Supporting Information (SI)

Computational assessment of the radical scavenging activity of natural cleomiscosins

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Table S1. The method to calculate rate constant following the conventional transition state theory

The rate constant (k) was calculated by using the conventional transition state theory (TST) (at 298.15 K, 1M standard state) according to the equation (1):[1-5]

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

Where: σ is the reaction symmetry number ,[6,7]

κ contains the tunneling corrections calculated using the Eckart barrier,[8]

k_B is the Boltzmann constant,

h is the Planck constant,

$\Delta G^{\neq}$ is the Gibbs free energy of activation.

The Marcus Theory was used to estimate the reaction barriers of SET reactions.[9-12] The free energy of reaction $\Delta G^{\neq}$ for the SET pathway was computed following the equations (2,3).

$$\Delta G_{SET}^{\neq} = \frac{\lambda}{4}\left(1 + \frac{\Delta G_{SET}^{0}}{\lambda}\right)^2 \quad (2)$$

$$\lambda \approx \Delta E_{SET} - \Delta G_{SET}^{0} \quad (3)$$

where ΔG_{SET} is the Gibbs energy of reaction, ΔE_{SET} is the non-adiabatic energy difference between reactants and vertical products for SET ($\Delta E_{SET} = E_{vertical}$ (products) - $E_{adiabatic}$ (reactants))[13,14]

For rate constants that were close to the diffusion limit a correction was applied to yield realistic results[15]. The apparent rate constants (k_{app}) were calculated following the Collins–Kimball theory in the solvents at 298.15K;[16] the steady-state Smoluchowski rate constant (k_D) for an irreversible bimolecular diffusion–controlled reaction was calculated following the literature as corroding to equations (4,5).[15,17]

$$k_{app} = \frac{k_{TST} k_D}{k_{TST} + k_D} \quad (4)$$

$$k_D = 4\pi R_{AB} D_{AB} N_A \quad (5)$$

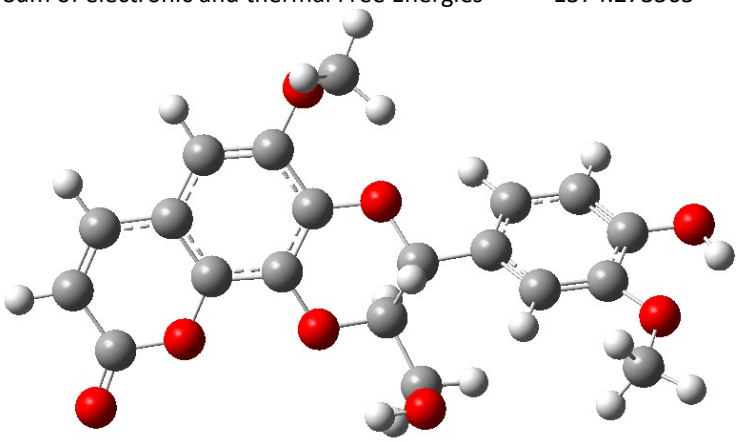
where R_{AB} is the reaction distance, N_A is the Avogadro constant, and $D_{AB} = D_A + D_B$ (D_{AB} is the mutual diffusion coefficient of the reactants A and B),[16,18] where D_A or D_B is estimated using the Stokes–Einstein formulation (6).[19,20]

$$D_{A\ or\ B} = \frac{k_B T}{6\pi\eta a_{A\ or\ B}} \quad (6)$$

η is the viscosity of the solvents (i.e. $\eta(H_2O) = 8.91\times10^{-4}$ Pa s, η(pentyl ethanoate) = 8.62×10^{-4} Pa s) and a is the radius of the solute.

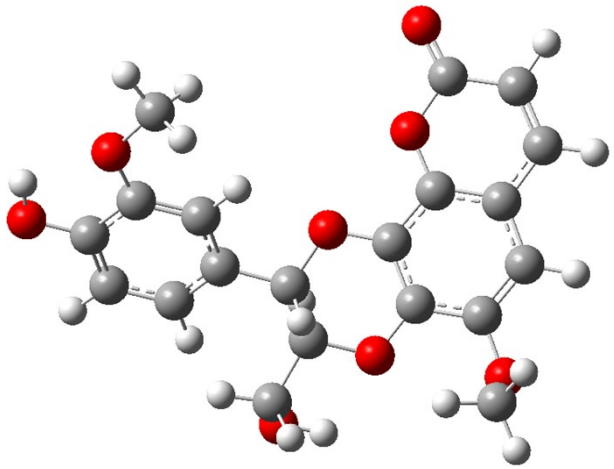
The kinetic study requires different considerations. Water and pentyl ethanoate are the *de facto* standard solvents in the literature to mimic the polar and nonpolar environments in the human body.[15,21-23] Thus, these solvents were used to model the physiological environments. The solvent cage effects were included following the corrections proposed by Okuno,[24] adjusted with the free volume theory according to the Benson correction[15,25-27] to reduce over-penalizing entropy losses in solution. For the species that have multiple conformers, all of these were investigated and the conformer with the lowest electronic energy was included in the analysis.[22,23] The hindered internal rotation treatment was also applied to the single bonds to ensure that the obtained conformer has the lowest electronic energy.[23,28] All transition states were characterized by the existence of only one single imaginary frequency. Intrinsic coordinate calculations (IRCs) were performed to ensure that each transition state is connected correctly with the pre-complex and post-complex. The kinetic calculations were performed by the *Eyringpy* code[29,30]

Table S2: The Cartesian coordinates **and energies** of CMs, ANIONs, TSs in the studied media (G: gas phase; P: pentyl ethanoate; H: water)

Name				**CMA-G**
Cartesian Coordinates				Energy
O	0.08395500	1.22354200	-0.04499100	Zero-point correction= 0.359109 (Hartree/Particle)
O	-1.11653100	-1.31339600	-0.34213000	Thermal correction to Energy= 0.383556
O	1.01400800	-2.85686400	0.68803600	Thermal correction to Enthalpy= 0.384500
O	-3.76529400	-1.54519900	-0.20653200	Thermal correction to Gibbs Free Energy= 0.304077
O	-1.48017200	3.44836100	0.20367800	Sum of electronic and zero-point Energies= -1374.218534
O	5.62901500	-0.96540500	0.75873900	Sum of electronic and thermal Energies= -1374.194087
O	6.27932900	0.85250200	-1.04229900	Sum of electronic and thermal Enthalpies= -1374.193142
O	-5.49944000	-2.91612300	-0.27363300	Sum of electronic and thermal Free Energies= -1374.273565
C	0.82894300	0.01794800	0.14942600	
C	0.23147600	-1.06907300	-0.74910000	
C	2.27580700	0.29251100	-0.15065000	
C	-1.85213600	-0.18811400	-0.14641500	
C	-1.26258400	1.06560600	-0.01176000	
C	0.93450400	-2.40929900	-0.65124500	
C	-3.24479200	-0.29809700	-0.08999100	
C	-2.06265600	2.21708300	0.14165200	
C	-4.04112000	0.83387900	0.06719200	
C	3.24874300	-0.46986700	0.50782700	
C	2.65336600	1.23399800	-1.09663800	
C	-3.43378400	2.09429000	0.17744800	
C	4.58585800	-0.28610700	0.20205100	
C	4.00295300	1.42582500	-1.39328400	
C	-5.46783200	0.62472500	0.09728300	
C	4.96892400	0.67098500	-0.75410000	
C	-5.98352700	-0.61065400	-0.01637100	
C	-5.12448900	-1.78455200	-0.17345800	
C	-0.78747300	3.71694800	1.42111300	
C	5.31975200	-1.96983100	1.70808400	
H	0.70985500	-0.30259200	1.19042800	
H	0.23878200	-0.70969600	-1.78658900	
H	0.39689900	-3.12789200	-1.27786100	
H	1.95549100	-2.31707300	-1.02132000	
H	2.93761600	-1.21224900	1.23389000	
H	1.89796700	1.83291700	-1.58979800	
H	-4.03537200	2.98868000	0.28670300	
H	4.32123800	2.16117000	-2.12168600	
H	-6.11589300	1.48737800	0.21270400	
H	0.11614400	-3.02236500	0.99410400	
H	-7.04549800	-0.81162600	0.00130400	
H	-0.41694700	4.73689500	1.34175700	
H	0.05109200	3.03117300	1.55302700	
H	-1.47458800	3.64010800	2.26912700	
H	6.79330500	0.24073400	-0.50141800	
H	4.82274200	-1.53753900	2.58100500	
H	4.67976000	-2.73886900	1.26615600	
H	6.26884300	-2.40770600	2.00715200	
Name				**CMB-G**
Cartesian Coordinates				Energy
O	0.07256800	0.31177600	-0.28937800	Zero-point correction= 0.359150 (Hartree/Particle)
O	1.04501500	-2.28917600	0.19781000	Thermal correction to Energy= 0.383540

O	1.77236600	2.35619800	-0.41070600
O	-0.95562500	-3.72020300	-1.15596400
O	3.72899200	-2.73753200	0.32788900
O	-4.42939700	1.92147100	1.20118600
O	-6.18160900	0.52212300	-0.18833500
O	2.00941200	4.54322000	-0.63820300
C	-0.71922300	-0.83868100	-0.59388400
C	-0.33777900	-1.95599500	0.38272100
C	-2.17035200	-0.45145800	-0.50290300
C	1.39515900	0.05546300	-0.14721900
C	1.88337300	-1.22773100	0.07738200
C	-1.08874400	-3.25695400	0.17068200
C	2.29930100	1.12039000	-0.22723500
C	3.26974800	-1.46120100	0.17206200
C	3.67117300	0.89926900	-0.12791500
C	-2.56649700	0.59156500	0.33964900
C	-3.11991200	-1.15344500	-1.23481100
C	4.14817300	-0.40645800	0.06616800
C	-3.90973600	0.91713800	0.43778500
C	-4.47069400	-0.83262000	-1.12314600
C	4.52541200	2.05613000	-0.24243300
C	-4.87076100	0.19816600	-0.29071200
C	4.00274400	3.28055100	-0.42138100
C	2.55644400	3.48807600	-0.50225700
C	3.57185500	-3.25331100	1.64671300
C	-3.51755500	2.75667800	1.89175200
H	-0.47938300	-1.17462700	-1.60837200
H	-0.48490500	-1.59084800	1.40766500
H	-0.71187800	-3.99384100	0.88862100
H	-2.15170100	-3.10434400	0.35496300
H	-1.81408000	1.15418300	0.87560300
H	-2.80547200	-1.95922500	-1.89006000
H	5.21197800	-0.60144100	0.13085500
H	-5.22650300	-1.36484400	-1.68703800
H	5.59962600	1.91541900	-0.18121900
H	-0.02147700	-3.89064500	-1.31538200
H	4.60570200	4.17329800	-0.51063900
H	3.97815000	-4.26271400	1.63304500
H	2.51734200	-3.28498800	1.92935800
H	4.13045800	-2.64095600	2.36089100
H	-6.25703300	1.27566600	0.40968900
H	-4.11801600	3.50981000	2.39601800
H	-2.95111600	2.18425500	2.63173400
H	-2.82824400	3.23939500	1.19377600

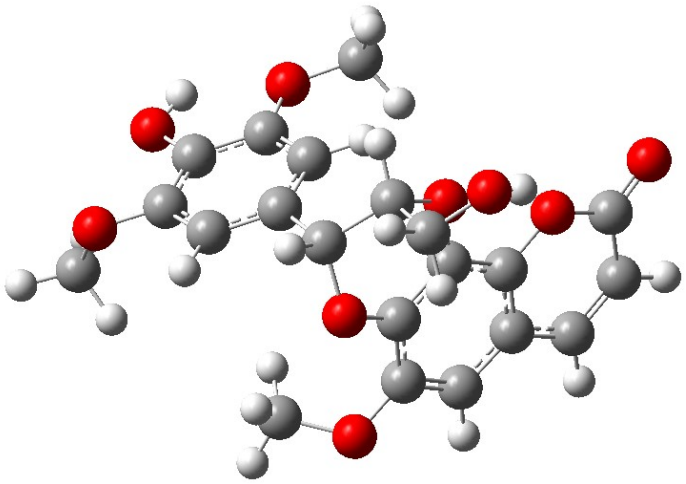
Thermal correction to Enthalpy= 0.384484
Thermal correction to Gibbs Free Energy= 0.304214
Sum of electronic and zero-point Energies= -1374.217304
Sum of electronic and thermal Energies= -1374.192914
Sum of electronic and thermal Enthalpies= -1374.191970
Sum of electronic and thermal Free Energies= -1374.272239



Name			**CMC-G**
Cartesian Coordinates			Energy
O	-0.13292900	-2.21086700	0.43785400
O	1.39941600	-0.14676600	1.60267800
O	2.37179900	-1.57807400	3.79718400
O	3.24585500	1.10096300	0.16986800
O	0.22808200	-2.82507300	-2.24046700
O	-2.00975000	3.17412600	0.27776800
O	-5.03865300	-0.39655800	-0.25797200
O	-4.37147600	2.29469700	-0.48000800

Zero-point correction= 0.391894 (Hartree/Particle)
Thermal correction to Energy= 0.419069
Thermal correction to Enthalpy= 0.420013
Thermal correction to Gibbs Free Energy= 0.333301
Sum of electronic and zero-point Energies= -1488.687765
Sum of electronic and thermal Energies= -1488.660590
Sum of electronic and thermal Enthalpies= -1488.659646
Sum of electronic and thermal Free Energies= -1488.746358

O	4.80175200	2.67181000	0.14118700
C	-0.65710100	-1.46266000	1.55222600
C	0.51353600	-0.95762400	2.38828900
C	-1.62906000	-0.41184000	1.06123200
C	1.56202200	-0.52925500	0.30710900
C	0.78996400	-1.52467300	-0.28586200
C	1.32777100	-2.08785600	3.00389300
C	2.53311100	0.12602400	-0.45311400
C	0.97164600	-1.85801700	-1.64258900
C	-2.88042300	-0.84095400	0.63355800
C	-1.28796200	0.94031700	0.95624300
C	2.74659900	-0.22487300	-1.78409000
C	1.95505300	-1.22137900	-2.37139000
C	-2.20950700	1.83449600	0.43013600
C	-3.80411200	0.05507300	0.10403300
C	-3.47377100	1.40572600	0.00593000
C	3.78203900	0.49462500	-2.48587000
C	4.48737200	1.45811300	-1.87018300
C	4.23318000	1.81795200	-0.47477100
C	-1.19244400	-2.71226500	-2.12851500
C	-0.75132500	3.69989100	0.66705200
C	-5.32874600	-0.29313800	-1.64969600
H	-1.19963200	-2.20768600	2.13688800
H	0.15448800	-0.29677700	3.17989200
H	0.68874200	-2.68231900	3.66005900
H	1.70706900	-2.74150700	2.20798800
H	-3.16951100	-1.88403100	0.70368000
H	-0.31785800	1.28925700	1.28120800
H	2.09313800	-1.49611100	-3.40990400
H	3.97870300	0.24018800	-3.52221400
H	2.88953800	-0.97422000	3.25405500
H	5.27057300	2.02055600	-2.35889000
H	-1.60355600	-3.11240800	-3.05446600
H	-1.48978300	-1.66602800	-2.01219600
H	-1.55793300	-3.28504600	-1.27694700
H	-3.96569700	3.17041500	-0.44780800
H	-0.58178400	3.54838800	1.73623500
H	-0.78810000	4.76425600	0.44961300
H	0.05735000	3.23435500	0.09700100
H	-6.31894200	-0.72290600	-1.78637300
H	-4.59765700	-0.86631500	-2.22904600
H	-5.32898100	0.74779500	-1.97524800

