Supplementary information (SI)

Antioxidant Motifs in Flavonoids: O-H versus C-H Bond Dissociation

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Table S1: BDE values of the X–H (X = O, C) bond breaking of different compounds in the gas phase using B3LYP/3-21g and ROB3LYP/6-311G++G(2df,2p)//B3LYP/6-311G(d,p) methods.

Comp. No	X-H (X = O, C) position	BDEs kcal/mol	
		B3LYP/3-21G	ROB3LYP/6-311G++G(2df,2p)//B3LYP/6-311G(d,p)
1	1		
	O5-H	83.6	
	O7-H	**82.6**	93.6
	O4'-H	**82.8**	87.5
	O3-H	90.5	
	C2-H	81.3	
	C3-H	**66.5**	73.0
2	2		
	O5-H	79.9	
	O7-H	81.7	
	O3'-H	71.9	
	O4'-H	**64.9**	79.0
	O3-H	90.5	
	2-C2-H	79.9	
	2-C3-H	**65.7**	73.4
3	3		
	3-O5-H	84.0	
	3-O7-H	84.0	
	3-O3-H	**76.8**	85.2
	3-O4'-H	**77.1**	85.4
4	4		
	O7-H	**71.4**	79.3
	O8-H	78.0	
	O4'-H	78.9	
	O3-H	98.6	
	C2-H	82.0	
	C3-H	**74.1**	76.1
5	5		
	5-O5-H	80.0	
	5-O7-H	81.6	
	5-O4'-H	**79.4**	88.0
	5-C2-H	**79.8**	80.5
	5-C3-H	91.5	
6	6		
	6-O5-H	97.5	

	6-O7-H	**85.7**	94.0
	6-O3-H	93.7	
	6-C2-H	74.6	
	6-C3-H	**66.5**	73.5
7	7		
	7-O5-H	98.9	
	7-O7-H	**85.5**	93.5
	7-C2-H	**81.4**	82.9
	7-C3-H	91.8	
8	8		
	8-O5-H	78.0	
	8-O7-H	79.6	
	8-O4'-H	**69.4**	77.2
	8-O3'-H	83.8	
	8-O3-H	95.1	
	8-C2-H	**81.9**	82.5
	8-C3-H	92.0	
	8-C4-H	86.2	
9	9		
	O7-H	**68.8**	77.0
	O8-H	76.7	
	O3'-H	81.4	
	O4'-H	**70.4**	77.8
	O3-H	92.7	
	O4-H	89.7	
	C2-H	78.8	
	C3-H	93.9	
	C4-H	**77.2**	80.3
10	10		
	O7-H	**69.0**	77.1
	O8-H	76.9	
	O4'-H	80.0	
	O3-H	92.7	
	O4-H	89.4	
	C2-H	78.4	
	C3-H	94.0	
	C4-H	**77.4**	80.1
11	11		
	O7-H	**70.1**	77.7
	O8-H	77.2	
	O4'-H	**69.3**	77.3
	O5'-H	80.9	

	O3-H	99.2	
	O4-H	96.2	
	C2-H	**82.0**	82.6
	C3-H	91.0	
	C4-H	84.6	
12	12		
	O5-H	81.9	
	O7-H	69.2	
	O4'-H	**69.8**	78.2
	O5'-H	81.0	
	O3-H	90.4	
	C2-H	80.7	
	C3-H	**65.5**	73.7
13	13		
	O7-H	**70.3**	77.8
	O8-H	77.3	
	O4'-H	79.0	
	O3-H	99.0	
	O4-H	96.3	
	C2-H	**81.5**	82.2
	C3-H	91.1	
	C4-H	84.7	

Table S2: Proton affinities (PA) of the X–H (X = O, C) bond breaking in the gas phase calculated using B3LYP/3-21g and ROB3LYP/6-311G++G(2df,2p)//B3LYP/6-311G(d,p) methods.

Comp. No	X-H (X = O, C) position	PAs kcal/mol	
		B3LYP/3-21G	ROB3LYP/6-311G++G(2df,2p)//B3LYP/6-311G(d,p)
1			
	O5-H	340.1	
	O7-H	**337.6**	326.8
	O4'-H	348.0	
	O3-H	373.5	
	C2-H	370.0	
	C3-H	360.9	
2	2		
	O5-H	340.6	
	O7-H	323.2	
	O3'-H	356.0	
	O4'-H	**321.5**	323.4
	O3-H	361.3	
	2-C2-H	362.7	
	2-C3-H	341.9	
3	3		
	3-O5-H	351.1	
	3-O7-H	336.1	
	3-O3-H	342.0	
	3-O4'-H	**335.5**	327.3
4	4		
	O7-H	**324.8**	318.6
	O8-H	348.4	
	O4'-H	353.6	
	O3-H	373.2	
	C2-H	374.6	
	C3-H	364.2	
5	5		
	5-O5-H	337.6	
	5-O7-H	**335.1**	330.0
	5-O4'-H	345.2	
	5-C2-H	373.0	
	5-C3-H	369.0	
6	6		
	6-O5-H	337.5	
	6-O7-H	**320.8**	320.0
	6-O3-H	372.1	

	6-C2-H	366.4	
	6-C3-H	359.5	
7	7		
	7-O5-H	360.2	
	7-O7-H	**338.9**	329.4
	7-C2-H	371.3	
	7-C3-H	355.9	
8	8		
	8-O5-H	351.0	
	8-O7-H	347.1	
	8-O4'-H	**345.3**	333.4
	8-O3'-H	383.6	
	8-O3-H	361.7	
	8-C2-H	381.1	
	8-C3-H	347.1	
	8-C4-H	388.7	
9	9		
	O7-H	345.3	
	O8-H	361.6	
	O3'-H	353.0	
	O4'-H	**336.2**	328.1
	O3-H	358.5	
	O4-H	358.5	
	C2-H	375.9	
	C3-H	399.4	
	C4-H	384.5	
	10		
10	O7-H	**345.0**	334.6
	O8-H	361.2	
	O4'-H	348.1	
	O3-H	357.0	
	O4-H	357.0	
	C2-H	377.2	
	C3-H	399.0	
	C4-H	383.5	
11	11		
	O7-H	**336.0**	330.5
	O8-H	353.5	
	O4'-H	340.3	
	O5'-H	359.0	
	O3-H	358.8	
	O4-H	358.9	
	C2-H	377.8	

	C3-H	405.1	
	C4-H	386.1	
12	12		
	O5-H	341.5	
	O7-H	**324.1**	328.1
	O4'-H	338.7	
	O5'-H	362.7	
	O3-H	356.3	
	C2-H	362.7	
	C3-H	342.9	
13	13		
	O7-H	**335.5**	330.1
	O8-H	352.9	
	O4'-H	352.1	
	O3-H	357.5	
	O4-H	357.5	
	C2-H	378.4	
	C3-H	404.3	
	C4-H	385.3	

Table S3: The calculated thermal properties (in Kcal/mol) of the reaction between the studied compounds (for the lowest PAs(X–H)) with HOO• radical *via* sequential proton process in the studied solvents using the ROB3LYP/6-311G++G(2df,2p)//B3LYP/6-311G(d,p) methods

Comp.	Thermal properties of the reaction between the studied compounds with HOO• radical *via* sequential proton process (in Kcal/mol)					
	GAS		**WATER**		**ETHANOL**	
	ΔH	**ΔG**	**ΔH**	**ΔG**	**ΔH**	**ΔG**
1	171.6	120.4	63.2	62.8	66.2	65.9
2	169.0	119.3	62.2	62.7	65.2	65.8
3	172.9	125.9	66.0	66.0	69.0	69.0
4	164.2	116.7	58.7	59.5	61.6	62.4
5	175.6	122.4	63.9	63.6	67.1	66.8
6	165.6	119.5	59.1	59.5	62.0	62.5
7	175.0	124.7	63.8	63.7	66.9	66.9
8	179.0	122.0	66.8	67.0	70.0	70.2
9	174.4	121.7	65.7	66.0	68.7	69.0
10	180.2	124.3	67.1	67.7	70.4	70.9
11	176.1	123.2	66.5	66.8	69.5	69.9
12	173.7	122.7	65.2	65.8	68.3	68.9
13	175.7	124.4	66.3	66.9	69.4	70.0

Table S4: Cartesian coordinates and molecular enthalpies of all parent molecules, radicals and anions optimized at B3LYP/6-311G(d,p) level of theory in the gas phase.

Name of compound (1)	**Dihydrokaempferol**
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)	
C -2.60442300 -0.06541200 1.11605500	
C -3.22242000 -1.28621900 0.88546900	
C -1.83082600 -1.61342900 -1.09979400	
H -3.99857500 -1.64159800 1.54871800	
C -0.99022800 1.70107000 0.42567900	
C 0.68639700 1.02153900 -1.34981200	
C -0.01724500 2.17656800 -0.65183000	
O -0.26387800 -0.01028600 -1.75265400	
O -1.27772500 2.47260300 1.35488900	
C 1.83658400 0.39353200 -0.58701400	
C 2.73288400 -0.41296400 -1.29595000	
C 2.04225000 0.54906600 0.78910600	
C 3.79464400 -1.04605100 -0.66279800	
H 2.59348200 -0.55326300 -2.36250200	
C 3.10268900 -0.07504300 1.43515900	
H 1.37955000 1.16686400 1.38282500	
C 3.98395100 -0.87854400 0.71174000	
H 4.47951700 -1.66498500 -1.23515100	
O 5.00701300 -1.46654700 1.39387700	
H 5.53713700 -1.99242300 0.78601600	
C -1.20829300 -0.39637700 -0.86854900	
C -1.58061100 0.40820500 0.23790800	
O -0.76056500 2.88094800 -1.64590500	
H -1.22487100 3.60037800 -1.20306300	
H -1.52367400 -2.21226500 -1.94894200	
O -2.98661900 0.66836700 2.16642800	
H -2.46050900 1.50298600 2.14825000	
H 3.26049400 0.04925400 2.49929800	
C -2.83493000 -2.04179400 -0.22191200	
O -3.47159100 -3.22475700 -0.40476500	
H -3.13267100 -3.65193000 -1.19883700	
H 1.04794200 1.39830800 -2.30764600	
H 0.72656200 2.83116200 -0.18466800	
Frequency and Energy at B3LYP/6-311G(d,p) in gas phase	
Zero-point correction= 0.248814 (Hartree/Particle)	
Thermal correction to Energy= 0.266037	
Thermal correction to Enthalpy= 0.266981	
Thermal correction to Gibbs Free Energy= 0.203157	
Sum of electronic and zero-point Energies= -1030.181779	
Sum of electronic and thermal Energies= -1030.164555	
Sum of electronic and thermal Enthalpies= -1030.163611	
Sum of electronic and thermal Free Energies= -1030.227436	
Name of radical	C3-H
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)	
C 3.45108800 0.58783800 -0.25918400	
C 4.23779100 -0.55822900 -0.23542300	
C 2.25696400 -1.90748500 0.24803600	
H 5.30142400 -0.49558000 -0.41887100	
C 1.21165700 1.67433100 -0.05843000	

C	-0.69334400	0.18817300	0.81524200
C	-0.15595700	1.48543200	0.29243200
O	0.13516400	-0.92343800	0.40123900
O	1.60683900	2.83832600	-0.35774600
C	-2.11589200	-0.10534800	0.39531100
C	-3.15407400	-0.04322600	1.32029900
C	-2.41383500	-0.43136000	-0.93258900
C	-4.46945500	-0.29265700	0.93630500
H	-2.94151400	0.20299700	2.35527400
C	-3.71715100	-0.68962100	-1.32602400
H	-1.61374800	-0.49392400	-1.66101900
C	-4.75413500	-0.61785000	-0.38993700
H	-5.26958400	-0.24040200	1.66865300
O	-6.01651100	-0.87950700	-0.83351700
H	-6.63696200	-0.79299400	-0.10232700
C	1.47862400	-0.76109500	0.23040000
C	2.05363800	0.50291500	-0.01402700
O	-0.94350200	2.55785500	0.31813100
H	-0.35972200	3.29389300	0.03615600
H	1.78888800	-2.86628600	0.43707400
O	4.02287500	1.77159100	-0.51869300
H	3.30788100	2.45061900	-0.53211000
H	-3.95626700	-0.94738100	-2.35042000
C	3.63465900	-1.79075100	0.01283800
O	4.44668300	-2.87928300	0.02163700
H	3.92230900	-3.66912800	0.19108700
H	-0.65855800	0.22743200	1.91659300

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.235990 (Hartree/Particle)
Thermal correction to Energy= 0.253108
Thermal correction to Enthalpy= 0.254053
Thermal correction to Gibbs Free Energy= 0.189238
Sum of electronic and zero-point Energies= -1029.569276
Sum of electronic and thermal Energies= -1029.552157
Sum of electronic and thermal Enthalpies= -1029.551213
Sum of electronic and thermal Free Energies= -1029.616028

Name of radical	O4’-H

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

C	-2.60784400	0.12613600	1.15842000
C	-3.42977400	-0.94576000	0.83867700
C	-2.11413000	-1.35121100	-1.18359200
H	-4.25855700	-1.21008600	1.48042600
C	-0.72204700	1.64699800	0.57537000
C	0.78867500	0.85612200	-1.31000900
C	0.27864300	2.05556900	-0.50346000
O	-0.26718600	-0.02883300	-1.71207400
O	-0.87276700	2.38324800	1.55986100
C	1.91468400	0.11266200	-0.61406400
C	1.76229900	-1.19562100	-0.11245200
C	3.17037000	0.75809500	-0.49972200
C	2.80986700	-1.83576600	0.50683000
H	0.81157800	-1.70117800	-0.21818600
C	4.23116900	0.14124300	0.11045300
H	3.29283400	1.75517100	-0.91191700

C	4.10423900	-1.19899600	0.65544300
H	2.70831000	-2.83906100	0.90333100
O	5.06212700	-1.77449100	1.21527500
C	-1.28935400	-0.28627500	-0.85888600
C	-1.51370700	0.48057500	0.30900300
O	-0.37419500	2.93136000	-1.41844100
H	-0.72081400	3.67597300	-0.91337000
H	-1.91780000	-1.92029100	-2.08443700
O	-2.85998100	0.82974400	2.26502000
H	-2.19866500	1.56008800	2.31000600
H	5.19795000	0.62174500	0.20229200
C	-3.18214900	-1.66511600	-0.33054800
O	-4.01877100	-2.69495600	-0.59962100
H	-3.76605300	-3.11145400	-1.43079200
H	1.16868100	1.25773600	-2.25337900
H	1.12307300	2.55085300	-0.01290500

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.235446 (Hartree/Particle)
Thermal correction to Energy= 0.252461
Thermal correction to Enthalpy= 0.253405
Thermal correction to Gibbs Free Energy= 0.189005
Sum of electronic and zero-point Energies= -1029.549816
Sum of electronic and thermal Energies= -1029.532801
Sum of electronic and thermal Enthalpies= -1029.531857
Sum of electronic and thermal Free Energies= -1029.596257

Name of anion	C3-H

Cartesian Coordinates optimized at B3LYP/6-311G(d,p

C	3.37596700	0.61224000	-0.38163300
C	4.20828100	-0.51391900	-0.30933700
C	2.31475200	-1.86392900	0.41186400
H	5.25753300	-0.43297500	-0.56345300
C	1.11988700	1.67415800	-0.13140300
C	-0.67769600	0.23748800	0.89452400
C	-0.16620100	1.49462300	0.26932600
O	0.16737300	-0.90292500	0.61305100
O	1.58674300	2.83620700	-0.53001600
C	-2.08777000	-0.12322300	0.43746200
C	-3.18919700	0.48085100	1.04147600
C	-2.31474700	-1.02317400	-0.60524300
C	-4.48666900	0.19851700	0.61792700
H	-3.02842300	1.19537000	1.84122000
C	-3.60539200	-1.32429400	-1.02991000
H	-1.46310500	-1.49462700	-1.07907000
C	-4.69674200	-0.70924800	-0.41878300
H	-5.33507600	0.68561900	1.09394700
O	-5.95862800	-1.03381000	-0.87087200
H	-6.59493700	-0.50892800	-0.37576500
C	1.50013900	-0.73185700	0.33599500
C	2.00672300	0.50603600	-0.05143500
O	-1.01029700	2.60018500	0.35438000
H	-0.42062800	3.31116100	0.04572400
H	1.88779900	-2.81273500	0.72161700
O	3.86490100	1.80051100	-0.76997500
H	3.04361600	2.42786100	-0.74539700

H	-3.78346100	-2.02891600	-1.83449400
C	3.66652400	-1.73392200	0.08214800
O	4.51961200	-2.82268800	0.14213300
H	3.99402900	-3.58315400	0.40739600
H	-0.72212300	0.33940800	2.00080400

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.232475 (Hartree/Particle)
Thermal correction to Energy= 0.249968
Thermal correction to Enthalpy= 0.250912
Thermal correction to Gibbs Free Energy= 0.186056
Sum of electronic and zero-point Energies= -1029.635092
Sum of electronic and thermal Energies= -1029.617599
Sum of electronic and thermal Enthalpies= -1029.616655
Sum of electronic and thermal Free Energies= -1029.681510

Name of anion	O7-H

Cartesian Coordinates optimized at B3LYP/6-311G(d,p

C	-2.53452900	-0.13729000	1.21752700
C	-3.28176800	-1.21883600	0.83922600
C	-2.08099800	-1.28831500	-1.31479700
H	-4.02806500	-1.62134500	1.51439700
C	-0.80884500	1.59111300	0.70410400
C	0.65663100	1.09201000	-1.29878000
C	0.07524000	2.18802600	-0.39184500
O	-0.39151100	0.26649800	-1.81714500
O	-0.88589800	2.18647700	1.80833700
C	1.78212600	0.29019900	-0.65895500
C	1.65919000	-1.06711100	-0.36084900
C	3.00327300	0.91663200	-0.38203500
C	2.71750500	-1.77148600	0.20947000
H	0.73085000	-1.58168800	-0.57102600
C	4.06632900	0.22455800	0.18633500
H	3.13119400	1.96893400	-0.61755800
C	3.92204500	-1.12917900	0.48811800
H	2.59807700	-2.82689900	0.44119600
O	4.99501600	-1.77952600	1.04954600
H	4.73472000	-2.68817000	1.23080600
C	-1.34747500	-0.20879700	-0.92737800
C	-1.53438300	0.43547100	0.34040200
O	-0.66437200	3.13145800	-1.17760400
H	-1.44193600	2.66114000	-1.50045800
H	-1.90428300	-1.75424200	-2.27707000
O	-2.72220800	0.43826500	2.43021600
H	-2.08486200	1.19453600	2.47750900
H	5.00861500	0.71478400	0.40135200
C	-3.11865400	-1.85853500	-0.45488200
O	-3.79690000	-2.83968700	-0.81468000
H	1.05375200	1.59663500	-2.18522300
H	0.87479900	2.75766800	0.08274700

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.235296 (Hartree/Particle)
Thermal correction to Energy= 0.252330
Thermal correction to Enthalpy= 0.253274
Thermal correction to Gibbs Free Energy= 0.189799
Sum of electronic and zero-point Energies= -1029.657324

Sum of electronic and thermal Energies=	-1029.640291
Sum of electronic and thermal Enthalpies=	-1029.639347
Sum of electronic and thermal Free Energies=	-1029.702822
Name of anion	O4'-H

Cartesian Coordinates optimized at B3LYP/6-311G(d,p

C	-2.54809700	-0.10643100	1.11501700
C	-3.18753200	-1.30111400	0.80740400
C	-1.85081700	-1.48486700	-1.23011000
H	-3.93713200	-1.70980800	1.47089500
C	-0.91184900	1.68740300	0.54695000
C	0.82402400	1.14703400	-1.22615100
C	0.03331700	2.24084600	-0.52187300
O	-0.30913800	0.18925500	-1.80105700
O	-1.13674500	2.33922000	1.57860800
C	1.88910400	0.43346400	-0.52250800
C	2.92369500	-0.16767500	-1.28403200
C	1.96026500	0.26399300	0.88398100
C	3.94548000	-0.88084800	-0.70904500
H	2.89679200	-0.05342800	-2.36756300
C	2.97853400	-0.44042100	1.48107400
H	1.20440100	0.71390300	1.52198400
C	4.04876000	-1.07669900	0.72911100
H	4.73092000	-1.32196700	-1.31667200
O	4.97745800	-1.71968300	1.26700700
C	-1.21285400	-0.27920800	-0.93578500
C	-1.55704400	0.43329500	0.24427500
O	-0.76418600	2.96767700	-1.46943100
H	-1.15424600	2.29922400	-2.04714900
H	-1.55859600	-2.02626800	-2.12291100
O	-2.88199200	0.54171400	2.24123500
H	-2.30946000	1.35032000	2.27482400
H	3.02081300	-0.54138500	2.56179000
C	-2.82724900	-1.97380500	-0.36165000
O	-3.47445200	-3.14945800	-0.61891600
H	-3.10109100	-3.53041300	-1.42047900
H	1.17460500	1.53612000	-2.18230500
H	0.69901400	2.96409500	-0.05192200

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction=	0.234318 (Hartree/Particle)
Thermal correction to Energy=	0.251383
Thermal correction to Enthalpy=	0.252327
Thermal correction to Gibbs Free Energy=	0.189323
Sum of electronic and zero-point Energies=	-1029.644080
Sum of electronic and thermal Energies=	-1029.627015
Sum of electronic and thermal Enthalpies=	-1029.626071
Sum of electronic and thermal Free Energies=	-1029.689075
Name of cationic radical	

Cartesian Coordinates optimized at B3LYP/6-311G(d,p

C	2.66110900	-0.02557200	1.06857200
C	3.34066300	1.19468000	0.82091700
C	1.87553600	1.62823200	-1.06572100
H	4.15933000	1.49094600	1.46378600
C	0.94834700	-1.72547300	0.44424700
C	-0.74463900	-0.99633900	-1.30804400

C	-0.00919800	-2.17280700	-0.66150700
O	0.21300800	0.10976600	-1.64615900
O	1.20552200	-2.44118700	1.40917700
C	-1.88335200	-0.35970000	-0.56314800
C	-2.88500200	0.29035200	-1.31201000
C	-1.98318700	-0.35602500	0.84140600
C	-3.95343600	0.90918900	-0.69503400
H	-2.82127000	0.29807700	-2.39419800
C	-3.04771000	0.25375200	1.47376300
H	-1.24528300	-0.85822000	1.45422600
C	-4.04292500	0.89649300	0.70926700
H	-4.72424200	1.39271300	-1.28552400
O	-5.04490000	1.46719000	1.38600700
H	-5.68887300	1.87400300	0.79146800
C	1.20940600	0.40238400	-0.82219000
C	1.59743700	-0.44631200	0.23073200
O	0.71659700	-2.91883000	-1.62393200
H	1.41295600	-2.37561800	-2.01204300
H	1.52508600	2.25177400	-1.87941600
O	3.05842000	-0.75346000	2.08352100
H	2.48380000	-1.56887400	2.12381000
H	-3.15001600	0.24159200	2.55133000
C	2.95096600	2.00449700	-0.25356200
O	3.64220600	3.13782400	-0.42602200
H	3.32595600	3.64042100	-1.18685500
H	-1.06959400	-1.31771400	-2.29612200
H	-0.73876000	-2.86363800	-0.23732500

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.247249 (Hartree/Particle)
Thermal correction to Energy= 0.264739
Thermal correction to Enthalpy= 0.265683
Thermal correction to Gibbs Free Energy= 0.200510
Sum of electronic and zero-point Energies= -1029.898406
Sum of electronic and thermal Energies= -1029.880915
Sum of electronic and thermal Enthalpies= -1029.879971
Sum of electronic and thermal Free Energies= -1029.945144

Name of compound (2)	**Dihydromyricetin**

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

C	2.95448900	-0.03544300	1.21481500
C	3.72505900	1.06903000	0.86831500
C	3.49610800	1.70113600	-0.35623300
C	2.49891300	1.27109800	-1.23859900
H	4.49723100	1.40821700	1.54920800
C	1.20127000	-1.70251100	0.63788700
C	-0.25919700	-1.11972100	-1.35330400
C	0.28959400	-2.23535400	-0.46271300
O	0.77180300	-0.20393000	-1.76954200
O	1.34828300	-2.36335800	1.67608300
O	4.22332300	2.77719800	-0.74652000
H	4.88098300	2.98070900	-0.07250500
C	-1.44177900	-0.38624000	-0.73031300
C	-1.39010600	0.98073700	-0.45396800
C	-2.61522800	-1.10127000	-0.47462400

C	-2.50210700	1.61426200	0.09508000
H	-0.49975000	1.55705800	-0.67093200
C	-3.72466700	-0.46177800	0.07082000
H	-2.70052400	-2.15734500	-0.70153700
C	-3.66736100	0.90292000	0.36147700
H	-0.57783100	-1.58814600	-2.28696900
O	-4.78589500	1.48747400	0.89808400
H	-4.59655900	2.42266300	1.04355300
C	1.72563700	0.17568300	-0.88831700
C	1.93490200	-0.50541800	0.33692500
H	-0.54221400	-2.76599000	0.00943600
O	1.05705200	-3.10802700	-1.29169900
H	1.40277100	-3.81189300	-0.73122200
O	-4.86246200	-1.16491300	0.31605600
H	-5.51318800	-0.55529500	0.68793400
H	2.34024900	1.78069600	-2.17858500
O	3.19079100	-0.65370200	2.37544500
H	2.57072100	-1.42140900	2.42780200
O	-2.55628900	2.95197900	0.40913200
H	-1.70788800	3.36618400	0.22402400

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.257141 (Hartree/Particle)
Thermal correction to Energy= 0.276962
Thermal correction to Enthalpy= 0.277906
Thermal correction to Gibbs Free Energy= 0.208744
Sum of electronic and zero-point Energies= -1180.662895
Sum of electronic and thermal Energies= -1180.643075
Sum of electronic and thermal Enthalpies= -1180.642130
Sum of electronic and thermal Free Energies= -1180.711292

Name of radical	C3-H

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

C	-3.43062100	0.15272200	0.72961200
C	-4.05832100	-1.05883700	0.45327900
C	-3.51506600	-1.90142900	-0.51905400
C	-2.34985100	-1.56870100	-1.22061800
H	-4.96503100	-1.31694000	0.98836200
C	-1.59227700	1.77590300	0.29242800
C	0.29503500	0.98331500	-1.26404500
C	-0.37193500	2.00334200	-0.40026800
O	-0.62902200	-0.05115200	-1.68108500
O	-2.02500100	2.66898400	1.07969200
O	-4.08793700	-3.09255300	-0.83107900
H	-4.87781000	-3.21714000	-0.29402200
C	1.52886000	0.37352000	-0.61457300
C	1.42467400	-0.30572000	0.60550000
C	2.76182200	0.48785400	-1.25066700
C	2.56088100	-0.87235600	1.16793700
H	0.46949600	-0.40031600	1.11063600
C	3.90194800	-0.07302000	-0.67567400
H	2.86226300	1.00718600	-2.19581500
C	3.79969500	-0.75669800	0.53557200
H	0.60776100	1.46506700	-2.19510800
O	4.94381600	-1.29638300	1.06086300
H	4.71719000	-1.73996100	1.88780300

C	-1.72657100	-0.36472100	-0.93988100
C	-2.24342300	0.51242700	0.04180100
O	0.25379500	3.16218600	-0.21054400
H	-0.31349300	3.64819500	0.42363800
O	5.10445100	0.04252900	-1.29881100
H	5.76480900	-0.41003600	-0.75804700
H	-1.95048100	-2.23551800	-1.97150800
O	-3.96069900	0.97202400	1.64834800
H	-3.40625300	1.78942200	1.66864700
O	2.58590900	-1.56772700	2.35295400
H	1.69993700	-1.61882500	2.72462600

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.244637 (Hartree/Particle)
Thermal correction to Energy= 0.264327
Thermal correction to Enthalpy= 0.265271
Thermal correction to Gibbs Free Energy= 0.194928
Sum of electronic and zero-point Energies= -1180.049653
Sum of electronic and thermal Energies= -1180.029963
Sum of electronic and thermal Enthalpies= -1180.029019
Sum of electronic and thermal Free Energies= -1180.099363

Name of radical	O4'-H

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

C	-2.94407400	0.07879900	1.19478300
C	-3.72867800	-1.01465400	0.84481900
C	-3.49329700	-1.66087400	-0.37074600
C	-2.47475400	-1.25503000	-1.24210200
H	-4.51656900	-1.33451900	1.51688200
C	-1.15282700	1.70938700	0.63144800
C	0.32324300	1.08413100	-1.33746400
C	-0.21192000	2.21772500	-0.45711900
O	-0.71252300	0.18354500	-1.75910000
O	-1.30153900	2.38175900	1.66130900
O	-4.23158200	-2.72590500	-0.76464200
H	-4.90187200	-2.91756500	-0.09943100
C	1.49562100	0.34471300	-0.70801000
C	1.40810600	-1.02263800	-0.39594200
C	2.68462300	1.06225200	-0.48716200
C	2.48143900	-1.69421200	0.16258800
H	0.49253500	-1.56337500	-0.60154200
C	3.76983900	0.41561700	0.06400900
H	2.77076900	2.10939600	-0.75162000
C	3.72965300	-1.00099400	0.42567800
H	0.66336000	1.54543000	-2.26813400
O	4.75000000	-1.52307800	0.92108200
C	-1.68948400	-0.17142400	-0.88816900
C	-1.90257000	0.52364200	0.32838100
H	0.62385800	2.73115100	0.02739400
O	-0.94181100	3.10089800	-1.30549200
H	-1.28774600	3.81391500	-0.75655300
O	4.93080400	1.03005700	0.30114500
H	5.50499900	0.33630500	0.68555300
H	-2.31159400	-1.77504300	-2.17557100
O	-3.18725600	0.70943700	2.34605400
H	-2.55564000	1.46684300	2.40518600

