Supporting information

A DFT analysis on the radical scavenging activity of oxygenated terpenoids present in the extract of the buds of *Cleistocalyx operculatus*

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List of supporting information:

Table S1*:* Cartesian coordinates and molecular enthalpies of all parent molecules and resulted radicals, anions optimized at B3LYP/6-311G(d,p) level of theory in the gas phase, water and ethanol.

Figure S2*:* IRC plots for all transition states related to reaction of $CH_3OO^{\bullet}$ and $HO^{\bullet}$ radical with falcarinol at B3LYP/6-311G(d,p) level of theory in the gas phase.

Figure S3: IRC plots for all transition states related to reaction of $CH_3OO^{\bullet}$ and $HO^{\bullet}$ radical with α-vetivone at B3LYP/6-311G(d,p) level of theory in the gas phase.

Figure S4: Optimized structures of transition state for H-atom abstraction reactions between (A) falcarinol and DPPH• radical; (B) α-vetivone and DPPH• radical calculated at B3LYP/3-21G level of theory

Table S1: Cartesian coordinates and molecular enthalpies of all parent molecules and resulted radicals, anions optimized at B3LYP/6-311G(d,p) level of theory in the gas phase, water and ethanol.

Name of compound	cis-Linalool oxide		
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	1.27631500	1.44313400	0.20331800
C	1.46496200	-0.08786900	0.11478900
C	-0.21635700	1.68597200	-0.04805800
O	0.30592200	-0.59474200	-0.62148000
C	2.65638900	-0.50533500	-0.71519000
C	1.44944600	-0.78319900	1.47654000
C	-0.73236500	0.41309600	-0.73686400
C	-2.01855800	-0.18385700	-0.08403000
C	-2.28419300	-1.59205300	-0.61500900
C	-3.21606600	0.74687000	-0.26066200
O	-1.83565600	-0.24859100	1.34586100
C	3.91296500	-0.17945800	-0.42835600
H	1.59671900	1.83996200	1.17994800
H	1.89371500	1.95719500	-0.55550400
H	-0.38887500	2.58118200	-0.66582700
H	-0.75146400	1.85462500	0.90947600
H	2.38670700	-1.11078700	-1.58547000
H	1.54306600	-1.87063700	1.35953600
H	2.26853400	-0.44583200	2.11862200
H	0.49911800	-0.59029000	2.00088200
H	-0.87257200	0.54061100	-1.82972700
H	-2.66767400	-1.58194600	-1.63886500
H	-1.36170600	-2.19190200	-0.61808000
H	-3.01486500	-2.11174400	0.01549100
H	-3.46550200	0.90207800	-1.31340400
H	-4.09983300	0.32706400	0.23979100
H	-3.03601900	1.72321300	0.20509100
H	-1.00309500	-0.74659300	1.55142900
H	4.75419500	-0.49017100	-1.03228200
H	4.20220500	0.41683300	0.42498400
Frequency and Energy at B3LYP/6-311G (d,p) (gas)			
Zero-point correction=		0.265040	(Hartree/Particle)
Thermal correction to Energy=		0.278428	
Thermal correction to Enthalpy=		0.279372	
Thermal correction to Gibbs Free Energy=		0.226005	
Sum of electronic and zero-point Energies=		-542.215015	
Sum of electronic and thermal Energies=		-542.201627	
Sum of electronic and thermal Enthalpies=		-542.200683	
Sum of electronic and thermal Free Energies=		-542.254050	
Frequency and Energy at B3LYP/6-311G (d,p) (water)			
Zero-point correction=		0.264493	(Hartree/Particle)

Thermal correction to Energy=	0.277915
Thermal correction to Enthalpy=	0.278859
Thermal correction to Gibbs Free Energy=	0.225511
Sum of electronic and zero-point Energies=	-542.221289
Sum of electronic and thermal Energies=	-542.207867
Sum of electronic and thermal Enthalpies=	-542.206923
Sum of electronic and thermal Free Energies=	-542.260272
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.264528 (Hartree/Particle)
Thermal correction to Energy=	0.277947
Thermal correction to Enthalpy=	0.278891
Thermal correction to Gibbs Free Energy=	0.225550
Sum of electronic and zero-point Energies=	-542.220962
Sum of electronic and thermal Energies=	-542.207543
Sum of electronic and thermal Enthalpies=	-542.206599
Sum of electronic and thermal Free Energies=	-542.259940

Name of radical	cis-Linalool oxide-C7-H

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

0 2

C	1.35981700	1.41192300	-0.16136100
C	1.55089500	-0.04958300	0.30706500
C	-0.16288500	1.59535500	-0.16456800
O	0.27415000	-0.70162700	0.03677300
C	2.61168000	-0.83757700	-0.42905300
C	1.79146100	-0.14696600	1.82083600
C	-0.65482200	0.20820700	-0.58025700
C	-2.06819900	-0.19231600	-0.10057300
C	-2.41574600	-1.59948100	-0.60978400
C	-3.11415600	0.82407100	-0.55381000
O	-2.08702700	-0.17835100	1.33128900
C	3.64815100	-0.35247800	-1.10422000
H	1.87501500	2.12088600	0.48933700
H	1.75088400	1.53850100	-1.17335600
H	-0.48831400	2.38202800	-0.84745500
H	-0.54101800	1.82574200	0.83419900
H	2.48417600	-1.91410600	-0.34023800
H	1.76031700	-1.19184800	2.13933200
H	2.76842000	0.26481900	2.08541500
H	1.01737600	0.40116500	2.36462200
H	-2.47622400	-1.62423200	-1.70214500
H	-1.65402900	-2.31636900	-0.29677200
H	-3.37946000	-1.90889700	-0.19954900
H	-3.12738400	0.91601600	-1.64326000
H	-4.10406500	0.50167900	-0.22369700
H	-2.91784200	1.80548200	-0.11870700
H	-1.33648700	-0.72231600	1.60290900
H	4.37051500	-1.01242600	-1.57116900
H	3.82565300	0.71193100	-1.21650900

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

Zero-point correction=	0.251504 (Hartree/Particle)
Thermal correction to Energy=	0.265191
Thermal correction to Enthalpy=	0.266136
Thermal correction to Gibbs Free Energy=	0.211240
Sum of electronic and zero-point Energies=	-541.571378
Sum of electronic and thermal Energies=	-541.557691
Sum of electronic and thermal Enthalpies=	-541.556746
Sum of electronic and thermal Free Energies=	-541.611641
Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.250995 (Hartree/Particle)
Thermal correction to Energy=	0.264710
Thermal correction to Enthalpy=	0.265654
Thermal correction to Gibbs Free Energy=	0.210741
Sum of electronic and zero-point Energies=	-541.578156
Sum of electronic and thermal Energies=	-541.564442
Sum of electronic and thermal Enthalpies=	-541.563497
Sum of electronic and thermal Free Energies=	-541.618410
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.251026 (Hartree/Particle)
Thermal correction to Energy=	0.264738
Thermal correction to Enthalpy=	0.265682
Thermal correction to Gibbs Free Energy=	0.210781
Sum of electronic and zero-point Energies=	-541.577809
Sum of electronic and thermal Energies=	-541.564097
Sum of electronic and thermal Enthalpies=	-541.563153
Sum of electronic and thermal Free Energies=	-541.618054

Name of anion	cis-Linalool oxide-O-H

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

C	1.35981700	1.41192300	-0.16136100
C	1.55089500	-0.04958300	0.30706500
C	-0.16288500	1.59535500	-0.16456800
O	0.27415000	-0.70162700	0.03677300
C	2.61168000	-0.83757700	-0.42905300
C	1.79146100	-0.14696600	1.82083600
C	-0.65482200	0.20820700	-0.58025700
C	-2.06819900	-0.19231600	-0.10057300
C	-2.41574600	-1.59948100	-0.60978400
C	-3.11415600	0.82407100	-0.55381000
O	-2.08702700	-0.17835100	1.33128900
C	3.64815100	-0.35247800	-1.10422000
H	1.87501500	2.12088600	0.48933700
H	1.75088400	1.53850100	-1.17335600
H	-0.48831400	2.38202800	-0.84745500
H	-0.54101800	1.82574200	0.83419900
H	2.48417600	-1.91410600	-0.34023800
H	1.76031700	-1.19184800	2.13933200
H	2.76842000	0.26481900	2.08541500
H	1.01737600	0.40116500	2.36462200
H	-0.60169200	0.09484600	-1.67311800

H	-2.47622400	-1.62423200	-1.70214500
H	-1.65402900	-2.31636900	-0.29677200
H	-3.37946000	-1.90889700	-0.19954900
H	-3.12738400	0.91601600	-1.64326000
H	-4.10406500	0.50167900	-0.22369700
H	-2.91784200	1.80548200	-0.11870700
H	4.37051500	-1.01242600	-1.57116900
H	3.82565300	0.71193100	-1.21650900

Frequency and Energy at B3LYP/6-311G (d,p) (gas)		
Zero-point correction=	0.249140	(Hartree/Particle)
Thermal correction to Energy=	0.262112	
Thermal correction to Enthalpy=	0.263056	
Thermal correction to Gibbs Free Energy=	0.211254	
Sum of electronic and zero-point Energies=	-541.622083	
Sum of electronic and thermal Energies=	-541.609111	
Sum of electronic and thermal Enthalpies=	-541.608167	
Sum of electronic and thermal Free Energies=	-541.659969	

Frequency and Energy at B3LYP/6-311G (d,p) (water)		
Zero-point correction=	0.249616	(Hartree/Particle)
Thermal correction to Energy=	0.262676	
Thermal correction to Enthalpy=	0.263620	
Thermal correction to Gibbs Free Energy=	0.211448	
Sum of electronic and zero-point Energies=	-541.707480	
Sum of electronic and thermal Energies=	-541.694421	
Sum of electronic and thermal Enthalpies=	-541.693476	
Sum of electronic and thermal Free Energies=	-541.745648	

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)		
Zero-point correction=	0.249690	(Hartree/Particle)
Thermal correction to Energy=	0.262722	
Thermal correction to Enthalpy=	0.263666	
Thermal correction to Gibbs Free Energy=	0.211550	
Sum of electronic and zero-point Energies=	-541.704389	
Sum of electronic and thermal Energies=	-541.691357	
Sum of electronic and thermal Enthalpies=	-541.690413	
Sum of electronic and thermal Free Energies=	-541.742529	

Name of cationic radical	cis-Linalool oxide

Cartesian Coordinates optimized at B3LYP/6-311G (d,p) (gas)			
C	1.27631500	1.44313400	0.20331800
C	1.46496200	-0.08786900	0.11478900
C	-0.21635700	1.68597200	-0.04805800
O	0.30592200	-0.59474200	-0.62148000
C	2.65638900	-0.50533500	-0.71519000
C	1.44944600	-0.78319900	1.47654000
C	-0.73236500	0.41309600	-0.73686400
C	-2.01855800	-0.18385700	-0.08403000
C	-2.28419300	-1.59205300	-0.61500900
C	-3.21606600	0.74687000	-0.26066200
O	-1.83565600	-0.24859100	1.34586100

C	3.91296500	-0.17945800	-0.42835600
H	1.59671900	1.83996200	1.17994800
H	1.89371500	1.95719500	-0.55550400
H	-0.38887500	2.58118200	-0.66582700
H	-0.75146400	1.85462500	0.90947600
H	2.38670700	-1.11078700	-1.58547000
H	1.54306600	-1.87063700	1.35953600
H	2.26853400	-0.44583200	2.11862200
H	0.49911800	-0.59029000	2.00088200
H	-0.87257200	0.54061100	-1.82972700
H	-2.66767400	-1.58194600	-1.63886500
H	-1.36170600	-2.19190200	-0.61808000
H	-3.01486500	-2.11174400	0.01549100
H	-3.46550200	0.90207800	-1.31340400
H	-4.09983300	0.32706400	0.23979100
H	-3.03601900	1.72321300	0.20509100
H	-1.00309500	-0.74659300	1.55142900
H	4.75419500	-0.49017100	-1.03228200
H	4.20220500	0.41683300	0.42498400

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.262676 (Hartree/Particle)
Thermal correction to Energy=	0.277190
Thermal correction to Enthalpy=	0.278134
Thermal correction to Gibbs Free Energy=	0.221348
Sum of electronic and zero-point Energies=	-541.918837
Sum of electronic and thermal Energies=	-541.904324
Sum of electronic and thermal Enthalpies=	-541.903379
Sum of electronic and thermal Free Energies=	-541.960165

Name of compound	cis-Verbenol	
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)		
C	33.69720000	7.80970000	-0.07740000
C	33.66310000	8.80480000	-0.97760000
C	34.98250000	6.99590000	-0.00440000
C	32.55820000	7.45290000	0.83440000
C	34.87630000	9.09080000	-1.84240000
C	36.01410000	8.11140000	-1.48550000
O	35.27400000	10.46600000	-1.79650000
C	36.23110000	7.96020000	0.06730000
C	35.40690000	6.67830000	-1.47150000
C	37.53320000	7.20490000	0.38520000
C	36.17760000	9.18880000	0.98460000
H	32.78680000	9.43700000	-1.11140000
H	34.92480000	6.17690000	0.72150000
H	31.69150000	8.10250000	0.67530000
H	32.23890000	6.41260000	0.68050000
H	32.85650000	7.53190000	1.88940000
H	34.61970000	8.93770000	-2.90000000
H	36.89700000	8.31150000	-2.10300000
H	35.37460000	10.70660000	-0.86340000
H	36.15610000	5.88840000	-1.55570000

H	34.59410000	6.47530000	-2.17590000
H	38.39880000	7.86220000	0.23390000
H	37.54330000	6.88360000	1.43450000
H	37.68430000	6.31690000	-0.23380000
H	36.32820000	8.88960000	2.02990000
H	36.98200000	9.89250000	0.73410000
H	35.22140000	9.71690000	0.93880000

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.239559 (Hartree/Particle)
Thermal correction to Energy=	0.250548
Thermal correction to Enthalpy=	0.251492
Thermal correction to Gibbs Free Energy=	0.204555
Sum of electronic and zero-point Energies=	-465.757360
Sum of electronic and thermal Energies=	-465.746370
Sum of electronic and thermal Enthalpies=	-465.745426
Sum of electronic and thermal Free Energies=	-465.792364

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.238771 (Hartree/Particle)
Thermal correction to Energy=	0.249872
Thermal correction to Enthalpy=	0.250816
Thermal correction to Gibbs Free Energy=	0.203629
Sum of electronic and zero-point Energies=	-465.762857
Sum of electronic and thermal Energies=	-465.751756
Sum of electronic and thermal Enthalpies=	-465.750812
Sum of electronic and thermal Free Energies=	-465.797999

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.239061 (Hartree/Particle)
Thermal correction to Energy=	0.250092
Thermal correction to Enthalpy=	0.251036
Thermal correction to Gibbs Free Energy=	0.204017
Sum of electronic and zero-point Energies=	-465.762316
Sum of electronic and thermal Energies=	-465.751285
Sum of electronic and thermal Enthalpies=	-465.750340
Sum of electronic and thermal Free Energies=	-465.797359

Name of radical	cis-Verbenol-C5-H

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	33.69720000	7.80970000	-0.07740000
C	33.66310000	8.80480000	-0.97760000
C	34.98250000	6.99590000	-0.00440000
C	32.55820000	7.45290000	0.83440000
C	34.87630000	9.09080000	-1.84240000
C	36.01410000	8.11140000	-1.48550000
O	35.27400000	10.46600000	-1.79650000
C	36.23110000	7.96020000	0.06730000
C	35.40690000	6.67830000	-1.47150000
C	37.53320000	7.20490000	0.38520000
C	36.17760000	9.18880000	0.98460000
H	32.78680000	9.43700000	-1.11140000

H	34.92480000	6.17690000	0.72150000
H	31.69150000	8.10250000	0.67530000
H	32.23890000	6.41260000	0.68050000
H	32.85650000	7.53190000	1.88940000
H	36.89700000	8.31150000	-2.10300000
H	35.37460000	10.70660000	-0.86340000
H	36.15610000	5.88840000	-1.55570000
H	34.59410000	6.47530000	-2.17590000
H	38.39880000	7.86220000	0.23390000
H	37.54330000	6.88360000	1.43450000
H	37.68430000	6.31690000	-0.23380000
H	36.32820000	8.88960000	2.02990000
H	36.98200000	9.89250000	0.73410000
H	35.22140000	9.71690000	0.93880000

Frequency and Energy at B3LYP/6-311G (d,p) (gas)		
Zero-point correction=	0.225705	(Hartree/Particle)
Thermal correction to Energy=	0.236971	
Thermal correction to Enthalpy=	0.237915	
Thermal correction to Gibbs Free Energy=	0.189393	
Sum of electronic and zero-point Energies=	-465.137596	
Sum of electronic and thermal Energies=	-465.126331	
Sum of electronic and thermal Enthalpies=	-465.125386	
Sum of electronic and thermal Free Energies=	-465.173908	

Frequency and Energy at B3LYP/6-311G (d,p) (water)		
Zero-point correction=	0.224914	(Hartree/Particle)
Thermal correction to Energy=	0.236195	
Thermal correction to Enthalpy=	0.237139	
Thermal correction to Gibbs Free Energy=	0.188580	
Sum of electronic and zero-point Energies=	-465.145200	
Sum of electronic and thermal Energies=	-465.133919	
Sum of electronic and thermal Enthalpies=	-465.132975	
Sum of electronic and thermal Free Energies=	-465.181534	

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)		
Zero-point correction=	0.225224	(Hartree/Particle)
Thermal correction to Energy=	0.236507	
Thermal correction to Enthalpy=	0.237451	
Thermal correction to Gibbs Free Energy=	0.188896	
Sum of electronic and zero-point Energies=	-465.142606	
Sum of electronic and thermal Energies=	-465.131322	
Sum of electronic and thermal Enthalpies=	-465.130378	
Sum of electronic and thermal Free Energies=	-465.178933	

Name of anion	cis-Verbenol-O-H	
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)		
C	-1.44774400	-0.55380200	0.02371400
C	-1.51392600	0.77999800	-0.06873800
C	-0.13580800	-1.20622000	-0.38758500
C	-2.57481300	-1.42724600	0.49060600
C	-0.30922900	1.56933200	-0.54004500
C	0.86116100	0.61194400	-0.83677300

O	0.04092600	2.62793400	0.36155500
C	1.07648900	-0.46056100	0.29550100
C	0.30574100	-0.53817800	-1.72682600
C	2.40159700	-1.21617600	0.10768100
C	0.97545900	-0.06744700	1.77257100
H	-2.40989400	1.33603500	0.19249000
H	-0.16747300	-2.29678300	-0.32350400
H	-3.46092200	-0.84188200	0.74476300
H	-2.85252500	-2.15417100	-0.28171400
H	-2.28018400	-2.00788400	1.37292000
H	-0.55608900	2.09810200	-1.46823400
H	1.73586600	1.17384300	-1.17377000
H	1.08248400	-1.08626700	-2.25823700
H	-0.49464400	-0.28411600	-2.42407000
H	3.24183100	-0.58203900	0.40867200
H	2.42265600	-2.11188700	0.73709900
H	2.58027700	-1.53052100	-0.92112900
H	1.11701400	-0.94863500	2.40755800
H	1.76306600	0.64695700	2.03359800
H	0.00931200	0.36437600	2.03659500

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.222935 (Hartree/Particle)
Thermal correction to Energy=	0.233671
Thermal correction to Enthalpy=	0.234615
Thermal correction to Gibbs Free Energy=	0.188024
Sum of electronic and zero-point Energies=	-465.160190
Sum of electronic and thermal Energies=	-465.149454
Sum of electronic and thermal Enthalpies=	-465.148510
Sum of electronic and thermal Free Energies=	-465.195101

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.223792 (Hartree/Particle)
Thermal correction to Energy=	0.234462
Thermal correction to Enthalpy=	0.235406
Thermal correction to Gibbs Free Energy=	0.188970
Sum of electronic and zero-point Energies=	-465.249198
Sum of electronic and thermal Energies=	-465.238528
Sum of electronic and thermal Enthalpies=	-465.237584
Sum of electronic and thermal Free Energies=	-465.284021

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.223788 (Hartree/Particle)
Thermal correction to Energy=	0.234457
Thermal correction to Enthalpy=	0.235401
Thermal correction to Gibbs Free Energy=	0.188964
Sum of electronic and zero-point Energies=	-465.246131
Sum of electronic and thermal Energies=	-465.235462
Sum of electronic and thermal Enthalpies=	-465.234518
Sum of electronic and thermal Free Energies=	-465.280955

Name of cationic radical	cis-Verbenol
Cartesian Coordinates optimized at B3LYP/6-311G (d,p) (gas)	

C	-1.44748100	-0.52167700	0.01391000
C	-1.48206800	0.82288400	-0.05090800
C	-0.16275000	-1.20647500	-0.41230100
C	-2.57497100	-1.37861300	0.46786600
C	-0.26410400	1.58145600	-0.55005900
C	0.90099600	0.59776000	-0.83553700
O	0.12276900	2.60247200	0.37526500
C	1.05717600	-0.48785200	0.29821300
C	0.29727400	-0.52082200	-1.73970300
C	2.35582700	-1.28532100	0.16399000
C	0.88476200	-0.07936800	1.75284100
H	-2.33132700	1.42905900	0.23227100
H	-0.18452900	-2.29626100	-0.38378500
H	-3.45557400	-0.79508000	0.76879000
H	-2.89811300	-2.06454100	-0.32868700
H	-2.28353400	-1.99552800	1.32999200
H	-0.50667900	2.17973000	-1.45938000
H	1.81153800	1.10196800	-1.16308100
H	0.31605800	2.21282200	1.25836500
H	1.03508900	-1.09000900	-2.31275500
H	-0.49722900	-0.21998100	-2.42725500
H	3.22460000	-0.66607200	0.41584100
H	2.35962100	-2.15083900	0.83567400
H	2.51746500	-1.66386800	-0.85115900
H	0.60099300	-0.94260900	2.36682400
H	1.81551000	0.32738500	2.16676900
H	0.10599400	0.68222600	1.89958400

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.236321 (Hartree/Particle)
Thermal correction to Energy=	0.248085
Thermal correction to Enthalpy=	0.249029
Thermal correction to Gibbs Free Energy=	0.199078
Sum of electronic and zero-point Energies=	-465.463134
Sum of electronic and thermal Energies=	-465.451371
Sum of electronic and thermal Enthalpies=	-465.450427
Sum of electronic and thermal Free Energies=	-465.500377

Name of compound	Isomenthone

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	0.77490000	4.45490000	2.18780000
C	2.05640000	3.68260000	1.91730000
C	1.79180000	2.53560000	0.95630000
C	2.73320000	3.22490000	3.22310000
C	2.08630000	2.02570000	3.90800000
C	4.21480000	2.94140000	2.96890000
O	0.88380000	1.88950000	4.02910000
C	3.04420000	1.00840000	4.49690000
C	4.97310000	2.62910000	4.24850000
C	4.20500000	1.70490000	5.19940000
C	5.13230000	0.67730000	5.82620000
H	0.95030000	5.30280000	2.86320000

H	0.35900000	4.85880000	1.25510000
H	0.00000000	3.82420000	2.64360000
H	2.77070000	4.38730000	1.41870000
H	2.70920000	1.97080000	0.74040000
H	1.40110000	2.90780000	0.00000000
H	1.05350000	1.82740000	1.35600000
H	2.66190000	4.06620000	3.95890000
H	4.68320000	3.81330000	2.46940000
H	4.31330000	2.10210000	2.24870000
H	2.52320000	0.33300000	5.20530000
H	3.41270000	0.35650000	3.67860000
H	5.95300000	2.18470000	3.98110000
H	5.21560000	3.57040000	4.78020000
H	3.77440000	2.33020000	6.02030000
H	4.60330000	0.05800000	6.56250000
H	5.55840000	0.00000000	5.07350000
H	5.96980000	1.16270000	6.34410000

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.262317 (Hartree/Particle)
Thermal correction to Energy=	0.274491
Thermal correction to Enthalpy=	0.275435
Thermal correction to Gibbs Free Energy=	0.224660
Sum of electronic and zero-point Energies=	-467.004015
Sum of electronic and thermal Energies=	-466.991841
Sum of electronic and thermal Enthalpies=	-466.990897
Sum of electronic and thermal Free Energies=	-467.041673

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.261854 (Hartree/Particle)
Thermal correction to Energy=	0.274053
Thermal correction to Enthalpy=	0.274997
Thermal correction to Gibbs Free Energy=	0.224203
Sum of electronic and zero-point Energies=	-467.009650
Sum of electronic and thermal Energies=	-466.997451
Sum of electronic and thermal Enthalpies=	-466.996506
Sum of electronic and thermal Free Energies=	-467.047301

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.261883 (Hartree/Particle)
Thermal correction to Energy=	0.274078
Thermal correction to Enthalpy=	0.275022
Thermal correction to Gibbs Free Energy=	0.224247
Sum of electronic and zero-point Energies=	-467.009360
Sum of electronic and thermal Energies=	-466.997166
Sum of electronic and thermal Enthalpies=	-466.996222
Sum of electronic and thermal Free Energies=	-467.046996

Name of radical	Isomenthone-C4-H	
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)		
C	-2.99359800	0.20520300	-1.06522500
C	-2.12053800	-0.64670500	-0.13766200
C	-2.47317400	-0.37925600	1.32947800

C	-0.61565900	-0.39597500	-0.42866300
C	-0.13243000	0.97382800	0.03484200
C	0.25511800	-1.50513200	0.18492700
O	-0.83559600	1.96027100	0.06339900
C	1.32570600	1.05791800	0.43875900
C	1.74059700	-1.37353800	-0.17870000
C	2.19993500	0.08835700	-0.37261900
C	3.67640500	0.25248400	0.00059900
H	-2.82359200	-0.02832200	-2.11951500
H	-4.05817300	0.05729300	-0.85919700
H	-2.78170300	1.27796800	-0.92429700
H	-2.32643100	-1.72519900	-0.35760300
H	-1.84060200	-0.95116100	2.01408700
H	-3.51463500	-0.64455700	1.53992400
H	-2.35854100	0.68590500	1.57614300
H	-0.11810000	-2.49456300	-0.14301300
H	0.13911500	-1.49356400	1.28729800
H	1.68446200	2.10038200	0.32415100
H	1.40702900	0.84307300	1.52357000
H	2.34310900	-1.86197800	0.61139100
H	1.95478900	-1.94059000	-1.10414400
H	2.08395400	0.34876500	-1.45558400
H	4.02958000	1.26980400	-0.20363100
H	3.85529200	0.05458700	1.06330700
H	4.31109800	-0.43280100	-0.57228800

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.249168 (Hartree/Particle)
Thermal correction to Energy=	0.261340
Thermal correction to Enthalpy=	0.262284
Thermal correction to Gibbs Free Energy=	0.210814
Sum of electronic and zero-point Energies=	-466.379193
Sum of electronic and thermal Energies=	-466.367021
Sum of electronic and thermal Enthalpies=	-466.366077
Sum of electronic and thermal Free Energies=	-466.417547
Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.248803 (Hartree/Particle)
Thermal correction to Energy=	0.261005
Thermal correction to Enthalpy=	0.261950
Thermal correction to Gibbs Free Energy=	0.210379
Sum of electronic and zero-point Energies=	-466.385528
Sum of electronic and thermal Energies=	-466.373325
Sum of electronic and thermal Enthalpies=	-466.372381
Sum of electronic and thermal Free Energies=	-466.423952
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.248830 (Hartree/Particle)
Thermal correction to Energy=	0.261028
Thermal correction to Enthalpy=	0.261972
Thermal correction to Gibbs Free Energy=	0.210405
Sum of electronic and zero-point Energies=	-466.385195
Sum of electronic and thermal Energies=	-466.372996
Sum of electronic and thermal Enthalpies=	-466.372052

Sum of electronic and thermal Free Energies=	-466.423619

Name of anion	Isomenthone-C4-H

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

C	2.93569900	0.27789200	1.21079000
C	2.13330300	-0.60132400	0.23888200
C	2.66570800	-0.46916000	-1.19712300
C	0.60616700	-0.36652500	0.35462400
C	0.10524700	0.99351600	-0.14358600
C	-0.24520800	-1.47747000	-0.29964200
O	0.82073700	1.95630100	-0.31427900
C	-1.39368100	1.06916900	-0.42656900
C	-1.74266100	-1.38908900	0.07379200
C	-2.21467800	0.05323400	0.38027000
C	-3.72000100	0.21953800	0.15399200
H	2.57911000	0.15645500	2.23896500
H	3.99352100	-0.00130000	1.19322400
H	2.85212600	1.33136900	0.94314000
H	2.28505300	-1.64436800	0.54800400
H	2.13822700	-1.12891200	-1.89182400
H	3.72468300	-0.74038700	-1.23239300
H	2.56963600	0.55710300	-1.55610000
H	0.15440800	-2.45403600	-0.01288600
H	-0.13392700	-1.41358800	-1.38677100
H	-1.71363400	2.09881700	-0.24835400
H	-1.52613600	0.88521900	-1.50270500
H	-2.34031100	-1.79766500	-0.74839900
H	-1.95098200	-2.01996400	0.94380400
H	-2.01969600	0.25429400	1.44134600
H	-4.05951100	1.21762700	0.44523100
H	-3.97519700	0.07262100	-0.90083000
H	-4.28827600	-0.51045100	0.73814400

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

Zero-point correction=	0.246811 (Hartree/Particle)
Thermal correction to Energy=	0.258925
Thermal correction to Enthalpy=	0.259869
Thermal correction to Gibbs Free Energy=	0.208934
Sum of electronic and zero-point Energies=	-466.420473
Sum of electronic and thermal Energies=	-466.408359
Sum of electronic and thermal Enthalpies=	-466.407415
Sum of electronic and thermal Free Energies=	-466.458349

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction=	0.247204 (Hartree/Particle)
Thermal correction to Energy=	0.259226
Thermal correction to Enthalpy=	0.260170
Thermal correction to Gibbs Free Energy=	0.209937
Sum of electronic and zero-point Energies=	-466.508375
Sum of electronic and thermal Energies=	-466.496353
Sum of electronic and thermal Enthalpies=	-466.495409
Sum of electronic and thermal Free Energies=	-466.545642

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.247187 (Hartree/Particle)
Thermal correction to Energy=	0.259218
Thermal correction to Enthalpy=	0.260162
Thermal correction to Gibbs Free Energy=	0.209817
Sum of electronic and zero-point Energies=	-466.505669
Sum of electronic and thermal Energies=	-466.493638
Sum of electronic and thermal Enthalpies=	-466.492694
Sum of electronic and thermal Free Energies=	-466.543039

Name of cationic radical	Isomenthone

Cartesian Coordinates optimized at B3LYP/6-311G (d,p) (gas)			
C	-2.99359800	0.20520300	-1.06522500
C	-2.12053800	-0.64670500	-0.13766200
C	-2.47317400	-0.37925600	1.32947800
C	-0.61565900	-0.39597500	-0.42866300
C	-0.13243000	0.97382800	0.03484200
C	0.25511800	-1.50513200	0.18492700
O	-0.83559600	1.96027100	0.06339900
C	1.32570600	1.05791800	0.43875900
C	1.74059700	-1.37353800	-0.17870000
C	2.19993500	0.08835700	-0.37261900
C	3.67640500	0.25248400	0.00059900
H	-2.82359200	-0.02832200	-2.11951500
H	-4.05817300	0.05729300	-0.85919700
H	-2.78170300	1.27796800	-0.92429700
H	-2.32643100	-1.72519900	-0.35760300
H	-1.84060200	-0.95116100	2.01408700
H	-3.51463500	-0.64455700	1.53992400
H	-2.35854100	0.68590500	1.57614300
H	-0.47606600	-0.41032200	-1.54220700
H	-0.11810000	-2.49456300	-0.14301300
H	0.13911500	-1.49356400	1.28729800
H	1.68446200	2.10038200	0.32415100
H	1.40702900	0.84307300	1.52357000
H	2.34310900	-1.86197800	0.61139100
H	1.95478900	-1.94059000	-1.10414400
H	2.08395400	0.34876500	-1.45558400
H	4.02958000	1.26980400	-0.20363100
H	3.85529200	0.05458700	1.06330700
H	4.31109800	-0.43280100	-0.57228800

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.258706 (Hartree/Particle)
Thermal correction to Energy=	0.271327
Thermal correction to Enthalpy=	0.272271
Thermal correction to Gibbs Free Energy=	0.219548
Sum of electronic and zero-point Energies=	-466.695347
Sum of electronic and thermal Energies=	-466.682726
Sum of electronic and thermal Enthalpies=	-466.681782
Sum of electronic and thermal Free Energies=	-466.734505

Name of compound	trans-Dihydrocarvone

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

C	-1.96374200	-0.40796200	-0.33044300
C	-1.19042600	-1.44344900	0.50558800
C	0.29825300	-1.45903000	0.14968000
C	0.92925600	-0.07212800	0.35717400
C	0.19339100	1.00012800	-0.45733800
C	-1.30437800	0.96389600	-0.19808900
H	0.82792200	-2.21185300	0.76443200
H	-1.32499400	-1.23245500	1.58474300
H	-1.62720200	-2.44800300	0.34163000
H	-1.89906200	-0.69679200	-1.41221600
H	0.86806300	0.19392300	1.44110900
H	0.58437200	2.01112100	-0.22311800
H	0.37017600	0.85402000	-1.54466700
H	0.44633900	-1.78193300	-0.90264300
C	-3.43359000	-0.34998100	0.07708500
H	-3.96546800	0.43641100	-0.47733600
H	-3.94344200	-1.29992400	-0.11135900
H	-3.55230200	-0.10734400	1.14072400
O	-1.91293300	1.97733900	0.05415800
C	2.39748500	-0.08852500	-0.08895600
C	3.33110600	0.76248200	0.72135700
H	4.31965100	0.83509600	0.24164800
H	2.95535000	1.78448900	0.85695900
H	3.49379700	0.33964100	1.72204400
O	2.77576600	-0.74096100	-1.03394300

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

Zero-point correction=	0.215100 (Hartree/Particle)
Thermal correction to Energy=	0.226747
Thermal correction to Enthalpy=	0.227691
Thermal correction to Gibbs Free Energy=	0.176608
Sum of electronic and zero-point Energies=	-501.767947
Sum of electronic and thermal Energies=	-501.756300
Sum of electronic and thermal Enthalpies=	-501.755355
Sum of electronic and thermal Free Energies=	-501.806439

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction=	0.214947 (Hartree/Particle)
Thermal correction to Energy=	0.226534
Thermal correction to Enthalpy=	0.227478
Thermal correction to Gibbs Free Energy=	0.177075
Sum of electronic and zero-point Energies=	-501.779094
Sum of electronic and thermal Energies=	-501.767507
Sum of electronic and thermal Enthalpies=	-501.766563
Sum of electronic and thermal Free Energies=	-501.816966

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction=	0.214871 (Hartree/Particle)
Thermal correction to Energy=	0.226485
Thermal correction to Enthalpy=	0.227429

Thermal correction to Gibbs Free Energy=	0.176882
Sum of electronic and zero-point Energies=	-501.778616
Sum of electronic and thermal Energies=	-501.767002
Sum of electronic and thermal Enthalpies=	-501.766058
Sum of electronic and thermal Free Energies=	-501.816605

Name of radical	trans-Dihydrocarvone-C1-H

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

C	-1.98582400	-0.39536500	-0.32024900
C	-1.20463000	-1.42666800	0.52891900
C	0.28901700	-1.46563400	0.18858400
C	0.94272600	-0.08584500	0.34636600
C	0.19104800	0.97052900	-0.50864900
C	-1.30323300	0.96594300	-0.20919000
H	0.79857400	-2.18962200	0.83218500
H	-1.33808700	-1.17998500	1.59002100
H	-1.64814800	-2.41652600	0.38400000
H	0.88449100	0.22950500	1.39561000
H	0.56547000	1.98149600	-0.33828800
H	0.33643100	0.72147000	-1.56694300
H	0.44117700	-1.80597200	-0.83986700
C	-3.46936900	-0.33149000	0.03456700
H	-3.99207600	0.39580100	-0.58864700
H	-3.93929600	-1.30898300	-0.10282100
H	-3.60777600	-0.02592000	1.07462000
O	-1.89098700	1.97539000	0.10724200
C	2.41513500	-0.09313900	-0.08198000
C	3.36094200	0.79510800	0.69962200
H	4.32995000	0.83695700	0.20405500
H	2.95035600	1.80284400	0.81257100
H	3.48726700	0.38891200	1.70931300
O	2.79003000	-0.76690700	-1.01492100

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

Zero-point correction=	0.201392 (Hartree/Particle)
Thermal correction to Energy=	0.213193
Thermal correction to Enthalpy=	0.214137
Thermal correction to Gibbs Free Energy=	0.162251
Sum of electronic and zero-point Energies=	-501.137143
Sum of electronic and thermal Energies=	-501.125342
Sum of electronic and thermal Enthalpies=	-501.124398
Sum of electronic and thermal Free Energies=	-501.176284

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction=	0.201322 (Hartree/Particle)
Thermal correction to Energy=	0.213109
Thermal correction to Enthalpy=	0.214054
Thermal correction to Gibbs Free Energy=	0.162212
Sum of electronic and zero-point Energies=	-501.149041
Sum of electronic and thermal Energies=	-501.137254
Sum of electronic and thermal Enthalpies=	-501.136309
Sum of electronic and thermal Free Energies=	-501.188151

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)		
Zero-point correction=	0.201312	(Hartree/Particle)
Thermal correction to Energy=	0.213092	
Thermal correction to Enthalpy=	0.214037	
Thermal correction to Gibbs Free Energy=	0.162248	
Sum of electronic and zero-point Energies=	-501.148453	
Sum of electronic and thermal Energies=	-501.136672	
Sum of electronic and thermal Enthalpies=	-501.135728	
Sum of electronic and thermal Free Energies=	-501.187517	

