Supporting Information (SI)

The Radical Scavenging Activity of Moracins: Theoretical Insights

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Table of Contents

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.[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) $= 8.62\times10^{-4}$ Pa s) and a is the radius of the solute.

The kinetic study requires different considerations. Water (dielectric constants, $\varepsilon = 78.35$) and pentyl ethanoate ($\varepsilon = 4.73$) 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.

Table S2: The Cartesian coordinates and energies of TS of the reaction between MM with HO•/HOO• at the M06-2X/6-311++G(d,p) calculating method following the FHT and FHT mechanisms

Name				**1-C1-OH-RAF (gas)**
Cartesian Coordinates				Frequency and Energy
O	-0.84823900	0.75309300	0.20423000	Zero-point correction= 0.222324 (Hartree/Particle)
O	-5.59591100	1.22969700	0.01747000	Thermal correction to Energy= 0.239053
O	4.53650100	-2.01511900	-0.21029400	Thermal correction to Enthalpy= 0.239998
O	3.79609600	2.59020100	-0.63563000	Thermal correction to Gibbs Free Energy= 0.177201
C	-2.14217500	-1.04844800	-0.23703900	Sum of electronic and zero-point Energies= -915.805912
C	-0.04118400	-0.33982500	0.03717000	Sum of electronic and thermal Energies= -915.789183
C	-2.12457700	0.32359500	0.04344300	Sum of electronic and thermal Enthalpies= -915.788239
C	1.40156600	-0.10279300	0.16645700	Sum of electronic and thermal Free Energies= -915.851036
C	-0.75791800	-1.45321800	-0.23913700	
C	-3.37586900	-1.67030500	-0.43994000	
C	-3.25719000	1.11376500	0.13552300	
C	1.90055400	1.19598200	-0.13959300	
C	2.28639600	-1.21354600	0.07144500	
C	-4.46855400	0.46815500	-0.06998200	
C	-4.52879000	-0.90714500	-0.35472800	
C	3.62837500	-1.00329100	-0.17446300	
C	3.24772800	1.37116000	-0.38626800	
C	4.12366900	0.28247500	-0.40221200	
H	-0.36184300	-2.43636000	-0.43332700	
H	-3.43838000	-2.72918200	-0.65898200	
H	-3.21883100	2.17116400	0.35832600	
H	1.21083200	2.03152100	-0.13970000	
H	1.90675500	-2.20788500	0.27549200	
H	-5.49741900	-1.37165500	-0.50827800	
H	5.17830800	0.43426500	-0.59118800	
H	-6.37082000	0.68104600	-0.12728300	
H	4.10812700	-2.84708800	0.00834400	
H	3.11760100	3.26924600	-0.58584100	
O	1.33999100	0.00110700	2.12677900	
H	2.18598000	0.43372600	2.31793200	
Name				**1-C2-OH-RAF (gas)**
Cartesian Coordinates				Frequency and Energy
O	0.82116200	0.60397600	-0.04220600	Zero-point correction= 0.223662 (Hartree/Particle)
O	5.54293300	1.29923400	0.05072900	Thermal correction to Energy= 0.239930
O	-3.81262100	2.30727500	-0.63293500	Thermal correction to Enthalpy= 0.240874
O	-4.48524500	-2.23064300	0.34364300	Thermal correction to Gibbs Free Energy= 0.178965
C	2.22042000	-1.17327900	-0.08562200	Sum of electronic and zero-point Energies= -915.821560
C	0.06889400	-0.54794300	-0.09513100	Sum of electronic and thermal Energies= -915.805293
C	2.12412000	0.22345100	-0.03711700	Sum of electronic and thermal Enthalpies= -915.804348
C	-1.37400300	-0.36439600	-0.11291200	Sum of electronic and thermal Free Energies= -915.866257
C	0.86227100	-1.64850000	-0.12493100	
C	3.49253500	-1.75227300	-0.09137600	
C	3.21084500	1.07867400	0.01083600	
C	-2.22903300	-1.42280600	0.17019400	
C	-1.90065900	0.90337900	-0.42765000	
C	4.46088100	0.47470400	0.00535300	
C	4.60074600	-0.92413900	-0.04524500	
C	-3.30459700	1.07932600	-0.43293100	
C	-3.61080800	-1.22900900	0.09425800	
C	-4.15810100	0.01957400	-0.20048800	