O	2.46286900	-2.99930300	0.49226700
H	1.59667300	-3.37044700	0.28690400

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.245446 (Hartree/Particle)
Thermal correction to Energy= 0.264444
Thermal correction to Enthalpy= 0.265388
Thermal correction to Gibbs Free Energy= 0.197017
Sum of electronic and zero-point Energies= -1180.043581
Sum of electronic and thermal Energies= -1180.024584
Sum of electronic and thermal Enthalpies= -1180.023640
Sum of electronic and thermal Free Energies= -1180.092010

Name of anion C3-H

Cartesian Coordinates optimized at B3LYP/6-311G(d,p

C	3.30092300	-0.33836200	0.89479500
C	4.00412000	0.86726400	0.74029400
C	3.58787700	1.78557200	-0.22128700
C	2.47963900	1.54316400	-1.03383800
H	4.87453100	1.05231300	1.36362200
C	1.44594900	-1.87124400	0.21828200
C	-0.24657600	-0.90707000	-1.37651100
C	0.33013200	-2.00475200	-0.54017000
O	0.72751200	0.10808900	-1.70489900
O	1.89816500	-2.81066600	1.02132200
O	4.25670900	2.98334600	-0.40723100
H	4.99167500	2.99693300	0.21307200
C	-1.48437900	-0.25546300	-0.74185800
C	-1.45327800	1.06952700	-0.30135400
C	-2.65770800	-1.00440400	-0.60048700
C	-2.57882200	1.62271700	0.29761600
H	-0.55531400	1.66271200	-0.42634600
C	-3.78091900	-0.43901700	-0.00614600
H	-2.68919200	-2.04030900	-0.91209200
C	-3.74424200	0.88105100	0.44517400
H	-0.56243300	-1.31357400	-2.34932600
O	-4.88258400	1.40323100	1.03618900
H	-4.64982300	2.28228000	1.35796200
C	1.78884600	0.34161300	-0.86323200
C	2.16622900	-0.59546700	0.09777100
O	-0.41443700	-3.18155800	-0.49204300
H	0.06843900	-3.69368700	0.17900200
O	-4.93174400	-1.17012500	0.14391200
H	-5.56322700	-0.60472700	0.60544900
H	2.17942100	2.25531900	-1.79142800
O	3.69683200	-1.25549500	1.78821100
H	3.03753100	-2.04982100	1.63279000
O	-2.64151400	2.92286800	0.77550900
H	-1.74987900	3.28427400	0.78523700

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.241209 (Hartree/Particle)
Thermal correction to Energy= 0.261174
Thermal correction to Enthalpy= 0.262118
Thermal correction to Gibbs Free Energy= 0.192237
Sum of electronic and zero-point Energies= -1180.116646
Sum of electronic and thermal Energies= -1180.096681

Sum of electronic and thermal Enthalpies=	-1180.095737
Sum of electronic and thermal Free Energies=	-1180.165618
Name of anion	O4'-H
Cartesian Coordinates optimized at B3LYP/6-311G(d,p	
C	3.07880200 0.08615400 0.99945100
C	3.64982400 1.33492700 0.79555200
C	3.18600100 2.12780700 -0.26215700
C	2.16905400 1.70978800 -1.11390200
H	4.44387000 1.66978800 1.45395100
C	1.48594200 -1.68938600 0.31503900
C	-0.31088200 -1.03534200 -1.38366000
C	0.46324100 -2.16111200 -0.71082600
O	0.63946900 0.07565800 -1.76707600
O	1.86714900 -2.49379600 1.18874700
O	3.72301200 3.36127900 -0.49647600
H	4.37451200 3.54449300 0.18802200
C	-1.49696400 -0.51816300 -0.64756400
C	-1.56334900 -0.47002100 0.76280900
C	-2.57514100 -0.00700400 -1.40114300
C	-2.67672900 0.06739200 1.38469700
H	-0.76467400 -0.85521800 1.38762700
C	-3.67966500 0.53077000 -0.76673300
H	-2.54466300 -0.03071200 -2.48657300
C	-3.77575600 0.59430400 0.65090300
H	-0.60583200 -1.38856600 -2.37157000
O	-4.81204400 1.08098900 1.23905500
C	1.58754900 0.45684400 -0.91573100
C	2.03386500 -0.37718200 0.14819300
H	-0.24698800 -2.82195100 -0.20560500
O	1.18889400 -2.88032500 -1.72332800
H	1.67963200 -3.57073500 -1.26339700
O	-4.76824500 1.02786300 -1.43998700
H	-5.34177400 1.30449900 -0.69668400
H	1.81618300 2.34974600 -1.91007800
O	3.53122000 -0.68548800 1.99908800
H	3.01388300 -1.53069000 1.95182900
O	-2.81714000 0.12465000 2.74869600
H	-3.69742700 0.54403800 2.83314200
Frequency and Energy at B3LYP/6-311G(d,p) in gas phase	
Zero-point correction=	0.244264 (Hartree/Particle)
Thermal correction to Energy=	0.263300
Thermal correction to Enthalpy=	0.264244
Thermal correction to Gibbs Free Energy=	0.196454
Sum of electronic and zero-point Energies=	-1180.141513
Sum of electronic and thermal Energies=	-1180.122477
Sum of electronic and thermal Enthalpies=	-1180.121533
Sum of electronic and thermal Free Energies=	-1180.189322
Name of anion	O7-H
Cartesian Coordinates optimized at B3LYP/6-311G(d,p	
C	4.06027700 -0.43858400 0.02742700
C	4.72741200 0.74325100 -0.15597200
C	4.04960000 2.02011900 -0.30673900
C	2.59933500 1.93722800 -0.27420900
H	5.81484500 0.76061800 -0.19616400

C	1.87799800	-1.68485700	0.36152400
C	-0.15372100	-0.38324000	-0.35307000
C	0.35347800	-1.49430800	0.56971700
O	0.56790500	0.81019200	-0.04624800
O	2.27212200	-2.85919100	0.43878800
O	4.66338500	3.09294100	-0.46944400
C	-1.63453200	-0.07813500	-0.22137700
C	-2.05868900	1.14969500	0.29332900
C	-2.58055500	-1.02630700	-0.62317400
C	-3.41807500	1.41745300	0.40183700
H	-1.32184500	1.88512600	0.59189000
C	-3.93858700	-0.74815600	-0.50905300
H	-2.26654500	-1.99288400	-0.99212500
C	-4.36198000	0.47909500	0.00335200
H	0.05934100	-0.68184200	-1.39004000
O	-5.72125000	0.71376500	0.09296600
H	-5.83205700	1.59826000	0.46130900
C	1.95079300	0.75190500	-0.08001600
C	2.62695600	-0.50347100	0.09889700
H	0.18394800	-1.16724800	1.60878700
O	-0.28113600	-2.72860500	0.32669000
H	0.48258300	-3.34390000	0.33389600
O	-4.86962900	-1.67325900	-0.90066500
H	-5.73838100	-1.28826800	-0.73190700
H	2.03057800	2.84700700	-0.42548800
O	4.74550900	-1.61641800	0.17495800
H	5.68097800	-1.39027500	0.13590000
O	-3.93748800	2.60297000	0.89335400
H	-3.20704700	3.18412400	1.12591900

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.243114 (Hartree/Particle)
Thermal correction to Energy= 0.262885
Thermal correction to Enthalpy= 0.263829
Thermal correction to Gibbs Free Energy= 0.194772
Sum of electronic and zero-point Energies= -1180.131212
Sum of electronic and thermal Energies= -1180.111441
Sum of electronic and thermal Enthalpies= -1180.110496
Sum of electronic and thermal Free Energies= -1180.179554

Name of cationic radical

Cartesian Coordinates optimized at B3LYP/6-311G(d,p

C	3.09880700	-0.03283500	1.13304100
C	3.93034600	0.99851600	0.66049600
C	3.66711300	1.58696200	-0.57997400
C	2.56654200	1.18369100	-1.34962000
H	4.77486200	1.30064600	1.26868200
C	1.20604200	-1.60761200	0.78581500
C	-0.29902000	-1.10020300	-1.19882100
C	0.25905200	-2.18236600	-0.26547400
O	0.69071600	-0.15475000	-1.64850200
O	1.35026700	-2.17369700	1.87032200
O	4.42354600	2.56895800	-1.09486100
H	5.16948400	2.77419300	-0.51814600
C	-1.50957900	-0.36916500	-0.65551200
C	-1.41118600	0.94984000	-0.15627700

C	-2.73787100	-1.03462500	-0.69144000
C	-2.53444900	1.57285500	0.34533200
H	-0.46639300	1.47649100	-0.17340700
C	-3.87557900	-0.42433600	-0.18438600
H	-2.82976000	-2.03269800	-1.10151100
C	-3.77729400	0.89611200	0.34051100
H	-0.59550800	-1.61517000	-2.11649500
O	-4.89395500	1.45183400	0.80889900
H	-4.71610700	2.34922900	1.13527200
C	1.74276000	0.15846400	-0.87328000
C	1.99142200	-0.47590300	0.36381500
H	-0.56950700	-2.68642800	0.24245200
O	1.00147300	-3.06745000	-1.08943700
H	1.29961400	-3.81513300	-0.55745900
O	-5.04634500	-1.06272700	-0.19241100
H	-5.74267200	-0.51060600	0.19321300
H	2.36101700	1.65344800	-2.30162800
O	3.38737300	-0.58211800	2.29997800
H	2.72406800	-1.29562900	2.47909100
O	-2.60719400	2.82081000	0.86659700
H	-1.75878300	3.27838500	0.83990700

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.256219 (Hartree/Particle)
Thermal correction to Energy= 0.275914
Thermal correction to Enthalpy= 0.276858
Thermal correction to Gibbs Free Energy= 0.206914
Sum of electronic and zero-point Energies= -1180.389697
Sum of electronic and thermal Energies= -1180.370002
Sum of electronic and thermal Enthalpies= -1180.369058
Sum of electronic and thermal Free Energies= -1180.439002

Name of compound (3)	**Kaempferol**

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

O	-0.08738100	-0.79878200	-0.00002400
O	0.79482200	2.72780500	-0.00002700
O	-4.19202800	1.67639100	0.00002400
O	-1.82237600	2.86039100	0.00000500
O	-4.17887100	-3.09038200	0.00000600
O	6.16874300	-1.06104800	0.00002800
C	-2.10545400	0.49628800	0.00000200
C	-1.44453700	-0.74362500	-0.00000900
C	0.70323600	0.32623100	-0.00001900
C	-1.33375500	1.70356500	-0.00000500
C	0.10897800	1.55801300	-0.00001800
C	2.13001100	0.00352800	-0.00001200
C	-3.52743600	0.51428600	0.00001400
C	-2.13452200	-1.94771100	-0.00000700
C	-3.52840400	-1.89870700	0.00000500
C	-4.22836600	-0.68348100	0.00001500
C	3.12193800	1.00095500	0.00000800
C	2.54962800	-1.34188800	-0.00002500
C	4.46843200	0.66488800	0.00002400
C	3.89169100	-1.67844500	-0.00001300
C	4.86376800	-0.67443700	0.00001300

H	-1.61413600	-2.89469100	-0.00001500
H	-5.31223100	-0.65781900	0.00002400
H	2.83753200	2.04170500	0.00001600
H	1.80909000	-2.12907700	-0.00004400
H	5.21720400	1.45167800	0.00004200
H	4.20886800	-2.71399100	-0.00002200
H	0.09535600	3.40989400	-0.00002500
H	-3.52045700	2.39935100	0.00002100
H	-5.12983100	-2.93754100	0.00001500
H	6.73409500	-0.28127400	0.00005200

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.225588 (Hartree/Particle)
Thermal correction to Energy= 0.242263
Thermal correction to Enthalpy= 0.243207
Thermal correction to Gibbs Free Energy= 0.181008
Sum of electronic and zero-point Energies= -1029.017202
Sum of electronic and thermal Energies= -1029.000527
Sum of electronic and thermal Enthalpies= -1028.999583
Sum of electronic and thermal Free Energies= -1029.061782

Name of radical	O3-H

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

C	-3.54341700	0.50276100	0.00001900
C	-4.22251200	-0.71080900	0.00000100
C	-2.09696800	-1.91462000	-0.00000200
H	-5.30362500	-0.72894900	0.00000000
C	-1.38854100	1.77382600	-0.00001000
C	0.71816700	0.36415900	0.00000300
C	0.12664700	1.68677100	-0.00001500
O	-0.07015900	-0.74654400	0.00001100
O	-1.94345600	2.87623400	-0.00003600
C	2.12696300	0.05257800	0.00000500
C	2.55098900	-1.29755100	0.00000100
C	3.12881900	1.05625800	0.00001000
C	3.89265400	-1.62812100	0.00000100
H	1.81250800	-2.08639700	-0.00000300
C	4.46879800	0.72343700	0.00001100
H	2.82752100	2.09216400	0.00001200
C	4.86459900	-0.61905400	0.00000600
H	4.19421800	-2.67147000	-0.00000300
O	6.19453500	-0.88178700	0.00000600
H	6.33889000	-1.83447800	0.00000000
C	-1.43566900	-0.69733800	0.00000700
C	-2.11576500	0.52693900	0.00000800
O	0.79291900	2.72704400	-0.00004000
H	-1.53199300	-2.83872500	-0.00001000
O	-4.23463100	1.64192000	0.00007200
H	-3.57503900	2.38162400	-0.00004500
H	5.23206000	1.49161000	0.00001500
C	-3.49911100	-1.90329000	-0.00001000
O	-4.21750800	-3.05322500	-0.00002900
H	-3.62205400	-3.81019400	-0.00004100

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.212461 (Hartree/Particle)
Thermal correction to Energy= 0.229042

Thermal correction to Enthalpy= 0.229987	
Thermal correction to Gibbs Free Energy= 0.167225	
Sum of electronic and zero-point Energies= -1028.388147	
Sum of electronic and thermal Energies= -1028.371566	
Sum of electronic and thermal Enthalpies= -1028.370622	
Sum of electronic and thermal Free Energies= -1028.433383	
Name of radical	O4'-H
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)	
C -3.47733100 0.52810200 -0.00005900	
C -4.18416400 -0.66544700 -0.00010400	
C -2.09362500 -1.93976400 -0.00006300	
H -5.26767600 -0.63444300 -0.00013700	
C -1.27915800 1.70250000 0.00006700	
C 0.76796000 0.30671600 0.00007900	
C 0.17077600 1.55161000 0.00015900	
O -0.04016500 -0.80884900 0.00001000	
O -1.74920700 2.86474100 0.00010400	
C 2.17204300 -0.01357100 0.00006600	
C 2.58285800 -1.38370500 0.00046600	
C 3.18091700 0.99952500 -0.00041100	
C 3.90241800 -1.72623100 0.00039700	
H 1.82404000 -2.15348200 0.00083500	
C 4.50514900 0.66920000 -0.00049300	
H 2.88570500 2.03729900 -0.00071900	
C 4.95391600 -0.71665300 -0.00008300	
H 4.21948600 -2.76256500 0.00072700	
O 6.15784500 -1.02091100 -0.00014100	
C -1.39728300 -0.74264600 -0.00001900	
C -2.05379100 0.50265000 -0.00000800	
O 0.84623000 2.71244800 0.00028300	
H 0.14559700 3.39752900 0.00043700	
H -1.57988700 -2.89030300 -0.00006700	
O -4.13713700 1.69137500 -0.00005900	
H -3.47025700 2.41583500 0.00000500	
H 5.27556000 1.43132400 -0.00086400	
C -3.48954200 -1.88347000 -0.00009900	
O -4.14091800 -3.07053400 -0.00012800	
H -5.09260900 -2.92023900 -0.00014100	
Frequency and Energy at B3LYP/6-311G(d,p) in gas phase	
Zero-point correction= 0.212600 (Hartree/Particle)	
Thermal correction to Energy= 0.228993	
Thermal correction to Enthalpy= 0.229938	
Thermal correction to Gibbs Free Energy= 0.167670	
Sum of electronic and zero-point Energies= -1028.388635	
Sum of electronic and thermal Energies= -1028.372241	
Sum of electronic and thermal Enthalpies= -1028.371297	
Sum of electronic and thermal Free Energies= -1028.433565	
Name of anion	O3-H
Cartesian Coordinates optimized at B3LYP/6-311G(d,p	
C -3.52662500 0.51539500 0.00012400	
C -4.23076400 -0.68222900 0.00008600	
C -2.13531300 -1.93163900 -0.00007800	
H -5.31262400 -0.68105500 0.00014300	
C -1.35259800 1.76016500 -0.00009800	

C	0.70013300	0.38189600	-0.00003500
C	0.14768100	1.68901100	-0.00004900
O	-0.09783300	-0.77368400	-0.00008900
O	-1.94597800	2.86391900	-0.00023300
C	2.10974500	0.04472700	-0.00000800
C	2.54766500	-1.29877700	-0.00001100
C	3.11678300	1.04301200	0.00002300
C	3.89978100	-1.62469900	0.00001400
H	1.81408100	-2.09348200	-0.00003500
C	4.46464700	0.71102400	0.00004800
H	2.79260900	2.07454100	0.00002600
C	4.86907800	-0.62316400	0.00004400
H	4.20189100	-2.67096700	0.00001100
O	6.22539200	-0.90104900	0.00007100
H	6.32641800	-1.85760400	0.00007400
C	-1.42987300	-0.71693300	-0.00004200
C	-2.09646600	0.51742100	0.00004800
O	0.81006000	2.75435600	-0.00003200
H	-1.58703600	-2.86758000	-0.00014600
O	-4.18274400	1.68236000	0.00023000
H	-3.45470100	2.38360400	0.00045100
H	5.22279500	1.48705300	0.00007200
C	-3.52222200	-1.89119600	-0.00001900
O	-4.27240700	-3.04436400	-0.00004400
H	-3.66527400	-3.79088700	-0.00009600

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.210458 (Hartree/Particle)
Thermal correction to Energy= 0.227151
Thermal correction to Enthalpy= 0.228095
Thermal correction to Gibbs Free Energy= 0.166194
Sum of electronic and zero-point Energies= -1028.477277
Sum of electronic and thermal Energies= -1028.460585
Sum of electronic and thermal Enthalpies= -1028.459640
Sum of electronic and thermal Free Energies= -1028.521542

Name of anion	O4'-H

Cartesian Coordinates optimized at B3LYP/6-311G(d,p

C	-3.46755400	0.52490700	-0.00009300
C	-4.18577300	-0.66869400	-0.00008100
C	-2.10699900	-1.94873600	-0.00003800
H	-5.27038000	-0.63216600	-0.00007400
C	-1.26294700	1.70184400	-0.00006300
C	0.77271800	0.31056000	0.00006200
C	0.14265300	1.55780900	0.00011600
O	-0.04930900	-0.81056200	-0.00005900
O	-1.79290400	2.86612400	0.00000000
C	2.15689100	-0.01016500	0.00014200
C	2.59347400	-1.37320400	0.00046700
C	3.18402400	0.98713300	-0.00020900
C	3.91609000	-1.71266000	0.00032300
H	1.84406200	-2.15552700	0.00082700
C	4.50986100	0.65516400	-0.00033200
H	2.89506500	2.02829000	-0.00033900
C	4.98437900	-0.72115500	-0.00012700
H	4.22325400	-2.75452700	0.00054300

O	6.19315000	-1.02728700	-0.00030200
C	-1.40182500	-0.74548800	-0.00005600
C	-2.05292100	0.49205000	-0.00007800
O	0.84461500	2.73666900	0.00039300
H	0.13461500	3.40532500	0.00041000
H	-1.59016700	-2.89811200	-0.00000800
O	-4.11053100	1.70499900	-0.00009400
H	-3.39027800	2.40010900	-0.00001100
H	5.27257500	1.42841600	-0.00053100
C	-3.49725000	-1.88809900	-0.00004900
O	-4.17384300	-3.08206500	-0.00002200
H	-5.11709200	-2.89242900	-0.00004600

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.211526 (Hartree/Particle)
Thermal correction to Energy= 0.228046
Thermal correction to Enthalpy= 0.228990
Thermal correction to Gibbs Free Energy= 0.167304
Sum of electronic and zero-point Energies= -1028.490912
Sum of electronic and thermal Energies= -1028.474391
Sum of electronic and thermal Enthalpies= -1028.473447
Sum of electronic and thermal Free Energies= -1028.535134

Name of cationic radical

Cartesian Coordinates optimized at B3LYP/6-311G(d,p

O	-0.07233900	-0.79629900	0.00007000
O	0.77391400	2.69355000	-0.00015000
O	-4.20615800	1.66016000	0.00007800
O	-1.79947000	2.86940700	-0.00002200
O	-4.14075700	-3.08542500	-0.00000500
O	6.13580400	-1.04236900	0.00015300
C	-2.10767300	0.50541900	0.00003000
C	-1.44418500	-0.73674500	0.00002100
C	0.72989500	0.29212900	-0.00005600
C	-1.35306300	1.70686200	-0.00001500
C	0.11233900	1.55613500	-0.00010200
C	2.13065300	-0.00295600	-0.00006000
C	-3.53911900	0.51615400	0.00006300
C	-2.12182600	-1.93161400	0.00001100
C	-3.53762800	-1.89202300	0.00002000
C	-4.23992500	-0.68613800	0.00005600
C	3.12538300	1.01465900	0.00007800
C	2.55932800	-1.36237400	-0.00024800
C	4.46149000	0.69181300	0.00013500
C	3.89022200	-1.68557300	-0.00014700
C	4.86174400	-0.65971500	0.00006200
H	-1.60679700	-2.88179300	0.00001000
H	-5.32296800	-0.66028400	0.00006900
H	2.83934500	2.05442400	0.00015300
H	1.82120000	-2.15123800	-0.00043200
H	5.20901100	1.47766600	0.00024300
H	4.22441900	-2.71507800	-0.00026400
H	0.07895900	3.39625900	-0.00023400
H	-3.57340200	2.41200600	0.00010500
H	-5.10221700	-2.99383300	0.00001000

H	6.73869000	-0.28650700 0.00026800

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.226088 (Hartree/Particle)
Thermal correction to Energy= 0.242625
Thermal correction to Enthalpy= 0.243569
Thermal correction to Gibbs Free Energy= 0.181061
Sum of electronic and zero-point Energies= -1028.756281
Sum of electronic and thermal Energies= -1028.739744
Sum of electronic and thermal Enthalpies= -1028.738800
Sum of electronic and thermal Free Energies= -1028.801308

Name of compound (4)	**Keto-teracacidin**

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

C	-2.25762900	0.78511500	1.63933100
C	-3.18735000	-0.23798800	1.60742900
C	-3.24627900	-1.07112300	0.48605800
C	-2.38471100	-0.90065500	-0.60175200
H	-2.18282800	1.45313200	2.48780100
H	-3.86938200	-0.39888300	2.43591500
C	-0.43289100	2.09483500	0.54287400
C	0.61875500	0.96544100	-1.43284700
C	0.25745000	2.32328300	-0.79755200
O	-0.63798900	0.27248400	-1.64784500
O	-0.18659600	2.83327600	1.48236300
O	-2.41835900	-1.74107800	-1.67101800
H	-3.10728700	-2.39685300	-1.50304200
O	-4.11811800	-2.12052600	0.35930800
H	-4.64747600	-2.21063000	1.15781100
O	1.34352700	3.20182000	-0.66895000
H	1.24553900	3.59010300	0.21719800
H	-0.50671700	2.75997200	-1.46286800
C	1.60391900	0.07089500	-0.68737800
C	1.43683200	-1.31698300	-0.71467600
C	2.73657000	0.58711300	-0.04314900
C	2.35315400	-2.16325600	-0.09819700
H	0.58171800	-1.74425400	-1.22315100
C	3.65591200	-0.25165500	0.57443900
H	2.90048600	1.65507800	-0.03058100
C	3.46753900	-1.63352900	0.55283600
H	2.19964800	-3.23845900	-0.12746500
H	4.52793200	0.15022500	1.07592200
H	0.98475800	1.14936300	-2.44534700
O	4.40091200	-2.41189100	1.17657400
H	4.15652600	-3.33788000	1.07846800
C	-1.45310300	0.14150200	-0.56775700
C	-1.39315900	0.98974200	0.55632200

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

ero-point correction= 0.248282 (Hartree/Particle)
Thermal correction to Energy= 0.265733
Thermal correction to Enthalpy= 0.266677
Thermal correction to Gibbs Free Energy= 0.202780
Sum of electronic and zero-point Energies= -1030.169811
Sum of electronic and thermal Energies= -1030.152360
Sum of electronic and thermal Enthalpies= -1030.151416

Sum of electronic and thermal Free Energies=	-1030.215313
Name of radical	O7-H
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)	
C	-2.29327100 0.68859100 1.65722500
C	-3.19133900 -0.33098600 1.68015500
C	-3.28325500 -1.22386500 0.54835500
C	-2.37610300 -0.98260500 -0.58550600
H	-2.19817500 1.37732000 2.48810600
H	-3.85036800 -0.50985500 2.51975700
C	-0.51970900 2.06568800 0.51267900
C	0.57938500 0.96840300 -1.45481500
C	0.16535300 2.31253400 -0.82726800
O	-0.66014200 0.22808200 -1.66628300
O	-0.32072100 2.82125700 1.44951600
O	-2.46192400 -1.83668100 -1.59361600
H	-3.17006400 -2.46067400 -1.31598900
O	-4.05246300 -2.19828000 0.44220400
O	1.21975400 3.22878400 -0.70693600
H	1.09135900 3.65464200 0.15683700
H	-0.61525900 2.71723600 -1.49455800
C	1.58162700 0.10350700 -0.69970600
C	1.52913400 -1.28686400 -0.84549800
C	2.61321100 0.64740900 0.07669400
C	2.45698400 -2.11126500 -0.21909100
H	0.75043900 -1.73342000 -1.45141200
C	3.54511400 -0.16935000 0.70478700
H	2.69463600 1.71953100 0.18096200
C	3.47101300 -1.55500800 0.56295700
H	2.39198400 -3.18868700 -0.34107700
H	4.33904600 0.25329100 1.30825700
H	0.93583200 1.15577400 -2.46958000
O	4.41003500 -2.30867600 1.20358200
H	4.24747300 -3.24075000 1.02503200
C	-1.46065100 0.08302000 -0.58345200
C	-1.43302700 0.92074000 0.53347400
Frequency and Energy at B3LYP/6-311G(d,p) in gas phase	
ero-point correction=	0.236271 (Hartree/Particle)
Thermal correction to Energy=	0.253150
Thermal correction to Enthalpy=	0.254095
Thermal correction to Gibbs Free Energy=	0.189885
Sum of electronic and zero-point Energies=	-1029.550398
Sum of electronic and thermal Energies=	-1029.533519
Sum of electronic and thermal Enthalpies=	-1029.532574
Sum of electronic and thermal Free Energies=	-1029.596784
Name of radical	C3-H
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)	
C	2.74030300 0.82115700 -1.33473200
C	3.49696500 -0.34030500 -1.34922800
C	3.22805300 -1.34319600 -0.41729700
C	2.20926700 -1.20374200 0.53204500
H	2.92519900 1.62310000 -2.03773600
H	4.29400600 -0.47598900 -2.07322000
C	0.91854600 2.21357700 -0.33041600
C	-0.62047300 0.93493500 1.28898700

C	-0.20296900	2.16750600	0.55137300
O	0.52035100	0.09452000	1.53109300
O	1.14002700	3.26538100	-0.96649300
O	1.93919400	-2.19200300	1.42961500
H	2.56306300	-2.91027600	1.26288700
O	3.90721000	-2.53437700	-0.34974700
H	4.58271600	-2.56796900	-1.03393500
O	-0.94429000	3.26938900	0.66052100
H	-0.50474600	3.90532200	0.05268600
C	-1.73718000	0.15133200	0.58447600
C	-1.70163700	-1.24250400	0.54224200
C	-2.83703200	0.81337900	0.02659300
C	-2.73445800	-1.96005600	-0.05596500
H	-0.86484400	-1.77255500	0.97912500
C	-3.87274400	0.10408000	-0.56640100
H	-2.88869300	1.89505600	0.05355400
C	-3.82420900	-1.29055200	-0.61259500
H	-2.69002600	-3.04516100	-0.08573700
H	-4.72413100	0.61353900	-1.00082300
H	-0.96052500	1.22122900	2.28965100
O	-4.86581600	-1.93916200	-1.21155900
H	-4.71072800	-2.88862800	-1.17491200
C	1.45640600	-0.02840100	0.54315100
C	1.71538000	0.98484900	-0.39873000

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction=	0.235811 (Hartree/Particle)
Thermal correction to Energy=	0.253256
Thermal correction to Enthalpy=	0.254200
Thermal correction to Gibbs Free Energy=	0.189316
Sum of electronic and zero-point Energies=	-1029.551374
Sum of electronic and thermal Energies=	-1029.533929
Sum of electronic and thermal Enthalpies=	-1029.532985
Sum of electronic and thermal Free Energies=	-1029.597868

Name of anion	O7-H

Cartesian Coordinates optimized at B3LYP/6-311G(d,p

C	2.33296600	0.72279000	-1.62092800
C	3.20178900	-0.34085500	-1.60853900
C	3.24717500	-1.24326000	-0.49164400
C	2.33776300	-0.96240400	0.60595300
H	2.28932600	1.40057700	-2.46690600
H	3.86948300	-0.54023500	-2.44031200
C	0.56870200	2.10286300	-0.53806800
C	-0.57036700	0.99363400	1.42635800
C	-0.19047200	2.33855900	0.77729700
O	0.65958500	0.30460200	1.68864700
O	0.33944000	2.90099700	-1.46266800
O	2.37904800	-1.88403000	1.61526800
H	3.07076700	-2.49112500	1.26595700
O	3.98056100	-2.26726000	-0.38744600
O	-1.27465900	3.21279200	0.54715100
H	-1.08842700	3.52448000	-0.36218800
H	0.51896900	2.80407200	1.48048300
C	-1.56524300	0.10391000	0.68303500
C	-1.34816900	-1.27535600	0.61515700

