

Supporting information (SI)

A theoretical study of the radical scavenging activity of natural stilbenes

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Table S1: The calculated thermal properties (in Kcal/mol) of the reaction between the studied compounds (for the lowest PAs(X–H)) with CH₃OO[•] radical *via* the sequential proton, SET processes and HAT mechanism using the ROB3LYP/6-311G++G(2df,2p)//B3LYP/6-311G(d,p) methods in the gas phase.

comp.	PA mechanism		SET mechanism		HAT mechanism	
	ΔH	ΔG	ΔH	ΔG	ΔH	ΔG
1	167.4	164.6	141.0	139.9	4.0	1.1
2	169.4	166.3	139.1	137.8	5.4	2.6
3	170.3	169.4	155.2	155.4	3.1	2.6
4	161.1	158.7	134.3	133.2	-1.5	-3.7
5	148.4	149.2	134.2	135.4	-10.4	-9.9
6	162.2	159.7	131.3	129.9	-1.1	-3.4
7	161.7	161.1	130.7	131.6	2.1	1.7
8	162.6	162.9	130.5	132.1	-2.5	-1.8
9	168.8	168.5	129.0	130.8	3.0	3.3
10	165.1	164.8	129.6	130.7	-2.3	-2.2
11	152.2	152.7	133.0	134.4	-10.7	-10.1
12	158.6	159.1	129.8	131.9	-3.9	-4.3

Table S2: The calculated Gibb energies (in kcal/mol) of the reaction between the studied compounds with CH₃OO[•] radical *via* RAF mechanism using the ROB3LYP/6-311G++G(2df,2p)//B3LYP/6-311G(d,p) methods in the gas phase.

comp.	C=C position	ΔG
1	C7	10.1
	C8	9.6
2	C7	9.8
	C8	10.0
3		
4	C7	9.6
	C8	9.6
5	C7	11.6
	C8	10.6
6	C7	13.9
	C8	11.5
7	C7	11.4
	C8	10.4
8	C7	11.8
	C8	12.8
9	C7	11.7
	C8	12.7
10	C7	10.6
	C8	10.9
11	C7	11.4
	C8	12.2
12	C7	9.5
	C8	8.8

Table S3: Cartesian coordinates and molecular enthalpies of all parent molecules, radicals and anions optimized at B3LYP/6-311G(d,p) level in the gas phase.

Name of compound (1)		Pinosylvin		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)			Energies at B3LYP/6-311G(d,p) in gas phase	
C	4.04960200	0.17936800	-0.00013600	Zero-point correction= 0.221958 (Hartree/Particle)
C	3.52080100	-1.11013100	-0.00090500	Thermal correction to Energy= 0.234890
C	2.14208100	-1.30923600	-0.00070300	Thermal correction to Enthalpy= 0.235835
C	1.26320300	-0.21224300	0.00022200	Thermal correction to Gibbs Free Energy= 0.182011
C	1.79666000	1.08288400	0.00104900	Sum of electronic and zero-point Energies= -691.106438
C	3.17658600	1.26807700	0.00084800	Sum of electronic and thermal Energies= -691.093505
H	5.12610700	0.31058300	-0.00027600	Sum of electronic and thermal Enthalpies= -691.092561
H	1.74219200	-2.31893900	-0.00129700	Sum of electronic and thermal Free Energies= -691.146385
H	1.16549700	1.96110600	0.00197700	
C	-1.17038500	0.42251500	-0.00019500	
H	-0.91075200	1.47770500	-0.00097400	
C	-2.61155500	0.15827800	-0.00004600	
C	-3.49713200	1.24922300	-0.00238400	
C	-3.16677800	-1.13439100	0.00238800	
C	-4.87571300	1.06282500	-0.00242900	
H	-3.09189900	2.25591000	-0.00422600	
C	-4.54230800	-1.32107400	0.00234400	
H	-2.51819300	-2.00243000	0.00446500	
C	-5.40616200	-0.22436800	-0.00007900	
H	-5.53527800	1.92350700	-0.00428500	
H	-4.94624100	-2.32751800	0.00427400	
H	-6.47969400	-0.37461700	-0.00007800	
H	-0.43318500	-1.54027600	0.00068400	
C	-0.17765500	-0.48408900	0.00031700	
O	4.41303200	-2.14462600	-0.00182500	
H	3.92952300	-2.97702800	-0.00252300	
O	3.63084800	2.55622600	0.00169900	
H	4.59341300	2.55337300	0.00153100	
Name of radical		1-O3		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)			Energies at B3LYP/6-311G(d,p) in gas phase	
C	-4.11388400	0.15174600	-0.00000200	Zero-point correction= 0.208868 (Hartree/Particle)
C	-3.60593800	-1.20496500	0.00002700	Thermal correction to Energy= 0.222423
C	-2.16527000	-1.37735000	0.00003500	Thermal correction to Enthalpy= 0.223367
C	-1.29398200	-0.29922800	0.00001500	Thermal correction to Gibbs Free Energy= 0.165056
C	-1.84674500	1.00483500	-0.00001000	Sum of electronic and zero-point Energies= -690.475106
C	-3.24288600	1.21535900	-0.00002000	Sum of electronic and thermal Energies= -690.461551

H	-5.19082400	0.28088100	-0.00000600	Sum of electronic and thermal Enthalpies=	-690.460607
H	-1.80181300	-2.39831300	0.00005600	Sum of electronic and thermal Free Energies=	-690.518919
H	-1.21586400	1.88414500	-0.00001600		
C	1.12454800	0.38473400	-0.00003800		
H	0.84595900	1.43530000	-0.00009700		
C	2.57091400	0.15122400	-0.00002600		
C	3.43191400	1.26125400	0.00005000		
C	3.15111200	-1.13010800	-0.00008700		
C	4.81398600	1.10375000	0.00007800		
H	3.00592800	2.25933100	0.00009100		
C	4.53013400	-1.28767600	-0.00006000		
H	2.52087300	-2.01141700	-0.00016800		
C	5.37009600	-0.17252500	0.00002500		
H	5.45580100	1.97756600	0.00014000		
H	4.95530900	-2.28512300	-0.00011000		
H	6.44645900	-0.30044500	0.00004500		
H	0.42233100	-1.59454400	0.00008700		
C	0.15140300	-0.54298700	0.00002400		
O	-4.37453100	-2.19011500	0.00003700		
O	-3.63754700	2.52027000	-0.00004100		
H	-4.59994800	2.56300400	-0.00006100		
Name of radical			1-O5		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase	
C	4.12174200	0.23181300	0.02006500	Zero-point correction=	0.208582 (Hartree/Particle)
C	3.59866900	-1.03788300	0.09773000	Thermal correction to Energy=	0.222206
C	2.20124900	-1.23337800	0.06505500	Thermal correction to Enthalpy=	0.223151
C	1.29063500	-0.15479500	-0.04250000	Thermal correction to Gibbs Free Energy=	0.165318
C	1.81223600	1.12735200	-0.13315700	Sum of electronic and zero-point Energies=	-690.472389
C	3.24025000	1.37153600	-0.09990000	Sum of electronic and thermal Energies=	-690.458764
H	5.19009300	0.40156300	0.04300100	Sum of electronic and thermal Enthalpies=	-690.457820
H	1.80968500	-2.24527400	0.12981500	Sum of electronic and thermal Free Energies=	-690.515653
H	1.18482300	2.00237800	-0.24317900		
C	-1.14634300	0.43219800	0.03094800		
H	-0.89401800	1.48297600	0.14698900		
C	-2.58456700	0.15580600	0.01162700		
C	-3.47594800	1.21415400	0.25439100		
C	-3.12816300	-1.11649600	-0.24147800		
C	-4.85232500	1.01316000	0.25547500		
H	-3.07763000	2.20503300	0.44657900		
C	-4.50163700	-1.31741500	-0.24060400		

H	-2.47357500	-1.95440600	-0.45057400	
C	-5.37194600	-0.25474200	0.00907400	
H	-5.51825500	1.84688700	0.44727700	
H	-4.89905300	-2.30636700	-0.44010500	
H	-6.44384600	-0.41580100	0.00679600	
H	-0.38454000	-1.51673000	-0.13581300	
C	-0.14481500	-0.45972000	-0.05934000	
O	4.45891000	-2.09078600	0.20579400	
H	3.96203300	-2.91377400	0.25617900	
O	3.68984600	2.53878100	-0.17720500	
Name of anion			1-O3	
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	4.09026500	0.20614900	0.00003200	Zero-point correction= 0.207454 (Hartree/Particle)
C	3.54599300	-1.06374600	-0.00003700	Thermal correction to Energy= 0.221193
C	2.16380700	-1.27440900	-0.00003300	Thermal correction to Enthalpy= 0.222137
C	1.30801300	-0.14536800	0.00003100	Thermal correction to Gibbs Free Energy= 0.165160
C	1.84521900	1.13981300	0.00008800	Sum of electronic and zero-point Energies= -690.555245
C	3.26905200	1.40290000	0.00003500	Sum of electronic and thermal Energies= -690.541506
H	5.16846800	0.32851800	0.00013600	Sum of electronic and thermal Enthalpies= -690.540562
H	1.75116200	-2.28068200	-0.00018200	Sum of electronic and thermal Free Energies= -690.597539
H	1.20406600	2.01546500	0.00016400	
C	-1.14338600	0.47886700	-0.00001500	
H	-0.89783500	1.53701000	-0.00006600	
C	-2.57226600	0.17954900	-0.00000700	
C	-3.49761300	1.24340700	-0.00009000	
C	-3.10791600	-1.12630800	0.00008100	
C	-4.87046100	1.02205300	-0.00008800	
H	-3.11790100	2.26040000	-0.00015800	
C	-4.47856600	-1.34708300	0.00008200	
H	-2.43781500	-1.97807000	0.00015000	
C	-5.37604100	-0.27678800	-0.00000200	
H	-5.54943300	1.86934400	-0.00015400	
H	-4.85367700	-2.36614200	0.00015200	
H	-6.44620500	-0.45388900	0.00000100	
H	-0.38091100	-1.47217200	0.00006300	
C	-0.12825300	-0.41233900	0.00002500	
O	4.42128500	-2.14713200	-0.00011700	
H	3.87977100	-2.94202100	0.00013000	
O	3.75286800	2.56239100	0.00001100	
Name of anion			1-O5	

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase	
C	-4.08143300	0.09579100	0.00009600	Zero-point correction=	0.207822 (Hartree/Particle)
C	-3.58426100	-1.26149900	0.00026800	Thermal correction to Energy=	0.221391
C	-2.13696800	-1.33795700	0.00005100	Thermal correction to Enthalpy=	0.222335
C	-1.30320100	-0.21774000	-0.00021300	Thermal correction to Gibbs Free Energy=	0.165712
C	-1.85205200	1.08579500	-0.00028200	Sum of electronic and zero-point Energies=	-690.557679
C	-3.23965500	1.20044000	-0.00015400	Sum of electronic and thermal Energies=	-690.544110
H	-5.16331800	0.22649800	0.00005900	Sum of electronic and thermal Enthalpies=	-690.543166
H	-1.70694200	-2.33631300	0.00011200	Sum of electronic and thermal Free Energies=	-690.599788
H	-1.24232900	1.97943100	-0.00050000		
C	1.13412000	0.45446000	0.00008400		
H	0.87191200	1.50893500	0.00037900		
C	2.56902100	0.18226300	0.00004300		
C	3.47546200	1.26193200	0.00050700		
C	3.12672700	-1.11415700	-0.00042400		
C	4.85214500	1.06463400	0.00049100		
H	3.07870000	2.27256700	0.00088000		
C	4.50096200	-1.31090000	-0.00043000		
H	2.47119700	-1.97697200	-0.00079500		
C	5.37983100	-0.22520000	0.00002400		
H	5.51653400	1.92348700	0.00085000		
H	4.89333100	-2.32333300	-0.00080400		
H	6.45288900	-0.38390700	0.00000900		
H	0.40363500	-1.51200800	-0.00056800		
C	0.13670600	-0.45686200	-0.00024200		
O	-4.32661200	-2.27634300	0.00052300		
O	-3.76332500	2.48923600	-0.00034800		
H	-4.72053600	2.39246200	0.00006600		
Name of cationic radical				Energies at B3LYP/6-311G(d,p) in gas phase	
C	4.00115100	0.20262900	0.00001600	Zero-point correction=	0.222313 (Hartree/Particle)
C	3.50114200	-1.12014600	0.00000200	Thermal correction to Energy=	0.236010
C	2.13566400	-1.34724800	-0.00000600	Thermal correction to Enthalpy=	0.236954
C	1.24180400	-0.24851200	-0.00001800	Thermal correction to Gibbs Free Energy=	0.180243
C	1.75276600	1.07723600	-0.00001400	Sum of electronic and zero-point Energies=	-690.844122
C	3.12499600	1.29518400	0.00001000	Sum of electronic and thermal Energies=	-690.830425
H	5.07705400	0.34008500	0.00002800	Sum of electronic and thermal Enthalpies=	-690.829481
H	1.74586300	-2.35860200	0.00002700	Sum of electronic and thermal Free Energies=	-690.886192
H	1.10436700	1.94163300	-0.00002300		
C	-1.17414100	0.41432700	-0.00001500		
H	-0.90165800	1.46444600	-0.00002200		

C	-2.57666900	0.15179200	-0.00000700
C	-3.46379500	1.26289300	-0.00001800
C	-3.13240400	-1.15804900	0.00001500
C	-4.83210800	1.07645000	-0.00000800
H	-3.05197800	2.26567800	-0.00003400
C	-4.49973100	-1.33553400	0.00002500
H	-2.48640700	-2.02645200	0.00002500
C	-5.35451900	-0.22240700	0.00001300
H	-5.49903300	1.92946100	-0.00001700
H	-4.91737200	-2.33462800	0.00004300
H	-6.42800100	-0.37070200	0.00002200
H	-0.42827100	-1.57445000	-0.00001000
C	-0.15940600	-0.52360400	-0.00001500
O	4.43500100	-2.08640700	0.00001700
H	4.03343900	-2.96382300	-0.00022300
O	3.54674200	2.57489000	0.00001700
H	4.50955100	2.62942600	0.00003700

Name of compound (2)		Pinosylvin monomethyl ether			
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)		Energies at B3LYP/6-311G(d,p) in gas phase			
C	-3.83232100	-0.38112300	-0.01021800	Zero-point correction=	0.250156 (Hartree/Particle)
C	-3.20603100	-1.61967000	-0.02032100	Thermal correction to Energy=	0.264474
C	-1.81160700	-1.70901900	-0.01358500	Thermal correction to Enthalpy=	0.265418
C	-1.03056300	-0.55083700	0.00261400	Thermal correction to Gibbs Free Energy=	0.208311
C	-1.66375300	0.70937700	0.01456900	Sum of electronic and zero-point Energies=	-730.388250
C	-3.05221400	0.78440700	0.00761500	Sum of electronic and thermal Energies=	-730.373932
H	-4.91250700	-0.28453500	-0.01433100	Sum of electronic and thermal Enthalpies=	-730.372987
H	-1.35345500	-2.69028900	-0.02233900	Sum of electronic and thermal Free Energies=	-730.430095
H	-1.06898300	1.61008900	0.03267800		
C	1.35016800	0.27133100	-0.00893900		
H	1.01659200	1.30548500	-0.03330300		
C	2.80708400	0.11346700	-0.00291800		
C	3.61119800	1.26423600	-0.06347900		
C	3.45542300	-1.13348300	0.06202100		
C	4.99970900	1.17943200	-0.06257100		
H	3.13388300	2.23769100	-0.11310100		
C	4.84097600	-1.21887700	0.06278900		
H	2.87244700	-2.04512800	0.11554700		
C	5.62277600	-0.06398900	0.00019100		
H	5.59456600	2.08479400	-0.11078900		

H	5.31713100	-2.19188400	0.11410800	
H	6.70438800	-0.13575800	0.00165600	
H	0.76112600	-1.74011600	0.02131600	
C	0.42723900	-0.70638800	0.00714400	
O	-3.90371500	-2.79388300	-0.03682300	
H	-4.84694300	-2.60135500	-0.03989900	
C	-3.05307700	3.17764800	0.03694800	
H	-3.81191900	3.95844300	0.04194400	
H	-2.42328600	3.29107300	-0.85236500	
H	-2.43334300	3.26985800	0.93572500	
O	-3.76375400	1.94795300	0.01832100	
Name of radical		2-O3		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	-3.89302400	-0.40700700	-0.00000700	Zero-point correction= 0.236849 (Hartree/Particle)
C	-3.28316000	-1.71504500	-0.00011500	Thermal correction to Energy= 0.251860
C	-1.83526600	-1.77777300	-0.00014200	Thermal correction to Enthalpy= 0.252804
C	-1.05929200	-0.63622900	-0.00005800	Thermal correction to Gibbs Free Energy= 0.191593
C	-1.71081000	0.63260500	0.00006100	Sum of electronic and zero-point Energies= -729.754606
C	-3.11125000	0.73713700	0.00007400	Sum of electronic and thermal Energies= -729.739595
H	-4.97299400	-0.33714500	0.00001500	Sum of electronic and thermal Enthalpies= -729.738651
H	-1.39071600	-2.76594200	-0.00022800	Sum of electronic and thermal Free Energies= -729.799861
H	-1.11016800	1.53028700	0.00016600	
C	1.30340200	0.23314400	-0.00004200	
H	0.95199000	1.26168200	-0.00006300	
C	2.76308900	0.10548600	-0.00001100	
C	3.54128300	1.27517800	-0.00035500	
C	3.43585000	-1.12984200	0.00038600	
C	4.93115000	1.21968400	-0.00034800	
H	3.04352900	2.23963000	-0.00065500	
C	4.82278100	-1.18573400	0.00038700	
H	2.87247300	-2.05524900	0.00076300	
C	5.57926900	-0.01241000	0.00001500	
H	5.50715800	2.13823000	-0.00063000	
H	5.31972700	-2.14945000	0.00071100	
H	6.66207600	-0.06146200	0.00002600	
H	0.75106900	-1.79115300	-0.00015500	
C	0.40042200	-0.76341900	-0.00007900	
O	-3.97953500	-2.75685200	-0.00018400	
C	-3.04028800	3.13651000	0.00016600	
H	-3.78193800	3.93309600	0.00017200	

H	-2.41525100	3.22743300	-0.89514100	
H	-2.41523200	3.22744200	0.89545800	
O	-3.78129700	1.92296300	0.00018100	
Name of anion			2-O3	
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	-3.86118100	-0.46418800	0.00004800	Zero-point correction= 0.235743 (Hartree/Particle)
C	-3.25753600	-1.77423000	0.00001700	Thermal correction to Energy= 0.250745
C	-1.80698300	-1.73740100	0.00009800	Thermal correction to Enthalpy= 0.251689
C	-1.06420000	-0.55846600	0.00016600	Thermal correction to Gibbs Free Energy= 0.191333
C	-1.71461100	0.70186600	0.00016700	Sum of electronic and zero-point Energies= -729.836856
C	-3.11155600	0.70587100	0.00011100	Sum of electronic and thermal Energies= -729.821853
H	-4.94396100	-0.39572200	0.00001100	Sum of electronic and thermal Enthalpies= -729.820909
H	-1.29977600	-2.69915400	0.00007900	Sum of electronic and thermal Free Energies= -729.881266
H	-1.14171100	1.61682000	0.00053300	
C	1.31540500	0.30263100	-0.00015400	
H	0.97668700	1.33523900	-0.00057100	
C	2.76646900	0.14088100	-0.00010900	
C	3.58756600	1.28704700	0.00019300	
C	3.42275100	-1.10873800	-0.00035700	
C	4.97522800	1.19693300	0.00028300	
H	3.11453900	2.26436400	0.00037600	
C	4.80807500	-1.19846800	-0.00025700	
H	2.83637400	-2.01986700	-0.00064400	
C	5.60084800	-0.04838200	0.00006800	
H	5.57122500	2.10457000	0.00052400	
H	5.27739900	-2.17759100	-0.00044800	
H	6.68289800	-0.12411400	0.00013600	
H	0.73619100	-1.71320600	0.00055600	
C	0.38893600	-0.68176300	0.00019500	
O	-3.91064800	-2.84852800	-0.00007300	
C	-3.16227500	3.10457000	-0.00044000	
H	-3.92195800	3.88958700	-0.00091800	
H	-2.52928200	3.22141100	-0.89117000	
H	-2.52934700	3.22249300	0.89018900	
O	-3.85821200	1.88180300	0.00022000	
Name of cationic radical				Energies at B3LYP/6-311G(d,p) in gas phase
C	-3.78895800	-0.39867900	0.00010000	Zero-point correction= 0.250384 (Hartree/Particle)
C	-3.16993100	-1.65209000	-0.00026400	Thermal correction to Energy= 0.265577
C	-1.78125000	-1.72024400	-0.00040000	Thermal correction to Enthalpy= 0.266521
C	-1.00207800	-0.53426100	-0.00012800	Thermal correction to Gibbs Free Energy= 0.206210

C	-1.63730400	0.73627300	0.00020500	Sum of electronic and zero-point Energies=	-730.128791
C	-3.01949000	0.79615900	0.00031400	Sum of electronic and thermal Energies=	-730.113599
H	-4.86909600	-0.29928500	0.00028000	Sum of electronic and thermal Enthalpies=	-730.112654
H	-1.30543200	-2.69250100	-0.00067800	Sum of electronic and thermal Free Energies=	-730.172965
H	-1.05146100	1.64200200	0.00036400		
C	1.36435700	0.29695900	-0.00028500		
H	1.02308000	1.32721100	-0.00058600		
C	2.78250400	0.12773100	-0.00007400		
C	3.59564900	1.29312400	-0.00075000		
C	3.42225200	-1.14254800	0.00076900		
C	4.97352600	1.19644900	-0.00067000		
H	3.11985400	2.26724800	-0.00136000		
C	4.79865900	-1.23078300	0.00087900		
H	2.83466600	-2.05139100	0.00139300		
C	5.57960000	-0.06525200	0.00014400		
H	5.58333000	2.09121500	-0.00122700		
H	5.27969500	-2.20098400	0.00156100		
H	6.66041700	-0.14362500	0.00022400		
H	0.75541100	-1.73573200	-0.00010900		
C	0.41566100	-0.70604800	-0.00018100		
O	-3.85074800	-2.81397300	-0.00040900		
H	-4.80351900	-2.66449200	-0.00046000		
C	-3.10785500	3.18962900	0.00011000		
H	-3.90924800	3.92350200	0.00017700		
H	-2.49650200	3.31212800	-0.89840300		
H	-2.49596300	3.31270200	0.89818200		
O	-3.75891300	1.91315900	0.00066200		

Name of compound (3)		Dihyropinosylvin			
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase	
C	-4.00453200	-0.00175700	-0.15301600	Zero-point correction=	0.232301 (Hartree/Particle)
C	-3.31237300	1.20049900	-0.00726300	Thermal correction to Energy=	0.246243
C	-1.94631700	1.20335100	0.27285300	Thermal correction to Enthalpy=	0.247187
C	-1.25636700	-0.00652600	0.41271200	Thermal correction to Gibbs Free Energy=	0.188544
C	-1.94430300	-1.20966200	0.26912900	Sum of electronic and zero-point Energies=	-691.672723
C	-3.31278500	-1.20240300	-0.01264900	Sum of electronic and thermal Energies=	-691.658781
H	-5.06758500	0.02303000	-0.36685300	Sum of electronic and thermal Enthalpies=	-691.657836
H	-1.42015200	2.14661300	0.39150300	Sum of electronic and thermal Free Energies=	-691.716480
H	-1.44024000	-2.16231900	0.37936600		
C	1.07218800	-0.00545500	-0.62492700		

H	0.79984500	0.87120200	-1.22064800	
C	2.56083500	-0.00433100	-0.36055600	
C	3.26712700	1.19658800	-0.23301000	
C	3.26317400	-1.20445800	-0.20527800	
C	4.63269600	1.20064000	0.04217600	
H	2.74241100	2.13896200	-0.35815000	
C	4.62860600	-1.20623600	0.07006300	
H	2.73528600	-2.14763900	-0.30817500	
C	5.31857200	-0.00228000	0.19556200	
H	5.16204200	2.14302400	0.13168200	
H	5.15477900	-2.14801100	0.18160900	
H	6.38202500	-0.00162400	0.40650700	
H	0.50445100	0.87077900	1.27373200	
C	0.23246300	-0.00587100	0.67779000	
O	-4.03670500	2.35072700	-0.14760800	
H	-3.45311400	3.10568000	-0.02079700	
O	-3.92980200	-2.41437800	-0.13746800	
H	-4.86411300	-2.27606900	-0.32368600	
H	0.50278700	-0.88386600	1.27167100	
H	0.79974000	-0.88314500	-1.21866100	
Name of radical				3-O3
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	-4.07720000	-0.01777000	-0.15976900	Zero-point correction= 0.245714 (Hartree/Particle)
C	-3.36739100	1.15298100	-0.02157100	Thermal correction to Energy= 0.259852
C	-1.98309600	1.11478600	0.25731300	Thermal correction to Enthalpy= 0.260796
C	-1.28706800	-0.10478200	0.40646300	Thermal correction to Gibbs Free Energy= 0.202623
C	-1.98780600	-1.28363500	0.27381900	Sum of electronic and zero-point Energies= -692.305922
C	-3.41215500	-1.29331500	-0.01666300	Sum of electronic and thermal Energies= -692.291784
H	-5.13838700	-0.00764900	-0.37142800	Sum of electronic and thermal Enthalpies= -692.290840
H	-1.44141900	2.05094900	0.36950800	Sum of electronic and thermal Free Energies= -692.349013
H	-1.50878100	-2.24960900	0.38542700	
C	1.04002800	0.00386000	-0.62785100	
H	0.75560600	0.91089400	-1.17085700	
C	2.52832900	0.01280800	-0.36055100	
C	3.21860300	1.21537200	-0.17635100	
C	3.24410200	-1.18507200	-0.26012200	
C	4.58357900	1.22311200	0.10191600	
H	2.68341600	2.15654500	-0.25965500	
C	4.60883900	-1.18271200	0.01794100	
H	2.72850400	-2.12888600	-0.40892300	