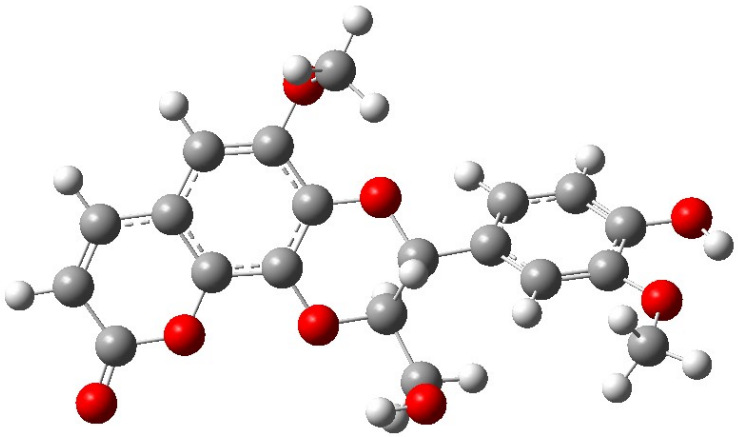


Name	**CMA-P**
Cartesian Coordinates	Energy

O	0.09574500	1.19540000	-0.05276900
O	-1.13200600	-1.33200300	-0.33025400
O	0.98412600	-2.89452700	0.72589800
O	-3.78838700	-1.52682800	-0.20359200
O	-1.42899400	3.42982900	0.19672800
O	5.65662800	-0.84188400	0.83346800
O	6.26929700	0.78922600	-1.14735200
O	-5.53000600	-2.87810500	-0.27233300
C	0.83538000	-0.01803600	0.14317900
C	0.22453000	-1.11056900	-0.73800800

Zero-point correction=	0.358295 (Hartree/Particle)
Thermal correction to Energy=	0.382904
Thermal correction to Enthalpy=	0.383849
Thermal correction to Gibbs Free Energy=	0.302844
Sum of electronic and zero-point Energies=	-1374.247999
Sum of electronic and thermal Energies=	-1374.223390
Sum of electronic and thermal Enthalpies=	-1374.222446
Sum of electronic and thermal Free Energies=	-1374.303450

C	2.27817700	0.24806700	-0.18529300
C	-1.85271700	-0.19796300	-0.14550800
C	-1.24948500	1.05030600	-0.01717800
C	0.91308100	-2.45574100	-0.61867100
C	-3.24678300	-0.28584300	-0.08936600
C	-2.03776100	2.21130600	0.13209100
C	-4.03168600	0.85437700	0.06522300
C	3.26728500	-0.42561100	0.54120300
C	2.63536100	1.09315600	-1.22693700
C	-3.41022700	2.10884600	0.17113500
C	4.60176900	-0.24847300	0.21409900
C	3.98027500	1.27946000	-1.54859700
C	-5.45951900	0.66401500	0.09861100
C	4.96178600	0.61271900	-0.83767200
C	-5.99119900	-0.56681000	-0.01210400
C	-5.14539700	-1.74326700	-0.16980400
C	-0.82463000	3.70732800	1.46230100
C	5.37159100	-1.74307100	1.89534400
H	0.73327500	-0.32069800	1.19056600
H	0.23633500	-0.77433700	-1.78251200
H	0.37403500	-3.17649400	-1.24197600
H	1.93548300	-2.37850600	-0.98918700
H	2.97737400	-1.09263200	1.34432300
H	1.87029000	1.62236600	-1.78211600
H	-4.00674200	3.00692600	0.28262400
H	4.27726700	1.94275900	-2.35245600
H	-6.09640500	1.53502400	0.21398800
H	0.08364900	-3.05434800	1.03042700
H	-7.05689600	-0.74987300	0.00842800
H	-0.37321000	4.69470600	1.37997100
H	-0.05195200	2.97227500	1.69725300
H	-1.58492000	3.71534900	2.24919000
H	6.79781700	0.24466200	-0.54899200
H	4.86237500	-1.22790900	2.71427500
H	4.75892400	-2.57730000	1.54221400
H	6.33310100	-2.11600700	2.24134500

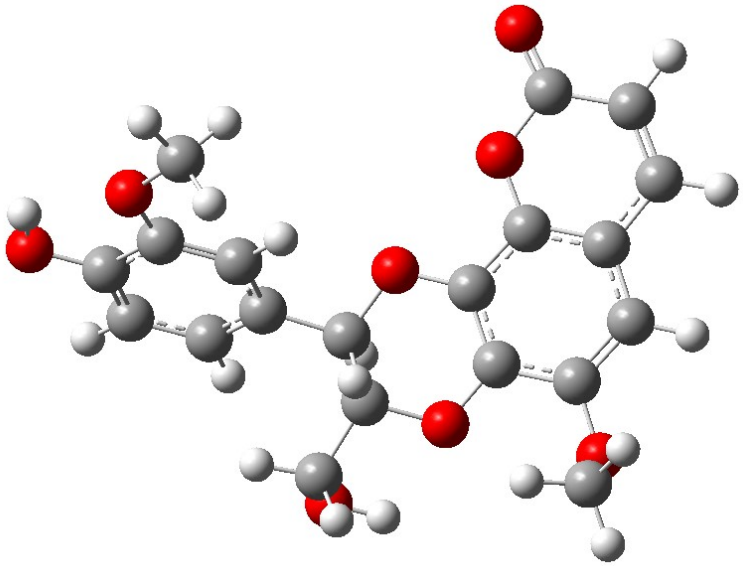


Name	**CMB-P**
Cartesian Coordinates	Energy

O	0.10107500	0.37070000	-0.35582100
O	0.96068500	-2.26818100	0.15932800
O	1.89313700	2.34247700	-0.45410700
O	-1.03446800	-3.63190700	-1.27824300
O	3.60728700	-2.81656100	0.40863500
O	-4.45810200	1.68808800	1.47987200
O	-6.15688300	0.73366700	-0.29226200
O	2.22072900	4.50772600	-0.71821100
C	-0.72878100	-0.75366200	-0.68227600
C	-0.41734600	-1.88958200	0.29539500
C	-2.16439300	-0.31624200	-0.60729500
C	1.40752800	0.06133000	-0.17364300
C	1.83783400	-1.23935900	0.07246800
C	-1.20969200	-3.15756900	0.04236800
C	2.35874000	1.08529700	-0.23355800
C	3.21087000	-1.52434100	0.22211100

Zero-point correction= 0.358205 (Hartree/Particle)
Thermal correction to Energy= 0.382848
Thermal correction to Enthalpy= 0.383793
Thermal correction to Gibbs Free Energy= 0.302254
Sum of electronic and zero-point Energies= -1374.247414
Sum of electronic and thermal Energies= -1374.222770
Sum of electronic and thermal Enthalpies= -1374.221826
Sum of electronic and thermal Free Energies= -1374.303365

C	3.71649200	0.81408200	-0.08023900
C	-2.58286600	0.52117400	0.43389500
C	-3.08593600	-0.79181600	-1.52964200
C	4.13516800	-0.50705900	0.14449000
C	-3.91898000	0.87455800	0.53289000
C	-4.43261500	-0.44484300	-1.42268400
C	4.62009500	1.93307400	-0.17190700
C	-4.85190200	0.38421900	-0.39795100
C	4.15395500	3.17611000	-0.38756200
C	2.72647500	3.43241600	-0.53441800
C	3.40559700	-3.29081600	1.74163800
C	-3.57307800	2.27720500	2.42289000
H	-0.48516500	-1.08653000	-1.69613700
H	-0.59031600	-1.53753800	1.32026000
H	-0.90194400	-3.90956100	0.77700900
H	-2.27302200	-2.95929500	0.17849100
H	-1.85651400	0.90564300	1.13887700
H	-2.75841400	-1.44158000	-2.33368700
H	5.18876300	-0.73552800	0.25691200
H	-5.16376200	-0.80513900	-2.13661700
H	5.68430200	1.75045300	-0.06365000
H	-0.10322800	-3.85511700	-1.38863000
H	4.79967400	4.04055600	-0.46112600
H	3.74214500	-4.32619300	1.75720000
H	2.34947300	-3.24558900	2.01740500
H	3.99950700	-2.70092400	2.44612900
H	-6.24957700	1.32837400	0.46384900
H	-4.18897500	2.90294300	3.06513500
H	-3.07999100	1.50918200	3.02491800
H	-2.82362300	2.89271000	1.91831100

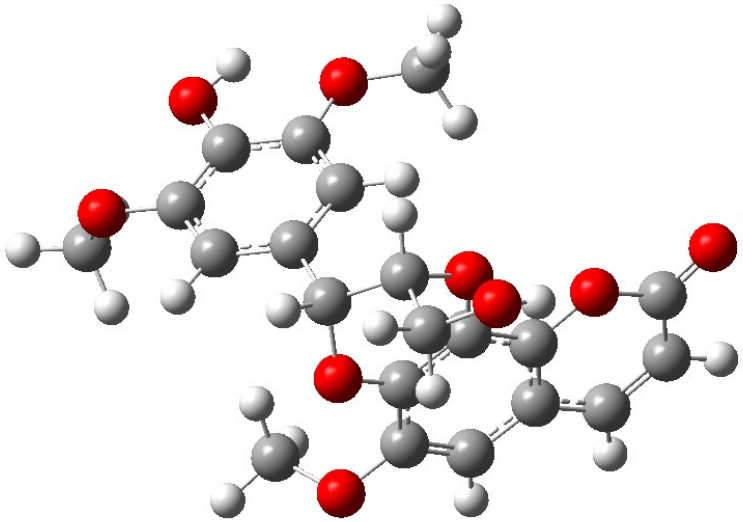


Name	**CMC-P**
Cartesian Coordinates	Energy

O	-0.12427600	-2.12104800	0.71019500
O	1.37177500	0.10588600	1.61349100
O	2.33886000	-1.02442400	3.99542000
O	3.23635600	1.15776400	0.04222900
O	0.34163800	-3.16360900	-1.75546100
O	-2.12323100	3.17544500	-0.10093300
O	-5.06439600	-0.49301500	-0.22387500
O	-4.45932300	2.14921900	-0.75927100
O	4.77052500	2.72739500	-0.17398900
C	-0.66484500	-1.24362300	1.72137800
C	0.48889700	-0.61282300	2.49254600
C	-1.65491500	-0.28339800	1.09610300
C	1.56901800	-0.45886000	0.39359900
C	0.82546500	-1.54327400	-0.06386500
C	1.30690000	-1.64343000	3.25710900
C	2.54865300	0.08880900	-0.44007300
C	1.06868100	-2.08664100	-1.34204000
C	-2.89613700	-0.79168100	0.72521000
C	-1.34774700	1.05515400	0.83141000
C	2.80258200	-0.44970500	-1.69929900
C	2.05128700	-1.54911600	-2.14304800
C	-2.28914900	1.86133800	0.20476900

Zero-point correction= 0.391050 (Hartree/Particle)
Thermal correction to Energy= 0.417458
Thermal correction to Enthalpy= 0.418402
Thermal correction to Gibbs Free Energy= 0.334685
Sum of electronic and zero-point Energies= -1488.719027
Sum of electronic and thermal Energies= -1488.692618
Sum of electronic and thermal Enthalpies= -1488.691674
Sum of electronic and thermal Free Energies= -1488.775392

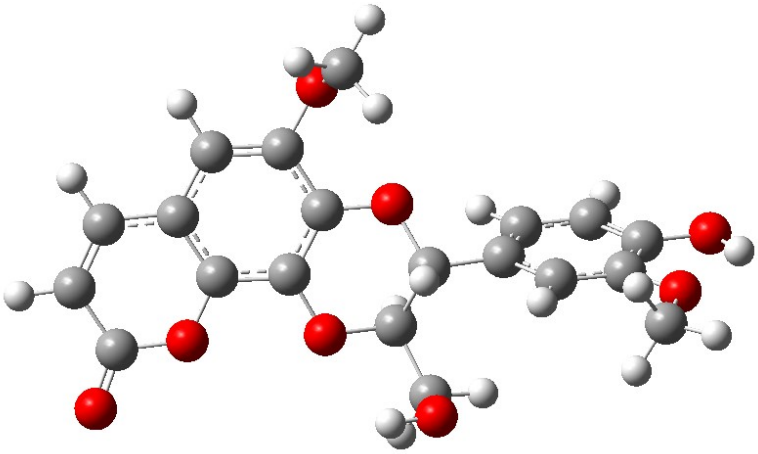
C	-3.83725400	0.01522700	0.09303000
C	-3.54010200	1.35139800	-0.16736600
C	3.84014100	0.17605400	-2.47953000
C	4.51638000	1.23515100	-1.99925400
C	4.22505700	1.78292700	-0.68039200
C	-0.98610600	-2.82534500	-2.16572300
C	-0.88075300	3.78057500	0.23676600
C	-5.27024200	-0.67162100	-1.62612000
H	-1.19709100	-1.91475000	2.39671900
H	0.10641600	0.13749600	3.18672500
H	0.66111900	-2.15472200	3.97338900
H	1.71127200	-2.39049300	2.56266700
H	-3.15749100	-1.82602400	0.92363200
H	-0.39101000	1.46913500	1.11734900
H	2.23454100	-1.97887400	-3.12112300
H	4.06410400	-0.22511000	-3.46249400
H	2.87963300	-0.51787500	3.37878900
H	5.30043500	1.73194200	-2.55428000
H	-1.48314200	-3.76195600	-2.41393500
H	-0.95366100	-2.17993100	-3.04888500
H	-1.52864500	-2.32308200	-1.36096400
H	-4.07509000	3.03246300	-0.84546100
H	-0.71565200	3.75122300	1.31694100
H	-0.94984400	4.81447100	-0.09375500
H	-0.05434200	3.28446700	-0.27971300
H	-6.27510600	-1.07452700	-1.74324000
H	-4.54178300	-1.38366000	-2.02704800
H	-5.19296100	0.27821700	-2.15900200