C	-2.75186700	0.61283800	0.13893800
C	-2.27512400	-2.11698200	0.00547700
H	-0.44478700	-1.69381300	1.04032300
C	-3.68307400	-0.22278600	-0.47030100
H	-2.93371000	1.67787300	0.18504100
C	-3.44458200	-1.59350900	-0.54196100
H	-2.07986700	-3.18552500	-0.04706700
H	-4.59556700	0.17535000	-0.89935300
H	-0.97655600	1.19834000	2.42264400
O	-4.39052000	-2.38417700	-1.15495000
H	-4.06330800	-3.28913800	-1.15942400
C	1.49156900	0.11257600	0.59208500
C	1.46327200	0.99394200	-0.53739500

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.235981 (Hartree/Particle)
Thermal correction to Energy= 0.252601
Thermal correction to Enthalpy= 0.253546
Thermal correction to Gibbs Free Energy= 0.191362
Sum of electronic and zero-point Energies= -1029.657494
Sum of electronic and thermal Energies= -1029.640874
Sum of electronic and thermal Enthalpies= -1029.639929
Sum of electronic and thermal Free Energies= -1029.702114

Name of anion	C3-H

Cartesian Coordinates optimized at B3LYP/6-311G(d,p

C	2.74396700	0.84932700	-1.28015400
C	3.51033000	-0.31485600	-1.33686900
C	3.23595200	-1.34846700	-0.45110200
C	2.20876100	-1.23945300	0.49417400
H	2.92467800	1.69146900	-1.93736800
H	4.32720100	-0.41601400	-2.04749800
C	0.91839700	2.23344800	-0.25297900
C	-0.60131000	0.92135400	1.29763900
C	-0.15173800	2.15667500	0.59917700
O	0.50938400	0.02369500	1.53365400
O	1.20290300	3.29643400	-0.91956000
O	1.94279800	-2.28540100	1.34957100
H	2.54529200	-2.99116700	1.08249100
O	3.94162800	-2.55923600	-0.42470000
H	4.24555300	-2.73985000	-1.31818800
O	-0.96509500	3.28594200	0.71175700
H	-0.49084600	3.88336000	0.09498200
C	-1.73830800	0.14845900	0.60238500
C	-1.84526400	-1.23804800	0.72083100
C	-2.70540500	0.82767400	-0.14763100
C	-2.88675800	-1.93202700	0.10282400
H	-1.08981200	-1.77867900	1.27862400
C	-3.75834400	0.14658700	-0.75122900
H	-2.61610900	1.90239800	-0.25419600
C	-3.84894300	-1.23953000	-0.62840100
H	-2.94464700	-3.01585300	0.18620700
H	-4.50731800	0.67206700	-1.33318700
H	-0.95393300	1.17242400	2.30937900
O	-4.90227100	-1.87793300	-1.25198600
H	-4.80466700	-2.82266700	-1.09840900

C	1.46053500	-0.06391600 0.55349600
C	1.71309900	0.98852300 -0.34761700

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.233380 (Hartree/Particle)
Thermal correction to Energy= 0.251213
Thermal correction to Enthalpy= 0.252157
Thermal correction to Gibbs Free Energy= 0.187172
Sum of electronic and zero-point Energies= -1029.604323
Sum of electronic and thermal Energies= -1029.586490
Sum of electronic and thermal Enthalpies= -1029.585546
Sum of electronic and thermal Free Energies= -1029.650532

Name of cationic radical

Cartesian Coordinates optimized at B3LYP/6-311G(d,p

C	-2.53558800	0.92134200	1.48343200
C	-3.57542900	-0.01103300	1.40336200
C	-3.59939300	-0.91899800	0.35687200
C	-2.57270400	-0.92053000	-0.62102300
H	-2.50827000	1.64454500	2.28941900
H	-4.36264100	-0.01655700	2.14841600
C	-0.46003800	1.98469000	0.56243700
C	0.62529500	0.74367500	-1.34736600
C	0.29893900	2.13465100	-0.75050100
O	-0.57469600	-0.05627400	-1.46805100
O	-0.20610800	2.69973600	1.50738900
O	-2.55671400	-1.80651500	-1.61134000
H	-3.33584700	-2.38227400	-1.54031200
O	-4.53377700	-1.87300700	0.14811000
H	-5.23153200	-1.85367400	0.81418300
O	1.46496400	2.88298700	-0.60218800
H	1.39571200	3.34290500	0.25012000
H	-0.39812000	2.62335600	-1.45206300
C	1.71430400	-0.03900500	-0.65003100
C	1.45378400	-1.20279400	0.09937700
C	3.05242600	0.38966400	-0.80681000
C	2.47842100	-1.88372400	0.72644800
H	0.44596700	-1.58428200	0.18276800
C	4.08104200	-0.27398800	-0.18082700
H	3.26227800	1.27219400	-1.39563300
C	3.80295600	-1.42161900	0.59636500
H	2.27016600	-2.77619700	1.30664800
H	5.10829900	0.05608400	-0.26805200
H	0.93761500	0.88821200	-2.38518800
O	4.84638200	-2.02488800	1.16890100
H	4.57570100	-2.80236100	1.67560300
C	-1.52264100	0.03464100	-0.52870900
C	-1.52132900	0.96498500	0.52889300

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.247782 (Hartree/Particle)
Thermal correction to Energy= 0.265228
Thermal correction to Enthalpy= 0.266172
Thermal correction to Gibbs Free Energy= 0.201566
Sum of electronic and zero-point Energies= -1029.895164
Sum of electronic and thermal Energies= -1029.877718
Sum of electronic and thermal Enthalpies= -1029.876774

Sum of electronic and thermal Free Energies= -1029.941380

Name of compound (5)	**Naringenin**
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)	
C 2.52246200 0.46348200 -0.97294500	
C 3.18880400 -0.75353500 -1.08099000	
C 2.88942700 -1.77745300 -0.18088600	
C 1.92479400 -1.62372000 0.82177000	
H 3.93118400 -0.87920400 -1.86082500	
C 0.91603000 1.94630900 0.22282700	
C -0.66703900 0.74786300 1.77305700	
C 0.00848700 2.07246700 1.43005800	
O 0.34655700 -0.29081300 1.92319300	
O 1.11801200 2.91342800 -0.52316400	
O 3.50967600 -2.98261900 -0.24200800	
H 4.13689100 -2.98198600 -0.97323400	
H 0.63752400 2.37195800 2.27625000	
C -1.75424000 0.28284700 0.81722500	
C -2.40361700 -0.92600300 1.09189100	
C -2.15584600 1.00182700 -0.31293100	
C -3.41381200 -1.40612800 0.26939500	
H -2.10354000 -1.50631400 1.95738400	
C -3.16880800 0.53404500 -1.14339900	
H -1.68118700 1.94110000 -0.56905500	
C -3.80256100 -0.67379100 -0.85629200	
H -3.90309300 -2.34786200 0.50125500	
H -3.47584500 1.09160500 -2.01958200	
H -1.08739400 0.80916900 2.77859800	
O -4.78929200 -1.08808600 -1.70167700	
H -5.13616900 -1.93317300 -1.39757900	
C 1.26191400 -0.41387900 0.92746200	
C 1.54754600 0.66053000 0.04629000	
H 1.69634200 -2.43965200 1.49259900	
O 2.82380800 1.44424700 -1.82936500	
H 2.26791000 2.22371700 -1.58112800	
H -0.71396700 2.87221800 1.26428600	
Frequency and Energy at B3LYP/6-311G(d,p) in gas phase	
Zero-point correction= 0.244238 (Hartree/Particle)	
Thermal correction to Energy= 0.260163	
Thermal correction to Enthalpy= 0.261108	
Thermal correction to Gibbs Free Energy= 0.200128	
Sum of electronic and zero-point Energies= -954.955241	
Sum of electronic and thermal Energies= -954.939316	
Sum of electronic and thermal Enthalpies= -954.938372	
Sum of electronic and thermal Free Energies= -954.999351	
Name of radical	O4'-H
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)	
C 2.49901400 0.55642400 -1.01953200	
C 3.32825600 -0.56056100 -0.97319900	
C 3.14183200 -1.50824500 0.03388100	
C 2.12744900 -1.38063300 0.99240600	
H 4.10936900 -0.66637300 -1.71716300	
C 0.68353200 1.93718700 -0.01457200	
C -0.76634600 0.72223500 1.65708800	

C	-0.23919000	2.08255800	1.17824200
O	0.32181000	-0.19014500	1.88394700
O	0.78141700	2.83881800	-0.85332800
O	3.92224600	-2.61146100	0.12916200
H	4.57373500	-2.60782500	-0.58076200
H	0.33981900	2.54223500	1.98753200
C	-1.83667100	0.11797500	0.75946900
C	-1.72863100	-1.19198500	0.24814800
C	-3.00753200	0.86920100	0.49223300
C	-2.72865200	-1.72965400	-0.52687200
H	-0.84766100	-1.77764700	0.47363900
C	-4.02128900	0.35416100	-0.27332900
H	-3.10767900	1.86789100	0.90432500
C	-3.93225800	-0.98215800	-0.83406200
H	-2.65638900	-2.73218800	-0.93174700
H	-4.92123400	0.91906400	-0.48555500
H	-1.20473100	0.84554600	2.65176000
O	-4.84775700	-1.46302600	-1.53655600
C	1.30169500	-0.27295500	0.93883800
C	1.46859800	0.72640500	-0.05058800
H	1.99149200	-2.13864900	1.75095900
O	2.69667500	1.46963400	-1.97274300
H	2.03591900	2.19039400	-1.82700600
H	-1.04661000	2.76726400	0.92126000

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.231174 (Hartree/Particle)
Thermal correction to Energy= 0.246805
Thermal correction to Enthalpy= 0.247749
Thermal correction to Gibbs Free Energy= 0.186620
Sum of electronic and zero-point Energies= -954.322437
Sum of electronic and thermal Energies= -954.306806
Sum of electronic and thermal Enthalpies= -954.305862
Sum of electronic and thermal Free Energies= -954.366991

Name of radical	C2-H

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

C	3.43347700	0.63169800	-0.26980700
C	4.15455200	-0.55836000	-0.25889500
C	3.49102700	-1.75964500	0.00211600
C	2.11354800	-1.80598200	0.24422700
H	5.22078400	-0.52774800	-0.45146100
C	1.29071800	1.85474300	0.08029000
C	-0.75240200	0.40286100	0.32186400
C	-0.14593100	1.74615000	0.56133400
O	0.06102100	-0.70660100	0.42968000
O	1.78296900	2.96424100	-0.15371900
O	4.14681500	-2.94646400	0.02282300
H	5.08030400	-2.80081200	-0.16565700
H	-0.13329500	2.00025200	1.63664100
C	-2.13173900	0.12687100	0.14967500
C	-2.60265100	-1.20066800	-0.04000500
C	-3.10846000	1.16123200	0.15771300
C	-3.94821700	-1.46660200	-0.21592700
H	-1.89111400	-2.01465900	-0.04874300
C	-4.45053700	0.88961100	-0.02162100

H	-2.80814900	2.18963500	0.31317700
C	-4.88616300	-0.42717100	-0.21107300
H	-4.27907800	-2.49143300	-0.36070000
H	-5.18579900	1.68508200	-0.01423300
O	-6.22435100	-0.63275200	-0.38093400
H	-6.38930500	-1.57398100	-0.49928700
C	1.40330800	-0.61881400	0.22855100
C	2.03240600	0.62392800	-0.01094400
H	1.61833200	-2.75010700	0.42085100
O	4.07461900	1.77788600	-0.51052900
H	3.40081300	2.50094400	-0.46508500
H	-0.71969500	2.53323700	0.07093700

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.230239 (Hartree/Particle)
Thermal correction to Energy= 0.246497
Thermal correction to Enthalpy= 0.247442
Thermal correction to Gibbs Free Energy= 0.185336
Sum of electronic and zero-point Energies= -954.331541
Sum of electronic and thermal Energies= -954.315283
Sum of electronic and thermal Enthalpies= -954.314338
Sum of electronic and thermal Free Energies= -954.376444

Name of anion	O4'-H

Cartesian Coordinates optimized at B3LYP/6-311G(d,p

C	2.64522200	0.50139000	-0.84697700
C	3.33135800	-0.70154000	-0.96774100
C	2.96507100	-1.77667300	-0.14992900
C	1.93217600	-1.68459700	0.77712100
H	4.13330000	-0.78373500	-1.69348300
C	0.92429200	1.90402600	0.27562500
C	-0.81960100	0.66560000	1.66698000
C	-0.09756400	1.98436100	1.38646000
O	0.27495000	-0.41091400	1.82413300
O	1.19525800	2.91090100	-0.40526900
O	3.61594600	-2.97637200	-0.23913000
H	4.26160000	-2.91705200	-0.95047100
H	0.45423400	2.28860100	2.28556600
C	-1.89384700	0.26062500	0.74022600
C	-2.90561700	-0.61483400	1.20246600
C	-1.97730200	0.66164000	-0.61481500
C	-3.92091000	-1.06436400	0.39244800
H	-2.86895200	-0.94199900	2.24174000
C	-2.98765000	0.22798500	-1.44322900
H	-1.23621900	1.34534800	-1.02175400
C	-4.03727500	-0.67638900	-1.00422800
H	-4.69029400	-1.72857900	0.77720900
H	-3.03867500	0.56390300	-2.47524900
H	-1.19247100	0.66059600	2.69196200
O	-4.96224500	-1.07174500	-1.75104900
C	1.24145400	-0.47825600	0.90991600
C	1.59337300	0.63906800	0.10198200
H	1.64872700	-2.53883600	1.37564000
O	2.99888300	1.53596300	-1.62500800
H	2.39718000	2.28511400	-1.36880200
H	-0.80985000	2.77572500	1.15039200

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase	
Zero-point correction= 0.229611 (Hartree/Particle) Thermal correction to Energy= 0.245429 Thermal correction to Enthalpy= 0.246373 Thermal correction to Gibbs Free Energy= 0.185826 Sum of electronic and zero-point Energies= -954.413247 Sum of electronic and thermal Energies= -954.397428 Sum of electronic and thermal Enthalpies= -954.396484 Sum of electronic and thermal Free Energies= -954.457031	
Name of anion	O7-H
Cartesian Coordinates optimized at B3LYP/6-311G(d,p	
C 2.59802600 0.36215900 -1.05001300 C 3.33000800 -0.79036000 -0.95573900 C 3.13250300 -1.74771600 0.11828700 C 2.08118800 -1.40972000 1.07724000 H 4.09376000 -1.00563300 -1.69426600 C 0.87946500 1.91762000 -0.12687600 C -0.65404300 0.89732200 1.62300600 C -0.08412800 2.18811600 1.02033600 O 0.39118100 -0.02363300 1.93798600 O 1.02657600 2.80580700 -1.00626200 O 3.79643500 -2.79837800 0.21965700 H 0.46109900 2.73486300 1.79954200 C -1.75504400 0.25796700 0.77784600 C -1.63822300 -1.03156700 0.25909600 C -2.95003300 0.95089800 0.55000100 C -2.67362600 -1.60209300 -0.47894800 H -0.72882000 -1.59445900 0.42272100 C -3.99208000 0.39097200 -0.18029800 H -3.07496000 1.95262200 0.95006000 C -3.85208300 -0.89409200 -0.70301300 H -2.55593700 -2.60385400 -0.88481700 H -4.91328400 0.93413000 -0.35650400 H -1.09329400 1.12839800 2.59972300 O -4.90281500 -1.41338400 -1.42244900 H -4.64385400 -2.28185600 -1.74627000 C 1.36027400 -0.25861200 0.97061800 C 1.57412800 0.69005400 -0.08126000 H 1.88586900 -2.10590400 1.88466900 O 2.82595200 1.23889500 -2.05984800 H 2.21088700 1.99892600 -1.90392100 H -0.87808200 2.84262000 0.65470300	
Frequency and Energy at B3LYP/6-311G(d,p) in gas phase	
Zero-point correction= 0.230715 (Hartree/Particle) Thermal correction to Energy= 0.246433 Thermal correction to Enthalpy= 0.247377 Thermal correction to Gibbs Free Energy= 0.186497 Sum of electronic and zero-point Energies= -954.423991 Sum of electronic and thermal Energies= -954.408273 Sum of electronic and thermal Enthalpies= -954.407329 Sum of electronic and thermal Free Energies= -954.468209	
Name of anion	C2-H
Cartesian Coordinates optimized at B3LYP/6-311G(d,p	
C 3.32305200 0.67786000 -0.41885400	

C	4.11478000	-0.46154600	-0.39105200
C	3.54803700	-1.68528500	0.01469600
C	2.21664300	-1.79526700	0.37671400
H	5.15710800	-0.39049300	-0.68609000
C	1.18682300	1.82140300	0.15557000
C	-0.71237800	0.38078800	0.44956200
C	-0.10284800	1.64983500	0.93306300
O	0.10936900	-0.76408000	0.58367600
O	1.57668600	2.94319000	-0.25404200
O	4.31433200	-2.83203100	0.03978600
H	5.19458700	-2.59892100	-0.26968700
H	0.10315100	1.69429200	2.02980000
C	-2.07503000	0.10805900	0.21877300
C	-2.54638100	-1.20402100	-0.10475100
C	-3.09063200	1.11552200	0.28071900
C	-3.88654800	-1.46270300	-0.35312700
H	-1.83018500	-2.01344900	-0.15978700
C	-4.42409700	0.84420400	0.01367700
H	-2.81830500	2.13106800	0.54410600
C	-4.84307900	-0.44696300	-0.30619900
H	-4.19450200	-2.48006100	-0.59532200
H	-5.16503200	1.63632600	0.06412500
O	-6.19791100	-0.66956500	-0.55768700
H	-6.29643200	-1.60390600	-0.76129700
C	1.41447200	-0.64396900	0.33907300
C	1.95757300	0.61894100	-0.01502900
H	1.78953500	-2.75372800	0.63958500
O	3.85019000	1.85547700	-0.80391800
H	3.10059400	2.51303300	-0.72580200
H	-0.74417800	2.50075100	0.70084300

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.227208 (Hartree/Particle)
Thermal correction to Energy= 0.243896
Thermal correction to Enthalpy= 0.244840
Thermal correction to Gibbs Free Energy= 0.182773
Sum of electronic and zero-point Energies= -954.374859
Sum of electronic and thermal Energies= -954.358171
Sum of electronic and thermal Enthalpies= -954.357227
Sum of electronic and thermal Free Energies= -954.419294

Name of cationic radical

Cartesian Coordinates optimized at B3LYP/6-311G(d,p

C	2.64621700	0.50090900	-0.86004100
C	3.34636400	-0.72662600	-0.98774100
C	2.98901800	-1.80467700	-0.18850500
C	1.91665400	-1.69230300	0.72315900
H	4.15345300	-0.78273400	-1.70848500
C	0.94676500	1.93633800	0.27327000
C	-0.73240700	0.69660300	1.71753500
C	-0.01820800	2.01604100	1.43492100
O	0.24392000	-0.43604900	1.74001100
O	1.22013600	2.91464500	-0.42184600
O	3.59045600	-2.99987400	-0.22940200
H	4.30831800	-3.01604600	-0.87503200
H	0.57367200	2.29815300	2.31344500

C	-1.83537300	0.28325100	0.77832000
C	-2.71844400	-0.73028600	1.20281200
C	-2.00727800	0.83238100	-0.50534500
C	-3.73892100	-1.17734400	0.38857300
H	-2.59821600	-1.16490900	2.18874200
C	-3.02756300	0.40042200	-1.33011200
H	-1.36371800	1.62718800	-0.86077800
C	-3.90093400	-0.61370700	-0.89118300
H	-4.41903600	-1.94922800	0.73278800
H	-3.18528900	0.83169500	-2.31035700
H	-1.10024500	0.68749200	2.74166800
O	-4.86668400	-0.98701700	-1.73894100
H	-5.42567900	-1.67579100	-1.35637600
C	1.22789300	-0.46375500	0.84980700
C	1.58328100	0.64771300	0.07308400
H	1.61915300	-2.54367100	1.32081100
O	3.02064700	1.50202100	-1.61634000
H	2.44506000	2.28975900	-1.39096800
H	-0.73765000	2.81853700	1.26537200

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.243180 (Hartree/Particle)
Thermal correction to Energy= 0.259192
Thermal correction to Enthalpy= 0.260136
Thermal correction to Gibbs Free Energy= 0.198576
Sum of electronic and zero-point Energies= -954.678244
Sum of electronic and thermal Energies= -954.662232
Sum of electronic and thermal Enthalpies= -954.661288
Sum of electronic and thermal Free Energies= -954.722848

Name of compound (6)	**Pinobanksin**

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

C	-2.37957200	0.43636500	1.03762200
C	-3.30557300	-0.56660100	0.77532100
C	-3.08468000	-1.43315400	-0.29827600
C	-1.94829600	-1.33615500	-1.10883700
H	-4.18660600	-0.64777100	1.40131900
C	-0.30429300	1.66097500	0.42550700
C	1.19995800	0.50816500	-1.26285700
C	0.78708600	1.83611900	-0.62541400
O	0.06530200	-0.28995000	-1.64587300
O	-0.41999900	2.50984800	1.32197400
O	-3.95801100	-2.42391500	-0.60252000
H	-4.69437000	-2.40533900	0.01852100
C	2.18115200	-0.27966900	-0.40219300
C	1.85775800	-1.51085000	0.16863900
C	3.46675200	0.23860200	-0.20520200
C	2.79420600	-2.19867800	0.93982500
H	0.87882800	-1.94250000	0.00898000
C	4.40129700	-0.44835300	0.56230600
H	3.74526300	1.18240100	-0.66375800
C	4.06531900	-1.67058100	1.14217700
H	2.52588100	-3.15277300	1.37925300
H	5.39251800	-0.03232900	0.70292600
H	1.67707300	0.75132700	-2.21480400

C	-1.02128700	-0.34269300	-0.84082000
C	-1.21343800	0.56926700	0.22816100
H	4.79170200	-2.20822700	1.74077200
H	1.65644600	2.29146700	-0.14087500
O	0.27827200	2.67254200	-1.66366400
H	0.00218000	3.50255400	-1.25850700
H	-1.79611400	-2.02631900	-1.92654300
O	-2.60439800	1.27915400	2.04985500
H	-1.86046000	1.92952500	2.05878400

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.244614 (Hartree/Particle)
Thermal correction to Energy= 0.260606
Thermal correction to Enthalpy= 0.261550
Thermal correction to Gibbs Free Energy= 0.200421
Sum of electronic and zero-point Energies= -954.943046
Sum of electronic and thermal Energies= -954.927054
Sum of electronic and thermal Enthalpies= -954.926110
Sum of electronic and thermal Free Energies= -954.987239

Name of radical	O7-H

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

C	-2.37101900	0.35984000	1.09154700
C	-3.28801000	-0.63983500	0.83815900
C	-3.11765900	-1.52837100	-0.29054800
C	-1.95361300	-1.36206700	-1.13763800
H	-4.15365500	-0.76984200	1.47362100
C	-0.31981600	1.62997300	0.41732000
C	1.16099500	0.53003900	-1.30509100
C	0.71332600	1.85046200	-0.68107700
O	0.03220100	-0.27074100	-1.69471900
O	-0.40644000	2.43594300	1.34840400
O	-3.95194600	-2.43199200	-0.52340500
C	2.13594400	-0.24417700	-0.42337000
C	1.86894200	-1.54317800	0.01133700
C	3.35981300	0.34360400	-0.08009400
C	2.79554300	-2.23060600	0.79433900
H	0.94360700	-2.02828700	-0.26807300
C	4.28483000	-0.34354400	0.69881700
H	3.60319300	1.34043100	-0.43329000
C	4.00246400	-1.63381500	1.14396300
H	2.57052400	-3.23774700	1.12617300
H	5.22742000	0.12701200	0.95412400
H	1.64346100	0.77179500	-2.25483700
C	-1.04282800	-0.37096300	-0.87290900
C	-1.23736600	0.52226500	0.22865600
H	4.72165900	-2.17041400	1.75189900
H	1.57161500	2.36762600	-0.24348300
O	0.10307600	2.62588600	-1.71001300
H	-0.13919500	3.48028100	-1.33531900
H	-1.81936800	-2.03522400	-1.97337900
O	-2.56298500	1.17670500	2.13627300
H	-1.82978900	1.83019300	2.14977600

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.230634 (Hartree/Particle)
Thermal correction to Energy= 0.246507

Thermal correction to Enthalpy=	0.247451		
Thermal correction to Gibbs Free Energy=	0.185428		
Sum of electronic and zero-point Energies=	-954.301216		
Sum of electronic and thermal Energies=	-954.285344		
Sum of electronic and thermal Enthalpies=	-954.284400		
Sum of electronic and thermal Free Energies=	-954.346423		
Name of radical	C3-H		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)			
C	2.74942800	0.66094300	-0.60774000
C	3.60505300	-0.43480300	-0.53570200
C	3.19693500	-1.57321800	0.16211600
C	1.94667600	-1.64988800	0.78831900
H	4.57583900	-0.37776000	-1.01450000
C	0.58345900	1.74366000	-0.02676600
C	-1.16052800	0.28177300	1.18121800
C	-0.68189100	1.57204200	0.59664700
O	-0.09359900	-0.66609900	1.36305400
O	0.85192100	2.85829600	-0.56373000
O	3.99170200	-2.66893600	0.26762200
H	4.81948200	-2.50913400	-0.19838900
C	-2.29063000	-0.32790500	0.35402300
C	-2.01875800	-1.16383900	-0.73108300
C	-3.61464000	-0.02010300	0.66956900
C	-3.06330400	-1.68383400	-1.49034200
H	-0.99524600	-1.41943100	-0.97740500
C	-4.65835400	-0.53585100	-0.09505600
H	-3.83115400	0.62578700	1.51384100
C	-4.38447600	-1.36951100	-1.17651700
H	-2.84453600	-2.33696300	-2.32753100
H	-5.68371200	-0.29273100	0.15951400
H	-1.54612200	0.47905700	2.18809400
C	1.09840800	-0.55858600	0.71067800
C	1.47371100	0.60976100	0.01070800
H	-5.19582900	-1.77643700	-1.76918400
O	-1.52270000	2.60396900	0.60697700
H	-1.04511600	3.31476800	0.12991100
H	1.65527200	-2.54042800	1.32687500
O	3.14510600	1.76010500	-1.26319900
H	2.42514700	2.43074500	-1.17745000
Frequency and Energy at B3LYP/6-311G(d,p) in gas phase			
Zero-point correction=	0.231982 (Hartree/Particle)		
Thermal correction to Energy=	0.247885		
Thermal correction to Enthalpy=	0.248830		
Thermal correction to Gibbs Free Energy=	0.186273		
Sum of electronic and zero-point Energies=	-954.329999		
Sum of electronic and thermal Energies=	-954.314096		
Sum of electronic and thermal Enthalpies=	-954.313152		
Sum of electronic and thermal Free Energies=	-954.375708		
Name of anion	O7-H		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p			
C	3.18995100	0.59947100	0.00959200
C	3.97787000	-0.51138100	0.11170600
C	3.42063600	-1.85526900	0.14498900
C	1.95962500	-1.94131100	0.09096400

H	5.05519800	-0.40851100	0.16922200
C	0.93044700	1.61138300	-0.25954500
C	-0.98376100	0.11764800	0.34838400
C	-0.57361500	1.37206200	-0.43879200
O	-0.18600300	-0.98384700	-0.09019500
O	1.29959700	2.82315900	-0.27650700
O	4.12987400	-2.87409700	0.23262100
C	-2.44329700	-0.25967500	0.18760900
C	-2.82558300	-1.41303300	-0.50187000
C	-3.43718600	0.55912500	0.73782200
C	-4.17410300	-1.74066000	-0.63993000
H	-2.05719700	-2.05092600	-0.91724800
C	-4.78221600	0.23145200	0.59645700
H	-3.14495500	1.46523600	1.25322900
C	-5.15771700	-0.92179600	-0.09221500
H	-4.45368800	-2.64212000	-1.17587100
H	-5.53994800	0.87881000	1.02617000
H	-0.77818900	0.31515500	1.41047300
C	1.18884000	-0.82817000	-0.01729000
C	1.74966700	0.49231900	-0.07952600
H	-6.20674400	-1.17858000	-0.19875800
H	-0.77438900	1.18245600	-1.50568200
O	-1.27146000	2.52222600	-0.00258800
H	-0.56916600	3.20030500	0.00594400
H	1.50665000	-2.92355400	0.15128200
O	3.74377900	1.83903400	-0.02592500
H	2.99879500	2.47693500	-0.10814600

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.231581 (Hartree/Particle)
Thermal correction to Energy= 0.247061
Thermal correction to Enthalpy= 0.248005
Thermal correction to Gibbs Free Energy= 0.188089
Sum of electronic and zero-point Energies= -954.430528
Sum of electronic and thermal Energies= -954.415049
Sum of electronic and thermal Enthalpies= -954.414104
Sum of electronic and thermal Free Energies= -954.474021

