Polyketides and a Dihydroquinolone Alkaloid from a Marine-Derived Strain of the Fungus *Metarhizium marquandii*

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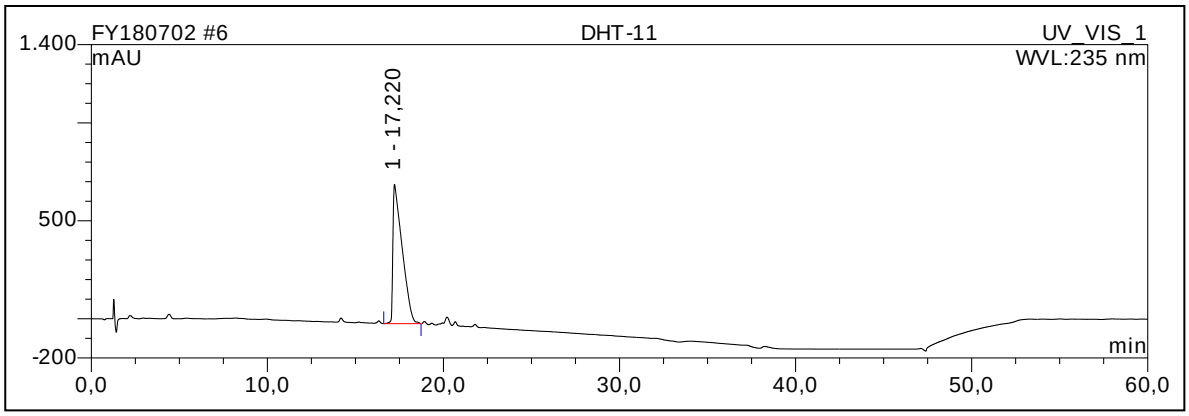
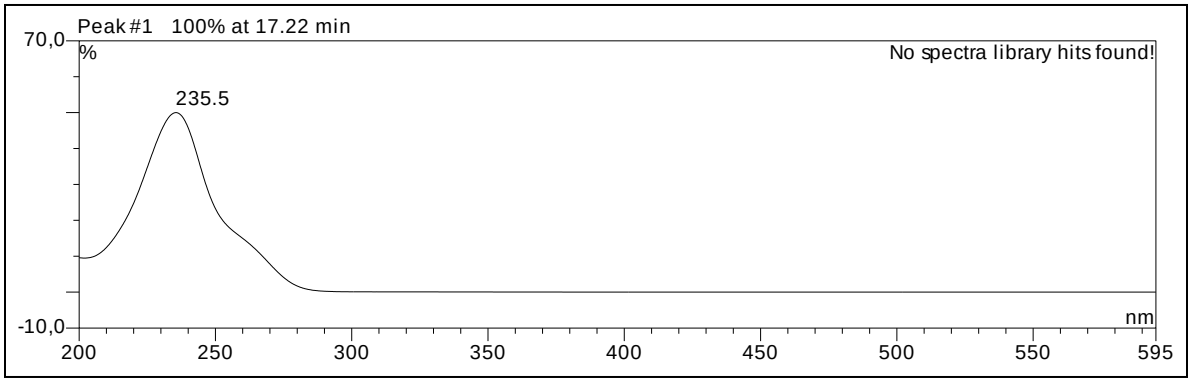
* The ^{1}H and ^{13}C NMR spectra for this study were recorded at 600 MHz and 150 MHz, respectively.

Figure S1. HPLC chromatogram (A), UV (B) and HRESIMS spectrum (C) of compound **1**.



A)



B)

C)

Mass Spectrum SmartFormula Report

Analysis Info

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Method	tune_low_new.m	Operator	Peter Tommes
Sample Name	D. Hassouna Mm-8-2-P5 (CH3OH)	Instrument	maXis 288882.20213
Comment	10 ul in 1 ml		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
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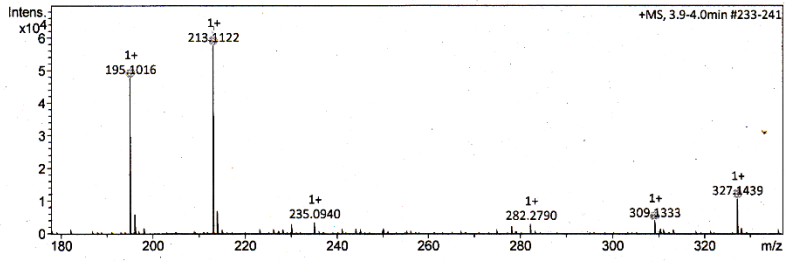
Scan End	1500 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
195.1016	1	C11H15O3	195.1016	-0.3	3.3	1	100.00	4.5	even	ok
213.1122	1	C11H17O4	213.1121	-0.1	0.9	1	100.00	3.5	even	ok
309.1333	1	C16H21O6	309.1333	0.0	15.5	1	100.00	6.5	even	ok
327.1439	1	C16H23O7	327.1438	-0.1	4.1	1	100.00	5.5	even	ok

Figure S2. ^{1}H NMR spectrum of compound **1** in DMSO-d_6

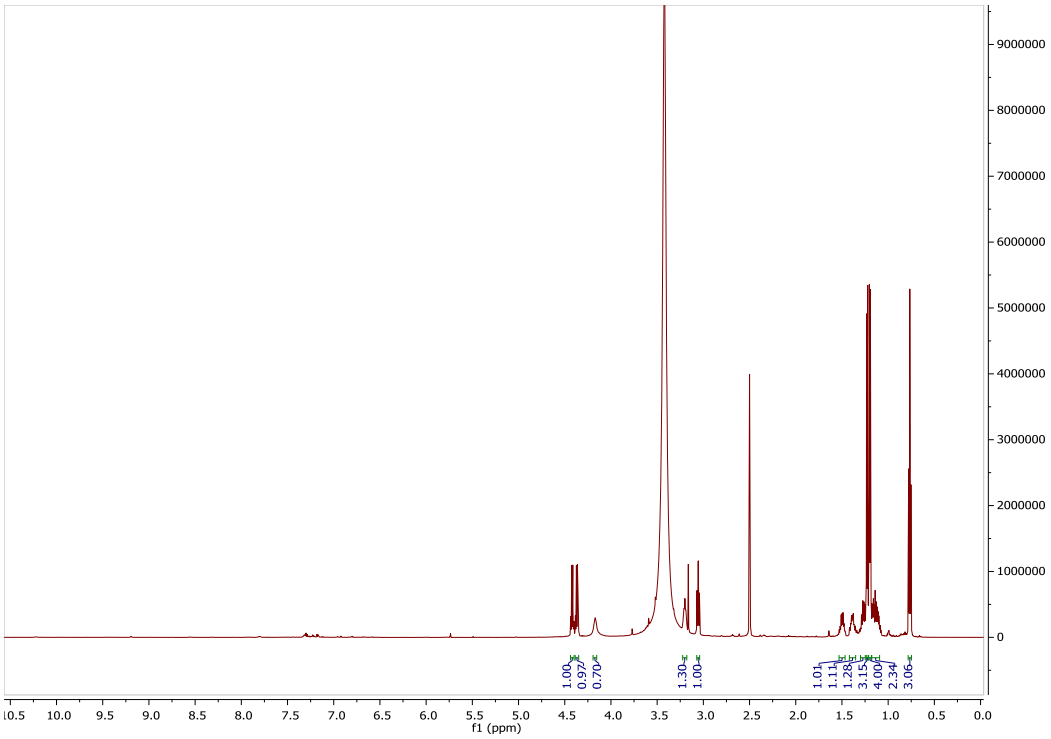


Figure S3. ^{13}C NMR spectrum of compound **1** in DMSO-d_6

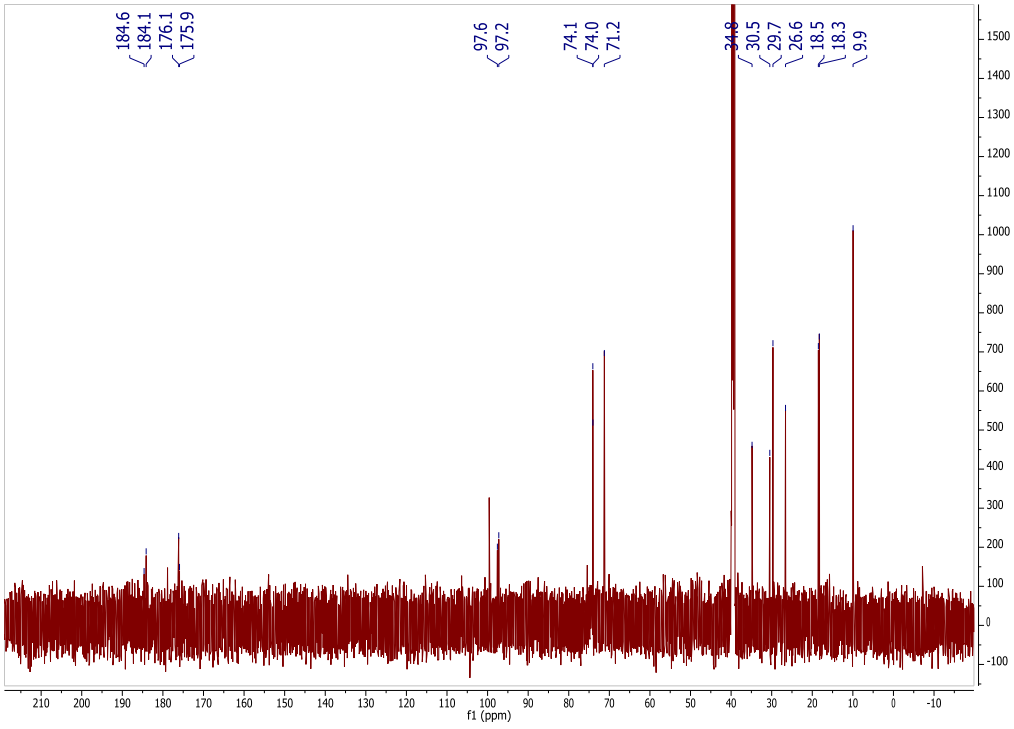


Figure S4. COSY spectrum of compound **1** in DMSO-d_6

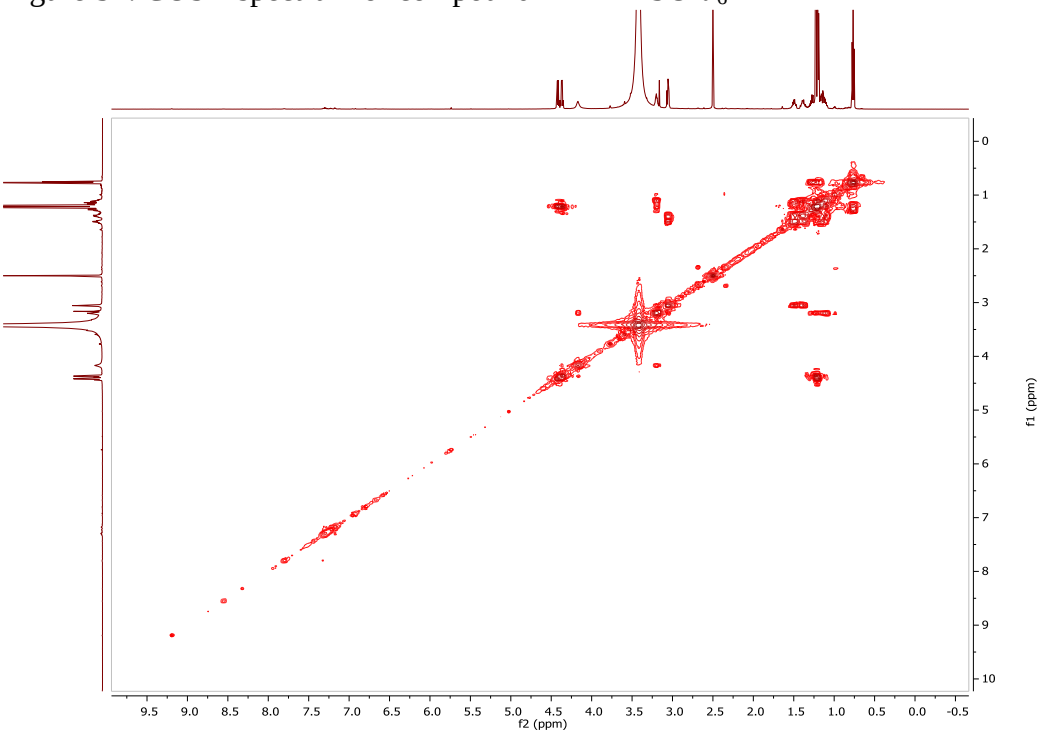


Figure S5. HSQC spectrum of compound **1** in DMSO-d_6

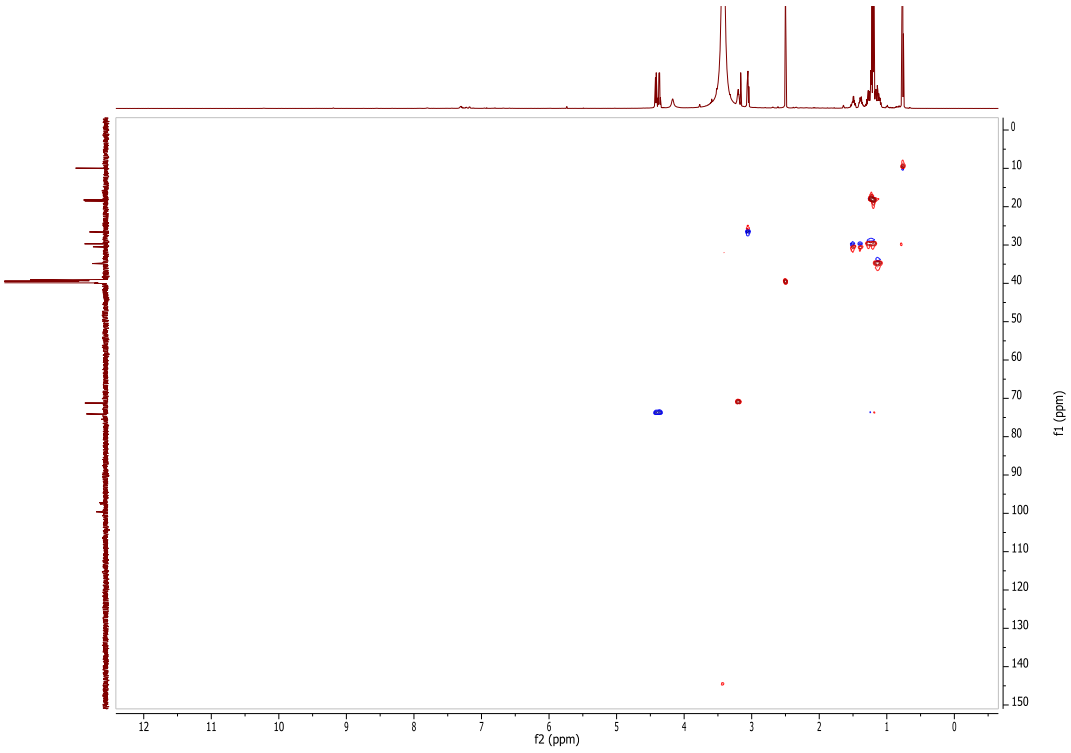


Figure S6. HMBC spectrum of compound **1** in DMSO-d_6

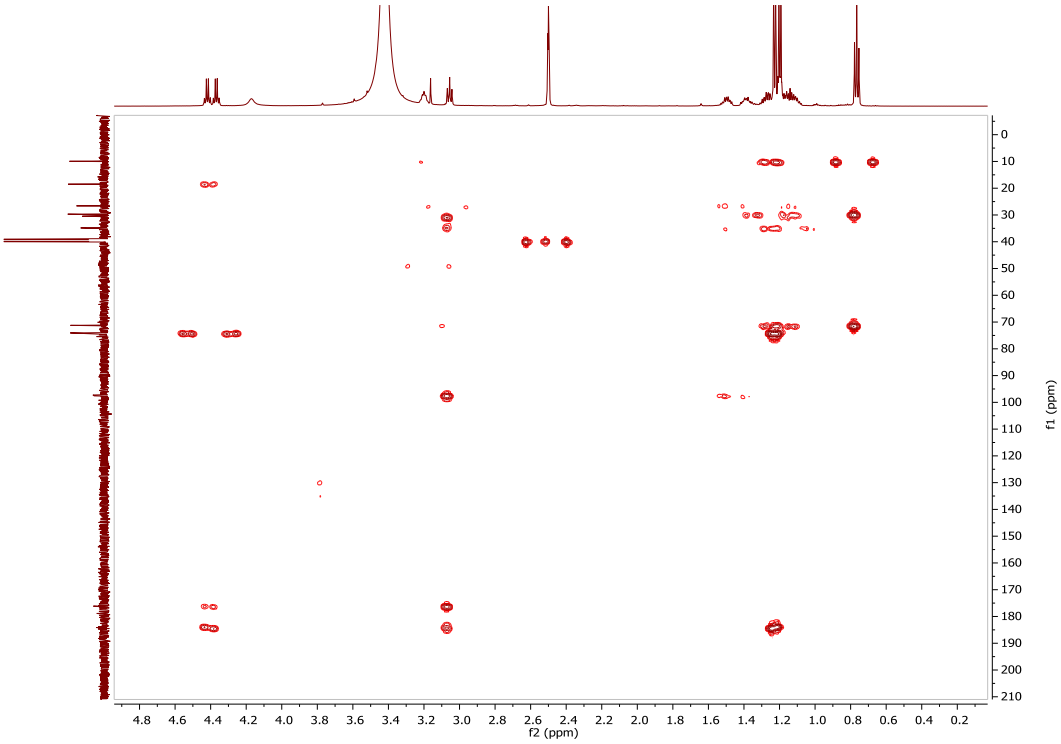


Figure S7. Comparison of ^{1}H NMR spectra of (*S*)-MPA and (*R*)-MPA esters of compound **1**

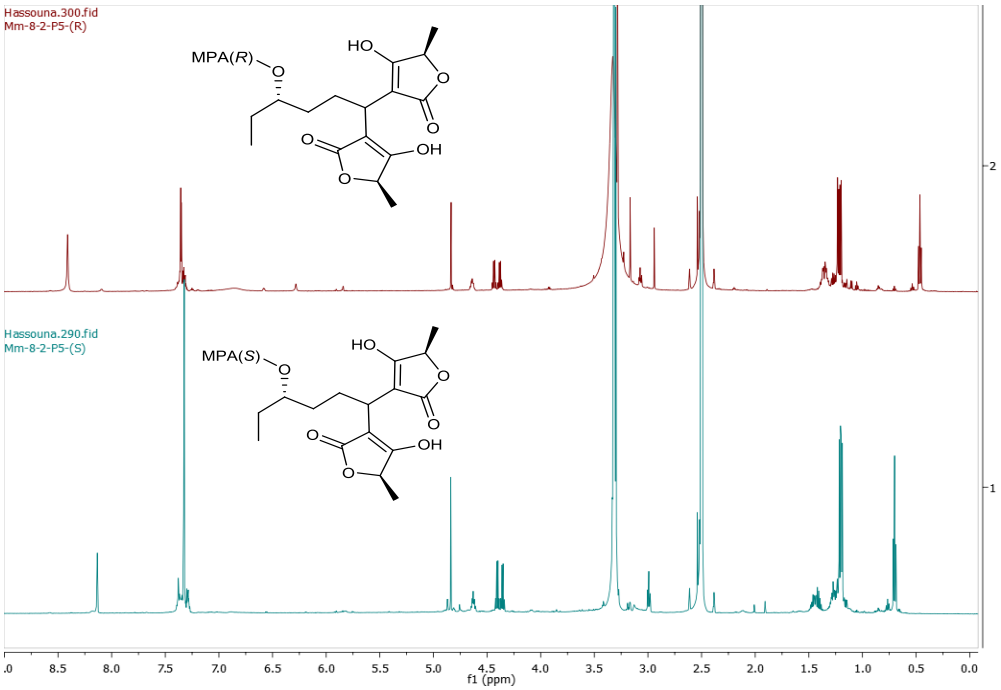
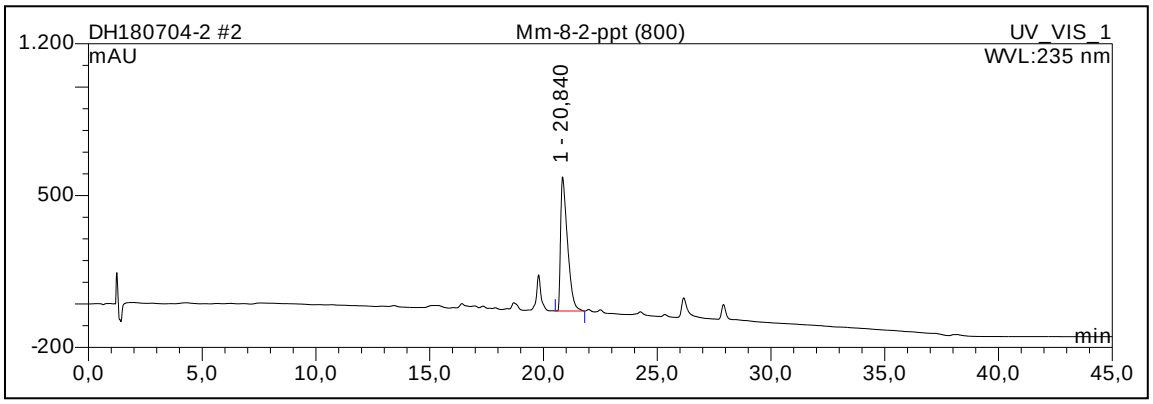


Figure S8. HPLC chromatogram (A), UV (B) and HRESIMS spectrum (C) of compound **2**

A)



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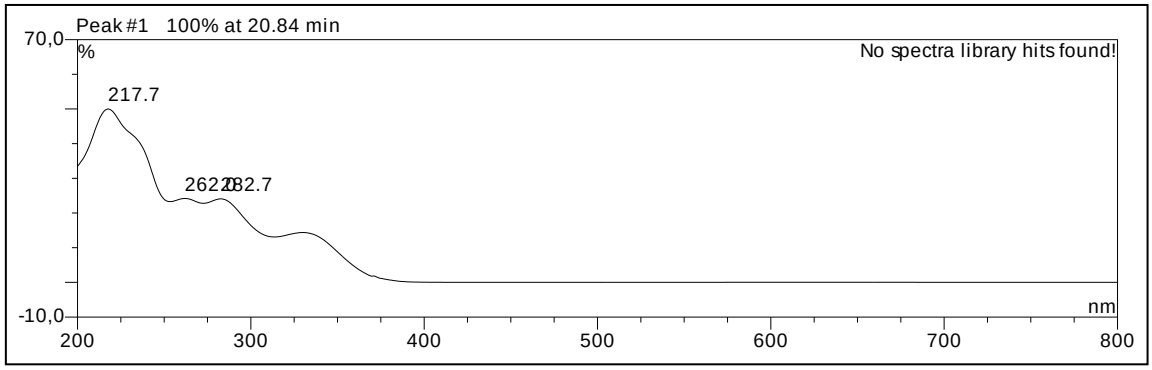
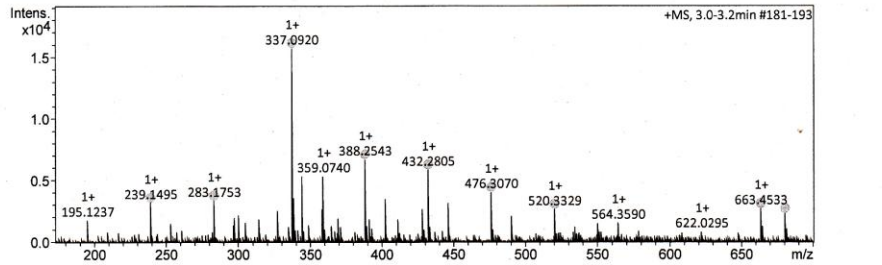


C)



Mass Spectrum SmartFormula Report

Analysis Info

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Sample Name	D. Hassouna Mm-8-2-PPt in H2O (CH3OH)	Instrument	maXis 288882.20213
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
239.1495	1	C11H19N4O2	239.1503	3.2	20.8	1	100.00	4.5	even	ok
	2	C10H23O6	239.1489	-2.4	32.3	2	83.57	-0.5	even	ok
	3	C9H20N4NaO2	239.1478	-6.9	32.7	3	43.96	1.5	even	ok
283.1753	1	C9H19N10O	283.1738	-5.4	6.5	1	54.24	5.5	even	ok
	2	C11H24N4NaO3	283.1741	-4.4	9.0	2	62.12	1.5	even	ok
	3	C12H27O7	283.1751	-0.7	13.3	3	100.00	-0.5	even	ok
	4	C13H23N4O3	283.1765	4.1	18.2	4	55.42	4.5	even	ok
337.0920	1	C16H17O8	337.0918	-0.6	7.1	1	100.00	8.5	even	ok
	2	C15H14N4NaO4	337.0907	-3.8	10.8	2	53.44	10.5	even	ok

