Supplementary Material
ORGANIC CHEMISTRY FRONTIERS

Going Beyond Structural Effects: Explicit Solvation Influence on the Rotational Isomerism of C-Glycosylated Flavonoids

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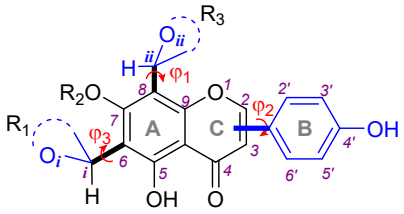
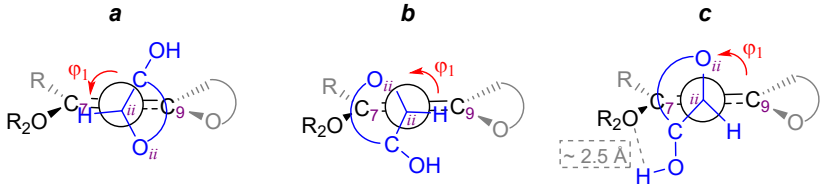
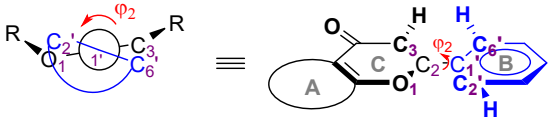
CONFORMATIONAL ANALYSIS



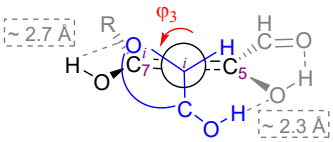
8-C projection: three most stable rotamers



B ring projection: ***a***, ***b***, and ***c*** have a similar dihedral angle



6-C projection: ***a***, ***b***, and ***c*** are equivalents



Flavonoid	Rotamer	Dihedral angle	ΔG
1	*a*	$\varphi_1 = 120.8°$; $\varphi_2 = 20.4°$; $\varphi_3 = -35.3°$	0.0
	b	$\varphi_1 = -63.3°$; $\varphi_2 = 18.3°$; $\varphi_3 = -35.0°$	1.2
	c	$\varphi_1 = -99.9°$; $\varphi_2 = 28.2°$; $\varphi_3 = -35.3°$	2.1
2	*a*	$\varphi_1 = 124.9°$; $\varphi_2 = 20.1°$; $\varphi_3 = -34.4°$	0.0
	b	$\varphi_1 = -62.7°$; $\varphi_2 = 16.2°$; $\varphi_3 = -33.6°$	1.7
	c	$\varphi_1 = 124.9°$; $\varphi_2 = 20.1°$; $\varphi_3 = -34.4°$	0.0 [a]
3	*a*	$\varphi_1 = 123.6°$; $\varphi_2 = 21.4°$	0.0
	b	$\varphi_1 = -63.7°$; $\varphi_2 = 20.2°$	1.6
	c	$\varphi_1 = -98.1°$; $\varphi_2 = 27.5°$	2.8
4	*a*	$\varphi_1 = 120.3°$; $\varphi_2 = 45.14°$	0.0
	b	$\varphi_1 = -62.3°$; $\varphi_2 = 46.4°$	0.3
	c	$\varphi_1 = -104.6°$; $\varphi_2 = 46.7°$	1.2
5	*a*	$\varphi_1 = 119.8°$; $\varphi_2 = 44.8°$	0.0
	b	$\varphi_1 = -63.2°$; $\varphi_2 = 45.8°$	0.1
	c	$\varphi_1 = -102.2°$; $\varphi_2 = 45.5°$	0.9

[a] optimization yield rotamer *a*.

Figure S1: Simplification of Newman projections along the 8-C-glycosyl, C–B ring, and 6-C-glycosyl (for 6,8-di-C-glycosyl flavonoids **1** and **2**) bonds for the three most stable rotamers (*a*, *b*, and *c*). Glycosyl group and B ring highlighted in blue and the flavonoid core in black. Energies relative to rotamer a (kcal mol^{-1}). Values computed at B3LYP-D3/6-311++G(d,p).

ROTATIONAL ISOMERISM

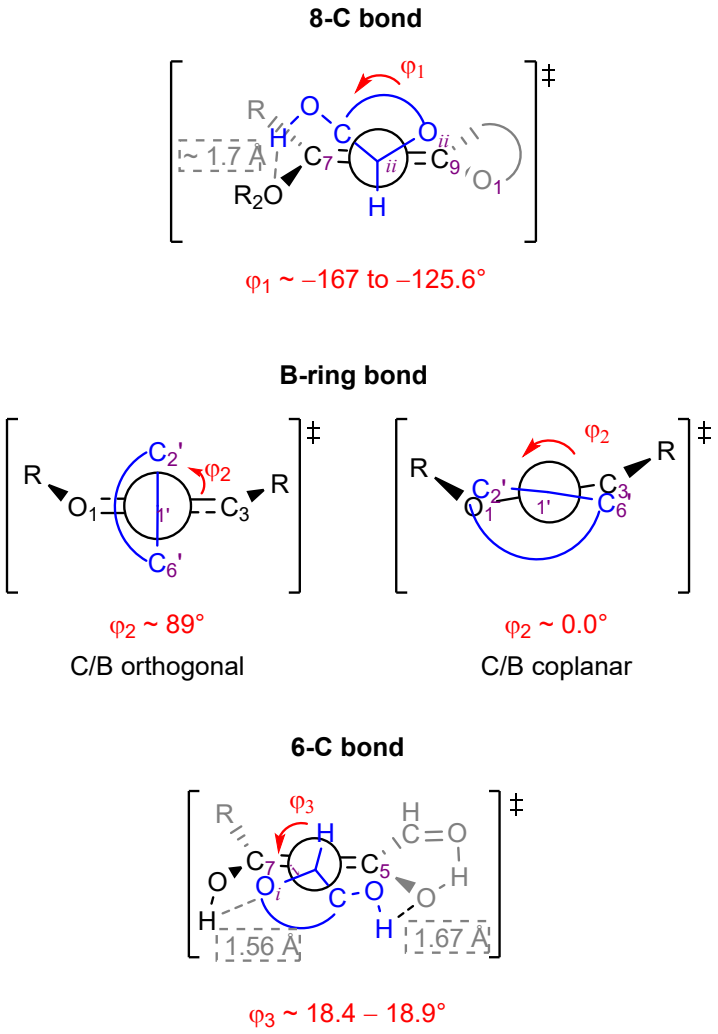


Figure S2: Newman projections of the transition state structures along the 8-C, B-ring and 6-C glycosyl bond calculated with B3LYP-D3/6-311++G(d,p).

Theoretical Rotational Barrier for NMR Signal Duplication

The rotational barrier ($\Delta G^{\ddagger}$) for identifying NMR signal duplication of 1 and 2 Hz can be calculated from the Eyring equation (1):

$$k = \frac{\kappa k_B T}{h} e^{-\frac{\Delta G^{\ddagger}}{RT}} \quad (1)$$

where k is the rate constant, k_B is the Boltzmann constant ($1.3807x10^{-23}$ J K^{-1}), T is temperature (K), h is Planck constant ($6.6262x10^{-34}$ J.s), R is the ideal gas constant (R = 8.314 J $K^{-1}mol^{-1}$) and κ is the transmission coefficient, which is usually taken as unity for monomolecular processes (such as isomerization).

Thus, to obtain $\Delta G^{\ddagger}$ value, we need to calculate the rate constant k. According to the IUPAC Gold Book[1], for a process that follows a first-order kinects, the lifetime of a molecular entity can be associated with the rate constant by $t = \frac{1}{k}$.

From Planck equation, we can correlate the lifetime with the frequency (Δv):

$$\Delta\Delta E \sim \frac{h}{2\pi} x \frac{1}{\Delta t} \sim h\Delta v \quad (2)$$

$$\Delta t = \frac{1}{2\pi\,\Delta v} \quad (3)$$

According to equation (3), the lifetime of a specie separated by Δv = 1 *Hz* and Δv = 2 *Hz* is 0.1592 and 0.0796 s, respectively. Its rate constant (k) of the isomerization processes is 6.2832 and 12.5664 s^{-1}. Aimed to confirm the veracity and reproducibility of this protocol, we also calculated the rate constant for an isomerization process with temperature-dependent first-order half-life time ($t_{1/2}$) of approximately 1000 s, which is reported with a barrier height of 20 kcal mol^{-1} — thus, $k = \frac{1}{t} =$ 0.001 s^{-1}. Rearranging equation (1) in terms of the rotational barrier, we have:

1. IUPAC. Compendium of Chemical Terminology, 2nd ed. (the "Gold Book"). Compiled by A. D. McNaught and A. Wilkinson. Blackwell Scientific Publications, Oxford (1997). Online version (2019-) created by S. J. Chalk. ISBN 0-9678550-9-8. https://doi.org/10.1351/goldbook.

$$\Delta G^{\ddagger} = -RT\left[\ln\left(\frac{kh}{\kappa k_B T}\right)\right] \quad (4)$$

1. IUPAC. Compendium of Chemical Terminology, 2nd ed. (the "Gold Book"). Compiled by A. D. McNaught and A. Wilkinson. Blackwell Scientific Publications, Oxford (1997). Online version (2019-) created by S. J. Chalk. ISBN 0-9678550-9-8. https://doi.org/10.1351/goldbook.

Therefore, according to the calculated rate constants, we have that the barrier heights will be 68.5, 66.7 and 90. kJ mol^{-1} for lifetime of 0.1592, 0.0796, and 1000 s, respectively. Converting to kcal mol^{-1}, the minimum rotational barrier for identify the isomerization processes with NMR signal separation of 1 and 2 Hz is 16.4 and 16.0 kcal mol^{-1}, respectively. For 1000 s, the rotational barrier is 21.6 kcal mol^{-1}, in agreement with IUPAC definition (20 kcal mol^{-1}) of isomerization and experimental isolation of individual isomers.

EXPLICIT SOLVATION

Table S1: Rotational barrier (kcal mol^{-1}) relative to the most stable conformer (*a*) calculated at B3LYP-D3/6-311++G(d,p)/IEFPCM//B3LYP/6-31G(d,p) for 8-C bond rotation using hybrid cluster-continuum solvation model with H_2O as solvent for **1** and DMSO as solvent for **2–5**. Minimum-energy pathway for the rotational isomerism of each system highlighted in bold.

Flavonoid	Number of explicit solvent molecules (*n*)	TS dihedral angle	8-C bond rotation	
1	8	–	$\Delta G_1^{\ddagger}$	[a]
		φ_1 = 37.0°; φ_2 = 39.4°; φ_3 = – 48.9°	$\Delta G_2^{\ddagger}$	**20.9**
2	6	φ_1 = – 164.0°; φ_2 = –11.0°; φ_3 = –35.6°	$\Delta G_1^{\ddagger}$	24.6
		φ_1 = 21.7°; φ_2 = –25.8°; φ_3 = –35.7°	$\Delta G_2^{\ddagger}$	**20.4**
3	4	φ_1 = – 168.8°; φ_2 = 17.4°	$\Delta G_1^{\ddagger}$	21.3
		φ_1 = 20.6°; φ_2 = –11.9°	$\Delta G_2^{\ddagger}$	**19.8**
4	3	**φ_1 = –171.4°**; φ_2 = 35.5°	$\Delta G_1^{\ddagger}$	**17.3**
		φ_1 = 22.7°; φ_2 = 37.2°	$\Delta G_2^{\ddagger}$	20.9
5	3	φ_1 = –164.7°; φ_2 = 37.3°	$\Delta G_1^{\ddagger}$	19.3
		φ_1 = 15.0°; φ_2 = 37.3°	$\Delta G_2^{\ddagger}$	**19.3**

[a] TS not found.

Table S2: Absolute values of the Solvation Electronic Energy (kcal mol^{-1}) calculated for the minimum-energy point (rotamer *a*) and transition state structures of 8-C bond rotation with C_9-O_{ii} eclipsed (TS1, $\varphi_1 = -171$ to $-164°$) and C_7–O_{ii} (TS2, $\varphi_1 = 15$ to $22°$). Solvation energy was obtained from $\Delta E = E_{AB} - (E_A + E_B)$, where AB is the interacting solute-solvent complex, A and B is respectively the solute and solvent configuration in the stationary point. Fragments electronic energy calculated at B3LYP-D3/6-311++G(d,p)/IEFPCM level.

	Stationary Points	C-Glycosylated Flavonoids				
		1	**2**	**3**	**4**	**5**
ΔE	Rotamer *a*	– 68.3	– 58.4	– 50.8	– 55.1	– 35.2
	TS1 C_9-O_{ii}	[*a*]	– 54.8	– 44.3	– 51.6	– 31.7
	TS2 C_7-O_{ii}	– 65.1	– 55.7	– 49.2	– 46.9	– 36.5

[*a*] TS not found.

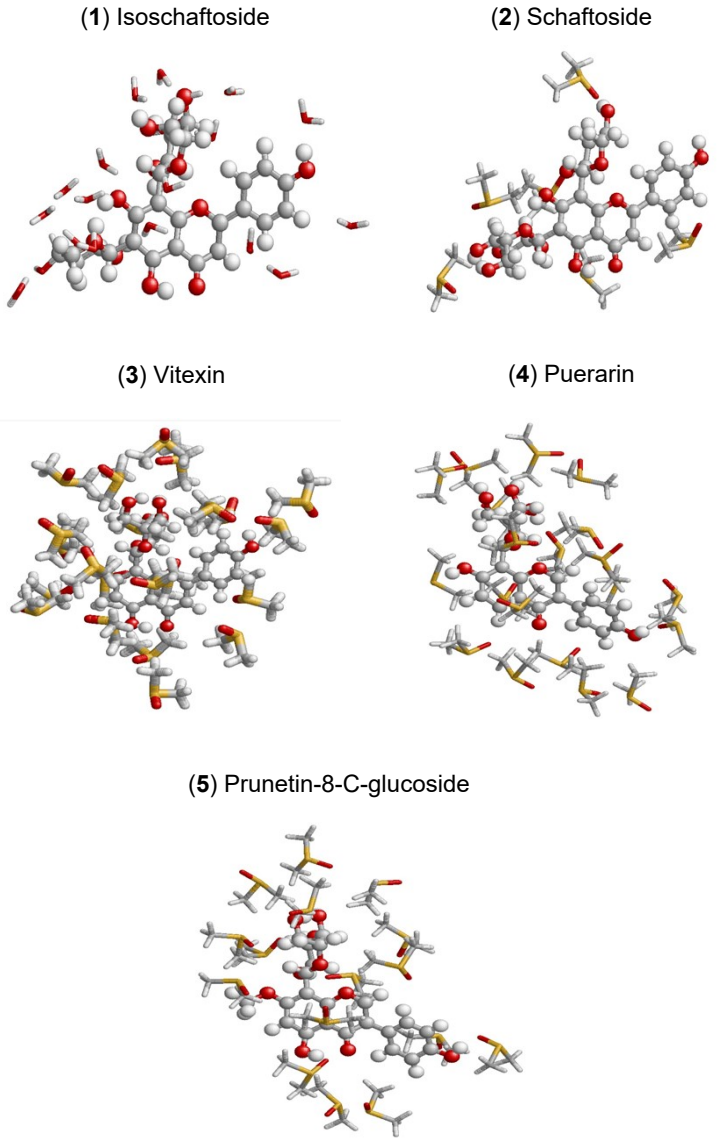


Figure S3: Frames generated from molecular dynamics simulations, including all solvent molecules within a 3.0 Å radius from each flavonoid.

XTB Pre-optimization

1 Isoschaftoside

H	2.589699027	10.269860959	1.108217389
O	1.717088240	10.475771156	1.466387241
C	1.385015294	9.573831044	2.433922912
C	0.179944718	9.732128381	3.114916889
C	2.220573553	8.507605910	2.745980366
H	-0.455244342	10.569655942	2.875112547
C	-0.183574423	8.840743606	4.102959708
H	3.171709338	8.391496821	2.243972858
C	1.846991157	7.610560692	3.724476137
H	-1.114318642	8.988624007	4.626003118
C	0.645227118	7.761388598	4.416509302
H	2.503683888	6.795043266	3.977298713
C	0.318167295	6.803150322	5.474185760
O	0.958661063	5.632562312	5.338405140
C	-0.502977894	7.071870414	6.523860106
C	0.856631931	4.690517867	6.293919353
H	-1.007245654	8.019558620	6.597481977
C	-0.675884436	6.121729336	7.584706435
C	0.088538044	4.896097053	7.448292330
C	1.566609044	3.506917316	6.115889627
O	-1.410181453	6.335906481	8.574071461
C	0.104885696	3.921915840	8.476092623
C	1.625674902	2.579043244	7.159067784
C	2.353383470	3.232693165	4.864098613
O	-0.613864368	4.098855057	9.583865027
C	0.902714854	2.787433541	8.342088423
O	2.418133405	1.517525094	6.971330732
H	2.621525748	2.171080239	4.860504684
O	1.566974698	3.531856853	3.725625405
C	3.662298821	4.044246583	4.900275475
H	-1.089080481	4.970286722	9.483533422
C	1.078323533	1.861024963	9.514732020
H	2.312843860	0.836484693	7.666926109
C	2.225924061	3.263928274	2.510463839
H	3.437395107	5.098652757	5.107618391
O	4.511373572	3.528444519	5.909533246
C	4.426585106	3.956131740	3.578535190
H	0.288395213	2.058200953	10.252297087
O	1.008418332	0.511482689	9.067956537
C	2.453348626	2.133686405	10.180819761
H	1.516989865	3.591611999	1.740650064
C	2.476060361	1.761706663	2.230702910
C	3.484512055	4.150697738	2.386996000
H	4.069438456	3.652950143	6.783993453
H	4.899214669	2.970520535	3.508994580
O	5.433885112	4.962124925	3.513007714
C	1.206844351	-0.436855557	10.089482429
H	3.243406553	1.943274065	9.439485819
O	2.571062011	3.438511458	10.681918922
C	2.637643828	1.152716518	11.340580738

O	3.308392875	1.092657551	3.145276407
H	1.499287783	1.265949017	2.264851621
H	2.869499893	1.684660803	1.213654277
H	4.225986796	0.991946185	2.788260090
H	3.141825298	5.193796794	2.417435078
O	4.175401191	3.893781667	1.187841573
H	5.849771407	5.049690732	4.380978865
H	0.418346892	-0.360910105	10.849507945
H	1.152383757	-1.410986915	9.602899834
C	2.571903815	-0.259489293	10.763537186
H	2.717005600	4.026279482	9.918608679
H	1.831503937	1.295659008	12.075322196
O	3.887613294	1.355101029	11.973628939
H	3.888692789	4.550130989	0.521412473
H	3.365846794	-0.363038145	10.012360952
O	2.727245763	-1.257366418	11.752907051
H	3.898535487	2.285784215	12.234312561
H	3.428401101	-0.955788097	12.344001206
O	2.594586321	-0.848264503	5.085105533
H	1.666928523	-0.678671059	5.324195403
H	2.784662034	-0.240715813	4.355797398
O	3.390537353	6.165924480	-0.077609727
H	2.523935552	6.555816516	0.047976984
H	4.004457606	6.637354643	0.520727521
O	6.125015697	4.404258708	9.379283436
H	6.355655339	4.933409530	10.143837154
H	6.198189139	3.453266099	9.680338692
O	3.095993372	-3.220688125	9.615570612
H	2.916612896	-2.738658462	10.434599996
H	3.793290967	-3.848283501	9.811598322
O	-2.897538450	8.627801564	8.776731020
H	-2.317856025	7.838825715	8.760768722
H	-3.778651956	8.301973552	8.966198576
O	6.483682817	5.214126584	6.717678429
H	6.622487074	5.017259818	7.657136987
H	6.006593154	4.433981813	6.383255823
O	3.635074474	4.440540304	8.319691826
H	3.595790762	5.318004475	7.900855545
H	4.521030868	4.401065431	8.741098711
O	5.475456316	0.931345159	5.388784026
H	4.771561271	0.326461566	5.132642259
H	5.062389561	1.800585476	5.520424473
O	0.125981716	-0.176378282	6.252254383
H	0.295318297	-0.139481361	7.201702420
H	-0.131060764	0.707723629	5.982659311
O	0.134725942	12.950872413	1.658215148
H	0.664634886	12.148688897	1.584943098
H	-0.071183048	13.226844616	0.763759335
O	4.225560717	6.695637497	6.878966372
H	5.104588171	6.273607202	6.740617754
H	4.390657786	7.592890328	7.168520120
O	5.233074854	0.598005894	8.121545364
H	4.527738696	-0.069860050	8.030192556
H	5.565494213	0.709445564	7.218105479
O	5.918518672	0.855458141	2.582385510

H	6.155038475	0.781498383	3.517580750
H	6.393478645	1.622128483	2.207372155
O	6.855697685	3.229875111	1.547588618
H	5.959118690	3.442697682	1.238533348
H	7.017921213	3.832394305	2.278831468
O	6.155738440	1.933852465	10.231012889
H	5.931144159	1.407510358	9.435432255
H	5.476066020	1.710073012	10.881524578
O	-2.433219843	9.759078245	6.324044040
H	-2.652099710	9.405760250	7.208595920
H	-2.473456323	10.712787919	6.404327930
O	5.179376343	7.141604627	1.748379419
H	6.050336528	7.171545715	1.347648069
H	5.207233749	6.414094837	2.394617373
O	3.144364263	-1.054124960	7.745776196
H	3.089055840	-1.948512284	8.105500272
H	3.044202264	-1.114549025	6.776136843

2 Schaftoside

H	-7.073261902	-1.235309083	-2.360050148
O	-7.066956732	-2.105560769	-1.942446682
C	-5.805922616	-2.417164622	-1.548158743
C	-5.595588264	-3.632417426	-0.899969207
C	-4.728228031	-1.565291913	-1.769262767
H	-6.442056212	-4.277974021	-0.727431896
C	-4.331256429	-3.986942979	-0.483613365
H	-4.887148348	-0.617153516	-2.266882092
C	-3.463769754	-1.922995243	-1.352579805
H	-4.196177407	-4.920761198	0.036688933
C	-3.243169194	-3.141665660	-0.706146859
H	-2.630146479	-1.260236813	-1.523673875
C	-1.890371737	-3.467817878	-0.257322871
O	-1.054883394	-2.428793223	-0.349741407
C	-1.483792238	-4.687770977	0.194164110
C	0.217510785	-2.533769529	0.057818594
H	-2.165427536	-5.518267770	0.250156774
C	-0.143965328	-4.902536850	0.652490311
C	0.727868571	-3.741258486	0.546557275
C	1.011700290	-1.385558171	-0.000319001
O	0.260191897	-5.983924713	1.122818745
C	2.056762810	-3.791002596	1.015075393
C	2.343328798	-1.472499949	0.399027723
C	0.388446740	-0.032269711	-0.203240576
O	2.522638810	-4.909302134	1.600045846
C	2.870170206	-2.670147589	0.905594502
O	3.124066639	-0.371417008	0.321368083
H	1.187715700	0.709278654	-0.356141177
O	-0.514546632	0.013407877	-1.284673435
C	-0.342334748	0.290281737	1.116778635
H	1.772024741	-5.582525652	1.517090671
C	4.245049722	-2.717320262	1.531169592
H	4.043710927	-0.672738427	0.467138651
C	-1.072631812	1.292859655	-1.435661336

H	-1.134700794	-0.460331329	1.261524957
O	0.588145579	0.232740308	2.170898884
C	-1.012029342	1.656843674	1.045974963
H	4.563115149	-3.767442255	1.598732904
O	5.180088192	-1.983438043	0.754466023
C	4.144222097	-2.135274212	2.953418743
H	-0.285380915	2.040531270	-1.619955911
H	-1.721191401	1.248171461	-2.311916342
C	-1.882637776	1.755704670	-0.214778368
H	0.322189326	0.875050529	2.858743075
H	-0.233992672	2.440609662	0.995343524
O	-1.760286344	1.785313606	2.228566610
C	6.503478464	-2.004643484	1.258986917
H	3.751410782	-1.111651754	2.907367270
O	3.232801555	-2.878320949	3.734302747
C	5.526341481	-2.077442526	3.623078498
H	-2.755027806	1.096937996	-0.074963399
O	-2.290772256	3.079706653	-0.471094749
H	-2.224112360	2.650233229	2.213444837
H	7.055255526	-1.332957606	0.589331245
C	7.184987074	-3.383810859	1.150893607
C	6.570405961	-1.434898157	2.694942292
H	3.218939198	-3.787109185	3.403958625
H	5.842205864	-3.093714627	3.886127331
O	5.455197920	-1.367053348	4.839531883
H	-2.612306080	3.485966702	0.350306797
O	8.573545514	-3.240823993	1.023601890
H	6.836987623	-3.880819197	0.241304364
H	6.942850263	-4.013984269	2.017637013
H	8.878209152	-2.725332616	1.785772125
H	6.348318338	-0.359732889	2.653981121
O	7.872243595	-1.556402376	3.212215323
H	5.171073431	-0.462156346	4.623297804
H	7.923547247	-2.386054235	3.739702030
C	1.011319599	1.654242479	6.997508824
S	0.506293342	0.792524278	5.448473055
C	2.126631997	0.005107225	5.156330660
O	0.441465727	1.893022008	4.437135623
H	0.232660310	2.363253411	7.259000360
H	1.101393473	0.900424132	7.769882311
H	1.950395311	2.173354549	6.842658824
H	2.003908948	-0.715536819	4.355696728
H	2.436280026	-0.502277032	6.061085475
H	2.854870898	0.753345010	4.865289706
C	8.226412776	-1.844452790	6.490813316
S	8.028816911	-3.648010522	6.210302370
C	6.302292177	-3.726637890	6.848909799
O	7.912340239	-3.798943596	4.742717798
H	8.219778447	-1.662877500	7.559293383
H	7.413374596	-1.322062203	5.995515145
H	9.177140049	-1.541007026	6.064640597
H	5.701371435	-2.969511470	6.355761318
H	5.914384117	-4.717536820	6.635435448
H	6.335412417	-3.562915832	7.919911871
C	5.358969238	2.226271962	1.310844690

S	4.523394233	2.403843893	2.942679635
C	2.821994487	2.411223440	2.271453555
O	4.679598225	1.093434623	3.619120406
H	4.864236332	1.461996098	0.722326184
H	6.395515891	1.956580012	1.487312681
H	5.309442672	3.187338674	0.810886417
H	2.124948830	2.488764390	3.102028392
H	2.724758301	3.273770417	1.621878694
H	2.632262163	1.485947930	1.734801362
C	-2.448819749	-0.782762416	4.285174868
S	-2.156280601	-2.449290523	3.554810782
C	-0.329325756	-2.404611644	3.753272916
O	-2.415520156	-2.312515943	2.112101468
H	-2.005129976	-0.762079430	5.273593606
H	-2.019531920	-0.022128469	3.642019024
H	-3.522895313	-0.638801854	4.348631921
H	0.089976179	-1.640166182	3.107923174
H	-0.121208969	-2.190497932	4.793799730
H	0.067554379	-3.375271773	3.473615265
C	-2.323431202	3.871586720	4.789354235
S	-2.150080188	5.003311448	3.354428783
C	-0.331289452	4.795204830	3.195327232
O	-2.735835319	4.267109270	2.204827584
H	-1.809138828	2.937501899	4.582574925
H	-3.380920880	3.691098817	4.951528915
H	-1.892755440	4.367623148	5.651813621
H	-0.054548871	3.761563269	3.381458760
H	0.136524117	5.448775191	3.923249607
H	-0.048827267	5.096320808	2.191755306
C	0.118479796	-3.433668812	8.703125595
S	1.108108044	-2.291924405	7.647965160
C	1.736213028	-3.597191267	6.518685908
O	0.110724061	-1.516823811	6.882941942
H	-0.385032092	-2.839444129	9.458779517
H	0.789745702	-4.142234172	9.174052472
H	-0.616668342	-3.940895873	8.088159280
H	0.909347941	-4.181818621	6.131698919
H	2.416657395	-4.220472499	7.087897304
H	2.266573083	-3.124019933	5.696324322

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H	4.713213561	2.169596030	0.890483162
O	4.118576973	2.912751146	0.597755182
C	2.856846169	2.467043477	0.529297453
C	1.814499836	3.374962671	0.325153616
C	2.549322382	1.108689653	0.643796906
H	2.057699669	4.413022573	0.164522250
C	0.503853971	2.957172007	0.338855511
H	3.356610778	0.395126779	0.711510612
C	1.240832312	0.691929662	0.671091323
H	-0.281193556	3.672721624	0.174666544
C	0.194123421	1.612735276	0.554072885