Name of anion	C3-H

Cartesian Coordinates optimized at B3LYP/6-311G(d,p

C	-2.58155800	0.59348300	0.71189900
C	-3.37712400	-0.56128900	0.75465400
C	-2.98655500	-1.68997400	0.03629600
C	-1.81637200	-1.70639700	-0.72194300
H	-4.29734900	-0.54631100	1.33211700
C	-0.57133800	1.81557700	-0.13417700
C	1.13938700	0.39077200	-1.28286600
C	0.60192500	1.69678700	-0.80438500
O	0.08080700	-0.56278400	-1.55508100
O	-0.99682100	2.94323400	0.39030900
O	-3.74655600	-2.84684000	0.05124600
H	-4.49777100	-2.68490800	0.62959600
C	2.18759000	-0.26551000	-0.36299200
C	2.46436000	-1.63219900	-0.46720500
C	2.90244800	0.49583500	0.56564500
C	3.42822600	-2.22869000	0.34311700

H	1.89885800	-2.22795100	-1.17407400
C	3.87758700	-0.09728300	1.36671900
H	2.69004000	1.55497300	0.64190400
C	4.14255900	-1.46157200	1.26214500
H	3.61742700	-3.29492500	0.26150200
H	4.42440200	0.50825900	2.08304100
H	1.62409200	0.53056900	-2.26032400
C	-1.03199100	-0.55283600	-0.74761600
C	-1.38347700	0.59323800	-0.03090900
H	4.89404200	-1.92410900	1.89454200
O	1.43378700	2.81225900	-0.95207500
H	0.90683600	3.49990300	-0.50790300
H	-1.52863200	-2.58818200	-1.27898100
O	-2.95482800	1.70779400	1.36076000
H	-2.23705300	2.40373100	1.08701500

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.229093 (Hartree/Particle)
Thermal correction to Energy= 0.245077
Thermal correction to Enthalpy= 0.246022
Thermal correction to Gibbs Free Energy= 0.184838
Sum of electronic and zero-point Energies= -954.396863
Sum of electronic and thermal Energies= -954.380878
Sum of electronic and thermal Enthalpies= -954.379934
Sum of electronic and thermal Free Energies= -954.441118

Name of cationic radical

Cartesian Coordinates optimized at B3LYP/6-311G(d,p

C	-2.43805600	0.42911400	0.89399900
C	-3.28182600	-0.72163900	0.80041400
C	-2.94666100	-1.75224500	-0.06842200
C	-1.76275100	-1.66936100	-0.83193400
H	-4.17444400	-0.74718700	1.41466700
C	-0.45863100	1.75170900	0.16130200
C	1.23771400	0.50254900	-1.26221700
C	0.62414200	1.85312300	-0.91032400
O	0.16301400	-0.53787200	-1.46098400
O	-0.71398000	2.68301600	0.92412700
O	-3.66872200	-2.86300300	-0.23916000
H	-4.46487300	-2.86812200	0.30794900
C	2.24597800	-0.08410400	-0.31160900
C	2.30400800	0.25945300	1.04555700
C	3.15177100	-1.02793400	-0.81881800
C	3.25623800	-0.32572100	1.87433500
H	1.63736600	1.00267500	1.46685000
C	4.09702800	-1.61533600	0.01219200
H	3.11658500	-1.29549300	-1.86929400
C	4.14961600	-1.26574000	1.36130500
H	3.30775800	-0.04106700	2.91826000
H	4.79723500	-2.33645100	-0.39149100
H	1.64606400	0.57879300	-2.26812400
C	-0.91759900	-0.51668400	-0.72733500
C	-1.25489100	0.54183900	0.12496800
H	4.89055100	-1.71763200	2.00989800
H	1.41675100	2.52747300	-0.57349600
O	-0.02344900	2.31932700	-2.08741000

H	-0.22276200	3.25815900	-1.98888900
H	-1.48108500	-2.47753400	-1.49486600
O	-2.80464000	1.37942200	1.70778500
H	-2.12341500	2.11512100	1.65318500

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.242985 (Hartree/Particle)
Thermal correction to Energy= 0.259255
Thermal correction to Enthalpy= 0.260199
Thermal correction to Gibbs Free Energy= 0.198067
Sum of electronic and zero-point Energies= -954.659910
Sum of electronic and thermal Energies= -954.643640
Sum of electronic and thermal Enthalpies= -954.642696
Sum of electronic and thermal Free Energies= -954.704829

Name of compound (7)	**Pinocembrin**	

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

O	-0.28454800	-0.83259600	0.00847400
O	1.27142300	2.95043100	-0.32298800
O	3.65455200	1.93966200	-0.08083200
O	3.96337500	-2.79360600	0.21471200
C	-1.09042600	0.29835600	0.40529800
C	-0.67144800	1.54440400	-0.38037700
C	1.64125100	0.63466300	-0.03978800
C	-2.54482500	-0.06202800	0.21247600
C	0.81487000	1.80420900	-0.23780800
C	1.06307700	-0.65823800	0.03283300
C	3.06100400	0.74513100	-0.00936400
C	1.84686100	-1.79504600	0.11446600
C	-3.50770900	0.48720800	1.06266600
C	-2.95303300	-0.89896400	-0.82892900
C	3.85192900	-0.39683500	0.07823400
C	3.23944400	-1.65007800	0.13087100
C	-4.85993200	0.21634300	0.86925700
C	-4.30488200	-1.17606100	-1.01684300
C	-5.26175500	-0.61687700	-0.17226100
H	-0.90016300	0.47352400	1.47225100
H	-1.22279700	2.42374000	-0.04330600
H	-0.89631000	1.40055100	-1.44399800
H	1.39545100	-2.77487500	0.17940000
H	-3.19938400	1.12674000	1.88398300
H	-2.20865000	-1.34480500	-1.47662300
H	4.93040100	-0.28891100	0.09465800
H	-5.59697000	0.64784300	1.53703100
H	-4.61075600	-1.83276500	-1.82357400
H	-6.31335300	-0.83448500	-0.32059900
H	2.93537200	2.61316900	-0.17249200
H	4.90217700	-2.57798000	0.23395700

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.239768 (Hartree/Particle)
Thermal correction to Energy= 0.254630
Thermal correction to Enthalpy= 0.255574
Thermal correction to Gibbs Free Energy= 0.196995
Sum of electronic and zero-point Energies= -879.719598
Sum of electronic and thermal Energies= -879.704737

Sum of electronic and thermal Enthalpies=	-879.703792		
Sum of electronic and thermal Free Energies=	-879.762372		
Name of radical	O7-H		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)			
O	-0.27083000	-0.85261300	-0.02335700
O	1.34227600	2.89634900	-0.32085400
O	3.72629900	1.88194200	-0.05947400
O	3.99214900	-2.79411900	0.23070900
C	-1.05551100	0.28471700	0.39401500
C	-0.61815000	1.52201400	-0.39496800
C	1.69764000	0.57454500	-0.05239600
C	-2.51720200	-0.04790900	0.20985900
C	0.86794700	1.76096800	-0.24988800
C	1.08292900	-0.71809600	0.02351100
C	3.12468900	0.68724300	-0.00071100
C	1.84075800	-1.85493600	0.11624200
C	-3.46092900	0.49490900	1.08495600
C	-2.94876100	-0.85254100	-0.84748100
C	3.89912700	-0.45367700	0.09456100
C	3.28759800	-1.76309500	0.14735100
C	-4.81922400	0.24928600	0.90033500
C	-4.30660400	-1.10466700	-1.02599700
C	-5.24490400	-0.55179000	-0.15666200
H	-0.85517900	0.45103500	1.46052600
H	-1.15523300	2.41385300	-0.06855700
H	-0.84103800	1.37120600	-1.45819400
H	1.38021200	-2.83155700	0.17561200
H	-3.13383100	1.10836900	1.91877800
H	-2.21925400	-1.29482800	-1.51438500
H	4.97836600	-0.38523600	0.12475500
H	-5.54205300	0.67469000	1.58709100
H	-4.63165000	-1.73711700	-1.84435000
H	-6.30118400	-0.75010600	-0.29793700
H	3.02526900	2.56538500	-0.15589000
Frequency and Energy at B3LYP/6-311G(d,p) in gas phase			
Zero-point correction=	0.225823 (Hartree/Particle)		
Thermal correction to Energy=	0.240571		
Thermal correction to Enthalpy=	0.241516		
Thermal correction to Gibbs Free Energy=	0.182244		
Sum of electronic and zero-point Energies=	-879.078281		
Sum of electronic and thermal Energies=	-879.063532		
Sum of electronic and thermal Enthalpies=	-879.062588		
Sum of electronic and thermal Free Energies=	-879.121860		
Name of radical	C2-H		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)			
O	0.29372200	-0.76729600	0.35404600
O	-1.29124300	2.98078700	-0.11801500
O	-3.64245700	1.89655600	-0.41168800
O	-3.89042700	-2.83011600	0.03532900
C	1.15251800	0.30340500	0.25583400
C	0.61130700	1.67484300	0.49790600
C	-1.63435000	0.65163500	0.00013600
C	2.51986600	-0.03038900	0.07376600
C	-0.83799800	1.84815100	0.07952300

C	-1.05052800	-0.61989200	0.19644100
C	-3.04131200	0.72148900	-0.21254400
C	-1.80664800	-1.77738200	0.21230200
C	3.53155000	0.96777400	0.08121900
C	2.92937200	-1.37819100	-0.12296500
C	-3.80992300	-0.43870100	-0.20041100
C	-3.18870200	-1.67074300	0.01553900
C	4.86250800	0.63309100	-0.10664100
C	4.26385900	-1.69420700	-0.30636400
C	5.24390600	-0.69655500	-0.30247600
H	1.19984700	2.42955500	-0.02540400
H	0.65798300	1.94124400	1.56866200
H	-1.34487500	-2.74380700	0.35566700
H	3.26969000	2.00598200	0.24192600
H	2.18032800	-2.15802000	-0.13034600
H	-4.87955600	-0.36095600	-0.35747700
H	5.61351400	1.41527300	-0.09696400
H	4.54910700	-2.72978700	-0.45601100
H	6.28690800	-0.95153400	-0.44799700
H	-2.93918800	2.59138100	-0.37713000
H	-4.82306000	-2.64476100	-0.11988600

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.226153 (Hartree/Particle)
Thermal correction to Energy= 0.241175
Thermal correction to Enthalpy= 0.242119
Thermal correction to Gibbs Free Energy= 0.182621
Sum of electronic and zero-point Energies= -879.092199
Sum of electronic and thermal Energies= -879.077177
Sum of electronic and thermal Enthalpies= -879.076233
Sum of electronic and thermal Free Energies= -879.135731

Name of anion	O7-H

Cartesian Coordinates optimized at B3LYP/6-311G(d,p

O	-0.27732600	-0.85060800	-0.08759900
O	1.32484500	2.93615100	-0.35334500
O	3.70245900	1.90493200	-0.05638500
O	4.00417800	-2.81260100	0.25250300
C	-1.03881800	0.26214200	0.37362700
C	-0.61709300	1.53515600	-0.36690300
C	1.67836100	0.60597300	-0.06375000
C	-2.50964000	-0.05830500	0.20388600
C	0.88703400	1.75948000	-0.25593000
C	1.10198600	-0.70667400	-0.00353900
C	3.12184500	0.68004000	0.00235500
C	1.85283600	-1.83526100	0.10495400
C	-3.46850300	0.70711000	0.87656000
C	-2.94168800	-1.09194600	-0.63051000
C	3.89097200	-0.44677700	0.11055000
C	3.31376700	-1.77883200	0.15929000
C	-4.82755600	0.45489000	0.71249600
C	-4.30265800	-1.34665500	-0.79373600
C	-5.25111900	-0.57497200	-0.12666500
H	-0.83052500	0.40347400	1.44532900
H	-1.12795300	2.41383500	0.03546700
H	-0.89194600	1.44777400	-1.42523100

H	1.37908500	-2.80832800	0.15859100
H	-3.14626900	1.50568700	1.53794900
H	-2.19907200	-1.69552200	-1.13523600
H	4.97066500	-0.35971900	0.15345100
H	-5.55596500	1.05853700	1.24416900
H	-4.62147900	-2.15551300	-1.44326500
H	-6.30965500	-0.77626400	-0.25378500
H	2.96151900	2.55082200	-0.17493800

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.226410 (Hartree/Particle)
Thermal correction to Energy= 0.240981
Thermal correction to Enthalpy= 0.241925
Thermal correction to Gibbs Free Energy= 0.183834
Sum of electronic and zero-point Energies= -879.189832
Sum of electronic and thermal Energies= -879.175261
Sum of electronic and thermal Enthalpies= -879.174317
Sum of electronic and thermal Free Energies= -879.232408

Name of anion	C2-H

Cartesian Coordinates optimized at B3LYP/6-311G(d,p

O	0.23934300	-0.83548300	0.55891900
O	-1.06407700	2.95265600	-0.19941900
O	-3.39548500	1.98274800	-0.73007100
O	-4.06317000	-2.68954000	0.04388300
C	1.12034600	0.26620400	0.43125600
C	0.57623100	1.56148300	0.92690700
C	-1.54941200	0.64543600	0.00395600
C	2.45088600	-0.05973400	0.13472700
C	-0.71973600	1.80785600	0.18069800
C	-1.06008200	-0.64674000	0.33087200
C	-2.91693100	0.77595900	-0.37447300
C	-1.91568400	-1.75844400	0.36375900
C	3.50956600	0.90947800	0.15531900
C	2.85195100	-1.39345500	-0.21780800
C	-3.76134400	-0.32523400	-0.35197300
C	-3.24610500	-1.57996700	0.02455200
C	4.81237400	0.57617500	-0.17245800
C	4.16361200	-1.70220400	-0.52704300
C	5.17520800	-0.73120900	-0.51959600
H	1.25483800	2.38233100	0.69410600
H	0.38836700	1.60313000	2.02532200
H	-1.53041700	-2.73998900	0.60469500
H	3.28862900	1.93352100	0.43523300
H	2.09627900	-2.16840100	-0.24313300
H	-4.80366400	-0.20066900	-0.62831200
H	5.57150400	1.35522200	-0.14573000
H	4.40946800	-2.72984900	-0.78722900
H	6.19998300	-0.98338300	-0.76966000
H	-2.61686500	2.60462800	-0.65387000
H	-4.93627800	-2.41320600	-0.25008900

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.223504 (Hartree/Particle)
Thermal correction to Energy= 0.238650
Thermal correction to Enthalpy= 0.239594
Thermal correction to Gibbs Free Energy= 0.181006

Sum of electronic and zero-point Energies=	-879.141089		
Sum of electronic and thermal Energies=	-879.125943		
Sum of electronic and thermal Enthalpies=	-879.124999		
Sum of electronic and thermal Free Energies=	-879.183587		
Name of cationic radical			
Cartesian Coordinates optimized at B3LYP/6-311G(d,p			
O	-0.27548700	-0.77511700	0.18267000
O	1.37724900	2.97241700	-0.12626100
O	3.67494100	1.83911800	-0.05056500
O	3.85341400	-2.90545900	-0.01210200
C	-1.14013100	0.41232100	0.50219500
C	-0.64484000	1.65773400	-0.23737300
C	1.63229500	0.64937300	0.04049800
C	-2.55774600	0.01992300	0.21183700
C	0.84173500	1.86753400	-0.08291000
C	1.02044400	-0.60587400	0.08590900
C	3.04863600	0.70036000	-0.00261800
C	1.80433900	-1.80735400	0.04589700
C	-3.48398100	-0.03525500	1.25482100
C	-2.96650200	-0.28307400	-1.09331600
C	3.83892300	-0.49335900	-0.00869400
C	3.21306500	-1.73365000	0.00609800
C	-4.81050900	-0.37480600	0.99679200
C	-4.28770600	-0.63542200	-1.34643800
C	-5.21170100	-0.67642900	-0.30276600
H	-0.99918900	0.54171000	1.57908700
H	-1.17986000	2.53359500	0.13361700
H	-0.85917900	1.58376700	-1.30985500
H	1.30621200	-2.76860400	0.06468100
H	-3.17378800	0.18935900	2.26987200
H	-2.25629400	-0.25776700	-1.91277400
H	4.91713400	-0.38655500	-0.03708000
H	-5.52599200	-0.40868100	1.80934900
H	-4.59761800	-0.87572100	-2.35623800
H	-6.24218500	-0.94448300	-0.50282700
H	2.97884400	2.57092800	-0.06851300
H	4.81306100	-2.79736300	-0.03886500
Frequency and Energy at B3LYP/6-311G(d,p) in gas phase			
Zero-point correction=	0.237985 (Hartree/Particle)		
Thermal correction to Energy=	0.253101		
Thermal correction to Enthalpy=	0.254045		
Thermal correction to Gibbs Free Energy=	0.194228		
Sum of electronic and zero-point Energies=	-879.433957		
Sum of electronic and thermal Energies=	-879.418841		
Sum of electronic and thermal Enthalpies=	-879.417897		
Sum of electronic and thermal Free Energies=	-879.477714		

Name of compound (8)		**Catechin**	
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)			
C	-2.94473800	0.16853700	1.28940700
C	-3.91373800	-0.72221000	0.82868600
C	-3.75871400	-1.29649200	-0.43694100
C	-2.65575200	-0.99191200	-1.22305600
H	-4.77510800	-0.96493100	1.44554300

C	-0.77706000	1.46793600	1.01057600
C	0.43158500	0.99467600	-1.14676600
C	-0.04374900	2.08719200	-0.17879600
O	-0.64628900	0.14287200	-1.56474300
O	-4.67167600	-2.17602600	-0.94892800
H	-5.38615100	-2.29442300	-0.31547400
C	1.59976800	0.18826200	-0.60101000
C	1.47421500	-1.15387300	-0.25199800
C	2.84627300	0.81410900	-0.46610600
C	2.57442900	-1.85829600	0.24359900
H	0.52770800	-1.66148100	-0.37495300
C	3.94266400	0.12090900	0.02536200
H	2.99104900	1.84981800	-0.75363000
C	3.80036500	-1.22851000	0.38530900
H	2.47203700	-2.90506700	0.51500600
H	0.74191700	1.49598500	-2.06684500
O	4.94583300	-1.82910800	0.85914700
H	4.77627200	-2.75723200	1.04608700
C	-1.69836700	-0.10112900	-0.73289700
C	-1.82003600	0.49602300	0.52731000
H	0.83906400	2.63379800	0.17483000
O	-0.88276100	2.94846400	-0.94513500
H	-1.38287300	3.49974600	-0.33585900
O	5.14707800	0.74517300	0.14836100
H	5.77903700	0.09760100	0.48614300
H	-2.53839900	-1.43016300	-2.20448200
O	-3.04595800	0.76837300	2.51818700
H	-3.87117300	0.49873000	2.93292500
H	-0.04701100	0.97423900	1.66316300
H	-1.23903300	2.25405300	1.61636500

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.270012 (Hartree/Particle)
Thermal correction to Energy= 0.288697
Thermal correction to Enthalpy= 0.289642
Thermal correction to Gibbs Free Energy= 0.223079
Sum of electronic and zero-point Energies= -1031.353587
Sum of electronic and thermal Energies= -1031.334902
Sum of electronic and thermal Enthalpies= -1031.333958
Sum of electronic and thermal Free Energies= -1031.400521

Name of radical	O4'-H

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

C	-2.91495000	0.18118800	1.27451500
C	-3.88414600	-0.70268400	0.80258100
C	-3.72158000	-1.27629200	-0.46256800
C	-2.60909400	-0.97690500	-1.23838900
H	-4.75262200	-0.94107900	1.41081600
C	-0.73851600	1.46938400	1.01937100
C	0.48819600	0.98393200	-1.12711200
C	0.01704900	2.08287400	-0.15868000
O	-0.58609300	0.14249100	-1.55803100
O	-4.63317100	-2.14814400	-0.98503200
H	-5.35208000	-2.27183900	-0.35747100
C	1.64899900	0.17507000	-0.57861600
C	1.47905600	-1.17538000	-0.16533000

C	2.90561300	0.78390800	-0.49841800
C	2.52471800	-1.90280500	0.34085900
H	0.50279700	-1.63027800	-0.26446400
C	3.97747800	0.07008000	0.00783100
H	3.06003100	1.80316700	-0.83495200
C	3.83360300	-1.31919900	0.45845500
H	2.40515300	-2.93140800	0.65890400
H	0.81625000	1.48827300	-2.04002000
O	4.85454300	-1.89198900	0.90263800
C	-1.65302100	-0.09331700	-0.73647300
C	-1.78100100	0.50322700	0.52241300
H	0.90304300	2.61753400	0.20531200
O	-0.79929900	2.95074200	-0.93770800
H	-1.31686100	3.49736100	-0.33867100
O	5.20059300	0.58654600	0.11435100
H	5.73760300	-0.14117700	0.49444600
H	-2.48447600	-1.41550100	-2.21868800
O	-3.02127900	0.78035000	2.50157100
H	-3.84683800	0.51075600	2.91595200
H	-0.02383700	0.97516300	1.68898200
H	-1.20493400	2.26058200	1.61490700

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.258209 (Hartree/Particle)
Thermal correction to Energy= 0.276185
Thermal correction to Enthalpy= 0.277129
Thermal correction to Gibbs Free Energy= 0.211058
Sum of electronic and zero-point Energies= -1030.737363
Sum of electronic and thermal Energies= -1030.719388
Sum of electronic and thermal Enthalpies= -1030.718444
Sum of electronic and thermal Free Energies= -1030.784514

Name of radical	C2-H

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

C	-3.74147100	-0.81810200	-0.36712000
C	-4.57210900	0.27040700	-0.09694800
C	-4.00215600	1.51302500	0.19870000
C	-2.62155800	1.66916700	0.23145300
H	-5.65228600	0.15318300	-0.12318700
C	-1.41069300	-1.83417000	-0.65678100
C	0.42578700	-0.27833400	-0.00654700
C	-0.11314900	-1.66748300	0.14331500
O	-0.46893800	0.77409300	-0.01020200
O	-4.76277500	2.61346600	0.47052300
H	-5.69447100	2.37729300	0.42362700
C	1.79442500	0.09961800	-0.04893500
C	2.17443000	1.45281700	-0.24611700
C	2.82865300	-0.86362200	0.10232700
C	3.51307900	1.81107200	-0.30233800
H	1.40946200	2.20723800	-0.35954400
C	4.15837700	-0.49751700	0.04273000
H	2.60654300	-1.90352400	0.29949600
C	4.50865200	0.84980300	-0.16356600
H	3.78958600	2.85013000	-0.45877200
O	5.86095800	1.10602900	-0.20491100
H	6.01228700	2.04850400	-0.32322300

C	-1.82236500	0.56143000	-0.04465600
C	-2.34786000	-0.69770500	-0.34673200
H	0.62742900	-2.37691300	-0.22295000
O	-0.30372200	-2.03750100	1.52321100
H	-0.97652300	-1.45328600	1.89181900
O	5.13109900	-1.44098700	0.19414900
H	5.98467400	-0.99305600	0.14024400
H	-2.17756200	2.62619100	0.46721800
O	-4.24555600	-2.05061000	-0.67360800
H	-5.20647800	-2.02288800	-0.63004000
H	-1.17737200	-1.85934000	-1.72908800
H	-1.86608100	-2.79187400	-0.40159700

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.256818 (Hartree/Particle)
Thermal correction to Energy= 0.275669
Thermal correction to Enthalpy= 0.276613
Thermal correction to Gibbs Free Energy= 0.209328
Sum of electronic and zero-point Energies= -1030.729196
Sum of electronic and thermal Energies= -1030.710345
Sum of electronic and thermal Enthalpies= -1030.709401
Sum of electronic and thermal Free Energies= -1030.776687

Name of anion	O4'-H

Cartesian Coordinates optimized at B3LYP/6-311G(d,p

C	-3.01038300	0.01029500	1.21546800
C	-3.95374900	-0.82262000	0.60906700
C	-3.73324100	-1.24246400	-0.70561300
C	-2.59932100	-0.84653400	-1.39496700
H	-4.84179900	-1.13794800	1.15268000
C	-0.84746800	1.34353900	1.20351000
C	0.50448500	1.09517400	-0.91500400
C	-0.04346100	2.07360200	0.13669300
O	-0.58944600	0.32560200	-1.50533800
O	-4.62683700	-2.06112100	-1.35833600
H	-5.33405800	-2.28303700	-0.74574200
C	1.65182900	0.24005400	-0.44764100
C	1.48999800	-0.95783200	0.24988100
C	2.97188600	0.70203400	-0.69149300
C	2.58763000	-1.69284900	0.71231400
H	0.49134100	-1.34773900	0.42413300
C	4.05197400	-0.00859200	-0.22589600
H	3.14248100	1.62045400	-1.25047800
C	3.92021900	-1.25422700	0.50729800
H	2.43810600	-2.63031600	1.24036100
H	0.85964000	1.69881900	-1.76052400
O	5.00410800	-1.82407200	0.87509200
C	-1.66547900	-0.01365400	-0.76239500
C	-1.85738700	0.43312100	0.55502800
H	0.82060700	2.57120000	0.59245300
O	-0.91974200	3.04874100	-0.45271400
H	-0.51278600	3.33389000	-1.27672300
O	5.35177100	0.36243300	-0.41504100
H	5.79718800	-0.39538700	0.04541300
H	-2.42066200	-1.18009300	-2.40797600
O	-3.18495800	0.45354800	2.50621600

H	-4.01902200	0.10646100	2.83535500
H	-0.15642900	0.77379200	1.83328900
H	-1.34896900	2.07459100	1.84121800

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.256653 (Hartree/Particle)
Thermal correction to Energy= 0.274705
Thermal correction to Enthalpy= 0.275649
Thermal correction to Gibbs Free Energy= 0.209950
Sum of electronic and zero-point Energies= -1030.816671
Sum of electronic and thermal Energies= -1030.798619
Sum of electronic and thermal Enthalpies= -1030.797675
Sum of electronic and thermal Free Energies= -1030.863374

Name of cationic radical

Cartesian Coordinates optimized at B3LYP/6-311G(d,p

C	-2.68105900	-0.09065400	1.41809300
C	-3.62912800	-0.96147600	0.92461400
C	-3.59541300	-1.30497900	-0.44906500
C	-2.60933300	-0.80540500	-1.30606200
H	-4.40003700	-1.36973000	1.56994600
C	-0.74205300	1.51567000	1.08540300
C	0.40266800	1.24783000	-1.13722000
C	-0.07594300	2.25432600	-0.06899400
O	-0.71106600	0.49426600	-1.64946100
O	-4.49240400	-2.13456700	-0.98798200
H	-5.14149800	-2.43055700	-0.33694900
C	1.51188100	0.32588300	-0.66427000
C	1.34628300	-1.07219300	-0.62056100
C	2.73606600	0.87928000	-0.29655500
C	2.37939200	-1.89958100	-0.18543500
H	0.42320000	-1.52157000	-0.95567400
C	3.77800900	0.06284700	0.13712800
H	2.92305700	1.94548000	-0.34081700
C	3.59228000	-1.34733100	0.19663700
H	2.24176400	-2.97509000	-0.15956100
H	0.75303300	1.80109100	-2.01310400
O	4.67507900	-2.03117000	0.63180500
H	4.52374200	-2.98382400	0.63418400
C	-1.65635900	0.05929000	-0.79606000
C	-1.67581100	0.46545400	0.57075500
H	0.78768600	2.81785800	0.29984700
O	-1.06587900	3.11458000	-0.60527200
H	-0.68145400	3.66836100	-1.29335200
O	4.94437500	0.61041100	0.49454800
H	5.56216500	-0.08494500	0.76660600
H	-2.59821400	-1.08964900	-2.34899100
O	-2.62839500	0.32000900	2.69974400
H	-3.35508400	-0.04849200	3.21656600
H	0.00018000	1.07161500	1.75755000
H	-1.30110400	2.23745700	1.68624200

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.270590 (Hartree/Particle)
Thermal correction to Energy= 0.288688
Thermal correction to Enthalpy= 0.289632
Thermal correction to Gibbs Free Energy= 0.223837

Sum of electronic and zero-point Energies= -1031.092889
Sum of electronic and thermal Energies= -1031.074792
Sum of electronic and thermal Enthalpies= -1031.073848
Sum of electronic and thermal Free Energies= -1031.139643

Name of compound (9)	**Isomelacacidin**
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)	
C -2.95018900 0.92141700 1.36325000	
C -3.99407500 0.00935100 1.25439100	
C -3.92980200 -0.98474800 0.28285500	
C -2.84000900 -1.07698400 -0.58549300	
H -2.98738400 1.71506200 2.09734300	
H -4.85409700 0.07050400 1.91373900	
C -0.69744300 1.81699600 0.61961000	
C 0.37050300 0.55910900 -1.30638900	
C -0.01396200 1.94470000 -0.73823000	
O -0.77878200 -0.29696200 -1.37307400	
O -2.77950400 -2.04661400 -1.54073600	
H -3.59539400 -2.55902700 -1.47432800	
O -4.90110100 -1.94326200 0.08533000	
H -5.63666200 -1.78694000 0.68455200	
O 1.09133400 2.83882100 -0.66794400	
H 1.78833000 2.40964600 -0.15438700	
H -0.72188100 2.41367600 -1.42617000	
C 1.52369800 -0.11210600 -0.57506200	
C 1.31588600 -1.12210700 0.36352800	
C 2.83626700 0.29238100 -0.86182400	
C 2.40000100 -1.70506300 1.02134800	
H 0.31521900 -1.47520700 0.57100300	
C 3.91861300 -0.28123700 -0.20561900	
H 3.03985400 1.03897800 -1.62121400	
C 3.69342100 -1.28639600 0.74697300	
H 2.23311800 -2.49476300 1.74807100	
H 0.66610000 0.70320100 -2.34795100	
O 4.82798200 -1.79456600 1.33639700	
H 4.59760600 -2.51622400 1.92928000	
C -1.79655700 -0.14900200 -0.46870200	
C -1.84594600 0.84715200 0.51498200	
O 5.18379600 0.12319700 -0.49897400	
H 5.79317800 -0.40375800 0.03410200	
H 0.04456600 1.43227100 1.33993600	
O -1.16747500 3.08363600 1.06198700	
H -0.43498800 3.69779900 0.92841300	
Frequency and Energy at B3LYP/6-311G(d,p) in gas phase	
Zero-point correction= 0.275406 (Hartree/Particle)	
Thermal correction to Energy= 0.294976	
Thermal correction to Enthalpy= 0.295921	
Thermal correction to Gibbs Free Energy= 0.227811	
Sum of electronic and zero-point Energies= -1106.582499	
Sum of electronic and thermal Energies= -1106.562929	
Sum of electronic and thermal Enthalpies= -1106.561985	
Sum of electronic and thermal Free Energies= -1106.630094	
Name of radical	O7-H
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)	