Figure S9. ^{1}H NMR spectrum of compound **2** in DMSO-d_6

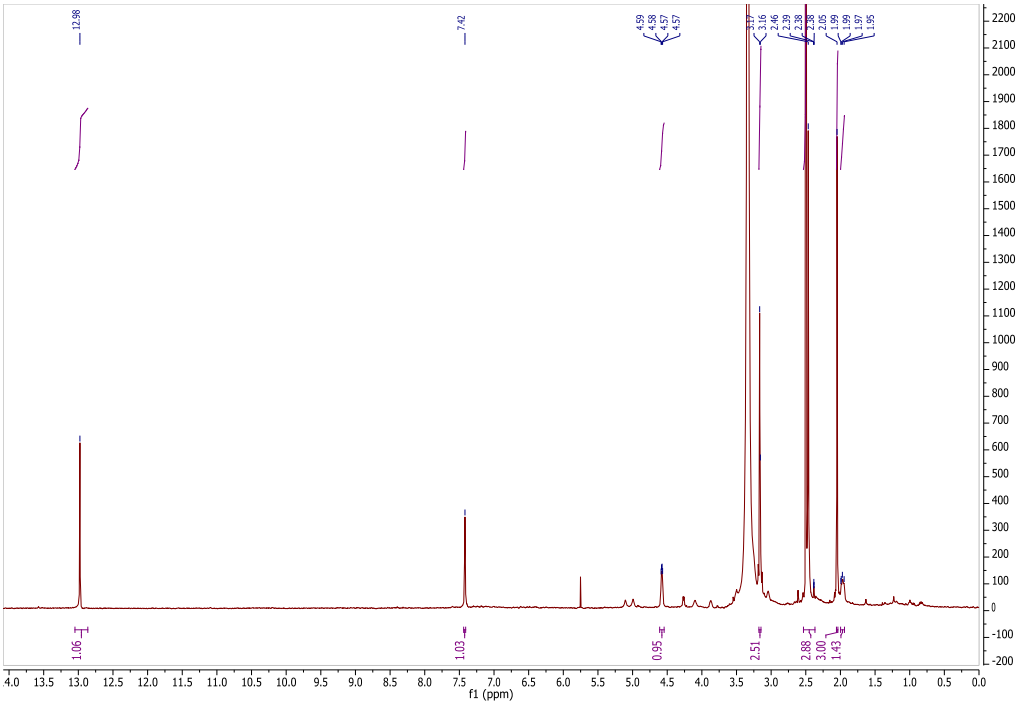


Figure S10. COSY spectrum of compound **2** in DMSO-d_6

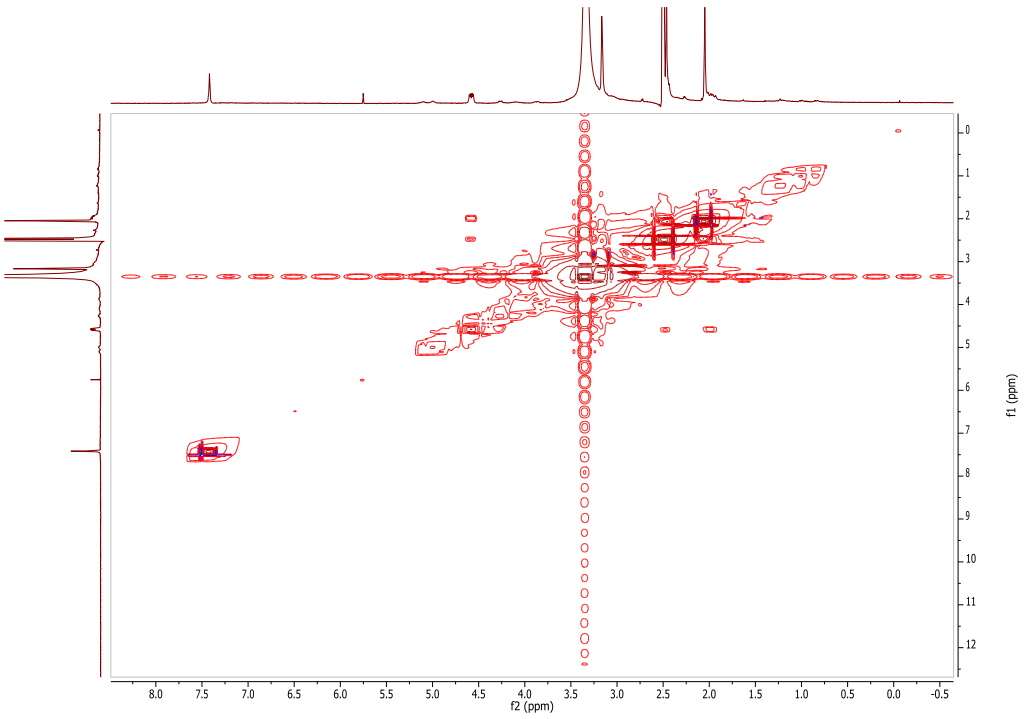


Figure S11. HSQC spectrum of compound **2** in DMSO-*d*6

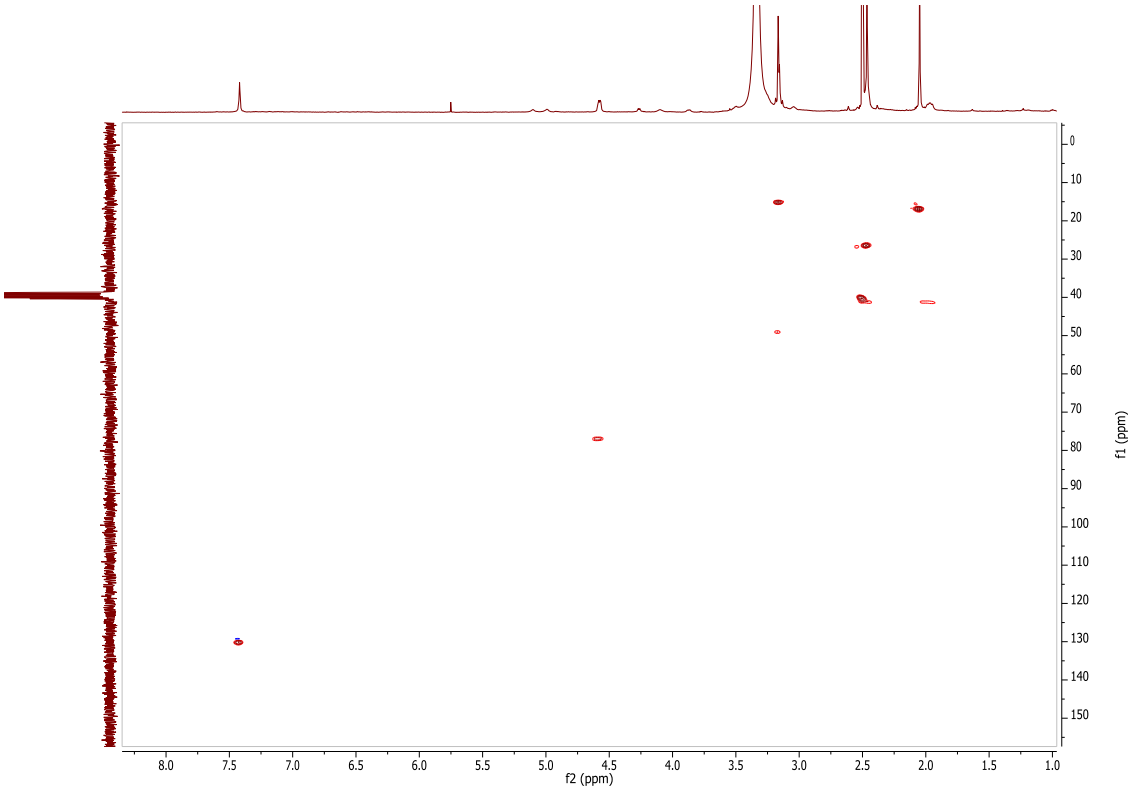


Figure S12. HMBC spectrum of compound **2** in DMSO-*d*6

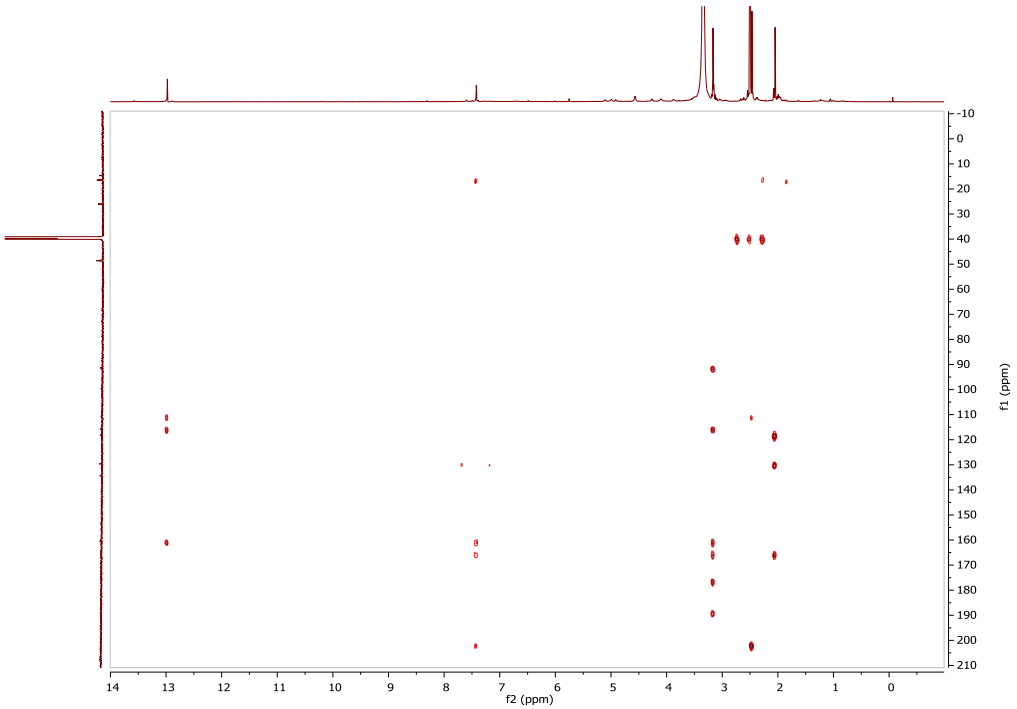


Figure S13. HMBC spectrum of compound **2** in D_2O

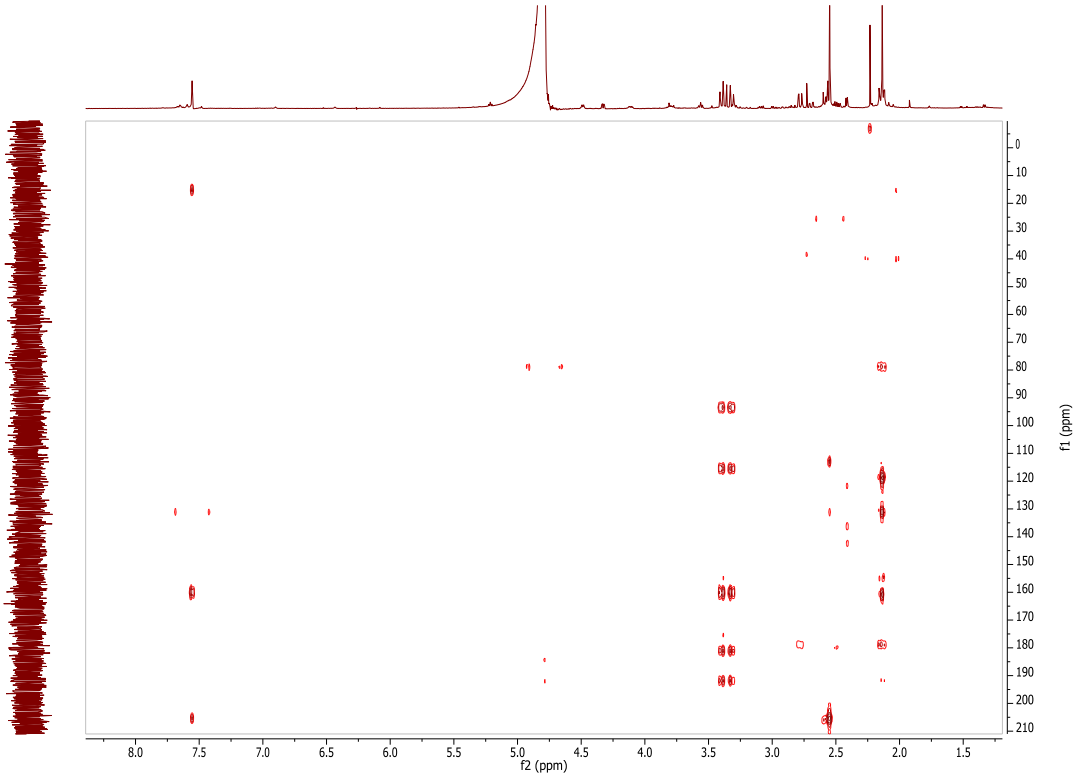
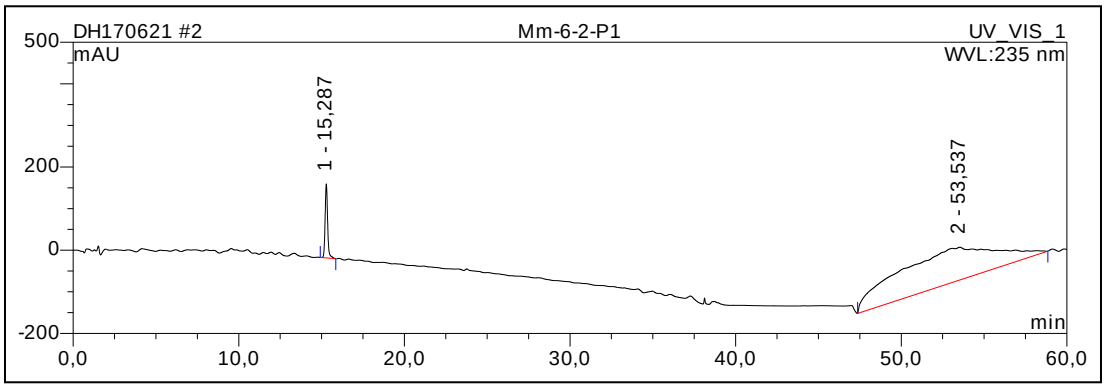
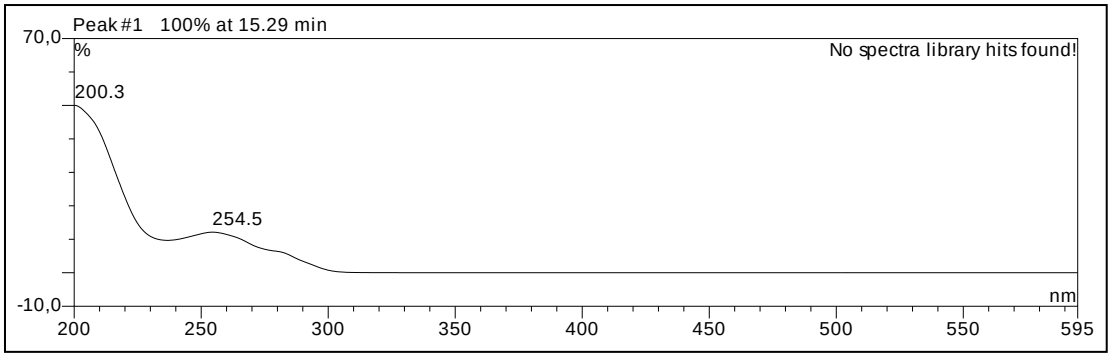


Figure S14. HPLC chromatogram (A), UV (B) and HRESIMS spectrum (C) of compound **3**



A)



B)

Mass Spectrum SmartFormula Report

Analysis Info

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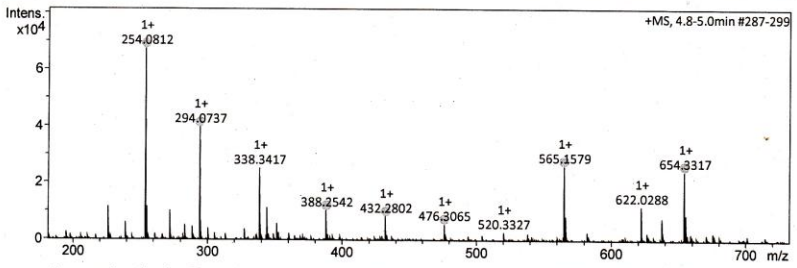
Method	tune_low_new.m	Operator	Peter Tommes
Sample Name	D. Hassouna Mm-6-2-P1 (CH3OH)	Instrument	maXis 288882.20213
Comment	5 ul in 1 ml		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
254.0812	1	C15H12NO3	254.0812	-0.2	3.8	1	100.00	10.5	even	ok
294.0737	1	C15H13NNaO4	294.0737	-0.2	1.3	1	100.00	9.5	even	ok
	2	C13H8N7O2	294.0734	-1.1	1.6	2	88.24	13.5	even	ok
388.2542	1	C16H31N9NaO	388.2544	0.6	16.6	1	100.00	5.5	even	ok
432.2802	1	C18H35N9NaO2	432.2806	1.0	20.5	1	90.38	5.5	even	ok
	2	C16H30N15	432.2803	0.3	21.6	2	100.00	9.5	even	ok
476.3065	1	C19H43N5NaO7	476.3055	-2.1	13.7	1	85.70	0.5	even	ok
	2	C20H39N9NaO3	476.3068	0.7	27.2	2	88.71	5.5	even	ok
	3	C18H34N15O	476.3065	0.2	27.2	3	100.00	9.5	even	ok
	4	C33H38N3	476.3060	-0.9	82.4	4	19.31	16.5	even	ok
565.1579	1	C30H26N2NaO8	565.1581	0.4	8.3	1	94.66	18.5	even	ok
	2	C28H21N8O6	565.1579	-0.1	8.3	2	100.00	22.5	even	ok
	3	C27H18N12NaO2	565.1568	-2.0	11.1	3	55.49	24.5	even	ok
	4	C44H21O	565.1587	1.3	81.4	4	8.65	34.5	even	ok

C)

Figure S15.[1]H NMR spectrum of compound **3** in DMSO-*d*6

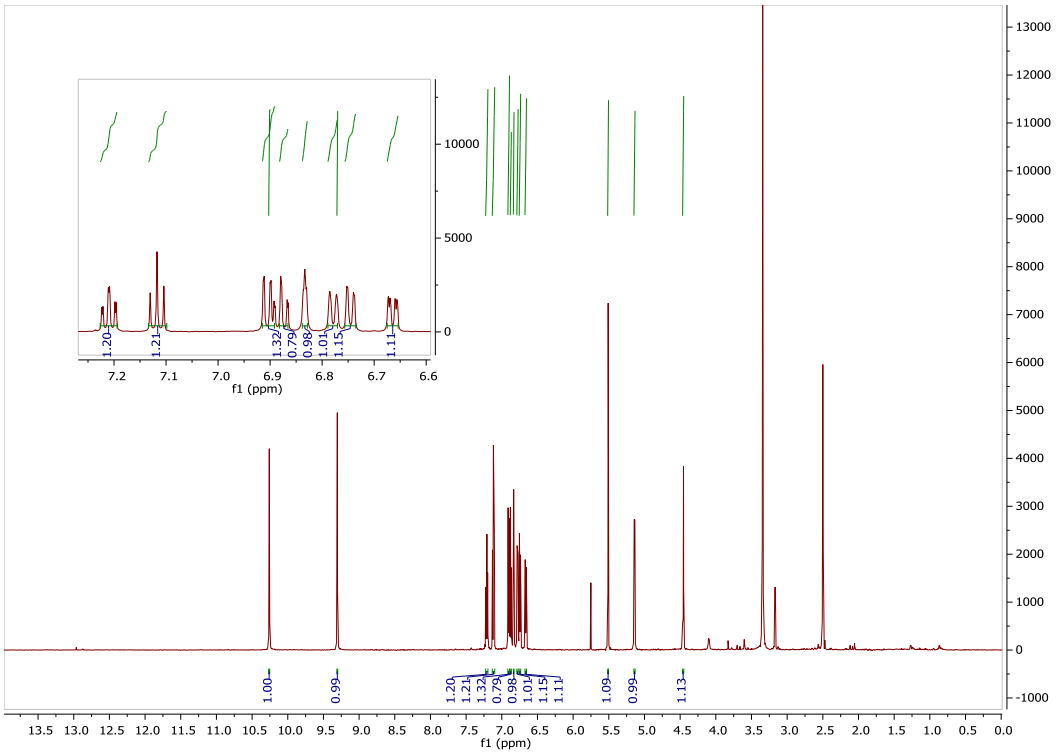


Figure S16.[13]C NMR spectrum of compound **3** in DMSO-*d*6

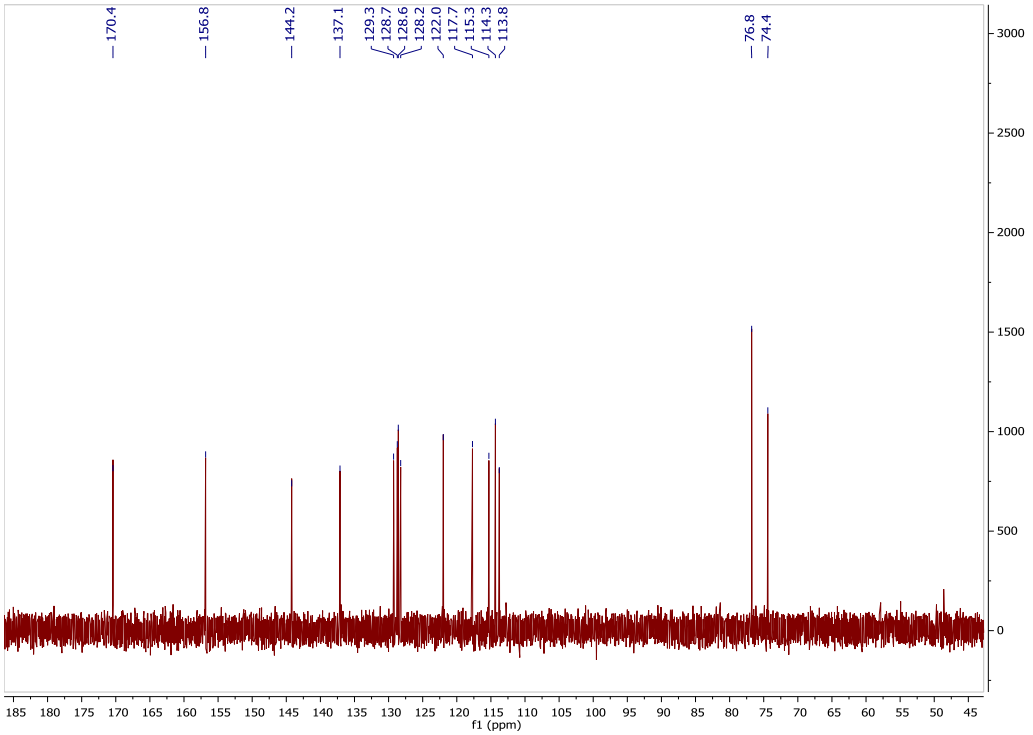


Figure S17. COSY spectrum of compound **3** in DMSO-d_6

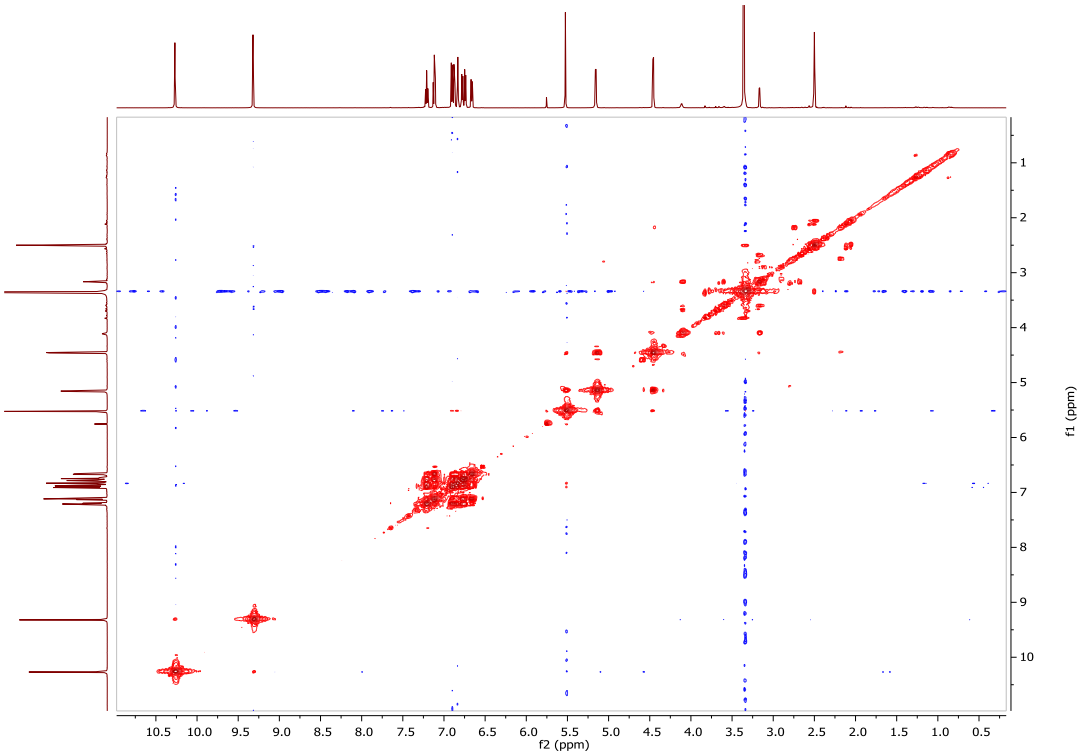


Figure S18. HSQC spectrum of compound **3** in DMSO-d_6

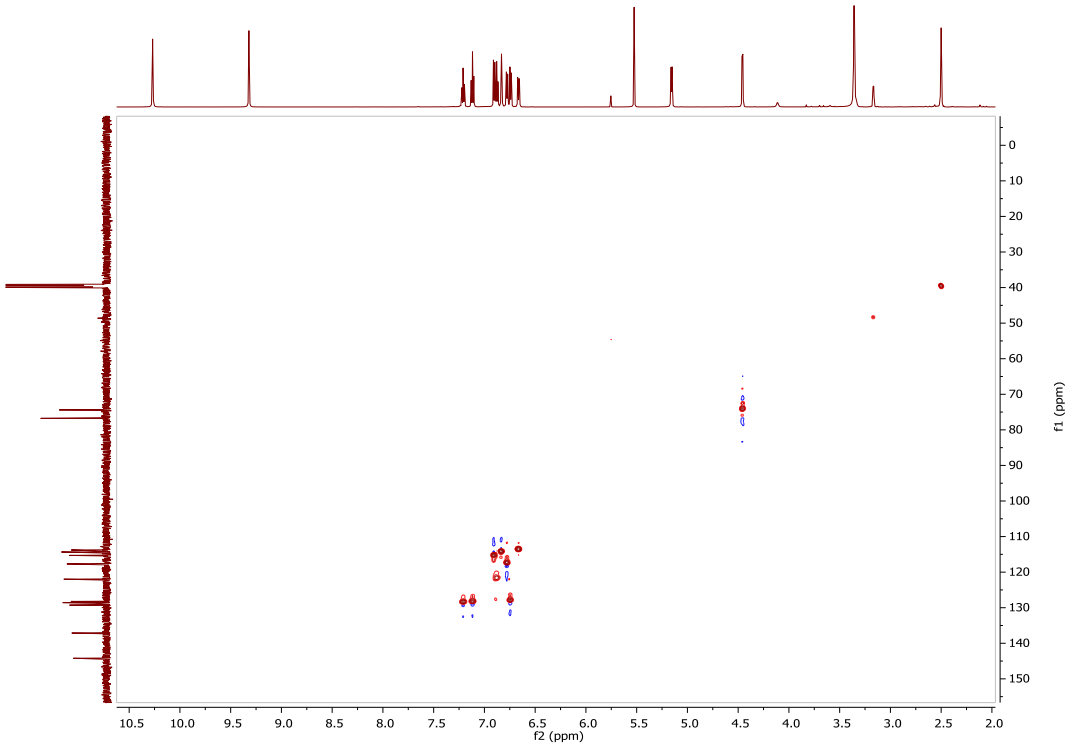


Figure S19. HMBC spectrum of compound **3** in DMSO-d_6

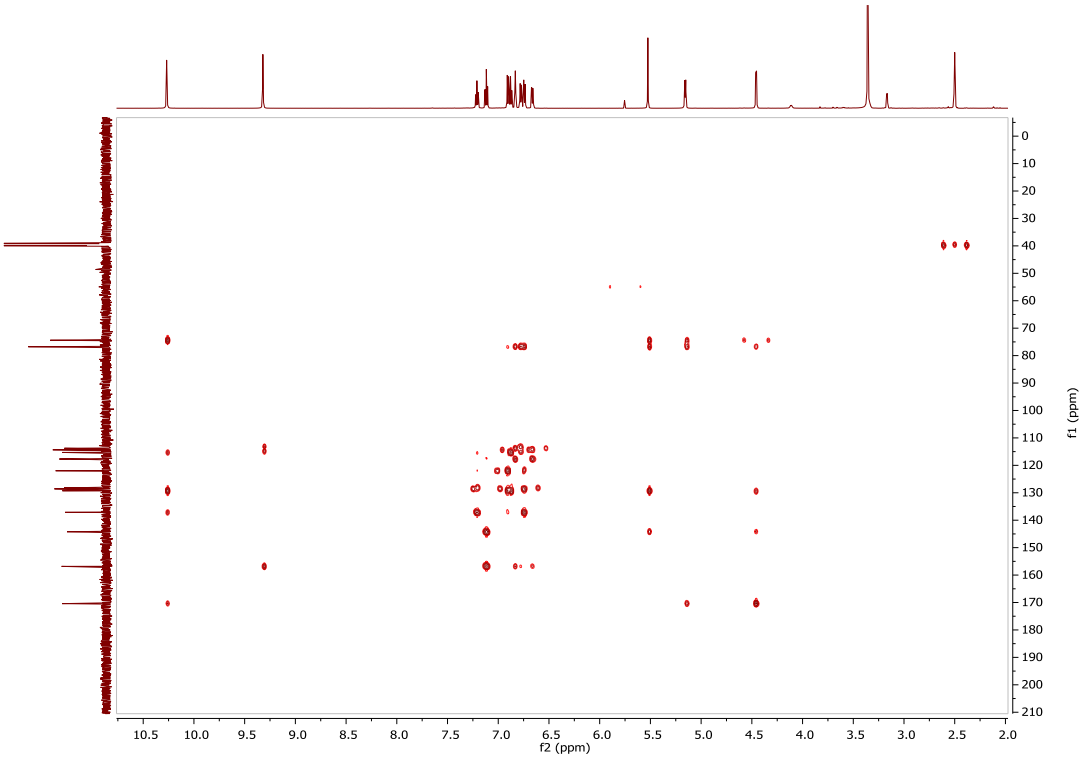


Figure S20. ROESY spectrum of compound **3** in DMSO-d_6

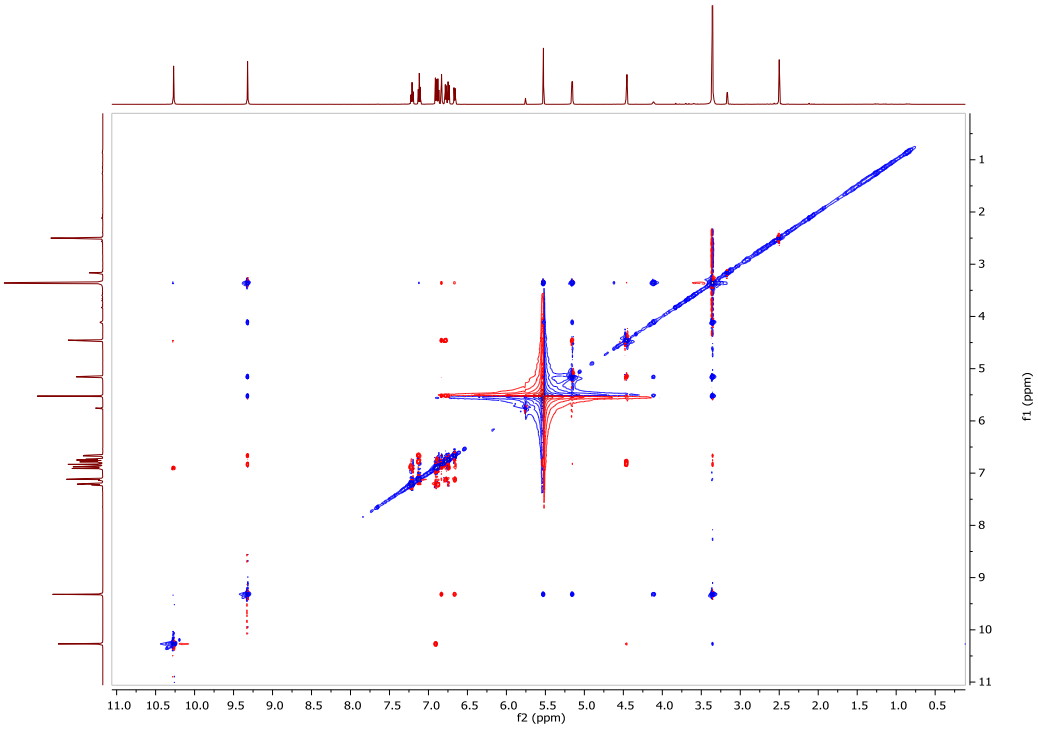


Figure S21. Experimental ECD spectrum of **1** in MeCN compared with the Boltzmann-weighted BH&HLYP/TZVP PCM/MeCN spectra of (5*R*,9*S*,5'*R*)-**1** and (5*S*,9*S*,5'*S*)-**1** computed for the gas-phase B3LYP/6-31+G(d,p) conformers.

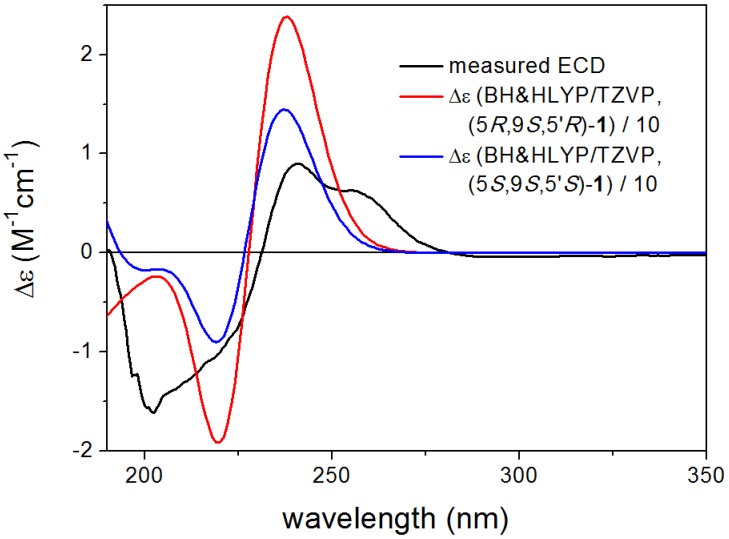


Figure S22. Low-energy conformers (≥ 1%) of (3*S*,4*S*)-**3** obtained at the B97D/TZVP PCM/MeCN level of theory.

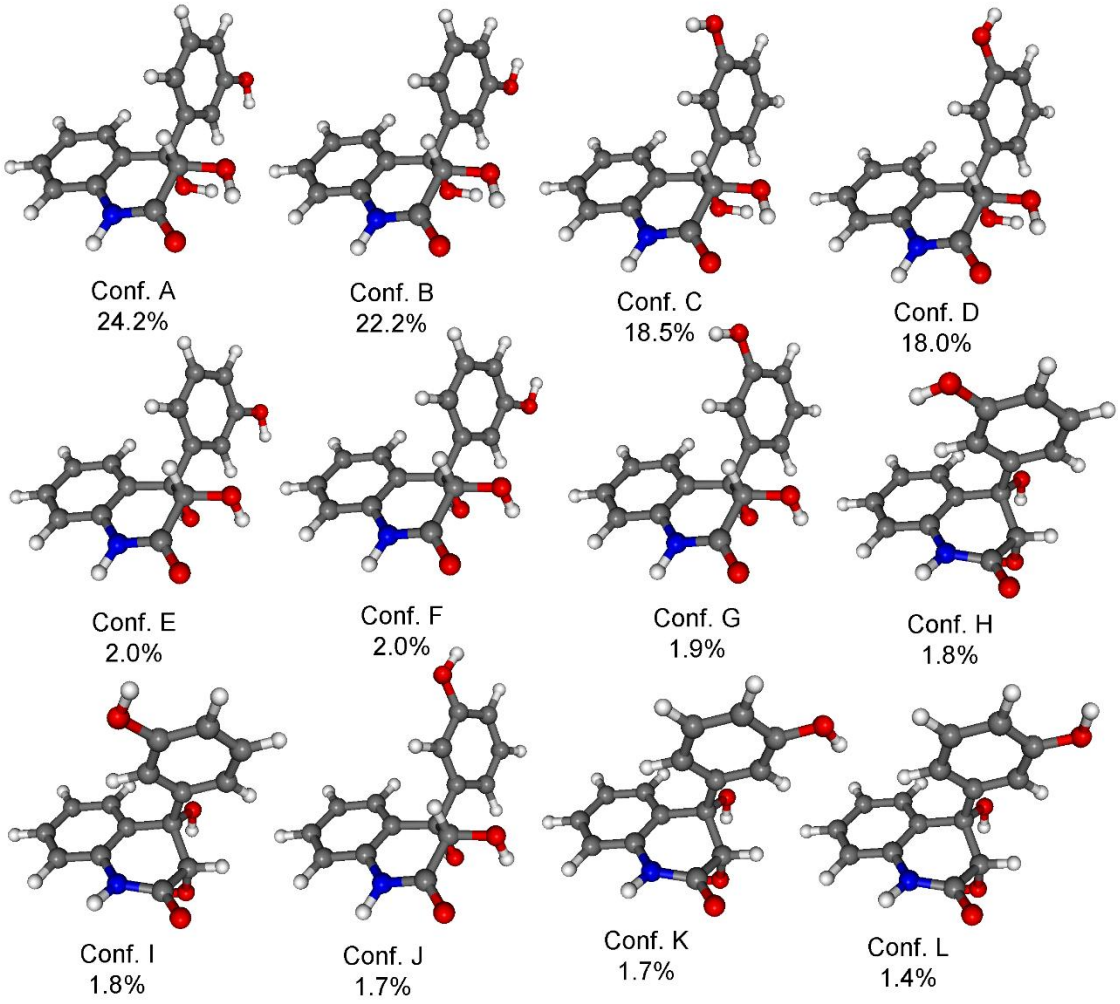


Figure S23. Experimental VCD spectrum (black) of 3 in MeOH-d_4 compared with the B3LYP/TZVP PCM/MeOH spectrum (red) of (3*S*,4*S*)-3 computed for the B3LYP/TZVP PCM/MeOH conformers; generated with Gaussian broadening and a manual scaling factor of 0.98.

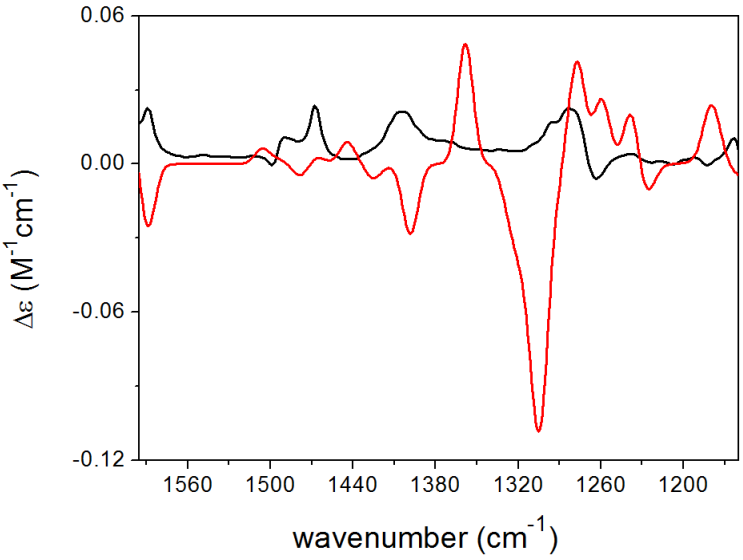


Table S1. Boltzmann populations and optical rotations of the low-energy conformers of (3*S*,4*S*)-**3** computed at various levels for the B97D/TZVP PCM/MeCN optimized MMFF conformers.

Conformer	Boltzmann population	B3LYP/TZVP	BH&HLYP/TZVP	CAM-B3LYP/TZVP	PBE0/TZVP
Conf. A	24.30	-157.50	-122.98	-136.90	-153.78
Conf. B	22.24	-153.00	-119.13	-133.32	-149.56
Conf. C	18.55	-98.02	-79.90	-90.18	-97.52
Conf. D	18.04	-102.64	-83.68	-93.86	-101.81
Conf. E	1.95	-81.88	-85.77	-87.95	-80.27
Conf. F	1.95	-84.79	-87.41	-90.02	-82.80
Conf. G	1.85	-43.13	-58.33	-58.77	-43.81
Conf. H	1.80	8.29	3.55	5.91	7.00
Conf. I	1.76	14.11	7.98	10.40	12.44
Conf. J	1.72	-46.95	-61.59	-61.55	-47.27
Conf. K	1.68	37.50	21.85	28.74	35.50
Conf. L	1.43	27.88	14.29	20.57	26.23
Average	N/A	-115.59	-93.60	-103.97	-113.69

Table S2. Boltzmann populations and optical rotations of the low-energy conformers of (3*S*,4*S*)-**3** computed at various levels for the CAM-B3LYP/TZVP PCM/MeCN optimized MMFF conformers.