C	5.28336300	0.02263700	0.20097700	
H	5.10133500	2.16651600	0.23598100	
H	5.14647000	-2.12197200	0.08632600	
H	6.34627200	0.02640200	0.41413400	
H	0.45904900	0.74723800	1.32395300	
C	0.20167400	-0.09331800	0.67161000	
O	-4.03198600	2.33650600	-0.15762900	
H	-3.42010800	3.06926500	-0.03368800	
O	-4.03554900	-2.37231700	-0.13584200	
H	0.48366500	-1.00282800	1.20864500	
H	0.78186900	-0.84009500	-1.27461800	
Name of radical		3-O5		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	-4.07312900	-0.01693800	0.15711600	Zero-point correction= 0.232591 (Hartree/Particle)
C	-3.40738400	-1.29554600	0.01267600	Thermal correction to Energy= 0.246445
C	-1.98258300	-1.27826800	-0.27700100	Thermal correction to Enthalpy= 0.247389
C	-1.28191800	-0.09514800	-0.40878100	Thermal correction to Gibbs Free Energy= 0.188878
C	-1.97581300	1.11976800	-0.25931600	Sum of electronic and zero-point Energies= -691.674933
C	-3.36480000	1.15044500	0.02123900	Sum of electronic and thermal Energies= -691.661079
H	-5.13675100	-0.03115300	0.36960100	Sum of electronic and thermal Enthalpies= -691.660135
H	-1.50136300	-2.24316800	-0.38965600	Sum of electronic and thermal Free Energies= -691.718646
H	-1.46162300	2.06854300	-0.36455100	
C	1.04378300	0.00645300	0.62654000	
H	0.78509700	-0.83963800	1.27049500	
C	2.53229900	0.01540400	0.36053900	
C	3.25034300	-1.18180200	0.26955000	
C	3.22038200	1.21802300	0.16803900	
C	4.61539300	-1.17905200	-0.00733000	
H	2.73623700	-2.12542800	0.42477800	
C	4.58552000	1.22605200	-0.10916200	
H	2.68309100	2.15858200	0.24353400	
C	5.28774200	0.02616200	-0.19869900	
H	5.15483100	-2.11781700	-0.06837400	
H	5.10151200	2.16943900	-0.25000000	
H	6.35083500	0.03039800	-0.41106500	
H	0.48856400	-0.99248900	-1.21511300	
C	0.20691200	-0.08502100	-0.67416900	
O	-4.02739700	-2.37398300	0.12992300	
O	-3.91136200	2.39360700	0.13652800	
H	-4.85327500	2.31156600	0.32179300	

H	0.46373600	0.75888900	-1.32177000	
H	0.75869600	0.91208100	1.17126600	
Name of anion		3-O3		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	-4.04421200	-0.04454000	-0.17257100	Zero-point correction= 0.231116 (Hartree/Particle)
C	-3.35335000	1.13968400	-0.01604100	Thermal correction to Energy= 0.245193
C	-1.98204400	1.17325300	0.28189700	Thermal correction to Enthalpy= 0.246137
C	-1.30621000	-0.05378300	0.42667500	Thermal correction to Gibbs Free Energy= 0.187963
C	-1.98056100	-1.25308600	0.27529800	Sum of electronic and zero-point Energies= -691.749403
C	-3.39798600	-1.33424300	-0.03571100	Sum of electronic and thermal Energies= -691.735326
H	-5.10516900	-0.02463500	-0.40007800	Sum of electronic and thermal Enthalpies= -691.734382
H	-1.46281200	2.12069000	0.41736700	Sum of electronic and thermal Free Energies= -691.792556
H	-1.45775400	-2.20006800	0.39401800	
C	1.02725300	0.00413000	-0.60492300	
H	0.73998300	0.89811000	-1.16637100	
C	2.51643000	0.00826100	-0.35628000	
C	3.22612800	1.20768600	-0.21700900	
C	3.22900000	-1.19002100	-0.21787400	
C	4.59409300	1.21331000	0.04767500	
H	2.69444800	2.14864200	-0.32146500	
C	4.59659300	-1.19179700	0.04670800	
H	2.69908000	-2.13171400	-0.32236300	
C	5.28720600	0.01163400	0.18065200	
H	5.12025700	2.15757900	0.14721100	
H	5.12492300	-2.13480900	0.14565300	
H	6.35286500	0.01270400	0.38454500	
H	0.45681000	0.81180600	1.32171300	
C	0.18493600	-0.04846400	0.69721300	
O	-4.06161700	2.33355100	-0.15800700	
H	-3.42879500	3.04439000	-0.01959200	
O	-4.00531600	-2.42752400	-0.17095700	
H	0.46595000	-0.94658600	1.25797100	
H	0.75203200	-0.85648100	-1.22115600	
Name of anion		3-O5		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	-4.02591200	-0.04024100	0.16623500	Zero-point correction= 0.231402 (Hartree/Particle)
C	-3.38833400	-1.33357300	0.02687500	Thermal correction to Energy= 0.245335
C	-1.97299500	-1.24984100	-0.28317500	Thermal correction to Enthalpy= 0.246280
C	-1.29974500	-0.04703200	-0.43002200	Thermal correction to Gibbs Free Energy= 0.188364
C	-1.96776500	1.18309000	-0.28345800	Sum of electronic and zero-point Energies= -691.751284

C	-3.33413800	1.14847100	0.01426100	Sum of electronic and thermal Energies=	-691.737351
H	-5.09170900	-0.03691600	0.39520400	Sum of electronic and thermal Enthalpies=	-691.736407
H	-1.44887600	-2.19559800	-0.40559700	Sum of electronic and thermal Free Energies=	-691.794322
H	-1.46170600	2.13428500	-0.40744200		
C	1.03232100	0.01594400	0.60255500		
H	0.75584100	-0.83991700	1.22498200		
C	2.52184300	0.01636600	0.35585000		
C	3.23068800	1.21378800	0.19564500		
C	3.23560400	-1.18358600	0.24047700		
C	4.59901800	1.21551100	-0.06698700		
H	2.69780400	2.15587200	0.28150400		
C	4.60369100	-1.18917900	-0.02186500		
H	2.70618400	-2.12365000	0.36122600		
C	5.29346400	0.01216200	-0.17673800		
H	5.12445700	2.15826800	-0.18330700		
H	5.13293700	-2.13344400	-0.10276700		
H	6.35946100	0.01045600	-0.37902800		
H	0.47305000	-0.94721700	-1.25474900		
C	0.19202900	-0.04509400	-0.70032300		
O	-4.00325300	-2.42357100	0.15974600		
O	-3.98094800	2.37604300	0.14843400		
H	-4.90103800	2.17139000	0.34172900		
H	0.46365200	0.81140200	-1.32943300		
H	0.74493300	0.91457100	1.15626700		
Name of cationic radical				Energies at B3LYP/6-311G(d,p) in gas phase	
C	-4.06680200	-0.02469200	-0.15840200	Zero-point correction=	0.245741 (Hartree/Particle)
C	-3.38194700	1.17653400	0.01633300	Thermal correction to Energy=	0.259804
C	-1.96637300	1.20633200	0.30118800	Thermal correction to Enthalpy=	0.260748
C	-1.22974300	0.03577000	0.41431800	Thermal correction to Gibbs Free Energy=	0.201834
C	-1.91961100	-1.17044800	0.23961400	Sum of electronic and zero-point Energies=	-692.021416
C	-3.33713900	-1.19518200	-0.04642200	Sum of electronic and thermal Energies=	-692.007354
H	-5.12881100	-0.01239800	-0.36872400	Sum of electronic and thermal Enthalpies=	-692.006410
H	-1.48474700	2.17044700	0.43472100	Sum of electronic and thermal Free Energies=	-692.065324
H	-1.41626400	-2.12697200	0.32239000		
C	1.08453100	-0.04231100	-0.63523000		
H	0.81321800	0.79236500	-1.28955700		
C	2.57202300	-0.02322800	-0.36232000		
C	3.27336100	1.18601900	-0.33446000		
C	3.26563600	-1.21024600	-0.10712700		
C	4.63729500	1.20995700	-0.05390600		

H	2.75460600	2.11602400	-0.54721600
C	4.62948700	-1.18922200	0.17358000
H	2.74150800	-2.16074500	-0.14090900
C	5.31773800	0.02183400	0.20273400
H	5.16945900	2.15403100	-0.04384500
H	5.15572500	-2.11785000	0.36132000
H	6.37986800	0.03859000	0.41635100
H	0.52474300	0.96491700	1.20862500
C	0.25402200	0.05094500	0.67470900
O	-4.07704000	2.29449100	-0.08672600
H	-3.53792000	3.08721600	0.04999200
O	-3.83681000	-2.41278600	-0.18063500
H	-4.78707600	-2.40644600	-0.37056500
H	0.51837900	-0.78542800	1.32692400
H	0.81325200	-0.95977700	-1.16826800

Name of compound (4)				<i>trans</i> -Resveratrol	
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase	
C	4.51009800	0.14910900	0.00005700	Zero-point correction=	0.226064 (Hartree/Particle)
C	3.96591700	-1.13397600	0.00043100	Thermal correction to Energy=	0.240201
C	2.58514700	-1.31738400	0.00028300	Thermal correction to Enthalpy=	0.241145
C	1.71762200	-0.21105400	-0.00012700	Thermal correction to Gibbs Free Energy=	0.184786
C	2.26706900	1.07784500	-0.00051200	Sum of electronic and zero-point Energies=	-766.346047
C	3.64881400	1.24714000	-0.00043900	Sum of electronic and thermal Energies=	-766.331910
H	5.58800300	0.26823800	0.00013300	Sum of electronic and thermal Enthalpies=	-766.330966
H	2.17432900	-2.32274700	0.00038500	Sum of electronic and thermal Free Energies=	-766.387325
H	1.64652900	1.96365200	-0.00097300		
C	-0.70793400	0.45265900	0.00019000		
H	-0.43243000	1.50407500	0.00071800		
C	-2.15054600	0.21222600	0.00007800		
C	-3.02444800	1.31030900	0.00121300		
C	-2.73224200	-1.07073300	-0.00114700		
C	-4.40530600	1.14862700	0.00119000		
H	-2.61205400	2.31385700	0.00215100		
C	-4.10489700	-1.24579300	-0.00118600		
H	-2.09997400	-1.95060500	-0.00214400		
C	-4.95399500	-0.13359600	-0.00000500		
H	-5.05514600	2.01912800	0.00209600		
H	-4.54467200	-2.23580700	-0.00215100		
H	0.00630000	-1.51977300	-0.00053200		

C	0.27415400	-0.46650700	-0.00020100	
O	4.84598200	-2.17945600	0.00087800	
H	4.35174100	-3.00551100	0.00222600	
O	4.11813100	2.53054700	-0.00086500	
H	5.08054500	2.51548300	-0.00083200	
O	-6.29816800	-0.36807900	-0.00011000	
H	-6.76746200	0.47266400	0.00075700	
Name of radical		4-O3		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	4.58480800	0.19729100	0.01903900	Zero-point correction= 0.212719 (Hartree/Particle)
C	4.04515000	-1.06592700	0.08551400	Thermal correction to Energy= 0.227532
C	2.64532900	-1.24310500	0.05524000	Thermal correction to Enthalpy= 0.228476
C	1.74694200	-0.15238600	-0.03966100	Thermal correction to Gibbs Free Energy= 0.168231
C	2.28618800	1.12347500	-0.11892200	Sum of electronic and zero-point Energies= -765.712387
C	3.71697600	1.34918000	-0.08707400	Sum of electronic and thermal Energies= -765.697574
H	5.65526500	0.35324600	0.04068600	Sum of electronic and thermal Enthalpies= -765.696630
H	2.24153400	-2.25073900	0.11159700	Sum of electronic and thermal Free Energies= -765.756875
H	1.67054000	2.00811200	-0.21816800	
C	-0.68236500	0.46534600	0.03273500	
H	-0.41337600	1.51277200	0.14367000	
C	-2.12174700	0.21459400	0.01331400	
C	-3.00157900	1.28878200	0.21763600	
C	-2.69326200	-1.05446900	-0.20365400	
C	-4.38046000	1.11574100	0.21567200	
H	-2.59530900	2.28096600	0.38356500	
C	-4.06396000	-1.24046400	-0.20826000	
H	-2.05540200	-1.91251700	-0.37955100	
C	-4.91998100	-0.15325300	0.00340700	
H	-5.03600800	1.96636500	0.37776600	
H	-4.49801300	-2.21827200	-0.37795900	
H	0.05639000	-1.49419700	-0.13153300	
C	0.30868100	-0.44001100	-0.05556000	
O	4.89163500	-2.13173500	0.18070200	
H	4.38303700	-2.94794600	0.22344500	
O	4.18167500	2.51129300	-0.15396000	
O	-6.26017900	-0.39830000	-0.01316500	
H	-6.73803400	0.42338500	0.14131600	
Name of radical		4-O5		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	4.57431300	0.12858700	-0.00007200	Zero-point correction= 0.213001 (Hartree/Particle)

C	4.05468600	-1.22411500	-0.00034000	Thermal correction to Energy=	0.227742
C	2.61306900	-1.38464000	-0.00020800	Thermal correction to Enthalpy=	0.228686
C	1.74941900	-0.30005100	0.00012600	Thermal correction to Gibbs Free Energy=	0.168247
C	2.31407400	0.99959500	0.00043300	Sum of electronic and zero-point Energies=	-765.714986
C	3.71170400	1.19879300	0.00030300	Sum of electronic and thermal Energies=	-765.700245
H	5.65229000	0.24887700	-0.00015100	Sum of electronic and thermal Enthalpies=	-765.699301
H	2.24169500	-2.40275700	-0.00041200	Sum of electronic and thermal Free Energies=	-765.759740
H	1.69087400	1.88438500	0.00085500		
C	-0.66231300	0.40697000	-0.00028900		
H	-0.37077100	1.45426000	-0.00087900		
C	-2.10835800	0.19346200	-0.00017700		
C	-2.96094300	1.30807900	-0.00084400		
C	-2.71185600	-1.07945800	0.00060400		
C	-4.34407400	1.17189300	-0.00073200		
H	-2.53047000	2.30401700	-0.00145700		
C	-4.08694100	-1.22903700	0.00071700		
H	-2.09588300	-1.97068800	0.00114600		
C	-4.91553600	-0.10082100	0.00004400		
H	-4.97807800	2.05378400	-0.00125600		
H	-4.54501400	-2.21057900	0.00132400		
H	0.02205000	-1.57984300	0.00067900		
C	0.30269600	-0.53073000	0.00021800		
O	4.81610400	-2.21500100	-0.00067000		
O	4.11724400	2.50101400	0.00061300		
H	5.07996300	2.53482200	0.00053500		
O	-6.26181400	-0.31147800	0.00021000		
H	-6.71857100	0.53627000	-0.00032100		
Name of radical				4-O4'	
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase	
C	-4.43183700	0.15042400	0.00000000	Zero-point correction=	0.213311 (Hartree/Particle)
C	-3.89230900	-1.13665000	0.00000000	Thermal correction to Energy=	0.227976
C	-2.51332300	-1.32268900	0.00000100	Thermal correction to Enthalpy=	0.228920
C	-1.64488700	-0.21325800	0.00000000	Thermal correction to Gibbs Free Energy=	0.169561
C	-2.19105700	1.07947900	0.00000000	Sum of electronic and zero-point Energies=	-765.722549
C	-3.57246300	1.25048800	0.00000100	Sum of electronic and thermal Energies=	-765.707885
H	-5.50967200	0.26983400	0.00000000	Sum of electronic and thermal Enthalpies=	-765.706941
H	-2.10196300	-2.32733900	0.00000300	Sum of electronic and thermal Free Energies=	-765.766300
H	-1.56927700	1.96405200	0.00000000		
C	0.78223600	0.46453800	-0.00000100		
H	0.50163900	1.51383700	-0.00000200		

C	2.19198800	0.21846000	0.00000000	
C	3.08391800	1.33513000	-0.00000200	
C	2.76754400	-1.09308800	0.00000200	
C	4.43818600	1.17662300	-0.00000200	
H	2.65463200	2.33234700	-0.00000300	
C	4.11585500	-1.27686000	0.00000200	
H	2.11492100	-1.95838800	0.00000300	
C	5.04618900	-0.14946500	0.00000000	
H	5.11405000	2.02379100	-0.00000300	
H	4.55640300	-2.26719000	0.00000300	
H	0.06079300	-1.51884700	0.00000200	
C	-0.21250100	-0.46809500	0.00000100	
O	-4.77786100	-2.17366500	-0.00000100	
H	-4.29447100	-3.00632700	-0.00001700	
O	-4.03893000	2.53164700	0.00000100	
H	-5.00162700	2.52358400	0.00000200	
O	6.27545900	-0.31292900	0.00000000	
Name of anion			4-O3	
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	4.55485800	0.16906700	0.00007900	Zero-point correction= 0.211456 (Hartree/Particle)
C	3.99275700	-1.09270000	-0.00019300	Thermal correction to Energy= 0.226519
C	2.60745300	-1.28472900	-0.00023900	Thermal correction to Enthalpy= 0.227463
C	1.76689400	-0.14492900	0.00000100	Thermal correction to Gibbs Free Energy= 0.167272
C	2.32206300	1.13225600	0.00028000	Sum of electronic and zero-point Energies= -765.792922
C	3.74936700	1.37619000	0.00032800	Sum of electronic and thermal Energies= -765.777859
H	5.63465100	0.27681100	0.00011400	Sum of electronic and thermal Enthalpies= -765.776915
H	2.18186700	-2.28572600	-0.00048500	Sum of electronic and thermal Free Energies= -765.837106
H	1.69357000	2.01719000	0.00048100	
C	-0.67477300	0.51456400	0.00005000	
H	-0.41084900	1.56849000	0.00018200	
C	-2.11082200	0.24284000	0.00000500	
C	-3.01783400	1.31783600	0.00012400	
C	-2.67541200	-1.05057700	-0.00015500	
C	-4.39651400	1.12431700	0.00008700	
H	-2.62718500	2.33030700	0.00024900	
C	-4.04699600	-1.25547400	-0.00019300	
H	-2.02383800	-1.91642900	-0.00025000	
C	-4.92044400	-0.16617700	-0.00007100	
H	-5.06499900	1.98255000	0.00018400	
H	-4.46196000	-2.25720900	-0.00031500	

H	0.05714200	-1.44811000	-0.00019700	
C	0.32514900	-0.39175900	-0.00005300	
O	4.85246100	-2.18910400	-0.00042600	
H	4.29870500	-2.97549800	-0.00047900	
O	4.24818200	2.52980300	0.00057000	
O	-6.27476100	-0.42279700	-0.00011400	
H	-6.73862300	0.42006000	-0.00001700	
Name of anion			4-O5	
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	4.54447900	0.06460500	0.00008500	Zero-point correction= 0.211838 (Hartree/Particle)
C	4.03081300	-1.28650200	0.00027000	Thermal correction to Energy= 0.226722
C	2.58256600	-1.34619500	0.00024600	Thermal correction to Enthalpy= 0.227666
C	1.76173500	-0.21718600	0.00006300	Thermal correction to Gibbs Free Energy= 0.167935
C	2.32612900	1.07956200	-0.00011400	Sum of electronic and zero-point Energies= -765.795236
C	3.71514500	1.17827500	-0.00009700	Sum of electronic and thermal Energies= -765.780353
H	5.62785000	0.18277200	0.00009200	Sum of electronic and thermal Enthalpies= -765.779408
H	2.14147000	-2.33980700	0.00038100	Sum of electronic and thermal Free Energies= -765.839140
H	1.72732500	1.98067800	-0.00025600	
C	-0.66694700	0.48487800	-0.00008900	
H	-0.38945600	1.53565100	-0.00024000	
C	-2.10778200	0.23611800	-0.00008000	
C	-2.99922600	1.32359900	-0.00025300	
C	-2.69014000	-1.04939400	0.00009600	
C	-4.38081900	1.14972100	-0.00025300	
H	-2.59495000	2.33087200	-0.00039200	
C	-4.06432500	-1.23471300	0.00009800	
H	-2.05057500	-1.92395500	0.00023400	
C	-4.92252600	-0.13324500	-0.00007700	
H	-5.03741500	2.01714100	-0.00039000	
H	-4.49294800	-2.23061100	0.00023400	
H	0.03745600	-1.49093200	0.00021700	
C	0.31727700	-0.43886000	0.00006600	
O	4.76124700	-2.31029700	0.00043600	
O	4.25351500	2.46169800	-0.00027100	
H	5.20947500	2.35329000	-0.00023400	
O	-6.28025600	-0.37104200	-0.00006700	
H	-6.73255700	0.47804000	-0.00019700	
Name of anion			4-O4'	
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	-4.46934500	0.18138300	0.00001200	Zero-point correction= 0.212096 (Hartree/Particle)

C	-3.93637300	-1.10828000	0.00004500	Thermal correction to Energy=	0.226822
C	-2.56545300	-1.32002800	0.00000900	Thermal correction to Enthalpy=	0.227766
C	-1.65095600	-0.23711700	-0.00002000	Thermal correction to Gibbs Free Energy=	0.169216
C	-2.20007000	1.06628400	-0.00005700	Sum of electronic and zero-point Energies=	-765.808758
C	-3.57339400	1.25574900	-0.00005800	Sum of electronic and thermal Energies=	-765.794032
H	-5.54461300	0.32412800	0.00001700	Sum of electronic and thermal Enthalpies=	-765.793088
H	-2.17972100	-2.33685800	-0.00005300	Sum of electronic and thermal Free Energies=	-765.851638
H	-1.56600500	1.94289800	-0.00011900		
C	0.78235900	0.39788100	0.00002700		
H	0.49629500	1.44959400	0.00010900		
C	2.19481300	0.18663600	0.00000900		
C	3.07785400	1.30316300	0.00016600		
C	2.81469400	-1.09684200	-0.00016400		
C	4.44292800	1.17284100	0.00017000		
H	2.63685200	2.29945500	0.00029300		
C	4.17511600	-1.25147900	-0.00016600		
H	2.18505000	-1.98329800	-0.00031000		
C	5.10001500	-0.12396300	0.00000600		
H	5.09031900	2.04531200	0.00029400		
H	4.62529100	-2.24055000	-0.00030600		
H	0.02220900	-1.57587300	-0.00006700		
C	-0.23323200	-0.51930300	-0.00003100		
O	-4.83390100	-2.15472900	0.00011900		
H	-4.32657700	-2.97248500	0.00057500		
O	-4.03333000	2.55554300	-0.00012300		
H	-4.99468300	2.52924700	-0.00012200		
O	6.34246300	-0.26620300	0.00000400		
Name of cationic radical				Energies at B3LYP/6-311G(d,p) in gas phase	
C	4.45789200	0.16338200	0.00001100	Zero-point correction=	0.227064 (Hartree/Particle)
C	3.93739900	-1.14613600	0.00000000	Thermal correction to Energy=	0.241799
C	2.56647500	-1.34842600	-0.00000500	Thermal correction to Enthalpy=	0.242743
C	1.69036800	-0.23528500	-0.00001200	Thermal correction to Gibbs Free Energy=	0.183660
C	2.22192500	1.07720700	-0.00000700	Sum of electronic and zero-point Energies=	-766.094631
C	3.59833900	1.26871300	0.00000900	Sum of electronic and thermal Energies=	-766.079896
H	5.53552000	0.28572000	0.00001600	Sum of electronic and thermal Enthalpies=	-766.078952
H	2.15997400	-2.35343700	0.00001800	Sum of electronic and thermal Free Energies=	-766.138034
H	1.58986500	1.95373600	-0.00001200		
C	-0.72059900	0.45700900	-0.00001200		
H	-0.43428700	1.50341000	-0.00001700		
C	-2.12029300	0.21138200	-0.00000700		

C	-3.00430500	1.32871300	-0.00001900
C	-2.70074800	-1.09271500	0.00001200
C	-4.36790600	1.16758100	-0.00001300
H	-2.58614200	2.32864300	-0.00003300
C	-4.05846000	-1.26423200	0.00001900
H	-2.06682900	-1.96973500	0.00002300
C	-4.91144400	-0.13469500	0.00000600
H	-5.02585100	2.02993800	-0.00002300
H	-4.50948000	-2.24825800	0.00003400
H	0.00238400	-1.53982800	-0.00000700
C	0.28283600	-0.49170400	-0.00001100
O	4.85119100	-2.13624300	0.00001600
H	4.42591900	-3.00178000	-0.00020500
O	4.04432600	2.54243900	0.00001500
H	5.00792000	2.57441000	0.00003400
O	-6.21938600	-0.37709100	0.00001300
H	-6.73694400	0.43958300	0.00000400

Name of compound (5)		Astringin		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
O	-0.72741600	3.32295100	1.05886200	Zero-point correction= 0.403425 (Hartree/Particle)
C	-0.36772200	2.18436500	0.39683200	Thermal correction to Energy= 0.431154
C	0.95228700	1.75423200	0.31748600	Thermal correction to Enthalpy= 0.432098
C	-1.40309600	1.46968000	-0.21542600	Thermal correction to Gibbs Free Energy= 0.342785
C	1.27489200	0.58046500	-0.38536700	Sum of electronic and zero-point Energies= -1452.328102
H	1.73040300	2.34509200	0.78863700	Sum of electronic and thermal Energies= -1452.300372
C	-1.08355300	0.30290900	-0.90062200	Sum of electronic and thermal Enthalpies= -1452.299428
H	-2.41570800	1.84096600	-0.17722700	Sum of electronic and thermal Free Energies= -1452.388742
C	0.23629000	-0.14161100	-0.98880300	
H	0.44312800	-1.04260000	-1.55393500	
O	-2.01382700	-0.45886100	-1.58497100	
C	3.74780900	0.56891500	0.06969300	
H	3.64688300	1.42511700	0.73158700	
C	2.64329300	0.07384800	-0.51668500	
H	2.73532200	-0.79933200	-1.15659600	
C	5.12003000	0.07651500	-0.06437000	
C	6.12128700	0.66536100	0.72825200	
C	5.49346000	-0.95032300	-0.94601500	
C	7.44185600	0.24812300	0.65702900	
H	5.87826900	1.46373800	1.42013200	

C	6.81560500	-1.37372600	-1.02320300	
H	4.75749900	-1.41983000	-1.58592100	
C	7.79022200	-0.78267000	-0.22737400	
O	9.12123600	-1.12766000	-0.23077600	
H	9.27846600	-1.83431600	-0.86423200	
C	-3.19112700	-1.35051500	0.38563900	
C	-4.60061300	-1.64956300	0.87962400	
C	-5.47786100	-0.41193700	0.76556500	
C	-5.44913500	0.12256200	-0.67205800	
C	-3.26912500	-0.75779000	-1.03036600	
H	-5.03005600	-2.44228500	0.24908400	
H	-2.72723300	-0.62307800	1.06110700	
H	-5.86775400	-0.63853100	-1.34653700	
H	-3.68465100	-1.50820100	-1.71434200	
H	-5.07487600	0.36334200	1.43273900	
O	-4.09033100	0.40065500	-1.03103500	
H	-7.82072000	0.66390600	-0.00300600	
C	-6.25397200	1.41017200	-0.85401700	
H	-6.02684000	1.82190200	-1.83900300	
H	-5.93592100	2.14590200	-0.09991700	
O	-7.64775600	1.17058700	-0.80747900	
O	-6.82653800	-0.70937100	1.11983500	
H	-6.80081700	-1.15636900	1.97451500	
O	-4.61428600	-2.05494500	2.24316800	
H	-4.02108000	-2.81123300	2.31811600	
O	-2.48114400	-2.58460300	0.40652500	
H	-1.55008500	-2.39886600	0.24424600	
H	0.06096400	3.74670700	1.41353900	
H	7.09399200	-2.16681200	-1.71119600	
O	8.38653500	0.83800200	1.44023400	
H	9.23408200	0.41667100	1.24842000	
Name of radical		5-O3		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
O	-0.61687300	3.01607800	1.40478500	Zero-point correction= 0.390163 (Hartree/Particle)
C	-0.33566700	1.98346700	0.75522500	Thermal correction to Energy= 0.417671
C	1.04010700	1.58455600	0.55529500	Thermal correction to Enthalpy= 0.418615
C	-1.38271800	1.16178400	0.17508000	Thermal correction to Gibbs Free Energy= 0.329070
C	1.37107000	0.44181000	-0.16371400	Sum of electronic and zero-point Energies= -1451.694915
H	1.78883300	2.23605900	0.98715900	Sum of electronic and thermal Energies= -1451.667406
C	-1.04501600	0.03020500	-0.52436200	Sum of electronic and thermal Enthalpies= -1451.666462