C	-3.03353200	0.88014400	1.35031000
C	-4.06775700	-0.00761600	1.27491900
C	-4.03000900	-1.06187800	0.29547500
C	-2.86326800	-1.11987900	-0.58750500
H	-3.04880300	1.69174500	2.06622900
H	-4.93142400	0.05061700	1.92484800
C	-0.76335800	1.77560600	0.61049900
C	0.34696200	0.53803300	-1.30883200
C	-0.06395600	1.91637400	-0.74098900
O	-0.79000800	-0.34041400	-1.37498300
O	-2.85694900	-2.09907500	-1.48686500
H	-3.70292400	-2.57016400	-1.31998700
O	-4.90818600	-1.93897900	0.12428300
O	1.02489700	2.82498100	-0.65064600
H	1.73455700	2.39517200	-0.15474500
H	-0.77035400	2.37908500	-1.43474100
C	1.50913100	-0.11283100	-0.57557500
C	1.31777700	-1.11191000	0.37805600
C	2.81515200	0.30443800	-0.87410900
C	2.41194000	-1.67339200	1.03813500
H	0.32352400	-1.47757600	0.59492000
C	3.90742500	-0.24718700	-0.21546900
H	3.00652300	1.04235100	-1.64511100
C	3.69877700	-1.24277700	0.75187600
H	2.25780000	-2.45564100	1.77539100
H	0.63867100	0.68676500	-2.35046500
O	4.84169100	-1.72789900	1.34082100
H	4.62685300	-2.44668300	1.94316700
C	-1.81813000	-0.19228500	-0.48629500
C	-1.90011300	0.79844200	0.48807800
O	5.16461900	0.16857600	-0.52030800
H	5.78485000	-0.34369300	0.01481200
H	-0.03019300	1.38094100	1.33569300
O	-1.24715600	3.03163700	1.05850900
H	-0.52257800	3.65677600	0.93206200

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.263644 (Hartree/Particle)
Thermal correction to Energy= 0.282449
Thermal correction to Enthalpy= 0.283394
Thermal correction to Gibbs Free Energy= 0.215905
Sum of electronic and zero-point Energies= -1105.966692
Sum of electronic and thermal Energies= -1105.947887
Sum of electronic and thermal Enthalpies= -1105.946943
Sum of electronic and thermal Free Energies= -1106.014431

Name of radical	C4-H

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

C	-2.90679900	0.86009500	1.38697700
C	-3.82997500	-0.17014200	1.30901000
C	-3.74062700	-1.10851900	0.28212200
C	-2.71588700	-1.04070100	-0.67774000
H	-2.96985600	1.60114600	2.17211300
H	-4.62878400	-0.24736600	2.04055300
C	-0.91325400	1.99759400	0.42031200
C	0.37626700	0.78197000	-1.35005500

C	0.03569200	2.16171700	-0.72244100
O	-0.82070300	0.02621500	-1.57488500
O	-2.62514600	-1.97369900	-1.66692900
H	-3.36435400	-2.58331700	-1.54786300
O	-4.60617000	-2.17038900	0.11910000
H	-5.28758600	-2.13953900	0.79681900
O	1.19651000	2.89465400	-0.31610400
H	1.76772000	2.28554300	0.17305200
H	-0.41279200	2.78768300	-1.50603900
C	1.43753100	0.01237000	-0.57928400
C	1.12938900	-0.88969300	0.44065000
C	2.78337800	0.22667500	-0.91263500
C	2.14880500	-1.56296400	1.11400100
H	0.10106600	-1.08699200	0.70812300
C	3.80296100	-0.43450000	-0.23918500
H	3.05887100	0.89994200	-1.71656200
C	3.47726600	-1.33742600	0.78337200
H	1.90369400	-2.26897500	1.90205100
H	0.76304400	0.96139900	-2.35445300
O	4.55223600	-1.94859400	1.38546600
H	4.24705400	-2.58871000	2.03548400
C	-1.78918700	-0.00884800	-0.60488100
C	-1.86898500	0.97010400	0.42805900
O	5.10107000	-0.21346900	-0.58205400
H	5.65316500	-0.77964300	-0.02738800
O	-0.95131700	2.99486300	1.34426900
H	-0.16252000	3.53578200	1.18352600

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.262250 (Hartree/Particle)
Thermal correction to Energy= 0.281904
Thermal correction to Enthalpy= 0.282848
Thermal correction to Gibbs Free Energy= 0.213695
Sum of electronic and zero-point Energies= -1105.959632
Sum of electronic and thermal Energies= -1105.939978
Sum of electronic and thermal Enthalpies= -1105.939034
Sum of electronic and thermal Free Energies= -1106.008188

Name of anion	O7-H

Cartesian Coordinates optimized at B3LYP/6-311G(d,p

C	2.78707600	0.68248200	-1.51958400
C	3.74365900	-0.32562900	-1.43412400
C	3.75426000	-1.23882000	-0.34447000
C	2.72098000	-1.04355300	0.64958400
H	2.80169300	1.37154400	-2.35855100
H	4.50529400	-0.43793000	-2.20005400
C	0.73579200	1.90676200	-0.67286800
C	-0.32909500	0.80616500	1.35550800
C	0.03402700	2.13624400	0.65997900
O	0.84911100	0.05844500	1.59616500
O	2.76045900	-1.95764400	1.66570100
H	3.54537300	-2.48150900	1.36288100
O	4.55808800	-2.21349900	-0.15000200
O	-1.09024500	3.01536100	0.50355500
H	-1.70279600	2.57582100	-0.09912200
H	0.72620700	2.66927900	1.31534900

C	-1.41152300	-0.00230900	0.64337900
C	-1.10722000	-1.17534100	-0.04983300
C	-2.74985500	0.41411600	0.71640000
C	-2.11764800	-1.89863100	-0.68291000
H	-0.08533800	-1.52657100	-0.08858500
C	-3.75832400	-0.30401000	0.08508600
H	-3.02896200	1.29232100	1.28775500
C	-3.43423900	-1.46557000	-0.62382400
H	-1.87352300	-2.80901600	-1.22432300
H	-0.71212500	1.05776200	2.34982400
O	-4.50238500	-2.11806600	-1.21828500
H	-4.18044300	-2.91479500	-1.64959400
C	1.79042100	-0.03114500	0.55660100
C	1.80369100	0.86283100	-0.54250800
O	-5.06067500	0.11547800	0.16698800
H	-5.59223000	-0.52477100	-0.32205200
H	-0.03972800	1.58391300	-1.39722400
O	1.27610300	3.15311500	-1.14601700
H	0.54092100	3.77688000	-1.09964000

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.262209 (Hartree/Particle)
Thermal correction to Energy= 0.281093
Thermal correction to Enthalpy= 0.282037
Thermal correction to Gibbs Free Energy= 0.215202
Sum of electronic and zero-point Energies= -1106.042885
Sum of electronic and thermal Energies= -1106.024001
Sum of electronic and thermal Enthalpies= -1106.023057
Sum of electronic and thermal Free Energies= -1106.089893

Name of anion	O4'-H

Cartesian Coordinates optimized at B3LYP/6-311G(d,p

C	-3.03137400	1.09067500	1.18852700
C	-4.11147200	0.21624800	1.12248100
C	-4.02936900	-0.89057900	0.28254500
C	-2.89727900	-1.13294300	-0.49352300
H	-3.06815400	1.96753000	1.82164800
H	-5.01081800	0.39280300	1.70542200
C	-0.68994800	1.78009800	0.49424200
C	0.41216600	0.33654100	-1.26987800
C	0.01517500	1.77238700	-0.85822000
O	-0.75587200	-0.53806800	-1.22157700
O	-2.83599700	-2.21930900	-1.32142900
H	-3.65160300	-2.71529700	-1.18006700
O	-5.04860600	-1.82216900	0.13439600
H	-5.69492700	-1.68407200	0.83193700
O	1.14499800	2.63848700	-0.83072300
H	1.88488500	2.10896800	-0.48782600
H	-0.67489400	2.19618800	-1.59604500
C	1.58741200	-0.21390400	-0.50350600
C	1.46455700	-0.87303200	0.72188000
C	2.89568300	0.00342300	-1.02147200
C	2.58291600	-1.30824400	1.43907200
H	0.47497500	-1.08145100	1.11790700
C	3.99863400	-0.40886500	-0.30891600
H	3.03537500	0.47427200	-1.99194000

C	3.90416700	-1.08779800	0.97085100
H	2.46119600	-1.83561100	2.38066100
H	0.67195500	0.36578600	-2.33165700
O	5.00255700	-1.42656800	1.52592300
C	-1.81198500	-0.24166100	-0.42785300
C	-1.88358400	0.86933900	0.42968800
O	5.28374300	-0.24471500	-0.73056800
H	5.75548300	-0.66939600	0.03185300
H	0.02170200	1.40465300	1.24393900
O	-1.08372200	3.10805600	0.84266900
H	-0.29617900	3.63980300	0.66913200

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.262272 (Hartree/Particle)
Thermal correction to Energy= 0.281158
Thermal correction to Enthalpy= 0.282102
Thermal correction to Gibbs Free Energy= 0.214999
Sum of electronic and zero-point Energies= -1106.053375
Sum of electronic and thermal Energies= -1106.034489
Sum of electronic and thermal Enthalpies= -1106.033545
Sum of electronic and thermal Free Energies= -1106.100648

Name of cationic radical

Cartesian Coordinates optimized at B3LYP/6-311G(d,p

C	3.10959200	0.98437300	-1.18182700
C	4.16305100	0.05233500	-1.06600000
C	4.02286900	-1.02578300	-0.22434000
C	2.82346600	-1.18557400	0.52808800
H	3.22593800	1.84166300	-1.83219700
H	5.07409500	0.19269400	-1.63587800
C	0.79518900	1.85311600	-0.59351800
C	-0.39140900	0.50836500	1.21743300
C	0.05081500	1.91358900	0.74261800
O	0.71224100	-0.44224500	1.18360800
O	2.66583700	-2.20411900	1.35535900
H	3.46765500	-2.75488900	1.34355900
O	4.92213200	-2.01236100	0.00285800
H	5.73704400	-1.88505700	-0.49744900
O	-1.03315400	2.81723300	0.69365000
H	-1.72367000	2.45641900	0.12246400
H	0.73968900	2.32867900	1.48298900
C	-1.57739100	-0.08805600	0.49103200
C	-1.42072000	-0.93523800	-0.62051400
C	-2.86074000	0.20318300	0.95910500
C	-2.53247500	-1.46051700	-1.27015800
H	-0.43426900	-1.20682100	-0.97080200
C	-3.98050700	-0.31330400	0.31431600
H	-3.01735400	0.82622200	1.83158500
C	-3.81015000	-1.15595600	-0.81477700
H	-2.40681000	-2.11638400	-2.12488100
H	-0.63579800	0.57508500	2.27847500
O	-4.96636200	-1.60561700	-1.35560500
H	-4.81056500	-2.18836200	-2.10805300
C	1.77268900	-0.21971100	0.40564000
C	1.92066200	0.85604800	-0.47528900
O	-5.20617100	-0.01418500	0.76676700

H	-5.87176400	-0.45172900	0.21606300
H	0.08937700	1.51418300	-1.37095500
O	1.33414800	3.10936100	-0.93958900
H	0.62742900	3.76253600	-0.86215700

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.275585 (Hartree/Particle)
Thermal correction to Energy= 0.294851
Thermal correction to Enthalpy= 0.295795
Thermal correction to Gibbs Free Energy= 0.227724
Sum of electronic and zero-point Energies= -1106.322779
Sum of electronic and thermal Energies= -1106.303513
Sum of electronic and thermal Enthalpies= -1106.302569
Sum of electronic and thermal Free Energies= -1106.370639

Name of compound (10)	**Isoteracacidin**	

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

C	2.66019300	0.91745200	-1.38057100
C	3.69996000	-0.00135600	-1.29199300
C	3.64445800	-0.99990500	-0.32440800
C	2.56740300	-1.08995700	0.55990200
H	2.69108400	1.71438200	-2.11137300
H	4.55014000	0.05788800	-1.96411200
C	0.42439200	1.82268200	-0.59933100
C	-0.62049800	0.56463600	1.34114300
C	-0.23859400	1.94891200	0.76858900
O	0.52212800	-0.30313200	1.38117200
O	2.51563500	-2.06335700	1.51160100
H	3.32675500	-2.58114300	1.43002600
O	4.61272000	-1.96487800	-0.14602600
H	5.33957000	-1.81137600	-0.75651700
O	-1.34580600	2.84288900	0.71539600
H	-2.04374600	2.41753000	0.20017300
H	0.47939900	2.41767900	1.44602800
C	-1.79552000	-0.09357500	0.63568500
C	-1.62260600	-1.07695300	-0.34089200
C	-3.10451600	0.27832700	0.97382900
C	-2.71755100	-1.65161600	-0.97909900
H	-0.62636400	-1.41481700	-0.59600200
C	-4.20517800	-0.28385900	0.33799300
H	-3.26764700	1.00818600	1.76005400
C	-4.01415000	-1.25299200	-0.64803000
H	-2.56190900	-2.41941600	-1.73163300
H	-5.21553000	0.00088100	0.60504100
H	-0.89153300	0.70977800	2.38927800
O	-5.12522300	-1.77920000	-1.23992700
H	-4.85913500	-2.44559700	-1.88191400
C	1.52755700	-0.15548800	0.46322800
C	1.56844000	0.84565200	-0.51590700
H	-0.33051800	1.44582700	-1.31057400
O	0.89543100	3.08800900	-1.04431500
H	0.16762700	3.70579600	-0.90251400

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.271187 (Hartree/Particle)
Thermal correction to Energy= 0.289469

Thermal correction to Enthalpy=	0.290413		
Thermal correction to Gibbs Free Energy=	0.224975		
Sum of electronic and zero-point Energies=	-1031.342477		
Sum of electronic and thermal Energies=	-1031.324195		
Sum of electronic and thermal Enthalpies=	-1031.323251		
Sum of electronic and thermal Free Energies=	-1031.388689		
Name of radical	O7-H		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)			
C	2.74737700	0.87716300	-1.36582700
C	3.77641500	-0.01812400	-1.31282200
C	3.74514800	-1.08094700	-0.34239600
C	2.59010200	-1.13946700	0.55586800
H	2.75844900	1.69507000	-2.07459500
H	4.63135100	0.04022800	-1.97416200
C	0.49401700	1.78150900	-0.58654300
C	-0.59475100	0.53961200	1.34439800
C	-0.18319300	1.91749400	0.77650900
O	0.53182400	-0.35536400	1.37700500
O	2.58960300	-2.12603400	1.44688500
H	3.43001700	-2.60140300	1.26472400
O	4.62001000	-1.96482400	-0.19074200
O	-1.27225600	2.82876200	0.70800900
H	-1.98462900	2.40541800	0.21067600
H	0.53532400	2.37581700	1.46053200
C	-1.78300700	-0.09028900	0.63780000
C	-1.63313900	-1.05511800	-0.36106100
C	-3.08327900	0.29402200	0.99578500
C	-2.74165900	-1.60112100	-1.00049500
H	-0.64513800	-1.40468100	-0.63251900
C	-4.19720800	-0.23878500	0.35859900
H	-3.22888300	1.00944300	1.79858700
C	-4.02945800	-1.19055200	-0.64896800
H	-2.60388300	-2.35570900	-1.76943300
H	-5.20080000	0.05481100	0.64072600
H	-0.85861400	0.68580900	2.39384900
O	-5.15272400	-1.68711400	-1.23954000
H	-4.90579300	-2.34597500	-1.89695900
C	1.54944300	-0.20431300	0.47707800
C	1.62529400	0.79523700	-0.48877400
H	-0.25338300	1.39823900	-1.30345800
O	0.98002600	3.03689700	-1.03379700
H	0.26149900	3.66641900	-0.89542800
Frequency and Energy at B3LYP/6-311G(d,p) in gas phase			
Zero-point correction=	0.259406 (Hartree/Particle)		
Thermal correction to Energy=	0.276942		
Thermal correction to Enthalpy=	0.277887		
Thermal correction to Gibbs Free Energy=	0.212975		
Sum of electronic and zero-point Energies=	-1030.726525		
Sum of electronic and thermal Energies=	-1030.708989		
Sum of electronic and thermal Enthalpies=	-1030.708045		
Sum of electronic and thermal Free Energies=	-1030.772956		
Name of radical	C4-H		
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)			
C	2.59027200	0.87504100	-1.41951700

C	3.52458000	-0.14632000	-1.36027400
C	3.46789700	-1.08274300	-0.32910800
C	2.46516400	-1.02190500	0.65408200
H	2.62801700	1.61425000	-2.20799900
H	4.30672000	-0.21803900	-2.11010300
C	0.60697100	1.99518900	-0.41178200
C	-0.62915500	0.77167300	1.39076300
C	-0.32155100	2.15137900	0.74836000
O	0.58341200	0.03168100	1.59364600
O	2.40733500	-1.95141200	1.64863900
H	3.14802000	-2.55583400	1.51333100
O	4.34708500	-2.13535600	-0.18300600
H	5.00985900	-2.10327100	-0.87893600
O	-1.50539500	2.85782400	0.35941400
H	-2.06585300	2.23444300	-0.12408000
H	0.12983400	2.79275900	1.51760000
C	-1.69893100	-0.01334800	0.65191300
C	-1.42373600	-0.83973700	-0.44311000
C	-3.03069600	0.09274000	1.07683900
C	-2.44295300	-1.53265400	-1.08836100
H	-0.40719400	-0.96072100	-0.79268100
C	-4.05834400	-0.58442200	0.43234600
H	-3.26776500	0.71422400	1.93417200
C	-3.76518500	-1.40591200	-0.65700900
H	-2.20719600	-2.17680400	-1.93066100
H	-5.08492400	-0.50206800	0.76753700
H	-0.99463500	0.95245100	2.40281400
O	-4.80377900	-2.05879400	-1.25315100
H	-4.46755700	-2.60155800	-1.97389600
C	1.52706600	0.00095500	0.60023900
C	1.57404400	0.97819300	-0.43686100
O	0.61369800	2.98871300	-1.34061900
H	-0.17884700	3.52015000	-1.16760600

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.258074 (Hartree/Particle)
Thermal correction to Energy= 0.276429
Thermal correction to Enthalpy= 0.277373
Thermal correction to Gibbs Free Energy= 0.210608
Sum of electronic and zero-point Energies= -1030.719887
Sum of electronic and thermal Energies= -1030.701532
Sum of electronic and thermal Enthalpies= -1030.700588
Sum of electronic and thermal Free Energies= -1030.767353

Name of anion	O7-H

Cartesian Coordinates optimized at B3LYP/6-311G(d,p

C	2.50718700	0.66785200	-1.52804600
C	3.45852900	-0.34510700	-1.44487200
C	3.47124400	-1.25416600	-0.35157300
C	2.44470700	-1.05020400	0.64782700
H	2.52069600	1.35404500	-2.36936500
H	4.21480600	-0.46440500	-2.21499700
C	0.47027400	1.90899700	-0.67254500
C	-0.59069300	0.81955300	1.36419400
C	-0.22526900	2.14508300	0.66232400
O	0.58441700	0.06490600	1.60125700

O	2.48620300	-1.95980500	1.66767800
H	3.26652400	-2.48903000	1.36269700
O	4.27162700	-2.23152300	-0.15819800
O	-1.35113800	3.02340200	0.50566000
H	-1.95935000	2.58320200	-0.10088500
H	0.46951400	2.68135500	1.31222300
C	-1.68266200	0.01751300	0.66117400
C	-1.39357400	-1.14707600	-0.05583400
C	-3.02353400	0.41427500	0.75838000
C	-2.40691700	-1.86763300	-0.68197300
H	-0.37051100	-1.49463200	-0.11762200
C	-4.04385900	-0.29857000	0.13379500
H	-3.27729300	1.28933400	1.34806400
C	-3.73300500	-1.44392800	-0.59628200
H	-2.16049600	-2.76978700	-1.23655200
H	-5.07981100	0.00953600	0.21606100
H	-0.96567900	1.07738800	2.36002700
O	-4.76560400	-2.12309900	-1.19829900
H	-4.39779400	-2.88808900	-1.65198600
C	1.51899700	-0.03313500	0.55684100
C	1.53076400	0.85729500	-0.54544900
H	-0.31052100	1.59158500	-1.39378700
O	1.01825600	3.15063600	-1.14984800
H	0.28669000	3.77886900	-1.10763000

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.258015 (Hartree/Particle)
Thermal correction to Energy= 0.275546
Thermal correction to Enthalpy= 0.276490
Thermal correction to Gibbs Free Energy= 0.212493
Sum of electronic and zero-point Energies= -1030.803570
Sum of electronic and thermal Energies= -1030.786039
Sum of electronic and thermal Enthalpies= -1030.785095
Sum of electronic and thermal Free Energies= -1030.849092

Name of cationic radical

Cartesian Coordinates optimized at B3LYP/6-311G(d,p

C	2.80473100	0.99402800	-1.20234200
C	3.86383100	0.05740200	-1.12404800
C	3.74644700	-1.03000900	-0.29508900
C	2.56294800	-1.19578200	0.48652300
H	2.90842400	1.85806700	-1.84631700
H	4.75889000	0.20671900	-1.71648800
C	0.50544600	1.86116000	-0.55635600
C	-0.64154100	0.50073800	1.27256100
C	-0.21282200	1.90766100	0.79522600
O	0.47649400	-0.44708300	1.20618600
O	2.42287100	-2.21860900	1.30302800
H	3.21907500	-2.77806900	1.26481600
O	4.64407100	-2.02214000	-0.10008600
H	5.44538600	-1.90216400	-0.62425000
O	-1.30644000	2.79928800	0.77080300
H	-2.01343600	2.41964400	0.23213700
H	0.48788600	2.32715100	1.52229700
C	-1.84043600	-0.10042100	0.57921300
C	-1.73900300	-0.83618100	-0.61060000

C	-3.11205400	0.08020200	1.15023300
C	-2.86845900	-1.35281700	-1.22687100
H	-0.77189500	-1.02754000	-1.05957500
C	-4.24772300	-0.41874100	0.53821400
H	-3.20985000	0.62197700	2.08439700
C	-4.13353700	-1.14368300	-0.65847800
H	-2.77371500	-1.92506000	-2.14378700
H	-5.23049800	-0.27578400	0.96911000
H	-0.85177700	0.55608800	2.34132800
O	-5.27287500	-1.61356800	-1.19861400
H	-5.09527200	-2.10806100	-2.00767300
C	1.50576300	-0.22165300	0.40410700
C	1.63327300	0.86288800	-0.47255000
H	-0.21390200	1.53073400	-1.32376000
O	1.04151600	3.11911000	-0.90030500
H	0.33441500	3.77156000	-0.81877700

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.271254 (Hartree/Particle)
Thermal correction to Energy= 0.289375
Thermal correction to Enthalpy= 0.290319
Thermal correction to Gibbs Free Energy= 0.224592
Sum of electronic and zero-point Energies= -1031.079795
Sum of electronic and thermal Energies= -1031.061674
Sum of electronic and thermal Enthalpies= -1031.060730
Sum of electronic and thermal Free Energies= -1031.126457

Name of compound (11)	**Melacacidin**

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

C	-2.75773300	0.89294600	1.56077400
C	-3.77060800	-0.05228200	1.46667600
C	-3.80801400	-0.89605900	0.35881000
C	-2.84237500	-0.81274400	-0.64592500
H	-2.71417500	1.55734900	2.41589000
H	-4.53017100	-0.13242800	2.23765800
C	-0.69028600	2.04224300	0.66720500
H	-1.11330900	3.00095700	0.97731800
C	0.31007800	0.88100200	-1.36882500
C	0.00414300	2.24051100	-0.68591400
O	-0.92420000	0.16929700	-1.56391700
O	0.28678000	1.75169400	1.68462100
H	0.55471900	0.82983100	1.57893500
O	-2.86297100	-1.65533900	-1.71536400
H	-3.63468000	-2.22690000	-1.61243800
O	-4.76002100	-1.87012900	0.15783000
H	-5.39003500	-1.86629700	0.88438700
O	1.15524600	3.04468400	-0.54411000
H	1.50618500	2.84133000	0.33560700
H	-0.68403500	2.76814100	-1.35442300
C	1.36529500	0.01071400	-0.69381600
C	1.05838100	-1.24004000	-0.15597400
C	2.69765000	0.45188200	-0.66999800
C	2.05887300	-2.02220900	0.42889300
H	0.05173500	-1.62852900	-0.21477600
C	3.69299100	-0.32177700	-0.09111600

H	2.97348400	1.40422400	-1.10309600
C	3.36686200	-1.56800000	0.46831700
H	1.81297900	-2.99602900	0.84236200
H	0.65166100	1.09803100	-2.38282600
O	4.42507600	-2.25655300	1.01654500
H	4.13061800	-3.11622800	1.33195900
C	-1.82431300	0.14565500	-0.53762100
C	-1.78108500	1.00608700	0.56783000
O	4.97837800	0.12509200	-0.07387700
H	5.51957300	-0.55098800	0.35372800

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.275927 (Hartree/Particle)
Thermal correction to Energy= 0.295276
Thermal correction to Enthalpy= 0.296220
Thermal correction to Gibbs Free Energy= 0.228997
Sum of electronic and zero-point Energies= -1106.585525
Sum of electronic and thermal Energies= -1106.566176
Sum of electronic and thermal Enthalpies= -1106.565232
Sum of electronic and thermal Free Energies= -1106.632456

Name of radical	O7-H

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

C	-2.79230200	0.80211500	1.59093900
C	-3.79914100	-0.11507700	1.52573100
C	-3.89039900	-0.98442300	0.38051300
C	-2.87028200	-0.83631800	-0.65989900
H	-2.70730800	1.46113100	2.44808500
H	-4.54419200	-0.21945800	2.30388900
C	-0.74331300	1.99730000	0.67556000
H	-1.18967300	2.94239000	0.99646600
C	0.28126500	0.88319400	-1.37557300
C	-0.04590600	2.22739000	-0.67168200
O	-0.94864100	0.16069900	-1.58558300
O	0.22013000	1.70253100	1.70076900
H	0.53425400	0.79919200	1.56172200
O	-2.96045200	-1.66754600	-1.69162400
H	-3.75729600	-2.20567300	-1.48817300
O	-4.75724500	-1.86821900	0.19561300
O	1.09048100	3.04672300	-0.51416300
H	1.45087000	2.83714300	0.35973300
H	-0.74006200	2.75622100	-1.33306900
C	1.34145100	0.01701600	-0.70445400
C	1.04738200	-1.23747800	-0.16818000
C	2.66891200	0.47313500	-0.67760900
C	2.05551800	-2.01027700	0.41641300
H	0.04634200	-1.63981200	-0.22839900
C	3.67185400	-0.29079500	-0.09879300
H	2.93618500	1.42826800	-1.11004700
C	3.35839100	-1.54213000	0.45828800
H	1.81910300	-2.98726600	0.82735500
H	0.62261500	1.11877300	-2.38499000
O	4.42293800	-2.21812400	1.00540800
H	4.14139200	-3.08267200	1.31977800
C	-1.84491300	0.11857800	-0.56002200
C	-1.81447500	0.94479700	0.55785900

O	4.95059200	0.17015200	-0.07950100
H	5.50109400	-0.50011400	0.34574800

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.264206 (Hartree/Particle)
Thermal correction to Energy= 0.282807
Thermal correction to Enthalpy= 0.283751
Thermal correction to Gibbs Free Energy= 0.217121
Sum of electronic and zero-point Energies= -1105.968466
Sum of electronic and thermal Energies= -1105.949865
Sum of electronic and thermal Enthalpies= -1105.948921
Sum of electronic and thermal Free Energies= -1106.015551

Name of radical	O4'-H

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

C	-2.72697600	0.94508200	1.52851400
C	-3.74607100	0.00603200	1.44430100
C	-3.78184500	-0.86093400	0.35430900
C	-2.80682300	-0.80600600	-0.64423800
H	-2.68665900	1.62721000	2.36959300
H	-4.51260000	-0.05146800	2.21013400
C	-0.64228400	2.05677100	0.63057900
H	-1.05843900	3.02832000	0.90880100
C	0.36588000	0.83821900	-1.37121000
C	0.07693300	2.21897300	-0.71410200
O	-0.87048600	0.13815900	-1.56456300
O	0.31944600	1.78015100	1.66690600
H	0.49433200	0.83127300	1.66969800
O	-2.82188800	-1.66963300	-1.69473500
H	-3.59337300	-2.24078000	-1.58608200
O	-4.73783600	-1.83010100	0.16417800
H	-5.36324900	-1.82504100	0.89491600
O	1.23944000	3.00098000	-0.56971900
H	1.57436100	2.80858600	0.31895400
H	-0.59049000	2.74345300	-1.40518400
C	1.41096900	-0.02442800	-0.68268100
C	1.06461600	-1.27693700	-0.09621900
C	2.74503200	0.40113500	-0.68910600
C	2.00562900	-2.06617300	0.51373000
H	0.04097800	-1.61856200	-0.16127100
C	3.71150300	-0.38135100	-0.08093000
H	3.02681900	1.33561200	-1.15572900
C	3.38350300	-1.65846400	0.56255400
H	1.74947600	-3.02128300	0.95616500
H	0.72192400	1.03680400	-2.38476600
O	4.31899400	-2.30099000	1.09107500
C	-1.78316100	0.14649800	-0.54574100
C	-1.74067200	1.02979800	0.54159000
O	4.99564500	-0.03095800	-0.04124300
H	5.43299100	-0.76426800	0.44147200