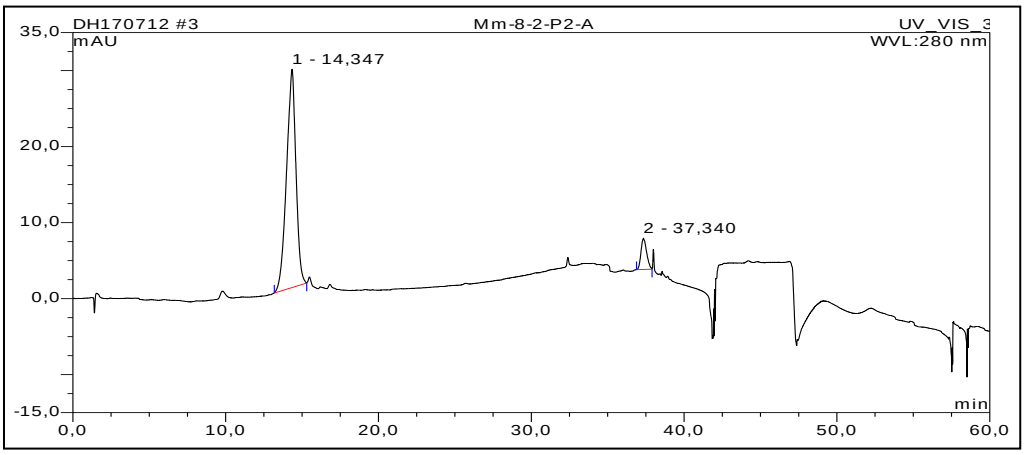
Conformer	Boltzmann population	B3LYP/TZVP	BH&HLYP/TZVP	CAM-B3LYP/TZVP	PBE0/TZVP
Conf. A	27.89	-153.03	-118.05	-131.82	-149.17
Conf. B	27.03	-148.93	-114.56	-128.62	-145.34
Conf. C	21.37	-102.69	-81.83	-91.65	-101.12
Conf. D	19.25	-96.52	-76.63	-86.70	-95.33
Conf. E	1.47	-57.04	-60.30	-61.24	-56.96
Conf. F	1.21	-27.49	-39.84	-37.60	-28.98
Conf. G	1.10	-24.21	-37.17	-35.36	-26.13
Average	N/A	-125.75	-98.57	-110.30	-123.16

Table S3. Boltzmann populations and optical rotations of the low-energy conformers of (3*S*,4*S*)-**3** computed at various levels for the CAM-B3LYP/TZVP SMD/MeCN optimized MMFF conformers.

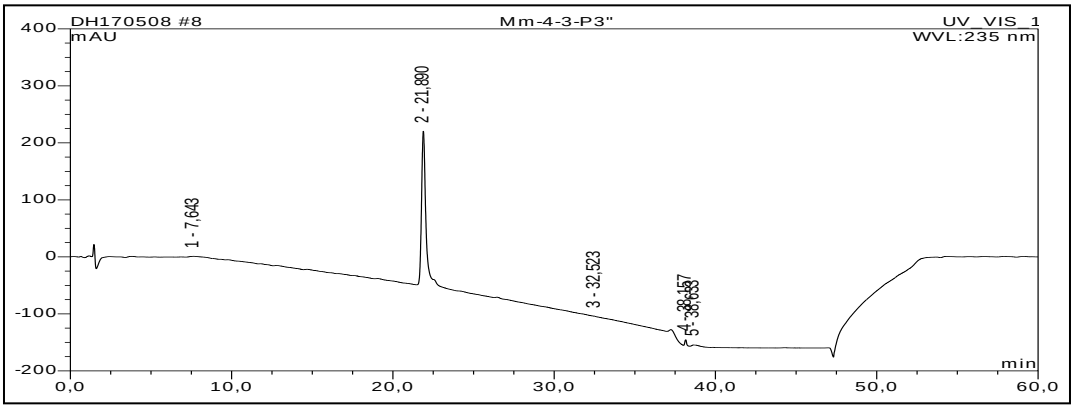
Conformer	Boltzmann population	B3LYP/TZVP	BH&HLYP/TZVP	CAM-B3LYP/TZVP	PBE0/TZVP
Conf. A	21.48	-156.95	-119.74	-134.06	-154.12
Conf. B	21.09	-147.03	-114.03	-127.94	-144.53
Conf. C	18.07	-126.17	-99.89	-111.52	-124.31
Conf. D	17.66	-124.55	-98.14	-110.18	-122.93
Conf. E	4.72	-69.63	-70.20	-72.53	-70.24
Conf. F	4.11	-86.52	-83.91	-88.14	-85.54
Conf. G	3.93	-51.91	-58.52	-59.30	-53.71
Conf. H	3.58	-66.90	-71.20	-73.75	-67.29
Conf. I	3.52	-66.24	-70.88	-73.88	-66.95
Average	N/A	-125.44	-101.12	-112.07	-123.75

Figure S24. HPLC chromatograms of the known compounds isolated from *M. marquandii*

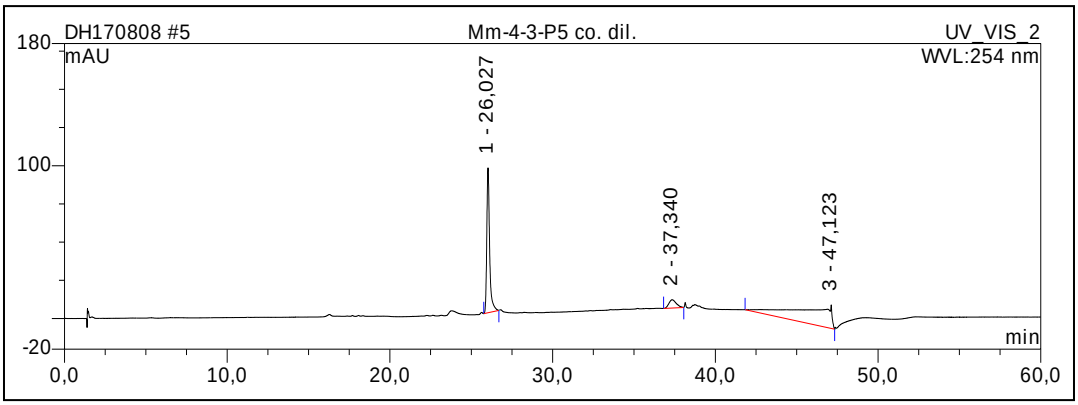
Terrestric acid hydrate (**4**)



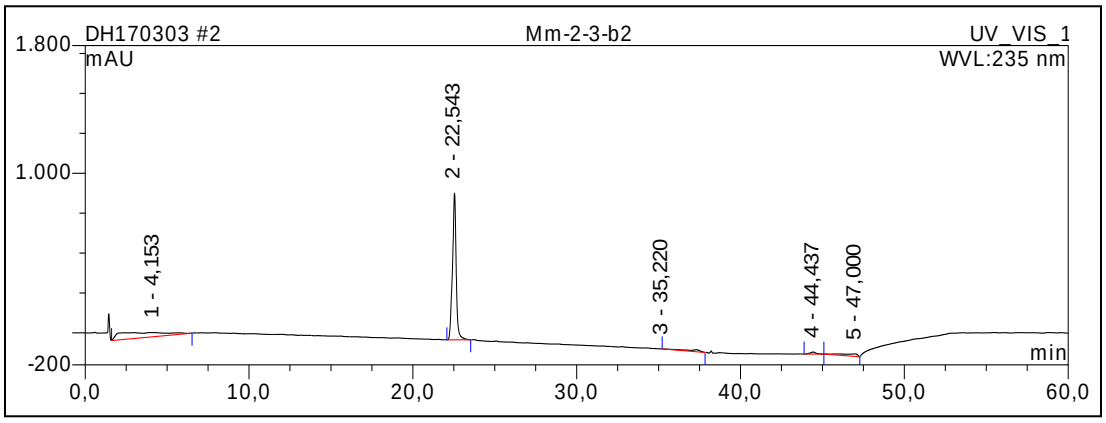
Peniphenone D (**5**)



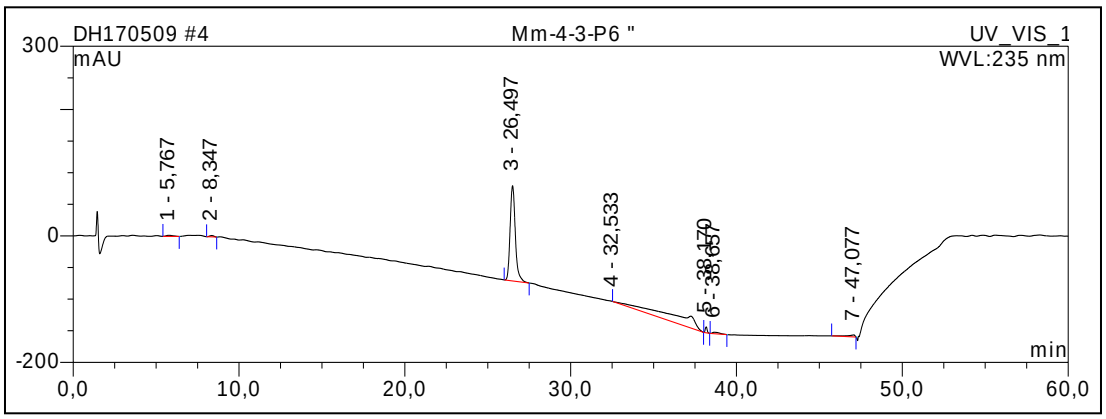
Viridicatin



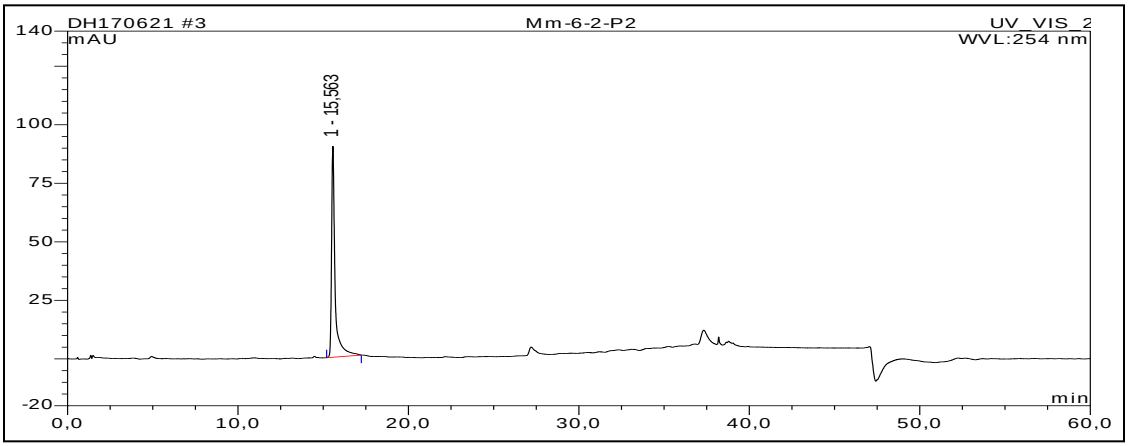
Clavatol



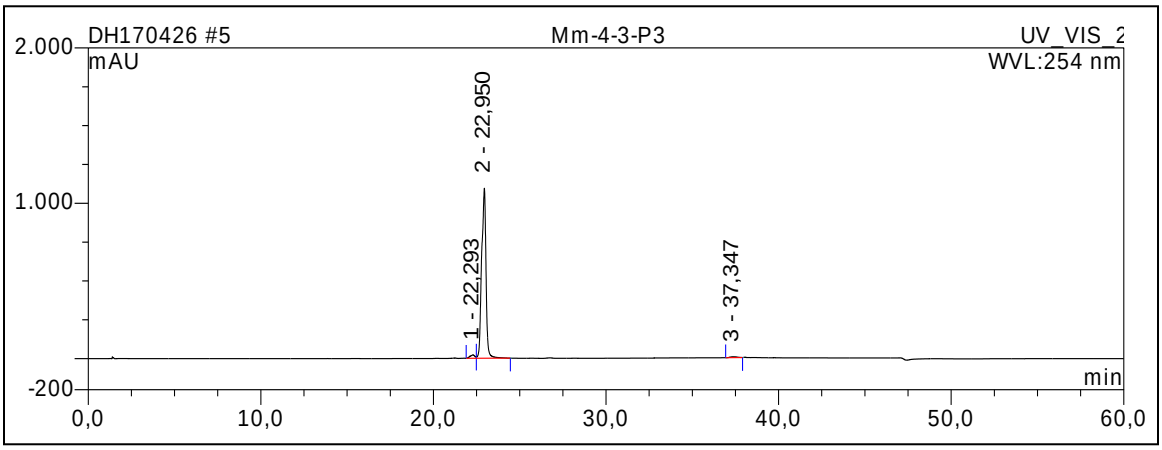
Penilactone A



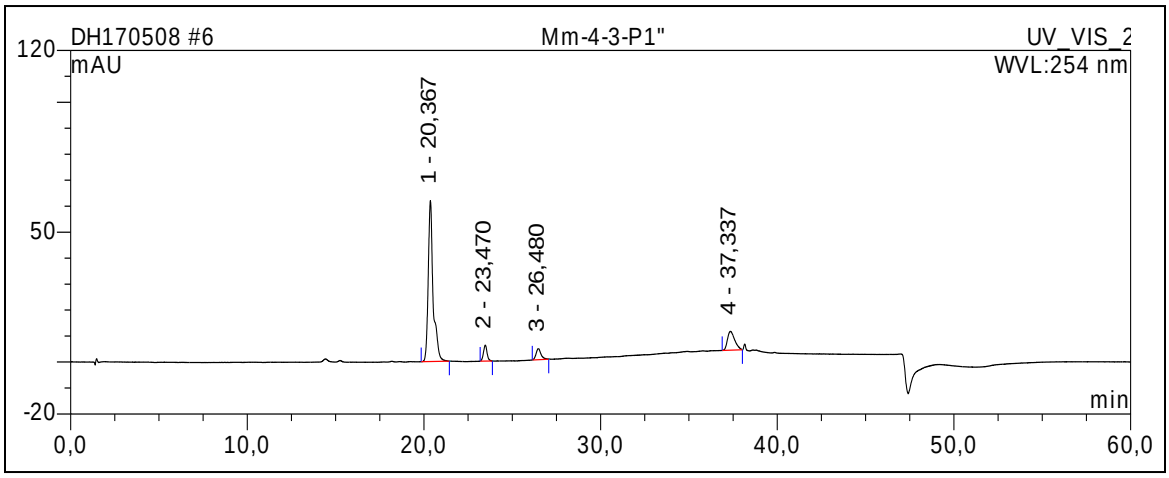
Cyclopenol



Dehydrocyclopeptine



Chaetobutenolide C



WF-3681

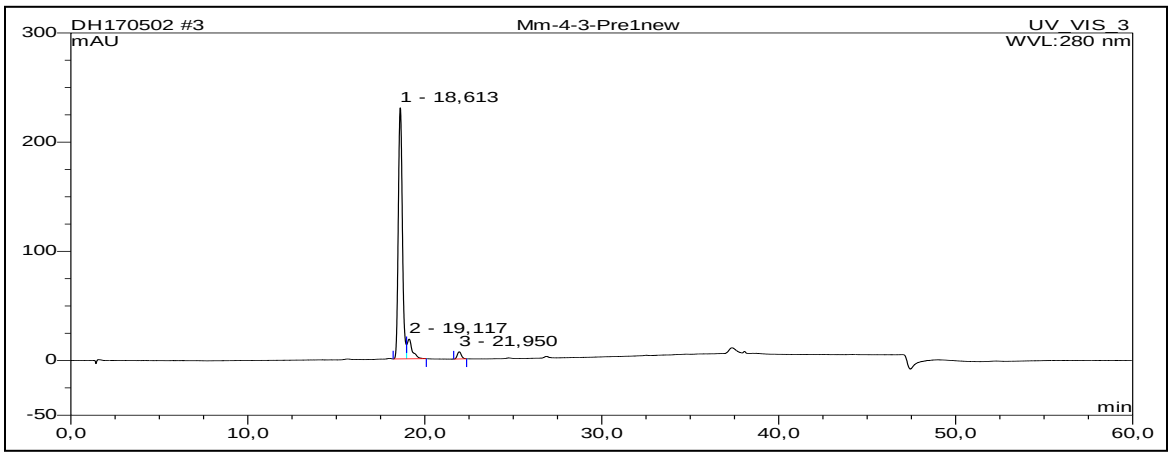


Figure S25. IR spectrum of compound **1**

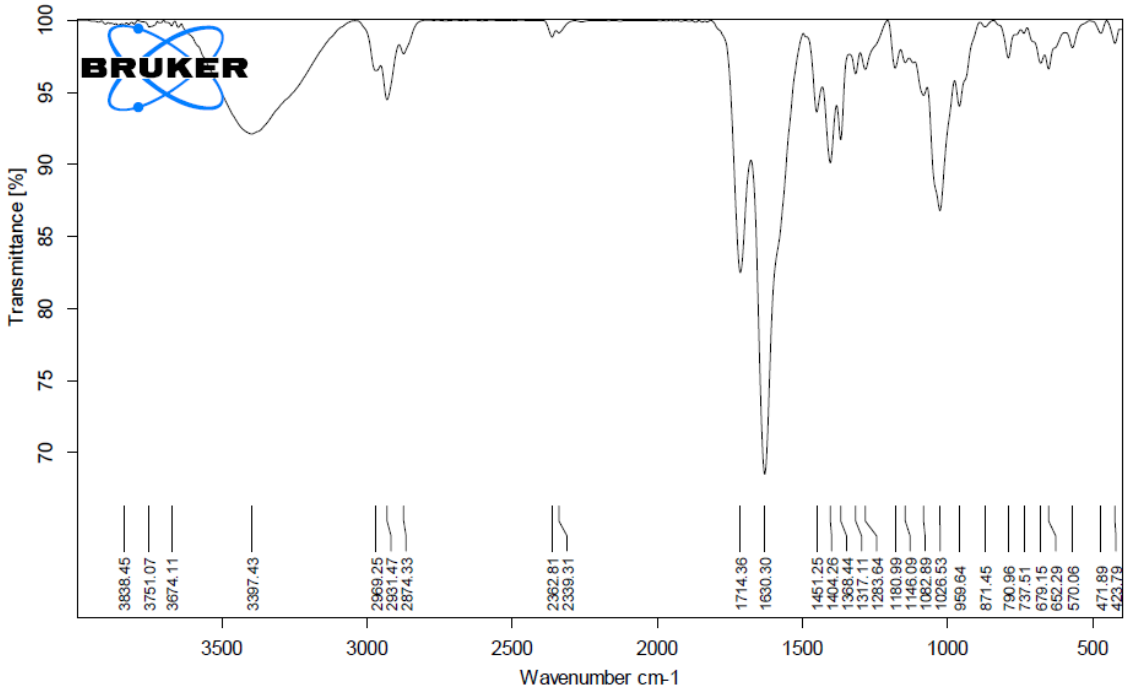


Figure S26. IR spectrum of compound **3**

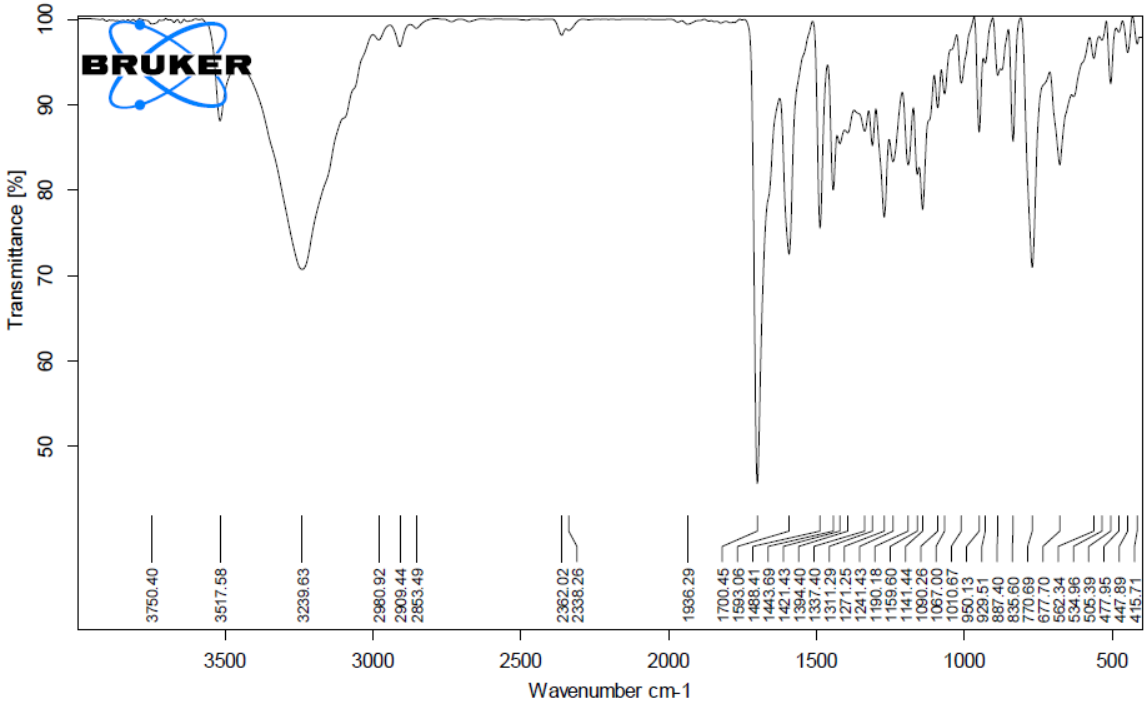


Figure S27. ITS sequence and identification of *Metarhizium marquandii*.

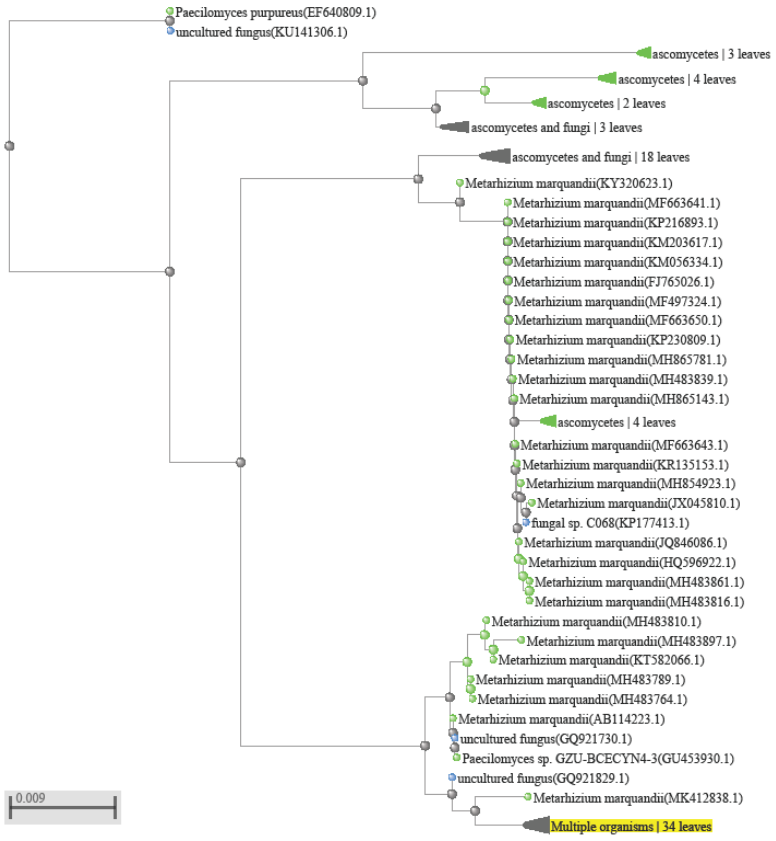
ITS 1 sequencing results

CTCCCAACCNACTGTGACATATACCATTTGTTTATTCGTTGCCTCGGCGGGTTCTACCCCCTGGAGACA
GGGCGGCCAGCCCCCGCCGGCGTAACACCAAAAACCCTGAATGTGTACCCGTTACACGGCAGTATTAC
TCTGAGTCACATCATTTTAAATGAATCAAAACTTTCAACAACGGATCTCTTGGTTCTGGCATCGATGAA
GAACGCAGCGAAATGCGATAAGTAATGTGAATTGCAGAATTCAGTGAATCATCGAATCTTTGAACGCA
CATTGCGCCCGCCAGTATTCTGGCGGGCATGCCTGTTCGAGCGTCATTTCAACCCTCAGGTCCCCCTTT
TCGGAGGGGGAGACACCCTGGTGTTGGGGGACGGCATCCTGGCCCGCTGTCTCACAGTGTGCCACGCC
GCCCCCGAAATGAATTGGCGGCCTCGTCGCGTGCCACCCCTGCGTAGTAGCACAACCTCGCAACGGGA
GCCCGACGCGGCCACTGCCGTAAAACGCCCAACTTTTACCGAGTTGACCTCGAATCAGGTAGGAATAC
CCGCTGAACTTAAGCATATCAATAAGCNGGAGGAA

Strain Identification Information

Sample No.	Sequencing Primer Name	Sequencing No.
SW2-B	ITS1	24AH61

Phylogenic Tree of the Fungus



Scheme S1. Proposed biosynthetic pathway of **1**

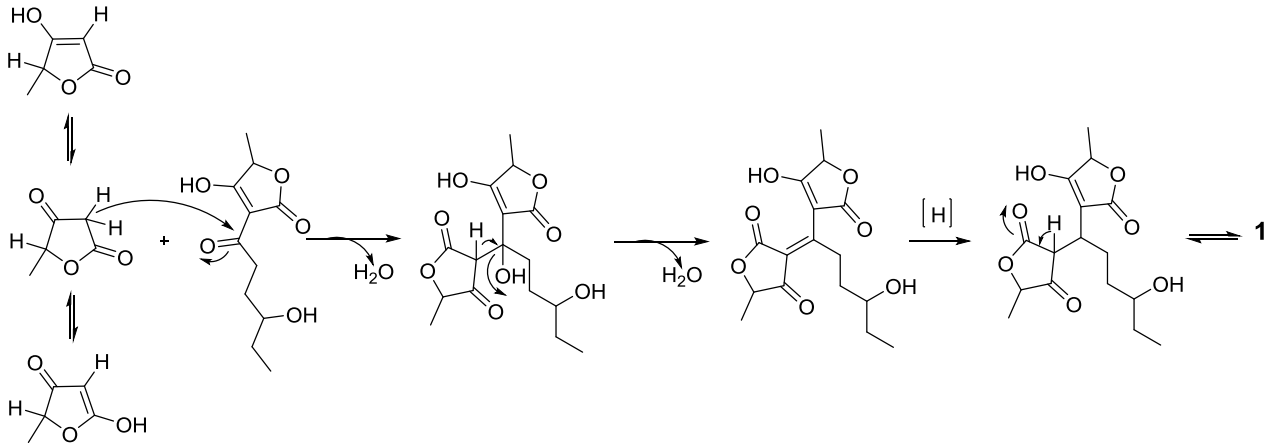


Table S4. Cartesian coordinates and energies of the low-energy conformers calculated at the B3LYP/6-31+G(d,p) level.

(5*R*,9*S*,5'*R*)-**1**, Conf A

C	-3.603890	-1.846819	-0.045894
C	-2.749262	-0.722490	0.493441
C	-1.470459	-0.867635	0.059215
C	-1.434652	-2.098859	-0.738326
O	-2.680171	-2.661650	-0.800425
C	-4.758905	-1.393590	-0.930666
O	-3.349329	0.174151	1.257501
O	-0.468207	-2.610831	-1.285088
C	-0.136080	-0.198491	0.279500
C	0.580181	-0.754149	1.550155
C	2.112838	-0.614494	1.536696
C	2.863048	-1.501268	0.527206
C	4.382326	-1.382446	0.669184
O	2.526058	-1.155376	-0.851244
C	5.165833	-2.348654	-0.224624
C	0.779372	3.439322	-0.427642
C	0.950389	1.948888	-0.549254
C	-0.019450	1.297661	0.148837
C	-0.822365	2.331188	0.787323
O	-0.366132	3.569363	0.445376
C	0.532759	4.170426	-1.741822
O	1.972813	1.496254	-1.263862
O	-1.787191	2.222619	1.541686
H	-3.977708	-2.460167	0.783913
H	-4.385845	-0.808184	-1.776280
H	-5.300088	-2.262207	-1.314869
H	-5.447249	-0.774349	-0.348587
H	-2.737305	0.942157	1.466073
H	0.429398	-0.578515	-0.566598
H	0.175506	-0.253845	2.438060
H	0.322386	-1.816063	1.645798
H	2.404825	0.432688	1.381295
H	2.486628	-0.882480	2.533023
H	2.566034	-2.547768	0.680569
H	4.640275	-1.556046	1.721611
H	4.669609	-0.346432	0.444029
H	1.848978	-1.769507	-1.181557
H	6.244032	-2.217622	-0.087143
H	4.935400	-2.180336	-1.280247
H	4.924870	-3.391768	0.012565
H	1.638446	3.875306	0.097377
H	1.404983	4.059933	-2.392463
H	-0.342941	3.758464	-2.251354
H	0.364465	5.233497	-1.552080
H	2.122468	0.515471	-1.164660

B3LYP Energy = -1149.63573883 a.u.

(5*R*,9*S*,5'*R*)-**1**, Conf B

C	-3.666887	-1.721933	0.076169
C	-2.715316	-0.674186	0.606951
C	-1.494319	-0.827999	0.031942
C	-1.591448	-1.992243	-0.855920
O	-2.859806	-2.504971	-0.830579
C	-4.885929	-1.160919	-0.645712
O	-3.196593	0.179144	1.494758
O	-0.707709	-2.491999	-1.537390
C	-0.117115	-0.226034	0.164465
C	0.697665	-0.904606	1.309587
C	2.226361	-0.819362	1.147375
C	2.829083	-1.653647	0.004483
C	4.360772	-1.618028	-0.037270
O	2.370650	-1.182700	-1.300868
C	5.049837	-2.272180	1.167019
C	0.876480	3.422511	-0.359119
C	0.972119	1.941344	-0.608533
C	0.050657	1.270617	0.135020
C	-0.639917	2.277472	0.928866
O	-0.168492	3.522391	0.635517
C	0.528436	4.261195	-1.583054
O	1.897259	1.512673	-1.457846
O	-1.528512	2.142935	1.767993
H	-3.979527	-2.386544	0.891716
H	-4.576662	-0.524584	-1.480212
H	-5.500579	-1.977253	-1.034007
H	-5.483575	-0.565213	0.050025
H	-2.534933	0.907394	1.694771
H	0.345135	-0.557338	-0.760817
H	0.406416	-0.460817	2.269096
H	0.405435	-1.961013	1.353447
H	2.546223	0.225342	1.033529
H	2.681723	-1.170234	2.080714
H	2.497685	-2.695761	0.109661
H	4.685318	-0.573750	-0.137892
H	4.668588	-2.127680	-0.957091
H	1.636197	-1.742919	-1.603656
H	4.862931	-1.731036	2.100091
H	6.133817	-2.297122	1.017334
H	4.712903	-3.306421	1.305709
H	1.801517	3.787337	0.104458
H	0.423132	5.311258	-1.298924
H	1.325373	4.173249	-2.327027
H	-0.410079	3.918673	-2.028085
H	2.015713	0.522634	-1.449126

B3LYP Energy = -1149.63438777 a.u.

(5*R*,9*S*,5'*R*)-**1**, Conf C

C	-3.886016	-1.238698	-0.000336
C	-2.823758	-0.307264	0.537185
C	-1.606706	-0.670396	0.055675
C	-1.822023	-1.857360	-0.779941
O	-3.151167	-2.181167	-0.811872
C	-4.968255	-0.555487	-0.827495
O	-3.225916	0.659155	1.345002
O	-0.984166	-2.516304	-1.378803
C	-0.166850	-0.263728	0.251546
C	0.469731	-0.962802	1.493321
C	1.995546	-1.149131	1.400796
C	2.468199	-2.159769	0.340334
C	3.950978	-2.535613	0.454734
O	2.235924	-1.659546	-1.015741
C	4.939411	-1.377226	0.271406
C	1.374651	3.164131	-0.419418
C	1.265760	1.671455	-0.579227
C	0.217796	1.188585	0.141681
C	-0.361585	2.332876	0.831197
O	0.300920	3.476663	0.497556
C	1.226349	3.965551	-1.706934
O	2.163413	1.059608	-1.341343
O	-1.303905	2.380086	1.619417
H	-4.337770	-1.802165	0.826111
H	-5.512875	0.158654	-0.203373
H	-4.524131	-0.019895	-1.671852
H	-5.670898	-1.299145	-1.212555
H	-2.478247	1.296685	1.549599
H	0.300214	-0.725301	-0.613937
H	0.221064	-0.393366	2.396902
H	0.000804	-1.947999	1.606069
H	2.490904	-0.183943	1.239908
H	2.355389	-1.511831	2.372257
H	1.875137	-3.076608	0.449463
H	4.152391	-3.306298	-0.298596
H	4.104808	-3.007079	1.434414
H	1.466941	-2.119630	-1.390769
H	4.843193	-0.623395	1.060010
H	4.792859	-0.881761	-0.693160
H	5.968527	-1.749470	0.300427
H	2.315324	3.420149	0.084019
H	0.273624	3.737932	-2.193515
H	1.264935	5.035497	-1.487482
H	2.041766	3.714256	-2.391240
H	2.135838	0.066000	-1.263581

B3LYP Energy = -1149.63388069 a.u.

