures for the determination of diastereo- and regioisomeric ratio, before reduction (Table S1, Table 1 and Table 2 in the manuscript).

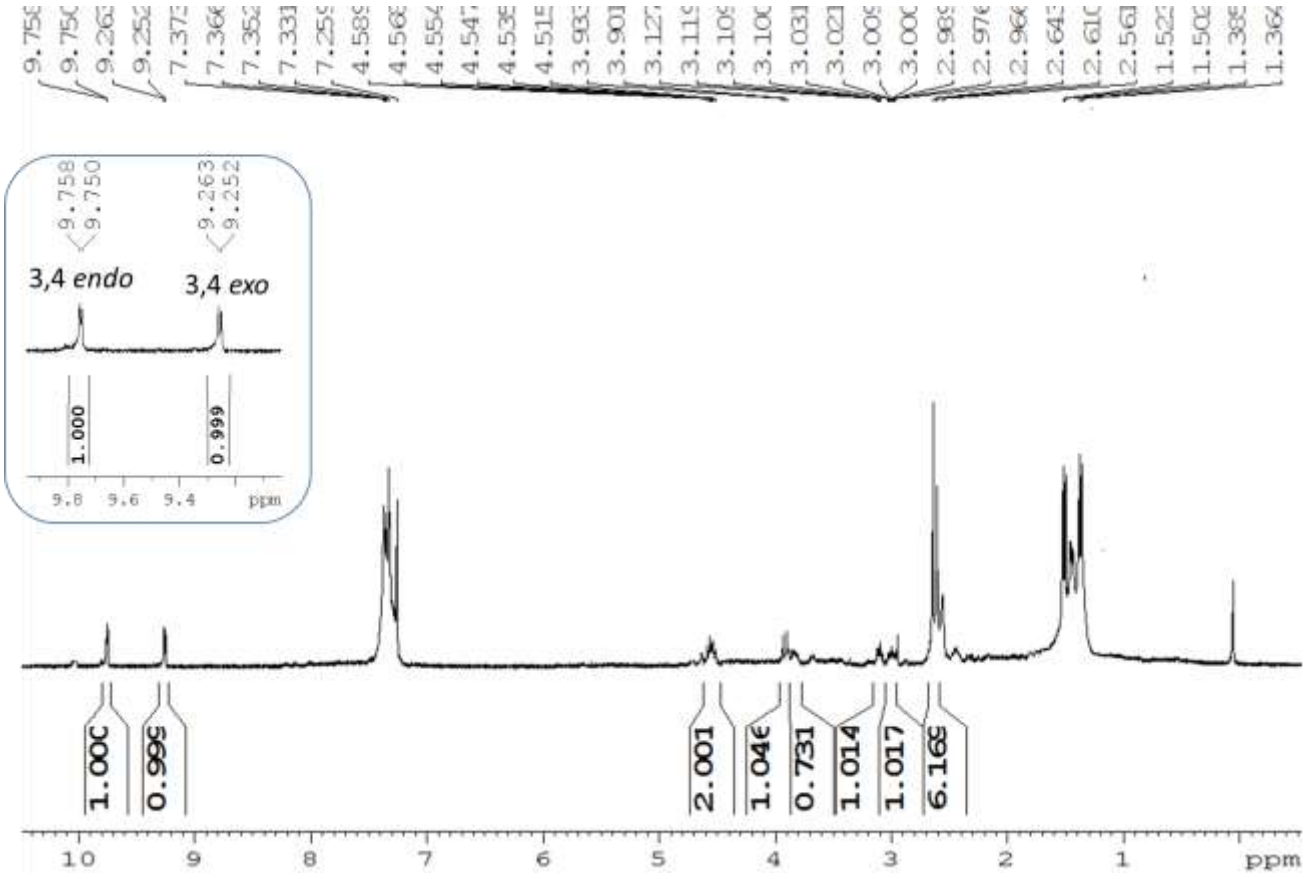


Figure S52. ^{1}H NMR spectrum (300 MHz, $CDCl_3$, 298 K) for entry 1, Table S1.

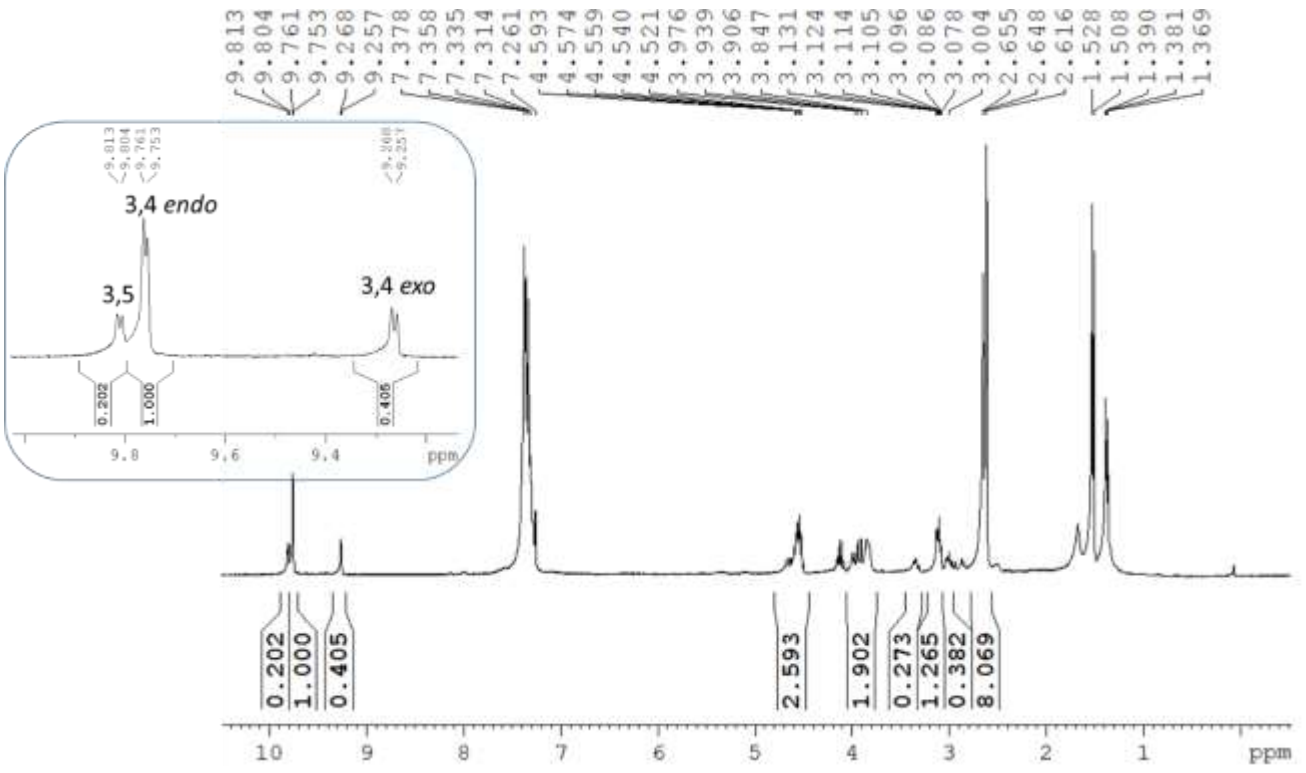


Figure S53. ^{1}H NMR spectrum (300 MHz, $CDCl_3$, 298 K) for entry 2, Table S1.

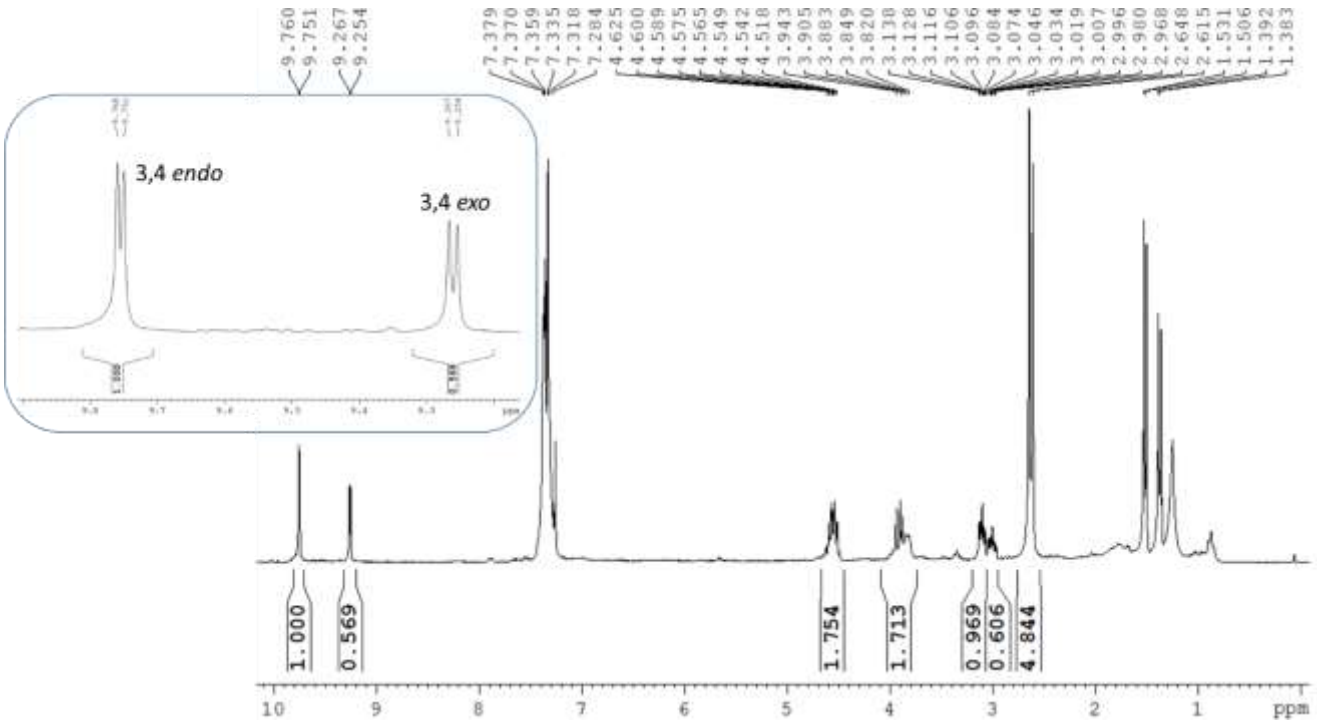


Figure S54. ^{1}H NMR spectrum (250 MHz, $CDCl_3$, 298 K) for entry 3, Table S1.

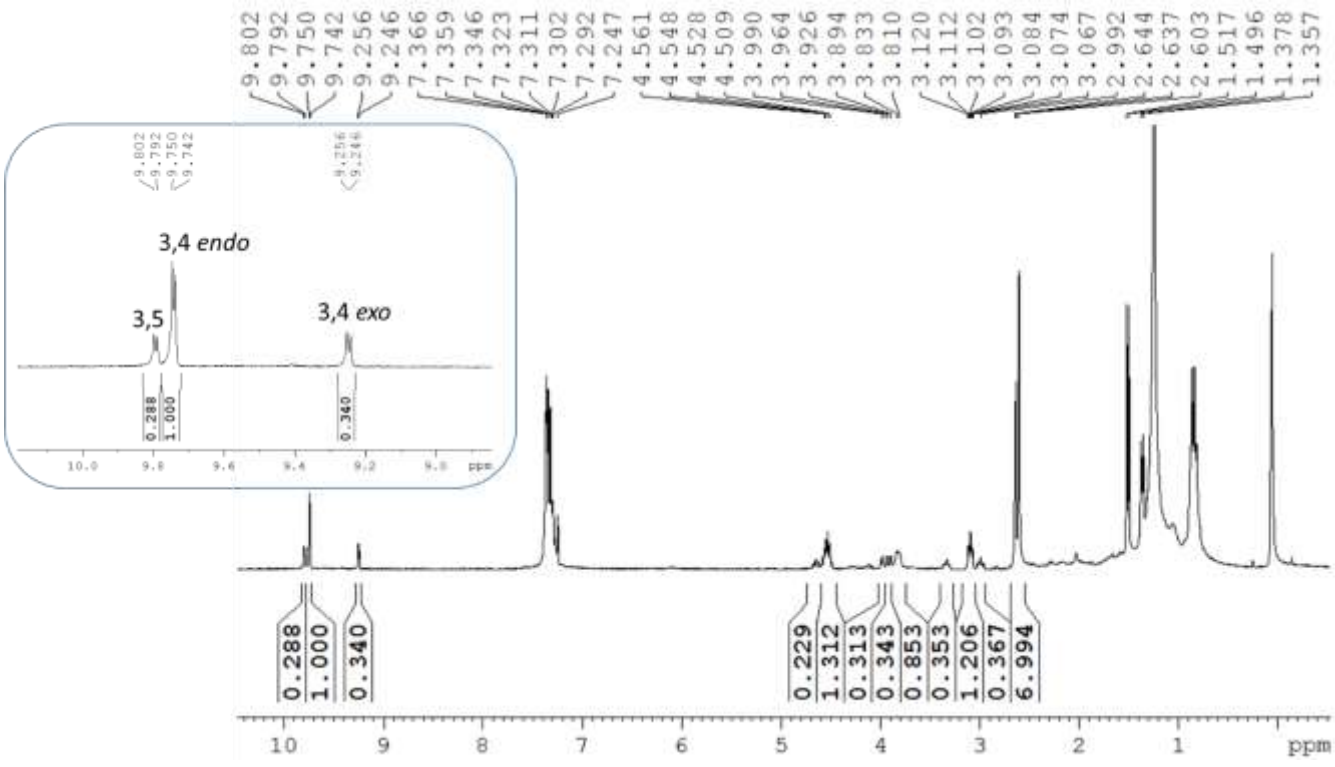


Figure S55. ^{1}H NMR spectrum (250 MHz, $CDCl_3$, 298 K) for entry 4, Table S1.

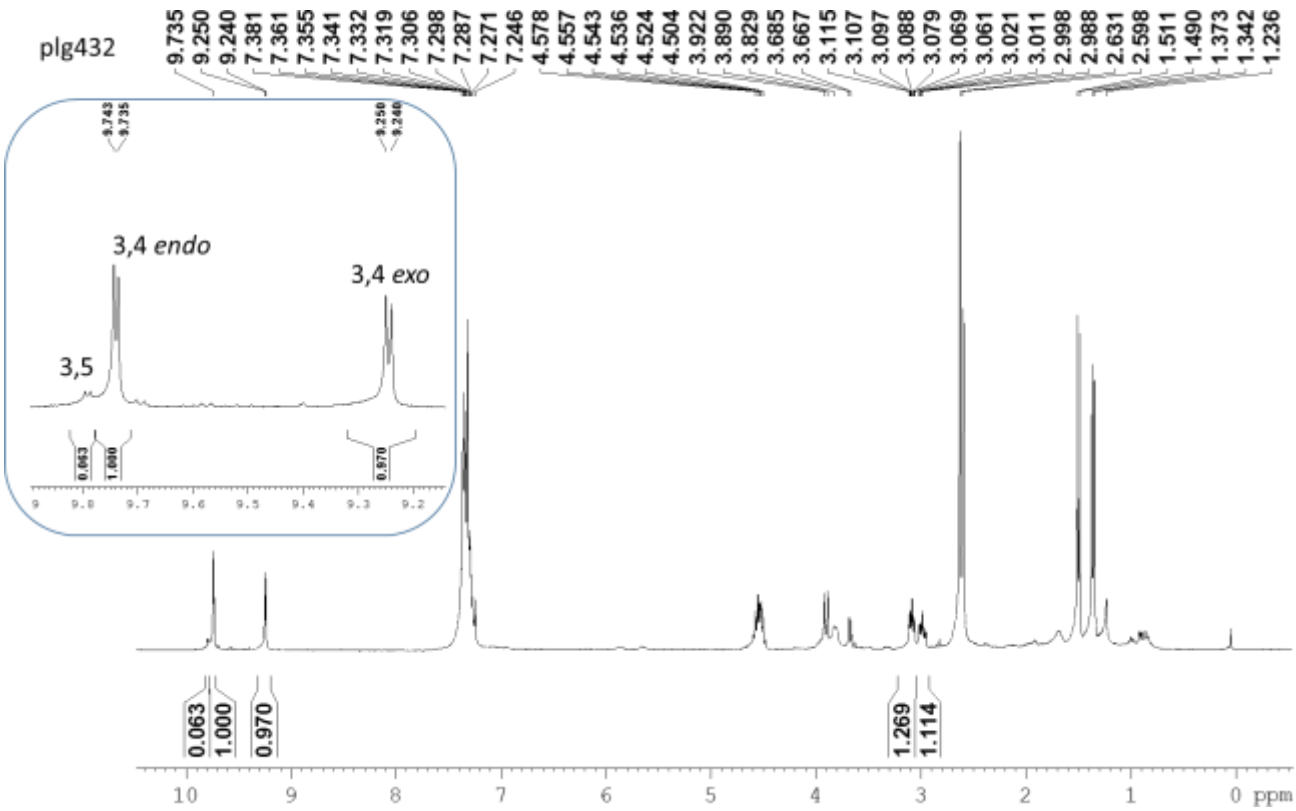


Figure S56. ^{1}H NMR spectrum (300 MHz, $CDCl_3$, 298 K) for entry 5, Table S1.

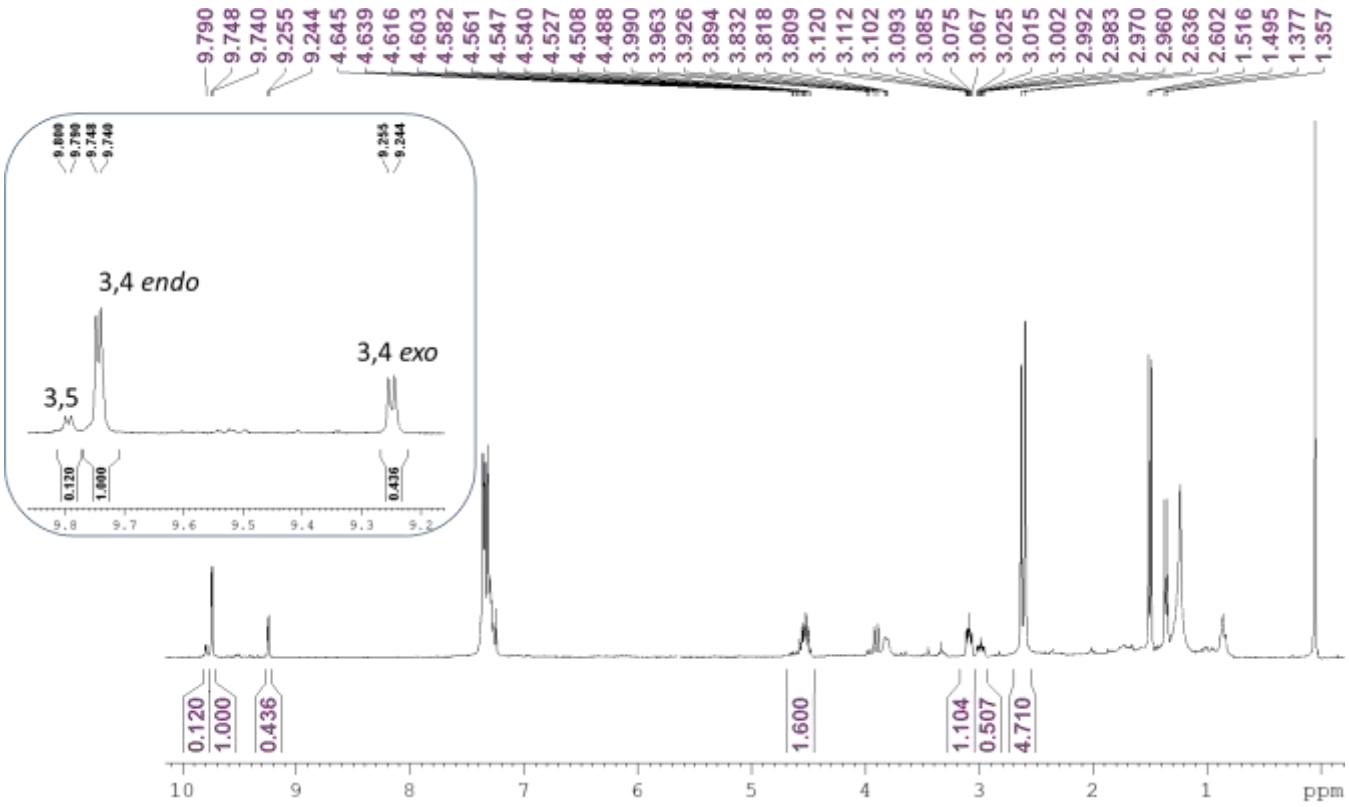


Figure S57. ^{1}H NMR spectrum (300 MHz, $CDCl_3$, 298 K) for entry 6, Table S1.

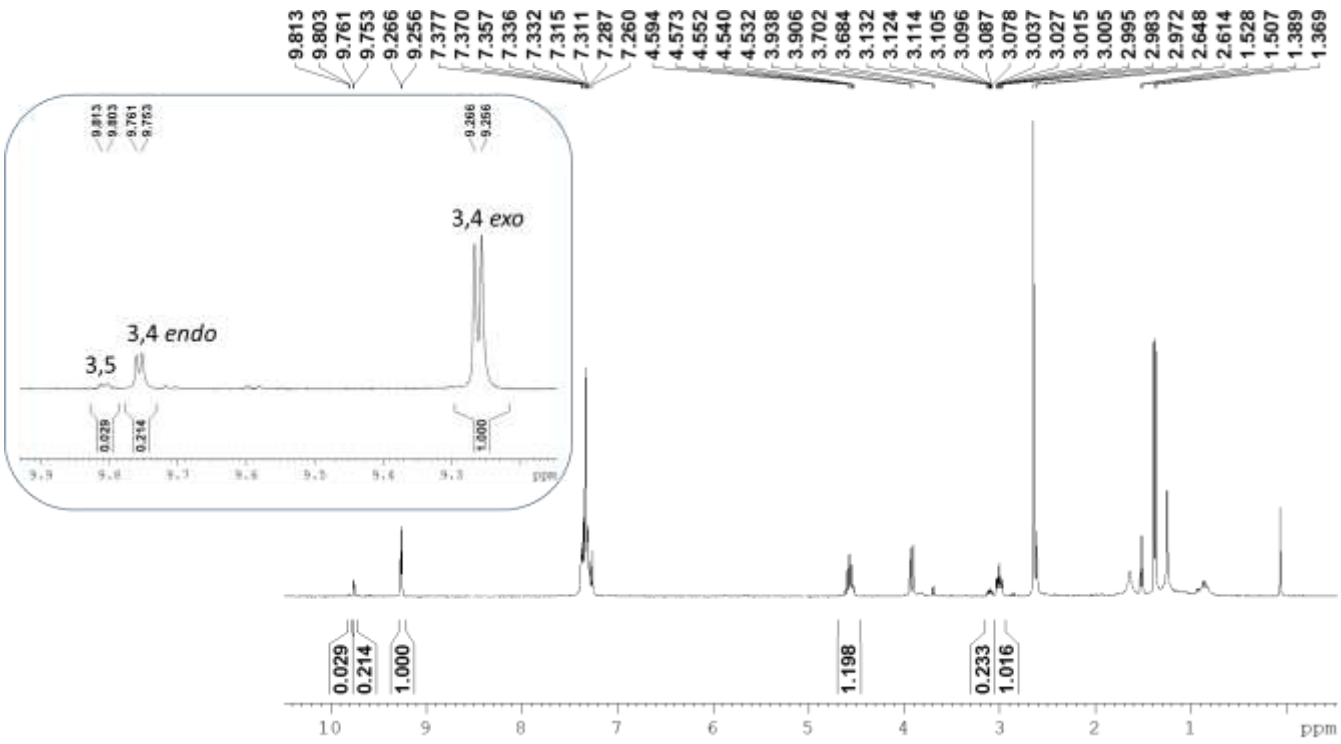


Figure S58. ^{1}H NMR spectrum (300 MHz, $CDCl_3$, 298 K) for entry 7, Table S1.

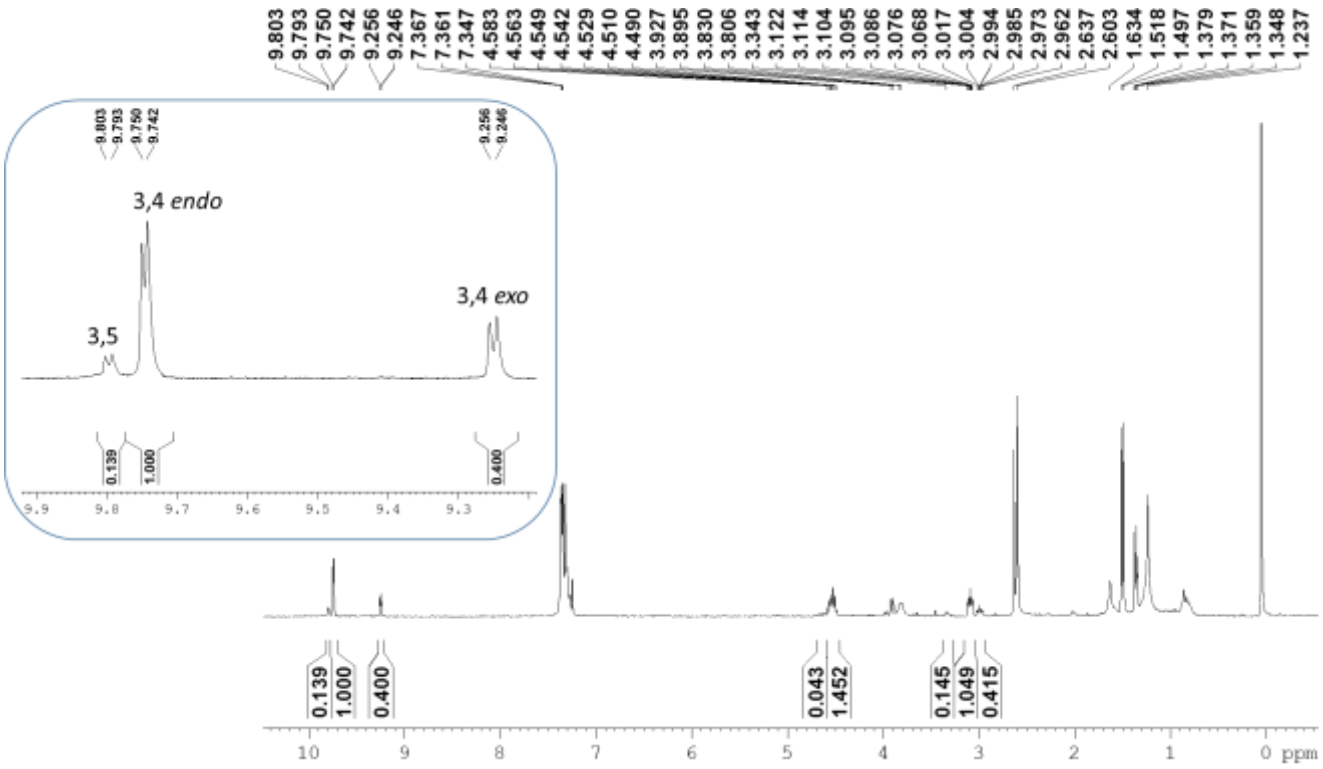


Figure S59. ^{1}H NMR spectrum (300 MHz, $CDCl_3$, 298 K) for entry 8, Table S1.

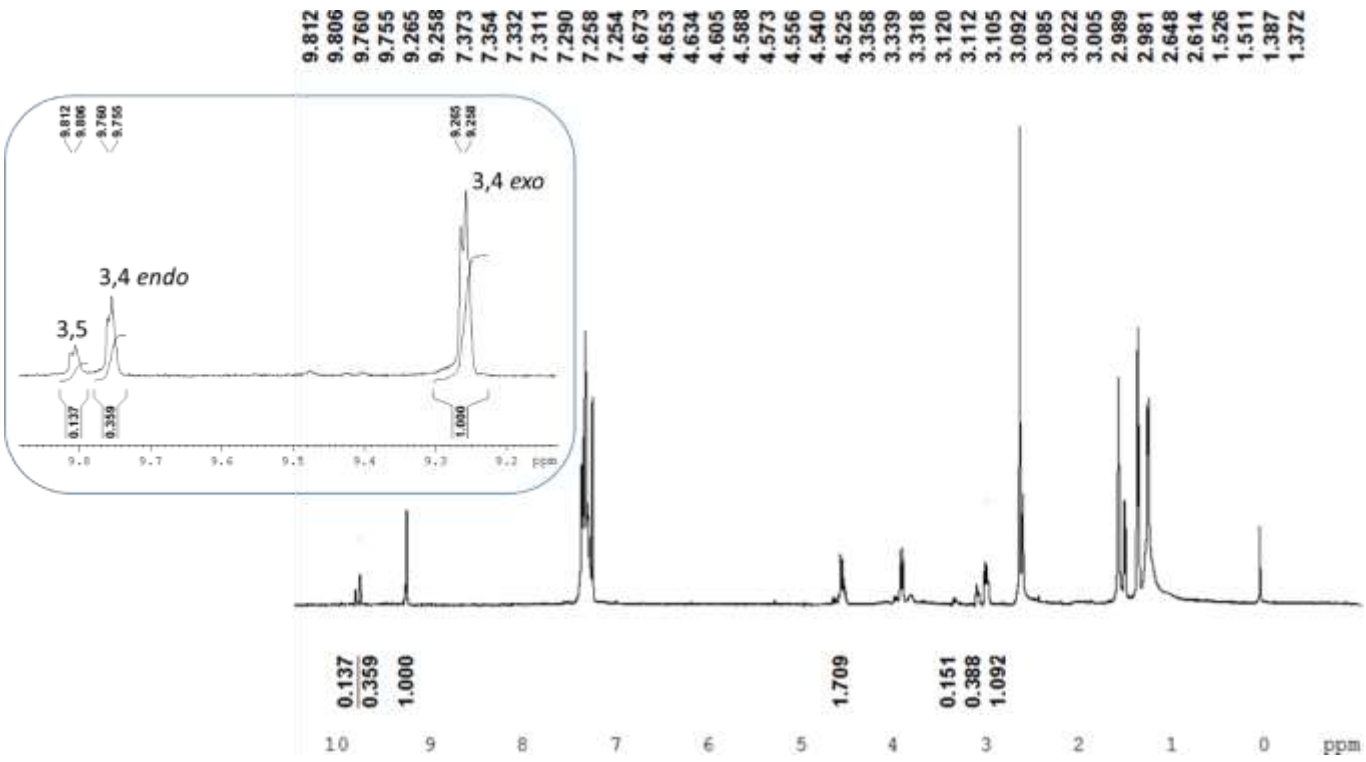


Figure S60. ^{1}H NMR spectrum (250 MHz, $CDCl_3$, 298 K) for entry 9, Table S1.

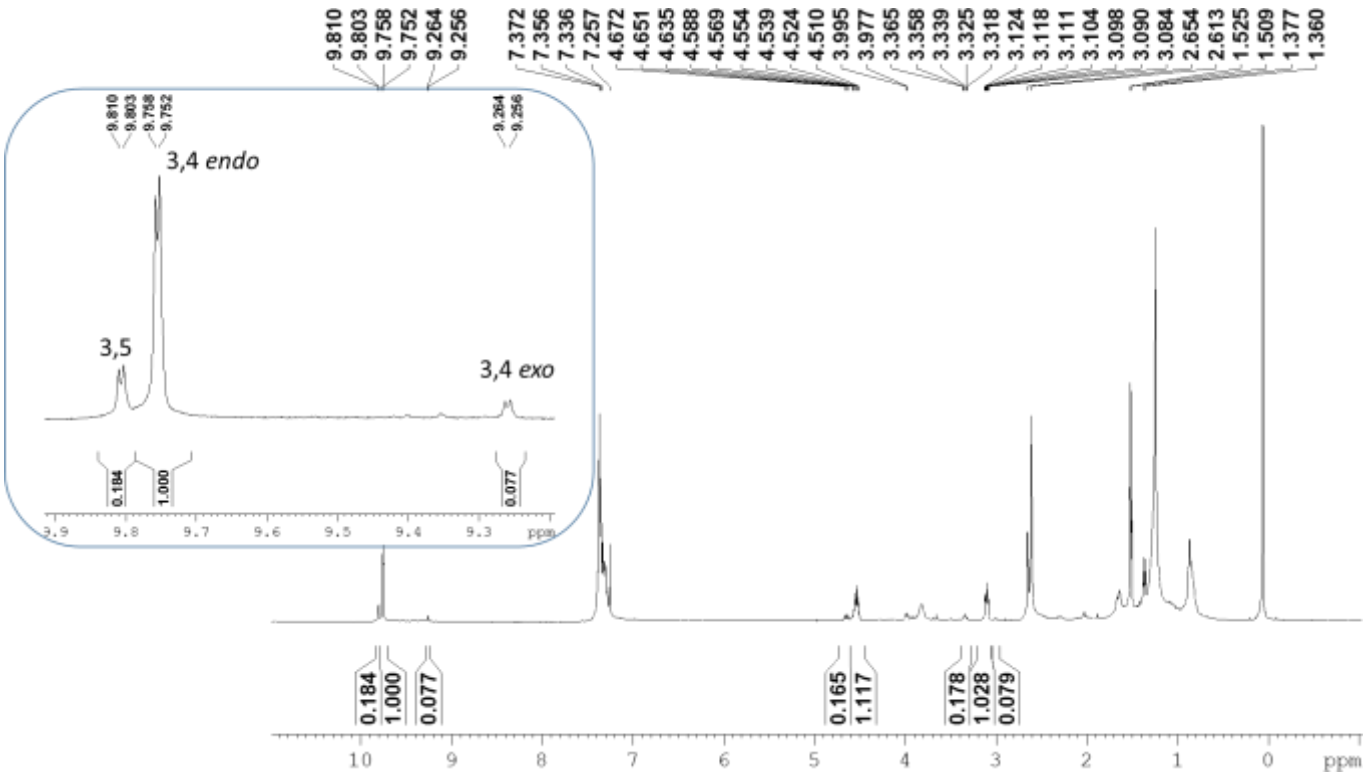


Figure S61. ^{1}H NMR spectrum (250 MHz, $CDCl_3$, 298 K) for entry 10, Table S1.

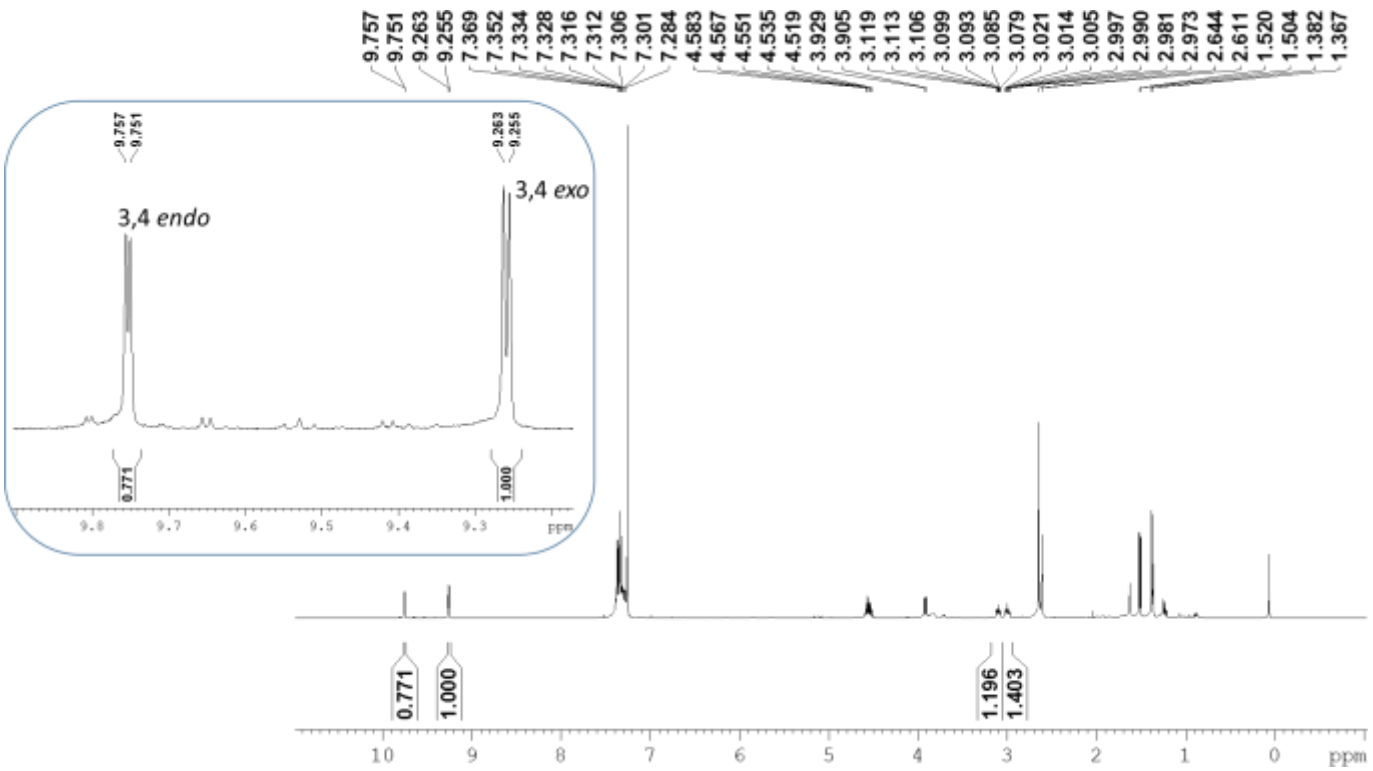


Figure S62. ^{1}H NMR spectrum (300 MHz, $CDCl_3$, 298 K) for entry 2, Table 1 in the manuscript. Reaction was performed without capsule.