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.264032 (Hartree/Particle)
Thermal correction to Energy= 0.282688
Thermal correction to Enthalpy= 0.283633
Thermal correction to Gibbs Free Energy= 0.216856
Sum of electronic and zero-point Energies= -1105.968998

Sum of electronic and thermal Energies=	-1105.950342
Sum of electronic and thermal Enthalpies=	-1105.949398
Sum of electronic and thermal Free Energies=	-1106.016174
Name of radical	C2-H
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)	
C	-3.77881100 1.29574600 0.11334000
C	-4.67719100 0.23548700 0.09622700
C	-4.19455900 -1.06616100 -0.02794500
C	-2.82588100 -1.32298200 -0.13641000
H	-4.14235800 2.31184800 0.21198600
H	-5.74496100 0.41204900 0.17494600
C	-1.40014200 2.18470000 0.04229300
H	-1.79808900 3.08454200 -0.43068100
C	0.36427400 0.42318700 -0.24920100
C	-0.09920900 1.79502700 -0.69235200
O	-0.61510900 -0.55469700 -0.21522700
O	-1.06764100 2.60479100 1.38102100
H	-0.94804600 1.81026600 1.91515600
O	-2.34897000 -2.59054300 -0.25467700
H	-3.10986200 -3.18565200 -0.24914900
O	-4.98820300 -2.18917400 -0.05625100
H	-5.91378000 -1.94029000 0.02323600
O	0.85078600 2.82292000 -0.49831700
H	0.75616800 3.08353900 0.43024400
H	-0.31113900 1.76844700 -1.77177700
C	1.68521900 -0.09334000 -0.10482900
C	1.86685700 -1.46301800 0.23314700
C	2.85004400 0.70225700 -0.28973200
C	3.13848100 -1.99361700 0.38298800
H	1.00190600 -2.09622900 0.36592000
C	4.11095600 0.16053600 -0.13677400
H	2.76529700 1.74278800 -0.56189400
C	4.26341800 -1.19526900 0.20455400
H	3.25965400 -3.04228000 0.64061300
O	5.56307900 -1.63049300 0.33383500
H	5.57378600 -2.56864900 0.54599900
C	-1.93702800 -0.24078100 -0.11907200
C	-2.40482700 1.07228200 0.00678600
O	5.21233700 0.94501300 -0.32175000
H	5.99160400 0.39277400 -0.18178200
Frequency and Energy at B3LYP/6-311G(d,p) in gas phase	
ero-point correction=	0.261903 (Hartree/Particle)
Thermal correction to Energy=	0.281672
Thermal correction to Enthalpy=	0.282617
Thermal correction to Gibbs Free Energy=	0.213455
Sum of electronic and zero-point Energies=	-1105.958588
Sum of electronic and thermal Energies=	-1105.938819
Sum of electronic and thermal Enthalpies=	-1105.937875
Sum of electronic and thermal Free Energies=	-1106.007037
Name of anion	O7-H
Cartesian Coordinates optimized at B3LYP/6-311G(d,p	
C	-2.76301500 0.87059200 1.54374900
C	-3.70066100 -0.15384100 1.51327100
C	-3.73452800 -1.08407500 0.43483900

C	-2.74830700	-0.87987500	-0.60391300
H	-2.74853800	1.56137500	2.38394800
H	-4.42748500	-0.27278400	2.31096900
C	-0.79008600	2.13643700	0.60138800
H	-1.23829200	3.09866900	0.87197500
C	0.26650100	0.95017400	-1.40425500
C	-0.04681400	2.31251800	-0.72989600
O	-0.95560300	0.26511700	-1.64651600
O	0.21295100	1.93624300	1.65295800
H	0.32501900	0.98045600	1.72343500
O	-2.80206900	-1.81319500	-1.60256800
H	-3.55868600	-2.35477600	-1.26500900
O	-4.52440500	-2.07512500	0.29109200
O	1.11351100	3.11204200	-0.54479600
H	1.38543700	2.90655100	0.36469600
H	-0.70509000	2.84052100	-1.42742900
C	1.30129600	0.05609000	-0.71816600
C	0.97451600	-1.24716900	-0.33603000
C	2.62390400	0.49676600	-0.55642000
C	1.94023700	-2.07796500	0.23487500
H	-0.02648600	-1.62060700	-0.50016700
C	3.58586400	-0.32878300	0.00861500
H	2.91237200	1.49247600	-0.86593400
C	3.23713600	-1.62266000	0.41315900
H	1.67580000	-3.08894900	0.53448200
H	0.65513200	1.17842400	-2.40206800
O	4.26362600	-2.37364400	0.96607400
H	3.91040000	-3.22309300	1.24531000
C	-1.83323000	0.14825500	-0.56475100
C	-1.80993300	1.04914400	0.53036100
O	4.87373900	0.11704500	0.16446300
H	5.36915000	-0.59977800	0.57917100

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.262953 (Hartree/Particle)
Thermal correction to Energy= 0.281569
Thermal correction to Enthalpy= 0.282514
Thermal correction to Gibbs Free Energy= 0.216417
Sum of electronic and zero-point Energies= -1106.054203
Sum of electronic and thermal Energies= -1106.035587
Sum of electronic and thermal Enthalpies= -1106.034643
Sum of electronic and thermal Free Energies= -1106.100739

Name of cationic radical

Cartesian Coordinates optimized at B3LYP/6-311G(d,p

C	-2.89930300	0.98617300	1.42526100
C	-3.93247300	0.03633400	1.33191800
C	-3.91568600	-0.89242900	0.31052100
C	-2.85720600	-0.89023000	-0.62688700
H	-2.92877200	1.71385700	2.22776500
H	-4.74130500	0.04289600	2.05347800
C	-0.74849700	2.06276400	0.62246700
H	-1.18291100	3.03624100	0.85900600
C	0.33035900	0.80095500	-1.32357000
C	-0.00843400	2.18978100	-0.71587800
O	-0.86527800	-0.00872300	-1.45167500

O	0.17689400	1.82203200	1.68918400
H	0.41304900	0.88698100	1.69965700
O	-2.80366200	-1.77806900	-1.61418200
H	-3.58780300	-2.35004300	-1.56812600
O	-4.83474800	-1.86418800	0.08155100
H	-5.56573800	-1.82650200	0.70915500
O	1.14718100	2.97483200	-0.58975800
H	1.45978400	2.86813900	0.32096200
H	-0.67240200	2.68575700	-1.43154000
C	1.41846100	-0.00377400	-0.63734400
C	1.13692800	-1.20517600	0.05261400
C	2.74047300	0.41841700	-0.76549500
C	2.15480500	-1.93628400	0.65534800
H	0.12860400	-1.59132900	0.08793400
C	3.76828500	-0.30425200	-0.16733000
H	2.99224200	1.32125400	-1.30545300
C	3.46950600	-1.49791500	0.55461200
H	1.92970400	-2.85820900	1.18023100
H	0.63892900	0.96021300	-2.35837300
O	4.54830800	-2.11200600	1.08158400
H	4.31500400	-2.92329300	1.54935000
C	-1.81313300	0.07889300	-0.51309800
C	-1.84319000	1.02755700	0.52426200
O	5.02786900	0.12649400	-0.27055500
H	5.62373500	-0.47382200	0.20235600

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.275931 (Hartree/Particle)
Thermal correction to Energy= 0.295028
Thermal correction to Enthalpy= 0.295973
Thermal correction to Gibbs Free Energy= 0.228439
Sum of electronic and zero-point Energies= -1106.321351
Sum of electronic and thermal Energies= -1106.302253
Sum of electronic and thermal Enthalpies= -1106.301309
Sum of electronic and thermal Free Energies= -1106.368843

Name of compound (12)	**Taxifolin**

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

C	-2.85814400	0.13780700	1.20254000
C	-3.70750100	-0.91816200	0.89260500
C	-3.51221400	-1.62110900	-0.29900800
C	-2.47451900	-1.30864400	-1.18375100
H	-4.51178500	-1.16593100	1.57567900
C	-0.97478400	1.63746000	0.58049200
C	0.45895600	0.85872100	-1.36361900
C	-0.01322200	2.05091000	-0.52925700
O	-0.63076500	0.00121700	-1.75061500
O	-1.08103100	2.35357300	1.58720000
O	-4.31529000	-2.65468500	-0.65277900
H	-4.98910000	-2.78292500	0.02380200
C	1.58087900	0.07331200	-0.69502600
C	1.43220100	-1.25229200	-0.29794100
C	2.81763400	0.70631600	-0.50983000
C	2.49768900	-1.93200000	0.29806300
H	0.49735400	-1.77165700	-0.45314500

C	3.87960400	0.03733200	0.07975900
H	2.98344000	1.72931500	-0.82941800
C	3.71239100	-1.29520500	0.49075300
H	2.37512600	-2.96512900	0.60941400
H	0.81857200	1.26189500	-2.31298900
O	4.82320000	-1.87002800	1.06309900
H	4.63346900	-2.77939600	1.31290800
C	-1.62262200	-0.26218500	-0.86966700
C	-1.79430000	0.48851800	0.32094200
H	0.85191700	2.53683000	-0.06795200
O	-0.70125000	2.94384700	-1.40502700
H	-1.00708900	3.68994500	-0.87687100
O	5.07280800	0.66819200	0.24985100
H	5.67950600	0.04328700	0.66750000
H	-2.33987800	-1.87520400	-2.09426300
O	-3.06033700	0.82428600	2.33114500
H	-2.38250400	1.54308200	2.36002500

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.252822 (Hartree/Particle)
Thermal correction to Energy= 0.271372
Thermal correction to Enthalpy= 0.272316
Thermal correction to Gibbs Free Energy= 0.205506
Sum of electronic and zero-point Energies= -1105.422487
Sum of electronic and thermal Energies= -1105.403937
Sum of electronic and thermal Enthalpies= -1105.402993
Sum of electronic and thermal Free Energies= -1105.469803

Name of radical	O4'-H

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

C	-2.84434300	0.17399000	1.17869900
C	-3.69643900	-0.88071000	0.87210200
C	-3.48780600	-1.60606400	-0.30330300
C	-2.43224600	-1.31610900	-1.17670900
H	-4.51357500	-1.11015300	1.54610200
C	-0.93956500	1.64894900	0.56233900
C	0.51702800	0.82298000	-1.34724700
C	0.04813000	2.03510300	-0.53521500
O	-0.56730300	-0.03252700	-1.73565000
O	-1.05631400	2.38518800	1.55221600
O	-4.29049000	-2.63822800	-0.65412600
H	-4.97532000	-2.75675100	0.01335700
C	1.63357400	0.04697800	-0.66373900
C	1.44838300	-1.28858400	-0.21283400
C	2.87563100	0.67382400	-0.51976900
C	2.46280200	-1.98259400	0.39408200
H	0.48893600	-1.76496900	-0.35904100
C	3.91632700	-0.00640700	0.08801000
H	3.04642100	1.68159100	-0.88183600
C	3.75420200	-1.37906200	0.58174800
H	2.32974900	-2.99920200	0.74334300
H	0.89545900	1.21271300	-2.29574300
O	4.74562800	-1.92239700	1.11767600
C	-1.57984700	-0.27174300	-0.86557700
C	-1.76206800	0.50116300	0.30912200
H	0.91144700	2.51508100	-0.06383200

O	-0.60670800	2.92069100	-1.43994900
H	-0.91994700	3.67791100	-0.93199400
O	5.12196200	0.53033900	0.25749300
H	5.64149300	-0.17163400	0.70423400
H	-2.28721800	-1.89960500	-2.07482300
O	-3.06160600	0.88054400	2.29073800
H	-2.38137900	1.59585700	2.32279900

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.240889 (Hartree/Particle)
Thermal correction to Energy= 0.258767
Thermal correction to Enthalpy= 0.259711
Thermal correction to Gibbs Free Energy= 0.193188
Sum of electronic and zero-point Energies= -1104.804775
Sum of electronic and thermal Energies= -1104.786898
Sum of electronic and thermal Enthalpies= -1104.785954
Sum of electronic and thermal Free Energies= -1104.852477

Name of radical	C3-H

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

C	-3.28425500	0.47043300	0.80388900
C	-4.07375300	-0.66990300	0.68013000
C	-3.66501900	-1.69146800	-0.17896300
C	-2.47704400	-1.60795800	-0.91580500
H	-4.99694700	-0.73484800	1.24438300
C	-1.25592500	1.76609200	0.16215900
C	0.46676100	0.55241500	-1.31606300
C	-0.04457700	1.75053000	-0.57984100
O	-0.56653600	-0.41826400	-1.55009700
O	-1.54838000	2.79882600	0.83373200
O	-4.39786300	-2.82311800	-0.34338400
H	-5.18838300	-2.77384200	0.20483400
C	1.66277800	-0.07956400	-0.60154300
C	1.52028500	-1.22029600	0.18348300
C	2.91855900	0.52200900	-0.73352000
C	2.63044800	-1.75631000	0.83886800
H	0.55937000	-1.70679800	0.27929600
C	4.02319600	-0.00441700	-0.07940800
H	3.05647700	1.41054200	-1.33798400
C	3.87279200	-1.15397700	0.71321400
H	2.52373700	-2.64982800	1.44678600
H	0.79244700	0.86893800	-2.31334100
O	5.02725200	-1.60036500	1.31278800
H	4.84623800	-2.38831000	1.83403400
C	-1.69351500	-0.47404300	-0.78413500
C	-2.07107900	0.57875600	0.07768700
O	0.71980600	2.84005500	-0.55814900
H	0.24348600	3.46435400	0.02841900
O	5.24092300	0.58642100	-0.21472600
H	5.87588200	0.07602000	0.30419800
H	-2.18623800	-2.40790400	-1.58196000
O	-3.68530900	1.46117600	1.61167600
H	-3.02311100	2.19003100	1.53570800

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.240395 (Hartree/Particle)
Thermal correction to Energy= 0.258760

Thermal correction to Enthalpy= 0.259705	
Thermal correction to Gibbs Free Energy= 0.192368	
Sum of electronic and zero-point Energies= -1104.809134	
Sum of electronic and thermal Energies= -1104.790769	
Sum of electronic and thermal Enthalpies= -1104.789824	
Sum of electronic and thermal Free Energies= -1104.857161	
Name of anion	O4'-H
Cartesian Coordinates optimized at B3LYP/6-311G(d,p	
C -2.95724900 -0.07443000 0.97856200	
C -3.49616700 -1.34190000 0.80552100	
C -2.96940800 -2.17231900 -0.19240500	
C -1.92017900 -1.77335500 -1.01342000	
H -4.31497700 -1.66218600 1.44049700	
C -1.36606400 1.70041000 0.28771500	
C 0.52316100 1.00504600 -1.27916000	
C -0.30693900 2.14685400 -0.71198400	
O -0.39251500 -0.13686700 -1.66904800	
O -1.80143400 2.53475600 1.10731500	
O -3.47414800 -3.42511400 -0.39529000	
H -4.15517200 -3.58921100 0.26485300	
C 1.65824400 0.53483500 -0.44084300	
C 1.71426600 0.68729600 0.95160200	
C 2.72771000 -0.15065000 -1.08138100	
C 2.78019800 0.19664600 1.70403600	
H 0.92065500 1.21270900 1.47562200	
C 3.77530400 -0.64173700 -0.34657900	
H 2.71861400 -0.29133500 -2.15918100	
C 3.86195700 -0.49716600 1.09855200	
H 2.81072100 0.34243600 2.77950500	
H 0.87153000 1.30966900 -2.26688300	
O 4.89106400 -0.98474100 1.66796700	
C -1.37161200 -0.50103200 -0.84680600	
C -1.88168800 0.37078900 0.15652200	
H 0.36064200 2.85302400 -0.21032900	
O -0.99617000 2.79208100 -1.79698700	
H -1.52431500 3.49418300 -1.40081300	
O 4.84403600 -1.29720900 -0.88226700	
H 5.36055800 -1.47115800 -0.05629000	
H -1.51836700 -2.44148300 -1.76185700	
O -3.46983900 0.73239200 1.92068800	
H -2.96705900 1.58524800 1.85626700	
Frequency and Energy at B3LYP/6-311G(d,p) in gas phase	
Zero-point correction= 0.239448 (Hartree/Particle)	
Thermal correction to Energy= 0.257330	
Thermal correction to Enthalpy= 0.258274	
Thermal correction to Gibbs Free Energy= 0.193046	
Sum of electronic and zero-point Energies= -1104.894720	
Sum of electronic and thermal Energies= -1104.876838	
Sum of electronic and thermal Enthalpies= -1104.875894	
Sum of electronic and thermal Free Energies= -1104.941122	
Name of anion	C3-H
Cartesian Coordinates optimized at B3LYP/6-311G(d,p	
C -3.00451000 0.37293800 0.98127700	
C -3.69668200 -0.84830300 1.00063100	

C	-3.35624100	-1.86144400	0.11050000
C	-2.31184100	-1.67622900	-0.78527900
H	-4.50586700	-0.99500800	1.71602400
C	-1.23883600	1.91090800	-0.08818100
C	0.40710300	0.62281000	-1.53341400
C	-0.13048100	1.84372400	-0.89607400
O	-0.64142500	-0.35718600	-1.72794700
O	-1.60465200	3.02270700	0.43737000
O	-4.01838100	-3.07678400	0.09603800
H	-4.69484400	-3.04571700	0.77869800
C	1.59954400	-0.04153600	-0.81472300
C	1.85218000	-1.40826500	-0.94486900
C	2.46154600	0.74297500	-0.04186600
C	2.94548500	-1.98994400	-0.29961900
H	1.17984200	-2.01943000	-1.53299200
C	3.56115000	0.17194300	0.58721100
H	2.26658700	1.80281200	0.07086500
C	3.79760100	-1.20172900	0.45959000
H	3.13364800	-3.05824900	-0.38509400
H	0.74712500	0.85425300	-2.55547900
O	4.91598800	-1.68637900	1.13171900
H	4.86501600	-2.64580900	1.15486600
C	-1.62950100	-0.45896700	-0.78729500
C	-1.95411000	0.61271300	0.07564200
O	0.57591000	3.03274700	-1.08994000
H	0.01258800	3.62697400	-0.54355200
O	4.40981000	0.94411000	1.34097100
H	5.05693300	0.34376500	1.73061800
H	-2.02743900	-2.45799500	-1.47729100
O	-3.35770200	1.35096700	1.87448800
H	-4.08439700	1.00337100	2.40055400

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.236355 (Hartree/Particle)
Thermal correction to Energy= 0.255794
Thermal correction to Enthalpy= 0.256738
Thermal correction to Gibbs Free Energy= 0.187954
Sum of electronic and zero-point Energies= -1104.833513
Sum of electronic and thermal Energies= -1104.814075
Sum of electronic and thermal Enthalpies= -1104.813130
Sum of electronic and thermal Free Energies= -1104.881915

Name of cationic radical

Cartesian Coordinates optimized at B3LYP/6-311G(d,p

C	-3.04889200	0.14844500	1.06057300
C	-3.89631000	-0.90590500	0.66107300
C	-3.58956900	-1.64813300	-0.48363800
C	-2.43253200	-1.37394000	-1.22541000
H	-4.78249800	-1.10540700	1.25211600
C	-1.07545900	1.60505900	0.65424800
C	0.50803800	0.83771600	-1.19043700
C	-0.05286900	2.02473500	-0.39900200
O	-0.49530200	-0.14286500	-1.56242900
O	-1.26022000	2.29309300	1.65890800
O	-4.35326000	-2.65831200	-0.92486100
H	-5.13325800	-2.77842400	-0.36947500

C	1.67073400	0.12421100	-0.53622700
C	1.47795500	-0.97394100	0.33558000
C	2.96044300	0.55806000	-0.81949100
C	2.55571700	-1.59279500	0.94950400
H	0.48285900	-1.35033400	0.52782800
C	4.05572300	-0.05088000	-0.21096900
H	3.15013800	1.37697600	-1.50307500
C	3.84694300	-1.14295900	0.68734900
H	2.39989000	-2.43090000	1.61949800
H	0.83494100	1.24090100	-2.15054800
O	4.97706200	-1.65269900	1.20624600
H	4.80864400	-2.38867900	1.80857800
C	-1.59303200	-0.32320600	-0.82266400
C	-1.88539000	0.46117600	0.31447000
H	0.77317300	2.54933800	0.09210700
O	-0.72448400	2.84569100	-1.34371600
H	-0.99481800	3.66490700	-0.91154100
O	5.28632400	0.38721000	-0.47128400
H	5.93958500	-0.12693700	0.02776800
H	-2.18601900	-1.96433900	-2.09716900
O	-3.38068200	0.83821000	2.13496900
H	-2.69712700	1.54440300	2.27148500

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.252154 (Hartree/Particle)
Thermal correction to Energy= 0.270615
Thermal correction to Enthalpy= 0.271559
Thermal correction to Gibbs Free Energy= 0.203921
Sum of electronic and zero-point Energies= -1105.148623
Sum of electronic and thermal Energies= -1105.130162
Sum of electronic and thermal Enthalpies= -1105.129218
Sum of electronic and thermal Free Energies= -1105.196855

Name of compound (13)	**Teracacidin**

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

C	-2.47775100	0.87887300	1.56833400
C	-3.48087700	-0.07685000	1.47687800
C	-3.51762600	-0.91554000	0.36508400
C	-2.56049000	-0.81650800	-0.64633800
H	-2.43488700	1.53910600	2.42667900
H	-4.23357000	-0.16921800	2.25319000
C	-0.43186400	2.05739100	0.66481000
H	-0.86687000	3.01174900	0.97183000
C	0.57294100	0.90468200	-1.37513700
C	0.26291100	2.26048100	-0.68784100
O	-0.66095400	0.19286500	-1.57454300
O	0.54775400	1.78367800	1.68507000
H	0.83091400	0.86608100	1.58305000
O	-2.57832400	-1.65503300	-1.71891400
H	-3.34121000	-2.23770300	-1.61231200
O	-4.45985800	-1.89919900	0.16648800
H	-5.08047700	-1.91097100	0.90102800
O	1.41387900	3.06533900	-0.53967000
H	1.74572900	2.87627700	0.35083400
H	-0.42570600	2.78938100	-1.35498300

C	1.62676300	0.03218100	-0.70164600
C	1.32956200	-1.23459600	-0.19434300
C	2.96136500	0.46641400	-0.64682400
C	2.31833100	-2.02553600	0.39043100
H	0.32471700	-1.62683300	-0.27402500
C	3.95166100	-0.31419000	-0.06817300
H	3.22225700	1.43044900	-1.06448500
C	3.63249300	-1.56661600	0.46234800
H	2.06316000	-3.00859800	0.77604200
H	4.97991500	0.02429200	-0.02802500
H	0.91390000	1.12693900	-2.38841000
O	4.64458600	-2.29277700	1.02164100
H	4.29698400	-3.13600900	1.32997600
C	-1.55267000	0.15293400	-0.54121800
C	-1.51000300	1.00789200	0.56847300

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

zero-point correction= 0.271795 (Hartree/Particle)
Thermal correction to Energy= 0.289820
Thermal correction to Enthalpy= 0.290764
Thermal correction to Gibbs Free Energy= 0.226216
Sum of electronic and zero-point Energies= -1031.345607
Sum of electronic and thermal Energies= -1031.327581
Sum of electronic and thermal Enthalpies= -1031.326637
Sum of electronic and thermal Free Energies= -1031.391186

Name of radical	O7-H

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

C	-2.51498000	0.78358300	1.59797500
C	-3.51066800	-0.14582800	1.53576400
C	-3.59892300	-1.01189900	0.38774700
C	-2.58761800	-0.84717400	-0.65874600
H	-2.43239800	1.44013500	2.45721800
H	-4.24897600	-0.26262000	2.31856300
C	-0.49070300	2.01123400	0.67235100
H	-0.95183600	2.95039900	0.98987100
C	0.54064400	0.90765800	-1.38216400
C	0.20488500	2.24753000	-0.67510800
O	-0.68584200	0.17932100	-1.59426400
O	0.47710400	1.73727200	1.69979100
H	0.80994500	0.84024700	1.56447800
O	-2.67324800	-1.67611300	-1.69257100
H	-3.46161900	-2.22557100	-1.48626300
O	-4.45569100	-1.90576400	0.20525800
O	1.33863600	3.07121400	-0.51292200
H	1.67977700	2.87904000	0.37285700
H	-0.49212500	2.77457500	-1.33500500
C	1.60409100	0.04490200	-0.71279200
C	1.32585300	-1.22487100	-0.20194200
C	2.93268400	0.49849300	-0.66055600
C	2.32622700	-2.00103700	0.38255300
H	0.32762600	-1.63420800	-0.27810800
C	3.93432600	-0.26694400	-0.08204300
H	3.18026900	1.46484900	-1.08107800
C	3.63409100	-1.52329200	0.45147400
H	2.08510100	-2.98673900	0.76979700

H	4.95778400	0.08580800	-0.04476200
H	0.87915500	1.14868300	-2.39144200
O	4.65684600	-2.23183800	1.00940600
H	4.32568400	-3.08079000	1.32055400
C	-1.57401600	0.12061400	-0.56231400
C	-1.54603300	0.94260400	0.55875600

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.260068 (Hartree/Particle)
Thermal correction to Energy= 0.277353
Thermal correction to Enthalpy= 0.278297
Thermal correction to Gibbs Free Energy= 0.214355
Sum of electronic and zero-point Energies= -1030.728346
Sum of electronic and thermal Energies= -1030.711061
Sum of electronic and thermal Enthalpies= -1030.710117
Sum of electronic and thermal Free Energies= -1030.774059

Name of radical	C2-H

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

C	-3.54948200	1.20047600	0.11576700
C	-4.40226800	0.10321900	0.11514000
C	-3.86600600	-1.17807800	-0.00154500
C	-2.48861800	-1.37791400	-0.11896700
H	-3.95473600	2.20118200	0.20904900
H	-5.47591100	0.23525500	0.20096700
C	-1.21168800	2.18833800	0.02071400
H	-1.65080100	3.06711700	-0.45557500
C	0.62411200	0.50098200	-0.27403600
C	0.10112000	1.85047700	-0.71879700
O	-0.31303800	-0.51749000	-0.22229900
O	-0.88908600	2.63170600	1.35485900
H	-0.74334200	1.84645300	1.89607300
O	-1.95937100	-2.62512800	-0.23000300
H	-2.69423800	-3.25189500	-0.21320400
O	-4.61168800	-2.33362800	-0.01351800
H	-5.54638700	-2.12335500	0.07071300
O	1.00981200	2.91702900	-0.52734600
H	0.90111100	3.17611700	0.40031200
H	-0.11317900	1.81588700	-1.79754800
C	1.96609700	0.04081900	-0.14195200
C	2.21610500	-1.31484200	0.21082100
C	3.10424200	0.87022800	-0.35334300
C	3.50542000	-1.79679500	0.35138700
H	1.37844800	-1.98063800	0.36504300
C	4.38754000	0.37891100	-0.21156000
H	2.95625000	1.90109400	-0.63626000
C	4.60448200	-0.95665300	0.14546600
H	3.66296300	-2.83775200	0.62155700
H	5.24611800	1.01826600	-0.37956700
O	5.89728600	-1.38010100	0.27320000
H	5.90068500	-2.31240700	0.51360600
C	-1.64608500	-0.25907800	-0.11816200
C	-2.16802000	1.03417100	0.00001400

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction= 0.257916 (Hartree/Particle)
Thermal correction to Energy= 0.276300

Thermal correction to Enthalpy= 0.277245	
Thermal correction to Gibbs Free Energy= 0.211082	
Sum of electronic and zero-point Energies= -1030.719241	
Sum of electronic and thermal Energies= -1030.700856	
Sum of electronic and thermal Enthalpies= -1030.699912	
Sum of electronic and thermal Free Energies= -1030.766075	
Name of anion	O7-H
Cartesian Coordinates optimized at B3LYP/6-311G(d,p	
C -2.50726200 0.85648000 1.53165400	
C -3.43110000 -0.18008400 1.49299000	
C -3.44651700 -1.10790400 0.41204200	
C -2.45765200 -0.88710400 -0.62079600	
H -2.50628700 1.54423200 2.37443300	
H -4.16005400 -0.31132600 2.28677100	
C -0.54606200 2.15098600 0.60460900	
H -1.00916700 3.10865900 0.86634300	
C 0.54160200 0.97357700 -1.39098600	
C 0.21412300 2.33227500 -0.71712100	
O -0.67694300 0.28771600 -1.65193700	
O 0.44481400 1.96706800 1.67122100	
H 0.56922700 1.01312900 1.74670700	
O -2.49186800 -1.81910300 -1.62150900	
H -3.24207500 -2.37283900 -1.28921600	
O -4.22132000 -2.10955600 0.26154800	
O 1.36965200 3.13565900 -0.51262400	
H 1.61758600 2.93873000 0.40584400	
H -0.43681400 2.86002400 -1.42177500	
C 1.56610300 0.07751900 -0.69282400	
C 1.24599500 -1.23794800 -0.34538500	
C 2.88356600 0.50999300 -0.48054600	
C 2.19531700 -2.07685700 0.23620700	
H 0.25177400 -1.61499200 -0.54479100	
C 3.83750100 -0.32161500 0.09639100	
H 3.15969500 1.51541400 -0.77152500	
C 3.49130100 -1.62084100 0.46565400	
H 1.92013600 -3.09399700 0.50484800	
H 4.85310400 0.01945100 0.26212500	
H 0.94167400 1.20665400 -2.38334800	
O 4.46321400 -2.41009300 1.03691400	
H 4.06967600 -3.26321600 1.24555800	
C -1.55739200 0.15355300 -0.57443000	
C -1.55100100 1.05072900 0.52405700	
Frequency and Energy at B3LYP/6-311G(d,p) in gas phase	
Zero-point correction= 0.258881 (Hartree/Particle)	
Thermal correction to Energy= 0.276095	
Thermal correction to Enthalpy= 0.277039	
Thermal correction to Gibbs Free Energy= 0.213939	
Sum of electronic and zero-point Energies= -1030.815109	
Sum of electronic and thermal Energies= -1030.797895	
Sum of electronic and thermal Enthalpies= -1030.796951	
Sum of electronic and thermal Free Energies= -1030.860051	
Name of cationic radical	
Cartesian Coordinates optimized at B3LYP/6-311G(d,p	