(5*R*,9*S*,5'*R*)-**1**, Conf D

C	-1.366756	3.523930	-0.663657
C	-1.329947	2.019587	-0.652195
C	-0.174132	1.574112	-0.092717
C	0.557633	2.755298	0.332898
O	-0.125659	3.884637	-0.010679
C	-2.550063	4.146865	0.065947
O	-2.372915	1.352360	-1.134936
O	1.631217	2.845063	0.925826
C	0.126519	0.114755	0.121104
C	-0.429275	-0.405642	1.490648
C	-1.047443	-1.813831	1.410359
C	-2.394692	-1.904732	0.667095
C	-2.980064	-3.321268	0.702458
O	-2.315151	-1.433899	-0.706489
C	-4.379955	-3.428231	0.088716
C	3.720464	-1.126751	-0.492186
C	2.777219	-0.109371	0.106146
C	1.494292	-0.423745	-0.215423
C	1.552713	-1.640205	-1.032765
O	2.849311	-2.050817	-1.180460
C	4.586875	-1.864922	0.520862
O	3.314239	0.878799	0.800090
O	0.624960	-2.260485	-1.534378
H	-1.310630	3.900048	-1.692899
H	-2.460012	5.236014	0.061608
H	-3.480000	3.865386	-0.436188
H	-2.589151	3.800559	1.102810
H	-2.304759	0.368416	-1.015996
H	-0.483498	-0.367990	-0.635770
H	0.372372	-0.396194	2.237606
H	-1.194045	0.294493	1.850503
H	-0.338604	-2.517189	0.956436
H	-1.226006	-2.173695	2.431602
H	-3.107343	-1.211637	1.133737
H	-3.006573	-3.653445	1.748537
H	-2.287276	-3.997254	0.181883
H	-1.599935	-1.919462	-1.159501
H	-4.743971	-4.459987	0.127738
H	-4.377751	-3.107263	-0.956702
H	-5.097786	-2.800827	0.630484
H	4.349203	-0.643884	-1.250894
H	5.206596	-2.608122	0.012429
H	5.237113	-1.152982	1.036978
H	3.962386	-2.374084	1.261016
H	2.651326	1.618749	0.959069

B3LYP Energy = -1149.63371319 a.u.

(5*R*,9*S*,5'*R*)-**1**, Conf E

C	3.059518	-2.122076	-0.728605
C	2.207686	-0.880579	-0.762576

C	1.027706	-1.093146	-0.117122
C	1.088929	-2.452895	0.400258
O	2.260129	-3.049434	0.040562
C	4.430302	-1.945677	-0.087644
O	2.700590	0.192846	-1.365009
O	0.271272	-3.074904	1.076083
C	-0.059467	-0.066790	0.077407
C	0.065262	0.696872	1.433902
C	1.304143	1.606159	1.526134
C	1.341538	2.856814	0.621883
C	0.220280	3.866821	0.886965
O	1.385201	2.505639	-0.794877
C	0.425233	5.214497	0.183313
C	-3.726922	-1.112800	-0.485253
C	-2.362466	-1.427433	0.084390
C	-1.491167	-0.433734	-0.231326
C	-2.253331	0.568169	-0.985552
O	-3.553448	0.167111	-1.131309
C	-4.843613	-1.039879	0.548860
O	-2.241666	-2.557715	0.758830
O	-1.853741	1.632114	-1.436221
H	3.161144	-2.541725	-1.737442
H	4.952303	-2.905245	-0.053453
H	5.022908	-1.239748	-0.676201
H	4.332292	-1.562075	0.932155
H	2.167754	1.022095	-1.205752
H	0.136878	0.672658	-0.694595
H	-0.843594	1.291491	1.576028
H	0.089110	-0.029594	2.255079
H	1.400200	1.965370	2.559092
H	2.209953	1.016838	1.335946
H	2.304663	3.351973	0.797474
H	0.161262	4.024848	1.971445
H	-0.741090	3.431916	0.584274
H	0.483881	2.541807	-1.159443
H	-0.397748	5.898627	0.412216
H	0.469956	5.100371	-0.904034
H	1.358342	5.690087	0.506799
H	-3.978639	-1.841843	-1.265894
H	-4.611468	-0.291898	1.312899
H	-5.784956	-0.767309	0.064565
H	-4.961147	-2.013537	1.032733
H	-1.280484	-2.746303	0.981432

B3LYP Energy = -1149.63342782 a.u.

(5*R*,9*S*,5'*R*)-**1**, Conf F

C	3.218721	-1.942807	-0.580788
C	2.279634	-0.781457	-0.775340
C	1.113937	-0.991305	-0.103485
C	1.272048	-2.261031	0.591832
O	2.483892	-2.815505	0.307265
C	4.568419	-1.581915	0.026765
O	2.699279	0.236455	-1.513950
O	0.500722	-2.842640	1.352713
C	-0.045888	-0.029276	-0.035758
C	0.016397	0.900725	1.216595
C	1.192895	1.892503	1.202968
C	1.150727	3.027853	0.158675
C	-0.053856	3.972244	0.248445
O	1.252240	2.509399	-1.203188
C	-0.183178	4.701629	1.591459
C	-3.625066	-1.408987	-0.426343
C	-2.242660	-1.540386	0.170760
C	-1.445232	-0.539797	-0.286990
C	-2.277627	0.289677	-1.167023
O	-3.544242	-0.223677	-1.246487
C	-4.745596	-1.272053	0.597359
O	-2.042574	-2.553545	0.996065
O	-1.958507	1.308083	-1.761991
H	3.357567	-2.483962	-1.525227
H	5.159153	-2.487088	0.188431
H	5.111563	-0.919868	-0.653358
H	4.435306	-1.072496	0.985624
H	2.115061	1.043865	-1.450295
H	0.098525	0.622121	-0.894435
H	-0.929930	1.449049	1.279844
H	0.075018	0.282543	2.120487
H	1.265377	2.367654	2.188947
H	2.137163	1.348412	1.076503
H	2.065343	3.619414	0.287768
H	-0.974997	3.414732	0.035393
H	0.053384	4.711275	-0.555188
H	0.363893	2.473723	-1.596486
H	-0.997954	5.430888	1.550603
H	0.735511	5.245186	1.841591
H	-0.400642	4.013083	2.414344
H	-3.821962	-2.257217	-1.094183
H	-4.569689	-0.408162	1.245295
H	-5.703819	-1.140276	0.088032
H	-4.791808	-2.173084	1.215376
H	-1.070621	-2.642050	1.232750

B3LYP Energy = -1149.63296515 a.u.

(5*R*,9*S*,5'*R*)-**1**, Conf G

C	-3.540932	-1.513077	0.569053
C	-2.431659	-0.503058	0.685386
C	-1.302353	-0.961918	0.084164
C	-1.642176	-2.249692	-0.497701
O	-2.932983	-2.576579	-0.202880
C	-4.801717	-1.011033	-0.123355
O	-2.681426	0.649462	1.297792
O	-0.957419	-3.011737	-1.177839

C	-0.040832	-0.147736	-0.028229
C	-0.043973	0.762221	-1.304031
C	0.543010	2.166333	-1.065074
C	-0.337507	3.113845	-0.229145
C	0.255775	4.520161	-0.068733
O	-0.640914	2.577440	1.088582
C	0.347603	5.329392	-1.369143
C	3.343700	-1.936539	0.396240
C	1.959318	-1.892100	-0.207119
C	1.293982	-0.795290	0.242808
C	2.207044	-0.094690	1.152486
O	3.401712	-0.757584	1.228537
C	4.481165	-1.929675	-0.617501
O	1.623843	-2.875664	-1.023543
O	2.008388	0.937960	1.777366
H	-3.785980	-1.928743	1.554517
H	-4.567131	-0.627584	-1.120623
H	-5.523679	-1.825735	-0.220249
H	-5.250030	-0.207692	0.468087
H	-1.926247	1.293553	1.255301
H	-0.120641	0.536561	0.810722
H	0.506876	0.263078	-2.109057
H	-1.076963	0.869710	-1.658916
H	1.533644	2.094790	-0.598728
H	0.695272	2.643925	-2.039998
H	-1.323650	3.197289	-0.705099
H	1.250523	4.434901	0.390258
H	-0.376616	5.053904	0.649899
H	0.197256	2.362671	1.538819
H	0.684307	6.349763	-1.160530
H	-0.628745	5.399453	-1.863651
H	1.054377	4.892818	-2.082005
H	3.428898	-2.808009	1.057739
H	4.424124	-2.826247	-1.241245
H	4.416737	-1.046950	-1.260760
H	5.443777	-1.918032	-0.099640
H	0.631581	-2.892686	-1.189583

B3LYP Energy = -1149.63270258 a.u.

(5*R*,9*S*,5'*R*)-**1**, Conf H

C	-3.759679	-1.276709	-0.053552
C	-2.718679	-0.356109	0.539692
C	-1.496006	-0.646433	0.021958
C	-1.689773	-1.756052	-0.917358
O	-3.008337	-2.120507	-0.953781
C	-4.879687	-0.564544	-0.802189
O	-3.132122	0.544349	1.414830
O	-0.848463	-2.331070	-1.593871
C	-0.082846	-0.176886	0.259465
C	0.594460	-0.850838	1.502546
C	1.153078	-2.253034	1.194111
C	2.411589	-2.318152	0.299109
C	3.661392	-1.691367	0.920746
O	2.218558	-1.684764	-0.996153
C	4.940336	-1.941991	0.113178
C	1.395477	3.276953	-0.338332
C	1.320460	1.781863	-0.485545
C	0.234446	1.290998	0.166108
C	-0.403399	2.426284	0.812881
O	0.256556	3.579165	0.503386
C	1.317829	4.061818	-1.641871
O	2.277407	1.160915	-1.169197
O	-1.385005	2.459392	1.552343
H	-4.176593	-1.923511	0.729200
H	-5.566794	-1.296967	-1.233879
H	-5.432300	0.078551	-0.111531
H	-4.470109	0.051947	-1.607862
H	-2.431131	1.246301	1.577912
H	0.428969	-0.590183	-0.603934
H	1.400798	-0.202243	1.862657
H	-0.130303	-0.918522	2.321475
H	1.414791	-2.750535	2.137041
H	0.368792	-2.866901	0.736330
H	2.623103	-3.381320	0.111722
H	3.774092	-2.105925	1.930491
H	3.508471	-0.611891	1.044279
H	1.446771	-2.091923	-1.429862
H	5.806562	-1.489057	0.606393
H	4.862671	-1.520406	-0.892750
H	5.137210	-3.015711	0.011752
H	2.294813	3.557172	0.224361
H	2.181159	3.819309	-2.268263
H	0.403759	3.810620	-2.187396
H	1.322153	5.134577	-1.433138
H	2.210389	0.171960	-1.131142

B3LYP Energy = -1149.63187458 a.u.

(5*S*,9*S*,5'*S*)-**1**, Conf A

C	-3.994022	-0.845493	-0.418941
C	-2.928245	0.087548	0.109473
C	-1.697939	-0.402084	-0.193232
C	-1.911473	-1.671166	-0.897370
O	-3.249270	-1.924537	-1.026335
C	-4.943994	-1.386883	0.642240
O	-3.339779	1.171870	0.743988
O	-1.064770	-2.444182	-1.323878
C	-0.257530	-0.054018	0.089936
C	0.226595	-0.654290	1.446655
C	1.742408	-0.910754	1.525623
C	2.281805	-2.043136	0.633041
C	3.771916	-2.304238	0.865553
O	2.109050	-1.744158	-0.785689

C	4.313518	-3.516545	0.101745
C	1.569141	3.176480	-0.799648
C	1.369582	1.684069	-0.804639
C	0.230522	1.352318	-0.138061
C	-0.330180	2.601708	0.355734
O	0.441590	3.656511	-0.031335
C	2.876326	3.648879	-0.175849
O	2.283763	0.933696	-1.407055
O	-1.339964	2.797433	1.029371
H	-4.559081	-0.348522	-1.217638
H	-5.497293	-0.560143	1.096531
H	-5.654039	-2.083476	0.188904
H	-4.386809	-1.910909	1.424486
H	-2.572963	1.786088	0.950542
H	0.248833	-0.629021	-0.679324
H	-0.076461	0.010705	2.264271
H	-0.300282	-1.603241	1.604975
H	2.302107	0.010214	1.314708
H	1.988524	-1.178211	2.561045
H	1.716363	-2.961612	0.842429
H	3.930515	-2.440613	1.942812
H	4.328133	-1.401344	0.579316
H	1.307765	-2.188015	-1.112796
H	5.382433	-3.652814	0.295251
H	4.176440	-3.393071	-0.976069
H	3.800648	-4.437105	0.405022
H	1.462704	3.578778	-1.814957
H	3.719547	3.274353	-0.762939
H	2.910488	4.741134	-0.162425
H	2.968386	3.281298	0.850380
H	2.168502	-0.041918	-1.240627

B3LYP Energy = -1149.63543318 a.u.

(5*S*,9*S*,5'*S*)-**1**, Conf B

C	-4.060487	-0.613199	-0.280690
C	-2.903817	0.210048	0.239347
C	-1.731756	-0.307014	-0.212701
C	-2.074312	-1.487098	-1.014406
O	-3.430643	-1.660632	-1.050600
C	-4.947565	-1.211698	0.803873
O	-3.200690	1.244928	1.006388
O	-1.310969	-2.254615	-1.583861
C	-0.255374	-0.066186	-0.016183
C	0.288212	-0.830119	1.231827
C	1.787710	-1.174495	1.172089
C	2.192682	-2.236337	0.135155
C	3.673953	-2.624321	0.201214
O	1.948329	-1.772222	-1.228676
C	4.090245	-3.344906	1.489836
C	1.700374	3.135568	-0.717584
C	1.410812	1.664206	-0.852895
C	0.301214	1.328062	-0.139879
C	-0.148491	2.549918	0.511561
O	0.658157	3.595433	0.173324
C	3.072553	3.470879	-0.147171
O	2.235791	0.931596	-1.589901
O	-1.096544	2.732018	1.273082
H	-4.660791	-0.012434	-0.975585
H	-4.356689	-1.836651	1.480148
H	-5.414203	-0.409185	1.381944
H	-5.730419	-1.825654	0.350948
H	-2.385922	1.798505	1.202124
H	0.155597	-0.584660	-0.877248
H	0.083967	-0.238842	2.132510
H	-0.282762	-1.761019	1.334149
H	2.388144	-0.269223	1.008861
H	2.082367	-1.553598	2.157507
H	1.580441	-3.135554	0.287984
H	4.281582	-1.720612	0.059329
H	3.874571	-3.270291	-0.660760
H	1.103505	-2.136855	-1.543739
H	5.131924	-3.674101	1.422035
H	3.474365	-4.235155	1.664777
H	4.009010	-2.702667	2.372679
H	1.551351	3.643678	-1.678687
H	3.209312	2.997679	0.829650
H	3.850293	3.111488	-0.826815
H	3.174749	4.552770	-0.031055
H	2.076457	-0.049530	-1.509164

B3LYP Energy = -1149.63415359 a.u.

(5*S*,9*S*,5'*S*)-**1**, Conf C

C	0.542820	3.711962	-0.269786
C	-0.181026	2.397870	-0.379227
C	0.541513	1.404249	0.201878
C	1.723455	2.034311	0.766785
O	1.736397	3.366176	0.473438
C	0.911064	4.361623	-1.597847
O	-1.372090	2.376004	-0.967990
O	2.634151	1.544232	1.432190
C	0.051034	-0.014113	0.318473
C	-0.801206	-0.233238	1.615896
C	-2.042365	-1.118698	1.397014
C	-3.183244	-0.466434	0.593270
C	-4.418368	-1.369778	0.498283
O	-2.768116	-0.050767	-0.737770
C	-5.621649	-0.703694	-0.176778
C	2.574281	-2.883543	-0.161493
C	2.216467	-1.550426	0.453531
C	0.988976	-1.157096	0.022181
C	0.503427	-2.207554	-0.878726
O	1.427917	-3.211597	-0.977411

C	3.842230	-2.867985	-1.006696
O	3.103843	-0.997600	1.262015
O	-0.561094	-2.257383	-1.479254
H	-0.032420	4.409782	0.351558
H	1.481618	5.276847	-1.420961
H	1.513862	3.679727	-2.204330
H	-0.000089	4.612917	-2.148418
H	-1.824511	1.492791	-0.916188
H	-0.652257	-0.095418	-0.504451
H	-0.169737	-0.669240	2.398007
H	-1.129065	0.743671	1.993737
H	-1.759561	-2.064149	0.917927
H	-2.458254	-1.382843	2.377518
H	-3.466611	0.477402	1.077709
H	-4.689595	-1.684181	1.514535
H	-4.140224	-2.284929	-0.043126
H	-2.375125	-0.818157	-1.193912
H	-6.469502	-1.394240	-0.229890
H	-5.377313	-0.385985	-1.194285
H	-5.947285	0.181779	0.382021
H	2.648367	-3.649619	0.621055
H	3.758863	-2.128750	-1.808825
H	4.699571	-2.611297	-0.378134
H	4.008599	-3.852775	-1.451019
H	2.888160	-0.030585	1.437181

B3LYP Energy = -1149.63387683 a.u.

(5*S*,9*S*,5'*S*)-**1**, Conf D

C	-4.108621	-0.362298	-0.367701
C	-2.911188	0.395141	0.159186
C	-1.768144	-0.249057	-0.192575
C	-2.172798	-1.448914	-0.934045
O	-3.536062	-1.509470	-1.033071
C	-5.095993	-0.807869	0.703836
O	-3.153137	1.503415	0.838346
O	-1.453298	-2.314790	-1.411602
C	-0.288302	-0.113985	0.069403
C	0.130816	-0.795900	1.408992
C	1.589274	-1.289464	1.436147
C	1.898137	-2.475062	0.503844
C	3.271186	-3.115467	0.745331
O	1.829037	-2.081621	-0.904093
C	4.476489	-2.198036	0.504105
C	1.942081	2.856975	-0.812824
C	1.542387	1.405537	-0.839184
C	0.386450	1.215362	-0.146850
C	0.013230	2.518190	0.385574
O	0.911156	3.467458	-0.002926
C	3.317230	3.134606	-0.218995
O	2.331502	0.552787	-1.480294
O	-0.942606	2.834040	1.091429
H	-4.619834	0.237157	-1.131548
H	-4.595853	-1.433409	1.449286
H	-5.517086	0.068773	1.203966
H	-5.907518	-1.382571	0.249838
H	-2.304273	2.002186	1.034376
H	0.120035	-0.744201	-0.715321
H	-0.039746	-0.100689	2.239784
H	-0.534350	-1.651790	1.576438
H	2.277171	-0.462393	1.223270
H	1.820807	-1.616495	2.458028
H	1.131298	-3.244452	0.659567
H	3.345199	-3.989841	0.088101
H	3.290103	-3.494986	1.775479
H	0.996839	-2.412694	-1.280986
H	5.409173	-2.755705	0.636868
H	4.499621	-1.353609	1.201200
H	4.470737	-1.798762	-0.514646
H	1.864636	3.292638	-1.816996
H	3.498196	4.211841	-0.184072
H	3.386027	2.733004	0.796212
H	4.086551	2.665073	-0.838372
H	2.096136	-0.402196	-1.318251

B3LYP Energy = -1149.63354237 a.u.

(5*S*,9*S*,5'*S*)-**1**, Conf E

C	0.556289	3.678582	-0.231438
C	-0.160038	2.390510	-0.536927
C	0.383985	1.361549	0.169408
C	1.427174	1.949191	0.998962
O	1.536217	3.285619	0.756218
C	1.236543	4.338384	-1.424794
O	-1.176212	2.436545	-1.387511
O	2.160335	1.419703	1.832305
C	-0.094642	-0.068586	0.148617
C	-1.109338	-0.377840	1.295190
C	-2.453856	0.357961	1.153207
C	-3.376079	-0.067557	-0.007866
C	-3.820336	-1.534972	-0.002792
O	-2.787761	0.251370	-1.306561
C	-4.607706	-1.948848	1.246924
C	2.526071	-2.888935	-0.054255
C	2.079405	-1.573545	0.541301
C	0.910907	-1.181045	-0.030542
C	0.535622	-2.234243	-0.981669
O	1.481899	-3.223477	-0.993551
C	3.877458	-2.836103	-0.757121
O	2.856542	-1.042803	1.469719
O	-0.463884	-2.292727	-1.682127
H	-0.130036	4.382880	0.255120
H	1.775457	5.232103	-1.100297
H	1.944192	3.648339	-1.893098

H	0.482929	4.627061	-2.163038
H	-1.721393	1.600275	-1.402969
H	-0.663280	-0.145457	-0.774901
H	-1.278343	-1.460123	1.318077
H	-0.655023	-0.117143	2.258548
H	-3.025897	0.228369	2.080081
H	-2.278995	1.438074	1.072144
H	-4.270555	0.565437	0.041796
H	-2.944792	-2.185184	-0.126031
H	-4.446717	-1.686816	-0.890497
H	-2.389198	-0.552641	-1.680496
H	-4.978867	-2.972698	1.140357
H	-5.474660	-1.297082	1.406693
H	-3.991802	-1.916516	2.151418
H	2.530689	-3.666060	0.720722
H	4.109506	-3.809674	-1.196848
H	3.866368	-2.084195	-1.551820
H	4.657632	-2.576184	-0.036108
H	2.556932	-0.113616	1.705981

B3LYP Energy = -1149.63328503 a.u.

(5*S*,9*S*,5'*S*)-**1**, Conf F

C	1.446175	3.524445	-0.193264
C	0.443627	2.426094	-0.419868
C	0.838739	1.282732	0.199517
C	2.068825	1.603484	0.904556
O	2.434055	2.894062	0.656885
C	2.100905	4.075318	-1.453974
O	-0.647633	2.697631	-1.127933
O	2.756205	0.903657	1.646057
C	0.011063	0.025400	0.218190
C	-1.007297	0.014211	1.409660
C	-2.391358	-0.549507	1.035245
C	-3.252055	0.362959	0.142535
C	-4.650654	-0.200369	-0.145330
O	-2.603220	0.679763	-1.120653
C	-5.567900	-0.296458	1.080845
C	1.807771	-3.368267	-0.077122
C	1.712179	-1.991961	0.539199
C	0.673751	-1.309609	-0.011719
C	0.055656	-2.206745	-0.994080
O	0.717150	-3.404507	-1.023667
C	3.130294	-3.654115	-0.778264
O	2.607506	-1.676345	1.458989
O	-0.914290	-1.994434	-1.708169
H	0.992242	4.336509	0.388519
H	1.341690	4.544133	-2.086652
H	2.851971	4.823587	-1.188588
H	2.584216	3.272345	-2.017701
H	-1.301025	1.949548	-1.151279
H	-0.595996	0.121332	-0.676928
H	-0.587316	-0.560490	2.242617
H	-1.134033	1.040710	1.776941
H	-2.288764	-1.529038	0.551673
H	-2.953881	-0.719590	1.960584
H	-3.357968	1.341658	0.629001
H	-4.545162	-1.189553	-0.612110
H	-5.110445	0.453291	-0.895360
H	-2.364773	-0.154099	-1.566163
H	-6.572882	-0.610700	0.781943
H	-5.662216	0.673559	1.583892
H	-5.205377	-1.021918	1.816146
H	1.607021	-4.134402	0.682850
H	3.316707	-2.912733	-1.560893
H	3.947180	-3.613940	-0.052285
H	3.106437	-4.647936	-1.232895
H	2.615873	-0.686556	1.637868

B3LYP Energy = -1149.63286847 a.u.

(5*S*,9*S*,5'*S*)-**1**, Conf G

C	0.565204	3.634942	-0.424827
C	-0.219635	2.358998	-0.567375
C	0.360205	1.352024	0.140972
C	1.483864	1.963115	0.844727
O	1.614944	3.274595	0.498704
C	1.156071	4.176420	-1.720988
O	-1.321594	2.398280	-1.304426
O	2.259342	1.475072	1.664386
C	-0.117307	-0.080225	0.252643
C	-0.905936	-0.337289	1.572589
C	-2.278565	0.355968	1.653082
C	-3.364178	-0.096956	0.662198
C	-3.533119	-1.615218	0.546564
O	-3.076792	0.493340	-0.640780
C	-4.764789	-2.042944	-0.264198
C	2.550771	-2.850323	-0.093929
C	2.092930	-1.547352	0.517105
C	0.897494	-1.175587	-0.013487
C	0.510031	-2.242558	-0.949736
O	1.487840	-3.206724	-0.997894
C	3.879768	-2.764663	-0.835936
O	2.890313	-1.008374	1.425564
O	-0.511851	-2.341566	-1.604205
H	-0.049885	4.400065	0.064968
H	1.752270	5.069206	-1.515613
H	1.794526	3.424612	-2.193656
H	0.349446	4.440137	-2.411054
H	-1.920842	1.626293	-1.123846
H	-0.832423	-0.217252	-0.562254
H	-1.036722	-1.418496	1.685044
H	-0.299299	-0.013591	2.426711
H	-2.686136	0.186796	2.657899

H	-2.164875	1.443921	1.560622
H	-4.316591	0.339827	0.997622
H	-3.619968	-2.016031	1.564755
H	-2.632020	-2.051611	0.101938
H	-3.535517	-0.001173	-1.332752
H	-4.864178	-3.132386	-0.264153
H	-4.699770	-1.742582	-1.318035
H	-5.687266	-1.619083	0.149499
H	2.599575	-3.626419	0.681216
H	3.827024	-2.012508	-1.628771
H	4.674901	-2.487374	-0.138072
H	4.121300	-3.732048	-1.284348
H	2.611972	-0.067389	1.635059

B3LYP Energy = -1149.63233902 a.u.

(5*S*,9*S*,5'*S*)-**1**, Conf H

C	-2.399234	-2.977303	-0.297092
C	-1.096099	-2.234088	-0.410280
C	-1.183738	-1.021481	0.197036
C	-2.512879	-0.950855	0.781440
O	-3.225163	-2.073030	0.475355
C	-3.072117	-3.312207	-1.622307
O	-0.079105	-2.827553	-1.026285
O	-3.022564	-0.069499	1.470924
C	-0.023847	-0.070216	0.320193
C	0.821400	-0.338789	1.612766
C	2.341607	-0.251142	1.378453
C	2.939758	-1.415975	0.565750
C	4.475724	-1.412381	0.508161
O	2.389067	-1.507949	-0.778410
C	5.115099	-0.184113	-0.153181
C	-0.694420	3.694631	-0.136840
C	-1.071905	2.367363	0.478768
C	-0.231305	1.395923	0.034740
C	0.720467	2.046208	-0.872129
O	0.448570	3.384367	-0.964042
C	-1.795750	4.337818	-0.970864
O	-2.108603	2.352703	1.298909
O	1.651208	1.539416	-1.482594
H	-2.265470	-3.884903	0.304808
H	-2.435561	-3.992386	-2.195568
H	-4.034843	-3.796612	-1.440769
H	-3.237213	-2.403981	-2.208852
H	0.770502	-2.314636	-0.975883
H	0.617327	-0.361386	-0.506044
H	0.526289	0.367108	2.396992
H	0.580382	-1.340086	1.991835
H	2.594919	0.702809	0.902787
H	2.846297	-0.254444	2.353243
H	2.625412	-2.358475	1.031424
H	4.782289	-2.316902	-0.030436
H	4.851198	-1.517088	1.534945
H	2.462597	-0.639176	-1.213648
H	6.202081	-0.304777	-0.200783
H	4.911128	0.738320	0.399411
H	4.760256	-0.043566	-1.179719
H	-0.354803	4.387553	0.643765
H	-2.111332	3.664082	-1.773036
H	-2.657834	4.557030	-0.334700
H	-1.434451	5.269114	-1.414761
H	-2.423016	1.414396	1.476440

B3LYP Energy = -1149.63198948 a.u.

(5*S*,9*S*,5'*S*)-**1**, Conf I

C	-4.006110	-0.156691	-0.383613
C	-2.784261	0.522822	0.188502
C	-1.662294	-0.135538	-0.205425
C	-2.104604	-1.252437	-1.047000
O	-3.469655	-1.264593	-1.139385
C	-5.002526	-0.653916	0.656570
O	-2.981172	1.597221	0.932866
O	-1.418557	-2.095752	-1.608220
C	-0.185412	-0.024015	0.078176
C	0.246572	-0.713697	1.417940
C	0.414168	-2.238983	1.280236
C	1.628647	-2.735700	0.461574
C	2.986582	-2.406148	1.085197
O	1.647844	-2.217035	-0.896670
C	4.168406	-3.067366	0.366297
C	2.178466	2.838357	-0.752109
C	1.710737	1.408198	-0.763049
C	0.511419	1.292357	-0.135562
C	0.174221	2.619191	0.353693
O	1.132407	3.516906	-0.015493
C	3.529121	3.069823	-0.086335
O	2.488537	0.486820	-1.324206
O	-0.793285	2.990386	1.015266
H	-4.502043	0.515016	-1.095603
H	-4.518752	-1.349202	1.349096
H	-5.395551	0.194194	1.224313
H	-5.832638	-1.167664	0.164754
H	-2.126193	2.106577	1.075662
H	0.230514	-0.646752	-0.707216
H	1.187546	-0.268003	1.758988
H	-0.493203	-0.496485	2.196569
H	0.510381	-2.680855	2.280532
H	-0.495734	-2.669411	0.846617
H	1.545761	-3.830409	0.389950
H	2.959791	-2.733943	2.132109
H	3.128335	-1.318110	1.104435
H	0.802770	-2.441233	-1.328127
H	5.113262	-2.816901	0.859581

H	4.230904	-2.740721	-0.675304
H	4.069148	-4.159153	0.369005
H	2.177065	3.251043	-1.768716
H	3.757720	4.138335	-0.067562
H	3.521315	2.693196	0.940597
H	4.309798	2.549530	-0.648478
H	2.152046	-0.438202	-1.205012

B3LYP Energy = -1149.63165134 a.u.

Table S5. Cartesian coordinates and energies of the low-energy conformers calculated at the B97D/TZVP PCM/MeCN level.

(5*R*,9*S*,5'*R*)-**1**, Conf A

C	-3.118302	-2.036432	0.531679
C	-2.242124	-0.844064	0.817917
C	-1.060359	-0.946269	0.145275
C	-1.162476	-2.139218	-0.671121
O	-2.326997	-2.810850	-0.419088
C	-4.465408	-1.675332	-0.084764
O	-2.721564	0.114021	1.595511
O	-0.391240	-2.588882	-1.526304
C	0.069953	0.053809	0.126722
C	0.021841	0.919241	-1.164019
C	-1.230117	1.806179	-1.254956
C	-1.317999	2.972936	-0.261448
C	-0.055457	3.835442	-0.179129
O	-1.629697	2.442007	1.069456
C	0.317595	4.463922	-1.528928
C	3.660493	-1.323055	0.250747
C	2.288892	-1.267017	-0.373358
C	1.455382	-0.497918	0.378202
C	2.230439	-0.039382	1.531549
O	3.522989	-0.536542	1.464914
C	4.762242	-0.744535	-0.633164
O	2.098348	-1.927471	-1.507799
O	1.893317	0.677761	2.460515
H	-3.248867	-2.657381	1.427541
H	-5.022973	-2.586160	-0.327666
H	-5.041468	-1.085545	0.637170
H	-4.317954	-1.081811	-0.994779
H	-2.240246	0.988189	1.443625
H	-0.105125	0.727971	0.969950
H	0.924609	1.540563	-1.198770
H	0.054707	0.261685	-2.041553
H	-1.267063	2.252688	-2.256170
H	-2.136972	1.194419	-1.158880
H	-2.163879	3.605456	-0.569243
H	0.771787	3.222645	0.201415
H	-0.232240	4.629653	0.560461
H	-1.794930	3.180084	1.671902
H	1.173869	5.139796	-1.415655
H	-0.523324	5.041552	-1.936639
H	0.586118	3.692662	-2.261386
H	3.900653	-2.352566	0.548948
H	4.522953	0.291332	-0.902601
H	5.720732	-0.770911	-0.103065
H	4.845679	-1.342823	-1.547960
H	1.105108	-2.081689	-1.631497

B97D Energy = -1149.23634677 a.u.

(5*R*,9*S*,5'*R*)-**1**, Conf B

C	4.006962	-1.012165	-0.148820
C	2.735587	-0.437033	-0.722583
C	1.687117	-0.675663	0.111024
C	2.215673	-1.431680	1.247042
O	3.577200	-1.637878	1.090676
C	5.081522	0.035039	0.129523
O	2.815308	0.198937	-1.884449
O	1.634342	-1.873119	2.225880
C	0.196335	-0.468374	-0.033146
C	-0.370145	-1.251834	-1.252240
C	-1.906255	-1.273284	-1.318433
C	-2.600869	-2.189458	-0.309661
C	-4.105129	-2.345443	-0.571399
O	-2.369284	-1.671002	1.044161
C	-4.895964	-1.029304	-0.552184
C	-1.477031	2.946613	0.419773
C	-1.314871	1.476096	0.697989
C	-0.281713	0.962614	-0.029120
C	0.161897	2.028737	-0.904117
O	-0.494794	3.197617	-0.630007
C	-1.215779	3.848238	1.620780
O	-2.159077	0.899780	1.539218
O	0.987041	2.013510	-1.824457
H	4.398369	-1.805902	-0.800105
H	5.384241	0.501955	-0.814880
H	4.689107	0.808179	0.801165
H	5.956837	-0.437156	0.589155
H	2.023166	0.823616	-1.971369
H	-0.225662	-0.929049	0.864010
H	0.018702	-0.802528	-2.174745
H	0.010957	-2.280989	-1.205285
H	-2.302270	-0.254199	-1.226437

H	-2.206105	-1.633686	-2.310998
H	-2.128968	-3.182208	-0.353098
H	-4.511821	-3.034750	0.183911
H	-4.219915	-2.845312	-1.543260
H	-2.888417	-2.194811	1.670473
H	-4.585763	-0.365281	-1.368304
H	-4.745945	-0.497962	0.395964
H	-5.968743	-1.228135	-0.665956
H	-2.465803	3.143650	-0.014031
H	-0.211121	3.663864	2.018980
H	-1.307169	4.899699	1.327618
H	-1.956148	3.631581	2.399706
H	-2.187440	-0.101920	1.402735

B97D Energy = -1149.23603277 a.u.