H	1.005048718	-0.355094750	0.768312867
C	-1.170275800	1.110248748	0.622371833
O	-1.232106119	-0.122521920	1.146759152
C	-2.280090124	1.773108683	0.186656677
C	-2.389579675	-0.806216549	1.159052675
H	-2.190637506	2.764076479	-0.227998978
C	-3.562572654	1.147794198	0.221006482
C	-3.578806085	-0.215851659	0.709542070
C	-2.357343501	-2.119974690	1.614964186
O	-4.618177948	1.719287209	-0.156980823
C	-4.769002454	-0.976004388	0.733523406
C	-3.551525840	-2.849015842	1.632766509
C	-1.072087492	-2.767803133	2.065701456
O	-5.917603510	-0.426727769	0.301332348
C	-4.744477928	-2.275158582	1.191712661
O	-3.504132143	-4.110010613	2.055080995
H	-1.257001892	-3.844368240	2.160137564
O	-0.082198906	-2.524231727	1.074086506
C	-0.623162179	-2.250690183	3.450503497
H	-5.667326991	0.505713826	0.017523805
H	-5.656725368	-2.849951466	1.217898976
H	-4.409688635	-4.516803353	2.163255591
C	1.169478866	-3.125637405	1.328121878
H	-0.564245313	-1.152845840	3.424492725
O	-1.505036454	-2.678413023	4.459405228
C	0.766060182	-2.807900723	3.804361619
H	1.813796094	-2.790473121	0.505773313
C	1.755539702	-2.600346781	2.653899542
C	1.112340396	-4.663777164	1.256349685
H	-2.391819613	-2.301367262	4.276240307
H	0.665877820	-3.880601848	3.999723731
O	1.285321319	-2.156843852	4.935010354
H	1.896987791	-1.510540180	2.552187679
O	2.983258931	-3.232269941	2.894788825
O	2.386241051	-5.236103216	1.159563305
H	0.563695948	-4.946611778	0.352725689
H	0.581218153	-5.067807143	2.130025833
H	2.938129755	-4.800059274	1.831752341
H	0.788838209	-2.472549389	5.726524725
H	3.281644655	-3.050508193	3.829895842
C	0.801840083	0.922497295	5.231030541
S	1.551972278	1.385753885	6.828107865
H	1.158078615	-0.066641158	4.962576374
H	-0.273674488	0.924351824	5.364765568
H	1.094777792	1.661077956	4.489578520
C	0.567582684	0.196347160	7.823889407
H	0.648447830	-0.800033465	7.403860882
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S	-2.959514181	5.056385100	-2.032435569
H	-3.629332952	2.799333475	-2.595590878
H	-4.600261764	4.044158369	-3.447341873
H	-2.951299575	3.654044753	-3.996603944
C	-4.326718579	4.953163233	-0.826037415
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H	-4.471258806	3.918828350	-0.530146256
H	-5.200661899	5.347313829	-1.332107554
O	-1.778366527	4.448958812	-1.355442374
C	3.273579566	-2.142648666	7.702604744
S	3.711104645	-1.543897277	6.036039594
H	4.030190980	-2.849930906	8.018837116
H	2.298002260	-2.610802302	7.651174199
H	3.243072284	-1.279540832	8.355484750
C	5.357731480	-0.922073155	6.543370652
H	5.215244395	-0.228447114	7.360767506
H	5.820523184	-0.405303344	5.709822547
H	5.955289138	-1.783931897	6.828328517
O	4.050863394	-2.796609353	5.272172811
C	-0.527962123	6.358281235	0.881642403
S	-1.657524932	5.235672963	1.807503977
H	-0.712875430	6.208103706	-0.177081126
H	-0.745482455	7.383348342	1.160720503
H	0.490994645	6.087046817	1.127559098
C	-0.799161711	5.468159467	3.422421221
H	-1.472528236	5.145585944	4.208247052
H	-0.550567596	6.513683809	3.565627820
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O	-2.935281807	5.965508312	1.923239429
C	1.156605632	-0.313223479	-2.784826745
S	-0.408746971	0.503456587	-2.250366824
H	1.064242969	-1.375399825	-2.582535392
H	1.315630134	-0.149668943	-3.844599563
H	1.964192444	0.106628437	-2.197137939
C	0.043323656	2.172976048	-2.859271694
H	-0.655249213	2.893469948	-2.441852640
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H	-0.012750180	2.175631918	-3.942148545
O	-1.438241116	0.006225937	-3.190901202
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S	-5.258983591	-1.929770755	-2.291807726
H	-5.058397945	-0.288496765	-4.066378509
H	-4.946102100	0.441740570	-2.439653680
H	-3.559585172	-0.424297845	-3.127298172
C	-7.047783058	-1.531881196	-2.489508001

H	-7.288267296	-0.706401056	-1.831284934
H	-7.612033606	-2.412014428	-2.199420795
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O	-5.004892852	-3.010184748	-3.271487735
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H	-8.161458935	0.372743526	3.186717361
H	-9.296810958	-0.357562054	2.031276386
H	-7.630492071	-0.017043169	1.519358776
C	-7.359709037	2.794001072	1.816256508
H	-6.651195912	2.366853244	1.115292535
H	-7.033709232	2.651817100	2.839276217
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O	-9.240515133	1.903571715	0.168429989
C	-2.028809859	-6.727493746	0.805387730
S	-0.918332891	-7.646310465	1.923633407
H	-2.875692951	-7.347325180	0.527858687
H	-2.374470357	-5.839659730	1.325049516
H	-1.463743147	-6.440760172	-0.075737465
C	-0.952284969	-9.204864641	0.951845457
H	-0.473525898	-9.000283799	0.001541106
H	-1.980959796	-9.516493258	0.806479066
H	-0.397220671	-9.966768872	1.488994250
O	-1.725605760	-7.915322697	3.146024050
C	3.625102147	5.372413566	3.026092396
S	3.238097013	3.652043281	3.571659368
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C	3.603824965	3.966565058	5.343583613
H	2.911092894	4.707115051	5.726519799
H	4.630603578	4.297780847	5.421506731
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O	1.757346312	3.564692115	3.515811085
C	-4.667329543	1.091313265	3.729493048
S	-2.918113929	0.598514740	4.045621777
H	-5.003288738	1.732210882	4.537208004
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H	-5.252777862	0.181543464	3.684179572
C	-2.269539037	2.292592433	3.667550857
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H	-1.185765893	2.267722862	3.656426636
H	-2.613232160	2.963418798	4.446199579
O	-2.790860560	0.505914006	5.516492497
C	0.695118451	-6.151972847	5.242972246
S	2.462267532	-5.657038502	5.515232523
H	0.487510573	-7.057346743	5.801233701
H	0.061904116	-5.335031244	5.569174891

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C	2.247839136	-5.552664142	7.339452375
H	1.523728426	-4.771155380	7.536532311
H	3.204903112	-5.295704755	7.777714219
H	1.912481307	-6.510613281	7.721645978
O	3.218946817	-6.905281761	5.288291658
C	-2.050834445	-3.953179925	-4.109355751
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H	-1.750642389	-1.909797757	-2.270562373
H	-1.254991849	-2.672764725	-0.742004027
H	-2.834667853	-3.070886934	-1.461924157
O	-1.473357809	-5.415305419	-1.959582821
C	-3.558629952	-7.565355689	-2.873623351
S	-5.010284363	-7.326628981	-1.780655577
H	-3.345425829	-8.627803764	-2.925580333
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C	-4.701511546	-5.552310197	-1.458484719
H	-4.877868609	-5.004929297	-2.379135303
H	-5.388633521	-5.206328934	-0.694481046
H	-3.676599914	-5.425024006	-1.127397266
O	-4.685075716	-8.030121671	-0.508350650
C	-5.453831605	-1.249343875	6.314793225
S	-4.685555206	-2.555167574	5.267080004
H	-6.310495300	-0.803351059	5.822859848
H	-5.751074269	-1.706022248	7.251539637
H	-4.687526437	-0.498834119	6.484281260
C	-6.276535405	-3.182205199	4.590943973
H	-6.887264558	-3.509338571	5.424119208
H	-6.074052121	-4.023967942	3.935422037
H	-6.770726178	-2.397405050	4.028877331
O	-4.064159221	-1.804282240	4.138029058
C	5.784258880	-5.065340210	4.475040009
S	5.364321846	-4.740166364	6.226220760
H	5.420610708	-4.233467532	3.885946978
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H	5.264210421	-7.140497822	6.401559369
H	6.958927710	-6.576221930	6.468664034
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O	6.399515760	-3.819062356	6.743283840
C	8.438887395	2.495162118	3.486901101
S	7.040803293	3.661292569	3.211918237

H	8.287001443	1.604783593	2.889280918
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C	7.116599889	3.594712335	1.382375503
H	8.079535230	3.974320253	1.062140538
H	6.316233835	4.212133912	0.988990502
H	6.963303628	2.567815810	1.066898652
O	5.823430305	2.920362584	3.599291846
C	-7.081594843	-7.302569743	1.203164837
S	-5.390097336	-6.689881161	1.553413987
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H	-6.988243779	-8.204997898	0.612797513
H	-7.597442792	-7.487271387	2.138546667
C	-4.909448985	-8.084927445	2.621605163
H	-4.992598660	-8.981484799	2.019807760
H	-5.559610528	-8.123464074	3.487984112
H	-3.876477050	-7.947660945	2.932060506
O	-5.639259180	-5.542864210	2.502981325
C	-1.439586227	-4.171322395	8.906028170
S	-1.320162021	-3.502655239	7.190281331
H	-2.478268017	-4.410229851	9.092061812
H	-0.827507682	-5.064468376	8.977814701
H	-1.072003233	-3.427568510	9.603566736
C	-2.270921736	-1.998692641	7.551439141
H	-2.264322614	-1.355205270	6.677078369
H	-3.275828000	-2.328939968	7.777643906
H	-1.825000155	-1.485421536	8.396242170
O	0.113390763	-3.058563728	7.148343441
C	4.011311219	0.483616015	3.581055605
S	5.703530432	0.420827486	2.888474004
H	3.418101380	1.164883018	2.984717984
H	3.570682168	-0.504124628	3.589360906
H	4.082839264	0.863524932	4.592929245
C	5.792323497	-1.410532207	2.747235876
H	6.753618099	-1.671313694	2.315432982
H	4.994651877	-1.775157671	2.109645471
H	5.702708612	-1.838012930	3.738889047
O	5.588747295	0.861238117	1.461132205
C	-8.331661069	4.715954454	-1.267369159
S	-7.810246316	4.024977172	-2.892778059
H	-8.816570177	5.670279146	-1.444797343
H	-9.024242128	4.015549939	-0.814961982
H	-7.453351580	4.857202139	-0.647485959
C	-7.197694506	2.431873019	-2.206663268
H	-6.309862833	2.610632316	-1.610532842
H	-7.990487526	1.998085857	-1.606591139
H	-6.960135098	1.787604371	-3.046759328
O	-6.600608812	4.781730161	-3.272776903

C	-3.079907286	-5.553485928	4.758400134
S	-3.851316884	-5.904881403	6.370145168
H	-3.880465846	-5.309530618	4.071760360
H	-2.410172547	-4.706006827	4.851788677
H	-2.557612991	-6.433191567	4.396619257
C	-2.483536686	-6.959975445	7.013192343
H	-1.561987064	-6.393592496	6.989879245
H	-2.415587709	-7.833637522	6.375624523
H	-2.720549395	-7.256433939	8.029736770
O	-3.765789753	-4.633847785	7.135590550
C	3.068658409	-8.237810738	2.340586316
S	2.231207286	-9.863435070	2.542954696
H	3.894665894	-8.387377860	1.653598232
H	2.365886002	-7.529481371	1.917646165
H	3.438722715	-7.884919455	3.296948111
C	1.414629279	-9.471671062	4.153479143
H	0.503123066	-8.922713207	3.946386566
H	2.090365560	-8.892472543	4.772876704
H	1.182260456	-10.416815579	4.633532506
O	3.284859403	-10.838328390	2.852990089

4 Puerarin

H	8.639609739	-4.254635785	-3.296340862
O	8.930564350	-3.512568204	-2.715675063
C	7.885935658	-2.662225967	-2.570079833
C	7.972965191	-1.613116819	-1.657233550
C	6.711271439	-2.834836804	-3.298003797
H	8.887891357	-1.475888850	-1.101955656
C	6.893352862	-0.775892142	-1.453457349
H	6.664592710	-3.641428248	-4.013528539
C	5.629104178	-2.008630602	-3.077360056
H	6.966840434	0.033995362	-0.744993751
C	5.705088344	-0.977455830	-2.147133356
H	4.714561848	-2.162428685	-3.631868784
C	4.519698068	-0.136207554	-1.908986232
C	3.365821631	-0.713342647	-1.512370097
C	4.550724202	1.297307553	-2.152724915
H	3.300198366	-1.777719282	-1.324791826
O	2.204900044	-0.086144791	-1.308341024
O	5.566751340	1.923475475	-2.464954098
C	3.235372542	1.933723845	-2.076795097
C	2.110348252	1.223851669	-1.628387309
C	3.074676215	3.256155272	-2.504572306
C	0.851562401	1.834245816	-1.578492933
H	3.947414102	3.795305632	-2.830194125
C	1.837134941	3.836119988	-2.543617897
C	0.717776715	3.129701090	-2.085383968

C	-0.414576203	1.147554961	-1.125375113
H	1.702314607	4.838750977	-2.917843003
O	-0.509584018	3.684380703	-2.149059380
H	-1.134349303	1.939089488	-0.887619103
O	-0.899138345	0.370035989	-2.214388841
C	-0.292139377	0.289088506	0.133137432
H	-0.573061112	4.230250386	-2.975590896
C	-2.238532448	-0.042304015	-2.023430547
H	0.431407577	-0.518852914	-0.029163358
O	0.131254535	1.128301407	1.171656163
C	-1.654811062	-0.348217582	0.454426029
H	-2.467113380	-0.641164595	-2.912655742
C	-3.232951860	1.142893125	-2.012617407
C	-2.350975796	-0.940300993	-0.776902974
H	0.116131703	0.620248622	2.009768056
H	-2.297410810	0.419154783	0.908672519
O	-1.468600604	-1.428298448	1.365657048
O	-4.320040686	0.926734554	-2.870614399
H	-2.719940401	2.029490446	-2.396283456
H	-3.571610284	1.348354977	-0.991380222
H	-4.944335682	0.293574551	-2.449841504
H	-1.851748232	-1.896897659	-1.001371021
O	-3.711972591	-1.165980122	-0.524706467
H	-0.947692464	-1.093810267	2.134333260
H	-3.810837502	-1.577644121	0.358124198
S	6.975248391	-4.980134766	1.129469702
O	7.059510482	-3.623200618	1.712016171
C	8.593739796	-5.258852440	0.287563576
H	8.552085944	-6.235422323	-0.180510176
H	8.767692727	-4.484818865	-0.451530709
H	9.373363844	-5.234282179	1.042113844
C	6.016094757	-4.816387827	-0.414945438
H	6.411694929	-3.992605906	-0.997546382
H	4.982207869	-4.606902483	-0.160172156
H	6.081662104	-5.745534759	-0.971978591
S	-7.495569376	-0.128053773	1.367367996
O	-8.262049403	0.514554427	0.269016287
C	-5.772292438	0.453226969	1.181634855
H	-5.462265083	0.275654174	0.157897225
H	-5.715491306	1.507812853	1.429296861
H	-5.151951202	-0.118306758	1.860121512
C	-7.148530236	-1.829728151	0.783132016
H	-6.359351946	-2.245415410	1.397327902
H	-6.834594723	-1.747743095	-0.252717631
H	-8.056634661	-2.417403125	0.866917111
S	5.282728683	1.970799321	1.315827496
O	3.961044339	1.332478037	1.080373746
C	5.226135877	3.560423604	0.431548676

H	5.277516534	3.336497409	-0.625105932
H	4.302992727	4.085907872	0.641675000
H	6.101551504	4.120592064	0.737692813
C	5.127632217	2.762579064	2.985217160
H	5.957767249	3.449419250	3.090593407
H	5.176143503	1.996362489	3.751128971
H	4.179549309	3.282503332	3.053867804
S	4.952885558	-2.463655335	2.915263711
O	3.713813912	-2.066975090	3.662666103
C	4.710962521	-1.839309628	1.223256704
H	5.686855946	-1.799701851	0.756965931
H	4.091137513	-2.550163246	0.690076917
H	4.253002893	-0.855223001	1.246471149
C	6.203959567	-1.193987571	3.364313596
H	7.125291846	-1.519947340	2.898722986
H	6.309739055	-1.176377847	4.444360826
H	5.901621579	-0.224032746	2.985410987
S	-7.673274674	0.366159724	-2.149362344
O	-6.450308416	-0.433417751	-1.877587500
C	-7.637965069	0.492281334	-4.001144508
H	-6.655748869	0.824633443	-4.316132924
H	-7.837099063	-0.494662337	-4.405018837
H	-8.408204885	1.182091884	-4.324571026
C	-7.184613813	2.115352274	-1.913177147
H	-6.201265436	2.269255565	-2.344652379
H	-7.176269061	2.311116487	-0.847898877
H	-7.929200229	2.739522256	-2.392917962
S	8.254604003	2.152671551	2.207816238
O	8.194632060	3.620792013	2.110254346
C	8.585295188	1.866300568	4.022521637
H	9.478164040	2.395990624	4.331132807
H	7.734543601	2.241569505	4.579656617
H	8.690548953	0.800613491	4.186618971
C	9.969898133	1.671900158	1.739670269
H	10.202506107	0.723882144	2.209443138
H	10.657156516	2.447906486	2.057108761
H	9.988486451	1.561344678	0.663417803
S	-3.019149262	-2.908661159	2.644569456
O	-4.207828270	-2.490757706	1.864677677
C	-2.290790930	-4.294615613	1.679700798
H	-2.120839688	-3.943597645	0.667489802
H	-1.353217854	-4.572053601	2.146766044
H	-2.972378887	-5.137096159	1.664837930
C	-3.745742879	-4.021227688	3.943253493
H	-2.943265903	-4.583222277	4.405959849
H	-4.478660433	-4.685364028	3.500028594
H	-4.229181145	-3.394567806	4.685281201
S	0.191165973	5.127391606	1.863221830

O	0.010969370	4.921864868	3.319358958
C	-1.229941426	4.326437821	1.041730708
H	-2.118560103	4.910943915	1.260919165
H	-1.036717279	4.324178232	-0.024279090
H	-1.355195625	3.314779073	1.414474311
C	1.473745444	3.924320208	1.340665911
H	1.888799538	4.269303982	0.399137026
H	2.236889658	3.923217075	2.111925931
H	1.055182287	2.930881420	1.233996677
S	4.138909001	-6.885288286	-3.350413206
O	5.432785224	-7.081699755	-2.646553219
C	2.856286254	-7.032627302	-2.040556440
H	2.833764105	-8.059296171	-1.691104243
H	3.110539095	-6.361737279	-1.228780042
H	1.903339393	-6.759873942	-2.477666886
C	3.934462114	-5.088189790	-3.579654357
H	4.006306390	-4.583845196	-2.621580621
H	4.724031876	-4.753348796	-4.242058180
H	2.964578641	-4.916421044	-4.036121250
S	1.590510374	-4.236394407	-0.279962201
O	3.002672341	-3.956589021	-0.654604651
C	1.251538098	-3.066553621	1.089360510
H	1.739933006	-2.124887491	0.866267108
H	0.182084629	-2.926666766	1.184453194
H	1.672501455	-3.474153690	2.002781137
C	0.577809976	-3.400249317	-1.548857781
H	0.710618862	-2.325134144	-1.506086984
H	0.897683725	-3.775413678	-2.518066258
H	-0.459226093	-3.669590187	-1.377652436
S	3.329857037	7.263451259	-0.044374255
O	3.117718076	5.917381702	-0.592797359
C	3.503734125	7.055419665	1.780355220
H	2.644520729	6.527750326	2.180247357
H	4.412171121	6.490656005	1.964037734
H	3.588844889	8.041289081	2.222204796
C	1.659552749	8.041474139	0.041529486
H	1.760490913	9.008210438	0.520616516
H	0.984935045	7.397646396	0.596437636
H	1.300022001	8.167510518	-0.974476941
S	7.822766418	2.873284930	-1.314709292
O	7.771451786	1.913298332	-0.176099695
C	8.662746242	1.987386996	-2.678524872
H	9.530656943	1.457834581	-2.302502302
H	7.949728394	1.286265457	-3.097409956
H	8.942001858	2.737189646	-3.410101022
C	9.242625506	3.973839870	-0.926161246
H	10.167320540	3.410220035	-0.894097300
H	9.044863896	4.420567498	0.042720223

H	9.282963582	4.725227690	-1.705821119
S	1.531872123	-1.017197476	3.556154685
O	0.109023841	-0.510221075	3.343154734
C	1.497554841	-1.426460059	5.339486790
H	1.200201882	-0.551608870	5.906569409
H	0.777033015	-2.224646850	5.483558889
H	2.490228206	-1.763816222	5.605043086
C	2.467185080	0.534950617	3.714784558
H	1.848686896	1.280515798	4.202975175
H	2.740667612	0.866946974	2.714927359
H	3.357171091	0.314498941	4.288588958
S	-0.310508118	-4.672045311	-5.271789521
O	0.951900337	-4.293858750	-4.585396435
C	-1.481634589	-3.304976819	-4.953429027
H	-1.549397016	-3.123604549	-3.885998018
H	-1.122973606	-2.416477021	-5.471351151
H	-2.439502712	-3.605755565	-5.362903463
C	-1.126078068	-5.881128890	-4.148890628
H	-2.030313059	-6.223516451	-4.639214394
H	-1.364629080	-5.410523897	-3.200127479
H	-0.447935042	-6.715248151	-4.001221244
S	7.081946283	5.584906524	-4.133020414
O	8.395867542	5.059364991	-3.728072363
C	6.119164643	4.128284546	-4.714049268
H	6.620175635	3.735221829	-5.593048990
H	6.080741925	3.367242184	-3.939620825
H	5.125619614	4.471181479	-4.981140615
C	6.136645310	5.816352308	-2.569266134
H	5.121971117	6.112133951	-2.807536112
H	6.622698110	6.602797038	-2.001500228
H	6.150447979	4.893664730	-2.001763104
S	7.931558797	-6.823954850	-3.064382530
O	7.885256558	-5.673034321	-3.993969707
C	9.756636547	-7.101431282	-2.841022679
H	10.236988800	-7.213133044	-3.805739809
H	10.162710953	-6.232117031	-2.334774096
H	9.904354094	-7.986524729	-2.233335685
C	7.708527453	-8.299320461	-4.131734321
H	7.996555531	-9.180279308	-3.570305998
H	8.313791963	-8.185646308	-5.024259504
H	6.657617047	-8.352073009	-4.391054837
S	1.314894413	-0.604193386	-6.049697160
O	-0.077254285	-0.899330128	-6.447758540
C	2.332878899	-2.019422770	-6.641478858
H	2.248482068	-2.069209857	-7.721888171
H	3.360426756	-1.823605370	-6.356088913
H	1.977600754	-2.941912014	-6.193723726
C	1.443420080	-1.040071335	-4.275537220

H	0.689778794	-0.488211202	-3.720099905
H	1.292531196	-2.107248608	-4.154626489
H	2.439899730	-0.757181409	-3.954923653
S	-0.618987654	3.554991142	-5.742179793
O	-0.602350489	4.539951521	-4.630703909
C	-1.318213362	2.007419799	-5.063132394
H	-0.863184451	1.762552424	-4.108965602
H	-2.386734177	2.144703809	-4.928620190
H	-1.139597082	1.212659094	-5.779962292
C	1.112200040	2.931554854	-5.854021079
H	1.747907928	3.762122945	-6.142784047
H	1.428554010	2.542634146	-4.892458864
H	1.137056624	2.157465056	-6.611266640
S	-2.986834038	1.915181578	3.829785262
O	-2.912169078	1.863682428	2.360061734
C	-1.289262116	2.260401574	4.429650994
H	-0.624678740	1.495351553	4.043750275
H	-1.316959373	2.245399862	5.513975870
H	-0.973627778	3.242755260	4.083707823
C	-2.977777154	0.149320355	4.390160185
H	-3.096666896	0.142506918	5.467911867
H	-2.043167807	-0.317276670	4.097754301
H	-3.810268822	-0.360950244	3.917944127
S	-3.972534112	-4.464801166	-2.224247387
O	-2.588552838	-4.155983769	-1.780981789
C	-4.690973586	-2.907468875	-2.856093352
H	-5.727998246	-3.101310525	-3.104110244
H	-4.617298477	-2.132698288	-2.097011274
H	-4.149679919	-2.607743058	-3.747462340
C	-4.988278154	-4.520889528	-0.697123886
H	-6.031996618	-4.506377197	-0.987738872
H	-4.753622260	-3.664912286	-0.072538635
H	-4.763807751	-5.447158530	-0.176403312

5 Prunetin-8-C-glucoside

H	6.287197251	-1.295019665	1.992509094
O	5.966630850	-0.470940339	2.436356769
C	4.688956142	-0.232905722	2.050481713
C	3.997498681	0.831772146	2.619570955
C	4.044925663	-1.038015077	1.114679117
H	4.496589145	1.444285211	3.354801079
C	2.695303143	1.093097039	2.244246680
H	4.579888058	-1.874214053	0.684383714
C	2.742721837	-0.768391913	0.743532448
H	2.174446061	1.918879510	2.699536897
C	2.046328403	0.305798446	1.294986304
H	2.259110188	-1.401569328	0.017690786
C	0.651810974	0.574832845	0.925911901

C	-0.191461892	-0.447974470	0.646532183
C	0.132106597	1.933721059	0.872877656
H	0.125360557	-1.480339338	0.612389778
O	-1.488068313	-0.336912308	0.382861572
O	0.834317028	2.941215868	1.070565502
C	-1.284649583	2.032610163	0.580953552
C	-2.062545449	0.885586043	0.379798642
C	-1.918611171	3.293321926	0.504132068
C	-3.441009626	0.952015858	0.180044366
O	-1.220717888	4.419269948	0.644091663
C	-3.285703831	3.364260734	0.287471091
C	-4.049851723	2.210743029	0.149722435
C	-4.250859676	-0.316619443	0.072692318
H	-0.273238797	4.134648523	0.788557971
H	-3.725593556	4.345947481	0.242822307
O	-5.398715395	2.226707894	-0.008488085
H	-5.301272911	-0.044596440	-0.095665601
O	-3.755653699	-1.063124112	-1.026642880
C	-4.188120544	-1.077502895	1.422007507
C	-6.052524945	3.475480681	-0.078239909
C	-4.284090091	-2.354587426	-1.191294876
H	-3.144381054	-1.167437338	1.744448336
O	-4.944154253	-0.380943373	2.382202329
C	-4.743699866	-2.499079802	1.277164738
H	-7.111091518	3.246818032	-0.196652047
H	-5.906522796	4.052576195	0.838437454
H	-5.707078638	4.053756777	-0.939412845
H	-3.692393371	-2.785598506	-2.007320752
C	-5.757337148	-2.351816568	-1.642142370
C	-4.062638339	-3.180567683	0.090496730
H	-4.357171563	0.324873584	2.756956507
H	-5.822596224	-2.433059042	1.098951916
O	-4.496993663	-3.276280133	2.421537779
O	-6.194822397	-3.635088233	-2.027285079
H	-5.857769807	-1.693117369	-2.507153051
H	-6.398144260	-1.964860240	-0.840043609
H	-5.814193486	-4.256441632	-1.378257680
H	-2.983280287	-3.204414094	0.301193087
O	-4.535825546	-4.499647065	-0.092046256
H	-5.177777078	-3.030886132	3.087119685
H	-4.804061483	-4.853041553	0.774394340
S	-6.611846546	-0.998646852	4.252042385
C	-7.786298672	-0.971590117	5.686705909
H	-7.862524779	0.047550209	6.047072122
H	-8.757886835	-1.342846408	5.381598753
H	-7.377807726	-1.607653972	6.464851914
C	-7.791213475	-0.201835010	3.101843484
H	-8.134634900	0.723296558	3.548757285
H	-8.625041910	-0.870266641	2.902186912
H	-7.241790845	0.011130803	2.192530468
O	-6.605815123	-2.436979388	3.867922451
S	-1.856133891	0.251235710	3.476919448
C	-2.320673438	-0.747886393	4.950830334
H	-2.741302856	-0.085558943	5.698622826
H	-3.070614692	-1.466367261	4.635861820

H	-1.439568040	-1.258434022	5.314893782
C	-0.610108690	1.282243021	4.330910087
H	-1.020924258	1.671252214	5.255266742
H	-0.358866865	2.101552966	3.665941940
H	0.257328274	0.658737631	4.502396530
O	-3.032336028	1.163840805	3.325482412
S	-0.673663979	2.961724059	-3.325994637
C	0.419370495	4.187787308	-4.150033110
H	0.334185233	5.165177979	-3.689054444
H	1.427106135	3.797096101	-4.060403810
H	0.128813828	4.226083397	-5.193224513
C	-2.010448548	4.182218436	-2.931962789
H	-1.714322521	4.792618323	-2.087347379
H	-2.204673890	4.789225383	-3.807917617
H	-2.895713621	3.605534120	-2.687149582
O	-0.046185648	2.692806135	-2.004255466
S	-5.043907262	-2.179576677	-5.082115928
C	-4.350109597	-3.868379384	-4.858227279
H	-4.626891957	-4.493100491	-5.699008727
H	-3.271229413	-3.762721905	-4.816731833
H	-4.735926068	-4.268794565	-3.929049514
C	-6.803597396	-2.733990930	-5.122878548
H	-7.033531594	-3.112300374	-4.135767172
H	-6.946858601	-3.483157326	-5.890976808
H	-7.422328466	-1.867940745	-5.330039699
O	-4.707320146	-1.788271622	-6.460001725
S	0.136839770	-2.950063692	3.514020811
C	1.507418639	-3.551594328	2.447538274
H	1.183994448	-3.598994742	1.412365636
H	2.336659097	-2.861266949	2.542813732
H	1.791989731	-4.534342814	2.805827100
C	-1.195203550	-3.749509242	2.543263743
H	-1.139816553	-4.812398784	2.750891212
H	-1.031377896	-3.563710669	1.486389047
H	-2.163059004	-3.368931816	2.853469157
O	0.034951143	-1.490679379	3.259789554
S	-9.756390625	-3.821367599	2.054812161
C	-8.052599666	-3.927366240	1.409424028
H	-8.047613259	-3.559730668	0.387659783
H	-7.432456239	-3.311549482	2.052063262
H	-7.708383388	-4.956522968	1.437756272
C	-9.298009033	-4.281287959	3.772939493
H	-9.061013564	-5.338964297	3.772806445
H	-10.146228777	-4.083685992	4.420299770
H	-8.431470028	-3.701956280	4.078246034
O	-10.055106597	-2.365627219	2.086835171
S	8.453865388	-2.781404950	2.003598573
C	8.309256889	-2.437156477	3.805969667
H	7.706407905	-1.547392010	3.953348486
H	9.305765155	-2.308877186	4.211366912
H	7.827254510	-3.290641848	4.271596862
C	9.193316336	-1.150367648	1.581109263
H	10.169512558	-1.083287421	2.046739306
H	8.539086229	-0.356218036	1.925413455
H	9.294484692	-1.101342982	0.501665716