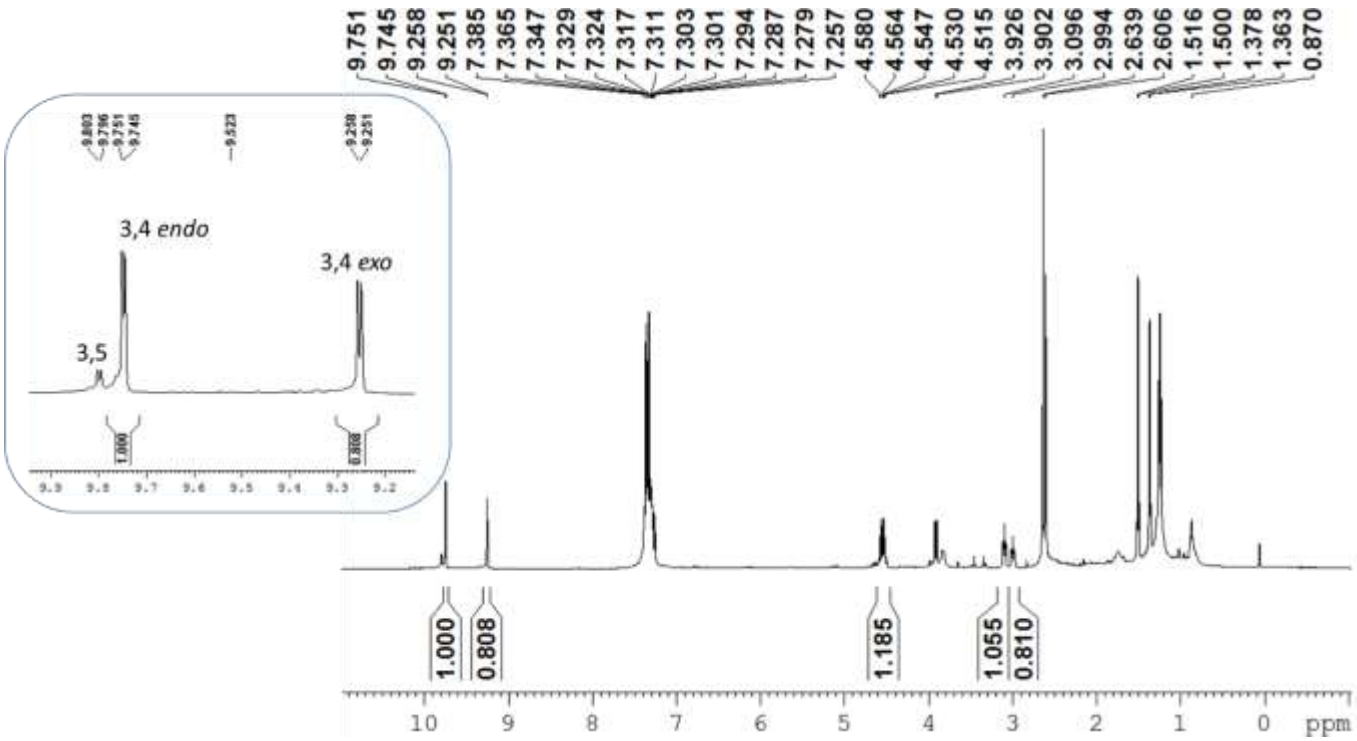


Figure S63. ^{1}H NMR spectrum (300 MHz, $CDCl_3$, 298 K) for entry 2, Table 1 in the manuscript. The reaction was performed with the capsule.

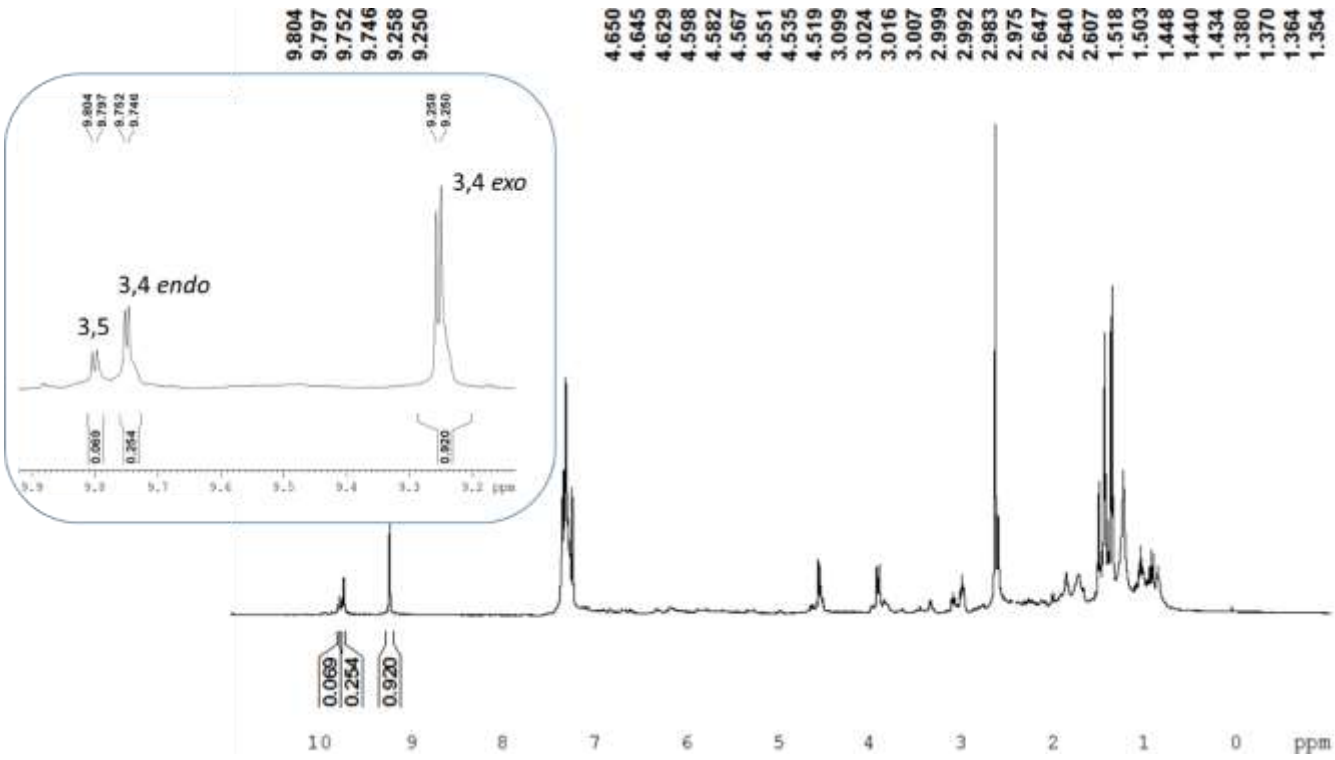


Figure S64. ^{1}H NMR spectrum (250 MHz, $CDCl_3$, 298 K) for entry 3, Table 1 in the manuscript. The reaction was performed with the capsule.

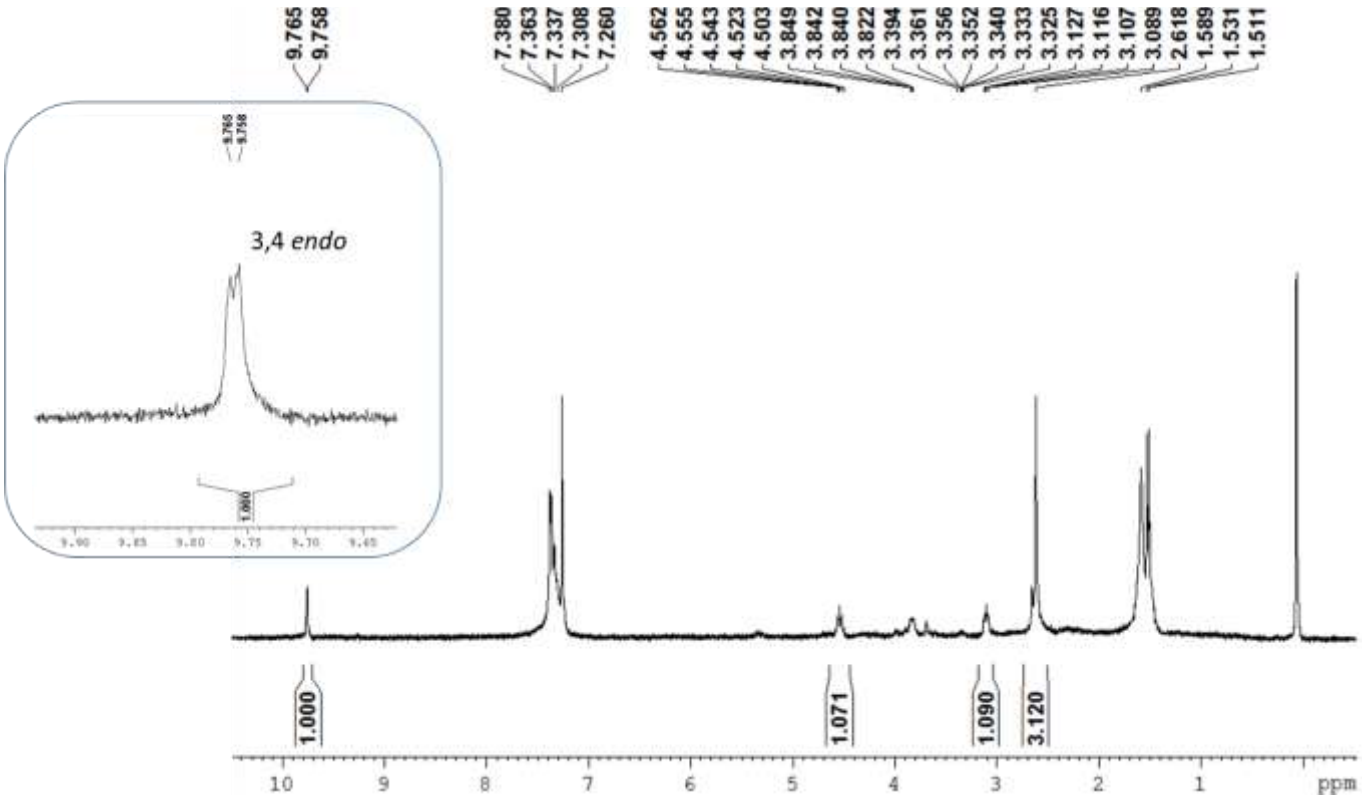


Figure S65. ^{1}H NMR spectrum (250 MHz, $CDCl_3$, 298 K) for entry 4, Table 1 in the manuscript. The reaction was performed with the capsule.

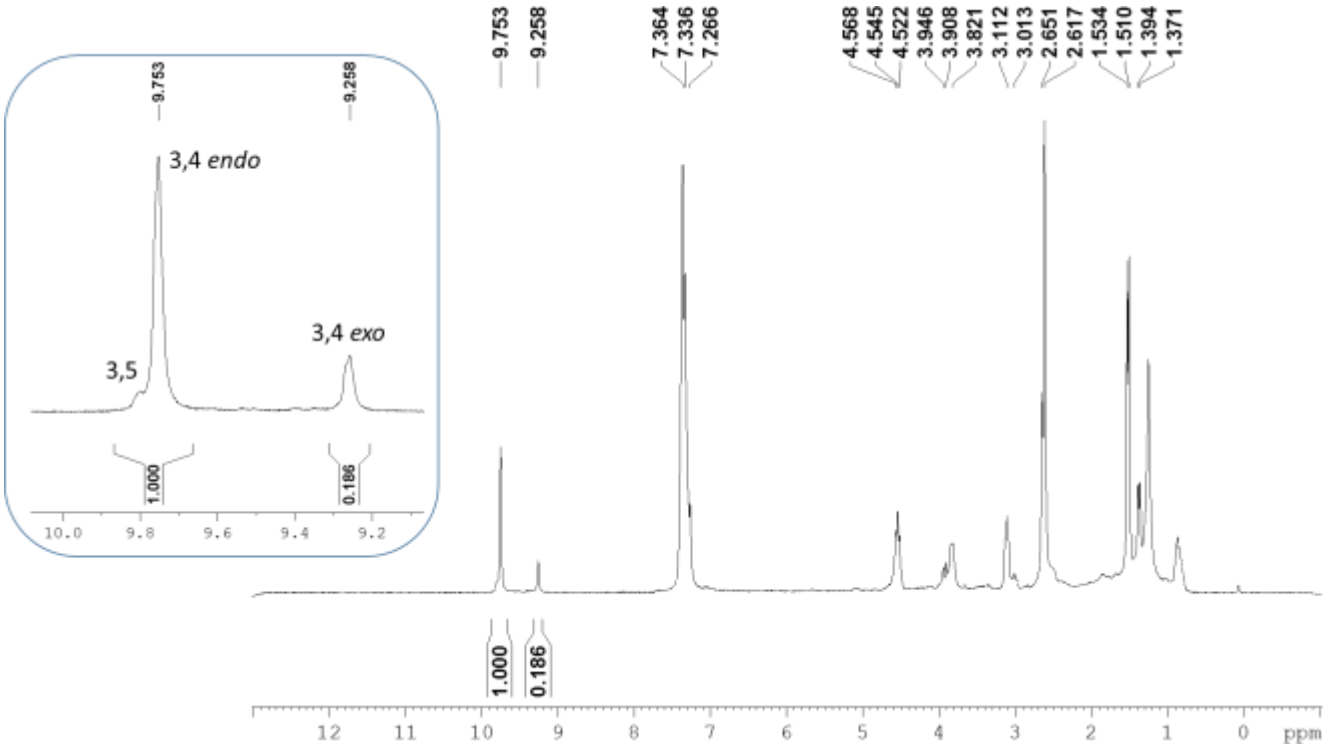


Figure S66. ^{1}H NMR spectrum (250 MHz, $CDCl_3$, 298 K) for entry 5, Table 1 in the manuscript. The reaction was performed with the capsule.

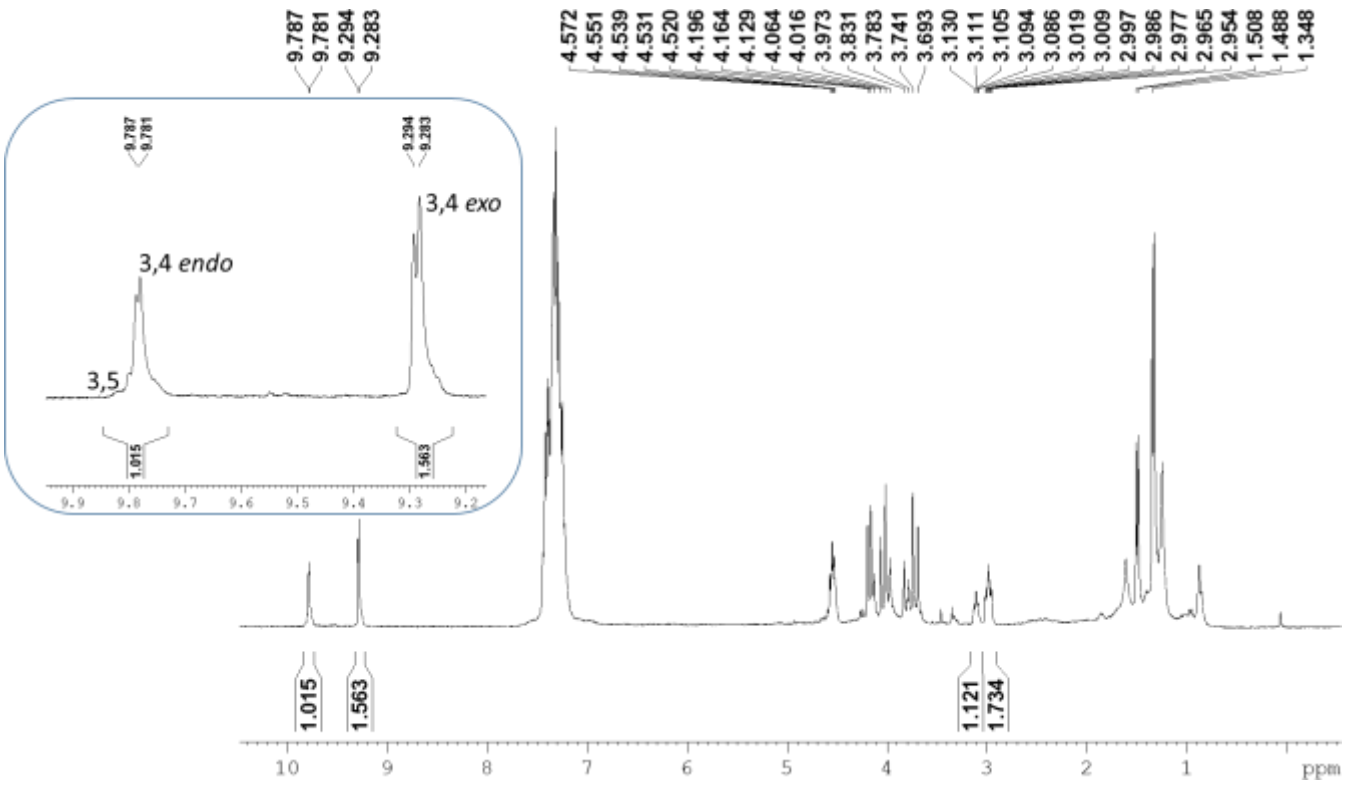


Figure S67. ^{1}H NMR spectrum (300 MHz, $CDCl_3$, 298 K) for entry 2, Table 2 in the manuscript. The reaction was performed with the capsule.

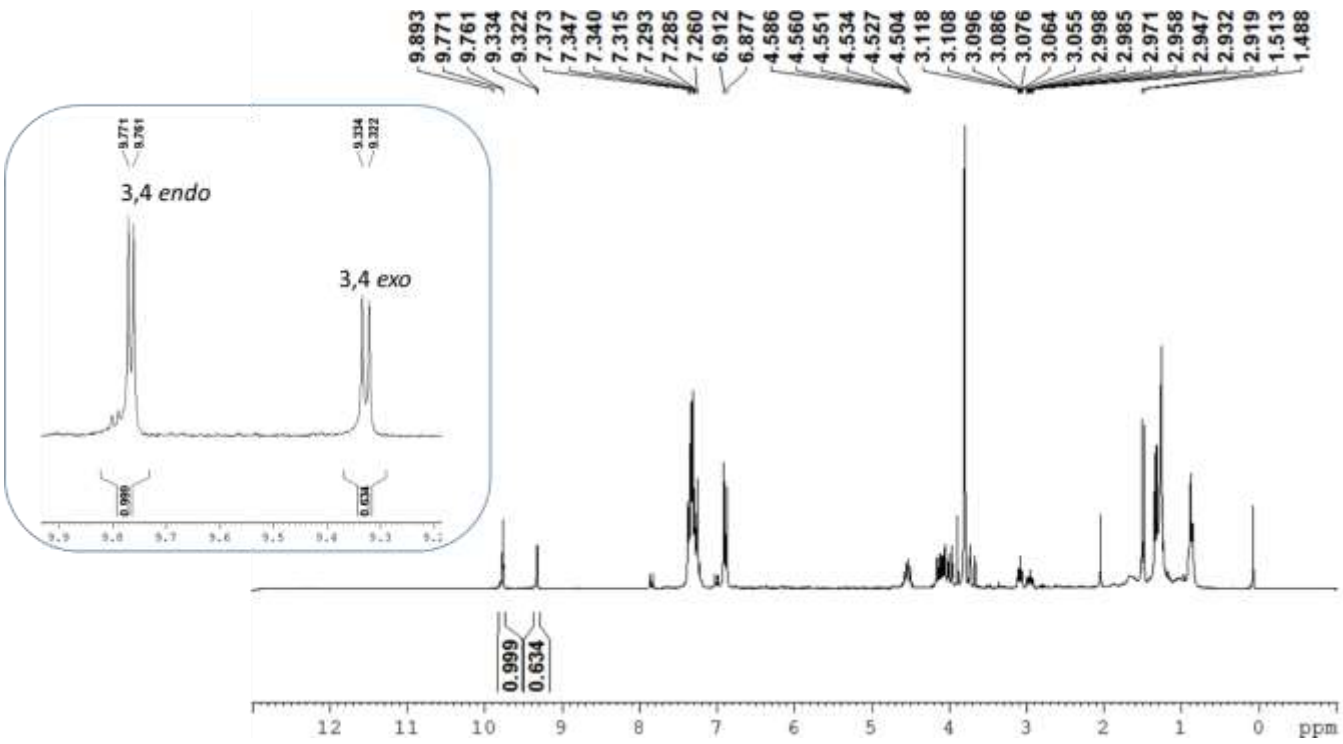


Figure S68. ^{1}H NMR spectrum (300 MHz, $CDCl_3$, 298 K) for entry 3, Table 2 in the manuscript. The reaction was performed with the capsule.

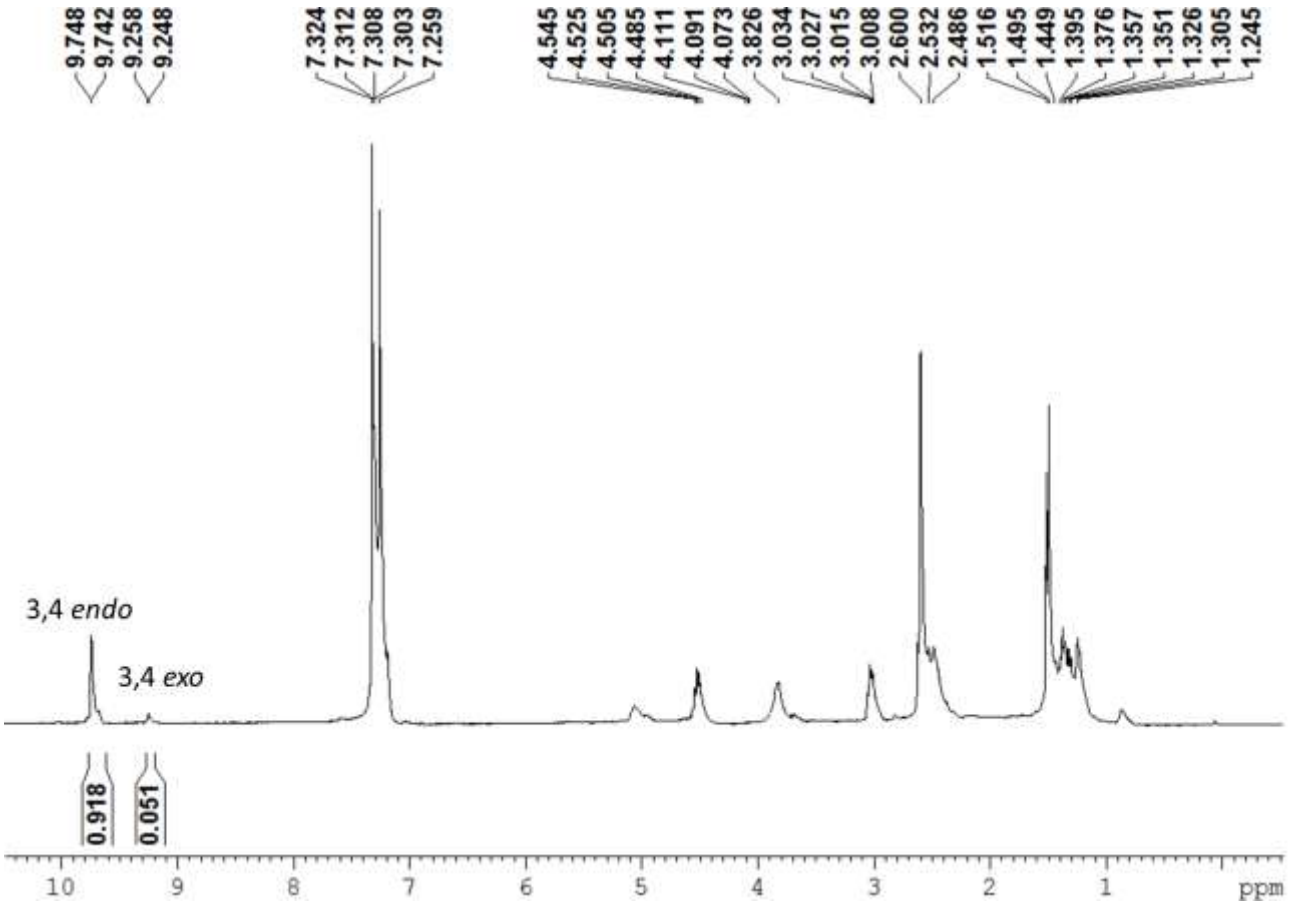


Figure S69. ^{1}H NMR spectrum (250 MHz, $CDCl_3$, 298 K) for entry 4, Table 2 in the manuscript. The reaction was performed with the capsule.

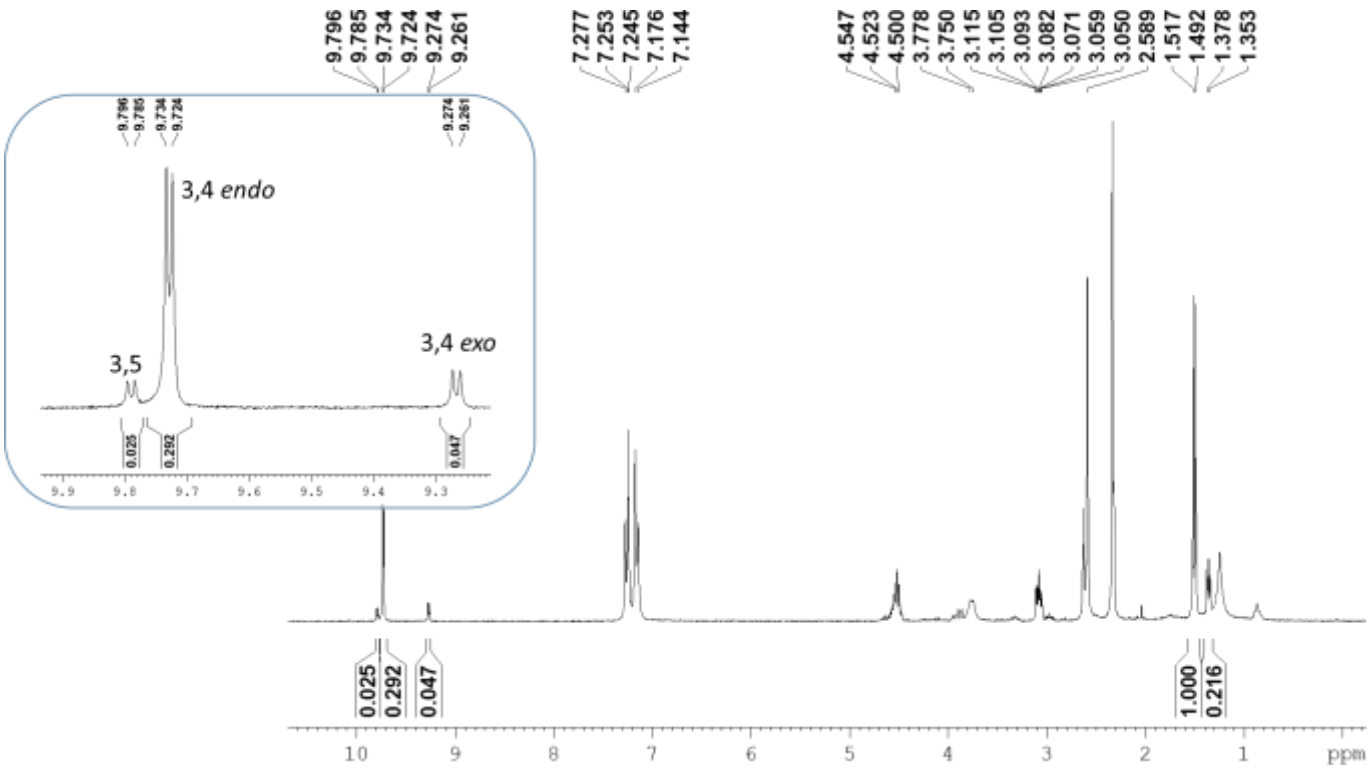


Figure S70. ^{1}H NMR spectrum (300 MHz, $CDCl_3$, 298 K) for entry 5, Table 2 in the manuscript. The reaction was performed with the capsule.

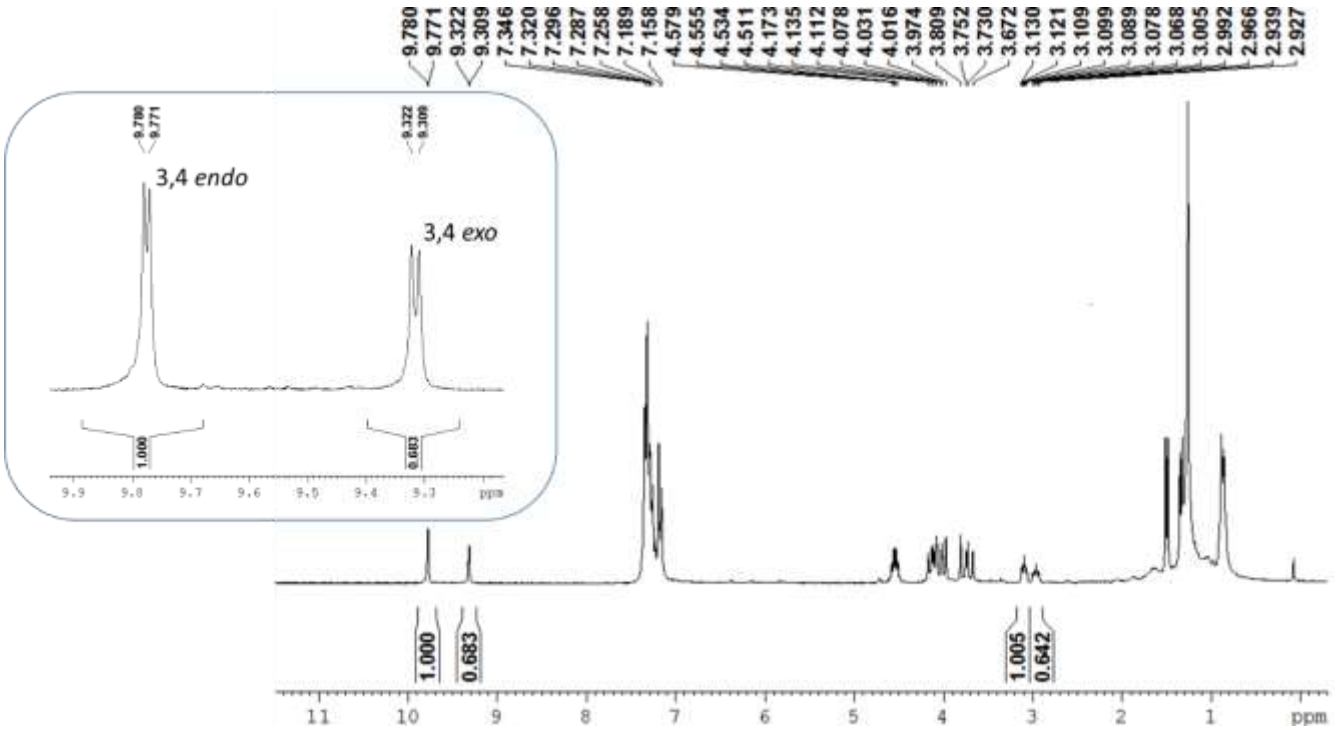


Figure S71. ^{1}H NMR spectrum (300 MHz, $CDCl_3$, 298 K) for entry 6, Table 2 in the manuscript. The reaction was performed with the capsule.

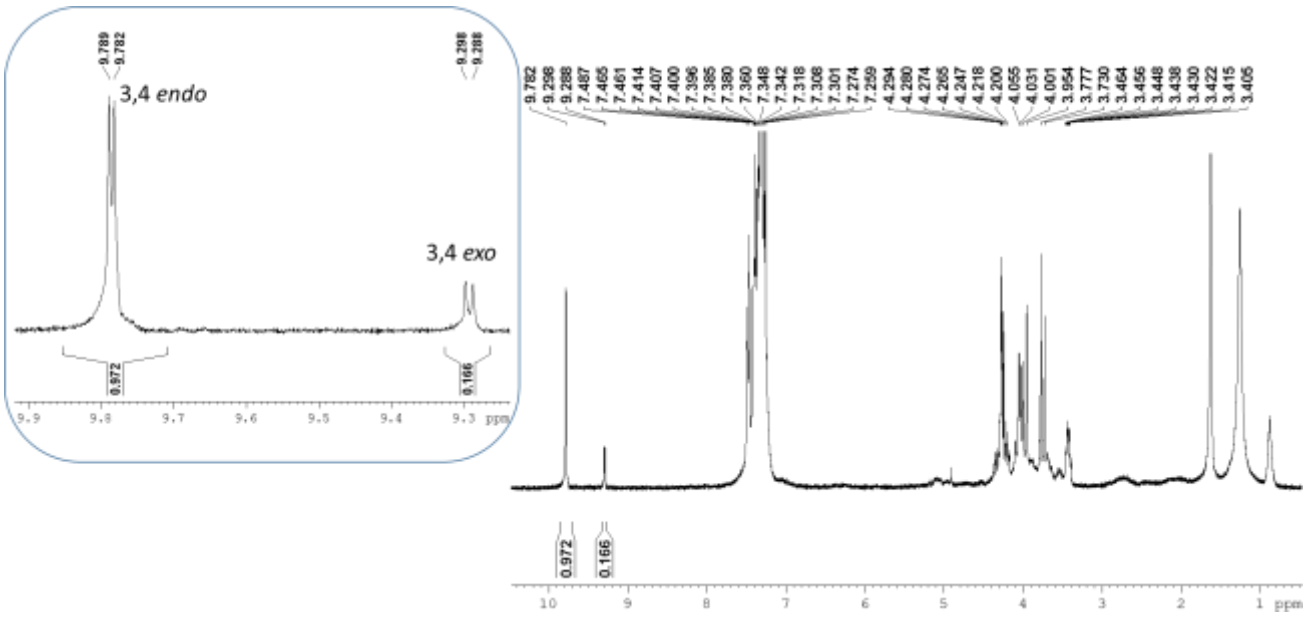


Figure S72. ^{1}H NMR spectrum (300 MHz, $CDCl_3$, 298 K) for entry 8, Table 2 in the manuscript. The reaction was performed with the capsule.