H	0.52580600	-2.67049200	-0.19250800	
H	3.61631500	-2.82748500	-0.13042600	
H	3.11147200	2.15484400	0.04806900	
H	-1.83158100	-2.39145100	0.45354400	
H	-1.26936000	1.64756100	-0.89148000	
H	5.59716800	-1.35372200	-0.04836600	
H	-5.22975700	0.16399600	-0.18942400	
H	6.35094500	0.77970000	0.04886000	
H	-3.16855500	2.93343100	-0.26809700	
H	-4.01173800	-3.03435100	0.57578300	
O	-1.77294200	2.28508000	1.21702200	
H	-0.81808100	2.17802500	1.34058800	
Name				**1-C2-OH-RAF (water)**
Cartesian Coordinates				Frequency and Energy
O	0.83818500	0.66051400	-0.18298000	Zero-point correction= 0.221999 (Hartree/Particle)
O	5.58604000	1.27794600	-0.07411100	Thermal correction to Energy= 0.238526
O	-3.85503000	2.37771800	-0.62832200	Thermal correction to Enthalpy= 0.239470
O	-4.48465300	-2.20178600	0.15732900	Thermal correction to Gibbs Free Energy= 0.176749
C	2.21045100	-1.13375700	-0.02288500	Sum of electronic and zero-point Energies= -915.860109
C	0.06809400	-0.48706000	-0.13078800	Sum of electronic and thermal Energies= -915.843582
C	2.13824900	0.26110300	-0.11664300	Sum of electronic and thermal Enthalpies= -915.842638
C	-1.37562200	-0.29817900	-0.17681800	Sum of electronic and thermal Free Energies= -915.905359
C	0.84639500	-1.59387200	-0.03403700	
C	3.47286000	-1.73377100	0.05395700	
C	3.23890300	1.10177800	-0.13645800	
C	-2.22620000	-1.38373500	0.01523500	
C	-1.90224800	0.98961900	-0.38178300	
C	4.47561300	0.47485900	-0.05785300	
C	4.59530800	-0.92392200	0.03592800	
C	-3.29549400	1.15639200	-0.42232600	
C	-3.60499400	-1.17922000	-0.02206400	
C	-4.15214800	0.08454300	-0.23662200	
H	0.49760400	-2.61348500	0.02001700	
H	3.57498900	-2.80970700	0.12721800	
H	3.15193600	2.17827600	-0.20944300	
H	-1.83704600	-2.37972300	0.19397000	
H	-1.25685100	1.82645900	-0.61714800	
H	5.58831400	-1.35620700	0.09493600	
H	-5.22582000	0.22332000	-0.25668500	
H	6.38132700	0.73335100	-0.01653300	
H	-3.16800900	3.05049300	-0.72412500	
H	-4.00966200	-3.03104100	0.29827800	
O	-1.80836300	1.70039300	1.86665600	
H	-0.84122600	1.65132300	1.77988200	
Name				**1-C2-OH-RAF (pentyl ethanoate)**
Cartesian Coordinates				Frequency and Energy
O	0.82246500	0.60696800	-0.08941000	Zero-point correction= 0.222917 (Hartree/Particle)
O	5.54354500	1.29972700	0.02715000	Thermal correction to Energy= 0.239382
O	-3.82333000	2.30616800	-0.63842800	Thermal correction to Enthalpy= 0.240326
O	-4.47769000	-2.23478600	0.32728800	Thermal correction to Gibbs Free Energy= 0.177062
C	2.22097100	-1.17085100	-0.06788200	Sum of electronic and zero-point Energies= -915.848912
C	0.07059500	-0.54655100	-0.11091500	Sum of electronic and thermal Energies= -915.832448
C	2.12493400	0.22659300	-0.06250300	Sum of electronic and thermal Enthalpies= -915.831504
C	-1.37360900	-0.36431100	-0.13385400	Sum of electronic and thermal Free Energies= -915.894768