(5*R*,9*S*,5'*R*)-**1**, Conf C

C	-2.729904	-2.441244	0.745658
C	-2.049579	-1.100486	0.848710
C	-0.854351	-1.117902	0.191981
C	-0.763206	-2.416917	-0.443449
O	-1.816054	-3.214880	-0.088668
C	-4.108211	-2.384894	0.096169
O	-2.681768	-0.123482	1.479285
O	0.079199	-2.862752	-1.230981
C	0.107951	0.033055	0.024858
C	-0.058861	0.699012	-1.370745
C	-1.442737	1.335260	-1.582012
C	-1.756154	2.601625	-0.775035
C	-0.699254	3.701006	-0.907473
O	-1.928871	2.242780	0.638764
C	-1.109445	5.016618	-0.231540
C	3.869471	-0.731475	0.297034
C	2.510975	-0.988333	-0.305280
C	1.560551	-0.253528	0.333687
C	2.244863	0.491755	1.390851
O	3.600397	0.200940	1.378579
C	4.871467	-0.129912	-0.684713
O	2.438045	-1.836217	-1.322463
O	1.791529	1.280111	2.205738
H	-2.775963	-2.937729	1.723733
H	-4.519806	-3.395311	0.000633
H	-4.774969	-1.785842	0.726649
H	-4.041669	-1.921574	-0.895313
H	-2.332909	0.783514	1.200526
H	-0.178029	0.779152	0.771450
H	0.725406	1.455456	-1.490854
H	0.104871	-0.055873	-2.150052
H	-1.535198	1.621807	-2.637738
H	-2.229669	0.592716	-1.392598
H	-2.722187	2.990667	-1.130056
H	-0.532821	3.869484	-1.980693
H	0.246552	3.340935	-0.482971
H	-2.317711	2.995237	1.104618
H	-0.352169	5.791990	-0.400099
H	-1.212883	4.894265	0.855718
H	-2.066901	5.379901	-0.630369
H	4.267994	-1.651983	0.744671
H	4.472835	0.801409	-1.104846
H	5.818897	0.076300	-0.174620
H	5.053566	-0.841225	-1.498709
H	1.481485	-2.157127	-1.413304

B97D Energy = -1149.23595243 a.u.

(5*R*,9*S*,5'*R*)-**1**, Conf D

C	3.816367	-1.534647	-0.073845
C	2.684183	-0.735513	-0.670420
C	1.572680	-0.830388	0.108997
C	1.915947	-1.712323	1.225547
O	3.231920	-2.133124	1.114080
C	5.030411	-0.689209	0.300470
O	2.921867	-0.077176	-1.797024
O	1.224667	-2.094846	2.156589
C	0.142674	-0.377468	-0.083422
C	-0.493539	-1.036326	-1.341758
C	-2.009354	-0.811033	-1.470173
C	-2.894192	-1.618651	-0.519827
C	-4.381012	-1.440442	-0.843366
O	-2.606013	-1.204529	0.856796
C	-5.312722	-2.272822	0.049098
C	-0.992599	3.246761	0.406837
C	-1.078945	1.762188	0.638118
C	-0.101738	1.111433	-0.056194
C	0.548455	2.118310	-0.870800
O	0.068285	3.367933	-0.587594
C	-0.650602	4.057577	1.651937
O	-2.046661	1.305467	1.417539
O	1.408758	1.999874	-1.750847
H	4.106081	-2.352875	-0.747735
H	4.735368	0.102554	0.999667
H	5.798200	-1.318026	0.764781
H	5.445087	-0.231098	-0.604901
H	2.244387	0.671096	-1.890144
H	-0.384128	-0.782437	0.784260
H	0.000655	-0.640336	-2.237993
H	-0.284331	-2.114107	-1.305498
H	-2.249308	0.256602	-1.364066
H	-2.315609	-1.096239	-2.484738
H	-2.627218	-2.684347	-0.593665
H	-4.521577	-1.732938	-1.892806
H	-4.629509	-0.372139	-0.765814
H	-3.192992	-1.680054	1.460511
H	-6.354257	-2.168670	-0.278350

H	-5.273091	-1.947601	1.098554
H	-5.045265	-3.337681	0.007597
H	-1.914343	3.613591	-0.062521
H	-1.455662	3.943352	2.387212
H	0.288369	3.698196	2.089002
H	-0.553666	5.117801	1.394399
H	-2.215843	0.321875	1.258738

B97D Energy = -1149.23590359 a.u.

(5*R*,9*S*,5'*R*)-**1**, Conf E

C	3.827329	-1.453222	-0.186379
C	2.608645	-0.763109	-0.747149
C	1.591736	-0.784917	0.156597
C	2.086003	-1.506868	1.329762
O	3.397493	-1.906749	1.125587
C	5.043869	-0.540746	-0.059767
O	2.697765	-0.245465	-1.965314
O	1.513487	-1.782398	2.372473
C	0.134760	-0.390254	0.067593
C	-0.604260	-1.199304	-1.036917
C	-2.130868	-1.009969	-1.041773
C	-2.901072	-1.719324	0.071645
C	-4.421409	-1.589273	-0.079125
O	-2.483331	-1.161543	1.362896
C	-4.977567	-2.337057	-1.299810
C	-1.061736	3.241993	0.261827
C	-1.074782	1.792921	0.667813
C	-0.153428	1.086528	-0.047438
C	0.375305	2.004491	-1.036358
O	-0.111717	3.269172	-0.845562
C	-0.623844	4.200341	1.363603
O	-1.943225	1.406596	1.589498
O	1.140259	1.800537	-1.985903
H	4.071113	-2.345220	-0.779980
H	4.799326	0.328372	0.562999
H	5.879438	-1.088015	0.390520
H	5.341312	-0.194198	-1.056211
H	1.991145	0.473791	-2.067963
H	-0.285945	-0.704550	1.025978
H	-0.207966	-0.903381	-2.016609
H	-0.367082	-2.263007	-0.899332
H	-2.387489	0.059062	-1.029274
H	-2.517178	-1.409001	-1.986743
H	-2.625173	-2.785197	0.077321
H	-4.679743	-0.521912	-0.127908
H	-4.887288	-1.995489	0.831402
H	-3.048246	-1.532199	2.055969
H	-4.633644	-1.886746	-2.238771
H	-6.074119	-2.311893	-1.296162
H	-4.659694	-3.388745	-1.288421
H	-2.038224	3.530754	-0.147736
H	-0.591744	5.225292	0.978555
H	-1.345432	4.153186	2.187539
H	0.366998	3.916726	1.737329
H	-2.098294	0.407801	1.553354

B97D Energy = -1149.23571721 a.u.

(5*R*,9*S*,5'*R*)-**1**, Conf F

C	3.292242	-2.142278	0.022990
C	2.305542	-1.212866	-0.639210
C	1.246065	-0.984690	0.182688
C	1.474005	-1.766498	1.396840
O	2.673399	-2.453696	1.301228
C	4.670301	-1.522818	0.236430
O	2.597534	-0.766675	-1.853691
O	0.773885	-1.879074	2.390883
C	-0.067623	-0.266645	-0.029750
C	-0.880292	-0.885535	-1.199136
C	-2.368515	-0.509283	-1.145980
C	-3.076653	-1.022510	0.128672
C	-4.469067	-1.603011	-0.135945
O	-3.169911	0.028600	1.151942
C	-4.416167	-2.918970	-0.925795
C	-0.209585	3.554999	0.166780
C	-0.610247	2.169188	0.595673
C	0.032167	1.232104	-0.153726
C	0.781594	1.959334	-1.159174
O	0.666892	3.309586	-0.975514
C	0.521817	4.360972	1.234420
O	-1.493382	2.036220	1.575522
O	1.451320	1.537700	-2.108358
H	3.371779	-3.081773	-0.541204
H	4.582623	-0.601745	0.825254
H	5.323290	-2.229567	0.760338
H	5.113448	-1.283909	-0.737284
H	2.048506	0.059732	-2.049027
H	-0.628877	-0.460611	0.892884
H	-0.445519	-0.574839	-2.156868
H	-0.789447	-1.978293	-1.137391
H	-2.489356	0.581433	-1.201826
H	-2.863262	-0.924362	-2.032229
H	-2.460447	-1.792888	0.608949
H	-5.068303	-0.857150	-0.681045
H	-4.956083	-1.776041	0.832895
H	-3.902640	0.610121	0.895150
H	-5.426751	-3.319691	-1.071001
H	-3.823709	-3.668844	-0.384308
H	-3.963265	-2.778358	-1.915352
H	-1.082622	4.101869	-0.211746
H	-0.150956	4.522389	2.084796
H	1.409065	3.815904	1.577157
H	0.821760	5.333704	0.830046

H	-1.970634	1.152674	1.501057

B97D Energy = -1149.23351005 a.u.

(5*R*,9*S*,5'*R*)-**1**, Conf G

C	-3.367077	-2.122565	-0.032248
C	-2.427265	-1.148442	0.634092
C	-1.286205	-1.018471	-0.094559
C	-1.412506	-1.912832	-1.244446
O	-2.631873	-2.569159	-1.204430
C	-4.698934	-1.502197	-0.444766
O	-2.828725	-0.579252	1.763138
O	-0.621123	-2.132722	-2.147989
C	0.013909	-0.293958	0.171585
C	0.703816	-0.795886	1.469352
C	2.199076	-0.446024	1.519985
C	3.011252	-1.095217	0.375977
C	4.379032	-1.605702	0.836050
O	3.176631	-0.175712	-0.759425
C	5.167345	-2.333609	-0.260247
C	0.235659	3.486261	-0.397222
C	0.649758	2.060565	-0.644621
C	-0.072854	1.210318	0.134762
C	-0.896146	2.042344	0.989458
O	-0.741892	3.366039	0.681432
C	-0.387357	4.181218	-1.602627
O	1.613366	1.818698	-1.521957
O	-1.656860	1.725150	1.910358
H	-3.529047	-3.000249	0.608484
H	-5.314740	-2.244617	-0.964347
H	-5.231626	-1.162210	0.450900
H	-4.526668	-0.644012	-1.105677
H	-2.282066	0.253682	1.933091
H	0.655750	-0.584484	-0.669295
H	0.188789	-0.381697	2.344787
H	0.595553	-1.888100	1.512814
H	2.340963	0.643183	1.485261
H	2.601050	-0.786057	2.483116
H	2.443333	-1.930768	-0.052789
H	4.204425	-2.279896	1.685150
H	4.955980	-0.752089	1.227224
H	3.919540	0.409228	-0.542910
H	6.128611	-2.692884	0.128044
H	5.366741	-1.670554	-1.110885
H	4.599839	-3.198623	-0.629910
H	1.080320	4.064111	-0.000825
H	-1.251281	3.610023	-1.962054
H	-0.704158	5.193587	-1.329801
H	0.358485	4.246340	-2.403413
H	2.054980	0.936941	-1.319133

B97D Energy = -1149.23339628 a.u.

(5*S*,9*S*,5'*S*)-**1**, Conf A

C	4.216266	-0.066882	0.060272
C	2.865449	0.366526	-0.451791
C	1.872623	-0.200884	0.286330
C	2.524217	-1.005195	1.320627
O	3.902002	-0.915011	1.197596
C	5.043237	-0.838636	-0.964731
O	2.836299	1.184539	-1.495305
O	2.028338	-1.692576	2.199624
C	0.373662	-0.274884	0.100859
C	0.007983	-0.971378	-1.242526
C	-1.490762	-1.274229	-1.402362
C	-2.027123	-2.445095	-0.577995
C	-3.479083	-2.806940	-0.920159
O	-1.904836	-2.122679	0.849454
C	-4.486191	-1.664262	-0.722812
C	-2.025224	2.605732	0.889363
C	-1.530643	1.187564	1.009098
C	-0.392787	1.012911	0.277263
C	-0.166029	2.263240	-0.418451
O	-1.069998	3.214123	-0.030934
C	-3.437319	2.716541	0.323923
O	-2.246891	0.328603	1.717371
O	0.672270	2.557684	-1.278095
H	4.775175	0.799774	0.438352
H	4.486317	-1.716943	-1.312867
H	5.258355	-0.188597	-1.820869
H	5.989809	-1.161265	-0.517173
H	1.933566	1.644140	-1.528202
H	0.037667	-0.936382	0.903679
H	0.330203	-0.329195	-2.072069
H	0.583477	-1.904491	-1.310845
H	-2.081237	-0.373740	-1.193467
H	-1.683769	-1.532744	-2.451649
H	-1.389973	-3.323348	-0.758208
H	-3.768965	-3.668387	-0.299711
H	-3.495577	-3.154380	-1.962510
H	-2.337948	-2.819886	1.362118
H	-5.507689	-2.023962	-0.897372
H	-4.295124	-0.837688	-1.417885
H	-4.433506	-1.268836	0.299185
H	-1.940654	3.139267	1.845058
H	-3.712064	3.769966	0.204523
H	-3.497506	2.209907	-0.646412
H	-4.138149	2.240682	1.019081
H	-2.059545	-0.626128	1.438106

B97D Energy = -1149.23645245 a.u.

(5*S*,9*S*,5'*S*)-**1**, Conf B

C	0.867835	3.549450	0.135287
C	1.089444	2.114736	0.534491
C	0.225421	1.294891	-0.129401
C	-0.478285	2.135975	-1.076705
O	-0.144012	3.452410	-0.911635
C	0.380718	4.449368	1.265296
O	2.049463	1.849567	1.406155
O	-1.273480	1.833142	-1.973553
C	0.118826	-0.206015	-0.013104
C	0.843301	-0.910633	-1.194551
C	2.358154	-0.651708	-1.217501
C	3.185308	-1.310554	-0.104957
C	2.918261	-2.806084	0.088195
O	2.931919	-0.608206	1.157902
C	3.216590	-3.627059	-1.174424
C	-3.439474	-1.675930	0.050361
C	-2.358333	-0.858535	-0.612180
C	-1.272123	-0.758840	0.200797
C	-1.580246	-1.521120	1.411298
O	-2.851261	-2.066335	1.320666
C	-4.736167	-0.904802	0.279800
O	-2.607576	-0.366999	-1.819094
O	-0.892593	-1.722766	2.399916
H	1.773141	3.957744	-0.332042
H	-0.541980	4.045137	1.697916
H	1.151365	4.496819	2.043524
H	0.196411	5.460463	0.886469
H	2.330205	0.880494	1.359412
H	0.657799	-0.479903	0.898511
H	0.647866	-1.987338	-1.126819
H	0.410292	-0.566552	-2.142132
H	2.761947	-1.030595	-2.164252
H	2.558015	0.428194	-1.210406
H	4.247159	-1.166520	-0.354150
H	1.875139	-2.945978	0.399673
H	3.550271	-3.160880	0.915010
H	3.544638	-0.939439	1.828826
H	3.100092	-4.698799	-0.972747
H	4.245232	-3.453284	-1.518909
H	2.535193	-3.358258	-1.990983
H	-3.630079	-2.595164	-0.520738
H	-4.539123	-0.006704	0.877699
H	-5.154723	-0.605453	-0.688087
H	-5.463013	-1.537560	0.801106
H	-1.990899	0.418215	-1.985957

B97D Energy = -1149.23611314 a.u.

(5*S*,9*S*,5'*S*)-**1**, Conf C

C	4.168280	-0.499319	0.124423
C	2.899288	0.119991	-0.405616
C	1.822372	-0.325892	0.297068
C	2.337076	-1.231883	1.324897
O	3.717279	-1.324181	1.232363
C	4.911817	-1.349740	-0.901971
O	3.004425	0.956414	-1.429297
O	1.734184	-1.865847	2.176677
C	0.331052	-0.203106	0.078294
C	-0.090068	-0.840572	-1.278673
C	-1.610942	-0.949008	-1.480065
C	-2.324975	-2.040942	-0.682659
C	-3.811692	-2.120435	-1.044021
O	-2.149086	-1.773003	0.748237
C	-4.571755	-3.230118	-0.303396
C	-1.709719	2.946152	0.845100
C	-1.401714	1.475258	0.952572
C	-0.271232	1.169525	0.252593
C	0.135088	2.392460	-0.409450
O	-0.654190	3.443707	-0.030875
C	-3.075313	3.243507	0.235126
O	-2.244567	0.704693	1.622478
O	1.032124	2.593589	-1.236210
H	4.826790	0.277335	0.536415
H	5.236350	-0.713985	-1.734052
H	5.793724	-1.808310	-0.441061
H	4.251785	-2.135872	-1.288191
H	2.170454	1.531275	-1.471476
H	-0.105146	-0.822801	0.865616
H	0.332220	-0.242142	-2.095905
H	0.362774	-1.839456	-1.341610
H	-2.092099	0.017921	-1.276843
H	-1.803993	-1.172820	-2.536937
H	-1.844139	-3.010646	-0.884282
H	-3.873770	-2.293875	-2.126989
H	-4.271597	-1.142082	-0.843063
H	-2.627933	-2.442925	1.255508
H	-5.607981	-3.289436	-0.657723
H	-4.614277	-3.045473	0.779685
H	-4.097096	-4.207122	-0.468584
H	-1.592681	3.449117	1.813870
H	-3.854765	2.846133	0.894951
H	-3.212388	4.325022	0.130571
H	-3.162093	2.766452	-0.748298
H	-2.160865	-0.264553	1.346086

B97D Energy = -1149.23608864 a.u.

(5*S*,9*S*,5'*S*)-**1**, Conf D

C	4.164701	-0.329521	-0.042818
C	2.826707	0.142433	-0.553656
C	1.833977	-0.225681	0.301146
C	2.474906	-0.932039	1.411178
O	3.846653	-0.982337	1.215741
C	4.874511	-1.302156	-0.980714

O	2.804123	0.806612	-1.701513
O	1.975103	-1.443938	2.400648
C	0.326025	-0.192586	0.193286
C	-0.168851	-1.030716	-1.020742
C	-1.693368	-1.225522	-1.075318
C	-2.282024	-2.223688	-0.079049
C	-3.784023	-2.452527	-0.286317
O	-2.039974	-1.731843	1.281954
C	-4.112234	-3.171822	-1.603220
C	-1.782496	2.967882	0.677803
C	-1.403398	1.538383	0.965544
C	-0.321621	1.170105	0.220874
C	-0.027388	2.293589	-0.645203
O	-0.828749	3.363421	-0.353676
C	-3.207553	3.132624	0.160823
O	-2.154035	0.844278	1.806749
O	0.787365	2.397521	-1.569362
H	4.808212	0.531347	0.184243
H	4.233376	-2.169524	-1.179375
H	5.096701	-0.796548	-1.927744
H	5.814295	-1.639572	-0.529731
H	1.944450	1.340976	-1.753354
H	-0.017377	-0.706458	1.094809
H	0.158032	-0.539645	-1.946098
H	0.324846	-2.011275	-0.982499
H	-2.210546	-0.261778	-0.964467
H	-1.949506	-1.600117	-2.073095
H	-1.750229	-3.183232	-0.173018
H	-4.297625	-1.481888	-0.236711
H	-4.152808	-3.059827	0.553937
H	-2.513558	-2.302146	1.904407
H	-5.180575	-3.415840	-1.649305
H	-3.543471	-4.108142	-1.685246
H	-3.871256	-2.548686	-2.472983
H	-1.602984	3.610271	1.549716
H	-3.360889	2.511719	-0.729777
H	-3.908602	2.816746	0.941674
H	-3.398077	4.182207	-0.087162
H	-2.053541	-0.150854	1.655758

B97D Energy = -1149.23590417 a.u.

(5*S*,9*S*,5'*S*)-**1**, Conf E

C	0.393305	3.604745	0.362209
C	0.821506	2.176611	0.570316
C	-0.011268	1.325205	-0.094072
C	-0.912164	2.162830	-0.860563
O	-0.715633	3.487177	-0.578781
C	-0.054820	4.321345	1.630806
O	1.899530	1.949629	1.303598
O	-1.764660	1.856187	-1.701837
C	0.084504	-0.180030	-0.150800
C	0.769052	-0.641299	-1.469726
C	2.229651	-0.178220	-1.593620
C	3.249656	-0.834656	-0.654157
C	3.211148	-2.364416	-0.667780
O	3.035373	-0.340062	0.712407
C	4.347187	-3.003396	0.142869
C	-3.225836	-2.138144	0.044722
C	-2.340974	-1.099462	-0.598649
C	-1.191975	-0.946434	0.113927
C	-1.259645	-1.890456	1.230085
O	-2.450924	-2.596999	1.185507
C	-4.575541	-1.592941	0.503049
O	-2.787631	-0.503998	-1.696369
O	-0.444357	-2.112875	2.111580
H	1.186590	4.165847	-0.148386
H	-0.391813	5.335353	1.389962
H	-0.870488	3.767266	2.109968
H	0.791892	4.384153	2.324256
H	2.285952	1.033620	1.121488
H	0.743908	-0.473015	0.670952
H	0.714928	-1.734853	-1.525608
H	0.201696	-0.250888	-2.323985
H	2.576251	-0.396411	-2.612216
H	2.289878	0.911959	-1.473223
H	4.250486	-0.499753	-0.965280
H	3.275432	-2.685204	-1.717003
H	2.240295	-2.700832	-0.282170
H	3.796335	-0.586207	1.255243
H	4.321350	-4.096231	0.052469
H	4.261177	-2.763225	1.211586
H	5.326174	-2.652886	-0.212433
H	-3.362498	-2.996518	-0.627528
H	-4.428397	-0.754850	1.195034
H	-5.137695	-1.241012	-0.369704
H	-5.150094	-2.381244	1.001918
H	-2.297646	0.374778	-1.815865

B97D Energy = -1149.23570579 a.u.

(5*S*,9*S*,5'*S*)-**1**, Conf F

C	-4.015773	0.068428	0.204380
C	-2.706225	-0.326291	-0.431230
C	-1.663331	0.082054	0.340386
C	-2.235704	0.738495	1.514862
O	-3.619716	0.718993	1.442607
C	-4.852332	1.017186	-0.649392
O	-2.751955	-0.967252	-1.591739
O	-1.673306	1.262558	2.463474
C	-0.170827	0.107326	0.098835
C	0.195474	0.936849	-1.160928
C	1.670658	1.363566	-1.178908
C	2.054039	2.275154	0.008885

C	2.975463	3.434103	-0.383734
O	2.672068	1.506521	1.098644
C	2.265093	4.481270	-1.254089
C	1.921491	-3.072651	0.526595
C	1.535280	-1.657775	0.869304
C	0.500211	-1.242131	0.089802
C	0.212969	-2.331067	-0.822934
O	1.004627	-3.413981	-0.558202
C	3.364578	-3.213080	0.054497
O	2.231735	-1.010141	1.793603
O	-0.595887	-2.391852	-1.755316
H	-4.593231	-0.826823	0.471810
H	-4.271345	1.914366	-0.894720
H	-5.139940	0.511352	-1.578492
H	-5.759552	1.306979	-0.107910
H	-1.863052	-1.417773	-1.761276
H	0.230136	0.644503	0.967312
H	-0.043596	0.362486	-2.064233
H	-0.432575	1.837778	-1.169860
H	2.325901	0.481172	-1.171022
H	1.866765	1.889469	-2.121003
H	1.146583	2.686362	0.469033
H	3.849545	3.028830	-0.916722
H	3.338727	3.907978	0.537820
H	3.587849	1.327068	0.833679
H	2.945210	5.308812	-1.489764
H	1.393502	4.892197	-0.726893
H	1.916820	4.050274	-2.201314
H	1.708733	-3.758656	1.356653
H	3.550498	-2.544495	-0.794457
H	4.036644	-2.942606	0.876832
H	3.563413	-4.248117	-0.243083
H	2.196053	-0.018546	1.625064

B97D Energy = -1149.23362640 a.u.

(5*S*,9*S*,5'*S*)-**1**, Conf G

C	4.009181	-0.631258	0.274494
C	2.804098	0.015289	-0.361494
C	1.670104	-0.348385	0.295480
C	2.077427	-1.225513	1.392041
O	3.454252	-1.383317	1.387963
C	4.776726	-1.559558	-0.662665
O	3.006758	0.792942	-1.416886
O	1.392691	-1.789768	2.230859
C	0.204787	-0.139627	-0.013634
C	-0.187358	-0.738763	-1.390900
C	-1.701323	-0.959458	-1.531795
C	-2.263553	-1.965664	-0.501475
C	-3.312127	-2.905746	-1.101776
O	-2.819355	-1.281248	0.675082
C	-3.814852	-3.974632	-0.123597
C	-1.478496	3.211102	0.766629
C	-1.303597	1.722981	0.919826
C	-0.285503	1.277324	0.134671
C	0.196208	2.428496	-0.602396
O	-0.462184	3.564722	-0.221225
C	-2.859838	3.618297	0.265742
O	-2.133480	1.058502	1.712619
O	1.061268	2.502108	-1.481822
H	4.674478	0.136086	0.692946
H	5.177745	-0.977926	-1.500924
H	5.608644	-2.029264	-0.126426
H	4.108920	-2.336978	-1.053073
H	2.195034	1.376654	-1.564363
H	-0.314219	-0.726253	0.754284
H	0.175520	-0.086120	-2.194353
H	0.321692	-1.705886	-1.500292
H	-2.238875	-0.006071	-1.430479
H	-1.904468	-1.330649	-2.544524
H	-1.443985	-2.564748	-0.084365
H	-2.854379	-3.383315	-1.978518
H	-4.150689	-2.298158	-1.478695
H	-3.704871	-0.970991	0.428674
H	-4.548227	-4.629922	-0.610038
H	-4.290317	-3.517484	0.752718
H	-2.978939	-4.594464	0.228655
H	-1.224046	3.740031	1.694340
H	-2.900988	4.702689	0.118144
H	-3.084962	3.110787	-0.679804
H	-3.608267	3.331147	1.013095
H	-2.205712	0.099994	1.415377

B97D Energy = -1149.23354201 a.u.

(3*S*,4*S*)-**3**, Conf A

O	-2.570965	-3.059396	0.141152
O	-0.209398	-0.794446	-1.720921
O	4.714924	0.192606	-1.247577
O	0.112093	-2.756263	0.290344
C	1.538167	0.279000	1.449688
C	2.836612	0.595980	1.855962
C	3.900306	0.562241	0.949694
C	3.647705	0.209980	-0.381615
C	2.344649	-0.107098	-0.797851
C	1.287884	-0.078054	0.115297
C	-2.471877	0.519262	-0.002577
C	-3.385367	1.579384	0.070720
C	-2.930013	2.894892	-0.034103
C	-1.565608	3.156042	-0.203168
C	-0.660856	2.091623	-0.267799
C	-1.094195	0.766268	-0.168528
C	-0.142343	-0.417099	-0.329079
C	-0.679913	-1.601401	0.522498

C	-2.155476	-1.900408	0.209226
N	-2.948117	-0.806175	0.068338
H	0.207988	-1.670829	-1.782906
H	4.410231	-0.068787	-2.129513
H	-0.515284	-3.501274	0.237008
H	0.720873	0.328456	2.164707
H	3.025826	0.874592	2.890754
H	4.913475	0.807651	1.259139
H	2.159520	-0.364224	-1.838344
H	-4.444010	1.367331	0.206375
H	-3.643635	3.713992	0.021923
H	-1.207636	4.179716	-0.282665
H	0.400768	2.286341	-0.395593
H	-0.639414	-1.304975	1.584134
H	-3.943166	-0.968447	-0.047557

B97D Energy = -934.780396684 a.u.

(3*S*,4*S*)-**3**, Conf B

O	-2.568382	-3.061703	0.144994
O	-0.217735	-0.793681	-1.725643
O	4.632479	0.141506	-1.344640
O	0.114467	-2.754711	0.287906
C	1.534839	0.288755	1.440054
C	2.831900	0.604090	1.846120
C	3.896195	0.560931	0.938435
C	3.643755	0.201479	-0.391539
C	2.340481	-0.114005	-0.806862
C	1.285634	-0.075522	0.105532
C	-2.475291	0.517034	0.000973
C	-3.389997	1.575938	0.077162
C	-2.937030	2.891987	-0.031161
C	-1.573794	3.154913	-0.206822
C	-0.667852	2.091693	-0.274355
C	-1.098728	0.765842	-0.171187
C	-0.145531	-0.416056	-0.334622
C	-0.678476	-1.600593	0.520117
C	-2.154428	-1.902067	0.212105
N	-2.949402	-0.809043	0.074755
H	0.211625	-1.663871	-1.791418
H	5.481243	0.381042	-0.942977
H	-0.512490	-3.500019	0.233514
H	0.716652	0.344452	2.153575
H	3.022605	0.888592	2.878983
H	4.908738	0.806827	1.255366
H	2.164684	-0.375505	-1.845976
H	-4.447742	1.362506	0.217559
H	-3.651593	3.710115	0.027095
H	-1.217705	4.179004	-0.289455
H	0.392898	2.287633	-0.407516
H	-0.635233	-1.302436	1.581234
H	-3.944567	-0.972853	-0.037907

B97D Energy = -934.780316629 a.u.

(3*S*,4*S*)-**3**, Conf C

O	2.601333	-2.928835	-0.642610
O	0.569095	-0.967560	1.842731
O	-3.768793	0.926899	-2.099202
O	-0.068521	-2.795103	-0.227666
C	-2.172387	-0.427868	1.509554
C	-3.545170	-0.178173	1.369892
C	-4.074485	0.270394	0.160985
C	-3.211382	0.475403	-0.927175
C	-1.840931	0.226798	-0.795353
C	-1.315418	-0.229198	0.422968
C	2.353244	0.615378	-0.178562
C	3.176118	1.737547	-0.344932
C	2.684664	3.008522	-0.041426
C	1.372629	3.164745	0.419238
C	0.557039	2.039596	0.576072
C	1.028261	0.756996	0.281527
C	0.192524	-0.496782	0.532095
C	0.601158	-1.576173	-0.510309
C	2.122205	-1.798564	-0.526990
N	2.870919	-0.666984	-0.454963
H	0.206231	-1.866377	1.921931
H	-3.075941	1.025860	-2.769450
H	0.593741	-3.498740	-0.360887
H	-1.773416	-0.764199	2.461266
H	-4.209094	-0.334346	2.217916
H	-5.137927	0.467108	0.047003
H	-1.183040	0.409016	-1.643934
H	4.194398	1.609379	-0.706634
H	3.328409	3.875731	-0.171312
H	0.986193	4.153602	0.654124
H	-0.463854	2.152757	0.931314
H	0.329304	-1.203947	-1.512612
H	3.875237	-0.771895	-0.555504

B97D Energy = -934.780145811 a.u.

(3*S*,4*S*)-**3**, Conf D

O	2.607027	-2.925405	-0.648992
O	0.575475	-0.966958	1.841318
O	-3.646627	0.926999	-2.146874
O	-0.061984	-2.794858	-0.228614
C	-2.168560	-0.436605	1.509144
C	-3.540399	-0.190993	1.370041
C	-4.068809	0.261336	0.160140
C	-3.204934	0.473542	-0.926803
C	-1.834512	0.228336	-0.793976
C	-1.311353	-0.230656	0.421963

C	2.356053	0.618251	-0.182118
C	3.177559	1.741249	-0.349708
C	2.685391	3.011695	-0.045236
C	1.373887	3.166498	0.417404
C	0.559585	2.040540	0.575079
C	1.031652	0.758388	0.279973
C	0.197222	-0.496189	0.530911
C	0.605680	-1.574809	-0.512233
C	2.126825	-1.795680	-0.531760
N	2.874589	-0.663496	-0.459956
H	0.215227	-1.866884	1.919781
H	-4.604434	1.068425	-2.110544
H	0.600755	-3.497576	-0.364221
H	-1.769254	-0.775543	2.459769
H	-4.206042	-0.352097	2.215737
H	-5.136000	0.451716	0.054188
H	-1.183929	0.416667	-1.644695
H	4.195272	1.614107	-0.713363
H	3.328019	3.879576	-0.176208
H	0.986725	4.154977	0.652715
H	-0.461107	2.152786	0.931121
H	0.331002	-1.202092	-1.513532
H	3.878800	-0.767245	-0.562689

B97D Energy = -934.780118121 a.u.

(3*S*,4*S*)-**3**, Conf E

O	2.442720	3.157309	0.201266
O	0.191400	0.914853	-1.664587
O	-4.748137	-0.052644	-1.196024
O	-0.282874	2.708579	0.486217
C	-1.505377	-0.548330	1.375214
C	-2.796704	-0.907556	1.768150
C	-3.881679	-0.741141	0.902496
C	-3.659177	-0.203985	-0.371210
C	-2.364875	0.166506	-0.770134
C	-1.284630	-0.010327	0.097591
C	2.505471	-0.416189	0.002293
C	3.478090	-1.425476	0.036224
C	3.098815	-2.761623	-0.105370
C	1.750792	-3.096730	-0.275935
C	0.785903	-2.084716	-0.303822
C	1.142914	-0.739106	-0.164870
C	0.132708	0.399050	-0.310345
C	0.588610	1.601099	0.567508
C	2.054882	1.994287	0.258316
N	2.902004	0.928996	0.106972
H	0.014689	0.178329	-2.268179
H	-4.461892	0.322711	-2.042313
H	-0.259710	3.025328	-0.429640
H	-0.668571	-0.699057	2.052682
H	-2.963605	-1.325833	2.758772
H	-4.889277	-1.021976	1.199815
H	-2.210988	0.600183	-1.755687
H	4.523951	-1.157032	0.172425
H	3.858938	-3.539383	-0.078201
H	1.451647	-4.136616	-0.383489
H	-0.263375	-2.337986	-0.431786
H	0.568260	1.261344	1.611174
H	3.886577	1.147670	-0.006011

B97D Energy = -934.778034430 a.u.