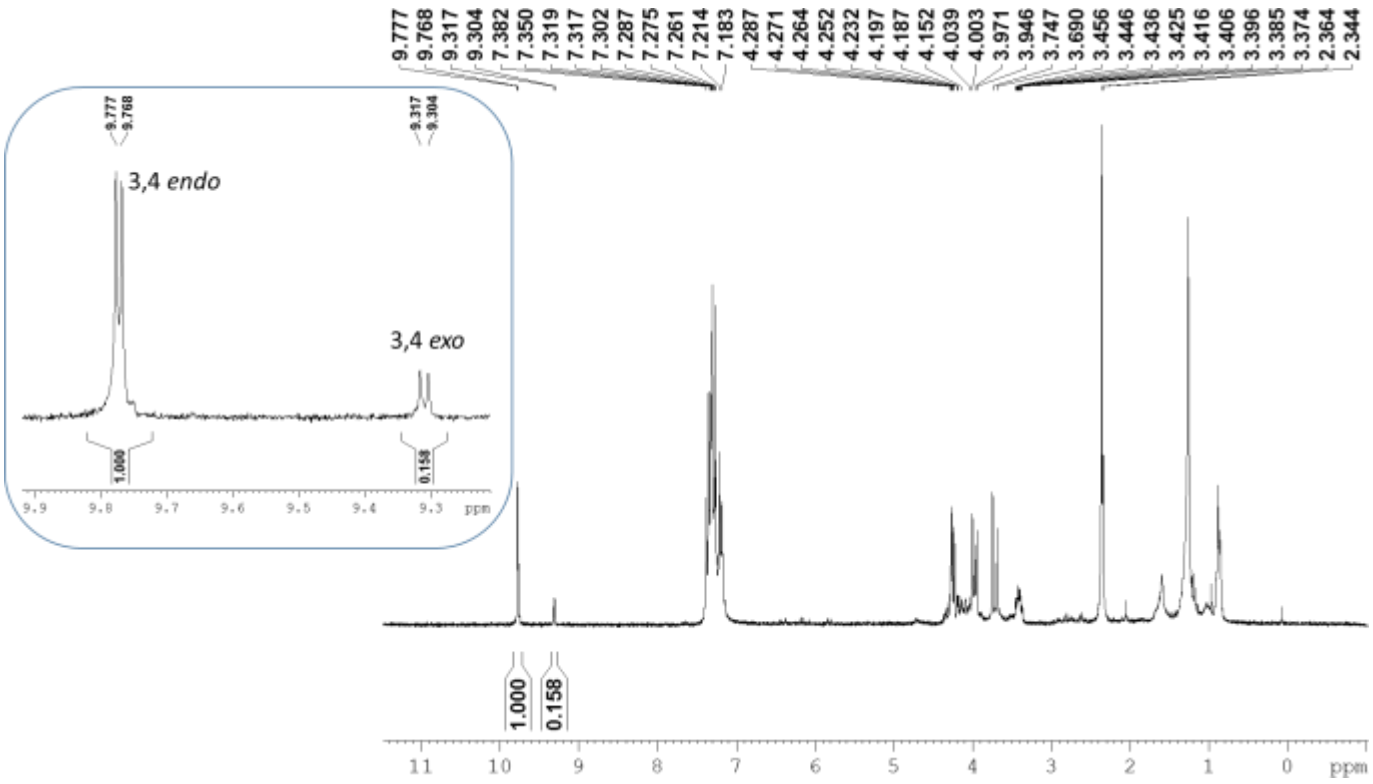


Figure S73. ^{1}H NMR spectrum (250 MHz, $CDCl_3$, 298 K) for entry 9, Table 2 in the manuscript. The reaction was performed with the capsule.

8. Computational studies for 1,3 dipolar cycloaddition

Table S5. Total (ΔH and ΔG) and relative ($\Delta\Delta H$ and $\Delta\Delta G$) enthalpies and energies (in kcal/mol) for all reactants, (4*R*)-*endo*-**5a** and P1a products, and their combinations within the capsule.

Guest/Host-guest complex	ΔH	$\Delta\Delta H$[a]	ΔG	$\Delta\Delta G$[a]
$\mathbf{1_R}$	–223.37	—	–567.21	—
(*Z*)-**3a**	124.69	—	96.08	—
(*E*)-**4**	33.36	—	9.98	—
7e	10.76	—	–15.76	—
s-trans-(*E*,*E*)-**8**	74.23	—	39.49	—
P1a	171.75	—	124.93	—
(4*R*)-*endo*-**5a**	130.79	—	93.57	—
(*Z*)-**3a**@$\mathbf{2_R}$	–112.01	–0.20	–470.98	0.20
(*E*)-**4**@$\mathbf{2_R}$	–200.24	–10.23	–555.95	1.28
7e@$\mathbf{2_R}$	–243.66	–31.04	–598.44	–15.46
s-trans-(*E*,*E*)-**8**@$\mathbf{2_R}$	–179.87	–30.72	–541.31	–13.59
(*Z*)-**3a**&**7e**@$\mathbf{2_R}$	–133.81	–45.88	–503.21	–16.32
(*E*)-**4**&**7e**@$\mathbf{2_R}$	–223.13	–43.88	–587.66	–14.67
(*Z*)-**3a**&*s-trans*-(*E*,*E*)-**8**@$\mathbf{2_R}$	–64.33	–39.87	–441.83	–10.20
(*Z*)-**3a**&(*E*)-**4**&**7e**@$\mathbf{2_R}$	–110.48	–22.56	–490.84	–3.95
(4*R*)-*endo*-**5a**&**7e**@$\mathbf{2_R}$	–128.25	–35.67	–507.45	–33.80

[a] Referred to those of the host and the corresponding non-encapsulated guests.

To prove the catalytic effect of the iminium species upon the 1,3-DC reactivity and the enhanced enantioselectivity (due to the intermediate's diastereoselectivity) observed into the capsule we performed an *in silico* study of the 1,3-DC, in the absence of the capsule, between the nitrone (*Z*)-**3a** and the free aldehyde (*E*)-**4** or the iminium *s-trans*-(*E*,*E*)-**8**, respectively (Table S6).

From this study emerged that the iminium ion significantly reduces the reaction-limiting free activation energy (from 29.03 kcal/mol to 10.72–11.22 kcal/mol, see TS2a, TS2c, and TSa-CHO), causing the reaction to easily proceed even at room temperature. Moreover, the two diastereomeric TSs are relatively close to energy, thus justifying the low stereoselectivity observed in the absence of the capsule. Finally, the reaction with the iminium ion conducted without the capsule results lower in energy (about 5 kcal/mol), and so much faster, respect to the same conducted into the capsule; this observation leads to the logical conclusion that, if the iminium ion was formed outside the capsule, the 1,3-DC would proceed faster, leading to a low enantioselectivity. Therefore, the fact that without the capsule the reaction does not occur is an indirect proof that the iminium ion is formed inside, either because the L-proline is quickly seized from the capsule either because the latter, being acidic, catalyses its formation.

Table S6. Total (ΔH and ΔG) and relative ($\Delta\Delta H$ and $\Delta\Delta G$) enthalpies and free energies, and activation free energies (in kcal/mol) of the stationary points involved in the 1,3-DC in the absence of the capsule.

Stationary point	ΔH	$\Delta\Delta H$	ΔG	$\Delta\Delta G$	$\Delta G^{\#}$
MC1a	184.18	–14.74[a]	134.21	–1.37[a]	—
TS1a	188.35	–10.56[a]	141.80	6.23[a]	7.59
IN1a	186.77	–12.15[a]	139.28	3.70[a]	—
TS2a	195.98	–2.93[a]	150.00	14.42[a]	10.72
P1a	171.75	–27.17[a]	124.93	–10.65[a]	—
MC1c	186.39	–12.53	134.43	–1.15	—
TS1c	189.68	–9.24	141.93	6.35	7.50
IN1c	188.86	–10.06	141.48	5.90	—
TS2c	198.92	0.00	152.70	17.12	11.22
P1c	174.33	–24.59	125.61	–9.97	—
TSa-CHO	172.41	14.37[b]	135.09	29.03[b]	29.03

[a] Relative to the (*Z*)-)-**3a**+*s-trans*-(*E*,*E*)-**8**. [b] Relative to the (*Z*)-**3a**+(*E*)-**4**.

Table S7. Total (ΔH and ΔG) and relative[a] ($\Delta\Delta H$ and $\Delta\Delta G$) enthalpies and free energies, and activation free energies (in kcal/mol) of the stationary points involved in the 1,3-DC within the capsule (i.e. @$\mathbf{2_R}$).

Stationary point	ΔH	$\Delta\Delta H$	ΔG	$\Delta\Delta G$	$\Delta G^{\#}$
MC1a	–64.09	0.24	-443.48	–1.65	—
TS1a	–61.91	2.42	-437.16	4.67	6.32
IN1a	–68.28	–3.95	-443.33	–1.50	—
TS2a	–52.64	11.69	-427.45	14.38	15.88
P1a	–75.59	–11.26	–450.83	–9.00	—
MC1b	–63.98	0.35	–443.25	–1.42	—
TS1b	–61.57	2.76	–436.78	5.05	6.47
IN1b	–64.48	–0.15	–439.20	2.63	—
TS2b	–48.67	15.66	–421.11	20.72	18.09
P1b	–75.20	–10.87	–450.25	–8.42	—
MC1c	–64.64	–0.31	–442.85	–1.02	—
TS1c	–61.32	3.01	–435.94	5.89	6.91
IN1c	–67.17	–2.84	–442.32	–0.49	—
TS2c	–51.87	12.46	–425.00	16.83	17.32
P1c	–73.85	–9.52	–449.65	–7.82	—
MC1d	–64.47	–0.14	–443.07	–1.24	—
TS1d	–62.50	1.83	–437.62	4.21	5.45
IN1d	–65.17	–0.84	–439.68	2.15	—
TS2d	–48.24	16.09	–422.27	19.56	17.41
P1d	–74.88	–10.55	–450.67	–8.84	—
MC2a	–64.15	0.18	–443.30	–1.47	—
TS3a	–34.85	29.48	–409.25	32.58	34.02
P2a	–77.57	–13.24	–450.46	–8.63	—
MC2b	–65.16	–0.83	–443.18	–1.35	—
TS3b	–36.19	28.14	–409.59	32.24	33.88
P2b	–75.32	–10.99	–449.84	–8.01	—
MC2c	–65.43	–1.10	–443.36	–1.53	—
TS3c	–35.94	28.39	–409.79	32.04	33.57
P2c	–75.59	–11.26	–450.67	–8.84	—
MC2d	–65.37	–1.04	–443.30	–1.47	—
TS3d	–35.37	28.96	–408.94	32.89	34.51
P2d	–76.92	–12.59	–450.57	–8.74	—

[a] Relative to the (*Z*)-**3a**&*s-trans*-(*E*,*E*)-**8**@$\mathbf{2_R}$ complex.

Table S8. Partitioned Mulliken atomic charges (e) at selected stationary points related to the *meta*-channel.

Stationary point	Nitrone fragment	Iminium fragment	Capsule
MC1a	–0.002	0.102	–0.100
TS1a	0.144	–0.011	–0.133
IN1a	0.571	–0.101	–0.470
TS2a	0.370	–0.250	–0.120
P1a	–0.086	0.166	–0.079

9. Cartesian coordinates, energies, and frequencies for selected fully optimized compounds and transition states

(*Z*)-**3a**&*s-trans*-(*E*,*E*)-**8**@$\mathbf{2_R}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.456208	-0.992184	7.416341
2	6	0	-3.817683	-2.213662	7.179657
3	6	0	-2.585373	-2.421275	7.808063
4	6	0	-1.993639	-1.464220	8.658498
5	6	0	-2.652858	-0.237839	8.816123
6	6	0	-3.885668	0.025798	8.212671
7	6	0	-0.691079	-1.775321	9.363022
8	6	0	-0.762955	-1.458981	10.860528
9	6	0	2.662272	3.764539	6.886425
10	6	0	2.134137	4.698686	5.990020
11	6	0	0.819567	5.120123	6.209342
12	6	0	0.040301	4.650075	7.287648
13	6	0	0.602389	3.674844	8.120763
14	6	0	1.912161	3.214993	7.948471
15	6	0	-1.354051	5.195517	7.508146
16	6	0	-1.570722	5.633329	8.960537
17	6	0	1.140879	-1.746365	7.619735
18	6	0	2.250799	-1.196388	6.972462
19	6	0	2.671568	0.073369	7.384855
20	6	0	2.026510	0.786233	8.420897
21	6	0	0.919410	0.184775	9.030045
22	6	0	0.466523	-1.089901	8.670131
23	6	0	2.531968	2.153304	8.832500
24	6	0	2.326826	2.453006	10.320482
25	6	0	-2.815985	4.226561	5.682268
26	6	0	-3.809625	3.377874	5.187561
27	6	0	-4.371010	2.457492	6.081165
28	6	0	-3.968403	2.371977	7.434067
29	6	0	-2.968119	3.247180	7.869491
30	6	0	-2.390864	4.204471	7.026556
31	6	0	-4.604041	1.351538	8.355160
32	6	0	-4.680093	1.811225	9.814124
33	1	0	-5.205666	1.066471	10.425551
34	8	0	-5.691623	-0.711696	6.887957
35	8	0	-1.889126	-3.596307	7.629148
36	1	0	-4.259054	-2.960772	6.527250
37	1	0	-2.186744	0.536548	9.428886
38	1	0	-0.517550	-2.891832	9.282190
39	1	0	-0.959462	-0.400796	11.059875
40	1	0	0.176294	-1.720744	11.362457
41	1	0	-1.567382	-2.032290	11.338735
42	8	0	3.960095	3.325414	6.776594
43	8	0	0.221696	6.035114	5.372412
44	1	0	2.721407	5.067857	5.153348
45	1	0	-0.002235	3.259818	8.929845
46	1	0	-1.461286	6.129048	6.876828
47	1	0	-1.459048	4.808835	9.671731
48	1	0	-2.574147	6.054197	9.097564
49	1	0	-0.844087	6.405310	9.244045
50	8	0	0.769724	-2.989264	7.160826
51	8	0	3.758864	0.555209	6.701954
52	1	0	2.749097	-1.717282	6.154375
53	1	0	0.395023	0.724377	9.822445
54	1	0	3.650410	2.166508	8.657986
55	1	0	2.807408	1.689607	10.944307
56	1	0	1.270058	2.493826	10.602435
57	1	0	2.769469	3.422595	10.582744

58	8	0	-2.294742	5.100588	4.752139
59	8	0	-5.344259	1.663864	5.532986
60	1	0	-4.107214	3.404898	4.142849
61	1	0	-2.631415	3.189867	8.907385
62	1	0	-5.673175	1.206610	8.012873
63	1	0	-5.229318	2.756817	9.898936
64	1	0	-3.693225	1.960008	10.263330
65	6	0	3.399047	-0.995406	3.738712
66	6	0	3.391424	-1.735876	2.456062
67	6	0	2.720595	-1.307534	1.368828
68	6	0	2.809805	-2.011877	0.106550
69	6	0	3.845684	-2.559164	-2.626769
70	6	0	1.606703	-1.517677	-3.338360
71	6	0	2.340731	-2.364985	-2.286995
72	7	0	2.174804	-1.644322	-0.987546
73	6	0	1.321283	-0.427122	-1.136408
74	6	0	1.149894	-0.221885	-2.647179
75	1	0	4.278389	-0.327908	3.788798
76	1	0	3.449702	-1.672088	4.611771
77	1	0	2.520750	-0.344846	3.877170
78	1	0	3.986238	-2.658792	2.443200
79	1	0	2.153979	-0.366376	1.396905
80	1	0	3.473969	-2.908311	0.057807
81	1	0	0.748546	-2.078205	-3.756902
82	1	0	2.268131	-1.302076	-4.204846
83	1	0	1.885074	-3.390490	-2.220842
84	1	0	0.350012	-0.588580	-0.621313
85	1	0	1.818498	0.455098	-0.645631
86	1	0	1.755935	0.637410	-2.996230
87	1	0	0.102435	0.019693	-2.903202
88	8	0	4.124633	-2.941335	-3.784856
89	8	0	4.696073	-2.380267	-1.726503
90	6	0	4.488753	-0.150165	-7.047024
91	6	0	5.101552	-1.136026	-6.273468
92	6	0	4.648061	-2.453044	-6.433459
93	6	0	3.580112	-2.775245	-7.309615
94	6	0	3.002755	-1.746053	-8.054753
95	6	0	3.450739	-0.421094	-7.960057
96	6	0	3.107428	-4.208504	-7.401890
97	6	0	3.285170	-4.753804	-8.825290
98	6	0	-3.776695	-3.118128	-7.249632
99	6	0	-4.407994	-1.898996	-6.981882
100	6	0	-3.861138	-0.756058	-7.572859
101	6	0	-2.737746	-0.801423	-8.422734
102	6	0	-2.117475	-2.042895	-8.617093
103	6	0	-2.613336	-3.217762	-8.044435
104	6	0	-2.228807	0.465707	-9.075081
105	6	0	-2.074756	0.298428	-10.590267
106	6	0	-1.033385	1.745951	-7.247039
107	6	0	0.098926	2.244636	-6.596138
108	6	0	1.348840	1.886929	-7.117098
109	6	0	1.484296	1.058018	-8.255131
110	6	0	0.315028	0.583557	-8.855751
111	6	0	-0.960975	0.930950	-8.393007
112	6	0	2.860148	0.704139	-8.779906
113	6	0	2.882103	0.379031	-10.277574
114	6	0	1.453424	-4.586397	-5.511418
115	6	0	0.181313	-4.898341	-5.014991
116	6	0	-0.882656	-4.914550	-5.921438
117	6	0	-0.719388	-4.605738	-7.288436
118	6	0	0.580434	-4.334868	-7.735971
119	6	0	1.691457	-4.359581	-6.885884
120	6	0	-1.924435	-4.558547	-8.204333
121	6	0	-1.600740	-4.865966	-9.668845
122	1	0	-0.921796	-4.131573	-10.114140
123	8	0	4.862097	1.176311	-6.950393
124	8	0	5.216836	-3.496382	-5.769799

125	1	0	5.885252	-0.899411	-5.560308
126	1	0	2.170794	-1.975208	-8.722596
127	1	0	3.770395	-4.838309	-6.735675
128	1	0	4.345276	-4.731962	-9.109427
129	1	0	2.741232	-4.166989	-9.571110
130	1	0	2.943635	-5.792395	-8.895826
131	8	0	-4.260752	-4.301026	-6.744626
132	8	0	-4.402404	0.491498	-7.344494
133	1	0	-5.273347	-1.846591	-6.328877
134	1	0	-1.212663	-2.091406	-9.227181
135	1	0	-3.008577	1.271624	-8.921850
136	1	0	-3.036196	0.036336	-11.049638
137	1	0	-1.365342	-0.491801	-10.857040
138	1	0	-1.724897	1.227932	-11.054934
139	8	0	-2.233847	2.133769	-6.684515
140	8	0	2.413840	2.420676	-6.437355
141	1	0	0.014496	2.855456	-5.702620
142	1	0	0.396104	-0.074589	-9.724668
143	1	0	3.513600	1.617903	-8.646565
144	1	0	3.912765	0.201955	-10.612449
145	1	0	2.477937	1.208011	-10.869055
146	1	0	2.309535	-0.521385	-10.521172
147	8	0	2.429714	-4.544375	-4.554552
148	8	0	-2.090484	-5.264358	-5.362348
149	1	0	0.032340	-5.098371	-3.957973
150	1	0	0.734990	-4.108248	-8.793734
151	1	0	-2.642076	-5.362947	-7.861151
152	1	0	-2.516071	-4.871114	-10.273797
153	1	0	-1.131435	-5.852501	-9.767256
154	6	0	4.092248	-6.665825	-2.382204
155	6	0	5.058589	-5.660035	-2.449903
156	6	0	6.012814	-5.612736	-1.427379
157	6	0	6.026174	-6.531945	-0.355634
158	6	0	5.024346	-7.511159	-0.329235
159	6	0	4.058684	-7.614908	-1.333006
160	6	0	7.104328	-6.457755	0.704701
161	6	0	7.678052	-7.836007	1.049977
162	6	0	2.384538	-5.584401	5.611783
163	6	0	1.003151	-5.661829	5.409885
164	6	0	0.531753	-6.709662	4.610382
165	6	0	1.384606	-7.677890	4.043796
166	6	0	2.763638	-7.520355	4.239330
167	6	0	3.293133	-6.490874	5.022361
168	6	0	0.816654	-8.843304	3.259443
169	6	0	1.540320	-10.159819	3.560004
170	6	0	6.826807	-4.323930	2.032173
171	6	0	6.323244	-3.558148	3.088293
172	6	0	5.615089	-4.232853	4.090464
173	6	0	5.431146	-5.629994	4.078777
174	6	0	5.898441	-6.337360	2.960480
175	6	0	6.596094	-5.716214	1.923124
176	6	0	4.778203	-6.321375	5.256115
177	6	0	5.462389	-7.645566	5.612009
178	6	0	-0.380897	-7.999081	1.204361
179	6	0	-0.456708	-7.589636	-0.128406
180	6	0	0.689286	-7.759621	-0.917360
181	6	0	1.862215	-8.370562	-0.417249
182	6	0	1.902205	-8.691240	0.943988
183	6	0	0.797474	-8.513283	1.784235
184	6	0	3.006312	-8.699485	-1.351689
185	6	0	3.602882	-10.084781	-1.073627
186	1	0	2.830761	-10.861286	-1.130261
187	8	0	3.118209	-6.798571	-3.336411
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189	1	0	5.075341	-4.927002	-3.261831
190	1	0	5.003160	-8.221436	0.499160
191	1	0	7.962635	-5.853471	0.277894

192	1	0	8.080967	-8.323080	0.152958
193	1	0	6.928832	-8.510929	1.475057
194	1	0	8.494063	-7.748085	1.777160
195	8	0	2.932155	-4.609218	6.409043
196	8	0	-0.835836	-6.724275	4.432882
197	1	0	0.326943	-4.931960	5.844315
198	1	0	3.447434	-8.231520	3.769743
199	1	0	-0.256080	-8.988183	3.590654
200	1	0	1.506985	-10.390249	4.631476
201	1	0	2.593198	-10.141640	3.260978
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205	1	0	6.476924	-2.482962	3.133557
206	1	0	5.718194	-7.413317	2.905841
207	1	0	4.905219	-5.646086	6.157296
208	1	0	5.384939	-8.389805	4.813112
209	1	0	5.014661	-8.085081	6.511834
210	1	0	6.530104	-7.491577	5.811934
211	8	0	-1.476500	-7.920593	2.034447
212	8	0	0.572467	-7.301521	-2.201910
213	1	0	-1.360334	-7.147418	-0.539516
214	1	0	2.821132	-9.107778	1.361652
215	1	0	2.582308	-8.744248	-2.401424
216	1	0	4.068728	-10.154359	-0.086307
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218	6	0	-3.467301	7.183170	2.309244
219	6	0	-2.070243	7.242905	2.313304
220	6	0	-1.456730	7.957834	1.277309
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223	6	0	-4.250699	7.789117	1.299945
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225	6	0	-2.224742	10.743086	-1.117096
226	6	0	-3.534064	5.012273	-5.419895
227	6	0	-4.385078	3.938471	-5.140010
228	6	0	-5.530411	4.209363	-4.382412
229	6	0	-5.854690	5.501704	-3.925373
230	6	0	-4.940357	6.530543	-4.194671
231	6	0	-3.780487	6.320894	-4.943926
232	6	0	-7.150856	5.752592	-3.183086
233	6	0	-7.796186	7.091111	-3.557325
234	6	0	-7.266737	4.404658	-1.047473
235	6	0	-7.041528	4.182934	0.312621
236	6	0	-6.497050	5.241143	1.051441
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238	6	0	-6.408444	6.643694	-0.902897
239	6	0	-6.934126	5.615846	-1.692266
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243	6	0	0.465569	7.251406	-3.239407
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245	6	0	-1.808525	7.602319	-4.124757
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250	1	0	-4.145179	8.594115	-6.503277
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262	1	0	-5.148899	7.532894	-3.813793
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293	6	0	8.430673	1.306799	-1.803415
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295	6	0	8.575468	1.021927	0.622596
296	6	0	8.614429	2.127317	-3.060400
297	6	0	9.953421	2.871289	-3.091961
298	6	0	6.325984	2.638083	-4.027152
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318	1	0	7.495967	6.059926	0.063783
319	1	0	6.153160	6.428713	3.593095
320	1	0	7.968901	7.762380	2.576859
321	1	0	8.704108	6.333024	1.846537
322	1	0	8.632438	6.479792	3.603495
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325	1	0	7.036717	-1.701778	-0.836292

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328	1	0	10.059633	3.588039	-2.272185
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335	1	0	5.569220	7.217156	-2.996025
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343	1	0	9.157659	0.578140	2.639000
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364	6	0	-8.122793	-0.562582	2.712851
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413	1	0	3.232530	-3.895185	-4.786191
414	1	0	-2.863367	-5.198883	-6.024418
415	1	0	3.094940	-6.007304	-3.998415
416	1	0	7.460646	-4.469905	-0.679440
417	1	0	2.222863	-3.994669	6.804327
418	1	0	-1.116805	-7.373526	3.688038
419	1	0	7.690284	-2.749456	1.162594
420	1	0	4.554355	-3.946065	5.758201
421	1	0	-2.313658	-7.624399	1.533863
422	1	0	1.467609	-7.308123	-2.704394
423	1	0	-3.535553	6.036512	3.945666
424	1	0	0.335397	8.362293	0.476102
425	1	0	-2.263241	3.870043	-6.456516
426	1	0	-1.483318	5.612326	5.114038
427	1	0	-8.071973	2.595255	-1.308371
428	1	0	-5.746522	5.699888	2.840953
429	1	0	1.963964	7.981004	-1.387403
430	1	0	-0.944030	5.908915	-5.806446
431	1	0	-6.027102	-1.450002	6.265625
432	1	0	3.872918	6.843370	-2.733056
433	1	0	2.971173	6.683709	2.872192
434	1	0	7.831375	-0.570226	2.449619
435	1	0	7.204391	-1.486993	-3.161878
436	1	0	6.935935	0.726819	-4.200415
437	1	0	3.574518	5.328572	-4.750056
438	1	0	4.767340	5.467527	4.063013
439	1	0	6.674718	0.099605	4.641685
440	1	0	-2.288346	-4.175705	6.885147
441	1	0	-3.935624	-7.364940	-0.410830
442	1	0	-4.069766	-5.134963	4.827578
443	1	0	4.446641	3.763490	5.996088
444	1	0	-6.962076	-0.380440	-4.576284
445	1	0	-5.995310	-3.599087	5.047078
446	1	0	-7.836438	1.427661	3.023501
447	1	0	-6.706967	-2.843549	-4.769348
448	1	0	-3.329795	-7.026197	-2.766349
449	1	0	0.774882	6.203535	4.519570
450	1	0	-7.035564	3.297542	-3.422251
451	1	0	-0.099051	-3.319472	7.590818
452	1	0	3.990022	1.516282	6.957685
453	1	0	-5.672452	0.938896	6.174873
454	1	0	5.556370	1.321354	-6.221666
455	1	0	5.676144	-3.192032	-4.890762
456	1	0	-5.038338	-4.155378	-6.101041
457	1	0	-8.600976	1.073051	0.679827
458	6	0	3.366318	3.436780	-0.092837
459	6	0	-0.624001	4.522118	0.977321

460	6	0	1.994527	3.790479	0.287998
461	7	0	3.886619	2.229998	0.054048
462	6	0	5.292666	1.976553	-0.344332
463	6	0	0.045501	3.541583	1.714614
464	6	0	0.017322	5.142027	-0.101369
465	6	0	1.322932	4.788344	-0.443103
466	6	0	1.347044	3.170037	1.370325
467	1	0	-1.649009	4.793043	1.229925
468	1	0	-0.511787	5.897965	-0.684024
469	1	0	1.818940	5.275541	-1.285090
470	1	0	5.993682	2.277537	0.459635
471	1	0	5.580480	2.508402	-1.268658
472	1	0	5.455558	0.889498	-0.513478
473	1	0	3.972615	4.242768	-0.525616
474	8	0	3.270359	1.242408	0.518812
475	1	0	-0.453505	3.056193	2.553703
476	1	0	1.863329	2.387156	1.931261
477	1	0	-1.898877	-6.746995	-4.258272
478	8	0	-2.051204	-7.409578	-3.550696
479	1	0	-1.246750	-7.399724	-2.997501
480	8	0	6.089546	-0.831643	5.794477
481	1	0	5.980967	-1.753522	5.496575
482	1	0	5.227584	-0.552027	6.151206
483	8	0	-7.365115	2.689615	3.821641
484	1	0	-6.572840	2.491505	4.359375
485	1	0	-7.112155	3.419761	3.226546
486	8	0	2.509529	5.193726	-5.863921
487	1	0	1.663683	5.583301	-5.574982
488	1	0	2.321776	4.252403	-6.066866
489	8	0	-6.051569	0.947412	-5.206607
490	1	0	-5.479844	1.319108	-4.499288
491	1	0	-6.637251	1.695441	-5.454534
492	8	0	1.251768	6.717175	2.968226
493	1	0	0.919191	7.638047	2.868257
494	1	0	0.817169	6.216496	2.237078
495	8	0	-2.436249	-5.210567	5.476613
496	1	0	-2.203853	-6.129229	5.731410
497	1	0	-1.776220	-4.985857	4.784049
498	8	0	6.770425	-2.859098	-3.329609
499	1	0	6.085357	-2.950346	-2.559068
500	1	0	7.478581	-3.483314	-3.103661

Sum of electronic and thermal Free Energies= -0.704102
0 imaginary frequency

MC1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.448292	1.952418	-2.398796
2	1	0	0.443553	1.501854	-3.953963
3	1	0	2.727592	1.152203	-3.067277
4	1	0	6.018533	1.524989	0.456248
5	1	0	5.573465	-0.177802	0.832622
6	1	0	5.550183	1.071787	2.118431
7	1	0	4.262563	1.019071	-1.305913
8	1	0	1.398868	1.545871	4.093934
9	1	0	0.002001	0.458220	3.946096
10	1	0	1.204450	0.195880	5.222426
11	1	0	2.993002	-0.252271	3.421076
12	1	0	0.323108	-1.252394	2.163160
13	1	0	3.275950	-2.264523	1.911485
14	1	0	1.858419	-4.350320	-2.076776
15	1	0	2.924026	-3.109825	-2.768627
16	1	0	3.083766	-4.156333	-0.094087

17	1	0	-0.126436	-2.490530	-0.082208
18	6	0	1.039769	-2.315887	-1.949681
19	6	0	0.752763	-1.945356	-0.487410
20	7	0	1.982413	-2.339247	0.268590
21	8	0	3.165411	1.320940	1.741075
22	6	0	3.511371	1.181830	-0.518864
23	6	0	-0.447324	1.794760	-2.005147
24	6	0	4.304994	-2.451096	-0.660371
25	8	0	4.806908	-2.336796	-1.799047
26	6	0	2.143907	1.402670	-0.988705
27	8	0	4.809551	-2.083285	0.421728
28	6	0	2.275807	-1.969069	1.497919
29	6	0	1.397898	-1.182020	2.334189
30	6	0	1.905495	-0.356728	3.277121
31	7	0	3.906633	1.163664	0.745685
32	6	0	5.333261	0.893742	1.047453
33	6	0	-0.215191	1.858706	-0.629327
34	1	0	1.310289	-1.410309	-2.532815
35	6	0	2.911265	-3.157295	-0.575378
36	6	0	2.210086	-3.312355	-1.931595
37	6	0	0.617846	1.539431	-2.877993
38	6	0	1.904121	1.343000	-2.378457
39	6	0	1.071404	1.664009	-0.119340
40	1	0	0.563582	-0.850326	-0.369012
41	1	0	0.149795	-2.744750	-2.441957
42	6	0	1.077933	0.489637	4.161956
43	1	0	-1.037973	2.071555	0.051467
44	1	0	1.252236	1.727225	0.959275
45	8	0	2.249381	1.727705	8.025396
46	8	0	-0.983920	5.052539	6.676146
47	6	0	0.983477	2.256374	7.987695
48	6	0	0.700712	3.435985	7.291853
49	6	0	-0.617072	3.902325	7.337239
50	6	0	-1.637960	3.236901	8.047987
51	6	0	-1.305580	2.040884	8.696330
52	6	0	-0.003966	1.530447	8.689618
53	6	0	-3.038721	3.809879	8.080710
54	6	0	-3.582549	3.899675	9.510120
55	1	0	1.471350	3.960142	6.734873
56	1	0	-2.089287	1.487239	9.217715
57	1	0	-2.984980	4.872781	7.694227
58	1	0	-3.647738	2.922786	9.999556
59	1	0	-4.585255	4.343662	9.521591
60	1	0	-2.932761	4.529121	10.131560
61	8	0	-7.309569	-1.442487	5.090588
62	8	0	-3.936469	-4.772570	6.029110
63	6	0	-6.256481	-1.944151	5.814710
64	6	0	-5.646102	-3.156093	5.475188
65	6	0	-4.599840	-3.592866	6.293171
66	6	0	-4.160820	-2.870360	7.421786
67	6	0	-4.782574	-1.643977	7.691009
68	6	0	-5.836442	-1.158961	6.911274
69	6	0	-3.045678	-3.413924	8.289519
70	6	0	-3.430346	-3.415953	9.772344
71	1	0	-5.967258	-3.721052	4.605457
72	1	0	-4.428069	-1.046398	8.533643
73	1	0	-2.881915	-4.496633	8.003118
74	1	0	-3.645935	-2.413064	10.154498
75	1	0	-2.626316	-3.839114	10.386506
76	1	0	-4.329472	-4.023577	9.937048
77	8	0	-3.248927	4.403066	5.236953
78	8	0	-6.450576	1.121475	4.412339
79	6	0	-4.003532	3.386544	5.779478
80	6	0	-4.846035	2.743464	4.868212
81	6	0	-5.643776	1.701661	5.356126
82	6	0	-5.618391	1.299109	6.711475
83	6	0	-4.746085	1.973311	7.572612

84	6	0	-3.943442	3.037630	7.144705
85	6	0	-6.509907	0.170013	7.183777
86	6	0	-6.939322	0.301991	8.648100
87	1	0	-4.856353	3.016378	3.816538
88	1	0	-4.696655	1.666301	8.620116
89	1	0	-7.460209	0.211837	6.570268
90	1	0	-7.448870	1.257424	8.822738
91	1	0	-6.096263	0.243575	9.343554
92	1	0	-7.637922	-0.500350	8.918284
93	8	0	-1.249411	-4.145706	6.118216
94	8	0	1.869837	-0.820848	7.078055
95	6	0	-0.932516	-3.082500	6.937105
96	6	0	0.284795	-2.465570	6.635369
97	6	0	0.674399	-1.389406	7.441127
98	6	0	-0.108272	-0.933356	8.526141
99	6	0	-1.323693	-1.582459	8.769130
100	6	0	-1.755638	-2.674062	8.006547
101	6	0	0.368471	0.230081	9.370184
102	6	0	-0.125141	0.180055	10.818921
103	1	0	0.889414	-2.789778	5.790849
104	1	0	-1.954626	-1.231293	9.589361
105	1	0	1.497958	0.171190	9.418261
106	1	0	0.175932	-0.756057	11.304607
107	1	0	-1.213692	0.261099	10.898747
108	1	0	0.303685	1.007152	11.399667
109	1	0	2.906618	2.239745	7.426456
110	1	0	-0.231882	5.413926	6.076804
111	1	0	-7.532720	-2.020129	4.279352
112	1	0	-4.193618	-5.171236	5.122689
113	1	0	-2.594507	4.806982	5.912035
114	1	0	-6.967338	0.318515	4.771883
115	1	0	-2.193113	-4.503574	6.293729
116	1	0	2.133486	-0.032968	7.678339
117	8	0	-2.397307	-2.471763	-8.125242
118	8	0	-2.294418	2.348828	-7.810245
119	6	0	-1.787233	-1.249445	-8.274543
120	6	0	-2.439152	-0.060624	-7.931784
121	6	0	-1.738573	1.131125	-8.140276
122	6	0	-0.438035	1.167226	-8.683613
123	6	0	0.180701	-0.056235	-8.971952
124	6	0	-0.470199	-1.279193	-8.782695
125	6	0	0.250712	2.494612	-8.920887
126	6	0	0.769586	2.610073	-10.357787
127	1	0	-3.437879	-0.070246	-7.506477
128	1	0	1.206583	-0.053813	-9.347081
129	1	0	-0.521010	3.312857	-8.795349
130	1	0	-0.055085	2.511553	-11.075047
131	1	0	1.504037	1.836456	-10.604221
132	1	0	1.243928	3.584110	-10.527381
133	8	0	6.593656	2.270082	-5.053057
134	8	0	6.279326	-2.540116	-4.808211
135	6	0	6.208323	1.040257	-5.538558
136	6	0	6.510806	-0.139660	-4.854996
137	6	0	6.069964	-1.339714	-5.424386
138	6	0	5.368261	-1.380062	-6.652516
139	6	0	5.068111	-0.166839	-7.277142
140	6	0	5.476533	1.061783	-6.743952
141	6	0	4.960384	-2.714682	-7.235634
142	6	0	5.431061	-2.860642	-8.687600
143	1	0	7.046960	-0.128891	-3.909179
144	1	0	4.489640	-0.175252	-8.202717
145	1	0	5.487640	-3.526937	-6.651604
146	1	0	6.523875	-2.773793	-8.744892
147	1	0	5.013352	-2.093143	-9.346275
148	1	0	5.153681	-3.839712	-9.094809
149	8	0	3.746107	-3.738174	-4.763295
150	8	0	-0.571241	-3.813997	-6.498037