H	-2.40133600	1.49832600	0.28372400	Sum of electronic and thermal Free Energies=	-1451.756007
C	0.31375600	-0.32562800	-0.69826900		
H	0.52558300	-1.21970100	-1.27349700		
O	-1.91294500	-0.84208200	-1.14421600		
C	3.85958900	0.51218800	0.14025800		
H	3.75637400	1.34509000	0.83083500		
C	2.74553400	-0.01350400	-0.39910300		
H	2.83150100	-0.86596600	-1.06701700		
C	5.24086200	0.08252000	-0.07989400		
C	6.25610200	0.69042800	0.67982600		
C	5.60784100	-0.90285500	-1.01008600		
C	7.58662700	0.32942600	0.53068700		
H	6.01634700	1.45843100	1.40621300		
C	6.93975900	-1.26934500	-1.16580600		
H	4.85916600	-1.38370900	-1.62646900		
C	7.92919400	-0.66153100	-0.40098800		
O	9.26960500	-0.95213600	-0.47997800		
H	9.42379300	-1.63293400	-1.14196800		
C	-3.52292800	-1.38130500	0.63795300		
C	-5.02341400	-1.43368800	0.90129900		
C	-5.68090400	-0.11514200	0.52032100		
C	-5.34790800	0.23632600	-0.93479000		
C	-3.28180000	-0.92706000	-0.81152900		
H	-5.45597900	-2.23116300	0.27919900		
H	-3.06635900	-0.67038800	1.33543400		
H	-5.75114400	-0.54368300	-1.59647500		
H	-3.65840100	-1.70254600	-1.49029300		
H	-5.28112400	0.67658900	1.16994300		
O	-3.92145500	0.30433700	-1.07310600		
H	-7.70316300	1.14320700	-0.76256100		
C	-5.92472000	1.58099800	-1.38040200		
H	-5.47774800	1.84625100	-2.34006600		
H	-5.64379800	2.35626400	-0.65208300		
O	-7.32450000	1.51181200	-1.57149000		
O	-7.09644400	-0.19448700	0.66010700		
H	-7.27402300	-0.53193700	1.54648400		
O	-5.31698000	-1.67320500	2.27161400		
H	-4.88692500	-2.50060900	2.51570000		
O	-3.02786400	-2.69743000	0.86110900		
H	-2.06823200	-2.67830400	0.78666800		

H	7.21435500	-2.03048600	-1.89030300	
O	8.54517400	0.93419100	1.28335700	
H	9.39832200	0.55270200	1.03991700	
Name of radical		5-O3'		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
O	-0.70499000	3.29042200	1.11803300	Zero-point correction= 0.391763 (Hartree/Particle)
C	-0.32650400	2.15948800	0.45648000	Thermal correction to Energy= 0.418755
C	0.99900900	1.74681300	0.37892400	Thermal correction to Enthalpy= 0.419699
C	-1.35105400	1.43040100	-0.15830200	Thermal correction to Gibbs Free Energy= 0.331471
C	1.33393900	0.57817800	-0.32683200	Sum of electronic and zero-point Energies= -1451.711841
H	1.76891800	2.34454900	0.85432900	Sum of electronic and thermal Energies= -1451.684848
C	-1.01904600	0.26777900	-0.84474200	Sum of electronic and thermal Enthalpies= -1451.683904
H	-2.36772800	1.79027800	-0.12074800	Sum of electronic and thermal Free Energies= -1451.772132
C	0.30775800	-0.15751200	-0.93321700	
H	0.52722700	-1.05598400	-1.49733900	
O	-1.93400300	-0.50838800	-1.52846900	
C	3.80840800	0.60120700	0.12204300	
H	3.70485400	1.46869300	0.76747700	
C	2.70694500	0.08654500	-0.45669000	
H	2.80408600	-0.79073300	-1.08938300	
C	5.18026200	0.11638400	-0.00494000	
C	6.18637200	0.74801700	0.70136800	
C	5.51961200	-0.99887400	-0.84470200	
C	7.54917600	0.31457600	0.61812800	
H	5.97601300	1.59405500	1.34544000	
C	6.81552900	-1.46478200	-0.96809300	
H	4.73866500	-1.49443300	-1.40683800	
C	7.82946200	-0.83122200	-0.25439900	
O	9.09945600	-1.21180600	-0.31286600	
H	9.56326700	-0.58514100	0.28638700	
C	-3.18360000	-1.36700100	0.41208100	
C	-4.61147200	-1.63272300	0.87270500	
C	-5.46213200	-0.38009300	0.72272100	
C	-5.38538400	0.13766900	-0.71903400	
C	-3.21248600	-0.78076700	-1.00864000	
H	-5.03949800	-2.42374200	0.23921000	
H	-2.72055000	-0.64733800	1.09672400	
H	-5.79578400	-0.62418300	-1.39741000	
H	-3.61813200	-1.52951100	-1.70007700	
H	-5.06255300	0.39524400	1.39201500	

O	-4.01168200	0.39034300	-1.04183100	
H	-7.76923700	0.72366700	-0.12779000	
C	-6.16505700	1.43505600	-0.93803400	
H	-5.90099500	1.83387500	-1.91910200	
H	-5.86067400	2.17353600	-0.18097600	
O	-7.56233100	1.21485000	-0.93386300	
O	-6.82462800	-0.64848800	1.04328400	
H	-6.83135700	-1.08511800	1.90368600	
O	-4.66738700	-2.02231900	2.23933200	
H	-4.10172800	-2.79693800	2.33603900	
O	-2.50339700	-2.61696400	0.45568900	
H	-1.56655600	-2.45714200	0.30071700	
H	0.07405100	3.72897300	1.47557800	
H	7.05415100	-2.30620500	-1.60706100	
O	8.52210400	0.82344800	1.22171200	
Name of radical		5-O4'		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
O	-0.67450600	3.27203500	1.10226400	Zero-point correction= 0.391719 (Hartree/Particle)
C	-0.30326400	2.13715800	0.44451900	Thermal correction to Energy= 0.418678
C	1.01854500	1.71545000	0.36609300	Thermal correction to Enthalpy= 0.419622
C	-1.33432900	1.41192900	-0.16547100	Thermal correction to Gibbs Free Energy= 0.331603
C	1.34414800	0.54065500	-0.33793100	Sum of electronic and zero-point Energies= -1451.717372
H	1.79310700	2.30821900	0.83974400	Sum of electronic and thermal Energies= -1451.690413
C	-1.01350200	0.24331900	-0.84870200	Sum of electronic and thermal Enthalpies= -1451.689469
H	-2.34840300	1.77893900	-0.12619100	Sum of electronic and thermal Free Energies= -1451.777489
C	0.30928400	-0.19104000	-0.93946200	
H	0.52175300	-1.09304900	-1.50042400	
O	-1.93584600	-0.52811000	-1.52579000	
C	3.82509700	0.56476100	0.09371200	
H	3.72387200	1.44775400	0.71823200	
C	2.70602000	0.03962500	-0.46934000	
H	2.79737000	-0.85049200	-1.08378300	
C	5.17288600	0.07507900	-0.03279100	
C	6.20442700	0.75122400	0.65589200	
C	5.50890800	-1.07219900	-0.83039400	
C	7.50483300	0.31256500	0.56299900	
H	5.97864600	1.61968200	1.26413300	
C	6.78970100	-1.52422600	-0.93784200	
H	4.72218700	-1.59103500	-1.36369600	
C	7.86883000	-0.85924400	-0.24575300	

O	9.06845100	-1.19502200	-0.27938400	
C	-3.19356300	-1.36879300	0.41758800	
C	-4.62389100	-1.61551600	0.88170200	
C	-5.46016200	-0.35343700	0.72915400	
C	-5.37938600	0.15897800	-0.71422600	
C	-3.21774500	-0.78469600	-1.00411800	
H	-5.06233800	-2.40344400	0.25155700	
H	-2.72024000	-0.65392700	1.10042900	
H	-5.79848900	-0.60028800	-1.39004800	
H	-3.63177000	-1.53018900	-1.69396600	
H	-5.05062200	0.41928100	1.39551100	
O	-4.00285500	0.39532500	-1.03894700	
H	-7.75694800	0.77323000	-0.12392800	
C	-6.14504200	1.46412000	-0.93668100	
H	-5.87679400	1.85741200	-1.91885000	
H	-5.83282600	2.20137900	-0.18159300	
O	-7.54437900	1.25863000	-0.93202400	
O	-6.82508100	-0.60487400	1.05214500	
H	-6.83609600	-1.03882300	1.91386900	
O	-4.68169400	-1.99962800	2.24964900	
H	-4.12904500	-2.78343000	2.34748600	
O	-2.53000600	-2.62741100	0.46215600	
H	-1.59163800	-2.48165200	0.30301200	
H	0.10687100	3.70909700	1.45660100	
H	7.04398900	-2.38811500	-1.54007800	
O	8.51981700	0.90961200	1.19224000	
H	9.30543200	0.38072000	0.93983500	
Name of anion		5-O3		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
O	-0.63192400	3.60119800	1.16057200	Zero-point correction= 0.390221 (Hartree/Particle)
C	-0.35686700	2.50508700	0.38272500	Thermal correction to Energy= 0.416907
C	0.92133000	1.96815100	0.30159600	Thermal correction to Enthalpy= 0.417852
C	-1.43109100	1.95427900	-0.32630300	Thermal correction to Gibbs Free Energy= 0.330989
C	1.19457600	0.84603700	-0.51152200	Sum of electronic and zero-point Energies= -1451.802386
H	1.72272000	2.43440900	0.86559600	Sum of electronic and thermal Energies= -1451.775700
C	-1.16744000	0.84498300	-1.12158500	Sum of electronic and thermal Enthalpies= -1451.774756
H	-2.42013500	2.38414900	-0.26754100	Sum of electronic and thermal Free Energies= -1451.861618
C	0.10526200	0.29365800	-1.22328100	
H	0.26154900	-0.53857400	-1.90110600	
O	-2.17348100	0.25291100	-1.88867100	

C	3.63478900	0.60654800	0.02043700
H	3.55667000	1.43648200	0.72156000
C	2.50641100	0.23992200	-0.64202000
H	2.55492700	-0.59408300	-1.33640400
C	4.96467700	0.04306600	-0.05484300
C	5.96994300	0.59723700	0.78064800
C	5.28676400	-1.02408500	-0.91561900
C	7.29450700	0.11899600	0.79052400
H	5.72198700	1.42122100	1.44469900
C	6.58947200	-1.53208700	-0.94200900
H	4.53368300	-1.45535500	-1.56489700
C	7.55767100	-0.98188500	-0.11886700
O	8.84185000	-1.40104300	-0.07097100
H	9.18428100	-0.76514400	0.61900100
C	-2.81072000	-1.19063600	0.01021300
C	-4.04179700	-1.86044100	0.60295600
C	-5.11954200	-0.82738200	0.88385100
C	-5.42664200	-0.03494400	-0.39375200
C	-3.22442800	-0.39452000	-1.23907000
H	-4.43301400	-2.58642300	-0.12635400
H	-2.39617400	-0.49507500	0.74750400
H	-5.83199600	-0.72548600	-1.14937800
H	-3.64496500	-1.07494200	-1.99128100
H	-4.74363200	-0.12882500	1.64420100
O	-4.22113900	0.56434000	-0.86718900
H	-7.67760700	-0.11589400	0.71397900
C	-6.44875800	1.08080600	-0.17627100
H	-6.48286700	1.69792100	-1.07606400
H	-6.11469100	1.71852600	0.65586400
O	-7.75489000	0.57136900	0.03862700
O	-6.31847600	-1.45374200	1.34839200
H	-6.05855400	-2.04984600	2.06099900
O	-3.74745900	-2.52367000	1.82774500
H	-2.95783800	-3.05369900	1.66331200
O	-1.88151000	-2.22781200	-0.28163900
H	-1.01441700	-1.81659000	-0.39553700
H	0.18629000	3.88662400	1.58009200
H	6.85594200	-2.35359500	-1.60076000
O	8.28817100	0.52363000	1.48884400
Name of anion		5-O3'	

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase	
O	-0.64584800	3.72209700	1.27581900	Zero-point correction=	0.389552 (Hartree/Particle)
C	-0.43262100	2.72066500	0.55546600	Thermal correction to Energy=	0.416845
C	0.86180600	2.07391700	0.46165800	Thermal correction to Enthalpy=	0.417789
C	-1.46920100	2.10008000	-0.25782400	Thermal correction to Gibbs Free Energy=	0.329454
C	1.11140400	0.97088700	-0.34533800	Sum of electronic and zero-point Energies=	-1451.790191
H	1.64767400	2.51555300	1.06569200	Sum of electronic and thermal Energies=	-1451.762899
C	-1.20397200	0.99973700	-1.04071200	Sum of electronic and thermal Enthalpies=	-1451.761955
H	-2.46288800	2.53090700	-0.23890900	Sum of electronic and thermal Free Energies=	-1451.850290
C	0.05836200	0.39557800	-1.10523700		
H	0.24700000	-0.38666100	-1.83251000		
O	-2.21122100	0.41701500	-1.84666100		
C	3.58405200	0.72453300	0.11871300		
H	3.57571800	1.61045000	0.74707600		
C	2.43015700	0.34080300	-0.46113900		
H	2.44433500	-0.53877300	-1.10317500		
C	4.88934700	0.07300600	-0.00668100		
C	6.00193100	0.65626100	0.62960500		
C	5.10593600	-1.11534700	-0.72829800		
C	7.26721700	0.09235400	0.55209400		
H	5.88591900	1.57133900	1.19930900		
C	6.37249400	-1.68446400	-0.81013300		
H	4.28021100	-1.60534800	-1.22794500		
C	7.45464900	-1.08791800	-0.17502000		
O	8.75093300	-1.58000500	-0.19826200		
H	8.77043100	-2.39040800	-0.71471500		
C	-2.78948400	-1.03857900	0.06262700		
C	-3.97599700	-1.81476200	0.61067800		
C	-5.15196800	-0.88166200	0.83208600		
C	-5.47748700	-0.14281000	-0.47387800		
C	-3.21321800	-0.31416500	-1.22689500		
H	-4.26918700	-2.58055600	-0.12442800		
H	-2.48413700	-0.28237700	0.79317100		
H	-5.79479200	-0.88439300	-1.22522500		
H	-3.55119100	-1.04962200	-1.97217400		
H	-4.87290400	-0.13959100	1.59198700		
O	-4.31967800	0.55388100	-0.91667700		
H	-7.73862600	-0.40954900	0.56690300		
C	-6.60224200	0.88045800	-0.31409000		
H	-6.66561100	1.47014700	-1.23052300		

H	-6.34896900	1.56511500	0.50839900	
O	-7.86645700	0.26158500	-0.11711800	
O	-6.30823300	-1.61062300	1.26739200	
H	-6.01798300	-2.16165800	2.00384900	
O	-3.66700000	-2.44556300	1.85199500	
H	-2.78142800	-2.81354400	1.73752600	
O	-1.74341600	-1.98097800	-0.14663400	
H	-0.93277100	-1.45677700	-0.27780400	
H	6.52052800	-2.60360800	-1.37194600	
O	8.32578500	0.68818800	1.18391800	
H	9.10276000	0.14313100	1.00918000	
Name of anion		5-O4'		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
O	-0.61531300	3.60499500	1.15642100	Zero-point correction= 0.390682 (Hartree/Particle)
C	-0.34931200	2.50402700	0.37877200	Thermal correction to Energy= 0.417307
C	0.92346100	1.95667300	0.30321100	Thermal correction to Enthalpy= 0.418251
C	-1.42936400	1.96370100	-0.33082500	Thermal correction to Gibbs Free Energy= 0.332020
C	1.19563200	0.82839800	-0.50946500	Sum of electronic and zero-point Energies= -1451.811138
H	1.72455400	2.41833400	0.87190000	Sum of electronic and thermal Energies= -1451.784513
C	-1.17006300	0.85020400	-1.12331100	Sum of electronic and thermal Enthalpies= -1451.783569
H	-2.41461800	2.40223700	-0.27552500	Sum of electronic and thermal Free Energies= -1451.869801
C	0.09547900	0.28551900	-1.22137300	
H	0.24449100	-0.54600000	-1.90200100	
O	-2.18294000	0.26511000	-1.89099300	
C	3.64001700	0.59464600	0.01127200	
H	3.56422200	1.44344100	0.69057500	
C	2.49499900	0.21638800	-0.63776900	
H	2.53587000	-0.63108900	-1.31644800	
C	4.95269300	0.03553000	-0.05685700	
C	5.99487700	0.60520800	0.74254600	
C	5.29483400	-1.06865800	-0.87620500	
C	7.26240900	0.09740400	0.71228300	
H	5.77672100	1.45399200	1.38553400	
C	6.57259000	-1.58823300	-0.91388000	
H	4.52789800	-1.52196000	-1.49702800	
C	7.63043900	-1.03732900	-0.12242000	
O	8.83067000	-1.43506600	-0.08081100	
C	-2.80964000	-1.17057400	0.01712000	
C	-4.03533700	-1.84806100	0.61146800	
C	-5.12162700	-0.82261400	0.88585500	

C	-5.43417300	-0.04050800	-0.39699200	
C	-3.22755200	-0.38706600	-1.23876400	
H	-4.41985900	-2.58098200	-0.11450900	
H	-2.40404500	-0.46453700	0.74937700	
H	-5.83396300	-0.73957900	-1.14796500	
H	-3.64393900	-1.07599100	-1.98589100	
H	-4.75220300	-0.11638000	1.64219500	
O	-4.23443400	0.56597100	-0.87352000	
H	-7.68262300	-0.13437800	0.71195000	
C	-6.46546400	1.06810100	-0.18633400	
H	-6.50570900	1.67849900	-1.09045600	
H	-6.13529600	1.71442300	0.64068000	
O	-7.76756900	0.54995000	0.03450700	
O	-6.31585800	-1.45648300	1.35410500	
H	-6.05016100	-2.04761700	2.06868400	
O	-3.73595400	-2.50383200	1.83952000	
H	-2.93428400	-3.01699200	1.67929900	
O	-1.86871800	-2.20000300	-0.26367400	
H	-1.00805700	-1.77582200	-0.38579700	
H	0.20688500	3.88114800	1.57405700	
H	6.81473700	-2.43472600	-1.54902900	
O	8.29962800	0.59080400	1.44844200	
H	9.02389700	-0.01412300	1.16841700	
Name of cationic radical				Energies at B3LYP/6-311G(d,p) in gas phase
O	-0.72045300	2.78493700	1.64439700	Zero-point correction= 0.403876 (Hartree/Particle)
C	-0.28413600	1.69393400	0.97901200	Thermal correction to Energy= 0.431339
C	1.04929600	1.37170900	0.81008600	Thermal correction to Enthalpy= 0.432283
C	-1.30509800	0.87885600	0.44126500	Thermal correction to Gibbs Free Energy= 0.343849
C	1.39002400	0.20341300	0.08315500	Sum of electronic and zero-point Energies= -1452.076365
H	1.81452900	2.01573300	1.22457700	Sum of electronic and thermal Energies= -1452.048903
C	-0.97720900	-0.28430700	-0.26412400	Sum of electronic and thermal Enthalpies= -1452.047959
H	-2.32852900	1.19936300	0.55336700	Sum of electronic and thermal Free Energies= -1452.136392
C	0.36573700	-0.61526500	-0.44144000	
H	0.60759300	-1.50773400	-1.00432600	
O	-1.85593500	-1.14769700	-0.83181900	
C	3.88128800	0.44919500	0.24411500	
H	3.77285500	1.36313300	0.81847800	
C	2.74100900	-0.20381300	-0.16472400	
H	2.84392600	-1.11795400	-0.73947600	
C	5.22799700	0.05264400	-0.01247300	

C	6.27648900	0.85984000	0.48677300
C	5.56353300	-1.12168600	-0.75407900
C	7.59720800	0.53205300	0.26834300
H	6.05912300	1.75724400	1.05271300
C	6.87764500	-1.45998800	-0.97858800
H	4.78633200	-1.76020400	-1.15045300
C	7.90284000	-0.64595500	-0.47593300
O	9.21265300	-0.88028600	-0.63585700
H	9.38606500	-1.68295200	-1.14468900
C	-3.76962500	-1.48050500	0.68719600
C	-5.28807900	-1.31806700	0.74283000
C	-5.70108800	0.07786900	0.29368800
C	-5.12332800	0.38530800	-1.09294700
C	-3.27577600	-1.05119200	-0.70301200
H	-5.73704900	-2.05162600	0.05806700
H	-3.32237800	-0.84388200	1.46153900
H	-5.52310700	-0.32899500	-1.82481600
H	-3.63438200	-1.77230800	-1.44645900
H	-5.29460200	0.80794600	1.00984900
O	-3.68722300	0.25156200	-1.02461200
H	-7.33939500	1.61820900	-1.26891400
C	-5.43984200	1.79843900	-1.58604700
H	-4.81288300	2.00905700	-2.45451400
H	-5.18367600	2.52466600	-0.79940300
O	-6.78254800	1.91230000	-2.00170000
O	-7.11399300	0.19452100	0.22414400
H	-7.47124800	-0.10565000	1.06915000
O	-5.79159700	-1.49627200	2.05681900
H	-5.61561000	-2.40579600	2.32269300
O	-3.50035000	-2.85150900	0.93652700
H	-2.54927400	-2.97763500	1.01246400
H	0.01923900	3.31072000	1.96962900
H	7.12984300	-2.35156700	-1.54231600
O	8.57674400	1.30985800	0.74885700
H	9.44093400	0.94603400	0.51022800

Name of compound (6)		Isorhapontin		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)			Energies at B3LYP/6-311G(d,p) in gas phase	
C	-3.89490700	-1.83338600	-0.29088200	Zero-point correction= 0.431856 (Hartree/Particle)
C	-5.38709700	-1.75994500	-0.57925300	Thermal correction to Energy= 0.459930

C	-6.06835100	-0.82180000	0.40577800	Thermal correction to Enthalpy=	0.460874
C	-5.38175100	0.55040000	0.39340400	Thermal correction to Gibbs Free Energy=	0.371960
C	-3.30887000	-0.42095500	-0.24840100	Sum of electronic and zero-point Energies=	-1491.616740
H	-5.52860000	-1.36413400	-1.59579000	Sum of electronic and thermal Energies=	-1491.588666
H	-3.73661800	-2.28688000	0.69616000	Sum of electronic and thermal Enthalpies=	-1491.587722
H	-5.49305100	0.99933500	-0.60460000	Sum of electronic and thermal Free Energies=	-1491.676636
H	-3.36668000	0.04792500	-1.24305400		
H	-5.97161900	-1.24718400	1.41473100		
O	-3.99413100	0.36998500	0.70632300		
H	-7.78011400	1.20890400	0.82608100		
C	-5.96693800	1.52229200	1.41935000		
H	-5.31164800	2.39279300	1.48568400		
H	-5.98128400	1.03744500	2.40686600		
O	-7.24662300	1.98736200	1.03405700		
O	-7.44503500	-0.65102000	0.07633300		
H	-7.82045300	-1.53387600	-0.02651000		
O	-6.02011200	-3.02880500	-0.46085600		
H	-5.56106200	-3.63207100	-1.05624200		
O	-3.30981900	-2.62335200	-1.31668500		
H	-2.36898500	-2.69798600	-1.12271700		
O	-1.97070500	-0.55767600	0.14216800		
C	-1.07578400	0.46523500	-0.10396400		
C	0.26700400	0.11352200	-0.00729900		
C	-1.46964400	1.76414200	-0.41591900		
C	1.26349600	1.07082800	-0.23700400		
H	0.50809600	-0.90861400	0.25136300		
C	-0.47696100	2.71591100	-0.65388100		
H	-2.50627100	2.06497800	-0.43420300		
C	0.87116200	2.37979400	-0.56684400		
H	1.62854400	3.13621300	-0.75173500		
O	-0.90044400	3.97778200	-0.95996500		
H	-0.13420700	4.54825700	-1.07834200		
C	3.25945300	-0.42503100	0.08254600		
H	2.60791600	-1.28240400	0.22953300		
C	2.69607500	0.77312800	-0.15818400		
H	3.33992000	1.63271700	-0.32527900		
C	4.68312300	-0.74306200	0.16537500		
C	5.07071500	-2.07715800	0.34309000		
C	5.69780000	0.23492400	0.07284400		
C	6.41232500	-2.44359500	0.42015600		

H	4.30802100	-2.84410300	0.41962100	
C	7.03037200	-0.12599300	0.14991700	
H	5.43108800	1.27509700	-0.05321400	
C	7.40154400	-1.47738100	0.32383400	
H	6.70814200	-3.47663400	0.55617500	
O	8.71291500	-1.82029300	0.39920600	
H	9.22707100	-1.00595800	0.31317200	
C	7.86066700	2.11635300	-0.09303700	
H	8.83939600	2.59187900	-0.12473100	
H	7.28600600	2.52175500	0.74641300	
H	7.32961500	2.31372100	-1.03027900	
O	8.10472800	0.72595200	0.07581100	
Name of radical				6-O3
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	-3.91146900	-1.77042600	-0.53062500	Zero-point correction= 0.418854 (Hartree/Particle)
C	-5.42274000	-1.67477400	-0.68822300	Thermal correction to Energy= 0.447528
C	-6.02043700	-0.84749900	0.44062900	Thermal correction to Enthalpy= 0.448472
C	-5.33564300	0.52356600	0.51512900	Thermal correction to Gibbs Free Energy= 0.356129
C	-3.32439200	-0.36546100	-0.38538500	Sum of electronic and zero-point Energies= -1490.985156
H	-5.64465400	-1.17633200	-1.64329000	Sum of electronic and thermal Energies= -1490.956482
H	-3.67646800	-2.32604700	0.38627800	Sum of electronic and thermal Enthalpies= -1490.955538
H	-5.52550400	1.07338000	-0.41809300	Sum of electronic and thermal Free Energies= -1491.047880
H	-3.45306500	0.20018000	-1.32141900	
H	-5.84293800	-1.37427800	1.38900700	
O	-3.92603300	0.31858800	0.69362400	
H	-7.68912800	1.11707400	1.21390400	
C	-5.83144400	1.38026600	1.68134400	
H	-5.17137200	2.24365100	1.78265300	
H	-5.76487200	0.79561800	2.61099900	
O	-7.13705400	1.87341400	1.45231800	
O	-7.41795100	-0.65223800	0.24238400	
H	-7.80373400	-1.52183900	0.08122500	
O	-6.04630800	-2.95239300	-0.65071900	
H	-5.65084000	-3.48403400	-1.35075400	
O	-3.41445700	-2.44219100	-1.67956100	
H	-2.46623900	-2.56293600	-1.56113500	
O	-1.95567300	-0.52930300	-0.11144700	
C	-1.10417400	0.54317700	-0.25497100	
C	0.26026800	0.20442000	-0.15585800	