Name of anion	trans-Dihydrocarvone-C4-H

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	-1.98582400	-0.39536500	-0.32024900
C	-1.20463000	-1.42666800	0.52891900
C	0.28901700	-1.46563400	0.18858400
C	0.94272600	-0.08584500	0.34636600
C	0.19104800	0.97052900	-0.50864900
C	-1.30323300	0.96594300	-0.20919000
H	0.79857400	-2.18962200	0.83218500
H	-1.33808700	-1.17998500	1.59002100
H	-1.64814800	-2.41652600	0.38400000
H	-1.87554400	-0.69847000	-1.37231900
H	0.56547000	1.98149600	-0.33828800
H	0.33643100	0.72147000	-1.56694300
H	0.44117700	-1.80597200	-0.83986700
C	-3.46936900	-0.33149000	0.03456700
H	-3.99207600	0.39580100	-0.58864700
H	-3.93929600	-1.30898300	-0.10282100
H	-3.60777600	-0.02592000	1.07462000
O	-1.89098700	1.97539000	0.10724200
C	2.41513500	-0.09313900	-0.08198000
C	3.36094200	0.79510800	0.69962200
H	4.32995000	0.83695700	0.20405500
H	2.95035600	1.80284400	0.81257100
H	3.48726700	0.38891200	1.70931300
O	2.79003000	-0.76690700	-1.01492100

Frequency and Energy at B3LYP/6-311G (d,p) (gas)		
Zero-point correction=	0.199784	(Hartree/Particle)
Thermal correction to Energy=	0.210454	
Thermal correction to Enthalpy=	0.211398	
Thermal correction to Gibbs Free Energy=	0.163342	
Sum of electronic and zero-point Energies=	-501.192362	
Sum of electronic and thermal Energies=	-501.181692	
Sum of electronic and thermal Enthalpies=	-501.180748	
Sum of electronic and thermal Free Energies=	-501.228804	

Frequency and Energy at B3LYP/6-311G (d,p) (water)		
Zero-point correction=	0.200912	(Hartree/Particle)
Thermal correction to Energy=	0.212184	
Thermal correction to Enthalpy=	0.213128	
Thermal correction to Gibbs Free Energy=	0.163803	

Sum of electronic and zero-point Energies=	-501.275772
Sum of electronic and thermal Energies=	-501.264500
Sum of electronic and thermal Enthalpies=	-501.263556
Sum of electronic and thermal Free Energies=	-501.312880

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.200904 (Hartree/Particle)
Thermal correction to Energy=	0.212162
Thermal correction to Enthalpy=	0.213107
Thermal correction to Gibbs Free Energy=	0.163788
Sum of electronic and zero-point Energies=	-501.272826
Sum of electronic and thermal Energies=	-501.261567
Sum of electronic and thermal Enthalpies=	-501.260623
Sum of electronic and thermal Free Energies=	-501.309941

Name of cationic radical	trans-Dihydrocarvone

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

C	-1.94078200	0.38987700	0.41733800
C	-1.07926700	1.54341100	-0.12555700
C	0.39797900	1.35779300	0.23417100
C	0.93496400	0.03186800	-0.33578100
C	0.10480800	-1.16137800	0.14893600
C	-1.38216800	-0.95110600	-0.06083800
H	0.98986600	2.20830100	-0.15380100
H	-1.20052000	1.61983900	-1.22405800
H	-1.44948700	2.50368500	0.28349800
H	-1.87630100	0.38487000	1.53695700
H	0.88705300	0.06958400	-1.45170600
H	0.42513700	-2.09287200	-0.36237500
H	0.29968300	-1.34890500	1.23000500
H	0.52592200	1.37270000	1.33625200
C	-3.40288900	0.55017000	0.00916500
H	-3.99807600	-0.31588900	0.33370400
H	-3.84927800	1.44930100	0.44463800
H	-3.51821900	0.60750500	-1.08049800
O	-2.07215700	-1.82150500	-0.53907400
C	2.39141800	-0.13752000	0.11698200
C	3.43271000	0.30980400	-0.86715100
H	4.43375000	0.32009500	-0.40822500
H	3.48645600	-0.37067100	-1.72840700
H	3.23822400	1.31593800	-1.25737800
O	2.68030100	-0.59362000	1.19879900

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.213167 (Hartree/Particle)
Thermal correction to Energy=	0.225075
Thermal correction to Enthalpy=	0.226019
Thermal correction to Gibbs Free Energy=	0.174224
Sum of electronic and zero-point Energies=	-501.458450
Sum of electronic and thermal Energies=	-501.446542
Sum of electronic and thermal Enthalpies=	-501.445598
Sum of electronic and thermal Free Energies=	-501.497393

Name of compound	Terpinen-4-ol

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

C	-0.94250000	3.39010000	0.74760000
C	-0.15870000	2.12270000	1.13280000
C	-1.04320000	0.88510000	0.89880000
C	1.20720000	2.02320000	0.39810000
C	5.48310000	1.69060000	-0.63440000
C	2.15150000	3.18720000	0.77380000
C	1.93680000	0.69950000	0.71740000
C	3.45760000	3.15140000	-0.03270000
C	3.36630000	0.68110000	0.22580000
C	4.06800000	1.76950000	-0.12290000
O	0.91130000	2.07630000	-1.01010000
H	-0.41350000	4.31040000	1.01390000
H	-1.13540000	3.41010000	-0.32950000
H	-1.90700000	3.40720000	1.26810000
H	0.07420000	2.17760000	2.20700000
H	-0.60020000	-0.03020000	1.30480000
H	-2.01680000	1.01790000	1.38420000
H	-1.21530000	0.73560000	-0.17230000
H	6.17190000	2.23870000	0.02350000
H	5.83380000	0.65600000	-0.70740000
H	5.57290000	2.15110000	-1.62840000
H	2.38110000	3.11910000	1.84600000
H	1.65520000	4.14750000	0.60880000
H	1.91210000	0.51210000	1.80230000
H	1.38680000	-0.13000000	0.25700000
H	4.18520000	3.84650000	0.40950000
H	3.27680000	3.53470000	-1.04930000
H	3.83910000	-0.29850000	0.15100000
H	1.69540000	1.74480000	-1.47640000

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

Zero-point correction=	0.261674 (Hartree/Particle)
Thermal correction to Energy=	0.273949
Thermal correction to Enthalpy=	0.274893
Thermal correction to Gibbs Free Energy=	0.224699
Sum of electronic and zero-point Energies=	-466.990439
Sum of electronic and thermal Energies=	-466.978165
Sum of electronic and thermal Enthalpies=	-466.977220
Sum of electronic and thermal Free Energies=	-467.027414

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction=	0.261082 (Hartree/Particle)
Thermal correction to Energy=	0.273417
Thermal correction to Enthalpy=	0.274361
Thermal correction to Gibbs Free Energy=	0.224013
Sum of electronic and zero-point Energies=	-466.994884
Sum of electronic and thermal Energies=	-466.982550
Sum of electronic and thermal Enthalpies=	-466.981606

Sum of electronic and thermal Free Energies=	-467.031954
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.261112 (Hartree/Particle)
Thermal correction to Energy=	0.273443
Thermal correction to Enthalpy=	0.274387
Thermal correction to Gibbs Free Energy=	0.224045
Sum of electronic and zero-point Energies=	-466.994650
Sum of electronic and thermal Energies=	-466.982319
Sum of electronic and thermal Enthalpies=	-466.981375
Sum of electronic and thermal Free Energies=	-467.031717

Name of radical	Terpinen-4-ol-C7-H		
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	-2.85782000	-1.24243000	0.00436500
C	-2.09732100	0.01459600	-0.45124400
C	-2.84314100	1.26782400	0.03635600
C	-0.61005500	0.00081200	-0.00310200
C	3.79403500	0.06120000	0.15111300
C	0.16715600	-1.18171600	-0.61842700
C	0.11943500	1.30261200	-0.39340800
C	1.60704900	-1.25676800	-0.09514100
C	1.61576000	1.22154200	-0.20610500
C	2.30419600	0.08434200	-0.06250500
O	-0.62641300	-0.12725200	1.43218400
H	-2.45007100	-2.15987800	-0.42481200
H	-2.82539500	-1.33354700	1.09203500
H	-3.90542100	-1.17793500	-0.30239100
H	-2.08520500	0.02865400	-1.54910900
H	-2.43834300	2.18872300	-0.38893200
H	-3.89734500	1.21398700	-0.24861700
H	-2.78887100	1.34086500	1.12512500
H	4.29751200	-0.47704100	-0.66046300
H	4.21204700	1.06861400	0.20341700
H	4.05106200	-0.46329500	1.07914700
H	0.17961400	-1.06040700	-1.70779900
H	-0.34446600	-2.12019000	-0.40072800
H	-0.27437000	2.12369800	0.21253400
H	2.18829600	-1.95368500	-0.71048500
H	1.61472200	-1.69061000	0.91429200
H	2.15142700	2.16818500	-0.18270400
H	0.24227300	0.13184700	1.75726500

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.247526 (Hartree/Particle)
Thermal correction to Energy=	0.260277
Thermal correction to Enthalpy=	0.261221
Thermal correction to Gibbs Free Energy=	0.208752
Sum of electronic and zero-point Energies=	-466.363140
Sum of electronic and thermal Energies=	-466.350390

Sum of electronic and thermal Enthalpies=	-466.349446
Sum of electronic and thermal Free Energies=	-466.401914
Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.247167 (Hartree/Particle)
Thermal correction to Energy=	0.259841
Thermal correction to Enthalpy=	0.260785
Thermal correction to Gibbs Free Energy=	0.208712
Sum of electronic and zero-point Energies=	-466.367694
Sum of electronic and thermal Energies=	-466.355020
Sum of electronic and thermal Enthalpies=	-466.354076
Sum of electronic and thermal Free Energies=	-466.406149
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.247209 (Hartree/Particle)
Thermal correction to Energy=	0.259870
Thermal correction to Enthalpy=	0.260814
Thermal correction to Gibbs Free Energy=	0.208783
Sum of electronic and zero-point Energies=	-466.367432
Sum of electronic and thermal Energies=	-466.354771
Sum of electronic and thermal Enthalpies=	-466.353827
Sum of electronic and thermal Free Energies=	-466.405858

Name of anion	Terpinen-4-ol-O-H		
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	-2.85782000	-1.24243000	0.00436500
C	-2.09732100	0.01459600	-0.45124400
C	-2.84314100	1.26782400	0.03635600
C	-0.61005500	0.00081200	-0.00310200
C	3.79403500	0.06120000	0.15111300
C	0.16715600	-1.18171600	-0.61842700
C	0.11943500	1.30261200	-0.39340800
C	1.60704900	-1.25676800	-0.09514100
C	1.61576000	1.22154200	-0.20610500
C	2.30419600	0.08434200	-0.06250500
O	-0.62641300	-0.12725200	1.43218400
H	-2.45007100	-2.15987800	-0.42481200
H	-2.82539500	-1.33354700	1.09203500
H	-3.90542100	-1.17793500	-0.30239100
H	-2.08520500	0.02865400	-1.54910900
H	-2.43834300	2.18872300	-0.38893200
H	-3.89734500	1.21398700	-0.24861700
H	-2.78887100	1.34086500	1.12512500
H	4.29751200	-0.47704100	-0.66046300
H	4.21204700	1.06861400	0.20341700
H	4.05106200	-0.46329500	1.07914700
H	0.17961400	-1.06040700	-1.70779900
H	-0.34446600	-2.12019000	-0.40072800
H	-0.11192100	1.55794700	-1.43665200
H	-0.27437000	2.12369800	0.21253400
H	2.18829600	-1.95368500	-0.71048500
H	1.61472200	-1.69061000	0.91429200

H	2.15142700	2.16818500	-0.18270400

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.245374 (Hartree/Particle)
Thermal correction to Energy=	0.257327
Thermal correction to Enthalpy=	0.258271
Thermal correction to Gibbs Free Energy=	0.208792
Sum of electronic and zero-point Energies=	-466.396058
Sum of electronic and thermal Energies=	-466.384105
Sum of electronic and thermal Enthalpies=	-466.383161
Sum of electronic and thermal Free Energies=	-466.432640
Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction= (Hartree/Particle)	0.245901
Thermal correction to Energy=	0.257916
Thermal correction to Enthalpy=	0.258860
Thermal correction to Gibbs Free Energy=	0.209288
Sum of electronic and zero-point Energies=	-466.481370
Sum of electronic and thermal Energies=	-466.469355
Sum of electronic and thermal Enthalpies=	-466.468410
Sum of electronic and thermal Free Energies=	-466.517983
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.245905 (Hartree/Particle)
Thermal correction to Energy=	0.257917
Thermal correction to Enthalpy=	0.258861
Thermal correction to Gibbs Free Energy=	0.209302
Sum of electronic and zero-point Energies=	-466.478364
Sum of electronic and thermal Energies=	-466.466351
Sum of electronic and thermal Enthalpies=	-466.465407
Sum of electronic and thermal Free Energies=	-466.514966

Name of cationic radical	Terpinen-4-ol	
Cartesian Coordinates optimized at B3LYP/6-311G (d,p) (gas)		
C	-2.81769300	-1.25110800	-0.10938300
C	-2.07610600	0.02805700	-0.51463200
C	-2.83300500	1.25481000	0.00728300
C	-0.60789500	0.00963700	0.01451900
C	3.79646900	0.04916700	0.04133600
C	0.17823000	-1.20362900	-0.52876000
C	0.13698000	1.32703300	-0.30367500
C	1.61867900	-1.25000800	-0.00770900
C	1.62553300	1.23849500	-0.18329500
C	2.30385300	0.08869400	-0.06385200
O	-0.74517800	-0.11415200	1.44614400
H	-2.39618400	-2.14028200	-0.58737800
H	-2.75498200	-1.39876300	0.97931100
H	-3.87760500	-1.20175200	-0.37687400
H	-2.03111500	0.07995000	-1.62998600
H	-2.45311400	2.18808300	-0.41675600
H	-3.89992900	1.19683100	-0.23139700

H	-2.74321400	1.32102400	1.10160700
H	4.24143900	-0.38893600	-0.86318200
H	4.23805400	1.04639900	0.16519600
H	4.12636100	-0.55707900	0.89521900
H	0.18063400	-1.16775500	-1.63427600
H	-0.34334400	-2.13832100	-0.24499100
H	-0.11777800	1.66345100	-1.32990400
H	-0.24174000	2.11870100	0.37800100
H	2.19303000	-2.00028400	-0.58795500
H	1.62860200	-1.61729900	1.04053300
H	2.13466000	2.20022400	-0.21515800
H	0.12739400	-0.03786100	1.87784900

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.258043 (Hartree/Particle)
Thermal correction to Energy=	0.271045
Thermal correction to Enthalpy=	0.271989
Thermal correction to Gibbs Free Energy=	0.219378
Sum of electronic and zero-point Energies=	-466.687937
Sum of electronic and thermal Energies=	-466.674935
Sum of electronic and thermal Enthalpies=	-466.673991
Sum of electronic and thermal Free Energies=	-466.726602

Name of compound	trans-Carveol

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	-0.32720000	0.34470000	1.86140000
C	0.33570000	1.61990000	1.38980000
C	0.46540000	2.64870000	2.23980000
C	0.70970000	1.69640000	-0.09600000
C	1.73460000	2.78540000	-0.47620000
C	1.21890000	0.36470000	-0.69600000
C	3.16910000	2.51200000	0.02310000
C	2.66930000	0.09910000	-0.38020000
C	5.00540000	0.73760000	0.24130000
C	3.56270000	1.04690000	-0.06430000
O	4.22861217	2.76755668	-0.91127609
H	-0.71970000	0.45730000	2.87630000
H	-1.16100000	0.06010000	1.20520000
H	0.37410000	-0.49920000	1.86530000
H	0.91240000	3.59680000	1.96190000
H	0.10320000	2.57380000	3.26260000
H	-0.23440000	1.93140000	-0.61350000
H	1.42800000	3.77950000	-0.13510000
H	1.76170000	2.83080000	-1.57360000
H	0.60340000	-0.48070000	-0.37120000
H	1.08800000	0.41080000	-1.78890000
H	3.32960828	3.27396825	0.79749735
H	3.00090000	-0.93800000	-0.44180000
H	5.67260000	1.20810000	-0.49500000
H	5.28730000	1.14220000	1.21980000
H	5.19910000	-0.33990000	0.23540000

H	4.12013786	2.12181806	-1.63025226

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.239106 (Hartree/Particle)
Thermal correction to Energy=	0.250778
Thermal correction to Enthalpy=	0.251722
Thermal correction to Gibbs Free Energy=	0.201882
Sum of electronic and zero-point Energies=	-465.772729
Sum of electronic and thermal Energies=	-465.761058
Sum of electronic and thermal Enthalpies=	-465.760113
Sum of electronic and thermal Free Energies=	-465.809953
Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.238676 (Hartree/Particle)
Thermal correction to Energy=	0.250378
Thermal correction to Enthalpy=	0.251322
Thermal correction to Gibbs Free Energy=	0.201441
Sum of electronic and zero-point Energies=	-465.779102
Sum of electronic and thermal Energies=	-465.767400
Sum of electronic and thermal Enthalpies=	-465.766456
Sum of electronic and thermal Free Energies=	-465.816338
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.238695 (Hartree/Particle)
Thermal correction to Energy=	0.250398
Thermal correction to Enthalpy=	0.251343
Thermal correction to Gibbs Free Energy=	0.201448
Sum of electronic and zero-point Energies=	-465.778778
Sum of electronic and thermal Energies=	-465.767075
Sum of electronic and thermal Enthalpies=	-465.766131
Sum of electronic and thermal Free Energies=	-465.816026

Name of radical	trans-Carveol-C7-H		
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	-0.32720000	0.34470000	1.86140000
C	0.33570000	1.61990000	1.38980000
C	0.46540000	2.64870000	2.23980000
C	0.70970000	1.69640000	-0.09600000
C	1.73460000	2.78540000	-0.47620000
C	1.21890000	0.36470000	-0.69600000
C	3.16910000	2.51200000	0.02310000
C	2.66930000	0.09910000	-0.38020000
C	5.00540000	0.73760000	0.24130000
C	3.56270000	1.04690000	-0.06430000
O	4.22861217	2.76755668	-0.91127609
H	-0.71970000	0.45730000	2.87630000
H	-1.16100000	0.06010000	1.20520000
H	0.37410000	-0.49920000	1.86530000
H	0.91240000	3.59680000	1.96190000
H	0.10320000	2.57380000	3.26260000
H	-0.23440000	1.93140000	-0.61350000
H	1.42800000	3.77950000	-0.13510000
H	1.76170000	2.83080000	-1.57360000

H	0.60340000	-0.48070000	-0.37120000
H	1.08800000	0.41080000	-1.78890000
H	3.00090000	-0.93800000	-0.44180000
H	5.67260000	1.20810000	-0.49500000
H	5.28730000	1.14220000	1.21980000
H	5.19910000	-0.33990000	0.23540000
H	4.12013786	2.12181806	-1.63025226

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.224918 (Hartree/Particle)
Thermal correction to Energy=	0.236909
Thermal correction to Enthalpy=	0.237853
Thermal correction to Gibbs Free Energy=	0.186549
Sum of electronic and zero-point Energies=	-465.155550
Sum of electronic and thermal Energies=	-465.143560
Sum of electronic and thermal Enthalpies=	-465.142615
Sum of electronic and thermal Free Energies=	-465.193920

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.224648 (Hartree/Particle)
Thermal correction to Energy=	0.236592
Thermal correction to Enthalpy=	0.237536
Thermal correction to Gibbs Free Energy=	0.186552
Sum of electronic and zero-point Energies=	-465.161485
Sum of electronic and thermal Energies=	-465.149541
Sum of electronic and thermal Enthalpies=	-465.148597
Sum of electronic and thermal Free Energies=	-465.199581

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.224673 (Hartree/Particle)
Thermal correction to Energy=	0.236613
Thermal correction to Enthalpy=	0.237557
Thermal correction to Gibbs Free Energy=	0.186575
Sum of electronic and zero-point Energies=	-465.161161
Sum of electronic and thermal Energies=	-465.149221
Sum of electronic and thermal Enthalpies=	-465.148277
Sum of electronic and thermal Free Energies=	-465.199260

Name of anion	trans-Carveol-O-H

Cartesian Coordinates optimzied at B3LYP/6-311G (d,p)			
C	-3.08042600	0.66500400	-0.51779200
C	-1.98793200	-0.35681100	-0.30199100
C	-1.90401600	-1.42214900	-1.10081000
C	-1.08949000	-0.14026800	0.91598600
C	0.13039300	-1.07138700	1.00519100
C	-0.58162000	1.31257200	1.07783700
C	1.20048500	-0.79674300	-0.06061300
C	0.63051300	1.60973900	0.23328800
C	2.61921700	1.03683100	-1.15958500
C	1.44286200	0.68493100	-0.28765100
O	2.41516500	-1.49211600	0.26361600
H	-3.80314300	0.31440300	-1.25642300
H	-3.61887000	0.87447300	0.41353000

H	-2.67741700	1.61856800	-0.87366800
H	-1.15267900	-2.19220500	-0.98190000
H	-2.60846000	-1.56547000	-1.91313500
H	-1.73144300	-0.34851800	1.78412200
H	-0.15519700	-2.12517700	0.96914400
H	0.59498300	-0.91275800	1.98709800
H	-1.37161300	2.03374500	0.85439000
H	-0.33526300	1.47909000	2.13589500
H	0.90429000	-1.24012700	-1.01582900
H	0.84465700	2.66011800	0.04564400
H	3.54926200	0.62900200	-0.75576600
H	2.50246700	0.60088500	-2.15887400
H	2.72450200	2.11816100	-1.26827000

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.222423 (Hartree/Particle)
Thermal correction to Energy=	0.233922
Thermal correction to Enthalpy=	0.234867
Thermal correction to Gibbs Free Energy=	0.185416
Sum of electronic and zero-point Energies=	-465.172892
Sum of electronic and thermal Energies=	-465.161392
Sum of electronic and thermal Enthalpies=	-465.160448
Sum of electronic and thermal Free Energies=	-465.209899

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.223482 (Hartree/Particle)
Thermal correction to Energy=	0.234877
Thermal correction to Enthalpy=	0.235821
Thermal correction to Gibbs Free Energy=	0.186507
Sum of electronic and zero-point Energies=	-465.264757
Sum of electronic and thermal Energies=	-465.253361
Sum of electronic and thermal Enthalpies=	-465.252417
Sum of electronic and thermal Free Energies=	-465.301731

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.223446 (Hartree/Particle)
Thermal correction to Energy=	0.234843
Thermal correction to Enthalpy=	0.235787
Thermal correction to Gibbs Free Energy=	0.186447
Sum of electronic and zero-point Energies=	-465.261571
Sum of electronic and thermal Energies=	-465.250174
Sum of electronic and thermal Enthalpies=	-465.249230
Sum of electronic and thermal Free Energies=	-465.298570

Name of cationic radical	trans-Carveol

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C 0	-0.327200	0.344700	1.861400
C 0	0.335700	1.619900	1.389800
C 0	0.465400	2.648700	2.239800
C 0	0.709700	1.696400	-0.096000
C 0	1.734600	2.785400	-0.476200
C 0	1.218900	0.364700	-0.696000
C 0	3.169100	2.512000	0.023100

C 0	2.669300	0.099100	-0.380200
C 0	5.005400	0.737600	0.241300
C 0	3.562700	1.046900	-0.064300
O 0	4.228612	2.767557	-0.911276
H 0	-0.719700	0.457300	2.876300
H 0	-1.161000	0.060100	1.205200
H 0	0.374100	-0.499200	1.865300
H 0	0.912400	3.596800	1.961900
H 0	0.103200	2.573800	3.262600
H 0	-0.234400	1.931400	-0.613500
H 0	1.428000	3.779500	-0.135100
H 0	1.761700	2.830800	-1.573600
H 0	0.603400	-0.480700	-0.371200
H 0	1.088000	0.410800	-1.788900
H 0	3.329608	3.273968	0.797497
H 0	3.000900	-0.938000	-0.441800
H 0	5.672600	1.208100	-0.495000
H 0	5.287300	1.142200	1.219800
H 0	5.199100	-0.339900	0.235400
H 0	4.120138	2.121818	-1.630252

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

Zero-point correction=	0.235734 (Hartree/Particle)
Thermal correction to Energy=	0.247652
Thermal correction to Enthalpy=	0.248596
Thermal correction to Gibbs Free Energy=	0.197955
Sum of electronic and zero-point Energies=	-465.476783
Sum of electronic and thermal Energies=	-465.464866
Sum of electronic and thermal Enthalpies=	-465.463922
Sum of electronic and thermal Free Energies=	-465.514562

Name of compound	Nerol	
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)		
C	0.12183900	0.82354300	-0.69391600
C	1.52567700	0.75027400	-0.15123100
C	2.25538000	-0.36898000	-0.26722000
C	2.04259700	1.98723800	0.51472800
C	-0.91172700	0.60440100	0.42508000
C	3.64847300	-0.53053400	0.25197900
C	-2.30937200	0.66878200	-0.11027500
O	4.27799900	-1.70262800	-0.29472600
C	-3.23692000	-0.29034600	0.03171800
C	-3.00537800	-1.58359600	0.74955600
C	-4.61747100	-0.12752800	-0.53223200
H	-0.03622700	0.06803700	-1.49078000
H	-0.04857800	1.80201000	-1.18586500
H	1.85278900	-1.26523600	-0.74079200
H	1.26762900	2.75381500	0.64380200
H	2.44513800	1.77080300	1.51389800
H	2.85214400	2.44309800	-0.07282700
H	-0.78647100	1.37270500	1.21603300
H	-0.71406800	-0.37032400	0.92231800

H	3.66211100	-0.73890200	1.34156400
H	4.29305100	0.34169000	0.03331600
H	-2.54012900	1.59009200	-0.64436600
H	4.26325200	-1.67332700	-1.27061400
H	-1.94686800	-1.73039300	1.01379000
H	-3.58216400	-1.62446100	1.68321900
H	-3.30870200	-2.44332200	0.13826900
H	-5.38392500	-0.28388500	0.23837700
H	-4.78789300	0.86809000	-0.96020500
H	-4.80366800	-0.85899100	-1.33045500

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.258715 (Hartree/Particle)
Thermal correction to Energy=	0.272993
Thermal correction to Enthalpy=	0.273937
Thermal correction to Gibbs Free Energy=	0.216078
Sum of electronic and zero-point Energies=	-466.962765
Sum of electronic and thermal Energies=	-466.948487
Sum of electronic and thermal Enthalpies=	-466.947542
Sum of electronic and thermal Free Energies=	-467.005402

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.258219 (Hartree/Particle)
Thermal correction to Energy=	0.272560
Thermal correction to Enthalpy=	0.273504
Thermal correction to Gibbs Free Energy=	0.215468
Sum of electronic and zero-point Energies=	-466.969377
Sum of electronic and thermal Energies=	-466.955035
Sum of electronic and thermal Enthalpies=	-466.954091
Sum of electronic and thermal Free Energies=	-467.012127

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.258239 (Hartree/Particle)
Thermal correction to Energy=	0.272582
Thermal correction to Enthalpy=	0.273526
Thermal correction to Gibbs Free Energy=	0.215481
Sum of electronic and zero-point Energies=	-466.969069
Sum of electronic and thermal Energies=	-466.954727
Sum of electronic and thermal Enthalpies=	-466.953783
Sum of electronic and thermal Free Energies=	-467.011827

Name of radical	Nerol-C6-H	
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)		
C	0.14364300	0.59043100	-0.62463100
C	1.57170500	0.61927000	-0.12134500
C	2.33992400	-0.47445700	-0.22116700
C	2.02057100	1.92578500	0.48749600
C	-0.92309900	0.66302800	0.49728800
C	3.76689600	-0.65967000	0.20267000
C	-2.32337900	0.67210700	-0.05039100
O	4.56612900	-1.20144100	-0.85533300
C	-3.27554900	-0.25986000	0.07724900
C	-3.12214700	-1.55150200	0.84047800

C	-4.63119700	-0.07196800	-0.55962700
H	-0.02331500	-0.32188000	-1.20358600
H	-0.01545500	1.43343800	-1.31049600
H	1.91108000	-1.36233600	-0.68330600
H	1.76206500	2.76226900	-0.17107000
H	1.51600100	2.11141500	1.44182100
H	3.09324400	1.96164800	0.67651000
H	-0.76775700	1.57915200	1.07981500
H	-0.76528000	-0.17059300	1.18537000
H	3.82906800	-1.40065700	1.00564800
H	-2.57044700	1.55613300	-0.63824600
H	4.46190300	-0.61720500	-1.61344700
H	-2.13200200	-1.68202700	1.27580900
H	-3.85758100	-1.60883400	1.65167200
H	-3.31689100	-2.40814200	0.18474100
H	-5.42596800	-0.09189900	0.19572400
H	-4.69917500	0.87445500	-1.09948000
H	-4.85044500	-0.88352100	-1.26372500

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

Zero-point correction=	0.244864 (Hartree/Particle)
Thermal correction to Energy=	0.259146
Thermal correction to Enthalpy=	0.260090
Thermal correction to Gibbs Free Energy=	0.201797
Sum of electronic and zero-point Energies=	-466.343470
Sum of electronic and thermal Energies=	-466.329188
Sum of electronic and thermal Enthalpies=	-466.328244
Sum of electronic and thermal Free Energies=	-466.386537

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction=	0.244524 (Hartree/Particle)
Thermal correction to Energy=	0.258773
Thermal correction to Enthalpy=	0.259717
Thermal correction to Gibbs Free Energy=	0.201591
Sum of electronic and zero-point Energies=	-466.349997
Sum of electronic and thermal Energies=	-466.335747
Sum of electronic and thermal Enthalpies=	-466.334803
Sum of electronic and thermal Free Energies=	-466.392929

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction=	0.244543 (Hartree/Particle)
Thermal correction to Energy=	0.258793
Thermal correction to Enthalpy=	0.259737
Thermal correction to Gibbs Free Energy=	0.201609
Sum of electronic and zero-point Energies=	-466.349677
Sum of electronic and thermal Energies=	-466.335426
Sum of electronic and thermal Enthalpies=	-466.334482
Sum of electronic and thermal Free Energies=	-466.392610

Name of anion	Nerol-C1-H

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

C	0.14364300	0.59043100	-0.62463100
C	1.57170500	0.61927000	-0.12134500
C	2.33992400	-0.47445700	-0.22116700
C	2.02057100	1.92578500	0.48749600
C	-0.92309900	0.66302800	0.49728800
C	3.76689600	-0.65967000	0.20267000
C	-2.32337900	0.67210700	-0.05039100
O	4.56612900	-1.20144100	-0.85533300
C	-3.27554900	-0.25986000	0.07724900
C	-3.12214700	-1.55150200	0.84047800
C	-4.63119700	-0.07196800	-0.55962700
H	-0.02331500	-0.32188000	-1.20358600
H	1.91108000	-1.36233600	-0.68330600
H	1.76206500	2.76226900	-0.17107000
H	1.51600100	2.11141500	1.44182100
H	3.09324400	1.96164800	0.67651000
H	-0.76775700	1.57915200	1.07981500
H	-0.76528000	-0.17059300	1.18537000
H	3.82906800	-1.40065700	1.00564800
H	4.20597500	0.26898300	0.58570300
H	-2.57044700	1.55613300	-0.63824600
H	4.46190300	-0.61720500	-1.61344700
H	-2.13200200	-1.68202700	1.27580900
H	-3.85758100	-1.60883400	1.65167200
H	-3.31689100	-2.40814200	0.18474100
H	-5.42596800	-0.09189900	0.19572400
H	-4.69917500	0.87445500	-1.09948000
H	-4.85044500	-0.88352100	-1.26372500

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

Zero-point correction= (Hartree/Particle)	0.241727
Thermal correction to Energy=	0.256068
Thermal correction to Enthalpy=	0.257012
Thermal correction to Gibbs Free Energy=	0.199362
Sum of electronic and zero-point Energies=	-466.355826
Sum of electronic and thermal Energies=	-466.341485
Sum of electronic and thermal Enthalpies=	-466.340541
Sum of electronic and thermal Free Energies=	-466.398191

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction=	0.241501 (Hartree/Particle)
Thermal correction to Energy=	0.256038
Thermal correction to Enthalpy=	0.256982
Thermal correction to Gibbs Free Energy=	0.199759
Sum of electronic and zero-point Energies=	-466.437157
Sum of electronic and thermal Energies=	-466.422620
Sum of electronic and thermal Enthalpies=	-466.421676
Sum of electronic and thermal Free Energies=	-466.478899

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.241030 (Hartree/Particle)
Thermal correction to Energy=	0.254786
Thermal correction to Enthalpy=	0.255730
Thermal correction to Gibbs Free Energy=	0.200651
Sum of electronic and zero-point Energies=	-466.433768
Sum of electronic and thermal Energies=	-466.420012
Sum of electronic and thermal Enthalpies=	-466.419068
Sum of electronic and thermal Free Energies=	-466.474146

Name of cationic radical	Nerol		
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	0.14364300	0.59043100	-0.62463100
C	1.57170500	0.61927000	-0.12134500
C	2.33992400	-0.47445700	-0.22116700
C	2.02057100	1.92578500	0.48749600
C	-0.92309900	0.66302800	0.49728800
C	3.76689600	-0.65967000	0.20267000
C	-2.32337900	0.67210700	-0.05039100
O	4.56612900	-1.20144100	-0.85533300
C	-3.27554900	-0.25986000	0.07724900
C	-3.12214700	-1.55150200	0.84047800
C	-4.63119700	-0.07196800	-0.55962700
H	-0.02331500	-0.32188000	-1.20358600
H	-0.01545500	1.43343800	-1.31049600
H	1.91108000	-1.36233600	-0.68330600
H	1.76206500	2.76226900	-0.17107000
H	1.51600100	2.11141500	1.44182100
H	3.09324400	1.96164800	0.67651000
H	-0.76775700	1.57915200	1.07981500
H	-0.76528000	-0.17059300	1.18537000
H	3.82906800	-1.40065700	1.00564800
H	4.20597500	0.26898300	0.58570300
H	-2.57044700	1.55613300	-0.63824600
H	4.46190300	-0.61720500	-1.61344700
H	-2.13200200	-1.68202700	1.27580900
H	-3.85758100	-1.60883400	1.65167200
H	-3.31689100	-2.40814200	0.18474100
H	-5.42596800	-0.09189900	0.19572400
H	-4.69917500	0.87445500	-1.09948000
H	-4.85044500	-0.88352100	-1.26372500

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.255628 (Hartree/Particle)
Thermal correction to Energy=	0.270588
Thermal correction to Enthalpy=	0.271532
Thermal correction to Gibbs Free Energy=	0.210721
Sum of electronic and zero-point Energies=	-466.680145
Sum of electronic and thermal Energies=	-466.665185
Sum of electronic and thermal Enthalpies=	-466.664241

Sum of electronic and thermal Free Energies=	-466.725052

Name of compound	2,3-Dehydro-1,4-cineol		
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	4.19532	0.46152	-1.21681
C	3.70072	0.95765	0.15716
C	3.2513	-0.24082	1.02001
C	4.24341	-1.36391	0.98868
C	5.19641	-1.4874	0.05337
C	5.39736	-0.47784	-1.04746
C	2.59122	1.97878	-0.00123
C	2.75551	3.24029	0.40776
C	6.15664	-2.63713	0.04214
C	1.30807	1.52437	-0.6488
C	0.15487	1.46393	0.36913
C	-1.08974	0.92506	-0.26756
C	-1.64111	-0.26933	-0.00428
C	-2.90704	-0.7068	-0.70175
C	-4.14931	-0.247	0.07944
C	-5.42814	-0.67054	-0.57574
C	-6.64679	-0.35894	-0.10555
C	-7.894	-0.81096	-0.80232
C	-1.07908	-1.25471	0.97172
C	-6.85631	0.45388	1.13493
H	4.46985	1.32078	-1.85519
H	3.37805	-0.06844	-1.74302
H	4.56834	1.43988	0.67783
H	2.27042	-0.62516	0.66688
H	3.08845	0.09786	2.06201
H	4.12321	-2.09731	1.78241
H	6.30954	0.11366	-0.8225
H	5.60189	-0.99262	-2.00695
H	1.99669	4.00033	0.30713
H	3.65509	3.60879	0.87361
H	6.07143	-3.26657	0.93701
H	5.98133	-3.28649	-0.82651
H	7.19746	-2.29186	-0.01017
H	1.04189	2.21196	-1.47715
H	1.43043	0.52976	-1.12451
H	0.45968	0.84929	1.2429
H	-0.04326	2.47698	0.77609
H	-1.54273	1.59667	-0.99718
H	-2.94264	-0.30135	-1.73298
H	-2.92227	-1.80837	-0.82026
H	-4.10702	-0.64723	1.11454
H	-4.127	0.85858	0.18793
H	-5.31724	-1.26363	-1.48148
H	-7.68771	-1.40178	-1.70346
H	-8.51131	-1.43396	-0.14098
H	-8.5057	0.04756	-1.11134
H	-0.29011	-0.81638	1.6007

H	-1.85553	-1.64391	1.64318
H	-0.63605	-2.11317	0.44844
H	-6.39695	1.44789	1.03858
H	-7.91588	0.6086	1.36931
H	-6.39807	-0.03111	2.00821

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.238854 (Hartree/Particle)
Thermal correction to Energy=	0.249789
Thermal correction to Enthalpy=	0.250733
Thermal correction to Gibbs Free Energy=	0.203462
Sum of electronic and zero-point Energies=	-465.774445
Sum of electronic and thermal Energies=	-465.763510
Sum of electronic and thermal Enthalpies=	-465.762565
Sum of electronic and thermal Free Energies=	-465.809837

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.238445 (Hartree/Particle)
Thermal correction to Energy=	0.249395
Thermal correction to Enthalpy=	0.250339
Thermal correction to Gibbs Free Energy=	0.203029
Sum of electronic and zero-point Energies=	-465.778936
Sum of electronic and thermal Energies=	-465.767986
Sum of electronic and thermal Enthalpies=	-465.767042
Sum of electronic and thermal Free Energies=	-465.814352