151	6	0	2.962722	-3.453165	-5.857380
152	6	0	1.607926	-3.756571	-5.678999
153	6	0	0.740207	-3.481672	-6.741174
154	6	0	1.184946	-2.916843	-7.956821
155	6	0	2.552412	-2.645119	-8.080814
156	6	0	3.471885	-2.931578	-7.065184
157	6	0	0.195612	-2.611218	-9.061502
158	6	0	0.804905	-2.660297	-10.465677
159	1	0	1.243197	-4.160055	-4.738486
160	1	0	2.918829	-2.201775	-9.010135
161	1	0	-0.600926	-3.414213	-9.033079
162	1	0	0.031809	-2.495689	-11.226964
163	1	0	1.260806	-3.638411	-10.661533
164	1	0	1.576008	-1.898464	-10.618488
165	8	0	-0.326418	3.578021	-6.274773
166	8	0	4.118189	3.528548	-4.883349
167	6	0	0.972003	3.254729	-6.617066
168	6	0	1.911600	3.518901	-5.616966
169	6	0	3.251443	3.229512	-5.901839
170	6	0	3.660946	2.686225	-7.142209
171	6	0	2.671802	2.427546	-8.095348
172	6	0	1.319879	2.723256	-7.874562
173	6	0	5.125110	2.384703	-7.389354
174	6	0	5.521328	2.420965	-8.868451
175	1	0	1.612140	3.898392	-4.642461
176	1	0	2.963016	1.987214	-9.052171
177	1	0	5.726742	3.196204	-6.880192
178	1	0	6.601903	2.259950	-8.977810
179	1	0	5.283432	3.392405	-9.316988
180	1	0	5.021045	1.646804	-9.458555
181	1	0	-3.320262	-2.391868	-7.700033
182	1	0	-3.176659	2.246629	-7.303404
183	1	0	7.078566	2.193531	-4.158175
184	1	0	6.729976	-2.421836	-3.843954
185	1	0	4.679204	-3.300064	-4.799807
186	1	0	-1.194302	-3.538572	-7.256367
187	1	0	-0.995419	3.317613	-7.002225
188	1	0	5.084542	3.258596	-5.086673
189	8	0	-0.566984	6.166088	-5.325788
190	8	0	-4.932467	4.410754	-4.701360
191	6	0	-1.841077	6.277320	-4.837030
192	6	0	-2.770335	5.244281	-4.995684
193	6	0	-4.065010	5.467556	-4.512494
194	6	0	-4.455815	6.677060	-3.906886
195	6	0	-3.469423	7.659582	-3.731754
196	6	0	-2.161811	7.495026	-4.192628
197	6	0	-5.891978	6.894348	-3.477788
198	6	0	-6.368272	8.332119	-3.710838
199	1	0	-2.492796	4.302688	-5.458845
200	1	0	-3.737744	8.589872	-3.225841
201	1	0	-6.544005	6.236587	-4.128035
202	1	0	-6.251624	8.617548	-4.763285
203	1	0	-5.818037	9.062798	-3.109705
204	1	0	-7.430212	8.433568	-3.453540
205	8	0	-4.652216	6.103764	3.544190
206	8	0	-0.144309	7.476523	2.950762
207	6	0	-3.704481	6.858159	2.901456
208	6	0	-2.351987	6.768079	3.245323
209	6	0	-1.463606	7.615883	2.573381
210	6	0	-1.884512	8.550988	1.607478
211	6	0	-3.244690	8.559937	1.266466
212	6	0	-4.177930	7.734510	1.898562
213	6	0	-0.891667	9.509879	0.983789
214	6	0	-1.483618	10.904490	0.752574
215	1	0	-2.004093	6.058581	3.989322
216	1	0	-3.587510	9.243889	0.486684
217	1	0	-0.042655	9.645638	1.719844

218	1	0	-1.867337	11.327665	1.688569
219	1	0	-2.306843	10.900453	0.031375
220	1	0	-0.717603	11.589069	0.366407
221	8	0	-7.010998	4.438748	-2.866001
222	8	0	-6.553325	4.974158	1.829627
223	6	0	-6.627376	5.180050	-1.770732
224	6	0	-6.780921	4.681329	-0.475518
225	6	0	-6.404261	5.520136	0.580940
226	6	0	-5.923791	6.831939	0.372174
227	6	0	-5.736732	7.254084	-0.949609
228	6	0	-6.082480	6.453281	-2.043196
229	6	0	-5.650538	7.739263	1.552922
230	6	0	-6.198718	9.153620	1.335142
231	1	0	-7.160362	3.680267	-0.289749
232	1	0	-5.315265	8.244461	-1.133434
233	1	0	-6.207446	7.315986	2.444475
234	1	0	-5.724488	9.665984	0.492333
235	1	0	-6.041523	9.773504	2.226335
236	1	0	-7.276971	9.126259	1.134167
237	8	0	1.606178	8.313459	0.970116
238	8	0	1.430166	7.126727	-3.621703
239	6	0	0.956171	8.296580	-0.244253
240	6	0	1.538774	7.693413	-1.360342
241	6	0	0.823807	7.749525	-2.563371
242	6	0	-0.417346	8.415771	-2.676090
243	6	0	-0.974797	8.955946	-1.511534
244	6	0	-0.310370	8.918115	-0.280776
245	6	0	-1.088965	8.548467	-4.026225
246	6	0	-1.612688	9.967077	-4.274591
247	1	0	2.498356	7.186197	-1.300555
248	1	0	-1.956242	9.430982	-1.566533
249	1	0	-0.302680	8.356093	-4.819381
250	1	0	-2.386815	10.263395	-3.560161
251	1	0	-2.042546	10.053154	-5.279981
252	1	0	-0.800063	10.700203	-4.195898
253	1	0	-0.373506	5.231862	-5.699806
254	1	0	-5.800060	4.522347	-4.166619
255	1	0	-4.239849	5.451643	4.212980
256	1	0	0.494873	7.957912	2.307985
257	1	0	-7.403857	3.536592	-2.597236
258	1	0	-6.125413	5.548570	2.554825
259	1	0	2.523907	7.871299	0.915812
260	1	0	0.808899	7.035571	-4.424190
261	8	0	0.860220	-5.884895	5.887265
262	8	0	-2.297099	-7.517538	2.732939
263	6	0	0.533935	-6.673716	4.811240
264	6	0	-0.766793	-6.704649	4.301190
265	6	0	-1.003919	-7.554177	3.214238
266	6	0	-0.006491	-8.377811	2.658025
267	6	0	1.289646	-8.274039	3.185193
268	6	0	1.589003	-7.435690	4.261719
269	6	0	-0.339682	-9.331682	1.528875
270	6	0	0.294273	-10.711448	1.729197
271	1	0	-1.555366	-6.088872	4.720703
272	1	0	2.091016	-8.866691	2.737962
273	1	0	-1.461161	-9.491309	1.533927
274	1	0	-0.005286	-11.396727	0.926291
275	1	0	-0.023517	-11.153632	2.681254
276	1	0	1.388523	-10.676702	1.736206
277	8	0	3.563545	-6.293979	-3.893123
278	8	0	6.944080	-4.691420	-0.945485
279	6	0	4.279902	-6.370940	-2.722555
280	6	0	5.260416	-5.427868	-2.404860
281	6	0	5.943042	-5.596246	-1.194937
282	6	0	5.636492	-6.640890	-0.294047
283	6	0	4.636880	-7.549041	-0.656710
284	6	0	3.957701	-7.453869	-1.875533

285	6	0	6.354754	-6.725675	1.036086
286	6	0	6.871970	-8.136019	1.329060
287	1	0	5.473412	-4.574246	-3.046369
288	1	0	4.379376	-8.355726	0.031909
289	1	0	7.265278	-6.051249	0.985978
290	1	0	7.417221	-8.163636	2.280183
291	1	0	7.560622	-8.466048	0.540837
292	1	0	6.068527	-8.877050	1.384893
293	8	0	6.166094	-4.018561	1.459351
294	8	0	3.020232	-4.362334	4.987585
295	6	0	5.390926	-4.758348	2.289707
296	6	0	4.570634	-4.167553	3.257461
297	6	0	3.798217	-5.018874	4.057905
298	6	0	3.824349	-6.420325	3.929304
299	6	0	4.656551	-6.961859	2.935410
300	6	0	5.453815	-6.167365	2.116321
301	6	0	2.984953	-7.295403	4.834302
302	6	0	3.620628	-8.658425	5.125772
303	1	0	4.549228	-3.090936	3.398963
304	1	0	4.679761	-8.046552	2.805776
305	1	0	2.900140	-6.767119	5.831253
306	1	0	4.619672	-8.537735	5.562817
307	1	0	3.726677	-9.276403	4.228558
308	1	0	3.011136	-9.224811	5.840820
309	8	0	-2.221549	-7.964423	0.036911
310	8	0	0.837009	-6.670600	-3.350305
311	6	0	-0.957871	-7.970019	-0.504851
312	6	0	-0.682597	-7.284667	-1.690562
313	6	0	0.612412	-7.401231	-2.212529
314	6	0	1.596511	-8.216821	-1.610553
315	6	0	1.286105	-8.813394	-0.382719
316	6	0	0.019067	-8.705376	0.200074
317	6	0	2.916109	-8.458238	-2.311470
318	6	0	3.412066	-9.900186	-2.149744
319	1	0	-1.436036	-6.678675	-2.186970
320	1	0	2.054851	-9.396064	0.129922
321	1	0	2.738889	-8.308813	-3.420241
322	1	0	2.658093	-10.615775	-2.498364
323	1	0	3.651956	-10.150932	-1.112053
324	1	0	4.323215	-10.061452	-2.740041
325	1	0	0.082089	-5.286618	6.173591
326	1	0	-2.378265	-8.004171	1.834612
327	1	0	3.756184	-5.427667	-4.406884
328	1	0	7.191689	-4.672172	0.045856
329	1	0	5.992720	-2.997493	1.524456
330	1	0	2.389865	-4.992938	5.484025
331	1	0	-2.896013	-7.502413	-0.570866
332	1	0	1.812336	-6.720464	-3.665225
333	8	0	-3.923993	-6.684181	-1.745025
334	8	0	-6.302557	-5.395090	2.146473
335	6	0	-5.106622	-6.252286	-1.206273
336	6	0	-5.071803	-6.049465	0.180374
337	6	0	-6.238098	-5.571572	0.783552
338	6	0	-7.403002	-5.261034	0.049015
339	6	0	-7.387245	-5.510110	-1.327927
340	6	0	-6.269233	-6.046417	-1.977491
341	6	0	-8.598975	-4.659579	0.753547
342	6	0	-9.927389	-5.251981	0.272969
343	1	0	-4.167326	-6.243797	0.745926
344	1	0	-8.281240	-5.285679	-1.914253
345	1	0	-8.511289	-4.922307	1.852142
346	1	0	-9.945353	-6.338702	0.420447
347	1	0	-10.113741	-5.063537	-0.789156
348	1	0	-10.769266	-4.824584	0.831565
349	8	0	-7.858316	1.934822	-1.963314
350	8	0	-6.077648	0.305855	-6.047448
351	6	0	-7.842683	0.935276	-2.901952

352	6	0	-6.956317	1.149407	-3.966373
353	6	0	-6.882721	0.153439	-4.944113
354	6	0	-7.630219	-1.042659	-4.870336
355	6	0	-8.510028	-1.193103	-3.793493
356	6	0	-8.668828	-0.204289	-2.814855
357	6	0	-7.444322	-2.110057	-5.926238
358	6	0	-8.769494	-2.739099	-6.368175
359	1	0	-6.347099	2.045414	-4.007952
360	1	0	-9.099635	-2.109558	-3.718403
361	1	0	-7.009347	-1.606164	-6.843108
362	1	0	-9.287045	-3.251002	-5.550731
363	1	0	-8.604140	-3.478053	-7.161946
364	1	0	-9.451754	-1.974755	-6.759771
365	8	0	-4.611553	-1.966638	-6.552203
366	8	0	-3.695400	-6.090879	-4.385895
367	6	0	-5.086139	-3.031908	-5.821214
368	6	0	-4.123749	-3.993130	-5.491039
369	6	0	-4.550541	-5.090493	-4.735696
370	6	0	-5.890214	-5.224057	-4.291713
371	6	0	-6.805702	-4.235987	-4.657829
372	6	0	-6.442036	-3.142193	-5.454965
373	6	0	-6.277605	-6.415965	-3.446021
374	6	0	-7.606315	-7.039697	-3.886347
375	1	0	-3.087164	-3.871887	-5.793001
376	1	0	-7.840687	-4.321712	-4.320752
377	1	0	-5.486777	-7.212540	-3.600252
378	1	0	-7.842015	-7.924672	-3.283266
379	1	0	-7.554272	-7.356116	-4.935921
380	1	0	-8.449036	-6.347291	-3.797435
381	8	0	-7.408304	-2.952954	2.777622
382	8	0	-8.656802	1.015668	0.490855
383	6	0	-7.998900	-2.377346	1.674964
384	6	0	-8.005318	-0.978042	1.675026
385	6	0	-8.580178	-0.342232	0.569087
386	6	0	-9.113895	-1.068415	-0.524951
387	6	0	-9.083623	-2.462785	-0.464309
388	6	0	-8.563646	-3.149938	0.641428
389	6	0	-9.691220	-0.316890	-1.703493
390	6	0	-11.016805	-0.915498	-2.186486
391	1	0	-7.561613	-0.416628	2.491828
392	1	0	-9.486173	-3.038131	-1.300482
393	1	0	-9.927360	0.733888	-1.351560
394	1	0	-10.912145	-1.946338	-2.538590
395	1	0	-11.433413	-0.326837	-3.012665
396	1	0	-11.755962	-0.921329	-1.375508
397	1	0	-3.938266	-6.732607	-2.772889
398	1	0	-5.411961	-5.597489	2.605910
399	1	0	-8.406413	1.691184	-1.129603
400	1	0	-5.505759	1.155537	-6.001713
401	1	0	-5.311327	-1.231039	-6.660780
402	1	0	-2.718664	-5.987934	-4.797296
403	1	0	-7.310729	-3.963350	2.680246
404	1	0	-8.299987	1.511020	1.359103
405	8	0	4.122551	7.083860	0.702253
406	8	0	3.329501	5.528169	5.119850
407	6	0	4.626428	6.496465	1.834041
408	6	0	3.701465	6.322705	2.872002
409	6	0	4.165699	5.709563	4.038820
410	6	0	5.492932	5.255564	4.188840
411	6	0	6.376354	5.472201	3.124946
412	6	0	5.981529	6.122633	1.951049
413	6	0	5.913422	4.549742	5.458901
414	6	0	7.259258	5.058961	5.986550
415	1	0	2.669839	6.633633	2.754150
416	1	0	7.408340	5.126437	3.216505
417	1	0	5.147500	4.796747	6.254979
418	1	0	8.080017	4.889040	5.282370

419	1	0	7.525157	4.558345	6.925504
420	1	0	7.216297	6.137329	6.182592
421	8	0	7.254113	-2.156042	2.778868
422	8	0	8.678110	-0.348577	-1.364843
423	6	0	7.842971	-1.111594	2.117683
424	6	0	7.961530	-1.293068	0.732935
425	6	0	8.510105	-0.246144	-0.010576
426	6	0	8.903657	0.976724	0.582141
427	6	0	8.786679	1.096637	1.969564
428	6	0	8.286885	0.060355	2.767597
429	6	0	9.412906	2.099406	-0.294501
430	6	0	10.686633	2.741091	0.265660
431	1	0	7.612369	-2.213504	0.269967
432	1	0	9.094640	2.029160	2.446454
433	1	0	9.697923	1.651409	-1.294598
434	1	0	11.053638	3.529564	-0.402147
435	1	0	11.481943	1.991804	0.366723
436	1	0	10.535360	3.188111	1.252984
437	8	0	3.565481	2.909549	5.981772
438	8	0	5.896241	-1.115904	5.055298
439	6	0	4.741134	2.306868	5.581138
440	6	0	4.694688	0.909551	5.544236
441	6	0	5.850066	0.241185	5.120565
442	6	0	7.018894	0.939324	4.724959
443	6	0	7.008652	2.332913	4.799725
444	6	0	5.895129	3.048403	5.263975
445	6	0	8.230895	0.153342	4.275962
446	6	0	9.535372	0.698075	4.868880
447	1	0	3.789693	0.376154	5.818456
448	1	0	7.903364	2.884967	4.504031
449	1	0	8.112189	-0.900540	4.678563
450	1	0	9.752393	1.720027	4.543872
451	1	0	10.386853	0.074238	4.570070
452	1	0	9.492437	0.702639	5.964618
453	8	0	7.469470	1.833894	-2.459858
454	8	0	5.435604	5.991960	-1.441826
455	6	0	7.428912	2.933217	-1.638195
456	6	0	6.444019	3.871223	-1.973950
457	6	0	6.335223	5.009263	-1.167715
458	6	0	7.155804	5.201133	-0.027482
459	6	0	8.121091	4.234500	0.256639
460	6	0	8.307261	3.102647	-0.549105
461	6	0	6.951331	6.429312	0.828992
462	6	0	8.264426	7.024010	1.348183
463	1	0	5.786330	3.707364	-2.823040
464	1	0	8.762795	4.369106	1.130303
465	1	0	6.479340	7.222227	0.171333
466	1	0	8.930173	7.279160	0.514198
467	1	0	8.809707	6.337359	2.003121
468	1	0	8.078123	7.941433	1.919315
469	1	0	4.745461	6.973170	-0.106759
470	1	0	2.365271	5.798113	4.912262
471	1	0	7.045143	-1.928951	3.750607
472	1	0	8.280957	-1.245391	-1.754248
473	1	0	3.593618	3.925411	5.864135
474	1	0	5.122491	-1.583224	5.612646
475	1	0	8.159650	1.132301	-2.160541
476	1	0	4.911971	5.847585	-2.356624
477	8	0	0.655526	6.096422	4.770645
478	1	0	0.463676	7.060344	4.755327
479	1	0	0.331930	5.778560	3.896921
480	8	0	-4.427898	2.494844	-6.099995
481	1	0	-4.053151	2.676415	-5.209456
482	1	0	-4.915162	3.319065	-6.321813
483	8	0	-4.010097	-5.991546	3.580390
484	1	0	-3.934072	-6.958384	3.725070
485	1	0	-3.175064	-5.757044	3.118443

486	8	0	7.193427	-2.231252	-2.367888
487	1	0	6.267558	-1.905876	-1.961132
488	1	0	7.257946	-3.151178	-2.017339
489	8	0	-1.268070	-6.265442	-5.287641
490	1	0	-0.677110	-6.526349	-4.554871
491	1	0	-0.867903	-5.461008	-5.679773
492	8	0	4.181183	-2.426504	6.526706
493	1	0	3.295513	-2.021834	6.606484
494	1	0	4.041919	-3.280254	6.063970
495	8	0	-7.980831	2.546811	2.489640
496	1	0	-7.612589	3.371833	2.120954
497	1	0	-7.312432	2.210600	3.118700
498	8	0	4.119908	6.057144	-3.677532
499	1	0	3.267031	6.500172	-3.510176
500	1	0	3.898439	5.194398	-4.087118

Sum of electronic and thermal Free Energies= -0.706733
0 imaginary frequency

TS1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.465967	-4.642339	-1.346173
2	1	0	-0.067559	-2.933538	-3.078123
3	1	0	-2.164392	-1.614206	-2.922889
4	1	0	-6.710754	-1.100672	-0.500955
5	1	0	-5.695721	0.373344	-0.541971
6	1	0	-6.251647	-0.314548	1.033430
7	1	0	-4.404965	-1.358465	-1.981808
8	1	0	-3.347642	-2.383019	3.062818
9	1	0	-1.847188	-1.561278	3.545698
10	1	0	-3.412594	-1.073882	4.253959
11	1	0	-4.032381	0.196672	2.313463
12	1	0	-1.221322	-0.688767	1.297924
13	1	0	-3.338063	1.407596	0.297548
14	1	0	-0.119987	2.962635	-2.749892
15	1	0	-1.075403	1.948950	-3.841575
16	1	0	-2.009445	3.112862	-1.388233
17	1	0	0.524212	0.787769	-0.222595
18	6	0	0.156455	0.814208	-2.400472
19	6	0	-0.230050	0.438960	-0.960863
20	7	0	-1.528254	1.130554	-0.703049
21	8	0	-4.290341	-1.731374	1.275931
22	6	0	-4.022838	-1.737586	-1.011023
23	6	0	-0.448884	-4.056312	-1.269641
24	6	0	-3.237530	1.677890	-2.454200
25	8	0	-3.390552	2.061500	-3.651901
26	6	0	-2.802010	-2.548922	-1.069529
27	8	0	-4.077537	1.068534	-1.778082
28	6	0	-2.377107	0.843014	0.288164
29	6	0	-2.149417	-0.120581	1.293283
30	6	0	-3.139033	-0.437467	2.213015
31	7	0	-4.669741	-1.405459	0.085991
32	6	0	-5.888564	-0.572451	0.020914
33	6	0	-1.326603	-4.266562	-0.202337
34	1	0	-0.031318	-0.031997	-3.089439
35	6	0	-1.880802	2.079745	-1.803444
36	6	0	-0.704995	2.026565	-2.791618
37	6	0	-0.748987	-3.094911	-2.241993
38	6	0	-1.925101	-2.349837	-2.153210
39	6	0	-2.499067	-3.513895	-0.095431
40	1	0	-0.344804	-0.662231	-0.835161
41	1	0	1.233173	1.044400	-2.481924
42	6	0	-2.909622	-1.396961	3.326503
43	1	0	-1.097344	-5.023230	0.547816

44	1	0	-3.184553	-3.667848	0.743798
45	8	0	-4.666481	0.667616	7.239090
46	8	0	-1.743203	-3.156539	7.660464
47	6	0	-3.524983	0.044442	7.677201
48	6	0	-3.261215	-1.297099	7.380854
49	6	0	-2.085536	-1.844515	7.904801
50	6	0	-1.189647	-1.106270	8.704787
51	6	0	-1.484186	0.244040	8.934736
52	6	0	-2.646146	0.844188	8.440929
53	6	0	0.045087	-1.772894	9.272708
54	6	0	0.179342	-1.529200	10.779282
55	1	0	-3.939967	-1.883576	6.770659
56	1	0	-0.781060	0.846575	9.513751
57	1	0	-0.076032	-2.891080	9.141612
58	1	0	0.269938	-0.467245	11.028937
59	1	0	1.061797	-2.040378	11.182608
60	1	0	-0.700111	-1.912041	11.312593
61	8	0	5.705273	2.112188	6.529677
62	8	0	2.757065	5.827240	5.611640
63	6	0	4.587832	2.873939	6.769572
64	6	0	4.281871	3.991283	5.986249
65	6	0	3.138210	4.717645	6.332526
66	6	0	2.316070	4.369497	7.424770
67	6	0	2.647143	3.216115	8.147217
68	6	0	3.779487	2.452411	7.848050
69	6	0	1.117846	5.224748	7.776375
70	6	0	1.105689	5.601138	9.261561
71	1	0	4.901228	4.269409	5.138855
72	1	0	1.997648	2.901994	8.966907
73	1	0	1.208998	6.197129	7.203440
74	1	0	1.054057	4.727103	9.918416
75	1	0	0.248629	6.243601	9.496763
76	1	0	2.017215	6.151350	9.527833
77	8	0	0.898704	-3.125376	6.837047
78	8	0	4.674851	-0.458620	6.247643
79	6	0	1.634778	-2.066286	7.324222
80	6	0	2.776719	-1.763047	6.577688
81	6	0	3.568471	-0.696110	7.020109
82	6	0	3.249230	0.056527	8.174222
83	6	0	2.087823	-0.288305	8.872748
84	6	0	1.272181	-1.360014	8.489453
85	6	0	4.145435	1.196432	8.610864
86	6	0	4.145705	1.427851	10.125058
87	1	0	3.022275	-2.306971	5.669947
88	1	0	1.811260	0.292125	9.756331
89	1	0	5.206401	0.916181	8.333677
90	1	0	4.438857	0.517203	10.661241
91	1	0	3.167640	1.737661	10.506136
92	1	0	4.861523	2.215573	10.393391
93	8	0	0.049269	5.520890	5.083862
94	8	0	-3.723258	2.910009	5.895669
95	6	0	-0.625767	4.750301	6.004442
96	6	0	-1.820758	4.199627	5.532478
97	6	0	-2.558765	3.409027	6.421420
98	6	0	-2.135319	3.164522	7.747948
99	6	0	-0.925703	3.734992	8.159101
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101	6	0	-2.975133	2.304950	8.668957
102	6	0	-2.855703	2.693873	10.145580
103	1	0	-2.145396	4.349040	4.506582
104	1	0	-0.570626	3.544254	9.174743
105	1	0	-4.059131	2.466889	8.385870
106	1	0	-3.123578	3.746728	10.296583
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108	1	0	-3.534425	2.087943	10.759508
109	1	0	-5.223664	0.073713	6.620356
110	1	0	-2.352411	-3.594287	6.966937

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112	1	0	3.311673	5.946729	4.757174
113	1	0	0.039775	-3.278373	7.370267
114	1	0	5.191433	0.372872	6.538684
115	1	0	0.958956	5.835468	5.431745
116	1	0	-4.209287	2.282316	6.539081
117	8	0	5.063130	0.106706	-7.355658
118	8	0	3.993052	-4.442462	-6.128845
119	6	0	4.301857	-1.033788	-7.433879
120	6	0	4.602939	-2.170299	-6.676928
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122	6	0	2.699762	-3.305871	-7.757447
123	6	0	2.417459	-2.123951	-8.456006
124	6	0	3.200729	-0.974784	-8.316593
125	6	0	1.883525	-4.566745	-7.945524
126	6	0	1.770057	-4.948071	-9.425315
127	1	0	5.429716	-2.174591	-5.973806
128	1	0	1.552433	-2.098332	-9.122525
129	1	0	2.439244	-5.414286	-7.440833
130	1	0	2.764708	-5.105145	-9.861361
131	1	0	1.275574	-4.175332	-10.022859
132	1	0	1.200970	-5.877149	-9.549294
133	8	0	-5.140942	-2.735543	-6.296932
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135	6	0	-4.427958	-1.700241	-6.862508
136	6	0	-4.710471	-0.369290	-6.544325
137	6	0	-3.925764	0.614373	-7.155394
138	6	0	-2.893720	0.294813	-8.070677
139	6	0	-2.642926	-1.052709	-8.335916
140	6	0	-3.399803	-2.076209	-7.750751
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142	6	0	-2.132069	1.309220	-10.241992
143	1	0	-5.491196	-0.107060	-5.833794
144	1	0	-1.827498	-1.317969	-9.011252
145	1	0	-2.593102	2.391938	-8.451003
146	1	0	-3.166767	1.368890	-10.603978
147	1	0	-1.716508	0.367471	-10.612938
148	1	0	-1.571385	2.130291	-10.703228
149	8	0	-1.417907	2.629363	-6.109580
150	8	0	3.149868	1.953459	-6.595346
151	6	0	-0.442015	2.097260	-6.915555
152	6	0	0.852534	2.268275	-6.409460
153	6	0	1.909605	1.713835	-7.137555
154	6	0	1.707460	0.982487	-8.328700
155	6	0	0.394977	0.870494	-8.801725
156	6	0	-0.695986	1.449422	-8.143057
157	6	0	2.879963	0.325769	-9.026103
158	6	0	2.675336	0.121923	-10.529530
159	1	0	1.022946	2.783895	-5.468837
160	1	0	0.214757	0.316021	-9.726169
161	1	0	3.769717	1.015531	-8.916866
162	1	0	3.577059	-0.305294	-10.986412
163	1	0	2.469948	1.075940	-11.030257
164	1	0	1.846276	-0.556417	-10.755078
165	8	0	1.494479	-5.159152	-5.121408
166	8	0	-3.083466	-4.280886	-5.194489
167	6	0	0.418804	-4.763794	-5.892483
168	6	0	-0.798461	-4.722938	-5.207326
169	6	0	-1.926153	-4.310294	-5.927242
170	6	0	-1.865123	-3.964197	-7.297347
171	6	0	-0.618129	-4.022587	-7.926247
172	6	0	0.540983	-4.441287	-7.258231
173	6	0	-3.126188	-3.539244	-8.021816
174	6	0	-3.101783	-3.844610	-9.522856
175	1	0	-0.865387	-4.968956	-4.150215
176	1	0	-0.543910	-3.741054	-8.979514
177	1	0	-3.981053	-4.141431	-7.589442

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179	1	0	-2.926592	-4.910905	-9.706041
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183	1	0	-5.837111	-2.397268	-5.635226
184	1	0	-4.836975	2.117033	-6.150815
185	1	0	-2.373952	2.387850	-6.390642
186	1	0	3.898566	1.477789	-7.099872
187	1	0	2.376558	-5.115689	-5.636670
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189	8	0	1.027315	-7.368581	-3.529452
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195	6	0	3.062795	-8.585124	-0.778847
196	6	0	1.986885	-8.446889	-1.658136
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205	8	0	2.415998	-5.308007	5.997732
206	8	0	-1.909421	-6.351087	4.339371
207	6	0	1.573596	-6.107389	5.270247
208	6	0	0.212977	-5.807405	5.151009
209	6	0	-0.580623	-6.710205	4.433010
210	6	0	-0.069450	-7.894530	3.868618
211	6	0	1.311656	-8.116314	3.974465
212	6	0	2.155481	-7.248454	4.671065
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214	6	0	-0.605853	-10.340965	3.476989
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219	1	0	0.376640	-10.604172	3.072831
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237	8	0	-3.136016	-7.489909	2.130736
238	8	0	-1.478474	-7.573614	-2.313525
239	6	0	-2.179360	-7.857881	1.211224
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253	1	0	1.123240	-6.591665	-4.190356
254	1	0	5.902735	-5.902007	-1.179539
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258	1	0	4.172434	-5.155869	5.391876
259	1	0	-3.907266	-6.982421	1.693780
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261	8	0	-1.577740	7.318947	3.711652
262	8	0	2.577433	7.579159	1.428109
263	6	0	-0.813016	7.769019	2.665376
264	6	0	0.535703	7.416693	2.553125
265	6	0	1.253782	7.965752	1.484352
266	6	0	0.677472	8.854908	0.556507
267	6	0	-0.691388	9.131015	0.689300
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273	1	0	2.588788	9.519998	-0.158124
274	1	0	1.799181	11.374311	-1.573176
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278	8	0	-5.256433	4.922547	-3.454903
279	6	0	-2.048619	5.825865	-4.829477
280	6	0	-3.158165	5.063960	-4.461069
281	6	0	-4.163683	5.703916	-3.726701
282	6	0	-4.062053	7.054445	-3.321425
283	6	0	-2.903338	7.754897	-3.678661
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334	8	0	6.291162	5.272040	2.662830
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340	6	0	7.580196	4.837136	-1.285474
341	6	0	8.714868	3.954129	2.282702
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343	1	0	4.871915	6.005170	0.496567
344	1	0	9.292809	3.871833	-0.410942
345	1	0	8.356406	4.492728	3.212761
346	1	0	10.372034	5.350862	2.070163
347	1	0	10.661832	3.804172	1.270112
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357	6	0	9.099706	-0.122324	-3.688796
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370	6	0	7.733976	3.456255	-3.344762
371	6	0	8.526879	2.319234	-3.183957
372	6	0	8.202418	1.093319	-3.781994
373	6	0	8.078562	4.786995	-2.714777
374	6	0	9.569367	5.123404	-2.826544
375	1	0	5.233974	2.038175	-5.263956
376	1	0	9.434976	2.387406	-2.581678
377	1	0	7.527490	5.588594	-3.295988
378	1	0	9.780041	6.111472	-2.400064

379	1	0	9.883085	5.140490	-3.877965
380	1	0	10.206341	4.399905	-2.308571
381	8	0	6.676386	2.945856	4.086265
382	8	0	7.877222	-1.574808	3.279916
383	6	0	7.471592	2.053806	3.403178
384	6	0	7.240966	0.707894	3.709278
385	6	0	8.008298	-0.242297	3.026829
386	6	0	8.959975	0.122802	2.042267
387	6	0	9.153053	1.482192	1.788806
388	6	0	8.449981	2.476909	2.482260
389	6	0	9.721519	-0.959280	1.310232
390	6	0	11.209912	-0.628581	1.156374
391	1	0	6.481493	0.420777	4.430356
392	1	0	9.882245	1.781759	1.033294
393	1	0	9.668492	-1.897377	1.943312
394	1	0	11.383219	0.277974	0.568310
395	1	0	11.743287	-1.448527	0.660586
396	1	0	11.674587	-0.474132	2.138362
397	1	0	5.765429	5.577558	-2.919176
398	1	0	5.350835	5.663865	2.753850
399	1	0	8.018861	-2.634815	1.869916
400	1	0	6.750793	-3.109783	-3.664037
401	1	0	7.115337	-0.949056	-4.799115
402	1	0	5.011678	4.373598	-4.976334
403	1	0	6.792734	3.903884	3.753040
404	1	0	7.210258	-1.790386	4.076463
405	8	0	-4.986460	-5.896482	0.781020
406	8	0	-5.359120	-3.595264	4.911789
407	6	0	-5.751528	-5.106689	1.599723
408	6	0	-5.143991	-4.774057	2.818625
409	6	0	-5.864470	-3.939812	3.676368
410	6	0	-7.134930	-3.419724	3.351269
411	6	0	-7.702371	-3.810241	2.133466
412	6	0	-7.053703	-4.687076	1.256652
413	6	0	-7.820855	-2.457765	4.295229
414	6	0	-9.310216	-2.771045	4.470758
415	1	0	-4.150315	-5.133983	3.058745
416	1	0	-8.687878	-3.424749	1.862692
417	1	0	-7.347253	-2.585237	5.315601
418	1	0	-9.870934	-2.696593	3.533420
419	1	0	-9.773759	-2.078699	5.184211
420	1	0	-9.450358	-3.789350	4.853866
421	8	0	-7.240583	3.443950	0.287067
422	8	0	-7.495049	0.962601	-3.747221
423	6	0	-7.764178	2.366773	-0.387584
424	6	0	-7.337707	2.238071	-1.713457
425	6	0	-7.813625	1.140558	-2.441227
426	6	0	-8.660343	0.163483	-1.853966
427	6	0	-9.069552	0.355745	-0.534297
428	6	0	-8.656193	1.461399	0.222327
429	6	0	-9.062613	-1.046265	-2.669002
430	6	0	-10.532069	-1.431523	-2.469367
431	1	0	-6.635325	2.947213	-2.145441
432	1	0	-9.733479	-0.378501	-0.073358
433	1	0	-8.952705	-0.769793	-3.761773
434	1	0	-10.800166	-2.285460	-3.103307
435	1	0	-11.189820	-0.595939	-2.739546
436	1	0	-10.761235	-1.706150	-1.435350
437	8	0	-5.543918	-0.883705	5.204267
438	8	0	-7.066996	3.006091	2.958732
439	6	0	-6.481789	-0.307763	4.371587
440	6	0	-6.265148	1.047562	4.101066
441	6	0	-7.171706	1.682106	3.243517
442	6	0	-8.233658	0.978436	2.619222
443	6	0	-8.409302	-0.366689	2.944626
444	6	0	-7.573330	-1.030410	3.854760
445	6	0	-9.130978	1.703312	1.638702