C	-1.49776800	1.84090600	-0.47561700	
C	1.28196200	1.17748400	-0.29017100	
H	0.49785900	-0.83570600	0.02518600	
C	-0.49213100	2.87468700	-0.64216600	
H	-2.53232100	2.14918600	-0.50568100	
C	0.89915000	2.48573600	-0.54048900	
H	1.63120700	3.27572200	-0.66124100	
O	-0.81959900	4.06116100	-0.85978400	
C	3.23041800	-0.35153700	0.13617900	
H	2.55543800	-1.17749000	0.34521500	
C	2.70414700	0.84601400	-0.18208500	
H	3.36807500	1.68361100	-0.37512000	
C	4.64270900	-0.70313400	0.25387800	
C	4.98637200	-2.00433900	0.64144500	
C	5.68729900	0.21154400	-0.00523400	
C	6.31544100	-2.39818400	0.77436400	
H	4.19948300	-2.72202900	0.84526200	
C	7.00757300	-0.17649800	0.12607200	
H	5.45409800	1.22200200	-0.31099700	
C	7.33469800	-1.49354000	0.51987300	
H	6.57864600	-3.40476300	1.07524400	
O	8.63307900	-1.86374700	0.64468800	
H	9.17431900	-1.09284200	0.42534900	
C	7.91097800	1.96256600	-0.49429900	
H	8.90529200	2.39061700	-0.60726800	
H	7.35753000	2.52237600	0.26673200	
H	7.37975900	2.01768000	-1.45014400	
O	8.10831300	0.61138100	-0.09458700	
Name of radical			6-O4'	
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	-3.86726400	-1.80567400	-0.46292100	Zero-point correction= 0.418994 (Hartree/Particle)
C	-5.36720800	-1.69118300	-0.69509500	Thermal correction to Energy= 0.447665
C	-6.00280500	-0.82627900	0.38340100	Thermal correction to Enthalpy= 0.448609
C	-5.29962700	0.53550000	0.45453200	Thermal correction to Gibbs Free Energy= 0.356498
C	-3.26155000	-0.40727400	-0.32805700	Sum of electronic and zero-point Energies= -1490.991772
H	-5.53525300	-1.21366100	-1.67165300	Sum of electronic and thermal Energies= -1490.963101
H	-3.68463400	-2.33901000	0.47880700	Sum of electronic and thermal Enthalpies= -1490.962157
H	-5.43850300	1.06261300	-0.50076600	Sum of electronic and thermal Free Energies= -1491.054269
H	-3.33977100	0.13506900	-1.28326600	
H	-5.87788700	-1.33089800	1.35195300	

O	-3.90367400	0.31660800	0.70385000
H	-7.67295700	1.18160400	1.02428900
C	-5.83623800	1.42987000	1.57344200
H	-5.16794700	2.28590600	1.68413600
H	-5.82269900	0.86941900	2.52005900
O	-7.12168200	1.93627600	1.27021300
O	-7.38669300	-0.61436000	0.11601000
H	-7.77888100	-1.48185200	-0.04109900
O	-6.01396800	-2.95722800	-0.65599500
H	-5.58965100	-3.51518100	-1.31765200
O	-3.32735100	-2.51655100	-1.56796600
H	-2.38600000	-2.63895700	-1.40397000
O	-1.91249700	-0.58805200	0.01275800
C	-1.01851900	0.44766500	-0.14985600
C	0.32384900	0.08982600	-0.06997700
C	-1.40564200	1.76737000	-0.37285100
C	1.32165200	1.06334100	-0.22373000
H	0.56371800	-0.94982200	0.10547700
C	-0.41242500	2.73523300	-0.54238500
H	-2.44147600	2.07150900	-0.37953300
C	0.93420100	2.39395000	-0.47310700
H	1.69402800	3.15945900	-0.59876800
O	-0.83917300	4.01128300	-0.76412000
H	-0.07750600	4.59542400	-0.83833500
C	3.30640200	-0.43288900	0.18333000
H	2.64608800	-1.26215200	0.41982400
C	2.74450800	0.76286800	-0.14270700
H	3.39652900	1.60440500	-0.35760600
C	4.70570000	-0.74137800	0.26981600
C	5.08123700	-2.06079700	0.67038500
C	5.73347600	0.19777700	-0.02138700
C	6.38765600	-2.43059200	0.78085700
H	4.29341300	-2.77371600	0.89115900
C	7.06031100	-0.14500700	0.07995000
H	5.45815000	1.19648400	-0.33061700
C	7.47561100	-1.50912600	0.49668600
H	6.67823600	-3.42890700	1.08570300
O	8.66427800	-1.82431800	0.58988400
C	7.83841400	2.00559400	-0.58165300
H	8.81467300	2.46446600	-0.72272900

H	7.28361300	2.55376800	0.18732000	
H	7.28198500	2.03104000	-1.52471300	
O	8.09729800	0.66761900	-0.17339200	
Name of anion			6-O3	
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	3.76581300	-1.73391300	0.14574900	Zero-point correction= 0.417964 (Hartree/Particle)
C	5.17898000	-1.76497500	0.69623200	Thermal correction to Energy= 0.446634
C	6.09012100	-0.91094900	-0.16857500	Thermal correction to Enthalpy= 0.447578
C	5.51620200	0.50999900	-0.29502000	Thermal correction to Gibbs Free Energy= 0.354840
C	3.29134800	-0.28424400	0.01155700	Sum of electronic and zero-point Energies= -1491.074335
H	5.16817300	-1.34946600	1.71422100	Sum of electronic and thermal Energies= -1491.045665
H	3.75197800	-2.17739900	-0.85930300	Sum of electronic and thermal Enthalpies= -1491.044721
H	5.49809300	0.97595900	0.70187600	Sum of electronic and thermal Free Energies= -1491.137459
H	3.25226700	0.20839900	0.99409000	
H	6.13465900	-1.35447700	-1.17316700	
O	4.20155500	0.42531700	-0.83786500	
H	7.98797100	0.90082900	-0.35205100	
C	6.33757300	1.40200500	-1.22675200	
H	5.79605300	2.33794200	-1.37303300	
H	6.42313300	0.90683500	-2.20624500	
O	7.60988900	1.72516200	-0.68556300	
O	7.40684800	-0.85007500	0.39177600	
H	7.65533400	-1.75866100	0.59948200	
O	5.72662700	-3.08598100	0.72655700	
H	5.07808800	-3.63623300	1.18034900	
O	2.94103500	-2.47719200	1.03455900	
H	2.02996800	-2.28958700	0.77322600	
O	2.03688700	-0.33169200	-0.56336700	
C	1.07675300	0.64532800	-0.20026900	
C	-0.23987700	0.19682200	-0.24804900	
C	1.43998100	1.92974100	0.15909700	
C	-1.25394600	1.12064500	0.09370500	
H	-0.44950300	-0.81913600	-0.55513800	
C	0.44328200	2.91376500	0.53791500	
H	2.47281600	2.25484800	0.12848400	
C	-0.91721500	2.41880600	0.47407900	
H	-1.69835700	3.12769500	0.73650600	
O	0.73037800	4.08683400	0.87771700	
C	-3.23274800	-0.42609700	-0.20863300	
H	-2.58158500	-1.26106300	-0.45308900	

C	-2.67288300	0.76659200	0.07861000	
H	-3.32742800	1.59428100	0.34607300	
C	-4.66003800	-0.74821000	-0.21741000	
C	-5.07411500	-2.07237900	-0.42463800	
C	-5.66909900	0.22251200	-0.02644200	
C	-6.42239400	-2.42968000	-0.43413700	
H	-4.32249700	-2.83935200	-0.57745500	
C	-7.00667800	-0.13203500	-0.03425000	
H	-5.38685000	1.25571300	0.12021700	
C	-7.40006700	-1.46803400	-0.23809700	
H	-6.73025800	-3.45687200	-0.59323900	
O	-8.72885000	-1.80124700	-0.24555600	
H	-9.21417800	-0.98006300	-0.09261200	
C	-7.78693900	2.10680100	0.35609300	
H	-8.75174300	2.59945700	0.47326100	
H	-7.25705600	2.54293100	-0.49760900	
H	-7.19027200	2.25417600	1.26273600	
O	-8.06976000	0.73240500	0.14147400	
Name of anion		6-O4'		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	-3.68832200	-1.80056000	-0.19288700	Zero-point correction= 0.417796 (Hartree/Particle)
C	-5.11561300	-1.83175800	-0.71125200	Thermal correction to Energy= 0.446335
C	-6.00463200	-0.95566000	0.15522800	Thermal correction to Enthalpy= 0.447279
C	-5.42313300	0.46338000	0.23972200	Thermal correction to Gibbs Free Energy= 0.356238
C	-3.20705600	-0.35188300	-0.08206500	Sum of electronic and zero-point Energies= -1491.077617
H	-5.12412000	-1.43561000	-1.73727900	Sum of electronic and thermal Energies= -1491.049078
H	-3.65400600	-2.23527400	0.81503400	Sum of electronic and thermal Enthalpies= -1491.048134
H	-5.41947800	0.90727700	-0.76728900	Sum of electronic and thermal Free Energies= -1491.139176
H	-3.16449700	0.12100500	-1.07488600	
H	-6.03058000	-1.37905200	1.16902400	
O	-4.09539400	0.38390800	0.75977800	
H	-7.89438600	0.89645300	0.32104600	
C	-6.22394900	1.38194700	1.16380900	
H	-5.66617000	2.31052700	1.29731800	
H	-6.31700400	0.90249700	2.14996300	
O	-7.48763800	1.72148900	0.61732200	
O	-7.32959700	-0.89261300	-0.37914200	
H	-7.59836800	-1.80244700	-0.55413100	
O	-5.66858600	-3.14689600	-0.70025800	
H	-5.04252200	-3.71251500	-1.16688700	

O	-2.89678000	-2.55603400	-1.09897800	
H	-1.98028700	-2.47205000	-0.80911600	
O	-1.94380800	-0.39781400	0.49183300	
C	-1.02998500	0.62422300	0.21053300	
C	0.30217300	0.25035200	0.22989100	
C	-1.44802900	1.92813200	-0.05526600	
C	1.32140000	1.19892400	-0.02886200	
H	0.54021300	-0.78327400	0.44313500	
C	-0.44756100	2.86699600	-0.32530000	
H	-2.48350900	2.22972900	-0.00517400	
C	0.89508100	2.52035100	-0.31659100	
H	1.64448400	3.27940400	-0.52909600	
O	-0.86348800	4.15276300	-0.58832100	
H	-0.07920400	4.69364300	-0.72426500	
C	3.30018100	-0.32386000	0.24995800	
H	2.62500100	-1.13871200	0.50956600	
C	2.72960300	0.89184400	-0.03115800	
H	3.37961100	1.72590000	-0.28225800	
C	4.67313800	-0.69838500	0.25908000	
C	5.03788100	-2.02635400	0.59391400	
C	5.74283900	0.19904100	-0.05697600	
C	6.34524700	-2.44678000	0.61897300	
H	4.24344500	-2.72932500	0.83879200	
C	7.05253600	-0.20142500	-0.03768300	
H	5.49404300	1.22017600	-0.31903000	
C	7.45870700	-1.57809600	0.30763200	
H	6.60269500	-3.46907100	0.87860300	
O	8.65040500	-1.93626700	0.32283500	
C	7.84321600	1.95164300	-0.67276200	
H	8.80792900	2.42455300	-0.86524500	
H	7.33635500	2.48934900	0.14165900	
H	7.21984400	2.02857300	-1.57545500	
O	8.11965800	0.61594100	-0.33277600	
Name of cationic radical				Energies at B3LYP/6-311G(d,p) in gas phase
C	-3.98665100	-1.83812600	-0.51131500	Zero-point correction= 0.432430 (Hartree/Particle)
C	-5.50215100	-1.66866600	-0.56743600	Thermal correction to Energy= 0.461306
C	-5.98009300	-0.76480000	0.56178700	Thermal correction to Enthalpy= 0.462250
C	-5.23154800	0.57177800	0.52779100	Thermal correction to Gibbs Free Energy= 0.370048
C	-3.32633900	-0.45964300	-0.45223800	Sum of electronic and zero-point Energies= -1491.370397
H	-5.76728800	-1.20057400	-1.52682000	Sum of electronic and thermal Energies= -1491.341521

H	-3.71997100	-2.38051800	0.40409600	Sum of electronic and thermal Enthalpies=	-1491.340577
H	-5.45440000	1.08970200	-0.41578300	Sum of electronic and thermal Free Energies=	-1491.432779
H	-3.46622500	0.06383600	-1.41129200		
H	-5.76208000	-1.26071700	1.51859200		
O	-3.81647700	0.30509200	0.61947200		
H	-7.50576100	1.37250700	1.33326500		
C	-5.60824400	1.50567200	1.68010100		
H	-4.88079600	2.31911900	1.72145100		
H	-5.54851500	0.95368300	2.62959900		
O	-6.87582300	2.09115900	1.47672700		
O	-7.37084500	-0.49728500	0.44943100		
H	-7.82283200	-1.34688400	0.37587000		
O	-6.17702800	-2.90729600	-0.42184300		
H	-5.92150800	-3.47201300	-1.15991600		
O	-3.60483200	-2.55848700	-1.67308500		
H	-2.69783200	-2.85993100	-1.56137400		
O	-1.93925700	-0.67466900	-0.23508100		
C	-1.06808000	0.36032800	-0.35951000		
C	0.27873300	0.03755000	-0.23504100		
C	-1.45237000	1.68540200	-0.59335800		
C	1.26553000	1.04267800	-0.35809800		
H	0.53435200	-0.99477200	-0.04276700		
C	-0.47318900	2.68846300	-0.72968300		
H	-2.49058200	1.97766100	-0.64216600		
C	0.87219400	2.37723900	-0.61591200		
H	1.62500700	3.15175700	-0.71256900		
O	-0.94474200	3.93143300	-0.96161300		
H	-0.22369300	4.56803400	-1.02616700		
C	3.23917500	-0.45262800	0.05354600		
H	2.58378400	-1.30432600	0.19903700		
C	2.66624800	0.76687300	-0.22939700		
H	3.31727800	1.62481500	-0.36522900		
C	4.62832400	-0.73355100	0.19056900		
C	5.00277100	-2.07280700	0.50933800		
C	5.65405300	0.24077200	0.03021800		
C	6.31842300	-2.43704800	0.66522400		
H	4.22467100	-2.81639200	0.63224400		
C	6.97156800	-0.11451500	0.18340100		
H	5.39954100	1.26180900	-0.21395900		
C	7.31997500	-1.46986800	0.50622200		

H	6.61084000	-3.45032600	0.90831200
O	8.59093600	-1.80665800	0.65368500
H	9.14885400	-1.02346900	0.51081200
C	7.88934300	2.06875800	-0.25044700
H	8.89311800	2.48350100	-0.28449800
H	7.30756700	2.56947600	0.52752700
H	7.40814300	2.18255200	-1.22506700
O	8.05585700	0.67774800	0.06633500

Name of compound (7)		Rhapontin		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)			Energies at B3LYP/6-311G(d,p) in gas phase	
O	-1.19928600	3.44389400	0.86145600	Zero-point correction= 0.431955 (Hartree/Particle)
C	-0.79353900	2.28226200	0.26956600	Thermal correction to Energy= 0.460923
C	0.54316100	1.90195600	0.21371500	Thermal correction to Enthalpy= 0.461868
C	-1.79808400	1.49153800	-0.29859000	Thermal correction to Gibbs Free Energy= 0.369411
C	0.91300900	0.70254500	-0.41877500	Sum of electronic and zero-point Energies= -1491.610790
H	1.29875600	2.55372100	0.63924100	Sum of electronic and thermal Energies= -1491.581821
C	-1.43051400	0.30158200	-0.91715500	Sum of electronic and thermal Enthalpies= -1491.580877
H	-2.82472200	1.82403500	-0.28244000	Sum of electronic and thermal Free Energies= -1491.673333
C	-0.09370600	-0.09292400	-0.98230500	
H	0.15052500	-1.01639200	-1.49360300	
O	-2.32810300	-0.53629400	-1.55463100	
C	3.36354000	0.75168800	0.13590600	
H	3.20348900	1.56559400	0.83846800	
C	2.30159700	0.24477600	-0.51549700	
H	2.44840100	-0.60624000	-1.17487500	
C	4.75577900	0.30985200	0.03281500	
C	5.68780300	0.80557100	0.96351600	
C	5.21346500	-0.57784700	-0.95054400	
C	7.01756100	0.42139000	0.92627700	
H	5.37973300	1.49849200	1.73822200	
C	6.54927500	-0.97055600	-0.99787900	
H	4.53384500	-0.95823800	-1.70253900	
C	7.45489300	-0.47842100	-0.06334900	
O	8.79209900	-0.77527800	0.00625600	
C	-3.48829000	-1.33770700	0.46513700	
C	-4.89020800	-1.65652600	0.96861900	
C	-5.81334800	-0.46468700	0.76478900	
C	-5.79032700	-0.02730500	-0.70551700	
C	-3.57546200	-0.84486400	-0.98812500	

H	-5.28311400	-2.50578900	0.39003800	
H	-3.05789000	-0.54973200	1.09309000	
H	-6.17210100	-0.84800700	-1.33018700	
H	-3.95728900	-1.65454900	-1.62229500	
H	-5.44810800	0.36918600	1.38103600	
O	-4.43966800	0.27886500	-1.07176900	
H	-8.18995600	0.46277100	-0.09606500	
C	-6.64270100	1.21253200	-0.97928300	
H	-6.41970200	1.56833200	-1.98674400	
H	-6.36331100	2.00761600	-0.27156200	
O	-8.02656500	0.92102000	-0.93099500	
O	-7.15321700	-0.79042300	1.12772800	
H	-7.11923800	-1.17747900	2.01089000	
O	-4.90100200	-1.96975100	2.35624100	
H	-4.27922100	-2.69512900	2.48559000	
O	-2.73316000	-2.54003100	0.57414800	
H	-1.80810200	-2.33067600	0.40629000	
H	-0.42881800	3.91870600	1.18984100	
H	6.87617500	-1.65319600	-1.77139600	
O	7.89662600	0.91271500	1.84129200	
H	8.76084000	0.52837000	1.64272800	
C	9.33992200	-1.66973300	-0.95447100	
H	10.39739800	-1.76020400	-0.71259300	
H	8.86644900	-2.65516000	-0.89215700	
H	9.23120600	-1.27447700	-1.96988700	
Name of radical		7-O3		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
O	-1.08867600	3.25145400	1.02077000	Zero-point correction= 0.418661 (Hartree/Particle)
C	-0.76612900	2.16155000	0.49625200	Thermal correction to Energy= 0.447433
C	0.62446000	1.79015100	0.35042400	Thermal correction to Enthalpy= 0.448377
C	-1.77924700	1.24315200	0.00745500	Thermal correction to Gibbs Free Energy= 0.355563
C	0.99962000	0.58400700	-0.22892300	Sum of electronic and zero-point Energies= -1490.977679
H	1.34856300	2.51449900	0.70086100	Sum of electronic and thermal Energies= -1490.948907
C	-1.39684000	0.05238300	-0.55826200	Sum of electronic and thermal Enthalpies= -1490.947963
H	-2.81014400	1.55304500	0.07212300	Sum of electronic and thermal Free Energies= -1491.040777
C	-0.02571300	-0.27373200	-0.68334700	
H	0.22214800	-1.21915300	-1.15223000	
O	-2.23020500	-0.91308900	-1.08006300	
C	3.46906700	0.70872900	0.18247200	
H	3.31685800	1.54242900	0.86319400	

C	2.39116100	0.15099200	-0.39673700
H	2.52331500	-0.71834800	-1.03486300
C	4.86618000	0.30205700	0.02655900
C	5.82566100	0.86137300	0.89089100
C	5.30067400	-0.61379900	-0.94130600
C	7.16218500	0.51002900	0.80586400
H	5.53446100	1.57853300	1.64974700
C	6.64303000	-0.97290800	-1.03717100
H	4.59729000	-1.04364200	-1.64320900
C	7.57700200	-0.41923600	-0.16671300
O	8.92215200	-0.67969600	-0.14788200
C	-3.80475000	-1.31643900	0.76879800
C	-5.29978200	-1.41067600	1.04876100
C	-6.02036200	-0.17553000	0.52887900
C	-5.71047500	0.02456600	-0.95997100
C	-3.59135000	-1.02162700	-0.72550400
H	-5.69545100	-2.29215700	0.52280300
H	-3.38198600	-0.50814700	1.37568900
H	-6.07977200	-0.84331500	-1.52495700
H	-3.93576500	-1.88576900	-1.30733500
H	-5.65560600	0.70231000	1.08112900
O	-4.28927000	0.14188500	-1.11940800
H	-8.10532300	0.83386000	-0.86787400
C	-6.35249400	1.28155300	-1.54875000
H	-5.92295900	1.45723200	-2.53659000
H	-6.10595500	2.14683700	-0.91559200
O	-7.74825500	1.12538400	-1.71709200
O	-7.42997000	-0.30427400	0.69050500
H	-7.58702500	-0.54997800	1.61031200
O	-5.57740200	-1.50944400	2.43961600
H	-5.10448000	-2.28113600	2.77122900
O	-3.24494200	-2.57233000	1.13816700
H	-2.28747100	-2.51470100	1.05608200
H	6.95286100	-1.67817800	-1.79725300
O	8.06825400	1.06053900	1.65721100
H	8.93311300	0.69063500	1.43538500
C	9.45081300	-1.59907300	-1.09645100
H	10.51945600	-1.65480700	-0.89738500
H	9.00524800	-2.59178800	-0.97473800
H	9.28886500	-1.24683200	-2.12043900

Name of radical		7-O3'			
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase	
O	-1.18217000	3.45019200	0.82863800	Zero-point correction=	0.418970 (Hartree/Particle)
C	-0.76041800	2.28044800	0.26753400	Thermal correction to Energy=	0.447744
C	0.57962600	1.90995300	0.23134700	Thermal correction to Enthalpy=	0.448688
C	-1.75391400	1.46685400	-0.28881100	Thermal correction to Gibbs Free Energy=	0.356108
C	0.96142300	0.69930400	-0.37152500	Sum of electronic and zero-point Energies=	-1490.979951
H	1.32572500	2.57503700	0.65251500	Sum of electronic and thermal Energies=	-1490.951178
C	-1.37448100	0.26491300	-0.87578500	Sum of electronic and thermal Enthalpies=	-1490.950234
H	-2.78299300	1.79193600	-0.28687900	Sum of electronic and thermal Free Energies=	-1491.042813
C	-0.03308200	-0.11867300	-0.92247000		
H	0.22242500	-1.05243800	-1.40882100		
O	-2.25712700	-0.59721900	-1.49803200		
C	3.41599900	0.80271300	0.16159200		
H	3.26230000	1.66846200	0.79950800		
C	2.35343000	0.24791600	-0.44855600		
H	2.49893000	-0.63781100	-1.06040400		
C	4.80831400	0.35897400	0.08740300		
C	5.76549000	0.99396900	0.85320300		
C	5.23080400	-0.71251300	-0.75435700		
C	7.16164600	0.62234800	0.85007000		
H	5.50422300	1.81722500	1.50885500		
C	6.55627900	-1.12774000	-0.81250600		
H	4.50745800	-1.22155300	-1.37882500		
C	7.52866200	-0.49766300	-0.03855800		
O	8.82541600	-0.81469800	-0.01693400		
C	-3.47260300	-1.34024800	0.51125300		
C	-4.88876500	-1.63236900	0.99095500		
C	-5.79475300	-0.43703200	0.73662300		
C	-5.73509800	-0.03737800	-0.74324400		
C	-3.52228200	-0.88069200	-0.95465300		
H	-5.27725300	-2.49205000	0.42504700		
H	-3.04701800	-0.54304100	1.13099700		
H	-6.11010200	-0.87003900	-1.35585100		
H	-3.89430200	-1.70282300	-1.57838000		
H	-5.43432400	0.40851200	1.33973000		
O	-4.37296000	0.24726200	-1.08669800		
H	-8.14557800	0.48969300	-0.20429500		
C	-6.56975600	1.20235600	-1.06769700		
H	-6.31888300	1.53190600	-2.07753800		

H	-6.30164900	2.01230600	-0.37256400	
O	-7.95633200	0.92228200	-1.04740000	
O	-7.14537900	-0.73992400	1.07711100	
H	-7.13593500	-1.10369400	1.97073100	
O	-4.93328800	-1.90968600	2.38521200	
H	-4.32835200	-2.64278800	2.54653800	
O	-2.73429900	-2.54825000	0.66373300	
H	-1.80414300	-2.35533900	0.50584700	
H	-0.42079300	3.94203300	1.15337000	
H	6.81936400	-1.94492300	-1.47150900	
O	8.01175400	1.20047300	1.54706100	
C	9.29566400	-1.88319400	-0.83701400	
H	10.36399000	-1.95012300	-0.64474400	
H	8.81337500	-2.82760100	-0.56696500	
H	9.12550600	-1.66981400	-1.89671400	
Name of anion			7-O3	
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
O	-1.13856700	3.86902600	1.03903300	Zero-point correction= 0.418275 (Hartree/Particle)
C	-0.87683100	2.83088800	0.39011100	Thermal correction to Energy= 0.446663
C	0.44526900	2.23675100	0.34617200	Thermal correction to Enthalpy= 0.447608
C	-1.87919100	2.11278600	-0.38519600	Thermal correction to Gibbs Free Energy= 0.355964
C	0.74736600	1.09096600	-0.37929500	Sum of electronic and zero-point Energies= -1491.072138
H	1.20844700	2.75641300	0.91624800	Sum of electronic and thermal Energies= -1491.043750
C	-1.56109400	0.97292800	-1.08793400	Sum of electronic and thermal Enthalpies= -1491.042805
H	-2.88957100	2.50304700	-0.40376400	Sum of electronic and thermal Free Energies= -1491.134449
C	-0.27423100	0.41994700	-1.10234500	
H	-0.04751300	-0.40365300	-1.77054400	
O	-2.53428600	0.29368700	-1.85943800	
C	3.21819900	0.96025100	0.14164300	
H	3.15813800	1.85334400	0.75707400	
C	2.09259000	0.51213100	-0.44760100	
H	2.15407200	-0.39078500	-1.05338400	
C	4.55227900	0.36322200	0.05282100	
C	5.59649200	0.92125100	0.81712500	
C	4.86514600	-0.74083200	-0.75777600	
C	6.88095000	0.40398900	0.78125600	
H	5.40797700	1.77577300	1.45714600	
C	6.15398100	-1.26892100	-0.80036800	
H	4.09900200	-1.19553200	-1.37269900	
C	7.16661500	-0.70274300	-0.03349100	