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.238449 (Hartree/Particle)
Thermal correction to Energy=	0.249405
Thermal correction to Enthalpy=	0.250350
Thermal correction to Gibbs Free Energy=	0.203019
Sum of electronic and zero-point Energies=	-465.778693
Sum of electronic and thermal Energies=	-465.767737
Sum of electronic and thermal Enthalpies=	-465.766792
Sum of electronic and thermal Free Energies=	-465.814123

Name of radical	2,3-Dehydro-1,4-cineol-C8-H

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	1.35640800	-0.44901900	1.40618100
C	0.02974900	-0.65038400	1.42726300
C	-0.50657400	-0.19060200	0.05591300
C	-0.01957100	-1.24358700	-1.00108100
C	1.51182700	-1.01151800	-1.02079300
C	1.68740700	0.14054900	0.02372100
C	2.87978000	1.03952600	-0.10666200
C	-1.90761200	0.26223000	-0.02586000
C	-2.99436800	-0.73208100	0.08900800
C	-2.21142900	1.69186500	-0.21476900
O	0.44526800	0.91317700	-0.22752300
H	2.10204600	-0.63589000	2.14915700
H	-0.60746700	-1.04296500	2.19100400
H	-0.29047800	-2.26804400	-0.71831200
H	-0.47441600	-1.03498300	-1.98064700

H	1.85827600	-0.69142200	-2.01394400
H	2.07902300	-1.90968200	-0.74599800
H	3.82100000	0.48612700	-0.01844500
H	2.87794300	1.55953100	-1.07563500
H	2.87037800	1.82217000	0.66589100
H	-3.41863200	-0.95615200	-0.90289700
H	-2.66278600	-1.68339300	0.52447700
H	-3.81955400	-0.35536700	0.71131100
H	-3.11420500	1.85498700	-0.81559800
H	-1.37497900	2.22096600	-0.70578500
H	-2.36200600	2.18682900	0.75807100

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.224125 (Hartree/Particle)
Thermal correction to Energy=	0.235651
Thermal correction to Enthalpy=	0.236595
Thermal correction to Gibbs Free Energy=	0.186588
Sum of electronic and zero-point Energies=	-465.126987
Sum of electronic and thermal Energies=	-465.115460
Sum of electronic and thermal Enthalpies=	-465.114516
Sum of electronic and thermal Free Energies=	-465.164523

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.223814 (Hartree/Particle)
Thermal correction to Energy=	0.235370
Thermal correction to Enthalpy=	0.236314
Thermal correction to Gibbs Free Energy=	0.186048
Sum of electronic and zero-point Energies=	-465.131067
Sum of electronic and thermal Energies=	-465.119511
Sum of electronic and thermal Enthalpies=	-465.118567
Sum of electronic and thermal Free Energies=	-465.168833

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.223823 (Hartree/Particle)
Thermal correction to Energy=	0.235373
Thermal correction to Enthalpy=	0.236318
Thermal correction to Gibbs Free Energy=	0.186048
Sum of electronic and zero-point Energies=	-465.131367
Sum of electronic and thermal Energies=	-465.119816
Sum of electronic and thermal Enthalpies=	-465.118872
Sum of electronic and thermal Free Energies=	-465.169142

Name of anion	2,3-Dehydro-1,4-cineol-C4-H

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	-1.22894700	-0.30018700	1.43609800
C	0.08499900	-0.08565100	1.43320900
C	0.46423000	0.17736100	-0.02715200
C	-0.09239800	1.61020400	-0.35525500
C	-1.62319000	1.35356900	-0.35449500
C	-1.68063400	-0.17692100	-0.01859200
C	-2.91464400	-0.93086900	-0.45349700
C	1.87859500	-0.14428300	-0.50124900

C	2.92022700	0.78433000	0.13976100
C	2.22674400	-1.62176900	-0.27488900
O	-0.50705900	-0.63730700	-0.71884800
H	-1.88996900	-0.42195000	2.28471200
H	0.74676100	0.01011500	2.28349200
H	0.22155000	2.36213400	0.37035000
H	-2.05392200	1.52520000	-1.34369900
H	-2.16949500	1.96214300	0.36883200
H	-3.80074400	-0.54425600	0.05741400
H	-3.06388700	-0.82448100	-1.53059500
H	-2.81526800	-1.99338300	-0.22056600
H	1.87844500	0.04103300	-1.58282100
H	3.91564700	0.56894200	-0.25753300
H	2.70587000	1.83790300	-0.05628700
H	2.96587500	0.64604100	1.22464900
H	3.20667100	-1.85521300	-0.70112400
H	1.48201200	-2.26942500	-0.73887700
H	2.26062200	-1.85989400	0.79295800

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.221608 (Hartree/Particle)
Thermal correction to Energy=	0.232623
Thermal correction to Enthalpy=	0.233567
Thermal correction to Gibbs Free Energy=	0.186339
Sum of electronic and zero-point Energies=	-465.129045
Sum of electronic and thermal Energies=	-465.118030
Sum of electronic and thermal Enthalpies=	-465.117086
Sum of electronic and thermal Free Energies=	-465.164315

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.222164 (Hartree/Particle)
Thermal correction to Energy=	0.233144
Thermal correction to Enthalpy=	0.234088
Thermal correction to Gibbs Free Energy=	0.186915
Sum of electronic and zero-point Energies=	-465.213247
Sum of electronic and thermal Energies=	-465.202268
Sum of electronic and thermal Enthalpies=	-465.201323
Sum of electronic and thermal Free Energies=	-465.248497

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.222147 (Hartree/Particle)
Thermal correction to Energy=	0.233122
Thermal correction to Enthalpy=	0.234066
Thermal correction to Gibbs Free Energy=	0.186910
Sum of electronic and zero-point Energies=	-465.210315
Sum of electronic and thermal Energies=	-465.199340
Sum of electronic and thermal Enthalpies=	-465.198396
Sum of electronic and thermal Free Energies=	-465.245552

Name of cationic radical	2,3-Dehydro-1,4-cineol

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	-1.23419700	-0.40794900	1.42166000
C	0.09191400	-0.19846700	1.42955400

C	0.48429300	0.19211500	-0.00546400
C	-0.08117800	1.63231600	-0.25158400
C	-1.61265100	1.39170300	-0.26400200
C	-1.70803900	-0.15140600	-0.02012800
C	-2.92319700	-0.87420100	-0.51752700
C	1.88169500	-0.12604900	-0.52584600
C	2.92387400	0.78871500	0.12444200
C	2.21515100	-1.60351800	-0.29699000
O	-0.50898100	-0.60564800	-0.76713700
H	-1.90102500	-0.68858300	2.20847300
H	0.80291400	-0.26089800	2.22589000
H	0.22754600	2.33626500	0.53168600
H	0.27096700	2.02959900	-1.21424700
H	-2.05525700	1.65982800	-1.23389700
H	-2.13663100	1.96678800	0.50959200
H	-3.84216900	-0.49405900	-0.05832400
H	-3.02029800	-0.77770100	-1.60875100
H	-2.85628200	-1.95126900	-0.30603100
H	1.87486000	0.06025100	-1.63245600
H	3.93049800	0.55342000	-0.24064700
H	2.73343400	1.84387600	-0.09799600
H	2.94113300	0.67594300	1.21404400
H	3.14396100	-1.88674000	-0.80047200
H	1.40854800	-2.24031600	-0.69064400
H	2.32366300	-1.84077900	0.76617700

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.237967 (Hartree/Particle)
Thermal correction to Energy=	0.249311
Thermal correction to Enthalpy=	0.250255
Thermal correction to Gibbs Free Energy=	0.201557
Sum of electronic and zero-point Energies=	-465.464811
Sum of electronic and thermal Energies=	-465.453468
Sum of electronic and thermal Enthalpies=	-465.452524
Sum of electronic and thermal Free Energies=	-465.501221

Name of compound	Lavandulyl acetate

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	-1.17822457	0.21676636	0.32092541
O	-0.20036698	-0.49026937	0.08122388
O	-0.99859604	1.56180319	0.31651020
C	-2.63262627	-0.17737766	0.63867717
H	-2.89965193	0.19415978	1.60591924
H	-3.28515334	0.24330881	-0.09761850
H	-2.72359897	-1.24345483	0.62850624
C	0.36161446	1.88695877	0.01817944
H	1.00225639	1.45435006	0.75799538
H	0.61770613	1.49973488	-0.94586139
C	0.53583001	3.41707213	0.01961641
H	0.12770272	3.46261222	1.00767421
C	0.71004555	4.94718548	0.02105339
H	1.25346955	5.24510242	-0.85120567

H	1.24964616	5.24389731	0.89609239
C	2.06594035	3.24285410	0.02284402
C	2.46777509	2.21456504	-1.05081815
H	3.32180065	2.57333626	-1.58637725
H	2.70667250	1.28332935	-0.58110747
H	1.65404884	2.07256924	-1.73095547
C	2.61945690	4.35749527	-0.23032489
H	2.11406584	4.82937326	-1.04690988
H	2.56611723	4.98657784	0.63356746
C	-0.67448466	5.62147735	0.01848936
H	-1.38925933	4.97014837	0.47649342
C	-0.61112076	6.80485459	0.72559850
C	-1.94662283	7.55876327	0.58539894
H	-1.89573085	8.47866412	1.12954269
H	-2.13280159	7.76537545	-0.44782363
H	-2.73924947	6.95606966	0.97706643
C	0.53064934	7.67524329	0.16847683
H	1.46412247	7.33723140	0.56757064
H	0.55001026	7.59791781	-0.89854984
H	0.37112272	8.69533104	0.44931886

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.295756 (Hartree/Particle)
Thermal correction to Energy=	0.312464
Thermal correction to Enthalpy=	0.313408
Thermal correction to Gibbs Free Energy=	0.250063
Sum of electronic and zero-point Energies=	-619.627327
Sum of electronic and thermal Energies=	-619.610619
Sum of electronic and thermal Enthalpies=	-619.609675
Sum of electronic and thermal Free Energies=	-619.673020

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.295050 (Hartree/Particle)
Thermal correction to Energy=	0.312785
Thermal correction to Enthalpy=	0.313729
Thermal correction to Gibbs Free Energy=	0.246368
Sum of electronic and zero-point Energies=	-619.635132
Sum of electronic and thermal Energies=	-619.617397
Sum of electronic and thermal Enthalpies=	-619.616452
Sum of electronic and thermal Free Energies=	-619.683814

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.295077 (Hartree/Particle)
Thermal correction to Energy=	0.312813
Thermal correction to Enthalpy=	0.313757
Thermal correction to Gibbs Free Energy=	0.246395
Sum of electronic and zero-point Energies=	-619.634767
Sum of electronic and thermal Energies=	-619.617031
Sum of electronic and thermal Enthalpies=	-619.616087
Sum of electronic and thermal Free Energies=	-619.683449

Name of radical	Lavandulyl acetate-C13-H
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)	

C	-1.17822457	0.21676636	0.32092541
O	-0.20036698	-0.49026937	0.08122388
O	-0.99859604	1.56180319	0.31651020
C	-2.63262627	-0.17737766	0.63867717
H	-2.89965193	0.19415978	1.60591924
H	-3.28515334	0.24330881	-0.09761850
H	-2.72359897	-1.24345483	0.62850624
C	0.36161446	1.88695877	0.01817944
H	1.00225639	1.45435006	0.75799538
H	0.61770613	1.49973488	-0.94586139
C	0.53583001	3.41707213	0.01961641
H	0.12770272	3.46261222	1.00767421
C	0.71004555	4.94718548	0.02105339
H	1.24964616	5.24389731	0.89609239
C	2.06594035	3.24285410	0.02284402
C	2.46777509	2.21456504	-1.05081815
H	3.32180065	2.57333626	-1.58637725
H	2.70667250	1.28332935	-0.58110747
H	1.65404884	2.07256924	-1.73095547
C	2.61945690	4.35749527	-0.23032489
H	2.11406584	4.82937326	-1.04690988
H	2.56611723	4.98657784	0.63356746
C	-0.67448466	5.62147735	0.01848936
H	-1.38925933	4.97014837	0.47649342
C	-0.61112076	6.80485459	0.72559850
C	-1.94662283	7.55876327	0.58539894
H	-1.89573085	8.47866412	1.12954269
H	-2.13280159	7.76537545	-0.44782363
H	-2.73924947	6.95606966	0.97706643
C	0.53064934	7.67524329	0.16847683
H	1.46412247	7.33723140	0.56757064
H	0.55001026	7.59791781	-0.89854984
H	0.37112272	8.69533104	0.44931886

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.281945 (Hartree/Particle)
Thermal correction to Energy=	0.299768
Thermal correction to Enthalpy=	0.300712
Thermal correction to Gibbs Free Energy=	0.232669
Sum of electronic and zero-point Energies=	-619.002224
Sum of electronic and thermal Energies=	-618.984401
Sum of electronic and thermal Enthalpies=	-618.983457
Sum of electronic and thermal Free Energies=	-619.051500

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.281407 (Hartree/Particle)
Thermal correction to Energy=	0.299268
Thermal correction to Enthalpy=	0.300212
Thermal correction to Gibbs Free Energy=	0.231961
Sum of electronic and zero-point Energies=	-619.010184
Sum of electronic and thermal Energies=	-618.992323
Sum of electronic and thermal Enthalpies=	-618.991379
Sum of electronic and thermal Free Energies=	-619.059630

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.281434 (Hartree/Particle)
Thermal correction to Energy=	0.299295
Thermal correction to Enthalpy=	0.300239
Thermal correction to Gibbs Free Energy=	0.231968
Sum of electronic and zero-point Energies=	-619.009808
Sum of electronic and thermal Energies=	-618.991947
Sum of electronic and thermal Enthalpies=	-618.991003
Sum of electronic and thermal Free Energies=	-619.059274

Name of anion	Lavandulyl acetate-C4-H

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	-2.68222600	-1.31561900	0.21920400
O	-2.75719100	-1.00015300	1.38081500
O	-1.55664500	-1.23333600	-0.52539700
C	-3.82282700	-1.85263000	-0.60861700
H	-3.51328400	-2.74932000	-1.14793700
H	-4.10993600	-1.10343900	-1.35063300
C	-0.37035500	-0.67732700	0.08562500
H	-0.51322400	-0.63368900	1.16542800
H	0.43546800	-1.37447500	-0.14568700
C	-0.05061900	0.69975800	-0.51076300
H	-0.01496900	0.57241800	-1.59825100
C	1.36250900	1.15334400	-0.04477900
H	1.41326600	1.14519900	1.04648400
H	1.48448400	2.19951100	-0.35070600
C	-1.11725800	1.74169900	-0.21051700
C	-1.34230000	2.13709600	1.22852500
H	-2.10177500	2.91754800	1.30138400
H	-1.68073300	1.28253400	1.82147800
H	-0.42475200	2.51709700	1.68970700
C	-1.82379900	2.28592300	-1.20320000
H	-2.57988100	3.04105500	-1.01468100
H	-1.66787000	1.99705800	-2.23736900
C	2.47297800	0.34006300	-0.65283300
H	2.48511900	0.34962800	-1.74269300
C	3.43208900	-0.36509300	-0.03989500
C	4.47778000	-1.10279500	-0.84055900
H	5.48456200	-0.74594700	-0.59299400
H	4.46270100	-2.17522500	-0.61282500
H	4.32845300	-0.98039000	-1.91494800
C	3.58851700	-0.49460100	1.45437200
H	2.80912100	0.01693400	2.01806900
H	3.58208600	-1.54986500	1.75076600
H	4.55530200	-0.08866400	1.77437900

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.281126 (Hartree/Particle)
Thermal correction to Energy=	0.297941
Thermal correction to Enthalpy=	0.298885
Thermal correction to Gibbs Free Energy=	0.235307
Sum of electronic and zero-point Energies=	-619.034837

Sum of electronic and thermal Energies=	-619.018022
Sum of electronic and thermal Enthalpies=	-619.017078
Sum of electronic and thermal Free Energies=	-619.080656
Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.281106 (Hartree/Particle)
Thermal correction to Energy=	0.298181
Thermal correction to Enthalpy=	0.299125
Thermal correction to Gibbs Free Energy=	0.233968
Sum of electronic and zero-point Energies=	-619.125919
Sum of electronic and thermal Energies=	-619.108845
Sum of electronic and thermal Enthalpies=	-619.107901
Sum of electronic and thermal Free Energies=	-619.173058
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.281225 (Hartree/Particle)
Thermal correction to Energy=	0.298213
Thermal correction to Enthalpy=	0.299157
Thermal correction to Gibbs Free Energy=	0.234792
Sum of electronic and zero-point Energies=	-619.122667
Sum of electronic and thermal Energies=	-619.105679
Sum of electronic and thermal Enthalpies=	-619.104735
Sum of electronic and thermal Free Energies=	-619.169100

Name of cationic radical	Lavandulyl acetate	
Cartesian Coordinates optimized at B3LYP/6-311G		
C	-2.73669500	-1.22708000	0.28707300
O	-2.85093200	-0.68400100	1.36232000
O	-1.52626800	-1.33678700	-0.35590600
C	-3.78368900	-1.88858200	-0.53985100
H	-3.35963500	-2.42986600	-1.40052800
H	-4.36596800	-2.60271000	0.06229400
H	-4.49094500	-1.14124500	-0.93462800
C	-0.35922400	-0.68668800	0.23708800
H	-0.53249200	-0.50439800	1.31104700
H	0.42924800	-1.44981200	0.09816600
C	-0.07154400	0.58779900	-0.56845700
H	-0.14224700	0.31100900	-1.65458100
C	1.36371000	1.08008300	-0.27869100
H	1.48173100	1.28129000	0.80752400
H	1.51764600	2.06169200	-0.77793600
C	-1.06551400	1.70162600	-0.28669000
C	-1.30249000	2.06223100	1.14400200
H	-1.79442600	3.03636500	1.25588300
H	-1.96723400	1.31572500	1.62173100
H	-0.37656200	2.09456000	1.72881700
C	-1.69506800	2.32213500	-1.28878800
H	-2.40146500	3.12327300	-1.14015800
H	-1.55631000	2.07904600	-2.32946800
C	2.39925900	0.11697000	-0.77115300
H	2.28821600	-0.15853800	-1.82026700
C	3.40440100	-0.38233000	-0.03552200

C	4.40491200	-1.32980900	-0.62738900
H	5.43092400	-0.96341400	-0.48823400
H	4.34401900	-2.31696300	-0.14927200
H	4.26108100	-1.48344400	-1.70435100
C	3.63341400	-0.05474800	1.40728100
H	2.80144400	0.51662300	1.84487500
H	3.75934900	-0.96223900	2.01197500
H	4.54239000	0.54970200	1.53238200

Frequency and Energy at B3LYP/6-311G (gas)

Zero-point correction=	0.293832 (Hartree/Particle)
Thermal correction to Energy=	0.311632
Thermal correction to Enthalpy=	0.312576
Thermal correction to Gibbs Free Energy=	0.245635
Sum of electronic and zero-point Energies=	-619.338432
Sum of electronic and thermal Energies=	-619.320631
Sum of electronic and thermal Enthalpies=	-619.319687
Sum of electronic and thermal Free Energies=	-619.386629

Name of compound	cis-Carvyl acetate

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

C	-0.31060000	2.28460000	0.51060000
C	5.21530000	-0.31190000	2.49680000
C	2.09650000	2.18400000	0.30080000
C	-1.42970000	2.65790000	1.45990000
C	5.63350000	-1.21240000	0.21680000
C	2.87120000	1.13910000	1.10380000
C	2.88720000	3.44920000	0.03550000
C	4.29150000	0.95870000	0.53790000
C	2.10920000	4.64090000	-0.46030000
C	4.21780000	3.46860000	0.19180000
C	5.05490000	-0.20000000	1.17420000
C	5.05130000	2.29900000	0.65190000
O	-0.48660000	1.82110000	-0.61730000
O	0.90250000	2.52470000	1.07150000
H	5.77080000	-1.13770000	2.93420000
H	4.80220000	0.41100000	3.19610000
H	1.74420000	1.76350000	-0.64730000
H	-1.05320000	3.09200000	2.38740000
H	-2.09830000	3.36570000	0.96050000
H	-2.01570000	1.76100000	1.68530000
H	6.30750000	-0.73260000	-0.50660000
H	6.19490000	-1.99410000	0.73800000
H	4.84090000	-1.69530000	-0.37170000
H	2.32480000	0.18920000	1.09520000
H	2.92450000	1.47190000	2.14750000
H	4.18960000	0.74060000	-0.53530000
H	1.50180000	4.37920000	-1.33740000
H	1.41550000	5.00910000	0.30540000
H	2.77710000	5.46180000	-0.73860000
H	4.75590000	4.38930000	-0.03500000
H	5.36630000	2.45210000	1.69500000

H	5.98180000	2.25310000	0.06940000

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.276074 (Hartree/Particle)
Thermal correction to Energy=	0.291515
Thermal correction to Enthalpy=	0.292459
Thermal correction to Gibbs Free Energy=	0.232130
Sum of electronic and zero-point Energies=	-618.446173
Sum of electronic and thermal Energies=	-618.430732
Sum of electronic and thermal Enthalpies=	-618.429788
Sum of electronic and thermal Free Energies=	-618.490117
Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.275530 (Hartree/Particle)
Thermal correction to Energy=	0.291008
Thermal correction to Enthalpy=	0.291952
Thermal correction to Gibbs Free Energy=	0.231393
Sum of electronic and zero-point Energies=	-618.453349
Sum of electronic and thermal Energies=	-618.437872
Sum of electronic and thermal Enthalpies=	-618.436928
Sum of electronic and thermal Free Energies=	-618.497487
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.275551 (Hartree/Particle)
Thermal correction to Energy=	0.291028
Thermal correction to Enthalpy=	0.291972
Thermal correction to Gibbs Free Energy=	0.231423
Sum of electronic and zero-point Energies=	-618.453018
Sum of electronic and thermal Energies=	-618.437540
Sum of electronic and thermal Enthalpies=	-618.436596
Sum of electronic and thermal Free Energies=	-618.497145

Name of radical	cis-Carvyl acetate-C12-H		
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	2.74718500	-1.08646200	0.19361500
C	-2.86229100	-1.98109400	-0.82763900
C	0.78108200	0.29530400	0.29563700
C	3.97876000	-1.37893200	-0.62856800
C	-4.19913800	-0.51496400	0.65604900
C	-0.36617900	-0.58805600	-0.19027900
C	0.56845700	1.76580900	0.01509400
C	-1.71928800	-0.01386800	0.24487400
C	1.76882800	2.66433400	0.14940300
C	-0.64855700	2.22690500	-0.28579800
C	-2.91521200	-0.91091000	-0.03342700
C	-1.89439900	1.38652500	-0.38758900
O	2.45329200	-1.63613700	1.22502800
O	2.01073800	-0.10882800	-0.38401800
H	-3.74210700	-2.59102200	-1.00269200
H	-1.95415300	-2.29217500	-1.32873700
H	0.95131500	0.13651200	1.36528900
H	4.62539800	-0.49839300	-0.65124500

H	4.51469700	-2.21824400	-0.19054500
H	3.69777200	-1.60489500	-1.65903500
H	-4.54570600	0.47200000	0.33173100
H	-4.99650700	-1.23180600	0.45291500
H	-4.05795600	-0.45863100	1.74141900
H	-0.22821100	-1.59872600	0.19951400
H	-0.31312900	-0.63812800	-1.28307000
H	-1.68069400	0.13312500	1.33454800
H	2.22149500	2.56800300	1.14341300
H	2.54138700	2.39865800	-0.57681400
H	1.49515800	3.71044500	0.00044400
H	-0.77148600	3.29329600	-0.46189700
H	-2.72306700	1.91894600	0.09073500

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

Zero-point correction=	0.262334 (Hartree/Particle)
Thermal correction to Energy=	0.277782
Thermal correction to Enthalpy=	0.278726
Thermal correction to Gibbs Free Energy=	0.217866
Sum of electronic and zero-point Energies=	-617.818491
Sum of electronic and thermal Energies=	-617.803043
Sum of electronic and thermal Enthalpies=	-617.802099
Sum of electronic and thermal Free Energies=	-617.862959

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction=	0.261870 (Hartree/Particle)
Thermal correction to Energy=	0.277335
Thermal correction to Enthalpy=	0.278279
Thermal correction to Gibbs Free Energy=	0.217303
Sum of electronic and zero-point Energies=	-617.825804
Sum of electronic and thermal Energies=	-617.810338
Sum of electronic and thermal Enthalpies=	-617.809394
Sum of electronic and thermal Free Energies=	-617.870370

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction=	0.261912 (Hartree/Particle)
Thermal correction to Energy=	0.277371
Thermal correction to Enthalpy=	0.278315
Thermal correction to Gibbs Free Energy=	0.217394
Sum of electronic and zero-point Energies=	-617.825441
Sum of electronic and thermal Energies=	-617.809982
Sum of electronic and thermal Enthalpies=	-617.809038
Sum of electronic and thermal Free Energies=	-617.869959

Name of anion	cis-Carvyl acetate-C4-H

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

C	2.74718500	-1.08646200	0.19361500
C	-2.86229100	-1.98109400	-0.82763900
C	0.78108200	0.29530400	0.29563700
C	3.97876000	-1.37893200	-0.62856800
C	-4.19913800	-0.51496400	0.65604900
C	-0.36617900	-0.58805600	-0.19027900

C	0.56845700	1.76580900	0.01509400
C	-1.71928800	-0.01386800	0.24487400
C	1.76882800	2.66433400	0.14940300
C	-0.64855700	2.22690500	-0.28579800
C	-2.91521200	-0.91091000	-0.03342700
C	-1.89439900	1.38652500	-0.38758900
O	2.45329200	-1.63613700	1.22502800
O	2.01073800	-0.10882800	-0.38401800
H	-3.74210700	-2.59102200	-1.00269200
H	-1.95415300	-2.29217500	-1.32873700
H	0.95131500	0.13651200	1.36528900
H	4.51469700	-2.21824400	-0.19054500
H	3.69777200	-1.60489500	-1.65903500
H	-4.54570600	0.47200000	0.33173100
H	-4.99650700	-1.23180600	0.45291500
H	-4.05795600	-0.45863100	1.74141900
H	-0.22821100	-1.59872600	0.19951400
H	-0.31312900	-0.63812800	-1.28307000
H	-1.68069400	0.13312500	1.33454800
H	2.22149500	2.56800300	1.14341300
H	2.54138700	2.39865800	-0.57681400
H	1.49515800	3.71044500	0.00044400
H	-0.77148600	3.29329600	-0.46189700
H	-2.18192200	1.27321600	-1.44227900
H	-2.72306700	1.91894600	0.09073500

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

Zero-point correction=	0.261007 (Hartree/Particle)
Thermal correction to Energy=	0.276014
Thermal correction to Enthalpy=	0.276958
Thermal correction to Gibbs Free Energy=	0.218166
Sum of electronic and zero-point Energies=	-617.853211
Sum of electronic and thermal Energies=	-617.838205
Sum of electronic and thermal Enthalpies=	-617.837260
Sum of electronic and thermal Free Energies=	-617.896053

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction=	0.261251 (Hartree/Particle)
Thermal correction to Energy=	0.276256
Thermal correction to Enthalpy=	0.277201
Thermal correction to Gibbs Free Energy=	0.218388
Sum of electronic and zero-point Energies=	-617.941977
Sum of electronic and thermal Energies=	-617.926972
Sum of electronic and thermal Enthalpies=	-617.926028
Sum of electronic and thermal Free Energies=	-617.984841

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction=	0.261351 (Hartree/Particle)
Thermal correction to Energy=	0.276312
Thermal correction to Enthalpy=	0.277257
Thermal correction to Gibbs Free Energy=	0.218710
Sum of electronic and zero-point Energies=	-617.938886

Sum of electronic and thermal Energies=	-617.923924
Sum of electronic and thermal Enthalpies=	-617.922980
Sum of electronic and thermal Free Energies=	-617.981527

Name of cationic radical	cis-Carvyl acetate		
Cartesian Coordinates optimized at B3LYP/6-311G			
C	2.93677000	-0.88116400	0.19003600
C	-3.37708900	-1.18228500	-1.20429700
C	0.67004800	0.03171200	0.37778700
C	3.81499800	-1.60782700	-0.76916900
C	-4.07054300	-0.78874700	1.14459700
C	-0.59820100	-0.73752000	-0.00303600
C	0.66329100	1.48648500	-0.03664700
C	-1.84569600	0.11029700	0.30423100
C	1.98287600	2.18248400	0.02521700
C	-0.46760200	2.10793300	-0.39993800
C	-3.11752900	-0.65994600	-0.00324800
C	-1.79963600	1.42976500	-0.49646400
O	3.18551400	-0.51389200	1.31593000
O	1.71508100	-0.66555900	-0.39746400
H	-4.27706600	-1.72941200	-1.43524700
H	-2.70850500	-1.10399800	-2.04730600
H	0.91701700	-0.06278900	1.46179200
H	3.32444700	-1.77841000	-1.74087300
H	4.74284200	-1.04412900	-0.95212000
H	4.10649000	-2.58893600	-0.36251700
H	-4.37274900	0.19628100	1.52576800
H	-4.98981400	-1.32302200	0.87061300
H	-3.61579200	-1.34003900	1.97925900
H	-0.63945900	-1.70383300	0.53152600
H	-0.55780900	-0.99567800	-1.08229500
H	-1.82327600	0.37187400	1.39332200
H	2.56258400	1.87927600	0.91246400
H	2.59070500	1.93359100	-0.85714400
H	1.88525600	3.27423000	0.05874400
H	-0.47346500	3.16391200	-0.66769100
H	-2.02274700	1.23455500	-1.56816100
H	-2.60354200	2.10502600	-0.14228400

Frequency and Energy at B3LYP/6-311G (gas)	
Zero-point correction=	0.272801 (Hartree/Particle)
Thermal correction to Energy=	0.288501
Thermal correction to Enthalpy=	0.289446
Thermal correction to Gibbs Free Energy=	0.228333
Sum of electronic and zero-point Energies=	-618.150229
Sum of electronic and thermal Energies=	-618.134529
Sum of electronic and thermal Enthalpies=	-618.133585
Sum of electronic and thermal Free Energies=	-618.194697

Name of compound	Geranyl acetate
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)	

C	0.96382900	-1.47801900	-0.15946100
C	-0.47441400	-1.35724000	0.27959400
C	-1.47140200	-1.44424000	-0.61789700
C	-0.69641100	-1.14364700	1.74011300
C	1.58385200	-0.08578500	-0.37269400
C	-2.92168600	-1.34569700	-0.29532800
C	3.03354600	-0.18576900	-0.73593200
O	-3.43589300	-0.06325000	-0.79951300
C	4.02559500	0.50248800	-0.15064600
C	-3.37060400	1.03299700	0.02076000
C	3.82484100	1.47679700	0.96840500
C	5.44987000	0.34479100	-0.59445600
C	-3.87492900	2.22435800	-0.71995600
O	-2.97730300	0.97115100	1.16443000
H	1.55283600	-2.03828600	0.59499900
H	1.04611300	-2.07246500	-1.09132200
H	-1.25963000	-1.57172900	-1.67937100
H	-1.09269100	-2.04567500	2.22394300
H	0.21751300	-0.86104900	2.27587400
H	-1.43149200	-0.33229600	1.91829600
H	1.03888100	0.44732100	-1.18049100
H	1.43867100	0.53139000	0.54061300
H	-3.15774800	-1.42248400	0.78090600
H	-3.53682100	-2.05880500	-0.87604600
H	3.24354600	-0.87868300	-1.55040000
H	4.53124400	1.30074300	1.78954400
H	3.97435000	2.50819100	0.62151500
H	2.81084300	1.42061700	1.39286200
H	5.54947900	-0.28076700	-1.49018000
H	5.90536800	1.31655200	-0.82643700
H	6.05674400	-0.12042300	0.19424500
H	-4.24769500	1.96687300	-1.72400700
H	-4.69230100	2.71124200	-0.16654000
H	-3.07416700	2.97031900	-0.84234200

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.296398 (Hartree/Particle)
Thermal correction to Energy=	0.313962
Thermal correction to Enthalpy=	0.314906
Thermal correction to Gibbs Free Energy=	0.247789
Sum of electronic and zero-point Energies=	-619.632323
Sum of electronic and thermal Energies=	-619.614759
Sum of electronic and thermal Enthalpies=	-619.613815
Sum of electronic and thermal Free Energies=	-619.680931

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.295723 (Hartree/Particle)
Thermal correction to Energy=	0.313342
Thermal correction to Enthalpy=	0.314286
Thermal correction to Gibbs Free Energy=	0.247049
Sum of electronic and zero-point Energies=	-619.639484
Sum of electronic and thermal Energies=	-619.621865
Sum of electronic and thermal Enthalpies=	-619.620921

Sum of electronic and thermal Free Energies=	-619.688158
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.295760 (Hartree/Particle)
Thermal correction to Energy=	0.313376
Thermal correction to Enthalpy=	0.314320
Thermal correction to Gibbs Free Energy=	0.247120
Sum of electronic and zero-point Energies=	-619.639131
Sum of electronic and thermal Energies=	-619.621515
Sum of electronic and thermal Enthalpies=	-619.620571
Sum of electronic and thermal Free Energies=	-619.687771

Name of radical	Geranyl acetate-C5-H		
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	0.97640800	-1.20528500	-0.13714000
C	-0.46359000	-1.15668300	0.32876500
C	-1.45893400	-1.32982200	-0.55124800
C	-0.66897100	-0.91816300	1.80536100
C	1.63842500	0.19258900	-0.24191800
C	-2.92720500	-1.33237900	-0.26080900
C	3.05527500	0.11457000	-0.73973000
O	-3.59638000	-0.20437400	-0.90668000
C	4.18533900	0.44023300	-0.10065200
C	-3.73339400	0.92308100	-0.17735200
C	4.25666600	0.98591700	1.30350300
C	5.52690300	0.28295500	-0.77480400
C	-4.37108400	2.01463600	-1.00202100
O	-3.39085500	1.03599900	0.97398500
H	1.56584300	-1.81637000	0.55712200
H	1.03261700	-1.69556300	-1.11366700
H	-1.20187500	-1.49977200	-1.59477200
H	-0.53559300	-1.85145500	2.36543800
H	0.07582400	-0.21519200	2.18837000
H	-1.65231800	-0.50778300	2.03017500
H	1.58472500	0.70022500	0.72293500
H	-3.14826500	-1.30612500	0.80373600
H	-3.40868600	-2.20359700	-0.70809300
H	3.15407800	-0.27154700	-1.75416600
H	4.88402500	0.34372300	1.93262300
H	4.72570900	1.97691500	1.30694900
H	3.28240300	1.07505300	1.78274600
H	5.42892000	-0.11525600	-1.78659700
H	6.05103200	1.24425700	-0.83598800
H	6.17717100	-0.39056500	-0.20383200
H	-5.26776000	1.64112700	-1.49937700
H	-4.61440200	2.85884000	-0.36026400
H	-3.67326500	2.33479800	-1.78002200
Frequency and Energy at B3LYP/6-311G (d,p) (gas)			
Zero-point correction=	0.282400 (Hartree/Particle)		
Thermal correction to Energy=	0.300157		
Thermal correction to Enthalpy=	0.301102		

Thermal correction to Gibbs Free Energy=	0.232349
Sum of electronic and zero-point Energies=	-619.005779
Sum of electronic and thermal Energies=	-618.988021
Sum of electronic and thermal Enthalpies=	-618.987077
Sum of electronic and thermal Free Energies=	-619.055830
Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.281754 (Hartree/Particle)
Thermal correction to Energy=	0.299604
Thermal correction to Enthalpy=	0.300548
Thermal correction to Gibbs Free Energy=	0.231331
Sum of electronic and zero-point Energies=	-619.013553
Sum of electronic and thermal Energies=	-618.995703
Sum of electronic and thermal Enthalpies=	-618.994759
Sum of electronic and thermal Free Energies=	-619.063976
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.281813 (Hartree/Particle)
Thermal correction to Energy=	0.299640
Thermal correction to Enthalpy=	0.300584
Thermal correction to Gibbs Free Energy=	0.231665
Sum of electronic and zero-point Energies=	-619.013118
Sum of electronic and thermal Energies=	-618.995291
Sum of electronic and thermal Enthalpies=	-618.994347
Sum of electronic and thermal Free Energies=	-619.063266

Name of anion	Geranyl acetate-C13-H		
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	0.97640800	-1.20528500	-0.13714000
C	-0.46359000	-1.15668300	0.32876500
C	-1.45893400	-1.32982200	-0.55124800
C	-0.66897100	-0.91816300	1.80536100
C	1.63842500	0.19258900	-0.24191800
C	-2.92720500	-1.33237900	-0.26080900
C	3.05527500	0.11457000	-0.73973000
O	-3.59638000	-0.20437400	-0.90668000
C	4.18533900	0.44023300	-0.10065200
C	-3.73339400	0.92308100	-0.17735200
C	4.25666600	0.98591700	1.30350300
C	5.52690300	0.28295500	-0.77480400
C	-4.37108400	2.01463600	-1.00202100
O	-3.39085500	1.03599900	0.97398500
H	1.56584300	-1.81637000	0.55712200
H	1.03261700	-1.69556300	-1.11366700
H	-1.20187500	-1.49977200	-1.59477200
H	-0.53559300	-1.85145500	2.36543800
H	0.07582400	-0.21519200	2.18837000
H	-1.65231800	-0.50778300	2.03017500
H	1.04314800	0.79453500	-0.93949500
H	1.58472500	0.70022500	0.72293500

H	-3.14826500	-1.30612500	0.80373600
H	-3.40868600	-2.20359700	-0.70809300
H	3.15407800	-0.27154700	-1.75416600
H	4.88402500	0.34372300	1.93262300
H	4.72570900	1.97691500	1.30694900
H	3.28240300	1.07505300	1.78274600
H	5.42892000	-0.11525600	-1.78659700
H	6.05103200	1.24425700	-0.83598800
H	6.17717100	-0.39056500	-0.20383200
H	-5.26776000	1.64112700	-1.49937700
H	-3.67326500	2.33479800	-1.78002200