446	6	0	-10.611656	1.361885	1.832190
447	1	0	-5.424905	1.577428	4.541623
448	1	0	-9.232207	-0.919187	2.485424
449	1	0	-9.029753	2.813071	1.847362
450	1	0	-10.826478	0.301762	1.665944
451	1	0	-11.236342	1.934091	1.134969
452	1	0	-10.937154	1.607346	2.850491
453	8	0	-6.652409	-1.558536	-4.236597
454	8	0	-5.653754	-5.513757	-1.826306
455	6	0	-6.990743	-2.406468	-3.217898
456	6	0	-6.130844	-3.502921	-3.062629
457	6	0	-6.411623	-4.402836	-2.030353
458	6	0	-7.495773	-4.207043	-1.138149
459	6	0	-8.325497	-3.104108	-1.345462
460	6	0	-8.116960	-2.198004	-2.393894
461	6	0	-7.708666	-5.192313	-0.012143
462	6	0	-9.185705	-5.544101	0.194888
463	1	0	-5.277436	-3.636335	-3.721645
464	1	0	-9.172183	-2.945514	-0.673870
465	1	0	-7.190643	-6.156546	-0.303815
466	1	0	-9.614222	-5.963179	-0.724521
467	1	0	-9.793172	-4.676299	0.469698
468	1	0	-9.302600	-6.291902	0.988141
469	1	0	-5.382548	-5.988890	-0.166443
470	1	0	-4.415476	-3.963138	5.062689
471	1	0	-7.512583	3.463249	1.271887
472	1	0	-6.754741	1.673710	-4.116804
473	1	0	-5.680572	-1.895804	5.294267
474	1	0	-6.357428	3.516519	3.569561
475	1	0	-7.185738	-0.672183	-4.216081
476	1	0	-4.893277	-5.661023	-2.562980
477	8	0	-2.860997	-4.483523	5.551223
478	1	0	-2.882376	-5.442868	5.766225
479	1	0	-2.229872	-4.424465	4.799995
480	8	0	5.522954	-4.331516	-3.838435
481	1	0	4.882144	-4.244674	-3.098709
482	1	0	5.908940	-5.225400	-3.710883
483	8	0	3.757704	6.296096	3.117333
484	1	0	3.720067	7.269862	2.991003
485	1	0	3.091053	5.952585	2.481102
486	8	0	-5.570138	2.301079	-4.756903
487	1	0	-4.730893	1.893876	-4.167353
488	1	0	-5.542051	3.251237	-4.513845
489	8	0	3.869303	4.602105	-5.980818
490	1	0	3.187816	5.188396	-5.595734
491	1	0	3.415651	3.753956	-6.174764
492	8	0	-5.568224	4.522272	4.441831
493	1	0	-4.778645	4.111019	4.845263
494	1	0	-5.237662	5.250855	3.878418
495	8	0	6.431028	-2.460500	5.257610
496	1	0	6.043547	-3.311810	4.981033
497	1	0	5.683101	-1.910180	5.563910
498	8	0	-3.834992	-6.336651	-3.452289
499	1	0	-3.136379	-6.744132	-2.905935
500	1	0	-3.383276	-5.663814	-4.005590

Sum of electronic and thermal Free Energies= -0.696659
1 imaginary frequency: -248.3198

IN1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.933999	4.066972	-2.538977
2	1	0	0.898096	1.817769	-3.608300
3	1	0	2.514988	0.066207	-2.885378

4	1	0	6.726971	-0.950242	-0.028064
5	1	0	5.329544	-2.014944	0.327557
6	1	0	6.057301	-0.992955	1.625674
7	1	0	4.686962	-0.444600	-1.818077
8	1	0	3.435070	2.487872	2.612969
9	1	0	2.509108	1.489102	3.755298
10	1	0	4.285370	1.518880	3.844235
11	1	0	3.933453	-0.545597	2.651869
12	1	0	1.608171	0.953685	1.234177
13	1	0	2.650557	-1.986321	1.146894
14	1	0	-1.159898	-3.156016	-1.239923
15	1	0	-0.089508	-2.947411	-2.631820
16	1	0	0.824352	-3.606369	-0.042790
17	1	0	-0.820341	-0.180030	0.370594
18	6	0	-0.674875	-1.058122	-1.650133
19	6	0	-0.050328	-0.434926	-0.389575
20	7	0	0.838855	-1.482581	0.204869
21	8	0	4.547326	0.914812	1.239553
22	6	0	4.380520	0.271544	-1.006336
23	6	0	1.641440	3.300468	-2.218702
24	6	0	2.211287	-2.766706	-1.472855
25	8	0	2.188473	-3.773014	-2.336864
26	6	0	3.454255	1.338245	-1.395879
27	8	0	3.187988	-2.042676	-1.332644
28	6	0	1.977327	-1.137764	0.932238
29	6	0	2.249351	0.098020	1.420904
30	6	0	3.478070	0.358413	2.192103
31	7	0	4.857585	0.068066	0.198359
32	6	0	5.778505	-1.020335	0.552899
33	6	0	2.572890	3.586756	-1.216001
34	1	0	-0.280752	-0.577215	-2.564123
35	6	0	0.896613	-2.682113	-0.677302
36	6	0	-0.314839	-2.552440	-1.621786
37	6	0	1.617472	2.034262	-2.816589
38	6	0	2.525731	1.054385	-2.416649
39	6	0	3.480087	2.609714	-0.798949
40	1	0	0.508692	0.495271	-0.629134
41	1	0	-1.769086	-0.912601	-1.672053
42	6	0	3.428319	1.531097	3.151828
43	1	0	2.594756	4.578231	-0.760458
44	1	0	4.210869	2.832241	-0.014751
45	8	0	4.095421	-0.408294	7.568103
46	8	0	2.482445	4.102403	6.943553
47	6	0	3.192933	0.605248	7.772740
48	6	0	3.358811	1.863389	7.184067
49	6	0	2.400104	2.836607	7.482821
50	6	0	1.305956	2.593286	8.337788
51	6	0	1.167637	1.302878	8.866088
52	6	0	2.098345	0.292209	8.608867
53	6	0	0.321828	3.700922	8.647590
54	6	0	0.097898	3.855139	10.155280
55	1	0	4.191645	2.066976	6.518717
56	1	0	0.302524	1.079655	9.494231
57	1	0	0.776479	4.675237	8.292753
58	1	0	-0.311761	2.950557	10.616004
59	1	0	-0.595520	4.677850	10.367322
60	1	0	1.043801	4.076803	10.665744
61	8	0	-6.219946	1.139722	6.330743
62	8	0	-4.538824	-3.387072	6.473300
63	6	0	-5.393422	0.157691	6.820736
64	6	0	-5.433380	-1.147880	6.321170
65	6	0	-4.572134	-2.080433	6.907558
66	6	0	-3.698861	-1.751158	7.965507
67	6	0	-3.671446	-0.418825	8.396386
68	6	0	-4.510732	0.556115	7.848330
69	6	0	-2.821764	-2.816774	8.587108
70	6	0	-2.943518	-2.832451	10.114280

71	1	0	-6.095898	-1.415985	5.503716
72	1	0	-2.968631	-0.132265	9.181499
73	1	0	-3.196099	-3.823390	8.228563
74	1	0	-2.637219	-1.886633	10.572172
75	1	0	-2.325122	-3.626888	10.549176
76	1	0	-3.982390	-3.015945	10.416883
77	8	0	-0.033715	4.629095	5.910357
78	8	0	-4.440028	3.145939	5.592811
79	6	0	-1.069132	3.981984	6.552155
80	6	0	-2.236858	3.865900	5.793341
81	6	0	-3.326056	3.216534	6.387240
82	6	0	-3.272314	2.694107	7.700604
83	6	0	-2.072791	2.833738	8.405872
84	6	0	-0.960532	3.495455	7.870757
85	6	0	-4.482931	2.003464	8.293129
86	6	0	-4.576988	2.134372	9.816346
87	1	0	-2.287942	4.229172	4.770631
88	1	0	-2.002806	2.421321	9.415363
89	1	0	-5.401438	2.515221	7.874364
90	1	0	-4.583385	3.188062	10.120238
91	1	0	-3.747782	1.643582	10.335385
92	1	0	-5.504569	1.677421	10.184804
93	8	0	-1.865339	-4.004479	6.107228
94	8	0	2.510410	-2.498113	6.639991
95	6	0	-0.998657	-3.279600	6.894577
96	6	0	0.310728	-3.220064	6.409117
97	6	0	1.244805	-2.505898	7.168623
98	6	0	0.903804	-1.863676	8.381058
99	6	0	-0.425554	-1.948819	8.809128
100	6	0	-1.395347	-2.670181	8.103291
101	6	0	1.958199	-1.110142	9.163755
102	6	0	1.709971	-1.103503	10.675133
103	1	0	0.583579	-3.676640	5.461323
104	1	0	-0.715582	-1.444044	9.733739
105	1	0	2.942197	-1.647384	9.006853
106	1	0	1.637854	-2.126195	11.065004
107	1	0	0.790430	-0.577908	10.950866
108	1	0	2.536573	-0.606684	11.199099
109	1	0	4.827658	-0.149360	6.903703
110	1	0	3.222103	4.178764	6.242947
111	1	0	-6.799981	0.807811	5.559642
112	1	0	-5.077593	-3.525856	5.612629
113	1	0	0.820825	4.645653	6.471001
114	1	0	-5.192277	2.596188	6.011014
115	1	0	-2.830222	-3.958899	6.445201
116	1	0	3.161060	-1.928197	7.181713
117	8	0	-4.549714	-0.377908	-7.548258
118	8	0	-2.247438	3.848064	-7.124867
119	6	0	-3.492350	0.466011	-7.783132
120	6	0	-3.467278	1.767457	-7.271626
121	6	0	-2.359615	2.556875	-7.596025
122	6	0	-1.304954	2.094861	-8.408983
123	6	0	-1.361038	0.767223	-8.854897
124	6	0	-2.443492	-0.067903	-8.564323
125	6	0	-0.162266	3.019625	-8.769416
126	6	0	0.090133	3.043399	-10.280622
127	1	0	-4.269214	2.137607	-6.640425
128	1	0	-0.530054	0.372358	-9.443644
129	1	0	-0.467333	4.071340	-8.481939
130	1	0	-0.808586	3.371972	-10.817663
131	1	0	0.360822	2.059892	-10.678307
132	1	0	0.901670	3.736494	-10.532590
133	8	0	5.855350	-0.342412	-6.164874
134	8	0	3.530311	-4.565450	-6.068779
135	6	0	4.905426	-1.221317	-6.623863
136	6	0	4.740758	-2.479734	-6.038861
137	6	0	3.764138	-3.316729	-6.585752

138	6	0	2.964240	-2.931118	-7.685211
139	6	0	3.148746	-1.647579	-8.209765
140	6	0	4.115754	-0.771797	-7.704537
141	6	0	1.934491	-3.891184	-8.238979
142	6	0	2.054404	-4.040579	-9.759465
143	1	0	5.340553	-2.788086	-5.182716
144	1	0	2.514136	-1.317199	-9.033928
145	1	0	2.144339	-4.914289	-7.803430
146	1	0	3.053000	-4.407140	-10.030363
147	1	0	1.904069	-3.095300	-10.289847
148	1	0	1.320697	-4.759295	-10.142637
149	8	0	0.809843	-4.653265	-5.649923
150	8	0	-3.294224	-2.595604	-6.414645
151	6	0	0.064823	-3.908739	-6.528310
152	6	0	-1.227593	-3.613527	-6.079667
153	6	0	-2.038696	-2.839432	-6.916492
154	6	0	-1.597465	-2.358893	-8.169124
155	6	0	-0.295934	-2.688937	-8.566296
156	6	0	0.548805	-3.483869	-7.785018
157	6	0	-2.512951	-1.509823	-9.024811
158	6	0	-2.245877	-1.640674	-10.527331
159	1	0	-1.574376	-3.946107	-5.105815
160	1	0	0.071300	-2.319422	-9.526861
161	1	0	-3.569409	-1.879440	-8.857404
162	1	0	-2.978056	-1.058881	-11.101323
163	1	0	-2.326243	-2.686067	-10.849580
164	1	0	-1.251879	-1.281942	-10.812645
165	8	0	0.333242	4.076044	-6.099523
166	8	0	4.458519	1.955076	-5.634087
167	6	0	1.261839	3.238685	-6.688855
168	6	0	2.402628	3.005533	-5.916824
169	6	0	3.372711	2.144388	-6.445899
170	6	0	3.233077	1.539765	-7.717326
171	6	0	2.068291	1.810911	-8.440684
172	6	0	1.072820	2.675913	-7.965749
173	6	0	4.319172	0.625708	-8.247596
174	6	0	4.432757	0.638109	-9.775290
175	1	0	2.520679	3.444124	-4.929562
176	1	0	1.931303	1.339041	-9.416911
177	1	0	5.307308	1.012045	-7.853981
178	1	0	5.274343	0.012397	-10.100482
179	1	0	4.609679	1.653240	-10.148991
180	1	0	3.535877	0.251238	-10.268936
181	1	0	-5.254160	0.043231	-6.943472
182	1	0	-2.981121	4.078116	-6.451341
183	1	0	6.326929	-0.700197	-5.313416
184	1	0	4.050148	-4.720913	-5.171180
185	1	0	1.792379	-4.763057	-5.938323
186	1	0	-3.844575	-1.982117	-7.013104
187	1	0	-0.519144	4.159051	-6.658995
188	1	0	5.102145	1.228297	-5.983151
189	8	0	1.366468	6.383508	-4.993937
190	8	0	-3.153488	6.509475	-3.543433
191	6	0	0.365614	6.941734	-4.244929
192	6	0	-0.928857	6.412183	-4.252748
193	6	0	-1.899483	7.081379	-3.497329
194	6	0	-1.622858	8.253375	-2.766627
195	6	0	-0.296297	8.707952	-2.752515
196	6	0	0.715136	8.081229	-3.483637
197	6	0	-2.730543	8.989652	-2.042099
198	6	0	-2.576600	10.512295	-2.119181
199	1	0	-1.169262	5.516009	-4.816149
200	1	0	-0.048400	9.589822	-2.157034
201	1	0	-3.702382	8.743826	-2.567735
202	1	0	-2.530680	10.849386	-3.161818
203	1	0	-1.673229	10.872833	-1.617415
204	1	0	-3.431843	11.011046	-1.645474

205	8	0	-0.795566	6.923763	4.557722
206	8	0	3.689314	6.327648	3.112628
207	6	0	0.262751	7.276850	3.763416
208	6	0	1.477870	6.587000	3.823670
209	6	0	2.520702	7.056118	3.015908
210	6	0	2.394028	8.187648	2.187617
211	6	0	1.136482	8.807013	2.127253
212	6	0	0.057342	8.381489	2.904269
213	6	0	3.584619	8.712509	1.412357
214	6	0	3.632306	10.243534	1.370123
215	1	0	1.600762	5.717206	4.461238
216	1	0	1.001215	9.658672	1.456452
217	1	0	4.518694	8.382689	1.960244
218	1	0	3.637262	10.663843	2.383081
219	1	0	2.780945	10.679498	0.838126
220	1	0	4.542587	10.587530	0.862453
221	8	0	-4.666844	7.159342	-1.309629
222	8	0	-3.247500	6.891863	3.212576
223	6	0	-3.827143	7.538728	-0.287499
224	6	0	-3.959829	6.997098	0.992543
225	6	0	-3.088706	7.472005	1.981195
226	6	0	-2.133021	8.481026	1.727727
227	6	0	-2.008921	8.944425	0.412350
228	6	0	-2.843117	8.495959	-0.616822
229	6	0	-1.302135	9.043889	2.861127
230	6	0	-1.209400	10.572487	2.808708
231	1	0	-4.695383	6.228271	1.214545
232	1	0	-1.242296	9.687595	0.184023
233	1	0	-1.831602	8.790536	3.830620
234	1	0	-0.705982	10.935686	1.907456
235	1	0	-0.654941	10.958965	3.672719
236	1	0	-2.209570	11.023555	2.826520
237	8	0	5.261656	6.593630	0.833470
238	8	0	3.790489	6.167955	-3.661456
239	6	0	4.476491	7.001949	-0.219984
240	6	0	4.530298	6.351097	-1.454277
241	6	0	3.723183	6.857452	-2.481140
242	6	0	2.905798	7.997182	-2.309141
243	6	0	2.850541	8.572865	-1.034638
244	6	0	3.624766	8.099470	0.030243
245	6	0	2.147156	8.568489	-3.488207
246	6	0	2.250187	10.095411	-3.559580
247	1	0	5.165655	5.484046	-1.619474
248	1	0	2.188244	9.424780	-0.867553
249	1	0	2.634505	8.172244	-4.432069
250	1	0	1.803787	10.591371	-2.692224
251	1	0	1.743131	10.478633	-4.453768
252	1	0	3.299521	10.412395	-3.611153
253	1	0	1.066125	5.535399	-5.485267
254	1	0	-3.784971	6.904824	-2.837752
255	1	0	-0.602695	6.089025	5.116822
256	1	0	4.365185	6.585348	2.385338
257	1	0	-5.369439	6.486938	-0.997826
258	1	0	-2.506395	7.152618	3.861464
259	1	0	5.874499	5.816266	0.577405
260	1	0	3.096581	6.486162	-4.337881
261	8	0	-0.819768	-6.445287	5.268592
262	8	0	-4.816007	-6.016294	2.739280
263	6	0	-1.660477	-6.878849	4.274443
264	6	0	-2.845254	-6.196385	3.981891
265	6	0	-3.668021	-6.740596	2.988670
266	6	0	-3.358126	-7.937347	2.314062
267	6	0	-2.131190	-8.548807	2.611792
268	6	0	-1.266956	-8.050850	3.589778
269	6	0	-4.327821	-8.531224	1.313006
270	6	0	-4.389239	-10.060468	1.388091
271	1	0	-3.106673	-5.274686	4.491767

272	1	0	-1.845917	-9.450884	2.065334
273	1	0	-5.362900	-8.159473	1.579280
274	1	0	-5.147346	-10.450523	0.697171
275	1	0	-4.655291	-10.393139	2.398437
276	1	0	-3.438162	-10.534991	1.126006
277	8	0	-0.504433	-6.808569	-4.517276
278	8	0	3.576093	-7.037273	-2.105939
279	6	0	0.267547	-7.338182	-3.511730
280	6	0	1.562578	-6.873273	-3.273802
281	6	0	2.299427	-7.509628	-2.266956
282	6	0	1.773343	-8.573918	-1.500601
283	6	0	0.453537	-8.966628	-1.753763
284	6	0	-0.318937	-8.381851	-2.761775
285	6	0	2.625371	-9.249686	-0.446875
286	6	0	2.414287	-10.766335	-0.395687
287	1	0	1.980419	-6.030221	-3.820852
288	1	0	0.015875	-9.764730	-1.150956
289	1	0	3.709848	-9.089384	-0.730941
290	1	0	3.091101	-11.227079	0.334222
291	1	0	2.618591	-11.220069	-1.373313
292	1	0	1.393167	-11.041535	-0.114545
293	8	0	4.372492	-7.340917	0.516035
294	8	0	1.853084	-6.461700	4.444091
295	6	0	3.291788	-7.574513	1.325468
296	6	0	3.099931	-6.856359	2.508813
297	6	0	2.005253	-7.214879	3.305002
298	6	0	1.136106	-8.274121	2.970296
299	6	0	1.336629	-8.912193	1.737729
300	6	0	2.402226	-8.587161	0.895805
301	6	0	0.052488	-8.706954	3.934090
302	6	0	-0.064597	-10.232068	4.032108
303	1	0	3.760727	-6.042648	2.795058
304	1	0	0.640746	-9.695410	1.430267
305	1	0	0.351159	-8.344682	4.965095
306	1	0	0.894721	-10.677341	4.324086
307	1	0	-0.361972	-10.694574	3.085739
308	1	0	-0.808590	-10.518070	4.785284
309	8	0	-5.746441	-6.450551	0.169835
310	8	0	-3.150742	-6.367144	-3.805226
311	6	0	-4.724310	-6.944140	-0.612177
312	6	0	-4.437007	-6.381010	-1.857324
313	6	0	-3.415152	-6.976843	-2.607508
314	6	0	-2.724231	-8.127277	-2.163891
315	6	0	-3.010752	-8.604556	-0.880443
316	6	0	-4.006650	-8.034475	-0.078703
317	6	0	-1.731658	-8.817578	-3.075753
318	6	0	-1.893357	-10.341942	-3.056205
319	1	0	-4.968426	-5.508232	-2.226579
320	1	0	-2.445847	-9.455873	-0.495030
321	1	0	-1.958215	-8.488269	-4.135941
322	1	0	-2.914211	-10.629888	-3.334392
323	1	0	-1.686925	-10.775878	-2.073132
324	1	0	-1.206699	-10.812240	-3.771124
325	1	0	-1.128077	-5.561575	5.675014
326	1	0	-5.287392	-6.326212	1.881879
327	1	0	-0.048219	-6.019504	-4.979884
328	1	0	4.023904	-7.396523	-1.263372
329	1	0	4.956502	-6.568527	0.851551
330	1	0	0.980685	-6.665018	4.928171
331	1	0	-6.240169	-5.687275	-0.289819
332	1	0	-2.296741	-6.725871	-4.242378
333	8	0	-6.831609	-4.270833	-1.193303
334	8	0	-7.608810	-2.491488	3.131888
335	6	0	-7.556824	-3.409857	-0.412220
336	6	0	-7.187480	-3.400854	0.939849
337	6	0	-7.876883	-2.525565	1.783122
338	6	0	-8.882610	-1.651850	1.315640

339	6	0	-9.220833	-1.717983	-0.040513
340	6	0	-8.604653	-2.614530	-0.921253
341	6	0	-9.536318	-0.677185	2.269913
342	6	0	-11.050547	-0.573245	2.061587
343	1	0	-6.386291	-4.037565	1.298765
344	1	0	-9.998422	-1.052784	-0.422682
345	1	0	-9.385674	-1.078838	3.318555
346	1	0	-11.527858	-1.553669	2.180360
347	1	0	-11.315021	-0.199958	1.067143
348	1	0	-11.498901	0.108152	2.795048
349	8	0	-6.391667	5.202252	-0.334015
350	8	0	-6.244403	3.459989	-4.743505
351	6	0	-6.987080	4.417671	-1.288279
352	6	0	-6.289657	4.348209	-2.502152
353	6	0	-6.837100	3.544298	-3.505837
354	6	0	-8.020344	2.795866	-3.321217
355	6	0	-8.681615	2.918931	-2.094811
356	6	0	-8.212149	3.753647	-1.073219
357	6	0	-8.514379	1.886202	-4.424625
358	6	0	-10.033209	1.958036	-4.611635
359	1	0	-5.358268	4.885934	-2.637254
360	1	0	-9.600139	2.350470	-1.931823
361	1	0	-8.056128	2.251840	-5.394311
362	1	0	-10.583609	1.632551	-3.723195
363	1	0	-10.353348	1.319429	-5.444291
364	1	0	-10.350190	2.983771	-4.835811
365	8	0	-6.063798	0.852368	-5.589517
366	8	0	-6.779539	-3.486392	-3.802881
367	6	0	-6.845963	0.021335	-4.819297
368	6	0	-6.384459	-1.296226	-4.722795
369	6	0	-7.132142	-2.178990	-3.935699
370	6	0	-8.293199	-1.763999	-3.235091
371	6	0	-8.708402	-0.439258	-3.377547
372	6	0	-8.025163	0.472216	-4.194716
373	6	0	-9.030752	-2.758753	-2.367297
374	6	0	-10.550936	-2.675875	-2.541895
375	1	0	-5.472115	-1.607402	-5.223688
376	1	0	-9.599245	-0.102894	-2.843371
377	1	0	-8.728132	-3.795813	-2.709066
378	1	0	-11.056327	-3.435073	-1.933012
379	1	0	-10.828685	-2.849759	-3.589230
380	1	0	-10.957292	-1.701100	-2.255295
381	8	0	-7.372292	0.091673	4.044967
382	8	0	-7.102332	4.455900	2.197263
383	6	0	-7.827583	0.993011	3.110233
384	6	0	-7.211383	2.248711	3.155624
385	6	0	-7.625032	3.196936	2.213869
386	6	0	-8.603737	2.907152	1.231141
387	6	0	-9.188962	1.639336	1.241997
388	6	0	-8.848331	0.669506	2.194606
389	6	0	-8.974670	3.966524	0.217817
390	6	0	-10.488073	4.060152	-0.004303
391	1	0	-6.430719	2.462526	3.879470
392	1	0	-9.943139	1.397736	0.490282
393	1	0	-8.653668	4.967163	0.641012
394	1	0	-10.915738	3.133609	-0.399675
395	1	0	-10.730752	4.862287	-0.711543
396	1	0	-11.003547	4.280192	0.939128
397	1	0	-7.033339	-4.169674	-2.196797
398	1	0	-6.824786	-3.098223	3.388242
399	1	0	-6.845684	5.129327	0.585122
400	1	0	-5.352817	3.959908	-4.785479
401	1	0	-6.373613	1.823347	-5.547262
402	1	0	-5.948131	-3.771449	-4.407902
403	1	0	-7.749913	-0.845102	3.896591
404	1	0	-6.424375	4.642224	2.991593
405	8	0	6.566779	4.292322	0.042330

406	8	0	6.230461	2.881216	4.556037
407	6	0	7.070746	3.509892	1.049204
408	6	0	6.392261	3.625088	2.269887
409	6	0	6.822535	2.803462	3.315485
410	6	0	7.869640	1.868445	3.171441
411	6	0	8.533217	1.825316	1.940013
412	6	0	8.183446	2.661168	0.873905
413	6	0	8.229400	0.948821	4.317620
414	6	0	9.742488	0.796207	4.497454
415	1	0	5.559957	4.310651	2.378986
416	1	0	9.356508	1.118634	1.808683
417	1	0	7.841585	1.429417	5.268660
418	1	0	10.228330	0.348287	3.624234
419	1	0	9.971056	0.157024	5.359367
420	1	0	10.215361	1.770935	4.669311
421	8	0	5.632302	-5.133864	1.558415
422	8	0	6.414254	-3.571189	-2.803279
423	6	0	6.459758	-4.429080	0.705860
424	6	0	6.027604	-4.388497	-0.619859
425	6	0	6.790434	-3.647580	-1.547281
426	6	0	7.970501	-2.959239	-1.109203
427	6	0	8.358799	-3.052255	0.219512
428	6	0	7.619354	-3.781491	1.166955
429	6	0	8.740468	-2.146247	-2.124239
430	6	0	10.259354	-2.249470	-1.950042
431	1	0	5.124358	-4.900886	-0.929131
432	1	0	9.264129	-2.537919	0.548809
433	1	0	8.507291	-2.576371	-3.145797
434	1	0	10.779746	-1.681179	-2.729964
435	1	0	10.582976	-3.295077	-2.026161
436	1	0	10.601565	-1.871671	-0.982256
437	8	0	5.611425	0.423174	5.444527
438	8	0	5.676634	-4.113845	4.057237
439	6	0	6.273969	-0.587142	4.776157
440	6	0	5.604640	-1.815519	4.760461
441	6	0	6.225450	-2.875481	4.088192
442	6	0	7.451875	-2.705036	3.391142
443	6	0	8.072779	-1.458862	3.448891
444	6	0	7.523603	-0.382364	4.164974
445	6	0	8.028182	-3.875149	2.618165
446	6	0	9.542090	-4.013399	2.805599
447	1	0	4.645315	-1.936724	5.256455
448	1	0	9.023067	-1.315527	2.929296
449	1	0	7.565543	-4.818823	3.043810
450	1	0	10.094468	-3.145143	2.433274
451	1	0	9.918691	-4.891803	2.266273
452	1	0	9.795064	-4.137015	3.865120
453	8	0	6.505397	-1.225818	-3.722061
454	8	0	7.087751	3.279034	-2.383216
455	6	0	7.191776	-0.334187	-2.979963
456	6	0	6.776671	1.003050	-3.099949
457	6	0	7.412716	1.956390	-2.301901
458	6	0	8.396269	1.605695	-1.348923
459	6	0	8.805161	0.268986	-1.293643
460	6	0	8.246665	-0.713582	-2.113704
461	6	0	8.951673	2.669938	-0.432929
462	6	0	10.464581	2.551960	-0.226059
463	1	0	5.992153	1.272897	-3.801546
464	1	0	9.591343	-0.013137	-0.589846
465	1	0	8.774648	3.672935	-0.928056
466	1	0	10.989334	2.620133	-1.188008
467	1	0	10.756275	1.602183	0.233194
468	1	0	10.838128	3.358089	0.415849
469	1	0	7.017117	4.110367	-0.871034
470	1	0	5.464488	3.558793	4.580426
471	1	0	5.950814	-5.096352	2.526277
472	1	0	5.140435	-4.217268	-3.196970

473	1	0	6.141999	1.298013	5.435765
474	1	0	4.849048	-4.235264	4.723076
475	1	0	6.677816	-2.310606	-3.420358
476	1	0	6.464722	3.511152	-3.218797
477	8	0	4.072854	4.584804	4.762135
478	1	0	4.331527	5.531981	4.795220
479	1	0	3.490028	4.528068	3.973279
480	8	0	-3.806680	4.715682	-5.041355
481	1	0	-3.258060	4.631646	-4.231075
482	1	0	-3.907540	5.685189	-5.158883
483	8	0	-5.543053	-4.087273	4.028881
484	1	0	-5.823097	-5.026799	4.096108
485	1	0	-4.782570	-4.114474	3.405883
486	8	0	4.224308	-4.658455	-3.553571
487	1	0	3.132029	-3.918620	-2.886638
488	1	0	4.194295	-5.545393	-3.137587
489	8	0	-4.912353	-4.583063	-5.225751
490	1	0	-4.472440	-5.253673	-4.667309
491	1	0	-4.196132	-4.011841	-5.573348
492	8	0	3.797581	-4.818888	5.683297
493	1	0	3.133165	-4.141545	5.922557
494	1	0	3.304951	-5.525241	5.215865
495	8	0	-5.495480	5.296308	4.071742
496	1	0	-4.863857	5.917162	3.663640
497	1	0	-4.953517	4.631832	4.542298
498	8	0	5.733658	4.159224	-4.406066
499	1	0	5.111436	4.832884	-4.074323
500	1	0	5.186955	3.486295	-4.866163

Sum of electronic and thermal Free Energies= -0.706492
0 imaginary frequency

TS2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.067641	-6.211194	-5.920654
2	6	0	-3.573136	-3.593698	-7.372685
3	6	0	-2.379764	-5.501702	-6.330371
4	6	0	-0.458629	-0.509148	-8.390906
5	6	0	1.855532	-1.250412	-8.059448
6	6	0	-3.495878	-5.103214	-7.271754
7	6	0	-1.090955	-5.808091	-6.784328
8	6	0	-1.719101	-1.173131	-10.496180
9	6	0	-2.753381	-1.443623	-8.212341
10	6	0	-1.626385	-5.954199	-4.027122
11	6	0	-0.359580	-6.257031	-4.539366
12	6	0	-0.222920	0.524237	-7.463013
13	6	0	2.231125	-5.396578	-6.384322
14	6	0	-3.756760	-0.801395	-7.458823
15	6	0	-4.682842	-1.501515	-6.679925
16	6	0	-4.579191	-2.896480	-6.667732
17	6	0	3.048894	-3.295683	-7.337255
18	6	0	2.174261	-4.389251	-7.351005
19	6	0	-2.616363	-5.575631	-4.939943
20	6	0	3.182184	-5.268257	-5.343093
21	6	0	4.072631	-4.188435	-5.278623
22	6	0	3.991780	-3.230249	-6.291412
23	6	0	-3.391837	-5.761524	-8.651253
24	6	0	2.034486	-0.189334	-7.141031
25	6	0	0.596042	-1.394603	-8.648396
26	6	0	1.009725	0.714043	-6.832578
27	6	0	1.290311	-7.268520	-7.791271
28	6	0	1.310700	-6.597232	-6.413409
29	6	0	2.961218	-2.744389	-9.799610

30	6	0	3.000808	-2.191969	-8.370975
31	6	0	-2.669522	-2.839922	-8.127309
32	6	0	-1.807176	-0.627912	-9.066973
33	1	0	4.791965	-4.106457	-4.468170
34	1	0	3.845257	-3.365501	-9.993923
35	1	0	2.956504	-1.932224	-10.535693
36	1	0	0.429776	-2.221652	-9.343129
37	8	0	3.216009	0.054705	-6.491794
38	1	0	1.157196	1.505332	-6.103239
39	1	0	-3.365215	-6.854427	-8.561506
40	8	0	4.846655	-2.150098	-6.326522
41	1	0	0.934125	-6.600661	-8.581408
42	8	0	3.190622	-6.243244	-4.393326
43	8	0	-5.464525	-3.673749	-5.961958
44	1	0	1.724472	-7.365955	-5.693422
45	1	0	-1.870479	-3.354494	-8.665569
46	1	0	-1.344404	-2.201201	-10.532909
47	1	0	-2.708043	-1.172967	-10.971611
48	1	0	-1.818265	-5.980955	-2.958149
49	1	0	-1.052787	-0.556551	-11.111212
50	8	0	-3.786561	0.575492	-7.530534
51	8	0	-1.191136	1.445729	-7.115330
52	8	0	-3.831932	-5.286628	-4.369199
53	1	0	-4.465843	-5.470304	-6.817891
54	1	0	-4.258469	-5.499383	-9.270848
55	1	0	3.959046	-1.595884	-8.289676
56	1	0	2.082415	-3.369454	-9.986488
57	1	0	-2.495920	-5.453761	-9.199544
58	1	0	-0.879686	-5.740571	-7.854086
59	1	0	1.422710	-4.454012	-8.139965
60	1	0	2.299339	-7.594981	-8.073579
61	1	0	-2.234152	0.417108	-9.151701
62	1	0	-5.443870	-0.991163	-6.097660
63	1	0	0.643038	-8.153335	-7.786129
64	8	0	0.561832	-6.620572	-3.592401
65	6	0	0.945768	-0.392795	-2.483333
66	7	0	4.241779	1.283533	-0.210587
67	6	0	0.675191	-1.516128	1.124679
68	6	0	4.204293	-0.029824	-0.593120
69	6	0	3.085918	-0.593649	-1.349642
70	6	0	-0.270147	-2.469182	0.378311
71	7	0	1.954993	-2.263704	1.282838
72	6	0	1.931861	0.153205	-1.663183
73	6	0	3.102322	1.697864	2.867146
74	6	0	0.304578	-3.885424	0.550385
75	6	0	2.803457	0.812422	1.673201
76	6	0	3.222528	-1.900543	-1.860767
77	6	0	5.501134	1.886070	0.272664
78	6	0	1.741188	-3.736266	1.073487
79	6	0	2.222773	-2.444751	-2.668271
80	6	0	2.813350	-4.295142	0.102281
81	6	0	3.595968	-0.420952	1.585255
82	6	0	1.088940	-1.691311	-2.988202
83	6	0	3.175699	-1.747182	1.485474
84	1	0	0.281513	-1.258590	2.133546
85	1	0	0.318217	-2.115929	-3.634513
86	1	0	6.155703	2.100816	-0.595327
87	1	0	2.322176	-3.471109	-3.035980
88	1	0	0.065449	0.195578	-2.740861
89	8	0	4.011767	-4.154078	0.444515
90	1	0	-0.305001	-4.486913	1.247433
91	1	0	6.054888	1.243646	0.983028
92	1	0	2.925681	1.164060	3.814583
93	1	0	-1.300461	-2.402294	0.766938
94	1	0	1.820265	1.170221	-1.274330
95	1	0	0.838333	-0.565422	0.569002
96	1	0	0.301139	-4.436627	-0.417472