(3*S*,4*S*)-**3**, Conf F

O	-2.470109	-3.144503	0.190302
O	-0.203836	-0.914962	-1.669927
O	4.660434	0.006176	-1.299799
O	0.260235	-2.718813	0.473625
C	1.507357	0.518765	1.376928
C	2.798419	0.872286	1.769743
C	3.880250	0.714111	0.895944
C	3.652661	0.192228	-0.383731
C	2.356965	-0.172865	-0.781865
C	1.282696	-0.005225	0.092248
C	-2.503511	0.430214	0.005487
C	-3.467464	1.447560	0.045212
C	-3.077357	2.780939	-0.093316
C	-1.727014	3.105253	-0.266326
C	-0.770778	2.085191	-0.299542
C	-1.138727	0.742217	-0.163884
C	-0.138078	-0.403757	-0.314649
C	-0.602471	-1.604900	0.559804
C	-2.072438	-1.985050	0.251423
N	-2.911090	-0.912027	0.106551
H	-0.002478	-0.182755	-2.271051
H	5.502415	0.290697	-0.913637
H	0.242067	-3.025026	-0.445956
H	0.672886	0.662740	2.058717
H	2.970779	1.279019	2.764178
H	4.887682	0.993583	1.201178
H	2.208593	-0.592981	-1.772166
H	-4.515173	1.187539	0.183341
H	-3.830910	3.564916	-0.061841
H	-1.419402	4.142898	-0.371699
H	0.280316	2.329868	-0.429488
H	-0.578457	-1.269204	1.604692
H	-3.897553	-1.122103	-0.006584

B97D Energy = -934.778031351 a.u.

(3*S*,4*S*)-**3**, Conf G

O	2.633792	-2.927523	-0.703577
O	0.563749	-1.122646	1.759910

O	-3.733924	1.220861	-1.981168
O	-0.127377	-2.798430	-0.419259
C	-2.196309	-0.651807	1.416106
C	-3.570272	-0.407279	1.279493
C	-4.079244	0.217285	0.141955
C	-3.194851	0.606538	-0.876685
C	-1.822172	0.371785	-0.743807
C	-1.316591	-0.255551	0.404309
C	2.355967	0.601245	-0.173812
C	3.192355	1.720965	-0.287654
C	2.713208	2.985277	0.060058
C	1.399523	3.139447	0.517144
C	0.569546	2.018736	0.622135
C	1.027857	0.741973	0.278896
C	0.188837	-0.517785	0.496837
C	0.587676	-1.589540	-0.560168
C	2.119716	-1.820854	-0.573143
N	2.862082	-0.673324	-0.484496
H	0.382595	-0.478166	2.459756
H	-3.027641	1.435060	-2.609188
H	0.085437	-3.155722	0.456457
H	-1.818545	-1.156107	2.300072
H	-4.252505	-0.714562	2.069658
H	-5.144023	0.407801	0.029919
H	-1.143935	0.697336	-1.531074
H	4.212698	1.594392	-0.644504
H	3.368346	3.849020	-0.030358
H	1.022361	4.122899	0.787246
H	-0.453075	2.131718	0.972760
H	0.325478	-1.182353	-1.545343
H	3.866837	-0.778737	-0.581172

B97D Energy = -934.777981608 a.u.

(3*S*,4*S*)-**3**, Conf H

O	0.001923	-2.331314	2.341563
O	-0.221610	-1.093242	-2.297095
O	2.956982	2.607213	1.074736
O	-1.637833	-2.674082	-0.421668
C	2.315212	-0.954788	-0.995309
C	3.607883	-0.520676	-0.689528
C	3.817919	0.671900	0.007069
C	2.711739	1.438401	0.395254
C	1.410581	1.013392	0.087994
C	1.206674	-0.183263	-0.608561
C	-1.755541	0.368390	0.758280
C	-2.713999	1.322689	1.125147
C	-3.230417	2.190176	0.160341
C	-2.801280	2.103660	-1.169199
C	-1.839297	1.152712	-1.525907
C	-1.304412	0.281589	-0.574530
C	-0.198921	-0.718498	-0.912221
C	-0.434470	-1.986026	-0.034925
C	-0.495796	-1.631568	1.463680
N	-1.222346	-0.500616	1.734855
H	-1.018667	-1.634747	-2.423175
H	2.116718	3.041568	1.285036
H	-2.389585	-2.076602	-0.275050
H	2.162907	-1.879603	-1.543998
H	4.464611	-1.117509	-0.996008
H	4.821029	1.014371	0.250180
H	0.565684	1.626988	0.392756
H	-3.049788	1.379287	2.158651
H	-3.974573	2.928925	0.449682
H	-3.207766	2.775401	-1.921560
H	-1.486661	1.078070	-2.551173
H	0.379169	-2.696531	-0.187723
H	-1.397618	-0.292448	2.712587

B97D Energy = -934.777949925 a.u.

(3*S*,4*S*)-**3**, Conf I

O	0.001808	-2.316988	2.348767
O	-0.238400	-1.097814	-2.293846
O	2.840550	2.603047	1.085461
O	-1.650718	-2.667751	-0.406854
C	2.304505	-0.959801	-1.013077
C	3.598841	-0.532249	-0.712899
C	3.814499	0.656674	-0.008281
C	2.712335	1.423383	0.392056
C	1.408818	1.004025	0.088818
C	1.199759	-0.185927	-0.613890
C	-1.757556	0.378914	0.761115
C	-2.713241	1.336174	1.127333
C	-3.230479	2.201582	0.161101
C	-2.804911	2.109862	-1.169213
C	-1.845728	1.155820	-1.525239
C	-1.310047	0.286797	-0.572468
C	-0.208601	-0.717633	-0.910586
C	-0.444134	-1.981184	-0.027295
C	-0.499023	-1.620344	1.470022
N	-1.223612	-0.487954	1.739295
H	-1.037359	-1.637726	-2.414198
H	3.779980	2.789190	1.233022
H	-2.400166	-2.067338	-0.260363
H	2.146088	-1.880571	-1.566725
H	4.453184	-1.127928	-1.028019
H	4.824702	0.988455	0.227571
H	0.574735	1.622661	0.406173
H	-3.045927	1.397024	2.161598
H	-3.972273	2.942883	0.449987
H	-3.211874	2.780035	-1.922732
H	-1.495976	1.077215	-2.551197
H	0.367151	-2.694409	-0.180245

H	-1.393120	-0.274313	2.716853

B97D Energy = -934.777927721 a.u.

(3*S*,4*S*)-**3**, Conf J

O	2.646196	-2.921736	-0.698833
O	0.572659	-1.116592	1.759575
O	-3.618949	1.203718	-2.032511
O	-0.115144	-2.799976	-0.415125
C	-2.188125	-0.647040	1.422723
C	-3.561028	-0.404011	1.290095
C	-4.072600	0.212420	0.147301
C	-3.191594	0.591731	-0.878658
C	-1.818975	0.358744	-0.748042
C	-1.311845	-0.258044	0.402816
C	2.358389	0.607562	-0.178029
C	3.191398	1.729463	-0.294916
C	2.707879	2.993475	0.047875
C	1.393147	3.145095	0.502756
C	0.566519	2.022170	0.610692
C	1.029569	0.745610	0.273325
C	0.194603	-0.516153	0.495006
C	0.596306	-1.589093	-0.559344
C	2.128969	-1.816109	-0.571419
N	2.868280	-0.666498	-0.484837
H	0.395019	-0.468938	2.457338
H	-4.581630	1.308967	-2.002641
H	0.101814	-3.155942	0.460083
H	-1.807107	-1.143660	2.309579
H	-4.241689	-0.703725	2.084448
H	-5.140643	0.400217	0.045257
H	-1.151538	0.679277	-1.544282
H	4.212403	1.604986	-0.650609
H	3.360357	3.858984	-0.044919
H	1.012419	4.128389	0.768420
H	-0.456942	2.133204	0.959382
H	0.332462	-1.184992	-1.545298
H	3.873348	-0.769499	-0.580831

B97D Energy = -934.777916770 a.u.

(3*S*,4*S*)-**3**, Conf K

O	0.102168	2.739082	-1.730821
O	0.086752	0.198110	2.348675
O	4.793579	-0.105223	0.420613
O	-1.138606	2.499840	1.242396
C	0.985958	-1.344719	-0.754051
C	2.138066	-1.864620	-1.358004
C	3.408064	-1.446285	-0.962488
C	3.525605	-0.490300	0.058151
C	2.380124	0.035164	0.666361
C	1.103834	-0.390383	0.264200
C	-2.023484	0.032989	-0.709920
C	-3.195373	-0.580176	-1.172644
C	-3.788330	-1.595599	-0.419247
C	-3.222572	-1.994240	0.797411
C	-2.048254	-1.382089	1.248703
C	-1.435104	-0.371795	0.505215
C	-0.112405	0.266994	0.928962
C	-0.157411	1.762983	0.490634
C	-0.442795	1.900913	-1.017423
N	-1.416928	1.052127	-1.475499
H	-0.554700	0.809407	2.747620
H	4.740003	0.566845	1.116664
H	-2.012408	2.116228	1.060436
H	0.007231	-1.686782	-1.075615
H	2.042315	-2.607391	-2.147333
H	4.305256	-1.847126	-1.428378
H	2.480975	0.766455	1.465962
H	-3.635366	-0.259259	-2.114747
H	-4.698054	-2.068671	-0.782390
H	-3.688001	-2.780414	1.387220
H	-1.587987	-1.686274	2.185067
H	0.801041	2.238811	0.703986
H	-1.728497	1.185780	-2.432056

B97D Energy = -934.777884110 a.u.

(3*S*,4*S*)-**3**, Conf L

O	0.077958	2.756632	-1.713281
O	0.080715	0.189192	2.350402
O	4.738703	-0.022696	0.539533
O	-1.157273	2.489442	1.258861
C	0.994213	-1.316621	-0.772848
C	2.148768	-1.824125	-1.378602
C	3.416498	-1.410553	-0.965238
C	3.526794	-0.473193	0.073975
C	2.376706	0.043833	0.680023
C	1.106127	-0.378088	0.263050
C	-2.026786	0.027968	-0.708913
C	-3.193549	-0.591954	-1.175722
C	-3.777048	-1.618417	-0.429942
C	-3.206879	-2.021631	0.783172
C	-2.037690	-1.402686	1.238383
C	-1.433969	-0.381118	0.502562
C	-0.116373	0.265354	0.930964
C	-0.171577	1.763574	0.501942
C	-0.459977	1.909848	-1.004741
N	-1.429458	1.057976	-1.467227
H	-0.564388	0.795104	2.751579
H	5.453601	-0.452251	0.046226
H	-2.028744	2.101811	1.074338
H	0.018045	-1.655538	-1.105145

H	2.060562	-2.552835	-2.181740
H	4.313436	-1.808298	-1.438135
H	2.479316	0.763173	1.487638
H	-3.636846	-0.267868	-2.115187
H	-4.682794	-2.096687	-0.796219
H	-3.664847	-2.816546	1.367096
H	-1.574010	-1.710035	2.172019
H	0.784183	2.243699	0.717815
H	-1.743684	1.196724	-2.422189

B97D Energy = -934.777731755 a.u.

Table S6. Cartesian coordinates and energies of the low-energy conformers calculated at the CAM-B3LYP/TZVP PCM/MeCN level.

(5*R*,9*S*,5'*R*)-**1**, Conf A

C	3.677991	-1.712283	-0.027723
C	2.617293	-0.851840	-0.647395
C	1.493177	-0.875938	0.092101
C	1.767431	-1.759314	1.222029
O	3.038247	-2.237695	1.145408
C	4.941687	-0.969819	0.343295
O	2.923796	-0.224762	-1.765104
O	1.038614	-2.085503	2.129126
C	0.095913	-0.348733	-0.114229
C	-0.568135	-0.978739	-1.357494
C	-2.075756	-0.755730	-1.468153
C	-2.938314	-1.517157	-0.474006
C	-4.411430	-1.490639	-0.853855
O	-2.745042	-0.938103	0.839111
C	-5.312651	-2.240970	0.117280
C	-0.764527	3.335026	0.369992
C	-0.949546	1.870692	0.616960
C	-0.056799	1.147938	-0.088149
C	0.669342	2.104305	-0.896904
O	0.290490	3.363368	-0.610500
C	-0.382036	4.141211	1.589428
O	-1.920555	1.499842	1.423628
O	1.513580	1.914836	-1.760243
H	3.903917	-2.554499	-0.685524
H	4.716366	-0.144683	1.019152
H	5.643472	-1.645396	0.829812
H	5.410390	-0.570874	-0.555338
H	2.308250	0.552250	-1.900540
H	-0.446528	-0.718073	0.754147
H	-0.089690	-0.585911	-2.257348
H	-0.365247	-2.052154	-1.342945
H	-2.316173	0.309450	-1.404135
H	-2.389980	-1.072881	-2.464122
H	-2.595861	-2.556062	-0.425224
H	-4.502770	-1.931052	-1.849288
H	-4.732143	-0.448588	-0.936740
H	-3.103288	-1.519894	1.517731
H	-6.341971	-2.250684	-0.241134
H	-5.323021	-1.775915	1.104550
H	-4.992003	-3.278670	0.233142
H	-1.657103	3.744411	-0.105983
H	-1.187992	4.100355	2.321258
H	0.526280	3.744167	2.042012
H	-0.218145	5.181288	1.312992
H	-2.181642	0.549497	1.283063

CAM-B3LYP Energy = -1149.47524903 a.u.

(5*R*,9*S*,5'*R*)-**1**, Conf B

C	3.659114	-1.698334	-0.112258
C	2.532915	-0.906619	-0.707477
C	1.489506	-0.851781	0.140676
C	1.885544	-1.611705	1.323352
O	3.146417	-2.097442	1.167928
C	4.946002	-0.921271	0.049240
O	2.719830	-0.400357	-1.909715
O	1.255967	-1.839322	2.329405
C	0.073754	-0.346692	0.023942
C	-0.708428	-1.102685	-1.071537
C	-2.221619	-0.886814	-1.053138
C	-2.974536	-1.540095	0.094542
C	-4.486687	-1.529249	-0.089691
O	-2.634258	-0.839391	1.314844
C	-4.985046	-2.461103	-1.187022
C	-0.769085	3.368401	0.207157
C	-0.916990	1.937378	0.619375
C	-0.088830	1.144994	-0.090292
C	0.546693	2.012187	-1.059710
O	0.186671	3.294668	-0.868006
C	-0.278198	4.295226	1.294933
O	-1.803305	1.652230	1.548658
O	1.304393	1.734309	-1.977723
H	3.826032	-2.604890	-0.698210
H	4.782298	-0.033149	0.659808
H	5.702337	-1.543950	0.524439
H	5.313980	-0.613234	-0.928567
H	2.089282	0.361505	-2.060823
H	-0.374427	-0.622681	0.976561
H	-0.326116	-0.810240	-2.051947

H	-0.498360	-2.169316	-0.963389
H	-2.463138	0.179991	-1.071177
H	-2.625165	-1.299786	-1.978026
H	-2.632176	-2.574434	0.204123
H	-4.810436	-0.502963	-0.281976
H	-4.940988	-1.828065	0.859019
H	-3.050122	-1.273147	2.068392
H	-4.644683	-2.151856	-2.175373
H	-6.074767	-2.475608	-1.207564
H	-4.642782	-3.484189	-1.019157
H	-1.706671	3.728028	-0.220013
H	-0.152044	5.301428	0.899100
H	-1.008887	4.329799	2.102230
H	0.673632	3.946549	1.694851
H	-2.067170	0.691613	1.532020

CAM-B3LYP Energy = -1149.47464178 a.u.

(5*R*,9*S*,5'*R*)-**1**, Conf C

C	3.905683	-1.201631	-0.118509
C	2.692578	-0.543790	-0.706168
C	1.622014	-0.723181	0.089485
C	2.087009	-1.511930	1.226950
O	3.413316	-1.783370	1.098291
C	5.047120	-0.252909	0.169615
O	2.843199	0.087382	-1.852989
O	1.463111	-1.918842	2.178566
C	0.150436	-0.430818	-0.058248
C	-0.463399	-1.196148	-1.250405
C	-1.991374	-1.224974	-1.276324
C	-2.648987	-2.089279	-0.210848
C	-4.117095	-2.393090	-0.486199
O	-2.506651	-1.428452	1.070406
C	-5.013657	-1.170424	-0.629869
C	-1.264951	3.083677	0.379289
C	-1.200702	1.617525	0.672638
C	-0.237575	1.023098	-0.059830
C	0.286473	2.055381	-0.928988
O	-0.276178	3.246812	-0.655447
C	-0.958318	3.980870	1.555702
O	-2.060113	1.124231	1.537709
O	1.108767	1.974715	-1.829747
H	4.235911	-2.018070	-0.764469
H	5.402146	0.187376	-0.761255
H	4.721393	0.546238	0.835589
H	5.871482	-0.789793	0.636247
H	2.105891	0.752155	-1.976403
H	-0.284939	-0.854199	0.845267
H	-0.105209	-0.755737	-2.183473
H	-0.086254	-2.221167	-1.226126
H	-2.393875	-0.210765	-1.225419
H	-2.304691	-1.624150	-2.243047
H	-2.106231	-3.037142	-0.148422
H	-4.487945	-3.026897	0.324527
H	-4.164688	-3.003557	-1.391377
H	-2.834122	-2.001144	1.772946
H	-4.753582	-0.577400	-1.507202
H	-4.944500	-0.524485	0.246209
H	-6.055265	-1.474239	-0.736903
H	-2.233396	3.329797	-0.059297
H	0.023689	3.749969	1.967786
H	-0.978748	5.023973	1.244864
H	-1.709679	3.835776	2.331070
H	-2.172540	0.139387	1.434837

CAM-B3LYP Energy = -1149.47448879 a.u.

(5*R*,9*S*,5'*R*)-**1**, Conf D

C	-2.524686	-2.609751	0.743548
C	-1.954923	-1.226857	0.824206
C	-0.789481	-1.148240	0.151179
C	-0.607184	-2.441915	-0.471418
O	-1.583974	-3.292820	-0.107817
C	-3.913668	-2.680096	0.152720
O	-2.640971	-0.311226	1.472530
O	0.258255	-2.820646	-1.247086
C	0.099393	0.055391	-0.011986
C	-0.103980	0.742424	-1.379802
C	-1.504152	1.315150	-1.600177
C	-1.910754	2.527564	-0.769620
C	-0.944979	3.698661	-0.858690
O	-2.079364	2.116762	0.610788
C	-1.449957	4.957967	-0.165534
C	3.871685	-0.535752	0.322252
C	2.550015	-0.834532	-0.319544
C	1.560228	-0.159656	0.293450
C	2.190424	0.599715	1.369906
O	3.532016	0.375110	1.378523
C	4.888610	0.085288	-0.608782
O	2.547250	-1.670375	-1.338416
O	1.684013	1.346321	2.173831
H	-2.490572	-3.093951	1.721219
H	-4.232780	-3.717618	0.071228
H	-4.611238	-2.151162	0.800557
H	-3.934606	-2.221907	-0.835989
H	-2.375830	0.613455	1.209606
H	-0.216363	0.766252	0.750066
H	0.641920	1.531551	-1.481101
H	0.102754	0.025242	-2.177125
H	-1.585904	1.620921	-2.645266
H	-2.255477	0.533982	-1.461473
H	-2.890914	2.853104	-1.131648
H	-0.777164	3.907775	-1.918020
H	0.017598	3.406194	-0.435289

H	-2.473393	2.835047	1.117895
H	-0.758948	5.786602	-0.319762
H	-1.541987	4.821294	0.913949
H	-2.424774	5.259845	-0.554188
H	4.270667	-1.442086	0.782255
H	4.496485	1.003957	-1.045318
H	5.803241	0.313829	-0.064039
H	5.127641	-0.612114	-1.410766
H	1.632297	-2.057374	-1.455862

CAM-B3LYP Energy = -1149.47366425 a.u.

(5*R*,9*S*,5'*R*)-**1**, Conf E

C	-2.854171	-2.332128	0.523355
C	-2.112811	-1.059762	0.796953
C	-0.953718	-1.022259	0.109242
C	-0.943712	-2.216588	-0.708310
O	-2.016950	-2.985914	-0.450176
C	-4.247230	-2.137955	-0.028412
O	-2.671354	-0.178640	1.597759
O	-0.141295	-2.574943	-1.557931
C	0.081923	0.070394	0.108238
C	-0.037329	0.982395	-1.132381
C	-1.361033	1.738295	-1.241479
C	-1.620286	2.853796	-0.235082
C	-0.533275	3.914787	-0.139299
O	-1.825400	2.259500	1.069829
C	-0.300777	4.664926	-1.444367
C	3.745711	-1.046911	0.245929
C	2.393060	-1.064379	-0.400132
C	1.504143	-0.374434	0.337846
C	2.235114	0.115416	1.503463
O	3.535553	-0.279025	1.440515
C	4.832876	-0.425556	-0.601697
O	2.274223	-1.719195	-1.537706
O	1.836433	0.782933	2.428469
H	-2.871079	-2.962439	1.414308
H	-4.696588	-3.102922	-0.256062
H	-4.864495	-1.632810	0.713120
H	-4.220857	-1.534176	-0.935432
H	-2.299959	0.737268	1.465675
H	-0.135946	0.688905	0.977310
H	0.795659	1.686724	-1.118122
H	0.089440	0.380626	-2.034898
H	-1.416493	2.191598	-2.232419
H	-2.198413	1.037965	-1.196667
H	-2.556920	3.339617	-0.525559
H	0.394132	3.454261	0.206878
H	-0.830834	4.627749	0.634979
H	-2.019505	2.950062	1.713716
H	0.405519	5.481428	-1.294925
H	-1.230126	5.094797	-1.823482
H	0.107204	4.014909	-2.219047
H	4.021415	-2.059410	0.547875
H	4.565888	0.594265	-0.879022
H	5.772183	-0.409001	-0.051276
H	4.972972	-1.012395	-1.508757
H	1.316208	-1.964965	-1.687464

CAM-B3LYP Energy = -1149.47365437 a.u.

(5*R*,9*S*,5'*R*)-**1**, Conf F

C	-3.400604	-2.058324	-0.043422
C	-2.451495	-1.107426	0.623412
C	-1.314457	-0.997113	-0.087246
C	-1.465213	-1.876358	-1.242067
O	-2.679949	-2.486298	-1.209654
C	-4.724648	-1.441166	-0.433211
O	-2.849658	-0.544802	1.746540
O	-0.682551	-2.101417	-2.134782
C	0.004550	-0.312409	0.167763
C	0.694857	-0.864248	1.430898
C	2.189156	-0.563291	1.519982
C	3.016785	-1.145004	0.370042
C	4.393409	-1.614234	0.813007
O	3.147181	-0.192200	-0.716208
C	5.218432	-2.252590	-0.295643
C	0.279308	3.452256	-0.371775
C	0.664520	2.030125	-0.634149
C	-0.045936	1.190078	0.141342
C	-0.862995	2.031159	0.990934
O	-0.692017	3.330138	0.686309
C	-0.314058	4.179411	-1.556085
O	1.604093	1.789419	-1.524949
O	-1.626389	1.717352	1.892002
H	-3.553964	-2.935217	0.589305
H	-5.340453	-2.173765	-0.952417
H	-5.254015	-1.113649	0.460618
H	-4.569269	-0.581551	-1.085368
H	-2.307278	0.271552	1.939162
H	0.612544	-0.609366	-0.689010
H	0.193256	-0.481913	2.322026
H	0.558068	-1.948002	1.438684
H	2.368671	0.513908	1.570004
H	2.556754	-0.976537	2.460939
H	2.485205	-1.987471	-0.077808
H	4.250055	-2.330915	1.623947
H	4.930578	-0.764283	1.249075
H	3.903509	0.377950	-0.527890
H	6.181203	-2.591049	0.087821
H	5.411753	-1.554186	-1.109863
H	4.701496	-3.117844	-0.715113
H	1.132785	3.996772	0.035464
H	-1.186630	3.647556	-1.934850

H	-0.607920	5.186757	-1.266490
H	0.428531	4.249905	-2.350077
H	2.049776	0.918636	-1.344912

CAM-B3LYP Energy = -1149.47199664 a.u.

(5*S*,9*S*,5'*S*)-**1**, Conf A

C	4.072780	-0.646833	0.194874
C	2.854822	-0.008921	-0.403193
C	1.746987	-0.380329	0.264666
C	2.194045	-1.270274	1.332553
O	3.545207	-1.419238	1.283883
C	4.844386	-1.530724	-0.759072
O	3.035193	0.781575	-1.441847
O	1.539841	-1.841968	2.172553
C	0.270526	-0.191645	0.025267
C	-0.175881	-0.835372	-1.304746
C	-1.687514	-0.975364	-1.479042
C	-2.366486	-2.018736	-0.605761
C	-3.787192	-2.314033	-1.063410
O	-2.365313	-1.543865	0.762325
C	-4.507130	-3.350074	-0.210949
C	-1.484320	3.107216	0.793817
C	-1.307470	1.623878	0.901371
C	-0.246830	1.213118	0.177896
C	0.245865	2.392605	-0.501091
O	-0.442849	3.486114	-0.127135
C	-2.833141	3.540933	0.268978
O	-2.178813	0.946703	1.617818
O	1.139611	2.501860	-1.327866
H	4.720458	0.123284	0.618684
H	5.230000	-0.933668	-1.584632
H	5.684903	-1.992384	-0.243343
H	4.200952	-2.313680	-1.160605
H	2.251914	1.395985	-1.542616
H	-0.192648	-0.767276	0.824417
H	0.219473	-0.249671	-2.137516
H	0.285295	-1.823270	-1.375382
H	-2.185461	-0.012345	-1.333751
H	-1.881211	-1.258307	-2.515194
H	-1.779052	-2.942468	-0.629780
H	-3.733873	-2.666006	-2.096108
H	-4.352019	-1.377897	-1.075464
H	-2.588752	-2.260920	1.365000
H	-5.488508	-3.577129	-0.627310
H	-4.667228	-2.997033	0.809283
H	-3.942841	-4.284120	-0.163459
H	-1.264155	3.587263	1.749079
H	-3.609781	3.239749	0.970518
H	-2.861595	4.623870	0.162447
H	-3.035523	3.082183	-0.698755
H	-2.194041	-0.018262	1.373690

CAM-B3LYP Energy = -1149.47519699 a.u.

(5*S*,9*S*,5'*S*)-**1**, Conf B

C	4.087682	-0.459117	0.046512
C	2.795278	0.040689	-0.526191
C	1.763968	-0.278211	0.277407
C	2.338829	-0.992731	1.413980
O	3.687818	-1.093017	1.270958
C	4.826231	-1.435761	-0.840803
O	2.852399	0.686984	-1.673243
O	1.783090	-1.467376	2.376349
C	0.265703	-0.182251	0.141470
C	-0.251333	-1.017914	-1.048863
C	-1.764843	-1.229137	-1.082301
C	-2.330043	-2.171665	-0.032321
C	-3.786120	-2.547328	-0.276341
O	-2.210082	-1.533139	1.261531
C	-4.002253	-3.448644	-1.485363
C	-1.592484	3.115840	0.611943
C	-1.332465	1.668715	0.896953
C	-0.308510	1.208770	0.150563
C	0.071315	2.305856	-0.713569
O	-0.642636	3.410722	-0.430931
C	-2.996986	3.418344	0.144621
O	-2.112815	1.057766	1.762167
O	0.894357	2.339721	-1.616733
H	4.726471	0.387703	0.305664
H	4.194285	-2.292008	-1.076981
H	5.115270	-0.944388	-1.769111
H	5.726926	-1.787283	-0.340089
H	2.035764	1.254067	-1.785159
H	-0.103588	-0.661968	1.045860
H	0.055296	-0.540763	-1.982236
H	0.244985	-1.990778	-1.021254
H	-2.292489	-0.272887	-1.019854
H	-2.018156	-1.646936	-2.056986
H	-1.722188	-3.082177	-0.006100
H	-4.373725	-1.630526	-0.372200
H	-4.152110	-3.061956	0.616464
H	-2.502362	-2.137727	1.952881
H	-5.045717	-3.757685	-1.547170
H	-3.392461	-4.351763	-1.416920
H	-3.755038	-2.947606	-2.421380
H	-1.327540	3.728299	1.475702
H	-3.245953	2.825445	-0.735309
H	-3.702693	3.181496	0.939592
H	-3.089987	4.474989	-0.099807
H	-2.095860	0.068441	1.647449

CAM-B3LYP Energy = -1149.47460832 a.u.

(5*S*,9*S*,5'*S*)-**1**, Conf C

C	4.147242	-0.225900	0.105488
C	2.840033	0.234440	-0.466605
C	1.809767	-0.250823	0.250559
C	2.399356	-1.042051	1.327109
O	3.756279	-1.021500	1.234668
C	4.993872	-1.037547	-0.848960
O	2.885992	1.007290	-1.532931
O	1.849972	-1.663358	2.206025
C	0.314319	-0.253145	0.059269
C	-0.093903	-0.982959	-1.238236
C	-1.579194	-1.329813	-1.337404
C	-2.059821	-2.427027	-0.399142
C	-3.415929	-3.009963	-0.779780
O	-2.105569	-1.893954	0.947246
C	-4.555735	-2.001689	-0.840105
C	-1.806460	2.827420	0.813487
C	-1.445326	1.380306	0.950273
C	-0.367393	1.081432	0.197655
C	-0.046716	2.292362	-0.527359
O	-0.851382	3.304064	-0.154304
C	-3.215153	3.078171	0.328433
O	-2.201223	0.623368	1.715633
O	0.797943	2.486483	-1.389360
H	4.705488	0.632950	0.483573
H	4.442108	-1.907856	-1.204355
H	5.274892	-0.424704	-1.704650
H	5.901683	-1.372805	-0.349942
H	2.030049	1.517715	-1.620561
H	-0.047097	-0.859560	0.887954
H	0.182059	-0.369625	-2.098801
H	0.493590	-1.901176	-1.310200
H	-2.191172	-0.435649	-1.198228
H	-1.777829	-1.674439	-2.354151
H	-1.322772	-3.235505	-0.402635
H	-3.659595	-3.796580	-0.059800
H	-3.302799	-3.509673	-1.745036
H	-2.318422	-2.596947	1.571087
H	-5.501982	-2.508871	-1.029992
H	-4.409499	-1.271454	-1.636560
H	-4.651921	-1.459251	0.101082
H	-1.614739	3.357711	1.748135
H	-3.380182	4.146083	0.197034
H	-3.391374	2.570974	-0.620020
H	-3.924993	2.704306	1.064919
H	-2.105349	-0.344069	1.497246

CAM-B3LYP Energy = -1149.47437819 a.u.

(5*S*,9*S*,5'*S*)-**1**, Conf D

C	0.541504	3.593243	0.131549
C	0.875803	2.189956	0.530428
C	0.104927	1.305570	-0.133929
C	-0.680636	2.091054	-1.062205
O	-0.460164	3.406943	-0.886686
C	0.012866	4.463270	1.248046
O	1.841109	2.012596	1.405837
O	-1.452523	1.725270	-1.936556
C	0.121486	-0.195316	-0.021229
C	0.916255	-0.852053	-1.171406
C	2.397459	-0.477749	-1.215995
C	3.295553	-1.022038	-0.110446
C	3.239802	-2.528861	0.094722
O	2.954525	-0.357435	1.130537
C	3.667812	-3.325569	-1.130832
C	-3.286833	-1.948795	0.048700
C	-2.295654	-1.034918	-0.608533
C	-1.217857	-0.858129	0.177755
C	-1.454664	-1.653415	1.379189
O	-2.658208	-2.281179	1.296069
C	-4.643386	-1.325102	0.286689
O	-2.608061	-0.557462	-1.796244
O	-0.745552	-1.803176	2.346129
H	1.406024	4.054799	-0.348637
H	-0.868069	4.010869	1.702807
H	0.780960	4.584596	2.011071
H	-0.249691	5.446717	0.862097
H	2.216832	1.089607	1.369829
H	0.656269	-0.419542	0.900340
H	0.805559	-1.934079	-1.087329
H	0.463659	-0.574022	-2.125602
H	2.812710	-0.833957	-2.160049
H	2.509682	0.608744	-1.242562
H	4.323022	-0.741324	-0.361749
H	2.232976	-2.815648	0.404550
H	3.900634	-2.776255	0.930406
H	3.534843	-0.667562	1.834969
H	3.712324	-4.389380	-0.898081
H	4.657669	-3.018990	-1.474884
H	2.971757	-3.199364	-1.960712
H	-3.381484	-2.871023	-0.528864
H	-4.548295	-0.419415	0.885853
H	-5.102181	-1.069313	-0.667486
H	-5.292497	-2.027909	0.806576
H	-2.078334	0.271107	-1.980241

CAM-B3LYP Energy = -1149.47371750 a.u.