O	7.068666278	-2.711311780	1.491301306
S	2.865768276	-2.928300524	5.388887316
C	4.534082751	-2.791754728	4.602583048
H	5.202059569	-2.287739829	5.292066198
H	4.895805077	-3.795548513	4.405254427
H	4.440781436	-2.239292548	3.677240306
C	2.542319213	-1.114265968	5.387774084
H	3.410907271	-0.577765648	5.752255647
H	2.293729167	-0.811181303	4.376806684
H	1.699051371	-0.942363840	6.048624392
O	3.127645389	-3.290801042	6.785461692
S	-9.068438573	-1.894516149	-1.533498433
C	-9.130848979	-0.479252308	-0.361513500
H	-8.136109429	-0.056013426	-0.269318669
H	-9.812836037	0.271693788	-0.744319891
H	-9.470494149	-0.861613787	0.595344954
C	-10.859697942	-2.296396723	-1.346160717
H	-11.085653473	-3.181683506	-1.930873555
H	-11.449474349	-1.459232281	-1.702655439
H	-11.043017818	-2.483811276	-0.294434380
O	-8.916722417	-1.302449901	-2.876003402
S	-6.436020734	-6.805709442	-0.482194689
C	-7.341220167	-8.408271215	-0.523744278
H	-7.342746757	-8.746849864	-1.551795548
H	-6.855005251	-9.121134409	0.132079779
H	-8.356376557	-8.229557562	-0.183752216
C	-4.811250125	-7.516489675	-0.939079957
H	-4.916837782	-7.930803272	-1.933463925
H	-4.526464006	-8.271312207	-0.214956371
H	-4.090639545	-6.706614671	-0.943345516
O	-6.331048366	-6.479693418	0.961979543
S	2.044816800	0.737988736	-4.173472086
C	1.741620987	-0.093371893	-2.562968046
H	2.706989633	-0.348787410	-2.142927446
H	1.242281702	0.628857666	-1.927379640
H	1.120856346	-0.970710054	-2.700454451
C	2.058071527	-0.868264890	-5.123712837
H	2.193748344	-0.630536747	-6.173336019
H	1.115101836	-1.386319728	-4.985769147
H	2.887714990	-1.471527119	-4.774864724
O	0.739381074	1.314058443	-4.569892066
S	2.293079751	2.821388572	-1.297572680
C	2.031516624	4.629516558	-1.108172386
H	2.731524396	5.149550465	-1.751927103
H	1.011011768	4.842522292	-1.397434618
H	2.178984906	4.884317770	-0.067045661
C	3.904319646	2.858978985	-0.383983811
H	4.574083889	3.571924148	-0.848656039
H	3.703333962	3.115733775	0.647130776
H	4.332376667	1.864188272	-0.435543231
O	2.748131601	2.645190742	-2.702314485
S	-2.188182480	-1.271503448	-4.145978882
C	-1.940550489	-0.150434045	-5.567011821
H	-2.131546562	-0.697969734	-6.483272159
H	-2.665155391	0.646489878	-5.449444758

H	-0.933923000	0.254989077	-5.539599411
C	-1.708338778	-0.044627050	-2.899908876
H	-0.784912860	0.430142742	-3.201249478
H	-1.603502080	-0.556332391	-1.953738111
H	-2.504837790	0.684961334	-2.835221159
O	-1.059836975	-2.255926535	-4.183528233
S	-0.329166845	-3.232242524	-1.795412409
C	-1.384879355	-4.674101926	-2.225397544
H	-0.880453064	-5.591745215	-1.943650113
H	-2.322113044	-4.591458338	-1.686323037
H	-1.556372761	-4.625439755	-3.292676056
C	1.119142110	-3.825724650	-2.762948233
H	1.978395886	-3.217449608	-2.501895899
H	1.324407143	-4.864617245	-2.531064354
H	0.863179925	-3.693056102	-3.806283941
O	0.060136939	-3.468343467	-0.375709038
S	-5.180887676	0.797290338	-3.736148086
C	-5.864951348	1.061503640	-5.431642480
H	-5.870588403	2.126199121	-5.637425102
H	-5.227940213	0.544066005	-6.141280797
H	-6.866501908	0.653556783	-5.477361914
C	-6.762688426	1.168454362	-2.870032740
H	-6.522728040	1.243740977	-1.815315631
H	-7.162513550	2.112282017	-3.224240496
H	-7.460224141	0.356521885	-3.049119279
O	-4.322182666	1.969411569	-3.481022132
S	-7.223713225	-5.760073101	-3.784309390
C	-8.154686865	-6.285296130	-5.298530698
H	-7.441585571	-6.686500043	-6.011186143
H	-8.868335282	-7.057678887	-5.035147421
H	-8.657633674	-5.425529180	-5.724716219
C	-8.725676092	-5.213615029	-2.873220167
H	-8.403221029	-4.928252347	-1.878761876
H	-9.442014424	-6.025529895	-2.822917475
H	-9.134647238	-4.355307675	-3.392557092
O	-6.819979258	-7.025317113	-3.146986421

MATRICES OF OPTIMIZED STRUCTURES

Pure Solvation model (IEFPCM)

1 Isoschaftoside

a Global Minimum Point H–C_7 eclipsed

C	-0.245203000	-0.973944000	-0.294899000
C	0.560082000	-2.108415000	-0.452679000
C	0.262429000	0.325614000	-0.251103000
C	1.958124000	-1.920668000	-0.571789000
C	1.655881000	0.466318000	-0.384931000

C	2.513975000	-0.645407000	-0.548978000
C	-2.196688000	-2.326489000	-0.211022000
C	-1.472598000	-3.469701000	-0.360327000
O	-1.593814000	-1.111061000	-0.163823000
C	-0.041170000	-3.431366000	-0.474610000
C	-3.651664000	-2.212321000	-0.105297000
C	-4.446346000	-3.303932000	0.283790000
C	-4.282037000	-0.992507000	-0.402216000
C	-5.823713000	-3.183739000	0.369147000
C	-5.661388000	-0.865887000	-0.322340000
C	-6.437839000	-1.963494000	0.064066000
O	0.660834000	-4.467967000	-0.602940000
C	-0.620304000	1.531195000	-0.049051000
C	4.017567000	-0.514147000	-0.597853000
O	2.155934000	1.721637000	-0.336383000
O	4.367616000	0.714301000	-1.262692000
C	5.779310000	0.896222000	-1.434274000
C	6.489343000	0.924666000	-0.082683000
O	7.884308000	1.047734000	-0.343768000
C	6.165519000	-0.344912000	0.695982000
C	4.650396000	-0.525844000	0.811482000
O	4.337010000	-1.708355000	1.543027000
H	4.428269000	-1.350456000	-1.175458000
O	6.778434000	-0.229148000	1.978336000
C	-1.312780000	1.547015000	1.330234000
C	-2.192230000	2.784505000	1.435316000
C	-3.173300000	2.838291000	0.270279000
C	-2.454856000	2.727524000	-1.087285000
O	-1.615086000	1.567150000	-1.093659000
C	-1.701097000	4.000794000	-1.513433000
O	-2.600736000	5.016529000	-1.957953000
O	-3.921416000	4.058889000	0.283857000
O	-2.976905000	2.786244000	2.629653000
O	-0.357069000	1.635095000	2.388303000
H	0.014008000	2.417969000	-0.107076000
O	-7.793419000	-1.907339000	0.165919000
O	2.769981000	-2.993066000	-0.683499000
H	-1.968256000	-4.427448000	-0.423903000
H	-3.987360000	-4.249698000	0.543639000
H	-3.682519000	-0.146472000	-0.712479000
H	-6.437082000	-4.020737000	0.679037000
H	-6.136538000	0.079334000	-0.561729000
H	3.087081000	1.699957000	-0.642983000
H	6.183834000	0.087562000	-2.054561000

H	5.906706000	1.842114000	-1.958439000
H	6.131108000	1.786850000	0.495238000
H	8.347308000	0.981415000	0.500404000
H	6.586700000	-1.205836000	0.156510000
H	4.238675000	0.304427000	1.392546000
H	4.316230000	-2.464711000	0.940929000
H	6.555752000	-1.020172000	2.484913000
H	-1.936273000	0.656338000	1.445797000
H	-1.549970000	3.674527000	1.418374000
H	-3.858144000	1.987998000	0.371183000
H	-3.204702000	2.533505000	-1.857544000
H	-1.060690000	4.384539000	-0.711556000
H	-1.062250000	3.743448000	-2.360259000
H	-3.222412000	5.167669000	-1.230982000
H	-4.247713000	4.200121000	1.181551000
H	-2.372328000	2.780643000	3.381536000
H	0.068202000	0.776974000	2.499571000
H	-8.114806000	-1.025324000	-0.059188000
H	2.175328000	-3.795922000	-0.683254000

E = – 2061.4685489 a. u.
H = – 2060.897848 a. u.
G = – 2061.003977 a. u.

b H–C_9 eclipsed

C	-0.458822000	-1.085340000	-0.227844000
C	0.299719000	-2.259551000	-0.320194000
C	0.104276000	0.192165000	-0.231341000
C	1.705872000	-2.137186000	-0.416410000
C	1.507475000	0.266583000	-0.327001000
C	2.317130000	-0.887093000	-0.429440000
C	-2.469683000	-2.355498000	-0.123955000
C	-1.789002000	-3.530725000	-0.219268000
O	-1.818390000	-1.162885000	-0.123218000
C	-0.356190000	-3.555610000	-0.309919000
C	-3.921616000	-2.192822000	-0.026124000
C	-4.746278000	-3.262872000	0.364367000
C	-4.524617000	-0.960036000	-0.325997000
C	-6.120330000	-3.111434000	0.444315000
C	-5.901143000	-0.800905000	-0.250799000
C	-6.705289000	-1.878318000	0.134422000
O	0.302659000	-4.625016000	-0.388511000
C	-0.770920000	1.415100000	-0.122362000

C	3.825775000	-0.825054000	-0.461680000
O	2.063400000	1.497230000	-0.310890000
O	4.239716000	0.359592000	-1.168131000
C	5.659916000	0.467259000	-1.331754000
C	6.358748000	0.512415000	0.025174000
O	7.760257000	0.558391000	-0.225546000
C	5.966843000	-0.709526000	0.847602000
C	4.443666000	-0.812610000	0.954007000
O	4.067301000	-1.949378000	1.726974000
H	4.203616000	-1.700224000	-1.002700000
O	6.573149000	-0.574985000	2.131258000
C	-0.651501000	2.376351000	-1.321828000
C	-1.552561000	3.580918000	-1.089189000
C	-1.232360000	4.230579000	0.251785000
C	-1.296585000	3.214559000	1.406981000
O	-0.453791000	2.097312000	1.106318000
C	-2.723230000	2.785205000	1.799476000
O	-3.398837000	3.815688000	2.521166000
O	-2.147713000	5.294589000	0.537821000
O	-1.370190000	4.588459000	-2.086788000
O	-1.109915000	1.748429000	-2.522257000
H	-1.808534000	1.077586000	-0.093755000
O	-8.059211000	-1.790338000	0.230493000
O	2.472674000	-3.246252000	-0.472912000
H	-2.319871000	-4.470782000	-0.248849000
H	-4.313232000	-4.219115000	0.629104000
H	-3.914966000	-0.121974000	-0.635493000
H	-6.753234000	-3.933855000	0.753866000
H	-6.352303000	0.155420000	-0.491895000
H	2.996828000	1.422040000	-0.601397000
H	6.030360000	-0.382388000	-1.917830000
H	5.837069000	1.385877000	-1.888967000
H	6.037425000	1.411919000	0.566754000
H	8.212173000	0.504738000	0.625493000
H	6.350352000	-1.609797000	0.345508000
H	4.067580000	0.058615000	1.498086000
H	4.015163000	-2.726817000	1.154298000
H	6.304906000	-1.333125000	2.665329000
H	0.379841000	2.716489000	-1.431543000
H	-2.598376000	3.247083000	-1.097119000
H	-0.210653000	4.625731000	0.199608000
H	-0.850820000	3.673634000	2.292183000
H	-3.314314000	2.482766000	0.927934000
H	-2.642965000	1.924045000	2.465460000

H	-3.366075000	4.605604000	1.961600000
H	-2.222455000	5.845272000	-0.251787000
H	-1.603028000	4.205511000	-2.941140000
H	-0.433868000	1.134233000	-2.830774000
H	-8.359261000	-0.901638000	0.002182000
H	1.844015000	-4.022870000	-0.458504000

E = – 2061.4661943 a. u.
H = – 2060.895495 a. u.
G = – 2061.001989 a. u.

c Gauche-like

C	-0.352223000	-1.016360000	-0.313459000
C	0.400873000	-2.195908000	-0.302292000
C	0.212664000	0.263382000	-0.373702000
C	1.809548000	-2.084926000	-0.370237000
C	1.614868000	0.320228000	-0.461180000
C	2.422265000	-0.840984000	-0.467376000
C	-2.367492000	-2.271926000	-0.193006000
C	-1.692168000	-3.452451000	-0.162976000
O	-1.715859000	-1.080404000	-0.253898000
C	-0.257946000	-3.487768000	-0.206219000
C	-3.822816000	-2.112689000	-0.182298000
C	-4.649620000	-3.068712000	0.431671000
C	-4.421736000	-1.002040000	-0.795727000
C	-6.026996000	-2.920283000	0.432782000
C	-5.800720000	-0.848773000	-0.804720000
C	-6.609000000	-1.808861000	-0.187172000
O	0.399817000	-4.559815000	-0.182107000
C	-0.724491000	1.445742000	-0.263859000
C	3.932402000	-0.786694000	-0.472748000
O	2.196101000	1.542013000	-0.551112000
O	4.368056000	0.340250000	-1.256611000
C	5.792652000	0.437345000	-1.390656000
C	6.454534000	0.587505000	-0.023196000
O	7.861922000	0.621395000	-0.239312000
C	6.043727000	-0.572895000	0.875624000
C	4.518183000	-0.670876000	0.952483000
O	4.123436000	-1.749071000	1.796471000
H	4.316810000	-1.701149000	-0.938781000
O	6.618178000	-0.344747000	2.160601000
C	-0.242549000	2.820355000	-0.751210000
C	-1.393531000	3.807800000	-0.593220000

C	-1.834183000	3.859695000	0.865942000
C	-2.163307000	2.459851000	1.416824000
O	-1.080540000	1.562614000	1.135387000
C	-3.521836000	1.901317000	0.957867000
O	-4.604482000	2.526284000	1.647878000
O	-2.990525000	4.688982000	1.028013000
O	-1.004762000	5.135272000	-0.948981000
O	0.122946000	2.806740000	-2.128772000
H	-1.617353000	1.196612000	-0.846363000
O	-7.966205000	-1.717785000	-0.152615000
O	2.573830000	-3.195936000	-0.322047000
H	-2.232689000	-4.387610000	-0.143810000
H	-4.213546000	-3.922282000	0.935863000
H	-3.804379000	-0.259872000	-1.283174000
H	-6.664560000	-3.648828000	0.918106000
H	-6.249822000	0.011306000	-1.289176000
H	3.137301000	1.424845000	-0.808403000
H	6.176755000	-0.454711000	-1.898966000
H	5.984463000	1.310347000	-2.012382000
H	6.115901000	1.523090000	0.441162000
H	8.291254000	0.623232000	0.625063000
H	6.440170000	-1.505824000	0.448914000
H	4.130011000	0.237101000	1.423206000
H	4.073231000	-2.564163000	1.278460000
H	6.341514000	-1.065655000	2.740010000
H	0.591213000	3.160193000	-0.135747000
H	-2.233045000	3.491090000	-1.226538000
H	-1.000799000	4.271640000	1.447770000
H	-2.200122000	2.518239000	2.506749000
H	-3.657667000	1.999037000	-0.124723000
H	-3.551451000	0.839844000	1.205132000
H	-4.519133000	3.476688000	1.483539000
H	-2.827071000	5.525167000	0.574364000
H	-0.684216000	5.111781000	-1.859109000
H	1.037549000	2.499958000	-2.173039000
H	-8.264949000	-0.914348000	-0.596578000
H	1.942718000	-3.968513000	-0.262329000

E = – 2061.4661317 a. u.
H = – 2060.895342 a. u.
G = – 2061.000563 a. u.

Transition state - 8-C bond rotation (φ_1 = 19.8°)

C	-0.481735000	-0.959879000	-0.364900000
C	0.251138000	-2.098542000	-0.741925000
C	0.074017000	0.315794000	-0.178897000
C	1.650208000	-1.974184000	-0.885987000
C	1.501338000	0.327139000	-0.146545000
C	2.278780000	-0.783369000	-0.560560000
C	-2.456014000	-2.325503000	-0.192774000
C	-1.793451000	-3.440694000	-0.584466000
O	-1.829412000	-1.110960000	-0.133056000
C	-0.399052000	-3.386053000	-0.916750000
C	-3.858952000	-2.253516000	0.219044000
C	-4.802147000	-3.164017000	-0.289191000
C	-4.283809000	-1.294824000	1.152813000
C	-6.122410000	-3.124033000	0.125918000
C	-5.604819000	-1.251433000	1.575665000
C	-6.528694000	-2.168816000	1.065070000
O	0.239666000	-4.400914000	-1.297329000
C	-0.771984000	1.600564000	0.038135000
C	3.791000000	-0.781134000	-0.526958000
O	2.154145000	1.397375000	0.345012000
O	4.285092000	0.532189000	-0.849947000
C	5.714514000	0.606543000	-0.936354000
C	6.360507000	0.218736000	0.391984000
O	7.771431000	0.255956000	0.198753000
C	5.879795000	-1.164299000	0.813666000
C	4.350681000	-1.206463000	0.850371000
O	3.892773000	-2.492149000	1.261228000
H	4.156818000	-1.480778000	-1.286864000
O	6.442131000	-1.441709000	2.094406000
C	-1.993678000	1.839454000	-0.918566000
C	-2.506349000	3.285819000	-0.803074000
C	-1.428002000	4.342300000	-0.916207000
C	-0.297546000	4.011986000	0.059509000
O	0.126431000	2.682765000	-0.221519000
C	-0.623842000	4.253756000	1.542919000
O	-0.651582000	5.649811000	1.842621000
O	-1.948694000	5.644066000	-0.619705000
O	-3.464070000	3.560376000	-1.828090000
O	-3.179826000	1.105208000	-0.638275000
H	-1.134840000	1.621510000	1.074532000
O	-7.836419000	-2.180988000	1.437884000
O	2.394027000	-3.040503000	-1.251037000
H	-2.295364000	-4.397008000	-0.603734000
H	-4.506563000	-3.895100000	-1.031399000

H	-3.574905000	-0.585200000	1.557928000
H	-6.852409000	-3.817712000	-0.272371000
H	-5.919167000	-0.511407000	2.303446000
H	3.089512000	1.356873000	0.055748000
H	6.071335000	-0.055762000	-1.734022000
H	5.953658000	1.636288000	-1.197337000
H	6.061973000	0.939992000	1.164196000
H	8.186406000	-0.072133000	1.005946000
H	6.239033000	-1.901525000	0.080523000
H	3.996000000	-0.505248000	1.611132000
H	3.820979000	-3.071068000	0.489746000
H	6.116659000	-2.305121000	2.378340000
H	-1.654420000	1.661059000	-1.946620000
H	-2.992592000	3.380016000	0.176047000
H	-1.021893000	4.326224000	-1.934279000
H	0.570850000	4.631936000	-0.175509000
H	-1.567804000	3.782607000	1.838250000
H	0.174136000	3.810625000	2.141684000
H	-1.282163000	6.050523000	1.225885000
H	-2.762160000	5.764244000	-1.125534000
H	-4.181492000	2.921620000	-1.732865000
H	-2.995646000	0.167458000	-0.736227000
H	-8.010276000	-1.491761000	2.091179000
H	1.751817000	-3.797340000	-1.377027000

E = – 2061.4374778 a. u.
H = – 2060.868794 a. u.
G = – 2060.972333 a. u.
f = 46.66i

Transition state - 8-C bond rotation (φ_1 = – 165.8°)

C	-0.383526000	-1.054912000	-0.158803000
C	0.374274000	-2.222471000	0.060739000
C	0.196510000	0.213077000	-0.401072000
C	1.781066000	-2.155728000	-0.037654000
C	1.591168000	0.173000000	-0.614207000
C	2.391659000	-0.973053000	-0.424126000
C	-2.389929000	-2.332225000	0.082667000
C	-1.709790000	-3.475582000	0.372093000
O	-1.740560000	-1.175651000	-0.177906000
C	-0.280983000	-3.485529000	0.370760000
C	-3.844828000	-2.177170000	-0.003807000
C	-4.719132000	-3.208172000	0.384647000

C	-4.399258000	-0.980018000	-0.484695000
C	-6.091725000	-3.049601000	0.293075000
C	-5.773103000	-0.813025000	-0.581738000
C	-6.626171000	-1.850367000	-0.192729000
O	0.387429000	-4.528461000	0.608517000
C	-0.610167000	1.540091000	-0.478218000
C	3.898832000	-0.945935000	-0.527932000
O	2.209963000	1.304766000	-1.044179000
O	4.290372000	-0.064668000	-1.600367000
C	5.706312000	-0.015896000	-1.828868000
C	6.438627000	0.471044000	-0.581332000
O	7.831889000	0.438208000	-0.874160000
C	6.084097000	-0.420440000	0.602855000
C	4.566285000	-0.481848000	0.785583000
O	4.221994000	-1.313191000	1.890705000
H	4.252199000	-1.955107000	-0.766075000
O	6.727126000	0.120265000	1.754790000
C	0.012234000	2.765061000	0.287459000
C	-1.021540000	3.861111000	0.589185000
C	-2.336191000	3.350998000	1.133020000
C	-2.869975000	2.264290000	0.199132000
O	-1.879768000	1.243854000	0.112742000
C	-3.354157000	2.761489000	-1.173550000
O	-4.593140000	3.460953000	-1.059809000
O	-3.300046000	4.407517000	1.224484000
O	-0.500533000	4.787528000	1.546394000
O	0.995359000	3.493765000	-0.439550000
H	-0.727327000	1.828460000	-1.531868000
O	-7.981568000	-1.755613000	-0.260201000
O	2.539430000	-3.237214000	0.228225000
H	-2.229505000	-4.399848000	0.574551000
H	-4.333638000	-4.142196000	0.772779000
H	-3.739138000	-0.180122000	-0.784549000
H	-6.764004000	-3.842422000	0.596896000
H	-6.183091000	0.118731000	-0.956658000
H	3.119776000	1.081780000	-1.354550000
H	6.066068000	-1.011291000	-2.113783000
H	5.859554000	0.668786000	-2.661385000
H	6.119736000	1.496448000	-0.351867000
H	8.307161000	0.656990000	-0.063151000
H	6.461576000	-1.434092000	0.404793000
H	4.201493000	0.518117000	1.038016000
H	4.179358000	-2.234781000	1.601039000
H	6.484638000	-0.426274000	2.512731000

H	0.416974000	2.398898000	1.239992000
H	-1.215409000	4.391827000	-0.350139000
H	-2.172752000	2.907166000	2.121933000
H	-3.722512000	1.775447000	0.676649000
H	-2.604497000	3.386226000	-1.671218000
H	-3.533170000	1.893071000	-1.810560000
H	-4.460481000	4.151887000	-0.393552000
H	-2.873768000	5.164135000	1.646747000
H	0.292620000	5.184333000	1.165847000
H	1.698221000	2.871755000	-0.682086000
H	-8.243821000	-0.895006000	-0.610055000
H	1.896631000	-3.978529000	0.437129000

E = – 2061.4471476 a. u.
H = – 2060.877963 a. u.
G = – 2060.980540 a. u.
f = 39.00i

Transition state – C_6 bond rotation (φ_3 = 18.9°)

C	-0.253100000	-0.900645000	-0.200551000
C	0.620436000	-1.980419000	-0.336834000
C	0.187548000	0.416304000	-0.202812000
C	2.010625000	-1.717422000	-0.463764000
C	1.573718000	0.639484000	-0.350818000
C	2.537146000	-0.421503000	-0.431909000
C	-2.124635000	-2.357224000	-0.101438000
C	-1.333777000	-3.456425000	-0.240411000
O	-1.590800000	-1.110728000	-0.061820000
C	0.090193000	-3.332016000	-0.356298000
C	-3.583643000	-2.325567000	-0.008373000
C	-4.317817000	-3.450684000	0.403345000
C	-4.279483000	-1.152887000	-0.346318000
C	-5.700615000	-3.407343000	0.472954000
C	-5.664368000	-1.103698000	-0.282668000
C	-6.380431000	-2.233214000	0.128121000
O	0.846064000	-4.335360000	-0.487985000
C	-0.769153000	1.575131000	-0.056121000
C	4.056230000	-0.149311000	-0.606291000
O	1.923192000	1.935413000	-0.428815000
O	4.263469000	1.225077000	-0.209610000
C	5.567177000	1.774542000	-0.419849000
C	6.521453000	1.082656000	0.535966000
O	7.824122000	1.621765000	0.331989000

C	6.476084000	-0.399208000	0.225476000
C	5.063201000	-1.011407000	0.228089000
O	5.305035000	-2.311044000	-0.289778000
H	4.318523000	-0.256860000	-1.668286000
O	7.304822000	-1.065679000	1.177719000
C	-1.468511000	1.608248000	1.319390000
C	-2.426660000	2.789921000	1.365383000
C	-3.401244000	2.730528000	0.195269000
C	-2.668971000	2.605413000	-1.153786000
O	-1.758185000	1.500955000	-1.104976000
C	-1.992886000	3.903243000	-1.633106000
O	-2.951198000	4.842757000	-2.120655000
O	-4.224801000	3.901002000	0.153803000
O	-3.218942000	2.793448000	2.555032000
O	-0.525409000	1.807711000	2.373848000
H	-0.195250000	2.497211000	-0.151743000
O	-7.737753000	-2.252838000	0.215959000
O	2.800652000	-2.795784000	-0.644280000
H	-1.769940000	-4.442661000	-0.302818000
H	-3.807542000	-4.360835000	0.693193000
H	-3.725181000	-0.284126000	-0.677248000
H	-6.268518000	-4.269351000	0.800387000
H	-6.190464000	-0.194859000	-0.553913000
H	2.908424000	1.977374000	-0.408579000
H	5.883651000	1.635849000	-1.460077000
H	5.488380000	2.840226000	-0.209008000
H	6.189588000	1.255614000	1.567412000
H	8.445894000	1.079270000	0.832741000
H	6.887237000	-0.540764000	-0.783735000
H	4.697188000	-1.056492000	1.262017000
H	4.447385000	-2.761253000	-0.373222000
H	7.317202000	-2.002983000	0.947413000
H	-2.034186000	0.686264000	1.477290000
H	-1.842962000	3.718033000	1.312790000
H	-4.031970000	1.844228000	0.331597000
H	-3.400650000	2.331159000	-1.917150000
H	-1.379319000	4.358717000	-0.847906000
H	-1.336963000	3.649672000	-2.467916000
H	-3.583761000	4.985160000	-1.401282000
H	-4.559726000	4.062071000	1.044999000
H	-2.621487000	2.861785000	3.309462000
H	-0.037362000	0.988425000	2.516133000
H	-8.107746000	-1.398454000	-0.039238000
H	2.196289000	-3.614972000	-0.612637000

E = – 2061.4569894 a. u.
H = – 2060.888164 a. u.
G = – 2060.991498 a. u.
f = 48.76i

Transition state – B ring rotation (φ_2 = 88.6°)

C	-0.224676000	-0.951095000	-0.335402000
C	0.584526000	-2.079798000	-0.528190000
C	0.281242000	0.346770000	-0.244807000
C	1.984814000	-1.884020000	-0.628478000
C	1.674959000	0.494274000	-0.359373000
C	2.537316000	-0.610223000	-0.552541000
C	-2.160428000	-2.319371000	-0.278619000
C	-1.444897000	-3.451195000	-0.458896000
O	-1.577416000	-1.094412000	-0.222437000
C	-0.007429000	-3.403587000	-0.596386000
C	-3.628058000	-2.227607000	-0.112720000
C	-4.195878000	-2.280613000	1.165288000
C	-4.455057000	-2.039486000	-1.223051000
C	-5.569269000	-2.154727000	1.332550000
C	-5.831802000	-1.912578000	-1.064142000
C	-6.389520000	-1.969857000	0.216269000
O	0.691652000	-4.433046000	-0.760331000
C	-0.613338000	1.544930000	-0.046475000
C	4.040948000	-0.473447000	-0.580656000
O	2.171353000	1.747624000	-0.265675000
O	4.393697000	0.777168000	-1.201715000
C	5.806647000	0.970081000	-1.350900000
C	6.501585000	0.955985000	0.008867000
O	7.898872000	1.090800000	-0.232989000
C	6.173012000	-0.338836000	0.742527000
C	4.657389000	-0.528018000	0.834734000
O	4.338606000	-1.733876000	1.524640000
H	4.461247000	-1.289267000	-1.180123000
O	6.770958000	-0.261931000	2.034817000
C	-1.382497000	1.510757000	1.292252000
C	-2.319865000	2.706020000	1.372430000
C	-3.230967000	2.740889000	0.151502000
C	-2.422533000	2.725775000	-1.157843000
O	-1.531234000	1.605995000	-1.157170000
C	-1.699076000	4.046774000	-1.477147000
O	-2.613181000	5.053843000	-1.912593000

O	-4.055109000	3.912164000	0.159641000
O	-3.172241000	2.640896000	2.518142000
O	-0.484182000	1.618411000	2.398853000
H	0.017959000	2.435947000	-0.033422000
O	-7.731008000	-1.852404000	0.441288000
O	2.801324000	-2.948479000	-0.772306000
H	-1.948641000	-4.406793000	-0.497609000
H	-3.560551000	-2.420135000	2.032160000
H	-4.024309000	-1.990769000	-2.216281000
H	-6.016964000	-2.197292000	2.317905000
H	-6.469682000	-1.769608000	-1.929754000
H	3.105881000	1.737773000	-0.563003000
H	6.221412000	0.184207000	-1.993251000
H	5.935774000	1.933408000	-1.841829000
H	6.134819000	1.798018000	0.610632000
H	8.353079000	0.998876000	0.613559000
H	6.603185000	-1.180922000	0.180885000
H	4.236184000	0.281721000	1.437427000
H	4.345039000	-2.473623000	0.902046000
H	6.545882000	-1.069338000	2.513711000
H	-1.975978000	0.596788000	1.365397000
H	-1.721011000	3.624887000	1.415408000
H	-3.862282000	1.844114000	0.175291000
H	-3.111731000	2.534643000	-1.983522000
H	-1.113105000	4.407074000	-0.624203000
H	-1.009609000	3.859363000	-2.302367000
H	-3.286828000	5.128780000	-1.220592000
H	-4.431074000	4.005457000	1.044192000
H	-2.613490000	2.650330000	3.304606000
H	-0.045864000	0.769903000	2.530516000
H	-8.202915000	-1.728735000	-0.391246000
H	2.213962000	-3.753614000	-0.808609000