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98	1	0	-0.321512	-2.204009	-0.696358
99	1	0	4.002586	-2.513531	1.560575
100	1	0	4.145841	2.043024	2.882819
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102	1	0	4.108157	-2.498283	-1.622287
103	1	0	4.617964	-0.311640	1.972698
104	1	0	5.174143	-0.558186	-0.699050
105	8	0	3.128749	1.717682	0.456587
106	1	0	2.471728	2.595360	2.872912
107	1	0	1.713135	0.696622	1.494727
108	1	0	5.291209	2.844214	0.784498
109	6	0	2.176265	4.906131	7.156829
110	6	0	3.204487	3.960430	7.106932
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112	6	0	3.345215	2.847883	8.124325
113	6	0	0.124508	0.761679	8.392260
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115	6	0	2.287611	1.794511	7.871384
116	6	0	2.485322	0.811099	6.875937
117	6	0	1.547880	-0.196600	6.620761
118	6	0	0.380618	-0.196796	7.389945
119	6	0	-3.422608	5.580703	8.870714
120	6	0	-3.539350	4.878287	7.514607
121	6	0	-0.374741	6.361117	5.900005
122	6	0	-1.286843	5.878234	6.846736
123	6	0	-2.540580	5.371848	6.488673
124	6	0	-2.860263	5.323301	5.111519
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126	6	0	-0.743741	6.272874	4.542360
127	6	0	0.948037	7.665604	7.638471
128	6	0	0.960804	6.965707	6.275759
129	6	0	2.051515	5.918960	6.197027
130	6	0	2.976019	5.930872	5.131833
131	6	0	4.025067	5.011103	5.031601
132	6	0	-2.378161	2.753667	8.330786
133	6	0	-1.156101	0.688073	9.195896
134	6	0	-3.429980	3.373697	7.649532
135	6	0	-2.279785	1.360540	8.436253
136	6	0	-3.260684	0.582564	7.786556
137	6	0	-4.333988	1.146736	7.090880
138	6	0	-4.401588	2.543218	7.048731
139	6	0	4.123844	4.047016	6.039264
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141	1	0	-0.218530	0.732355	11.163816
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144	1	0	1.707088	-0.933237	5.837907
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146	1	0	4.176542	4.092393	9.701531
147	1	0	-2.465064	5.389997	9.365227
148	1	0	-0.795172	2.317032	10.629654
149	1	0	-1.419869	-0.406750	9.308985
150	1	0	-5.077641	0.534219	6.589846
151	1	0	-1.950123	1.103285	11.177987
152	1	0	-1.604693	3.373888	8.788740
153	1	0	-1.012370	5.909289	7.903891
154	1	0	-2.227372	5.690982	3.065996
155	8	0	-4.053420	4.852955	4.629914
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157	8	0	0.076664	6.698858	3.519189
158	1	0	0.170662	8.438227	7.676179
159	1	0	0.767487	6.973322	8.466957
160	1	0	1.911953	8.153808	7.831004
161	1	0	1.194061	7.765720	5.509499
162	1	0	1.443011	4.850219	7.964361
163	1	0	0.904141	2.521598	9.350125

164	1	0	-3.530998	6.666529	8.761185
165	8	0	3.601641	0.747230	6.078625
166	1	0	-4.211940	5.236084	9.551331
167	1	0	-4.572769	5.119589	7.121115
168	1	0	4.724948	5.033374	4.202244
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173	6	0	2.685269	-8.487883	1.340093
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175	6	0	-3.698522	-6.857068	2.831479
176	6	0	1.383100	-8.941626	1.575468
177	6	0	-3.656805	-6.823371	1.435728
178	6	0	3.746111	-8.493544	2.421269
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182	6	0	3.570836	-7.283232	3.313580
183	6	0	2.804245	-7.292519	4.478372
184	6	0	2.643814	-6.152447	5.281843
185	6	0	3.251034	-4.957507	4.845485
186	6	0	4.033155	-4.888963	3.687918
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223	1	0	-1.201352	-9.053761	3.501241
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328	6	0	-9.236115	1.231538	-1.479285
329	6	0	-7.689149	1.370961	-3.315495
330	6	0	-8.207463	-3.331532	1.666993
331	6	0	-10.518623	-0.487201	4.039365
332	6	0	-6.984547	-3.752778	2.229932
333	1	0	-11.137503	-0.743397	-2.126630
334	1	0	-6.208637	3.406627	3.749637
335	8	0	-7.348250	4.485906	1.560866
336	8	0	-6.776726	1.232799	4.972104
337	1	0	-10.961930	0.387182	4.531569
338	1	0	-8.649377	-0.317578	5.081350
339	1	0	-5.513721	-3.539081	3.805467
340	1	0	-9.752845	-1.839288	1.790892
341	8	0	-7.056396	4.181135	-1.144595
342	1	0	-10.043337	0.712884	-0.957107
343	8	0	-6.712721	-1.517250	5.117080
344	1	0	-6.298306	3.046382	-3.291380
345	1	0	-11.250595	0.081284	-3.684179
346	1	0	-10.627339	-4.684512	1.518819
347	1	0	-10.828191	-3.232363	0.532517
348	1	0	-8.397135	-5.143136	0.532830
349	1	0	-9.787572	-1.882864	-0.836121
350	1	0	-5.909207	-3.944619	-3.218248
351	8	0	-6.706163	-5.169831	-0.952582
352	8	0	-6.887523	-1.885203	-4.376979
353	1	0	-11.231868	1.936005	0.373917
354	1	0	-11.302499	3.515902	1.157220
355	1	0	-10.711689	-4.811880	-0.245824
356	1	0	-11.331095	3.399493	-0.610162
357	1	0	-9.130235	4.198235	0.210929
358	1	0	-9.903739	0.772112	1.661159
359	8	0	-6.236077	-4.772043	1.703532
360	1	0	-10.960675	-0.555909	3.040274
361	1	0	-10.830102	-1.378869	4.596997
362	1	0	-11.104604	-1.683621	-3.619062
363	1	0	-8.974989	-0.635909	-4.335101
364	8	0	-7.256903	0.843861	-4.508553

365	6	0	10.511018	-1.488447	2.242333
366	6	0	8.173735	2.191490	2.478116
367	6	0	6.516702	0.956145	3.827242
368	6	0	9.975392	3.105728	-3.181713
369	6	0	7.823903	-0.669293	-3.050543
370	6	0	7.812187	1.770253	-3.267439
371	6	0	7.017284	2.140576	3.274227
372	6	0	8.797663	0.967622	2.175796
373	6	0	6.560048	1.682214	-3.924772
374	6	0	7.149217	-3.394039	-1.096865
375	6	0	6.764688	-3.809686	0.175923
376	6	0	7.350966	-3.184500	1.283433
377	6	0	8.713816	3.527771	2.015161
378	6	0	7.982404	3.720359	-1.752896
379	6	0	8.542769	3.362372	-0.523220
380	6	0	8.339968	-0.244846	2.684000
381	6	0	8.987097	-1.576998	2.367951
382	6	0	7.205835	-0.228624	3.543414
383	6	0	8.106721	3.920817	0.685215
384	6	0	7.065266	4.871797	0.629742
385	6	0	6.462556	5.261533	-0.570468
386	6	0	6.936353	4.668685	-1.747678
387	6	0	10.030916	-1.914998	-2.880545
388	6	0	8.511547	-1.969025	-2.689575
389	6	0	8.449017	3.126677	-3.066606
390	6	0	5.898652	0.460828	-4.097326
391	6	0	8.416239	0.582585	-2.846715
392	6	0	6.542541	-0.693511	-3.638447
393	6	0	10.244612	3.569999	1.980442
394	6	0	8.343342	-2.187772	1.142817
395	6	0	8.698376	-1.805317	-0.155479
396	6	0	8.125042	-2.387213	-1.289928
397	1	0	10.477577	-2.897111	-2.677880
398	1	0	10.830702	-0.850474	1.412797
399	1	0	10.600150	4.573497	1.714795
400	1	0	8.391323	4.301741	2.777268
401	1	0	5.666185	5.997535	-0.602693
402	8	0	6.323339	5.082240	-2.900377
403	1	0	10.665348	3.316261	2.961432
404	8	0	6.009824	2.845355	-4.367684
405	1	0	8.131586	-2.762403	-3.402341
406	1	0	9.676895	0.973670	1.527313
407	8	0	6.821896	-1.415877	4.060866
408	1	0	10.285497	2.711930	-4.158212
409	1	0	10.450106	2.486209	-2.414344
410	1	0	5.627912	0.961868	4.452841
411	1	0	10.957155	-1.088730	3.160660
412	1	0	8.073057	3.795981	-3.901812
413	8	0	5.827898	-1.853965	-3.811267
414	8	0	6.583203	-3.932455	-2.222539
415	8	0	6.875703	-3.610405	2.490428
416	1	0	9.448379	-1.023205	-0.288064
417	1	0	10.941702	-2.483003	2.068259
418	1	0	8.776334	-2.264591	3.245101
419	1	0	9.343406	2.618788	-0.502206
420	1	0	10.287286	-1.638626	-3.910113
421	8	0	6.641529	5.392290	1.831395
422	1	0	10.516229	-1.196544	-2.213160
423	1	0	5.994375	-4.577830	0.316422
424	8	0	6.266760	3.263562	3.560554
425	1	0	9.390980	0.629521	-2.355651
426	1	0	10.388078	4.117573	-3.085644
427	1	0	4.916226	0.397649	-4.561695
428	1	0	10.670832	2.872437	1.252278
429	1	0	3.436820	6.784623	3.379046
430	1	0	0.991720	7.004373	3.853378
431	1	0	-4.654568	4.470632	5.360095

432	1	0	-1.367225	-1.152905	7.619583
433	1	0	4.269526	1.493029	6.274744
434	1	0	0.442257	-2.745927	7.229674
435	1	0	-4.074877	-5.384869	5.027654
436	1	0	0.034167	-7.887143	-2.468908
437	1	0	4.804624	-7.351481	0.535113
438	1	0	-5.283543	-5.645263	2.905652
439	1	0	-1.887181	-8.036586	-0.976207
440	1	0	5.147051	-5.128061	1.454130
441	1	0	2.483708	-3.829508	6.306341
442	1	0	-0.594394	3.072743	-7.311823
443	1	0	-5.181939	5.010104	-4.567029
444	1	0	-0.825475	7.727300	2.418904
445	1	0	-2.104002	1.214497	-7.516816
446	1	0	4.858598	6.030613	-2.720097
447	1	0	1.381553	4.502034	-6.946510
448	1	0	-6.368402	5.200940	-2.421221
449	1	0	-2.986408	7.975870	1.199439
450	1	0	5.409585	-2.080021	-5.476053
451	1	0	-7.378166	4.452021	-0.207297
452	1	0	-6.456975	1.354373	-4.893711
453	1	0	-6.591173	-5.110597	0.798932
454	1	0	-5.826203	-1.910079	5.442557
455	1	0	-7.024871	0.284079	5.253152
456	1	0	-6.602339	5.025285	2.087174
457	1	0	-7.303708	-0.991139	-4.636757
458	1	0	-5.942073	-5.618021	-1.545139
459	1	0	3.880792	-6.027078	-3.585112
460	1	0	7.247653	-3.063004	3.262894
461	1	0	5.794715	-4.607517	-2.013547
462	1	0	-6.133200	-3.114788	-5.434920
463	1	0	5.810313	5.979899	1.729930
464	1	0	6.278869	-2.674882	-3.373334
465	1	0	5.230891	2.690429	-5.084603
466	1	0	6.659890	4.109983	3.145091
467	1	0	6.031756	-1.348372	4.777573
468	1	0	-4.440308	0.984910	-6.860460
469	1	0	3.603456	7.462972	-1.131534
470	1	0	1.528305	-6.623421	-3.945130
471	1	0	-4.514108	-4.951524	-5.046106
472	1	0	3.906767	-0.695703	-6.626125
473	1	0	-6.070237	2.544780	5.950841
474	1	0	-3.758638	-1.290393	7.265093
475	1	0	5.747778	3.205061	5.238698
476	1	0	6.496200	4.439965	-3.686631
477	1	0	-4.489536	-3.336478	6.637563
478	1	0	-3.692982	-2.724422	5.462260
479	8	0	-4.349011	-2.491545	6.156957
480	1	0	3.686085	-5.226079	-1.752059
481	1	0	4.701360	-6.461791	-1.788447
482	8	0	4.543068	-5.625923	-2.282922
483	1	0	-4.459463	2.417986	-5.041958
484	1	0	-5.403497	2.920548	-6.160205
485	8	0	-5.121311	2.102823	-5.695920
486	1	0	4.130235	7.592438	1.425389
487	1	0	3.540880	6.182484	1.198343
488	8	0	4.156486	6.678147	1.785090
489	1	0	-4.917453	5.743120	3.195512
490	1	0	-5.162308	6.584181	1.905904
491	8	0	-5.620998	6.123021	2.633089
492	1	0	3.692042	3.352262	-6.352215
493	1	0	3.874371	1.802017	-6.430582
494	8	0	4.368033	2.647469	-6.360147
495	1	0	-4.300986	-6.966275	-1.481554
496	8	0	-4.942961	-6.647280	-2.144950
497	1	0	-4.409695	-6.259702	-2.869022
498	8	0	5.005384	-1.706096	5.867876

499	1	0	4.582506	-2.562833	5.641044
500	1	0	4.285096	-1.046920	5.893377

Sum of electronic and thermal Free Energies= -0.672931
1 imaginary frequency: -401.3745

P1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.161900	-4.696320	0.400402
2	1	0	1.417824	-4.848359	-1.388712
3	1	0	-0.618143	-3.451393	-1.257131
4	1	0	-3.779413	-2.920482	1.735370
5	1	0	-3.879894	-1.364353	0.855846
6	1	0	-4.006011	-1.404782	2.631384
7	1	0	-1.951253	-1.875072	-0.211796
8	1	0	0.389052	0.843090	2.994346
9	1	0	-0.212803	2.275720	2.126857
10	1	0	-0.995539	1.727139	3.613893
11	1	0	-2.437243	0.989830	1.704254
12	1	0	0.263687	-0.033739	0.653227
13	1	0	-2.412833	0.955887	-0.589954
14	1	0	0.007602	1.692306	-4.594750
15	1	0	-0.911794	0.237476	-5.019197
16	1	0	-1.619397	2.125615	-2.963972
17	1	0	1.388749	0.574988	-1.600518
18	6	0	0.727880	-0.124266	-3.586888
19	6	0	0.599632	-0.063438	-2.056752
20	7	0	-0.744272	0.537238	-1.789823
21	8	0	-1.704463	-0.668230	2.746575
22	6	0	-1.277032	-1.624086	0.653769
23	6	0	2.250938	-4.091931	0.463779
24	6	0	-2.767692	0.280083	-3.225950
25	8	0	-3.199018	0.253040	-4.396839
26	6	0	-0.058075	-2.520373	0.623737
27	8	0	-3.279328	-0.162577	-2.192428
28	6	0	-1.382319	0.521884	-0.646526
29	6	0	-0.851545	-0.109765	0.597483
30	6	0	-1.457025	0.501750	1.891273
31	7	0	-2.014837	-1.799985	1.959285
32	6	0	-3.491552	-1.852204	1.762717
33	6	0	2.043241	-3.267415	1.574351
34	1	0	0.630844	-1.167979	-3.949952
35	6	0	-1.385663	1.035460	-3.043232
36	6	0	-0.392233	0.752343	-4.171967
37	6	0	1.286720	-4.164258	-0.546128
38	6	0	0.134207	-3.377123	-0.470670
39	6	0	0.887211	-2.486885	1.659150
40	1	0	0.678999	-1.076597	-1.596538
41	1	0	1.724072	0.220916	-3.918515
42	6	0	-0.517167	1.382498	2.683147
43	1	0	2.777049	-3.239767	2.380326
44	1	0	0.698942	-1.866709	2.539450
45	8	0	-4.615394	4.530560	5.902914
46	8	0	-1.957254	1.066984	7.967565
47	6	0	-3.510617	4.079867	6.581720
48	6	0	-3.346742	2.727475	6.897209
49	6	0	-2.204410	2.377195	7.623296
50	6	0	-1.249795	3.325627	8.046480
51	6	0	-1.438901	4.657752	7.657419
52	6	0	-2.558718	5.064873	6.926144
53	6	0	-0.066674	2.889004	8.883096
54	6	0	0.096800	3.759911	10.133031
55	1	0	-4.074330	1.985143	6.580528
56	1	0	-0.685314	5.399557	7.929795

57	1	0	-0.275374	1.839493	9.253256
58	1	0	0.271580	4.813672	9.894083
59	1	0	0.938711	3.414522	10.744968
60	1	0	-0.806651	3.715872	10.754758
61	8	0	5.863501	4.706451	4.878615
62	8	0	3.185666	7.767455	2.270114
63	6	0	4.805378	5.565200	4.708624
64	6	0	4.574281	6.211252	3.489921
65	6	0	3.491479	7.094476	3.432848
66	6	0	2.658287	7.351659	4.541303
67	6	0	2.909334	6.641677	5.722645
68	6	0	3.977028	5.746634	5.837994
69	6	0	1.533354	8.358307	4.430130
70	6	0	1.570873	9.378419	5.572642
71	1	0	5.203895	6.022619	2.626100
72	1	0	2.246465	6.789191	6.577957
73	1	0	1.690944	8.945627	3.474808
74	1	0	1.461006	8.913681	6.557612
75	1	0	0.768768	10.118522	5.464623
76	1	0	2.525375	9.920011	5.576158
77	8	0	0.656634	0.550191	7.303165
78	8	0	4.653799	2.374522	5.758481
79	6	0	1.482137	1.651590	7.309390
80	6	0	2.647055	1.505491	6.550565
81	6	0	3.526535	2.593927	6.508006
82	6	0	3.269163	3.803752	7.192260
83	6	0	2.084784	3.891114	7.931972
84	6	0	1.184124	2.824605	8.033807
85	6	0	4.249701	4.954021	7.099609
86	6	0	4.267034	5.846253	8.344185
87	1	0	2.845029	0.596931	5.989278
88	1	0	1.858527	4.821713	8.458262
89	1	0	5.286499	4.508235	7.015140
90	1	0	4.492421	5.260583	9.243716
91	1	0	3.314152	6.358050	8.511688
92	1	0	5.038656	6.621369	8.251374
93	8	0	0.459600	7.448961	1.882039
94	8	0	-3.497074	5.811230	3.712553
95	6	0	-0.264604	7.250155	3.037822
96	6	0	-1.505817	6.638058	2.842772
97	6	0	-2.293860	6.408529	3.977211
98	6	0	-1.872141	6.772528	5.277660
99	6	0	-0.616868	7.374843	5.408788
100	6	0	0.201290	7.651164	4.306304
101	6	0	-2.763503	6.494417	6.470175
102	6	0	-2.583345	7.493736	7.616516
103	1	0	-1.838216	6.328192	1.855871
104	1	0	-0.264645	7.649999	6.405929
105	1	0	-3.835517	6.600677	6.122943
106	1	0	-2.761447	8.520268	7.273919
107	1	0	-1.581394	7.458865	8.055431
108	1	0	-3.297508	7.285357	8.423749
109	1	0	-5.264322	3.776186	5.673803
110	1	0	-2.577112	0.411817	7.474200
111	1	0	6.387927	4.560203	4.014683
112	1	0	3.730930	7.433219	1.471975
113	1	0	-0.222671	0.716568	7.804990
114	1	0	5.242989	3.205411	5.676992
115	1	0	1.386271	7.840669	2.066852
116	1	0	-4.029503	5.598162	4.556967
117	8	0	4.789135	-3.725615	-6.464388
118	8	0	3.499340	-6.998188	-3.154573
119	6	0	3.969896	-4.717607	-5.981768
120	6	0	4.208370	-5.324671	-4.744674
121	6	0	3.339897	-6.351342	-4.361505
122	6	0	2.269304	-6.786329	-5.169076
123	6	0	2.049716	-6.110252	-6.376569

124	6	0	2.883854	-5.075193	-6.810358
125	6	0	1.394190	-7.934843	-4.713288
126	6	0	1.222814	-8.989389	-5.810960
127	1	0	5.026614	-5.002241	-4.108585
128	1	0	1.195271	-6.396490	-6.993943
129	1	0	1.924339	-8.451276	-3.856085
130	1	0	2.196877	-9.390913	-6.117655
131	1	0	0.741841	-8.589017	-6.709334
132	1	0	0.612751	-9.829104	-5.456565
133	8	0	-5.432552	-5.078079	-4.229001
134	8	0	-4.138527	-1.425137	-7.107193
135	6	0	-4.686452	-4.522574	-5.242223
136	6	0	-4.876191	-3.198218	-5.644238
137	6	0	-4.057779	-2.719611	-6.673305
138	6	0	-3.091875	-3.532391	-7.311451
139	6	0	-2.930553	-4.842905	-6.852680
140	6	0	-3.717190	-5.368578	-5.821367
141	6	0	-2.272840	-2.967534	-8.450412
142	6	0	-2.350233	-3.861029	-9.694131
143	1	0	-5.618979	-2.561670	-5.169183
144	1	0	-2.163763	-5.472946	-7.306872
145	1	0	-2.726694	-1.975016	-8.748091
146	1	0	-3.391386	-3.960563	-10.027895
147	1	0	-1.974034	-4.872265	-9.512154
148	1	0	-1.775338	-3.432643	-10.523179
149	8	0	-1.468392	-0.538136	-7.006696
150	8	0	3.045072	-1.641488	-6.932331
151	6	0	-0.535239	-1.480746	-7.355267
152	6	0	0.777821	-1.127930	-7.019409
153	6	0	1.785598	-2.059901	-7.288389
154	6	0	1.518394	-3.316431	-7.874053
155	6	0	0.190272	-3.601800	-8.213993
156	6	0	-0.853435	-2.694590	-8.000482
157	6	0	2.640496	-4.308855	-8.094782
158	6	0	2.410480	-5.242709	-9.286134
159	1	0	1.001168	-0.175931	-6.548851
160	1	0	-0.039505	-4.567627	-8.671330
161	1	0	3.575288	-3.716784	-8.331068
162	1	0	3.277929	-5.898040	-9.435784
163	1	0	2.263465	-4.670301	-10.210196
164	1	0	1.536268	-5.888448	-9.154819
165	8	0	1.047649	-7.060901	-1.956129
166	8	0	-3.457779	-5.993636	-2.476193
167	6	0	-0.020014	-7.006330	-2.831165
168	6	0	-1.205969	-6.532566	-2.264511
169	6	0	-2.331015	-6.463244	-3.095569
170	6	0	-2.292926	-6.858296	-4.454003
171	6	0	-1.071967	-7.303877	-4.967284
172	6	0	0.080188	-7.410336	-4.176718
173	6	0	-3.545156	-6.779381	-5.302583
174	6	0	-3.583457	-7.810959	-6.434763
175	1	0	-1.250359	-6.204483	-1.228629
176	1	0	-1.014012	-7.589777	-6.020406
177	1	0	-4.423643	-7.016244	-4.630071
178	1	0	-4.540661	-7.754717	-6.969696
179	1	0	-3.481607	-8.829711	-6.043173
180	1	0	-2.792897	-7.655318	-7.175239
181	1	0	5.508697	-3.458138	-5.792664
182	1	0	4.158670	-6.514347	-2.540307
183	1	0	-6.104115	-4.414188	-3.839122
184	1	0	-4.802575	-0.847189	-6.514486
185	1	0	-2.443827	-0.861133	-7.086418
186	1	0	3.751527	-2.366903	-7.064560
187	1	0	1.908297	-7.365773	-2.421779
188	1	0	-4.238408	-5.847683	-3.121623
189	8	0	0.351111	-8.311780	0.453693
190	8	0	4.645275	-6.458352	1.248188

191	6	0	1.380870	-8.003545	1.304177
192	6	0	2.539985	-7.379290	0.834156
193	6	0	3.555658	-7.131554	1.764505
194	6	0	3.474480	-7.534266	3.110380
195	6	0	2.271570	-8.120091	3.535248
196	6	0	1.211893	-8.368594	2.660185
197	6	0	4.658060	-7.349607	4.037242
198	6	0	4.835282	-8.525310	5.004188
199	1	0	2.635962	-7.082955	-0.205773
200	1	0	2.164128	-8.396279	4.586592
201	1	0	5.589952	-7.325510	3.394674
202	1	0	4.935692	-9.470546	4.457125
203	1	0	3.993669	-8.634759	5.695434
204	1	0	5.739699	-8.393730	5.611496
205	8	0	1.929657	-1.866869	7.770230
206	8	0	-2.454049	-3.249415	6.584825
207	6	0	1.020353	-2.854471	7.483860
208	6	0	-0.300529	-2.545589	7.147541
209	6	0	-1.172543	-3.618968	6.926949
210	6	0	-0.776554	-4.964281	7.070963
211	6	0	0.573784	-5.212944	7.352903
212	6	0	1.493500	-4.182894	7.567928
213	6	0	-1.789352	-6.082886	6.939748
214	6	0	-1.536843	-7.225212	7.930315
215	1	0	-0.630749	-1.517354	7.036571
216	1	0	0.916811	-6.248077	7.416152
217	1	0	-2.802822	-5.655031	7.204690
218	1	0	-1.525888	-6.853746	8.961952
219	1	0	-0.584864	-7.735416	7.753978
220	1	0	-2.328943	-7.981149	7.856470
221	8	0	6.109821	-5.141513	3.190898
222	8	0	4.370207	-2.248520	6.527180
223	6	0	5.301749	-4.914735	4.283323
224	6	0	5.230008	-3.648991	4.869163
225	6	0	4.421836	-3.514296	6.004821
226	6	0	3.725397	-4.605586	6.570693
227	6	0	3.786745	-5.834246	5.903285
228	6	0	4.569963	-6.023305	4.759137
229	6	0	2.955737	-4.431174	7.863194
230	6	0	3.173819	-5.596843	8.833151
231	1	0	5.768395	-2.798171	4.459882
232	1	0	3.211615	-6.676785	6.293286
233	1	0	3.359290	-3.507280	8.379781
234	1	0	2.810030	-6.550239	8.437470
235	1	0	2.652540	-5.415797	9.781296
236	1	0	4.240239	-5.722548	9.057745
237	8	0	-3.804100	-5.252790	5.234840
238	8	0	-2.185393	-7.699591	1.506566
239	6	0	-2.884905	-6.103517	4.661823
240	6	0	-2.990421	-6.476191	3.320834
241	6	0	-2.038914	-7.380300	2.831269
242	6	0	-1.027918	-7.932251	3.648987
243	6	0	-0.940694	-7.479268	4.971210
244	6	0	-1.858131	-6.571605	5.510128
245	6	0	-0.095446	-8.990744	3.099746
246	6	0	0.106797	-10.151613	4.079476
247	1	0	-3.760127	-6.066860	2.672551
248	1	0	-0.135354	-7.854145	5.605828
249	1	0	-0.585621	-9.432962	2.179089
250	1	0	0.582953	-9.838543	5.013709
251	1	0	0.736557	-10.931570	3.634554
252	1	0	-0.855017	-10.609650	4.342420
253	1	0	0.499826	-7.929436	-0.482784
254	1	0	5.309809	-6.180155	1.976773
255	1	0	1.543836	-0.931775	7.627491
256	1	0	-3.006224	-4.037483	6.223972
257	1	0	6.625806	-4.305700	2.920374

258	1	0	3.658611	-2.159611	7.254371
259	1	0	-4.497819	-4.929510	4.556566
260	1	0	-1.386506	-8.214711	1.142716
261	8	0	-1.124587	8.367197	-0.217398
262	8	0	3.009947	7.274051	-2.284030
263	6	0	-0.354218	8.198539	-1.338768
264	6	0	0.979440	7.787920	-1.245865
265	6	0	1.704106	7.694741	-2.439713
266	6	0	1.151567	8.017855	-3.693708
267	6	0	-0.206046	8.370705	-3.731428
268	6	0	-0.981385	8.477421	-2.574745
269	6	0	2.009074	7.990844	-4.942268
270	6	0	1.693714	9.146473	-5.897524
271	1	0	1.429137	7.542919	-0.289026
272	1	0	-0.669412	8.578512	-4.698848
273	1	0	3.085050	8.130714	-4.620081
274	1	0	2.375532	9.134139	-6.757348
275	1	0	1.808845	10.113914	-5.394192
276	1	0	0.673812	9.102196	-6.292861
277	8	0	-0.888619	2.049950	-7.693320
278	8	0	-5.029722	2.876993	-5.533489
279	6	0	-1.831447	2.917065	-7.195412
280	6	0	-2.967383	2.449450	-6.534686
281	6	0	-3.911526	3.399807	-6.126516
282	6	0	-3.727536	4.786158	-6.335444
283	6	0	-2.539821	5.199951	-6.949842
284	6	0	-1.579477	4.291013	-7.404682
285	6	0	-4.791182	5.770166	-5.896396
286	6	0	-4.972678	6.930085	-6.880593
287	1	0	-3.110009	1.391251	-6.298756
288	1	0	-2.362126	6.267926	-7.089866
289	1	0	-5.778750	5.216305	-5.872624
290	1	0	-5.792611	7.584755	-6.560478
291	1	0	-5.216820	6.555170	-7.882236
292	1	0	-4.076027	7.550433	-6.973058
293	8	0	-6.083715	4.673269	-3.715923
294	8	0	-3.685717	7.233975	-0.517917
295	6	0	-5.146135	5.620024	-3.397093
296	6	0	-4.863446	5.945825	-2.068022
297	6	0	-3.938032	6.972802	-1.842833
298	6	0	-3.325591	7.687790	-2.893106
299	6	0	-3.596150	7.271645	-4.204767
300	6	0	-4.499064	6.245188	-4.488955
301	6	0	-2.440649	8.878181	-2.593378
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303	1	0	-5.330056	5.418910	-1.240498
304	1	0	-3.090116	7.773476	-5.032030
305	1	0	-2.703750	9.242246	-1.552996
306	1	0	-3.762691	10.352226	-3.500872
307	1	0	-2.475998	9.817778	-4.583120
308	1	0	-2.103993	10.925453	-3.258696
309	8	0	3.955421	6.056522	-4.589402
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311	6	0	2.896424	5.665416	-5.379187
312	6	0	2.829919	4.372437	-5.903175
313	6	0	1.743729	4.075403	-6.736061
314	6	0	0.771025	5.040129	-7.082538
315	6	0	0.854664	6.296959	-6.473520
316	6	0	1.905314	6.640587	-5.615104
317	6	0	-0.304008	4.711298	-8.097673
318	6	0	-0.524396	5.851830	-9.097423
319	1	0	3.580159	3.621577	-5.670399
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321	1	0	0.059240	3.824598	-8.702564
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323	1	0	-0.890793	6.766404	-8.621189
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325	1	0	-0.624134	8.116370	0.635361
326	1	0	3.445548	7.038389	-3.181906
327	1	0	-1.125155	1.072059	-7.513940
328	1	0	-5.620812	3.592395	-5.114302
329	1	0	-6.490476	4.228822	-2.888394
330	1	0	-2.930665	7.904164	-0.393666
331	1	0	4.658007	5.324093	-4.507085
332	1	0	0.830984	2.574877	-7.686422
333	8	0	5.633820	3.838061	-4.360944
334	8	0	6.516543	5.519146	-0.015760
335	6	0	6.478324	3.864333	-3.281776
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337	6	0	6.847987	4.714669	-1.081039
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340	6	0	7.696653	3.155116	-3.248178
341	6	0	8.824682	3.999952	0.331699
342	6	0	10.335352	4.099301	0.097132
343	1	0	5.107445	5.216874	-2.289606
344	1	0	9.353363	2.608331	-1.987986
345	1	0	8.525324	4.943297	0.883255
346	1	0	10.580662	4.994311	-0.487638
347	1	0	10.736323	3.236209	-0.443740
348	1	0	10.874249	4.164852	1.050446
349	8	0	7.238872	-2.655815	2.511326
350	8	0	6.880733	-4.226884	-1.946128
351	6	0	7.678333	-2.564324	1.215714
352	6	0	7.034797	-3.431263	0.322273
353	6	0	7.432298	-3.377755	-1.016546
354	6	0	8.416880	-2.479814	-1.483571
355	6	0	9.030516	-1.644291	-0.544368
356	6	0	8.708979	-1.687796	0.817548
357	6	0	8.760534	-2.439031	-2.956085
358	6	0	10.267352	-2.318634	-3.205760
359	1	0	6.252313	-4.099240	0.665027
360	1	0	9.792699	-0.939437	-0.884417
361	1	0	8.441867	-3.430097	-3.403632
362	1	0	10.689363	-1.392357	-2.803217
363	1	0	10.486819	-2.335969	-4.280487
364	1	0	10.806958	-3.152962	-2.741095
365	8	0	6.217591	-2.925987	-4.266999
366	8	0	5.905210	1.548735	-5.820370
367	6	0	6.762741	-1.662394	-4.305545
368	6	0	6.032605	-0.729832	-5.050774
369	6	0	6.531959	0.576136	-5.103049
370	6	0	7.708045	0.961118	-4.411642
371	6	0	8.399087	-0.016865	-3.694192
372	6	0	7.971251	-1.350814	-3.652292
373	6	0	8.167268	2.400353	-4.473753
374	6	0	9.678108	2.525685	-4.695834
375	1	0	5.108888	-1.013003	-5.548125
376	1	0	9.307192	0.262739	-3.156282
377	1	0	7.672971	2.875039	-5.376301
378	1	0	9.975750	3.578055	-4.776881
379	1	0	9.974248	2.023457	-5.625639
380	1	0	10.263610	2.080445	-3.885580
381	8	0	6.744317	4.134254	2.351039
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383	6	0	7.459407	2.966899	2.197714
384	6	0	7.131644	1.954447	3.106274
385	6	0	7.812652	0.738745	2.979747
386	6	0	8.771170	0.515062	1.959092
387	6	0	9.063867	1.567565	1.090493
388	6	0	8.450694	2.823082	1.207739
389	6	0	9.428297	-0.842618	1.847950
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394	1	0	11.166763	-0.248097	0.636870
395	1	0	11.388634	-1.745236	1.547140
396	1	0	11.432197	-0.182967	2.380697
397	1	0	5.921723	3.161622	-5.079526
398	1	0	5.617032	5.989402	-0.146350
399	1	0	7.623120	-1.917555	3.114143
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412	6	0	-7.579790	-3.025156	3.202026
413	6	0	-8.230814	0.397264	4.841549
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422	8	0	-7.524339	-0.571443	-3.792364
423	6	0	-7.607372	2.273264	-1.499312
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425	6	0	-7.812893	0.236472	-2.731353
426	6	0	-8.787042	-0.240415	-1.819185
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428	6	0	-8.632340	1.886904	-0.613641
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430	6	0	-10.845958	-1.718129	-1.676659
431	1	0	-6.402566	1.814519	-3.242376
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435	1	0	-11.416609	-1.026372	-2.308130
436	1	0	-11.069894	-1.472048	-0.634201
437	8	0	-6.036560	2.264590	5.179277
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440	6	0	-6.523376	3.426079	3.208040
441	6	0	-7.297128	3.560873	2.050245
442	6	0	-8.344619	2.660314	1.733467
443	6	0	-8.614788	1.625612	2.630318
444	6	0	-7.899274	1.471018	3.826502
445	6	0	-9.122797	2.845685	0.449246
446	6	0	-10.636462	2.756323	0.674064
447	1	0	-5.703637	4.101533	3.429891
448	1	0	-9.411969	0.916772	2.397057
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453	8	0	-7.206889	-3.215899	-3.145696
454	8	0	-6.383321	-5.497061	0.940405
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456	6	0	-6.777372	-4.361503	-1.152042
457	6	0	-7.057230	-4.562750	0.202751
458	6	0	-8.038463	-3.811787	0.891105

459	6	0	-8.751099	-2.847416	0.171838
460	6	0	-8.535336	-2.627402	-1.193213
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463	1	0	-6.011271	-4.930180	-1.669480
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467	1	0	-10.332886	-3.279555	2.455269
468	1	0	-9.925867	-4.410427	3.751872
469	1	0	-5.977972	-4.900100	2.532056
470	1	0	-4.754389	-0.578691	6.028484
471	1	0	-7.214713	3.995259	-0.545384
472	1	0	-6.747707	-0.196858	-4.401732
473	1	0	-6.216944	1.410370	5.707828
474	1	0	-6.329395	5.248697	1.474158
475	1	0	-7.546561	-2.324337	-3.523813
476	1	0	-5.670198	-6.039097	0.382141
477	8	0	-3.198924	-0.936436	6.618024
478	1	0	-3.265004	-1.686919	7.253428
479	1	0	-2.617432	-1.279293	5.900639
480	8	0	4.838185	-5.828828	-1.089739
481	1	0	4.186611	-5.398134	-0.471941
482	1	0	5.207092	-6.575212	-0.564756
483	8	0	4.123820	6.894947	-0.154538
484	1	0	4.183470	7.679580	-0.741451
485	1	0	3.399346	6.362046	-0.551041
486	8	0	-5.428435	-0.062465	-5.266861
487	1	0	-4.669576	-0.318457	-4.590002
488	1	0	-5.231394	0.893529	-5.433303
489	8	0	3.965669	1.004015	-7.463130
490	1	0	3.297249	1.712361	-7.390420
491	1	0	3.485616	0.160568	-7.339851
492	8	0	-5.353342	6.483576	1.651936
493	1	0	-4.557549	6.273112	2.175622
494	1	0	-5.028422	6.793656	0.785350
495	8	0	6.147214	-0.028037	5.977429
496	1	0	5.660922	-0.865007	6.106412
497	1	0	5.473220	0.681032	5.975553
498	8	0	-4.531155	-7.045974	-0.085116
499	1	0	-3.908738	-7.282122	0.625260
500	1	0	-3.983061	-6.688945	-0.812079