O	8.48528500	-1.12007900	0.02000600	
C	-3.08371700	-1.03921600	0.14618200	
C	-4.24620800	-1.82241900	0.73376000	
C	-5.46529900	-0.92863700	0.86524400	
C	-5.79760500	-0.30645600	-0.49820400	
C	-3.51437300	-0.43241500	-1.20041500	
H	-4.49206800	-2.65430100	0.05510500	
H	-2.82307500	-0.21815600	0.82198500	
H	-6.06644300	-1.11638500	-1.19611200	
H	-3.80751000	-1.23599700	-1.89255300	
H	-5.23250100	-0.11952800	1.57041300	
O	-4.66285200	0.40671400	-0.97349900	
H	-8.06310000	-0.59495200	0.52603400	
C	-6.97006500	0.67275800	-0.43841800	
H	-7.04280400	1.18341500	-1.40049400	
H	-6.76460300	1.43293600	0.32939600	
O	-8.20843900	0.01311100	-0.21139400	
O	-6.59635800	-1.67370300	1.33805600	
H	-6.29501200	-2.15406600	2.11825100	
O	-3.93433100	-2.34315600	2.02452400	
H	-3.03257600	-2.68133900	1.95234300	
O	-1.99616000	-1.94942100	0.02386700	
H	-1.20547500	-1.40386500	-0.13779500	
H	6.35803600	-2.11999200	-1.43832600	
O	7.87173700	0.96846600	1.53716300	
H	8.67421000	0.46018800	1.36285400	
C	8.86254800	-2.22971000	-0.77402000	
H	9.92348500	-2.39338000	-0.58599300	
H	8.30263500	-3.13041500	-0.49599600	
H	8.71107800	-2.02903300	-1.84124000	
Name of anion		7-O3'		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
O	-1.12991700	3.73328800	0.93625800	Zero-point correction= 0.417450 (Hartree/Particle)
C	-0.80172400	2.60190000	0.23402700	Thermal correction to Energy= 0.445965
C	0.49741200	2.11147100	0.20141500	Thermal correction to Enthalpy= 0.446909
C	-1.84311400	1.96463600	-0.45067000	Thermal correction to Gibbs Free Energy= 0.355902
C	0.82335600	0.95200100	-0.53417500	Sum of electronic and zero-point Energies= -1491.060223
H	1.27326900	2.64352800	0.74223400	Sum of electronic and thermal Energies= -1491.031707
C	-1.52661000	0.81867700	-1.17045000	Sum of electronic and thermal Enthalpies= -1491.030763
H	-2.84912900	2.35697200	-0.42952800	Sum of electronic and thermal Free Energies= -1491.121770

C	-0.23145700	0.31352000	-1.22291200
H	-0.03280700	-0.55312800	-1.84412500
O	-2.49856200	0.14037200	-1.90918600
C	3.25957900	0.83671000	0.05190800
H	3.14188300	1.70021200	0.70490900
C	2.16196900	0.39049000	-0.60775000
H	2.25725400	-0.47921700	-1.25171200
C	4.61189100	0.31340600	0.02806700
C	5.57389200	0.94168500	0.84119900
C	4.98980900	-0.78706400	-0.76352500
C	6.94865000	0.54633200	0.94134700
H	5.28541400	1.79267700	1.45376100
C	6.31788400	-1.22555500	-0.71620900
H	4.28015700	-1.29234400	-1.40746300
C	7.26391200	-0.60376100	0.09038700
O	8.58067600	-1.00203200	0.16778800
C	-3.09834300	-1.22028700	0.06088800
C	-4.30979600	-1.89658800	0.68547100
C	-5.41905100	-0.88333800	0.91055100
C	-5.74829200	-0.17084600	-0.40805000
C	-3.53218600	-0.50537600	-1.23007200
H	-4.67680900	-2.67067300	-0.00582700
H	-2.70891600	-0.47425700	0.76161700
H	-6.13166400	-0.91300800	-1.12513800
H	-3.92500300	-1.23860200	-1.94675400
H	-5.06579700	-0.13365200	1.63207100
O	-4.56107100	0.43892500	-0.91398900
H	-7.99773500	-0.25761000	0.70440500
C	-6.80303200	0.92452200	-0.24944500
H	-6.85423600	1.49226000	-1.18037900
H	-6.48775900	1.61401500	0.54791100
O	-8.09390100	0.38941900	-0.00727100
O	-6.59900900	-1.52000600	1.40804000
H	-6.32221200	-2.06860100	2.15179300
O	-3.99960500	-2.48591500	1.94357500
H	-3.19297500	-2.99846500	1.80924100
O	-2.13542900	-2.24093200	-0.17455300
H	-1.28090300	-1.80927200	-0.30471400
H	-0.32985400	4.07728000	1.34687900
H	6.60237900	-2.07332400	-1.33104400

O	7.80183300	1.10768800	1.66855800	
C	8.98857400	-2.09482500	-0.61344300	
H	10.05073800	-2.24050100	-0.40629500	
H	8.44643600	-3.01732100	-0.35676100	
H	8.85821600	-1.90967600	-1.69020100	
Name of cationic radical				Energies at B3LYP/6-311G(d,p) in gas phase
C	-3.98669100	-1.83806000	-0.51175700	Zero-point correction= 0.432431 (Hartree/Particle)
C	-5.50220500	-1.66857400	-0.56743800	Thermal correction to Energy= 0.461307
C	-5.97992100	-0.76480100	0.56196200	Thermal correction to Enthalpy= 0.462251
C	-5.23128800	0.57174600	0.52808300	Thermal correction to Gibbs Free Energy= 0.370041
C	-3.32634200	-0.45961400	-0.45255900	Sum of electronic and zero-point Energies= -1491.370395
H	-5.76761200	-1.20041700	-1.52671500	Sum of electronic and thermal Energies= -1491.341520
H	-3.71978000	-2.38064100	0.40347500	Sum of electronic and thermal Enthalpies= -1491.340576
H	-5.45425200	1.08991800	-0.41532500	Sum of electronic and thermal Free Energies= -1491.432785
H	-3.46642300	0.06405600	-1.41148000	
H	-5.76176600	-1.26084600	1.51867200	
O	-3.81622000	0.30490600	0.61941500	
H	-7.50525100	1.37251500	1.33447700	
C	-5.60758700	1.50546900	1.68065400	
H	-4.88007300	2.31886900	1.72188400	
H	-5.54761100	0.95337500	2.63006000	
O	-6.87518300	2.09107700	1.47773800	
O	-7.37068800	-0.49728000	0.44990400	
H	-7.82263100	-1.34690300	0.37632600	
O	-6.17702800	-2.90723000	-0.42176200	
H	-5.92180400	-3.47184400	-1.16001400	
O	-3.60519800	-2.55817600	-1.67378600	
H	-2.69826400	-2.85989300	-1.56228000	
O	-1.93921300	-0.67471100	-0.23574000	
C	-1.06806400	0.36032400	-0.35992000	
C	0.27875100	0.03757400	-0.23537600	
C	-1.45236300	1.68541400	-0.59368500	
C	1.26553100	1.04273000	-0.35830500	
H	0.53438200	-0.99476200	-0.04319500	
C	-0.47319600	2.68850700	-0.72985800	
H	-2.49057400	1.97766200	-0.64258200	
C	0.87218800	2.37730100	-0.61605800	
H	1.62498500	3.15184500	-0.71261000	
O	-0.94476000	3.93148900	-0.96170000	
H	-0.22372200	4.56811900	-1.02610100	

C	3.23912500	-0.45256400	0.05355200
H	2.58370400	-1.30424200	0.19902700
C	2.66624400	0.76693100	-0.22951000
H	3.31729900	1.62484600	-0.36539800
C	4.62824900	-0.73350800	0.19066800
C	5.00267600	-2.07284400	0.50914800
C	5.65400400	0.24085900	0.03078500
C	6.31830300	-2.43713700	0.66515000
H	4.22456200	-2.81646400	0.63174800
C	6.97148600	-0.11451900	0.18401300
H	5.39961900	1.26203900	-0.21297100
C	7.31988600	-1.46991700	0.50654900
H	6.61065600	-3.45048400	0.90802600
O	8.59085600	-1.80668000	0.65406900
H	9.14875700	-1.02342700	0.51146800
C	7.88858000	2.06835700	-0.25172200
H	8.89223800	2.48321300	-0.28767700
H	7.30761000	2.57043700	0.52597600
H	7.40615900	2.18018500	-1.22598700
O	8.05563200	0.67795600	0.06747800

Name of compound (8)				<i>trans</i> -Pterostilbene			
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase			
C	3.81296400	0.07716100	0.00179200	Zero-point correction= 0.282380 (Hartree/Particle)			
C	3.25210200	-1.20367500	0.01219700	Thermal correction to Energy= 0.300268			
C	1.86835900	-1.37393800	0.00578400	Thermal correction to Enthalpy= 0.301212			
C	1.01220900	-0.26518400	-0.00995600	Thermal correction to Gibbs Free Energy= 0.233408			
C	1.57187800	1.02073600	-0.02205000	Sum of electronic and zero-point Energies= -844.908747			
C	2.95277400	1.18465300	-0.01560900	Sum of electronic and thermal Energies= -844.890858			
H	4.88297700	0.21154800	0.00586700	Sum of electronic and thermal Enthalpies= -844.889914			
H	1.47459100	-2.38282100	0.01479700	Sum of electronic and thermal Free Energies= -844.957719			
H	0.95974300	1.91228800	-0.03940500				
C	-1.40755500	0.41953400	0.00717300				
H	-1.12295700	1.46827000	0.03412000				
C	-2.85262800	0.19150300	0.00256900				
C	-3.71746000	1.29482000	0.06525800				
C	-3.44500400	-1.08481000	-0.06328800				
C	-5.09978000	1.14439000	0.06592700				
H	-3.29672300	2.29367600	0.11566400				
C	-4.81921000	-1.24862000	-0.06346600				

H	-2.81989800	-1.96802300	-0.11822800	
C	-5.65902300	-0.13150700	0.00186500	
H	-5.74242000	2.01886000	0.11602400	
H	-5.26697400	-2.23371700	-0.11521000	
H	-0.70906400	-1.55925800	-0.03038400	
C	-0.43409200	-0.50813200	-0.01341300	
O	3.98748200	-2.35414200	0.02893000	
O	3.39210000	2.47864500	-0.02862100	
O	-7.00573800	-0.35470500	-0.00188000	
H	-7.46711000	0.48898000	0.04627900	
C	4.78824000	2.72936100	-0.02525400	
H	5.27674800	2.31065900	-0.91270700	
H	4.89518700	3.81300100	-0.03741100	
H	5.26868300	2.33151200	0.87608300	
C	5.40293600	-2.26035200	0.03901800	
H	5.78093000	-1.75635200	-0.85797300	
H	5.76666100	-1.73670700	0.93063700	
H	5.76862100	-3.28593500	0.05313000	
Name of radical				8-O4'
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	3.73886600	0.07721500	0.00006700	Zero-point correction= 0.269635 (Hartree/Particle)
C	3.18244000	-1.20676900	0.00007100	Thermal correction to Energy= 0.287137
C	1.79944100	-1.37813800	0.00008300	Thermal correction to Enthalpy= 0.288082
C	0.94324900	-0.26597800	0.00007300	Thermal correction to Gibbs Free Energy= 0.221819
C	1.50019100	1.02355000	0.00005100	Sum of electronic and zero-point Energies= -844.285757
C	2.88096000	1.18761500	0.00005200	Sum of electronic and thermal Energies= -844.268254
H	4.80890000	0.21227000	0.00012600	Sum of electronic and thermal Enthalpies= -844.267310
H	1.40483500	-2.38648900	0.00008900	Sum of electronic and thermal Free Energies= -844.333573
H	0.88749800	1.91450800	0.00003900	
C	-1.47844700	0.43171600	-0.00002700	
H	-1.18882500	1.47864200	-0.00011700	
C	-2.89080100	0.19774600	-0.00002300	
C	-3.77324900	1.32168900	-0.00004900	
C	-3.47755600	-1.10864000	0.00000300	
C	-5.12896900	1.17474100	-0.00004800	
H	-3.33548300	2.31525900	-0.00006900	
C	-4.82761800	-1.28074700	0.00000600	
H	-2.83214400	-1.97928200	0.00001900	
C	-5.74830000	-0.14585500	-0.00002100	

H	-5.79759200	2.02768800	-0.00006700	
H	-5.27632300	-2.26743100	0.00002600	
H	-0.77192300	-1.55814800	0.00015900	
C	-0.49220800	-0.50921200	0.00007300	
O	3.91864000	-2.35301200	0.00009400	
O	3.32019600	2.47808400	0.00004800	
O	-6.97935000	-0.29852700	-0.00002200	
C	4.71773300	2.73155000	-0.00006900	
H	5.20117500	2.32452300	-0.89524400	
H	4.82130800	3.81521500	0.00018800	
H	5.20141800	2.32407700	0.89477600	
C	5.33597100	-2.25959400	-0.00023300	
H	5.70534700	-1.74675700	-0.89537200	
H	5.70575200	-1.74627400	0.89446500	
H	5.69995700	-3.28550600	-0.00002600	
Name of anion			8-O4'	
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	3.77264300	0.10064200	0.00000400	Zero-point correction= 0.268332 (Hartree/Particle)
C	3.22579100	-1.19000000	-0.00005400	Thermal correction to Energy= 0.285824
C	1.85397900	-1.39486400	-0.00003500	Thermal correction to Enthalpy= 0.286768
C	0.94695900	-0.31073100	0.00003800	Thermal correction to Gibbs Free Energy= 0.221265
C	1.50238700	0.98997900	0.00009800	Sum of electronic and zero-point Energies= -844.368730
C	2.87457800	1.18013500	0.00008600	Sum of electronic and thermal Energies= -844.351237
H	4.83883800	0.25911800	-0.00001700	Sum of electronic and thermal Enthalpies= -844.350293
H	1.48722300	-2.41463500	-0.00008400	Sum of electronic and thermal Free Energies= -844.415797
H	0.87411700	1.87079000	0.00017000	
C	-1.47908900	0.34736000	-0.00006000	
H	-1.18109000	1.39585400	-0.00019500	
C	-2.89489900	0.15493100	-0.00003500	
C	-3.76197900	1.28353400	-0.00027400	
C	-3.53262700	-1.11950100	0.00022800	
C	-5.12903600	1.17267200	-0.00026200	
H	-3.30695700	2.27360700	-0.00047400	
C	-4.89540000	-1.25464500	0.00024800	
H	-2.91542800	-2.01461800	0.00043000	
C	-5.80438000	-0.11449600	0.00000400	
H	-5.76394700	2.05435200	-0.00044900	
H	-5.35933500	-2.23736400	0.00045600	
H	-0.73814900	-1.63510500	0.00014800	
C	-0.47428200	-0.58089700	0.00005100	

O	3.99865800	-2.33319400	-0.00014400	
O	3.29032100	2.49621000	0.00014100	
O	-7.04906900	-0.23896500	0.00002400	
C	4.67520400	2.76571100	0.00008400	
H	5.17242600	2.36423200	-0.89261000	
H	4.77101800	3.85210900	-0.00002400	
H	5.17247000	2.36439500	0.89283000	
C	5.40277100	-2.19402600	-0.00012000	
H	5.76355000	-1.66636300	-0.89266500	
H	5.76353100	-1.66648900	0.89250800	
H	5.80672600	-3.20711300	-0.00019000	
Name of cationic radical				Energies at B3LYP/6-311G(d,p) in gas phase
C	3.76531500	0.08016100	0.00002300	Zero-point correction= 0.282889 (Hartree/Particle)
C	3.22466900	-1.22253500	0.00001800	Thermal correction to Energy= 0.300643
C	1.84572100	-1.39897400	-0.00001600	Thermal correction to Enthalpy= 0.301587
C	0.98773800	-0.27904300	-0.00003100	Thermal correction to Gibbs Free Energy= 0.235293
C	1.53564600	1.02822200	-0.00003100	Sum of electronic and zero-point Energies= -844.661960
C	2.91387800	1.20191800	0.00002600	Sum of electronic and thermal Energies= -844.644207
H	4.83575800	0.21797100	-0.00003200	Sum of electronic and thermal Enthalpies= -844.643262
H	1.45056500	-2.40640400	-0.00001700	Sum of electronic and thermal Free Energies= -844.709557
H	0.91746000	1.91458200	-0.00006800	
C	-1.41792200	0.43500700	0.00002500	
H	-1.12298500	1.47902400	0.00012700	
C	-2.81914900	0.19751000	0.00000700	
C	-3.69771300	1.31898700	0.00015300	
C	-3.40635500	-1.10363600	-0.00015000	
C	-5.06221400	1.16441600	0.00015300	
H	-3.27444300	2.31675600	0.00027000	
C	-4.76509800	-1.26831500	-0.00015500	
H	-2.77672700	-1.98369200	-0.00027500	
C	-5.61225700	-0.13493700	-0.00000100	
H	-5.71598100	2.02998800	0.00026900	
H	-5.22065100	-2.25025800	-0.00027700	
H	-0.70954100	-1.56843600	-0.00010500	
C	-0.42205400	-0.52224400	-0.00005100	
O	3.96756600	-2.34316000	0.00005500	
O	3.34918900	2.47725000	0.00012800	
O	-6.92231500	-0.37033800	-0.00001400	
H	-7.43432300	0.44966000	0.00009800	
C	4.75364200	2.75013800	-0.00022500	

H	5.23361800	2.35047000	-0.89846100
H	4.83707400	3.83404600	0.00036400
H	5.23432600	2.34935300	0.89715600
C	5.39647800	-2.25654800	0.00012200
H	5.76072400	-1.74884700	-0.89765500
H	5.76064900	-1.74950300	0.89829600
H	5.74702000	-3.28548900	-0.00024900

Name of compound (9)		Rhapontigenin		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)			Energies at B3LYP/6-311G(d,p) in gas phase	
C	-5.24484700	0.13272000	0.00027300	Zero-point correction= 0.281723 (Hartree/Particle)
C	-4.71135900	-1.15476900	0.00786500	Thermal correction to Energy= 0.299933
C	-3.33230200	-1.35000700	0.00721600	Thermal correction to Enthalpy= 0.300877
C	-2.45493200	-0.25129800	-0.00091400	Thermal correction to Gibbs Free Energy= 0.232659
C	-2.99377200	1.04217300	-0.00889800	Sum of electronic and zero-point Energies= -844.928728
C	-4.37396600	1.22320900	-0.00808800	Sum of electronic and thermal Energies= -844.910518
H	-6.32169100	0.26108000	0.00076000	Sum of electronic and thermal Enthalpies= -844.909574
H	-2.93013700	-2.35890900	0.01334200	Sum of electronic and thermal Free Energies= -844.977792
H	-2.36558300	1.92254000	-0.01654000	
C	-0.02372100	0.39186900	-0.00018100	
H	-0.29075000	1.44549000	0.00188000	
C	1.41726600	0.13965000	-0.00089600	
C	2.29942100	1.23695200	0.00856900	
C	1.98859300	-1.13930100	-0.01096600	
C	3.68102100	1.09990500	0.00886000	
H	1.88194300	2.23953900	0.01619500	
C	3.36775500	-1.31274700	-0.01095100	
H	1.35739700	-2.01990500	-0.01970200	
C	4.21643800	-0.20228600	-0.00105600	
H	3.77242200	-2.31601000	-0.01908200	
H	-0.75458100	-1.57439900	-0.00063600	
C	-1.01377800	-0.51887100	-0.00090300	
O	-5.60020300	-2.19319200	0.01573700	
O	-4.83248200	2.51064700	-0.01615900	
O	5.57928200	-0.27623200	-0.00045600	
H	-5.79496800	2.50347800	-0.01508000	
H	-5.11221800	-3.02291100	0.02075800	
C	4.60274100	2.29101500	0.01925600	
H	5.25607600	2.27707500	0.89647900	
H	5.25797000	2.29089200	-0.85665800	

H	4.03399000	3.22235200	0.02600600	
C	6.19464100	-1.55630200	-0.00986900	
H	5.92645800	-2.13766600	0.87928800	
H	5.92827000	-2.12368200	-0.90855400	
H	7.26742100	-1.37021000	-0.00733600	
Name of radical		9-O3		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	-5.32288300	0.17563200	-0.00806300	Zero-point correction= 0.268326 (Hartree/Particle)
C	-4.78986500	-1.08797500	-0.10784100	Thermal correction to Energy= 0.286304
C	-3.39079600	-1.27276000	-0.08923600	Thermal correction to Enthalpy= 0.287249
C	-2.48563500	-0.18977900	0.02828100	Thermal correction to Gibbs Free Energy= 0.218771
C	-3.01853300	1.08681300	0.13847300	Sum of electronic and zero-point Energies= -844.295262
C	-4.44818400	1.32022900	0.12017900	Sum of electronic and thermal Energies= -844.277284
H	-6.39258800	0.33758800	-0.02035500	Sum of electronic and thermal Enthalpies= -844.276340
H	-2.99265600	-2.28093000	-0.17140600	Sum of electronic and thermal Free Energies= -844.344818
H	-2.39825700	1.96659300	0.25081700	
C	-0.05056400	0.41385500	0.00363500	
H	-0.31049300	1.46850700	-0.04094600	
C	1.38698100	0.15068200	0.01285100	
C	2.27590100	1.23547800	-0.11296400	
C	1.94739200	-1.12644500	0.14346200	
C	3.65578400	1.08699000	-0.11875400	
H	1.86515100	2.23589400	-0.21192900	
C	3.32458900	-1.31108300	0.14171300	
H	1.30987000	-1.99535400	0.25577500	
C	4.18109000	-0.21370100	0.01053800	
H	3.72272700	-2.31139400	0.24660500	
H	-0.80501100	-1.54564900	0.04701500	
C	-1.04955100	-0.48692500	0.03198100	
O	-5.64196100	-2.14764200	-0.22411600	
O	-4.90675500	2.48278300	0.21643500	
O	5.54111600	-0.29929100	-0.00031200	
H	-5.13677200	-2.96448800	-0.28878000	
C	4.58645300	2.26287300	-0.25632200	
H	5.25569200	2.33902000	0.60541800	
H	5.22489300	2.15962300	-1.13843200	
H	4.02525500	3.19471000	-0.34252300	
C	6.14976700	-1.57733100	0.12779600	
H	5.89174500	-2.05038100	1.08151200	
H	5.86640100	-2.24070300	-0.69659700	

H	7.22315600	-1.39913700	0.09340100	
Name of radical			9-O5	
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)			Energies at B3LYP/6-311G(d,p) in gas phase	
C	-5.30834800	0.11493700	0.00000000	Zero-point correction= 0.268627 (Hartree/Particle)
C	-4.80221200	-1.24301000	-0.00000200	Thermal correction to Energy= 0.286516
C	-3.36240400	-1.41780100	-0.00000100	Thermal correction to Enthalpy= 0.287461
C	-2.48751800	-0.34216200	-0.00000100	Thermal correction to Gibbs Free Energy= 0.220063
C	-3.03939200	0.96322900	-0.00000100	Sum of electronic and zero-point Energies= -844.297998
C	-4.43498500	1.17633700	0.00000100	Sum of electronic and thermal Energies= -844.280109
H	-6.38507200	0.24600500	0.00000100	Sum of electronic and thermal Enthalpies= -844.279165
H	-3.00116600	-2.43958100	-0.00000100	Sum of electronic and thermal Free Energies= -844.346563
H	-2.40714300	1.84157800	-0.00000600	
C	-0.06865000	0.34094100	0.00000300	
H	-0.34992100	1.39107400	0.00000700	
C	1.37542700	0.11287500	0.00000300	
C	2.23901800	1.22489000	0.00000000	
C	1.96543600	-1.15764100	0.00000600	
C	3.62220700	1.10984900	-0.00000100	
H	1.80584300	2.22083800	-0.00000200	
C	3.34657700	-1.30898000	0.00000500	
H	1.34832000	-2.04807100	0.00001000	
C	4.17766300	-0.18461400	0.00000100	
H	3.76709700	-2.30559500	0.00000700	
H	-0.77291100	-1.63878200	-0.00000400	
C	-1.04339100	-0.58692100	0.00000000	
O	-5.57381800	-2.22609900	-0.00000300	
O	-4.82768900	2.48263700	0.00000200	
O	5.53951500	-0.23719200	0.00000000	
H	-5.79002100	2.52566300	0.00000300	
C	4.52566300	2.31468200	-0.00000400	
H	5.17987000	2.31719800	0.87657900	
H	5.17986900	2.31719500	-0.87658700	
H	3.94312000	3.23744700	-0.00000500	
C	6.17708800	-1.50762100	-0.00000400	
H	5.91937700	-2.08556200	0.89415800	
H	5.91937100	-2.08556100	-0.89416500	
H	7.24623700	-1.30254400	-0.00000700	
Name of anion			9-O3	
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)			Energies at B3LYP/6-311G(d,p) in gas phase	
C	-5.29216200	0.14381600	-0.00003400	Zero-point correction= 0.267153 (Hartree/Particle)

C	-4.73445500	-1.11984900	0.00077400	Thermal correction to Energy=	0.285294
C	-3.34990700	-1.31671500	0.00079400	Thermal correction to Enthalpy=	0.286238
C	-2.50516100	-0.17986600	-0.00002800	Thermal correction to Gibbs Free Energy=	0.218784
C	-3.05578900	1.09920800	-0.00087000	Sum of electronic and zero-point Energies=	-844.374528
C	-4.48233500	1.34813900	-0.00091600	Sum of electronic and thermal Energies=	-844.356387
H	-6.37156000	0.25545900	-0.00003800	Sum of electronic and thermal Enthalpies=	-844.355443
H	-2.92786200	-2.31925300	0.00145000	Sum of electronic and thermal Free Energies=	-844.422898
H	-2.42394400	1.98172500	-0.00158800		
C	-0.05933800	0.46838600	-0.00017700		
H	-0.31635300	1.52397200	-0.00028000		
C	1.37501800	0.18542000	-0.00017700		
C	2.28968900	1.25920000	0.00080100		
C	1.93053400	-1.10394100	-0.00117500		
C	3.66968000	1.09158600	0.00088600		
H	1.89392500	2.27090100	0.00154900		
C	3.30813400	-1.30592900	-0.00110100		
H	1.28120400	-1.97138400	-0.00212900		
C	4.18057900	-0.21713800	-0.00007900		
H	3.68901300	-2.31950500	-0.00191000		
H	-0.80105200	-1.48987100	0.00042700		
C	-1.06440400	-0.43226700	0.00005100		
O	-5.59799900	-2.21344000	0.00156300		
O	-4.97720000	2.50340300	-0.00166800		
O	5.55622200	-0.32095600	0.00002200		
H	-5.04669700	-3.00154900	0.00213700		
C	4.61272700	2.26790200	0.00197700		
H	5.26752800	2.25212200	0.87906700		
H	5.26788900	2.25345700	-0.87486400		
H	4.05751100	3.20792200	0.00258400		
C	6.12612300	-1.61400200	-0.00103200		
H	5.84090600	-2.18646700	0.89067600		
H	5.84104400	-2.18494700	-0.89375700		
H	7.20666700	-1.46833100	-0.00082100		
Name of anion			9-O5		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase	
C	-5.28127800	0.04168300	0.00003500	Zero-point correction=	0.267542 (Hartree/Particle)
C	-4.77386900	-1.31174400	0.00026400	Thermal correction to Energy=	0.285502
C	-3.32606400	-1.37794700	0.00021400	Thermal correction to Enthalpy=	0.286447
C	-2.49986700	-0.25272400	-0.00002800	Thermal correction to Gibbs Free Energy=	0.219554
C	-3.05823300	1.04655700	-0.00025800	Sum of electronic and zero-point Energies=	-844.377049