C	0.86308400	-1.64819100	-0.10059500
C	3.49414700	-1.75116300	-0.04430000
C	3.21128700	1.08416900	-0.03012400
C	-2.22548000	-1.42855700	0.13989900
C	-1.90213000	0.90572300	-0.43284500
C	4.46095600	0.47843700	-0.00531200
C	4.60247900	-0.92238900	-0.01312200
C	-3.30151100	1.08208400	-0.42896200
C	-3.60770100	-1.23111700	0.08336000
C	-4.15624100	0.02216400	-0.19178100
H	0.52621900	-2.67274800	-0.12778200
H	3.61706500	-2.82755000	-0.04928300
H	3.10784600	2.16154000	-0.02470200
H	-1.82827000	-2.40389200	0.39972200
H	-1.26748300	1.67431800	-0.85185000
H	5.60056100	-1.34910200	0.00547900
H	-5.22881600	0.16744600	-0.17641000
H	6.35184300	0.77506900	0.04912400
H	-3.16147600	2.95449700	-0.35706700
H	-3.99935500	-3.04598900	0.53695200
O	-1.78747400	2.27219000	1.32127300
H	-0.82894300	2.14804100	1.40644800

Name			**1-C3-OH-RAF (gas)**
Cartesian Coordinates			Frequency and Energy
O	-0.92865000	-0.66776400	-0.08408300
O	-5.64697700	-1.38809200	0.00443500
O	3.79526400	-2.25233500	-0.81783600
O	4.34862100	2.31494900	0.07699700
C	-2.33378800	1.10199300	-0.00393700
C	-0.18185000	0.48392300	-0.06947000
C	-2.23211100	-0.29413200	-0.04438600
C	1.26736100	0.30895400	-0.11522900
C	-0.97577800	1.58270700	-0.02448200
C	-3.60730500	1.67495000	0.03909800
C	-3.31546400	-1.15522900	-0.04161800
C	2.11415800	1.41110700	0.04708900
C	1.81246100	-0.94924700	-0.34095500
C	-4.56753600	-0.55746000	0.00181300
C	-4.71270400	0.84077800	0.04107100
C	3.22765700	-1.12058500	-0.33147900
C	3.50492300	1.25577600	-0.04505500
C	4.06527200	0.01680100	-0.26223500
H	-0.64710300	2.60930000	-0.01885200
H	-3.73562700	2.74995000	0.06973800
H	-3.21078900	-2.23106200	-0.07121600
H	1.69632300	2.39429900	0.23699500
H	1.17867700	-1.81357500	-0.48706200
H	-5.71054600	1.26593800	0.07333500
H	5.13673400	-0.10851700	-0.33495300
H	-6.45614200	-0.87226500	0.04697300
H	3.41822600	-2.99970100	-0.33833000
H	3.84759300	3.12933100	0.16912700
O	3.11252200	-1.82552800	1.50816100
H	2.64463400	-1.17556600	2.05150200

Zero-point correction= 0.222196 (Hartree/Particle)
Thermal correction to Energy= 0.238892
Thermal correction to Enthalpy= 0.239836
Thermal correction to Gibbs Free Energy= 0.176811
Sum of electronic and zero-point Energies= -915.811165
Sum of electronic and thermal Energies= -915.794469
Sum of electronic and thermal Enthalpies= -915.793525
Sum of electronic and thermal Free Energies= -915.856550