E = – 2061.4595302 a. u.
H = – 2060.890006 a. u.
G = – 2060.994751 a. u.
f = 52.15i

2 Schaftoside

a Global Minimum Point H–C_7 eclipsed

C	-0.769975000	-0.735901000	-0.169566000
C	-0.018059000	-1.916022000	-0.112403000

C	-0.197490000	0.531708000	-0.269178000
C	1.391940000	-1.808578000	-0.152746000
C	1.205989000	0.592076000	-0.303241000
C	2.013192000	-0.567883000	-0.255455000
C	-2.792304000	-1.977352000	-0.059849000
C	-2.122354000	-3.161453000	-0.000263000
O	-2.129939000	-0.794557000	-0.118341000
C	-0.686599000	-3.201886000	-0.005481000
C	-4.242874000	-1.787060000	-0.095940000
C	-5.125327000	-2.785373000	0.350476000
C	-4.779168000	-0.588601000	-0.595940000
C	-6.496516000	-2.596990000	0.294526000
C	-6.151669000	-0.394417000	-0.657449000
C	-7.015974000	-1.400345000	-0.212677000
O	-0.033787000	-4.276300000	0.057324000
C	3.522461000	-0.518559000	-0.217119000
C	-1.027642000	1.788904000	-0.317481000
O	1.767569000	1.821782000	-0.368795000
O	-1.963104000	1.703053000	-1.405928000
C	-2.685707000	2.917105000	-1.603310000
C	-3.523929000	3.255633000	-0.371838000
O	-4.184439000	4.493594000	-0.627996000
C	-2.623941000	3.339670000	0.853737000
C	-1.787537000	2.067292000	0.999110000
O	-0.907477000	2.165370000	2.120010000
H	-0.354049000	2.634061000	-0.501932000
O	-3.462060000	3.554317000	1.989420000
C	4.070466000	-0.387525000	1.218911000
C	5.595008000	-0.292588000	1.168888000
C	6.021587000	0.871878000	0.282145000
C	5.401660000	0.770726000	-1.121923000
O	3.975359000	0.604655000	-1.003631000
C	6.021205000	-0.307740000	-2.027261000
O	7.301413000	0.095057000	-2.507727000
O	7.443106000	0.919530000	0.133952000
O	6.151697000	-0.048647000	2.459550000
O	3.660050000	-1.458279000	2.063776000
H	3.906782000	-1.443221000	-0.657601000
O	-8.370453000	-1.274485000	-0.244130000
O	2.151274000	-2.922295000	-0.062887000
H	-2.663382000	-4.096223000	0.020628000
H	-4.741775000	-3.709565000	0.764453000
H	-4.110977000	0.185213000	-0.951497000
H	-7.178138000	-3.361334000	0.646593000

H	-6.553961000	0.532209000	-1.052718000
H	2.714023000	1.719202000	-0.602628000
H	-1.999770000	3.747717000	-1.820394000
H	-3.329640000	2.761270000	-2.468824000
H	-4.262389000	2.461201000	-0.203975000
H	-4.643864000	4.753326000	0.179956000
H	-1.946263000	4.197631000	0.724712000
H	-2.450075000	1.230598000	1.221277000
H	-0.238770000	2.839547000	1.942271000
H	-2.900844000	3.569066000	2.774565000
H	3.673922000	0.526282000	1.671341000
H	5.998447000	-1.231728000	0.767474000
H	5.665574000	1.797874000	0.750264000
H	5.525157000	1.728150000	-1.630551000
H	6.089101000	-1.276049000	-1.519154000
H	5.373115000	-0.428131000	-2.897071000
H	7.840675000	0.288881000	-1.726938000
H	7.838896000	0.830989000	1.010248000
H	5.894914000	-0.779180000	3.035875000
H	3.589152000	-2.272166000	1.545928000
H	-8.623001000	-0.417759000	-0.610219000
H	1.514819000	-3.690517000	-0.000887000

E = – 2061.4665527 a. u.
H = – 2060.895733 a. u.
G = – 2061.001176 a. u.

b H–C_9 eclipsed

C	-1.051617000	-0.826978000	-0.027143000
C	-0.354302000	-2.028117000	-0.216164000
C	-0.420276000	0.409138000	0.108769000
C	1.057469000	-1.976296000	-0.266660000
C	0.986693000	0.414219000	0.051750000
C	1.736349000	-0.767929000	-0.143278000
C	-3.130512000	-1.987063000	-0.116993000
C	-2.508648000	-3.183274000	-0.307620000
O	-2.418036000	-0.838481000	0.026599000
C	-1.077257000	-3.279362000	-0.356595000
C	-4.575910000	-1.757686000	-0.054950000
C	-5.470807000	-2.823822000	0.148599000
C	-5.104494000	-0.465039000	-0.205677000
C	-6.837964000	-2.610021000	0.189612000
C	-6.473993000	-0.242493000	-0.168624000

C	-7.347497000	-1.316618000	0.027553000
O	-0.473842000	-4.371153000	-0.524926000
C	3.247278000	-0.796526000	-0.154358000
C	-1.225240000	1.671044000	0.287889000
O	1.605552000	1.606055000	0.192911000
O	-0.904375000	2.261800000	1.556931000
C	-1.734902000	3.378901000	1.865667000
C	-1.551185000	4.491074000	0.834879000
O	-2.426646000	5.559474000	1.191279000
C	-1.857226000	3.951829000	-0.556971000
C	-1.025566000	2.701788000	-0.845640000
O	-1.354085000	2.160240000	-2.127694000
H	-2.287491000	1.400292000	0.297623000
O	-1.586791000	4.994508000	-1.494289000
C	3.848889000	-0.980443000	1.253659000
C	5.374185000	-0.959038000	1.152236000
C	5.840646000	0.335163000	0.493802000
C	5.163909000	0.553463000	-0.870340000
O	3.736249000	0.437570000	-0.721158000
C	5.686279000	-0.345566000	-2.004114000
O	6.965914000	0.088129000	-2.458397000
O	7.255818000	0.333407000	0.287582000
O	5.989045000	-1.010708000	2.438220000
O	3.404611000	-2.174273000	1.891560000
H	3.567385000	-1.631924000	-0.784172000
O	-8.698745000	-1.170261000	0.074922000
O	1.765158000	-3.117484000	-0.414393000
H	-3.084586000	-4.085879000	-0.447621000
H	-5.100287000	-3.830260000	0.295056000
H	-4.441939000	0.374458000	-0.364925000
H	-7.524269000	-3.431430000	0.353973000
H	-6.865570000	0.761232000	-0.293663000
H	2.540260000	1.504409000	-0.084333000
H	-2.792324000	3.080228000	1.900530000
H	-1.438735000	3.726778000	2.855260000
H	-0.507421000	4.830661000	0.854319000
H	-2.375938000	6.224661000	0.494070000
H	-2.925407000	3.686938000	-0.595878000
H	0.025504000	2.977876000	-0.906501000
H	-2.268508000	1.848732000	-2.120172000
H	-1.726114000	4.639995000	-2.381146000
H	3.524771000	-0.153792000	1.892985000
H	5.703909000	-1.818931000	0.553886000
H	5.563160000	1.166112000	1.154020000

H	5.324529000	1.587349000	-1.179983000
H	5.721645000	-1.398886000	-1.705031000
H	4.997621000	-0.256949000	-2.846151000
H	7.546528000	0.093184000	-1.683322000
H	7.678800000	0.055278000	1.109726000
H	5.700684000	-1.824442000	2.870200000
H	3.250313000	-2.859888000	1.226767000
H	-8.944937000	-0.243962000	-0.039767000
H	1.093978000	-3.854518000	-0.494636000

E = – 2061.4635294 a. u.
H = – 2060.892732 a. u.
G = – 2060.998529 a. u.

c Gauche-like – converge to **a** form

Transition state - 8-C bond rotation (φ_1 = 7.2°)

C	0.891883000	-0.729803000	-0.127350000
C	0.197450000	-1.923323000	0.140216000
C	0.280168000	0.515681000	-0.347971000
C	-1.209247000	-1.866333000	0.243830000
C	-1.135056000	0.522090000	-0.176065000
C	-1.869439000	-0.655548000	0.125162000
C	2.959265000	-1.942854000	0.034918000
C	2.329196000	-3.122663000	0.235271000
O	2.268676000	-0.783227000	-0.184265000
C	0.896603000	-3.187252000	0.290388000
C	4.414795000	-1.757850000	0.061680000
C	5.257920000	-2.675187000	-0.585010000
C	4.989044000	-0.703567000	0.786184000
C	6.635656000	-2.537854000	-0.519929000
C	6.368316000	-0.564064000	0.862074000
C	7.195822000	-1.480944000	0.205809000
O	0.281258000	-4.265163000	0.491825000
C	-3.380884000	-0.682692000	0.210628000
C	1.104180000	1.723002000	-0.872570000
O	-1.834053000	1.665402000	-0.308368000
O	0.219662000	2.828991000	-0.971368000
C	0.794961000	4.109492000	-1.152578000
C	1.585504000	4.462491000	0.096817000
O	2.001920000	5.824226000	0.015886000
C	2.773705000	3.528724000	0.135468000
C	2.427392000	2.037925000	-0.069416000

O	3.571922000	1.545538000	-0.772031000
H	1.448436000	1.461398000	-1.885754000
O	3.466962000	3.737058000	1.370927000
C	-4.046008000	-0.833878000	-1.172420000
C	-5.564856000	-0.811621000	-1.005849000
C	-5.998166000	0.466912000	-0.296778000
C	-5.268908000	0.645177000	1.045963000
O	-3.847767000	0.531190000	0.839528000
C	-5.749244000	-0.285509000	2.172448000
O	-7.009680000	0.136192000	2.687764000
O	-7.404324000	0.466776000	-0.037320000
O	-6.234576000	-0.828367000	-2.265323000
O	-3.630377000	-2.016279000	-1.850486000
H	-3.668914000	-1.535247000	0.831041000
O	8.554461000	-1.400207000	0.235750000
O	-1.923492000	-2.994417000	0.443807000
H	2.905459000	-4.016890000	0.424787000
H	4.829063000	-3.489806000	-1.156207000
H	4.357179000	0.001238000	1.310808000
H	7.289693000	-3.235059000	-1.028772000
H	6.801807000	0.248997000	1.434032000
H	-2.729306000	1.522627000	0.065220000
H	1.437743000	4.151961000	-2.043754000
H	-0.037079000	4.800477000	-1.292279000
H	0.945789000	4.307552000	0.974847000
H	2.640397000	5.975022000	0.723953000
H	3.423561000	3.818905000	-0.698108000
H	2.356585000	1.581066000	0.923031000
H	3.486396000	0.589884000	-0.851118000
H	4.347278000	3.351018000	1.296767000
H	-3.747869000	0.002300000	-1.811355000
H	-5.872498000	-1.685492000	-0.416083000
H	-5.740393000	1.313639000	-0.944923000
H	-5.414467000	1.669960000	1.391082000
H	-5.798628000	-1.329554000	1.844560000
H	-5.028776000	-0.222333000	2.989750000
H	-7.619337000	0.165295000	1.935878000
H	-7.858748000	0.207079000	-0.848715000
H	-5.974154000	-1.634379000	-2.728283000
H	-3.485923000	-2.724654000	-1.207870000
H	8.839607000	-0.641619000	0.760103000
H	-1.257946000	-3.738421000	0.511227000

$E = -2061.4319677$ a. u.

H = – 2060.862927 a. u.
G = – 2060.967008 a. u.
f = 47.93i

Transition state - 8-C bond rotation (φ_1 = – 166.1°)

C	-0.983309000	-0.804077000	-0.059062000
C	-0.277942000	-1.972637000	0.289020000
C	-0.352667000	0.431885000	-0.337436000
C	1.133114000	-1.945309000	0.289572000
C	1.050997000	0.343987000	-0.448919000
C	1.803217000	-0.806035000	-0.128092000
C	-3.036820000	-2.013338000	0.109151000
C	-2.414300000	-3.153914000	0.516044000
O	-2.337514000	-0.891741000	-0.169683000
C	-0.990001000	-3.197544000	0.626756000
C	-4.475387000	-1.826833000	-0.099300000
C	-5.410732000	-2.765538000	0.371127000
C	-4.950029000	-0.694643000	-0.782054000
C	-6.768002000	-2.583354000	0.164877000
C	-6.308191000	-0.507679000	-0.996965000
C	-7.223434000	-1.452754000	-0.522985000
O	-0.370081000	-4.238331000	0.977410000
C	3.314524000	-0.826027000	-0.119209000
C	-1.123679000	1.762686000	-0.558694000
O	1.729421000	1.429228000	-0.908403000
O	-2.438098000	1.540119000	-0.047650000
C	-3.373716000	2.592140000	-0.225763000
C	-2.967108000	3.759939000	0.654838000
O	-3.914344000	4.813413000	0.486001000
C	-1.582456000	4.179800000	0.216584000
C	-0.553722000	3.035478000	0.171880000
O	0.551390000	3.672313000	-0.459521000
H	-1.169990000	1.985943000	-1.635885000
O	-1.136410000	5.212047000	1.099121000
C	3.896966000	-0.292845000	1.205096000
C	5.422742000	-0.289830000	1.122241000
C	5.882288000	0.532428000	-0.077100000
C	5.236807000	0.038197000	-1.383414000
O	3.805618000	-0.023593000	-1.217294000
C	5.794360000	-1.291768000	-1.918082000
O	7.080216000	-1.112550000	-2.505537000
O	7.301356000	0.468729000	-0.238441000
O	6.012296000	0.304460000	2.276643000

O	3.451364000	-1.039227000	2.333278000
H	3.643056000	-1.859429000	-0.258635000
O	-8.567375000	-1.328386000	-0.695344000
O	1.839844000	-3.023711000	0.682572000
H	-2.974682000	-4.052715000	0.725359000
H	-5.084439000	-3.639991000	0.919338000
H	-4.244690000	0.039637000	-1.145118000
H	-7.488191000	-3.302445000	0.535077000
H	-6.659355000	0.368988000	-1.530521000
H	2.651330000	1.163137000	-1.137843000
H	-3.428478000	2.906364000	-1.277274000
H	-4.344732000	2.194646000	0.070837000
H	-2.941904000	3.430974000	1.701471000
H	-3.565135000	5.593930000	0.933450000
H	-1.663674000	4.580889000	-0.803411000
H	-0.304292000	2.745836000	1.201361000
H	1.241029000	3.005000000	-0.597704000
H	-0.269005000	5.501734000	0.790242000
H	3.549245000	0.732025000	1.364207000
H	5.777432000	-1.323986000	1.019298000
H	5.573694000	1.571898000	0.089541000
H	5.390575000	0.789617000	-2.159248000
H	5.831375000	-2.059934000	-1.137590000
H	5.125646000	-1.643557000	-2.705555000
H	7.642250000	-0.715064000	-1.824389000
H	7.708890000	0.634518000	0.621092000
H	5.729085000	-0.202375000	3.047892000
H	3.363244000	-1.971731000	2.092481000
H	-8.773863000	-0.515080000	-1.172542000
H	1.162991000	-3.735483000	0.888173000

E = – 2061.4455878 a. u.
H = – 2060.876703 a. u.
G = – 2060.979976 a. u.
f = 55.59i

Transition state – C_6 bond rotation (φ_3 = 18.4°)

C	0.821528000	0.723814000	-0.209315000
C	0.068030000	1.898574000	-0.224925000
C	0.239010000	-0.534221000	-0.285734000
C	-1.346390000	1.796635000	-0.297141000
C	-1.168696000	-0.595617000	-0.375128000
C	-2.011012000	0.565480000	-0.324973000

C	2.845242000	1.959110000	-0.097053000
C	2.175590000	3.144378000	-0.121296000
O	2.178775000	0.778030000	-0.120982000
C	0.743308000	3.183005000	-0.176802000
C	4.294481000	1.765148000	-0.072256000
C	5.163631000	2.784885000	0.351715000
C	4.844127000	0.541373000	-0.490014000
C	6.535142000	2.592169000	0.354090000
C	6.217131000	0.342855000	-0.493294000
C	7.068363000	1.369761000	-0.071296000
O	0.098231000	4.268687000	-0.200595000
C	-3.559634000	0.480325000	-0.422605000
C	1.068862000	-1.795462000	-0.279783000
O	-1.662086000	-1.836508000	-0.531745000
O	2.020712000	-1.752392000	-1.358181000
C	2.725327000	-2.984123000	-1.501200000
C	3.533618000	-3.299653000	-0.242882000
O	4.163096000	-4.563704000	-0.441853000
C	2.616536000	-3.316140000	0.973156000
C	1.812382000	-2.024236000	1.056193000
O	0.894994000	-2.186330000	2.140559000
H	0.400562000	-2.647527000	-0.429329000
O	3.439302000	-3.508230000	2.125497000
C	-4.400298000	1.381137000	0.541523000
C	-5.863300000	0.917495000	0.628324000
C	-6.037791000	-0.568145000	0.862299000
C	-5.255646000	-1.345398000	-0.196173000
O	-3.893543000	-0.896712000	-0.117496000
C	-5.818847000	-1.284574000	-1.624227000
O	-7.003769000	-2.068719000	-1.737668000
O	-7.415713000	-0.943225000	0.779165000
O	-6.533343000	1.584979000	1.698691000
O	-4.541582000	2.726946000	0.113904000
H	-3.859154000	0.714875000	-1.451570000
O	8.422330000	1.240907000	-0.048460000
O	-2.020404000	2.963745000	-0.361879000
H	2.714998000	4.080065000	-0.132510000
H	4.768560000	3.729985000	0.702858000
H	4.186469000	-0.248748000	-0.828957000
H	7.206388000	3.373039000	0.689355000
H	6.630444000	-0.603381000	-0.825663000
H	-2.642629000	-1.774706000	-0.457276000
H	2.028900000	-3.809458000	-1.704577000
H	3.389535000	-2.869086000	-2.357871000

H	4.292250000	-2.520667000	-0.092694000
H	4.592903000	-4.808979000	0.386732000
H	1.916077000	-4.157452000	0.872270000
H	2.494777000	-1.192665000	1.251443000
H	0.532347000	-1.324430000	2.375115000
H	2.863481000	-3.529446000	2.899422000
H	-3.952052000	1.324474000	1.542008000
H	-6.346508000	1.184049000	-0.319277000
H	-5.635967000	-0.825582000	1.849145000
H	-5.210754000	-2.397861000	0.089863000
H	-6.004641000	-0.254541000	-1.947309000
H	-5.078713000	-1.718316000	-2.299517000
H	-7.612368000	-1.755550000	-1.051972000
H	-7.927070000	-0.319187000	1.309962000
H	-6.496176000	2.532904000	1.520847000
H	-3.648605000	3.092367000	-0.005867000
H	8.685397000	0.365498000	-0.358762000
H	-1.328621000	3.709080000	-0.304742000

E = – 2061.4561232a. u.
H = – 2060.887350 a. u.
G = – 2060.990828 a. u.
f = 43.91i

Transition state – B ring rotation (φ_2 = 88.5°)

C	-0.752401000	-0.723789000	-0.223140000
C	0.002072000	-1.905290000	-0.187291000
C	-0.180136000	0.548118000	-0.283381000
C	1.414289000	-1.792608000	-0.206193000
C	1.224595000	0.611175000	-0.306678000
C	2.033179000	-0.549064000	-0.271010000
C	-2.761814000	-1.978268000	-0.121429000
C	-2.101348000	-3.156317000	-0.079473000
O	-2.115956000	-0.786335000	-0.196532000
C	-0.657771000	-3.196024000	-0.110143000
C	-4.230288000	-1.798674000	-0.088610000
C	-4.893057000	-1.642757000	1.133984000
C	-4.962092000	-1.739433000	-1.277334000
C	-6.266404000	-1.435432000	1.170422000
C	-6.338026000	-1.532456000	-1.249399000
C	-6.990881000	-1.378420000	-0.023259000
O	-0.008277000	-4.269415000	-0.070230000
C	3.541255000	-0.495655000	-0.204561000

C	-1.016483000	1.802272000	-0.340680000
O	1.785718000	1.839230000	-0.354468000
O	-1.852393000	1.745348000	-1.508087000
C	-2.606705000	2.939620000	-1.699904000
C	-3.543845000	3.185307000	-0.519055000
O	-4.247277000	4.400034000	-0.772096000
C	-2.734270000	3.264129000	0.768447000
C	-1.874773000	2.016670000	0.928056000
O	-1.046568000	2.231764000	2.074226000
H	-0.343529000	2.661792000	-0.423187000
O	-3.657287000	3.413452000	1.849108000
C	4.058533000	-0.376725000	1.244305000
C	5.582994000	-0.275599000	1.227628000
C	6.023218000	0.899211000	0.361250000
C	5.433576000	0.810430000	-1.056518000
O	4.005470000	0.637101000	-0.970560000
C	6.076518000	-0.255976000	-1.959779000
O	7.364640000	0.157103000	-2.409250000
O	7.447255000	0.953415000	0.243452000
O	6.111444000	-0.041366000	2.531774000
O	3.631414000	-1.456278000	2.069264000
H	3.937844000	-1.414362000	-0.646300000
O	-8.336740000	-1.170069000	0.073106000
O	2.176124000	-2.904095000	-0.131193000
H	-2.655419000	-4.082568000	-0.020443000
H	-4.332090000	-1.683179000	2.060426000
H	-4.457920000	-1.855002000	-2.229657000
H	-6.787061000	-1.315587000	2.112621000
H	-6.901696000	-1.490548000	-2.175055000
H	2.735859000	1.739188000	-0.575350000
H	-1.941181000	3.805279000	-1.826930000
H	-3.181065000	2.804624000	-2.616479000
H	-4.248171000	2.346952000	-0.438220000
H	-4.762222000	4.608902000	0.016990000
H	-2.076461000	4.143422000	0.717105000
H	-2.533200000	1.159547000	1.086553000
H	-0.671185000	1.387837000	2.350717000
H	-3.148530000	3.466594000	2.667189000
H	3.648620000	0.530525000	1.697673000
H	5.998619000	-1.209281000	0.825931000
H	5.653998000	1.819012000	0.831285000
H	5.563444000	1.773680000	-1.552329000
H	6.138066000	-1.229131000	-1.460194000
H	5.447276000	-0.370102000	-2.844138000

H	7.886946000	0.344666000	-1.615523000
H	7.824881000	0.861828000	1.127413000
H	5.845318000	-0.777476000	3.096630000
H	3.609217000	-2.272076000	1.550483000
H	-8.737349000	-1.142574000	-0.804417000
H	1.546856000	-3.677756000	-0.098444000

E = – 2061.4585911 a. u.
H = – 2060.889154 a. u.
G = – 2060.993749 a. u.
f = 50.71i

3 Vitexin

a Global Minimum Point H–C_7 eclipsed

C	-1.817486000	0.177964000	-0.076723000
C	-3.056682000	0.831216000	-0.136298000
C	-1.674185000	-1.212473000	-0.053010000
C	-4.229510000	0.032821000	-0.179477000
C	-2.865964000	-1.956297000	-0.105542000
C	-4.126492000	-1.349358000	-0.164357000
C	-0.677764000	2.263902000	-0.087740000
C	-1.844770000	2.960674000	-0.151705000
O	-0.668300000	0.907807000	-0.028507000
C	-3.113401000	2.283810000	-0.161861000
C	0.679483000	2.811665000	-0.096827000
C	0.937548000	4.139729000	0.281845000
C	1.756798000	2.003100000	-0.495747000
C	2.227613000	4.644463000	0.262355000
C	3.050799000	2.503406000	-0.522102000
C	3.290386000	3.827664000	-0.140438000
O	-4.210599000	2.895856000	-0.210821000
C	-0.328299000	-1.887200000	0.035993000
O	-2.750974000	-3.309220000	-0.092727000
C	0.397306000	-1.613883000	1.370694000
C	1.754347000	-2.303565000	1.355578000
C	2.557470000	-1.867143000	0.136603000
C	1.769076000	-2.076545000	-1.170159000
O	0.489212000	-1.442348000	-1.065891000
C	1.661527000	-3.545676000	-1.618779000
O	2.896207000	-4.020030000	-2.155727000
O	3.786461000	-2.595814000	0.043580000
O	2.538717000	-1.968703000	2.502111000

O	-0.325445000	-2.162141000	2.473996000
H	-0.490618000	-2.965192000	-0.031258000
O	4.534425000	4.379045000	-0.136584000
O	-5.442299000	0.609309000	-0.236318000
H	-1.835671000	4.038320000	-0.227271000
H	0.130558000	4.779803000	0.616287000
H	1.568885000	0.981553000	-0.800300000
H	2.430875000	5.664177000	0.565109000
H	3.873605000	1.871742000	-0.839577000
H	-3.621012000	-3.723729000	-0.142141000
H	0.546707000	-0.538845000	1.502401000
H	1.597183000	-3.389791000	1.325597000
H	2.773601000	-0.797704000	0.244670000
H	2.282328000	-1.539185000	-1.970888000
H	1.325189000	-4.196933000	-0.804358000
H	0.920803000	-3.597833000	-2.418810000
H	3.565126000	-3.871217000	-1.471341000
H	4.203835000	-2.589741000	0.914269000
H	2.060181000	-2.265419000	3.285595000
H	-1.077605000	-1.592508000	2.671394000
H	5.192806000	3.732172000	-0.419125000
H	-5.285687000	1.591606000	-0.238943000
H	-5.027128000	-1.951006000	-0.200015000

E = – 1565.0500957 a. u.
H = – 1564.628745 a. u.
G = – 1564.714904 a. u.

b H–C_9 eclipsed

C	-0.511811000	1.659915000	-0.079828000
C	-1.228255000	2.865043000	-0.135438000
C	0.884408000	1.586888000	-0.100189000
C	-0.492248000	4.074615000	-0.223278000
C	1.565729000	2.814847000	-0.199321000
C	0.892978000	4.040017000	-0.258541000
C	-2.544577000	0.423323000	0.029251000
C	-3.294567000	1.558074000	-0.000583000
O	-1.186881000	0.474070000	-0.007167000
C	-2.680783000	2.853881000	-0.097334000
C	-3.044507000	-0.950972000	0.109269000
C	-4.363740000	-1.263978000	-0.262943000
C	-2.212307000	-1.989836000	0.557457000
C	-4.836713000	-2.563361000	-0.186002000

C	-2.680064000	-3.293771000	0.641206000
C	-3.995857000	-3.585543000	0.268103000
O	-3.346610000	3.919562000	-0.137217000
C	1.587584000	0.255751000	-0.032198000
O	2.920944000	2.773624000	-0.236426000
C	2.540959000	0.116120000	1.171895000
C	3.206671000	-1.251462000	1.123328000
C	3.890671000	-1.461175000	-0.222338000
C	2.920482000	-1.235318000	-1.396092000
O	2.303941000	0.050815000	-1.265596000
C	1.889574000	-2.362409000	-1.596822000
O	2.488179000	-3.520967000	-2.178082000
O	4.420260000	-2.787978000	-0.326043000
O	4.217848000	-1.392971000	2.123519000
O	1.817620000	0.172790000	2.403918000
H	0.825464000	-0.517369000	0.081186000
O	-4.514865000	-4.841932000	0.320647000
O	-1.128431000	5.256970000	-0.274720000
H	-4.371418000	1.504894000	0.063689000
H	-5.023309000	-0.492322000	-0.639437000
H	-1.195429000	-1.775695000	0.857646000
H	-5.849458000	-2.804945000	-0.483902000
H	-2.028320000	-4.084534000	0.996525000
H	3.284710000	3.667489000	-0.260282000
H	3.309237000	0.891198000	1.136640000
H	2.438673000	-2.022049000	1.270476000
H	4.704701000	-0.730836000	-0.304333000
H	3.504231000	-1.175060000	-2.317173000
H	1.382544000	-2.625589000	-0.661830000
H	1.133823000	-2.003826000	-2.298106000
H	3.223960000	-3.767964000	-1.598833000
H	4.903714000	-2.981142000	0.487105000
H	3.797105000	-1.297495000	2.986401000
H	1.569120000	1.087545000	2.579580000
H	-3.852597000	-5.469418000	0.636053000
H	-2.101572000	5.053309000	-0.236919000
H	1.447022000	4.968051000	-0.334752000

E = – 1565.0477395 a. u.
H = – 1564.626232 a. u.
G = – 1564.712329 a. u.

c Gauche-like

C	0.513894000	1.706897000	0.013800000
C	0.452219000	3.101568000	-0.112195000
C	1.709554000	0.975688000	0.057543000
C	1.674529000	3.818336000	-0.182886000
C	2.887545000	1.738806000	-0.006255000
C	2.876459000	3.133496000	-0.121189000
C	-1.861535000	1.582011000	0.069089000
C	-1.988282000	2.930096000	-0.055579000
O	-0.641861000	0.981302000	0.091883000
C	-0.833650000	3.777841000	-0.164515000
C	-2.958177000	0.622032000	0.209780000
C	-4.228673000	0.892097000	-0.326239000
C	-2.762223000	-0.586666000	0.894574000
C	-5.267059000	-0.013731000	-0.182760000
C	-3.798101000	-1.496967000	1.047801000
C	-5.056034000	-1.213326000	0.506410000
O	-0.914044000	5.026823000	-0.278806000
C	1.615246000	-0.532019000	0.096215000
O	4.077759000	1.080884000	0.068111000
C	2.817886000	-1.328979000	0.624979000
C	2.433286000	-2.804163000	0.638798000
C	2.045355000	-3.250556000	-0.767376000
C	0.956403000	-2.349703000	-1.379204000
O	1.340813000	-0.973517000	-1.255521000
C	-0.461101000	-2.613107000	-0.840180000
O	-1.016813000	-3.806901000	-1.391793000
O	1.564227000	-4.599378000	-0.767463000
O	3.523852000	-3.633070000	1.042327000
O	3.163904000	-0.963941000	1.958991000
H	0.763437000	-0.778643000	0.738013000
O	-6.113160000	-2.063429000	0.613211000
O	1.675745000	5.156389000	-0.302452000
H	-2.966398000	3.388616000	-0.039652000
H	-4.401831000	1.804966000	-0.882591000
H	-1.795507000	-0.808714000	1.325267000
H	-6.242952000	0.186918000	-0.607269000
H	-3.632775000	-2.423220000	1.586926000
H	4.814782000	1.702373000	0.019109000
H	3.670925000	-1.200274000	-0.042329000
H	1.588602000	-2.951441000	1.325320000
H	2.942636000	-3.179576000	-1.393952000
H	0.921546000	-2.533239000	-2.455189000
H	-0.479005000	-2.659094000	0.254113000
H	-1.099667000	-1.785856000	-1.151658000

H	-0.399372000	-4.520196000	-1.174221000
H	2.194203000	-5.143491000	-0.278862000
H	3.808784000	-3.336583000	1.915560000
H	3.756650000	-0.204253000	1.904258000
H	-5.860410000	-2.861822000	1.093361000
H	0.721366000	5.436538000	-0.322995000
H	3.806357000	3.687785000	-0.164777000

E = – 1565.0477285 a. u.
H = – 1564.625878 a. u.
G = – 1564.710500 a. u.