Sum of electronic and thermal Free Energies= -0.718454
0 imaginary frequency

MC2c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	6.036535	2.977197	5.831613
2	8	0	3.947343	6.750449	3.654025
3	6	0	5.120083	3.996505	5.766530
4	6	0	5.049215	4.849585	4.660475
5	6	0	4.097547	5.872752	4.706009
6	6	0	3.242267	6.070491	5.809654
7	6	0	3.327348	5.159213	6.870401
8	6	0	4.257948	4.116354	6.879217
9	6	0	2.267878	7.228511	5.819203
10	6	0	2.382683	8.054007	7.104836
11	1	0	5.699074	4.708779	3.801602
12	1	0	2.641113	5.264656	7.713280
13	1	0	2.548945	7.922831	4.970280
14	1	0	2.165800	7.468126	8.003680
15	1	0	1.691476	8.905143	7.088638

16	1	0	3.399073	8.452583	7.217900
17	8	0	-4.427249	4.142768	6.539081
18	8	0	-2.410318	0.085949	8.217962
19	6	0	-3.434861	3.448871	7.187469
20	6	0	-3.491555	2.059431	7.336631
21	6	0	-2.444188	1.451408	8.035421
22	6	0	-1.371614	2.181530	8.588366
23	6	0	-1.345385	3.565109	8.371263
24	6	0	-2.364546	4.227231	7.680145
25	6	0	-0.291553	1.470368	9.375077
26	6	0	-0.060183	2.127237	10.739710
27	1	0	-4.308748	1.483036	6.913475
28	1	0	-0.499115	4.142792	8.749181
29	1	0	-0.654261	0.418911	9.586366
30	1	0	0.262353	3.170011	10.657269
31	1	0	0.705130	1.587711	11.310642
32	1	0	-0.983640	2.121403	11.332746
33	8	0	1.224108	6.825838	3.130453
34	8	0	-3.010638	5.524283	4.574467
35	6	0	0.417335	6.577739	4.220649
36	6	0	-0.881941	6.175815	3.898431
37	6	0	-1.751894	5.904888	4.961518
38	6	0	-1.357348	6.027434	6.313858
39	6	0	-0.042157	6.427744	6.572148
40	6	0	0.862507	6.736299	5.548987
41	6	0	-2.341830	5.719538	7.422631
42	6	0	-2.087819	6.515759	8.706110
43	1	0	-1.195792	6.045237	2.866550
44	1	0	0.289529	6.513616	7.609812
45	1	0	-3.367943	6.026990	7.057289
46	1	0	-2.100796	7.594396	8.508140
47	1	0	-1.126620	6.274613	9.170726
48	1	0	-2.867748	6.305966	9.449520
49	8	0	0.151094	-0.689508	7.473586
50	8	0	4.412923	0.747990	6.267440
51	6	0	1.122744	0.272495	7.653435
52	6	0	2.278315	0.073181	6.893192
53	6	0	3.308070	1.011970	7.032288
54	6	0	3.205117	2.124831	7.899541
55	6	0	2.020088	2.274073	8.627027
56	6	0	0.969512	1.351494	8.547169
57	6	0	4.349438	3.110730	8.007962
58	6	0	4.442669	3.794655	9.375191
59	1	0	2.364781	-0.757979	6.198914
60	1	0	1.912843	3.135436	9.290823
61	1	0	5.310670	2.527070	7.880001
62	1	0	4.534458	3.054205	10.179049
63	1	0	3.572027	4.419782	9.596355
64	1	0	5.326730	4.443822	9.420574
65	1	0	-0.254670	2.756386	0.513910
66	1	0	-0.024624	2.355622	-1.196494
67	1	0	-1.343509	1.615401	-0.299334
68	1	0	1.667888	1.134604	0.345593
69	1	0	-0.797744	-0.752244	0.037437
70	1	0	2.250902	-1.353846	0.344480
71	1	0	1.371353	-5.527577	2.637687
72	1	0	0.859796	-5.714286	0.959384
73	1	0	2.469911	-3.476568	2.228330
74	1	0	-1.093099	-2.304839	2.054002
75	6	0	-0.471884	-4.429354	2.137692
76	6	0	-0.588807	-3.072626	1.433244
77	7	0	0.814631	-2.662184	1.121879
78	6	0	2.651420	-4.061294	0.121366
79	8	0	3.480191	-5.006237	0.240789
80	8	0	2.480198	-3.353919	-0.875599
81	6	0	1.175411	-1.518583	0.583043
82	6	0	0.243063	-0.454378	0.255924

83	6	0	0.632162	0.829917	0.154685
84	1	0	-1.270109	-5.123175	1.808426
85	6	0	1.785026	-3.770540	1.390369
86	6	0	0.921100	-4.978376	1.787691
87	1	0	-1.165539	-3.152927	0.466298
88	1	0	-0.591249	-4.325878	3.232740
89	6	0	-0.289199	1.929632	-0.211412
90	8	0	-6.105606	-3.529902	-5.337878
91	8	0	-4.085408	0.380387	-7.319969
92	6	0	-5.180168	-2.910221	-6.143208
93	6	0	-5.127366	-1.517062	-6.251741
94	6	0	-4.193374	-0.981790	-7.144109
95	6	0	-3.334177	-1.786805	-7.920733
96	6	0	-3.394360	-3.173323	-7.730895
97	6	0	-4.308482	-3.764846	-6.853276
98	6	0	-2.384559	-1.143497	-8.908107
99	6	0	-2.429387	-1.830349	-10.276989
100	1	0	-5.776450	-0.882102	-5.656385
101	1	0	-2.702894	-3.812079	-8.284520
102	1	0	-2.735065	-0.079640	-9.075107
103	1	0	-3.444257	-1.799026	-10.692885
104	1	0	-2.131389	-2.882741	-10.231263
105	1	0	-1.761403	-1.329943	-10.988426
106	8	0	4.230695	-2.931637	-6.304325
107	8	0	2.291421	-6.507542	-3.732031
108	6	0	3.291717	-3.907722	-6.090612
109	6	0	3.327413	-4.715744	-4.952605
110	6	0	2.336733	-5.697905	-4.828979
111	6	0	1.340344	-5.889314	-5.814194
112	6	0	1.329674	-5.024781	-6.914112
113	6	0	2.293269	-4.025949	-7.082498
114	6	0	0.337275	-7.011094	-5.665258
115	6	0	0.229428	-7.854771	-6.940389
116	1	0	4.086844	-4.590471	-4.183690
117	1	0	0.544325	-5.133892	-7.664492
118	1	0	0.718123	-7.706510	-4.857974
119	1	0	1.205321	-8.286175	-7.198350
120	1	0	-0.103498	-7.273060	-7.805421
121	1	0	-0.475697	-8.683123	-6.804936
122	8	0	-0.318324	-6.591783	-2.852939
123	8	0	-4.669273	-5.172956	-3.700530
124	6	0	-1.255843	-6.322563	-3.825568
125	6	0	-2.490224	-5.896115	-3.326009
126	6	0	-3.482231	-5.571028	-4.257793
127	6	0	-3.268553	-5.657778	-5.652926
128	6	0	-2.016241	-6.101173	-6.091251
129	6	0	-0.997686	-6.467911	-5.202814
130	6	0	-4.368717	-5.259623	-6.615052
131	6	0	-4.351506	-6.056096	-7.922731
132	1	0	-2.657346	-5.789376	-2.256876
133	1	0	-1.826777	-6.171902	-7.165050
134	1	0	-5.357156	-5.491404	-6.114781
135	1	0	-5.200485	-5.773376	-8.558029
136	1	0	-4.427186	-7.132611	-7.726575
137	1	0	-3.440665	-5.890611	-8.506945
138	8	0	-1.446973	1.099280	-7.302020
139	8	0	2.844871	-0.620957	-6.745564
140	6	0	-0.596492	0.049393	-7.570495
141	6	0	0.690364	0.200013	-7.045937
142	6	0	1.606129	-0.831569	-7.286227
143	6	0	1.265658	-1.986951	-8.028495
144	6	0	-0.039394	-2.083735	-8.519456
145	6	0	-0.988717	-1.071689	-8.328604
146	6	0	2.294675	-3.074184	-8.258751
147	6	0	2.118538	-3.804648	-9.593671
148	1	0	0.969241	1.070351	-6.459021
149	1	0	-0.328005	-2.975533	-9.081212

150	1	0	3.310405	-2.576691	-8.302525
151	1	0	2.924905	-4.535324	-9.739213
152	1	0	2.152382	-3.100976	-10.433736
153	1	0	1.172900	-4.351894	-9.655245
154	1	0	-3.601737	3.382605	-2.366822
155	1	0	-1.603596	3.341546	-3.850118
156	1	0	-0.404020	1.212602	-4.269067
157	1	0	1.010468	-3.228874	-2.250520
158	1	0	0.125548	-3.540230	-3.782010
159	1	0	-0.403640	-4.307400	-2.254587
160	1	0	-0.325525	-1.204926	-4.134159
161	8	0	-1.524549	-2.301722	-1.314673
162	6	0	-0.922117	-1.184622	-3.211959
163	6	0	-3.084895	2.443066	-2.557548
164	6	0	-1.698152	0.037533	-2.981862
165	7	0	-0.882525	-2.222081	-2.390822
166	6	0	-0.005103	-3.372861	-2.701104
167	6	0	-3.528550	1.261537	-1.956340
168	6	0	-1.956269	2.419501	-3.385392
169	6	0	-1.272359	1.224990	-3.610611
170	6	0	-2.836794	0.064549	-2.158207
171	1	0	-4.414966	1.273862	-1.320074
172	1	0	-3.175181	-0.856866	-1.672615
173	8	0	-5.579092	-6.303101	-1.247411
174	1	0	-4.852896	-6.585218	-0.659389
175	1	0	-5.155928	-6.017389	-2.082459
176	8	0	5.586168	-1.847147	5.998130
177	1	0	4.986775	-1.081372	6.080518
178	1	0	5.014485	-2.619278	5.812739
179	8	0	-4.540871	6.824925	2.580180
180	1	0	-4.080386	7.165632	1.790028
181	1	0	-3.847531	6.424901	3.142705
182	8	0	4.488074	1.703661	-7.010187
183	1	0	4.023313	2.552446	-6.913664
184	1	0	3.809357	1.012900	-6.880002
185	1	0	0.636744	-6.705196	-3.234289
186	1	0	-5.342397	-4.843432	-4.395476
187	1	0	-2.408821	0.903991	-7.601656
188	1	0	3.456247	-1.440282	-6.823446
189	1	0	-0.585540	2.627930	-7.607296
190	1	0	-4.694327	5.147025	-4.593476
191	8	0	-0.203238	3.574995	-7.562851
192	8	0	-4.209572	4.457907	-5.174814
193	6	0	-1.022102	4.430721	-6.874161
194	6	0	-2.244388	3.999724	-6.350299
195	6	0	-3.037297	4.953985	-5.702260
196	6	0	-2.665458	6.308932	-5.599601
197	6	0	-1.404027	6.672705	-6.093965
198	6	0	-0.562462	5.760788	-6.735083
199	6	0	-3.614619	7.320570	-4.992239
200	6	0	-3.608506	8.655629	-5.744479
201	1	0	-2.558766	2.962185	-6.429778
202	1	0	-1.072930	7.707413	-5.980599
203	1	0	-4.663294	6.905236	-5.093259
204	1	0	-3.852020	8.508876	-6.803834
205	1	0	-2.639740	9.162821	-5.698830
206	1	0	-4.354806	9.340742	-5.322838
207	8	0	0.001605	8.344465	1.163809
208	8	0	4.042864	6.982556	-0.926519
209	6	0	0.808425	8.256643	0.058963
210	6	0	2.054438	7.625046	0.119283
211	6	0	2.831591	7.631388	-1.045320
212	6	0	2.418782	8.264166	-2.233963
213	6	0	1.137614	8.834616	-2.251609
214	6	0	0.313637	8.851960	-1.123853
215	6	0	3.343996	8.329773	-3.431363
216	6	0	3.275777	9.680433	-4.152132

217	1	0	2.398370	7.140146	1.027387
218	1	0	0.776401	9.289176	-3.176954
219	1	0	4.404385	8.229625	-3.047733
220	1	0	3.503554	10.503626	-3.464275
221	1	0	2.291244	9.879199	-4.586901
222	1	0	4.005905	9.718507	-4.970663
223	8	0	-5.135733	6.020749	-3.081289
224	8	0	-2.655294	7.708107	0.594982
225	6	0	-4.113577	6.787199	-2.572328
226	6	0	-3.881003	6.853759	-1.196902
227	6	0	-2.850729	7.696888	-0.761799
228	6	0	-2.087060	8.481764	-1.653778
229	6	0	-2.325692	8.326464	-3.024812
230	6	0	-3.333819	7.490831	-3.515914
231	6	0	-1.068378	9.467251	-1.121865
232	6	0	-1.113579	10.808823	-1.860798
233	1	0	-4.461809	6.266815	-0.490134
234	1	0	-1.711636	8.885037	-3.734350
235	1	0	-1.339250	9.688858	-0.044260
236	1	0	-0.855880	10.717614	-2.920504
237	1	0	-0.411274	11.523000	-1.413382
238	1	0	-2.116746	11.249852	-1.806122
239	8	0	4.944684	6.074622	-3.390031
240	8	0	2.489890	3.798505	-6.750996
241	6	0	3.907748	6.021674	-4.292595
242	6	0	3.702515	4.891915	-5.086835
243	6	0	2.652268	4.941174	-6.012906
244	6	0	1.841186	6.086297	-6.176886
245	6	0	2.057577	7.165834	-5.311863
246	6	0	3.085056	7.166938	-4.362885
247	6	0	0.800564	6.133061	-7.275617
248	6	0	0.790529	7.477462	-8.011054
249	1	0	4.319736	4.002772	-4.986081
250	1	0	1.409818	8.041564	-5.388338
251	1	0	1.084242	5.351809	-8.045878
252	1	0	0.515584	8.313740	-7.361095
253	1	0	0.075308	7.459979	-8.842718
254	1	0	1.780508	7.700277	-8.428365
255	1	0	0.389174	7.846599	1.968435
256	1	0	4.491712	6.834174	-1.837523
257	1	0	-5.682970	5.573155	-2.344799
258	1	0	-1.816733	8.223163	0.861805
259	1	0	5.517040	5.228341	-3.413584
260	1	0	1.642562	3.817736	-7.315843
261	1	0	0.907699	-2.281046	7.554865
262	1	0	-3.972045	-4.571261	5.746451
263	1	0	-0.813083	-7.970998	-1.902964
264	1	0	4.069347	-6.922081	0.633534
265	8	0	1.210951	-3.247753	7.419514
266	8	0	-3.339511	-3.921123	6.225992
267	6	0	0.193957	-4.053414	6.977306
268	6	0	-1.102909	-3.558447	6.808326
269	6	0	-2.084204	-4.468271	6.398341
270	6	0	-1.815203	-5.833321	6.183892
271	6	0	-0.485737	-6.261835	6.314651
272	6	0	0.537747	-5.398741	6.711296
273	6	0	-2.935575	-6.791519	5.835821
274	6	0	-2.834602	-8.109322	6.610110
275	1	0	-1.336244	-2.513077	6.983155
276	1	0	-0.245349	-7.306776	6.104741
277	1	0	-3.910369	-6.309657	6.152878
278	1	0	-3.687559	-8.760376	6.380101
279	1	0	-2.834620	-7.929106	7.691939
280	1	0	-1.924884	-8.670566	6.373652
281	8	0	-1.006035	-8.441023	-1.014953
282	8	0	3.561696	-7.439763	-0.114848
283	6	0	0.069153	-8.374835	-0.157150

284	6	0	1.317784	-7.924557	-0.592450
285	6	0	2.357843	-7.896395	0.345335
286	6	0	2.178704	-8.328855	1.681773
287	6	0	0.900796	-8.743714	2.067881
288	6	0	-0.173942	-8.780810	1.171358
289	6	0	3.356279	-8.360618	2.634744
290	6	0	3.407731	-9.660562	3.445770
291	1	0	1.491333	-7.596304	-1.614603
292	1	0	0.734370	-9.053928	3.101219
293	1	0	4.301946	-8.337676	2.014257
294	1	0	4.297875	-9.682352	4.086282
295	1	0	3.457138	-10.530054	2.778417
296	1	0	2.534123	-9.794018	4.090334
297	8	0	4.841216	-6.116922	1.964658
298	8	0	3.375791	-3.556619	5.677913
299	6	0	4.091460	-5.985416	3.101086
300	6	0	4.080284	-4.789667	3.826509
301	6	0	3.354431	-4.766002	5.022898
302	6	0	2.659846	-5.891318	5.511329
303	6	0	2.657804	-7.047063	4.715171
304	6	0	3.357484	-7.126169	3.510681
305	6	0	1.977298	-5.843533	6.861002
306	6	0	2.095363	-7.161182	7.634057
307	1	0	4.640900	-3.919995	3.488303
308	1	0	2.093369	-7.918193	5.055486
309	1	0	2.513380	-5.063030	7.482691
310	1	0	3.147865	-7.446327	7.757912
311	1	0	1.589589	-7.992782	7.133561
312	1	0	1.656590	-7.065703	8.634783
313	8	0	-4.667435	-5.321543	4.264218
314	8	0	-3.210986	-7.246051	0.181582
315	6	0	-3.868534	-6.196318	3.566998
316	6	0	-3.931142	-6.274734	2.173933
317	6	0	-3.126789	-7.236189	1.546521
318	6	0	-2.302519	-8.121861	2.278102
319	6	0	-2.229004	-7.948393	3.664385
320	6	0	-2.997944	-6.994079	4.339211
321	6	0	-1.559867	-9.235054	1.569044
322	6	0	-1.531367	-10.535348	2.380184
323	1	0	-4.576238	-5.620438	1.593452
324	1	0	-1.558824	-8.589421	4.241880
325	1	0	-2.130490	-9.468807	0.619236
326	1	0	-2.547179	-10.863667	2.630383
327	1	0	-0.974937	-10.437634	3.317300
328	1	0	-1.054221	-11.337715	1.802883
329	1	0	5.125212	1.475696	6.332402
330	1	0	2.781149	-3.553824	6.504905
331	1	0	-5.326052	-4.833928	3.656597
332	1	0	-2.529476	-7.880433	-0.252768
333	1	0	6.615919	2.921486	4.991716
334	1	0	-6.833071	-4.375296	1.670911
335	1	0	-5.406882	-0.954945	5.998565
336	1	0	-6.583316	5.114261	-0.017174
337	1	0	-6.224728	1.554534	-4.440141
338	1	0	-7.370232	-0.600183	-4.000074
339	8	0	-6.387996	-4.016924	2.527431
340	8	0	-6.265522	-0.491644	5.695595
341	6	0	-6.979105	-2.881935	3.014131
342	6	0	-6.301877	-2.289530	4.089371
343	6	0	-6.839294	-1.108338	4.608019
344	6	0	-7.991208	-0.495279	4.069411
345	6	0	-8.637738	-1.145084	3.012074
346	6	0	-8.180802	-2.360845	2.490416
347	6	0	-8.469508	0.827351	4.625954
348	6	0	-9.994104	0.897761	4.757581
349	1	0	-5.393604	-2.731855	4.482382
350	1	0	-9.535307	-0.691572	2.585186

351	1	0	-8.053792	0.921262	5.675953
352	1	0	-10.367458	0.091016	5.400099
353	1	0	-10.505307	0.810555	3.793520
354	1	0	-10.302953	1.851065	5.203967
355	8	0	-6.326878	4.720413	-0.931437
356	8	0	-7.085869	1.195232	-4.005200
357	6	0	-7.092207	3.635116	-1.278616
358	6	0	-6.674376	2.983865	-2.446644
359	6	0	-7.399057	1.856929	-2.844286
360	6	0	-8.489414	1.353692	-2.099524
361	6	0	-8.869697	2.054154	-0.950878
362	6	0	-8.215454	3.221069	-0.534850
363	6	0	-9.181784	0.085891	-2.548929
364	6	0	-10.704139	0.154718	-2.392042
365	1	0	-5.813089	3.338377	-3.003530
366	1	0	-9.711530	1.683190	-0.361660
367	1	0	-8.980414	-0.032549	-3.657668
368	1	0	-11.015978	0.274786	-1.349705
369	1	0	-11.175517	-0.761779	-2.768213
370	1	0	-11.116632	0.999127	-2.957419
371	8	0	-7.065673	-1.528518	-3.703222
372	8	0	-7.079134	-4.559695	-0.046475
373	6	0	-7.580282	-1.876488	-2.475491
374	6	0	-7.043891	-3.043318	-1.919623
375	6	0	-7.521683	-3.428050	-0.662558
376	6	0	-8.487115	-2.667003	0.043270
377	6	0	-8.991019	-1.516895	-0.566587
378	6	0	-8.582838	-1.113025	-1.844843
379	6	0	-8.931350	-3.119657	1.415924
380	6	0	-10.451583	-3.041170	1.593027
381	1	0	-6.268807	-3.603502	-2.437003
382	1	0	-9.732520	-0.916862	-0.035545
383	1	0	-8.656749	-4.213868	1.518743
384	1	0	-10.750137	-3.410651	2.581304
385	1	0	-10.958911	-3.657542	0.839868
386	1	0	-10.837585	-2.022261	1.491738
387	8	0	-6.029388	2.226525	5.338919
388	8	0	-6.461435	5.285819	1.733588
389	6	0	-6.736742	2.631671	4.229759
390	6	0	-6.210720	3.749912	3.572841
391	6	0	-6.882082	4.190879	2.427426
392	6	0	-8.029376	3.528865	1.923623
393	6	0	-8.512058	2.424145	2.627801
394	6	0	-7.907539	1.971429	3.808633
395	6	0	-8.680597	4.033652	0.655261
396	6	0	-10.207672	4.094240	0.767175
397	1	0	-5.308253	4.236099	3.930748
398	1	0	-9.393277	1.900119	2.252177
399	1	0	-8.331863	5.099501	0.495384
400	1	0	-10.658179	3.112807	0.944801
401	1	0	-10.651498	4.498851	-0.150365
402	1	0	-10.507949	4.745396	1.597876
403	1	0	-6.411745	-5.139655	-0.639900
404	1	0	-6.369820	1.339928	5.711381
405	1	0	-5.638747	5.784165	2.183656
406	1	0	4.496055	6.473047	2.835444
407	1	0	6.572640	3.065390	-4.253615
408	1	0	-5.153763	3.527261	6.173494
409	1	0	6.947106	-3.276761	2.846574
410	1	0	5.606677	-5.073458	-2.365728
411	1	0	7.486714	3.576428	2.703607
412	1	0	6.575945	-1.673883	4.792329
413	8	0	6.316433	3.647092	-3.444078
414	8	0	7.133730	4.493307	1.152395
415	6	0	7.110337	3.419625	-2.348555
416	6	0	6.688815	4.068336	-1.179391
417	6	0	7.441376	3.847828	-0.022213

418	6	0	8.555011	2.980385	0.008582
419	6	0	8.942992	2.381088	-1.194205
420	6	0	8.269156	2.618056	-2.398407
421	6	0	9.263589	2.712051	1.317965
422	6	0	10.785684	2.632954	1.165126
423	1	0	5.805737	4.696564	-1.182854
424	1	0	9.807447	1.712742	-1.195718
425	1	0	9.055825	3.593488	1.999301
426	1	0	11.101649	1.807517	0.518860
427	1	0	11.266980	2.482891	2.139493
428	1	0	11.183911	3.558936	0.733454
429	8	0	6.477543	-3.741111	2.069156
430	8	0	6.472216	-4.545204	-2.589770
431	6	0	7.116088	-3.548537	0.872797
432	6	0	6.456725	-4.121950	-0.221575
433	6	0	7.030448	-3.959210	-1.483239
434	6	0	8.213428	-3.208243	-1.681513
435	6	0	8.836359	-2.668025	-0.552583
436	6	0	8.336737	-2.853035	0.742655
437	6	0	8.747117	-3.001905	-3.080708
438	6	0	10.277380	-3.028916	-3.151555
439	1	0	5.509426	-4.651775	-0.077613
440	1	0	9.752881	-2.089016	-0.684353
441	1	0	8.383201	-3.871415	-3.709395
442	1	0	10.619648	-2.930430	-4.188951
443	1	0	10.667204	-3.976049	-2.759010
444	1	0	10.740287	-2.220389	-2.577467
445	8	0	7.168631	2.829825	3.320290
446	8	0	7.229474	-1.871699	3.983278
447	6	0	7.694274	1.605282	2.967366
448	6	0	7.173774	0.517213	3.676999
449	6	0	7.658402	-0.751951	3.341328
450	6	0	8.614736	-0.946129	2.312035
451	6	0	9.101483	0.178893	1.646755
452	6	0	8.685768	1.477890	1.977420
453	6	0	9.061082	-2.351837	1.972555
454	6	0	10.585255	-2.459670	1.850439
455	1	0	6.413861	0.656987	4.438724
456	1	0	9.833390	0.046814	0.847417
457	1	0	8.763740	-3.022432	2.835794
458	1	0	10.990692	-1.828872	1.053641
459	1	0	10.885867	-3.492733	1.637315
460	1	0	11.070134	-2.157077	2.786565
461	8	0	6.492056	-3.008440	-4.882923
462	8	0	6.584220	1.719189	-5.403863
463	6	0	7.068917	-1.804383	-4.547616
464	6	0	6.504987	-0.680076	-5.161094
465	6	0	7.072153	0.562455	-4.860017
466	6	0	8.172087	0.696926	-3.980803
467	6	0	8.687291	-0.461426	-3.390286
468	6	0	8.170726	-1.731516	-3.671895
469	6	0	8.755205	2.067374	-3.721984
470	6	0	10.284106	2.073439	-3.835020
471	1	0	5.667970	-0.777140	-5.845347
472	1	0	9.522399	-0.373891	-2.692708
473	1	0	8.375573	2.758471	-4.535022
474	1	0	10.596879	1.739148	-4.832557
475	1	0	10.764138	1.411065	-3.107951
476	1	0	10.685261	3.081698	-3.679787
477	1	0	6.701768	-3.740727	-4.197400
478	1	0	5.760183	1.562741	-6.039627
479	1	0	-3.138205	-0.396024	7.684216
480	1	0	5.112780	-5.206523	1.575080
481	1	0	2.186693	7.046464	3.400422
482	1	0	-3.605309	5.261864	5.361156
483	1	0	-0.704829	-0.479831	7.992581
484	1	0	-6.636491	-2.863946	-4.776205

485	1	0	-4.567989	0.905395	-6.582381
486	1	0	4.943968	-2.902803	-5.564728
487	8	0	-4.908774	2.095863	-5.380988
488	1	0	-4.135247	2.297736	-4.805680
489	1	0	-5.115652	2.946432	-5.827791
490	1	0	3.058757	-6.249188	-3.008880
491	1	0	6.284228	5.055616	1.079094
492	8	0	4.922722	6.136187	1.174024
493	1	0	5.129543	6.980375	0.717358
494	1	0	4.172232	5.767303	0.658445
495	8	0	-3.930863	-1.603566	6.688964
496	1	0	-4.110608	-2.396412	7.237948
497	1	0	-3.342807	-1.938930	5.977350
498	8	0	4.237287	-6.027221	-2.075129
499	1	0	3.816832	-5.582804	-1.218020
500	1	0	4.435696	-6.938679	-1.777874

Sum of electronic and thermal Free Energies= -0.706543
0 imaginary frequency

TS3c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	4.753992	4.100184	6.222894
2	8	0	1.258445	7.060834	4.689225
3	6	0	3.515127	4.681706	6.322484
4	6	0	3.059141	5.602198	5.373360
5	6	0	1.793001	6.157234	5.581746
6	6	0	0.993055	5.834085	6.697371
7	6	0	1.481865	4.873469	7.592423
8	6	0	2.739545	4.284441	7.434397
9	6	0	-0.347485	6.508546	6.893441
10	6	0	-0.481334	7.103677	8.298994
11	1	0	3.661933	5.858550	4.506850
12	1	0	0.857887	4.572730	8.436573
13	1	0	-0.403614	7.380191	6.173187
14	1	0	-0.404219	6.347535	9.086704
15	1	0	-1.445043	7.612479	8.420389
16	1	0	0.310343	7.841420	8.482412
17	8	0	-5.287538	0.999950	7.041143
18	8	0	-1.777608	-2.166408	8.040017
19	6	0	-4.069488	0.652683	7.573021
20	6	0	-3.579418	-0.654345	7.487097
21	6	0	-2.342021	-0.910467	8.086159
22	6	0	-1.603209	0.081363	8.763954
23	6	0	-2.123025	1.382010	8.781654
24	6	0	-3.355351	1.696655	8.200938
25	6	0	-0.290779	-0.270558	9.430974
26	6	0	-0.250395	0.204330	10.887035
27	1	0	-4.133453	-1.428230	6.964932
28	1	0	-1.544225	2.175368	9.259456
29	1	0	-0.212316	-1.399655	9.462880
30	1	0	-0.354938	1.289977	10.980155
31	1	0	0.694114	-0.079726	11.366615
32	1	0	-1.066404	-0.248930	11.464143
33	8	0	-1.320648	6.162731	4.170870
34	8	0	-4.638721	3.112556	5.353118
35	6	0	-1.901429	5.451732	5.198950
36	6	0	-2.964535	4.633304	4.807001
37	6	0	-3.599235	3.884134	5.804958
38	6	0	-3.200868	3.936093	7.160622
39	6	0	-2.125512	4.768367	7.489333
40	6	0	-1.471534	5.559775	6.537492
41	6	0	-3.923015	3.100846	8.197008

42	6	0	-3.917590	3.722335	9.596851
43	1	0	-3.262356	4.551514	3.765337
44	1	0	-1.789706	4.811584	8.528294
45	1	0	-5.008449	3.038178	7.882732
46	1	0	-4.356106	4.727468	9.581799
47	1	0	-2.911280	3.805273	10.019269
48	1	0	-4.510267	3.112458	10.290842
49	8	0	0.850720	-1.778996	7.216896
50	8	0	4.149821	1.372010	6.286170
51	6	0	1.381268	-0.551290	7.553316
52	6	0	2.479569	-0.166918	6.779409
53	6	0	3.072422	1.067283	7.073979
54	6	0	2.595549	1.908006	8.107019
55	6	0	1.486299	1.472657	8.838806
56	6	0	0.871416	0.236200	8.605073
57	6	0	3.275994	3.232477	8.382530
58	6	0	3.178280	3.679051	9.844419
59	1	0	2.841657	-0.783128	5.961609
60	1	0	1.090621	2.114257	9.629911
61	1	0	4.378652	3.096299	8.166484
62	1	0	3.594415	2.918252	10.515856
63	1	0	2.148607	3.874004	10.159744
64	1	0	3.745588	4.605557	10.001747
65	1	0	0.342471	2.425669	0.281055
66	1	0	-0.489729	2.525616	-1.274808
67	1	0	-1.200982	1.597687	0.049075
68	1	0	1.354950	0.868697	-1.563379
69	1	0	-0.126479	-0.614419	0.752587
70	1	0	2.706460	-0.839493	-0.590748
71	1	0	3.702276	-5.032337	1.685833
72	1	0	2.831872	-5.154075	0.153796
73	1	0	3.979404	-2.658125	1.533820
74	1	0	0.597993	-2.517768	2.287350
75	6	0	1.582454	-4.441020	1.812551
76	6	0	0.954725	-3.096906	1.410623
77	7	0	2.033701	-2.342529	0.699134
78	6	0	4.101737	-3.009691	-0.622171
79	8	0	5.289857	-3.444597	-0.584888
80	8	0	3.549457	-2.518415	-1.612524
81	6	0	1.847878	-1.233509	0.008527
82	6	0	0.616356	-0.474323	-0.033516
83	6	0	0.520007	0.644320	-0.887985
84	1	0	0.923250	-5.289619	1.546437
85	6	0	3.329618	-3.092784	0.726747
86	6	0	2.926878	-4.536225	1.070425
87	1	0	0.089557	-3.234060	0.714669
88	1	0	1.733109	-4.500415	2.907426
89	6	0	-0.249336	1.846250	-0.445282
90	8	0	-4.611094	-4.637507	-5.870908
91	8	0	-4.290259	0.023575	-7.095247
92	6	0	-4.030895	-3.587669	-6.540824
93	6	0	-4.515909	-2.282445	-6.412275
94	6	0	-3.886968	-1.292108	-7.172903
95	6	0	-2.822028	-1.569427	-8.054398
96	6	0	-2.342065	-2.884860	-8.101263
97	6	0	-2.924912	-3.914281	-7.356328
98	6	0	-2.232388	-0.464135	-8.903374
99	6	0	-2.154479	-0.865724	-10.380095
100	1	0	-5.334805	-2.051935	-5.737395
101	1	0	-1.481653	-3.110567	-8.735039
102	1	0	-2.935965	0.421290	-8.852381
103	1	0	-3.151736	-1.110145	-10.767344
104	1	0	-1.521069	-1.743089	-10.546122
105	1	0	-1.751752	-0.047380	-10.988967
106	8	0	4.876152	-0.095901	-6.973526
107	8	0	4.472059	-4.391818	-4.812157
108	6	0	4.336541	-1.354420	-6.837372

109	6	0	4.747351	-2.222497	-5.823856
110	6	0	4.160077	-3.493338	-5.788545
111	6	0	3.211233	-3.907412	-6.754750
112	6	0	2.797996	-2.977801	-7.713175
113	6	0	3.338182	-1.688658	-7.776650
114	6	0	2.680123	-5.322853	-6.728807
115	6	0	2.794545	-5.996656	-8.101334
116	1	0	5.478264	-1.920009	-5.076612
117	1	0	2.027745	-3.264196	-8.431484
118	1	0	3.333073	-5.924121	-6.027826
119	1	0	3.841872	-6.021355	-8.429194
120	1	0	2.227389	-5.474253	-8.877654
121	1	0	2.433470	-7.030893	-8.062650
122	8	0	2.098177	-5.486065	-3.870453
123	8	0	-2.513889	-5.689036	-4.450773
124	6	0	1.070057	-5.455424	-4.781137
125	6	0	-0.202535	-5.572158	-4.211654
126	6	0	-1.300767	-5.547881	-5.077841
127	6	0	-1.161118	-5.396483	-6.475514
128	6	0	0.137121	-5.292556	-6.988604
129	6	0	1.272753	-5.350433	-6.172868
130	6	0	-2.389553	-5.331597	-7.359152
131	6	0	-2.154921	-5.856741	-8.778020
132	1	0	-0.327223	-5.656963	-3.134549
133	1	0	0.270799	-5.172893	-8.066515
134	1	0	-3.175064	-6.002706	-6.897708
135	1	0	-3.088736	-5.841236	-9.354322
136	1	0	-1.794446	-6.892530	-8.757924
137	1	0	-1.422099	-5.262570	-9.333256
138	8	0	-1.998377	1.548122	-6.806428
139	8	0	2.658054	1.504066	-6.781069
140	6	0	-0.860100	0.981978	-7.344361
141	6	0	0.335221	1.490788	-6.828887
142	6	0	1.529761	0.950242	-7.321968
143	6	0	1.549171	-0.074957	-8.297245
144	6	0	0.320811	-0.540437	-8.774321
145	6	0	-0.902737	-0.013382	-8.339422
146	6	0	2.869036	-0.649633	-8.771846
147	6	0	2.822566	-1.197771	-10.201065
148	1	0	0.341285	2.259353	-6.062042
149	1	0	0.311801	-1.338991	-9.520570
150	1	0	3.622371	0.194189	-8.781090
151	1	0	3.817787	-1.545121	-10.508643
152	1	0	2.507510	-0.423622	-10.910308
153	1	0	2.140026	-2.046791	-10.306457
154	1	0	-5.471577	1.616375	-0.887246
155	1	0	-4.205947	2.815514	-2.671031
156	1	0	-2.007270	1.966093	-3.425636
157	1	0	1.824919	-2.131696	-2.618625
158	1	0	1.020957	-1.431669	-4.068961
159	1	0	0.551344	-3.042798	-3.446975
160	1	0	-0.267733	0.384658	-3.370711
161	8	0	-0.263720	-1.876864	-1.098843
162	6	0	-0.636277	-0.129470	-2.467920
163	6	0	-4.510260	1.231605	-1.233126
164	6	0	-1.992081	0.286750	-2.046195
165	7	0	-0.193218	-1.428508	-2.281995
166	6	0	0.846481	-2.014741	-3.153137
167	6	0	-3.981362	0.067659	-0.668012
168	6	0	-3.797213	1.904385	-2.230573
169	6	0	-2.550898	1.432997	-2.646132
170	6	0	-2.727128	-0.400815	-1.065543
171	1	0	-4.545711	-0.472897	0.092657
172	1	0	-2.311032	-1.303247	-0.608503
173	8	0	-2.824439	-7.568096	-2.375651
174	1	0	-2.035929	-7.683555	-1.811035
175	1	0	-2.544795	-6.979948	-3.108302