Name				**1-C4-OH-RAF (gas)**
Cartesian Coordinates				Frequency and Energy
O	1.04562400	0.74908600	-0.13498700	Zero-point correction= 0.222958 (Hartree/Particle)
O	5.78069300	1.30425400	0.08756300	Thermal correction to Energy= 0.239628
O	-3.62079300	2.56190100	-0.35383500	Thermal correction to Enthalpy= 0.240572
O	-4.31363000	-2.05885100	-0.38850400	Thermal correction to Gibbs Free Energy= 0.177395
C	2.38263700	-1.06629700	0.03737800	Sum of electronic and zero-point Energies= -915.815726
C	0.25566300	-0.37546800	-0.11458900	Sum of electronic and thermal Energies= -915.799056
C	2.33165600	0.33168200	-0.04337300	Sum of electronic and thermal Enthalpies= -915.798112
C	-1.18019800	-0.16056500	-0.19963300	Sum of electronic and thermal Free Energies= -915.861289
C	1.01223200	-1.49949000	-0.00962800	
C	3.63299300	-1.68254800	0.14063200	
C	3.44547300	1.15304200	-0.03028200	
C	-2.04560700	-1.26173200	-0.26107800	
C	-1.68852000	1.14230200	-0.22516500	
C	4.67282000	0.51279900	0.07259400	
C	4.76656500	-0.88843300	0.15702000	
C	-3.05672000	1.33970400	-0.29959600	
C	-3.40825800	-1.04826600	-0.33038300	
C	-3.95069700	0.25079900	-0.28562200	
H	0.64674100	-2.51232600	0.03696700	
H	3.72070900	-2.75998500	0.20694300	
H	3.38195100	2.23059300	-0.09367400	
H	-1.65170900	-2.27162500	-0.26146400	
H	-1.00948800	1.98552900	-0.19313100	
H	5.74692100	-1.34674400	0.23642300	
H	-4.99437500	0.41221900	-0.51495500	
H	6.56972300	0.76146300	0.16192700	
H	-2.94765600	3.24067200	-0.24994100	
H	-3.86124500	-2.90713100	-0.38478300	
O	-4.36705600	0.34296200	1.74269000	
H	-4.82050900	-0.51264500	1.78262800	

Name				**1-C5-OH-RAF (gas)**
Cartesian Coordinates				Frequency and Energy
O	1.01887100	0.83445900	-0.10155400	Zero-point correction= 0.222436 (Hartree/Particle)
O	5.78085200	1.16508500	0.01892300	Thermal correction to Energy= 0.239107
O	-3.57344600	2.85816700	0.16381600	Thermal correction to Enthalpy= 0.240051
O	-4.44590100	-1.63592300	-0.83768800	Thermal correction to Gibbs Free Energy= 0.177401
C	2.27497800	-1.04469600	-0.01561300	Sum of electronic and zero-point Energies= -915.812271
C	0.18183300	-0.25496700	-0.09563200	Sum of electronic and thermal Energies= -915.795601
C	2.28810600	0.35522300	-0.05455400	Sum of electronic and thermal Enthalpies= -915.794656
C	-1.24838300	0.02874200	-0.13677400	Sum of electronic and thermal Free Energies= -915.857307
C	0.88274700	-1.41421800	-0.03867800	
C	3.49667300	-1.72006600	0.04025700	
C	3.43865300	1.12398100	-0.04576900	
C	-2.15443700	-1.00144900	-0.38813500	
C	-1.71731000	1.32556000	0.06238300	
C	4.63721600	0.42532900	0.00890100	
C	4.66686700	-0.97979200	0.05176400	
C	-3.09906200	1.59553600	0.00546300	
C	-3.55465300	-0.74480500	-0.33385200	
C	-4.01011200	0.59125500	-0.21325700	
H	0.46628900	-2.40773300	0.00092200	
H	3.53513000	-2.80187300	0.07411700	

H	3.42440600	2.20470500	-0.07918700
H	-1.82179900	-2.00925300	-0.59938800
H	-1.01152600	2.12788800	0.24623000
H	5.62603100	-1.48535600	0.09495700
H	-5.07059300	0.79549100	-0.26281100
H	6.54546000	0.58419800	0.04390500
H	-2.84343800	3.47704600	0.24984000
H	-4.32413700	-2.47045100	-0.36959400
O	-3.52732100	-1.56738400	1.44321700
H	-3.04896800	-0.96368300	2.02827700