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.281569 (Hartree/Particle)
Thermal correction to Energy=	0.298521
Thermal correction to Enthalpy=	0.299465
Thermal correction to Gibbs Free Energy=	0.234753
Sum of electronic and zero-point Energies=	-619.034936
Sum of electronic and thermal Energies=	-619.017984
Sum of electronic and thermal Enthalpies=	-619.017040
Sum of electronic and thermal Free Energies=	-619.081752

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction= (Hartree/Particle)	0.281561
Thermal correction to Energy=	0.298746
Thermal correction to Enthalpy=	0.299690
Thermal correction to Gibbs Free Energy=	0.232790
Sum of electronic and zero-point Energies=	-619.126811
Sum of electronic and thermal Energies=	-619.109626
Sum of electronic and thermal Enthalpies=	-619.108682
Sum of electronic and thermal Free Energies=	-619.175582

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.281417 (Hartree/Particle)
Thermal correction to Energy=	0.298648
Thermal correction to Enthalpy=	0.299592
Thermal correction to Gibbs Free Energy=	0.232631
Sum of electronic and zero-point Energies=	-619.123788
Sum of electronic and thermal Energies=	-619.106557
Sum of electronic and thermal Enthalpies=	-619.105613
Sum of electronic and thermal Free Energies=	-619.172573

Name of cationic radical	Geranyl acetate	
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)		
C	0.97640800	-1.20528500	-0.13714000
C	-0.46359000	-1.15668300	0.32876500
C	-1.45893400	-1.32982200	-0.55124800
C	-0.66897100	-0.91816300	1.80536100

C	1.63842500	0.19258900	-0.24191800
C	-2.92720500	-1.33237900	-0.26080900
C	3.05527500	0.11457000	-0.73973000
O	-3.59638000	-0.20437400	-0.90668000
C	4.18533900	0.44023300	-0.10065200
C	-3.73339400	0.92308100	-0.17735200
C	4.25666600	0.98591700	1.30350300
C	5.52690300	0.28295500	-0.77480400
C	-4.37108400	2.01463600	-1.00202100
O	-3.39085500	1.03599900	0.97398500
H	1.56584300	-1.81637000	0.55712200
H	1.03261700	-1.69556300	-1.11366700
H	-1.20187500	-1.49977200	-1.59477200
H	-0.53559300	-1.85145500	2.36543800
H	0.07582400	-0.21519200	2.18837000
H	-1.65231800	-0.50778300	2.03017500
H	1.04314800	0.79453500	-0.93949500
H	1.58472500	0.70022500	0.72293500
H	-3.14826500	-1.30612500	0.80373600
H	-3.40868600	-2.20359700	-0.70809300
H	3.15407800	-0.27154700	-1.75416600
H	4.88402500	0.34372300	1.93262300
H	4.72570900	1.97691500	1.30694900
H	3.28240300	1.07505300	1.78274600
H	5.42892000	-0.11525600	-1.78659700
H	6.05103200	1.24425700	-0.83598800
H	6.17717100	-0.39056500	-0.20383200
H	-5.26776000	1.64112700	-1.49937700
H	-4.61440200	2.85884000	-0.36026400
H	-3.67326500	2.33479800	-1.78002200

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

Zero-point correction=	0.294563 (Hartree/Particle)
Thermal correction to Energy=	0.312502
Thermal correction to Enthalpy=	0.313446
Thermal correction to Gibbs Free Energy=	0.245149
Sum of electronic and zero-point Energies=	-619.349616
Sum of electronic and thermal Energies=	-619.331676
Sum of electronic and thermal Enthalpies=	-619.330732
Sum of electronic and thermal Free Energies=	-619.399029

Name of compound	Methyl jasmonate

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

C	-3.22928100	-1.41314900	-0.40541900
C	-3.25957300	0.02922800	0.05692800
C	-1.84173000	0.49922100	0.39813900
C	-0.90761400	-0.62311600	-0.12044800
C	-1.78627000	-1.89401200	-0.22930600
H	-3.95214500	-2.02684400	0.16260900
H	-3.56253500	-1.47671500	-1.45951400
H	-1.77716700	0.57581500	1.51144900
H	-0.54186700	-0.34775000	-1.13993300

H	-1.45006500	-2.53182700	-1.06656200
H	-1.68980500	-2.52556200	0.67206000
O	-4.25240700	0.70555500	0.15349600
C	-1.55419900	1.87712900	-0.21562500
H	-2.37823000	2.57523500	0.05737300
H	-1.58307600	1.81699000	-1.32244800
C	-0.24346300	2.41967100	0.27103500
H	-0.25041800	2.77294300	1.30185800
C	0.85755300	2.45764700	-0.48544200
H	0.85878400	2.10779700	-1.51871300
C	2.18215500	2.96388000	0.00423200
H	2.14877200	3.20129300	1.08704200
H	2.41432400	3.92559900	-0.50162800
C	3.29358500	1.95013300	-0.26623000
H	3.45695100	1.80459400	-1.33965700
H	4.24256500	2.27640300	0.17194400
H	3.05382900	0.96396500	0.16088100
C	0.30825700	-0.82264000	0.79483400
H	0.79749000	0.16355800	0.98974800
H	0.00249100	-1.20091300	1.79368400
C	1.29915200	-1.77882700	0.19840600
O	1.13044300	-2.83605600	-0.35975900
O	2.56560500	-1.26322900	0.40062300
C	3.68432500	-2.04782900	-0.09029700
H	4.54047500	-1.60660600	0.42999100
H	3.55126700	-3.10494600	0.16449100
H	3.75184800	-1.91720500	-1.17438900

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.309244 (Hartree/Particle)
Thermal correction to Energy=	0.327153
Thermal correction to Enthalpy=	0.328097
Thermal correction to Gibbs Free Energy=	0.260453
Sum of electronic and zero-point Energies=	-732.990705
Sum of electronic and thermal Energies=	-732.972796
Sum of electronic and thermal Enthalpies=	-732.971852
Sum of electronic and thermal Free Energies=	-733.039496

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.308809 (Hartree/Particle)
Thermal correction to Energy=	0.326730
Thermal correction to Enthalpy=	0.327674
Thermal correction to Gibbs Free Energy=	0.259847
Sum of electronic and zero-point Energies=	-733.001693
Sum of electronic and thermal Energies=	-732.983771
Sum of electronic and thermal Enthalpies=	-732.982827
Sum of electronic and thermal Free Energies=	-733.050655

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.308830 (Hartree/Particle)
Thermal correction to Energy=	0.326753
Thermal correction to Enthalpy=	0.327697
Thermal correction to Gibbs Free Energy=	0.259863

Sum of electronic and zero-point Energies=	-733.001172
Sum of electronic and thermal Energies=	-732.983250
Sum of electronic and thermal Enthalpies=	-732.982305
Sum of electronic and thermal Free Energies=	-733.050139

Name of radical	Methyl jasmonate-C20-H		
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	3.28380400	-1.35803000	0.22229900
C	3.19821400	0.13639900	-0.07626700
C	1.73111000	0.50807100	-0.35757700
C	0.93239300	-0.72323700	0.12269500
C	1.89537800	-1.91016800	-0.12255800
H	4.11768600	-1.81506000	-0.31370200
H	3.49877300	-1.45952200	1.29315400
H	1.66198600	0.56354600	-1.45650100
H	0.77812300	-0.63193300	1.20480500
H	1.61585000	-2.78451600	0.46409300
H	1.85841800	-2.19402300	-1.18139100
O	4.12064100	0.91269300	-0.07937800
C	1.37183100	1.88572500	0.22700400
H	2.21865700	2.54631500	0.00412700
H	1.31406500	1.81104900	1.31863700
C	0.10789500	2.49464700	-0.31181100
H	0.06912400	2.62574000	-1.39431700
C	-0.92836000	2.90639800	0.41867500
H	-0.88986600	2.77676500	1.50114000
C	-2.17754900	3.54682800	-0.11991300
H	-2.09212900	3.66289300	-1.20528300
C	-3.45347400	2.76012900	0.22289300
H	-3.56449400	2.64059600	1.30485200
H	-4.34381200	3.27520800	-0.14785900
H	-3.43151000	1.76121800	-0.22157400
C	-0.43527600	-0.88830400	-0.53705200
H	-1.01367000	0.03721000	-0.45968700
H	-0.33612700	-1.09086700	-1.60919800
C	-1.27540500	-1.98742400	0.07848500
O	-1.01444000	-2.60332200	1.08263700
O	-2.40011200	-2.18777200	-0.64220200
C	-3.29596100	-3.19447300	-0.13636500
H	-4.12754000	-3.22242900	-0.83687200
H	-2.79701000	-4.16379100	-0.09322300
H	-3.64453400	-2.93001200	0.86314900

Frequency and Energy at B3LYP/6-311G (d,p) (gas)		
Zero-point correction=	0.295401	(Hartree/Particle)
Thermal correction to Energy=	0.313297	
Thermal correction to Enthalpy=	0.314241	
Thermal correction to Gibbs Free Energy=	0.246498	
Sum of electronic and zero-point Energies=	-732.363586	
Sum of electronic and thermal Energies=	-732.345690	

Sum of electronic and thermal Enthalpies=	-732.344746
Sum of electronic and thermal Free Energies=	-732.412489
Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.294979 (Hartree/Particle)
Thermal correction to Energy=	0.312908
Thermal correction to Enthalpy=	0.313852
Thermal correction to Gibbs Free Energy=	0.245704
Sum of electronic and zero-point Energies=	-732.374929
Sum of electronic and thermal Energies=	-732.357001
Sum of electronic and thermal Enthalpies=	-732.356057
Sum of electronic and thermal Free Energies=	-732.424205
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction= (Hartree/Particle)	0.295010
Thermal correction to Energy=	0.312934
Thermal correction to Enthalpy=	0.313879
Thermal correction to Gibbs Free Energy=	0.245761
Sum of electronic and zero-point Energies=	-732.374381
Sum of electronic and thermal Energies=	-732.356457
Sum of electronic and thermal Enthalpies=	-732.355513
Sum of electronic and thermal Free Energies=	-732.423630

Name of anion	Methyl jasmonate-C3-H

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

C	3.28380400	-1.35803000	0.22229900
C	3.19821400	0.13639900	-0.07626700
C	1.73111000	0.50807100	-0.35757700
C	0.93239300	-0.72323700	0.12269500
C	1.89537800	-1.91016800	-0.12255800
H	4.11768600	-1.81506000	-0.31370200
H	3.49877300	-1.45952200	1.29315400
H	0.77812300	-0.63193300	1.20480500
H	1.61585000	-2.78451600	0.46409300
H	1.85841800	-2.19402300	-1.18139100
O	4.12064100	0.91269300	-0.07937800
C	1.37183100	1.88572500	0.22700400
H	2.21865700	2.54631500	0.00412700
H	1.31406500	1.81104900	1.31863700
C	0.10789500	2.49464700	-0.31181100
H	0.06912400	2.62574000	-1.39431700
C	-0.92836000	2.90639800	0.41867500
H	-0.88986600	2.77676500	1.50114000
C	-2.17754900	3.54682800	-0.11991300
H	-2.09212900	3.66289300	-1.20528300
H	-2.26829100	4.55946100	0.29414200
C	-3.45347400	2.76012900	0.22289300
H	-3.56449400	2.64059600	1.30485200
H	-4.34381200	3.27520800	-0.14785900
H	-3.43151000	1.76121800	-0.22157400
C	-0.43527600	-0.88830400	-0.53705200

H	-1.01367000	0.03721000	-0.45968700
H	-0.33612700	-1.09086700	-1.60919800
C	-1.27540500	-1.98742400	0.07848500
O	-1.01444000	-2.60332200	1.08263700
O	-2.40011200	-2.18777200	-0.64220200
C	-3.29596100	-3.19447300	-0.13636500
H	-4.12754000	-3.22242900	-0.83687200
H	-2.79701000	-4.16379100	-0.09322300
H	-3.64453400	-2.93001200	0.86314900

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

Zero-point correction= (Hartree/Particle)	0.294670
Thermal correction to Energy=	0.312435
Thermal correction to Enthalpy=	0.313379
Thermal correction to Gibbs Free Energy=	0.246411
Sum of electronic and zero-point Energies=	-732.416329
Sum of electronic and thermal Energies=	-732.398564
Sum of electronic and thermal Enthalpies=	-732.397620
Sum of electronic and thermal Free Energies=	-732.464588

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction=	0.295132 (Hartree/Particle)
Thermal correction to Energy=	0.312851
Thermal correction to Enthalpy=	0.313795
Thermal correction to Gibbs Free Energy=	0.246957
Sum of electronic and zero-point Energies=	-732.499804
Sum of electronic and thermal Energies=	-732.482085
Sum of electronic and thermal Enthalpies=	-732.481141
Sum of electronic and thermal Free Energies=	-732.547979

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction=	0.295173 (Hartree/Particle)
Thermal correction to Energy=	0.312884
Thermal correction to Enthalpy=	0.313828
Thermal correction to Gibbs Free Energy=	0.247045
Sum of electronic and zero-point Energies=	-732.496884
Sum of electronic and thermal Energies=	-732.479174
Sum of electronic and thermal Enthalpies=	-732.478230
Sum of electronic and thermal Free Energies=	-732.545012

Name of cationic radical	Methyl jasmonate

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

C	-3.22928100	-1.41314900	-0.40541900
C	-3.25957300	0.02922800	0.05692800
C	-1.84173000	0.49922100	0.39813900
C	-0.90761400	-0.62311600	-0.12044800
C	-1.78627000	-1.89401200	-0.22930600
H	-3.95214500	-2.02684400	0.16260900
H	-3.56253500	-1.47671500	-1.45951400

H	-1.77716700	0.57581500	1.51144900
H	-0.54186700	-0.34775000	-1.13993300
H	-1.45006500	-2.53182700	-1.06656200
H	-1.68980500	-2.52556200	0.67206000
O	-4.25240700	0.70555500	0.15349600
C	-1.55419900	1.87712900	-0.21562500
H	-2.37823000	2.57523500	0.05737300
H	-1.58307600	1.81699000	-1.32244800
C	-0.24346300	2.41967100	0.27103500
H	-0.25041800	2.77294300	1.30185800
C	0.85755300	2.45764700	-0.48544200
H	0.85878400	2.10779700	-1.51871300
C	2.18215500	2.96388000	0.00423200
H	2.14877200	3.20129300	1.08704200
H	2.41432400	3.92559900	-0.50162800
C	3.29358500	1.95013300	-0.26623000
H	3.45695100	1.80459400	-1.33965700
H	4.24256500	2.27640300	0.17194400
H	3.05382900	0.96396500	0.16088100
C	0.30825700	-0.82264000	0.79483400
H	0.79749000	0.16355800	0.98974800
H	0.00249100	-1.20091300	1.79368400
C	1.29915200	-1.77882700	0.19840600
O	1.13044300	-2.83605600	-0.35975900
O	2.56560500	-1.26322900	0.40062300
C	3.68432500	-2.04782900	-0.09029700
H	4.54047500	-1.60660600	0.42999100
H	3.55126700	-3.10494600	0.16449100
H	3.75184800	-1.91720500	-1.17438900

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.307408 (Hartree/Particle)
Thermal correction to Energy=	0.325597
Thermal correction to Enthalpy=	0.326541
Thermal correction to Gibbs Free Energy=	0.257524
Sum of electronic and zero-point Energies=	-732.690809
Sum of electronic and thermal Energies=	-732.672620
Sum of electronic and thermal Enthalpies=	-732.671676
Sum of electronic and thermal Free Energies=	-732.740693

Name of compound	Marsupellol

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	-0.25335790	0.53834762	-0.68698788
C	-0.41785290	-1.01265338	-0.68698788
C	0.13530210	-0.98021038	0.78331112
C	1.63442710	-1.13002138	1.03627712
C	2.48777610	0.04444362	0.57729312
C	2.30675110	0.37695362	-0.89500788
C	1.04359810	1.17858262	-1.17803688
C	-0.54041090	0.43011662	0.84836412
C	-2.05529490	0.37010562	1.10180612
C	-2.66055790	-0.89498538	0.47373412

C	-1.90634590	-1.38694638	-0.77139988
C	0.93405810	1.36920062	-2.68508588
C	-2.26633288	0.35644748	2.34393188
C	-0.14143990	-2.07617738	1.80399712
C	1.18921510	2.48562762	-0.40995088
O	-2.49396812	-2.08055948	-1.83610688
H	-0.83145490	1.20322562	-1.36706988
H	0.02718110	-1.68484338	-1.45436988
H	1.78762310	-1.25991738	2.13100412
H	1.96419610	-2.00651738	0.43479912
H	3.55776910	-0.20583838	0.75405212
H	2.16464510	0.93594362	1.16003012
H	2.25680910	-0.57543838	-1.46878888
H	3.17292010	1.00523362	-1.20124988
H	-0.21750790	1.18921162	1.59554412
H	-3.71195990	-0.67412938	0.18296712
H	-2.59156290	-1.70245838	1.23662012
H	0.83075110	0.37693262	-3.17854288
H	0.04120510	1.99240162	-2.91574588
H	1.84971310	1.87732062	-3.06212488
H	-1.29973488	0.39019948	2.89467488
H	-2.81251688	-0.57106452	2.62708188
H	-0.77560190	-2.86443038	1.34003212
H	0.82154410	-2.52390438	2.13712312
H	-0.67223990	-1.64133838	2.68031612
H	1.18604810	3.33886562	-1.12461488
H	0.33949510	2.59439662	0.30062212
H	2.14804510	2.47880662	0.15517412
H	-1.80677172	-2.44646511	-2.39777776
H	-2.62359953	-0.89387411	-1.39375586

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.360799 (Hartree/Particle)
Thermal correction to Energy=	0.376447
Thermal correction to Enthalpy=	0.377391
Thermal correction to Gibbs Free Energy=	0.320382
Sum of electronic and zero-point Energies=	-661.034135
Sum of electronic and thermal Energies=	-661.018487
Sum of electronic and thermal Enthalpies=	-661.017543
Sum of electronic and thermal Free Energies=	-661.074552

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.360217 (Hartree/Particle)
Thermal correction to Energy=	0.375890
Thermal correction to Enthalpy=	0.376834
Thermal correction to Gibbs Free Energy=	0.319832
Sum of electronic and zero-point Energies=	-661.040159
Sum of electronic and thermal Energies=	-661.024486
Sum of electronic and thermal Enthalpies=	-661.023542
Sum of electronic and thermal Free Energies=	-661.080544

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.360253 (Hartree/Particle)

Thermal correction to Energy=	0.375921
Thermal correction to Enthalpy=	0.376865
Thermal correction to Gibbs Free Energy=	0.319878
Sum of electronic and zero-point Energies=	-661.039862
Sum of electronic and thermal Energies=	-661.024195
Sum of electronic and thermal Enthalpies=	-661.023250
Sum of electronic and thermal Free Energies=	-661.080237

Name of radical	Marsupellol-C10-H		
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	-0.50537300	-0.74478600	-0.14286400
C	0.35728000	0.20036900	-1.03535700
C	0.55098800	1.15151400	0.20013200
C	-0.55744400	2.22434100	0.33213100
C	-1.99242500	1.78746900	0.65090600
C	-2.58382200	0.78579600	-0.34054100
C	-2.04758600	-0.65860500	-0.22009400
C	0.29632800	-0.13652100	1.06523900
C	1.58068500	-0.91554200	1.19252800
C	2.26521700	-1.24937400	-0.13748700
C	1.62340300	-0.58581100	-1.40202900
C	-2.49508600	-1.43413500	-1.47732800
C	2.08536300	-1.29374200	2.36642700
C	1.88653200	1.88642000	0.38692400
C	-2.65000800	-1.35384200	1.01722900
O	2.55774100	0.17174900	-2.17248400
H	-0.26556500	-1.80385600	-0.28863000
H	-0.08415600	0.63307300	-1.93730500
H	-0.24672600	2.92280200	1.11764700
H	-0.56296400	2.80611500	-0.59958400
H	-2.61468200	2.68907900	0.66147200
H	-2.04289100	1.38579000	1.66850200
H	-2.40339000	1.15202900	-1.35852100
H	-3.67299900	0.74973400	-0.22389900
H	-0.19558300	-0.01480200	2.03220600
H	3.31843600	-0.96021500	-0.10215600
H	-2.03188100	-1.02750300	-2.38127100
H	-2.22623500	-2.49246400	-1.40725900
H	-3.58043700	-1.37306900	-1.60401200
H	1.58344500	-1.06051800	3.29934100
H	3.01311500	-1.85320200	2.43643300
H	2.76308800	1.24084800	0.32414200
H	1.98997200	2.69264800	-0.34845000
H	1.92016500	2.35018400	1.37753600
H	-3.73884900	-1.41987600	0.92961700
H	-2.26064300	-2.37141700	1.11934500
H	-2.42295800	-0.82190300	1.94390100
H	2.82999500	0.93497600	-1.65537700
H	1.31850200	-1.37840100	-2.09041300
Frequency and Energy at B3LYP/6-311G (d,p) (gas)			

Zero-point correction=	0.347090 (Hartree/Particle)
Thermal correction to Energy=	0.362523
Thermal correction to Enthalpy=	0.363467
Thermal correction to Gibbs Free Energy=	0.306755
Sum of electronic and zero-point Energies=	-660.408410
Sum of electronic and thermal Energies=	-660.392977
Sum of electronic and thermal Enthalpies=	-660.392032
Sum of electronic and thermal Free Energies=	-660.448744
Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.346528 (Hartree/Particle)
Thermal correction to Energy=	0.361984
Thermal correction to Enthalpy=	0.362928
Thermal correction to Gibbs Free Energy=	0.306182
Sum of electronic and zero-point Energies=	-660.414081
Sum of electronic and thermal Energies=	-660.398625
Sum of electronic and thermal Enthalpies=	-660.397681
Sum of electronic and thermal Free Energies=	-660.454427
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.346557 (Hartree/Particle)
Thermal correction to Energy=	0.362012
Thermal correction to Enthalpy=	0.362957
Thermal correction to Gibbs Free Energy=	0.306210
Sum of electronic and zero-point Energies=	-660.413809
Sum of electronic and thermal Energies=	-660.398354
Sum of electronic and thermal Enthalpies=	-660.397410
Sum of electronic and thermal Free Energies=	-660.454156

Name of anion	Marsupellol-O-H		
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	-0.50537300	-0.74478600	-0.14286400
C	0.35728000	0.20036900	-1.03535700
C	0.55098800	1.15151400	0.20013200
C	-0.55744400	2.22434100	0.33213100
C	-1.99242500	1.78746900	0.65090600
C	-2.58382200	0.78579600	-0.34054100
C	-2.04758600	-0.65860500	-0.22009400
C	0.29632800	-0.13652100	1.06523900
C	1.58068500	-0.91554200	1.19252800
C	2.26521700	-1.24937400	-0.13748700
C	1.62340300	-0.58581100	-1.40202900
C	-2.49508600	-1.43413500	-1.47732800
C	2.08536300	-1.29374200	2.36642700
C	1.88653200	1.88642000	0.38692400
C	-2.65000800	-1.35384200	1.01722900
O	2.55774100	0.17174900	-2.17248400
H	-0.26556500	-1.80385600	-0.28863000
H	-0.08415600	0.63307300	-1.93730500
H	-0.24672600	2.92280200	1.11764700
H	-0.56296400	2.80611500	-0.59958400
H	-2.61468200	2.68907900	0.66147200

H	-2.04289100	1.38579000	1.66850200
H	-2.40339000	1.15202900	-1.35852100
H	-3.67299900	0.74973400	-0.22389900
H	-0.19558300	-0.01480200	2.03220600
H	2.26700700	-2.33534700	-0.26828900
H	3.31843600	-0.96021500	-0.10215600
H	-2.03188100	-1.02750300	-2.38127100
H	-2.22623500	-2.49246400	-1.40725900
H	-3.58043700	-1.37306900	-1.60401200
H	1.58344500	-1.06051800	3.29934100
H	3.01311500	-1.85320200	2.43643300
H	2.76308800	1.24084800	0.32414200
H	1.98997200	2.69264800	-0.34845000
H	1.92016500	2.35018400	1.37753600
H	-3.73884900	-1.41987600	0.92961700
H	-2.26064300	-2.37141700	1.11934500
H	-2.42295800	-0.82190300	1.94390100
H	1.31850200	-1.37840100	-2.09041300

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.344016 (Hartree/Particle)
Thermal correction to Energy=	0.359313
Thermal correction to Enthalpy=	0.360257
Thermal correction to Gibbs Free Energy=	0.304065
Sum of electronic and zero-point Energies=	-660.443696
Sum of electronic and thermal Energies=	-660.428399
Sum of electronic and thermal Enthalpies=	-660.427455
Sum of electronic and thermal Free Energies=	-660.483647

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.344721 (Hartree/Particle)
Thermal correction to Energy=	0.360030
Thermal correction to Enthalpy=	0.360975
Thermal correction to Gibbs Free Energy=	0.304211
Sum of electronic and zero-point Energies=	-660.529082
Sum of electronic and thermal Energies=	-660.513773
Sum of electronic and thermal Enthalpies=	-660.512829
Sum of electronic and thermal Free Energies=	-660.569592

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.344745 (Hartree/Particle)
Thermal correction to Energy=	0.360024
Thermal correction to Enthalpy=	0.360968
Thermal correction to Gibbs Free Energy=	0.304365
Sum of electronic and zero-point Energies=	-660.526045
Sum of electronic and thermal Energies=	-660.510766
Sum of electronic and thermal Enthalpies=	-660.509821
Sum of electronic and thermal Free Energies=	-660.566425

Name of cationic radical	Marsupellol

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C 0	-0.027287	0.481017	-0.704662
C 0	-0.191782	-1.069984	-0.704662

C 0	-0.053510	-0.993540	0.858620
C 0	1.322085	-1.130250	1.508898
C 0	2.271891	0.033985	1.262597
C 0	2.494045	0.323735	-0.213105
C 0	1.356368	1.112056	-0.847541
C 0	-0.716386	0.415426	0.699710
C 0	-2.243922	0.356757	0.538782
C 0	-2.663285	-0.928050	-0.192437
C 0	-1.604424	-1.452321	-1.174868
C 0	1.656157	1.259262	-2.333471
C 0	-3.091145	1.294572	0.975000
C 0	-0.598361	-2.061072	1.798323
C 0	1.295536	2.440997	-0.106094
O 0	-1.834733	-0.894339	-2.440260
H 0	-0.399003	1.124006	-1.533614
H 0	0.440298	-1.762012	-1.304947
H 0	1.797799	-2.022224	1.043231
H 0	1.175272	-1.228328	2.607805
H 0	1.807660	0.940450	1.711573
H 0	3.254175	-0.206995	1.727158
H 0	3.413070	0.946409	-0.293342
H 0	2.596259	-0.644794	-0.751875
H 0	-0.602962	1.196738	1.484220
H 0	-3.569010	-0.681669	-0.790540
H 0	-2.858136	-1.717159	0.567898
H 0	-1.678151	-2.561842	-1.222797
H 0	2.641390	1.760003	-2.465171
H 0	0.860432	1.872162	-2.812996
H 0	1.685248	0.252952	-2.808089
H 0	-2.706105	2.186674	1.490655
H 0	-4.173226	1.174046	0.818239
H 0	-1.343227	-1.603529	2.487234
H 0	0.238097	-2.495380	2.390340
H 0	-1.087759	-2.864679	1.203785
H 0	2.067430	2.454002	0.695642
H 0	0.286683	2.566643	0.346894
H 0	1.487658	3.273523	-0.819367
H 0	-2.705138	-1.147249	-2.696767

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.358328 (Hartree/Particle)
Thermal correction to Energy=	0.374831
Thermal correction to Enthalpy=	0.375775
Thermal correction to Gibbs Free Energy=	0.316396
Sum of electronic and zero-point Energies=	-660.746583
Sum of electronic and thermal Energies=	-660.730081
Sum of electronic and thermal Enthalpies=	-660.729137
Sum of electronic and thermal Free Energies=	-660.788515

Name of compound	Globulol

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
O	-2.01180000	0.32570000	-1.71740000

C	0.85040000	-0.56290000	-0.40730000
C	2.38880000	-0.55370000	-0.60030000
C	1.58110000	0.74590000	-0.80200000
C	-0.05110000	-0.30800000	0.83430000
C	-1.25090000	0.67790000	0.58090000
C	0.86250000	1.34570000	-2.02850000
C	-0.59570000	-1.63710000	1.44460000
C	-1.56250000	1.35010000	-0.82520000
C	-2.47890000	-0.04850000	1.20770000
C	-0.40190000	2.11430000	-1.56220000
C	3.23710000	-0.71390000	0.68900000
C	2.97180000	-1.22640000	-1.87280000
C	-2.04300000	-1.35030000	1.89710000
C	0.24700000	-2.24950000	2.59880000
C	-2.73420000	2.38160000	-0.67680000
H	0.34970000	-1.11450000	-1.20960000
H	1.77720000	1.47260000	-0.00770000
H	0.57190000	0.14310000	1.61450000
H	-1.04230000	1.53740000	1.23040000
H	1.55680000	2.04230000	-2.50450000
H	0.59500000	0.61040000	-2.79320000
H	-0.65110000	-2.40380000	0.66300000
H	-2.98780000	0.60110000	1.92760000
H	-3.22710000	-0.31290000	0.45640000
H	-0.07550000	2.95110000	-0.93750000
H	-0.79570000	2.56490000	-2.47980000
H	4.28900000	-0.51320000	0.48190000
H	3.15860000	-1.73820000	1.05180000
H	2.94250000	-0.03850000	1.49340000
H	2.71590000	-2.28650000	-1.87950000
H	4.06010000	-1.14230000	-1.88840000
H	2.61350000	-0.78400000	-2.80260000
H	-2.70340000	-2.18150000	1.62540000
H	-2.12680000	-1.22940000	2.98090000
H	-0.22280000	-3.15680000	2.98470000
H	0.34420000	-1.54440000	3.42820000
H	1.24700000	-2.51510000	2.26120000
H	-3.01860000	2.82520000	-1.63330000
H	-2.44840000	3.19850000	-0.00890000
H	-3.64520000	1.93990000	-0.27370000
H	-2.28500000	0.78340000	-2.54060000

Frequency and Energy at B3LYP/6-311G (d,p) (gas)		
Zero-point correction=	0.382870	(Hartree/Particle)
Thermal correction to Energy=	0.399623	
Thermal correction to Enthalpy=	0.400568	
Thermal correction to Gibbs Free Energy=	0.341124	
Sum of electronic and zero-point Energies=	-662.237299	
Sum of electronic and thermal Energies=	-662.220545	
Sum of electronic and thermal Enthalpies=	-662.219601	
Sum of electronic and thermal Free Energies=	-662.279044	
Frequency and Energy at B3LYP/6-311G (d,p) (water)		

Zero-point correction=	0.382082 (Hartree/Particle)
Thermal correction to Energy=	0.398893
Thermal correction to Enthalpy=	0.399837
Thermal correction to Gibbs Free Energy=	0.340288
Sum of electronic and zero-point Energies=	-662.241893
Sum of electronic and thermal Energies=	-662.225081
Sum of electronic and thermal Enthalpies=	-662.224137
Sum of electronic and thermal Free Energies=	-662.283686

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.382131
(Hartree/Particle)	
Thermal correction to Energy=	0.398939
Thermal correction to Enthalpy=	0.399883
Thermal correction to Gibbs Free Energy=	0.340342
Sum of electronic and zero-point Energies=	-662.241628
Sum of electronic and thermal Energies=	-662.224820
Sum of electronic and thermal Enthalpies=	-662.223876
Sum of electronic and thermal Free Energies=	-662.283417

Name of radical	Globulol-C5-H		
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
O	-1.52015600	-0.97777900	1.46086700
C	1.01299600	-0.04740500	0.23528700
C	2.45549400	-0.44390500	-0.04188300
C	1.30649800	-1.27506700	-0.58424200
C	0.06222200	0.94028300	-0.38025500
C	-1.36834300	0.27678900	-0.60723900
C	0.59838200	-2.51844600	-0.11486200
C	-0.19246700	2.23714100	0.41609700
C	-1.69812500	-1.12019800	0.03673700
C	-2.36882800	1.38107000	-0.15035000
C	-0.89169300	-2.35555100	-0.49327800
C	3.28647600	0.30944500	-1.06477600
C	3.26387000	-0.93814600	1.14472000
C	-1.56568200	2.68640100	-0.09705800
C	0.91825700	3.27739400	0.28824600
C	-3.18355200	-1.43894500	-0.24148600
H	0.71646600	-0.29793300	1.24871000
H	1.17111100	-1.11469000	-1.65427000
H	-1.48505700	0.11701500	-1.68421100
H	0.97678500	-3.43784100	-0.57897200
H	0.69728300	-2.64081100	0.96738900
H	-0.30090900	1.96365700	1.47421400
H	-3.24484100	1.45190500	-0.79942500
H	-2.72052200	1.14431900	0.85711400
H	-0.97515800	-2.35666400	-1.58715400
H	-1.43156500	-3.24991900	-0.15671300
H	4.06842600	-0.33493800	-1.48142700
H	3.77753900	1.17445600	-0.60604700
H	2.67941600	0.67565600	-1.89574400

H	3.71652700	-0.09871300	1.68375800
H	4.07358700	-1.59847900	0.81527600
H	2.64740100	-1.49399300	1.85431800
H	-2.03582600	3.44515100	0.53552800
H	-1.45869600	3.11962500	-1.10025200
H	0.69082300	4.17596900	0.87001400
H	1.05082200	3.58139500	-0.75610500
H	1.87469700	2.88454200	0.64490100
H	-3.45471000	-2.39382900	0.22111400
H	-3.37755100	-1.52784900	-1.31418100
H	-3.84009900	-0.67147000	0.16660500
H	-1.89757100	-1.75511200	1.88617300

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.368574 (Hartree/Particle)
Thermal correction to Energy=	0.385522
Thermal correction to Enthalpy=	0.386466
Thermal correction to Gibbs Free Energy=	0.325742
Sum of electronic and zero-point Energies=	-661.593260
Sum of electronic and thermal Energies=	-661.576311
Sum of electronic and thermal Enthalpies=	-661.575367
Sum of electronic and thermal Free Energies=	-661.636092

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.367829 (Hartree/Particle)
Thermal correction to Energy=	0.384826
Thermal correction to Enthalpy=	0.385770
Thermal correction to Gibbs Free Energy=	0.324962
Sum of electronic and zero-point Energies=	-661.598076
Sum of electronic and thermal Energies=	-661.581079
Sum of electronic and thermal Enthalpies=	-661.580135
Sum of electronic and thermal Free Energies=	-661.640942

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.367882 (Hartree/Particle)
Thermal correction to Energy=	0.384872
Thermal correction to Enthalpy=	0.385816
Thermal correction to Gibbs Free Energy=	0.325027
Sum of electronic and zero-point Energies=	-661.597794
Sum of electronic and thermal Energies=	-661.580804
Sum of electronic and thermal Enthalpies=	-661.579860
Sum of electronic and thermal Free Energies=	-661.640649

Name of anion	Globulol-O-H

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
O	-1.52015600	-0.97777900	1.46086700
C	1.01299600	-0.04740500	0.23528700
C	2.45549400	-0.44390500	-0.04188300
C	1.30649800	-1.27506700	-0.58424200
C	0.06222200	0.94028300	-0.38025500
C	-1.36834300	0.27678900	-0.60723900
C	0.59838200	-2.51844600	-0.11486200

C	-0.19246700	2.23714100	0.41609700
C	-1.69812500	-1.12019800	0.03673700
C	-2.36882800	1.38107000	-0.15035000
C	-0.89169300	-2.35555100	-0.49327800
C	3.28647600	0.30944500	-1.06477600
C	3.26387000	-0.93814600	1.14472000
C	-1.56568200	2.68640100	-0.09705800
C	0.91825700	3.27739400	0.28824600
C	-3.18355200	-1.43894500	-0.24148600
H	0.71646600	-0.29793300	1.24871000
H	1.17111100	-1.11469000	-1.65427000
H	0.42983500	1.23563100	-1.37150200
H	-1.48505700	0.11701500	-1.68421100
H	0.97678500	-3.43784100	-0.57897200
H	0.69728300	-2.64081100	0.96738900
H	-0.30090900	1.96365700	1.47421400
H	-3.24484100	1.45190500	-0.79942500
H	-2.72052200	1.14431900	0.85711400
H	-0.97515800	-2.35666400	-1.58715400
H	-1.43156500	-3.24991900	-0.15671300
H	4.06842600	-0.33493800	-1.48142700
H	3.77753900	1.17445600	-0.60604700
H	2.67941600	0.67565600	-1.89574400
H	3.71652700	-0.09871300	1.68375800
H	4.07358700	-1.59847900	0.81527600
H	2.64740100	-1.49399300	1.85431800
H	-2.03582600	3.44515100	0.53552800
H	-1.45869600	3.11962500	-1.10025200
H	0.69082300	4.17596900	0.87001400
H	1.05082200	3.58139500	-0.75610500
H	1.87469700	2.88454200	0.64490100
H	-3.45471000	-2.39382900	0.22111400
H	-3.37755100	-1.52784900	-1.31418100
H	-3.84009900	-0.67147000	0.16660500

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.366635 (Hartree/Particle)
Thermal correction to Energy=	0.383091
Thermal correction to Enthalpy=	0.384035
Thermal correction to Gibbs Free Energy=	0.325086
Sum of electronic and zero-point Energies=	-661.651124
Sum of electronic and thermal Energies=	-661.634668
Sum of electronic and thermal Enthalpies=	-661.633724
Sum of electronic and thermal Free Energies=	-661.692673

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.366991 (Hartree/Particle)
Thermal correction to Energy=	0.383413
Thermal correction to Enthalpy=	0.384357
Thermal correction to Gibbs Free Energy=	0.325470
Sum of electronic and zero-point Energies=	-661.729982
Sum of electronic and thermal Energies=	-661.713561
Sum of electronic and thermal Enthalpies=	-661.712617