Transition state - 8-C bond rotation (φ_1 = 20.6°)

C	-0.464917000	1.634763000	-0.032041000
C	-1.130635000	2.864797000	0.134616000
C	0.923283000	1.487778000	-0.203872000
C	-0.364896000	4.053639000	0.067558000
C	1.597508000	2.722333000	-0.434695000
C	0.974285000	3.964220000	-0.246398000
C	-2.597061000	0.516234000	0.014136000
C	-3.271914000	1.672498000	0.215643000
O	-1.231044000	0.491487000	-0.059022000
C	-2.570873000	2.921498000	0.320685000
C	-3.191070000	-0.811147000	-0.160711000
C	-4.401018000	-1.142215000	0.473470000
C	-2.578208000	-1.767660000	-0.985414000
C	-4.979569000	-2.387207000	0.291310000
C	-3.155755000	-3.015070000	-1.177079000
C	-4.358441000	-3.329600000	-0.536421000
O	-3.166931000	4.009691000	0.519148000
C	1.663641000	0.125689000	-0.216394000
O	2.873396000	2.743922000	-0.892636000
C	1.303100000	-0.920374000	0.894029000
C	2.353419000	-2.042690000	0.946912000
C	3.784733000	-1.554163000	1.012883000
C	4.026632000	-0.548801000	-0.114245000
O	3.035803000	0.466731000	0.005350000
C	4.114809000	-1.155401000	-1.524666000
O	5.345487000	-1.855876000	-1.708680000
O	4.706380000	-2.643829000	0.884259000
O	2.145669000	-2.869829000	2.093868000
O	0.107982000	-1.666439000	0.696958000
H	1.524539000	-0.352213000	-1.195480000

O	-4.972338000	-4.535635000	-0.673899000
O	-0.929679000	5.258492000	0.254321000
H	-4.351743000	1.675823000	0.248116000
H	-4.880115000	-0.429878000	1.133815000
H	-1.648878000	-1.531597000	-1.486778000
H	-5.903860000	-2.650106000	0.790596000
H	-2.677770000	-3.742662000	-1.823735000
H	3.135688000	3.661213000	-1.040688000
H	1.286995000	-0.398689000	1.859115000
H	2.226934000	-2.648461000	0.040560000
H	3.940815000	-1.044458000	1.970756000
H	4.971920000	-0.031196000	0.064478000
H	3.266174000	-1.813011000	-1.742838000
H	4.098257000	-0.336575000	-2.246444000
H	5.402762000	-2.503841000	-0.990842000
H	4.428273000	-3.344482000	1.487480000
H	1.249145000	-3.223213000	2.037993000
H	-0.638977000	-1.062141000	0.714968000
H	-4.458543000	-5.115419000	-1.249862000
H	-1.896856000	5.090392000	0.416292000
H	1.545127000	4.876073000	-0.380696000

E = – 1565.0210634 a. u.
H = – 1564.601085 a. u.
G = – 1564.683936 a. u.
f = 47.73i

Transition state - 8-C bond rotation (φ_1 = –165.6°)

C	-0.523712000	1.703908000	-0.136675000
C	-0.514690000	3.098558000	0.080386000
C	-1.702276000	0.950627000	-0.374026000
C	-1.731022000	3.816465000	-0.011787000
C	-2.846193000	1.754920000	-0.558707000
C	-2.879246000	3.136611000	-0.363455000
C	1.855950000	1.671819000	0.102445000
C	1.920144000	3.004867000	0.367490000
O	0.677322000	1.060307000	-0.151118000
C	0.730969000	3.798668000	0.366177000
C	2.984214000	0.738215000	0.037999000
C	4.262124000	1.096762000	0.502717000
C	2.805125000	-0.549217000	-0.492189000
C	5.319145000	0.204219000	0.437363000
C	3.858883000	-1.448788000	-0.564403000

C	5.122883000	-1.074064000	-0.098401000
O	0.748103000	5.039324000	0.585386000
C	-1.742206000	-0.600138000	-0.476231000
O	-4.004744000	1.163292000	-0.981651000
C	-2.921885000	-1.311537000	0.280943000
C	-2.646202000	-2.803138000	0.529233000
C	-1.259208000	-3.106422000	1.048668000
C	-0.230287000	-2.449524000	0.127945000
O	-0.511655000	-1.053234000	0.096825000
C	-0.109369000	-3.077929000	-1.271005000
O	0.539170000	-4.347617000	-1.211314000
O	-1.022127000	-4.519261000	1.087939000
O	-3.576580000	-3.330989000	1.478425000
O	-4.151079000	-1.366141000	-0.435330000
H	-1.806307000	-0.885667000	-1.535200000
O	6.199611000	-1.905234000	-0.134809000
O	-1.778415000	5.140777000	0.202319000
H	2.865101000	3.493318000	0.551896000
H	4.437438000	2.073449000	0.935405000
H	1.828018000	-0.837876000	-0.849277000
H	6.301018000	0.478279000	0.803001000
H	3.701470000	-2.438504000	-0.979347000
H	-4.709139000	1.817925000	-1.069328000
H	-3.052100000	-0.816483000	1.251852000
H	-2.781719000	-3.321179000	-0.427492000
H	-1.146021000	-2.680610000	2.052436000
H	0.755700000	-2.518249000	0.593324000
H	-1.083292000	-3.165874000	-1.764841000
H	0.513699000	-2.427945000	-1.888476000
H	0.055876000	-4.873930000	-0.556710000
H	-1.784488000	-4.938303000	1.506995000
H	-4.461942000	-3.223042000	1.109855000
H	-4.418445000	-0.457706000	-0.634513000
H	5.956567000	-2.759643000	-0.512753000
H	-0.841597000	5.419219000	0.406708000
H	-3.805538000	3.683739000	-0.493857000

E = – 1565.0282287 a. u.
H = – 1564.608119 a. u.
G = – 1564.690790 a. u.
f = 47.34i

Transition state – B ring rotation (φ_2 = 89.2°)

C	-1.797012000	0.361954000	-0.054259000
C	-2.952485000	1.154979000	-0.139537000
C	-1.819856000	-1.032562000	0.042805000
C	-4.212517000	0.498245000	-0.126293000
C	-3.091180000	-1.631111000	0.047707000
C	-4.272182000	-0.882373000	-0.030733000
C	-0.432596000	2.300607000	-0.148817000
C	-1.497855000	3.126204000	-0.239081000
O	-0.565727000	0.952180000	-0.061714000
C	-2.844341000	2.599582000	-0.240134000
C	0.990723000	2.705494000	-0.126595000
C	1.634450000	2.950918000	1.091518000
C	1.716482000	2.801704000	-1.316528000
C	2.980213000	3.294641000	1.121528000
C	3.064924000	3.145180000	-1.295196000
C	3.697757000	3.392151000	-0.073784000
O	-3.857566000	3.334337000	-0.320191000
C	-0.557533000	-1.855911000	0.101432000
O	-3.137729000	-2.984711000	0.133259000
C	0.303251000	-1.569376000	1.352202000
C	1.596618000	-2.366259000	1.274967000
C	2.316314000	-2.070272000	-0.034415000
C	1.408511000	-2.334417000	-1.248379000
O	0.190765000	-1.596317000	-1.103696000
C	1.154622000	-3.823455000	-1.545470000
O	2.306881000	-4.450098000	-2.110057000
O	3.493676000	-2.875378000	-0.165757000
O	2.500468000	-2.020887000	2.327238000
O	-0.370649000	-1.991480000	2.539771000
H	-0.843093000	-2.909603000	0.144196000
O	5.016535000	3.733877000	0.016265000
O	-5.351109000	1.207561000	-0.205675000
H	-1.347863000	4.194501000	-0.308214000
H	1.080221000	2.873091000	2.019617000
H	1.228870000	2.607421000	-2.264653000
H	3.484883000	3.489412000	2.059932000
H	3.622909000	3.220282000	-2.222257000
H	-4.051908000	-3.293916000	0.120579000
H	0.551519000	-0.507358000	1.407249000
H	1.359571000	-3.436148000	1.334601000
H	2.592141000	-1.008547000	-0.036897000
H	1.889073000	-1.911726000	-2.133589000
H	0.823822000	-4.366940000	-0.653087000
H	0.357895000	-3.884579000	-2.289080000

H	3.037206000	-4.283026000	-1.496004000
H	3.975583000	-2.835058000	0.670121000
H	2.075175000	-2.234802000	3.166353000
H	-1.049445000	-1.343920000	2.761438000
H	5.414936000	3.773878000	-0.861731000
H	-5.086065000	2.162735000	-0.268209000
H	-5.237626000	-1.373915000	-0.023566000

E = – 1565.0411556 a. u.
H = – 1564.620862 a. u.
G = – 1564.705471 a. u.
f = 55.29i

4 Puerarin

a Global Minimum Point H–C_7 eclipsed

C	-0.008094000	1.182700000	-0.074885000
C	1.041306000	2.105421000	-0.172654000
C	-1.362042000	1.560080000	-0.076595000
C	0.712571000	3.468002000	-0.277759000
C	-1.635836000	2.927905000	-0.182230000
C	-0.600498000	3.878452000	-0.280693000
C	1.534468000	-0.581788000	0.050642000
C	2.629655000	0.205691000	-0.062116000
O	0.256233000	-0.151469000	0.036767000
C	2.442773000	1.659969000	-0.174195000
C	3.978839000	-0.404198000	-0.080844000
C	5.022425000	0.118768000	0.699246000
C	4.243481000	-1.534886000	-0.864060000
C	6.277364000	-0.476032000	0.709494000
C	5.497955000	-2.140670000	-0.860772000
C	6.518765000	-1.610278000	-0.070440000
O	3.382565000	2.454776000	-0.271057000
C	-2.482640000	0.552633000	0.018318000
O	-2.938768000	3.312552000	-0.186688000
C	-2.491550000	-0.227488000	1.350215000
C	-3.612248000	-1.257609000	1.321239000
C	-3.477687000	-2.149170000	0.092872000
C	-3.407873000	-1.324717000	-1.205163000
O	-2.364602000	-0.349815000	-1.096830000
C	-4.746814000	-0.700603000	-1.640027000
O	-5.633745000	-1.683315000	-2.174722000
O	-4.583505000	-3.053448000	-0.008175000

O	-3.574512000	-2.119917000	2.459851000
O	-2.762373000	0.642400000	2.450884000
H	-3.427371000	1.097423000	-0.040384000
O	7.775653000	-2.150069000	-0.021578000
H	4.846970000	0.997498000	1.305620000
H	3.465331000	-1.942974000	-1.499294000
H	7.078473000	-0.073333000	1.317919000
H	-1.540402000	-0.745554000	1.491740000
H	-4.575341000	-0.731801000	1.293704000
H	-2.543967000	-2.716583000	0.189194000
H	-3.089941000	-1.985961000	-2.014177000
H	-5.230231000	-0.157198000	-0.820431000
H	-4.538423000	0.013412000	-2.438942000
H	-5.723551000	-2.368420000	-1.496016000
H	-4.719921000	-3.457112000	0.858321000
H	-3.694411000	-1.576390000	3.247902000
H	-1.959291000	1.124914000	2.677155000
H	7.830663000	-2.922470000	-0.597003000
H	-0.849945000	4.930369000	-0.362772000
H	1.575916000	-1.656423000	0.166726000
H	5.683103000	-3.013301000	-1.478305000
H	1.519190000	4.185872000	-0.355072000
H	-3.008359000	4.271392000	-0.271064000

E = – 1489.7767295 a. u.
H = – 1489.360348 a. u.
G = – 1489.444911 a. u.

b H–C_9 eclipsed

C	-0.163389000	0.945726000	-0.128360000
C	-1.165023000	1.918478000	-0.248443000
C	1.208650000	1.247617000	-0.146385000
C	-0.765450000	3.256606000	-0.397291000
C	1.554268000	2.596075000	-0.303755000
C	0.568302000	3.594083000	-0.426903000
C	-1.798006000	-0.733810000	0.039770000
C	-2.850176000	0.112849000	-0.044401000
O	-0.498001000	-0.371569000	0.013333000
C	-2.587901000	1.550188000	-0.211391000
C	-4.231681000	-0.412394000	0.044008000
C	-5.215871000	-0.018064000	-0.876143000
C	-4.587918000	-1.330974000	1.039200000
C	-6.503051000	-0.535512000	-0.814601000

C	-5.876000000	-1.857119000	1.110573000
C	-6.836960000	-1.458925000	0.180035000
O	-3.485693000	2.392402000	-0.304088000
C	2.239483000	0.152004000	-0.012535000
C	3.158741000	0.325922000	1.214248000
C	4.195771000	-0.788477000	1.225807000
C	4.946056000	-0.824714000	-0.100196000
C	3.983067000	-0.933706000	-1.296178000
O	3.013079000	0.117999000	-1.225656000
C	3.331031000	-2.318295000	-1.468658000
O	4.259178000	-3.274073000	-1.981773000
O	5.849049000	-1.935161000	-0.148127000
O	5.176704000	-0.595318000	2.246908000
O	2.413482000	0.207460000	2.428503000
H	1.712575000	-0.795534000	0.117541000
O	-8.121954000	-1.930376000	0.192728000
H	-4.967354000	0.697431000	-1.648883000
H	-3.855890000	-1.630727000	1.780677000
H	-7.258448000	-0.234556000	-1.530773000
H	3.673200000	1.287693000	1.167285000
H	3.685769000	-1.746828000	1.387308000
H	5.507323000	0.112631000	-0.196057000
H	4.547084000	-0.733901000	-2.209816000
H	2.888320000	-2.681095000	-0.534153000
H	2.529850000	-2.220870000	-2.203616000
H	5.017225000	-3.269721000	-1.378956000
H	6.346666000	-1.952032000	0.679174000
H	4.724560000	-0.606905000	3.099041000
H	1.944981000	1.033947000	2.591186000
H	-8.240262000	-2.559809000	0.914192000
H	0.873694000	4.627589000	-0.547317000
H	-1.895725000	-1.806707000	0.136519000
H	-6.133423000	-2.563170000	1.893161000
O	2.872267000	2.917220000	-0.333667000
H	2.983770000	3.873631000	-0.402814000
H	-1.532458000	4.014909000	-0.489390000

E = – 1489.7761858 a. u.
H = – 1489.359776 a. u.
G = – 1489.444391 a. u.

c Gauche-like

C	-0.004962000	1.135967000	-0.031697000

C	-1.011703000	2.090517000	-0.210186000
C	1.370559000	1.442642000	-0.025476000
C	-0.620492000	3.428241000	-0.387042000
C	1.701539000	2.789111000	-0.195814000
C	0.710134000	3.774032000	-0.376442000
C	-1.621189000	-0.554455000	0.169720000
C	-2.681163000	0.274575000	0.025008000
O	-0.325778000	-0.177670000	0.153364000
C	-2.431548000	1.706531000	-0.196433000
C	-4.057788000	-0.264249000	0.107556000
C	-5.029440000	0.080805000	-0.844919000
C	-4.421211000	-1.147193000	1.132125000
C	-6.311198000	-0.450465000	-0.785977000
C	-5.703745000	-1.686666000	1.201188000
C	-6.652070000	-1.338183000	0.238297000
O	-3.334781000	2.534098000	-0.347131000
C	2.332540000	0.283354000	0.130453000
C	3.790204000	0.574538000	0.518251000
C	4.510794000	-0.761331000	0.671729000
C	4.409322000	-1.570278000	-0.617259000
C	2.951834000	-1.716941000	-1.090564000
O	2.333914000	-0.424117000	-1.129807000
C	2.121077000	-2.742836000	-0.297089000
O	2.471243000	-4.080889000	-0.652857000
O	4.962549000	-2.880387000	-0.449241000
O	5.903574000	-0.584214000	0.932582000
O	3.894275000	1.252726000	1.767538000
H	1.915959000	-0.361705000	0.911384000
O	-7.931205000	-1.825293000	0.247028000
H	-4.775613000	0.768859000	-1.640485000
H	-3.699507000	-1.407827000	1.898123000
H	-7.056985000	-0.187311000	-1.526682000
H	4.277450000	1.146231000	-0.273856000
H	4.052919000	-1.321077000	1.498045000
H	4.968158000	-1.030372000	-1.391252000
H	2.958436000	-2.054941000	-2.128912000
H	2.218702000	-2.600425000	0.784798000
H	1.072465000	-2.600817000	-0.561991000
H	3.422009000	-4.165888000	-0.490551000
H	5.832283000	-2.790042000	-0.040345000
H	5.986387000	-0.059172000	1.738185000
H	3.793575000	2.195964000	1.586558000
H	-8.055531000	-2.425338000	0.992164000
H	1.012213000	4.807149000	-0.507350000

H	-1.708778000	-1.623295000	0.311009000
H	-5.967110000	-2.364242000	2.006587000
O	3.016517000	3.149273000	-0.166962000
H	3.110898000	4.102431000	-0.288038000
H	-1.389353000	4.177298000	-0.526058000

E = – 1489.7760101 a. u.
H = – 1489.359362 a. u.
G = – 1489.442978 a. u.

Transition state - 8-C bond rotation (φ_1 = 17.6°)

C	0.159407000	0.978852000	-0.032791000
C	1.159054000	1.908418000	-0.357165000
C	-1.227594000	1.260074000	-0.005695000
C	0.768076000	3.219979000	-0.654378000
C	-1.540551000	2.630843000	-0.188181000
C	-0.550870000	3.570027000	-0.554703000
C	1.866284000	-0.626583000	0.386119000
C	2.894631000	0.179555000	0.054163000
O	0.552585000	-0.288405000	0.323427000
C	2.586013000	1.550560000	-0.374250000
C	4.285420000	-0.322278000	0.116741000
C	5.302427000	0.440597000	0.711975000
C	4.618219000	-1.580961000	-0.399275000
C	6.601024000	-0.042635000	0.801444000
C	5.917231000	-2.076347000	-0.313692000
C	6.912583000	-1.304714000	0.288164000
O	3.454761000	2.355076000	-0.720413000
C	-2.308591000	0.182209000	0.285353000
O	-2.791262000	3.116601000	0.012092000
C	-2.208588000	-1.178664000	-0.489179000
C	-3.533839000	-1.959637000	-0.446423000
C	-4.764221000	-1.133271000	-0.751918000
C	-4.763058000	0.112301000	0.135871000
O	-3.537817000	0.796430000	-0.099822000
C	-5.041917000	-0.141043000	1.626982000
O	-6.410892000	-0.481683000	1.846211000
O	-5.959237000	-1.886764000	-0.511689000
O	-3.508798000	-3.036075000	-1.386965000
O	-1.306238000	-2.133305000	0.062470000
H	-2.295089000	-0.042574000	1.360761000
O	8.209727000	-1.724859000	0.399932000
H	5.071629000	1.419573000	1.110880000

H	3.859135000	-2.179940000	-0.889708000
H	7.382730000	0.546335000	1.266248000
H	-1.960973000	-0.961945000	-1.535914000
H	-3.633342000	-2.371455000	0.565079000
H	-4.730237000	-0.810717000	-1.799053000
H	-5.533598000	0.801995000	-0.216488000
H	-4.384630000	-0.913209000	2.042645000
H	-4.849352000	0.787172000	2.168504000
H	-6.607960000	-1.224739000	1.256460000
H	-5.861275000	-2.747280000	-0.938602000
H	-2.780692000	-3.620623000	-1.143288000
H	-0.429557000	-1.737799000	0.078033000
H	8.312768000	-2.599791000	0.006632000
H	-0.858876000	4.594727000	-0.734710000
H	1.982564000	-1.642240000	0.739517000
H	6.156659000	-3.052137000	-0.723085000
H	1.525985000	3.942546000	-0.926338000
H	-2.775358000	4.072278000	-0.124492000

E = – 1489.7509572 a. u.
H = – 1489.336085 a. u.
G = – 1489.418230 a. u.
f = 51.69i

Transition state - 8-C bond rotation (φ_1 = –167.0°)

C	0.045475000	1.100353000	-0.251417000
C	1.062649000	2.061804000	-0.100244000
C	-1.337935000	1.436512000	-0.350128000
C	0.722789000	3.419986000	-0.120837000
C	-1.580190000	2.814218000	-0.461828000
C	-0.579869000	3.791104000	-0.327060000
C	1.697045000	-0.583391000	-0.231042000
C	2.751389000	0.244406000	-0.043884000
O	0.413227000	-0.209411000	-0.343906000
C	2.480096000	1.679265000	0.047024000
C	4.124929000	-0.300069000	0.041948000
C	5.015320000	0.135457000	1.036284000
C	4.565875000	-1.284251000	-0.852003000
C	6.290727000	-0.403765000	1.144139000
C	5.842087000	-1.833707000	-0.752319000
C	6.707980000	-1.392992000	0.249800000
O	3.364608000	2.525618000	0.215083000
C	-2.480638000	0.384360000	-0.405714000

O	-2.847940000	3.248404000	-0.740455000
C	-3.741585000	0.646390000	0.493015000
C	-4.600094000	-0.621843000	0.632232000
C	-3.823299000	-1.870781000	0.986543000
C	-2.664111000	-2.035410000	0.001033000
O	-1.895052000	-0.837690000	0.044598000
C	-3.067869000	-2.447364000	-1.424273000
O	-3.481847000	-3.812978000	-1.468453000
O	-4.661744000	-3.031496000	0.929406000
O	-5.589975000	-0.444709000	1.648590000
O	-4.689420000	1.575938000	-0.017964000
H	-2.819296000	0.303044000	-1.447969000
O	7.976302000	-1.884810000	0.403161000
H	4.702214000	0.901040000	1.733720000
H	3.911633000	-1.620100000	-1.648713000
H	6.972180000	-0.069024000	1.917286000
H	-3.389978000	0.946867000	1.488655000
H	-5.100709000	-0.780529000	-0.330606000
H	-3.406967000	-1.760310000	1.994624000
H	-1.986537000	-2.807693000	0.372545000
H	-3.849900000	-1.798064000	-1.833477000
H	-2.188094000	-2.355345000	-2.064219000
H	-4.179052000	-3.910515000	-0.802820000
H	-5.476200000	-2.835735000	1.409668000
H	-6.135668000	0.309945000	1.395147000
H	-4.229345000	2.406717000	-0.205159000
H	8.157072000	-2.557170000	-0.264662000
H	-0.855481000	4.838043000	-0.392671000
H	1.786550000	-1.659366000	-0.304881000
H	6.165273000	-2.592147000	-1.457648000
H	1.507391000	4.155127000	-0.001091000
H	-2.874989000	4.212601000	-0.785823000

E = – 1489.7552978 a. u.
H = – 1489.340410 a. u.
G = – 1489.422057 a. u.
f = 51.95i

Transition state – B ring rotation (φ_2 = 179.8°)

C	-0.022405000	1.201257000	-0.033955000
C	1.023336000	2.126027000	-0.082730000
C	-1.378888000	1.567474000	-0.013357000
C	0.689037000	3.491777000	-0.111480000

C	-1.658684000	2.937245000	-0.044371000
C	-0.626101000	3.895142000	-0.091773000
C	1.537111000	-0.551158000	-0.016347000
C	2.649788000	0.229946000	-0.067411000
O	0.259038000	-0.130664000	0.000638000
C	2.430492000	1.692715000	-0.101310000
C	4.002248000	-0.402185000	-0.084021000
C	5.187954000	0.355530000	-0.139934000
C	4.155298000	-1.802796000	-0.046221000
C	6.443404000	-0.245115000	-0.156373000
C	5.403190000	-2.411440000	-0.062569000
C	6.561213000	-1.631490000	-0.117799000
O	3.336457000	2.532056000	-0.141728000
C	-2.492812000	0.550036000	0.034599000
O	-2.962956000	3.317175000	-0.026760000
C	-2.491990000	-0.295904000	1.325407000
C	-3.613883000	-1.322304000	1.250829000
C	-3.484345000	-2.154145000	-0.019541000
C	-3.416708000	-1.267842000	-1.276366000
O	-2.374602000	-0.298036000	-1.122586000
C	-4.757514000	-0.626549000	-1.679375000
O	-5.640856000	-1.583910000	-2.263733000
O	-4.591374000	-3.051203000	-0.161138000
O	-3.574350000	-2.238292000	2.346484000
O	-2.755104000	0.515820000	2.471285000
H	-3.440654000	1.091977000	0.005816000
O	7.818804000	-2.169349000	-0.136056000
H	5.124787000	1.430766000	-0.170579000
H	3.297914000	-2.460764000	-0.003007000
H	7.340013000	0.362150000	-0.199734000
H	-1.539687000	-0.820553000	1.432487000
H	-4.576025000	-0.793790000	1.251434000
H	-2.551051000	-2.726532000	0.047039000
H	-3.098964000	-1.888692000	-2.116860000
H	-5.243157000	-0.127560000	-0.833370000
H	-4.551459000	0.127922000	-2.440825000
H	-5.730931000	-2.301344000	-1.619383000
H	-4.724780000	-3.497702000	0.684534000
H	-3.689819000	-1.732595000	3.159991000
H	-1.949178000	0.981376000	2.721432000
H	7.770784000	-3.132402000	-0.105889000
H	-0.879963000	4.949059000	-0.115203000
H	1.552265000	-1.629625000	0.015829000
H	5.475342000	-3.493882000	-0.033332000

H	1.491407000	4.217096000	-0.148825000
H	-3.035725000	4.279002000	-0.058217000

E = – 1489.7712468 a. u.
H = – 1489.355875 a. u.
G = – 1489.438494 a. u.
f = 71.74i

5 Prunetin-8-C-glucoside

a Global Minimum Point H–C_7 eclipsed

C	0.019313000	0.863914000	-0.022898000
C	1.058002000	1.810233000	-0.093929000
C	-1.334534000	1.199825000	-0.015313000
C	0.693792000	3.181701000	-0.163368000
C	-1.642753000	2.576583000	-0.089340000
C	-0.641944000	3.554615000	-0.157948000
C	1.616916000	-0.862786000	0.048108000
C	2.691561000	-0.043241000	-0.040320000
O	0.330714000	-0.464355000	0.048583000
C	2.449207000	1.397057000	-0.106570000
C	4.059815000	-0.606610000	-0.079507000
C	5.088849000	-0.071758000	0.711677000
C	4.355803000	-1.707290000	-0.893554000
C	6.361370000	-0.627581000	0.702806000
C	5.628159000	-2.273505000	-0.909312000
C	6.634786000	-1.732917000	-0.107544000
O	3.377710000	2.234176000	-0.179419000
C	-2.427712000	0.163449000	0.051102000
O	-2.957324000	2.885648000	-0.088102000
C	-2.415793000	-0.660019000	1.355865000
C	-3.523602000	-1.702406000	1.303164000
C	-3.384795000	-2.555219000	0.048041000
C	-3.329258000	-1.691328000	-1.224959000
O	-2.298438000	-0.707302000	-1.091397000
C	-4.678025000	-1.072399000	-1.636577000
O	-5.553937000	-2.050073000	-2.198633000
O	-4.480687000	-3.469094000	-0.075683000
O	-3.470822000	-2.598593000	2.415379000
O	-2.689028000	0.168687000	2.487766000
H	-3.383928000	0.688510000	0.012201000
O	7.907159000	-2.235061000	-0.076201000
O	1.635865000	4.137115000	-0.234109000

H	4.888449000	0.784128000	1.342554000
H	3.588228000	-2.122488000	-1.536964000
H	7.151598000	-0.216655000	1.319795000
H	-1.456746000	-1.170182000	1.473274000
H	-4.493009000	-1.187496000	1.295856000
H	-2.444404000	-3.114719000	0.123804000
H	-3.007040000	-2.324833000	-2.054415000
H	-5.166033000	-0.561102000	-0.799323000
H	-4.481960000	-0.331386000	-2.413769000
H	-5.632120000	-2.756590000	-1.540758000
H	-4.608548000	-3.900102000	0.778836000
H	-3.591877000	-2.080204000	3.219950000
H	-1.905265000	0.692417000	2.689744000
H	7.982626000	-2.992608000	-0.668876000
H	2.512411000	3.668169000	-0.231488000
H	-0.877358000	4.606968000	-0.211552000
C	-3.367918000	4.258577000	-0.163126000
H	-2.999944000	4.823331000	0.697036000
H	-3.022967000	4.719654000	-1.091958000
H	-4.455027000	4.234694000	-0.147697000
H	1.687365000	-1.938994000	0.129706000
H	5.838410000	-3.123052000	-1.550410000

E = – 1604.3490242 a. u.
H = – 1603.897736 a. u.
G = – 1603.987184 a. u.