Name	**CMA-H**
Cartesian Coordinates	Energy

O	0.12543400	1.13834800	-0.11291400
O	-1.16903600	-1.37546600	-0.28016300
O	0.98010400	-2.94601400	0.80690700
O	-3.82745900	-1.49254200	-0.13741600
O	-1.32494700	3.40964300	0.07995700
O	5.68444900	-0.54318900	1.01414600
O	6.25732400	0.57934500	-1.33147800
O	-5.59577800	-2.80382600	-0.15987000
C	0.83935800	-0.09168100	0.12292200
C	0.19258100	-1.20144600	-0.70616700
C	2.27772200	0.12669800	-0.24984200
C	-1.85737400	-0.21169600	-0.13562300
C	-1.22405900	1.02427300	-0.05949800
C	0.86395800	-2.55033800	-0.55152500
C	-3.25037300	-0.25585000	-0.06686500
C	-1.98579100	2.20462700	0.05322700
C	-4.01055200	0.90424300	0.05189800
C	3.28365200	-0.30455800	0.62019100
C	2.61015400	0.69729000	-1.47288700
C	-3.35863400	2.14685100	0.10915600
C	4.61582600	-0.16210900	0.25850600
C	3.94798300	0.85229200	-1.83075600
C	-5.44020100	0.74930100	0.09564900
C	4.94675200	0.42427800	-0.97362200

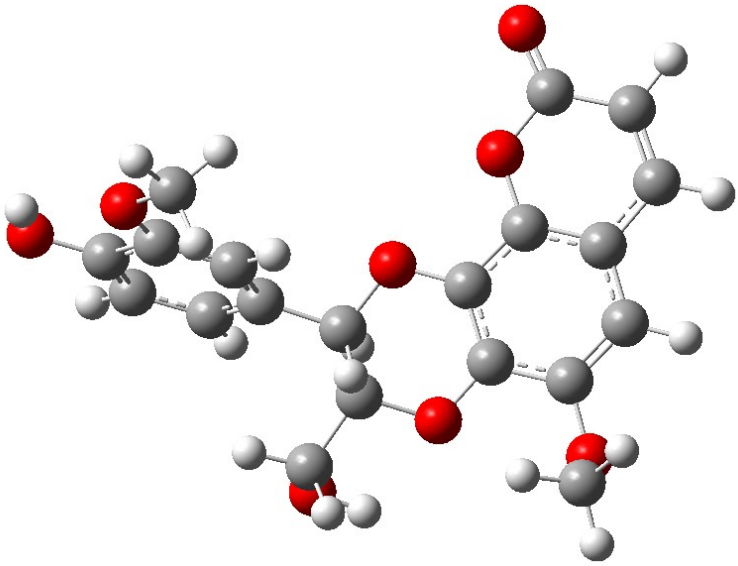
Zero-point correction= 0.357311 (Hartree/Particle)
Thermal correction to Energy= 0.381993
Thermal correction to Enthalpy= 0.382937
Thermal correction to Gibbs Free Energy= 0.301757
Sum of electronic and zero-point Energies= -1374.251454
Sum of electronic and thermal Energies= -1374.226772
Sum of electronic and thermal Enthalpies= -1374.225828
Sum of electronic and thermal Free Energies= -1374.307008



C	-6.00398800	-0.47249200	0.02503900
C	-5.18733500	-1.66325000	-0.09409000
C	-0.83835900	3.75100000	1.38681400
C	5.41011600	-1.15485100	2.27232900
H	0.74644300	-0.33788800	1.18440300
H	0.19522900	-0.90756900	-1.76224400
H	0.29490500	-3.28805600	-1.12430500
H	1.87336200	-2.49782300	-0.95998900
H	3.01505300	-0.74911100	1.57077700
H	1.83044600	1.02980700	-2.14848900
H	-3.93335600	3.06139100	0.19722200
H	4.22792000	1.30269900	-2.77582900
H	-6.05430600	1.63900300	0.18434200
H	0.09208700	-3.08599200	1.15707900
H	-7.07349400	-0.62827400	0.05402400
H	-0.30567800	4.69418900	1.28262200
H	-0.15851200	2.98012400	1.75620200
H	-1.67775300	3.87044600	2.07592500
H	6.81893200	0.23854800	-0.62099300
H	4.86838000	-0.46568800	2.92403700
H	4.83272600	-2.07195200	2.13485100
H	6.37827200	-1.38974800	2.70786800

Name			**CMB-H**
Cartesian Coordinates			Energy
O	0.12785900	0.42400800	-0.38233700
O	0.91456100	-2.25944400	0.06719500
O	1.97772900	2.34120300	-0.41296100
O	-1.25464800	-3.49808400	-1.37631800
O	3.52705500	-2.89027800	0.34314400
O	-4.50772000	1.43387200	1.66617700
O	-6.12815000	0.94480500	-0.38200700
O	2.35806400	4.49840700	-0.63089000
C	-0.73043900	-0.67916900	-0.73619400
C	-0.45148600	-1.83722100	0.22194200
C	-2.15283300	-0.20669200	-0.66160900
C	1.42705800	0.06734300	-0.19331900
C	1.81755000	-1.25034600	0.01999700
C	-1.30973700	-3.05976600	-0.02748900
C	2.40804600	1.05998500	-0.21170500
C	3.18049800	-1.57007800	0.18028600
C	3.75559500	0.75586700	-0.04091100
C	-2.61241100	0.41875900	0.50468600
C	-3.02282000	-0.43873000	-1.71731900
C	4.13659600	-0.58203700	0.15254800
C	-3.93845700	0.81001400	0.59644200
C	-4.36063400	-0.05423600	-1.62124800
C	4.68525600	1.85308800	-0.08187900
C	-4.81787200	0.56524700	-0.47312700
C	4.25498900	3.11502700	-0.27633800
C	2.84584000	3.40198900	-0.45164200
C	3.39437600	-3.33980000	1.70012200
C	-3.66752400	1.71381600	2.78330700
H	-0.48355500	-0.98990700	-1.75501100
H	-0.59398800	-1.49360100	1.25312700

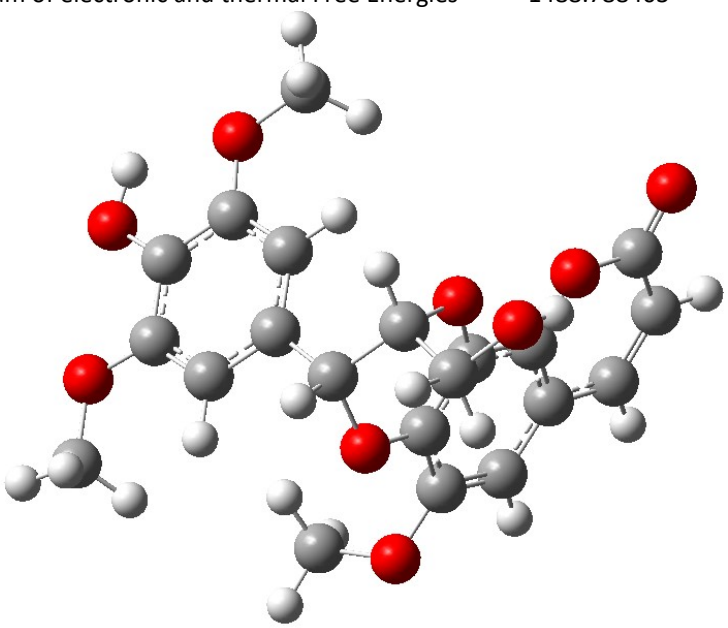
Zero-point correction= 0.357338 (Hartree/Particle)
Thermal correction to Energy= 0.382005
Thermal correction to Enthalpy= 0.382950
Thermal correction to Gibbs Free Energy= 0.301866
Sum of electronic and zero-point Energies= -1374.251610
Sum of electronic and thermal Energies= -1374.226943
Sum of electronic and thermal Enthalpies= -1374.225999
Sum of electronic and thermal Free Energies= -1374.307082



H	-0.98896800	-3.85349600	0.65315400
H	-2.34981900	-2.81591900	0.19015900
H	-1.92782100	0.59968500	1.32440400
H	-2.66278400	-0.92177300	-2.61853500
H	5.18143600	-0.83894600	0.28226300
H	-5.05454600	-0.22606700	-2.43558300
H	5.74122700	1.64118600	0.04744200
H	-0.36382600	-3.82301400	-1.55266600
H	4.92323600	3.96429100	-0.31134100
H	3.65253400	-4.39693500	1.70313300
H	2.36788700	-3.20792000	2.04929800
H	4.08201100	-2.78607400	2.34374100
H	-6.27375600	1.36078500	0.47959200
H	-4.29942100	2.21059300	3.51546700
H	-3.26908300	0.78827200	3.20506700
H	-2.84831800	2.37460000	2.49096300

Name			**CMC-H**
Cartesian Coordinates			Energy
O	-0.20490800	-1.75587200	1.30828100
O	1.30624800	0.64195000	1.45369800
O	2.28314500	0.25077000	4.08286600
O	3.21618800	1.09560800	-0.33497500
O	0.28808300	-3.55936500	-0.64638600
O	-2.28230200	3.32121300	-0.74001500
O	-4.71898400	-0.63057200	-0.90487400
O	-4.32607400	1.87279800	-1.64981000
O	4.78566200	2.48595800	-1.00540300
C	-0.73220400	-0.58461500	1.97288400
C	0.43051100	0.23201600	2.52017000
C	-1.66907300	0.14482500	1.02891600
C	1.51452800	-0.29740900	0.49256800
C	0.76986500	-1.46965200	0.40527100
C	1.23093200	-0.54112200	3.55654500
C	2.51373000	-0.07037700	-0.45540000
C	1.03562700	-2.40603900	-0.61236700
C	-2.75610700	-0.58499900	0.54401100
C	-1.46807700	1.46279600	0.62899600
C	2.78463600	-0.99133200	-1.46302100
C	2.03039500	-2.17362100	-1.53339700
C	-2.36569000	2.04439600	-0.26557800
C	-3.64022200	-0.00389400	-0.35849900
C	-3.44600500	1.31897700	-0.76348200
C	3.84380500	-0.66545800	-2.38109400
C	4.53213800	0.48587000	-2.25853500
C	4.22668200	1.42671500	-1.19975800
C	-0.95833000	-3.38655700	-1.33963300
C	-1.17723500	4.11220000	-0.30773900
C	-4.90987700	-2.00220600	-0.56639600
H	-1.29649500	-0.98721900	2.81468000
H	0.06336100	1.15897600	2.96158000
H	0.57279800	-0.79898300	4.38723900
H	1.62629000	-1.46578800	3.12302200
H	-2.89627100	-1.60744500	0.87119400
H	-0.62874700	2.03614200	0.99594000

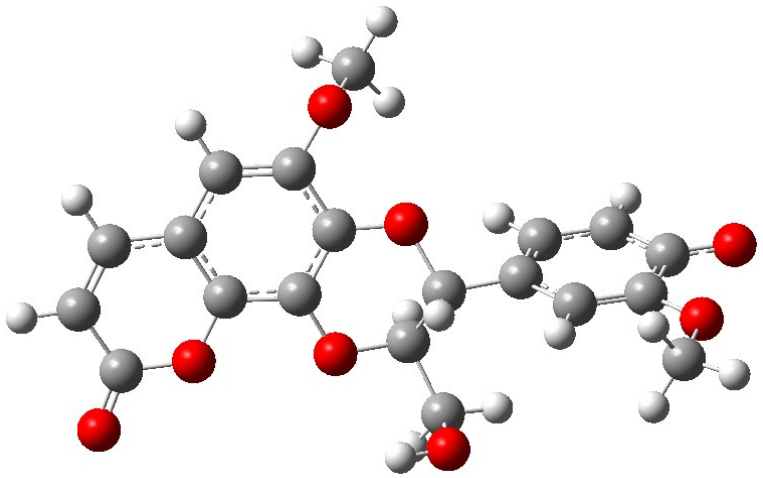
Zero-point correction= 0.390372 (Hartree/Particle)
Thermal correction to Energy= 0.417699
Thermal correction to Enthalpy= 0.418644
Thermal correction to Gibbs Free Energy= 0.330051
Sum of electronic and zero-point Energies= -1488.728082
Sum of electronic and thermal Energies= -1488.700755
Sum of electronic and thermal Enthalpies= -1488.699810
Sum of electronic and thermal Free Energies= -1488.788403



H	2.22504600	-2.90016800	-2.31356300
H	4.07503400	-1.36815100	-3.17429800
H	2.90020300	0.44109700	3.36605700
H	5.33369300	0.76479100	-2.92837400
H	-1.51429900	-4.31448000	-1.21875100
H	-0.76998800	-3.19791300	-2.39944700
H	-1.52112300	-2.55533000	-0.90874800
H	-4.04185500	2.77878700	-1.83765100
H	-1.20127600	4.24789100	0.77580300
H	-1.28902400	5.07442800	-0.80154700
H	-0.23354900	3.64988100	-0.60645400
H	-5.78903900	-2.32477700	-1.11923100
H	-5.08717700	-2.11626400	0.50553200
H	-4.04421400	-2.59848900	-0.86679900

Name			**CMA-anion**
Cartesian Coordinates			Energy
O	0.16898800	1.10195300	0.16610900
O	-1.15329500	-1.32229400	-0.46247300
O	0.95917700	-3.09724800	0.29009000
O	-3.80639800	-1.45775100	-0.26082600
O	-1.26008700	3.29841700	0.85205200
O	5.70664800	-0.66594300	1.10557900
O	6.32176300	0.71557900	-1.10450500
O	-5.58372900	-2.74062400	-0.46196700
C	0.88118400	-0.15992100	0.15462200
C	0.20931700	-1.08271400	-0.86043300
C	2.31642800	0.11356100	-0.17155300
C	-1.82670700	-0.20325100	-0.08628300
C	-1.17969300	0.99318000	0.20636800
C	0.86117200	-2.44555300	-0.96754600
C	-3.21706800	-0.25691000	0.01962200
C	-1.92993900	2.13467800	0.55847200
C	-3.96318700	0.85865400	0.38885400
C	3.32965200	-0.39446000	0.65708400
C	2.67247200	0.81684600	-1.31669100
C	-3.30053500	2.06950900	0.64821100
C	4.66256600	-0.19869100	0.33993100
C	4.01341800	1.02345100	-1.63141000
C	-5.38958000	0.69520700	0.47145800
C	5.06690500	0.52974400	-0.82885700
C	-5.96505800	-0.49225800	0.19787000
C	-5.16384200	-1.63463400	-0.19051400
C	-0.81890700	4.00516500	-0.31710900
C	5.37521900	-1.41616700	2.26388100
H	0.78621500	-0.60143100	1.15079400
H	0.20664100	-0.59741000	-1.84321300
H	0.28695500	-3.05159000	-1.67438400
H	1.87472300	-2.32950200	-1.35128200
H	3.04912000	-0.94314300	1.54892500
H	1.90003500	1.21592000	-1.96784300
H	-3.86453600	2.95150300	0.92813300
H	4.28438400	1.58237900	-2.52164700
H	-5.99230400	1.55017900	0.75863900
H	0.06460800	-3.25631100	0.61461700