Name			**1-C6-OH-RAF (gas)**
Cartesian Coordinates			Frequency and Energy
O	0.97116200	1.04344400	-0.25233200
O	5.80241200	1.10498900	-0.01344400
O	-3.80851200	2.90089800	0.45655300
O	-4.44067300	-1.73105800	-0.42478100
C	2.14194400	-0.90826100	0.02409400
C	0.07208800	-0.03904300	-0.18821400
C	2.24256600	0.49127800	-0.12707400
C	-1.34935400	0.23955300	-0.21967800
C	0.72522800	-1.21792600	-0.00855600
C	3.31669900	-1.65131000	0.17239600
C	3.44448600	1.17401700	-0.14391800
C	-2.22115500	-0.81971400	-0.52034100
C	-1.84923500	1.49707300	0.10278100
C	4.60326500	0.41429400	0.00328400
C	4.53478000	-0.98341400	0.16038900
C	-3.23701300	1.68365300	0.15908100
C	-3.60652100	-0.64671200	-0.33854300
C	-4.11061800	0.61028800	-0.02455800
H	0.23312200	-2.16596700	0.14522500
H	3.28119700	-2.72667600	0.29150200
H	3.50495400	2.24462000	-0.26490600
H	-1.84376800	-1.69724800	-1.02480600
H	-1.15881700	2.30542700	0.31194800
H	5.45436200	-1.54711800	0.27272800
H	-5.17295800	0.75753400	0.09750300
H	6.56601100	0.48542100	0.08969000
H	-3.11660800	3.59720500	0.57985300
H	-3.87882500	-2.51538200	-0.13251300
O	-2.25211400	-2.76687100	0.70654800
H	-2.28983400	-2.21169000	1.54655800

Zero-point correction= 0.221934 (Hartree/Particle)
Thermal correction to Energy= 0.238919
Thermal correction to Enthalpy= 0.239863
Thermal correction to Gibbs Free Energy= 0.175870
Sum of electronic and zero-point Energies= -915.821771
Sum of electronic and thermal Energies= -915.804786
Sum of electronic and thermal Enthalpies= -915.803842
Sum of electronic and thermal Free Energies= -915.867835

Name			**1-C6-OH-RAF (water)**
Cartesian Coordinates			Frequency and Energy
O	0.97116200	1.04344400	-0.25233200
O	5.80241200	1.10498900	-0.01344400
O	-3.80851200	2.90089800	0.45655300
O	-4.44067300	-1.73105800	-0.42478100
C	2.14194400	-0.90826100	0.02409400
C	0.07208800	-0.03904300	-0.18821400
C	2.24256600	0.49127800	-0.12707400
C	-1.34935400	0.23955300	-0.21967800
C	0.72522800	-1.21792600	-0.00855600
C	3.31669900	-1.65131000	0.17239600

Zero-point correction= 0.222248 (Hartree/Particle)
Thermal correction to Energy= 0.237504
Thermal correction to Enthalpy= 0.238448
Thermal correction to Gibbs Free Energy= 0.179806
Sum of electronic and zero-point Energies= -915.624171
Sum of electronic and thermal Energies= -915.608915
Sum of electronic and thermal Enthalpies= -915.607971
Sum of electronic and thermal Free Energies= -915.666613

C	3.44448600	1.17401700	-0.14391800
C	-2.22115500	-0.81971400	-0.52034100
C	-1.84923500	1.49707300	0.10278100
C	4.60326500	0.41429400	0.00328400
C	4.53478000	-0.98341400	0.16038900
C	-3.23701300	1.68365300	0.15908100
C	-3.60652100	-0.64671200	-0.33854300
C	-4.11061800	0.61028800	-0.02455800
H	0.23312200	-2.16596700	0.14522500
H	3.28119700	-2.72667600	0.29150200
H	3.50495400	2.24462000	-0.26490600
H	-1.84376800	-1.69724800	-1.02480600
H	-1.15881700	2.30542700	0.31194800
H	5.45436200	-1.54711800	0.27272800
H	-5.17295800	0.75753400	0.09750300
H	6.56601100	0.48542100	0.08969000
H	-3.11660800	3.59720500	0.57985300
H	-3.87882500	-2.51538200	-0.13251300
O	-1.73009788	-1.95525672	1.15707133
H	-1.76781788	-1.40007572	1.99708133

Name	**1-C1-OH-RAF (pentyl ethanoate)**
Cartesian Coordinates	Frequency and Energy