b H–C_9 eclipsed

C	-0.192630000	0.663376000	-0.058273000
C	-1.192482000	1.650448000	-0.142418000
C	1.174316000	0.939959000	-0.063414000
C	-0.771343000	3.002748000	-0.241538000
C	1.539798000	2.301584000	-0.174706000
C	0.579522000	3.317703000	-0.259474000
C	-1.864197000	-0.994339000	0.043090000
C	-2.903145000	-0.127930000	-0.010645000
O	-0.561262000	-0.650823000	0.032434000
C	-2.600018000	1.298312000	-0.121340000
C	-4.296141000	-0.624544000	0.052431000
C	-5.269952000	-0.166733000	-0.849155000
C	-4.672108000	-1.582589000	1.002156000
C	-6.567109000	-0.660748000	-0.813921000
C	-5.970148000	-2.085915000	1.045917000
C	-6.921076000	-1.624655000	0.134188000

O	-3.492912000	2.173703000	-0.186289000
C	2.186329000	-0.174764000	0.024829000
O	2.863545000	2.555587000	-0.192551000
C	3.126946000	-0.065796000	1.242803000
C	4.131516000	-1.208714000	1.206518000
C	4.864719000	-1.224869000	-0.129245000
C	3.883572000	-1.270888000	-1.314771000
O	2.946013000	-0.195543000	-1.200199000
C	3.191777000	-2.631778000	-1.518972000
O	4.086663000	-3.596805000	-2.072866000
O	5.737008000	-2.357189000	-0.222268000
O	5.130104000	-1.077329000	2.221057000
O	2.395591000	-0.203071000	2.464240000
H	1.640558000	-1.114509000	0.133912000
O	-8.214189000	-2.071601000	0.122191000
O	-1.671711000	3.996691000	-0.321247000
H	-5.006071000	0.579069000	-1.587354000
H	-3.948080000	-1.932066000	1.729531000
H	-7.314719000	-0.310797000	-1.515779000
H	3.666645000	0.882479000	1.219278000
H	3.595645000	-2.156725000	1.344381000
H	5.450023000	-0.300350000	-0.204219000
H	4.442152000	-1.060882000	-2.229674000
H	2.751405000	-3.010564000	-0.589697000
H	2.384015000	-2.490950000	-2.239599000
H	4.852712000	-3.629885000	-1.481150000
H	6.240749000	-2.414614000	0.599470000
H	4.686489000	-1.095500000	3.077535000
H	1.926744000	0.620297000	2.641626000
H	-8.344846000	-2.736076000	0.809335000
H	-2.567642000	3.567036000	-0.291996000
H	0.858859000	4.357395000	-0.342435000
C	3.332294000	3.909514000	-0.265721000
H	3.013540000	4.383190000	-1.197476000
H	2.984292000	4.491603000	0.591319000
H	4.417332000	3.838649000	-0.244350000
H	-1.979774000	-2.068275000	0.098389000
H	-6.243451000	-2.823775000	1.792907000

E = – 1604.348578 a. u.
H = – 1603.897312 a. u.
G = – 1603.987075 a. u.

c Gauche-like

C	-0.034977000	0.830161000	0.043765000
C	-1.031307000	1.808040000	-0.110326000
C	1.338041000	1.097374000	0.053381000
C	-0.606558000	3.154312000	-0.259648000
C	1.701601000	2.451966000	-0.093007000
C	0.744409000	3.463811000	-0.247200000
C	-1.702806000	-0.824722000	0.191152000
C	-2.742236000	0.034857000	0.069301000
O	-0.401301000	-0.478216000	0.189068000
C	-2.439443000	1.454231000	-0.105972000
C	-4.135356000	-0.461499000	0.128936000
C	-5.092794000	-0.049418000	-0.811344000
C	-4.527721000	-1.372969000	1.117186000
C	-6.390255000	-0.542700000	-0.775088000
C	-5.826022000	-1.875144000	1.162306000
C	-6.760746000	-1.459595000	0.212565000
O	-3.329959000	2.324362000	-0.234812000
C	2.269102000	-0.089514000	0.162700000
O	3.027425000	2.730780000	-0.054774000
C	3.727743000	0.138988000	0.585257000
C	4.403498000	-1.223990000	0.698462000
C	4.304789000	-1.975035000	-0.625861000
C	2.853929000	-2.052565000	-1.136891000
O	2.277172000	-0.740885000	-1.130690000
C	1.973328000	-3.085176000	-0.408469000
O	2.291544000	-4.417637000	-0.812534000
O	4.812257000	-3.308606000	-0.501977000
O	5.795526000	-1.102393000	0.994999000
O	3.832794000	0.765078000	1.861782000
H	1.826376000	-0.763817000	0.903109000
O	-8.053484000	-1.907424000	0.200033000
O	-1.502321000	4.144345000	-0.409387000
H	-4.816015000	0.660165000	-1.579856000
H	-3.816648000	-1.685592000	1.873546000
H	-7.125430000	-0.228112000	-1.506206000
H	4.246168000	0.724728000	-0.175656000
H	3.911080000	-1.803334000	1.490931000
H	4.898432000	-1.422081000	-1.363953000
H	2.874643000	-2.345134000	-2.188902000
H	2.047640000	-2.991263000	0.680541000
H	0.936416000	-2.899236000	-0.691987000
H	3.235808000	-4.537412000	-0.634759000
H	5.673656000	-3.264028000	-0.068706000

H	5.876237000	-0.604150000	1.817662000
H	3.732161000	1.714506000	1.717494000
H	-8.197599000	-2.534013000	0.919368000
H	-2.399364000	3.718001000	-0.383224000
H	1.029765000	4.499412000	-0.354802000
C	3.492028000	4.073436000	-0.272993000
H	3.186105000	4.432654000	-1.257960000
H	3.127000000	4.745218000	0.507294000
H	4.576643000	4.010440000	-0.224950000
H	-1.817623000	-1.894739000	0.299104000
H	-6.112160000	-2.576544000	1.938990000

E = – 1604.3481024 a. u.
H = – 1603.896739 a. u.
G = – 1603.985706 a. u.

Transition state - 8-C bond rotation (φ_1 = 16.8°)

C	0.182352000	0.690087000	0.036085000
C	1.184758000	1.635532000	-0.272106000
C	-1.195921000	0.944951000	0.068800000
C	0.768798000	2.959350000	-0.552282000
C	-1.523444000	2.336756000	-0.046108000
C	-0.562751000	3.292577000	-0.412068000
C	1.917425000	-0.902195000	0.426831000
C	2.935538000	-0.075757000	0.112449000
O	0.602469000	-0.577946000	0.365530000
C	2.594218000	1.289160000	-0.285211000
C	4.335750000	-0.550839000	0.163459000
C	5.340770000	0.220857000	0.767635000
C	4.688176000	-1.795948000	-0.372209000
C	6.647486000	-0.241459000	0.846460000
C	5.995379000	-2.270213000	-0.296737000
C	6.979110000	-1.490509000	0.314032000
O	3.467950000	2.122204000	-0.614956000
C	-2.258228000	-0.168403000	0.296237000
O	-2.771966000	2.740970000	0.248791000
C	-2.142300000	-1.466508000	-0.581057000
C	-3.440960000	-2.290465000	-0.545713000
C	-4.701917000	-1.486078000	-0.775450000
C	-4.712181000	-0.291406000	0.178556000
O	-3.508356000	0.434244000	-0.042825000
C	-4.959470000	-0.632887000	1.657608000
O	-6.319203000	-1.007975000	1.880204000

O	-5.869433000	-2.286430000	-0.550588000
O	-3.411649000	-3.313456000	-1.544446000
O	-1.190844000	-2.434884000	-0.147046000
H	-2.236116000	-0.469965000	1.352376000
O	8.283081000	-1.889856000	0.416858000
O	1.649273000	3.911328000	-0.904410000
H	5.094678000	1.189496000	1.182187000
H	3.938381000	-2.400456000	-0.869957000
H	7.420250000	0.353922000	1.317903000
H	-1.944650000	-1.158950000	-1.615702000
H	-3.499287000	-2.759303000	0.444176000
H	-4.701945000	-1.106684000	-1.803892000
H	-5.505130000	0.397784000	-0.121426000
H	-4.284061000	-1.416981000	2.017459000
H	-4.771696000	0.266244000	2.247690000
H	-6.511933000	-1.725659000	1.258518000
H	-5.756522000	-3.120069000	-1.024462000
H	-2.650843000	-3.878252000	-1.361425000
H	-0.327240000	-2.014174000	-0.110919000
H	8.400351000	-2.757976000	0.012489000
H	2.544220000	3.479713000	-0.898750000
H	-0.837009000	4.326053000	-0.555155000
C	-3.133603000	4.123159000	0.145740000
H	-2.539887000	4.742518000	0.823641000
H	-3.030840000	4.485329000	-0.880608000
H	-4.180252000	4.162186000	0.440061000
H	2.045025000	-1.923202000	0.760053000
H	6.250033000	-3.235735000	-0.720851000

E = – 1604.3203782 a. u.
H = – 1603.870837 a. u.
G = – 1603.958771 a. u.
f = 54.74i

Transition state - 8-C bond rotation (φ_1 = –165.5°)

C	0.053057000	0.814708000	-0.205089000
C	1.062383000	1.785850000	-0.003450000
C	-1.328964000	1.111082000	-0.270146000
C	0.681015000	3.148191000	0.056367000
C	-1.607960000	2.498922000	-0.335466000
C	-0.641909000	3.489917000	-0.147644000
C	1.749246000	-0.830632000	-0.294985000
C	2.784154000	0.007874000	-0.051302000

O	0.462029000	-0.474474000	-0.389681000
C	2.466702000	1.418501000	0.110294000
C	4.172157000	-0.500562000	0.013418000
C	5.043976000	-0.097072000	1.037141000
C	4.643728000	-1.421297000	-0.930816000
C	6.332918000	-0.606554000	1.123541000
C	5.933790000	-1.940405000	-0.852750000
C	6.781941000	-1.532614000	0.178248000
O	3.349885000	2.284740000	0.317213000
C	-2.432404000	0.019723000	-0.342934000
O	-2.888323000	2.866101000	-0.624944000
C	-3.696846000	0.208406000	0.566519000
C	-4.515060000	-1.089891000	0.648795000
C	-3.698941000	-2.320352000	0.981225000
C	-2.517451000	-2.413844000	0.013899000
O	-1.800992000	-1.186012000	0.098437000
C	-2.880286000	-2.811272000	-1.426654000
O	-3.229518000	-4.193455000	-1.507379000
O	-4.493030000	-3.508815000	0.877407000
O	-5.528627000	-0.980286000	1.651759000
O	-4.667815000	1.137886000	0.102912000
H	-2.770717000	-0.068971000	-1.384466000
O	8.061934000	-1.997476000	0.312801000
O	1.580966000	4.120994000	0.270608000
H	4.706470000	0.619271000	1.774503000
H	4.002759000	-1.730397000	-1.748830000
H	7.000615000	-0.297260000	1.918884000
H	-3.347069000	0.473224000	1.573243000
H	-4.992738000	-1.235470000	-0.327846000
H	-3.305208000	-2.222845000	1.999668000
H	-1.814256000	-3.165666000	0.379798000
H	-3.685735000	-2.190111000	-1.833971000
H	-1.996342000	-2.664293000	-2.050274000
H	-3.936362000	-4.336729000	-0.860439000
H	-5.321662000	-3.356488000	1.349002000
H	-6.090661000	-0.231620000	1.417041000
H	-4.200411000	1.959992000	-0.107922000
H	8.264480000	-2.627923000	-0.388851000
H	2.464310000	3.666240000	0.350621000
H	-0.900508000	4.537177000	-0.159488000
C	-3.221160000	4.249359000	-0.861470000
H	-3.087827000	4.842432000	0.044975000
H	-2.619509000	4.651035000	-1.678256000
H	-4.271014000	4.243007000	-1.145615000

H	1.863466000	-1.897064000	-0.438448000
H	6.281338000	-2.649367000	-1.596823000

E = – 1604.326888 a. u.
H = – 1603.877110 a. u.
G = – 1603.963428 a. u.
f = 49.05i

Transition state – B ring rotation (φ_2 = 179.8°)

C	0.005351000	0.885069000	-0.014540000
C	1.040528000	1.832341000	-0.057219000
C	-1.351394000	1.206525000	0.016727000
C	0.665031000	3.204967000	-0.068388000
C	-1.669687000	2.581888000	-0.002498000
C	-0.674010000	3.566437000	-0.040799000
C	1.616958000	-0.828460000	-0.023564000
C	2.709397000	-0.017785000	-0.065542000
O	0.332289000	-0.437990000	-0.000878000
C	2.436486000	1.427580000	-0.084637000
C	4.080138000	-0.606533000	-0.087823000
C	4.272167000	-2.004635000	-0.066058000
C	5.242105000	0.184348000	-0.131503000
C	5.534397000	-2.577085000	-0.086126000
C	6.515405000	-0.382139000	-0.152226000
C	6.670543000	-1.765464000	-0.129527000
O	3.335453000	2.300874000	-0.121347000
C	-2.434586000	0.158849000	0.053575000
O	-2.986021000	2.882533000	0.020399000
C	-2.399450000	-0.720669000	1.320662000
C	-3.503679000	-1.764839000	1.237502000
C	-3.378133000	-2.563434000	-0.054416000
C	-3.342233000	-1.645195000	-1.289529000
O	-2.314258000	-0.662752000	-1.126023000
C	-4.699444000	-1.017190000	-1.657407000
O	-5.575019000	-1.974581000	-2.253904000
O	-4.472140000	-3.475670000	-0.202824000
O	-3.433512000	-2.707034000	2.309951000
O	-2.660020000	0.055023000	2.492356000
H	-3.395019000	0.677794000	0.049220000
O	7.889973000	-2.383407000	-0.147698000
O	1.594113000	4.173650000	-0.105310000
H	3.432413000	-2.685547000	-0.032576000
H	5.153595000	1.257836000	-0.149716000

H	5.650921000	-3.654124000	-0.068758000
H	-1.436682000	-1.231171000	1.401411000
H	-4.474907000	-1.253866000	1.264106000
H	-2.434753000	-3.121629000	-0.014524000
H	-3.027459000	-2.240332000	-2.149699000
H	-5.181518000	-0.548616000	-0.792219000
H	-4.517314000	-0.239927000	-2.401892000
H	-5.643113000	-2.709604000	-1.626914000
H	-4.587223000	-3.943180000	0.634130000
H	-3.543061000	-2.223124000	3.137354000
H	-1.874624000	0.570060000	2.709542000
H	8.595575000	-1.725851000	-0.175000000
H	2.474526000	3.710229000	-0.121226000
H	-0.915090000	4.618867000	-0.051662000
C	-3.405120000	4.254747000	-0.002611000
H	-3.035664000	4.790353000	0.875378000
H	-3.068009000	4.751169000	-0.915940000
H	-4.491972000	4.223730000	0.017924000
H	1.659823000	-1.906300000	-0.004560000
H	7.388070000	0.262124000	-0.186462000

E = – 1604.3436251 a. u.
H = – 1603.893428 a. u.
G = – 1603.981241 a. u.
f = 71.89i

Hybrid cluster-continuum model (IEFPCM + Explicit Solvation)

1 Isoschaftoside, n = 8 (H_2O)

a H–C_7 eclipsed

H	8.139792000	1.596883000	0.741584000
O	7.913566000	2.465005000	0.381598000
C	6.563991000	2.543447000	0.220482000
C	6.045592000	3.738840000	-0.295780000
C	5.701817000	1.489709000	0.544298000
H	6.729391000	4.539058000	-0.556937000
C	4.677172000	3.876721000	-0.474415000
H	6.077952000	0.555748000	0.955618000
C	4.333447000	1.636480000	0.351951000
H	4.291863000	4.799209000	-0.895776000
C	3.792340000	2.831589000	-0.148341000
H	3.677851000	0.815375000	0.613312000

C	2.341208000	2.999628000	-0.296507000
O	1.685269000	1.812866000	-0.443257000
C	1.673918000	4.185265000	-0.264228000
C	0.320895000	1.764643000	-0.579390000
H	2.207066000	5.112821000	-0.104022000
C	0.237129000	4.238911000	-0.377767000
C	-0.425293000	2.952473000	-0.539000000
C	-0.263280000	0.501784000	-0.766138000
O	-0.407951000	5.313754000	-0.319495000
C	-1.844782000	2.877776000	-0.603048000
C	-1.664988000	0.484881000	-0.873351000
C	0.522416000	-0.786107000	-0.857791000
O	-2.575627000	3.991291000	-0.512011000
C	-2.470259000	1.635157000	-0.732722000
O	-2.277591000	-0.714860000	-1.102345000
H	-0.164742000	-1.589091000	-1.130484000
O	1.524238000	-0.640132000	-1.870395000
C	1.189134000	-1.186144000	0.481355000
H	-1.916356000	4.747463000	-0.423182000
C	-3.956110000	1.502469000	-0.519885000
H	-3.189512000	-0.515633000	-1.418781000
C	2.232674000	-1.846160000	-2.177388000
H	1.806292000	-0.359816000	0.850277000
O	0.183508000	-1.498243000	1.471859000
C	2.081217000	-2.425542000	0.314650000
H	-4.433461000	2.485581000	-0.592320000
O	-4.507994000	0.619208000	-1.531210000
C	-4.230757000	0.884577000	0.873978000
H	2.983434000	-1.533597000	-2.913182000
C	1.371551000	-2.908365000	-2.881469000
C	2.991063000	-2.314037000	-0.919895000
H	-0.317137000	-0.698215000	1.760887000
H	1.434794000	-3.300176000	0.184413000
O	2.935999000	-2.621208000	1.446884000
C	-5.919529000	0.407890000	-1.406312000
H	-3.700362000	-0.074105000	0.919058000
O	-3.823665000	1.722113000	1.938813000
C	-5.713018000	0.597506000	1.065372000
O	0.422232000	-3.566426000	-2.056805000
H	0.829910000	-2.390013000	-3.682879000
H	2.050420000	-3.630583000	-3.352697000
H	0.808287000	-4.430980000	-1.797422000
H	3.740876000	-1.540875000	-0.696657000
O	3.652421000	-3.540378000	-1.199163000

H	2.398157000	-2.891374000	2.228040000
H	-6.448580000	1.368001000	-1.479098000
H	-6.231299000	-0.233238000	-2.232316000
C	-6.248443000	-0.260902000	-0.067015000
H	-2.918370000	1.450246000	2.187541000
H	-6.268324000	1.547509000	1.078608000
O	-5.926193000	-0.097088000	2.303490000
H	4.508355000	-3.576292000	-0.701948000
H	-5.754537000	-1.245091000	-0.029941000
O	-7.663268000	-0.415204000	0.025838000
H	-5.586305000	0.504148000	2.985459000
H	-7.856791000	-0.663764000	0.941751000
O	6.048984000	-3.506786000	0.027124000
H	6.660312000	-3.108662000	-0.604902000
H	5.954110000	-2.843441000	0.750605000
O	-8.015829000	-1.865461000	-2.417348000
H	-8.162834000	-1.460624000	-1.545362000
H	-7.775678000	-2.778814000	-2.219035000
O	1.219735000	-3.015994000	3.508964000
H	0.735503000	-3.851340000	3.532433000
H	0.675008000	-2.420500000	2.951168000
O	-1.564783000	0.223870000	2.730949000
H	-1.226199000	0.476235000	3.600121000
H	-2.264180000	-0.481771000	2.901767000
O	-2.200823000	-2.905773000	0.851886000
H	-2.375237000	-2.425666000	0.025875000
H	-1.286138000	-2.625107000	1.048771000
O	1.979206000	-5.698276000	-1.303855000
H	2.705846000	-5.040505000	-1.209869000
H	1.834163000	-6.046166000	-0.415801000
O	-3.386896000	-1.660187000	2.943389000
H	-3.091542000	-2.222006000	2.181496000
H	-4.284992000	-1.353858000	2.729205000
O	5.398753000	-1.598228000	1.857935000
H	5.615507000	-1.780536000	2.781091000
H	4.446729000	-1.852269000	1.760912000

E = – 2673.3134522 a. u.
H = – 2673.3134522 + 0.799845 (thermal correction 6-31G(d,p)) a. u.
G = – 2673.3134522 + 0.652546 (thermal correction 6-31G(d,p)) a. u.

Transition state - 8-C bond rotation (φ_1 = 37.0°)

H	-7.946545000	-2.370381000	1.080948000

O	-7.477299000	-3.201923000	1.232188000
C	-6.202388000	-3.094879000	0.772720000
C	-5.359237000	-4.199644000	0.950340000
C	-5.716728000	-1.942848000	0.142647000
H	-5.747872000	-5.083144000	1.444631000
C	-4.041955000	-4.136398000	0.520200000
H	-6.366479000	-1.082076000	0.007769000
C	-4.397226000	-1.889251000	-0.294466000
H	-3.383951000	-4.981619000	0.693717000
C	-3.534917000	-2.981503000	-0.104871000
H	-4.058681000	-1.008392000	-0.828213000
C	-2.126622000	-2.941663000	-0.529430000
O	-1.534170000	-1.725786000	-0.295220000
C	-1.438186000	-3.977120000	-1.061934000
C	-0.188552000	-1.497524000	-0.557850000
H	-1.935116000	-4.914276000	-1.276267000
C	-0.025703000	-3.861174000	-1.349913000
C	0.578083000	-2.570505000	-1.054436000
C	0.332864000	-0.222335000	-0.281929000
O	0.634160000	-4.818686000	-1.815664000
C	1.979791000	-2.400965000	-1.204813000
C	1.749873000	-0.131312000	-0.403823000
C	-0.451017000	0.967476000	0.330900000
O	2.734685000	-3.398610000	-1.667807000
C	2.569973000	-1.193343000	-0.831236000
O	2.367632000	1.026025000	-0.056419000
H	-0.261434000	0.928178000	1.409169000
O	0.134876000	2.200881000	-0.078895000
C	-2.000948000	0.919960000	0.203928000
H	2.110717000	-4.166542000	-1.838092000
C	4.073031000	-1.095345000	-0.751669000
H	3.267876000	1.018437000	-0.458089000
C	-0.496591000	3.262849000	-0.788054000
H	-2.300301000	0.371569000	-0.692219000
O	-2.539176000	0.265932000	1.370296000
C	-2.642543000	2.303030000	0.084137000
H	4.510616000	-1.918547000	-1.326528000
O	4.495327000	0.166918000	-1.331794000
C	4.605833000	-1.155554000	0.706049000
H	0.032671000	3.393458000	-1.744742000
C	-0.232456000	4.542440000	0.022147000
C	-1.974740000	2.996349000	-1.108048000
H	-2.335377000	-0.676911000	1.265819000
H	-2.478517000	2.887658000	0.993549000

O	-4.044003000	2.213136000	-0.180568000
C	5.920118000	0.312659000	-1.411341000
H	4.222496000	-0.279672000	1.248166000
O	4.253804000	-2.338815000	1.383169000
C	6.130239000	-1.065696000	0.659781000
O	-0.815936000	4.548373000	1.321748000
H	0.852118000	4.615107000	0.151352000
H	-0.568842000	5.408795000	-0.556996000
H	-1.692507000	4.996555000	1.270470000
H	-2.032151000	2.299758000	-1.957438000
O	-2.600399000	4.210062000	-1.486964000
H	-4.514448000	1.877447000	0.619130000
H	6.336360000	-0.473482000	-2.056188000
H	6.123976000	1.286401000	-1.859659000
C	6.556143000	0.223992000	-0.022337000
H	3.472648000	-2.121361000	1.947668000
H	6.509804000	-1.917575000	0.069451000
O	6.693017000	-1.084241000	1.962268000
H	-3.202767000	4.013966000	-2.249257000
H	6.207993000	1.070334000	0.589969000
O	7.975652000	0.279999000	-0.174143000
H	6.242989000	-1.815884000	2.413859000
H	8.347903000	0.009714000	0.678868000
O	-4.055063000	3.410248000	-3.595747000
H	-3.490795000	3.329233000	-4.374579000
H	-4.306073000	2.487815000	-3.352879000
O	8.030069000	2.823054000	-1.449087000
H	8.272899000	1.991864000	-1.003569000
H	7.897799000	3.446290000	-0.724324000
O	-5.147256000	0.945313000	1.938530000
H	-5.180555000	1.388688000	2.795976000
H	-4.280108000	0.488701000	1.915306000
O	2.293491000	-1.440337000	3.055475000
H	2.703999000	-1.488563000	3.927818000
H	2.094796000	-0.474634000	2.941418000
O	-0.420823000	2.599313000	3.283798000
H	-0.503263000	3.299125000	2.597046000
H	-1.144386000	1.985857000	3.103271000
O	-3.277341000	5.573288000	0.755406000
H	-3.212137000	5.169301000	-0.140692000
H	-4.039183000	5.142185000	1.161413000
O	1.952332000	1.226376000	2.782689000
H	1.151100000	1.729204000	3.051386000
H	2.101456000	1.459441000	1.851945000

O	-4.587357000	0.964672000	-2.505553000
H	-5.514995000	0.707081000	-2.580628000
H	-4.490347000	1.379181000	-1.611610000

E = – 2673.2777982 a. u.
H = – 2673.2777982 + 0.798361 (thermal correction 6-31G(d,p)) a. u.
G = – 2673.2777982 + 0.65017 (thermal correction 6-31G(d,p)) a. u.
f = 122.69*i*

Transition state - 8-C bond rotation (φ_1 = about –166°): not found

2 Schaftoside, *n* = 6 (DMSO)

a H–C_7 eclipsed

H	-9.348942000	-2.911958000	-1.476289000
O	-9.004167000	-3.624203000	-0.921293000
C	-7.643360000	-3.550520000	-0.895603000
C	-6.961631000	-4.490280000	-0.111691000
C	-6.924073000	-2.585754000	-1.609404000
H	-7.534229000	-5.221715000	0.448005000
C	-5.577256000	-4.460130000	-0.050511000
H	-7.452023000	-1.853450000	-2.216541000
C	-5.536168000	-2.559840000	-1.542104000
H	-5.066842000	-5.176697000	0.583662000
C	-4.839127000	-3.502536000	-0.768408000
H	-4.978284000	-1.810442000	-2.092046000
C	-3.374181000	-3.482917000	-0.731964000
O	-2.867133000	-2.328875000	-1.234592000
C	-2.557907000	-4.493531000	-0.309313000
C	-1.524639000	-2.136627000	-1.383268000
H	-2.972739000	-5.418765000	0.066738000
C	-1.127816000	-4.369851000	-0.376853000
C	-0.634043000	-3.143700000	-0.981632000
C	-1.101887000	-0.917633000	-1.926230000
O	-0.334347000	-5.258632000	0.038088000
C	0.754451000	-2.914473000	-1.127120000
C	0.286297000	-0.761593000	-2.109713000
C	-2.021569000	0.262820000	-2.138234000
O	1.630635000	-3.828458000	-0.653268000
C	1.225532000	-1.748642000	-1.725343000
O	0.725128000	0.397208000	-2.667640000
H	-1.456679000	1.029946000	-2.683235000
O	-3.180617000	-0.091531000	-2.904552000

C	-2.464563000	0.868795000	-0.788960000
H	1.050126000	-4.584713000	-0.295135000
C	2.721428000	-1.526886000	-1.802495000
H	1.655647000	0.242850000	-2.946513000
C	-3.966462000	1.050385000	-3.223565000
H	-3.040552000	0.117943000	-0.230593000
O	-1.297739000	1.244061000	-0.060582000
C	-3.355794000	2.079801000	-1.029480000
H	3.209711000	-2.508129000	-1.856077000
O	3.021139000	-0.787615000	-3.001798000
C	3.256150000	-0.776594000	-0.563281000
H	-3.377079000	1.781191000	-3.801446000
H	-4.788193000	0.704281000	-3.855088000
C	-4.516291000	1.749425000	-1.972423000
H	-1.473491000	2.053390000	0.456789000
H	-2.746464000	2.849123000	-1.539486000
O	-3.761008000	2.534381000	0.254349000
C	4.425038000	-0.578589000	-3.260626000
H	2.699149000	0.163251000	-0.462814000
O	3.033225000	-1.541085000	0.621828000
C	4.746136000	-0.427428000	-0.709839000
H	-5.208448000	1.071737000	-1.449287000
O	-5.184323000	2.920053000	-2.432495000
H	-4.451387000	3.228345000	0.168595000
H	4.444006000	0.060423000	-4.149006000
C	5.161733000	-1.868665000	-3.665516000
C	5.076695000	0.182464000	-2.085579000
H	2.827996000	-2.456017000	0.368160000
H	5.331218000	-1.343510000	-0.569239000
O	5.162554000	0.455794000	0.330150000
H	-5.532011000	3.411285000	-1.668234000
O	6.312861000	-1.552877000	-4.425514000
H	4.496424000	-2.461529000	-4.301966000
H	5.416985000	-2.482017000	-2.786664000
H	6.801731000	-0.910985000	-3.881928000
H	4.658507000	1.197814000	-2.080696000
O	6.479521000	0.292503000	-2.305604000
H	4.640786000	1.276829000	0.241608000
H	6.968412000	-0.289085000	-1.672453000
C	0.893547000	3.262506000	4.004696000
S	-0.155943000	2.382379000	2.798754000
C	1.158262000	1.366819000	2.056831000
O	-0.604679000	3.408819000	1.738194000
H	0.266271000	3.991189000	4.521224000

H	1.269323000	2.514488000	4.707605000
H	1.711511000	3.767889000	3.485811000
H	0.695745000	0.808933000	1.241958000
H	1.508578000	0.690676000	2.837332000
H	1.958671000	1.999284000	1.666008000
C	8.454630000	1.148209000	0.425887000
S	8.678788000	-0.662324000	0.540026000
C	7.577851000	-0.934746000	1.974082000
O	7.983934000	-1.270119000	-0.684365000
H	8.837570000	1.614285000	1.337435000
H	7.390460000	1.347299000	0.282437000
H	9.029179000	1.488113000	-0.437400000
H	6.591972000	-0.515043000	1.757043000
H	7.518265000	-2.015036000	2.119775000
H	8.030249000	-0.470400000	2.854970000
C	3.336758000	3.848575000	-2.610927000
S	2.855445000	3.927615000	-0.847291000
C	1.067413000	3.674465000	-1.082781000
O	3.396379000	2.663464000	-0.173110000
H	2.952515000	2.929680000	-3.059165000
H	4.427276000	3.859684000	-2.652582000
H	2.936405000	4.725496000	-3.126347000
H	0.590466000	3.719336000	-0.098392000
H	0.690304000	4.476977000	-1.724073000
H	0.890648000	2.692732000	-1.530713000
C	-3.752613000	0.565570000	3.249449000
S	-3.445778000	-1.216650000	2.955616000
C	-1.651511000	-1.091639000	2.622180000
O	-4.118342000	-1.580305000	1.641419000
H	-3.096762000	0.921544000	4.048178000
H	-3.591617000	1.124006000	2.323203000
H	-4.797131000	0.659408000	3.554379000
H	-1.481294000	-0.401288000	1.791723000
H	-1.111380000	-0.772900000	3.518893000
H	-1.331021000	-2.094929000	2.331124000
C	-3.551279000	5.699600000	1.509584000
S	-4.635531000	5.912524000	0.054189000
C	-3.333331000	5.838224000	-1.227493000
O	-5.466214000	4.622049000	-0.067023000
H	-2.984953000	4.766795000	1.429017000
H	-4.202257000	5.676855000	2.385462000
H	-2.881572000	6.561555000	1.571054000
H	-2.645087000	5.019354000	-1.013078000
H	-2.809627000	6.797234000	-1.248934000

H	-3.840076000	5.657259000	-2.176896000
C	1.248677000	-2.426180000	6.360833000
S	2.077894000	-1.251008000	5.228679000
C	2.187664000	-2.372030000	3.789183000
O	1.050857000	-0.170289000	4.898952000
H	1.049083000	-1.890008000	7.290175000
H	1.908946000	-3.275242000	6.555192000
H	0.308227000	-2.757439000	5.913982000
H	1.191031000	-2.740962000	3.534758000
H	2.852981000	-3.202515000	4.041495000
H	2.597893000	-1.810282000	2.945576000

E = – 5381.2810927 a. u.
H = – 5381.2810927 + 1.105306 (thermal correction 6-31G(d,p)) a. u.
G = – 5381.2810927 + 0.896955 (thermal correction 6-31G(d,p)) a. u.