C	-2.64084100	0.99591600	1.42398800
C	-3.69205800	0.05849600	1.34014200
C	-3.69287600	-0.87728400	0.32903700
C	-2.62970100	-0.89818200	-0.60942200
H	-2.66184800	1.72935800	2.22170900
H	-4.49853200	0.08597700	2.06372600
C	-0.47443600	2.04246400	0.61252600
H	-0.89980900	3.02005900	0.84825900
C	0.58126100	0.76079800	-1.33382700
C	0.24629800	2.15514500	-0.73797100
O	-0.61475200	-0.06473800	-1.42141000
O	0.45548300	1.80155800	1.67072900
H	0.74796000	0.88244800	1.63995100
O	-2.59072400	-1.78668300	-1.58836500
H	-3.37995400	-2.35334000	-1.54064200
O	-4.62284700	-1.83489000	0.10073800
H	-5.35265700	-1.79470200	0.73019100
O	1.40510100	2.93821500	-0.63968400
H	1.73945400	2.83767100	0.26390800
H	-0.42772100	2.64694500	-1.44738900
C	1.69078300	-0.02515200	-0.66867800
C	1.45605800	-1.16704800	0.11586400
C	3.02359000	0.37663500	-0.89406400
C	2.50590700	-1.85188000	0.70914600
H	0.45132700	-1.54596700	0.24826400
C	4.07467200	-0.29145800	-0.30220200
H	3.22155000	1.23731100	-1.51977500
C	3.82504100	-1.41582200	0.50878600
H	2.31060800	-2.73377600	1.31005600
H	5.10000600	0.02164500	-0.45316500
H	0.85739700	0.90458500	-2.38090200
O	4.89302300	-2.02568700	1.04418800
H	4.63289500	-2.79303300	1.56921800
C	-1.56390300	0.05761800	-0.50051300
C	-1.58362100	1.01852300	0.52669300

Frequency and Energy at B3LYP/6-311G(d,p) in gas phase

Zero-point correction=	0.271531 (Hartree/Particle)
Thermal correction to Energy=	0.289476
Thermal correction to Enthalpy=	0.290420
Thermal correction to Gibbs Free Energy=	0.225418
Sum of electronic and zero-point Energies=	-1031.077110
Sum of electronic and thermal Energies=	-1031.059165
Sum of electronic and thermal Enthalpies=	-1031.058221
Sum of electronic and thermal Free Energies=	-1031.123223

Table S5: Cartesian coordinates of all of the Int, TS of the selective compounds and HOO• optimized at B3LYP/6-311G(d,p) level of theory in the gas phase

Name of compound			**Int1-1-C3-H-OOH**
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)			
C	2.58178500	-0.45584200	-1.11770800
C	3.32242500	-1.61158400	-0.92696500
C	1.98839600	-2.14330600	1.05438600
H	4.12857500	-1.86200900	-1.60207300
C	0.81874600	1.12078800	-0.32390200
C	-0.74304800	0.24777700	1.47057100
C	-0.12814900	1.48588700	0.81341000
O	0.24205200	-0.77092900	1.74073800
O	1.03051200	1.95101200	-1.24138700
C	-1.92905500	-0.31353900	0.70038300
C	-1.87615400	-1.50656100	-0.01770500
C	-3.14028100	0.39075300	0.72635400
C	-2.99241200	-1.97684300	-0.70666300
H	-0.96515500	-2.08973800	-0.04291300
C	-4.25803100	-0.06633700	0.04481300
H	-3.21682300	1.31085300	1.29763000
C	-4.18691700	-1.25801200	-0.68161000
H	-2.93044800	-2.90857600	-1.26129300
O	-5.31371300	-1.66504100	-1.33264100
H	-5.13656300	-2.49171200	-1.79343000
C	1.23639500	-0.99518000	0.86074700
C	1.51662600	-0.11541700	-0.22031300
O	0.62287100	2.19534900	1.78327900
H	0.76046800	3.09328500	1.42982800
H	1.75336100	-2.79347300	1.88850100
O	2.88581700	0.33894500	-2.14723600
H	2.28903500	1.11880900	-2.11133100
H	-5.19401400	0.47785500	0.06944000
C	3.02769400	-2.43513000	0.16130500
O	3.78930700	-3.54333600	0.30588000
H	3.51689500	-4.02528800	1.09460200
H	-1.07035500	0.56074900	2.46373100
H	-0.93951000	2.09888300	0.40646600
H	0.67290600	3.55534600	-1.11793200
O	0.58499900	4.67947700	0.36866100
O	0.52109200	4.53330900	-0.94527400
Frequency and Energy at B3LYP/6-311G(d,p)in gas phase			
Zero-point correction= 0.266154 (Hartree/Particle) Thermal correction to Energy= 0.286649 Thermal correction to Enthalpy= 0.287593 Thermal correction to Gibbs Free Energy= 0.214595 Sum of electronic and zero-point Energies= -1181.141475 Sum of electronic and thermal Energies= -1181.120981 Sum of electronic and thermal Enthalpies= -1181.120036 Sum of electronic and thermal Free Energies= -1181.193034			

Name of compound			**TS-1-C3-H-OOH**
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)			
C	3.56372000	0.17296300	0.34716500
C	4.28657300	-0.93966300	-0.05795600

C	2.19799200	-2.13692400	-0.50501800
H	5.36747100	-0.92349100	-0.05156400
C	1.37181000	1.31477600	0.66790100
C	-0.64431700	-0.20738000	0.70241800
C	-0.11199900	1.20512800	0.51059400
O	0.12285300	-1.11201300	-0.14527600
O	1.84776900	2.40610200	1.03538200
C	-2.10600300	-0.42124300	0.42343000
C	-2.72212700	0.07861900	-0.72765100
C	-2.87128100	-1.17498900	1.31841300
C	-4.06690100	-0.16982200	-0.97289400
H	-2.16004600	0.67684200	-1.43429400
C	-4.21595900	-1.42773800	1.08480200
H	-2.40793700	-1.57095400	2.21619500
C	-4.81945700	-0.92393300	-0.06857600
H	-4.53542000	0.22907800	-1.86796400
O	-6.14191500	-1.19541500	-0.25774500
H	-6.43599900	-0.78780700	-1.07908800
C	1.47511900	-1.02938900	-0.09412400
C	2.13701200	0.15001600	0.33101600
O	-0.80244600	2.15549200	1.21007800
H	-0.16735200	2.87520500	1.37405300
H	1.66902800	-3.02691500	-0.82435300
O	4.22178400	1.27036000	0.73958800
H	3.55496400	1.95661400	0.96569700
H	-4.81151900	-2.00720100	1.77924700
C	3.59875900	-2.07632100	-0.48767700
O	4.35375400	-3.13077700	-0.87695900
H	3.78150900	-3.85117800	-1.16306800
H	-0.43998700	-0.49237500	1.74444600
H	-0.20647600	1.51350900	-0.75000000
H	0.53822400	3.74874800	-1.61274500
O	-0.24658800	2.07262000	-1.88066200
O	-0.37822600	3.43054600	-1.59036100

Frequency and Energy at B3LYP/6-311G(d,p)in gas phase

Zero-point correction= 0.259641 (Hartree/Particle)
Thermal correction to Energy= 0.280178
Thermal correction to Enthalpy= 0.281122
Thermal correction to Gibbs Free Energy= 0.208429
Sum of electronic and zero-point Energies= -1181.116380
Sum of electronic and thermal Energies= -1181.095843
Sum of electronic and thermal Enthalpies= -1181.094899
Sum of electronic and thermal Free Energies= -1181.167591

Name of compound	**Int2-1-C3-H-OOH**

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

C	2.94332600	-0.17786400	-0.71512100
C	3.56996000	-1.41303500	-0.83710800
C	1.93548200	-2.39642700	0.68300300
H	4.44854200	-1.51560900	-1.45868800
C	1.13603200	1.25686500	0.26636000
C	-0.70588900	-0.02135700	1.49947000
C	-0.07593300	1.25597700	1.01844700
O	0.25645500	-1.09175800	1.65077200

O	1.63033200	2.31818600	-0.24724200
C	-1.88324600	-0.47282400	0.65032500
C	-1.82260000	-0.49882900	-0.74549100
C	-3.05286100	-0.91699800	1.27434800
C	-2.89722400	-0.96112700	-1.49626400
H	-0.93374700	-0.15410500	-1.26063300
C	-4.13473800	-1.37714600	0.53673700
H	-3.11910200	-0.90197500	2.35716600
C	-4.05887800	-1.40209100	-0.85730500
H	-2.83580900	-0.97343200	-2.58052100
O	-5.14637700	-1.86110200	-1.53853900
H	-4.97153600	-1.82138600	-2.48461500
C	1.30851900	-1.16653100	0.79736100
C	1.78154300	-0.03050100	0.10101300
O	-0.78863700	2.32901200	1.30895400
H	-0.42637000	3.17300800	0.92063700
H	1.53982700	-3.24372100	1.23020100
O	3.45423800	0.86769400	-1.37722500
H	2.92065600	1.65813000	-1.12219800
H	-5.04316800	-1.71714200	1.01845200
C	3.06638600	-2.50699600	-0.13672600
O	3.71836400	-3.68796900	-0.28775600
H	3.29040700	-4.36123100	0.25193100
H	-1.06852700	0.15636200	2.51476900
H	-0.35937500	5.70446700	-1.11391900
H	0.92872300	3.82995500	-0.15372400
O	-0.53502300	4.76274300	-0.98803400
O	0.28192400	4.50569300	0.18492800

Frequency and Energy at B3LYP/6-311G(d,p)in gas phase

Zero-point correction= 0.265174 (Hartree/Particle)
Thermal correction to Energy= 0.286155
Thermal correction to Enthalpy= 0.287099
Thermal correction to Gibbs Free Energy= 0.211872
Sum of electronic and zero-point Energies= -1181.153297
Sum of electronic and thermal Energies= -1181.132316
Sum of electronic and thermal Enthalpies= -1181.131372
Sum of electronic and thermal Free Energies= -1181.206599

Name of compound	**Int1-1-O4'-H-OOH**

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

C	3.39124100	0.44985000	1.05461800
C	3.73850000	1.77706900	0.84658500
C	2.22999700	1.86778200	-1.07689900
H	4.45243200	2.26512100	1.49519100
C	2.13508700	-1.58681400	0.36486800
C	0.28428700	-1.21438700	-1.33316000
C	1.22372500	-2.22119200	-0.68441200
O	0.99998100	-0.00416800	-1.73407300
O	2.61524200	-2.30905500	1.25367100
C	-0.94521000	-0.84631700	-0.52972600
C	-2.02385000	-0.26452800	-1.20448700
C	-1.06056000	-1.02576500	0.85438600
C	-3.17485100	0.12790200	-0.53444300
H	-1.95852700	-0.11084300	-2.27670300

C	-2.20743600	-0.64184700	1.53770100
H	-0.25638300	-1.47677600	1.42331600
C	-3.27522700	-0.05906300	0.84994600
H	-3.99942400	0.57450000	-1.07993000
O	-4.36970200	0.29559800	1.56530600
H	-5.04152300	0.68651400	0.98433400
C	1.87656900	0.54291100	-0.86791500
C	2.44855800	-0.19799700	0.19750100
O	2.04803600	-2.76096600	-1.71822700
H	2.65864500	-3.38101200	-1.30349800
H	1.77343000	2.41401600	-1.89370600
O	3.95818800	-0.21930400	2.06433800
H	3.61206500	-1.14307800	2.03433700
H	-2.29429100	-0.78531900	2.60774900
C	3.15968700	2.46805300	-0.21876300
O	3.53370500	3.76176300	-0.38035200
H	3.07784100	4.13344900	-1.14316500
H	-0.02052200	-1.63507500	-2.29232900
H	0.63679700	-3.01040900	-0.20228400
H	-8.17610200	0.89166000	-0.63279400
O	-6.51815500	1.44210500	-0.04926600
O	-7.42573800	0.48444000	-0.15831200

Frequency and Energy at B3LYP/6-311G(d,p)in gas phase

Zero-point correction= 0.264768 (Hartree/Particle)
Thermal correction to Energy= 0.286388
Thermal correction to Enthalpy= 0.287333
Thermal correction to Gibbs Free Energy= 0.208939
Sum of electronic and zero-point Energies= -1181.126198
Sum of electronic and thermal Energies= -1181.104577
Sum of electronic and thermal Enthalpies= -1181.103633
Sum of electronic and thermal Free Energies= -1181.182027

Name of compound	**TS-1-O4'-H-OOH**

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

C	3.08256500	0.78084700	1.16077600
C	3.27115900	2.12550400	0.87347400
C	1.95058700	1.87296900	-1.17033600
H	3.85102500	2.75112700	1.53753000
C	2.17889300	-1.45421600	0.53397900
C	0.46022800	-1.44928200	-1.32440900
C	1.46859400	-2.27651200	-0.54076500
O	1.03960200	-0.19208900	-1.77192200
O	2.65726100	-2.04023500	1.51751500
C	-0.85745800	-1.17007100	-0.62519700
C	-1.88890200	-0.59028900	-1.38877200
C	-1.09733000	-1.43977100	0.73391500
C	-3.11628000	-0.29744400	-0.83505100
H	-1.70981400	-0.37816200	-2.43713600
C	-2.31329800	-1.13546000	1.31490800
H	-0.32689700	-1.88467200	1.35161400
C	-3.35970200	-0.56033300	0.54536500
H	-3.91475700	0.12897500	-1.42988400
O	-4.50909200	-0.31103500	1.10293200
H	-5.07463600	0.57835300	0.57631400

C	1.75794500	0.53218200	-0.88205400
C	2.31826100	-0.04920300	0.28293100
O	2.44224200	-2.74081200	-1.47297400
H	3.09445800	-3.25199800	-0.98046900
H	1.50466600	2.29289800	-2.06399000
O	3.63414800	0.26968600	2.26554500
H	3.41669300	-0.69217100	2.28606100
H	-2.50309700	-1.32740100	2.36368700
C	2.71122200	2.65477300	-0.28951200
O	2.92726200	3.97111600	-0.52486600
H	2.50346200	4.22531900	-1.35182400
H	0.26828500	-1.97632300	-2.26096900
H	0.96029700	-3.11811600	-0.05737000
H	-7.28602400	2.19246900	0.45080700
O	-5.54848600	1.60191800	0.16947900
O	-6.91575800	1.34114400	0.17430700

Frequency and Energy at B3LYP/6-311G(d,p)in gas phase

Zero-point correction= 0.259849 (Hartree/Particle)
Thermal correction to Energy= 0.280485
Thermal correction to Enthalpy= 0.281429
Thermal correction to Gibbs Free Energy= 0.207169
Sum of electronic and zero-point Energies= -1181.113570
Sum of electronic and thermal Energies= -1181.092934
Sum of electronic and thermal Enthalpies= -1181.091990
Sum of electronic and thermal Free Energies= -1181.166250

Name of compound			**Int2-1-O4'-H-OOH**
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)			
C	3.27379500	0.49534300	1.06697300
C	3.55289900	1.84531000	0.90579900
C	2.04135000	1.92819800	-1.01634600
H	4.24113400	2.34514900	1.57295100
C	2.13163700	-1.57974700	0.29446300
C	0.26445800	-1.22702400	-1.37157100
C	1.26655800	-2.21520200	-0.79400900
O	0.90205500	0.02097900	-1.74135400
O	2.63854500	-2.30941600	1.15951300
C	-0.94916000	-0.92236700	-0.50961100
C	-1.94362100	-0.08436700	-1.07391200
C	-1.12670400	-1.41745100	0.80080000
C	-3.07577400	0.24857000	-0.38003300
H	-1.79122500	0.29790900	-2.07697600
C	-2.25171700	-1.09983200	1.52425500
H	-0.37470500	-2.05168900	1.25393400
C	-3.28470600	-0.25196100	0.96618000
H	-3.84768700	0.88133800	-0.80261500
O	-4.31225700	0.03066000	1.63065300
H	-5.55210400	1.05276000	0.74396500
C	1.75957000	0.58364200	-0.85242500
C	2.36583700	-0.16882000	0.18444200
O	2.10827200	-2.62413400	-1.86766900
H	2.76069800	-3.23725000	-1.51025800
H	1.55860600	2.47962600	-1.81419200
O	3.87396800	-0.17725600	2.05300000

H	3.57878900	-1.11604000	1.99544000
H	-2.40539000	-1.46673300	2.53181000
C	2.94241500	2.54476100	-0.13509400
O	3.25111400	3.85739800	-0.24926600
H	2.78000800	4.23895300	-0.99810200
H	-0.07281100	-1.62957900	-2.32954900
H	0.73836300	-3.07424700	-0.36560500
H	-7.74954000	0.89227300	-0.22812400
O	-6.04155100	1.61613300	0.10847100
O	-6.87829000	0.62478800	-0.54736500

Frequency and Energy at B3LYP/6-311G(d,p)in gas phase

Zero-point correction= 0.264537 (Hartree/Particle)
Thermal correction to Energy= 0.285966
Thermal correction to Enthalpy= 0.286910
Thermal correction to Gibbs Free Energy= 0.210413
Sum of electronic and zero-point Energies= -1181.127178
Sum of electronic and thermal Energies= -1181.105749
Sum of electronic and thermal Enthalpies= -1181.104805
Sum of electronic and thermal Free Energies= -1181.181303

Name of compound	**Int1-9-C4-H-OOH**

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

C	-2.90143200	0.62284000	1.26603500
C	-3.96459400	-0.11817200	0.74821000
C	-3.86507600	-0.64119600	-0.53890000
C	-2.72291300	-0.43176400	-1.31686500
H	-2.96879400	1.07429400	2.24707000
H	-4.86773700	-0.27021500	1.33029300
C	-0.57952600	1.62264600	1.05227100
C	0.56590700	1.21516200	-1.17660700
C	0.17928700	2.26301000	-0.10717300
O	-0.59311900	0.48305800	-1.61819700
O	-2.62608600	-0.93774900	-2.57299300
H	-3.45029800	-1.40632700	-2.75841900
O	-4.84377000	-1.38672200	-1.15394800
H	-5.60715800	-1.47078100	-0.57506200
O	1.30057600	2.99816000	0.36562400
H	1.97325000	2.36475600	0.64963600
H	-0.47969700	3.00356000	-0.56785700
C	1.68117200	0.27820100	-0.74370900
C	1.42196400	-0.97139900	-0.18232700
C	3.01181800	0.69483700	-0.89775000
C	2.47304600	-1.78563000	0.23896300
H	0.40777100	-1.32671800	-0.07152600
C	4.06304000	-0.11225400	-0.47917300
H	3.25235500	1.64265000	-1.36619300
C	3.78558200	-1.36088300	0.09794900
H	2.26041700	-2.75179500	0.68603500
H	0.89841900	1.75804100	-2.06356200
O	4.89134400	-2.08447900	0.47827300
H	4.62066400	-2.93122300	0.84624500
C	-1.65989900	0.31645500	-0.78717600
C	-1.74446400	0.83521100	0.51184200
O	5.34749600	0.30655100	-0.63842500

H	5.92788800	-0.39040100	-0.30581400
H	0.10210300	0.94046700	1.58378200
O	-1.04995800	2.61839800	1.95104400
H	-0.29244200	3.18739700	2.13505200
H	-2.15281500	-1.37866800	1.78311700
O	-0.49207100	-1.85626600	2.45494600
O	-1.69533900	-2.21688000	2.02538200

Frequency and Energy at B3LYP/6-311G(d,p)in gas phase

Zero-point correction= 0.291175 (Hartree/Particle)
Thermal correction to Energy= 0.315050
Thermal correction to Enthalpy= 0.315995
Thermal correction to Gibbs Free Energy= 0.235227
Sum of electronic and zero-point Energies= -1257.528541
Sum of electronic and thermal Energies= -1257.504666
Sum of electronic and thermal Enthalpies= -1257.503722
Sum of electronic and thermal Free Energies= -1257.584489

Name of compound	**TS-9-C4-H-OOH**

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

C	-3.09345600	1.05306300	0.84141600
C	-4.07089700	0.07561400	0.93899600
C	-3.92036800	-1.11251400	0.22309700
C	-2.80856000	-1.33357800	-0.59456700
H	-3.19480800	1.99088600	1.37116000
H	-4.94858700	0.22746200	1.55894800
C	-0.90403100	1.86648900	-0.07685800
C	0.35355200	0.24892200	-1.60945600
C	-0.02873800	1.72144400	-1.31340400
O	-0.80161800	-0.60903300	-1.54575300
O	-2.67157200	-2.48820300	-1.30038600
H	-3.45090800	-3.02895700	-1.11928400
O	-4.82376800	-2.14809900	0.24847500
H	-5.57200800	-1.91787800	0.80730100
O	1.09787400	2.58252000	-1.23153200
H	1.69146300	2.22626600	-0.55493200
H	-0.61056400	2.09592100	-2.16288800
C	1.50323000	-0.29960800	-0.78189800
C	1.30099400	-1.10761700	0.33343800
C	2.81352000	0.00946000	-1.17651500
C	2.39113600	-1.58488300	1.05935800
H	0.30209200	-1.36274900	0.65575400
C	3.90230000	-0.45902100	-0.45379400
H	3.00607100	0.61087100	-2.05748400
C	3.68331000	-1.26193400	0.67526300
H	2.22821200	-2.20293400	1.93694100
H	0.65271400	0.20710400	-2.65860500
O	4.82353300	-1.68284600	1.32119400
H	4.58794700	-2.19372200	2.10140900
C	-1.82653000	-0.34031100	-0.69307100
C	-1.96459700	0.85948700	0.03150700
O	5.16845700	-0.14855000	-0.84799800
H	5.77868400	-0.56378000	-0.22507200
H	-0.12770100	1.67510000	0.92967100

O	-1.36231600	3.17467100	0.09266000
H	-0.59874700	3.74908800	-0.05672300
H	-0.59238600	0.99391600	3.28655600
O	0.58066900	1.66874800	1.99298000
O	0.09665500	0.58620800	2.74113200

Frequency and Energy at B3LYP/6-311G(d,p)in gas phase

Zero-point correction= 0.286210 (Hartree/Particle)
Thermal correction to Energy= 0.309257
Thermal correction to Enthalpy= 0.310202
Thermal correction to Gibbs Free Energy= 0.232545
Sum of electronic and zero-point Energies= -1257.509754
Sum of electronic and thermal Energies= -1257.486707
Sum of electronic and thermal Enthalpies= -1257.485763
Sum of electronic and thermal Free Energies= -1257.563419

Name of compound	**Int2-9-C4-H-OOH**

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

C	-2.77950400	0.52707300	1.35849400
C	-3.73962000	-0.36020900	0.88831600
C	-3.69200800	-0.80268700	-0.43420100
C	-2.66942400	-0.38296400	-1.30370500
H	-2.81455500	0.89302500	2.37539600
H	-4.54198100	-0.69345500	1.53956500
C	-0.75626400	1.90245600	0.88886400
C	0.49211100	1.44067100	-1.22810600
C	0.18478700	2.48366500	-0.11760000
O	-0.73083600	0.87959600	-1.72366800
O	-2.61058400	-0.84260200	-2.58251000
H	-3.35661400	-1.44364900	-2.70439400
O	-4.59465800	-1.67639600	-0.99716200
H	-5.24072800	-1.95058500	-0.33957700
O	1.35666700	2.99536500	0.52158500
H	1.92624400	2.24322300	0.73748100
H	-0.26462500	3.36266600	-0.59892600
C	1.50647200	0.39024400	-0.80335700
C	1.13550800	-0.85888600	-0.30168100
C	2.87082600	0.69672200	-0.91935300
C	2.11056100	-1.77719500	0.09477800
H	0.09665400	-1.14813000	-0.22849000
C	3.84530500	-0.21246200	-0.52287100
H	3.19965100	1.64065900	-1.33969900
C	3.45679500	-1.45867300	-0.00795100
H	1.80774000	-2.74649200	0.47910700
H	0.90135100	1.97658400	-2.08597800
O	4.49108200	-2.28766200	0.35177400
H	4.14703800	-3.12711900	0.67275500
C	-1.70471900	0.50157400	-0.83753000
C	-1.74555100	0.98513300	0.50269300
O	5.16067300	0.10663600	-0.64504100
H	5.67871500	-0.65000000	-0.34067800
H	0.41936200	-1.07325800	2.09964200
O	-0.75770100	2.44654800	2.13233900
H	0.03279700	3.00654200	2.18245600
H	-1.79936100	-1.64484500	1.71558800

O	-0.19197800	-1.51762800	2.70692500
O	-1.03308100	-2.24035000	1.77263300

Frequency and Energy at B3LYP/6-311G(d,p)in gas phase

Zero-point correction= 0.290890 (Hartree/Particle)
Thermal correction to Energy= 0.314886
Thermal correction to Enthalpy= 0.315831
Thermal correction to Gibbs Free Energy= 0.236400
Sum of electronic and zero-point Energies= -1257.534007
Sum of electronic and thermal Energies= -1257.510011
Sum of electronic and thermal Enthalpies= -1257.509067
Sum of electronic and thermal Free Energies= -1257.588497

Name of compound	**Int1-9-O7-H-OOH**

Cartesian Coordinates optimized at B3LYP/6-311G(d,p)

C	-2.27086100	1.11487200	1.00747300
C	-3.36018000	0.30992700	0.69204100
C	-3.26146400	-0.58241500	-0.37355100
C	-2.08562000	-0.67029500	-1.12731800
H	-2.33265600	1.82730000	1.81947600
H	-4.27970100	0.37426900	1.26236300
C	0.10872400	1.89401300	0.60959800
C	1.29969700	0.74394500	-1.31198000
C	0.96102400	2.09433600	-0.63947200
O	0.10248800	0.01492600	-1.61054300
O	-1.99467200	-1.54109100	-2.17150900
H	-2.85183900	-1.98381000	-2.23147500
O	-4.25777800	-1.43103800	-0.77952100
H	-5.06883000	-1.29253000	-0.26528400
O	2.11737800	2.87206500	-0.34597900
H	2.70497200	2.33383700	0.20044900
H	0.38207200	2.69302900	-1.34697600
C	2.29285300	-0.10626600	-0.53270100
C	1.88667100	-1.19141600	0.24315200
C	3.65922500	0.20356800	-0.60870300
C	2.82740700	-1.94135300	0.95051900
H	0.84310500	-1.47138200	0.28382700
C	4.59914500	-0.53742600	0.09743300
H	4.01694600	1.00776000	-1.24182700
C	4.17416100	-1.61645700	0.88653800
H	2.50653600	-2.78801600	1.55051200
H	1.73673900	0.96606700	-2.28818400
O	5.17934300	-2.29060500	1.54206500
H	4.81812100	-3.05313700	2.00393700
C	-0.99889000	0.15018800	-0.80309100
C	-1.08631800	1.04032200	0.27514800
O	5.92018700	-0.22264300	0.00927200
H	6.41081100	-0.86102800	0.54295300
H	0.72834800	1.38131700	1.36521800
O	-0.31528800	3.14918800	1.12809800
H	0.47393300	3.70437100	1.14965800
H	-7.70750900	-0.32645400	1.90756200
O	-6.81555700	-1.19604800	0.54871800
O	-6.79291200	-0.34786000	1.56655700

Frequency and Energy at B3LYP/6-311G(d,p)in gas phase

Zero-point correction=	0.291630 (Hartree/Particle)
Thermal correction to Energy=	0.315356
Thermal correction to Enthalpy=	0.316300
Thermal correction to Gibbs Free Energy=	0.234768
Sum of electronic and zero-point Energies=	-1257.527001
Sum of electronic and thermal Energies=	-1257.503276
Sum of electronic and thermal Enthalpies=	-1257.502332
Sum of electronic and thermal Free Energies=	-1257.583864