Sum of electronic and thermal Free Energies= -661.771504

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.367082 (Hartree/Particle)
Thermal correction to Energy=	0.383449
Thermal correction to Enthalpy=	0.384393
Thermal correction to Gibbs Free Energy=	0.325673
Sum of electronic and zero-point Energies=	-661.727077
Sum of electronic and thermal Energies=	-661.710710
Sum of electronic and thermal Enthalpies=	-661.709766
Sum of electronic and thermal Free Energies=	-661.768486

Name of cationic radical	Globulol

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

O 0	-2.011800	0.325700	-1.717400
C 0	0.850400	-0.562900	-0.407300
C 0	2.388800	-0.553700	-0.600300
C 0	1.581100	0.745900	-0.802000
C 0	-0.051100	-0.308000	0.834300
C 0	-1.250900	0.677900	0.580900
C 0	0.862500	1.345700	-2.028500
C 0	-0.595700	-1.637100	1.444600
C 0	-1.562500	1.350100	-0.825200
C 0	-2.478900	-0.048500	1.207700
C 0	-0.401900	2.114300	-1.562200
C 0	3.237100	-0.713900	0.689000
C 0	2.971800	-1.226400	-1.872800
C 0	-2.043000	-1.350300	1.897100
C 0	0.247000	-2.249500	2.598800
C 0	-2.734200	2.381600	-0.676800
H 0	-2.285000	0.783400	-2.540600
H 0	0.349700	-1.114500	-1.209600
H 0	1.777200	1.472600	-0.007700
H 0	0.571900	0.143100	1.614500
H 0	-1.042300	1.537400	1.230400
H 0	1.556800	2.042300	-2.504500
H 0	0.595000	0.610400	-2.793200
H 0	-0.651100	-2.403800	0.663000
H 0	-2.987800	0.601100	1.927600
H 0	-3.227100	-0.312900	0.456400
H 0	-0.075500	2.951100	-0.937500
H 0	-0.795700	2.564900	-2.479800
H 0	4.289000	-0.513200	0.481900
H 0	3.158600	-1.738200	1.051800
H 0	2.942500	-0.038500	1.493400
H 0	2.715900	-2.286500	-1.879500
H 0	4.060100	-1.142300	-1.888400
H 0	2.613500	-0.784000	-2.802600
H 0	-2.703400	-2.181500	1.625400

H 0	-2.126800	-1.229400	2.980900
H 0	-0.222800	-3.156800	2.984700
H 0	0.344200	-1.544400	3.428200
H 0	1.247000	-2.515100	2.261200
H 0	-3.018600	2.825200	-1.633300
H 0	-2.448400	3.198500	-0.008900
H 0	-3.645200	1.939900	-0.273700

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

Zero-point correction=	0.380258 (Hartree/Particle)
Thermal correction to Energy=	0.397969
Thermal correction to Enthalpy=	0.398913
Thermal correction to Gibbs Free Energy=	0.336103
Sum of electronic and zero-point Energies=	-661.965853
Sum of electronic and thermal Energies=	-661.948142
Sum of electronic and thermal Enthalpies=	-661.947198
Sum of electronic and thermal Free Energies=	-662.010009

Name of compound	β-Himachalol

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

O	2.22530000	-0.51120000	1.54890000
C	0.19510000	-0.97710000	0.29270000
C	-0.40040000	0.39410000	0.74910000
C	0.04350000	1.74130000	0.05470000
C	1.73930000	-1.11660000	0.34200000
C	1.56320000	1.83540000	-0.24750000
C	-0.45770000	-1.47630000	-1.00440000
C	2.50230000	-0.50330000	-0.83860000
C	2.09770000	0.88770000	-1.31200000
C	-1.91750000	0.27440000	0.78450000
C	-1.97670000	-1.62100000	-0.84890000
C	-0.76030000	2.06440000	-1.23120000
C	-0.25610000	2.91010000	1.04310000
C	-2.62550000	-0.61770000	0.06970000
C	2.15060000	-2.60150000	0.44340000
C	-4.12280000	-0.68270000	0.15440000
H	-0.15300000	-1.67650000	1.07350000
H	-0.10120000	0.48380000	1.80450000
H	2.15010000	1.75400000	0.67410000
H	1.76690000	2.85300000	-0.61280000
H	-0.05410000	-2.45090000	-1.29970000
H	-0.23800000	-0.80320000	-1.83590000
H	2.44900000	-1.17090000	-1.70880000
H	3.56630000	-0.45350000	-0.56590000
H	1.39540000	0.79970000	-2.14560000
H	2.99120000	1.34650000	-1.75740000
H	-2.44470000	0.96520000	1.43790000
H	-2.18940000	-2.62330000	-0.45440000
H	-2.43740000	-1.56880000	-1.84270000
H	-0.36610000	2.96270000	-1.72160000
H	-0.73220000	1.25790000	-1.96470000
H	-1.81460000	2.26860000	-1.01290000

H	0.04670000	3.87520000	0.61940000
H	-1.32210000	2.98640000	1.28010000
H	0.28860000	2.77970000	1.98520000
H	1.89100000	-3.16930000	-0.45460000
H	3.23200000	-2.69260000	0.60200000
H	1.67690000	-3.08370000	1.30640000
H	1.77970000	-0.93800000	2.30060000
H	-4.56630000	-0.50280000	-0.83030000
H	-4.53150000	0.06280000	0.84480000
H	-4.44070000	-1.67030000	0.50420000

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.383406 (Hartree/Particle)
Thermal correction to Energy=	0.400124
Thermal correction to Enthalpy=	0.401068
Thermal correction to Gibbs Free Energy=	0.342073
Sum of electronic and zero-point Energies=	-662.256627
Sum of electronic and thermal Energies=	-662.239909
Sum of electronic and thermal Enthalpies=	-662.238965
Sum of electronic and thermal Free Energies=	-662.297961

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.382768 (Hartree/Particle)
Thermal correction to Energy=	0.399487
Thermal correction to Enthalpy=	0.400431
Thermal correction to Gibbs Free Energy=	0.341445
Sum of electronic and zero-point Energies=	-662.261730
Sum of electronic and thermal Energies=	-662.245010
Sum of electronic and thermal Enthalpies=	-662.244066
Sum of electronic and thermal Free Energies=	-662.303052

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.382800 (Hartree/Particle)
Thermal correction to Energy=	0.399520
Thermal correction to Enthalpy=	0.400465
Thermal correction to Gibbs Free Energy=	0.341480
Sum of electronic and zero-point Energies=	-662.261458
Sum of electronic and thermal Energies=	-662.244737
Sum of electronic and thermal Enthalpies=	-662.243793
Sum of electronic and thermal Free Energies=	-662.302778

Name of radical	β-Himachalol-C3-H	
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)		
O	2.22530000	-0.51120000	1.54890000
C	0.19510000	-0.97710000	0.29270000
C	-0.40040000	0.39410000	0.74910000
C	0.04350000	1.74130000	0.05470000
C	1.73930000	-1.11660000	0.34200000
C	1.56320000	1.83540000	-0.24750000
C	-0.45770000	-1.47630000	-1.00440000
C	2.50230000	-0.50330000	-0.83860000
C	2.09770000	0.88770000	-1.31200000
C	-1.91750000	0.27440000	0.78450000

C	-1.97670000	-1.62100000	-0.84890000
C	-0.76030000	2.06440000	-1.23120000
C	-0.25610000	2.91010000	1.04310000
C	-2.62550000	-0.61770000	0.06970000
C	2.15060000	-2.60150000	0.44340000
C	-4.12280000	-0.68270000	0.15440000
H	-0.15300000	-1.67650000	1.07350000
H	2.15010000	1.75400000	0.67410000
H	1.76690000	2.85300000	-0.61280000
H	-0.05410000	-2.45090000	-1.29970000
H	-0.23800000	-0.80320000	-1.83590000
H	2.44900000	-1.17090000	-1.70880000
H	3.56630000	-0.45350000	-0.56590000
H	1.39540000	0.79970000	-2.14560000
H	2.99120000	1.34650000	-1.75740000
H	-2.44470000	0.96520000	1.43790000
H	-2.18940000	-2.62330000	-0.45440000
H	-2.43740000	-1.56880000	-1.84270000
H	-0.36610000	2.96270000	-1.72160000
H	-0.73220000	1.25790000	-1.96470000
H	-1.81460000	2.26860000	-1.01290000
H	0.04670000	3.87520000	0.61940000
H	-1.32210000	2.98640000	1.28010000
H	0.28860000	2.77970000	1.98520000
H	1.89100000	-3.16930000	-0.45460000
H	3.23200000	-2.69260000	0.60200000
H	1.67690000	-3.08370000	1.30640000
H	1.77970000	-0.93800000	2.30060000
H	-4.56630000	-0.50280000	-0.83030000
H	-4.53150000	0.06280000	0.84480000
H	-4.44070000	-1.67030000	0.50420000

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

Zero-point correction=	0.369604	(Hartree/Particle)
Thermal correction to Energy=	0.386455	
Thermal correction to Enthalpy=	0.387399	
Thermal correction to Gibbs Free Energy=	0.326533	
Sum of electronic and zero-point Energies=	-661.631930	
Sum of electronic and thermal Energies=	-661.615080	
Sum of electronic and thermal Enthalpies=	-661.614136	
Sum of electronic and thermal Free Energies=	-661.675002	

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction=	0.369010	(Hartree/Particle)
Thermal correction to Energy=	0.385863	
Thermal correction to Enthalpy=	0.386808	
Thermal correction to Gibbs Free Energy=	0.325863	
Sum of electronic and zero-point Energies=	-661.636934	
Sum of electronic and thermal Energies=	-661.620081	
Sum of electronic and thermal Enthalpies=	-661.619137	
Sum of electronic and thermal Free Energies=	-661.680082	

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.369040 (Hartree/Particle)
Thermal correction to Energy=	0.385891
Thermal correction to Enthalpy=	0.386836
Thermal correction to Gibbs Free Energy=	0.325930
Sum of electronic and zero-point Energies=	-661.636661
Sum of electronic and thermal Energies=	-661.619809
Sum of electronic and thermal Enthalpies=	-661.618865
Sum of electronic and thermal Free Energies=	-661.679770

Name of anion	β-Himachalol-O-H		
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
O	-2.22507100	-0.46472500	-1.54523600
C	-0.19383400	-0.96332500	-0.27354100
C	0.41774300	0.39546800	-0.73408400
C	0.01352100	1.76739700	-0.04724500
C	-1.74100400	-1.10299400	-0.33989500
C	-1.50480400	1.88342700	0.24935000
C	0.45635900	-1.45646900	1.03038800
C	-2.52795100	-0.45154200	0.81030700
C	-2.07632600	0.93109800	1.31071400
C	1.92392100	0.22828300	-0.77256100
C	1.95709400	-1.70315500	0.81043800
C	0.82026400	2.06490400	1.23606800
C	0.34270700	2.89114600	-1.05864300
C	2.62048600	-0.69131900	-0.09691700
C	-2.13452800	-2.58924900	-0.42470500
C	4.11879200	-0.80276800	-0.21030300
H	0.16040700	-1.65916000	-1.05072400
H	0.08606100	0.51722900	-1.77092700
H	-2.06254700	1.76772800	-0.68275200
H	-1.67207900	2.91253000	0.58879500
H	-0.01015100	-2.38257800	1.37633400
H	0.31258200	-0.72390200	1.82656600
H	-2.54030300	-1.14460200	1.65762500
H	-3.55966800	-0.39007400	0.45074600
H	-1.35260200	0.81214800	2.12138700
H	-2.94591800	1.40722800	1.77567900
H	2.47300600	0.91960800	-1.40732300
H	2.10694000	-2.70265900	0.37628100
H	2.48243100	-1.72730300	1.77358300
H	0.48867400	3.01559800	1.66606200
H	0.70931000	1.30050000	2.00591900
H	1.88682100	2.14838600	1.02016800
H	0.11072600	3.87055700	-0.62934700
H	1.40015000	2.89888000	-1.33483900
H	-0.24707900	2.78041300	-1.97357600
H	-1.81218100	-3.15753700	0.45065700
H	-3.22011800	-2.67518000	-0.50906100
H	-1.68808800	-3.05505200	-1.30996200
H	4.60050400	-0.65658900	0.76385500

H	4.52751300	-0.06643600	-0.90543200
H	4.41493200	-1.79992200	-0.55815300

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.366862 (Hartree/Particle)
Thermal correction to Energy=	0.383335
Thermal correction to Enthalpy=	0.384280
Thermal correction to Gibbs Free Energy=	0.325719
Sum of electronic and zero-point Energies=	-661.666194
Sum of electronic and thermal Energies=	-661.649721
Sum of electronic and thermal Enthalpies=	-661.648776
Sum of electronic and thermal Free Energies=	-661.707337
Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.367468 (Hartree/Particle)
Thermal correction to Energy=	0.383923
Thermal correction to Enthalpy=	0.384867
Thermal correction to Gibbs Free Energy=	0.326290
Sum of electronic and zero-point Energies=	-661.747204
Sum of electronic and thermal Energies=	-661.730750
Sum of electronic and thermal Enthalpies=	-661.729805
Sum of electronic and thermal Free Energies=	-661.788382
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.367559 (Hartree/Particle)
Thermal correction to Energy=	0.383978
Thermal correction to Enthalpy=	0.384922
Thermal correction to Gibbs Free Energy=	0.326437
Sum of electronic and zero-point Energies=	-661.744224
Sum of electronic and thermal Energies=	-661.727804
Sum of electronic and thermal Enthalpies=	-661.726860
Sum of electronic and thermal Free Energies=	-661.785345

Name of cationic radical	β-Himachalol

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
O 0	2.225300	-0.511200	1.548900
C 0	0.195100	-0.977100	0.292700
C 0	-0.400400	0.394100	0.749100
C 0	0.043500	1.741300	0.054700
C 0	1.739300	-1.116600	0.342000
C 0	1.563200	1.835400	-0.247500
C 0	-0.457700	-1.476300	-1.004400
C 0	2.502300	-0.503300	-0.838600
C 0	2.097700	0.887700	-1.312000
C 0	-1.917500	0.274400	0.784500
C 0	-1.976700	-1.621000	-0.848900
C 0	-0.760300	2.064400	-1.231200
C 0	-0.256100	2.910100	1.043100
C 0	-2.625500	-0.617700	0.069700
C 0	2.150600	-2.601500	0.443400
C 0	-4.122800	-0.682700	0.154400
H 0	1.779700	-0.938000	2.300600
H 0	-0.153000	-1.676500	1.073500

H 0	-0.101200	0.483800	1.804500
H 0	2.150100	1.754000	0.674100
H 0	1.766900	2.853000	-0.612800
H 0	-0.054100	-2.450900	-1.299700
H 0	-0.238000	-0.803200	-1.835900
H 0	2.449000	-1.170900	-1.708800
H 0	3.566300	-0.453500	-0.565900
H 0	1.395400	0.799700	-2.145600
H 0	2.991200	1.346500	-1.757400
H 0	-2.444700	0.965200	1.437900
H 0	-2.189400	-2.623300	-0.454400
H 0	-2.437400	-1.568800	-1.842700
H 0	-0.366100	2.962700	-1.721600
H 0	-0.732200	1.257900	-1.964700
H 0	-1.814600	2.268600	-1.012900
H 0	0.046700	3.875200	0.619400
H 0	-1.322100	2.986400	1.280100
H 0	0.288600	2.779700	1.985200
H 0	1.891000	-3.169300	-0.454600
H 0	3.232000	-2.692600	0.602000
H 0	1.676900	-3.083700	1.306400
H 0	-4.566300	-0.502800	-0.830300
H 0	-4.531500	0.062800	0.844800
H 0	-4.440700	-1.670300	0.504200

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

Zero-point correction=	0.380192 (Hartree/Particle)
Thermal correction to Energy=	0.397714
Thermal correction to Enthalpy=	0.398658
Thermal correction to Gibbs Free Energy=	0.337221
Sum of electronic and zero-point Energies=	-661.973818
Sum of electronic and thermal Energies=	-661.956296
Sum of electronic and thermal Enthalpies=	-661.955352
Sum of electronic and thermal Free Energies=	-662.016789

Name of compound	α-Acorenol

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

O	1.96550000	1.52000000	1.15520000
C	-0.09100000	-0.29930000	-0.11320000
C	1.45270000	-0.32600000	-0.29140000
C	-0.38980000	-1.82420000	0.07620000
C	1.94060000	-1.36650000	0.72410000
C	0.76670000	-2.31710000	0.96520000
C	-0.79670000	0.34170000	-1.32680000
C	-0.52830000	0.50150000	1.15200000
C	2.19610000	0.99780000	-0.15500000
C	-2.32660000	0.32920000	-1.20320000
C	-0.43120000	-2.65810000	-1.21140000
C	-2.00900000	0.74500000	1.23340000
C	-2.83340000	0.66030000	0.17640000
C	1.69220000	2.01760000	-1.17730000
C	3.70280000	0.78980000	-0.30570000

C	-4.31060000	0.88830000	0.30170000
H	1.67220000	-0.72330000	-1.29360000
H	-1.34190000	-1.98350000	0.59600000
H	2.24330000	-0.92380000	1.67960000
H	2.80470000	-1.91680000	0.33460000
H	1.04550000	-3.35710000	0.76400000
H	0.47250000	-2.27040000	2.02070000
H	-0.49970000	-0.13730000	-2.26680000
H	-0.56000000	1.39470000	-1.43860000
H	-0.14200000	1.52090000	1.14700000
H	-0.19380000	0.01520000	2.07400000
H	-2.71420000	-0.65670000	-1.48340000
H	-2.73850000	1.04310000	-1.92750000
H	-0.57690000	-3.71730000	-0.97070000
H	-1.26210000	-2.36370000	-1.85730000
H	0.49400000	-2.57850000	-1.78980000
H	-2.40570000	1.00840000	2.21040000
H	2.45000000	2.80050000	-1.31830000
H	1.52590000	1.58280000	-2.16730000
H	0.82510000	2.57740000	-0.81720000
H	4.11450000	0.16760000	0.49590000
H	4.23690000	1.74510000	-0.23460000
H	3.95250000	0.33330000	-1.26920000
H	2.42820000	2.37270000	1.22420000
H	-4.85990000	-0.00290000	-0.01860000
H	-4.61950000	1.73130000	-0.32470000
H	-4.60850000	1.11130000	1.33160000

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.382588 (Hartree/Particle)
Thermal correction to Energy=	0.399648
Thermal correction to Enthalpy=	0.400592
Thermal correction to Gibbs Free Energy=	0.340237
Sum of electronic and zero-point Energies=	-662.261241
Sum of electronic and thermal Energies=	-662.244181
Sum of electronic and thermal Enthalpies=	-662.243237
Sum of electronic and thermal Free Energies=	-662.303592

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.381847 (Hartree/Particle)
Thermal correction to Energy=	0.398960
Thermal correction to Enthalpy=	0.399904
Thermal correction to Gibbs Free Energy=	0.339422
Sum of electronic and zero-point Energies=	-662.266498
Sum of electronic and thermal Energies=	-662.249385
Sum of electronic and thermal Enthalpies=	-662.248440
Sum of electronic and thermal Free Energies=	-662.308923

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.381896 (Hartree/Particle)
Thermal correction to Energy=	0.399002
Thermal correction to Enthalpy=	0.399946
Thermal correction to Gibbs Free Energy=	0.339491
Sum of electronic and zero-point Energies=	-662.266202

Sum of electronic and thermal Energies=	-662.249096
Sum of electronic and thermal Enthalpies=	-662.248152
Sum of electronic and thermal Free Energies=	-662.308607

Name of radical	α-Acorenol-C8-H		
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
O	1.96550000	1.52000000	1.15520000
C	-0.09100000	-0.29930000	-0.11320000
C	1.45270000	-0.32600000	-0.29140000
C	-0.38980000	-1.82420000	0.07620000
C	1.94060000	-1.36650000	0.72410000
C	0.76670000	-2.31710000	0.96520000
C	-0.79670000	0.34170000	-1.32680000
C	-0.52830000	0.50150000	1.15200000
C	2.19610000	0.99780000	-0.15500000
C	-2.32660000	0.32920000	-1.20320000
C	-0.43120000	-2.65810000	-1.21140000
C	-2.00900000	0.74500000	1.23340000
C	-2.83340000	0.66030000	0.17640000
C	1.69220000	2.01760000	-1.17730000
C	3.70280000	0.78980000	-0.30570000
C	-4.31060000	0.88830000	0.30170000
H	1.67220000	-0.72330000	-1.29360000
H	-1.34190000	-1.98350000	0.59600000
H	2.24330000	-0.92380000	1.67960000
H	2.80470000	-1.91680000	0.33460000
H	1.04550000	-3.35710000	0.76400000
H	0.47250000	-2.27040000	2.02070000
H	-0.49970000	-0.13730000	-2.26680000
H	-0.56000000	1.39470000	-1.43860000
H	-0.19380000	0.01520000	2.07400000
H	-2.71420000	-0.65670000	-1.48340000
H	-2.73850000	1.04310000	-1.92750000
H	-0.57690000	-3.71730000	-0.97070000
H	-1.26210000	-2.36370000	-1.85730000
H	0.49400000	-2.57850000	-1.78980000
H	-2.40570000	1.00840000	2.21040000
H	2.45000000	2.80050000	-1.31830000
H	1.52590000	1.58280000	-2.16730000
H	0.82510000	2.57740000	-0.81720000
H	4.11450000	0.16760000	0.49590000
H	4.23690000	1.74510000	-0.23460000
H	3.95250000	0.33330000	-1.26920000
H	2.42820000	2.37270000	1.22420000
H	-4.85990000	-0.00290000	-0.01860000
H	-4.61950000	1.73130000	-0.32470000
H	-4.60850000	1.11130000	1.33160000

Frequency and Energy at B3LYP/6-311G (d,p) (gas)		
Zero-point correction=	0.368735	(Hartree/Particle)
Thermal correction to Energy=	0.385874	
Thermal correction to Enthalpy=	0.386819	

Thermal correction to Gibbs Free Energy=	0.325397
Sum of electronic and zero-point Energies=	-661.637989
Sum of electronic and thermal Energies=	-661.620849
Sum of electronic and thermal Enthalpies=	-661.619905
Sum of electronic and thermal Free Energies=	-661.681327
Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.367994 (Hartree/Particle)
Thermal correction to Energy=	0.385212
Thermal correction to Enthalpy=	0.386156
Thermal correction to Gibbs Free Energy=	0.324434
Sum of electronic and zero-point Energies=	-661.643160
Sum of electronic and thermal Energies=	-661.625942
Sum of electronic and thermal Enthalpies=	-661.624998
Sum of electronic and thermal Free Energies=	-661.686720
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.368030 (Hartree/Particle)
Thermal correction to Energy=	0.385246
Thermal correction to Enthalpy=	0.386190
Thermal correction to Gibbs Free Energy=	0.324465
Sum of electronic and zero-point Energies=	-661.642871
Sum of electronic and thermal Energies=	-661.625655
Sum of electronic and thermal Enthalpies=	-661.624711
Sum of electronic and thermal Free Energies=	-661.686436

Name of anion	α-Acorenol-O-H	
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)		
O	2.30875700	-1.28124000	-1.24761900
C	-0.18769500	0.25805500	0.08547500
C	1.37314800	0.34935600	0.27342900
C	-0.55586100	1.76572900	-0.16598000
C	1.83478300	1.50506000	-0.66737500
C	0.55876700	2.25514800	-1.11106900
C	-0.92293500	-0.32259700	1.31381300
C	-0.61146700	-0.57809900	-1.15018400
C	2.29496300	-0.89849300	0.14329400
C	-2.45259700	-0.27885100	1.17202000
C	-0.60400500	2.64557400	1.09587300
C	-2.08916400	-0.87324500	-1.20412400
C	-2.93613300	-0.75012300	-0.17942100
C	1.85151700	-2.10355500	0.98724000
C	3.72786200	-0.51167300	0.55931000
C	-4.40700100	-1.04836900	-0.29867900
H	1.51511500	0.68123800	1.30869000
H	-1.53262500	1.82334000	-0.65502600
H	2.36707500	1.09896500	-1.52753500
H	2.52540800	2.17245700	-0.14627800
H	0.67690700	3.34115200	-1.06628800
H	0.31698000	2.01167700	-2.14827500
H	-0.61694000	0.20025400	2.22523000
H	-0.63175700	-1.36587900	1.44907800

H	-0.05384300	-1.51808300	-1.17530100
H	-0.31361500	-0.07091700	-2.07299200
H	-2.83576100	0.73478100	1.35174000
H	-2.90580700	-0.89928300	1.95585800
H	-0.83251700	3.67748300	0.81335800
H	-1.36982600	2.32798400	1.80623900
H	0.35386200	2.66173000	1.62533400
H	-2.47193500	-1.22202500	-2.16168100
H	2.60686400	-2.89455000	0.92276900
H	1.74049800	-1.83896900	2.04204300
H	0.90977600	-2.51765600	0.62945500
H	4.11349200	0.29838800	-0.06027700
H	4.39603900	-1.37228900	0.44408700
H	3.76896000	-0.20014600	1.60693100
H	-5.01040200	-0.17208600	-0.03129700
H	-4.70500300	-1.85219800	0.38534000
H	-4.67741600	-1.34769200	-1.31364300

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.366132 (Hartree/Particle)
Thermal correction to Energy=	0.382857
Thermal correction to Enthalpy=	0.383801
Thermal correction to Gibbs Free Energy=	0.323954
Sum of electronic and zero-point Energies=	-661.673128
Sum of electronic and thermal Energies=	-661.656404
Sum of electronic and thermal Enthalpies=	-661.655460
Sum of electronic and thermal Free Energies=	-661.715307

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.366586 (Hartree/Particle)
Thermal correction to Energy=	0.383400
Thermal correction to Enthalpy=	0.384344
Thermal correction to Gibbs Free Energy=	0.323974
Sum of electronic and zero-point Energies=	-661.754083
Sum of electronic and thermal Energies=	-661.737269
Sum of electronic and thermal Enthalpies=	-661.736325
Sum of electronic and thermal Free Energies=	-661.796695

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.366538 (Hartree/Particle)
Thermal correction to Energy=	0.383366
Thermal correction to Enthalpy=	0.384311
Thermal correction to Gibbs Free Energy=	0.323924
Sum of electronic and zero-point Energies=	-661.751209
Sum of electronic and thermal Energies=	-661.734380
Sum of electronic and thermal Enthalpies=	-661.733436
Sum of electronic and thermal Free Energies=	-661.793822

Name of cationic radical	α-Acorenol

Cartesian Coordinates optimized at B3LYP/6-311G (d,p) (d,p)			
O 0	1.965500	1.520000	1.155200
C 0	-0.091000	-0.299300	-0.113200
C 0	1.452700	-0.326000	-0.291400

C	0	-0.389800	-1.824200	0.076200
C	0	1.940600	-1.366500	0.724100
C	0	0.766700	-2.317100	0.965200
C	0	-0.796700	0.341700	-1.326800
C	0	-0.528300	0.501500	1.152000
C	0	2.196100	0.997800	-0.155000
C	0	-2.326600	0.329200	-1.203200
C	0	-0.431200	-2.658100	-1.211400
C	0	-2.009000	0.745000	1.233400
C	0	-2.833400	0.660300	0.176400
C	0	1.692200	2.017600	-1.177300
C	0	3.702800	0.789800	-0.305700
C	0	-4.310600	0.888300	0.301700
H	0	2.428200	2.372700	1.224200
H	0	1.672200	-0.723300	-1.293600
H	0	-1.341900	-1.983500	0.596000
H	0	2.243300	-0.923800	1.679600
H	0	2.804700	-1.916800	0.334600
H	0	1.045500	-3.357100	0.764000
H	0	0.472500	-2.270400	2.020700
H	0	-0.499700	-0.137300	-2.266800
H	0	-0.560000	1.394700	-1.438600
H	0	-0.142000	1.520900	1.147000
H	0	-0.193800	0.015200	2.074000
H	0	-2.714200	-0.656700	-1.483400
H	0	-2.738500	1.043100	-1.927500
H	0	-0.576900	-3.717300	-0.970700
H	0	-1.262100	-2.363700	-1.857300
H	0	0.494000	-2.578500	-1.789800
H	0	-2.405700	1.008400	2.210400
H	0	2.450000	2.800500	-1.318300
H	0	1.525900	1.582800	-2.167300
H	0	0.825100	2.577400	-0.817200
H	0	4.114500	0.167600	0.495900
H	0	4.236900	1.745100	-0.234600
H	0	3.952500	0.333300	-1.269200
H	0	-4.859900	-0.002900	-0.018600
H	0	-4.619500	1.731300	-0.324700
H	0	-4.608500	1.111300	1.331600

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

Zero-point correction=	0.379301 (Hartree/Particle)
Thermal correction to Energy=	0.396602
Thermal correction to Enthalpy=	0.397547
Thermal correction to Gibbs Free Energy=	0.335580
Sum of electronic and zero-point Energies=	-661.980410
Sum of electronic and thermal Energies=	-661.963108
Sum of electronic and thermal Enthalpies=	-661.962164
Sum of electronic and thermal Free Energies=	-662.024130

Name of compound	trans-Nuciferol

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
O	-5.29890000	-1.78960000	-0.23870000
C	0.77650000	2.03690000	-0.07810000
C	-0.71820000	1.71130000	0.14540000
C	1.67800000	0.81510000	-0.05940000
C	-1.35990000	0.81980000	-0.92990000
C	1.25390000	3.05660000	0.96400000
C	2.42400000	0.51450000	-1.18280000
C	1.72800000	0.03680000	1.08100000
C	-2.83220000	0.60630000	-0.71300000
C	3.25190000	-0.60800000	-1.16530000
C	2.55600000	-1.08580000	1.09840000
C	3.31780000	-1.40790000	-0.02460000
C	-3.44030000	-0.31350000	0.06140000
C	-4.92940000	-0.48780000	0.19890000
C	-2.61090000	-1.29720000	0.84840000
C	4.20380000	-2.60750000	-0.00560000
H	0.85900000	2.52360000	-1.05960000
H	-0.86120000	1.25350000	1.13250000
H	-1.27370000	2.65910000	0.17570000
H	-1.22690000	1.28900000	-1.91310000
H	-0.84250000	-0.14360000	-0.99640000
H	2.31140000	3.30380000	0.81710000
H	0.68140000	3.98690000	0.87970000
H	1.13480000	2.68890000	1.98890000
H	2.38090000	1.12970000	-2.07640000
H	1.14240000	0.27090000	1.96450000
H	-3.47160000	1.29710000	-1.26140000
H	3.84200000	-0.84780000	-2.04590000
H	2.60010000	-1.70050000	1.99360000
H	-5.48500000	0.24610000	-0.39390000
H	-5.23230000	-0.37410000	1.24450000
H	-2.93720000	-1.30280000	1.89440000
H	-2.73790000	-2.30750000	0.44570000
H	-1.54070000	-1.08010000	0.85910000
H	4.30160000	-3.04240000	-1.00620000
H	5.19950000	-2.33330000	0.35660000
H	3.79670000	-3.38920000	0.64470000
H	-5.05230000	-1.86650000	-1.17640000

Frequency and Energy at B3LYP/6-311G (d,p) (gas)		
Zero-point correction=	0.334458	(Hartree/Particle)
Thermal correction to Energy=	0.352521	
Thermal correction to Enthalpy=	0.353465	
Thermal correction to Gibbs Free Energy=	0.285532	
Sum of electronic and zero-point Energies=	-659.900395	
Sum of electronic and thermal Energies=	-659.882332	
Sum of electronic and thermal Enthalpies=	-659.881388	
Sum of electronic and thermal Free Energies=	-659.949321	

Frequency and Energy at B3LYP/6-311G (d,p) (water)		
Zero-point correction=	0.333900	(Hartree/Particle)
Thermal correction to Energy=	0.352052	

Thermal correction to Enthalpy=	0.352997
Thermal correction to Gibbs Free Energy=	0.284639
Sum of electronic and zero-point Energies=	-659.908143
Sum of electronic and thermal Energies=	-659.889991
Sum of electronic and thermal Enthalpies=	-659.889046
Sum of electronic and thermal Free Energies=	-659.957404

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.333947 (Hartree/Particle)
Thermal correction to Energy=	0.352084
Thermal correction to Enthalpy=	0.353028
Thermal correction to Gibbs Free Energy=	0.284763
Sum of electronic and zero-point Energies=	-659.907734
Sum of electronic and thermal Energies=	-659.889598
Sum of electronic and thermal Enthalpies=	-659.888654
Sum of electronic and thermal Free Energies=	-659.956919

Name of radical	trans-Nuciferol-C14-H

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
O	-5.29890000	-1.78960000	-0.23870000
C	0.77650000	2.03690000	-0.07810000
C	-0.71820000	1.71130000	0.14540000
C	1.67800000	0.81510000	-0.05940000
C	-1.35990000	0.81980000	-0.92990000
C	1.25390000	3.05660000	0.96400000
C	2.42400000	0.51450000	-1.18280000
C	1.72800000	0.03680000	1.08100000
C	-2.83220000	0.60630000	-0.71300000
C	3.25190000	-0.60800000	-1.16530000
C	2.55600000	-1.08580000	1.09840000
C	3.31780000	-1.40790000	-0.02460000
C	-3.44030000	-0.31350000	0.06140000
C	-4.92940000	-0.48780000	0.19890000
C	-2.61090000	-1.29720000	0.84840000
C	4.20380000	-2.60750000	-0.00560000
H	0.85900000	2.52360000	-1.05960000
H	-0.86120000	1.25350000	1.13250000
H	-1.27370000	2.65910000	0.17570000
H	-1.22690000	1.28900000	-1.91310000
H	-0.84250000	-0.14360000	-0.99640000
H	2.31140000	3.30380000	0.81710000
H	0.68140000	3.98690000	0.87970000
H	1.13480000	2.68890000	1.98890000
H	2.38090000	1.12970000	-2.07640000
H	1.14240000	0.27090000	1.96450000
H	-3.47160000	1.29710000	-1.26140000
H	3.84200000	-0.84780000	-2.04590000
H	2.60010000	-1.70050000	1.99360000
H	-5.23230000	-0.37410000	1.24450000
H	-2.93720000	-1.30280000	1.89440000

H	-2.73790000	-2.30750000	0.44570000
H	-1.54070000	-1.08010000	0.85910000
H	4.30160000	-3.04240000	-1.00620000
H	5.19950000	-2.33330000	0.35660000
H	3.79670000	-3.38920000	0.64470000
H	-5.05230000	-1.86650000	-1.17640000

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction= (Hartree/Particle)	0.320544
Thermal correction to Energy=	0.338659
Thermal correction to Enthalpy=	0.339604
Thermal correction to Gibbs Free Energy=	0.270989
Sum of electronic and zero-point Energies=	-659.275609
Sum of electronic and thermal Energies=	-659.257493
Sum of electronic and thermal Enthalpies=	-659.256549
Sum of electronic and thermal Free Energies=	-659.325163

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction= (Hartree/Particle)	0.320187
Thermal correction to Energy=	0.338265
Thermal correction to Enthalpy=	0.339210
Thermal correction to Gibbs Free Energy=	0.270925
Sum of electronic and zero-point Energies=	-659.283274
Sum of electronic and thermal Energies=	-659.265195
Sum of electronic and thermal Enthalpies=	-659.264251
Sum of electronic and thermal Free Energies=	-659.332535

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction= (Hartree/Particle)	0.320205
Thermal correction to Energy=	0.338288
Thermal correction to Enthalpy=	0.339232
Thermal correction to Gibbs Free Energy=	0.270882
Sum of electronic and zero-point Energies=	-659.282880
Sum of electronic and thermal Energies=	-659.264798
Sum of electronic and thermal Enthalpies=	-659.263853
Sum of electronic and thermal Free Energies=	-659.332204

Name of anion	trans-Nuciferol-O-H		
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
O	5.56439600	-1.32365900	0.35970800
C	-0.92991700	2.09181500	0.21063300
C	0.53683300	1.81430800	-0.18453600
C	-1.80892900	0.85179100	0.12928600
C	1.25030200	0.79070000	0.71832000
C	-1.51006100	3.24867900	-0.62436600
C	-2.47014400	0.36437300	1.25828600
C	-1.99565000	0.16319300	-1.07652600

C	2.69930100	0.62197100	0.35675700
C	-3.28662400	-0.76397100	1.19051600
C	-2.80846600	-0.96262100	-1.14424100
C	-3.47286700	-1.44798600	-0.01150300
C	3.31981600	-0.46604700	-0.11776200
C	4.79798800	-0.40689300	-0.43014600
C	2.67780000	-1.80582200	-0.37144200
C	-4.37357900	-2.65667000	-0.09884600
H	-0.92730100	2.41299700	1.25970400
H	0.58034600	1.46821100	-1.22339900
H	1.08679100	2.76272800	-0.15708300
H	1.18308700	1.14102700	1.75766200
H	0.71848500	-0.16154300	0.67996600
H	-2.53674300	3.47234600	-0.32431000
H	-0.91177100	4.15599100	-0.49826600
H	-1.52151200	3.00175700	-1.69004900
H	-2.34367600	0.87307200	2.20915600
H	-1.49808700	0.50694800	-1.97751400
H	3.30515200	1.52015200	0.48343400
H	-3.78353900	-1.11699600	2.08886300
H	-2.92971800	-1.47540800	-2.09379400
H	5.16731400	0.61977500	-0.31060500
H	4.98263500	-0.71085900	-1.46528100
H	2.66596100	-2.02457000	-1.44609000
H	3.26958100	-2.59454600	0.10070500
H	1.65407500	-1.86972900	-0.00442000
H	-4.59830300	-3.05780900	0.89166000
H	-5.32648300	-2.40565100	-0.57728900
H	-3.91519000	-3.45440400	-0.68971400