Transition state - 8-C bond rotation (φ_1 = 21.7°)

H	-7.073906000	6.290795000	-3.072285000
O	-6.706175000	6.920498000	-2.437646000
C	-5.564584000	6.407204000	-1.904567000
C	-4.915989000	7.165251000	-0.919973000
C	-5.034369000	5.172312000	-2.292180000
H	-5.348202000	8.112439000	-0.616560000
C	-3.753521000	6.686190000	-0.337262000
H	-5.538790000	4.574565000	-3.047412000
C	-3.864860000	4.699934000	-1.707675000
H	-3.279559000	7.268570000	0.445657000
C	-3.200964000	5.448151000	-0.720612000
H	-3.478747000	3.732756000	-2.004706000
C	-1.945669000	4.977615000	-0.116492000
O	-1.808779000	3.615189000	-0.155405000
C	-0.987455000	5.769418000	0.424917000
C	-0.655316000	2.967013000	0.261956000
H	-1.089039000	6.846199000	0.420427000
C	0.218991000	5.199444000	0.969443000
C	0.363383000	3.762453000	0.825715000
C	-0.562683000	1.574992000	0.080444000
O	1.107187000	5.911275000	1.503837000
C	1.582747000	3.143053000	1.187849000
C	0.758548000	1.049494000	0.290704000
C	-1.735869000	0.652182000	-0.364858000
O	2.572374000	3.878148000	1.735472000
C	1.791130000	1.800198000	0.910520000

O	1.062544000	-0.181462000	-0.147011000
H	-1.861277000	0.712865000	-1.461308000
O	-1.352540000	-0.668544000	0.008115000
C	-3.151820000	0.898589000	0.276725000
H	2.209818000	4.821856000	1.786527000
C	3.175901000	1.233435000	1.162552000
H	1.888873000	-0.484732000	0.303602000
C	-2.181834000	-1.705162000	-0.483361000
H	-3.013648000	1.014012000	1.362415000
O	-3.881378000	1.980633000	-0.273139000
C	-4.114128000	-0.288658000	0.035992000
H	3.602270000	1.769009000	2.021615000
O	3.042336000	-0.155803000	1.493431000
C	4.128493000	1.428224000	-0.042144000
H	-2.362365000	-1.596612000	-1.566060000
H	-1.658473000	-2.650014000	-0.321833000
C	-3.496940000	-1.656095000	0.276675000
H	-3.469673000	2.796981000	0.027032000
H	-4.390522000	-0.242092000	-1.028744000
O	-5.276864000	-0.156744000	0.836681000
C	4.257240000	-0.865993000	1.817846000
H	3.693729000	0.931305000	-0.919836000
O	4.272935000	2.799522000	-0.375128000
C	5.483714000	0.772953000	0.266753000
H	-3.268861000	-1.772980000	1.345342000
O	-4.362795000	-2.701909000	-0.156396000
H	-5.936857000	0.377708000	0.339957000
H	3.948896000	-1.913561000	1.832712000
C	4.775929000	-0.528020000	3.225702000
C	5.293960000	-0.690157000	0.690271000
H	4.105266000	3.329855000	0.419262000
H	5.954343000	1.331009000	1.086353000
O	6.384382000	0.871658000	-0.827528000
H	-5.009625000	-2.861675000	0.563615000
O	5.591782000	-1.578988000	3.715009000
H	3.915401000	-0.438286000	3.897450000
H	5.313113000	0.434284000	3.243122000
H	6.236489000	-1.744131000	3.005954000
H	4.902421000	-1.232380000	-0.175365000
O	6.535567000	-1.300630000	1.061096000
H	6.024496000	0.341880000	-1.575802000
H	7.181387000	-0.595030000	1.301400000
C	1.874741000	-5.336848000	-1.048248000
S	1.634770000	-3.606094000	-0.510350000

C	0.932689000	-2.983072000	-2.075215000
O	3.025601000	-2.985004000	-0.363891000
H	2.369047000	-5.861574000	-0.228277000
H	0.887907000	-5.762341000	-1.246029000
H	2.509712000	-5.357206000	-1.938067000
H	0.738266000	-1.921339000	-1.916612000
H	0.007414000	-3.528737000	-2.272617000
H	1.665593000	-3.121598000	-2.874700000
C	9.611598000	0.330992000	-0.404405000
S	9.422264000	1.286562000	1.142753000
C	8.670943000	2.773801000	0.386799000
O	8.340179000	0.576426000	1.960387000
H	10.285798000	0.862592000	-1.081005000
H	8.612839000	0.214987000	-0.833046000
H	10.040316000	-0.635387000	-0.132453000
H	7.806716000	2.485020000	-0.217751000
H	8.372462000	3.425779000	1.210008000
H	9.433962000	3.274694000	-0.216115000
C	7.621586000	-2.026161000	-3.614234000
S	5.835924000	-2.151759000	-3.229366000
C	5.992947000	-3.185093000	-1.733804000
O	5.379676000	-0.751413000	-2.822171000
H	8.151444000	-1.609973000	-2.754259000
H	7.719246000	-1.358166000	-4.471799000
H	8.010686000	-3.016074000	-3.866463000
H	4.980478000	-3.327720000	-1.340789000
H	6.427661000	-4.143764000	-2.033070000
H	6.610155000	-2.685305000	-0.981059000
C	-5.178853000	-1.551284000	3.737598000
S	-6.408862000	-2.821340000	3.292464000
C	-5.929793000	-4.066814000	4.542185000
O	-6.013210000	-3.423143000	1.941093000
H	-5.447793000	-1.134442000	4.712095000
H	-4.180125000	-1.994765000	3.767836000
H	-5.227300000	-0.788458000	2.955206000
H	-4.882020000	-4.338139000	4.393718000
H	-6.089806000	-3.658645000	5.543357000
H	-6.566534000	-4.939848000	4.390050000
C	-7.070544000	-1.503193000	-2.226124000
S	-8.164902000	-0.400860000	-1.258204000
C	-8.460349000	-1.554873000	0.129047000
O	-7.320018000	0.756256000	-0.729387000
H	-6.226034000	-1.838671000	-1.617356000
H	-6.716334000	-0.922085000	-3.079831000

H	-7.659672000	-2.353306000	-2.581899000
H	-7.510569000	-1.879909000	0.559414000
H	-9.034094000	-2.409636000	-0.239428000
H	-9.049227000	-1.010398000	0.869776000
C	-3.370294000	-5.957986000	0.343435000
S	-2.566636000	-6.107518000	-1.293428000
C	-3.889663000	-5.286800000	-2.254675000
O	-1.361791000	-5.171291000	-1.293303000
H	-2.643198000	-6.301064000	1.081922000
H	-4.252180000	-6.604290000	0.365451000
H	-3.645966000	-4.915998000	0.519970000
H	-4.095210000	-4.305421000	-1.819641000
H	-4.780989000	-5.920573000	-2.238904000
H	-3.522895000	-5.194216000	-3.278764000

E = – 5381.2480749 a. u.
H = – 5381.2480749 + 1.104003 (thermal correction 6-31G(d,p)) a. u.
G = – 5381.2480749 + 0.896436 (thermal correction 6-31G(d,p)) a. u.
f = 38.91*i*

Transition state - 8-C bond rotation (φ_1 = –164.0°)

H	-9.023721000	-3.591046000	-0.016197000
O	-8.637064000	-4.349943000	0.442392000
C	-7.280651000	-4.240893000	0.395240000
C	-6.527362000	-5.255744000	1.003158000
C	-6.638407000	-3.167917000	-0.232318000
H	-7.043932000	-6.087020000	1.470719000
C	-5.142551000	-5.185013000	0.993353000
H	-7.209453000	-2.362715000	-0.689850000
C	-5.251270000	-3.112398000	-0.242445000
H	-4.576638000	-5.986081000	1.457002000
C	-4.476469000	-4.106763000	0.378723000
H	-4.748855000	-2.288401000	-0.730268000
C	-3.014074000	-3.997699000	0.391108000
O	-2.564666000	-3.019054000	-0.434691000
C	-2.154894000	-4.747894000	1.139129000
C	-1.235503000	-2.727793000	-0.595175000
H	-2.518293000	-5.496025000	1.830025000
C	-0.739043000	-4.562136000	1.021604000
C	-0.302681000	-3.552730000	0.073941000
C	-0.848205000	-1.659018000	-1.433538000
O	0.091320000	-5.224393000	1.709616000
C	1.080255000	-3.354873000	-0.150051000

C	0.536438000	-1.640093000	-1.753882000
C	-1.808817000	-0.570734000	-1.988136000
O	1.982736000	-4.068629000	0.556848000
C	1.509858000	-2.434148000	-1.094581000
O	0.918689000	-0.819569000	-2.737782000
H	-2.051991000	-0.765819000	-3.045845000
O	-2.987026000	-0.676658000	-1.177547000
C	-1.291800000	0.913198000	-1.888721000
H	1.423919000	-4.684931000	1.148815000
C	3.003846000	-2.220796000	-1.259688000
H	1.872610000	-0.977929000	-2.920534000
C	-4.047292000	0.239219000	-1.414398000
H	-0.793852000	1.019299000	-0.911365000
O	-0.418210000	1.294127000	-2.946018000
C	-2.442175000	1.946544000	-1.951486000
H	3.509557000	-3.174481000	-1.058824000
O	3.284522000	-1.816650000	-2.611156000
C	3.532412000	-1.166666000	-0.259194000
H	-4.355540000	0.237711000	-2.471596000
H	-4.902026000	-0.091678000	-0.821521000
C	-3.578081000	1.626794000	-0.998663000
H	-0.487727000	2.262380000	-2.957174000
H	-2.848498000	1.919620000	-2.972081000
O	-1.869341000	3.246306000	-1.796337000
C	4.673344000	-1.596481000	-2.937992000
H	2.960351000	-0.240521000	-0.398703000
O	3.323174000	-1.583748000	1.087011000
C	5.016373000	-0.855430000	-0.505220000
H	-3.202740000	1.557392000	0.033295000
O	-4.639570000	2.569954000	-1.069667000
H	-2.011496000	3.543061000	-0.875724000
H	4.647205000	-1.183595000	-3.950759000
C	5.474897000	-2.906819000	-3.045328000
C	5.295273000	-0.547609000	-1.988114000
H	3.218169000	-2.549461000	1.100774000
H	5.607826000	-1.731277000	-0.210550000
O	5.462335000	0.208599000	0.325050000
H	-4.304521000	3.377437000	-0.634114000
O	6.601707000	-2.721819000	-3.880754000
H	4.835570000	-3.662922000	-3.513190000
H	5.768379000	-3.285920000	-2.053398000
H	7.056652000	-1.943438000	-3.514837000
H	4.824040000	0.421351000	-2.212728000
O	6.685761000	-0.424404000	-2.262640000

H	4.814860000	0.946445000	0.262182000
H	7.211825000	-0.832080000	-1.531027000
C	2.091712000	3.050123000	3.060860000
S	0.491631000	3.809966000	2.636639000
C	-0.322068000	2.317171000	1.991117000
O	0.719638000	4.759415000	1.438687000
H	2.703905000	3.827808000	3.522611000
H	1.889882000	2.241312000	3.770182000
H	2.568768000	2.675828000	2.149692000
H	-1.305649000	2.632481000	1.637464000
H	-0.393140000	1.593710000	2.809281000
H	0.275055000	1.914457000	1.169063000
C	8.672637000	0.994590000	0.298205000
S	8.962125000	-0.766263000	0.694943000
C	7.878778000	-0.850645000	2.164448000
O	8.285928000	-1.584007000	-0.412055000
H	9.042904000	1.611453000	1.121274000
H	7.600938000	1.131024000	0.135063000
H	9.232994000	1.212316000	-0.612719000
H	6.874463000	-0.515870000	1.890415000
H	7.868580000	-1.894193000	2.484920000
H	8.311327000	-0.229408000	2.953945000
C	1.844063000	3.427484000	-1.579927000
S	3.565661000	3.262307000	-1.011934000
C	3.700515000	4.894810000	-0.202693000
O	3.542620000	2.217996000	0.118360000
H	1.217417000	3.704490000	-0.728126000
H	1.538156000	2.464989000	-1.996813000
H	1.808234000	4.195561000	-2.358194000
H	4.657530000	4.909461000	0.322124000
H	3.694440000	5.667993000	-0.976106000
H	2.865152000	5.022348000	0.492212000
C	-7.704300000	2.146888000	-2.477901000
S	-8.334395000	1.053793000	-1.150435000
C	-7.736233000	2.068134000	0.251460000
O	-7.499295000	-0.219050000	-1.173460000
H	-8.270778000	3.082481000	-2.463303000
H	-6.637622000	2.330003000	-2.325751000
H	-7.879250000	1.627502000	-3.422036000
H	-6.660660000	2.228223000	0.139219000
H	-8.279375000	3.017419000	0.263920000
H	-7.953263000	1.507967000	1.162950000
C	-2.153391000	6.536847000	1.862007000
S	-2.900536000	5.959069000	0.303033000

C	-1.464827000	6.294431000	-0.773383000
O	-3.012149000	4.421963000	0.417621000
H	-1.162811000	6.086879000	1.970025000
H	-2.821569000	6.231172000	2.668782000
H	-2.091105000	7.628098000	1.826860000
H	-0.579237000	5.843149000	-0.317824000
H	-1.353934000	7.376788000	-0.878914000
H	-1.681960000	5.835065000	-1.739200000
C	-0.721270000	-1.656098000	5.483122000
S	0.800557000	-0.938445000	4.762328000
C	0.673650000	-1.743994000	3.131908000
O	0.521060000	0.549080000	4.560641000
H	-0.842529000	-1.222709000	6.477392000
H	-0.612428000	-2.741003000	5.558391000
H	-1.577113000	-1.393971000	4.856257000
H	-0.268795000	-1.451755000	2.661615000
H	0.717484000	-2.830066000	3.253145000
H	1.518143000	-1.408429000	2.524215000

E = – 5381.2463867 a. u.
H = – 5381.2463867 + 1.104574 (thermal correction 6-31G(d,p)) a. u.
G = – 5381.2463867 + 0.901486 (thermal correction 6-31G(d,p)) a. u.
f = 44.52i

3 Vitexin, *n* = 4 (DMSO)

a H–C_7 eclipsed

H	-6.245242000	-0.697886000	-2.484938000
O	-5.979938000	-1.633637000	-2.660000000
C	-4.635862000	-1.726410000	-2.662369000
C	-4.052830000	-3.005956000	-2.705308000
C	-3.803507000	-0.593524000	-2.611170000
H	-4.703302000	-3.872624000	-2.759128000
C	-2.674195000	-3.148999000	-2.630175000
H	-4.255974000	0.392028000	-2.606230000
C	-2.429540000	-0.746611000	-2.528665000
H	-2.244669000	-4.146208000	-2.612934000
C	-1.837685000	-2.023864000	-2.515939000
H	-1.792015000	0.127990000	-2.466055000
C	-0.393375000	-2.138808000	-2.309339000
O	0.086971000	-1.034474000	-1.675611000
C	0.430495000	-3.170065000	-2.651116000
C	1.403621000	-0.897741000	-1.341344000

H	0.043412000	-4.033445000	-3.176860000
C	1.837466000	-3.129866000	-2.332958000
C	2.307378000	-1.917038000	-1.684355000
C	1.756320000	0.259059000	-0.641257000
O	2.621745000	-4.086437000	-2.579515000
C	3.676914000	-1.736761000	-1.343497000
C	3.132722000	0.410361000	-0.351204000
C	0.747082000	1.290505000	-0.189838000
O	4.570280000	-2.697791000	-1.631024000
C	4.079420000	-0.572457000	-0.700817000
O	3.513167000	1.530044000	0.289557000
H	1.294808000	2.030345000	0.402236000
O	0.179132000	1.918875000	-1.361621000
C	-0.372385000	0.722027000	0.726535000
H	4.043669000	-3.424032000	-2.080484000
H	5.122968000	-0.434678000	-0.442531000
H	4.499459000	1.571401000	0.377256000
C	-0.700398000	3.017905000	-1.101941000
H	-0.928570000	-0.056873000	0.193800000
O	0.169264000	0.229260000	1.940252000
C	-1.344456000	1.850266000	1.067498000
H	-1.108673000	3.289329000	-2.081331000
C	-1.847927000	2.519329000	-0.209414000
C	0.018455000	4.276019000	-0.578595000
H	0.499284000	-0.685180000	1.810290000
H	-0.807253000	2.584938000	1.686787000
O	-2.521564000	1.422892000	1.745520000
H	-2.405736000	1.758678000	-0.774329000
O	-2.739961000	3.589586000	0.141782000
O	-0.807903000	5.422201000	-0.696430000
H	0.903145000	4.441208000	-1.201954000
H	0.369901000	4.141088000	0.456265000
H	-1.640531000	5.187445000	-0.254652000
H	-2.327097000	1.271378000	2.703171000
H	-3.141953000	3.282549000	0.973186000
C	2.802049000	-3.231669000	3.741512000
S	2.469032000	-2.724331000	2.015615000
H	2.126530000	-4.043371000	4.022952000
H	3.845902000	-3.541089000	3.837227000
H	2.617451000	-2.356983000	4.367677000
C	2.726173000	-4.363813000	1.251833000
H	3.742515000	-4.699474000	1.473070000
H	2.609146000	-4.260150000	0.172543000
H	1.985728000	-5.061809000	1.649948000

O	0.964916000	-2.438548000	1.946744000
C	8.099031000	1.986539000	-1.562530000
S	6.545153000	2.696026000	-0.921813000
H	7.854813000	1.002010000	-1.964781000
H	8.492628000	2.625598000	-2.356877000
H	8.814321000	1.887885000	-0.742820000
C	7.241857000	4.247805000	-0.258209000
H	7.643680000	4.847576000	-1.078742000
H	8.015767000	4.012279000	0.475973000
H	6.421597000	4.782169000	0.223882000
O	6.177439000	1.843669000	0.299660000
C	-1.778794000	-1.143065000	6.129383000
S	-1.241154000	-0.404940000	4.543209000
H	-1.294218000	-2.114175000	6.262730000
H	-1.472564000	-0.462942000	6.926173000
H	-2.866432000	-1.246415000	6.129024000
C	-1.901131000	-1.719011000	3.455625000
H	-1.976612000	-1.262093000	2.469761000
H	-1.184407000	-2.541824000	3.411195000
H	-2.884788000	-2.042894000	3.803077000
O	-2.150672000	0.816380000	4.360821000
C	-5.783408000	0.360112000	0.686380000
S	-6.891704000	1.258018000	-0.459717000
H	-5.881926000	-0.698894000	0.439302000
H	-4.741794000	0.676931000	0.593752000
H	-6.141159000	0.533516000	1.705163000
C	-6.275303000	2.942984000	-0.130092000
H	-6.822516000	3.615060000	-0.793352000
H	-5.203177000	3.005359000	-0.334982000
H	-6.490371000	3.197204000	0.911466000
O	-6.464886000	0.932880000	-1.896813000

E = – 3778.2733451 a. u.
H = – 3778.2733451 + 0.778534 (thermal correction 6-31G(d,p)) a. u.
G = – 3778.2733451 + 0.621077 (thermal correction 6-31G(d,p)) a. u.

Transition state - 8-C bond rotation (φ_1 = 20.6°)

H	-6.146638000	0.757255000	-0.680903000
O	-5.996867000	1.710492000	-0.453841000
C	-4.662746000	1.972342000	-0.419046000
C	-4.233213000	3.172180000	0.165773000
C	-3.711599000	1.074915000	-0.923858000
H	-4.974676000	3.858702000	0.560835000

C	-2.877442000	3.448623000	0.265612000
H	-4.040712000	0.146563000	-1.381068000
C	-2.354786000	1.356915000	-0.816069000
H	-2.570319000	4.367989000	0.752129000
C	-1.909423000	2.546196000	-0.215247000
H	-1.629024000	0.632772000	-1.160865000
C	-0.472857000	2.844706000	-0.113883000
O	0.309577000	1.771523000	-0.409189000
C	0.068739000	4.053183000	0.196541000
C	1.677771000	1.859956000	-0.504173000
H	-0.556076000	4.907705000	0.417131000
C	1.494992000	4.251979000	0.176595000
C	2.283041000	3.108592000	-0.245995000
C	2.387150000	0.704759000	-0.893951000
O	2.023645000	5.355539000	0.470000000
C	3.679320000	3.250730000	-0.467670000
C	3.724843000	0.979011000	-1.325029000
C	1.807433000	-0.732206000	-0.906142000
O	4.302153000	4.402052000	-0.186500000
C	4.369951000	2.197518000	-1.040895000
O	4.399277000	0.071940000	-2.053844000
H	1.196365000	-0.888762000	-1.808531000
O	2.960574000	-1.590948000	-0.919201000
C	0.957319000	-1.183113000	0.334455000
H	3.582909000	5.021285000	0.140731000
H	5.409767000	2.324684000	-1.321233000
H	5.337470000	0.354824000	-2.173669000
C	2.777375000	-2.990894000	-1.112902000
H	1.529147000	-0.905938000	1.232321000
O	-0.353742000	-0.663618000	0.373814000
C	0.767337000	-2.714485000	0.334085000
H	3.792703000	-3.401518000	-1.136190000
C	2.046539000	-3.505658000	0.127329000
C	2.139402000	-3.383324000	-2.456970000
H	-0.462401000	-0.094632000	1.164218000
H	0.075584000	-2.942658000	-0.491375000
O	0.221306000	-3.182848000	1.559223000
H	2.696523000	-3.333097000	0.999365000
O	1.746637000	-4.898909000	0.018291000
O	2.311098000	-4.768325000	-2.705149000
H	2.657056000	-2.836485000	-3.251577000
H	1.076574000	-3.098829000	-2.500760000
H	1.964916000	-5.218567000	-1.916540000
H	-0.749123000	-3.003877000	1.594173000

H	1.059573000	-5.050143000	0.688060000
C	-0.411201000	-1.470242000	4.304591000
S	-0.422649000	0.346642000	4.136000000
H	0.202687000	-1.931902000	3.526332000
H	-0.052074000	-1.718007000	5.307491000
H	-1.438191000	-1.815277000	4.171243000
C	1.385066000	0.604732000	4.198810000
H	1.752729000	0.327666000	5.190227000
H	1.563799000	1.665915000	4.017734000
H	1.869490000	0.006527000	3.423706000
O	-0.865900000	0.689673000	2.709674000
C	6.402308000	-0.925392000	0.315578000
S	7.570452000	-0.731250000	-1.079074000
H	5.441264000	-1.230695000	-0.104495000
H	6.789448000	-1.691460000	0.992591000
H	6.288189000	0.032785000	0.828556000
C	8.963013000	-0.041630000	-0.118894000
H	9.308074000	-0.782150000	0.607113000
H	8.635169000	0.875076000	0.376710000
H	9.760368000	0.184898000	-0.828504000
O	7.064300000	0.426759000	-1.946242000
C	-4.932464000	-2.991893000	0.969008000
S	-3.367766000	-2.056713000	1.094959000
H	-5.644602000	-2.413554000	0.372887000
H	-4.696234000	-3.928907000	0.461011000
H	-5.319721000	-3.203114000	1.968792000
C	-3.991346000	-0.694224000	2.134180000
H	-3.148010000	-0.023322000	2.313644000
H	-4.787834000	-0.166382000	1.606556000
H	-4.356654000	-1.118058000	3.073656000
O	-2.453160000	-2.891022000	2.004492000
C	-8.998551000	0.442010000	-1.606649000
S	-7.721643000	-0.676725000	-2.283311000
H	-9.466044000	-0.079819000	-0.770000000
H	-8.523074000	1.361824000	-1.257693000
H	-9.744068000	0.647395000	-2.378866000
C	-7.062375000	0.456759000	-3.555251000
H	-6.226672000	-0.054684000	-4.035586000
H	-6.715311000	1.371470000	-3.069404000
H	-7.842156000	0.667023000	-4.291335000
O	-6.633408000	-0.787813000	-1.202202000

E = – 3778.2453912 a. u.

H = – 3778.2453912 + 0.776692 (thermal correction 6-31G(d,p)) a. u.