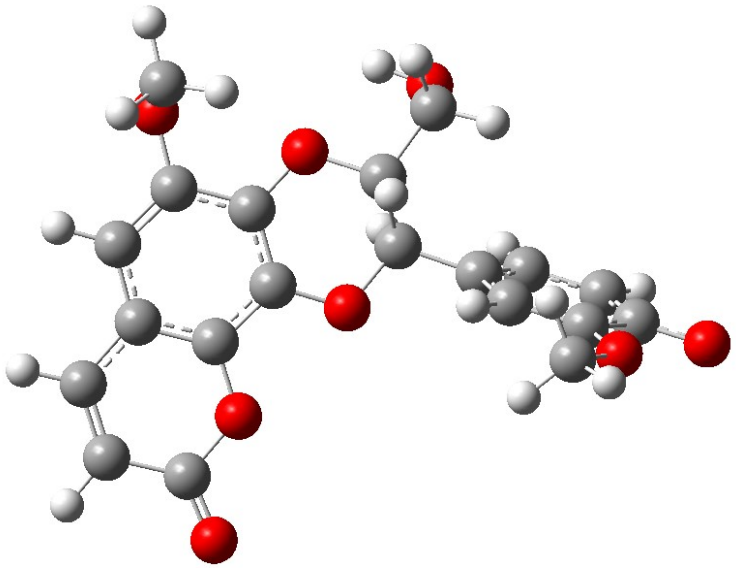
Zero-point correction= 0.344559 (Hartree/Particle)
Thermal correction to Energy= 0.368748
Thermal correction to Enthalpy= 0.369692
Thermal correction to Gibbs Free Energy= 0.289524
Sum of electronic and zero-point Energies= -1373.792021
Sum of electronic and thermal Energies= -1373.767833
Sum of electronic and thermal Enthalpies= -1373.766888
Sum of electronic and thermal Free Energies= -1373.847056



H	-7.03295800	-0.65317100	0.24918200
H	-0.28534400	4.88519700	0.03641700
H	-1.68229800	4.30749600	-0.91463000
H	-0.14979100	3.38269900	-0.91504500
H	4.80077900	-0.81328300	2.97285200
H	4.80566900	-2.31249800	2.00199600
H	6.32067700	-1.70636600	2.71814100

Name			**CMB-anion**
Cartesian Coordinates			Energy
O	-0.11792700	-0.47028400	-0.32266200
O	-0.85477800	2.24102500	0.03836300
O	-2.01071700	-2.34912700	-0.32376700
O	1.31888800	3.39423400	-1.46330300
O	-3.45540800	2.93425200	0.25785700
O	4.61826100	-1.27817100	1.74997600
O	6.14599800	-1.09801300	-0.44300200
O	-2.43608100	-4.50240300	-0.49087200
C	0.76582900	0.60706700	-0.72300700
C	0.50742700	1.79879200	0.19698800
C	2.17675700	0.11528300	-0.66612400
C	-1.41104000	-0.08261900	-0.16089100
C	-1.77647500	1.24947200	0.00766800
C	1.38106900	2.99940900	-0.10073600
C	-2.41469000	-1.05287500	-0.16558300
C	-3.13471800	1.60262900	0.13739800
C	-3.75813200	-0.71489500	-0.02736500
C	2.71092900	-0.37524300	0.54059500
C	2.99712000	0.18855800	-1.78239600
C	-4.11251900	0.63585600	0.12197100
C	4.02991800	-0.78185200	0.60952600
C	4.33046500	-0.21377800	-1.71299800
C	-4.71145300	-1.79152600	-0.05713800
C	4.90914500	-0.71480000	-0.52715500
C	-4.30681100	-3.06766600	-0.21018500
C	-2.90171100	-3.39048600	-0.35059500
C	-3.32554700	3.42057600	1.60217100
C	3.80799700	-1.36121600	2.91246100
H	0.50301800	0.88842600	-1.74692800
H	0.65050400	1.49292800	1.23965900
H	1.07989800	3.82140700	0.55512800
H	2.41921000	2.74561600	0.11394200
H	2.07177900	-0.43685300	1.41400500
H	2.59622600	0.56780800	-2.71761600
H	-5.15332300	0.91924300	0.22650700
H	4.96429900	-0.15434600	-2.59210600
H	-5.76458300	-1.55273100	0.04591000
H	0.42984100	3.72250700	-1.64200400
H	-4.99357000	-3.90235900	-0.23646000
H	-3.56144800	4.48252800	1.57199300
H	-2.30539700	3.27776000	1.96517700
H	-4.03054600	2.90048200	2.25505000
H	4.44384300	-1.76718300	3.69686500
H	3.44642700	-0.37308000	3.21089800
H	2.95655400	-2.02838800	2.75162800

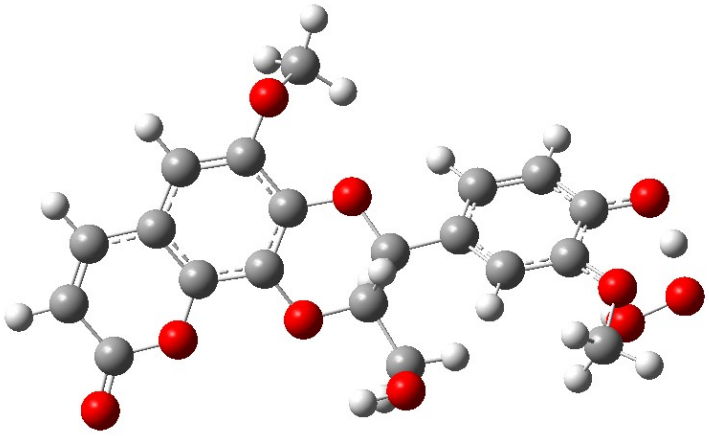
Zero-point correction= 0.344500 (Hartree/Particle)
Thermal correction to Energy= 0.368736
Thermal correction to Enthalpy= 0.369680
Thermal correction to Gibbs Free Energy= 0.289075
Sum of electronic and zero-point Energies= -1373.792099
Sum of electronic and thermal Energies= -1373.767863
Sum of electronic and thermal Enthalpies= -1373.766918
Sum of electronic and thermal Free Energies= -1373.847524



Name				**CMC-anion**
Cartesian Coordinates				Energy
O	-0.29165800	2.20128300	0.55365000	Zero-point correction= 0.377117 (Hartree/Particle)
O	1.47446000	1.04784900	-1.32042200	Thermal correction to Energy= 0.404118
O	2.33517600	3.43197400	-2.54814000	Thermal correction to Enthalpy= 0.405062
O	3.24977500	-0.75517200	-0.52294900	Thermal correction to Gibbs Free Energy= 0.318234
O	-0.22746400	1.41662900	3.15731500	Sum of electronic and zero-point Energies= -1488.268808
O	-1.58098000	-2.81780300	-1.61727800	Sum of electronic and thermal Energies= -1488.241807
O	-5.03545800	-0.03064700	0.10006800	Sum of electronic and thermal Enthalpies= -1488.240863
O	-4.08158900	-2.52370200	-0.67914500	Sum of electronic and thermal Free Energies= -1488.327692
O	4.87490400	-2.10456900	-1.14165700	
C	-0.72307500	2.03181900	-0.83136200	
C	0.51865300	2.05481800	-1.71552900	
C	-1.61311100	0.82276000	-0.93378700	
C	1.50198300	0.72745700	-0.00155100	
C	0.62510200	1.27346700	0.92947600	
C	1.20687500	3.40984200	-1.68792200	
C	2.42271300	-0.22826900	0.42966200	
C	0.67182000	0.86459600	2.27538500	
C	-2.91790800	0.93420500	-0.46171500	
C	-1.15205400	-0.44106800	-1.33689000	
C	2.49101300	-0.62281400	1.76322900	
C	1.59914600	-0.06308400	2.69225700	
C	-1.97755800	-1.55096600	-1.25325000	
C	-3.73877900	-0.18053100	-0.38176700	
C	-3.32034700	-1.48087700	-0.76295100	
C	3.47962900	-1.61197100	2.10274900	
C	4.29146700	-2.12817400	1.15958800	
C	4.19396400	-1.70118500	-0.22162900	
C	-1.52074200	0.79302200	3.08059000	
C	-0.22683200	-2.98255300	-2.01283900	
C	-5.11539900	-0.28686900	1.50366300	
H	-1.29897100	2.93540300	-1.03200000	
H	0.24723900	1.79839000	-2.74071400	
H	0.51084800	4.16682300	-2.05157500	
H	1.49849700	3.66156300	-0.66259300	
H	-3.30390400	1.89306800	-0.12643800	
H	-0.14668600	-0.55233000	-1.71983900	
H	1.62791300	-0.37082700	3.73088000	
H	3.55496400	-1.93465500	3.13563200	
H	2.97189100	2.78526600	-2.22080400	
H	5.04405400	-2.87341200	1.37673800	
H	-2.17619100	1.35246400	3.74563700	
H	-1.45033300	-0.24636500	3.41143000	
H	-1.90423000	0.83281300	2.05830200	
H	-0.01006000	-2.41866600	-2.92444800	
H	-0.09472500	-4.04555900	-2.20496900	
H	0.45551200	-2.66579900	-1.21725200	
H	-6.16351300	-0.19824400	1.78793900	
H	-4.52112000	0.44635700	2.05800800	
H	-4.75788100	-1.29477000	1.73208800	
Name				**CMA-O14-TS-G**
Cartesian Coordinates				Energy
O	-0.47593500	1.32416200	0.24417900	Zero-point correction= 0.370795 (Hartree/Particle)

O	-1.48954700	-1.24618900	-0.33514700
O	0.65608900	-2.73193900	0.75820100
O	-4.11305000	-1.66621400	-0.32830800
O	-2.21154500	3.39199500	0.72706800
O	5.08150900	-0.58506000	1.32656900
O	5.74944700	1.29602800	-0.41427400
O	-5.74071600	-3.14344000	-0.57288300
C	0.32338900	0.15246300	0.40802700
C	-0.13474900	-0.89761700	-0.61230000
C	1.76835500	0.52043000	0.22744800
C	-2.30669800	-0.18944300	-0.08533800
C	-1.81239000	1.08294700	0.18554300
C	0.64320100	-2.19926900	-0.55038200
C	-3.68869200	-0.40235000	-0.08139700
C	-2.69696600	2.15644800	0.42028200
C	-4.56760900	0.64862800	0.16685600
C	2.72741100	-0.21117600	0.92264500
C	2.14657100	1.52044800	-0.67905200
C	-4.05598700	1.93307800	0.40691800
C	4.07935400	0.04914000	0.72029500
C	3.48459200	1.77649600	-0.90118000
C	-5.97586800	0.33463400	0.15132500
C	4.48106600	1.05836900	-0.21283800
C	-6.39702700	-0.91735700	-0.09239700
C	-5.45192500	-2.00467800	-0.34980200
C	-1.55756400	4.06206400	-0.34693200
C	4.78440800	-1.78153300	2.02965300
H	0.15567100	-0.25125900	1.41186100
H	-0.06994700	-0.46074200	-1.61787200
H	0.19699400	-2.90115900	-1.26194400
H	1.68121500	-2.02436600	-0.83546000
H	2.40661000	-0.99219800	1.60171200
H	1.38303600	2.08506400	-1.19917300
H	-4.72215000	2.76401200	0.60530600
H	3.81264300	2.53678800	-1.59954600
H	-6.68698500	1.13190600	0.34108200
H	-0.24437100	-2.99108900	0.98004100
H	-7.44131200	-1.19588900	-0.11305300
H	-1.27190600	5.04059700	0.03311900
H	-2.24349500	4.18028900	-1.19109700
H	-0.66588100	3.51730600	-0.66192500
H	4.19081200	-1.57184700	2.92339900
H	4.24974500	-2.48008000	1.38045400
H	5.74424400	-2.20166700	2.31733000
O	5.24416400	-1.31494500	-1.41760100
H	5.02014700	-1.18388000	-2.35060800
O	6.48638200	-0.76108300	-1.29225000
H	6.25331800	0.34137100	-0.69232000

Thermal correction to Energy= 0.398146
Thermal correction to Enthalpy= 0.399090
Thermal correction to Gibbs Free Energy= 0.310922
Sum of electronic and zero-point Energies= -1525.082217
Sum of electronic and thermal Energies= -1525.054866
Sum of electronic and thermal Enthalpies= -1525.053921
Sum of electronic and thermal Free Energies= -1525.142090

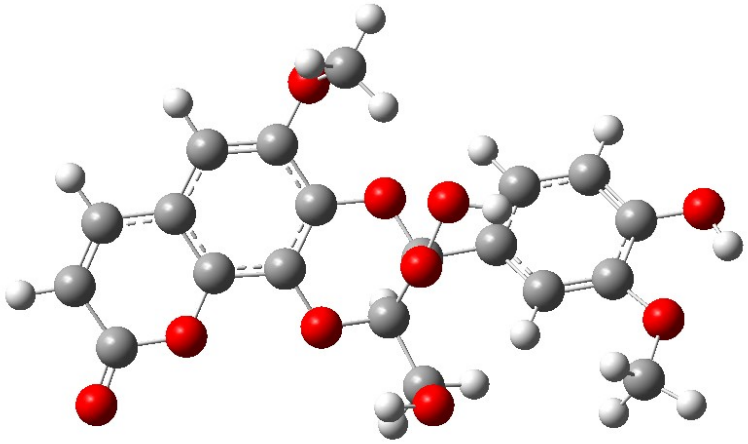


Name			**CMA-C18-TS-G**
Cartesian Coordinates			Energy
O	0.00530600	1.15269500	-0.45784100
O	-1.23747900	-1.37271900	-0.50609100
O	0.95226900	-2.89353300	0.44734800
O	-3.88413700	-1.54944100	-0.21639900

Zero-point correction= 0.370609 (Hartree/Particle)
Thermal correction to Energy= 0.398210
Thermal correction to Enthalpy= 0.399154
Thermal correction to Gibbs Free Energy= 0.311398