Frequency and Energy at B3LYP/6-311G (d,p) (gas)		
Zero-point correction=	0.317112	(Hartree/Particle)
Thermal correction to Energy=	0.334920	
Thermal correction to Enthalpy=	0.335864	
Thermal correction to Gibbs Free Energy=	0.267760	
Sum of electronic and zero-point Energies=	-659.295271	
Sum of electronic and thermal Energies=	-659.277462	
Sum of electronic and thermal Enthalpies=	-659.276518	
Sum of electronic and thermal Free Energies=	-659.344622	

Frequency and Energy at B3LYP/6-311G (d,p) (water)		
Zero-point correction=	0.318284	(Hartree/Particle)
Thermal correction to Energy=	0.336011	
Thermal correction to Enthalpy=	0.336956	
Thermal correction to Gibbs Free Energy=	0.269840	
Sum of electronic and zero-point Energies=	-659.393220	
Sum of electronic and thermal Energies=	-659.375493	
Sum of electronic and thermal Enthalpies=	-659.374549	
Sum of electronic and thermal Free Energies=	-659.441664	

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)		
Zero-point correction=	0.318282	(Hartree/Particle)
Thermal correction to Energy=	0.335999	

Thermal correction to Enthalpy=	0.336944
Thermal correction to Gibbs Free Energy=	0.269726
Sum of electronic and zero-point Energies=	-659.389852
Sum of electronic and thermal Energies=	-659.372134
Sum of electronic and thermal Enthalpies=	-659.371190
Sum of electronic and thermal Free Energies=	-659.438408

Name of cationic radical	trans-Nuciferol

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

O 0	-5.298900	-1.789600	-0.238700
C 0	0.776500	2.036900	-0.078100
C 0	-0.718200	1.711300	0.145400
C 0	1.678000	0.815100	-0.059400
C 0	-1.359900	0.819800	-0.929900
C 0	1.253900	3.056600	0.964000
C 0	2.424000	0.514500	-1.182800
C 0	1.728000	0.036800	1.081000
C 0	-2.832200	0.606300	-0.713000
C 0	3.251900	-0.608000	-1.165300
C 0	2.556000	-1.085800	1.098400
C 0	3.317800	-1.407900	-0.024600
C 0	-3.440300	-0.313500	0.061400
C 0	-4.929400	-0.487800	0.198900
C 0	-2.610900	-1.297200	0.848400
C 0	4.203800	-2.607500	-0.005600
H 0	-5.052300	-1.866500	-1.176400
H 0	0.859000	2.523600	-1.059600
H 0	-0.861200	1.253500	1.132500
H 0	-1.273700	2.659100	0.175700
H 0	-1.226900	1.289000	-1.913100
H 0	-0.842500	-0.143600	-0.996400
H 0	2.311400	3.303800	0.817100
H 0	0.681400	3.986900	0.879700
H 0	1.134800	2.688900	1.988900
H 0	2.380900	1.129700	-2.076400
H 0	1.142400	0.270900	1.964500
H 0	-3.471600	1.297100	-1.261400
H 0	3.842000	-0.847800	-2.045900
H 0	2.600100	-1.700500	1.993600
H 0	-5.485000	0.246100	-0.393900
H 0	-5.232300	-0.374100	1.244500
H 0	-2.937200	-1.302800	1.894400
H 0	-2.737900	-2.307500	0.445700
H 0	-1.540700	-1.080100	0.859100
H 0	4.301600	-3.042400	-1.006200
H 0	5.199500	-2.333300	0.356600
H 0	3.796700	-3.389200	0.644700

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

Zero-point correction=	0.332074 (Hartree/Particle)

Thermal correction to Energy=	0.350769
Thermal correction to Enthalpy=	0.351713
Thermal correction to Gibbs Free Energy=	0.281417
Sum of electronic and zero-point Energies=	-659.616138
Sum of electronic and thermal Energies=	-659.597443
Sum of electronic and thermal Enthalpies=	-659.596499
Sum of electronic and thermal Free Energies=	-659.666794

Name of compound	α-Santalol acetate

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

O	-3.20160000	-0.44180000	0.36720000
O	-3.22690000	-2.23080000	-1.09410000
C	2.71670000	-0.37050000	0.87820000
C	2.18450000	-1.69930000	0.43640000
C	3.54730000	-1.27000000	0.01510000
C	2.10380000	0.71080000	-0.00250000
C	1.99950000	-0.21700000	-1.28520000
C	1.25910000	-1.48710000	-0.74150000
C	3.44940000	-0.79710000	-1.41870000
C	3.07450000	-0.11990000	2.28910000
C	0.74600000	1.20090000	0.51430000
C	3.02810000	1.91930000	-0.19100000
C	-0.00130000	1.97640000	-0.56380000
C	-1.33570000	2.44500000	-0.05640000
C	-2.51320000	1.79360000	-0.11270000
C	-2.70050000	0.40420000	-0.65920000
C	-3.76300000	2.43940000	0.42720000
C	-3.42170000	-1.74380000	0.01130000
C	-3.94530000	-2.51240000	1.18650000
H	2.01870000	-2.52470000	1.10070000
H	4.43810000	-1.76270000	0.35270000
H	1.59780000	0.22210000	-2.19810000
H	1.29690000	-2.32470000	-1.44550000
H	0.22490000	-1.30770000	-0.44430000
H	4.20090000	-0.04640000	-1.67250000
H	3.50390000	-1.62850000	-2.12880000
H	3.80470000	0.69160000	2.36790000
H	3.51320000	-1.00610000	2.76050000
H	2.19100000	0.15990000	2.87120000
H	0.13000000	0.37120000	0.88050000
H	0.89410000	1.84080000	1.39540000
H	2.97030000	2.60020000	0.66620000
H	2.77360000	2.48500000	-1.09280000
H	4.08180000	1.63260000	-0.26970000
H	0.56120000	2.86380000	-0.87450000
H	-0.14500000	1.37970000	-1.46870000
H	-1.31860000	3.43700000	0.39330000
H	-1.76740000	-0.01780000	-1.04230000
H	-3.41950000	0.44070000	-1.48690000
H	-4.53290000	2.48050000	-0.35040000

H	-3.58690000	3.46490000	0.76900000
H	-4.15550000	1.87150000	1.27670000
H	-4.89100000	-2.07870000	1.52100000
H	-4.12320000	-3.55050000	0.89120000
H	-3.20900000	-2.50090000	1.99400000

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

Zero-point correction=	0.396537 (Hartree/Particle)
Thermal correction to Energy=	0.416874
Thermal correction to Enthalpy=	0.417818
Thermal correction to Gibbs Free Energy=	0.344693
Sum of electronic and zero-point Energies=	-813.703558
Sum of electronic and thermal Energies=	-813.683221
Sum of electronic and thermal Enthalpies=	-813.682277
Sum of electronic and thermal Free Energies=	-813.755402

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction=	0.395659 (Hartree/Particle)
Thermal correction to Energy=	0.416072
Thermal correction to Enthalpy=	0.417016
Thermal correction to Gibbs Free Energy=	0.343670
Sum of electronic and zero-point Energies=	-813.711238
Sum of electronic and thermal Energies=	-813.690825
Sum of electronic and thermal Enthalpies=	-813.689880
Sum of electronic and thermal Free Energies=	-813.763226

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction=	0.395709 (Hartree/Particle)
Thermal correction to Energy=	0.416119
Thermal correction to Enthalpy=	0.417064
Thermal correction to Gibbs Free Energy=	0.343718
Sum of electronic and zero-point Energies=	-813.710872
Sum of electronic and thermal Energies=	-813.690462
Sum of electronic and thermal Enthalpies=	-813.689518
Sum of electronic and thermal Free Energies=	-813.762863

Name of radical	α-Santalol acetate-C13-H

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

O	-3.20160000	-0.44180000	0.36720000
O	-3.22690000	-2.23080000	-1.09410000
C	2.71670000	-0.37050000	0.87820000
C	2.18450000	-1.69930000	0.43640000
C	3.54730000	-1.27000000	0.01510000
C	2.10380000	0.71080000	-0.00250000
C	1.99950000	-0.21700000	-1.28520000
C	1.25910000	-1.48710000	-0.74150000
C	3.44940000	-0.79710000	-1.41870000
C	3.07450000	-0.11990000	2.28910000
C	0.74600000	1.20090000	0.51430000
C	3.02810000	1.91930000	-0.19100000
C	-0.00130000	1.97640000	-0.56380000
C	-1.33570000	2.44500000	-0.05640000

C	-2.51320000	1.79360000	-0.11270000
C	-2.70050000	0.40420000	-0.65920000
C	-3.76300000	2.43940000	0.42720000
C	-3.42170000	-1.74380000	0.01130000
C	-3.94530000	-2.51240000	1.18650000
H	2.01870000	-2.52470000	1.10070000
H	4.43810000	-1.76270000	0.35270000
H	1.59780000	0.22210000	-2.19810000
H	1.29690000	-2.32470000	-1.44550000
H	0.22490000	-1.30770000	-0.44430000
H	4.20090000	-0.04640000	-1.67250000
H	3.50390000	-1.62850000	-2.12880000
H	3.80470000	0.69160000	2.36790000
H	3.51320000	-1.00610000	2.76050000
H	2.19100000	0.15990000	2.87120000
H	0.13000000	0.37120000	0.88050000
H	0.89410000	1.84080000	1.39540000
H	2.97030000	2.60020000	0.66620000
H	2.77360000	2.48500000	-1.09280000
H	4.08180000	1.63260000	-0.26970000
H	-0.14500000	1.37970000	-1.46870000
H	-1.31860000	3.43700000	0.39330000
H	-1.76740000	-0.01780000	-1.04230000
H	-3.41950000	0.44070000	-1.48690000
H	-4.53290000	2.48050000	-0.35040000
H	-3.58690000	3.46490000	0.76900000
H	-4.15550000	1.87150000	1.27670000
H	-4.89100000	-2.07870000	1.52100000
H	-4.12320000	-3.55050000	0.89120000
H	-3.20900000	-2.50090000	1.99400000

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.382610 (Hartree/Particle)
Thermal correction to Energy=	0.403039
Thermal correction to Enthalpy=	0.403983
Thermal correction to Gibbs Free Energy=	0.329865
Sum of electronic and zero-point Energies=	-813.078570
Sum of electronic and thermal Energies=	-813.058141
Sum of electronic and thermal Enthalpies=	-813.057197
Sum of electronic and thermal Free Energies=	-813.131315

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.381934 (Hartree/Particle)
Thermal correction to Energy=	0.402350
Thermal correction to Enthalpy=	0.403295
Thermal correction to Gibbs Free Energy=	0.329573
Sum of electronic and zero-point Energies=	-813.086331
Sum of electronic and thermal Energies=	-813.065915
Sum of electronic and thermal Enthalpies=	-813.064970
Sum of electronic and thermal Free Energies=	-813.138692

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.381963 (Hartree/Particle)
Thermal correction to Energy=	0.402382

Thermal correction to Enthalpy=	0.403327
Thermal correction to Gibbs Free Energy=	0.329576
Sum of electronic and zero-point Energies=	-813.085968
Sum of electronic and thermal Energies=	-813.065549
Sum of electronic and thermal Enthalpies=	-813.064605
Sum of electronic and thermal Free Energies=	-813.138356

Name of anion	α-Santalol acetate-C19-H		
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
O	-3.49120300	-0.32585500	0.36562200
O	-4.19105000	-1.78701800	-1.20199200
C	3.19689300	-0.14141900	0.81970200
C	2.68445700	-1.56106500	0.99921800
C	3.95223800	-1.30105800	0.19332800
C	2.34811300	0.49808700	-0.30572600
C	2.11562400	-0.83242300	-1.10282900
C	1.57205300	-1.79459000	-0.01826000
C	3.55065100	-1.38881800	-1.27449600
C	3.76111600	0.66582100	1.96088900
C	1.05553400	1.13087100	0.26217000
C	3.13464500	1.55599800	-1.10075300
C	-0.02022300	1.50899900	-0.77816400
C	-1.19228900	2.19500100	-0.13200300
C	-2.46780400	1.79714400	-0.05107800
C	-2.98542300	0.54041700	-0.69095700
C	-3.50693600	2.60805100	0.68312800
C	-4.08365900	-1.46918800	-0.04452200
C	-4.58682900	-2.26672000	1.13395800
H	2.71637800	-2.05606000	1.96157000
H	4.92619500	-1.60258500	0.55761500
H	1.52650100	-0.74628800	-2.01525500
H	1.53875800	-2.82885200	-0.37479300
H	0.57777500	-1.53334100	0.34856200
H	4.17856500	-0.79553600	-1.94129300
H	3.54138200	-2.41796000	-1.64725700
H	4.43340400	1.45278500	1.60321600
H	4.33523400	0.03006100	2.64072400
H	2.97016000	1.14252600	2.54907200
H	0.60254000	0.46362800	0.99956200
H	1.33655700	2.03410000	0.81699700
H	3.22699200	2.48064700	-0.52311200
H	2.63447700	1.80562700	-2.04101000
H	4.14531800	1.22461400	-1.34181900
H	0.41483100	2.18827900	-1.52107900
H	-0.33334200	0.61713900	-1.32453300
H	-0.94327300	3.14012700	0.35062400
H	-2.22904700	-0.00423500	-1.25262600

H	-3.81324600	0.75766600	-1.37327200
H	-4.32569000	2.89747100	0.01358500
H	-3.07806000	3.51623800	1.11026600
H	-3.95163000	2.02201400	1.49281700
H	-5.41106000	-1.73186200	1.61273800
H	-4.93387000	-3.23894100	0.79038600

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.381888 (Hartree/Particle)
Thermal correction to Energy=	0.401424
Thermal correction to Enthalpy=	0.402368
Thermal correction to Gibbs Free Energy=	0.333746
Sum of electronic and zero-point Energies=	-813.111599
Sum of electronic and thermal Energies=	-813.092063
Sum of electronic and thermal Enthalpies=	-813.091119
Sum of electronic and thermal Free Energies=	-813.159741

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.381641 (Hartree/Particle)
Thermal correction to Energy=	0.401475
Thermal correction to Enthalpy=	0.402419
Thermal correction to Gibbs Free Energy=	0.332358
Sum of electronic and zero-point Energies=	-813.198615
Sum of electronic and thermal Energies=	-813.178781
Sum of electronic and thermal Enthalpies=	-813.177837
Sum of electronic and thermal Free Energies=	-813.247898

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.381780 (Hartree/Particle)
Thermal correction to Energy=	0.401557
Thermal correction to Enthalpy=	0.402501
Thermal correction to Gibbs Free Energy=	0.332783
Sum of electronic and zero-point Energies=	-813.195301
Sum of electronic and thermal Energies=	-813.175524
Sum of electronic and thermal Enthalpies=	-813.174580
Sum of electronic and thermal Free Energies=	-813.244298

Name of cationic radical	α-Santalol acetate

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
O 0	-3.201600	-0.441800	0.367200
O 0	-3.226900	-2.230800	-1.094100
C 0	2.716700	-0.370500	0.878200
C 0	2.184500	-1.699300	0.436400
C 0	3.547300	-1.270000	0.015100
C 0	2.103800	0.710800	-0.002500
C 0	1.999500	-0.217000	-1.285200
C 0	1.259100	-1.487100	-0.741500
C 0	3.449400	-0.797100	-1.418700
C 0	3.074500	-0.119900	2.289100
C 0	0.746000	1.200900	0.514300
C 0	3.028100	1.919300	-0.191000
C 0	-0.001300	1.976400	-0.563800
C 0	-1.335700	2.445000	-0.056400

C 0	-2.513200	1.793600	-0.112700
C 0	-2.700500	0.404200	-0.659200
C 0	-3.763000	2.439400	0.427200
C 0	-3.421700	-1.743800	0.011300
C 0	-3.945300	-2.512400	1.186500
H 0	2.018700	-2.524700	1.100700
H 0	4.438100	-1.762700	0.352700
H 0	1.597800	0.222100	-2.198100
H 0	1.296900	-2.324700	-1.445500
H 0	0.224900	-1.307700	-0.444300
H 0	4.200900	-0.046400	-1.672500
H 0	3.503900	-1.628500	-2.128800
H 0	3.804700	0.691600	2.367900
H 0	3.513200	-1.006100	2.760500
H 0	2.191000	0.159900	2.871200
H 0	0.130000	0.371200	0.880500
H 0	0.894100	1.840800	1.395400
H 0	2.970300	2.600200	0.666200
H 0	2.773600	2.485000	-1.092800
H 0	4.081800	1.632600	-0.269700
H 0	0.561200	2.863800	-0.874500
H 0	-0.145000	1.379700	-1.468700
H 0	-1.318600	3.437000	0.393300
H 0	-1.767400	-0.017800	-1.042300
H 0	-3.419500	0.440700	-1.486900
H 0	-4.532900	2.480500	-0.350400
H 0	-3.586900	3.464900	0.769000
H 0	-4.155500	1.871500	1.276700
H 0	-4.891000	-2.078700	1.521000
H 0	-4.123200	-3.550500	0.891200
H 0	-3.209000	-2.500900	1.994000

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.394563 (Hartree/Particle)
Thermal correction to Energy=	0.415257
Thermal correction to Enthalpy=	0.416202
Thermal correction to Gibbs Free Energy=	0.343615
Sum of electronic and zero-point Energies=	-813.425728
Sum of electronic and thermal Energies=	-813.405033
Sum of electronic and thermal Enthalpies=	-813.404089
Sum of electronic and thermal Free Energies=	-813.476676

Name of compound	α-Vetivone		
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
O	4.32790000	-0.92960000	-0.07280000
C	0.38870000	0.42050000	-0.16020000
C	1.49530000	1.35770000	0.43390000
C	-0.98460000	0.72850000	0.50610000
C	0.78120000	-1.02800000	0.15580000
C	-0.32490000	-2.00900000	0.48790000
C	2.89190000	0.98440000	-0.08740000

C	-2.07890000	-0.24480000	0.12450000
C	0.27160000	0.59940000	-1.69480000
C	-1.66450000	-1.66510000	-0.16070000
C	1.26250000	2.85660000	0.20890000
C	2.05830000	-1.43780000	0.22320000
C	3.18070000	-0.49460000	0.01970000
C	-3.36210000	0.13690000	0.03890000
C	-3.79170000	1.54680000	0.31950000
C	-4.45150000	-0.82190000	-0.34240000
H	1.50680000	1.20440000	1.52420000
H	-1.26570000	1.74940000	0.23050000
H	-0.87540000	0.70500000	1.59910000
H	-0.04000000	-3.02570000	0.18920000
H	-0.45240000	-2.02120000	1.57900000
H	3.64820000	1.51220000	0.50650000
H	3.02290000	1.28090000	-1.13370000
H	1.22560000	0.43030000	-2.20460000
H	-0.44050000	-0.09870000	-2.14500000
H	-0.07000000	1.60720000	-1.95300000
H	-2.39670000	-2.38040000	0.23160000
H	-1.59740000	-1.82130000	-1.24380000
H	2.06530000	3.43930000	0.67510000
H	1.24930000	3.11410000	-0.85430000
H	0.32500000	3.19370000	0.65910000
H	2.31670000	-2.46550000	0.45580000
H	-3.76030000	2.14510000	-0.59650000
H	-4.82280000	1.55940000	0.69180000
H	-3.19540000	2.03650000	1.09480000
H	-4.99100000	-1.15430000	0.55020000
H	-5.16950000	-0.32240000	-1.00350000
H	-4.10760000	-1.70120000	-0.89260000

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

Zero-point correction=	0.335252 (Hartree/Particle)
Thermal correction to Energy=	0.352034
Thermal correction to Enthalpy=	0.352978
Thermal correction to Gibbs Free Energy=	0.291671
Sum of electronic and zero-point Energies=	-659.889020
Sum of electronic and thermal Energies=	-659.872238
Sum of electronic and thermal Enthalpies=	-659.871294
Sum of electronic and thermal Free Energies=	-659.932601

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction=	0.334836 (Hartree/Particle)
Thermal correction to Energy=	0.351599
Thermal correction to Enthalpy=	0.352543
Thermal correction to Gibbs Free Energy=	0.291315
Sum of electronic and zero-point Energies=	-659.897951
Sum of electronic and thermal Energies=	-659.881188
Sum of electronic and thermal Enthalpies=	-659.880244
Sum of electronic and thermal Free Energies=	-659.941471

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction=	0.334862 (Hartree/Particle)
Thermal correction to Energy=	0.351625
Thermal correction to Enthalpy=	0.352569
Thermal correction to Gibbs Free Energy=	0.291340
Sum of electronic and zero-point Energies=	-659.897539
Sum of electronic and thermal Energies=	-659.880776
Sum of electronic and thermal Enthalpies=	-659.879831
Sum of electronic and thermal Free Energies=	-659.941060

Name of radical	α-Vetivone-C6-H		
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
O	-4.44230100	-0.98758500	0.10141400
C	-0.46722500	0.34046900	0.09293800
C	-1.59239200	1.28612500	-0.44007100
C	0.87547500	0.62218300	-0.63730300
C	-0.87808400	-1.10338300	-0.19374300
C	0.22504700	-2.06241600	-0.57284300
C	-2.96300000	0.89483400	0.13750100
C	2.01026100	-0.29010600	-0.19948600
C	-0.26326400	0.51776700	1.61965800
C	1.59191800	-1.73776600	0.04430200
C	-1.34312000	2.78605600	-0.22816000
C	-2.16227700	-1.50288600	-0.16853500
C	-3.29301300	-0.58782800	0.03481400
C	3.27863800	0.12399700	-0.03321100
C	3.76756300	1.52979200	-0.29435200
C	4.38759700	-0.79074900	0.43537500
H	-1.63606100	1.11021600	-1.52323300
H	1.14445000	1.66354200	-0.47527100
H	0.70341000	0.51311600	-1.71779100
H	0.32480300	-2.02131500	-1.66671600
H	-3.76856600	1.44130000	-0.36031200
H	-3.02578600	1.17038800	1.19758100
H	-1.19087800	0.35392400	2.17016900
H	0.47438100	-0.18505900	2.00753300
H	0.09989400	1.52425900	1.84326000
H	2.32847400	-2.42680200	-0.37547900
H	1.55928700	-1.95059600	1.12033300
H	-2.16222900	3.36033100	-0.67021300
H	-1.30190600	3.04640000	0.83315000
H	-0.41884000	3.12857400	-0.69797700
H	-2.43075200	-2.54151800	-0.34009200
H	4.15415000	1.98316700	0.62648100
H	4.60462800	1.50987000	-1.00229300
H	3.01191700	2.19646700	-0.70559300
H	5.14437800	-0.91951100	-0.34847300
H	4.90573200	-0.34598900	1.29293100
H	4.04475400	-1.77920200	0.73613700
Frequency and Energy at B3LYP/6-311G (d,p) (gas)			

Zero-point correction=	0.322002 (Hartree/Particle)
Thermal correction to Energy=	0.338622
Thermal correction to Enthalpy=	0.339566
Thermal correction to Gibbs Free Energy=	0.278152
Sum of electronic and zero-point Energies=	-659.269715
Sum of electronic and thermal Energies=	-659.253095
Sum of electronic and thermal Enthalpies=	-659.252151
Sum of electronic and thermal Free Energies=	-659.313565
Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.321696 (Hartree/Particle)
Thermal correction to Energy=	0.338293
Thermal correction to Enthalpy=	0.339238
Thermal correction to Gibbs Free Energy=	0.277916
Sum of electronic and zero-point Energies=	-659.278969
Sum of electronic and thermal Energies=	-659.262371
Sum of electronic and thermal Enthalpies=	-659.261427
Sum of electronic and thermal Free Energies=	-659.322749
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.321723 (Hartree/Particle)
Thermal correction to Energy=	0.338317
Thermal correction to Enthalpy=	0.339261
Thermal correction to Gibbs Free Energy=	0.277961
Sum of electronic and zero-point Energies=	-659.278531
Sum of electronic and thermal Energies=	-659.261937
Sum of electronic and thermal Enthalpies=	-659.260993
Sum of electronic and thermal Free Energies=	-659.322293

Name of anion	α-Vetivone-C6-H		
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
O	-4.44230100	-0.98758500	0.10141400
C	-0.46722500	0.34046900	0.09293800
C	-1.59239200	1.28612500	-0.44007100
C	0.87547500	0.62218300	-0.63730300
C	-0.87808400	-1.10338300	-0.19374300
C	0.22504700	-2.06241600	-0.57284300
C	-2.96300000	0.89483400	0.13750100
C	2.01026100	-0.29010600	-0.19948600
C	-0.26326400	0.51776700	1.61965800
C	1.59191800	-1.73776600	0.04430200
C	-1.34312000	2.78605600	-0.22816000
C	-2.16227700	-1.50288600	-0.16853500
C	-3.29301300	-0.58782800	0.03481400
C	3.27863800	0.12399700	-0.03321100
C	3.76756300	1.52979200	-0.29435200
C	4.38759700	-0.79074900	0.43537500
H	-1.63606100	1.11021600	-1.52323300
H	1.14445000	1.66354200	-0.47527100
H	0.70341000	0.51311600	-1.71779100
H	0.32480300	-2.02131500	-1.66671600
H	-3.76856600	1.44130000	-0.36031200

H	-3.02578600	1.17038800	1.19758100
H	-1.19087800	0.35392400	2.17016900
H	0.47438100	-0.18505900	2.00753300
H	0.09989400	1.52425900	1.84326000
H	2.32847400	-2.42680200	-0.37547900
H	1.55928700	-1.95059600	1.12033300
H	-2.16222900	3.36033100	-0.67021300
H	-1.30190600	3.04640000	0.83315000
H	-0.41884000	3.12857400	-0.69797700
H	-2.43075200	-2.54151800	-0.34009200
H	4.15415000	1.98316700	0.62648100
H	4.60462800	1.50987000	-1.00229300
H	3.01191700	2.19646700	-0.70559300
H	5.14437800	-0.91951100	-0.34847300
H	4.90573200	-0.34598900	1.29293100
H	4.04475400	-1.77920200	0.73613700

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.320291 (Hartree/Particle)
Thermal correction to Energy=	0.336883
Thermal correction to Enthalpy=	0.337828
Thermal correction to Gibbs Free Energy=	0.277179
Sum of electronic and zero-point Energies=	-659.324107
Sum of electronic and thermal Energies=	-659.307514
Sum of electronic and thermal Enthalpies=	-659.306570
Sum of electronic and thermal Free Energies=	-659.367219

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.320750 (Hartree/Particle)
Thermal correction to Energy=	0.337229
Thermal correction to Enthalpy=	0.338173
Thermal correction to Gibbs Free Energy=	0.277942
Sum of electronic and zero-point Energies=	-659.406350
Sum of electronic and thermal Energies=	-659.389871
Sum of electronic and thermal Enthalpies=	-659.388926
Sum of electronic and thermal Free Energies=	-659.449157

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.320751 (Hartree/Particle)
Thermal correction to Energy=	0.337224
Thermal correction to Enthalpy=	0.338168
Thermal correction to Gibbs Free Energy=	0.277971
Sum of electronic and zero-point Energies=	-659.403517
Sum of electronic and thermal Energies=	-659.387044
Sum of electronic and thermal Enthalpies=	-659.386100
Sum of electronic and thermal Free Energies=	-659.446297

Name of cationic radical	α-Vetivone

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
O 0	4.327900	-0.929600	-0.072800
C 0	0.388700	0.420500	-0.160200
C 0	1.495300	1.357700	0.433900
C 0	-0.984600	0.728500	0.506100

C 0	0.781200	-1.028000	0.155800
C 0	-0.324900	-2.009000	0.487900
C 0	2.891900	0.984400	-0.087400
C 0	-2.078900	-0.244800	0.124500
C 0	0.271600	0.599400	-1.694800
C 0	-1.664500	-1.665100	-0.160700
C 0	1.262500	2.856600	0.208900
C 0	2.058300	-1.437800	0.223200
C 0	3.180700	-0.494600	0.019700
C 0	-3.362100	0.136900	0.038900
C 0	-3.791700	1.546800	0.319500
C 0	-4.451500	-0.821900	-0.342400
H 0	1.506800	1.204400	1.524200
H 0	-1.265700	1.749400	0.230500
H 0	-0.875400	0.705000	1.599100
H 0	-0.040000	-3.025700	0.189200
H 0	-0.452400	-2.021200	1.579000
H 0	3.648200	1.512200	0.506500
H 0	3.022900	1.280900	-1.133700
H 0	1.225600	0.430300	-2.204600
H 0	-0.440500	-0.098700	-2.145000
H 0	-0.070000	1.607200	-1.953000
H 0	-2.396700	-2.380400	0.231600
H 0	-1.597400	-1.821300	-1.243800
H 0	2.065300	3.439300	0.675100
H 0	1.249300	3.114100	-0.854300
H 0	0.325000	3.193700	0.659100
H 0	2.316700	-2.465500	0.455800
H 0	-3.760300	2.145100	-0.596500
H 0	-4.822800	1.559400	0.691800
H 0	-3.195400	2.036500	1.094800
H 0	-4.991000	-1.154300	0.550200
H 0	-5.169500	-0.322400	-1.003500
H 0	-4.107600	-1.701200	-0.892600

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.332832 (Hartree/Particle)
Thermal correction to Energy=	0.349965
Thermal correction to Enthalpy=	0.350909
Thermal correction to Gibbs Free Energy=	0.287315
Sum of electronic and zero-point Energies=	-659.602625
Sum of electronic and thermal Energies=	-659.585493
Sum of electronic and thermal Enthalpies=	-659.584548
Sum of electronic and thermal Free Energies=	-659.648142

Name of compound	Ethyl hexadecanoate	
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)		
O	-8.35294300	-0.56816200	-0.53913000
O	-7.54602600	1.34240000	0.36615300
C	2.74437100	0.39033100	-0.09284200
C	1.49454300	-0.48098800	0.09164700
C	4.03018300	-0.42768400	0.08828500

C	0.20897500	0.33732400	-0.08971300
C	5.27995600	0.44372300	-0.09617000
C	-1.04096800	-0.53380900	0.09490500
C	6.56585900	-0.37417800	0.08486800
C	-2.32578400	0.28538100	-0.08700400
C	7.81572100	0.49713000	-0.09954600
C	-3.57591800	-0.58548200	0.09794100
C	9.10136200	-0.32077400	0.08147600
C	-4.85609100	0.23834600	-0.08384600
C	10.35250700	0.54967200	-0.10273600
C	-6.10575400	-0.63128600	0.09288000
C	11.63529000	-0.25939200	0.07637400
C	-7.35487100	0.20130800	0.01956200
C	-9.68724300	0.01470200	-0.66803000
C	-10.38756200	0.00313200	0.67503300
H	2.73342800	0.85647500	-1.09696000
H	2.72784300	1.22977400	0.62880600
H	1.51154400	-1.32043100	-0.62991900
H	1.50585200	-0.94673000	1.09594600
H	4.04710000	-1.26704300	-0.63336800
H	4.04149600	-0.89363900	1.09246400
H	0.19834800	0.80345300	-1.09389700
H	0.19269800	1.17698800	0.63181500
H	5.26888600	0.90986400	-1.10026000
H	5.26332600	1.28308300	0.62551800
H	-1.02373600	-1.37347200	-0.62646100
H	-1.02955900	-0.99901800	1.09951600
H	6.58282000	-1.21352500	-0.63679100
H	6.57725300	-0.84024500	1.08898400
H	-2.33562200	0.75171000	-1.09131800
H	-2.34166300	1.12562400	0.63439600
H	7.80447300	0.96320600	-1.10365100
H	7.79891700	1.33642000	0.62219100
H	-3.55915100	-1.42512800	-0.62382900
H	-3.56358500	-1.05031700	1.10299900
H	9.11969700	-1.16040700	-0.63956900
H	9.11413800	-0.78739900	1.08513600
H	-4.86650800	0.71256400	-1.08546600
H	-4.88099800	1.07809600	0.64251300
H	10.34202000	1.01557800	-1.10751400
H	10.33644800	1.38909200	0.61967900
H	-6.13649500	-1.44213600	-0.66707900
H	-6.08695700	-1.15131700	1.07578400
H	12.52223600	0.36992100	-0.05685200
H	11.70119100	-1.07738100	-0.64995200
H	11.69561400	-0.70406900	1.07618900
H	-10.14427600	-0.67060200	-1.40480800
H	-9.58631600	1.03249200	-1.08522600
H	-11.43951300	0.29675900	0.58180400
H	-10.35620900	-0.99119300	1.13795600
H	-9.91044700	0.70431000	1.37653900

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.514869 (Hartree/Particle)
Thermal correction to Energy=	0.541173
Thermal correction to Enthalpy=	0.542117
Thermal correction to Gibbs Free Energy=	0.452652
Sum of electronic and zero-point Energies=	-857.821733
Sum of electronic and thermal Energies=	-857.795430
Sum of electronic and thermal Enthalpies=	-857.794486
Sum of electronic and thermal Free Energies=	-857.883950
Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.513675 (Hartree/Particle)
Thermal correction to Energy=	0.540040
Thermal correction to Enthalpy=	0.540984
Thermal correction to Gibbs Free Energy=	0.451338
Sum of electronic and zero-point Energies=	-857.828705
Sum of electronic and thermal Energies=	-857.802340
Sum of electronic and thermal Enthalpies=	-857.801396
Sum of electronic and thermal Free Energies=	-857.891043
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.513744 (Hartree/Particle)
Thermal correction to Energy=	0.540104
Thermal correction to Enthalpy=	0.541048
Thermal correction to Gibbs Free Energy=	0.451419
Sum of electronic and zero-point Energies=	-857.828357
Sum of electronic and thermal Energies=	-857.801996
Sum of electronic and thermal Enthalpies=	-857.801052
Sum of electronic and thermal Free Energies=	-857.890681

Name of radical	Ethyl hexadecanoate-C16-H	
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)		
O	-8.53278900	-0.71661400	-0.10148500
O	-7.54181200	1.27389000	-0.49714700
C	2.76514200	0.37653700	-0.01056600
C	1.50394500	-0.49412200	0.02600300
C	4.06939700	-0.42748500	0.03955600
C	0.20042000	0.31026800	-0.03546600
C	5.33008600	0.44391800	0.00315900
C	-1.06135000	-0.55950000	0.00240600
C	6.63482500	-0.35965400	0.04758000
C	-2.36343600	0.24535500	-0.07735000
C	7.89513700	0.51229900	0.01049400
C	-3.62600700	-0.62283000	-0.03567500
C	9.20019000	-0.29047600	0.05358400
C	-4.92134300	0.18865600	-0.14298100
C	10.46084100	0.58098100	0.01447900
C	-6.17387900	-0.68559400	-0.09232400
C	11.75945800	-0.22943600	0.05927500
C	-7.46152800	0.09513600	-0.25427200
C	-9.84176400	-0.11306300	-0.25572500
C	-10.33151600	0.49357800	1.04895800

H	2.75407700	0.99038800	-0.92051200
H	2.74228900	1.08152000	0.83045500
H	1.53022800	-1.20345700	-0.81130400
H	1.51105700	-1.10314200	0.93925500
H	4.09227700	-1.13144900	-0.80236600
H	4.08078700	-1.04237500	0.94882000
H	0.19339900	0.91703500	-0.95013700
H	0.17430200	1.02169200	0.79996000
H	5.31664800	1.06113400	-0.90449000
H	5.30888300	1.14578200	0.84684600
H	-1.02971900	-1.27804700	-0.82683700
H	-1.06067300	-1.15823800	0.92247200
H	6.65591300	-1.06135600	-0.79625900
H	6.64871100	-0.97697300	0.95515200
H	-2.36545400	0.83977900	-0.99985800
H	-2.39488900	0.96763700	0.74828000
H	7.88068600	1.12997300	-0.89685600
H	7.87438000	1.21371600	0.85459700
H	-3.58723900	-1.35575000	-0.85216000
H	-3.63365300	-1.20570200	0.89462700
H	9.22151800	-0.99288000	-0.78987800
H	9.21641900	-0.90746200	0.96153900
H	-4.92449900	0.76455300	-1.07353700
H	-4.96531700	0.92726200	0.66431600
H	10.44534600	1.19610000	-0.89347900
H	10.43964300	1.28325800	0.85664500
H	-6.23585100	-1.24296100	0.84845500
H	12.63832700	0.42044600	0.02789200
H	11.82524300	-0.91794700	-0.78907300
H	11.82106600	-0.82713400	0.97417000
H	-10.48025700	-0.93611900	-0.57782600
H	-9.79071100	0.63849100	-1.04452300
H	-11.35379300	0.86282500	0.92591900
H	-10.33018200	-0.25180100	1.84775300
H	-9.69953400	1.33231500	1.34545700

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.501468 (Hartree/Particle)
Thermal correction to Energy=	0.527698
Thermal correction to Enthalpy=	0.528643
Thermal correction to Gibbs Free Energy=	0.438153
Sum of electronic and zero-point Energies=	-857.178941
Sum of electronic and thermal Energies=	-857.152711
Sum of electronic and thermal Enthalpies=	-857.151767
Sum of electronic and thermal Free Energies=	-857.242257
Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.500589 (Hartree/Particle)
Thermal correction to Energy=	0.526825
Thermal correction to Enthalpy=	0.527769
Thermal correction to Gibbs Free Energy=	0.437033
Sum of electronic and zero-point Energies=	-857.185819
Sum of electronic and thermal Energies=	-857.159584

Sum of electronic and thermal Enthalpies=	-857.158640
Sum of electronic and thermal Free Energies=	-857.249376

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.500407 (Hartree/Particle)
Thermal correction to Energy=	0.526709
Thermal correction to Enthalpy=	0.527653
Thermal correction to Gibbs Free Energy=	0.436642
Sum of electronic and zero-point Energies=	-857.185652
Sum of electronic and thermal Energies=	-857.159350
Sum of electronic and thermal Enthalpies=	-857.158406
Sum of electronic and thermal Free Energies=	-857.249418