G = – 3778.2453912 + 0.624744 (thermal correction 6-31G(d,p)) a. u.
f = 29.18i

Transition state - 8-C bond rotation (φ_1 = –168.8°)

H	-7.472623000	-0.984639000	-0.685835000
O	-7.402383000	-1.797436000	-0.127359000
C	-6.111851000	-2.166791000	-0.020860000
C	-5.792309000	-3.257807000	0.808534000
C	-5.077739000	-1.496347000	-0.698257000
H	-6.596255000	-3.771618000	1.325039000
C	-4.470488000	-3.645139000	0.979072000
H	-5.328797000	-0.666878000	-1.350670000
C	-3.761334000	-1.885626000	-0.513817000
H	-4.245303000	-4.468857000	1.649767000
C	-3.425596000	-2.959890000	0.331221000
H	-2.966465000	-1.350655000	-1.017982000
C	-2.015489000	-3.304945000	0.531137000
O	-1.209713000	-2.281671000	0.151767000
C	-1.499285000	-4.469548000	1.016000000
C	0.152459000	-2.317614000	0.224559000
H	-2.142479000	-5.294535000	1.292547000
C	-0.075401000	-4.641820000	1.119918000
C	0.743007000	-3.514723000	0.684777000
C	0.887201000	-1.178864000	-0.195477000
O	0.451344000	-5.704366000	1.544097000
C	2.156262000	-3.623414000	0.692723000
C	2.283728000	-1.408333000	-0.282414000
C	0.262638000	0.199119000	-0.560891000
O	2.760882000	-4.739137000	1.123907000
C	2.907915000	-2.566308000	0.206258000
O	3.071785000	-0.485860000	-0.888462000
H	0.285206000	0.340301000	-1.653653000
O	-1.091958000	0.130973000	-0.101252000
C	1.037599000	1.432909000	0.047218000
H	2.007542000	-5.356088000	1.391251000
H	3.988300000	-2.627282000	0.198779000
H	3.983464000	-0.851395000	-1.050401000
C	-1.919574000	1.278437000	0.012475000
H	1.487189000	1.133591000	1.001645000
O	2.033442000	1.912577000	-0.841123000
C	0.142190000	2.654534000	0.298108000
H	-2.806992000	0.909055000	0.538650000
C	-1.205638000	2.299856000	0.894667000

C	-2.428955000	1.828382000	-1.331714000
H	2.689685000	1.196308000	-0.906058000
H	-0.020341000	3.136116000	-0.677188000
O	0.726925000	3.587589000	1.194638000
H	-1.044488000	1.841501000	1.882198000
O	-1.990702000	3.488475000	1.036831000
O	-3.511279000	2.733102000	-1.118351000
H	-2.814041000	0.995428000	-1.927100000
H	-1.626853000	2.305806000	-1.912754000
H	-3.182072000	3.371741000	-0.459003000
H	1.394970000	4.133434000	0.708216000
H	-1.342040000	4.163254000	1.303456000
C	3.005065000	2.836906000	3.713668000
S	3.845169000	1.255533000	3.327400000
H	2.149297000	2.971586000	3.044173000
H	2.703434000	2.841304000	4.764767000
H	3.730708000	3.634107000	3.539641000
C	2.465009000	0.152514000	3.814494000
H	2.347169000	0.181826000	4.901034000
H	2.740461000	-0.854336000	3.495710000
H	1.542934000	0.457258000	3.314973000
O	3.979500000	1.171086000	1.813876000
C	5.535507000	-4.307762000	-1.875015000
S	5.158009000	-2.700728000	-2.657837000
H	4.747043000	-4.514042000	-1.148971000
H	5.544574000	-5.084709000	-2.643892000
H	6.502383000	-4.241989000	-1.370448000
C	6.623101000	-2.614637000	-3.742327000
H	6.589827000	-3.431375000	-4.467599000
H	7.525803000	-2.667027000	-3.129530000
H	6.580049000	-1.654998000	-4.259763000
O	5.391794000	-1.622591000	-1.588671000
C	4.512015000	6.069111000	-1.530660000
S	3.497863000	4.623229000	-1.055875000
H	5.336682000	5.745210000	-2.170997000
H	3.861638000	6.751518000	-2.080615000
H	4.885875000	6.561031000	-0.629646000
C	4.787675000	3.740106000	-0.118225000
H	4.317143000	2.879949000	0.364845000
H	5.562131000	3.402731000	-0.813089000
H	5.211891000	4.411294000	0.633499000
O	2.505148000	5.185832000	-0.030938000
C	-6.495323000	2.067995000	0.530838000
S	-7.638969000	1.894793000	-0.885505000

H	-6.711033000	1.242800000	1.212190000
H	-5.459943000	2.030449000	0.182116000
H	-6.703655000	3.019829000	1.027524000
C	-6.843286000	3.132202000	-1.966315000
H	-7.319757000	3.047274000	-2.944413000
H	-5.770279000	2.933653000	-2.030708000
H	-7.028740000	4.126418000	-1.550204000
O	-7.364911000	0.533354000	-1.539037000

E = – 3778.2419366 a. u.
H = – 3778.2419366 + 0.777014 (thermal correction 6-31G(d,p)) a. u.
G = – 3778.2419366 + 0.623632 (thermal correction 6-31G(d,p)) a. u.
f = 31.21*i*

4 Puerarin, *n* = 4 (DMSO)

a H–C_7 eclipsed

H	-8.207588000	1.269601000	0.044598000
O	-8.091052000	0.289890000	-0.050968000
C	-6.770905000	-0.022832000	-0.138403000
C	-6.415673000	-1.370702000	-0.284468000
C	-5.762735000	0.951242000	-0.106991000
H	-7.203616000	-2.116551000	-0.318161000
C	-5.079869000	-1.740910000	-0.384152000
H	-6.033880000	1.999475000	-0.020587000
C	-4.427960000	0.568870000	-0.209477000
H	-4.819817000	-2.783532000	-0.515492000
C	-4.052819000	-0.779407000	-0.334452000
H	-3.662438000	1.340194000	-0.218218000
C	-2.624367000	-1.167360000	-0.381707000
C	-1.716257000	-0.502848000	0.374241000
C	-2.137262000	-2.270575000	-1.242849000
H	-1.977467000	0.291220000	1.064085000
O	-0.381069000	-0.724272000	0.395922000
O	-2.884615000	-2.970997000	-1.929667000
C	-0.678075000	-2.473723000	-1.220756000
C	0.161482000	-1.706898000	-0.397047000
C	-0.083489000	-3.447614000	-2.043757000
C	1.552750000	-1.891137000	-0.329982000
H	-0.738332000	-4.029815000	-2.683093000
C	1.279582000	-3.645753000	-2.030121000
C	2.101832000	-2.876150000	-1.173903000
C	2.488213000	-1.026034000	0.489722000

H	1.746870000	-4.386022000	-2.671329000
O	3.433064000	-3.071372000	-1.149277000
H	3.465521000	-1.517271000	0.465942000
O	2.559159000	0.251803000	-0.177734000
C	2.124983000	-0.857236000	1.978225000
H	3.775320000	-3.398387000	-2.040158000
C	3.481669000	1.203393000	0.378688000
H	1.132506000	-0.397527000	2.055720000
O	2.134891000	-2.146231000	2.574146000
C	3.129246000	0.096004000	2.627232000
H	3.267983000	2.127338000	-0.171421000
C	4.961024000	0.868735000	0.119939000
C	3.118405000	1.417826000	1.856079000
H	1.871987000	-2.014418000	3.502794000
H	4.131010000	-0.352454000	2.573565000
O	2.876557000	0.369064000	4.003834000
O	5.330846000	1.103151000	-1.229813000
H	5.158229000	-0.186357000	0.339116000
H	5.573001000	1.464362000	0.807299000
H	5.595014000	2.045758000	-1.283146000
H	2.087700000	1.808645000	1.883956000
O	4.002754000	2.352686000	2.467070000
H	1.978460000	0.072033000	4.247624000
H	3.862419000	2.227020000	3.420311000
S	5.096669000	4.846860000	-0.658173000
O	6.105441000	3.744727000	-0.980997000
C	5.863429000	6.399351000	-1.244353000
H	6.869274000	6.481134000	-0.825827000
H	5.918698000	6.338579000	-2.332483000
H	5.243802000	7.249787000	-0.948901000
C	5.225227000	5.180837000	1.131580000
H	6.276767000	5.327061000	1.391430000
H	4.820116000	4.307844000	1.651244000
H	4.635878000	6.070546000	1.370531000
S	-0.827712000	-1.243836000	4.200700000
O	0.602664000	-1.144411000	4.758006000
C	-1.896828000	-1.547628000	5.647754000
H	-1.487048000	-2.379950000	6.224330000
H	-1.893342000	-0.638163000	6.250578000
H	-2.911794000	-1.765715000	5.305942000
C	-0.967769000	-2.893828000	3.433627000
H	-0.799083000	-3.666414000	4.187444000
H	-0.183077000	-2.939069000	2.675333000
H	-1.955248000	-2.993014000	2.976596000

S	-9.536115000	3.037597000	-1.464469000
O	-8.644031000	2.910047000	-0.224210000
C	-10.863505000	1.792273000	-1.280108000
H	-11.468508000	1.770127000	-2.190080000
H	-10.412637000	0.818126000	-1.076196000
H	-11.477021000	2.107139000	-0.434259000
C	-8.652876000	2.226118000	-2.844972000
H	-9.298343000	2.214004000	-3.726868000
H	-8.368971000	1.215638000	-2.544462000
H	-7.761187000	2.822083000	-3.046131000
S	5.199874000	-2.104230000	-3.781668000
O	4.470093000	-3.432469000	-3.487175000
C	6.247975000	-1.752318000	-2.329722000
H	5.681376000	-2.029158000	-1.438732000
H	7.145808000	-2.366172000	-2.418938000
H	6.484039000	-0.686623000	-2.291583000
C	3.994097000	-0.748572000	-3.574123000
H	3.196917000	-0.936699000	-4.295875000
H	3.601330000	-0.710053000	-2.557519000
H	4.501157000	0.191711000	-3.798803000

E = – 3702.9932094 a. u.
H = – 3702.9932094 + 0.772933 (thermal correction 6-31G(d,p)) a. u.
G = – 3702.9932094 + 0.618271 (thermal correction 6-31G(d,p)) a. u.

Transition state - 8-C bond rotation (φ_1 = 22.7°)

H	9.111539000	-0.040734000	-1.219427000
O	8.819838000	-0.986507000	-1.204168000
C	7.470855000	-1.067162000	-1.036884000
C	6.885998000	-2.337740000	-0.959540000
C	6.659400000	0.069151000	-0.921210000
H	7.524184000	-3.211849000	-1.043469000
C	5.514509000	-2.472325000	-0.779918000
H	7.111735000	1.056389000	-0.955326000
C	5.286189000	-0.078118000	-0.741101000
H	5.075980000	-3.459008000	-0.704486000
C	4.679420000	-1.343488000	-0.679709000
H	4.674689000	0.812753000	-0.623771000
C	3.211603000	-1.473518000	-0.536733000
C	2.383970000	-0.605088000	-1.169882000
C	2.592624000	-2.542381000	0.276770000
H	2.723087000	0.171854000	-1.844841000
O	1.040672000	-0.585408000	-1.072792000

O	3.242610000	-3.426923000	0.842368000
C	1.123658000	-2.479684000	0.368758000
C	0.385364000	-1.470265000	-0.270258000
C	0.416252000	-3.447202000	1.099088000
C	-1.016210000	-1.317347000	-0.179531000
H	0.984554000	-4.219639000	1.605473000
C	-0.956425000	-3.419211000	1.117192000
C	-1.686662000	-2.405050000	0.442966000
C	-1.766576000	-0.108064000	-0.795040000
H	-1.523983000	-4.191193000	1.628940000
O	-3.018235000	-2.527799000	0.385061000
H	-1.881994000	-0.273594000	-1.877991000
O	-3.037742000	-0.087686000	-0.131598000
C	-1.192169000	1.338906000	-0.587910000
H	-3.362397000	-3.299324000	0.918830000
C	-4.069461000	0.779923000	-0.602575000
H	-1.051314000	1.464765000	0.495684000
O	0.007030000	1.669431000	-1.287626000
C	-2.238738000	2.364081000	-1.075624000
H	-4.905770000	0.588228000	0.077601000
C	-4.584535000	0.475774000	-2.021028000
C	-3.578133000	2.215303000	-0.382113000
H	-0.110014000	2.611058000	-1.504053000
H	-2.375817000	2.214467000	-2.155151000
O	-1.731057000	3.695964000	-0.958856000
O	-5.465586000	-0.632908000	-2.060751000
H	-3.759641000	0.237930000	-2.699552000
H	-5.059832000	1.388748000	-2.407365000
H	-6.205901000	-0.440840000	-1.452362000
H	-3.428407000	2.357259000	0.699164000
O	-4.516857000	3.170026000	-0.873459000
H	-1.507112000	3.855452000	-0.010426000
H	-4.009850000	3.990338000	-0.980309000
S	-8.478148000	1.154443000	-0.234254000
O	-7.467279000	0.006338000	-0.139530000
C	-9.830848000	0.556302000	-1.308488000
H	-9.407969000	0.174525000	-2.240855000
H	-10.336449000	-0.248091000	-0.771656000
H	-10.531933000	1.372405000	-1.500927000
C	-7.792749000	2.389373000	-1.390513000
H	-7.582549000	1.912619000	-2.351225000
H	-6.862907000	2.772836000	-0.962133000
H	-8.519472000	3.197833000	-1.508259000
S	0.326445000	3.737524000	2.326509000

O	-1.043808000	3.944038000	1.677732000
C	0.840431000	5.377944000	2.949565000
H	0.765205000	6.111100000	2.143081000
H	0.156397000	5.642491000	3.757559000
H	1.862577000	5.317532000	3.331934000
C	1.560626000	3.608485000	0.984248000
H	1.521024000	4.506973000	0.362722000
H	1.305706000	2.730786000	0.383607000
H	2.551723000	3.488441000	1.429512000
S	11.048361000	1.119693000	0.208410000
O	9.962198000	1.421163000	-0.829695000
C	11.993655000	-0.313705000	-0.423109000
H	12.715379000	-0.632129000	0.333465000
H	11.297566000	-1.117129000	-0.675173000
H	12.519317000	0.023763000	-1.318037000
C	10.231426000	0.256014000	1.598937000
H	10.988412000	-0.066169000	2.318541000
H	9.665238000	-0.590985000	1.206077000
H	9.556757000	0.974791000	2.067009000
S	-5.843957000	-3.522039000	1.668381000
O	-4.469886000	-4.210350000	1.761843000
C	-6.185551000	-3.226009000	-0.100354000
H	-5.389009000	-2.634655000	-0.558373000
H	-6.257878000	-4.207911000	-0.572075000
H	-7.137925000	-2.695619000	-0.178584000
C	-5.609957000	-1.777147000	2.160051000
H	-5.481181000	-1.761601000	3.243981000
H	-4.716047000	-1.396143000	1.660677000
H	-6.491915000	-1.204214000	1.862662000

E = – 3702.9613848 a. u.
H = – 3702.9613848 + 0.771807 (thermal correction 6-31G(d,p)) a. u.
G = – 3702.9613848 + 0.619813 (thermal correction 6-31G(d,p)) a. u.
f = 32.63*i*

Transition state - 8-C bond rotation (φ_1 = –171.4°)

H	8.783343000	-0.062504000	-0.860416000
O	8.385709000	-0.712942000	-1.491966000
C	7.042796000	-0.806475000	-1.290625000
C	6.312569000	-1.698971000	-2.086239000
C	6.375514000	-0.061700000	-0.308237000
H	6.839061000	-2.276998000	-2.839307000
C	4.940387000	-1.837178000	-1.913210000

H	6.940150000	0.614193000	0.327591000
C	5.001202000	-0.210579000	-0.141645000
H	4.389982000	-2.541443000	-2.523744000
C	4.249709000	-1.085586000	-0.944038000
H	4.507465000	0.350213000	0.647485000
C	2.781692000	-1.187917000	-0.782409000
C	2.046419000	-0.090744000	-0.472563000
C	2.055943000	-2.458314000	-0.941452000
H	2.468710000	0.903103000	-0.378710000
O	0.720230000	-0.051507000	-0.248674000
O	2.594994000	-3.518072000	-1.274374000
C	0.604792000	-2.390276000	-0.659382000
C	-0.042674000	-1.183303000	-0.323674000
C	-0.140695000	-3.575591000	-0.706007000
C	-1.438223000	-1.100431000	-0.050268000
H	0.382501000	-4.489252000	-0.965287000
C	-1.485422000	-3.550807000	-0.424076000
C	-2.120962000	-2.334808000	-0.096169000
C	-2.181089000	0.189692000	0.402209000
H	-2.084735000	-4.456279000	-0.441800000
O	-3.446472000	-2.356121000	0.185042000
H	-2.361916000	0.100710000	1.486145000
O	-1.295983000	1.269046000	0.148707000
C	-3.612545000	0.388746000	-0.227430000
H	-3.751645000	-3.255408000	0.493640000
C	-1.791028000	2.604534000	0.183379000
H	-3.692873000	-0.243001000	-1.120234000
O	-4.573280000	0.010274000	0.762418000
C	-3.968820000	1.833762000	-0.676294000
H	-0.906651000	3.214660000	-0.034893000
C	-2.331694000	3.052219000	1.552241000
C	-2.775815000	2.714625000	-0.979164000
H	-5.426864000	-0.071817000	0.298540000
H	-4.502171000	2.288994000	0.169624000
O	-4.803352000	1.854442000	-1.833287000
O	-1.306991000	3.189744000	2.512807000
H	-3.044969000	2.313529000	1.936701000
H	-2.883882000	3.990818000	1.403775000
H	-0.924700000	4.078301000	2.376082000
H	-2.267289000	2.340811000	-1.880463000
O	-3.196161000	4.064356000	-1.175592000
H	-5.634414000	1.394519000	-1.604778000
H	-3.979969000	4.002380000	-1.742642000
S	0.018533000	6.169291000	0.493283000

O	-0.636080000	5.836664000	1.830763000
C	0.896159000	7.754433000	0.747854000
H	0.203105000	8.484108000	1.173449000
H	1.707462000	7.560625000	1.451483000
H	1.303273000	8.106667000	-0.203361000
C	-1.295337000	6.806950000	-0.604240000
H	-1.854439000	7.583689000	-0.076063000
H	-1.949807000	5.965443000	-0.848210000
H	-0.837762000	7.205135000	-1.514284000
S	-6.885955000	-1.055276000	-2.178057000
O	-6.787767000	0.001892000	-1.063399000
C	-8.667276000	-1.417986000	-2.340712000
H	-9.077456000	-1.652693000	-1.355966000
H	-9.142906000	-0.520169000	-2.738563000
H	-8.805203000	-2.251365000	-3.034169000
C	-6.373987000	-2.638843000	-1.438080000
H	-6.985399000	-2.850995000	-0.558101000
H	-5.327899000	-2.531282000	-1.142691000
H	-6.478421000	-3.430165000	-2.184850000
S	10.667213000	-0.416819000	1.019427000
O	9.731641000	0.633280000	0.411408000
C	11.519481000	-1.230646000	-0.380118000
H	12.118797000	-2.063567000	-0.003680000
H	10.772877000	-1.569003000	-1.102518000
H	12.169665000	-0.480870000	-0.834134000
C	9.630089000	-1.841269000	1.510186000
H	10.274175000	-2.645190000	1.875557000
H	9.034912000	-2.164824000	0.654079000
H	8.975670000	-1.496212000	2.312312000
S	-4.606162000	-4.090343000	2.850681000
O	-4.470256000	-4.455799000	1.361746000
C	-5.404969000	-2.449931000	2.936645000
H	-4.901238000	-1.740874000	2.270622000
H	-6.442360000	-2.590396000	2.625696000
H	-5.383261000	-2.107346000	3.974756000
C	-2.951436000	-3.583001000	3.435436000
H	-2.298089000	-4.450867000	3.332272000
H	-2.577467000	-2.755479000	2.830179000
H	-3.023951000	-3.295234000	4.487223000

E = – 3702.9648026 a. u.
H = – 3702.9648026 + 0.771461 (thermal correction 6-31G(d,p)) a. u.
G = – 3702.9648026 + 0.617405 (thermal correction 6-31G(d,p)) a. u.
f = 32.85i

5 Prunetin-8-C-glucoside, *n* = 3 (DMSO)

a H–C_7 eclipsed

H	-7.844602000	-1.530509000	0.185672000
O	-7.512781000	-1.282792000	-0.715900000
C	-6.254400000	-0.777960000	-0.635741000
C	-5.628196000	-0.365395000	-1.820199000
C	-5.574267000	-0.640007000	0.582867000
H	-6.165430000	-0.469930000	-2.757503000
C	-4.344795000	0.165666000	-1.789856000
H	-6.064420000	-0.935660000	1.505878000
C	-4.289367000	-0.104730000	0.601407000
H	-3.878668000	0.490950000	-2.711630000
C	-3.641243000	0.297257000	-0.578165000
H	-3.789932000	0.026064000	1.557671000
C	-2.252887000	0.810237000	-0.537429000
C	-1.340264000	0.253317000	0.299588000
C	-1.801279000	1.928107000	-1.376179000
H	-1.554893000	-0.599843000	0.931919000
O	-0.064743000	0.658221000	0.465769000
O	-2.548461000	2.490811000	-2.211139000
C	-0.424810000	2.353419000	-1.185018000
C	0.424659000	1.712979000	-0.260255000
C	0.108463000	3.437747000	-1.935938000
C	1.754621000	2.076465000	-0.040930000
O	-0.644443000	4.086242000	-2.830811000
C	1.430135000	3.831924000	-1.741561000
C	2.233470000	3.160676000	-0.810891000
C	2.647470000	1.374392000	0.957571000
H	-1.539133000	3.638469000	-2.807622000
H	1.801812000	4.659229000	-2.330126000
O	3.527776000	3.512625000	-0.587967000
H	3.611486000	1.893081000	0.949705000
O	2.035692000	1.487277000	2.255928000
C	2.933540000	-0.105154000	0.606724000
C	4.079184000	4.614425000	-1.296316000
C	2.787901000	0.954075000	3.351090000
H	1.984290000	-0.651505000	0.566652000
O	3.599409000	-0.166181000	-0.643887000
C	3.790945000	-0.710593000	1.719892000
H	5.105464000	4.710411000	-0.939825000
H	4.085605000	4.434733000	-2.377825000

H	3.533958000	5.541954000	-1.086252000
H	2.110839000	1.013348000	4.209758000
C	4.017567000	1.806666000	3.718814000
C	3.101291000	-0.526318000	3.070455000
H	3.134117000	-0.826957000	-1.202375000
H	4.758303000	-0.187249000	1.729485000
O	4.022168000	-2.107127000	1.568108000
O	4.504721000	1.480196000	5.007805000
H	3.703290000	2.855345000	3.739883000
H	4.808755000	1.719217000	2.957063000
H	4.636612000	0.517461000	4.996771000
H	2.144270000	-1.070774000	3.031281000
O	3.918631000	-1.069688000	4.108105000
H	4.834250000	-2.217723000	1.013478000
H	4.306178000	-1.868301000	3.712184000
S	6.137037000	-2.032788000	-1.400975000
C	7.640085000	-2.784381000	-2.119540000
H	7.676171000	-2.579501000	-3.192566000
H	8.522301000	-2.385139000	-1.613770000
H	7.572984000	-3.860179000	-1.949023000
C	6.575775000	-0.290527000	-1.714194000
H	6.680773000	-0.136284000	-2.791611000
H	7.505402000	-0.054668000	-1.190249000
H	5.739507000	0.293348000	-1.327260000
O	6.279494000	-2.264988000	0.108360000
S	1.273425000	-2.974723000	-1.235745000
C	2.143720000	-4.212915000	-0.217986000
H	2.815068000	-4.796561000	-0.852977000
H	2.716311000	-3.649326000	0.525004000
H	1.406885000	-4.856890000	0.270002000
C	0.549309000	-4.122618000	-2.458129000
H	1.354076000	-4.671340000	-2.952952000
H	0.008423000	-3.517084000	-3.187104000
H	-0.140574000	-4.804404000	-1.954493000
O	2.342491000	-2.188723000	-1.998787000
S	-10.030386000	-0.778456000	1.522137000
C	-10.834791000	-1.248341000	-0.052016000
H	-10.105060000	-1.174565000	-0.861830000
H	-11.694290000	-0.596566000	-0.228232000
H	-11.169360000	-2.281106000	0.059621000
C	-9.513806000	0.902734000	1.020434000
H	-10.402065000	1.514078000	0.842078000
H	-8.890677000	0.833296000	0.126518000
H	-8.937616000	1.318835000	1.848506000

O	-8.756179000	-1.624521000	1.629219000

E = – 3264.2603266 a. u.
H = – 3264.2603266 + 0.719958 (thermal correction 6-31G(d,p)) a. u.
G = – 3264.2603266 + 0.575831 (thermal correction 6-31G(d,p)) a. u.

Transition state - 8-C bond rotation (φ_1 = 15.0°)

H	-7.169526000	-0.428804000	-0.820501000
O	-6.984779000	0.502340000	-1.106233000
C	-5.658000000	0.782114000	-1.008127000
C	-5.223455000	2.069452000	-1.351128000
C	-4.722010000	-0.163104000	-0.566443000
H	-5.957092000	2.795742000	-1.686493000
C	-3.877549000	2.404261000	-1.264609000
H	-5.058510000	-1.155352000	-0.278423000
C	-3.375153000	0.181078000	-0.481129000
H	-3.556570000	3.406058000	-1.521253000
C	-2.922425000	1.463291000	-0.838757000
H	-2.661976000	-0.551043000	-0.110353000
C	-1.478570000	1.782358000	-0.775947000
C	-0.557699000	0.848206000	-1.123996000
C	-0.966029000	3.076794000	-0.322293000
H	-0.813101000	-0.122896000	-1.527315000
O	0.776077000	0.979839000	-1.015404000
O	-1.717436000	4.042957000	-0.042897000
C	0.479040000	3.186459000	-0.194521000
C	1.339892000	2.106222000	-0.486212000
C	1.067867000	4.395237000	0.253974000
C	2.733567000	2.097147000	-0.306151000
O	0.319072000	5.455106000	0.577679000
C	2.450627000	4.481001000	0.323386000
C	3.275243000	3.385902000	0.012850000
C	3.584358000	0.805050000	-0.487626000
H	-0.627937000	5.170792000	0.419181000
H	2.873282000	5.434215000	0.605988000
O	4.617351000	3.558768000	-0.019801000
H	3.671055000	0.574433000	-1.562296000
O	4.854354000	1.135095000	0.073149000
C	3.047146000	-0.504686000	0.212005000
C	5.176800000	4.829231000	0.276966000
C	5.913589000	0.184653000	0.092788000
H	2.656498000	-0.221052000	1.199325000
O	2.070582000	-1.200425000	-0.547700000

C	4.166983000	-1.542865000	0.420225000
H	6.254407000	4.700922000	0.166537000
H	4.830457000	5.602315000	-0.419778000
H	4.955332000	5.143794000	1.303999000
H	6.740575000	0.711411000	0.580827000
C	6.430999000	-0.221680000	-1.298310000
C	5.454977000	-0.973030000	0.980906000
H	1.218486000	-1.191586000	-0.065695000
H	4.383704000	-1.974416000	-0.566147000
O	3.748946000	-2.588982000	1.292487000
O	7.672339000	-0.897127000	-1.201552000
H	6.597153000	0.692873000	-1.877429000
H	5.687941000	-0.822070000	-1.847321000
H	7.537087000	-1.603574000	-0.547635000
H	5.260515000	-0.572253000	1.987510000
O	6.447641000	-1.998146000	1.048942000
H	3.374585000	-3.310215000	0.730319000
H	5.962238000	-2.784068000	1.349922000
S	1.535936000	-4.378293000	-1.048391000
C	1.149140000	-6.043956000	-1.693739000
H	0.233668000	-6.003808000	-2.289521000
H	1.990531000	-6.403783000	-2.290452000
H	1.003054000	-6.696484000	-0.831331000
C	1.828051000	-3.569439000	-2.657322000
H	0.915001000	-3.622313000	-3.256537000
H	2.658763000	-4.067995000	-3.162953000
H	2.072512000	-2.532278000	-2.424012000
O	2.901115000	-4.537648000	-0.369675000
S	-0.023973000	-1.145981000	2.451217000
C	0.883797000	-2.564027000	3.152841000
H	0.353873000	-3.488074000	2.908766000
H	1.875653000	-2.562175000	2.689617000
H	0.968285000	-2.433823000	4.235175000
C	-1.642838000	-1.463388000	3.231660000
H	-1.983372000	-2.464627000	2.957638000
H	-2.335270000	-0.714600000	2.843070000
H	-1.550474000	-1.361872000	4.315908000
O	-0.226333000	-1.450192000	0.959839000
S	-9.257138000	-1.377503000	0.522302000
C	-10.181931000	-0.503204000	-0.791898000
H	-9.552819000	0.285067000	-1.212141000
H	-11.106115000	-0.095522000	-0.374278000
H	-10.417244000	-1.243976000	-1.558060000
C	-8.926071000	0.080286000	1.576773000

H	-9.873420000	0.485113000	1.941546000
H	-8.370021000	0.817688000	0.993508000
H	-8.323467000	-0.266979000	2.417840000
O	-7.916053000	-1.795651000	-0.090807000

E = – 3264.2318614 a. u.
H = – 3264.2318614 + 0.718417 (thermal correction 6-31G(d,p)) a. u.
G = – 3264.2318614 + 0.578095 (thermal correction 6-31G(d,p)) a. u.
f = 35.45*i*

Transition state - 8-C bond rotation (φ_1 = –164.7°)

H	-9.084880000	0.888741000	0.947194000
O	-8.704138000	0.073504000	1.362752000
C	-7.386247000	-0.047217000	1.054483000
C	-6.690028000	-1.159442000	1.547320000
C	-6.710551000	0.883855000	0.252739000
H	-7.222895000	-1.876496000	2.163701000
C	-5.343661000	-1.334320000	1.252970000
H	-7.249996000	1.737174000	-0.147715000
C	-5.362048000	0.696461000	-0.038228000
H	-4.821616000	-2.203437000	1.633129000
C	-4.645848000	-0.404001000	0.460558000
H	-4.862819000	1.411054000	-0.687111000
C	-3.200168000	-0.553484000	0.179735000
C	-2.381572000	0.528442000	0.146649000
C	-2.577872000	-1.847286000	-0.097761000
H	-2.717115000	1.537044000	0.358588000
O	-1.069259000	0.522225000	-0.137434000
O	-3.227862000	-2.922176000	-0.076771000
C	-1.156731000	-1.832221000	-0.416136000
C	-0.392884000	-0.637936000	-0.403091000
C	-0.516623000	-3.044060000	-0.790295000
C	0.995696000	-0.583575000	-0.672225000
O	-1.174628000	-4.206490000	-0.798785000
C	0.809838000	-3.006646000	-1.195001000
C	1.526747000	-1.804681000	-1.171896000
C	1.862546000	0.697288000	-0.504780000
H	-2.111321000	-3.983271000	-0.511202000
H	1.260030000	-3.926498000	-1.539883000
O	2.786346000	-1.750334000	-1.661969000
H	2.021163000	1.156643000	-1.494288000
O	1.079718000	1.547648000	0.339789000
C	3.282123000	0.536890000	0.161111000

C	3.414994000	-2.930833000	-2.147160000
C	1.532988000	2.857241000	0.667633000
H	3.179025000	-0.140860000	1.018003000
O	4.311190000	0.103881000	-0.714318000
C	3.815177000	1.886418000	0.679371000
H	4.408581000	-2.617110000	-2.467108000
H	3.521653000	-3.680803000	-1.357636000
H	2.867527000	-3.352410000	-2.998159000
H	0.744532000	3.265523000	1.308955000
C	1.640678000	3.811989000	-0.534741000
C	2.815040000	2.690785000	1.484631000
H	4.521557000	-0.828423000	-0.508975000
H	4.089280000	2.477558000	-0.208147000
O	4.956827000	1.712325000	1.505801000
O	1.783854000	5.154411000	-0.107170000
H	0.708603000	3.744207000	-1.105903000
H	2.457285000	3.516280000	-1.212762000
H	2.512900000	5.147916000	0.536049000
H	2.566912000	2.130685000	2.398533000
O	3.379219000	3.958423000	1.829367000
H	5.736483000	1.551689000	0.932537000
H	4.300063000	3.756035000	2.063412000
S	7.467186000	0.681179000	-1.285330000
C	9.110958000	1.221818000	-1.876651000
H	9.271841000	0.861613000	-2.895960000
H	9.170916000	2.311624000	-1.830940000
H	9.852300000	0.783128000	-1.206695000
C	6.467673000	1.636423000	-2.476130000
H	6.730908000	1.327812000	-3.491400000
H	6.658124000	2.702434000	-2.328603000
H	5.430115000	1.383219000	-2.255304000
O	7.313350000	1.350277000	0.085929000
S	5.444522000	-2.006369000	1.851404000
C	7.149953000	-1.407532000	2.095343000
H	7.849620000	-2.112833000	1.639196000
H	7.218995000	-0.431645000	1.606925000
H	7.339704000	-1.306319000	3.167310000
C	5.662202000	-3.656616000	2.606971000
H	6.445942000	-4.197868000	2.071580000
H	4.711598000	-4.182908000	2.505594000
H	5.913979000	-3.545521000	3.664714000
O	5.269537000	-2.270731000	0.351975000
S	-11.073907000	1.174127000	-0.828682000
C	-11.894687000	0.036983000	0.346489000

H	-11.130174000	-0.530305000	0.882771000
H	-12.572653000	-0.622145000	-0.201656000
H	-12.461684000	0.656417000	1.043498000
C	-10.174080000	-0.101839000	-1.781653000
H	-10.895114000	-0.737535000	-2.301900000
H	-9.549215000	-0.683414000	-1.100884000
H	-9.550484000	0.422897000	-2.507250000
O	-10.027422000	1.953248000	-0.024417000

E = – 3264.2314961 a. u.
H = – 3264.2314961 + 0.718163 (thermal correction 6-31G(d,p)) a. u.
G = – 3264.2314961 + 0.577767 (thermal correction 6-31G(d,p)) a. u.
f = 32.45*i*