O	-1.48405300	3.40769300	-0.19985500
O	5.46253800	-1.21019200	0.43217400
O	6.24746600	0.94479900	-0.87550600
O	-5.64230300	-2.88670500	-0.10618900
C	0.73982900	-0.02089000	-0.28723000
C	0.07784100	-1.17819500	-1.02984300
C	2.18636500	0.24025800	-0.47898500
C	-1.95128400	-0.22758700	-0.35114700
C	-1.34376700	1.02196500	-0.33580400
C	0.76556700	-2.52225100	-0.90095800
C	-3.33848100	-0.30830100	-0.20392400
C	-2.10530300	2.19680100	-0.18590000
C	-4.10399200	0.84732600	-0.06187500
C	3.11260600	-0.65773800	0.08381500
C	2.64004300	1.37938200	-1.13899400
C	-3.47314900	2.10124800	-0.05597800
C	4.46665700	-0.42089500	-0.05676400
C	4.00670100	1.61179500	-1.27620600
C	-5.52947100	0.66743700	0.07210200
C	4.92224300	0.72017600	-0.74508800
C	-6.07010900	-0.56202900	0.06173900
C	-5.24226800	-1.75985300	-0.08708200
C	-0.76712200	3.70123200	1.00417200
C	5.07882900	-2.38605100	1.12668000
H	-0.00153900	-0.90072800	-2.09153000
H	0.16100500	-3.26076200	-1.43734900
H	1.75179200	-2.47814400	-1.36417200
H	2.74593500	-1.51518500	0.63653800
H	1.92483000	2.08271000	-1.54527800
H	-4.05331900	3.00977200	0.05217300
H	4.37973800	2.48634700	-1.79444000
H	-6.15471500	1.54739200	0.18190300
H	0.08921400	-2.93056100	0.87451700
H	-7.13161300	-0.74132900	0.15987700
H	-0.27967300	4.66006300	0.83981900
H	-0.02220900	2.93243900	1.21689400
H	-1.46642800	3.78118900	1.84145000
H	6.72050900	0.22187000	-0.44478600
H	4.50162500	-2.13703400	2.02120000
H	4.48549000	-3.04078000	0.48244700
H	6.00198800	-2.88447700	1.41100800
O	1.24681500	1.07412000	2.37269100
H	2.20376900	0.94185500	2.29259300
O	0.71729200	-0.18492900	2.20700700
H	0.64347400	-0.29191900	0.97206000

Sum of electronic and zero-point Energies= -1525.079859
Sum of electronic and thermal Energies= -1525.052258
Sum of electronic and thermal Enthalpies= -1525.051314
Sum of electronic and thermal Free Energies= -1525.139070

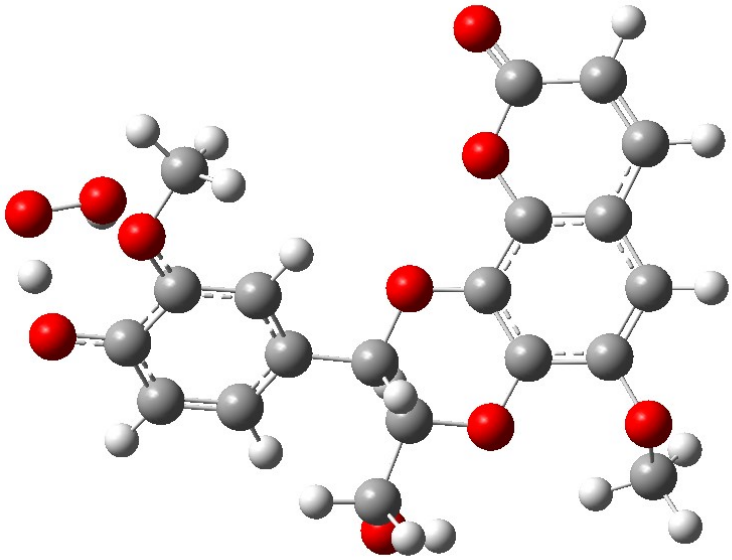


Name			**CMB-O14-TS-G**
Cartesian Coordinates			Energy
O	0.47141700	0.17582600	-0.16761300
O	1.87166700	-2.20676900	0.38997500
O	1.78584500	2.47738700	-0.32276200
O	0.03592900	-4.00911500	-0.78227500
O	4.59619500	-2.15882000	0.63511500
O	-4.15360800	1.07594600	1.44074800
O	-5.69472600	-0.65304400	0.15318800

Zero-point correction= 0.370593 (Hartree/Particle)
Thermal correction to Energy= 0.397984
Thermal correction to Enthalpy= 0.398928
Thermal correction to Gibbs Free Energy= 0.310728
Sum of electronic and zero-point Energies= -1525.081380
Sum of electronic and thermal Energies= -1525.053989
Sum of electronic and thermal Enthalpies= -1525.053045

O	1.63587900	4.66699800	-0.59557900
C	-0.12655700	-1.10064100	-0.38107700
C	0.46561200	-2.08917600	0.63234400
C	-1.61812400	-0.95274800	-0.24787900
C	1.81912000	0.15147700	-0.02070700
C	2.52078000	-1.02172800	0.23540000
C	-0.08365200	-3.49886200	0.53013700
C	2.52055000	1.35929900	-0.10541800
C	3.92493600	-1.00402400	0.35691400
C	3.90596200	1.38799800	0.03284400
C	-2.15072200	0.05756000	0.54402900
C	-2.45635800	-1.86665700	-0.90839600
C	4.60286800	0.18990100	0.25324900
C	-3.53290500	0.15839700	0.69949600
C	-3.82439000	-1.76229000	-0.77997300
C	4.54217000	2.67931200	-0.06947200
C	-4.39921700	-0.75939500	0.02653300
C	3.81426600	3.78762200	-0.28310700
C	2.35777700	3.73082900	-0.41633000
C	4.68037000	-3.06189800	-0.46175700
C	-3.41622900	2.22100100	1.84142900
H	0.12810800	-1.45118800	-1.38741500
H	0.30833400	-1.69050200	1.64294200
H	0.44634100	-4.12829600	1.25227500
H	-1.14435900	-3.50163800	0.78033300
H	-1.48547900	0.76900000	1.01375200
H	-2.01593600	-2.64811200	-1.51882700
H	5.68041700	0.19090200	0.36553900
H	-4.49917400	-2.44043800	-1.28788600
H	5.62115300	2.73516800	0.03057800
H	0.97303600	-4.09138400	-0.98333400
H	4.24949900	4.77375200	-0.36495300
H	5.22806500	-3.93155400	-0.10468100
H	5.22130800	-2.59974500	-1.29284500
H	3.68493200	-3.36620800	-0.79394300
H	-4.14003900	2.89667700	2.28899000
H	-2.65428200	1.95752400	2.57984300
H	-2.95216100	2.69372400	0.97245600
O	-4.82757100	1.70307900	-1.19501500
H	-4.83986900	1.49718100	-2.14123800
O	-6.10679000	1.46749400	-0.78062300
H	-6.00132900	0.38742800	-0.12241800

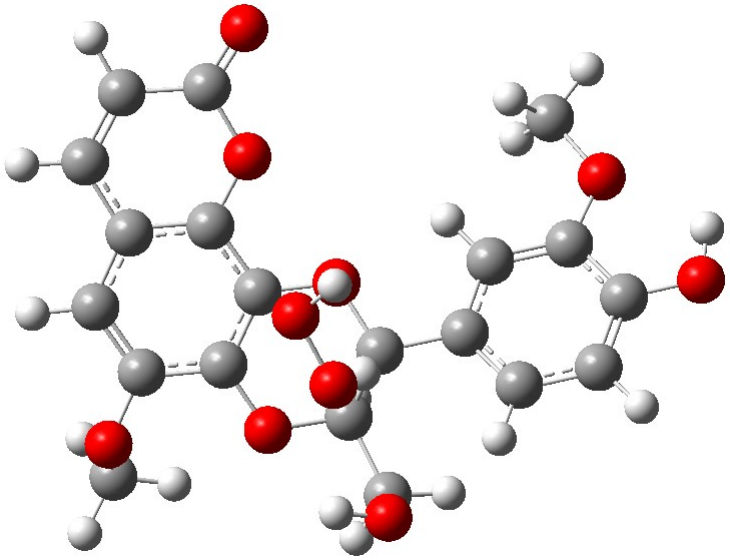
Sum of electronic and thermal Free Energies= -1525.141245



Name			**CMB-C17-TS-G**
Cartesian Coordinates			Energy
O	-0.01503800	0.28975400	-0.07310800
O	-1.19003100	-2.23209400	-0.48383400
O	-1.54097700	2.44586500	0.14288200
O	0.87212600	-3.72712700	0.78746800
O	-3.91414400	-2.48027300	-0.49627900
O	4.51911600	2.10062100	-0.96381300
O	6.21915300	0.33896000	0.01319300
O	-1.59474200	4.63819000	0.42108600
C	0.72748000	-0.87745800	0.10961500
C	0.19441000	-2.00445600	-0.77592700

Zero-point correction= 0.370307 (Hartree/Particle)
Thermal correction to Energy= 0.397980
Thermal correction to Enthalpy= 0.398924
Thermal correction to Gibbs Free Energy= 0.310591
Sum of electronic and zero-point Energies= -1525.078522
Sum of electronic and thermal Energies= -1525.050849
Sum of electronic and thermal Enthalpies= -1525.049905
Sum of electronic and thermal Free Energies= -1525.138238

C	2.17957600	-0.56832500	0.07119100
C	-1.36266700	0.12918900	-0.16382100
C	-1.94672700	-1.11545900	-0.34739900
C	0.86004300	-3.35076800	-0.56948600
C	-2.17179200	1.25835200	-0.02871000
C	-3.34968500	-1.24495700	-0.37116700
C	-3.55869400	1.14081600	-0.05105600
C	2.61433700	0.65654600	-0.45967600
C	3.10981900	-1.46139600	0.60391700
C	-4.13882600	-0.12626900	-0.22149000
C	3.96479200	0.95349000	-0.47889400
C	4.46650500	-1.15744600	0.57775300
C	-4.31386600	2.35757900	0.11844800
C	4.90159000	0.04054300	0.03547400
C	-3.68976900	3.53646300	0.28262700
C	-2.23043100	3.63202000	0.29396400
C	-3.83218100	-3.02968300	-1.80806400
C	3.63759900	3.10559400	-1.43517800
H	0.28430000	-1.69026500	-1.82628900
H	0.32580300	-4.08364000	-1.18470200
H	1.89661500	-3.30864400	-0.90441900
H	1.88412100	1.35862300	-0.83721300
H	2.76827600	-2.37989500	1.06764500
H	-5.21600400	-0.24256200	-0.23004900
H	5.20289100	-1.83477500	0.99167500
H	-5.39745600	2.30086900	0.11329300
H	-0.02178900	-3.64730600	1.14246700
H	-4.21733900	4.47088800	0.41286100
H	-4.32079000	-4.00095300	-1.76518300
H	-2.79144100	-3.15558400	-2.11407400
H	-4.35515400	-2.38502200	-2.52091200
H	6.32171800	1.21624200	-0.37631600
H	4.26474700	3.93918100	-1.74104600
H	3.06251300	2.74483200	-2.29231500
H	2.95533800	3.42681000	-0.64373600
O	-0.71345500	-0.28153900	2.71992700
H	-0.04749200	0.23861400	3.19068800
O	-0.06790400	-1.46121300	2.42258900
H	0.43921900	-1.26281300	1.30400800

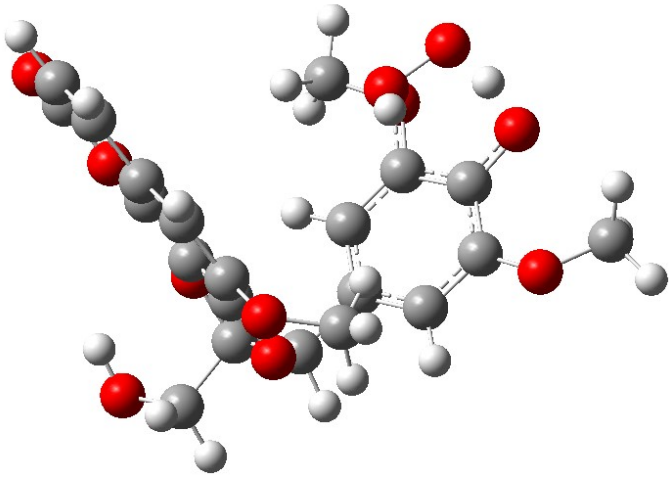


Name	**CMC-O14-TS-G**
Cartesian Coordinates	Energy

O	-0.28946400	-2.43923200	0.54786700
O	-1.73576300	-0.96806600	-1.37375400
O	-3.01577600	-3.12927700	-2.61364900
O	-3.24767900	1.07073300	-0.62603700
O	-0.45983700	-1.70279500	3.23137200
O	1.95168000	2.16423600	-1.91419100
O	4.53763100	-0.89252900	0.64601800
O	4.11366100	1.68046200	-0.50559400
O	-4.61295800	2.68423800	-1.27568500
C	0.19444000	-2.33995900	-0.80341800
C	-0.99884300	-2.14563000	-1.72948200
C	1.26939400	-1.27135100	-0.86685100
C	-1.78290200	-0.66951100	-0.04743100

Zero-point correction= 0.403434 (Hartree/Particle)
Thermal correction to Energy= 0.433551
Thermal correction to Enthalpy= 0.434495
Thermal correction to Gibbs Free Energy= 0.339554
Sum of electronic and zero-point Energies= -1639.554968
Sum of electronic and thermal Energies= -1639.524852
Sum of electronic and thermal Enthalpies= -1639.523907
Sum of electronic and thermal Free Energies= -1639.618848

C	-1.05974000	-1.37531500	0.91093700
C	-1.95561700	-3.33039400	-1.71167800
C	-2.58133400	0.40458100	0.35197900
C	-1.13060900	-1.01456700	2.27077400
C	2.46027600	-1.53889200	-0.19148900
C	1.06337200	-0.04154800	-1.49057800
C	-2.67816000	0.75208100	1.69702500
C	-1.94646700	0.03225300	2.65092300
C	2.04798500	0.93600000	-1.40100900
C	3.44930300	-0.57231100	-0.07982000
C	3.25066800	0.70626800	-0.66568500
C	-3.53912600	1.86540300	2.01902600
C	-4.19902800	2.52405000	1.05252600
C	-4.07120000	2.14533200	-0.35566500
C	0.94256100	-1.89596700	3.04383200
C	0.67438400	2.60257200	-2.35456300
C	5.80923200	-0.31463400	0.33492700
H	0.63789300	-3.31694600	-1.00428700
H	-0.66130300	-1.97096600	-2.75348400
H	-1.42807900	-4.23049900	-2.03429100
H	-2.31912600	-3.49196900	-0.68904800
H	2.62681100	-2.49808600	0.28526600
H	0.13798200	0.16822800	-2.00659000
H	-2.00431200	0.29028800	3.70129300
H	-3.64114500	2.15809300	3.05884900
H	-3.44042800	-2.29359600	-2.39248800
H	-4.85256100	3.36235200	1.24932900
H	1.38299100	-1.91699400	4.03949300
H	1.37412500	-1.07416100	2.46475500
H	1.13797800	-2.83561300	2.52835300
H	0.35741800	2.05481500	-3.24569700
H	0.78989000	3.65586700	-2.59490200
H	-0.06306100	2.47986700	-1.55688700
H	5.93149800	0.64807900	0.82601300
H	5.91914300	-0.18572700	-0.74289600
H	6.54535200	-1.02724200	0.70231200
O	1.75326000	2.41842400	0.91363000
H	1.81785000	2.04021600	1.80352500
O	2.86072000	3.20119500	0.79344500
H	3.59576400	2.53410700	-0.03168000