Name of compound			**TS-9-O7-H-OOH**
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)			
C	-2.28042600	1.06526900	1.24474300
C	-3.34978900	0.20153800	1.13117200
C	-3.30526100	-0.82219000	0.16220600
C	-2.16816900	-0.94526100	-0.68436800
H	-2.29614100	1.87027600	1.96736800
H	-4.22728600	0.29862500	1.75568100
C	0.03743500	1.86162600	0.56825000
C	1.12493700	0.56588400	-1.32451700
C	0.76906000	1.96454500	-0.76842700
O	-0.04907400	-0.25708900	-1.41496900
O	-2.14617800	-1.91498800	-1.61699200
H	-2.99640400	-2.37846100	-1.52932300
O	-4.24208300	-1.73748000	-0.02950300
H	-5.28332700	-1.41632400	0.11240600
O	1.89947300	2.82016100	-0.65971000
H	2.57245000	2.36127500	-0.13945200
H	0.09984700	2.45788500	-1.47778800
C	2.23880100	-0.13748500	-0.56409100
C	1.97808900	-1.13120100	0.37847000
C	3.56958500	0.22198700	-0.82621300
C	3.02832700	-1.74330900	1.06432900
H	0.96271800	-1.45154900	0.56697400
C	4.61841700	-0.38031800	-0.14185000
H	3.81358400	0.95414500	-1.58776500
C	4.34017900	-1.36919100	0.81441000
H	2.82011800	-2.52070200	1.79346000
H	1.44783700	0.69763200	-2.35937900
O	5.44451300	-1.90746900	1.43141900
H	5.18058300	-2.61632200	2.02590100
C	-1.08777900	-0.06422500	-0.54579700
C	-1.14157100	0.93717800	0.42565500
O	5.90108700	-0.01958000	-0.41122300
H	6.48275500	-0.56033200	0.13889500
H	0.73827500	1.44046400	1.30972300
O	-0.39658200	3.14197000	1.00105300
H	0.36134100	3.72959300	0.89168300
H	-7.05500100	0.77708600	-0.02104900
O	-6.50850600	-1.00003000	-0.01374600
O	-6.50919800	0.25045800	0.58227300
Frequency and Energy at B3LYP/6-311G(d,p)in gas phase			
Zero-point correction=	0.287443 (Hartree/Particle)		
Thermal correction to Energy=	0.309948		
Thermal correction to Enthalpy=	0.310892		

Thermal correction to Gibbs Free Energy= 0.233076
Sum of electronic and zero-point Energies= -1257.524122
Sum of electronic and thermal Energies= -1257.501618
Sum of electronic and thermal Enthalpies= -1257.500673
Sum of electronic and thermal Free Energies= -1257.578490

Name of compound	**Int2-9-O7-H-OOH**
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)	
C -2.32215300 1.14181300 1.00795800	
C -3.41973700 0.38578900 0.71349000	
C -3.35726900 -0.53508100 -0.38715100	
C -2.11182900 -0.61407100 -1.14869500	
H -2.34509100 1.85632100 1.82055200	
H -4.34732200 0.45000100 1.26950900	
C 0.09222500 1.87295700 0.63477300	
C 1.30487100 0.75696900 -1.29855900	
C 0.96421100 2.09459500 -0.60124700	
O 0.10214900 0.02719900 -1.60536200	
O -2.08557300 -1.47007100 -2.16435200	
H -2.97883000 -1.87482300 -2.16187100	
O -4.28773500 -1.29467800 -0.77037600	
H -5.85279000 -1.46317400 0.15382700	
O 2.11720400 2.85544900 -0.27173900	
H 2.71474000 2.29115400 0.23709900	
H 0.39788900 2.71446600 -1.30087400	
C 2.29818800 -0.10565700 -0.53702100	
C 1.89453300 -1.18174800 0.25241500	
C 3.66582600 0.19152000 -0.63842600	
C 2.83994500 -1.93880800 0.94615500	
H 0.85014400 -1.45534000 0.31381900	
C 4.61053000 -0.55540800 0.05496300	
H 4.02099800 0.98886800 -1.28161000	
C 4.18844600 -1.62779400 0.85673000	
H 2.52092700 -2.77964900 1.55470700	
H 1.73397400 0.99594700 -2.27355000	
O 5.19794800 -2.30652700 1.49471900	
H 4.84260800 -3.06163400 1.97355000	
C -1.00263100 0.17751200 -0.81736000	
C -1.10705000 1.04542200 0.26429600	
O 5.93008700 -0.25323900 -0.05784300	
H 6.42770300 -0.89194000 0.46941600	
H 0.68907100 1.31803700 1.37954000	
O -0.32484800 3.11151700 1.18461000	
H 0.46602900 3.66283200 1.23375300	
H -7.32472800 0.18442100 1.09231000	
O -6.67754800 -1.53928900 0.67727600	
O -6.60217900 -0.32830400 1.47630300	
Frequency and Energy at B3LYP/6-311G(d,p)in gas phase	
Zero-point correction= 0.290890 (Hartree/Particle)	
Thermal correction to Energy= 0.314886	
Thermal correction to Enthalpy= 0.315831	
Thermal correction to Gibbs Free Energy= 0.236400	
Sum of electronic and zero-point Energies= -1257.534007	
Sum of electronic and thermal Energies= -1257.510011	

Sum of electronic and thermal Enthalpies= -1257.509067
Sum of electronic and thermal Free Energies= -1257.588497

Name of compound	**Int1-9-O4'-H-OOH**
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)	
C 3.46282500 0.10024000 1.61567000	
C 4.21551500 1.21981100 1.27892500	
C 3.99456300 1.84338400 0.05487200	
C 3.03774600 1.36118300 -0.84048100	
H 3.62941800 -0.41296900 2.55325700	
H 4.97039500 1.60528700 1.95707600	
C 1.65732800 -1.60108200 1.09045700	
C 0.53781800 -1.31701800 -1.16738800	
C 1.22234100 -2.30199600 -0.19320300	
O 1.38964500 -0.19103400 -1.43403500	
O 2.82870500 1.96824200 -2.04270600	
H 3.45677800 2.69943900 -2.10101300	
O 4.67633200 2.96053000 -0.38207800	
H 5.36108800 3.18887100 0.25306700	
O 0.41405700 -3.43699700 0.09658600	
H -0.45054000 -3.11787500 0.38806400	
H 2.11892400 -2.69986900 -0.67551300	
C -0.84826200 -0.87408700 -0.72546100	
C -1.06482300 0.33723300 -0.07006700	
C -1.94385100 -1.71146500 -0.98815000	
C -2.35035900 0.70227500 0.33394700	
H -0.23934500 1.01218000 0.11121200	
C -3.22385000 -1.35413400 -0.58400800	
H -1.82209900 -2.63836700 -1.53770300	
C -3.42942100 -0.13613200 0.08565500	
H -2.51396300 1.64686500 0.84174700	
H 0.44292900 -1.82243200 -2.13096900	
O -4.72683400 0.12058500 0.43501300	
H -4.82064600 1.02126900 0.78606600	
C 2.28828800 0.22923600 -0.49173100	
C 2.49448100 -0.39727100 0.74453900	
O -4.27893200 -2.17150000 -0.84887900	
H -5.07131200 -1.73054600 -0.51345700	
H 0.74984800 -1.27658300 1.62669000	
O 2.39680700 -2.49116000 1.91667400	
H 1.88436000 -3.30874500 1.94347800	
H -5.53590400 4.43348000 0.57473300	
O -5.06372800 2.83543300 1.35913000	
O -5.44379600 3.50576600 0.28301900	
Frequency and Energy at B3LYP/6-311G(d,p)in gas phase	
Zero-point correction= 0.291785 (Hartree/Particle)	
Thermal correction to Energy= 0.315494	
Thermal correction to Enthalpy= 0.316439	
Thermal correction to Gibbs Free Energy= 0.234699	
Sum of electronic and zero-point Energies= -1257.527651	
Sum of electronic and thermal Energies= -1257.503942	
Sum of electronic and thermal Enthalpies= -1257.502998	
Sum of electronic and thermal Free Energies= -1257.584737	

Name of compound	TS-9-O4'-H-OOH
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)	

C	3.27935300	0.27283900	1.75075100
C	4.11748000	1.29730700	1.32442500
C	4.05891700	1.71807400	-0.00027700
C	3.17830300	1.12462500	-0.90816300
H	3.32154000	-0.08247500	2.77155600
H	4.81517000	1.76395900	2.01249100
C	1.46121600	-1.43673300	1.31160200
C	0.57368100	-1.45765000	-1.06451700
C	1.09775800	-2.31098100	0.11579400
O	1.52748800	-0.45267300	-1.42662200
O	3.12174600	1.53237500	-2.20569200
H	3.77709000	2.23404300	-2.31109200
O	4.83522200	2.72358300	-0.53321100
H	5.42712900	3.06989800	0.14090800
O	0.19764600	-3.34570600	0.49300000
H	-0.64797600	-2.93902700	0.72249400
H	2.00482500	-2.82315300	-0.21393600
C	-0.80473800	-0.86083000	-0.83606300
C	-0.97328200	0.48991700	-0.47004400
C	-1.93084300	-1.67450700	-1.01225800
C	-2.23475800	1.01804600	-0.26372600
H	-0.10604300	1.12913800	-0.37759100
C	-3.20208600	-1.16046400	-0.79133200
H	-1.83553400	-2.70427000	-1.33641800
C	-3.37558500	0.20595700	-0.41091500
H	-2.37092900	2.05816400	0.00550000
H	0.51717600	-2.11146900	-1.93786100
O	-4.61909800	0.61006300	-0.24903500
H	-4.69404300	1.43777700	0.50401600
C	2.34392400	0.08946400	-0.46699900
C	2.38574200	-0.33213100	0.86803500
O	-4.29713400	-1.92658200	-0.93839200
H	-5.05670700	-1.35559400	-0.73176000
H	0.52920700	-0.99917100	1.70991700
O	2.08529900	-2.21333800	2.32435700
H	1.53153900	-2.99500700	2.44148600
H	-6.13065200	3.46133100	1.85784500
O	-4.77864000	2.24755600	1.48104800
O	-5.68906500	3.19450300	1.03761800

Frequency and Energy at B3LYP/6-311G(d,p)in gas phase	
Zero-point correction=	0.287305 (Hartree/Particle)
Thermal correction to Energy=	0.309986
Thermal correction to Enthalpy=	0.310930
Thermal correction to Gibbs Free Energy=	0.232946
Sum of electronic and zero-point Energies=	-1257.522838
Sum of electronic and thermal Energies=	-1257.500157
Sum of electronic and thermal Enthalpies=	-1257.499213
Sum of electronic and thermal Free Energies=	-1257.577197

Name of compound	Int2-9-O4'-H-OOH
Cartesian Coordinates optimized at B3LYP/6-311G(d,p)	

C	3.32931300	0.14110200	1.64075900

C	4.05115900	1.28117700	1.30576500
C	3.85455200	1.87188600	0.06175700
C	2.94825700	1.33516200	-0.85671400
H	3.48115700	-0.34358400	2.59575000
H	4.76581700	1.70739400	2.00242200
C	1.61707800	-1.64416100	1.09450000
C	0.52052500	-1.39215300	-1.18080100
C	1.19729800	-2.36557300	-0.18232600
O	1.38021900	-0.29021700	-1.47617800
O	2.75169900	1.90979900	-2.07395000
H	3.33138300	2.68101100	-2.12223200
O	4.50707900	3.00136400	-0.37677700
H	5.10126400	3.32323400	0.30752400
O	0.40181700	-3.50716900	0.10738500
H	-0.42548200	-3.20796600	0.50542700
H	2.09923800	-2.75563400	-0.65968300
C	-0.86068900	-0.92513400	-0.75777200
C	-1.06150100	0.37228500	-0.20102600
C	-1.94627600	-1.78838200	-0.93879700
C	-2.29963200	0.79584200	0.20074700
H	-0.21306600	1.03682300	-0.11140400
C	-3.21198700	-1.38369800	-0.54088900
H	-1.82172300	-2.75808900	-1.40628200
C	-3.43923100	-0.06667100	0.05694600
H	-2.46550100	1.77955000	0.62361900
H	0.41501300	-1.92456500	-2.12913200
O	-4.62132900	0.21203300	0.39045300
H	-4.81292900	1.91146900	1.05886000
C	2.23331400	0.18286200	-0.50827200
C	2.41495400	-0.41310900	0.74566000
O	-4.28430600	-2.15763200	-0.68353700
H	-5.02845700	-1.62659900	-0.33188400
H	0.70105500	-1.34828100	1.63661200
O	2.39252100	-2.50246600	1.91783300
H	1.90714300	-3.33440900	1.97697000
H	-5.81355300	4.06027900	0.58400500
O	-4.67273300	2.81241300	1.41577000
O	-5.01798700	3.62072000	0.25802800

Frequency and Energy at B3LYP/6-311G(d,p)in gas phase

Zero-point correction=	0.292314 (Hartree/Particle)
Thermal correction to Energy=	0.315714
Thermal correction to Enthalpy=	0.316658
Thermal correction to Gibbs Free Energy=	0.236683
Sum of electronic and zero-point Energies=	-1257.543125
Sum of electronic and thermal Energies=	-1257.519726
Sum of electronic and thermal Enthalpies=	-1257.518781
Sum of electronic and thermal Free Energies=	-1257.598757

Table S6: The calculated ΔG≠ and rate constant *k* at the M05-2X/6-311G(d,p) level of theory at 298.15 K in the gas phase.

Reactions	**ΔG≠** (kcal/mol)	***k*** ($L.mol^{-1}.s^{-1}$)
1-C3-H + HOO•	14.1	4.10×10^{4}
1-O4'-H + HOO•	16.3	1.08×10^{3}
9-C4-H + HOO•	17.3	6.62×10^{2}
9-O7-H + HOO•	10.2	1.75×10^{7}
9-O4'-H + HOO•	11.3	8.96×10^{6}

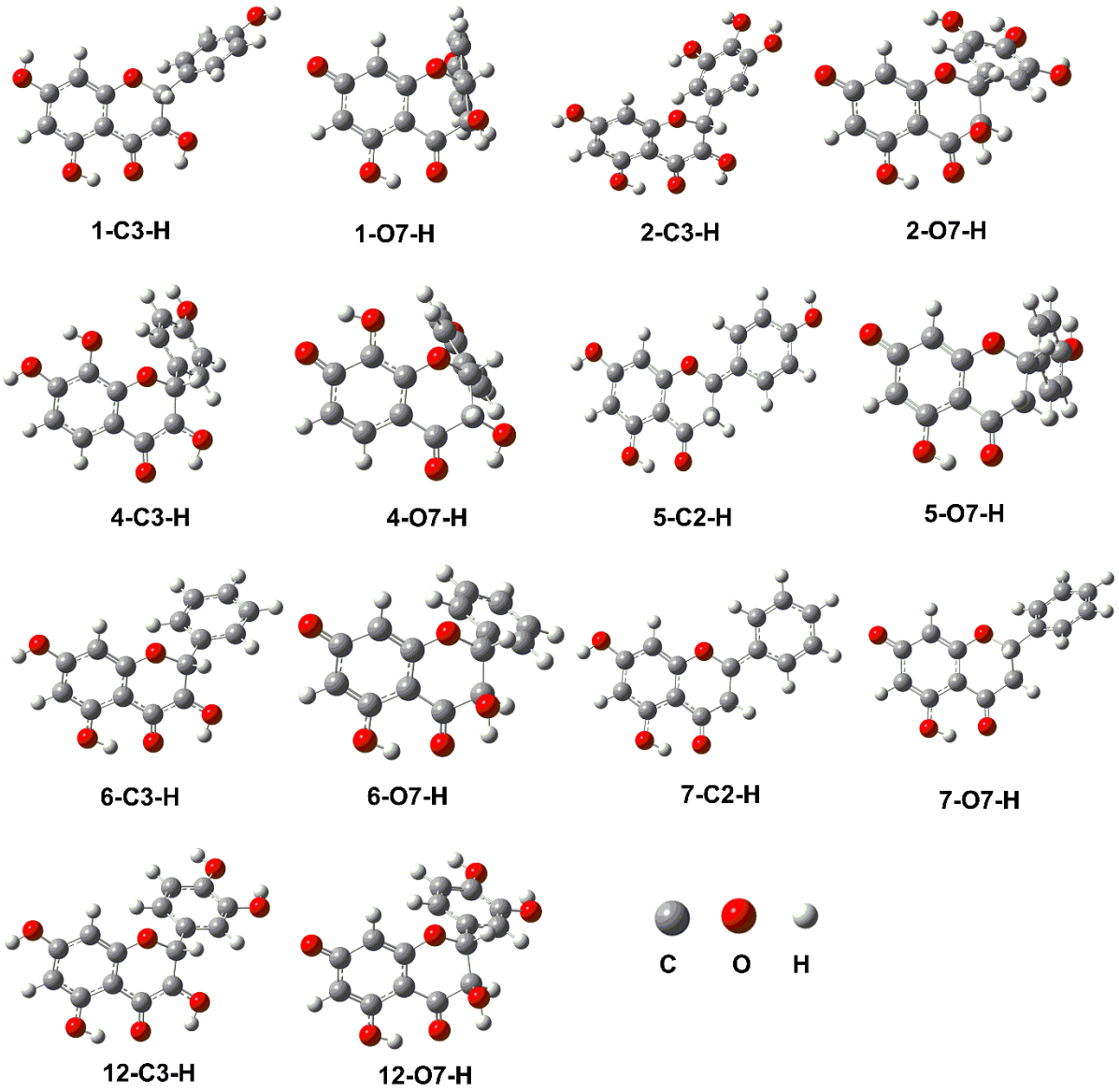


Figure S1: Optimized geometries of the radicals of the compounds **1, 2, 4, 5, 6, 7** and **12**.

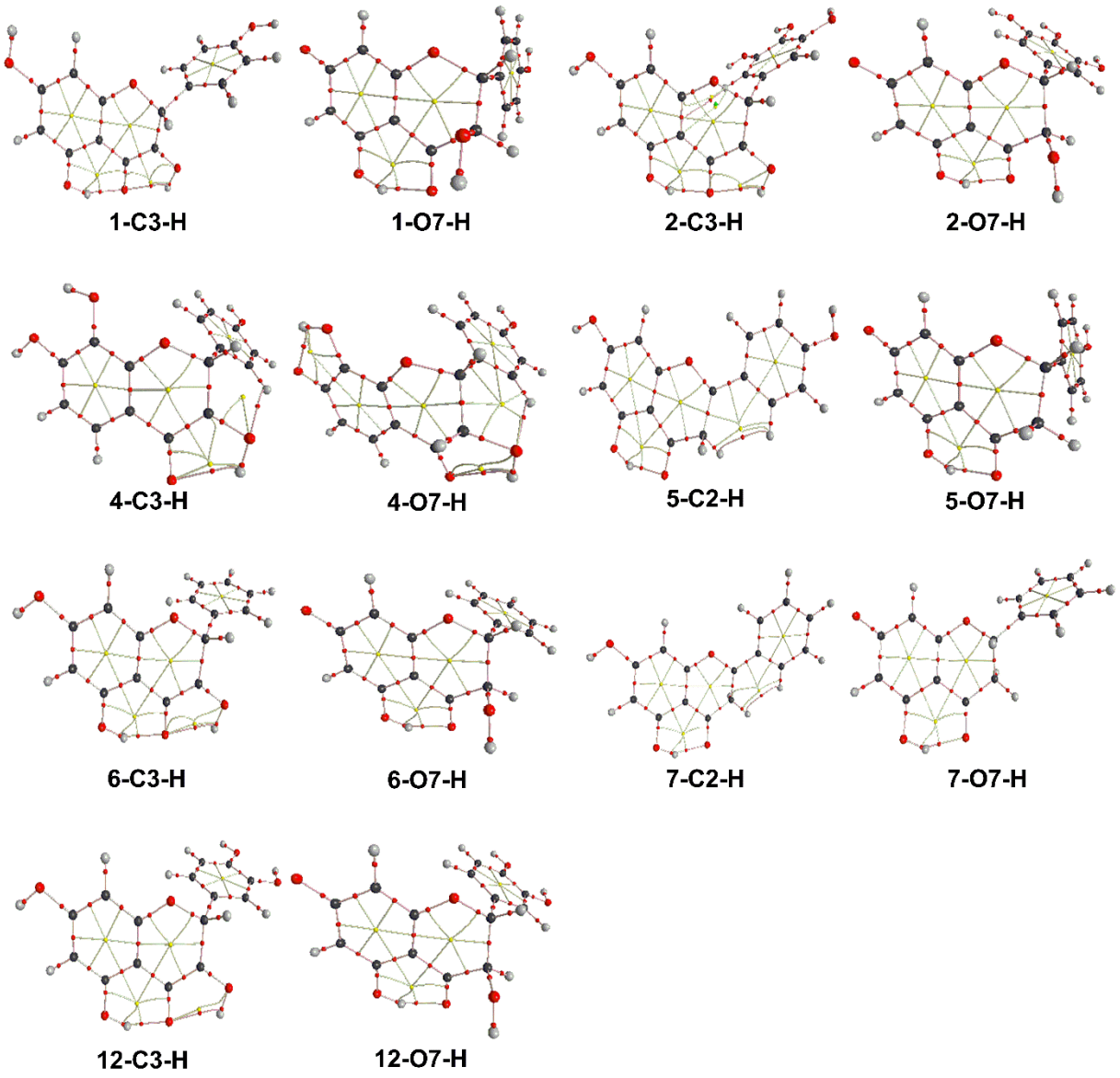
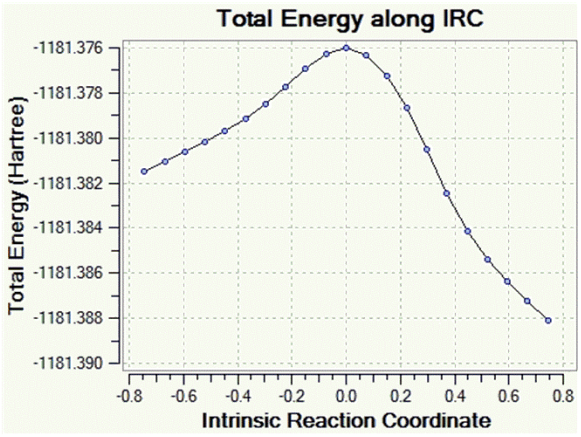
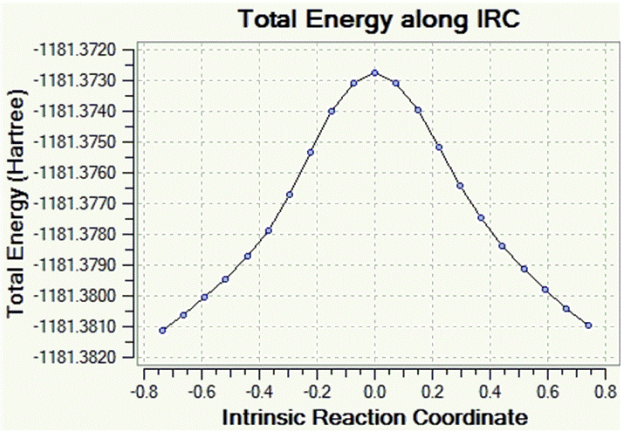


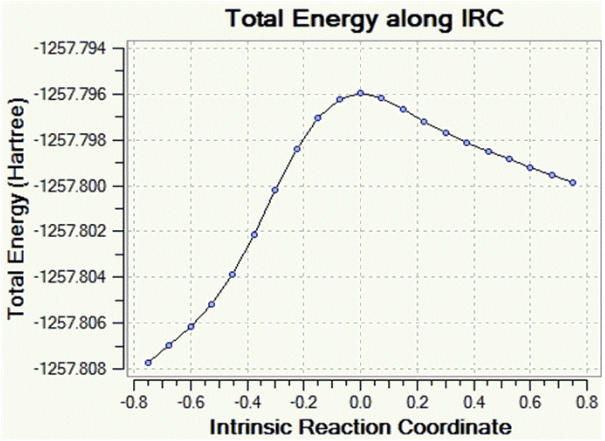
Figure S2: Topological shape of radicals formed by **1, 2, 4, 5, 6, 7** and **12** (B3LYP/6-311G(d,p))



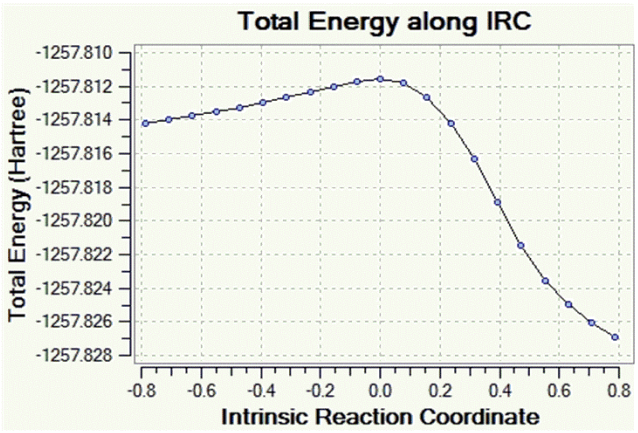
1-C3-H-OOH



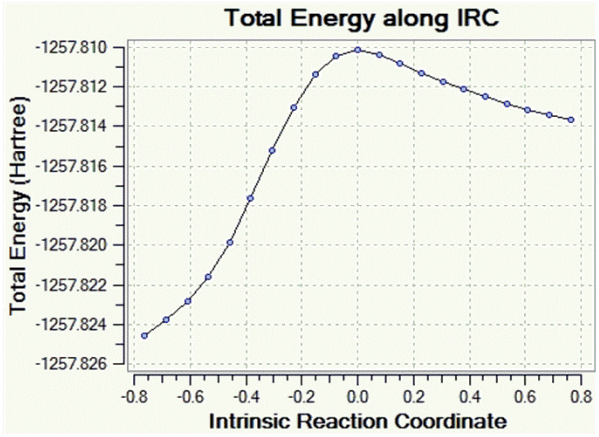
1-O4'-H-OOH



9-C4-H-OOH



9-O7-H-OOH



9-O4'-H-OOH

Figure S3: IRC plots for all transition states related to the reaction of HOO• radical with dihydrokaempferol **1**, and isomelacacidin **9** at B3LYP/6-311G(d,p) level of theory in the gas phase.

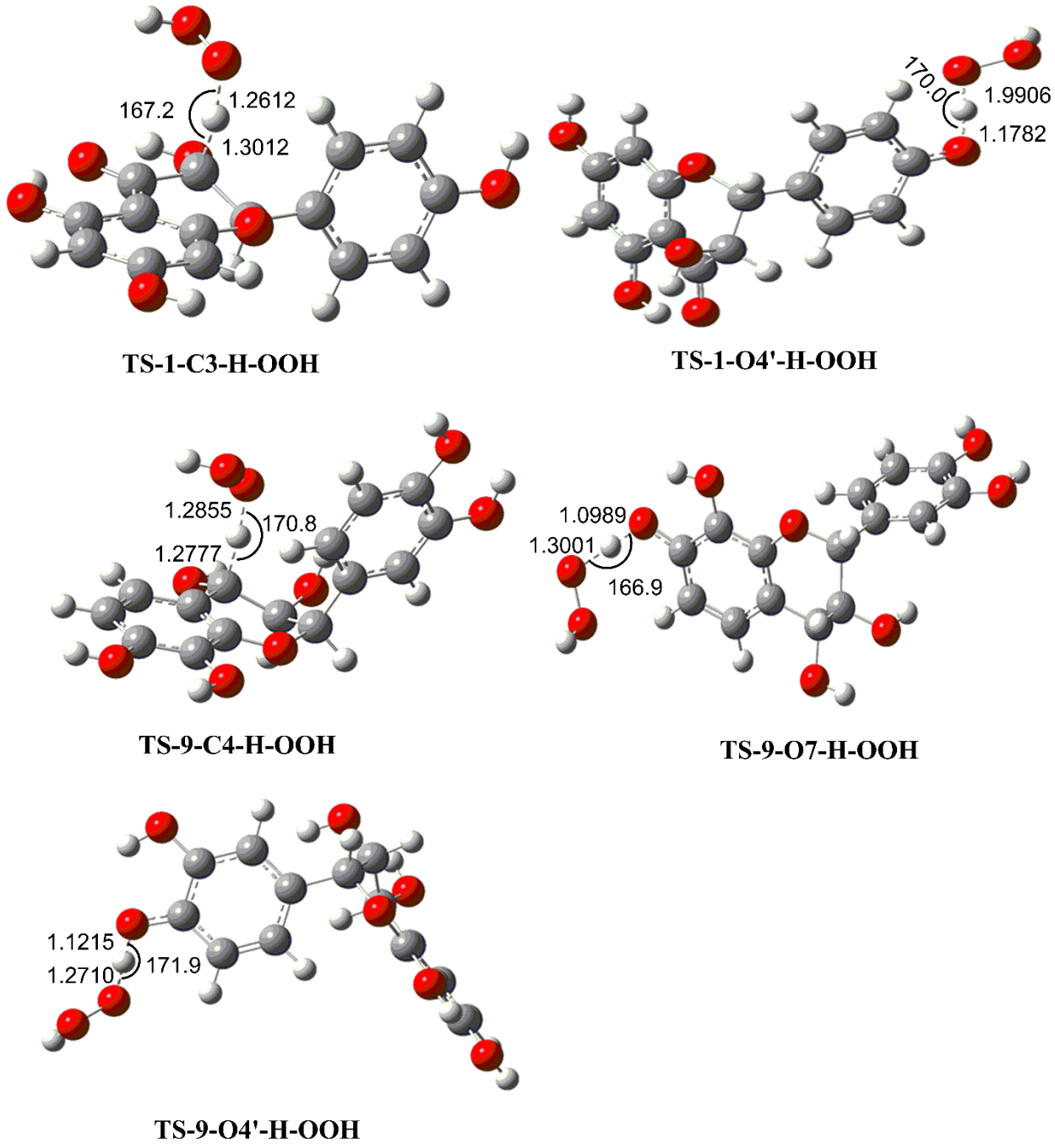


Figure S4. Optimized geometries of TS for the H abstraction channel of reaction between the selected phenolic compounds and the HOO• radical at the B3LYP/6-311G(d,p) level of theory (distances are given in angstroms)