O	0.97116200	1.04344400	-0.25233200
O	5.80241200	1.10498900	-0.01344400
O	-3.80851200	2.90089800	0.45655300
O	-4.44067300	-1.73105800	-0.42478100
C	2.14194400	-0.90826100	0.02409400
C	0.07208800	-0.03904300	-0.18821400
C	2.24256600	0.49127800	-0.12707400
C	-1.34935400	0.23955300	-0.21967800
C	0.72522800	-1.21792600	-0.00855600
C	3.31669900	-1.65131000	0.17239600
C	3.44448600	1.17401700	-0.14391800
C	-2.22115500	-0.81971400	-0.52034100
C	-1.84923500	1.49707300	0.10278100
C	4.60326500	0.41429400	0.00328400
C	4.53478000	-0.98341400	0.16038900
C	-3.23701300	1.68365300	0.15908100
C	-3.60652100	-0.64671200	-0.33854300
C	-4.11061800	0.61028800	-0.02455800
H	0.23312200	-2.16596700	0.14522500
H	3.28119700	-2.72667600	0.29150200
H	3.50495400	2.24462000	-0.26490600
H	-1.84376800	-1.69724800	-1.02480600
H	-1.15881700	2.30542700	0.31194800
H	5.45436200	-1.54711800	0.27272800
H	-5.17295800	0.75753400	0.09750300
H	6.56601100	0.48542100	0.08969000
H	-3.11660800	3.59720500	0.57985300
H	-3.87882500	-2.51538200	-0.13251300
O	-1.74391387	-1.67118853	1.26471426
H	-1.78163387	-1.11600753	2.10472426

Zero-point correction= 0.220939 (Hartree/Particle)
Thermal correction to Energy= 0.237619
Thermal correction to Enthalpy= 0.238563
Thermal correction to Gibbs Free Energy= 0.174115
Sum of electronic and zero-point Energies= -915.629751
Sum of electronic and thermal Energies= -915.613070
Sum of electronic and thermal Enthalpies= -915.612126
Sum of electronic and thermal Free Energies= -915.676574

Name	**1-C1'-OH-RAF (gas)**
Cartesian Coordinates	Frequency and Energy

O	-0.72842100	-0.78063300	-0.23240700	Zero-point correction= 0.222552 (Hartree/Particle)
O	-5.46043200	-1.23805300	-0.58876900	Thermal correction to Energy= 0.239210
O	4.02296700	-2.55138800	0.07713100	Thermal correction to Enthalpy= 0.240154
O	4.54699500	2.04564200	-0.65156100	Thermal correction to Gibbs Free Energy= 0.177411
C	-2.06520000	1.02172000	0.10291800	Sum of electronic and zero-point Energies= -915.817595
C	0.05710800	0.27848300	0.11964100	Sum of electronic and thermal Energies= -915.800936
C	-2.01392200	-0.34918500	-0.19745100	Sum of electronic and thermal Enthalpies= -915.799992
C	1.50379100	0.09954000	-0.03387100	Sum of electronic and thermal Free Energies= -915.862735
C	-0.70771400	1.42227300	0.27756400	
C	-3.31558700	1.64479600	0.17830300	
C	-3.12671000	-1.13150400	-0.43408100	
C	2.31897900	1.20289900	-0.28390400	
C	2.04867500	-1.17547600	0.08984200	
C	-4.35415900	-0.48349900	-0.35796400	
C	-4.44877800	0.88837600	-0.05616200	
C	3.42506900	-1.33711000	-0.03718400	
C	3.69483400	1.01512500	-0.40222300	
C	4.25571900	-0.24906500	-0.28176100	
H	-0.33163800	2.39776400	0.54086700	
H	-3.39994200	2.69771500	0.41685900	
H	-3.06583200	-2.18705900	-0.65961500	
H	1.88802700	2.18943400	-0.41504400	
H	1.40076600	-2.01524900	0.31216000	
H	-5.42942000	1.34974400	-0.00462600	
H	5.32432900	-0.38601600	-0.38014700	
H	-6.25098700	-0.70070200	-0.49188300	
H	3.35987200	-3.22405900	0.25494700	
H	4.05376700	2.86623900	-0.73014800	
O	-0.10803400	-0.04500000	2.20993400	
H	0.63382800	0.48339500	2.53999300	