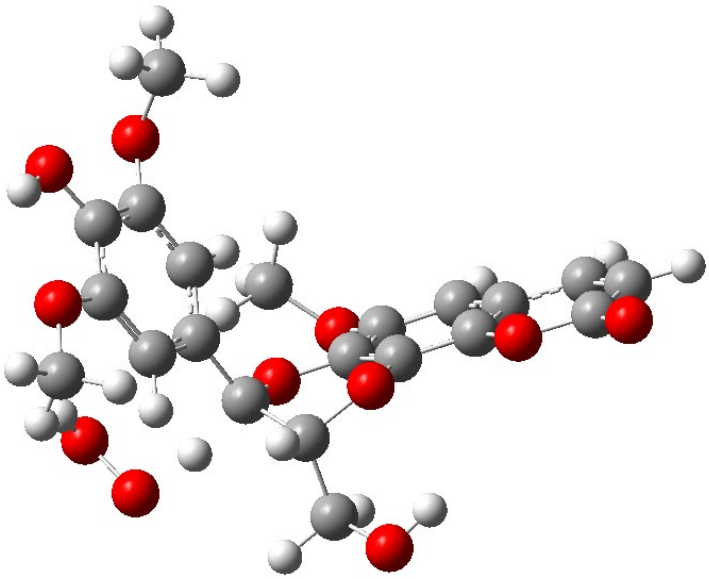


Name	**CMC-C18-TS-G**
Cartesian Coordinates	Energy

O	0.20490400	-0.02529900	-1.68920300
O	1.15190500	-1.33908500	0.61260000
O	1.71495200	-3.86440600	-0.49043900
O	3.51131900	-0.65851100	1.65403200
O	1.76613700	1.90270700	-2.90066800
O	-4.76624000	-1.11209700	1.63933300
O	-2.88707500	3.07852800	0.58795700
O	-4.85887300	1.50958100	1.76668800
O	5.00610200	-1.03539000	3.24021500
C	-0.59872300	-0.92811500	-0.98308600
C	0.22282200	-1.98518300	-0.27119600
C	-1.68731100	-0.27147500	-0.22535200

Zero-point correction=	0.402505 (Hartree/Particle)
Thermal correction to Energy=	0.433193
Thermal correction to Enthalpy=	0.434137
Thermal correction to Gibbs Free Energy=	0.337807
Sum of electronic and zero-point Energies=	-1639.544732
Sum of electronic and thermal Energies=	-1639.514044
Sum of electronic and thermal Enthalpies=	-1639.513099
Sum of electronic and thermal Free Energies=	-1639.609429

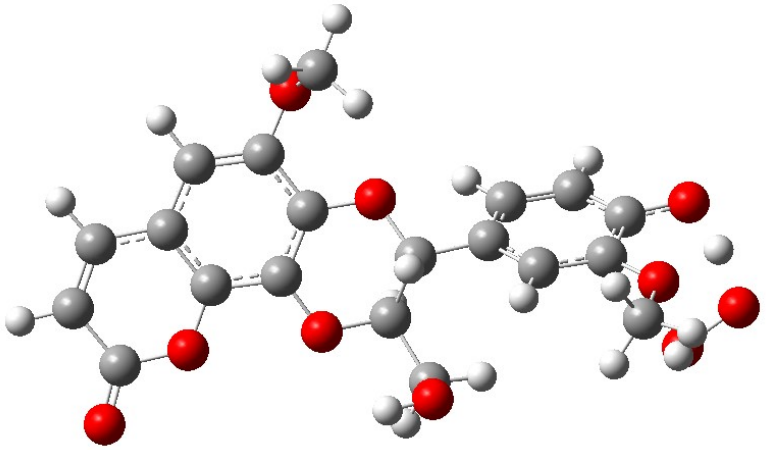
C	1.86138900	-0.34324400	0.01684300
C	1.39921700	0.30851100	-1.12245300
C	0.98154200	-2.90832700	-1.21673800
C	3.09757800	0.02140100	0.55521200
C	2.16585600	1.31647700	-1.74064300
C	-1.77289500	1.11370000	-0.13540300
C	-2.68491600	-1.07219800	0.36189600
C	3.85944300	1.02576900	-0.03763600
C	3.38090500	1.66635100	-1.18923800
C	-3.73136600	-0.46788500	1.03431400
C	-2.82274900	1.71984600	0.55035700
C	-3.81531600	0.93354200	1.13150700
C	5.12398700	1.33469900	0.58581300
C	5.52878500	0.67052700	1.68067800
C	4.71518800	-0.39054200	2.27649100
C	0.53233700	2.62133100	-2.86775000
C	-4.76774600	-2.52938500	1.61184400
C	-2.78445500	3.65597800	1.88977800
H	-0.40918900	-2.58266900	0.38469500
H	0.26545500	-3.44980400	-1.83821600
H	1.62944600	-2.32147300	-1.88060200
H	-1.02640900	1.75092200	-0.59025800
H	-2.63801900	-2.15007600	0.26874100
H	3.96489300	2.43987500	-1.67297300
H	5.74049400	2.11385600	0.14978100
H	2.26889600	-3.40071000	0.14718600
H	6.46753300	0.86912100	2.17855400
H	0.52563000	3.24399700	-3.75997700
H	0.49055500	3.26057400	-1.98024500
H	-0.32043400	1.94251400	-2.88580800
H	-5.43591900	0.80715100	2.09295300
H	-4.81585400	-2.89713100	0.58309600
H	-5.65707600	-2.84154400	2.15307900
H	-3.87688100	-2.92539700	2.10643800
H	-2.79221200	4.73368600	1.74194900
H	-1.84290400	3.35615400	2.35880800
H	-3.62621200	3.36229900	2.51739400
O	-2.89917700	-0.91732900	-2.92331400
H	-3.55092300	-0.92070000	-2.20526300
O	-2.10957300	-2.01033400	-2.67134500
H	-1.25736500	-1.56821800	-1.90761500



Name			**CMA-O14-TS-P**
Cartesian Coordinates			Energy
O	-0.48137300	1.30373300	-0.04022700
O	-1.53278800	-1.31329600	-0.18761900
O	0.63787500	-2.64209800	1.08797100
O	-4.17315700	-1.67477600	-0.18614500
O	-2.15566200	3.44383800	-0.02531100
O	5.09168300	-0.32852800	1.30571900
O	5.71318300	1.23759500	-0.77360100
O	-5.81970000	-3.14097000	-0.24913300
C	0.31118100	0.15840500	0.28979200
C	-0.17474400	-1.03456800	-0.54216300
C	1.75208000	0.48574600	0.01866300

Zero-point correction= 0.370117 (Hartree/Particle)
Thermal correction to Energy= 0.397510
Thermal correction to Enthalpy= 0.398455
Thermal correction to Gibbs Free Energy= 0.309994
Sum of electronic and zero-point Energies= -1525.120104
Sum of electronic and thermal Energies= -1525.092710
Sum of electronic and thermal Enthalpies= -1525.091766
Sum of electronic and thermal Free Energies= -1525.180227

C	-2.33225000	-0.21844200	-0.12670300
C	-1.81762700	1.07295700	-0.06090900
C	0.59426100	-2.31621000	-0.28923600
C	-3.71895500	-0.39565400	-0.13478400
C	-2.68310600	2.18664500	-0.03419000
C	-4.58080400	0.69774100	-0.10283500
C	2.72667600	-0.05083800	0.85709800
C	2.11001800	1.25019900	-1.10088300
C	-4.04651500	1.99537000	-0.05635200
C	4.07194600	0.16859800	0.58203900
C	3.44132600	1.47405500	-1.38104100
C	-5.99396900	0.41477200	-0.12926400
C	4.45331700	0.95846100	-0.54799100
C	-6.43956300	-0.85329700	-0.17864400
C	-5.51398100	-1.97896400	-0.20788600
C	-1.64674000	3.84653200	1.24875900
C	4.77677200	-1.05718100	2.49335500
H	0.16678100	-0.07554900	1.34944000
H	-0.12569000	-0.77138900	-1.60637200
H	0.13121800	-3.11806500	-0.87283000
H	1.62409200	-2.19822100	-0.62837000
H	2.42253700	-0.64749100	1.70827800
H	1.33786200	1.66682200	-1.73605200
H	-4.70405800	2.85687500	-0.03982800
H	3.74901900	2.06502600	-2.23559600
H	-6.69021400	1.24693400	-0.10981200
H	-0.25658400	-2.86933800	1.36637600
H	-7.49098900	-1.10550400	-0.20062100
H	-1.25098900	4.85263000	1.12021400
H	-0.84733800	3.17990200	1.57973000
H	-2.45222900	3.86010500	1.98910300
H	4.22060400	-0.42819200	3.19184000
H	4.20050800	-1.95632400	2.25864000
H	5.73280900	-1.33590100	2.92988800
O	5.59840300	-1.61974800	-1.20103100
H	5.50212700	-1.78842300	-0.24788600
O	6.70775200	-0.83602100	-1.28850600
H	6.30485700	0.30232100	-0.93403600

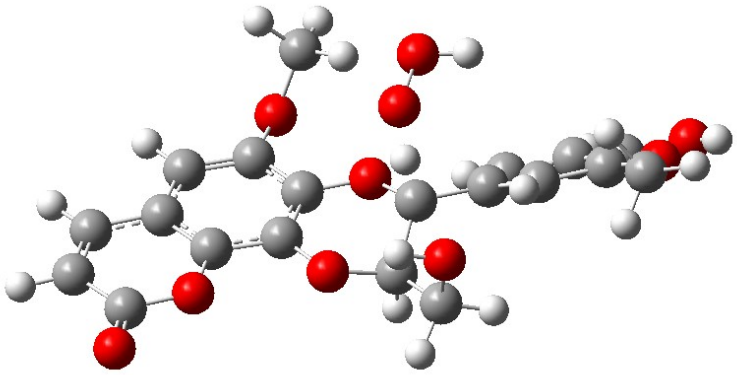


Name	**CMA-C18-TS-P**
Cartesian Coordinates	Energy

O	0.00264300	1.14736200	-0.42600000
O	-1.24297500	-1.37485500	-0.49083900
O	0.95020800	-2.92343800	0.43506600
O	-3.89842800	-1.54339400	-0.22066600
O	-1.48220500	3.40401900	-0.19813700
O	5.47883100	-1.18488600	0.40536600
O	6.23659700	0.96851600	-0.91210700
O	-5.65185300	-2.87765000	-0.12460900
C	0.74019600	-0.02808700	-0.26761000
C	0.07650900	-1.18065500	-1.01731300
C	2.18445900	0.23983700	-0.47388500
C	-1.95540400	-0.23096200	-0.33999700
C	-1.34606600	1.01817000	-0.31846100
C	0.76326500	-2.52520400	-0.90821800

Zero-point correction= 0.369658 (Hartree/Particle)
Thermal correction to Energy= 0.397448
Thermal correction to Enthalpy= 0.398392
Thermal correction to Gibbs Free Energy= 0.310043
Sum of electronic and zero-point Energies= -1525.113867
Sum of electronic and thermal Energies= -1525.086077
Sum of electronic and thermal Enthalpies= -1525.085133
Sum of electronic and thermal Free Energies= -1525.173481

C	-3.34395800	-0.30377300	-0.20279200
C	-2.10786800	2.19496300	-0.17879500
C	-4.10928500	0.85214700	-0.06464400
C	3.12172900	-0.65350600	0.07782100
C	2.62417300	1.37992800	-1.14252400
C	-3.47664700	2.10549000	-0.05550100
C	4.47394500	-0.40831900	-0.07406300
C	3.98813500	1.62017900	-1.29543700
C	-5.53532900	0.67787500	0.05870600
C	4.91328600	0.73574500	-0.76941000
C	-6.08003500	-0.55145500	0.04307500
C	-5.25311700	-1.74389900	-0.10082600
C	-0.78411300	3.70961700	1.01604200
C	5.11605200	-2.36058700	1.12015100
H	-0.00376900	-0.89451300	-2.07582500
H	0.16145200	-3.25535500	-1.45887100
H	1.74745700	-2.47423600	-1.37476600
H	2.77015200	-1.51792100	0.62909400
H	1.90539500	2.07956000	-1.54923900
H	-4.06051000	3.01242200	0.05003700
H	4.34516700	2.49728300	-1.82213700
H	-6.15800300	1.56014800	0.16467000
H	0.08355500	-3.01236200	0.84864300
H	-7.14409200	-0.72288300	0.13358300
H	-0.30493800	4.67476400	0.85967100
H	-0.02881000	2.95243800	1.23605600
H	-1.49306600	3.78087900	1.84615800
H	6.72076700	0.25021300	-0.48255100
H	4.54681200	-2.10736200	2.01864900
H	4.53027000	-3.03275600	0.48730400
H	6.04941100	-2.84271300	1.40182100
O	1.30687200	1.00914200	2.43481300
H	2.25922400	0.83548600	2.35608900
O	0.72030700	-0.22020000	2.23528500
H	0.65398900	-0.30504400	0.98833000