C	-4.44679300	1.15159900	-0.00021700	Sum of electronic and thermal Energies=	-844.359088
H	-6.36410400	0.16488500	0.00005800	Sum of electronic and thermal Enthalpies=	-844.358144
H	-2.88950300	-2.37359600	0.00038600	Sum of electronic and thermal Free Energies=	-844.425037
H	-2.45495400	1.94468500	-0.00049900		
C	-0.06576500	0.43504600	-0.00001200		
H	-0.33455100	1.48803600	0.00005900		
C	1.37301200	0.17204200	-0.00003600		
C	2.27488100	1.25618200	0.00023100		
C	1.94308800	-1.11088000	-0.00032100		
C	3.65698700	1.10453900	0.00024000		
H	1.86817000	2.26371800	0.00044800		
C	3.32271600	-1.29676300	-0.00031600		
H	1.30360100	-1.98538400	-0.00056600		
C	4.18276400	-0.19806600	-0.00003300		
H	3.71465500	-2.30604700	-0.00054400		
H	-0.78281400	-1.53534500	-0.00003300		
C	-1.05660900	-0.48162700	-0.00003400		
O	-5.50905600	-2.33233100	0.00048100		
O	-4.97944700	2.43739000	-0.00045000		
O	5.55946500	-0.28632300	-0.00000700		
H	-5.93587400	2.33322500	-0.00040000		
C	4.58680800	2.29138300	0.00053500		
H	5.24199700	2.28349400	0.87746800		
H	5.24204600	2.28389100	-0.87636500		
H	4.02115600	3.22529900	0.00073100		
C	6.14344500	-1.57340000	-0.00025800		
H	5.86435300	-2.14823800	0.89175700		
H	5.86445100	-2.14784700	-0.89255600		
H	7.22233500	-1.41594000	-0.00016500		
Name of cationic radical				Energies at B3LYP/6-311G(d,p) in gas phase	
C	-5.19192600	0.14086600	-0.00002400	Zero-point correction=	0.282573 (Hartree/Particle)
C	-4.67810700	-1.16855000	0.00000700	Thermal correction to Energy=	0.300593
C	-3.30706600	-1.37704900	0.00000800	Thermal correction to Enthalpy=	0.301538
C	-2.42547900	-0.26914300	0.00001200	Thermal correction to Gibbs Free Energy=	0.235160
C	-2.94988600	1.04351200	-0.00000100	Sum of electronic and zero-point Energies=	-844.684185
C	-4.32608900	1.24046200	-0.00002600	Sum of electronic and thermal Energies=	-844.666164
H	-6.26877500	0.26968800	-0.00004600	Sum of electronic and thermal Enthalpies=	-844.665220
H	-2.90600300	-2.38443000	-0.00004400	Sum of electronic and thermal Free Energies=	-844.731598
H	-2.31404400	1.91735600	-0.00000500		
C	-0.00842400	0.40642500	0.00002000		

H	-0.28776700	1.45473500	0.00005100
C	1.39054100	0.15277200	0.00000400
C	2.28497900	1.26164200	0.00002800
C	1.95614200	-1.15456200	-0.00003400
C	3.65127700	1.11908700	0.00002300
H	1.86513800	2.26163900	0.00005200
C	3.31596700	-1.33447400	-0.00003900
H	1.31615600	-2.02713500	-0.00006500
C	4.17740300	-0.21137400	-0.00000900
H	3.72506600	-2.33503500	-0.00007000
H	-0.74440000	-1.58451900	0.00002400
C	-1.01676500	-0.53409400	0.00001400
O	-5.59444600	-2.15914500	0.00003100
O	-4.76639300	2.51752100	-0.00005200
O	5.49999100	-0.29287500	-0.00000900
H	-5.72978000	2.55132500	-0.00005600
H	-5.16759500	-3.02355700	0.00030300
C	4.59173100	2.28950500	0.00004900
H	5.24396400	2.26598500	0.87703700
H	5.24396800	2.26602000	-0.87693600
H	4.04144400	3.23007000	0.00006700
C	6.17043300	-1.56935800	-0.00002800
H	5.91533300	-2.13423700	0.89876200
H	5.91536100	-2.13419500	-0.89885200
H	7.23034000	-1.33172200	-0.00000600

Name of compound (10)		Isorhapontigenin		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)			Energies at B3LYP/6-311G(d,p) in gas phase	
C	-5.09185000	0.41898800	0.00001500	Zero-point correction= 0.258875 (Hartree/Particle)
C	-4.71101000	-0.92170800	0.00010900	Thermal correction to Energy= 0.276466
C	-3.36356200	-1.27465100	0.00004100	Thermal correction to Enthalpy= 0.277410
C	-2.36504600	-0.28477200	-0.00002600	Thermal correction to Gibbs Free Energy= 0.211851
C	-2.75069700	1.06244700	-0.00009000	Sum of electronic and zero-point Energies= -880.868436
C	-4.10073700	1.40144500	-0.00010300	Sum of electronic and thermal Energies= -880.850845
H	-6.14656900	0.67149800	0.00000800	Sum of electronic and thermal Enthalpies= -880.849901
H	-3.08010100	-2.32311700	-0.00012700	Sum of electronic and thermal Free Energies= -880.915460
H	-2.02568000	1.86495000	-0.00018200	
C	0.12372500	0.07244300	-0.00003800	
H	-0.02173000	1.14964600	0.00002300	
C	1.52596800	-0.34371000	-0.00006200	

C	2.51895900	0.65836300	0.00003200	
C	1.94437200	-1.68218500	-0.00016000	
C	3.86536200	0.32947400	0.00003500	
H	2.21214300	1.69679400	0.00010700	
C	3.29408400	-2.01421900	-0.00015900	
H	1.21358000	-2.48116500	-0.00023900	
C	4.26483300	-1.01948600	-0.00006000	
H	3.61784300	-3.04810800	-0.00023600	
H	-0.82945000	-1.79604900	-0.00011100	
C	-0.96493300	-0.71790200	-0.00006600	
O	-5.71373700	-1.85026000	0.00025600	
O	-4.40773600	2.73337000	-0.00021900	
O	5.58390200	-1.34562500	-0.00005600	
H	-5.36467500	2.83681100	-0.00024200	
H	-5.32506500	-2.73091100	0.00097000	
H	6.08204700	-0.51701300	0.00002300	
O	4.91595400	1.21494800	0.00013000	
C	4.62932500	2.60747600	0.00024500	
H	4.06723600	2.89608600	-0.89422600	
H	4.06717400	2.89592500	0.89472900	
H	5.59342700	3.11316800	0.00032300	
Name of radical				10-O3
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	-5.16815400	0.46971900	0.00003100	Zero-point correction= 0.245405 (Hartree/Particle)
C	-4.78617300	-0.85124000	0.00000600	Thermal correction to Energy= 0.262795
C	-3.41719100	-1.19492900	-0.00001100	Thermal correction to Enthalpy= 0.263739
C	-2.39082000	-0.21862600	0.00000300	Thermal correction to Gibbs Free Energy= 0.197615
C	-2.77158200	1.11594600	0.00002600	Sum of electronic and zero-point Energies= -880.235065
C	-4.16496700	1.51139900	0.00004000	Sum of electronic and thermal Energies= -880.217675
H	-6.21221400	0.75359400	0.00004300	Sum of electronic and thermal Enthalpies= -880.216731
H	-3.13926600	-2.24581200	-0.00004200	Sum of electronic and thermal Free Energies= -880.282856
H	-2.05330000	1.92545900	0.00003500	
C	0.09874000	0.09610200	0.00000800	
H	-0.03655300	1.17476800	0.00003700	
C	1.49541400	-0.33317900	-0.00000800	
C	2.49697800	0.66066800	0.00000600	
C	1.89958200	-1.67603900	-0.00003700	
C	3.83980100	0.31921000	-0.00000800	
H	2.19998200	1.70187000	0.00002900	
C	3.24553800	-2.02095300	-0.00005100	

H	1.16120200	-2.46804900	-0.00004800	
C	4.22544100	-1.03467300	-0.00003700	
H	3.56000600	-3.05758700	-0.00007300	
H	-0.88056400	-1.76125700	-0.00004100	
C	-0.99951600	-0.68133200	-0.00001100	
O	-5.75646000	-1.81047600	-0.00001300	
O	-4.48422900	2.72355200	0.00006100	
O	5.53926600	-1.37347200	-0.00005100	
H	-5.35023500	-2.68318800	0.00001700	
H	6.04750100	-0.55074000	-0.00003700	
O	4.89864200	1.19224300	0.00000300	
C	4.62819400	2.58901300	0.00003400	
H	4.06986600	2.88343800	-0.89470000	
H	4.06987700	2.88340000	0.89478700	
H	5.59824000	3.08281400	0.00003900	
Name of radical		10-O5		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	-5.15173900	0.40438800	-0.00000900	Zero-point correction= 0.245730 (Hartree/Particle)
C	-4.80534800	-1.00291300	0.00001400	Thermal correction to Energy= 0.263020
C	-3.39500100	-1.34142900	-0.00001100	Thermal correction to Enthalpy= 0.263964
C	-2.40205700	-0.37371100	-0.00004300	Thermal correction to Gibbs Free Energy= 0.198373
C	-2.80047900	0.98658000	-0.00006400	Sum of electronic and zero-point Energies= -880.237419
C	-4.16238400	1.35852000	-0.00004700	Sum of electronic and thermal Energies= -880.220130
H	-6.20626300	0.65856200	0.00000600	Sum of electronic and thermal Enthalpies= -880.219186
H	-3.15389400	-2.39790300	-0.00000900	Sum of electronic and thermal Free Energies= -880.284776
H	-2.07215900	1.78701100	-0.00009900	
C	0.07882200	0.02713900	-0.00002200	
H	-0.08183700	1.10236200	0.00002100	
C	1.48721600	-0.36439500	-0.00002800	
C	2.46282700	0.65479200	0.00004900	
C	1.92567700	-1.69635800	-0.00010300	
C	3.81404300	0.34776100	0.00005300	
H	2.13952400	1.68826600	0.00010600	
C	3.28009000	-2.00650700	-0.00009900	
H	1.20785800	-2.50691000	-0.00016700	
C	4.23444400	-0.99557200	-0.00002100	
H	3.62055300	-3.03486700	-0.00015700	
H	-0.84759300	-1.85869400	-0.00008800	
C	-0.99587800	-0.78304400	-0.00005600	
O	-5.68451800	-1.89061900	0.00005600	

O	-4.40236600	2.70145100	-0.00007100	
O	5.55672000	-1.30049400	-0.00001700	
H	-5.35343700	2.85446700	-0.00006800	
H	6.04362700	-0.46506600	0.00004400	
O	4.85037800	1.24830200	0.00012600	
C	4.54393500	2.63698400	0.00021200	
H	3.97809500	2.91714600	-0.89452500	
H	3.97805700	2.91702600	0.89496300	
H	5.50075100	3.15606600	0.00026700	
Name of radical	10-O4'			
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	-5.02194900	0.42158800	0.00000600	Zero-point correction= 0.246035 (Hartree/Particle)
C	-4.64471100	-0.92155600	-0.00000800	Thermal correction to Energy= 0.263276
C	-3.29873100	-1.27599700	-0.00001100	Thermal correction to Enthalpy= 0.264220
C	-2.29959900	-0.28352500	-0.00000100	Thermal correction to Gibbs Free Energy= 0.199297
C	-2.68259900	1.06612500	0.00001400	Sum of electronic and zero-point Energies= -880.244376
C	-4.03238500	1.40599100	0.00001700	Sum of electronic and thermal Energies= -880.227134
H	-6.07664100	0.67406600	0.00000900	Sum of electronic and thermal Enthalpies= -880.226190
H	-3.01460700	-2.32393400	-0.00002000	Sum of electronic and thermal Free Energies= -880.291113
H	-1.95701000	1.86778500	0.00002200	
C	0.19187100	0.08550700	0.00000000	
H	0.04241700	1.16146000	0.00000900	
C	1.56669400	-0.33139400	-0.00000400	
C	2.57612100	0.66653100	0.00000400	
C	1.96741000	-1.70561500	-0.00001700	
C	3.91501700	0.34227200	0.00000100	
H	2.26256300	1.70315000	0.00001300	
C	3.28177000	-2.05641000	-0.00002000	
H	1.21070700	-2.48067300	-0.00002300	
C	4.35466900	-1.07191700	-0.00001200	
H	3.59600800	-3.09359700	-0.00003000	
H	-0.76876400	-1.79152200	-0.00001400	
C	-0.90771400	-0.71479700	-0.00000500	
O	-5.65050200	-1.84340300	-0.00001800	
O	-4.33772200	2.73585500	0.00003100	
O	5.54885300	-1.38414700	-0.00001500	
H	-5.29424400	2.84442800	0.00003300	
H	-5.27058400	-2.72801200	-0.00003500	
O	4.93034000	1.21963700	0.00000800	
C	4.63451800	2.61193900	0.00002100	

H	4.07108600	2.89679100	-0.89476800	
H	4.07108700	2.89677500	0.89481600	
H	5.59793600	3.11730300	0.00002600	
Name of anion		10-O3		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	-5.13743000	0.44958400	0.00002500	Zero-point correction= 0.244394 (Hartree/Particle)
C	-4.74125400	-0.87369000	0.00000300	Thermal correction to Energy= 0.261932
C	-3.39162800	-1.24099700	-0.00000700	Thermal correction to Enthalpy= 0.262876
C	-2.41236900	-0.21801700	0.00000600	Thermal correction to Gibbs Free Energy= 0.197395
C	-2.80014000	1.11970800	0.00002700	Sum of electronic and zero-point Energies= -880.315426
C	-4.18435200	1.54380800	0.00003500	Sum of electronic and thermal Energies= -880.297889
H	-6.19460000	0.69449300	0.00003600	Sum of electronic and thermal Enthalpies= -880.296945
H	-3.09647000	-2.28797200	-0.00003800	Sum of electronic and thermal Free Energies= -880.362425
H	-2.06475800	1.91808400	0.00003900	
C	0.09088300	0.12845000	-0.00000200	
H	-0.04369300	1.20661300	0.00001300	
C	1.48347200	-0.31562400	-0.00001400	
C	2.50168400	0.66361400	0.00000300	
C	1.89119700	-1.66118500	-0.00004100	
C	3.84298000	0.31082400	-0.00000700	
H	2.21073600	1.70664300	0.00002400	
C	3.23757000	-2.01384100	-0.00005100	
H	1.14728600	-2.44816600	-0.00005500	
C	4.22622700	-1.03854800	-0.00003400	
H	3.54207900	-3.05460200	-0.00007200	
H	-0.88033600	-1.72796300	-0.00002100	
C	-1.01374000	-0.64652600	-0.00000700	
O	-5.73385500	-1.85123800	-0.00000900	
O	-4.53143800	2.75193100	0.00005200	
O	5.55439500	-1.38348200	-0.00004300	
H	-5.28506300	-2.70188200	0.00003300	
H	6.04744500	-0.55301000	-0.00002800	
O	4.90950200	1.19227000	0.00000800	
C	4.62592700	2.58156900	0.00003900	
H	4.06175300	2.87442300	-0.89238500	
H	4.06175700	2.87438400	0.89247900	
H	5.59088700	3.08831500	0.00004800	
Name of anion		10-O5		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	-5.13467600	0.34661200	-0.00003700	Zero-point correction= 0.244730 (Hartree/Particle)

C	-4.80157000	-1.05994300	-0.00006800	Thermal correction to Energy=	0.262111
C	-3.37322200	-1.30825200	-0.00006400	Thermal correction to Enthalpy=	0.263055
C	-2.41220800	-0.29596600	-0.00003500	Thermal correction to Gibbs Free Energy=	0.198045
C	-2.80293900	1.06327100	-0.00000500	Sum of electronic and zero-point Energies=	-880.317556
C	-4.16712400	1.34245800	-0.00000700	Sum of electronic and thermal Energies=	-880.300175
H	-6.19331300	0.60561700	-0.00003800	Sum of electronic and thermal Enthalpies=	-880.299231
H	-3.06468400	-2.35072400	-0.00008700	Sum of electronic and thermal Free Energies=	-880.364241
H	-2.09250800	1.87926000	0.00001800		
C	0.08359700	0.09144100	-0.00000700		
H	-0.06407900	1.16818200	0.00002100		
C	1.48371400	-0.33028600	-0.00000600		
C	2.48740000	0.66356300	0.00004600		
C	1.91054400	-1.66976800	-0.00005400		
C	3.83386800	0.33016400	0.00005100		
H	2.18185200	1.70256500	0.00008300		
C	3.26180400	-2.00268000	-0.00004900		
H	1.17783300	-2.46702600	-0.00009700		
C	4.23648300	-1.01325200	0.00000400		
H	3.58090400	-3.03899000	-0.00008700		
H	-0.86363800	-1.78093200	-0.00006000		
C	-1.00821800	-0.70209300	-0.00003500		
O	-5.65923500	-1.97967000	-0.00009400		
O	-4.53325700	2.68530300	0.00002200		
O	5.56946300	-1.33923500	0.00000900		
H	-5.49519800	2.70234800	0.00001600		
H	6.05090300	-0.50207400	0.00005000		
O	4.88784000	1.22759800	0.00010200		
C	4.58424700	2.61191000	0.00015900		
H	4.01583000	2.89690800	-0.89231600		
H	4.01580300	2.89682900	0.89264300		
H	5.54161200	3.13300000	0.00019600		
Name of anion			10-O4'		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase	
C	-5.04595500	0.44953200	0.00001200	Zero-point correction=	0.244450 (Hartree/Particle)
C	-4.67792800	-0.89675900	-0.00000600	Thermal correction to Energy=	0.261753
C	-3.34437000	-1.27774900	-0.00001200	Thermal correction to Enthalpy=	0.262698
C	-2.30079000	-0.31768400	0.00000000	Thermal correction to Gibbs Free Energy=	0.198529
C	-2.68353900	1.04461000	0.00001900	Sum of electronic and zero-point Energies=	-880.323442
C	-4.02242200	1.40340300	0.00002400	Sum of electronic and thermal Energies=	-880.306139
H	-6.09483600	0.72612200	0.00001600	Sum of electronic and thermal Enthalpies=	-880.305195

H	-3.08872100	-2.33480900	-0.00002600	Sum of electronic and thermal Free Energies= -880.369363
H	-1.94576200	1.83588400	0.00002900	
C	0.19292200	0.00776700	0.00000100	
H	0.03919900	1.08673500	0.00001200	
C	1.56715300	-0.37883400	-0.00000600	
C	2.57900400	0.63256800	0.00000300	
C	2.01882900	-1.72225600	-0.00002100	
C	3.91848400	0.33587100	-0.00000200	
H	2.24681000	1.66610700	0.00001400	
C	3.35529400	-2.03705200	-0.00002600	
H	1.28803200	-2.52644000	-0.00002700	
C	4.41365900	-1.04693400	-0.00001800	
H	3.68584200	-3.07175800	-0.00003700	
H	-0.80957400	-1.85524800	-0.00001900	
C	-0.93084400	-0.77506600	-0.00000600	
O	-5.69904900	-1.82323400	-0.00001800	
O	-4.31716600	2.75064500	0.00004200	
O	5.62733700	-1.33073600	-0.00002300	
H	-5.27436900	2.84350400	0.00004300	
H	-5.29712500	-2.69758900	-0.00003100	
O	4.92732300	1.27876200	0.00000600	
C	4.55054500	2.63135400	0.00002200	
H	3.96272500	2.89929400	-0.89058700	
H	3.96272800	2.89927400	0.89063800	
H	5.47723900	3.20880900	0.00002600	
Name of cationic radical				Energies at B3LYP/6-311G(d,p) in gas phase
C	-5.04718400	0.42285600	-0.00001200	Zero-point correction= 0.259760 (Hartree/Particle)
C	-4.68130000	-0.93414700	0.00000300	Thermal correction to Energy= 0.277093
C	-3.34043400	-1.29161200	0.00000500	Thermal correction to Enthalpy= 0.278037
C	-2.34298800	-0.28782300	0.00000900	Thermal correction to Gibbs Free Energy= 0.213250
C	-2.71867000	1.07342800	0.00000300	Sum of electronic and zero-point Energies= -880.624086
C	-4.06515900	1.41992000	-0.00001100	Sum of electronic and thermal Energies= -880.606753
H	-6.10310200	0.67054700	-0.00002700	Sum of electronic and thermal Enthalpies= -880.605809
H	-3.05223900	-2.33699100	-0.00002500	Sum of electronic and thermal Free Energies= -880.670596
H	-1.99101800	1.87243100	0.00000300	
C	0.13562300	0.10862300	0.00000700	
H	-0.02224100	1.18184600	0.00001500	
C	1.49848800	-0.30653500	-0.00000100	
C	2.50939200	0.69361100	0.00000500	
C	1.89482400	-1.67919200	-0.00001500	

C	3.83973700	0.34478000	0.00000200
H	2.21531500	1.73471900	0.00001400
C	3.21943700	-2.03658700	-0.00001900
H	1.14626900	-2.45948300	-0.00002500
C	4.20958000	-1.04016500	-0.00000900
H	3.53391400	-3.07231100	-0.00003000
H	-0.82133900	-1.78391500	0.00001200
C	-0.97093300	-0.70933300	0.00000800
O	-5.69990500	-1.81950700	0.00001500
O	-4.36299100	2.73806900	-0.00002600
O	5.48653800	-1.38486300	-0.00001300
H	-5.31703300	2.87591000	-0.00002800
H	-5.36918600	-2.72503800	0.00015000
H	6.03599300	-0.58269200	-0.00000500
O	4.90600200	1.16589500	0.00000800
C	4.70551800	2.59021900	0.00002300
H	4.16538400	2.89739800	-0.89866300
H	4.16540000	2.89738000	0.89872500
H	5.70114700	3.02518800	0.00001800

Name of compound (11)		Piceatannol		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	4.81254300	-0.03128000	0.00000500	Zero-point correction= 0.230348 (Hartree/Particle)
C	4.19209200	1.21674200	-0.00001800	Thermal correction to Energy= 0.246669
C	2.80280300	1.31620700	-0.00003500	Thermal correction to Enthalpy= 0.247613
C	2.00383000	0.15950500	-0.00000700	Thermal correction to Gibbs Free Energy= 0.184965
C	2.62972100	-1.09402900	0.00001900	Sum of electronic and zero-point Energies= -841.586014
C	4.01915600	-1.17933600	0.00001600	Sum of electronic and thermal Energies= -841.569693
H	5.89570700	-0.08559200	0.00001200	Sum of electronic and thermal Enthalpies= -841.568749
H	2.33156700	2.29466500	-0.00009700	Sum of electronic and thermal Free Energies= -841.631397
H	2.06376500	-2.01558100	0.00003700	
C	-0.37861800	-0.64628000	-0.00000700	
H	-0.04567300	-1.68068300	-0.00000300	
C	-1.83311100	-0.48644500	-0.00000700	
C	-2.63777300	-1.63488500	-0.00002700	
C	-2.47034700	0.76894600	0.00001600	
C	-4.02820100	-1.54091000	-0.00002700	
H	-2.17183400	-2.61350100	-0.00004400	
C	-3.85005500	0.87099400	0.00001700	
H	-1.90337200	1.69112900	0.00003600	

C	-4.63644700	-0.29516200	-0.00000500	
H	-4.63781000	-2.43973400	-0.00004300	
H	0.21754600	1.36378500	-0.00002500	
C	0.54777300	0.32849900	-0.00001400	
O	5.00729300	2.31339300	-0.00003600	
O	4.56561200	-2.43197400	0.00003600	
O	-5.99510000	-0.08144500	-0.00000200	
H	-6.46141400	-0.92281800	-0.00001500	
H	5.52529900	-2.35817400	0.00002600	
H	4.46384100	3.10797200	0.00021100	
O	-4.44265900	2.09751500	0.00004000	
H	-5.39897800	1.96322100	0.00003800	
Name of radical		11-O3		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	4.89107300	-0.07301800	0.00000600	Zero-point correction= 0.216851 (Hartree/Particle)
C	4.27382100	1.15589800	-0.00003700	Thermal correction to Energy= 0.232989
C	2.86507700	1.24316400	-0.00004400	Thermal correction to Enthalpy= 0.233933
C	2.03583800	0.09524700	0.00000300	Thermal correction to Gibbs Free Energy= 0.169618
C	2.65408600	-1.14718200	0.00004900	Sum of electronic and zero-point Energies= -840.952568
C	4.09604200	-1.28065700	0.00004700	Sum of electronic and thermal Energies= -840.936430
H	5.96949100	-0.16040300	0.00001200	Sum of electronic and thermal Enthalpies= -840.935486
H	2.39925500	2.22522900	-0.00009700	Sum of electronic and thermal Free Energies= -840.999801
H	2.09528500	-2.07393300	0.00009000	
C	-0.35549600	-0.66837800	-0.00000600	
H	-0.03320000	-1.70629500	-0.00001400	
C	-1.80699900	-0.49315400	-0.00000800	
C	-2.62193000	-1.63413600	-0.00006900	
C	-2.43003500	0.76933900	0.00004900	
C	-4.01100800	-1.52595100	-0.00007700	
H	-2.16584900	-2.61727600	-0.00011200	
C	-3.80831700	0.88561700	0.00004100	
H	-1.85380500	1.68579100	0.00010500	
C	-4.60618500	-0.27368300	-0.00002300	
H	-4.62973100	-2.41830300	-0.00012600	
H	0.26870800	1.33513900	-0.00000700	
C	0.58288100	0.29502700	-0.00000200	
O	5.05230900	2.27625400	-0.00009300	
O	4.63190000	-2.41415600	0.00008700	
O	-5.96054100	-0.04578700	-0.00002500	
H	-6.43802200	-0.88106900	-0.00006400	

H	4.49358400	3.06019100	0.00004200	
O	-4.38779500	2.11713400	0.00009700	
H	-5.34579400	1.99457000	0.00008300	
Name of radical		11-O5		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	-4.87836000	-0.00795900	0.00000400	Zero-point correction= 0.217274 (Hartree/Particle)
C	-4.27953200	1.31162700	0.00002700	Thermal correction to Energy= 0.233259
C	-2.83080800	1.38542800	0.00002700	Thermal correction to Enthalpy= 0.234203
C	-2.03319200	0.25149200	0.00000400	Thermal correction to Gibbs Free Energy= 0.171798
C	-2.67407300	-1.01232500	-0.00001900	Sum of electronic and zero-point Energies= -840.954859
C	-4.08131100	-1.12772800	-0.00001800	Sum of electronic and thermal Energies= -840.938875
H	-5.96162100	-0.06404400	0.00000300	Sum of electronic and thermal Enthalpies= -840.937931
H	-2.39961000	2.37958000	0.00004700	Sum of electronic and thermal Free Energies= -841.000335
H	-2.10473500	-1.93262300	-0.00004000	
C	0.33301400	-0.59585300	0.00000000	
H	-0.01543000	-1.62529300	-0.00000200	
C	1.78963100	-0.46325300	0.00000000	
C	2.57133000	-1.62720200	0.00001900	
C	2.44836800	0.78081000	-0.00001900	
C	3.96303800	-1.55926600	0.00002100	
H	2.08720800	-2.59699400	0.00003300	
C	3.82962400	0.85708900	-0.00001700	
H	1.89863900	1.71333700	-0.00003700	
C	4.59388700	-0.32461300	0.00000400	
H	4.55591700	-2.46902100	0.00003700	
H	-0.23278000	1.42675300	0.00001100	
C	-0.57527900	0.39631400	0.00000500	
O	-4.98025200	2.34597700	0.00004600	
O	-4.56387700	-2.40345200	-0.00004100	
O	5.95443200	-0.13568900	0.00000400	
H	6.40764900	-0.98433300	0.00001600	
H	-5.52688500	-2.37933700	-0.00003600	
O	4.44412300	2.07106300	-0.00003500	
H	5.39822600	1.92141000	-0.00003100	
Name of radical		11-O3'		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	-4.76952700	-0.04880100	-0.00244500	Zero-point correction= 0.218588 (Hartree/Particle)
C	-4.16371300	1.20226800	-0.10973900	Thermal correction to Energy= 0.234189
C	-2.77546800	1.31684700	-0.10440700	Thermal correction to Enthalpy= 0.235133
C	-1.96777500	0.17156000	0.00609200	Thermal correction to Gibbs Free Energy= 0.173036