Name of anion	Ethyl hexadecanoate-C16-H

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
O	-8.53278900	-0.71661400	-0.10148500
O	-7.54181200	1.27389000	-0.49714700
C	2.76514200	0.37653700	-0.01056600
C	1.50394500	-0.49412200	0.02600300
C	4.06939700	-0.42748500	0.03955600
C	0.20042000	0.31026800	-0.03546600
C	5.33008600	0.44391800	0.00315900
C	-1.06135000	-0.55950000	0.00240600
C	6.63482500	-0.35965400	0.04758000
C	-2.36343600	0.24535500	-0.07735000
C	7.89513700	0.51229900	0.01049400
C	-3.62600700	-0.62283000	-0.03567500
C	9.20019000	-0.29047600	0.05358400
C	-4.92134300	0.18865600	-0.14298100
C	10.46084100	0.58098100	0.01447900
C	-6.17387900	-0.68559400	-0.09232400
C	11.75945800	-0.22943600	0.05927500
C	-7.46152800	0.09513600	-0.25427200
C	-9.84176400	-0.11306300	-0.25572500
C	-10.33151600	0.49357800	1.04895800
H	2.75407700	0.99038800	-0.92051200
H	2.74228900	1.08152000	0.83045500
H	1.53022800	-1.20345700	-0.81130400
H	1.51105700	-1.10314200	0.93925500
H	4.09227700	-1.13144900	-0.80236600
H	4.08078700	-1.04237500	0.94882000
H	0.19339900	0.91703500	-0.95013700
H	0.17430200	1.02169200	0.79996000
H	5.31664800	1.06113400	-0.90449000
H	5.30888300	1.14578200	0.84684600
H	-1.02971900	-1.27804700	-0.82683700
H	-1.06067300	-1.15823800	0.92247200
H	6.65591300	-1.06135600	-0.79625900
H	6.64871100	-0.97697300	0.95515200
H	-2.36545400	0.83977900	-0.99985800
H	-2.39488900	0.96763700	0.74828000
H	7.88068600	1.12997300	-0.89685600

H	7.87438000	1.21371600	0.85459700
H	-3.58723900	-1.35575000	-0.85216000
H	-3.63365300	-1.20570200	0.89462700
H	9.22151800	-0.99288000	-0.78987800
H	9.21641900	-0.90746200	0.96153900
H	-4.92449900	0.76455300	-1.07353700
H	-4.96531700	0.92726200	0.66431600
H	10.44534600	1.19610000	-0.89347900
H	10.43964300	1.28325800	0.85664500
H	-6.15433300	-1.44673000	-0.88125600
H	12.63832700	0.42044600	0.02789200
H	11.82524300	-0.91794700	-0.78907300
H	11.82106600	-0.82713400	0.97417000
H	-10.48025700	-0.93611900	-0.57782600
H	-9.79071100	0.63849100	-1.04452300
H	-11.35379300	0.86282500	0.92591900
H	-10.33018200	-0.25180100	1.84775300
H	-9.69953400	1.33231500	1.34545700

Frequency and Energy at B3LYP/6-311G (d,p) (gas)		
Zero-point correction=	0.499044	(Hartree/Particle)
Thermal correction to Energy=	0.525259	
Thermal correction to Enthalpy=	0.526203	
Thermal correction to Gibbs Free Energy=	0.436400	
Sum of electronic and zero-point Energies=	-857.227938	
Sum of electronic and thermal Energies=	-857.201723	
Sum of electronic and thermal Enthalpies=	-857.200779	
Sum of electronic and thermal Free Energies=	-857.290582	

Frequency and Energy at B3LYP/6-311G (d,p) (water)		
Zero-point correction=	0.498802	(Hartree/Particle)
Thermal correction to Energy=	0.524983	
Thermal correction to Enthalpy=	0.525928	
Thermal correction to Gibbs Free Energy=	0.437157	
Sum of electronic and zero-point Energies=	-857.314537	
Sum of electronic and thermal Energies=	-857.288355	
Sum of electronic and thermal Enthalpies=	-857.287411	
Sum of electronic and thermal Free Energies=	-857.376182	

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)		
Zero-point correction=	0.498808	(Hartree/Particle)
Thermal correction to Energy=	0.525024	
Thermal correction to Enthalpy=	0.525968	
Thermal correction to Gibbs Free Energy=	0.436505	
Sum of electronic and zero-point Energies=	-857.311604	
Sum of electronic and thermal Energies=	-857.285388	
Sum of electronic and thermal Enthalpies=	-857.284444	
Sum of electronic and thermal Free Energies=	-857.373907	

Name of cationic radical	Ethyl hexadecanoate	
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)		
O	-8.35294300	-0.56816200	-0.53913000
O	-7.54602600	1.34240000	0.36615300

C	2.74437100	0.39033100	-0.09284200
C	1.49454300	-0.48098800	0.09164700
C	4.03018300	-0.42768400	0.08828500
C	0.20897500	0.33732400	-0.08971300
C	5.27995600	0.44372300	-0.09617000
C	-1.04096800	-0.53380900	0.09490500
C	6.56585900	-0.37417800	0.08486800
C	-2.32578400	0.28538100	-0.08700400
C	7.81572100	0.49713000	-0.09954600
C	-3.57591800	-0.58548200	0.09794100
C	9.10136200	-0.32077400	0.08147600
C	-4.85609100	0.23834600	-0.08384600
C	10.35250700	0.54967200	-0.10273600
C	-6.10575400	-0.63128600	0.09288000
C	11.63529000	-0.25939200	0.07637400
C	-7.35487100	0.20130800	0.01956200
C	-9.68724300	0.01470200	-0.66803000
C	-10.38756200	0.00313200	0.67503300
H	2.73342800	0.85647500	-1.09696000
H	2.72784300	1.22977400	0.62880600
H	1.51154400	-1.32043100	-0.62991900
H	1.50585200	-0.94673000	1.09594600
H	4.04710000	-1.26704300	-0.63336800
H	4.04149600	-0.89363900	1.09246400
H	0.19834800	0.80345300	-1.09389700
H	0.19269800	1.17698800	0.63181500
H	5.26888600	0.90986400	-1.10026000
H	5.26332600	1.28308300	0.62551800
H	-1.02373600	-1.37347200	-0.62646100
H	-1.02955900	-0.99901800	1.09951600
H	6.58282000	-1.21352500	-0.63679100
H	6.57725300	-0.84024500	1.08898400
H	-2.33562200	0.75171000	-1.09131800
H	-2.34166300	1.12562400	0.63439600
H	7.80447300	0.96320600	-1.10365100
H	7.79891700	1.33642000	0.62219100
H	-3.55915100	-1.42512800	-0.62382900
H	-3.56358500	-1.05031700	1.10299900
H	9.11969700	-1.16040700	-0.63956900
H	9.11413800	-0.78739900	1.08513600
H	-4.86650800	0.71256400	-1.08546600
H	-4.88099800	1.07809600	0.64251300
H	10.34202000	1.01557800	-1.10751400
H	10.33644800	1.38909200	0.61967900
H	-6.13649500	-1.44213600	-0.66707900
H	-6.08695700	-1.15131700	1.07578400
H	12.52223600	0.36992100	-0.05685200
H	11.70119100	-1.07738100	-0.64995200
H	11.69561400	-0.70406900	1.07618900
H	-10.14427600	-0.67060200	-1.40480800
H	-9.58631600	1.03249200	-1.08522600

H	-11.43951300	0.29675900	0.58180400
H	-10.35620900	-0.99119300	1.13795600
H	-9.91044700	0.70431000	1.37653900

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.510552 (Hartree/Particle)
Thermal correction to Energy=	0.537371
Thermal correction to Enthalpy=	0.538315
Thermal correction to Gibbs Free Energy=	0.446214
Sum of electronic and zero-point Energies=	-857.507091
Sum of electronic and thermal Energies=	-857.480272
Sum of electronic and thermal Enthalpies=	-857.479328
Sum of electronic and thermal Free Energies=	-857.571429

Name of compound	Falcarinol	
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)		
C	0.28470600	2.50080900	-0.04000900
C	1.35429300	1.40589400	-0.13796600
C	-1.08114300	1.90906400	0.33113400
C	2.72965300	1.98022300	-0.50090600
C	-2.17430000	2.98481000	0.38195900
C	3.79108500	0.87547700	-0.63711200
C	-3.54827000	2.37918000	0.65809000
C	4.15681400	0.28061700	0.68879300
C	4.10804800	-1.01503700	1.01341600
C	3.65882800	-2.12919400	0.10200000
C	2.23531800	-2.08300200	-0.11063700
C	1.03832600	-2.00930300	-0.28099300
C	-2.91561300	-1.52000100	-0.84068800
C	-0.30539500	-1.88167900	-0.47177900
C	-1.49511800	-1.73358800	-0.63606600
H	0.21220400	3.04356300	-1.00236800
H	0.58270100	3.25674000	0.71161400
H	1.42258400	0.85056600	0.81860000
H	1.05173800	0.65203900	-0.89259300
H	-1.36337900	1.12146600	-0.40738700
H	-1.01481100	1.39016400	1.30727500
H	3.04479500	2.72009900	0.25938800
H	2.66326700	2.53787700	-1.45554700
H	-2.19888900	3.54464800	-0.57404700
H	-1.92971500	3.73266700	1.16144500
H	4.70658000	1.29804500	-1.10339300
H	3.42795300	0.10329900	-1.34559100
H	-4.32619600	3.15105800	0.67230800
H	-3.57885100	1.86584900	1.62563900
H	-3.83391200	1.64869500	-0.11469100
H	4.48964500	1.01540000	1.42803600
H	4.39619000	-1.34967900	2.01056700
H	3.94840800	-3.11883800	0.53083300
H	4.19560800	-2.06809600	-0.87711800
H	-3.32022600	-2.19061500	-1.64813800
C	-3.72018600	-1.67220400	0.43318800

C	-3.63817900	-2.72809100	1.23606800
H	-4.40291400	-0.83994900	0.61714000
H	-4.23599000	-2.83866800	2.13034200
H	-2.96617300	-3.55975100	1.06856400
O	-3.14909200	-0.21481300	-1.39610500
H	-2.65108500	0.48807200	-0.88298500

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction= (Hartree/Particle)	0.365217
Thermal correction to Energy=	0.386825
Thermal correction to Enthalpy=	0.387769
Thermal correction to Gibbs Free Energy=	0.311497
Sum of electronic and zero-point Energies=	-737.161060
Sum of electronic and thermal Energies=	-737.139452
Sum of electronic and thermal Enthalpies=	-737.138508
Sum of electronic and thermal Free Energies=	-737.214780

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.364300 (Hartree/Particle)
Thermal correction to Energy=	0.386147
Thermal correction to Enthalpy=	0.387091
Thermal correction to Gibbs Free Energy=	0.308728
Sum of electronic and zero-point Energies=	-737.169459
Sum of electronic and thermal Energies=	-737.147613
Sum of electronic and thermal Enthalpies=	-737.146669
Sum of electronic and thermal Free Energies=	-737.225031

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.364364 (Hartree/Particle)
Thermal correction to Energy=	0.386193
Thermal correction to Enthalpy=	0.387137
Thermal correction to Gibbs Free Energy=	0.308939
Sum of electronic and zero-point Energies=	-737.168989
Sum of electronic and thermal Energies=	-737.147161
Sum of electronic and thermal Enthalpies=	-737.146216
Sum of electronic and thermal Free Energies=	-737.224415

Name of radical	Falcarinol-C14-H	
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)		
C	1.14100300	2.69666900	-0.10867700
C	1.88966900	1.35903600	-0.13041800
C	-0.35259300	2.55250800	0.20729600
C	3.39626400	1.50354600	-0.37146900
C	-1.12641100	3.87473900	0.14788200
C	4.14583100	0.15805900	-0.49125900
C	-2.61229700	3.72151900	0.48691100
C	4.11256300	-0.65146100	0.77526700
C	3.62341100	-1.87882800	0.95249200
C	2.99694700	-2.75590500	-0.12198000
C	1.55734400	-2.54319000	-0.24294900
C	0.37662300	-2.29590300	-0.34421400

C	-3.46006200	-1.10818500	-0.71714500
C	-0.93739100	-1.95553100	-0.46755300
C	-2.09687600	-1.62401600	-0.57769900
H	1.25884800	3.19340700	-1.08063700
H	1.60375800	3.36392400	0.63052200
H	1.72175500	0.83071900	0.81489400
H	1.45893100	0.71817500	-0.90902300
H	-0.80893900	1.83782300	-0.48829300
H	-0.46468100	2.11391300	1.20818300
H	3.84284200	2.09324500	0.43933000
H	3.56605200	2.07373900	-1.29219200
H	-1.02628500	4.30308100	-0.85685400
H	-0.66591900	4.59707900	0.83327500
H	5.19263900	0.36957900	-0.74505100
H	3.72848200	-0.40862300	-1.32846000
H	-3.14026700	4.67637000	0.41273400
H	-2.74674200	3.35226800	1.50955500
H	-3.10094400	3.01572400	-0.19121200
H	4.52576100	-0.15071800	1.65012600
H	3.63991300	-2.31063900	1.94885200
H	3.18914600	-3.80922700	0.11133100
H	3.46379600	-2.57053000	-1.09496500
C	-4.48262900	-1.80126800	0.15898000
C	-4.24441300	-2.79000200	1.01286200
H	-5.48325300	-1.39199300	0.04797400
H	-5.04111500	-3.21676600	1.61129300
H	-3.25136600	-3.20815500	1.13689200
O	-3.50572600	0.31303700	-0.50214400
H	-3.21169200	0.47474300	0.40231500

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.352171 (Hartree/Particle)
Thermal correction to Energy=	0.373645
Thermal correction to Enthalpy=	0.374590
Thermal correction to Gibbs Free Energy=	0.297850
Sum of electronic and zero-point Energies=	-736.559894
Sum of electronic and thermal Energies=	-736.538420
Sum of electronic and thermal Enthalpies=	-736.537475
Sum of electronic and thermal Free Energies=	-736.614215

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.350595 (Hartree/Particle)
Thermal correction to Energy=	0.372484
Thermal correction to Enthalpy=	0.373428
Thermal correction to Gibbs Free Energy=	0.294658
Sum of electronic and zero-point Energies=	-736.566623
Sum of electronic and thermal Energies=	-736.544735
Sum of electronic and thermal Enthalpies=	-736.543790
Sum of electronic and thermal Free Energies=	-736.622560

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.350553 (Hartree/Particle)

Thermal correction to Energy=	0.372450
Thermal correction to Enthalpy=	0.373394
Thermal correction to Gibbs Free Energy=	0.293601
Sum of electronic and zero-point Energies=	-736.566579
Sum of electronic and thermal Energies=	-736.544682
Sum of electronic and thermal Enthalpies=	-736.543738
Sum of electronic and thermal Free Energies=	-736.623532

Name of anion	Falcarinol-C10-H	
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)		
C	1.14100300	2.69666900	-0.10867700
C	1.88966900	1.35903600	-0.13041800
C	-0.35259300	2.55250800	0.20729600
C	3.39626400	1.50354600	-0.37146900
C	-1.12641100	3.87473900	0.14788200
C	4.14583100	0.15805900	-0.49125900
C	-2.61229700	3.72151900	0.48691100
C	4.11256300	-0.65146100	0.77526700
C	3.62341100	-1.87882800	0.95249200
C	2.99694700	-2.75590500	-0.12198000
C	1.55734400	-2.54319000	-0.24294900
C	0.37662300	-2.29590300	-0.34421400
C	-3.46006200	-1.10818500	-0.71714500
C	-0.93739100	-1.95553100	-0.46755300
C	-2.09687600	-1.62401600	-0.57769900
H	1.25884800	3.19340700	-1.08063700
H	1.60375800	3.36392400	0.63052200
H	1.72175500	0.83071900	0.81489400
H	1.45893100	0.71817500	-0.90902300
H	-0.80893900	1.83782300	-0.48829300
H	-0.46468100	2.11391300	1.20818300
H	3.84284200	2.09324500	0.43933000
H	3.56605200	2.07373900	-1.29219200
H	-1.02628500	4.30308100	-0.85685400
H	-0.66591900	4.59707900	0.83327500
H	5.19263900	0.36957900	-0.74505100
H	3.72848200	-0.40862300	-1.32846000
H	-3.14026700	4.67637000	0.41273400
H	-2.74674200	3.35226800	1.50955500
H	-3.10094400	3.01572400	-0.19121200
H	4.52576100	-0.15071800	1.65012600
H	3.63991300	-2.31063900	1.94885200
H	3.46379600	-2.57053000	-1.09496500
H	-3.76680900	-1.22213600	-1.76339700
C	-4.48262900	-1.80126800	0.15898000
C	-4.24441300	-2.79000200	1.01286200
H	-5.48325300	-1.39199300	0.04797400
H	-5.04111500	-3.21676600	1.61129300
H	-3.25136600	-3.20815500	1.13689200
O	-3.50572600	0.31303700	-0.50214400
H	-3.21169200	0.47474300	0.40231500

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.349004 (Hartree/Particle)
Thermal correction to Energy=	0.371096
Thermal correction to Enthalpy=	0.372040
Thermal correction to Gibbs Free Energy=	0.292682
Sum of electronic and zero-point Energies=	-736.612314
Sum of electronic and thermal Energies=	-736.590223
Sum of electronic and thermal Enthalpies=	-736.589279
Sum of electronic and thermal Free Energies=	-736.668637
Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.349135 (Hartree/Particle)
Thermal correction to Energy=	0.371189
Thermal correction to Enthalpy=	0.372133
Thermal correction to Gibbs Free Energy=	0.292459
Sum of electronic and zero-point Energies=	-736.685573
Sum of electronic and thermal Energies=	-736.663519
Sum of electronic and thermal Enthalpies=	-736.662575
Sum of electronic and thermal Free Energies=	-736.742249
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.349193 (Hartree/Particle)
Thermal correction to Energy=	0.371238
Thermal correction to Enthalpy=	0.372183
Thermal correction to Gibbs Free Energy=	0.292367
Sum of electronic and zero-point Energies=	-736.682942
Sum of electronic and thermal Energies=	-736.660897
Sum of electronic and thermal Enthalpies=	-736.659953
Sum of electronic and thermal Free Energies=	-736.739768

Name of cationic radical	Falcarinol		
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	1.14100300	2.69666900	-0.10867700
C	1.88966900	1.35903600	-0.13041800
C	-0.35259300	2.55250800	0.20729600
C	3.39626400	1.50354600	-0.37146900
C	-1.12641100	3.87473900	0.14788200
C	4.14583100	0.15805900	-0.49125900
C	-2.61229700	3.72151900	0.48691100
C	4.11256300	-0.65146100	0.77526700
C	3.62341100	-1.87882800	0.95249200
C	2.99694700	-2.75590500	-0.12198000
C	1.55734400	-2.54319000	-0.24294900
C	0.37662300	-2.29590300	-0.34421400
C	-3.46006200	-1.10818500	-0.71714500
C	-0.93739100	-1.95553100	-0.46755300
C	-2.09687600	-1.62401600	-0.57769900
H	1.25884800	3.19340700	-1.08063700
H	1.60375800	3.36392400	0.63052200
H	1.72175500	0.83071900	0.81489400
H	1.45893100	0.71817500	-0.90902300
H	-0.80893900	1.83782300	-0.48829300

H	-0.46468100	2.11391300	1.20818300
H	3.84284200	2.09324500	0.43933000
H	3.56605200	2.07373900	-1.29219200
H	-1.02628500	4.30308100	-0.85685400
H	-0.66591900	4.59707900	0.83327500
H	5.19263900	0.36957900	-0.74505100
H	3.72848200	-0.40862300	-1.32846000
H	-3.14026700	4.67637000	0.41273400
H	-2.74674200	3.35226800	1.50955500
H	-3.10094400	3.01572400	-0.19121200
H	4.52576100	-0.15071800	1.65012600
H	3.63991300	-2.31063900	1.94885200
H	3.18914600	-3.80922700	0.11133100
H	3.46379600	-2.57053000	-1.09496500
H	-3.76680900	-1.22213600	-1.76339700
C	-4.48262900	-1.80126800	0.15898000
C	-4.24441300	-2.79000200	1.01286200
H	-5.48325300	-1.39199300	0.04797400
H	-5.04111500	-3.21676600	1.61129300
H	-3.25136600	-3.20815500	1.13689200
O	-3.50572600	0.31303700	-0.50214400
H	-3.21169200	0.47474300	0.40231500

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

Zero-point correction=	0.363494
(Hartree/Particle)	
Thermal correction to Energy=	0.384504
Thermal correction to Enthalpy=	0.385448
Thermal correction to Gibbs Free Energy=	0.310949
Sum of electronic and zero-point Energies=	-736.866673
Sum of electronic and thermal Energies=	-736.845663
Sum of electronic and thermal Enthalpies=	-736.844719
Sum of electronic and thermal Free Energies=	-736.919218

TS of abstraction reaction between falcarinol and $CH_3OO^{\bullet}$ at C14-H

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

O	-5.21300600	1.07110500	-1.57029300
C	3.79355900	0.94783900	-1.34559700
C	3.07226700	-0.22644000	-0.67434100
C	2.85004500	1.90985700	-2.07579800
C	4.02131000	-1.18974600	0.04658100
C	3.56812500	3.08824000	-2.74344900
C	3.31182700	-2.37412600	0.73362400
C	2.61732400	4.04422900	-3.46924500
C	2.45877900	-1.95687400	1.89983900
C	1.17203200	-2.21722800	2.13242900
C	0.23605700	-3.02906000	1.25929000
C	-0.97016600	-2.29374400	0.89351100
C	-1.97307900	-1.67520000	0.61064900
C	-5.25926500	0.42449200	-0.31098700

C	-3.09495400	-0.97978500	0.28615200
C	-4.11224400	-0.38223500	-0.00573400
C	-6.60933700	-0.15383600	-0.09592600
C	-6.88583700	-1.22252500	0.65089900
H	4.53586700	0.56098700	-2.05606400
H	4.36074600	1.50400100	-0.58791800
H	2.33235400	0.15928100	0.03648600
H	2.50352100	-0.78240500	-1.43127700
H	2.28399200	1.35523300	-2.83554100
H	2.10647900	2.29539900	-1.36621300
H	4.60341100	-0.63799300	0.79575100
H	4.74846200	-1.58741000	-0.67087800
H	4.31036900	2.70333900	-3.45340700
H	4.13355900	3.64243300	-1.98448200
H	4.07871000	-3.06927800	1.09947500
H	2.72847400	-2.92651600	-0.00901700
H	3.15991000	4.87143600	-3.93502600
H	1.88571400	4.47449600	-2.77805800
H	2.06132200	3.52639400	-4.25722400
H	2.98127200	-1.36446000	2.65019200
H	0.71666600	-1.82656800	3.03810700
H	-0.06499100	-3.93860600	1.79771700
H	0.73894100	-3.36841800	0.34936000
H	-5.20442800	1.35289500	0.54754800
H	-7.40310900	0.41423000	-0.57078400
H	-4.31898700	1.40987200	-1.69276100
H	-7.90807900	-1.54978600	0.79601300
H	-6.10496700	-1.79753800	1.13588800
O	-5.14369900	2.43055200	1.29539400
O	-6.37538600	3.04209700	1.21375700
C	-6.34259200	4.04473500	0.19033300
H	-7.32597100	4.51659400	0.22039600
H	-5.56192300	4.77738800	0.40849100
H	-6.17117400	3.58183100	-0.78419200

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

Zero-point correction= 0.403082 (Hartree/Particle)

Thermal correction to Energy= 0.429800

Thermal correction to Enthalpy= 0.430744

Thermal correction to Gibbs Free Energy= 0.338400

Sum of electronic and zero-point Energies= -927.381706

Sum of electronic and thermal Energies= -927.354988

Sum of electronic and thermal Enthalpies= -927.354044

Sum of electronic and thermal Free Energies= -927.446388

TS addition reaction between falcarinol and $CH_3OO^{\bullet}$ at C9

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

O	8.02214800	0.90181400	0.97098300
C	-6.02692600	-0.18940300	-0.24979800
C	-4.57836600	-0.50596800	0.13890300

C	-7.05876900	-0.68918800	0.76733300
C	-3.55071300	-0.00040000	-0.87872000
C	-8.50851500	-0.38236800	0.37479300
C	-2.10730300	-0.34420800	-0.49616300
C	-9.53224300	-0.88643000	1.39603300
C	-1.07915200	0.16984300	-1.47610300
C	0.27907100	-0.09389800	-1.34533000
C	0.90472300	-0.51100100	-0.03766100
C	2.35906200	-0.43412200	-0.02108700
C	3.56762300	-0.36837000	-0.01575900
C	7.59713500	-0.09164400	0.02727700
C	4.92873500	-0.28454800	-0.00638700
C	6.13795200	-0.22301600	-0.00255900
C	8.33061400	-1.39432800	0.27276200
C	7.77850000	-2.58678800	0.46453200
H	-6.24247400	-0.63240400	-1.23076200
H	-6.13745500	0.89511600	-0.37579300
H	-4.36263500	-0.06385500	1.11994600
H	-4.46748000	-1.59148200	0.26305800
H	-6.94307300	-1.77317600	0.89833700
H	-6.84823800	-0.24154500	1.74734800
H	-3.63312600	1.08498500	-0.98502200
H	-3.77453200	-0.43083000	-1.86341300
H	-8.71858200	-0.82965900	-0.60435900
H	-8.62527300	0.70037200	0.24480700
H	-1.99901700	-1.43522900	-0.42026500
H	-1.88226300	0.05744000	0.49763000
H	-10.55465100	-0.65225400	1.08694500
H	-9.36942300	-0.42985800	2.37740900
H	-9.46397600	-1.97161300	1.52210400
H	-1.43144200	0.31252400	-2.49419900
H	0.94021300	0.10488600	-2.17995900
H	0.59757100	-1.53673400	0.22027100
H	0.50140700	0.11544700	0.77150500
H	7.92247100	0.31071000	-0.93932000
H	9.40993100	-1.27079500	0.30443700
H	7.76774000	0.58479400	1.84557500
H	8.38964800	-3.46288400	0.64865700
H	6.70356900	-2.72833300	0.43705700
O	-0.84577600	2.37452300	0.10881200
O	-1.21313400	2.04299400	-1.19279600
C	0.37224500	3.11897100	0.06158600
H	0.25371400	3.99650800	-0.57811300
H	0.56397500	3.42615700	1.09175100
H	1.19390300	2.49810700	-0.30872500

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

Zero-point correction= 0.407669 (Hartree/Particle)

Thermal correction to Energy= 0.433129

Thermal correction to Enthalpy= 0.434073

Thermal correction to Gibbs Free Energy= 0.347126

Sum of electronic and zero-point Energies= -927.374213

Sum of electronic and thermal Energies=			-927.348754
Sum of electronic and thermal Enthalpies=			-927.347810
Sum of electronic and thermal Free Energies=			-927.434756

TS addition reaction between falcarinol and $CH_3OO^{\bullet}$ at C12

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

O	5.60564100	2.18386500	1.51018500
C	-5.13388400	0.43241700	0.55288400
C	-4.36075500	-0.34659800	-0.51715800
C	-6.18396700	1.38927200	-0.02299700
C	-3.29171800	-1.28087700	0.06002300
C	-6.96472600	2.16176100	1.04627800
C	-2.53008400	-2.07403400	-1.01811600
C	-8.00382400	3.12275000	0.46150300
C	-1.50712800	-3.00829200	-0.43393400
C	-0.19223400	-3.05141100	-0.65445500
C	0.59402900	-2.16475500	-1.59516300
C	1.70654500	-1.45899000	-0.92801600
C	2.21243200	-0.41125800	-0.48659000
C	4.32176600	2.64884200	1.06463900
C	2.91603500	0.61554400	0.02593600
C	3.52993900	1.56332200	0.48334000
C	4.48569200	3.85132200	0.15812400
C	4.00445500	3.98103300	-1.07281200
H	-4.42514100	1.00139400	1.16810200
H	-5.62415300	-0.27666100	1.23234300
H	-5.06714300	-0.93128000	-1.12058100
H	-3.88595100	0.36248100	-1.20765300
H	-5.69188800	2.10341600	-0.69614900
H	-6.88928200	0.82312000	-0.64524200
H	-3.76072500	-1.98398000	0.75967100
H	-2.57302300	-0.69873400	0.64830100
H	-6.25999000	2.72248800	1.67228200
H	-7.46252600	1.44857800	1.71455700
H	-2.07211400	-1.37494800	-1.72388900
H	-3.25655600	-2.66033200	-1.59745300
H	-8.54390100	3.65555500	1.24898600
H	-8.74227700	2.58688800	-0.14305800
H	-7.53173000	3.87163900	-0.18214400
H	-1.90929800	-3.73652800	0.26936500
H	0.40485400	-3.78783500	-0.12774000
H	-0.04552300	-1.41450100	-2.06597300
H	1.02323500	-2.77915800	-2.39529900
H	3.82899200	2.97573300	1.98787500
H	5.08246300	4.64070400	0.60738400
H	6.09008100	1.90451100	0.72417400
H	4.18818900	4.87747300	-1.65375000
H	3.40842100	3.20281700	-1.53697100
O	2.82667700	-3.47500300	0.53464800
O	2.97861400	-2.87112500	-0.69393600

C	3.86558300	-3.03464700	1.41396600
H	3.74308100	-3.62735200	2.32198300
H	4.84343600	-3.21957200	0.96366700
H	3.74751300	-1.97100100	1.63548000

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

Zero-point correction= 0.407809 (Hartree/Particle)
Thermal correction to Energy= 0.434350
Thermal correction to Enthalpy= 0.435294
Thermal correction to Gibbs Free Energy= 0.343135
Sum of electronic and zero-point Energies= -927.374851
Sum of electronic and thermal Energies= -927.348310
Sum of electronic and thermal Enthalpies= -927.347365
Sum of electronic and thermal Free Energies= -927.439525

TS addition reaction between falcarinol and $CH_3OO^{\bullet}$ at C13

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

O	-6.06233000	-2.89658400	-1.55797200
C	6.31686000	0.10351700	0.04051000
C	4.87303600	-0.33320600	0.31331500
C	7.33840400	-1.03131800	0.17572100
C	3.85856500	0.80929800	0.19248400
C	8.78191400	-0.59312600	-0.09692100
C	2.40805500	0.36803200	0.46633000
C	9.79762700	-1.72993500	0.04752600
C	1.43841800	1.51624300	0.43688500
C	0.41702600	1.72921400	-0.39420400
C	-0.02304500	0.83321400	-1.53841000
C	-1.42246800	0.43340100	-1.43131600
C	-2.63855500	0.41509700	-1.12408000
C	-6.20951900	-1.46898500	-1.51791900
C	-3.84552700	-0.24216400	-1.29673300
C	-4.91695400	-0.78933700	-1.40340900
C	-7.19688400	-1.07253600	-0.43901200
C	-6.97164600	-0.22971000	0.56327100
H	6.58499000	0.91447300	0.72992400
H	6.38106100	0.53009900	-0.96868600
H	4.60025200	-1.13722300	-0.38239000
H	4.80965100	-0.76771600	1.31927200
H	7.27553000	-1.45708100	1.18561700
H	7.07187400	-1.84390300	-0.51265800
H	3.91490500	1.24927100	-0.81003200
H	4.12863000	1.61037300	0.89162300
H	9.04627000	0.22155400	0.58820500
H	8.84576800	-0.17189600	-1.10754400
H	2.36848900	-0.09778900	1.46011700
H	2.12544800	-0.41210900	-0.24656500
H	10.81552900	-1.38459400	-0.15281500
H	9.58086400	-2.54560100	-0.64941600

H	9.78192900	-2.14775000	1.05901500
H	1.61839600	2.28029000	1.19229800
H	-0.19160000	2.61796800	-0.26441600
H	0.60885300	-0.05758200	-1.60425500
H	0.10542900	1.36970800	-2.48892900
H	-6.64339900	-1.22473400	-2.49442200
H	-8.15380300	-1.57880400	-0.53715600
H	-5.69971800	-3.16208200	-0.70474400
H	-7.74387100	-0.02538200	1.29684900
H	-6.02425300	0.28608300	0.68171700
O	-3.63494800	1.37384400	1.14027600
O	-3.00050500	1.83085700	-0.00786000
C	-2.67427800	1.22483500	2.18501000
H	-3.24710200	0.91024900	3.05933300
H	-1.93808600	0.46028500	1.92106300
H	-2.17179200	2.17522900	2.38165600

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

Zero-point correction= 0.407496 (Hartree/Particle)

Thermal correction to Energy= 0.434079

Thermal correction to Enthalpy= 0.435023

Thermal correction to Gibbs Free Energy= 0.341720

Sum of electronic and zero-point Energies= -927.362947

Sum of electronic and thermal Energies= -927.336364

Sum of electronic and thermal Enthalpies= -927.335420

Sum of electronic and thermal Free Energies= -927.428724

TS addition reaction between falcarinol and $CH_3OO^{\bullet}$ at C15

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

O	-5.81224700	-1.56353300	-0.27824100
C	5.68508100	-0.67095300	0.12133000
C	4.96972100	0.68086300	0.22522200
C	6.87762600	-0.66112500	-0.84170700
C	3.78248100	0.67079100	1.19434600
C	7.59390700	-2.01238600	-0.94725000
C	3.06706900	2.03153600	1.29179400
C	8.78590600	-1.99219700	-1.90842000
C	1.95664800	2.02957000	2.30486800
C	0.65532100	2.25016100	2.11646700
C	-0.03246600	2.58814100	0.80947600
C	-1.11693200	1.66363400	0.49150100
C	-2.01280000	0.89110100	0.24686100
C	-4.50516200	-2.15086200	-0.38113200
C	-3.06567800	0.04066600	-0.03331500
C	-3.46546800	-1.15136000	-0.10082000
C	-4.33578000	-2.84188400	-1.71984400
C	-3.35428100	-2.64225300	-2.59123700
H	4.96690800	-1.43630800	-0.19940500
H	6.02804700	-0.97556500	1.11850800
H	5.68846500	1.44774400	0.54180800
H	4.62243800	0.98298300	-0.77123700

H	6.53597600	-0.35585700	-1.83934300
H	7.59656900	0.10382200	-0.52052400
H	4.12911700	0.37451000	2.19216100
H	3.05809300	-0.09104300	0.88428000
H	6.87640300	-2.77616000	-1.27074500
H	7.93395400	-2.31865800	0.04950000
H	2.70339900	2.32037700	0.30151000
H	3.80412400	2.79305600	1.58041600
H	9.27469700	-2.96892900	-1.96003500
H	9.53672100	-1.26156000	-1.59154900
H	8.47240500	-1.72416900	-2.92226500
H	2.27263400	1.80422000	3.32251700
H	-0.01125700	2.19039100	2.97233300
H	0.68009100	2.60783200	-0.01972600
H	-0.45650500	3.59977500	0.87203200
H	-4.48643500	-2.91692600	0.40339600
H	-5.13582300	-3.54519500	-1.93451600
H	-5.75984500	-0.70584700	-0.72544500
H	-3.32224800	-3.18110200	-3.53128200
H	-2.55260000	-1.93767300	-2.39805600
O	-4.80538600	1.96275700	0.50235000
O	-4.48959000	1.09803300	-0.53505500
C	-5.94833800	1.47495000	1.20999800
H	-6.10761800	2.19420400	2.01476500
H	-6.82254200	1.44631500	0.55323900
H	-5.75454400	0.48021400	1.61707900

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

Zero-point correction=	0.408062 (Hartree/Particle)
Thermal correction to Energy=	0.434306
Thermal correction to Enthalpy=	0.435251
Thermal correction to Gibbs Free Energy=	0.343831
Sum of electronic and zero-point Energies=	-927.365103
Sum of electronic and thermal Energies=	-927.338859
Sum of electronic and thermal Enthalpies=	-927.337915
Sum of electronic and thermal Free Energies=	-927.429334

TS addition reaction between falcarinol and $CH_3OO^{\bullet}$ at C16

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

O	-6.34821300	1.98529000	-0.69968200
C	6.43070300	0.12311700	-0.36700500
C	4.92585000	-0.14995900	-0.47070700
C	7.25693300	-1.12530500	-0.03760600
C	4.09547800	1.09894200	-0.78620800
C	8.76334700	-0.85881300	0.06153000
C	2.58725000	0.80750800	-0.90034600
C	9.57833800	-2.11136100	0.39623500
C	1.78095100	2.02359400	-1.25977700
C	0.80918800	2.61235200	-0.56199300
C	0.27559100	2.18570300	0.79243500
C	-1.12598100	1.78414100	0.73550900

C	-2.29820500	1.46018700	0.66832300
C	-6.14414500	0.77646700	0.03545900
C	-3.59650400	1.11567300	0.57200500
C	-4.77413200	0.71837700	0.60719500
C	-6.51244000	-0.41854000	-0.81659900
C	-5.73136300	-1.44938600	-1.11723100
H	6.60841900	0.88719800	0.40066100
H	6.78625600	0.55368900	-1.31185700
H	4.74772200	-0.90711700	-1.24513600
H	4.57288700	-0.59033500	0.47073600
H	6.90362300	-1.55340400	0.90949000
H	7.07586300	-1.89168900	-0.80249700
H	4.44865500	1.54515900	-1.72398000
H	4.25654900	1.85531700	-0.00905800
H	8.94430800	-0.09122600	0.82378400
H	9.11749900	-0.43480300	-0.88588800
H	2.23276100	0.35754800	0.03138100
H	2.43754300	0.04868700	-1.68006200
H	10.64672500	-1.88801100	0.46055600
H	9.44623800	-2.88479600	-0.36685300
H	9.27002700	-2.53852600	1.35558100
H	2.04180300	2.47634500	-2.21528700
H	0.32053000	3.48658200	-0.98279900
H	0.37124000	3.02174300	1.49825800
H	0.86936200	1.36569100	1.20725900
H	-6.84361100	0.83848100	0.87442800
H	-7.52024800	-0.35220400	-1.21874700
H	-5.79895400	1.93126700	-1.49024900
H	-6.08494900	-2.24788900	-1.75977500
H	-4.73064900	-1.54548800	-0.71278400
O	-4.45111900	-1.61473700	2.03590000
O	-5.13700100	-0.42891200	2.10107400
C	-3.35555000	-1.58152800	2.95608500
H	-2.91872700	-2.58090200	2.91671400
H	-2.62337700	-0.83243400	2.64576100
H	-3.71665100	-1.36115800	3.96321700

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

Zero-point correction= 0.407510 (Hartree/Particle)

Thermal correction to Energy= 0.434092

Thermal correction to Enthalpy= 0.435036

Thermal correction to Gibbs Free Energy= 0.342875

Sum of electronic and zero-point Energies= -927.374885

Sum of electronic and thermal Energies= -927.348303

Sum of electronic and thermal Enthalpies= -927.347359

Sum of electronic and thermal Free Energies= -927.439520

TS addition reaction between falcarinol and CH3OO• at C18

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

O	-6.19279600	-1.18544000	0.72485100
C	7.39242700	-0.10376900	-0.06284800

C	5.91363100	0.12513100	-0.39548700
C	8.23782400	1.17383700	-0.11330100
C	5.06989000	-1.15302000	-0.33880300
C	9.71757200	0.94534700	0.21575700
C	3.58565300	-0.91678200	-0.67715300
C	10.55398700	2.22710300	0.16544000
C	2.78154000	-2.18641700	-0.68760000
C	1.75534700	-2.52850200	0.09178600
C	1.13972600	-1.70083800	1.20225400
C	-0.26617400	-1.39114400	0.95803100
C	-1.43235500	-1.14521500	0.74456300
C	-5.31336300	-0.25623600	0.06298700
C	-2.74245300	-0.85823400	0.50498300
C	-3.90684200	-0.60307400	0.28532900
C	-5.55827200	1.16986700	0.47607000
C	-6.01806000	2.15083700	-0.38538400
H	7.80966500	-0.84132900	-0.76046400
H	7.47310300	-0.55175400	0.93589400
H	5.49707900	0.86570500	0.29943600
H	5.83181600	0.56870300	-1.39609700
H	8.15603700	1.62385500	-1.11123900
H	7.82268800	1.91116800	0.58615500
H	5.14214700	-1.59871500	0.66031200
H	5.48399000	-1.89440400	-1.03336700
H	10.13297900	0.21049600	-0.48446600
H	9.79944600	0.49445100	1.21217100
H	3.52433800	-0.45808700	-1.67298600
H	3.16639400	-0.18511400	0.01937900
H	11.60284800	2.02998000	0.40326600
H	10.18496200	2.96848600	0.88109800
H	10.51917000	2.68314600	-0.82894100
H	3.09783000	-2.91769000	-1.43007500
H	1.28281700	-3.49438000	-0.06390400
H	1.69144400	-0.76860400	1.35283900
H	1.21260400	-2.25488700	2.14813700
H	-5.54829800	-0.36986100	-0.99932100
H	-5.41821500	1.39483600	1.52929100
H	-5.93335800	-1.22110600	1.65288400
H	-5.94968200	3.18711800	-0.07762300
H	-5.96257100	1.98551100	-1.45552000
O	-8.41391400	1.26364200	-1.17974700
O	-7.87257000	2.18393400	-0.29952100
C	-9.07145400	0.22886200	-0.43723100
H	-9.55306900	-0.39438900	-1.19344000
H	-8.34363700	-0.35417000	0.13151700
H	-9.82318200	0.66407800	0.22564100

Frequency and Energy at B3LYP/6-311G (d,p) (gas)
Zero-point correction= 0.408609 (Hartree/Particle)
Thermal correction to Energy= 0.434826
Thermal correction to Enthalpy= 0.435770
Thermal correction to Gibbs Free Energy= 0.344994

Sum of electronic and zero-point Energies=	-927.373658
Sum of electronic and thermal Energies=	-927.347441
Sum of electronic and thermal Enthalpies=	-927.346497
Sum of electronic and thermal Free Energies=	-927.437273

Figure S2*:* IRC plots for all transition states related to reaction of $CH_3OO^{\bullet}$ and $HO^{\bullet}$ radical with ***falcarinol*** at B3LYP/6-311G(d,p) level of theory in the gas phase.