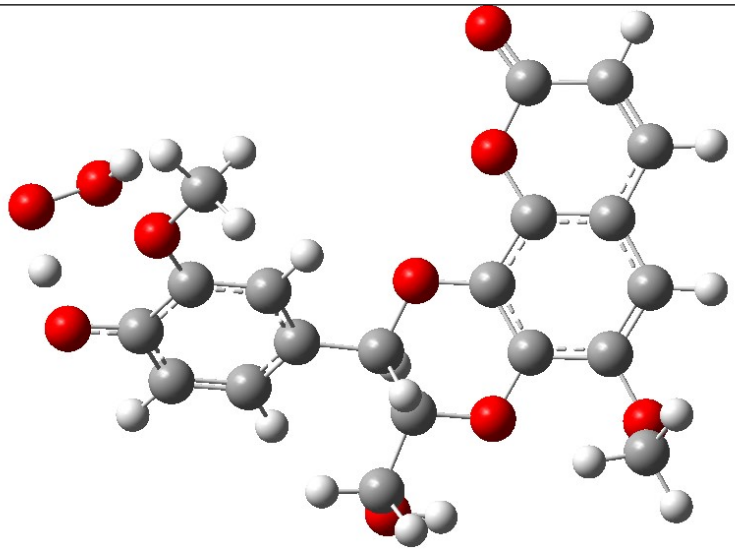


Name	**CMB-O14-TS-P**
Cartesian Coordinates	Energy

O	0.48448800	0.20199300	-0.22717000
O	1.84815000	-2.24294500	0.10423400
O	1.86703500	2.47908800	-0.33024900
O	-0.01388700	-3.91086800	-1.22571200
O	4.56416100	-2.29561400	0.14659700
O	-4.10546900	1.00457000	1.54288800
O	-5.69059700	-0.64617700	0.16337600
O	1.76695000	4.67591700	-0.49866200
C	-0.13780800	-1.04276600	-0.55435300
C	0.44182200	-2.13008800	0.36005700
C	-1.62423200	-0.88224400	-0.39050400
C	1.83700700	0.13841600	-0.14129900
C	2.51508000	-1.06660200	0.01090000
C	-0.12497900	-3.51659800	0.12765300
C	2.57300700	1.32526400	-0.20802500
C	3.92417200	-1.09469200	0.05428100
C	3.96478400	1.30813900	-0.15789800

Zero-point correction= 0.370143 (Hartree/Particle)
Thermal correction to Energy= 0.397478
Thermal correction to Enthalpy= 0.398422
Thermal correction to Gibbs Free Energy= 0.310244
Sum of electronic and zero-point Energies= -1525.119507
Sum of electronic and thermal Energies= -1525.092172
Sum of electronic and thermal Enthalpies= -1525.091228
Sum of electronic and thermal Free Energies= -1525.179406

C	-2.13129300	0.02333800	0.53663800
C	-2.48643600	-1.67793500	-1.16131900
C	4.63546700	0.08103100	-0.03120400
C	-3.50848100	0.13729200	0.70626200
C	-3.85019400	-1.57420700	-0.99773200
C	4.63628600	2.58043300	-0.24966200
C	-4.39814900	-0.68674700	-0.05028200
C	3.93336600	3.72086700	-0.36813100
C	2.47624200	3.70964600	-0.40680200
C	4.57255500	-2.84002800	1.46827900
C	-3.27532800	1.82153400	2.36945300
H	0.09964200	-1.29639800	-1.59306700
H	0.28993800	-1.83076000	1.40480000
H	0.39601200	-4.21612000	0.78974800
H	-1.18433800	-3.53032500	0.38488300
H	-1.45032500	0.64516200	1.10119400
H	-2.06930600	-2.37347400	-1.88150000
H	5.71856600	0.05099600	-0.00072500
H	-4.53850500	-2.17672800	-1.57849100
H	5.72096900	2.59739900	-0.22165200
H	0.92362300	-3.98146300	-1.43885700
H	4.40078000	4.69349400	-0.43894900
H	5.09677000	-3.79251100	1.40867600
H	3.55478300	-3.00478000	1.82982600
H	5.10489700	-2.16951900	2.14947200
H	-3.95634900	2.42257400	2.96728800
H	-2.65729600	1.20267900	3.02413500
H	-2.64071500	2.47364100	1.76319400
O	-5.12607900	1.92643300	-1.00699800
H	-4.65681100	2.25387700	-0.22063200
O	-6.33220500	1.51423000	-0.53134900
H	-6.09004000	0.37492900	-0.04286200

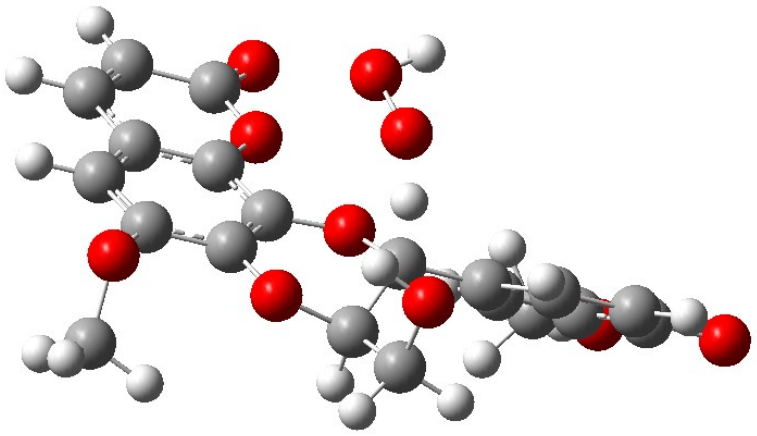


Name	**CMB-C17-TS-P**
Cartesian Coordinates	Energy

O	-0.02755200	0.29499500	-0.04261900
O	-1.17444800	-2.23851400	-0.46429400
O	-1.58972700	2.43613800	0.16416300
O	0.88843600	-3.74406400	0.77152300
O	-3.88228100	-2.52155600	-0.51447900
O	4.51529100	2.08976500	-1.03436500
O	6.21599100	0.37262100	0.00853300
O	-1.66911800	4.62150000	0.44868600
C	0.72738700	-0.86609500	0.12945800
C	0.20768900	-1.99344100	-0.76364100
C	2.17795300	-0.54279200	0.08748900
C	-1.37287200	0.11962200	-0.14176800
C	-1.94216700	-1.13163300	-0.33399100
C	0.89202100	-3.33169400	-0.57939700
C	-2.19961900	1.23732500	-0.01514400
C	-3.34393800	-1.27675600	-0.37445800
C	-3.58496100	1.10445900	-0.05523200
C	2.61082500	0.66403800	-0.48487600
C	3.10941400	-1.41718800	0.64724000
C	-4.14985000	-0.16880200	-0.23494700

Zero-point correction= 0.369493 (Hartree/Particle)
Thermal correction to Energy= 0.397294
Thermal correction to Enthalpy= 0.398238
Thermal correction to Gibbs Free Energy= 0.309476
Sum of electronic and zero-point Energies= -1525.112911
Sum of electronic and thermal Energies= -1525.085111
Sum of electronic and thermal Enthalpies= -1525.084167
Sum of electronic and thermal Free Energies= -1525.172929

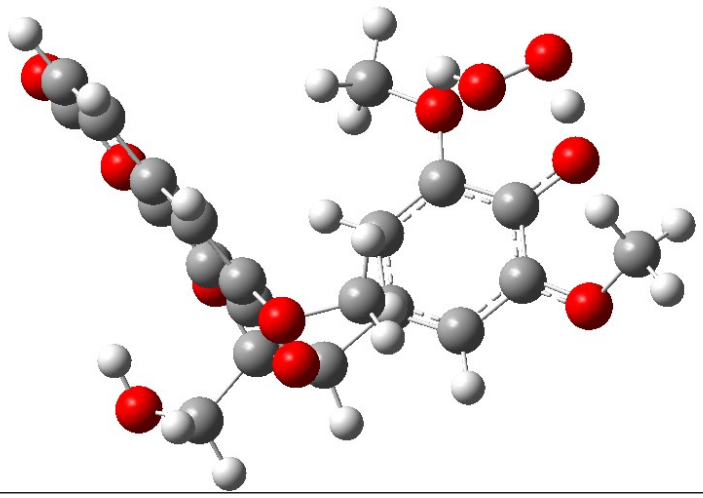
C	3.96194500	0.96427900	-0.51094300
C	4.46635000	-1.11154400	0.61668700
C	-4.35847000	2.30971100	0.10555600
C	4.89841800	0.07039600	0.03827200
C	-3.75110100	3.49745200	0.27924200
C	-2.29811500	3.60620200	0.30944200
C	-3.82924200	-3.02259800	-1.85202000
C	3.63483000	3.07835800	-1.55417500
H	0.28985300	-1.67054300	-1.81118300
H	0.38186800	-4.05918100	-1.22010100
H	1.93156000	-3.26628100	-0.89994400
H	1.88559300	1.35152000	-0.89837700
H	2.77238300	-2.32838400	1.12824400
H	-5.22665900	-0.28963600	-0.26123100
H	5.19975300	-1.77931900	1.05283900
H	-5.44092500	2.23855200	0.08597000
H	-0.02231500	-3.73616200	1.09092700
H	-4.29709900	4.42262900	0.40395300
H	-4.26639400	-4.01947100	-1.82773100
H	-2.79763200	-3.08552000	-2.20609300
H	-4.41304300	-2.38106100	-2.51883200
H	6.31919900	1.23743800	-0.41117500
H	4.26633000	3.89758700	-1.89065800
H	3.06557800	2.68390900	-2.39995900
H	2.95137500	3.43478200	-0.77907200
O	-0.57569200	-0.20448200	2.80007700
H	0.14501000	0.31387900	3.19036900
O	0.00707600	-1.41236500	2.48376200
H	0.45276900	-1.25284600	1.32741000



Name	**CMC-O14-TS-P**
Cartesian Coordinates	Energy

O	-0.41261200	-2.31651300	0.66233800
O	-1.80660900	-0.91313900	-1.36328300
O	-3.13938400	-3.10018500	-2.50748600
O	-3.39724100	1.10739900	-0.70270900
O	-0.65853700	-1.55608200	3.25792300
O	2.07172400	2.09234700	-1.77701700
O	4.66980600	-1.30927000	0.28823200
O	4.43852900	1.21878200	-0.96023000
O	-4.77569900	2.66340100	-1.43956900
C	0.07387500	-2.32828700	-0.69353100
C	-1.09709900	-2.13030500	-1.64866600
C	1.22111600	-1.34391100	-0.81583000
C	-1.91418500	-0.59138600	-0.04736700
C	-1.21330000	-1.26049600	0.95134100
C	-2.08371100	-3.28825000	-1.59045100
C	-2.74468100	0.47564000	0.30841400
C	-1.34418800	-0.87094200	2.30003800
C	2.44280800	-1.73381400	-0.27340000
C	1.05093100	-0.05976400	-1.34664100
C	-2.89156300	0.85710200	1.63976500
C	-2.18054500	0.17024800	2.63644000
C	2.12230700	0.81988300	-1.33789700
C	3.52023900	-0.85759600	-0.24018900

Zero-point correction= 0.403160 (Hartree/Particle)
Thermal correction to Energy= 0.433162
Thermal correction to Enthalpy= 0.434106
Thermal correction to Gibbs Free Energy= 0.339521
Sum of electronic and zero-point Energies= -1639.594315
Sum of electronic and thermal Energies= -1639.564314
Sum of electronic and thermal Enthalpies= -1639.563369
Sum of electronic and thermal Free Energies= -1639.657955



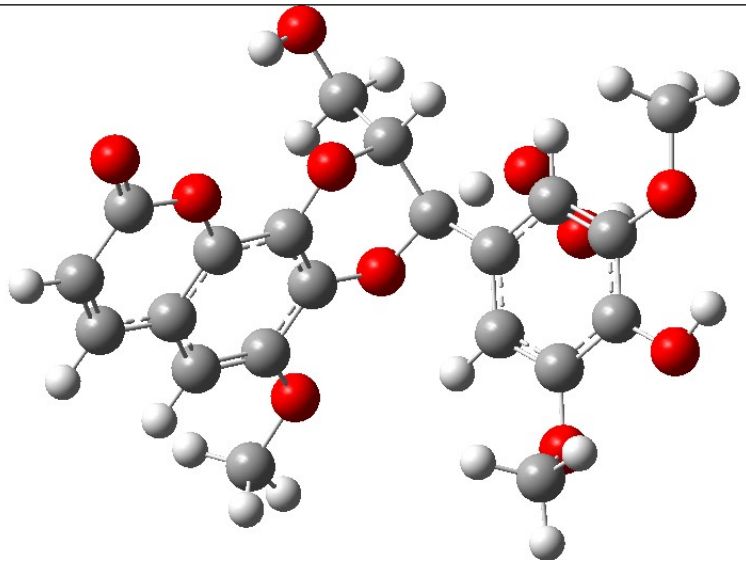
C	3.39676600	0.43205000	-0.82325000
C	-3.78262000	1.95814700	1.90802000
C	-4.42824000	2.57945500	0.90489000
C	-4.24909300	2.16458300	-0.48097800
C	0.72752100	-1.20568900	3.32013600
C	0.85123500	2.55031600	-2.35904200
C	5.50246800	-0.40597300	1.02973000
H	0.46026100	-3.33861700	-0.83434000
H	-0.72971100	-2.01254800	-2.66980400
H	-1.57195100	-4.20962000	-1.87413400
H	-2.46318900	-3.40520900	-0.56736400
H	2.56879200	-2.72068000	0.15804800
H	0.10047900	0.24355900	-1.76106100
H	-2.28089900	0.45760900	3.67670200
H	-3.92114800	2.27397700	2.93687500
H	-3.56533800	-2.26033400	-2.30128500
H	-5.10508100	3.40739000	1.06646900
H	1.17848100	-1.85361600	4.07009200
H	0.83768900	-0.15970200	3.62200800
H	1.21616200	-1.36492300	2.35545400
H	0.59544300	1.95352000	-3.23715200
H	1.03428000	3.58038700	-2.65517900
H	0.03433400	2.51398700	-1.63230000
H	6.02654500	-1.02451500	1.75705500
H	4.89534200	0.33731100	1.55088900
H	6.21707400	0.09044900	0.37613400
O	2.81379200	2.48834500	1.01721300
H	2.13514000	2.73528000	0.36430000
O	3.96629700	3.00246800	0.51744300
H	4.29653400	2.14977800	-0.39343700

Name	**CMC-C18-TS-P**
Cartesian Coordinates	Energy

O	-0.19038000	-0.13934100	-1.78158100
O	-1.01535900	1.60430900	0.28216200
O	-1.51209400	3.87454100	-1.31857200
O	-3.25409200	1.08259200	1.63739800
O	-1.61828100	-2.23024200	-2.43065100
O	4.63389800	1.14653300	1.70563300
O	2.84503200	-3.09269700	0.75537400
O	4.69492600	-1.46613100	1.98848700
O	-4.61368100	1.72672700	3.25095500
C	0.68200500	0.80644000	-1.22411200
C	-0.07675900	2.02271000	-0.72522800
C	1.70595800	0.20716700	-0.34258300
C	-1.73133000	0.50093300	-0.05827500
C	-1.33476600	-0.35602700	-1.07425400
C	-0.82058300	2.75704000	-1.83347000
C	-2.90571600	0.21613300	0.64937800
C	-2.10944100	-1.48835900	-1.41774400
C	1.77849800	-1.17583500	-0.17475600
C	2.66360300	1.03877000	0.27064400
C	-3.66796900	-0.89986800	0.33237500
C	-3.26651900	-1.75352000	-0.71280000
C	3.65315500	0.47360600	1.05426400