(5*S*,9*S*,5'*S*)-**1**, Conf E

C	-0.209946	3.594239	-0.350773
C	-0.703393	2.196716	-0.559022
C	0.059656	1.312776	0.114491
C	1.006311	2.107513	0.868197

O	0.878085	3.414930	0.576023
C	0.265325	4.293163	-1.603376
O	-1.771296	2.025643	-1.307054
O	1.836758	1.757795	1.694047
C	-0.094324	-0.183641	0.165278
C	-0.811171	-0.645842	1.452888
C	-2.246048	-0.139966	1.597603
C	-3.296090	-0.704730	0.646966
C	-3.372523	-2.223343	0.629089
O	-3.044410	-0.196154	-0.687681
C	-4.541231	-2.765282	-0.184339
C	3.130346	-2.245185	-0.059077
C	2.293925	-1.185861	0.594977
C	1.155725	-0.985571	-0.094524
C	1.194616	-1.910917	-1.223506
O	2.344759	-2.636138	-1.195410
C	4.498634	-1.772971	-0.495969
O	2.771263	-0.627774	1.689125
O	0.375041	-2.086533	-2.093991
H	-0.974090	4.182421	0.160131
H	0.648061	5.281971	-1.356764
H	1.052107	3.716592	-2.089408
H	-0.567908	4.407024	-2.295865
H	-2.213991	1.148285	-1.135710
H	-0.742022	-0.445899	-0.669976
H	-0.794351	-1.735916	1.481812
H	-0.240452	-0.310538	2.321638
H	-2.590119	-0.377965	2.606253
H	-2.268383	0.950232	1.527575
H	-4.265297	-0.308741	0.965637
H	-3.461940	-2.560878	1.664531
H	-2.435711	-2.628087	0.241901
H	-3.784109	-0.415967	-1.264592
H	-4.596045	-3.850876	-0.104128
H	-4.443174	-2.532438	-1.246663
H	-5.491056	-2.356651	0.166795
H	3.213098	-3.112805	0.599219
H	4.411783	-0.923463	-1.173548
H	5.078121	-1.470386	0.375241
H	5.028345	-2.578165	-1.002579
H	2.336671	0.261515	1.834615

CAM-B3LYP Energy = -1149.47369491 a.u.

(5*S*,9*S*,5'*S*)-**1**, Conf F

C	3.981114	-0.720505	0.287688
C	2.798114	-0.077676	-0.372349
C	1.661786	-0.406099	0.268795
C	2.051373	-1.271313	1.377372
O	3.399692	-1.448600	1.380254
C	4.767504	-1.648034	-0.610987
O	3.030700	0.673711	-1.429658
O	1.354780	-1.802936	2.209427
C	0.201506	-0.174772	-0.028371
C	-0.211059	-0.810207	-1.370612
C	-1.715436	-1.003708	-1.546935
C	-2.359442	-1.913662	-0.496935
C	-3.487059	-2.762700	-1.061880
O	-2.840125	-1.146557	0.636411
C	-4.104528	-3.723400	-0.055400
C	-1.322601	3.233096	0.753394
C	-1.219912	1.746191	0.898253
C	-0.249719	1.253113	0.106361
C	0.274985	2.384298	-0.629531
O	-0.328708	3.524441	-0.249865
C	-2.679778	3.725158	0.307161
O	-2.055309	1.133812	1.712184
O	1.134698	2.415713	-1.497301
H	4.628989	0.049570	0.711238
H	5.192070	-1.083897	-1.440558
H	5.580960	-2.108175	-0.052412
H	4.123303	-2.431437	-1.010371
H	2.257071	1.281757	-1.601127
H	-0.307992	-0.728805	0.762201
H	0.177172	-0.211472	-2.196865
H	0.274830	-1.786096	-1.439709
H	-2.235021	-0.041913	-1.542192
H	-1.882360	-1.434798	-2.535669
H	-1.603202	-2.574888	-0.068334
H	-3.082663	-3.324362	-1.906123
H	-4.254035	-2.098947	-1.476872
H	-3.723165	-0.817771	0.424765
H	-4.884340	-4.323267	-0.525072
H	-4.552719	-3.194927	0.785960
H	-3.350849	-4.405483	0.342944
H	-1.009628	3.730166	1.673335
H	-2.658138	4.804468	0.167604
H	-2.972402	3.250430	-0.629263
H	-3.420764	3.487935	1.069289
H	-2.184016	0.186572	1.439475

CAM-B3LYP Energy = -1149.47202426 a.u.

(5*R*,9*S*)-**4**, Conf A

O	2.571314	-1.062752	-0.915146
O	-0.568324	2.525207	0.149155
C	4.103641	-1.310789	1.591880
C	3.844006	-0.028805	0.814459
C	2.521418	-0.029981	0.066249
C	2.252153	1.325247	-0.581371
C	0.920780	1.424420	-1.341416
C	-0.263446	1.472504	-0.422081
O	-2.659855	1.450286	1.219211
C	-4.335963	-0.880124	0.115392

O	-0.174475	-1.612252	-1.316253
O	-2.080539	-1.750842	-0.170049
C	-1.011652	-1.061994	-0.639029
C	-1.097947	0.313828	-0.172850
C	-2.214413	0.401113	0.600521
C	-2.921638	-0.912141	0.648869
H	1.664137	-1.302103	-1.160892
H	4.113553	-2.174568	0.927970
H	5.064351	-1.267928	2.106620
H	3.329701	-1.474887	2.345063
H	4.644999	0.139541	0.088568
H	3.852207	0.825240	1.495734
H	1.722209	-0.257491	0.784486
H	3.059053	1.530018	-1.287884
H	2.286428	2.105035	0.182472
H	0.823650	0.600075	-2.045842
H	0.908243	2.357196	-1.905660
H	-2.002112	2.176137	1.015795
H	-4.949746	-0.238818	0.746756
H	-4.755224	-1.884137	0.128261
H	-4.355443	-0.497642	-0.904418
H	-2.892604	-1.312521	1.663907

CAM-B3LYP Energy = -804.893686572 a.u.

(5*R*,9*S*)-**4**, Conf B

O	2.364470	-1.794597	-0.410111
O	-0.229544	2.315451	-0.664194
C	4.123633	0.811125	1.653610
C	3.853479	-0.459338	0.858060
C	2.505031	-0.492280	0.154346
C	2.384338	0.581563	-0.922681
C	1.048054	0.587367	-1.680878
C	-0.088433	1.101415	-0.847402
O	-2.438816	1.957991	0.628990
C	-4.435703	-0.359951	0.293421
O	-0.436301	-2.085347	-0.645534
O	-2.328663	-1.571446	0.413252
C	-1.180921	-1.231795	-0.221750
C	-1.068874	0.218853	-0.246756
C	-2.152493	0.711612	0.412696
C	-3.037769	-0.400144	0.868285
H	1.423594	-1.964726	-0.575258
H	5.052859	0.718442	2.216465
H	4.218538	1.687326	1.011777
H	3.322112	1.006484	2.369390
H	3.888338	-1.322382	1.525588
H	4.636563	-0.610479	0.109424
H	1.722599	-0.342100	0.910320
H	3.183219	0.421275	-1.650002
H	2.541990	1.567232	-0.482581
H	0.821733	-0.406728	-2.062035
H	1.132991	1.265169	-2.530697
H	-1.687329	2.476546	0.220122
H	-4.949759	0.534034	0.644258
H	-4.992917	-1.233791	0.624906
H	-4.404813	-0.347938	-0.795494
H	-3.060934	-0.435346	1.958888

CAM-B3LYP Energy = -804.892794330 a.u.

(5*R*,9*S*)-**4**, Conf C

O	-2.826089	-0.626784	-1.103576
O	1.121472	2.624790	0.030356
C	-5.219817	-0.830340	0.648279
C	-3.850536	-0.331173	1.085098
C	-3.051611	0.304676	-0.045612
C	-1.735447	0.877926	0.466538
C	-0.899376	1.538524	-0.640449
C	0.550340	1.576501	-0.282743
O	3.373815	1.385308	0.394032
C	3.797322	-1.544220	1.240477
O	-0.065207	-1.507753	-0.954365
O	2.092283	-1.796294	-0.475160
C	0.986322	-1.020889	-0.612857
C	1.336921	0.354137	-0.283636
C	2.656406	0.362036	0.040067
C	3.228046	-1.013109	-0.055881
H	-1.960474	-1.046195	-0.977844
H	-5.757036	-1.282485	1.482962
H	-5.830716	-0.010205	0.264356
H	-5.129438	-1.577946	-0.139500
H	-3.264469	-1.157111	1.499767
H	-3.964408	0.406983	1.883844
H	-3.648972	1.110178	-0.485082
H	-1.174417	0.063737	0.932128
H	-1.939593	1.604872	1.253438
H	-1.234963	2.557511	-0.826055
H	-1.009239	0.962604	-1.560481
H	2.752744	2.166902	0.370579
H	4.648870	-0.935682	1.542467
H	4.135086	-2.569042	1.100288
H	3.046540	-1.520410	2.029608
H	3.968884	-1.052276	-0.856449

CAM-B3LYP Energy = -804.892643531 a.u.

(5*R*,9*S*)-**4**, Conf D

O	3.052274	-1.308709	-0.039475
O	0.344387	-1.173824	-0.505453
C	5.641984	-0.409290	0.843626
C	4.694612	0.411819	-0.018970
C	3.228143	0.083768	0.212518

C	2.317129	0.947214	-0.662400
C	0.880792	1.145223	-0.179589
C	-0.053048	-0.016728	-0.308045
O	-2.097545	-2.108151	-0.464720
C	-4.496724	-0.969881	1.064282
O	-1.908967	2.539219	0.168181
O	-3.579870	1.057035	0.081093
C	-2.260450	1.397418	0.034032
C	-1.481212	0.182674	-0.191578
C	-2.360442	-0.849599	-0.274980
C	-3.760427	-0.358936	-0.107025
H	2.107249	-1.457253	-0.206818
H	5.440229	-0.249996	1.905462
H	5.535068	-1.473839	0.638683
H	6.679991	-0.130671	0.656899
H	4.920312	0.255304	-1.078193
H	4.842227	1.475292	0.183681
H	2.993937	0.288636	1.267565
H	2.323701	0.544191	-1.678381
H	2.758250	1.943462	-0.722322
H	0.419484	1.986990	-0.698540
H	0.866953	1.437570	0.876915
H	-1.110063	-2.175480	-0.544050
H	-4.615503	-2.040893	0.904792
H	-5.483643	-0.519932	1.151519
H	-3.947642	-0.807674	1.991136
H	-4.314918	-0.502348	-1.036578

CAM-B3LYP Energy = -804.892406603 a.u.

(5*R*,9*S*)-**4**, Conf E

O	2.706753	-1.414814	-0.234478
O	-0.772645	2.524068	-0.215626
C	5.425139	-0.349609	-0.305168
C	4.158167	0.480162	-0.149756
C	3.036524	-0.268743	0.549613
C	1.800137	0.588027	0.813552
C	1.099633	1.062932	-0.470511
C	-0.342477	1.367232	-0.227097
O	-3.193490	1.710493	0.235007
C	-4.456671	-0.938856	-0.662869
O	-0.143567	-1.841704	-0.073620
O	-2.344411	-1.724040	0.253631
C	-1.129989	-1.154346	0.044719
C	-1.292782	0.292945	0.010462
C	-2.612928	0.549049	0.205955
C	-3.375365	-0.723028	0.371837
H	1.782090	-1.657522	-0.072521
H	6.210919	0.225081	-0.797072
H	5.804983	-0.668879	0.667951
H	5.237253	-1.242516	-0.900863
H	3.807992	0.807799	-1.131883
H	4.376167	1.381887	0.428576
H	3.406995	-0.603870	1.527193
H	2.082609	1.448132	1.422360
H	1.109605	-0.003595	1.417501
H	1.159943	0.272113	-1.220429
H	1.570374	1.958241	-0.871511
H	-2.464376	2.376145	0.083545
H	-4.923197	-1.909897	-0.509662
H	-5.218533	-0.166856	-0.561777
H	-4.040405	-0.897125	-1.668759
H	-3.779889	-0.785733	1.383624

CAM-B3LYP Energy = -804.892006353 a.u.

(5*R*,9*S*)-**4**, Conf F

O	-2.445808	-1.473028	0.334301
O	0.447423	2.447513	0.237721
C	-4.989734	-0.208819	-0.509577
C	-3.668057	-0.189275	-1.268288
C	-2.421650	-0.246065	-0.393617
C	-2.306732	0.949137	0.549349
C	-1.021945	0.975705	1.390631
C	0.200207	1.285475	0.578084
O	2.694864	1.751867	-0.835055
C	4.480036	-0.621598	-0.030733
O	0.305826	-1.912555	0.852230
O	2.295638	-1.691541	-0.127432
C	1.140867	-1.183990	0.368204
C	1.142971	0.259066	0.180007
C	2.299444	0.573465	-0.464379
C	3.120825	-0.651543	-0.692589
H	-1.540535	-1.686676	0.609300
H	-5.826480	-0.265953	-1.206850
H	-5.046824	-1.072139	0.153410
H	-5.129005	0.689362	0.093160
H	-3.608247	0.707476	-1.890150
H	-3.628014	-1.043214	-1.947967
H	-1.555943	-0.251693	-1.067721
H	-3.150542	0.934153	1.239413
H	-2.377366	1.873586	-0.028495
H	-0.896907	0.032239	1.919130
H	-1.105550	1.771077	2.131848
H	1.963416	2.375388	-0.558043
H	4.986476	-1.571330	-0.190648
H	4.384261	-0.443226	1.039752
H	5.082602	0.172290	-0.470300
H	3.207724	-0.848737	-1.762500

CAM-B3LYP Energy = -804.891972839 a.u.

(5*R*,9*S*)-**4**, Conf G

O	2.911399	-1.763105	0.205157
O	0.244599	-1.397966	-0.384854
C	5.313390	1.080377	0.572783
C	4.729198	-0.251357	0.121842
C	3.224753	-0.375711	0.317920
C	2.432275	0.470657	-0.680141
C	1.016755	0.873875	-0.270551
C	-0.031915	-0.193241	-0.297052
O	-2.280436	-2.069690	-0.298711
C	-4.555607	-0.566865	1.097470
O	-1.615038	2.570482	-0.059495
O	-3.430317	1.265710	-0.040100
C	-2.082495	1.463723	-0.100509
C	-1.432152	0.160814	-0.213103
C	-2.412806	-0.779180	-0.219433
C	-3.755325	-0.135096	-0.111029
H	1.964091	-1.834709	0.003471
H	4.915031	1.920903	0.002557
H	5.101017	1.264657	1.627954
H	6.396474	1.087717	0.446952
H	5.193284	-1.060740	0.689086
H	4.962276	-0.433596	-0.931378
H	2.982904	-0.035009	1.334770
H	2.416218	-0.052566	-1.639734
H	2.975937	1.400967	-0.846379
H	0.657292	1.690445	-0.899285
H	1.011770	1.290753	0.742983
H	-1.304687	-2.244211	-0.358350
H	-4.786607	-1.628900	1.023821
H	-5.489650	-0.009997	1.136108
H	-3.995622	-0.388186	2.014673
H	-4.317812	-0.298958	-1.032411

CAM-B3LYP Energy = -804.891918774 a.u.

(5*R*,9*S*)-**4**, Conf H

O	-2.699473	-1.179127	-1.263159
O	0.804035	2.588342	-0.282069
C	-4.643667	0.290821	1.639840
C	-3.953460	-0.742292	0.758100
C	-3.101895	-0.149519	-0.359203
C	-1.890247	0.608632	0.169195
C	-1.039755	1.223703	-0.953787
C	0.367683	1.456978	-0.510686
O	3.147962	1.647665	0.329793
C	3.830235	-1.112910	1.507953
O	0.113109	-1.729215	-0.854013
O	2.256076	-1.728827	-0.241105
C	1.086674	-1.097347	-0.518600
C	1.273341	0.334690	-0.328994
C	2.562806	0.520693	0.056298
C	3.279086	-0.786114	0.138398
H	-1.799341	-1.466293	-1.043435
H	-5.230532	0.989515	1.039416
H	-5.323970	-0.194386	2.340276
H	-3.932311	0.872159	2.227241
H	-4.705296	-1.376363	0.283863
H	-3.325816	-1.401888	1.365118
H	-3.725589	0.534715	-0.944160
H	-1.293567	-0.089091	0.762845
H	-2.213677	1.397633	0.847433
H	-1.458582	2.174030	-1.280756
H	-1.021061	0.540494	-1.804035
H	2.452396	2.349999	0.190552
H	4.594135	-0.384581	1.777399
H	4.282699	-2.102376	1.495068
H	3.039723	-1.091610	2.257302
H	4.062313	-0.826669	-0.620800

CAM-B3LYP Energy = -804.891876139 a.u.

(5*R*,9*S*)-**4**, Conf I

O	2.552129	-1.874531	-0.363432
O	-0.457109	2.442511	-0.286418
C	4.958762	0.932917	0.300509
C	4.199951	-0.166666	-0.429397
C	3.042800	-0.750245	0.365912
C	1.914899	0.233479	0.669165
C	1.221665	0.771559	-0.593234
C	-0.164166	1.243594	-0.296681
O	-2.934982	1.919218	0.274170
C	-4.527279	-0.575971	-0.539296
O	-0.327464	-1.963937	-0.096955
O	-2.486149	-1.590158	0.311206
C	-1.223549	-1.166616	0.047305
C	-1.220899	0.289226	-0.003785
C	-2.493731	0.698199	0.239783
C	-3.390230	-0.475839	0.452561
H	1.611750	-2.002100	-0.164376
H	5.827430	1.249785	-0.277106
H	4.339108	1.815129	0.467851
H	5.315659	0.587513	1.273119
H	4.878924	-0.990622	-0.659986
H	3.825829	0.200707	-1.388188
H	3.431774	-1.095782	1.332198
H	2.300211	1.062633	1.263014
H	1.191019	-0.282725	1.302405
H	1.159112	-0.027770	-1.334141
H	1.775556	1.602679	-1.025515
H	-2.141028	2.494311	0.083313
H	-5.193263	0.277641	-0.419324
H	-5.093788	-1.486987	-0.357338
H	-4.147710	-0.589239	-1.560508
H	-3.761313	-0.481819	1.478951

CAM-B3LYP Energy = -804.891768348 a.u.

(5*R*,9*S*)-**4**, Conf J

O	2.702649	-0.943596	0.806547
O	0.359591	-1.129970	-0.718602
C	5.632176	-0.492562	0.749782
C	4.644565	0.029131	-0.283450
C	3.250305	0.268228	0.282153
C	2.334561	0.908624	-0.754628
C	0.904122	1.167664	-0.291520
C	-0.034696	0.008514	-0.432832
O	-2.073989	-2.076759	-0.634547
C	-4.406183	-1.054456	1.074055
O	-1.871788	2.520102	0.287437
O	-3.542490	1.037509	0.182443
C	-2.226897	1.387420	0.096758
C	-1.456753	0.194288	-0.241133
C	-2.335444	-0.835142	-0.351848
C	-3.727705	-0.364607	-0.088340
H	2.080576	-1.303826	0.158008
H	6.614330	-0.658656	0.305267
H	5.753939	0.219732	1.569014
H	5.290403	-1.436241	1.174528
H	4.562625	-0.677871	-1.114645
H	5.013038	0.968956	-0.703900
H	3.334579	0.947423	1.137750
H	2.323058	0.290627	-1.656395
H	2.777929	1.863533	-1.039116
H	0.461514	2.000845	-0.840650
H	0.874596	1.482673	0.756888
H	-1.088974	-2.127238	-0.759346
H	-4.529726	-2.113481	0.850741
H	-5.389016	-0.616930	1.237270
H	-3.814097	-0.949867	1.982517
H	-4.324864	-0.450591	-0.998144

CAM-B3LYP Energy = -804.891718805 a.u.

(5*R*,9*S*)-**4**, Conf K

O	3.431607	1.008098	1.092661
O	-0.257650	-1.920526	-0.018316
C	6.037755	0.206364	-0.154018
C	4.766245	-0.631318	-0.133930
C	3.488536	0.195712	-0.085833
C	2.247635	-0.677735	-0.078210
C	0.965892	0.133014	-0.139848
C	-0.281926	-0.689971	-0.111751
O	-2.853930	-2.057630	-0.058897
C	-4.847834	0.051499	0.948293
O	-1.269177	2.346566	-0.368040
O	-3.314601	1.442792	-0.327768
C	-1.951867	1.358576	-0.303105
C	-1.581807	-0.047574	-0.193170
C	-2.731904	-0.765953	-0.159105
C	-3.917606	0.137891	-0.241040
H	4.099256	1.697996	1.030249
H	6.919783	-0.426942	-0.251185
H	6.036290	0.904933	-0.993849
H	6.156858	0.782640	0.765343
H	4.775575	-1.306144	0.726545
H	4.728301	-1.257001	-1.029214
H	3.459096	0.850019	-0.966785
H	2.258336	-1.292687	0.824253
H	2.295948	-1.361669	-0.926802
H	0.930269	0.753601	-1.040480
H	0.914163	0.843207	0.688938
H	-1.921330	-2.408796	-0.014818
H	-5.287778	-0.943844	0.998709
H	-5.648908	0.780291	0.841754
H	-4.308110	0.247966	1.874106
H	-4.456456	-0.040997	-1.173580

CAM-B3LYP Energy = -804.891560767 a.u.

(5*R*,9*S*)-**4**, Conf L

O	-3.476614	-1.082125	1.061942
O	0.253980	1.918015	-0.027024
C	-6.037623	-0.231191	-0.200034
C	-4.773968	0.613161	-0.121396
C	-3.493233	-0.208678	-0.072070
C	-2.250447	0.671648	-0.100434
C	-0.967031	-0.137348	-0.144991
C	0.280064	0.687284	-0.117482
O	2.850862	2.058072	-0.067697
C	4.847006	-0.045343	0.946435
O	1.270595	-2.348899	-0.361014
O	3.314986	-1.442773	-0.324234
C	1.952201	-1.359978	-0.300089
C	1.580662	0.046282	-0.195634
C	2.730064	0.766022	-0.163635
C	3.916592	-0.136974	-0.242345
H	-3.543566	-0.543735	1.859498
H	-6.927293	0.399031	-0.225806
H	-6.039339	-0.847964	-1.101289
H	-6.120829	-0.896060	0.659525
H	-4.807289	1.257802	0.763661
H	-4.719358	1.279538	-0.985656
H	-3.473178	-0.884545	-0.931257
H	-2.253045	1.318635	0.781064
H	-2.303499	1.331151	-0.968526
H	-0.925528	-0.768965	-1.037384
H	-0.918729	-0.838114	0.692543

H	1.918007	2.408788	-0.025048
H	5.286139	0.950510	0.993101
H	5.648593	-0.773921	0.842409
H	4.307621	-0.238918	1.873057
H	4.455100	0.039140	-1.175621

CAM-B3LYP Energy = -804.891546232 a.u.

(5*R*,9*S*)-**4**, Conf M

O	2.999552	-1.424881	0.507482
O	0.371237	-1.232722	-0.296751
C	5.341592	-0.035053	-0.725580
C	4.699792	0.235337	0.629229
C	3.199256	-0.024129	0.688815
C	2.412500	0.813514	-0.322546
C	0.944470	1.079113	0.009228
C	-0.009100	-0.060385	-0.166936
O	-2.088380	-2.103395	-0.441639
C	-4.574297	-0.858693	0.847659
O	-1.828231	2.555580	0.068178
O	-3.525472	1.112626	-0.116865
C	-2.198016	1.419001	-0.060788
C	-1.435742	0.178855	-0.181773
C	-2.332404	-0.833581	-0.310736
C	-3.727662	-0.303941	-0.276220
H	2.081794	-1.556508	0.219494
H	6.422874	0.097522	-0.670946
H	5.144151	-1.056087	-1.051746
H	4.967716	0.642784	-1.494483
H	4.879081	1.270820	0.929480
H	5.170862	-0.393759	1.388349
H	2.858309	0.254585	1.695181
H	2.495604	0.358100	-1.311544
H	2.893055	1.791149	-0.390662
H	0.564445	1.910288	-0.587182
H	0.836830	1.417407	1.046365
H	-1.099637	-2.196598	-0.435081
H	-4.709167	-1.930902	0.710605
H	-5.552248	-0.381636	0.839296
H	-4.098961	-0.681038	1.811694
H	-4.206696	-0.464017	-1.244176

CAM-B3LYP Energy = -804.891388692 a.u.

(5*R*,9*S*)-**4**, Conf N

O	3.184508	-0.490940	-1.053994
O	0.348687	-0.940604	-1.530834
C	4.598431	-1.138980	1.468884
C	3.909345	0.172064	1.119951
C	2.713836	0.004038	0.199859
C	1.949749	1.318066	0.035448
C	0.926907	1.326721	-1.114810
C	-0.000754	0.153783	-1.061135
O	-1.903549	-2.039343	-0.828578
C	-3.686698	-1.287133	1.554528
O	-1.648201	2.489039	0.372585
O	-3.210377	0.910025	0.625054
C	-1.993535	1.351178	0.195432
C	-1.304232	0.235863	-0.447594
C	-2.131271	-0.841169	-0.382842
C	-3.405560	-0.481056	0.306071
H	2.416516	-0.838023	-1.529824
H	3.914742	-1.814827	1.987223
H	4.953023	-1.644303	0.570926
H	5.455511	-0.968402	2.121583
H	4.616188	0.852806	0.636759
H	3.570433	0.668577	2.032609
H	2.042049	-0.743107	0.639704
H	2.657666	2.126974	-0.157301
H	1.448968	1.548671	0.978133
H	1.454413	1.273314	-2.066862
H	0.357916	2.253054	-1.078424
H	-0.992627	-2.009997	-1.231857
H	-3.823921	-2.335222	1.291127
H	-4.597874	-0.925309	2.026522
H	-2.861721	-1.203602	2.261261
H	-4.237139	-0.546270	-0.398209

CAM-B3LYP Energy = -804.891375812 a.u.

(5*R*,9*S*)-**4**, Conf O

O	-2.916819	-0.490977	-1.327820
O	0.988914	2.639549	0.301256
C	-3.586841	-1.510820	1.460775
C	-4.133960	-0.270454	0.766320
C	-3.181242	0.385241	-0.230508
C	-1.884244	0.860971	0.411734
C	-0.999661	1.641936	-0.573421
C	0.434090	1.635611	-0.153594
O	3.235164	1.364537	0.590350
C	3.653468	-1.644239	1.087438
O	-0.150642	-1.347215	-1.197589
O	1.991856	-1.691878	-0.688549
C	0.888524	-0.905178	-0.767867
C	1.223750	0.420772	-0.267136
C	2.532659	0.390502	0.095441
C	3.112938	-0.962631	-0.149058
H	-2.033059	-0.877710	-1.231579
H	-2.749894	-1.276919	2.120114
H	-4.359563	-1.980018	2.070685
H	-3.247045	-2.248877	0.732736
H	-4.422026	0.479307	1.508500
H	-5.043606	-0.531529	0.220577

H	-3.695755	1.252104	-0.656670
H	-1.346021	-0.008089	0.793547
H	-2.115820	1.489516	1.272878
H	-1.329807	2.676263	-0.654368
H	-1.066921	1.177513	-1.558618
H	2.613122	2.143619	0.640901
H	3.999241	-2.644317	0.833965
H	2.884197	-1.715891	1.855434
H	4.494876	-1.074383	1.479809
H	3.873410	-0.902983	-0.929827

CAM-B3LYP Energy = -804.891375684 a.u.

(5*R*,9*S*)-**4**, Conf P

O	-3.204953	-1.412255	-0.626006
O	-0.463836	-1.263139	-0.431879
C	-4.844656	-0.113269	1.510656
C	-3.607871	0.481633	0.853080
C	-3.409361	-0.000866	-0.579684
C	-2.325640	0.771549	-1.340701
C	-1.001653	1.069856	-0.636481
C	-0.089371	-0.083792	-0.366077
O	1.903364	-2.141101	0.251708
C	4.602680	-0.803384	-0.302841
O	1.686132	2.542403	0.024658
O	3.315081	1.091647	0.514348
C	2.035058	1.399907	0.159501
C	1.289621	0.153534	0.003344
C	2.146738	-0.864458	0.275411
C	3.498922	-0.332575	0.618035
H	-2.251277	-1.566272	-0.522334
H	-4.791815	-1.201906	1.520342
H	-4.947877	0.230021	2.540823
H	-5.749949	0.173568	0.970964
H	-2.722121	0.227684	1.442196
H	-3.680220	1.573393	0.848627
H	-4.345107	0.163647	-1.121089
H	-2.749796	1.740402	-1.611277
H	-2.132679	0.249645	-2.280497
H	-1.164347	1.568067	0.324704
H	-0.432874	1.797996	-1.217570
H	0.949613	-2.236112	-0.007145
H	4.722418	-1.882165	-0.210543
H	5.539846	-0.324863	-0.025757
H	4.370654	-0.559783	-1.339075
H	3.732424	-0.562574	1.659530

CAM-B3LYP Energy = -804.891208965 a.u.

(5*R*,9*S*)-**4**, Conf Q

O	3.224954	1.150016	-1.002153
O	0.277551	-1.391777	0.552679
C	5.327222	-0.953182	-0.837997
C	4.495186	-0.451594	0.333220
C	3.122503	0.068371	-0.069144
C	2.294921	0.477166	1.144964
C	0.879867	0.914395	0.804662
C	-0.056481	-0.206533	0.471690
O	-2.082056	-2.193999	-0.191392
C	-4.765112	-0.770118	0.266357
O	-1.737667	2.480357	0.005389
O	-3.395480	1.076613	-0.526606
C	-2.116070	1.347252	-0.133478
C	-1.416550	0.081237	0.052478
C	-2.295321	-0.911137	-0.236049
C	-3.620042	-0.342486	-0.624490
H	3.737186	1.857247	-0.592268
H	6.298282	-1.316572	-0.499663
H	4.823447	-1.775364	-1.350803
H	5.500232	-0.161666	-1.567075
H	5.030118	0.347189	0.858797
H	4.354788	-1.256538	1.058899
H	2.594886	-0.712959	-0.619322
H	2.804676	1.304387	1.646754
H	2.267724	-0.352806	1.852113
H	0.877360	1.617663	-0.030833
H	0.425888	1.464107	1.634252
H	-1.133269	-2.295217	0.098060
H	-4.912923	-1.846238	0.183175
H	-5.679630	-0.268971	-0.044602
H	-4.558116	-0.520212	1.306535
H	-3.829804	-0.573957	-1.670638

CAM-B3LYP Energy = -804.891107602 a.u.

(5*R*,9*S*)-**4**, Conf R

O	3.343674	1.496229	1.184136
O	-0.060097	-1.801613	0.230506
C	5.233249	-1.003722	-0.968177
C	4.876766	-0.124385	0.223739
C	3.525853	0.571268	0.106375
C	2.351070	-0.387834	0.155884
C	1.019963	0.318718	-0.028904
C	-0.166650	-0.589297	0.024700
O	-2.636885	-2.132516	0.107808
C	-4.818754	-0.091891	0.828001
O	-1.349964	2.328710	-0.558156
O	-3.327557	1.284567	-0.512245
C	-1.964847	1.303666	-0.425406
C	-1.503395	-0.054806	-0.165930
C	-2.600786	-0.849983	-0.109627
C	-3.841479	-0.047793	-0.325343
H	4.053027	2.146535	1.153429

H	6.248929	-1.388056	-0.871607
H	4.566758	-1.861956	-1.056941
H	5.179764	-0.440610	-1.902345
H	5.641304	0.650305	0.334363
H	4.888947	-0.709395	1.147355
H	3.495786	1.121329	-0.843453
H	2.369056	-0.910463	1.114917
H	2.473498	-1.144022	-0.619355
H	0.982210	0.852919	-0.983333
H	0.879425	1.093705	0.728362
H	-1.685048	-2.408630	0.220121
H	-5.186999	-1.108829	0.958537
H	-5.664800	0.559562	0.618116
H	-4.339558	0.232865	1.750991
H	-4.321591	-0.351918	-1.257408

CAM-B3LYP Energy = -804.890977161 a.u.

(5*R*,9*S*)-**4**, Conf S

O	3.188777	1.239217	-0.870639
O	0.260338	-1.415676	0.610970
C	5.317429	-0.867955	-0.912564
C	4.481136	-0.474637	0.297795
C	3.101290	0.060259	-0.059481
C	2.305445	0.440104	1.177846
C	0.882091	0.883396	0.881577
C	-0.059044	-0.226497	0.526017
O	-2.087489	-2.191581	-0.190034
C	-4.771173	-0.742945	0.193257
O	-1.704262	2.478807	0.029883
O	-3.359992	1.092402	-0.550637
C	-2.089110	1.349637	-0.122157
C	-1.407114	0.076234	0.078963
C	-2.287669	-0.906675	-0.235800
C	-3.595108	-0.324071	-0.660346
H	3.509574	0.993940	-1.743704
H	6.270123	-1.299504	-0.604738
H	4.799394	-1.609492	-1.525026
H	5.544298	-0.006791	-1.543813
H	5.006647	0.283108	0.886029
H	4.346779	-1.344354	0.946026
H	2.558142	-0.711583	-0.616027
H	2.829114	1.257708	1.678288
H	2.297470	-0.406323	1.864838
H	0.860593	1.621472	0.078171
H	0.443888	1.394040	1.744653
H	-1.147129	-2.301909	0.123582
H	-4.924655	-1.817880	0.105373
H	-5.671353	-0.234768	-0.146773
H	-4.595611	-0.494108	1.239336
H	-3.775281	-0.550013	-1.713195

CAM-B3LYP Energy = -804.890913518 a.u.