176	8	0	6.211194	-0.496361	5.623785
177	1	0	5.360636	-0.059120	5.816642
178	1	0	5.989679	-1.387979	5.288111
179	8	0	-6.654350	4.027662	3.590929
180	1	0	-6.404004	4.666843	2.896702
181	1	0	-5.832696	3.834011	4.086925
182	8	0	3.082783	4.310546	-6.565412
183	1	0	2.301761	4.843172	-6.333640
184	1	0	2.773125	3.385532	-6.624621
185	1	0	2.987496	-5.118519	-4.249102
186	1	0	-3.303216	-5.598911	-5.091937
187	1	0	-2.853141	1.092403	-7.142407
188	1	0	3.520360	1.031210	-7.077984
189	1	0	-1.883245	3.290413	-6.888017
190	1	0	-6.585416	3.633522	-3.696315
191	8	0	-1.925086	4.304305	-6.750544
192	8	0	-5.876885	3.259805	-4.336876
193	6	0	-2.986781	4.681934	-5.972654
194	6	0	-3.921508	3.747049	-5.517228
195	6	0	-5.005792	4.234422	-4.777998
196	6	0	-5.191200	5.603728	-4.507524
197	6	0	-4.192600	6.488925	-4.941167
198	6	0	-3.085164	6.061585	-5.676295
199	6	0	-6.431268	6.082233	-3.781439
200	6	0	-6.952666	7.419144	-4.318161
201	1	0	-3.805956	2.686053	-5.717234
202	1	0	-4.290288	7.550402	-4.701970
203	1	0	-7.250001	5.323935	-3.972059
204	1	0	-7.158039	7.356470	-5.393709
205	1	0	-6.245763	8.240952	-4.166568
206	1	0	-7.887761	7.698676	-3.816243
207	8	0	-3.150441	7.384742	2.484479
208	8	0	0.986849	8.067323	0.255496
209	6	0	-2.432527	7.803641	1.394273
210	6	0	-1.038405	7.699943	1.361663
211	6	0	-0.385404	8.203190	0.230323
212	6	0	-1.072074	8.816798	-0.835847
213	6	0	-2.472690	8.846294	-0.771585
214	6	0	-3.179607	8.357209	0.329490
215	6	0	-0.308437	9.427636	-1.992498
216	6	0	-0.934861	10.735692	-2.487273
217	1	0	-0.487241	7.235027	2.173134
218	1	0	-3.029005	9.276610	-1.607463
219	1	0	0.724460	9.695360	-1.614582
220	1	0	-1.013655	11.465248	-1.672268
221	1	0	-1.938604	10.594983	-2.900173
222	1	0	-0.318698	11.183965	-3.277180
223	8	0	-7.315324	4.051730	-2.125314
224	8	0	-5.449113	5.940221	1.812150
225	6	0	-6.617171	5.048350	-1.481577
226	6	0	-6.368103	4.983662	-0.109104
227	6	0	-5.689617	6.064534	0.468812
228	6	0	-5.299460	7.200008	-0.275678
229	6	0	-5.522304	7.179737	-1.657488
230	6	0	-6.180691	6.119876	-2.290093
231	6	0	-4.688775	8.395900	0.423697
232	6	0	-5.273714	9.720853	-0.077103
233	1	0	-6.670900	4.128505	0.488529
234	1	0	-5.179657	8.023050	-2.260679
235	1	0	-4.960261	8.323629	1.521536
236	1	0	-5.064759	9.902691	-1.135826
237	1	0	-4.861728	10.566095	0.487964
238	1	0	-6.363687	9.737033	0.047308
239	8	0	2.051688	8.023144	-2.306421
240	8	0	0.489682	5.474313	-5.993307
241	6	0	1.070092	7.695935	-3.212743
242	6	0	1.280049	6.708611	-4.177490

243	6	0	0.240920	6.470708	-5.086251
244	6	0	-0.962446	7.210581	-5.071935
245	6	0	-1.138123	8.146877	-4.045767
246	6	0	-0.140359	8.414831	-3.103157
247	6	0	-1.999228	6.999959	-6.154954
248	6	0	-2.558342	8.323258	-6.687961
249	1	0	2.204266	6.137899	-4.219943
250	1	0	-2.081546	8.693175	-3.985194
251	1	0	-1.481477	6.498177	-7.029449
252	1	0	-3.089698	8.897392	-5.922728
253	1	0	-3.260253	8.145780	-7.512025
254	1	0	-1.750890	8.960499	-7.070226
255	1	0	-2.558884	6.942238	3.191397
256	1	0	1.410585	8.262901	-0.658204
257	1	0	-7.616378	3.316349	-1.485126
258	1	0	-4.825351	6.667155	2.162959
259	1	0	2.911112	7.492399	-2.462262
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261	1	0	2.188987	-2.935254	7.003288
262	1	0	-1.587599	-6.567662	4.799478
263	1	0	2.212352	-7.111314	-3.215464
264	1	0	6.631585	-5.021416	-0.514788
265	8	0	2.821765	-3.681035	6.708944
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267	6	0	2.154027	-4.731458	6.135767
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269	6	0	0.161955	-5.868615	5.472944
270	6	0	0.903123	-6.987696	5.048683
271	6	0	2.301494	-6.908954	5.128480
272	6	0	2.954569	-5.799752	5.669972
273	6	0	0.197696	-8.225880	4.534656
274	6	0	0.826014	-9.518396	5.064166
275	1	0	0.167302	-3.884862	6.360582
276	1	0	2.898855	-7.747009	4.761170
277	1	0	-0.864377	-8.204064	4.926972
278	1	0	0.260043	-10.393438	4.720088
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281	8	0	2.237265	-7.791513	-2.451296
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284	6	0	4.283854	-6.628182	-1.908661
285	6	0	5.303191	-6.428964	-0.969685
286	6	0	5.330229	-7.111046	0.270995
287	6	0	4.283288	-7.993655	0.552179
288	6	0	3.246748	-8.235880	-0.357579
289	6	0	6.480383	-6.894073	1.233814
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291	1	0	4.287956	-6.080841	-2.848486
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293	1	0	7.339822	-6.448398	0.648695
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295	1	0	7.320578	-8.890396	1.023293
296	1	0	6.244771	-8.737729	2.414067
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303	6	0	5.451022	-6.251449	3.486831
304	6	0	6.087771	-5.891541	2.298317
305	6	0	4.462190	-5.707073	5.778028
306	6	0	5.077171	-6.989323	6.348662
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310	1	0	6.165132	-6.886389	6.450204
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317	6	0	-0.061404	-7.965629	0.234177
318	6	0	1.071530	-8.591877	0.803475
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325	1	0	1.633762	-9.452672	-1.077415
326	1	0	1.822203	-11.253451	0.621517
327	1	0	3.172721	-10.435531	1.416506
328	1	0	3.349063	-11.006439	-0.242507
329	1	0	4.524726	2.303806	6.466944
330	1	0	4.390007	-3.264262	5.799048
331	1	0	-2.886765	-7.011363	2.713942
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333	1	0	5.259425	4.404628	5.388036
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335	1	0	-4.291778	-3.910340	5.661392
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337	1	0	-6.885135	-0.276341	-4.328530
338	1	0	-6.970002	-2.736283	-4.163708
339	8	0	-4.246345	-6.516457	1.712175
340	8	0	-5.276820	-3.763696	5.432601
341	6	0	-5.191192	-5.784325	2.379496
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346	6	0	-6.527658	-5.680505	1.940494
347	6	0	-7.867490	-3.216923	4.574488
348	6	0	-9.294025	-3.755937	4.718666
349	1	0	-3.698745	-5.284313	3.868096
350	1	0	-8.400753	-4.685045	2.301960
351	1	0	-7.453189	-3.125887	5.625103
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358	6	0	-7.660744	0.550076	-2.113367
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366	1	0	-9.681320	-2.164575	-0.161075
367	1	0	-8.651765	-2.956672	-3.725318
368	1	0	-10.448697	-3.802415	-1.354804
369	1	0	-10.299583	-4.621610	-2.910647
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371	8	0	-6.276878	-3.469144	-4.006647
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373	6	0	-6.525314	-4.186606	-2.858867
374	6	0	-5.523231	-5.097995	-2.506558
375	6	0	-5.720328	-5.843892	-1.339658
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377	6	0	-7.833422	-4.753675	-0.928195
378	6	0	-7.709860	-4.017893	-2.114742
379	6	0	-6.997839	-6.485661	0.747122
380	6	0	-8.410273	-7.048004	0.940025
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385	1	0	-8.693252	-7.679343	0.088099
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394	6	0	-7.828592	-1.838914	3.948009
395	6	0	-9.560539	0.231058	1.207421
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405	1	0	-7.261424	2.744310	2.959051
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408	1	0	-5.733645	0.222367	6.554084
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411	1	0	5.691915	5.698735	3.254646
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419	6	0	7.287806	5.768885	-0.734123
420	6	0	6.511925	5.942725	-1.886254
421	6	0	7.617010	5.817187	1.797415
422	6	0	9.046458	6.345941	1.640477
423	1	0	3.564072	6.862358	-0.357987
424	1	0	8.323752	5.438118	-0.840398
425	1	0	7.138195	6.431471	2.620440
426	1	0	9.605576	5.822309	0.858244
427	1	0	9.609297	6.228951	2.574774
428	1	0	9.042222	7.411746	1.382648
429	8	0	7.721454	-1.356672	1.583652
430	8	0	7.680448	-1.452708	-3.148726
431	6	0	8.103663	-0.745565	0.420081
432	6	0	7.671748	-1.404449	-0.738803
433	6	0	8.003464	-0.835329	-1.968578
434	6	0	8.699683	0.392886	-2.066715
435	6	0	9.120183	0.999886	-0.880252
436	6	0	8.876360	0.434316	0.377525
437	6	0	8.940698	1.012029	-3.424660
438	6	0	10.351708	1.592816	-3.567220
439	1	0	7.072856	-2.318549	-0.663406
440	1	0	9.664982	1.944428	-0.936405
441	1	0	8.858155	0.186179	-4.194599
442	1	0	10.506157	2.000016	-4.573457
443	1	0	11.107187	0.814873	-3.400870

444	1	0	10.550583	2.397651	-2.852874
445	8	0	5.706387	4.796655	3.728892
446	8	0	7.636116	0.460439	3.678895
447	6	0	6.655173	3.945537	3.203656
448	6	0	6.628088	2.647222	3.725659
449	6	0	7.559641	1.736126	3.215568
450	6	0	8.474834	2.088318	2.190309
451	6	0	8.457615	3.399900	1.716889
452	6	0	7.581912	4.367938	2.233153
453	6	0	9.420371	1.035357	1.654734
454	6	0	10.849961	1.564581	1.493034
455	1	0	5.900675	2.361557	4.478443
456	1	0	9.153246	3.687235	0.925928
457	1	0	9.474000	0.204990	2.423870
458	1	0	10.916296	2.389053	0.776812
459	1	0	11.519871	0.770500	1.141112
460	1	0	11.238436	1.929511	2.451429
461	8	0	6.465255	0.337989	-4.793165
462	8	0	5.002780	4.849369	-4.863441
463	6	0	6.704921	1.640369	-4.438627
464	6	0	5.721582	2.549508	-4.849244
465	6	0	5.895658	3.887328	-4.482575
466	6	0	6.992710	4.319662	-3.700662
467	6	0	7.954453	3.371015	-3.340636
468	6	0	7.860577	2.029546	-3.729984
469	6	0	7.079149	5.769072	-3.280375
470	6	0	8.496132	6.337581	-3.410705
471	1	0	4.853938	2.215697	-5.409733
472	1	0	8.811690	3.687885	-2.743135
473	1	0	6.429969	6.367640	-3.989575
474	1	0	8.851435	6.252184	-4.445491
475	1	0	9.220056	5.817246	-2.775685
476	1	0	8.519520	7.398608	-3.135872
477	1	0	7.113859	-0.328488	-4.352866
478	1	0	4.252054	4.488447	-5.511140
479	1	0	-2.297524	-2.803695	7.431213
480	1	0	6.953127	-3.202546	0.710943
481	1	0	-0.496914	6.687789	4.476441
482	1	0	-5.039260	2.520636	6.082032
483	1	0	0.011573	-2.000216	7.757415
484	1	0	-5.357963	-4.332087	-5.246432
485	1	0	-4.945058	0.181798	-6.321431
486	1	0	5.581059	0.101440	-6.259337
487	8	0	-5.777140	0.892507	-4.984305
488	1	0	-5.168747	1.232249	-4.291455
489	1	0	-6.238144	1.693752	-5.321019
490	1	0	5.125809	-3.971758	-4.057599
491	1	0	3.995683	6.960268	1.934813
492	8	0	2.288491	7.324734	2.170170
493	1	0	2.080231	8.239909	1.883001
494	1	0	1.738119	6.762409	1.582254
495	8	0	-2.638579	-4.034583	6.236603
496	1	0	-2.458237	-4.910888	6.639255
497	1	0	-2.008904	-3.988084	5.484067
498	8	0	6.227151	-3.698318	-3.034630
499	1	0	5.720739	-3.638179	-2.106361
500	1	0	6.719679	-4.539070	-2.962532

Sum of electronic and thermal Free Energies= -0.653048
1 imaginary frequency: -630.9486

P2c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	4.812708	4.153455	6.170780

2	8	0	0.912543	6.817139	5.153390
3	6	0	3.532446	4.586123	6.410022
4	6	0	2.905842	5.518251	5.576602
5	6	0	1.610946	5.914262	5.924748
6	6	0	0.945351	5.423792	7.067512
7	6	0	1.603817	4.458911	7.840708
8	6	0	2.897984	4.024324	7.540059
9	6	0	-0.436447	5.931394	7.419131
10	6	0	-0.513186	6.402041	8.875192
11	1	0	3.404529	5.903104	4.691746
12	1	0	1.087274	4.030252	8.702018
13	1	0	-0.642054	6.842886	6.779808
14	1	0	-0.293287	5.602441	9.589632
15	1	0	-1.510944	6.791667	9.110118
16	1	0	0.210352	7.206516	9.059358
17	8	0	-4.745530	-0.089946	7.487035
18	8	0	-0.853085	-2.915218	7.946620
19	6	0	-3.457434	-0.339137	7.891902
20	6	0	-2.843922	-1.574867	7.662194
21	6	0	-1.539753	-1.736230	8.140005
22	6	0	-0.852211	-0.721406	8.837046
23	6	0	-1.499802	0.510207	9.000043
24	6	0	-2.802957	0.729229	8.544065
25	6	0	0.540570	-0.975777	9.371969
26	6	0	0.653058	-0.609541	10.855359
27	1	0	-3.358791	-2.364849	7.123906
28	1	0	-0.967121	1.325343	9.494486
29	1	0	0.738359	-2.088498	9.303778
30	1	0	0.443358	0.447711	11.046453
31	1	0	1.658758	-0.822201	11.237497
32	1	0	-0.060068	-1.192356	11.452272
33	8	0	-1.599949	5.692047	4.761159
34	8	0	-4.461009	2.204099	5.928416
35	6	0	-2.012155	4.842700	5.765421
36	6	0	-3.011816	3.941991	5.387694
37	6	0	-3.475626	3.051683	6.363742
38	6	0	-2.970648	3.044380	7.684557
39	6	0	-1.964932	3.964272	7.999466
40	6	0	-1.481980	4.894232	7.071083
41	6	0	-3.511550	2.058870	8.699085
42	6	0	-3.453341	2.570862	10.141476
43	1	0	-3.389074	3.908433	4.369123
44	1	0	-1.547938	3.965586	9.009479
45	1	0	-4.607222	1.900378	8.463612
46	1	0	-3.993632	3.519896	10.243105
47	1	0	-2.429323	2.732383	10.492412
48	1	0	-3.919477	1.849421	10.824909
49	8	0	1.643888	-2.178687	6.959824
50	8	0	4.507326	1.379644	6.051754
51	6	0	2.070966	-0.928951	7.357883
52	6	0	3.055821	-0.368769	6.539733
53	6	0	3.537252	0.898946	6.890334
54	6	0	3.061598	1.602718	8.021354
55	6	0	2.069058	0.993084	8.795228
56	6	0	1.570529	-0.283394	8.506247
57	6	0	3.618747	2.970851	8.354891
58	6	0	3.595650	3.293082	9.852110
59	1	0	3.413922	-0.879907	5.651252
60	1	0	1.674998	1.526036	9.664100
61	1	0	4.708010	2.975276	8.047389
62	1	0	4.144182	2.535900	10.425327
63	1	0	2.580797	3.347451	10.258121
64	1	0	4.072690	4.263078	10.043592
65	1	0	0.729183	2.158733	0.460958
66	1	0	-0.104742	2.685050	-1.003401
67	1	0	-0.978036	1.749036	0.203397
68	1	0	1.414037	0.754942	-1.491873

69	1	0	0.044126	-0.432050	0.964225
70	1	0	2.730644	-0.400570	-0.125334
71	1	0	4.315837	-4.786042	1.216162
72	1	0	3.675190	-4.877066	-0.425057
73	1	0	4.235514	-2.417968	1.268937
74	1	0	0.602175	-3.133841	1.617048
75	6	0	2.120457	-4.668721	1.110747
76	6	0	1.263825	-3.441383	0.780219
77	7	0	2.237026	-2.350827	0.458884
78	6	0	4.321350	-2.416716	-0.930393
79	8	0	5.500105	-2.817400	-1.101234
80	8	0	3.650741	-1.708054	-1.686961
81	6	0	1.924568	-1.131978	0.119237
82	6	0	0.506873	-0.626799	-0.029701
83	6	0	0.421652	0.576407	-1.003779
84	1	0	1.697095	-5.589410	0.662267
85	6	0	3.645173	-2.854850	0.422926
86	6	0	3.525227	-4.378987	0.555837
87	1	0	0.597399	-3.612314	-0.106235
88	1	0	2.157069	-4.853545	2.201858
89	6	0	-0.002337	1.850169	-0.294791
90	8	0	-4.556019	-4.714306	-5.856145
91	8	0	-4.846253	0.013194	-6.790360
92	6	0	-4.149122	-3.569850	-6.499432
93	6	0	-4.746985	-2.333851	-6.235775
94	6	0	-4.308878	-1.240508	-6.989574
95	6	0	-3.323802	-1.352584	-7.992330
96	6	0	-2.717126	-2.602991	-8.170542
97	6	0	-3.108080	-3.729444	-7.440340
98	6	0	-2.951865	-0.145656	-8.826119
99	6	0	-2.942487	-0.469290	-10.324080
100	1	0	-5.505825	-2.229356	-5.466260
101	1	0	-1.910778	-2.698649	-8.900718
102	1	0	-3.758131	0.634879	-8.675378
103	1	0	-3.926008	-0.832013	-10.647953
104	1	0	-2.211791	-1.241837	-10.584150
105	1	0	-2.703588	0.422444	-10.915949
106	8	0	4.166570	0.942328	-7.308591
107	8	0	4.416685	-3.498157	-5.435083
108	6	0	3.781679	-0.375635	-7.226968
109	6	0	4.356969	-1.248626	-6.300489
110	6	0	3.928988	-2.580947	-6.324100
111	6	0	2.977304	-3.048981	-7.259938
112	6	0	2.392880	-2.117651	-8.124440
113	6	0	2.772814	-0.771355	-8.130945
114	6	0	2.627823	-4.519313	-7.305522
115	6	0	2.714585	-5.079434	-8.730406
116	1	0	5.092630	-0.903513	-5.577022
117	1	0	1.615875	-2.451207	-8.814622
118	1	0	3.404279	-5.076722	-6.700853
119	1	0	3.726557	-4.946277	-9.133832
120	1	0	2.025194	-4.584981	-9.421565
121	1	0	2.488131	-6.151856	-8.744983
122	8	0	2.304468	-5.009553	-4.445346
123	8	0	-2.288537	-5.736403	-4.731008
124	6	0	1.205086	-5.030042	-5.274372
125	6	0	0.007035	-5.364309	-4.635672
126	6	0	-1.153797	-5.385168	-5.417385
127	6	0	-1.145038	-5.081205	-6.797522
128	6	0	0.086727	-4.769527	-7.383679
129	6	0	1.283392	-4.768705	-6.657603
130	6	0	-2.437748	-5.079954	-7.587205
131	6	0	-2.257514	-5.481637	-9.053810
132	1	0	-0.022379	-5.567680	-3.568777
133	1	0	0.118730	-4.528362	-8.448902
134	1	0	-3.118118	-5.857785	-7.126169
135	1	0	-3.227758	-5.521370	-9.564890

136	1	0	-1.798278	-6.474406	-9.134268
137	1	0	-1.626887	-4.780427	-9.609694
138	8	0	-2.818045	1.881797	-6.742059
139	8	0	1.816300	2.333988	-6.979420
140	6	0	-1.656677	1.447964	-7.345264
141	6	0	-0.494971	2.082745	-6.897220
142	6	0	0.718822	1.674360	-7.464569
143	6	0	0.791121	0.668941	-8.457055
144	6	0	-0.405503	0.069879	-8.861795
145	6	0	-1.649074	0.454482	-8.344957
146	6	0	2.131526	0.260445	-9.033596
147	6	0	2.050056	-0.215136	-10.487469
148	1	0	-0.526562	2.839445	-6.119274
149	1	0	-0.372297	-0.720721	-9.615381
150	1	0	2.792075	1.179168	-9.038038
151	1	0	3.053165	-0.436917	-10.874243
152	1	0	1.609268	0.556617	-11.129312
153	1	0	1.452534	-1.124937	-10.601546
154	1	0	-5.473805	2.239980	-1.472290
155	1	0	-3.735305	3.408416	-2.814109
156	1	0	-1.520187	2.367123	-3.164950
157	1	0	1.542551	-1.732368	-2.572946
158	1	0	0.304208	-1.924554	-3.854951
159	1	0	0.480612	-3.166470	-2.607480
160	1	0	-0.172810	0.364547	-3.126695
161	8	0	-0.326643	-1.675859	-0.606025
162	6	0	-0.562855	0.070711	-2.117248
163	6	0	-4.501858	1.771791	-1.628087
164	6	0	-1.966224	0.619147	-1.958751
165	7	0	-0.566106	-1.431870	-1.983177
166	6	0	0.510850	-2.076507	-2.781181
167	6	0	-4.214868	0.530546	-1.053052
168	6	0	-3.523554	2.430968	-2.379656
169	6	0	-2.266392	1.852224	-2.561841
170	6	0	-2.948682	-0.041779	-1.208957
171	1	0	-4.975803	0.009720	-0.469982
172	1	0	-2.724003	-1.008927	-0.750497
173	8	0	-2.201307	-7.732208	-2.731373
174	1	0	-1.340555	-7.762444	-2.274600
175	1	0	-2.091844	-7.098267	-3.470656
176	8	0	6.697553	-0.200863	5.114252
177	1	0	5.832202	0.130894	5.418343
178	1	0	6.533388	-1.085683	4.733950
179	8	0	-6.692467	3.015176	4.380908
180	1	0	-6.556937	3.685766	3.684107
181	1	0	-5.817147	2.879867	4.796530
182	8	0	2.003904	5.123151	-6.422178
183	1	0	1.187210	5.514834	-6.067144
184	1	0	1.795850	4.186689	-6.608127
185	1	0	3.099227	-4.493056	-4.854026
186	1	0	-3.136578	-5.637347	-5.293142
187	1	0	-3.622730	1.297637	-6.991361
188	1	0	2.699416	1.947584	-7.326483
189	1	0	-2.953064	3.634769	-6.683707
190	1	0	-7.348186	3.179693	-3.092207
191	8	0	-3.062467	4.616814	-6.413525
192	8	0	-6.699073	2.949175	-3.848143
193	6	0	-4.076720	4.800080	-5.510905
194	6	0	-4.911691	3.744763	-5.130638
195	6	0	-5.936502	4.034590	-4.221874
196	6	0	-6.166304	5.329932	-3.718380
197	6	0	-5.275095	6.341550	-4.104394
198	6	0	-4.228014	6.110148	-4.999486
199	6	0	-7.346579	5.596282	-2.807724
200	6	0	-8.063957	6.905518	-3.152616
201	1	0	-4.761871	2.738684	-5.511291
202	1	0	-5.408359	7.345189	-3.694653

203	1	0	-8.099885	4.766395	-2.977153
204	1	0	-8.396754	6.905546	-4.197790
205	1	0	-7.428076	7.785355	-3.012987
206	1	0	-8.950494	7.040363	-2.520299
207	8	0	-3.681817	6.824581	3.313201
208	8	0	0.158476	8.117654	0.834803
209	6	0	-3.105619	7.388788	2.203829
210	6	0	-1.715942	7.455412	2.064034
211	6	0	-1.218053	8.093885	0.922018
212	6	0	-2.053401	8.679936	-0.048992
213	6	0	-3.438490	8.538066	0.118547
214	6	0	-3.993880	7.906325	1.233730
215	6	0	-1.461396	9.439468	-1.218156
216	6	0	-2.251780	10.708572	-1.553755
217	1	0	-1.052146	7.017000	2.802402
218	1	0	-4.105510	8.943241	-0.645785
219	1	0	-0.426564	9.782631	-0.913137
220	1	0	-2.318040	11.370637	-0.681969
221	1	0	-3.274011	10.496298	-1.882199
222	1	0	-1.760526	11.267635	-2.360305
223	8	0	-7.717990	3.299328	-1.300201
224	8	0	-5.770082	5.100053	2.630629
225	6	0	-7.116424	4.337524	-0.627270
226	6	0	-6.723616	4.191386	0.705065
227	6	0	-6.151560	5.305822	1.330400
228	6	0	-5.999298	6.547071	0.672766
229	6	0	-6.359572	6.616041	-0.678289
230	6	0	-6.927253	5.531611	-1.356017
231	6	0	-5.485581	7.751575	1.432540
232	6	0	-6.256364	9.031048	1.090491
233	1	0	-6.836721	3.247580	1.233065
234	1	0	-6.204764	7.552269	-1.218657
235	1	0	-5.662957	7.559311	2.534852
236	1	0	-6.146356	9.324144	0.041845
237	1	0	-5.906403	9.870967	1.703317
238	1	0	-7.328852	8.902773	1.282894
239	8	0	0.967135	8.264130	-1.807187
240	8	0	-0.674517	5.838060	-5.540373
241	6	0	-0.054555	7.913726	-2.658117
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247	6	0	-3.266101	7.193041	-5.436255
248	6	0	-3.985886	8.499104	-5.790372
249	1	0	1.111863	6.517421	-3.848634
250	1	0	-3.318838	8.710712	-3.138007
251	1	0	-2.766335	6.838459	-6.389512
252	1	0	-4.523486	8.930394	-4.940510
253	1	0	-4.717756	8.334155	-6.590839
254	1	0	-3.271944	9.253945	-6.142907
255	1	0	-2.989810	6.408792	3.940015
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257	1	0	-7.910298	2.507921	-0.687229
258	1	0	-5.234773	5.881946	3.007362
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261	1	0	3.062418	-3.175706	6.574998
262	1	0	-0.477336	-7.036226	4.361789
263	1	0	2.705129	-6.622902	-3.926383
264	1	0	7.044209	-4.193652	-1.347931
265	8	0	3.744248	-3.826706	6.180223
266	8	0	-0.139797	-6.279188	4.967258
267	6	0	3.146579	-4.899440	5.572488
268	6	0	1.755458	-5.043378	5.560769
269	6	0	1.237322	-6.196059	4.959660

270	6	0	2.055476	-7.194200	4.397235
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272	6	0	4.015060	-5.838385	4.969427
273	6	0	1.444715	-8.463657	3.840260
274	6	0	2.242054	-9.713155	4.225949
275	1	0	1.105951	-4.292515	5.999774
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278	1	0	1.744502	-10.619290	3.857191
279	1	0	2.330021	-9.801333	5.315628
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281	8	0	2.869125	-7.340329	-3.212647
282	8	0	6.681450	-4.682577	-2.190655
283	6	0	3.930201	-7.017633	-2.398382
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293	1	0	8.017434	-5.621998	-0.393113
294	1	0	8.866948	-7.260282	1.248616
295	1	0	8.295374	-8.071273	-0.218030
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303	6	0	6.366485	-5.849612	2.588677
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322	6	0	3.808730	-10.220103	-0.552119
323	1	0	-1.180318	-7.304032	0.121578
324	1	0	3.222975	-8.975875	1.780972
325	1	0	2.566769	-9.150273	-1.934592
326	1	0	3.082820	-11.026424	-0.393216
327	1	0	4.390313	-10.112757	0.368444
328	1	0	4.502998	-10.546562	-1.337150
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330	1	0	5.188911	-3.178055	5.212403
331	1	0	-1.883134	-7.472761	2.342699
332	1	0	1.374224	-7.789971	-2.317836
333	1	0	5.214374	4.575755	5.330993
334	1	0	-3.742125	-7.397483	0.632115
335	1	0	-3.380926	-4.779256	5.678563
336	1	0	-8.209105	1.184625	1.526015

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340	8	0	-4.389909	-4.725759	5.535670
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342	6	0	-3.852443	-5.920544	3.511191
343	6	0	-4.780253	-5.282413	4.339063
344	6	0	-6.150226	-5.183916	4.014277
345	6	0	-6.584625	-5.808080	2.839354
346	6	0	-5.712872	-6.512422	2.001100
347	6	0	-7.084826	-4.407000	4.915055
348	6	0	-8.430538	-5.110923	5.116118
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350	1	0	-7.642314	-5.749766	2.572053
351	1	0	-6.598758	-4.350220	5.937051
352	1	0	-8.286932	-6.112308	5.539968
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354	1	0	-9.067639	-4.543817	5.805986
355	8	0	-7.973763	1.182344	0.526127
356	8	0	-7.442319	-1.503473	-3.339510
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361	6	0	-8.890152	-2.330395	-0.101915
362	6	0	-8.809694	-1.113069	0.586286
363	6	0	-8.501942	-3.794281	-2.157930
364	6	0	-9.837130	-4.514695	-1.944201
365	1	0	-7.210031	0.720811	-1.854525
366	1	0	-9.340397	-3.190463	0.399014
367	1	0	-8.441589	-3.556881	-3.264160
368	1	0	-10.006256	-4.788280	-0.897966
369	1	0	-9.878623	-5.439520	-2.532873
370	1	0	-10.676013	-3.881262	-2.257148
371	8	0	-6.069631	-3.839833	-3.736458
372	8	0	-4.126811	-7.246426	-1.058025
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374	6	0	-5.079772	-5.515897	-2.438652
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376	6	0	-6.222449	-6.360692	-0.424733
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378	6	0	-7.313423	-4.666382	-1.813520
379	6	0	-6.191829	-7.271938	0.781346
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384	1	0	-7.468733	-8.660259	1.873292
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387	8	0	-5.443897	-2.202849	5.849221
388	8	0	-7.822675	0.970852	3.240929
389	6	0	-6.439306	-1.958126	4.929656
390	6	0	-6.592623	-0.613254	4.574508
391	6	0	-7.578112	-0.311479	3.628226
392	6	0	-8.374417	-1.316029	3.022877
393	6	0	-8.180829	-2.638573	3.425243
394	6	0	-7.243704	-2.989428	4.407307
395	6	0	-9.389232	-0.923289	1.972318
396	6	0	-10.729423	-1.643861	2.152948
397	1	0	-5.955625	0.154723	5.002935
398	1	0	-8.784150	-3.425294	2.967723
399	1	0	-9.602466	0.181595	2.103494
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401	1	0	-11.456807	-1.310041	1.403194
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404	1	0	-5.291182	-3.200332	5.997495
405	1	0	-7.247815	1.692507	3.768897
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410	1	0	6.944350	-1.288225	-3.667339
411	1	0	5.314692	6.046987	3.275661
412	1	0	7.296767	0.723114	3.987049
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414	8	0	4.381445	7.065225	2.079309
415	6	0	4.275283	6.881557	-1.576506
416	6	0	3.806250	7.003146	-0.261192
417	6	0	4.751796	6.904720	0.763516
418	6	0	6.119262	6.656532	0.517561
419	6	0	6.531777	6.566699	-0.816652
420	6	0	5.641425	6.718063	-1.886060
421	6	0	7.074596	6.479021	1.677107
422	6	0	8.418380	7.177729	1.446368
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424	1	0	7.586723	6.379062	-1.030639
425	1	0	6.605403	6.979380	2.579086
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433	6	0	7.793149	0.201383	-2.600142
434	6	0	8.367133	1.493533	-2.664276
435	6	0	8.837291	2.056596	-1.475096
436	6	0	8.761756	1.385981	-0.247532
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438	6	0	9.758686	2.957187	-4.195926
439	1	0	7.124959	-1.450605	-1.336845
440	1	0	9.287351	3.050983	-1.504982
441	1	0	8.371246	1.438508	-4.806616
442	1	0	9.787701	3.437904	-5.181071
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444	1	0	9.929833	3.735703	-3.446127
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446	8	0	7.842205	1.046723	3.142603
447	6	0	6.453473	4.422193	3.015155
448	6	0	6.614084	3.097836	3.438847
449	6	0	7.587530	2.334195	2.785426
450	6	0	8.361445	2.854096	1.716491
451	6	0	8.160698	4.183762	1.346372
452	6	0	7.236903	5.009944	2.005197
453	6	0	9.358401	1.951851	1.022278
454	6	0	10.704092	2.645753	0.783516
455	1	0	5.994433	2.683282	4.227201
456	1	0	8.746003	4.599249	0.523584
457	1	0	9.568551	1.080682	1.715556
458	1	0	10.618033	3.521388	0.133046
459	1	0	11.417478	1.957638	0.313642
460	1	0	11.139681	2.982620	1.731938
461	8	0	5.959018	1.389299	-5.268498
462	8	0	4.015644	5.696029	-4.840900
463	6	0	6.078514	2.675669	-4.811168
464	6	0	4.976662	3.498294	-5.078544
465	6	0	5.032762	4.813168	-4.607391
466	6	0	6.132492	5.302896	-3.863969
467	6	0	7.212058	4.441775	-3.645835
468	6	0	7.232497	3.132782	-4.141270
469	6	0	6.098797	6.716684	-3.330307
470	6	0	7.429649	7.450789	-3.525368

471	1	0	4.111940	3.115735	-5.611696
472	1	0	8.070928	4.804164	-3.077367
473	1	0	5.329060	7.289596	-3.931810
474	1	0	7.696857	7.486163	-4.589248
475	1	0	8.259397	6.968417	-2.999259
476	1	0	7.364674	8.483362	-3.162889
477	1	0	6.695801	0.765391	-4.916155
478	1	0	3.252706	5.303846	-5.454307
479	1	0	-1.357335	-3.562992	7.336017
480	1	0	7.330268	-2.447726	-0.010059
481	1	0	-0.813145	6.280127	5.047410
482	1	0	-4.735700	1.519676	6.633330
483	1	0	0.875777	-2.528173	7.537917
484	1	0	-5.243442	-4.523419	-5.126633
485	1	0	-5.385121	0.065981	-5.918504
486	1	0	4.892791	1.173877	-6.629293
487	8	0	-6.141453	0.629769	-4.471689
488	1	0	-5.530194	1.112686	-3.869962
489	1	0	-6.803583	1.302207	-4.745137
490	1	0	5.052171	-3.053458	-4.699564
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494	1	0	1.118965	6.800381	1.998833
495	8	0	-1.666217	-4.749874	6.087712
496	1	0	-1.349405	-5.622831	6.402755
497	1	0	-1.126881	-4.578559	5.285856
498	8	0	6.186806	-2.736041	-3.679652
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500	1	0	6.784353	-3.510816	-3.717927

Sum of electronic and thermal Free Energies= -0.718181
0 imaginary frequency

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