Zero-point correction= 0.402034 (Hartree/Particle)
Thermal correction to Energy= 0.432729
Thermal correction to Enthalpy= 0.433673
Thermal correction to Gibbs Free Energy= 0.337433
Sum of electronic and zero-point Energies= -1639.585661
Sum of electronic and thermal Energies= -1639.554966
Sum of electronic and thermal Enthalpies= -1639.554022
Sum of electronic and thermal Free Energies= -1639.650262

C	2.77175700	-1.73820400	0.61974300
C	3.71811700	-0.92132200	1.23530200
C	-4.86178000	-1.11197800	1.11184200
C	-5.20316500	-0.25698000	2.09278000
C	-4.38462900	0.90974700	2.39846100
C	-2.36321500	-3.37785400	-2.81174400
C	4.63638900	2.56661200	1.61529700
C	2.46051000	-3.56672600	2.04849400
H	0.58853700	2.71744500	-0.21531700
H	-0.09762900	3.13345900	-2.55993000
H	-1.50291400	2.07543300	-2.35600000
H	1.07071800	-1.83580500	-0.66091100
H	2.62986200	2.11106300	0.12553000
H	-3.87832300	-2.61522000	-0.94400800
H	-5.48002100	-1.97579300	0.88980900
H	-2.10716300	3.56500700	-0.62605700
H	-6.09089900	-0.38350900	2.69744200
H	-1.81370300	-3.83058400	-3.63396100
H	-3.36514400	-3.09906400	-3.15074100
H	-2.43531700	-4.09015900	-1.98489100
H	5.24573300	-0.74970700	2.33410400
H	4.78193300	2.88806300	0.58055500
H	5.47218800	2.90564200	2.22293300
H	3.70363200	2.97863800	2.00884500
H	2.56676800	-4.65000900	2.02397700
H	1.41782000	-3.30428600	2.25100200
H	3.10595200	-3.15407000	2.82642000
O	3.14276700	0.48726800	-2.99244400
H	3.74472200	0.71693900	-2.26559700
O	2.26089200	1.53750900	-3.05425800
H	1.38950600	1.23307700	-2.22492300

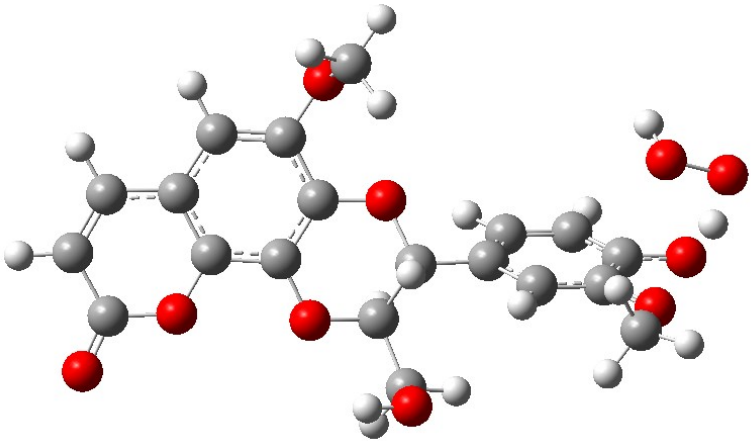


Name	**CMA-O14-TS-H**
Cartesian Coordinates	Energy

O	-0.26503300	0.96316700	-0.16940800
O	-1.77963500	-1.42839800	-0.24194600
O	0.25241800	-3.14115200	0.87828600
O	-4.43942000	-1.30016400	-0.08305300
O	-1.50200500	3.35978400	-0.02290200
O	5.10903600	-1.17489100	0.90909100
O	5.72652400	-0.16686700	-1.46169800
O	-6.32048100	-2.44414500	-0.06848700
C	0.33424000	-0.31530800	0.10215000
C	-0.41493100	-1.39254100	-0.68629300
C	1.78066000	-0.23660300	-0.29673600
C	-2.36080800	-0.20341900	-0.13057600
C	-1.61966600	0.97239500	-0.09817400
C	0.13908100	-2.78858000	-0.49151000
C	-3.75151100	-0.12032900	-0.04875000
C	-2.26905800	2.21950400	-0.00840700
C	-4.40152700	1.10659500	0.04939400
C	2.75001800	-0.73287900	0.56483300
C	2.12779600	0.28931700	-1.55385700
C	-3.64046900	2.28647800	0.06632600
C	4.08919500	-0.72046200	0.17348800

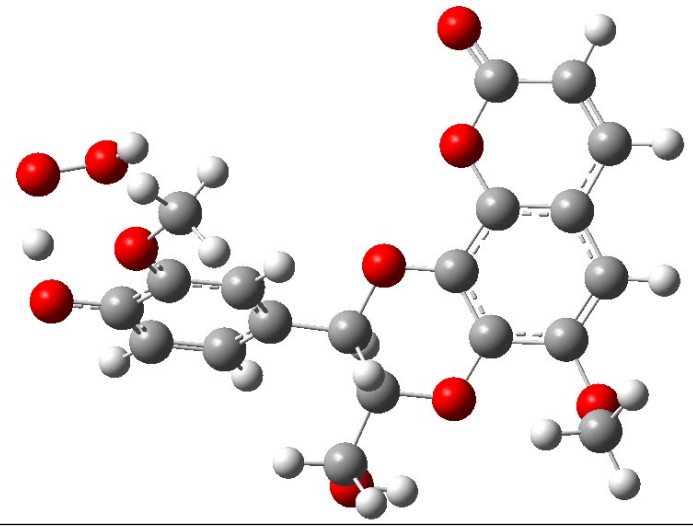
Zero-point correction= 0.368937 (Hartree/Particle)
Thermal correction to Energy= 0.396646
Thermal correction to Enthalpy= 0.397591
Thermal correction to Gibbs Free Energy= 0.308142
Sum of electronic and zero-point Energies= -1525.127556
Sum of electronic and thermal Energies= -1525.099846
Sum of electronic and thermal Enthalpies= -1525.098902
Sum of electronic and thermal Free Energies= -1525.188351

C	3.44976300	0.33361800	-1.93842000
C	-5.83848400	1.08383600	0.11574200
C	4.45192900	-0.17690100	-1.09575400
C	-6.51206200	-0.08240100	0.08040000
C	-5.80911400	-1.34476000	-0.02592200
C	-0.96291000	3.68768500	1.26697300
C	4.82855500	-1.62919300	2.23601600
H	0.23734700	-0.51967800	1.17180800
H	-0.39862700	-1.13355800	-1.75126700
H	-0.50541500	-3.49311000	-1.02467900
H	1.13944700	-2.84062700	-0.92214400
H	2.45815100	-1.12708300	1.52989600
H	1.35340600	0.66948400	-2.20953900
H	-4.12991000	3.25068900	0.13817400
H	3.75046900	0.74529700	-2.89449800
H	-6.36788500	2.02739800	0.19283100
H	-0.63519400	-3.18368600	1.25396500
H	-7.59079600	-0.13914600	0.12625200
H	-0.35130200	4.57724100	1.13005100
H	-0.34701700	2.86865100	1.64471900
H	-1.77577400	3.89750600	1.96621200
H	4.38080300	-0.82447300	2.82247000
H	4.16476000	-2.49534300	2.21025400
H	5.78924300	-1.90982700	2.65924800
H	6.26768000	0.48503400	-0.78255700
H	4.98053900	2.48033800	0.00809700
O	6.55571600	1.46790900	0.06660500
O	5.33236700	1.77083100	0.57415900



Name			**CMB-O14-TS-H**
Cartesian Coordinates			Energy
O	0.46283200	0.23358400	-0.30011100
O	1.76532200	-2.25349700	0.05622700
O	1.90922300	2.47226800	-0.36130800
O	-0.13954800	-3.86862900	-1.34805700
O	4.45957900	-2.37600100	0.21943700
O	-4.15731000	0.55149300	1.78516400
O	-5.73441400	-0.43402100	-0.10076200
O	1.86350500	4.66467600	-0.55394900
C	-0.17426200	-1.00371200	-0.65649100
C	0.35185700	-2.10831300	0.26454300
C	-1.65868500	-0.81666900	-0.51895100
C	1.81419100	0.13196900	-0.16884100
C	2.45693800	-1.08920100	-0.00052400
C	-0.25829100	-3.47038600	0.00833800
C	2.58414200	1.29518000	-0.20425900
C	3.86115400	-1.14447800	0.09886000
C	3.97102600	1.25184700	-0.09317100
C	-2.16783600	-0.17948300	0.60721200
C	-2.51311500	-1.32780000	-1.50949000
C	4.60813300	0.00921300	0.05578100
C	-3.54730000	-0.04818900	0.75364800
C	-3.87825600	-1.18919100	-1.38230300
C	4.67261100	2.50691900	-0.14796400
C	-4.42391700	-0.55700000	-0.25281300

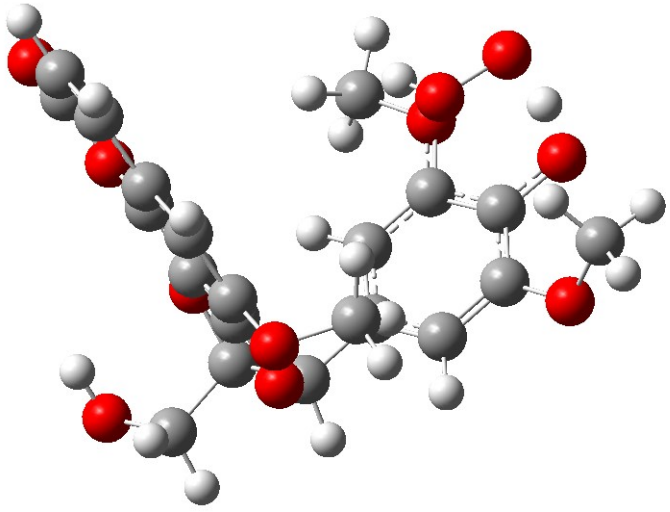
Zero-point correction= 0.369103 (Hartree/Particle)
Thermal correction to Energy= 0.396581
Thermal correction to Enthalpy= 0.397525
Thermal correction to Gibbs Free Energy= 0.309008
Sum of electronic and zero-point Energies= -1525.127689
Sum of electronic and thermal Energies= -1525.100211
Sum of electronic and thermal Enthalpies= -1525.099267
Sum of electronic and thermal Free Energies= -1525.187784



C	4.00179900	3.66528800	-0.29937500
C	2.55757700	3.67966300	-0.41387900
C	4.49313800	-2.84934500	1.57460700
C	-3.33744800	1.21274500	2.75368700
H	0.08778900	-1.24332300	-1.69062300
H	0.17855900	-1.81384800	1.30616700
H	0.22395200	-4.19413400	0.67157000
H	-1.32213800	-3.43977800	0.24551400
H	-1.49265200	0.20967900	1.35825300
H	-2.08959200	-1.81836000	-2.37807300
H	5.68732700	-0.04449800	0.13954100
H	-4.56021800	-1.55995500	-2.13806200
H	5.75407100	2.49920600	-0.06458600
H	0.79822400	-3.97289600	-1.54986700
H	4.49369300	4.62700300	-0.34456100
H	4.94589000	-3.83846900	1.54663400
H	3.48190000	-2.91579300	1.98201500
H	5.09957300	-2.17836300	2.18751000
H	-4.02701600	1.67225100	3.45661900
H	-2.70204000	0.49201600	3.27133100
H	-2.72715400	1.97855500	2.27002800
H	-5.98593800	0.62519800	-0.09576700
H	-4.22208300	2.42799800	0.08278500
O	-5.98364400	1.93051700	-0.31093100
O	-4.70840600	2.16375800	-0.71922500

Name			**CMC-O14-TS-H**
Cartesian Coordinates			Energy
O	-0.37282700	-2.44498500	0.51203100
O	-1.79748200	-0.87370700	-1.36926400
O	-3.24055900	-3.00920400	-2.56992100
O	-3.19578400	1.22277600	-0.53764700
O	-0.45167300	-1.81712300	3.14616100
O	2.15320100	1.93378900	-2.21791600
O	4.45838800	-1.07298300	0.63977300
O	4.32386900	1.31171300	-0.85599200
O	-4.48540200	2.90250800	-1.13852800
C	0.06077200	-2.37094400	-0.86314200
C	-1.14747700	-2.10105900	-1.74921000
C	1.19514400	-1.36668000	-0.95027500
C	-1.80713300	-0.60547000	-0.03683300
C	-1.10459400	-1.36220400	0.89537000
C	-2.15252400	-3.24087300	-1.69119400
C	-2.53575100	0.49684200	0.41339400
C	-1.14986800	-1.02993300	2.26185800
C	2.33628500	-1.65988100	-0.19607900
C	1.08945800	-0.17165000	-1.65874700
C	-2.58812300	0.83231000	1.76308100
C	-1.88570900	0.04982900	2.69304900
C	2.14131100	0.73747900	-1.60764400
C	3.37299500	-0.75114200	-0.11182700
C	3.31159000	0.45985600	-0.84435800
C	-3.37343000	1.98418500	2.12204700
C	-4.01874700	2.69857000	1.18021800
C	-3.94394500	2.32636100	-0.21857000

Zero-point correction= 0.402064 (Hartree/Particle)
Thermal correction to Energy= 0.432288
Thermal correction to Enthalpy= 0.433233
Thermal correction to Gibbs Free Energy= 0.338317
Sum of electronic and zero-point Energies= -1639.602701
Sum of electronic and thermal Energies= -1639.572476
Sum of electronic and thermal Enthalpies= -1639.571532
Sum of electronic and thermal Free Energies= -1639.666448



C	0.90331500	-1.37490200	3.32411100
C	0.95876500	2.35594600	-2.88102200
C	4.95625500	-0.07202300	1.54765900
H	0.44008500	-3.36840500	-1.08661100
H	-0.82744400	-1.94801800	-2.78084500
H	-1.66033900	-4.15724200	-2.01989800
H	-2.50836500	-3.38237300	-0.66524100
H	2.40264600	-2.58560900	0.36425500
H	0.20168100	0.05714300	-2.23052100
H	-1.91300900	0.29882500	3.74751500
H	-3.43207300	2.26426500	3.16829900
H	-3.73018700	-2.24402600	-2.24576000
H	-4.61594500	3.56991500	1.41084900
H	1.37769400	-2.08773400	3.99586600
H	0.91402400	-0.37697400	3.76937200
H	1.42864000	-1.35934000	2.36543900
H	0.73033500	1.69281400	-3.71729600
H	1.16550000	3.35773100	-3.24811800
H	0.12317500	2.37938900	-2.17726200
H	5.34641200	-0.61617200	2.40624000
H	4.14633500	0.58629400	1.86721000
H	5.75098400	0.50837300	1.08269200
O	2.29569200	2.31621800	0.86324700
H	1.61541900	2.59951900	0.22411200
O	3.41158500	3.01523200	0.54530900
H	4.03618200	2.19481800	-0.29707800

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