(5*R*,9*S*)-**4**, Conf T

O	1.729195	-0.561839	-0.773426
O	-0.049598	2.142547	-0.614078
C	4.520715	-1.672135	-0.949309
C	4.137475	-0.283902	-0.454920
C	2.751580	-0.220435	0.170775
C	2.419134	1.164944	0.692889
C	1.024440	1.243184	1.313274
C	-0.076334	1.306488	0.295279
O	-2.331669	1.366672	-1.526129
C	-3.546254	-1.448384	-1.381129
O	-0.990984	-1.091401	2.238159
O	-2.785477	-1.159889	0.910322
C	-1.579953	-0.642525	1.289588
C	-1.238596	0.442326	0.375985
C	-2.247904	0.538713	-0.526269
C	-3.304325	-0.477650	-0.246784
H	1.753797	-1.509305	-0.938512
H	4.474419	-2.405265	-0.140889
H	3.861414	-2.010411	-1.750757
H	5.536678	-1.678359	-1.344738
H	4.178429	0.432726	-1.279802
H	4.861117	0.049948	0.293172
H	2.706265	-0.929431	1.006858
H	2.503093	1.891776	-0.117539
H	3.158983	1.435103	1.447084
H	0.937844	2.165844	1.894519
H	0.852755	0.412654	1.995496
H	-1.492047	1.910248	-1.482390
H	-3.928150	-0.911190	-2.248561
H	-4.283252	-2.190217	-1.079883
H	-2.622269	-1.955525	-1.657148
H	-4.230683	0.018939	0.048043

CAM-B3LYP Energy = -804.890805322 a.u.

(5*S*,9*S*)-**4**, Conf A

O	2.548152	-0.849997	-1.042375
O	-0.614844	2.521657	0.535968
C	3.873286	-1.704726	1.447179
C	3.694689	-0.272588	0.965081
C	2.436326	-0.061613	0.139743
C	2.242700	1.412514	-0.204066
C	0.985486	1.722906	-1.030126
C	-0.277429	1.610901	-0.228387
O	-2.827397	1.329873	1.133006
C	-3.377833	-1.693881	1.243522
O	-0.157284	-1.205992	-1.769616
O	-2.166367	-1.518375	-0.858005

C	-1.047303	-0.783719	-1.068125
C	-1.156289	0.462281	-0.324281
C	-2.344787	0.425981	0.337860
C	-3.075128	-0.839262	0.033448
H	1.659740	-0.997973	-1.402564
H	4.789232	-1.809009	2.030243
H	3.038494	-2.011101	2.081539
H	3.926965	-2.395741	0.606577
H	4.553264	0.029105	0.357837
H	3.661624	0.404828	1.821652
H	1.577970	-0.415898	0.726506
H	3.111134	1.743677	-0.777146
H	2.220617	1.999761	0.716495
H	0.938724	1.078127	-1.906109
H	1.038016	2.756792	-1.372306
H	-2.136397	2.052972	1.160940
H	-4.058204	-1.160164	1.905974
H	-2.463937	-1.929279	1.787862
H	-3.854280	-2.620025	0.928758
H	-3.983348	-0.616151	-0.529165

CAM-B3LYP Energy = -804.893681769 a.u.

(5*S*,9*S*)-**4**, Conf B

O	2.325406	-1.731465	-0.554983
O	-0.234139	2.410463	-0.557636
C	3.833023	0.574831	2.004423
C	3.663417	-0.578883	1.024359
C	2.399418	-0.511400	0.180415
C	2.391706	0.689216	-0.761142
C	1.141802	0.806441	-1.646668
C	-0.074393	1.226946	-0.875776
O	-2.552025	1.917918	0.473012
C	-3.526320	-0.675794	1.808015
O	-0.439429	-1.954420	-1.114738
O	-2.418621	-1.558580	-0.169114
C	-1.220632	-1.153204	-0.656167
C	-1.110177	0.288362	-0.492762
C	-2.250686	0.706622	0.120611
C	-3.170118	-0.444866	0.357020
H	1.408527	-1.869288	-0.840570
H	3.985726	1.527908	1.497350
H	2.957363	0.675907	2.649307
H	4.697889	0.406086	2.646578
H	3.633480	-1.521987	1.573384
H	4.524647	-0.634378	0.352350
H	1.539123	-0.449333	0.860448
H	3.262469	0.609644	-1.415561
H	2.502281	1.610460	-0.187384
H	0.955673	-0.129059	-2.171060
H	1.314032	1.583853	-2.391548
H	-1.765800	2.474819	0.203471
H	-4.148751	-1.563844	1.896420
H	-4.084400	0.179557	2.186885
H	-2.627770	-0.808063	2.409516
H	-4.066252	-0.333232	-0.255879

CAM-B3LYP Energy = -804.892738292 a.u.

(5*S*,9*S*)-**4**, Conf C

O	-2.777444	-0.851660	-1.041809
O	1.074071	2.596659	-0.183036
C	-5.329634	-0.736456	0.479310
C	-4.001123	-0.159054	0.945020
C	-3.091732	0.260161	-0.203027
C	-1.822866	0.927830	0.313824
C	-0.885892	1.383679	-0.815412
C	0.526255	1.502508	-0.343202
O	3.284613	1.469996	0.582122
C	4.379461	-1.264320	-0.285816
O	-0.048137	-1.659395	-0.474114
O	2.066098	-1.831197	0.209878
C	0.974813	-1.106377	-0.146954
C	1.301769	0.309573	-0.045326
C	2.590954	0.391330	0.375448
C	3.166932	-0.971860	0.568778
H	-1.930098	-1.230740	-0.760392
H	-5.893283	-0.002010	-0.100407
H	-5.174936	-1.612561	-0.150184
H	-5.946823	-1.034884	1.327682
H	-3.467489	-0.891806	1.558041
H	-4.179979	0.713166	1.579765
H	-3.636101	0.965274	-0.839703
H	-1.312391	0.216383	0.967626
H	-2.091207	1.783995	0.933793
H	-1.197476	2.347881	-1.213636
H	-0.915484	0.648370	-1.620959
H	2.670687	2.227074	0.365658
H	4.699364	-2.292455	-0.129158
H	5.194664	-0.599381	-0.003197
H	4.152047	-1.118106	-1.341216
H	3.381269	-1.137515	1.626101

CAM-B3LYP Energy = -804.892683887 a.u.

(5*S*,9*S*)-**4**, Conf D

O	-3.079231	-1.309056	-0.029881
O	-0.340902	-1.228570	0.215238
C	-5.714869	-0.301711	-0.611518
C	-4.697777	0.407763	0.270602
C	-3.255973	0.104024	-0.104779
C	-2.272588	0.855301	0.795372
C	-0.877273	1.113288	0.228842

C	0.050913	-0.055991	0.129309
O	2.077990	-2.152127	-0.145179
C	4.713538	-0.800532	0.641482
O	1.888252	2.537900	-0.186577
O	3.546120	1.055387	-0.410957
C	2.237510	1.388112	-0.221794
C	1.465555	0.155291	-0.088174
C	2.337083	-0.880060	-0.206936
C	3.725024	-0.373148	-0.420317
H	-2.125513	-1.478774	0.038308
H	-5.608242	-1.383545	-0.540880
H	-6.733203	-0.041587	-0.319446
H	-5.586549	-0.019628	-1.659134
H	-4.848166	0.127999	1.317716
H	-4.846468	1.488336	0.205911
H	-3.096855	0.429886	-1.143140
H	-2.202859	0.330278	1.751514
H	-2.699224	1.835949	1.012187
H	-0.366561	1.880278	0.813288
H	-0.943880	1.540582	-0.778473
H	1.099612	-2.227574	0.007504
H	4.827631	-1.883704	0.621638
H	4.371657	-0.497290	1.630475
H	5.682204	-0.345597	0.444520
H	4.071731	-0.657907	-1.415649

CAM-B3LYP Energy = -804.892398115 a.u.

(5*S*,9*S*)-**4**, Conf E

O	2.715667	-1.373287	-0.332422
O	-0.777922	2.550684	-0.175698
C	5.422320	-0.324808	0.012992
C	4.139818	0.487328	0.129826
C	2.957181	-0.333550	0.614768
C	1.695467	0.492534	0.855231
C	1.119533	1.120632	-0.425046
C	-0.340931	1.401560	-0.284761
O	-3.223490	1.698106	-0.027269
C	-4.220746	-1.007588	1.055018
O	-0.135177	-1.802048	-0.503352
O	-2.355413	-1.718335	-0.334235
C	-1.132598	-1.130939	-0.383918
C	-1.302180	0.311063	-0.265814
C	-2.635550	0.546638	-0.151688
C	-3.399536	-0.735076	-0.185157
H	1.781720	-1.630604	-0.292668
H	5.303098	-1.143430	-0.696329
H	6.250572	0.298316	-0.326688
H	5.701867	-0.754324	0.977652
H	3.892371	0.929140	-0.838733
H	4.288016	1.313889	0.829585
H	3.228441	-0.787561	1.576840
H	1.911899	1.272678	1.586624
H	0.952992	-0.162836	1.314355
H	1.255206	0.424281	-1.254687
H	1.621700	2.054392	-0.669535
H	-2.488880	2.374579	-0.039967
H	-4.696287	-1.982849	0.972980
H	-4.996931	-0.249631	1.153464
H	-3.592939	-0.990387	1.945251
H	-4.018845	-0.773367	-1.083048

CAM-B3LYP Energy = -804.891979132 a.u.

(5*S*,9*S*)-**4**, Conf F

O	2.393552	-1.398752	-0.524909
O	-0.474486	2.519112	-0.028937
C	4.841647	-0.363261	0.780019
C	3.448931	-0.442449	1.393878
C	2.299630	-0.317326	0.401055
C	2.287390	1.026062	-0.323562
C	1.092711	1.229598	-1.267989
C	-0.201273	1.425078	-0.534930
O	-2.808902	1.697652	0.714889
C	-3.652199	-1.151045	1.504794
O	-0.298859	-1.678940	-1.354057
O	-2.358811	-1.591457	-0.507947
C	-1.168351	-1.026470	-0.824285
C	-1.183169	0.366867	-0.404770
C	-2.390460	0.591858	0.181642
C	-3.227979	-0.642826	0.145371
H	1.518446	-1.545822	-0.916261
H	5.049014	0.621890	0.360681
H	5.601771	-0.561519	1.536656
H	4.960156	-1.099961	-0.014580
H	3.330761	0.334634	2.153234
H	3.333057	-1.399798	1.906518
H	1.368969	-0.420724	0.972818
H	3.195861	1.111499	-0.920060
H	2.305593	1.833798	0.411759
H	1.013179	0.394546	-1.961998
H	1.255779	2.138404	-1.847905
H	-2.053179	2.344685	0.608152
H	-2.784789	-1.319323	2.141937
H	-4.200000	-2.084499	1.393265
H	-4.304580	-0.419343	1.979821
H	-4.091261	-0.485908	-0.503697

CAM-B3LYP Energy = -804.891942934 a.u.

(5*S*,9*S*)-**4**, Conf G

O	-2.636144	-1.357543	-1.179581
O	0.780481	2.540300	-0.442717

C	-4.813846	0.454980	1.339775
C	-4.052708	-0.675313	0.658242
C	-3.116021	-0.223457	-0.457086
C	-1.955555	0.617718	0.061244
C	-1.008818	1.079710	-1.058074
C	0.355525	1.385121	-0.531565
O	3.044579	1.720088	0.529032
C	4.459807	-0.946992	-0.035128
O	0.114217	-1.820223	-0.417118
O	2.189448	-1.710338	0.387066
C	1.054210	-1.136676	-0.087177
C	1.229355	0.309363	-0.092983
C	2.476818	0.561013	0.383133
C	3.174372	-0.713199	0.725644
H	-1.764704	-1.610028	-0.836141
H	-4.153075	1.118764	1.898279
H	-5.354788	1.060257	0.608895
H	-5.545183	0.056642	2.043623
H	-4.762816	-1.376080	0.214447
H	-3.473134	-1.241035	1.394046
H	-3.693067	0.366190	-1.177070
H	-1.412750	0.019453	0.797734
H	-2.339006	1.489799	0.589922
H	-1.394488	1.971119	-1.549927
H	-0.917324	0.285332	-1.800315
H	2.371707	2.387683	0.215295
H	4.282845	-0.915412	-1.109517
H	4.871218	-1.918776	0.229999
H	5.185510	-0.178414	0.227878
H	3.339584	-0.767375	1.803246

CAM-B3LYP Energy = -804.891924495 a.u.

(5*S*,9*S*)-**4**, Conf H

O	-2.954044	-1.748007	-0.241754
O	-0.241041	-1.419827	0.104918
C	-5.366354	1.110875	-0.189875
C	-4.748091	-0.247262	0.112137
C	-3.270209	-0.356810	-0.236268
C	-2.381743	0.426062	0.732261
C	-1.008174	0.854062	0.217350
C	0.033253	-0.211631	0.080464
O	2.268769	-2.081753	-0.210648
C	4.727672	-0.501244	0.706856
O	1.603844	2.563471	-0.098363
O	3.409733	1.264848	-0.322320
C	2.069392	1.456947	-0.161613
C	1.423534	0.148629	-0.093598
C	2.398574	-0.788588	-0.221484
C	3.733209	-0.137136	-0.372937
H	-1.991433	-1.830403	-0.142179
H	-4.912726	1.911434	0.396273
H	-5.253821	1.367352	-1.245314
H	-6.432710	1.107014	0.037860
H	-5.269524	-1.017236	-0.460191
H	-4.878775	-0.500094	1.168412
H	-3.125932	0.047685	-1.248378
H	-2.278827	-0.155092	1.652334
H	-2.901430	1.344673	1.005554
H	-0.588121	1.631432	0.857805
H	-1.095855	1.331102	-0.765519
H	1.299273	-2.261190	-0.092612
H	4.326723	-0.270151	1.693176
H	5.650544	0.055699	0.558035
H	4.951674	-1.566051	0.655206
H	4.136469	-0.349458	-1.364888

CAM-B3LYP Energy = -804.891907850 a.u.

(5*S*,9*S*)-**4**, Conf I

O	2.565307	-1.838160	-0.416398
O	-0.462958	2.464470	-0.345178
C	4.881006	0.907774	0.683982
C	4.205501	-0.137945	-0.192490
C	2.973864	-0.769408	0.436656
C	1.817768	0.195523	0.690702
C	1.251897	0.820806	-0.594909
C	-0.161111	1.269474	-0.410110
O	-2.979258	1.901466	-0.061168
C	-4.216920	-0.611092	1.212069
O	-0.320325	-1.944184	-0.456703
O	-2.507917	-1.602000	-0.206529
C	-1.231218	-1.159556	-0.337370
C	-1.235033	0.296462	-0.295360
C	-2.527969	0.686471	-0.143735
C	-3.429274	-0.500958	-0.073963
H	1.609972	-1.977012	-0.325369
H	4.245051	1.779956	0.842488
H	5.134281	0.497740	1.664008
H	5.805010	1.257753	0.223182
H	4.907618	-0.947112	-0.405448
H	3.932848	0.293977	-1.158612
H	3.262099	-1.183123	1.411414
H	2.139009	0.981236	1.374929
H	1.036505	-0.359848	1.212778
H	1.272020	0.076034	-1.392680
H	1.839809	1.681341	-0.908297
H	-2.175648	2.489459	-0.137874
H	-3.549632	-0.614519	2.073233
H	-4.799496	-1.530093	1.208489
H	-4.899822	0.233464	1.295612
H	-4.089476	-0.517301	-0.942886

CAM-B3LYP Energy = -804.891742855 a.u.

(5*S*,9*S*)-**4**, Conf J

O	-3.520058	1.014123	-0.976115
O	0.261267	-1.906979	-0.176870
C	-6.019930	0.175001	0.452481
C	-4.749125	-0.653481	0.320340
C	-3.483283	0.182867	0.189863
C	-2.241451	-0.681594	0.074159
C	-0.963364	0.136997	0.051108
C	0.283673	-0.676349	-0.084332
O	2.853159	-2.024059	-0.348859
C	4.897978	-0.083723	0.875133
O	1.265358	2.367442	0.095453
O	3.308523	1.478372	-0.097810
C	1.948153	1.384664	-0.024574
C	1.580546	-0.023442	-0.115264
C	2.729482	-0.732935	-0.243568
C	3.912019	0.178546	-0.241213
H	-4.186874	1.696845	-0.853970
H	-6.209753	0.770159	-0.442694
H	-6.889078	-0.466291	0.600278
H	-5.960479	0.855321	1.305095
H	-4.820614	-1.312898	-0.549176
H	-4.639927	-1.294713	1.198609
H	-3.391140	0.823126	1.076851
H	-2.317153	-1.281690	-0.835249
H	-2.221329	-1.379503	0.912407
H	-0.862989	0.743503	0.956581
H	-0.978296	0.860392	-0.767470
H	1.922867	-2.382451	-0.317707
H	5.695785	0.655596	0.842006
H	5.336027	-1.073696	0.753315
H	4.403860	-0.031584	1.844739
H	4.404918	0.147390	-1.214818

CAM-B3LYP Energy = -804.891546920 a.u.

(5*S*,9*S*)-**4**, Conf K

O	-3.567719	1.094581	-0.933251
O	0.257019	-1.903352	-0.178809
C	-6.014898	0.194524	0.510785
C	-4.755874	-0.636747	0.311381
C	-3.488458	0.196381	0.178504
C	-2.242130	-0.674436	0.088140
C	-0.963869	0.142941	0.047764
C	0.282111	-0.672664	-0.087540
O	2.849717	-2.026530	-0.340253
C	4.891603	-0.086588	0.888735
O	1.269097	2.369714	0.082896
O	3.311133	1.475669	-0.098419
C	1.950281	1.385160	-0.030621
C	1.580178	-0.022613	-0.118079
C	2.728220	-0.734944	-0.239561
C	3.912539	0.174104	-0.234106
H	-3.694426	0.573130	-1.734803
H	-5.946480	0.794196	1.420934
H	-6.174908	0.874560	-0.325768
H	-6.894490	-0.444292	0.598003
H	-4.856379	-1.261754	-0.582609
H	-4.627477	-1.321843	1.152932
H	-3.404343	0.853490	1.048373
H	-2.311310	-1.301548	-0.805022
H	-2.221936	-1.353260	0.942530
H	-0.857914	0.759850	0.945225
H	-0.983184	0.857610	-0.778896
H	1.918522	-2.383113	-0.311638
H	5.328153	-1.077889	0.772793
H	4.391995	-0.030026	1.855294
H	5.691102	0.650966	0.857706
H	4.410887	0.138557	-1.204779

CAM-B3LYP Energy = -804.891542387 a.u.

(5*S*,9*S*)-**4**, Conf L

O	-2.845307	-0.759748	-1.323617
O	0.946724	2.631022	0.026437
C	-3.788340	-1.205575	1.536621
C	-4.248461	-0.130841	0.560393
C	-3.196396	0.316580	-0.451985
C	-1.957722	0.913677	0.203932
C	-0.968787	1.482856	-0.826409
C	0.417260	1.557667	-0.274069
O	3.120873	1.434625	0.795303
C	4.283750	-1.193788	-0.289858
O	-0.124204	-1.571970	-0.767807
O	1.950145	-1.811531	0.011171
C	0.875540	-1.055017	-0.328255
C	1.185560	0.342607	-0.060676
C	2.448875	0.382183	0.437743
C	3.022927	-0.993123	0.520167
H	-1.979483	-1.115899	-1.071555
H	-4.623292	-1.549607	2.147963
H	-3.388729	-2.071020	1.006003
H	-3.017095	-0.840847	2.216411
H	-4.594450	0.750630	1.107530
H	-5.106217	-0.499458	-0.006877
H	-3.654685	1.080226	-1.087983
H	-1.473773	0.139955	0.802300
H	-2.259066	1.701508	0.895806
H	-1.268362	2.481013	-1.141459
H	-0.951760	0.832409	-1.702481
H	2.514153	2.208910	0.624392
H	5.076830	-0.560088	0.105147

H	4.114578	-0.939831	-1.335666
H	4.602162	-2.232033	-0.221994
H	3.178111	-1.268402	1.564950

CAM-B3LYP Energy = -804.891394434 a.u.

(5*S*,9*S*)-**4**, Conf M

O	-3.056310	-1.382094	-0.535455
O	-0.362256	-1.265047	0.037339
C	-5.309470	-0.077555	0.936287
C	-4.725837	0.308962	-0.416752
C	-3.235824	0.032714	-0.573955
C	-2.383310	0.754948	0.473501
C	-0.941539	1.066310	0.076597
C	0.012477	-0.084253	0.009266
O	2.094969	-2.137024	-0.161703
C	4.631277	-0.755191	0.859756
O	1.815650	2.548361	-0.116401
O	3.515370	1.101969	-0.245563
C	2.189784	1.406352	-0.148865
C	1.434832	0.157082	-0.100261
C	2.332849	-0.859262	-0.176241
C	3.722869	-0.322549	-0.269697
H	-2.120267	-1.551152	-0.341840
H	-4.878651	0.511660	1.747322
H	-6.387603	0.087433	0.949759
H	-5.128248	-1.130382	1.152174
H	-4.896675	1.371309	-0.608524
H	-5.245485	-0.236748	-1.208035
H	-2.937932	0.400661	-1.565182
H	-2.401881	0.187079	1.406100
H	-2.855369	1.715467	0.687599
H	-0.509254	1.799288	0.760498
H	-0.906622	1.557722	-0.902269
H	1.109708	-2.233657	-0.084195
H	4.204070	-0.482379	1.824290
H	5.602667	-0.276735	0.752550
H	4.769945	-1.835119	0.825584
H	4.153566	-0.579118	-1.239393

CAM-B3LYP Energy = -804.891346843 a.u.

(5*S*,9*S*)-**4**, Conf N

O	3.182069	-0.774962	-1.006828
O	0.321844	-1.320885	-1.061484
C	4.834850	-0.743763	1.453470
C	4.092186	0.433124	0.837847
C	2.819755	0.034377	0.112579
C	2.015750	1.261683	-0.316565
C	0.890490	0.971739	-1.325894
C	-0.007382	-0.138421	-0.877817
O	-1.861778	-2.175930	0.068506
C	-4.586037	-0.761559	0.153828
O	-1.570982	2.506609	0.005682
O	-3.100616	1.064497	0.765743
C	-1.916487	1.365521	0.159962
C	-1.258599	0.113659	-0.204534
C	-2.067064	-0.900739	0.202283
C	-3.301507	-0.359753	0.844190
H	2.381668	-1.235850	-1.296057
H	5.109045	-1.472754	0.691354
H	5.747986	-0.413775	1.950378
H	4.215998	-1.251259	2.196658
H	4.738001	0.956916	0.127161
H	3.830348	1.155594	1.614775
H	2.208381	-0.568416	0.794784
H	2.684926	1.988854	-0.781438
H	1.600408	1.734089	0.576223
H	1.328454	0.664520	-2.275310
H	0.310673	1.878656	-1.482419
H	-0.982003	-2.262097	-0.391691
H	-5.430502	-0.279500	0.642201
H	-4.716160	-1.841127	0.219338
H	-4.566506	-0.469376	-0.895580
H	-3.320742	-0.634320	1.900562

CAM-B3LYP Energy = -804.891341411 a.u.

(5*S*,9*S*)-**4**, Conf O

O	-3.233372	-1.268249	-0.759665
O	-0.486099	-1.138679	-0.759629
C	-4.672710	-0.425476	1.725237
C	-3.492208	0.295893	1.091119
C	-3.421691	0.104470	-0.419890
C	-2.401689	1.020907	-1.105228
C	-1.017687	1.187291	-0.475886
C	-0.094230	0.012177	-0.519285
O	1.927072	-2.107590	-0.494217
C	4.185223	-1.015184	1.266577
O	1.742686	2.537930	0.153907
O	3.393235	1.032063	0.218197
C	2.089454	1.391875	0.046325
C	1.318587	0.189856	-0.261464
C	2.187606	-0.854217	-0.269185
C	3.571647	-0.384926	0.036137
H	-2.275657	-1.432457	-0.761008
H	-4.626847	-1.495604	1.523334
H	-4.685402	-0.285501	2.806911
H	-5.618742	-0.049744	1.329113
H	-2.561361	-0.061075	1.540748
H	-3.554678	1.366962	1.305912
H	-4.399004	0.363551	-0.836459
H	-2.839267	2.020418	-1.141320

H	-2.296717	0.696534	-2.142902
H	-1.090805	1.483712	0.575665
H	-0.497853	2.021555	-0.949751
H	0.950640	-2.159735	-0.667533
H	3.553518	-0.853127	2.139293
H	5.165230	-0.579676	1.450900
H	4.304866	-2.086415	1.109179
H	4.210080	-0.529202	-0.837563

CAM-B3LYP Energy = -804.891214153 a.u.

(5*S*,9*S*)-**4**, Conf P

O	-3.029818	0.946459	1.287440
O	-0.293084	-1.247908	-0.973135
C	-5.171352	-1.098795	0.980064
C	-4.464185	-0.392019	-0.167274
C	-3.047404	0.051755	0.169431
C	-2.348245	0.674777	-1.034414
C	-0.902025	1.061578	-0.772769
C	0.052485	-0.091648	-0.714325
O	2.102131	-2.153184	-0.526847
C	4.196090	-1.001209	1.404540
O	1.782998	2.489145	0.067531
O	3.455941	1.019346	0.271568
C	2.159700	1.349158	-0.002535
C	1.441981	0.130010	-0.356638
C	2.329528	-0.894031	-0.290766
C	3.675698	-0.395757	0.119907
H	-3.558741	1.721851	1.064991
H	-5.250090	-0.451042	1.853046
H	-6.179463	-1.398975	0.691861
H	-4.627750	-1.997706	1.278576
H	-5.040940	0.485537	-0.479796
H	-4.415884	-1.053346	-1.035931
H	-2.476993	-0.814600	0.509091
H	-2.900844	1.571731	-1.327905
H	-2.401553	-0.018953	-1.874404
H	-0.808947	1.626703	0.156718
H	-0.528702	1.735707	-1.549411
H	1.136357	-2.206545	-0.770212
H	4.349492	-2.071390	1.270445
H	3.489076	-0.843399	2.218436
H	5.148225	-0.544049	1.666448
H	4.387778	-0.535301	-0.695744

CAM-B3LYP Energy = -804.891109996 a.u.

(5*S*,9*S*)-**4**, Conf Q

O	-3.455940	1.489961	-1.038123
O	0.067581	-1.752035	-0.483604
C	-5.123194	-1.086203	1.206350
C	-4.878398	-0.177779	0.008137
C	-3.534857	0.541233	0.031646
C	-2.351608	-0.394498	-0.132396
C	-1.021963	0.332751	-0.041408
C	0.170796	-0.547293	-0.235705
O	2.649733	-2.036538	-0.588954
C	4.769260	-0.424725	0.942133
O	1.352010	2.369315	0.363294
O	3.335238	1.362751	0.126270
C	1.969609	1.361589	0.140911
C	1.509766	0.007220	-0.142064
C	2.611352	-0.763331	-0.322711
C	3.852927	0.050442	-0.163258
H	-4.167288	2.130488	-0.934401
H	-4.437565	-1.933755	1.224659
H	-5.004761	-0.539977	2.144597
H	-6.136740	-1.487267	1.183279
H	-5.662870	0.583954	-0.025045
H	-4.954341	-0.744890	-0.923555
H	-3.438372	1.073251	0.987314
H	-2.438481	-0.898722	-1.097434
H	-2.397977	-1.167721	0.634317
H	-0.908022	0.835564	0.923742
H	-0.963623	1.135074	-0.780809
H	1.696207	-2.325869	-0.634529
H	5.615905	0.252680	1.034357
H	5.144440	-1.419703	0.705307
H	4.238502	-0.463170	1.892870
H	4.383873	0.105992	-1.115558

CAM-B3LYP Energy = -804.890941880 a.u.

(5*S*,9*S*)-**4**, Conf R

O	-3.063801	1.070885	1.167115
O	-0.280431	-1.268042	-0.969056
C	-5.199589	-1.025396	1.005177
C	-4.454838	-0.422148	-0.178124
C	-3.047725	0.050941	0.159473
C	-2.348008	0.645571	-1.051204
C	-0.902684	1.040332	-0.795845
C	0.057084	-0.107244	-0.719503
O	2.117313	-2.155450	-0.508419
C	4.200117	-0.977980	1.419597
O	1.770754	2.489282	0.050965
O	3.451000	1.030287	0.270841
C	2.153722	1.350878	-0.009819
C	1.443864	0.125115	-0.357058
C	2.337044	-0.893335	-0.280912
C	3.679261	-0.384468	0.129632
H	-3.312760	0.675910	2.008158
H	-5.369839	-0.289327	1.793076
H	-6.176888	-1.400459	0.700440

H	-4.643230	-1.860681	1.436556
H	-5.018017	0.423380	-0.583459
H	-4.377071	-1.164764	-0.976327
H	-2.468151	-0.802027	0.529314
H	-2.903809	1.534157	-1.358710
H	-2.399614	-0.068279	-1.873588
H	-0.812189	1.622630	0.122755
H	-0.532290	1.701481	-1.585183
H	1.152357	-2.215398	-0.754359
H	4.359972	-2.048161	1.293301
H	3.490323	-0.818533	2.230755
H	5.148983	-0.513551	1.680578
H	4.394057	-0.525670	-0.683370

CAM-B3LYP Energy = -804.890904569 a.u.

(5*S*,9*S*)-**4**, Conf S

O	1.966081	-0.045521	-0.966167
O	-0.018797	2.028058	0.501717
C	4.861307	-0.708714	-1.448856
C	4.311265	0.113123	-0.291002
C	2.891529	-0.265224	0.105694
C	2.392082	0.542465	1.289822
C	0.955714	0.194880	1.674708
C	-0.072602	0.826380	0.783118
O	-2.220862	1.914601	-0.833081
C	-4.604787	0.024798	-0.372296
O	-1.023150	-2.242749	0.981498
O	-2.745034	-1.537453	-0.254035
C	-1.571230	-1.334414	0.413528
C	-1.205155	0.071573	0.280114
C	-2.165152	0.665790	-0.473334
C	-3.216081	-0.320008	-0.861916
H	2.094086	-0.721472	-1.638662
H	5.893969	-0.434657	-1.665836
H	4.842103	-1.776349	-1.218691
H	4.286761	-0.549718	-2.363177
H	4.328186	1.176708	-0.544344
H	4.952132	-0.015369	0.585105
H	2.868715	-1.328856	0.374025
H	2.465717	1.608185	1.064481
H	3.046687	0.346167	2.139623
H	0.743729	0.578006	2.677679
H	0.806306	-0.882898	1.706007
H	-1.401748	2.333626	-0.438500
H	-4.939347	0.950656	-0.838882
H	-4.610201	0.151033	0.709857
H	-5.297704	-0.769933	-0.641648
H	-3.206634	-0.464526	-1.943979

CAM-B3LYP Energy = -804.890774346 a.u.

(5*S*,9*S*)-**4**, Conf T

O	-3.103185	-1.883026	-0.152354
O	-0.391457	-1.502294	-0.379361
C	-4.160367	1.493495	1.212098
C	-3.581781	0.084205	1.180770
C	-3.458416	-0.503118	-0.221194
C	-2.543351	0.286712	-1.164191
C	-1.179263	0.750912	-0.650705
C	-0.128321	-0.293329	-0.447130
O	2.121268	-2.112888	0.013220
C	4.258314	-0.378007	1.358881
O	1.419872	2.500154	-0.499685
O	3.231639	1.242489	-0.136199
C	1.893160	1.407223	-0.335959
C	1.259238	0.091508	-0.305395
C	2.240727	-0.822784	-0.090421
C	3.566496	-0.147468	0.033769
H	-2.133545	-1.937851	-0.183518
H	-5.127797	1.528964	0.706325
H	-4.311193	1.828535	2.238639
H	-3.506991	2.218365	0.724149
H	-4.225474	-0.587487	1.752185
H	-2.605966	0.061457	1.674117
H	-4.453303	-0.487702	-0.675423
H	-3.079747	1.187959	-1.464672
H	-2.411522	-0.301323	-2.075016
H	-1.268317	1.285585	0.300729
H	-0.764299	1.494726	-1.332712
H	1.155336	-2.311793	-0.100839
H	4.496631	-1.435163	1.469628
H	3.619482	-0.069485	2.185738
H	5.184504	0.192191	1.392391
H	4.208487	-0.438538	-0.799829

CAM-B3LYP Energy = -804.890755327 a.u.

(5*S*,9*S*)-**4**, Conf U

O	-3.629483	1.135488	-0.864366
O	0.255859	-1.908876	-0.194773
C	-6.014347	0.113653	0.544258
C	-4.754085	-0.668831	0.205124
C	-3.493986	0.178858	0.194821
C	-2.245215	-0.673937	0.008324
C	-0.965041	0.141699	-0.003442
C	0.282556	-0.678347	-0.113439
O	2.854139	-2.034461	-0.321415
C	4.877940	-0.086620	0.922677
O	1.266087	2.363745	0.050716
O	3.311007	1.469420	-0.095848
C	1.949760	1.378992	-0.046780
C	1.580915	-0.029243	-0.130267

C	2.730448	-0.742376	-0.230969
C	3.914460	0.167015	-0.215117
H	-3.079571	1.901651	-0.677030
H	-6.890655	-0.535725	0.536839
H	-5.941093	0.562271	1.537435
H	-6.182331	0.915045	-0.174615
H	-4.855843	-1.138588	-0.777527
H	-4.614022	-1.477276	0.926296
H	-3.421834	0.715508	1.148659
H	-2.337733	-1.233953	-0.924861
H	-2.202320	-1.407091	0.815769
H	-0.873607	0.754809	0.898932
H	-0.951430	0.855180	-0.832092
H	1.924149	-2.392859	-0.303425
H	5.316783	-1.078183	0.818009
H	4.365010	-0.025428	1.881979
H	5.677294	0.651341	0.898676
H	4.425906	0.125590	-1.178698

CAM-B3LYP Energy = -804.890722619 a.u.