C	-2.57819700	-1.08414900	0.11816100	Sum of electronic and zero-point Energies=	-840.969029
C	-3.96697200	-1.18479600	0.11154400	Sum of electronic and thermal Energies=	-840.953428
H	-5.85206700	-0.11404800	-0.00634900	Sum of electronic and thermal Enthalpies=	-840.952484
H	-2.31281000	2.29535700	-0.19007100	Sum of electronic and thermal Free Energies=	-841.014580
H	-2.00214200	-1.99356600	0.22110100		
C	0.42238000	-0.61161700	-0.01010400		
H	0.10359200	-1.64964700	-0.03694400		
C	1.87265600	-0.41729900	-0.01098000		
C	2.69122000	-1.57817900	-0.21646500		
C	2.49074000	0.80536900	0.17561200		
C	4.07464600	-1.52678000	-0.25163400		
H	2.19728700	-2.53383700	-0.35363100		
C	3.91527200	0.92942300	0.14857100		
H	1.93065700	1.71364300	0.35820900		
C	4.69565100	-0.29621500	-0.07538900		
H	4.67137400	-2.41646200	-0.41056700		
H	-0.19163600	1.39141400	-0.01194600		
C	-0.51517400	0.35403100	-0.00015600		
O	-4.99139200	2.28193500	-0.21673400		
O	-4.49960600	-2.43621600	0.22476000		
O	6.01346600	-0.13922900	-0.09071600		
H	6.13798800	0.82428900	0.06308300		
H	-5.46033100	-2.37650700	0.21255600		
H	-4.46093600	3.08247700	-0.28485600		
O	4.56310500	1.99187400	0.30362000		
Name of radical				11-O4'	
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase	
C	4.74597600	-0.03654100	0.00000400	Zero-point correction=	0.218614 (Hartree/Particle)
C	4.13462400	1.21778400	0.00000300	Thermal correction to Energy=	0.234133
C	2.74701900	1.32498000	0.00000100	Thermal correction to Enthalpy=	0.235077
C	1.94307300	0.16863900	-0.00000200	Thermal correction to Gibbs Free Energy=	0.173885
C	2.56104200	-1.09083900	0.00000100	Sum of electronic and zero-point Energies=	-840.975790
C	3.94993000	-1.18319600	0.00000500	Sum of electronic and thermal Energies=	-840.960271
H	5.82885700	-0.09522200	0.00000300	Sum of electronic and thermal Enthalpies=	-840.959326
H	2.27885600	2.30446700	0.00000400	Sum of electronic and thermal Free Energies=	-841.020519
H	1.99026800	-2.00912500	0.00000000		
C	-0.44350100	-0.63847100	-0.00000400		
H	-0.11141100	-1.67228600	-0.00000600		
C	-1.87023000	-0.46277100	-0.00000400		
C	-2.68754100	-1.64274900	-0.00000900		

C	-2.50215600	0.80483500	0.00000300	
C	-4.05081300	-1.58678600	-0.00000700	
H	-2.18767700	-2.60563800	-0.00001400	
C	-3.87090100	0.88642900	0.00000500	
H	-1.92714900	1.72188100	0.00000700	
C	-4.72692500	-0.31295600	-0.00000100	
H	-4.66478300	-2.47919200	-0.00001100	
H	0.16650400	1.37777100	0.00000000	
C	0.49727000	0.34346400	-0.00000200	
O	4.96002500	2.30360900	0.00001500	
O	4.48871500	-2.43608000	0.00000500	
O	-5.96183800	-0.14482300	0.00000100	
H	5.44931100	-2.37240100	0.00000900	
H	4.42959700	3.10714500	-0.00021100	
O	-4.52924000	2.04977400	0.00001100	
H	-5.47485600	1.79182300	0.00001100	
Name of anion			11-O3	
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	4.85584400	-0.05505700	0.00000700	Zero-point correction= 0.215560 (Hartree/Particle)
C	4.22224000	1.17252500	0.00001600	Thermal correction to Energy= 0.232063
C	2.82833600	1.28440600	0.00001500	Thermal correction to Enthalpy= 0.233007
C	2.05481400	0.09798000	0.00000400	Thermal correction to Gibbs Free Energy= 0.169671
C	2.68258400	-1.14538300	-0.00000600	Sum of electronic and zero-point Energies= -841.032452
C	4.12141800	-1.30664000	-0.00000600	Sum of electronic and thermal Energies= -841.015949
H	5.94005000	-0.10058700	0.00001000	Sum of electronic and thermal Enthalpies= -841.015005
H	2.34507100	2.25881100	0.00001700	Sum of electronic and thermal Free Energies= -841.078342
H	2.10630200	-2.06508300	-0.00001500	
C	-0.34439600	-0.70026500	-0.00000500	
H	-0.02168800	-1.73749100	-0.00001100	
C	-1.79308100	-0.51172600	-0.00000600	
C	-2.62983900	-1.64286700	-0.00001300	
C	-2.41906300	0.75299700	0.00000100	
C	-4.01819800	-1.52297000	-0.00001400	
H	-2.18128100	-2.62983100	-0.00001800	
C	-3.79772600	0.87767200	-0.00000100	
H	-1.83471700	1.66450100	0.00000600	
C	-4.60668400	-0.26783600	-0.00000800	
H	-4.64411500	-2.41230400	-0.00002000	
H	0.27334300	1.30113600	0.00000900	
C	0.60185400	0.26216900	0.00000300	

O	5.01763900	2.31624400	0.00002700	
O	4.68610200	-2.42955000	-0.00001600	
O	-5.97601900	-0.03588900	-0.00000900	
H	-6.43461100	-0.88047900	-0.00001500	
H	4.41971300	3.06960200	0.00005400	
O	-4.37587800	2.12105000	0.00000600	
H	-5.33144500	1.98685100	0.00000300	
Name of anion			11-O5	
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	-4.84246200	0.04381300	-0.00000100	Zero-point correction= 0.215939 (Hartree/Particle)
C	-4.25675100	1.36532400	0.00000100	Thermal correction to Energy= 0.232262
C	-2.80729400	1.34700900	0.00000100	Thermal correction to Enthalpy= 0.233206
C	-2.04860900	0.17516700	0.00000000	Thermal correction to Gibbs Free Energy= 0.170496
C	-2.68228100	-1.08933400	-0.00000200	Sum of electronic and zero-point Energies= -841.034538
C	-4.07442100	-1.11303300	-0.00000200	Sum of electronic and thermal Energies= -841.018215
H	-5.93066800	-0.01599500	-0.00000100	Sum of electronic and thermal Enthalpies= -841.017271
H	-2.31253000	2.31497900	0.00000200	Sum of electronic and thermal Free Energies= -841.079981
H	-2.13332500	-2.02153400	-0.00000300	
C	0.33578400	-0.66066100	-0.00000100	
H	-0.00019900	-1.69395000	-0.00000300	
C	1.78807900	-0.49686100	0.00000000	
C	2.60614200	-1.64138000	-0.00000300	
C	2.43377200	0.75764500	0.00000300	
C	3.99647100	-1.54428100	-0.00000300	
H	2.14198200	-2.62127500	-0.00000600	
C	3.81441000	0.85977500	0.00000300	
H	1.86371400	1.67807800	0.00000500	
C	4.60484500	-0.29885300	0.00000000	
H	4.60810800	-2.44354200	-0.00000500	
H	-0.25598200	1.35218300	0.00000200	
C	-0.59449600	0.31762400	0.00000000	
O	-4.93118700	2.42676200	0.00000200	
O	-4.68124600	-2.36558300	-0.00000400	
O	5.97771900	-0.08897600	0.00000100	
H	6.42278200	-0.94074100	-0.00000300	
H	-5.62997000	-2.20577800	-0.00000300	
O	4.41236700	2.09299800	0.00000600	
H	5.36573500	1.94424900	0.00000500	
Name of anion			11-O3'	
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase

C	-4.78282300	-0.04911200	-0.00001300	Zero-point correction=	0.216977 (Hartree/Particle)
C	-4.16973700	1.20348600	0.00006400	Thermal correction to Energy=	0.232490
C	-2.78611400	1.32250600	0.00008400	Thermal correction to Enthalpy=	0.233435
C	-1.95344500	0.18132500	0.00002800	Thermal correction to Gibbs Free Energy=	0.172969
C	-2.57943000	-1.08172700	-0.00004900	Sum of electronic and zero-point Energies=	-841.054372
C	-3.96376600	-1.18173400	-0.00006800	Sum of electronic and thermal Energies=	-841.038859
H	-5.86532300	-0.12049900	-0.00002900	Sum of electronic and thermal Enthalpies=	-841.037915
H	-2.33066500	2.30942400	0.00014300	Sum of electronic and thermal Free Energies=	-841.098381
H	-2.00141000	-1.99602400	-0.00009700		
C	0.43707100	-0.59733700	-0.00000200		
H	0.10335200	-1.63396400	-0.00005500		
C	1.87764700	-0.44294500	0.00001200		
C	2.64969000	-1.61953600	0.00004000		
C	2.52412500	0.81867700	0.00000500		
C	4.05014000	-1.55608500	0.00007700		
H	2.15087100	-2.58405700	0.00000000		
C	3.92545700	0.93615400	-0.00010700		
H	1.94758700	1.73760600	-0.00006900		
C	4.66528500	-0.31964300	0.00013800		
H	4.65513500	-2.45818600	0.00012100		
H	-0.18741100	1.40925100	0.00010800		
C	-0.51158700	0.37262600	0.00004900		
O	-4.99611200	2.30383300	0.00011700		
O	-4.50652400	-2.44691100	-0.00014600		
O	6.00325100	-0.12919300	0.00019300		
H	6.01074000	0.87147000	0.00013400		
H	-5.46455800	-2.36158700	-0.00015400		
H	-4.43986300	3.08928800	0.00016200		
O	4.64019400	1.99944000	-0.00039100		
Name of anion			11-O4'		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase	
C	4.78512800	-0.05507900	0.00000000	Zero-point correction=	0.217313 (Hartree/Particle)
C	4.17427300	1.19946800	0.00000100	Thermal correction to Energy=	0.232836
C	2.79254000	1.32530600	0.00000000	Thermal correction to Enthalpy=	0.233780
C	1.94892500	0.18773800	-0.00000100	Thermal correction to Gibbs Free Energy=	0.173568
C	2.57568300	-1.07894800	-0.00000100	Sum of electronic and zero-point Energies=	-841.061967
C	3.95848500	-1.18322400	-0.00000100	Sum of electronic and thermal Energies=	-841.046445
H	5.86721100	-0.13120300	0.00000100	Sum of electronic and thermal Enthalpies=	-841.045501
H	2.34374200	2.31567300	-0.00000100	Sum of electronic and thermal Free Energies=	-841.105712
H	1.99654100	-1.99265500	-0.00000300		

C	-0.44187500	-0.59257600	0.00000000	
H	-0.10110100	-1.62723400	0.00000200	
C	-1.86690400	-0.45412800	0.00000000	
C	-2.66930300	-1.61782000	0.00000300	
C	-2.54146700	0.80740900	-0.00000200	
C	-4.05332100	-1.57427900	0.00000300	
H	-2.16819100	-2.58368000	0.00000400	
C	-3.90623600	0.86088400	-0.00000100	
H	-1.98095300	1.73637400	-0.00000400	
C	-4.75021700	-0.33121900	0.00000100	
H	-4.64479200	-2.48468600	0.00000500	
H	0.19403700	1.42073200	-0.00000200	
C	0.51467600	0.38240600	-0.00000100	
O	5.00522900	2.29864000	0.00000300	
O	4.49776400	-2.45166200	-0.00000200	
O	-6.00564600	-0.15385600	0.00000100	
H	5.45574600	-2.36671000	-0.00000300	
H	4.44921100	3.08414700	0.00000800	
O	-4.62156500	2.02097400	-0.00000300	
H	-5.54002700	1.66084400	-0.00000200	
Name of cationic radical				Energies at B3LYP/6-311G(d,p) in gas phase
C	4.76298300	-0.04814500	0.00001300	Zero-point correction= 0.231235 (Hartree/Particle)
C	4.16554300	1.22677500	-0.00000100	Thermal correction to Energy= 0.247129
C	2.78428500	1.34587200	0.00000200	Thermal correction to Enthalpy= 0.248074
C	1.97713400	0.18268600	-0.00001000	Thermal correction to Gibbs Free Energy= 0.186570
C	2.58516000	-1.09464400	-0.00000800	Sum of electronic and zero-point Energies= -841.336234
C	3.97072900	-1.20259500	0.00001200	Sum of electronic and thermal Energies= -841.320340
H	5.84601200	-0.10673800	0.00001900	Sum of electronic and thermal Enthalpies= -841.319396
H	2.31787900	2.32457100	0.00004700	Sum of electronic and thermal Free Energies= -841.380899
H	2.00647400	-2.00728400	-0.00001600	
C	-0.39236500	-0.64324800	-0.00000900	
H	-0.05443800	-1.67370700	-0.00001400	
C	-1.80734300	-0.46696200	-0.00000600	
C	-2.61856800	-1.64236400	-0.00002000	
C	-2.44554500	0.79682900	0.00001000	
C	-3.99272500	-1.56079500	-0.00001800	
H	-2.13960800	-2.61372200	-0.00003200	
C	-3.81764300	0.89277300	0.00001200	
H	-1.88260400	1.72021100	0.00002200	
C	-4.60445500	-0.30160700	-0.00000200	

H	-4.60260700	-2.45744300	-0.00002900
H	0.21530100	1.38719800	0.00000000
C	0.55504400	0.35655100	-0.00000600
O	5.01691100	2.27193400	0.00000700
O	4.49338800	-2.44748200	0.00002000
O	-5.92734400	-0.09259900	0.00000100
H	-6.43291900	-0.91602200	-0.00000800
H	5.45702800	-2.41941800	0.00003900
H	4.53795600	3.10888000	-0.00030700
O	-4.41148900	2.09485100	0.00002700
H	-5.37360800	1.99308500	0.00002600

Name of compound (12)		Oxyresveratrol			
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)		Energies at B3LYP/6-311G(d,p) in gas phase			
C	4.66801300	0.13774300	-0.00001100	Zero-point correction=	0.230250 (Hartree/Particle)
C	4.16479300	-1.16181800	0.00007300	Thermal correction to Energy=	0.246626
C	2.79073300	-1.38916700	0.00008100	Thermal correction to Enthalpy=	0.247571
C	1.88774700	-0.31120300	0.00000500	Thermal correction to Gibbs Free Energy=	0.184017
C	2.39606300	0.99472900	-0.00007900	Sum of electronic and zero-point Energies=	-841.584261
C	3.77157900	1.20755900	-0.00008600	Sum of electronic and thermal Energies=	-841.567885
H	5.74157500	0.29130600	-0.00001600	Sum of electronic and thermal Enthalpies=	-841.566941
H	2.41212000	-2.40725800	0.00014700	Sum of electronic and thermal Free Energies=	-841.630494
H	1.74631200	1.85932100	-0.00014200		
C	-0.55327100	0.28128300	-0.00003000		
H	-0.31218300	1.33754400	-0.00006100		
C	-1.98505100	-0.00970000	-0.00003200		
C	-2.91090600	1.05546700	0.00008800		
C	-2.52470500	-1.30799500	-0.00015800		
C	-4.28712700	0.82354700	0.00009100		
C	-3.88616000	-1.55702700	-0.00015200		
H	-1.84874600	-2.15444800	-0.00027700		
C	-4.77757900	-0.48117100	-0.00002400		
H	-4.97527300	1.66598500	0.00017800		
H	-4.27832800	-2.56586200	-0.00025400		
H	0.22090800	-1.67383400	0.00008100		
C	0.45327100	-0.61214100	0.00001800		
O	5.07766900	-2.17965400	0.00014500		
H	4.60851500	-3.02016100	0.00019800		
O	4.20086900	2.50541400	-0.00017000		
H	5.16325500	2.51934100	-0.00016700		

O	-6.11152400	-0.76430600	-0.00002600	
H	-6.61508600	0.05611300	0.00006300	
O	-2.41292000	2.32776700	0.00019500	
H	-3.14020700	2.95754900	0.00038900	
Name of radical		12-O3		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	4.74480500	0.18463800	0.00000100	Zero-point correction= 0.216812 (Hartree/Particle)
C	4.24405000	-1.09566700	0.00022900	Thermal correction to Energy= 0.232967
C	2.84931500	-1.31367700	0.00019600	Thermal correction to Enthalpy= 0.233911
C	1.91609100	-0.24862900	-0.00006500	Thermal correction to Gibbs Free Energy= 0.170452
C	2.41651600	1.04636300	-0.00032300	Sum of electronic and zero-point Energies= -840.951103
C	3.84015700	1.31323700	-0.00028700	Sum of electronic and thermal Energies= -840.934948
H	5.81036500	0.37226000	0.00002400	Sum of electronic and thermal Enthalpies= -840.934004
H	2.47743200	-2.33523400	0.00038200	Sum of electronic and thermal Free Energies= -840.997463
H	1.77268100	1.91629000	-0.00057500	
C	-0.53025200	0.29860300	-0.00003800	
H	-0.30045500	1.35766000	0.00002100	
C	-1.95730400	-0.00649800	-0.00005900	
C	-2.89202400	1.05146700	0.00027900	
C	-2.48360100	-1.31060000	-0.00041500	
C	-4.26579400	0.80665100	0.00027600	
C	-3.84183200	-1.57174600	-0.00042300	
H	-1.79986100	-2.15083900	-0.00072300	
C	-4.74323100	-0.50296500	-0.00007100	
H	-4.96190000	1.64222800	0.00055100	
H	-4.22563900	-2.58368000	-0.00071000	
H	0.27361000	-1.64700400	-0.00003300	
C	0.48804800	-0.58174300	-0.00005700	
O	5.12271300	-2.14025300	0.00048000	
H	4.63752700	-2.97165000	0.00066300	
O	4.26910600	2.49122400	-0.00050700	
O	-6.07223800	-0.79974700	-0.00009300	
H	-6.58665600	0.01409500	0.00015700	
O	-2.40374800	2.32580800	0.00062100	
H	-3.13343700	2.95300300	0.00078400	
Name of radical		12-O5		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	-4.72719600	0.11583600	0.00000500	Zero-point correction= 0.217190 (Hartree/Particle)
C	-4.25156800	-1.25312500	-0.00002700	Thermal correction to Energy= 0.233218
C	-2.81609900	-1.45967400	-0.00003000	Thermal correction to Enthalpy= 0.234163

C	-1.91746600	-0.40385900	-0.00000600	Thermal correction to Gibbs Free Energy=	0.171293
C	-2.43988900	0.91403400	0.00002600	Sum of electronic and zero-point Energies=	-840.953764
C	-3.83045600	1.15765600	0.00002900	Sum of electronic and thermal Energies=	-840.937736
H	-5.80077500	0.27073400	0.00000800	Sum of electronic and thermal Enthalpies=	-840.936792
H	-2.47762200	-2.48926200	-0.00005500	Sum of electronic and thermal Free Energies=	-840.999661
H	-1.78708500	1.77721000	0.00005200		
C	0.50990500	0.23410800	0.00001300		
H	0.25158600	1.28649100	0.00003300		
C	1.94608700	-0.02759600	0.00001200		
C	2.84901900	1.05698100	-0.00003000		
C	2.51045400	-1.31576800	0.00005500		
C	4.22936700	0.85319800	-0.00003200		
C	3.87582300	-1.53654200	0.00005300		
H	1.85168100	-2.17555500	0.00009800		
C	4.74530800	-0.44184500	0.00000800		
H	4.90070800	1.70889600	-0.00006700		
H	4.28887000	-2.53687400	0.00008900		
H	-0.23270600	-1.73721600	-0.00004700		
C	-0.47901600	-0.67949700	-0.00001300		
O	-5.04549100	-2.21867000	-0.00005200		
O	-4.19519300	2.47231900	0.00005800		
H	-5.15641200	2.53509400	0.00005900		
O	6.08269400	-0.69896300	0.00000800		
H	6.57257200	0.12982600	-0.00002300		
O	2.32382200	2.31819200	-0.00007000		
H	3.03688900	2.96419300	-0.00009500		
Name of radical			12-O2'		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase	
C	-4.63025400	0.15243100	0.00002400	Zero-point correction=	0.217746 (Hartree/Particle)
C	-4.13832100	-1.15369000	0.00013500	Thermal correction to Energy=	0.233530
C	-2.76773500	-1.39002200	0.00015300	Thermal correction to Enthalpy=	0.234474
C	-1.85917500	-0.31226500	0.00006200	Thermal correction to Gibbs Free Energy=	0.172939
C	-2.35692300	1.00027700	-0.00004800	Sum of electronic and zero-point Energies=	-840.964367
C	-3.73128200	1.22085500	-0.00006800	Sum of electronic and thermal Energies=	-840.948583
H	-5.70307200	0.31107200	0.00001200	Sum of electronic and thermal Enthalpies=	-840.947639
H	-2.39258600	-2.40895400	0.00023600	Sum of electronic and thermal Free Energies=	-841.009174
H	-1.69977500	1.85882000	-0.00012000		
C	0.58479300	0.28854400	-0.00001600		
H	0.36398400	1.35070700	-0.00014600		
C	1.97927700	-0.00085900	0.00001100		

C	2.90533000	1.16685700	-0.00027400	
C	2.53400500	-1.30064900	0.00029300	
C	4.32807400	0.88612100	-0.00025400	
C	3.89019300	-1.50694200	0.00030000	
H	1.87908600	-2.16413200	0.00051900	
C	4.79480500	-0.39509600	0.00002100	
H	4.99272400	1.74354300	-0.00046700	
H	4.31275200	-2.50403000	0.00051900	
H	-0.20112900	-1.67637800	0.00018900	
C	-0.43743800	-0.61572500	0.00008500	
O	-5.06203200	-2.15838800	0.00022000	
H	-4.60770200	-3.00715000	0.00031500	
O	-4.15260100	2.51751300	-0.00017700	
H	-5.11492400	2.54271800	-0.00018300	
O	6.11200900	-0.73197700	0.00005800	
H	6.64494900	0.07131100	-0.00014000	
O	2.47182400	2.32828200	-0.00051200	
Name of radical				12-O4'
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	4.58989100	0.14797300	0.00000100	Zero-point correction= 0.217782 (Hartree/Particle)
C	4.09785100	-1.15826000	-0.00000100	Thermal correction to Energy= 0.233595
C	2.72708400	-1.39466000	-0.00000300	Thermal correction to Enthalpy= 0.234539
C	1.81796700	-0.31723800	-0.00000300	Thermal correction to Gibbs Free Energy= 0.172957
C	2.31668600	0.99524500	-0.00000100	Sum of electronic and zero-point Energies= -840.963473
C	3.69081200	1.21611200	0.00000100	Sum of electronic and thermal Energies= -840.947660
H	5.66267400	0.30655200	0.00000200	Sum of electronic and thermal Enthalpies= -840.946716
H	2.35224600	-2.41359700	-0.00000400	Sum of electronic and thermal Free Energies= -841.008298
H	1.66167300	1.85543400	-0.00000200	
C	-0.62732500	0.28232600	0.00000500	
H	-0.38435200	1.33751200	0.00001300	
C	-2.02056300	-0.01558100	0.00000200	
C	-2.97327800	1.07029800	-0.00000100	
C	-2.55183600	-1.34478400	0.00000400	
C	-4.31878800	0.84163300	-0.00000300	
C	-3.88758800	-1.59444500	0.00000300	
H	-1.85838800	-2.17698100	0.00000700	
C	-4.86627800	-0.50515400	0.00000000	
H	-5.03273200	1.65928400	-0.00000600	
H	-4.28311700	-2.60301500	0.00000400	
H	0.16290400	-1.68303700	-0.00001300	

C	0.39749500	-0.62314800	-0.00000400	
O	5.02133200	-2.16212500	0.00000000	
H	4.56846000	-3.01174100	-0.00000400	
O	4.11121800	2.51326500	0.00000200	
H	5.07357000	2.53929000	0.00000400	
O	-6.08493700	-0.72374900	-0.00000100	
O	-2.43803700	2.32478700	-0.00000400	
H	-3.15233100	2.97098500	0.00000200	
Name of anion		12-O3		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	4.71753300	0.14356700	-0.01099900	Zero-point correction= 0.215642 (Hartree/Particle)
C	4.18237400	-1.12391400	0.11136100	Thermal correction to Energy= 0.232002
C	2.80178800	-1.34590300	0.11623500	Thermal correction to Enthalpy= 0.232947
C	1.93679100	-0.23090500	-0.00738200	Thermal correction to Gibbs Free Energy= 0.170144
C	2.46440600	1.05154400	-0.13390900	Sum of electronic and zero-point Energies= -841.027778
C	3.88637800	1.32601200	-0.14214900	Sum of electronic and thermal Energies= -841.011418
H	5.79474400	0.27509900	-0.01207100	Sum of electronic and thermal Enthalpies= -841.010474
H	2.39741100	-2.35091400	0.21531200	Sum of electronic and thermal Free Energies= -841.073276
H	1.81576500	1.91561300	-0.23642300	
C	-0.52021200	0.37144100	-0.04787300	
H	-0.29180500	1.42958000	-0.07639100	
C	-1.94396600	0.03794900	-0.04953200	
C	-2.90966600	1.05357200	0.13349600	
C	-2.45428600	-1.25928300	-0.23621300	
C	-4.27773000	0.77614800	0.14119100	
C	-3.81214200	-1.55528300	-0.22693400	
H	-1.75327900	-2.06696000	-0.40944400	
C	-4.73355300	-0.52957600	-0.03609300	
H	-4.98885300	1.58733900	0.29216800	
H	-4.16955000	-2.56679600	-0.37747500	
H	0.25865400	-1.57039800	0.08132300	
C	0.50070400	-0.51027700	0.00587200	
O	5.06520400	-2.19590700	0.23071300	
H	4.52722300	-2.98941600	0.30791400	
O	4.36148300	2.48442400	-0.25446500	
O	-6.07405200	-0.84617500	-0.03599500	
H	-6.57707700	-0.03722700	0.09682900	
O	-2.45659800	2.33519800	0.31158900	
H	-3.21204000	2.92319000	0.40110000	
Name of anion		12-O5		