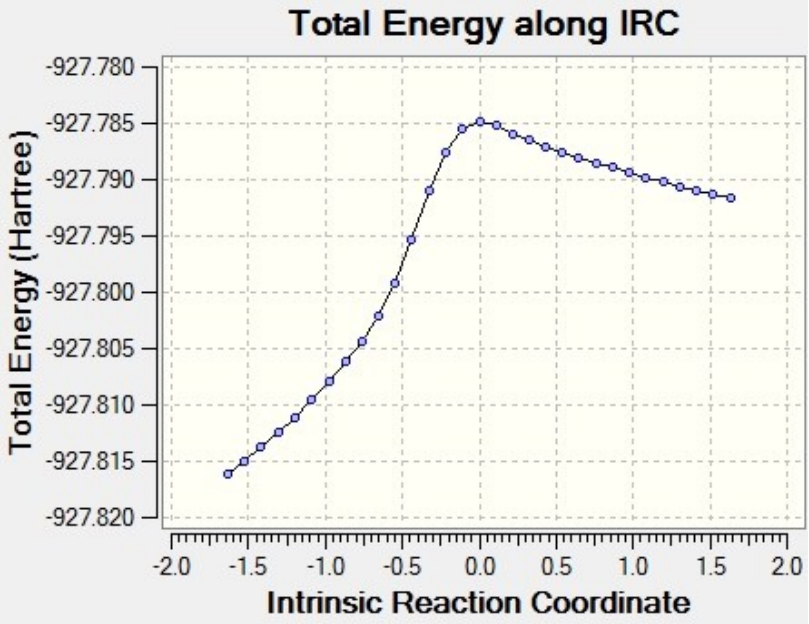


Figure S2-1. IRC of H-abstraction reaction by $CH_3OO^{\bullet}$ at C3-H

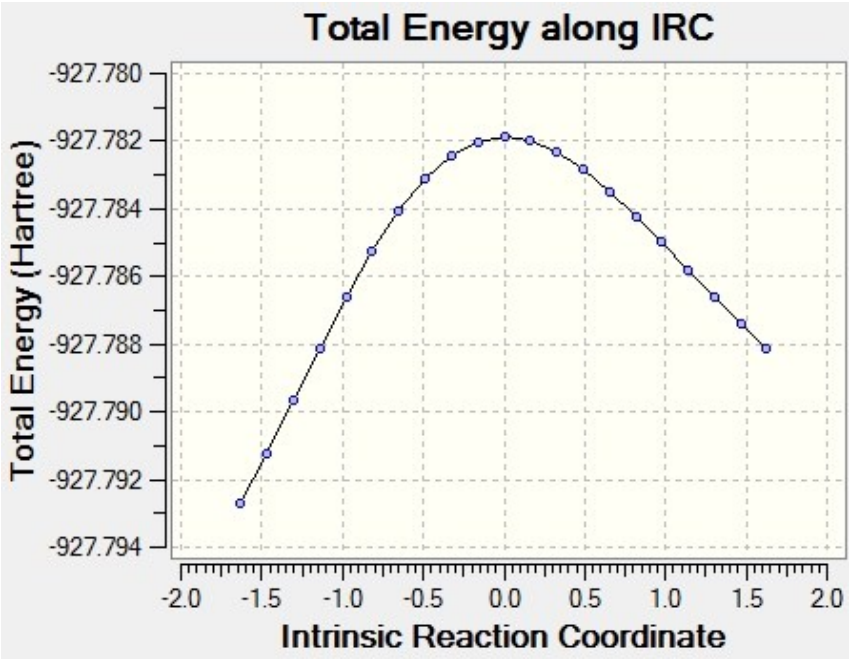


Figure S2-2. IRC of addition reaction by $CH_3OO^{\bullet}$ at C10 position

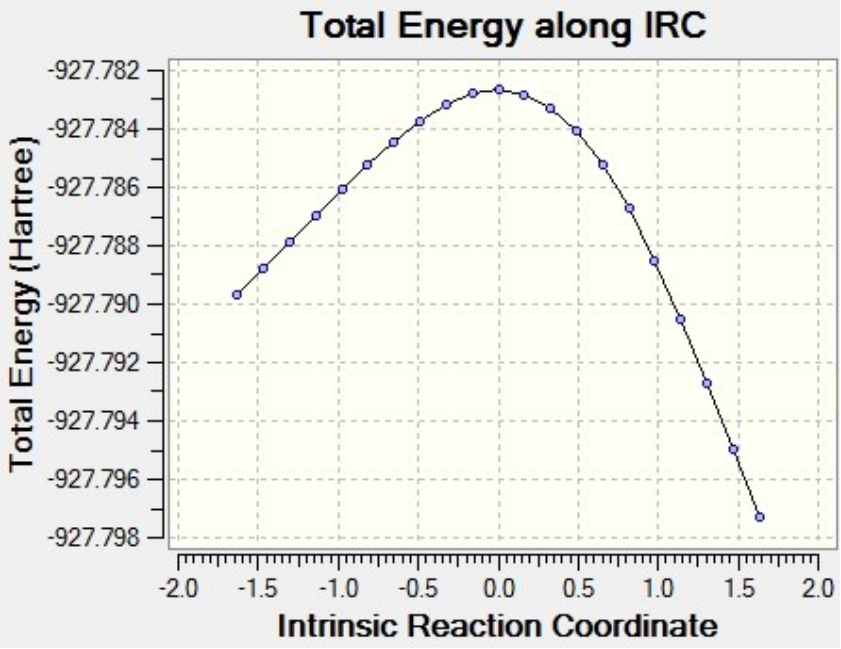


Figure S2-3. IRC of addition reaction by $CH_3OO^{\bullet}$ at C7 position

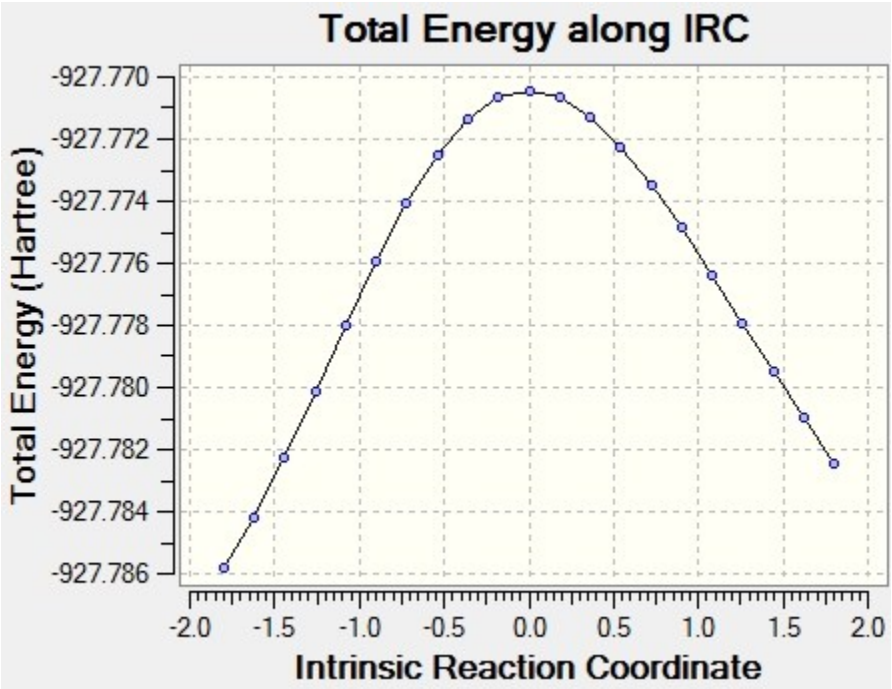


Figure S2-4. IRC of addition reaction by $CH_3OO^{\bullet}$ at C6 position

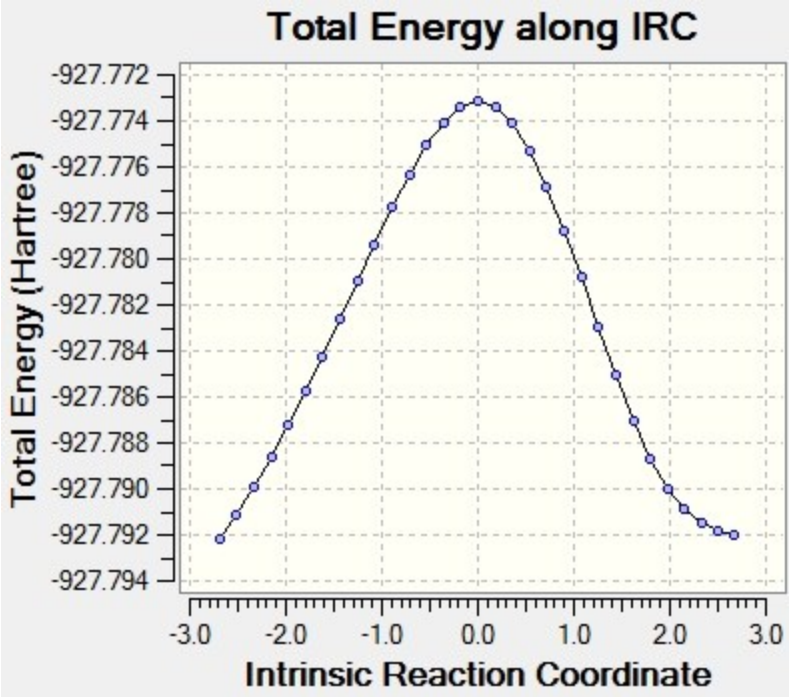


Figure S2-5. IRC of addition reaction by $CH_3OO^{\bullet}$ at C5 position

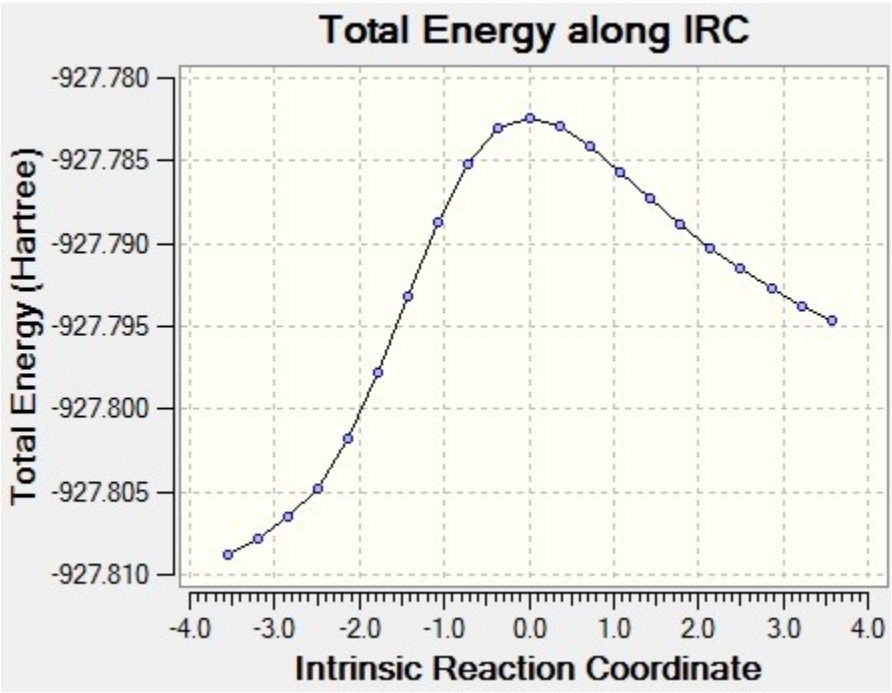


Figure S2-6. IRC of addition reaction by $CH_3OO^{\bullet}$ at C4 position

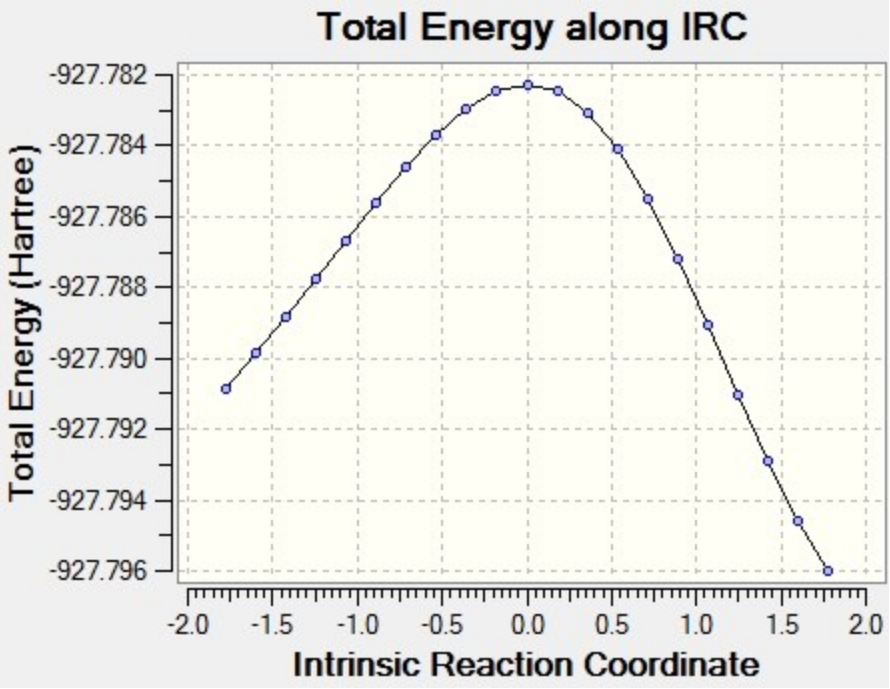


Figure S2-7. IRC of addition reaction by $CH_3OO^{\bullet}$ at C1 position

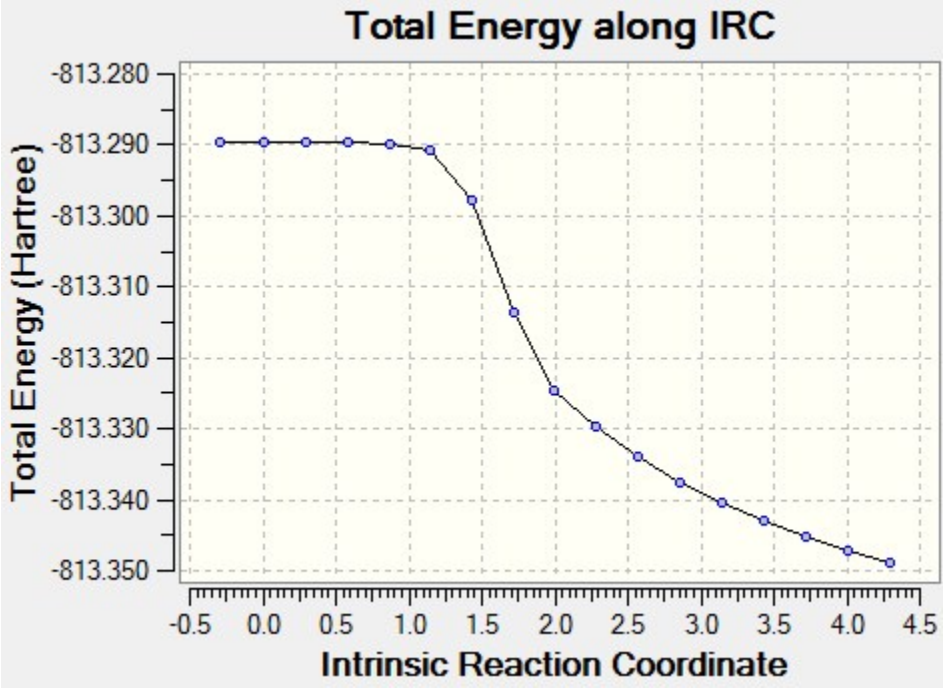


Figure S2-8: IRC of H-abstraction reaction by HO• radical at C3-H

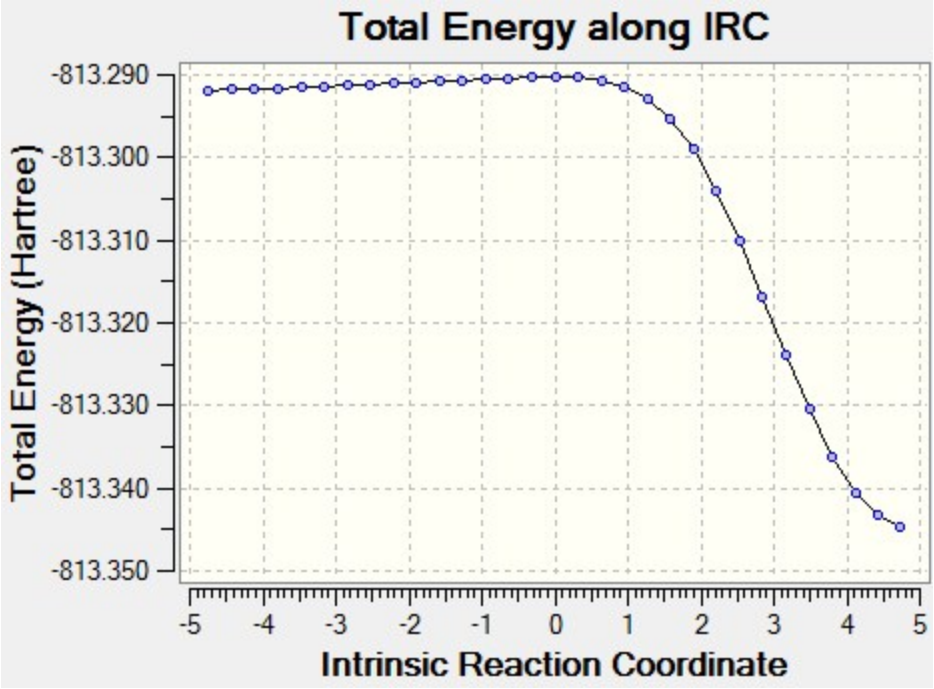


Figure S2-9: IRC of addition reaction by HO• radical at C4 position

Figure S3: IRC plots for all transition states related to reaction of $CH_3OO^{\bullet}$ and $HO^{\bullet}$ radical with ***α-vetivone*** at B3LYP/6-311G(d,p) level of theory in the gas phase.

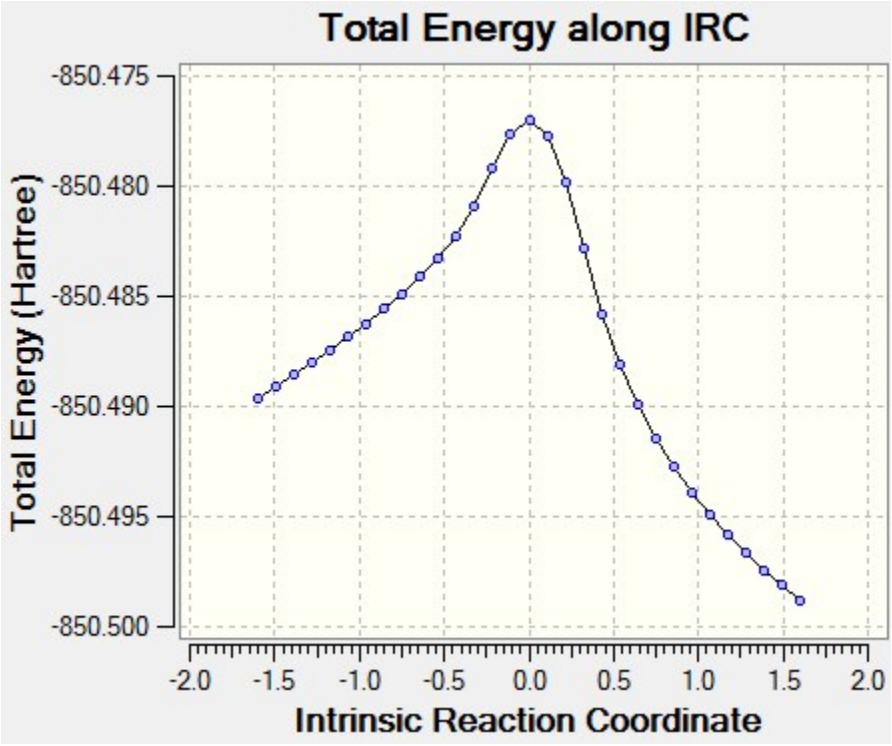


Figure S3-1: IRC of H-abstraction reaction at C8-H position by $CH_3OO\bullet$ radical

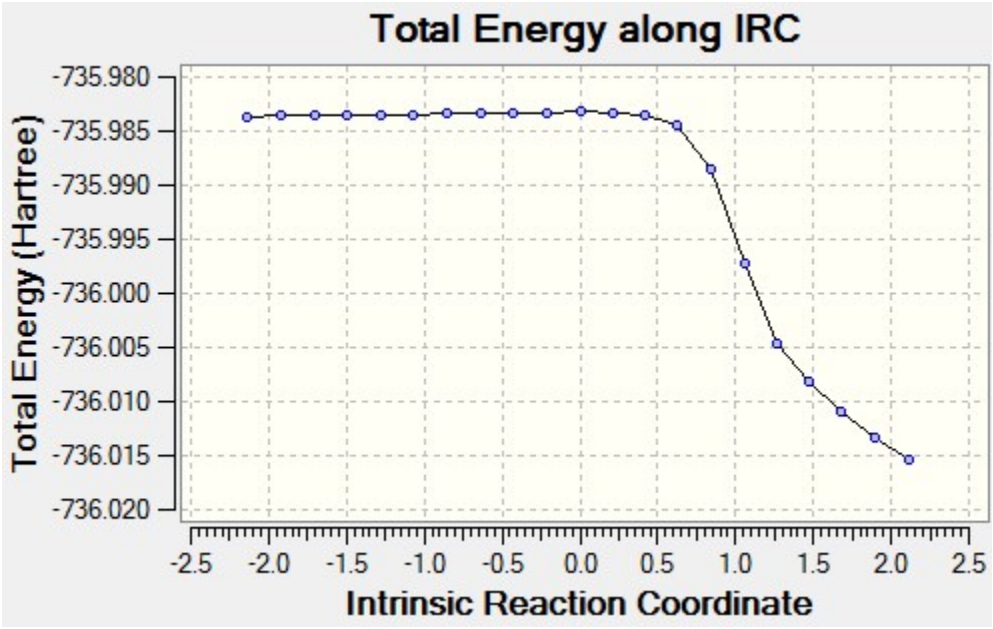


Figure S3-2: IRC of H-abstraction reaction at C8-H position by $HO\bullet$ radical

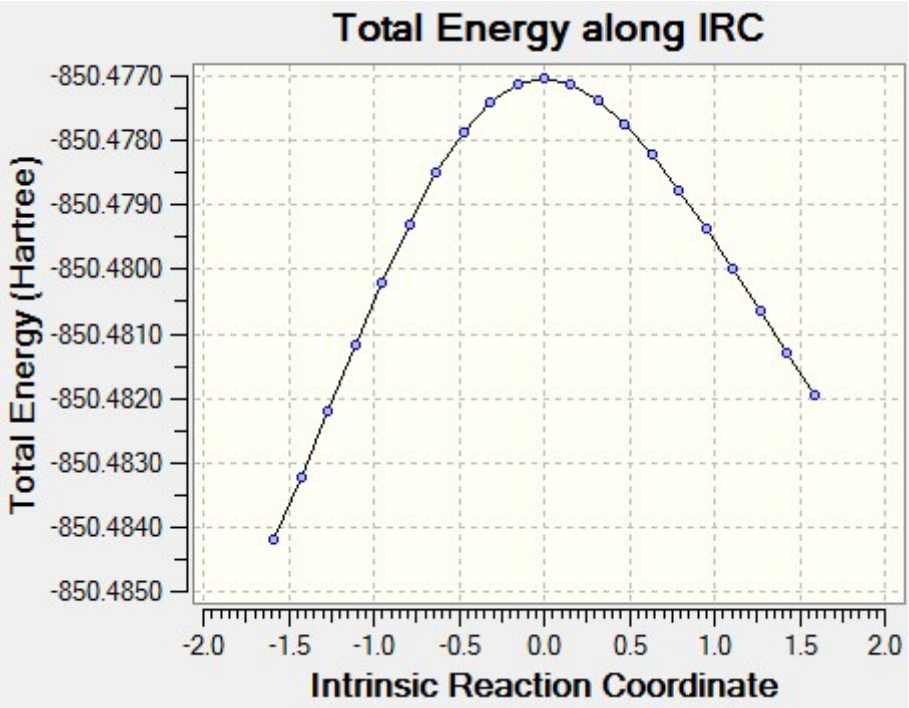


Figure S3-3: IRC of addition reaction at C9 position by $CH_3OO\bullet$ radical

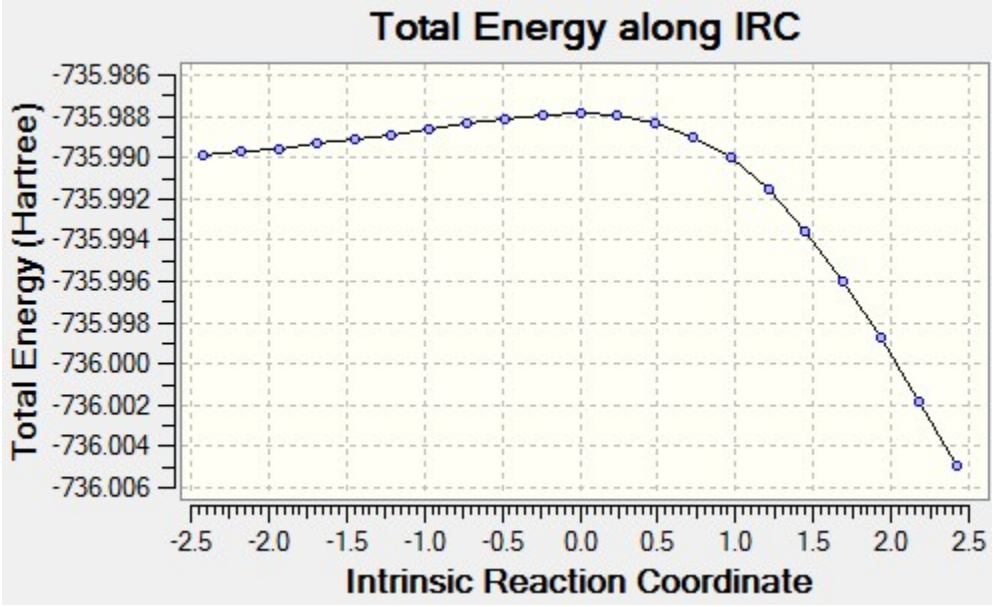
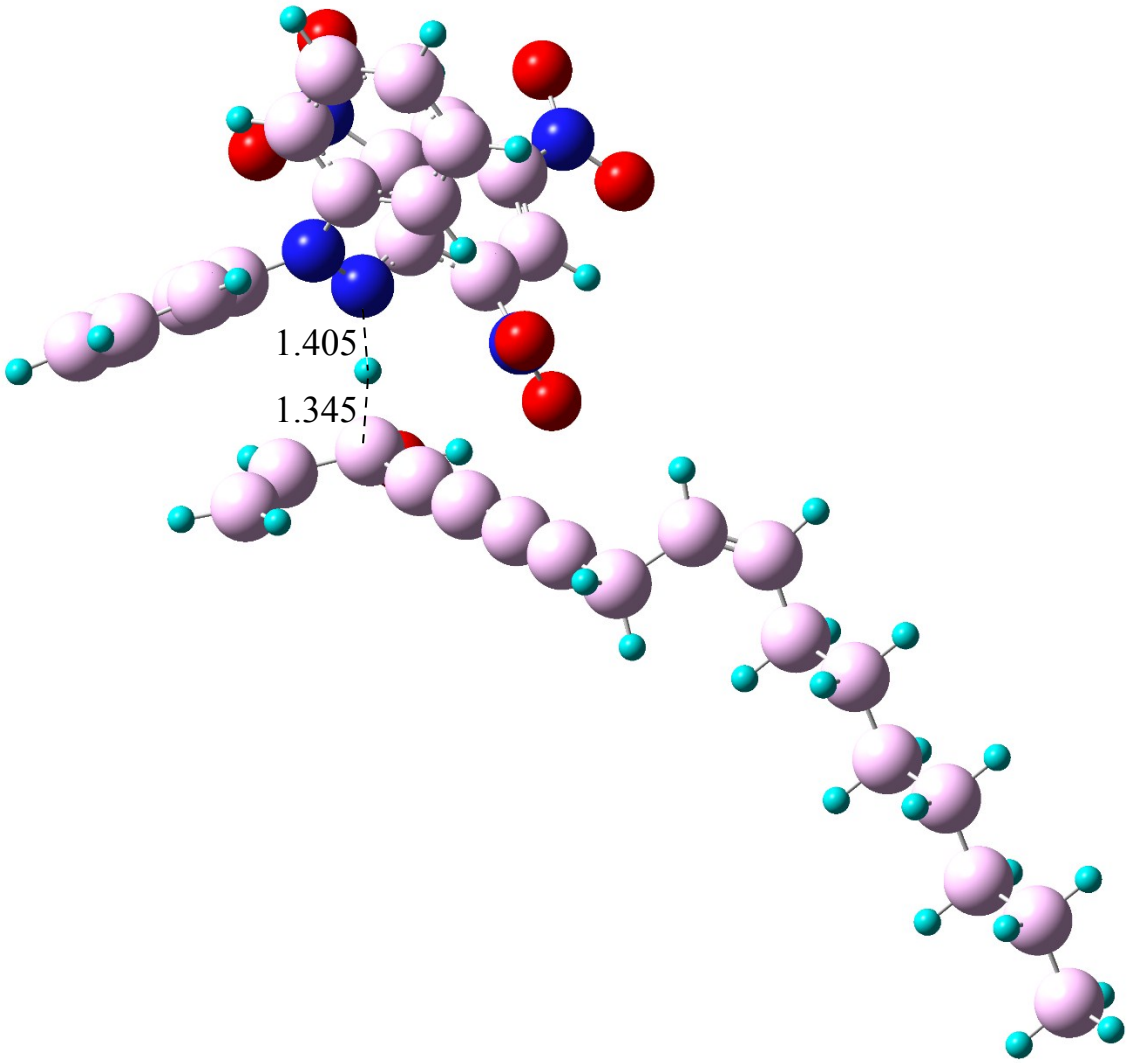
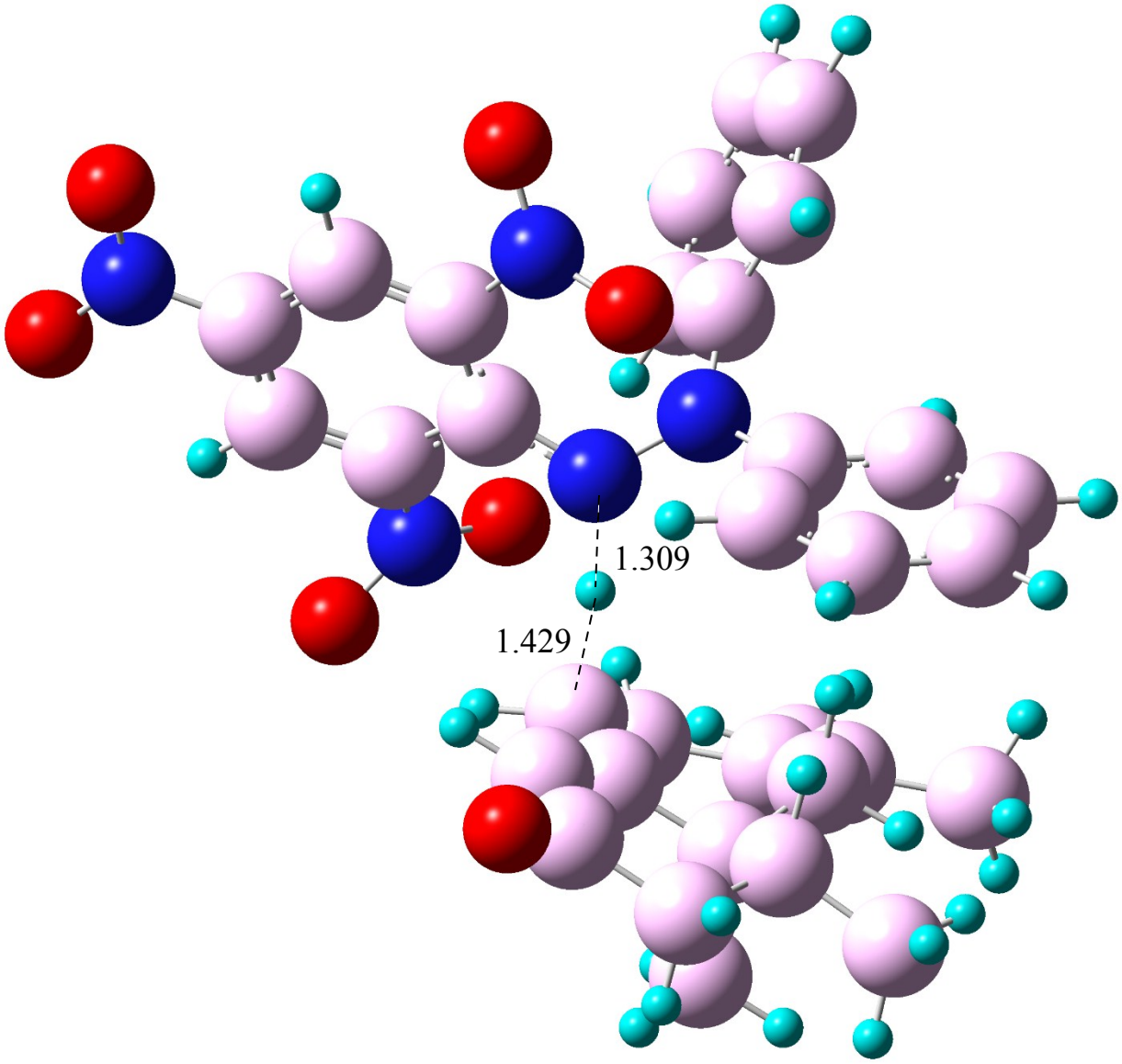


Figure S3-4: IRC of addition reaction at C9 position by HO• radical

Figure S4: Optimized structures of transition state for H-atom abstraction reactions between **(A)** falcarinol and DPPH• radical; **(B)** α-vetivone and DPPH• radical calculated at B3LYP/3-21G level of theory



(A)



(B)