Name				**1-C2'-OH-RAF (gas)**
Cartesian Coordinates				Frequency and Energy
O	0.71124800	0.89373600	0.22532200	Zero-point correction= 0.222849 (Hartree/Particle)
O	5.45929200	1.39517000	0.35095900	Thermal correction to Energy= 0.239588
O	-4.01068200	2.74520500	-0.05986000	Thermal correction to Enthalpy= 0.240532
O	-4.61246900	-1.89971900	0.01702300	Thermal correction to Gibbs Free Energy= 0.177742
C	2.04821700	-0.80827000	-0.45073600	Sum of electronic and zero-point Energies= -915.821460
C	-0.08378300	-0.14325200	-0.16920000	Sum of electronic and thermal Energies= -915.804721
C	2.00518500	0.49481800	0.05311800	Sum of electronic and thermal Enthalpies= -915.803776
C	-1.52112300	0.05750400	-0.10457500	Sum of electronic and thermal Free Energies= -915.866567
C	0.66993000	-1.22762700	-0.56562700	
C	3.29278400	-1.39018600	-0.68991100	
C	3.12081400	1.25966500	0.33476600	
C	-2.36036700	-1.05757700	-0.06757400	
C	-2.04675000	1.35144300	-0.09342300	
C	4.34844300	0.65707700	0.08258900	
C	4.43424800	-0.65040900	-0.42443500	
C	-3.42842100	1.51644700	-0.06355500	
C	-3.73724400	-0.86174000	-0.03425100	
C	-4.28003100	0.41853300	-0.03796100	
H	0.29237400	-2.08761800	-1.09062000	
H	3.36986600	-2.40168500	-1.06836200	
H	3.06270300	2.26589800	0.72631700	
H	-1.93102900	-2.05083700	0.00261800	

H	-1.38337100	2.20809600	-0.11961400	
H	5.41301000	-1.08305000	-0.60363200	
H	-5.35240400	0.55871400	-0.00730900	
H	6.24816500	0.88668900	0.14564600	
H	-3.33318000	3.42645600	-0.07136300	
H	-4.12880600	-2.72923500	0.06062900	
O	0.24476700	-2.48300700	1.16345000	
H	0.63399200	-1.90306900	1.83519400	
Name				**1- C2'-OH-RAF (water)**
Cartesian Coordinates				Frequency and Energy
O	0.72006200	0.85926600	-0.04192300	Zero-point correction= 0.221589 (Hartree/Particle)
O	5.48072000	1.36235400	-0.07736500	Thermal correction to Energy= 0.238228
O	-3.96716000	2.68354300	0.13200900	Thermal correction to Enthalpy= 0.239172
O	-4.64500600	-1.93640500	-0.40276900	Thermal correction to Gibbs Free Energy= 0.176201
C	2.05436800	-0.96103100	-0.26402500	Sum of electronic and zero-point Energies= -915.861192
C	-0.07640700	-0.25472700	-0.14705400	Sum of electronic and thermal Energies= -915.844552
C	2.01509600	0.42939400	-0.10837600	Sum of electronic and thermal Enthalpies= -915.843608
C	-1.51810100	-0.03363900	-0.14693900	Sum of electronic and thermal Free Energies= -915.906580
C	0.68112400	-1.38764300	-0.27918000	
C	3.30176500	-1.59070900	-0.34680900	
C	3.13278100	1.24038500	-0.03867100	
C	-2.37706900	-1.12868400	-0.27935200	
C	-2.02547200	1.25929600	-0.00724800	
C	4.35579900	0.58588400	-0.13343800	
C	4.44323800	-0.81060400	-0.28198400	
C	-3.40625700	1.44334200	-0.00319100	
C	-3.74938900	-0.91048700	-0.27368400	
C	-4.27741100	0.36989700	-0.13628400	
H	0.30571700	-2.39045100	-0.40956300	
H	3.37682600	-2.66506000	-0.46239700	
H	3.07180000	2.31468100	0.07810900	
H	-1.99280400	-2.13707200	-0.38465700	
H	-1.36687900	2.11271100	0.09872400	
H	5.42598200	-1.26482800	-0.34693200	
H	-5.34924800	0.52602500	-0.13272100	
H	6.26576000	0.80817300	-0.17182400	
H	-3.27507200	3.34958300	0.23033200	
H	-4.17413500	-2.77443200	-0.49399800	
O	0.07862600	-1.23311400	2.19519000	
H	1.04972500	-1.26852000	2.23121300	
Name				**1- C2'-OH-RAF (pentyl ethanoate)**
Cartesian Coordinates				Frequency and Energy
O	0.71107400	0.88804800	0.18858300	Zero-point correction= 0.222425 (Hartree/Particle)
O	5.46017900	1.39312000	0.26756100	Thermal correction to Energy= 0.239173
O	-4.00100000	2.73605400	0.00109500	Thermal correction to Enthalpy= 0.240117
O	-4.62062900	-1.90659300	-0.10044100	Thermal correction to Gibbs Free Energy= 0.177101
C	2.04583500	-0.83754400	-0.42696000	Sum of electronic and zero-point Energies= -915.848953
C	-0.08434200	-0.16255400	-0.15905400	Sum of electronic and thermal Energies= -915.832205
C	2.00456500	0.48421300	0.02724100	Sum of electronic and thermal Enthalpies= -915.831261
C	-1.52206500	0.04279100	-0.10602800	Sum of electronic and thermal Free Energies= -915.894277
C	0.66807900	-1.26195400	-0.51274200	
C	3.29127900	-1.42783900	-0.65220800	
C	3.12052600	1.26183300	0.27231300	
C	-2.36644800	-1.06994900	-0.11942500	