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase	
C	-4.70709600	0.04352300	0.00403400	Zero-point correction=	0.215972 (Hartree/Particle)
C	-4.22836600	-1.31693400	-0.08937600	Thermal correction to Energy=	0.232204
C	-2.78228800	-1.41371800	-0.08913200	Thermal correction to Enthalpy=	0.233148
C	-1.93248600	-0.30913900	-0.00640900	Thermal correction to Gibbs Free Energy=	0.170567
C	-2.46337300	0.99846600	0.08421000	Sum of electronic and zero-point Energies=	-841.030386
C	-3.84926400	1.13262200	0.08608400	Sum of electronic and thermal Energies=	-841.014154
H	-5.78715600	0.18961100	0.00921200	Sum of electronic and thermal Enthalpies=	-841.013210
H	-2.36665300	-2.41599600	-0.15791900	Sum of electronic and thermal Free Energies=	-841.075791
H	-1.84012500	1.87991500	0.15500800		
C	0.51258500	0.33116100	0.03256000		
H	0.26967200	1.38605000	0.06196900		
C	1.94259700	0.02377700	0.03422900		
C	2.89142500	1.06312300	-0.09066700		
C	2.47453800	-1.27195300	0.16392200		
C	4.26451900	0.81117200	-0.09500000		
C	3.83735300	-1.54245800	0.15827500		
H	1.78710900	-2.10052500	0.28362500		
C	4.74229200	-0.49281000	0.02716900		
H	4.96230700	1.64129200	-0.19837700		
H	4.21090100	-2.55392500	0.26242800		
H	-0.24311200	-1.62530700	-0.08031600		
C	-0.49385800	-0.56775700	-0.01671300		
O	-4.98525100	-2.31922900	-0.16339400		
O	-4.35602200	2.42613700	0.17629800		
H	-5.31425100	2.34082000	0.16596500		
O	6.08819100	-0.78534100	0.02818100		
H	6.57784500	0.03699500	-0.06690300		
O	2.41871200	2.34594900	-0.21337200		
H	3.16695400	2.94649700	-0.27549800		
Name of anion			12-O2'		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase	
C	-4.65482000	0.16961100	0.00001200	Zero-point correction=	0.216354 (Hartree/Particle)
C	-4.16062500	-1.13420000	0.00018200	Thermal correction to Energy=	0.232299
C	-2.79551000	-1.38399200	0.00020500	Thermal correction to Enthalpy=	0.233243
C	-1.85358600	-0.32675800	0.00005900	Thermal correction to Gibbs Free Energy=	0.172219
C	-2.36129600	0.99132600	-0.00011200	Sum of electronic and zero-point Energies=	-841.049389
C	-3.72905300	1.21928000	-0.00013400	Sum of electronic and thermal Energies=	-841.033445
H	-5.72569200	0.34356600	-0.00000400	Sum of electronic and thermal Enthalpies=	-841.032501
H	-2.43740800	-2.41111400	0.00033700	Sum of electronic and thermal Free Energies=	-841.093524

H	-1.69648200	1.84463500	-0.00023000	
C	0.59426900	0.23989700	-0.00003800	
H	0.37423300	1.30567600	-0.00018600	
C	2.00542000	-0.00979300	-0.00001200	
C	2.88887600	1.17183100	-0.00020500	
C	2.57079600	-1.29927400	0.00018900	
C	4.30782000	0.87377700	-0.00017000	
C	3.93338800	-1.53080100	0.00021400	
H	1.90523400	-2.15893800	0.00033300	
C	4.79456900	-0.41123900	0.00002900	
H	4.98205000	1.72853400	-0.00031200	
H	4.35369000	-2.52920300	0.00037100	
H	-0.22156400	-1.71439900	0.00022900	
C	-0.44026500	-0.64819300	0.00009000	
O	-5.08732400	-2.15614900	0.00032400	
H	-4.60139300	-2.98671900	0.00044500	
O	-4.15447000	2.53009300	-0.00030500	
H	-5.11613700	2.52937900	-0.00030200	
O	6.15338100	-0.67891700	0.00006000	
H	6.60276000	0.17239700	-0.00007800	
O	2.46101400	2.34839400	-0.00038700	
Name of anion			12-O4'	
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)				Energies at B3LYP/6-311G(d,p) in gas phase
C	4.63016200	0.16924900	-0.00000100	Zero-point correction= 0.216529 (Hartree/Particle)
C	4.13706300	-1.13583800	-0.00000500	Thermal correction to Energy= 0.232492
C	2.77303100	-1.38899200	-0.00000300	Thermal correction to Enthalpy= 0.233436
C	1.82636100	-0.33435900	0.00000300	Thermal correction to Gibbs Free Energy= 0.172408
C	2.33474300	0.98515500	0.00000600	Sum of electronic and zero-point Energies= -841.049687
C	3.70167800	1.21598300	0.00000400	Sum of electronic and thermal Energies= -841.033723
H	5.70059900	0.34504400	-0.00000100	Sum of electronic and thermal Enthalpies= -841.032779
H	2.41806800	-2.41708800	-0.00000600	Sum of electronic and thermal Free Energies= -841.093807
H	1.67260800	1.84069500	0.00001100	
C	-0.62157300	0.23056500	0.00000100	
H	-0.37183200	1.28737500	-0.00000300	
C	-2.02483100	-0.03287300	0.00000100	
C	-2.96569900	1.03947900	-0.00000500	
C	-2.59792600	-1.33942100	0.00000600	
C	-4.32543100	0.83496500	-0.00000500	
C	-3.94510600	-1.57045000	0.00000600	
H	-1.92144100	-2.18961300	0.00001000	

C	-4.92091100	-0.48628000	0.00000100	
H	-5.01091200	1.68117900	-0.00000900	
H	-4.34352300	-2.58068300	0.00001000	
H	0.19691000	-1.72420100	0.00000900	
C	0.41717400	-0.65979000	0.00000400	
O	5.06583900	-2.15515200	-0.00000900	
H	4.58267900	-2.98738700	-0.00001100	
O	4.12293600	2.52892300	0.00000900	
H	5.08462900	2.53066200	0.00000200	
O	-6.15566300	-0.68166300	0.00000200	
O	-2.44821400	2.32353300	-0.00001000	
H	-3.19937300	2.92453700	-0.00001700	
Name of cationic radical				Energies at B3LYP/6-311G(d,p) in gas phase
C	4.61376500	0.15301600	-0.00000400	Zero-point correction= 0.231571 (Hartree/Particle)
C	4.13699500	-1.17171800	-0.00001600	Thermal correction to Energy= 0.247426
C	2.77320600	-1.41894300	-0.00001600	Thermal correction to Enthalpy= 0.248370
C	1.86029000	-0.33562200	-0.00000500	Thermal correction to Gibbs Free Energy= 0.187027
C	2.34793900	0.99281900	0.00000700	Sum of electronic and zero-point Energies= -841.339551
C	3.71772800	1.22847800	0.00000800	Sum of electronic and thermal Energies= -841.323696
H	5.68667600	0.31140700	-0.00000300	Sum of electronic and thermal Enthalpies= -841.322752
H	2.40004000	-2.43696400	-0.00002600	Sum of electronic and thermal Free Energies= -841.384095
H	1.68672400	1.84758700	0.00001500	
C	-0.56912500	0.28135100	0.00000400	
H	-0.31802600	1.33425000	0.00001400	
C	-1.95459500	-0.01267200	0.00000200	
C	-2.89668700	1.07799300	0.00001400	
C	-2.49463700	-1.33291000	-0.00001100	
C	-4.26388000	0.84486800	0.00001300	
C	-3.83894600	-1.56750200	-0.00001200	
H	-1.82022600	-2.17867300	-0.00002100	
C	-4.74017600	-0.46989100	0.00000000	
H	-4.95935000	1.67846100	0.00002300	
H	-4.24860000	-2.56881400	-0.00002200	
H	0.21808600	-1.69633700	-0.00001600	
C	0.46180800	-0.63914300	-0.00000600	
O	5.08209000	-2.13390400	-0.00002600	
H	4.68210600	-3.01121500	-0.00003400	
O	4.12250200	2.51697300	0.00001900	
H	5.08457900	2.57799600	0.00001900	
O	-6.03593500	-0.77710300	-0.00000200	

H	-6.59563300	0.01062700	0.00000700	
O	-2.37749400	2.31429100	0.00002700	
H	-3.06778200	2.98888300	0.00003400	

Table S4: Cartesian coordinates and molecular enthalpies of the TS optimized at M05-2X/6-311++G(d,p) level in the studied environments.

Name of TS	4-O4'-H-OOCH ₃			Energies (in the gas phase)
C	-5.52195800	0.37483600	0.14070000	Zero-point correction= 0.270233 (Hartree/Particle)
C	-4.57901900	1.37670500	-0.05544000	Thermal correction to Energy= 0.289504
C	-3.22151300	1.09064400	-0.09670200	Thermal correction to Enthalpy= 0.290448
C	-2.79182100	-0.22689500	0.05455900	Thermal correction to Gibbs Free Energy= 0.218379
C	-3.73283200	-1.24098700	0.26530200	Sum of electronic and zero-point Energies= -956.453782
C	-5.08563000	-0.93352000	0.30301000	Sum of electronic and thermal Energies= -956.434511
H	-6.58212600	0.58755900	0.17946300	Sum of electronic and thermal Enthalpies= -956.433567
H	-2.52947700	1.90902000	-0.22369300	Sum of electronic and thermal Free Energies= -956.505636
H	-3.40420500	-2.26596400	0.38775100	
C	-0.38107900	0.16474200	-0.46685100	
H	-0.62093000	1.14045700	-0.87300500	
C	1.02661200	-0.19374800	-0.52418000	
C	1.91209500	0.66364200	-1.19644500	
C	1.55159500	-1.36265400	0.07165900	
C	3.25512700	0.37527600	-1.29685800	
H	1.52406200	1.56793700	-1.64681500	
C	2.88784100	-1.65684600	-0.00759200	
H	0.89767100	-2.03120000	0.61327500	
C	3.77428700	-0.80152900	-0.70849600	
H	3.93829400	1.03589800	-1.81138000	
H	3.30220500	-2.54610500	0.44684800	
H	-1.15847800	-1.60478600	0.35458400	
C	-1.37731700	-0.60366300	0.00287900	
O	-4.94230400	2.67981200	-0.20709200	
H	-5.89603400	2.76298300	-0.15019800	
O	-6.04365200	-1.88123600	0.49836400	
H	-5.63357500	-2.74284500	0.59437400	
O	5.03847100	-1.11948500	-0.80714200	
H	5.68122600	-0.26195400	-0.42263600	
O	6.11568800	0.68278900	0.25761100	
O	4.97673100	1.24632500	0.73510400	
C	4.79736400	0.85423100	2.09535700	
H	3.84440800	1.27892800	2.40028600	
H	4.78010400	-0.23276900	2.15909600	
H	5.61487600	1.25579300	2.69187100	

Name of TS		4-O4'-H-OOCH ₃		Energies (in the gas pentyl ethanoate)	
C	-5.47947700	0.09453300	0.31683700	Zero-point correction=	0.270525 (Hartree/Particle)
C	-4.84600700	1.29643300	0.02654600	Thermal correction to Energy=	0.289596
C	-3.48049200	1.34004800	-0.22465500	Thermal correction to Enthalpy=	0.290540
C	-2.72598300	0.16204600	-0.18064900	Thermal correction to Gibbs Free Energy=	0.219669
C	-3.35540200	-1.05195800	0.10159000	Sum of electronic and zero-point Energies=	-956.485498
C	-4.72131600	-1.07159300	0.34765900	Sum of electronic and thermal Energies=	-956.466428
H	-6.54548600	0.08063100	0.50622500	Sum of electronic and thermal Enthalpies=	-956.465483
H	-2.99855400	2.28435100	-0.44873500	Sum of electronic and thermal Free Energies=	-956.536355
H	-2.81404500	-1.98614700	0.12158600		
C	-0.38231300	-0.70718900	-0.24091800		
H	-0.70609800	-1.66095000	0.15911200		
C	1.04621900	-0.60310700	-0.48853900		
C	1.87214800	-1.66956000	-0.07874800		
C	1.64891300	0.50712900	-1.11470200		
C	3.23560100	-1.62753500	-0.25382300		
H	1.41555700	-2.53128200	0.39153900		
C	3.00751700	0.55556800	-1.30617300		
H	1.04178500	1.33268400	-1.45814600		
C	3.83432600	-0.51153900	-0.87682800		
H	3.87132900	-2.44209500	0.06609700		
H	3.47414800	1.40615100	-1.78502900		
H	-0.96090600	1.23756500	-0.79306600		
C	-1.28748600	0.26768600	-0.43716500		
O	-5.62142600	2.41348500	0.00082500		
H	-5.07885600	3.18086000	-0.20635600		
O	-5.28771900	-2.27908900	0.61564100		
H	-6.23310700	-2.17285000	0.76066900		
O	5.13374200	-0.49025700	-1.08628800		
H	5.57064500	0.35206700	-0.49779500		
O	5.79330800	1.20229000	0.42716600		
O	4.61317700	1.18372600	1.09303600		
C	4.73993300	0.37312600	2.26613100		
H	3.74170400	0.31372300	2.69321400		
H	5.10600700	-0.61430400	1.98968100		
H	5.43013600	0.85382500	2.95857900		
Name of TS		5-O3'-H-OOCH ₃		Energies (in pentyl ethanoate)	
O	-1.50155300	3.42145900	0.98439400	Zero-point correction=	0.450811 (Hartree/Particle)
C	-1.23470200	2.30680100	0.25256000	Thermal correction to Energy=	0.482312
C	0.04655900	1.77920700	0.16102700	Thermal correction to Enthalpy=	0.483256

C	-2.30917100	1.72628000	-0.41751100	Thermal correction to Gibbs Free Energy=	0.383124
C	0.27546300	0.63827700	-0.61377300	Sum of electronic and zero-point Energies=	-1642.444102
H	0.86286600	2.27574000	0.66997300	Sum of electronic and thermal Energies=	-1642.412601
C	-2.07005600	0.59097600	-1.17605600	Sum of electronic and thermal Enthalpies=	-1642.411657
H	-3.29569300	2.15872500	-0.35309700	Sum of electronic and thermal Free Energies=	-1642.511789
C	-0.79532200	0.05019500	-1.29089300		
H	-0.64485300	-0.82106200	-1.91560600		
O	-3.07142800	-0.02797900	-1.89666500		
C	2.64593500	0.24685900	0.05722900		
H	2.53126500	0.91236600	0.90547800		
C	1.60214300	0.02363800	-0.75054900		
H	1.69064100	-0.68342900	-1.56738500		
C	3.97448300	-0.35917500	-0.06510700		
C	4.88978000	-0.17676600	0.95570900		
C	4.37145800	-1.11935800	-1.18830700		
C	6.18404700	-0.72910200	0.90749500		
H	4.63203200	0.40615500	1.83103600		
C	5.62989600	-1.67987300	-1.26577200		
H	3.68973900	-1.26496300	-2.01398300		
C	6.54629800	-1.49772400	-0.23089700		
O	7.78497900	-2.01933400	-0.25430500		
H	7.91064700	-2.52803300	-1.06387400		
C	-3.85287200	-1.25257900	0.06913600		
C	-5.13923900	-1.73982000	0.70651300		
C	-6.06861600	-0.56651900	0.92822500		
C	-6.31216100	0.15277000	-0.39408100		
C	-4.20108800	-0.49750800	-1.21146600		
H	-5.62293100	-2.45832700	0.03468000		
H	-3.34396200	-0.58123900	0.76515600		
H	-6.78610700	-0.53512200	-1.10399100		
H	-4.69668600	-1.16965200	-1.91600200		
H	-5.59834100	0.13421400	1.62652900		
O	-5.05352400	0.58975700	-0.90624800		
H	-8.56032500	0.39682200	0.70502900		
C	-7.18757100	1.38562700	-0.23615700		
H	-7.14785000	1.96109800	-1.15885000		
H	-6.79830900	2.00526100	0.57801200		
O	-8.54424700	1.03763200	-0.01454100		
O	-7.32172200	-1.00110000	1.44122900		
H	-7.15056500	-1.54819000	2.21532100		

O	-4.90335100	-2.33794800	1.97065200	
H	-4.28991900	-3.06851500	1.84222500	
O	-3.06056900	-2.39653400	-0.20360000	
H	-2.15256000	-2.11488800	-0.35281600	
H	-0.69028600	3.75456900	1.38103400	
H	5.91554800	-2.25808100	-2.13653500	
O	7.03869400	-0.56694500	1.89259700	
H	7.45837800	0.47518300	1.80823900	
O	7.83330000	1.59287400	1.36035900	
O	7.40545700	1.52793600	0.07727400	
C	8.50140100	1.17176200	-0.77160200	
H	8.92878600	0.22849100	-0.43405700	
H	8.08175100	1.07680400	-1.77057000	
H	9.24845800	1.96372200	-0.73947800	
Name of TS	5-O4'-H-OOCH₃			Energies (in pentyl ethanoate)
O	-1.68657400	3.26563600	1.52515700	Zero-point correction= 0.451525 (Hartree/Particle)
C	-1.34245100	2.24963000	0.68983600	Thermal correction to Energy= 0.482718
C	-0.04560800	1.75925700	0.62493600	Thermal correction to Enthalpy= 0.483662
C	-2.35661400	1.73271900	-0.11369900	Thermal correction to Gibbs Free Energy= 0.385863
C	0.25992000	0.72032300	-0.26089600	Sum of electronic and zero-point Energies= -1642.452638
H	0.72031900	2.20735700	1.24529900	Sum of electronic and thermal Energies= -1642.421446
C	-2.04394400	0.69555100	-0.97841400	Sum of electronic and thermal Enthalpies= -1642.420502
H	-3.35450100	2.14023200	-0.06634400	Sum of electronic and thermal Free Energies= -1642.518301
C	-0.75154400	0.19278100	-1.06745700	
H	-0.53900400	-0.59892100	-1.77448000	
O	-2.97949400	0.14884500	-1.83183700	
C	2.62956500	0.36143600	0.44842600	
H	2.48355800	0.98579300	1.32210100	
C	1.60448500	0.15089200	-0.39166500	
H	1.73249600	-0.50705400	-1.24282600	
C	3.96973200	-0.20089100	0.31731000	
C	4.88314400	0.03912000	1.34872200	
C	4.37496600	-0.96715400	-0.79999700	
C	6.16647800	-0.46953800	1.27375900	
H	4.59478200	0.61788900	2.21632600	
C	5.64856300	-1.47289800	-0.87879400	
H	3.68530500	-1.15281700	-1.60994300	
C	6.57574700	-1.22804300	0.15055800	
O	7.81585500	-1.69555900	0.14948500	
H	8.40582100	-1.09760700	-0.56762800	

C	-3.90119200	-1.28142400	-0.07803600	
C	-5.22952600	-1.83034300	0.40399100	
C	-6.17506200	-0.68326300	0.68578000	
C	-6.32544600	0.17800700	-0.56329800	
C	-4.15642100	-0.38847300	-1.28989300	
H	-5.65915400	-2.46727700	-0.37785900	
H	-3.44820300	-0.69386500	0.72431600	
H	-6.74685800	-0.42421300	-1.37649400	
H	-4.59338200	-0.97770100	-2.09962000	
H	-5.75625200	-0.06558900	1.48767500	
O	-5.03433000	0.66207000	-0.93340400	
H	-8.64856200	0.31260500	0.39031200	
C	-7.21229600	1.39105500	-0.33220700	
H	-7.10628400	2.06615900	-1.17904200	
H	-6.88487100	1.91289400	0.57271600	
O	-8.58084000	1.02907600	-0.25059600	
O	-7.46056900	-1.16324200	1.05820100	
H	-7.34369600	-1.79481000	1.77604700	
O	-5.08593400	-2.56575100	1.60791300	
H	-4.46817200	-3.28533400	1.44329900	
O	-3.08661000	-2.39149800	-0.41592800	
H	-2.17139600	-2.09950900	-0.47130300	
H	-0.91398900	3.56250800	2.01642600	
H	5.97238200	-2.05170700	-1.73349200	
O	7.05468300	-0.24512300	2.25932300	
H	7.85768600	-0.74063500	2.03806300	
O	8.84048600	-0.10268600	-1.27986100	
O	7.76650600	0.71274100	-1.25957600	
C	8.01097300	1.82447400	-0.38912000	
H	8.82698800	2.41938600	-0.79634300	
H	7.08485800	2.39338000	-0.37413500	
H	8.26388500	1.46346200	0.60685600	
Name of TS	11-O4'-H-OOCH₃			Energies (in the gas phase)
C	5.67992200	-0.22161400	0.21213700	Zero-point correction= 0.275741 (Hartree/Particle)
C	4.80434000	-1.29892500	0.15239500	Thermal correction to Energy= 0.295790
C	3.43255700	-1.10797100	0.05910100	Thermal correction to Enthalpy= 0.296735
C	2.92090400	0.18760900	0.01615900	Thermal correction to Gibbs Free Energy= 0.223886
C	3.79283700	1.27918400	0.08931100	Sum of electronic and zero-point Energies= -1031.699964
C	5.16117600	1.06628800	0.18179700	Sum of electronic and thermal Energies= -1031.679915
H	6.75036400	-0.35889600	0.28993000	Sum of electronic and thermal Enthalpies= -1031.678971

H	2.79270500	-1.97712900	0.04804900	Sum of electronic and thermal Free Energies= -1031.751819
H	3.39922400	2.28807600	0.06141000	
C	0.56015600	-0.41882300	-0.51667000	
H	0.87594900	-1.40858300	-0.82468600	
C	-0.86958600	-0.16004000	-0.64198700	
C	-1.65776700	-1.11142300	-1.32303000	
C	-1.48075200	0.98565200	-0.11744800	
C	-3.00939900	-0.92611500	-1.49543600	
H	-1.18054400	-1.99776500	-1.71846900	
C	-2.83475300	1.17751900	-0.28833700	
H	-0.92303800	1.72737500	0.43523900	
C	-3.62871500	0.22224600	-0.97798800	
H	-3.62365500	-1.65097900	-2.01079000	
H	1.18788000	1.47378600	0.13493500	
C	1.48547600	0.45939800	-0.10368700	
O	5.24971900	-2.58483400	0.19260300	
H	6.20521000	-2.59807800	0.27393100	
O	6.05566700	2.09095100	0.24769700	
H	5.59179000	2.92969400	0.21402400	
O	-4.91662700	0.48915400	-1.10222500	
H	-5.48083300	-0.16754600	-0.39352200	
O	-5.77451700	-0.84479800	0.64641500	
O	-4.54751600	-1.16050000	1.11022500	
C	-4.27869800	-0.42173900	2.30461800	
H	-3.27099500	-0.70297400	2.59804100	
H	-4.33928500	0.64546600	2.09550200	
H	-5.00489300	-0.70570700	3.06372000	
O	-3.45122400	2.26160600	0.21939500	
H	-4.37007000	2.22314200	-0.08581100	
Name of TS	11-O3'-H-OOCH₃			Energies (in pentyl ethanoate)
C	5.58259800	0.09662900	0.24524500	Zero-point correction= 0.274873 (Hartree/Particle)
C	4.95491400	1.18289400	-0.35054300	Thermal correction to Energy= 0.295000
C	3.57748000	1.19952700	-0.53273800	Thermal correction to Enthalpy= 0.295944
C	2.80589800	0.10951500	-0.11710300	Thermal correction to Gibbs Free Energy= 0.222805
C	3.42624300	-0.98237300	0.49214300	Sum of electronic and zero-point Energies= -1031.722250
C	4.80399800	-0.97762300	0.66284100	Sum of electronic and thermal Energies= -1031.702124
H	6.65617700	0.10418500	0.38361500	Sum of electronic and thermal Enthalpies= -1031.701180
H	3.10072100	2.05291000	-1.00045400	Sum of electronic and thermal Free Energies= -1031.774319
H	2.86401000	-1.83147300	0.85198400	
C	0.49954900	-0.84620200	-0.22612400	

H	0.86950900	-1.82829400	0.04579200	
C	-0.94616500	-0.77962900	-0.46251200	
C	-1.66293100	-1.99133000	-0.55778700	
C	-1.64901200	0.40611600	-0.59338700	
C	-3.02435300	-2.01459600	-0.79757000	
H	-1.12926000	-2.92643000	-0.44771700	
C	-3.03405600	0.42131600	-0.83358800	
H	-1.16311300	1.36769900	-0.49847200	
C	-3.72281400	-0.82067600	-0.93945400	
H	-3.55185300	-2.95755700	-0.87618900	
H	0.99313000	1.14215200	-0.67423400	
C	1.35717500	0.17372700	-0.34985900	
O	5.74775900	2.21693200	-0.74233300	
O	5.36160300	-2.06523000	1.26211800	
O	-5.04617100	-0.77055500	-1.17330100	
H	-5.40016700	-1.66525600	-1.23680800	
H	6.31329700	-1.94476100	1.33688100	
H	5.20632700	2.90894400	-1.13489400	
O	-3.69305600	1.54924800	-0.97708600	
H	-3.85421200	1.98267900	0.05393000	
O	-3.99592900	2.11774600	1.29478800	
O	-3.74684300	0.86146200	1.73568200	
C	-4.98621300	0.19490100	1.99572500	
H	-5.59697700	0.20021300	1.09388900	
H	-4.71977600	-0.81981200	2.28285900	
H	-5.50057600	0.70480500	2.80914600	
Name of TS	11-O4'-H-OOCH₃			Energies (in pentyl ethanoate)
C	5.68350500	-0.13073800	0.26421900	Zero-point correction= 0.275532 (Hartree/Particle)
C	4.85108100	-1.24362800	0.20412600	Thermal correction to Energy= 0.295476
C	3.47668100	-1.11215400	0.05931600	Thermal correction to Enthalpy= 0.296420
C	2.91600200	0.16301900	-0.03363300	Thermal correction to Gibbs Free Energy= 0.224285
C	3.74278700	1.28988700	0.03396000	Sum of electronic and zero-point Energies= -1031.731481
C	5.11547000	1.13392100	0.17970300	Sum of electronic and thermal Energies= -1031.711537
H	6.75478800	-0.23399100	0.38129700	Sum of electronic and thermal Enthalpies= -1031.710593
H	2.87222700	-2.00692000	0.03594400	Sum of electronic and thermal Free Energies= -1031.782728
H	3.31318400	2.28215000	-0.03401400	
C	0.55974500	-0.55176000	-0.47439100	
H	0.87286500	-1.58043300	-0.60850800	
C	-0.87200000	-0.32588600	-0.63710500	
C	-1.66951200	-1.42387500	-1.02612700	

C	-1.47842900	0.91969400	-0.42647400
C	-3.02732200	-1.29159200	-1.20210300
H	-1.19507100	-2.38286600	-1.18623700
C	-2.83869200	1.05727900	-0.60251800
H	-0.90986900	1.78679100	-0.12196600
C	-3.64251700	-0.04917600	-0.98465200
H	-3.64508100	-2.13013300	-1.49406300
H	1.17056300	1.42421400	-0.10551000
C	1.47695000	0.38918600	-0.20040500
O	5.35036400	-2.50610400	0.29025400
H	6.30628100	-2.47379300	0.39597400
O	5.95996400	2.19790300	0.24720100
H	5.45811100	3.01581800	0.17446500
O	-4.94000600	0.16985000	-1.14407200
H	-5.47244900	-0.28045600	-0.28825700
O	-5.75405100	-0.69920500	0.90882100
O	-4.51695100	-0.82561200	1.43030300
C	-4.26558400	0.23452300	2.36127600
H	-3.23136100	0.11157100	2.67270000
H	-4.41528900	1.19611300	1.87242800
H	-4.94288500	0.12921600	3.20752000
O	-3.44071900	2.24508100	-0.40175100
H	-4.37382800	2.13523500	-0.63898200