C	-2.04350500	1.33786700	-0.05898400	
C	4.34766500	0.64931900	0.03642600	
C	4.43297900	-0.67762800	-0.42127400	
C	-3.42590900	1.50662100	-0.03804200	
C	-3.74282300	-0.87111500	-0.09728300	
C	-4.28204300	0.41150100	-0.06018500	
H	0.28831000	-2.15874700	-0.97191700	
H	3.36885500	-2.45145700	-0.99831600	
H	3.05905100	2.28346500	0.62418200	
H	-1.95153600	-2.07132800	-0.10347000	
H	-1.38309700	2.19742400	-0.05139600	
H	5.41233600	-1.11362500	-0.58974900	
H	-5.35534500	0.55436400	-0.03899100	
H	6.24846700	0.87361100	0.07211800	
H	-3.31786300	3.41600700	0.02393900	
H	-4.13953300	-2.74223000	-0.09571200	
O	0.22521600	-2.27480500	1.40956600	
H	0.90887200	-1.78744900	1.89563600	
Name				**1-C3'-OH-RAF (gas)**
Cartesian Coordinates				Frequency and Energy
O	0.57487700	0.83774500	0.20184600	Zero-point correction= 0.223092 (Hartree/Particle)
O	5.26085300	1.53418300	-0.18576500	Thermal correction to Energy= 0.239541
O	-4.10538900	2.63713100	0.09216100	Thermal correction to Enthalpy= 0.240485
O	-4.76401400	-1.98986500	-0.20308000	Thermal correction to Gibbs Free Energy= 0.178000
C	1.94525800	-0.95539100	-0.10925700	Sum of electronic and zero-point Energies= -915.807599
C	-0.19750000	-0.27856900	-0.08134700	Sum of electronic and thermal Energies= -915.791150
C	1.86340000	0.45888500	0.09339800	Sum of electronic and thermal Enthalpies= -915.790206
C	-1.64343600	-0.07115100	-0.06201800	Sum of electronic and thermal Free Energies= -915.852691
C	0.56412600	-1.35863500	-0.33673700	
C	3.19196400	-1.46596200	-0.57870300	
C	2.95070900	1.29874000	0.11271400	
C	-2.50064100	-1.17093800	-0.13413500	
C	-2.15988000	1.22081600	0.01852300	
C	4.18000900	0.71938800	-0.20594500	
C	4.29172700	-0.64234000	-0.57424000	
C	-3.54176600	1.40245400	0.01717700	
C	-3.87547200	-0.96278900	-0.13732000	
C	-4.40664600	0.32023700	-0.06305000	
H	0.22026700	-2.35206500	-0.57035400	
H	3.27446500	-2.50620400	-0.86583400	
H	2.87232100	2.35850400	0.31174100	
H	-2.10102400	-2.17820500	-0.16762900	
H	-1.48980800	2.06989600	0.07923400	
H	5.26225400	-1.02719600	-0.86978200	
H	-5.47789100	0.47063600	-0.05973500	
H	6.04832100	1.04714700	-0.44439600	
H	-3.41760600	3.30428700	0.16388600	
H	-4.29381700	-2.82726000	-0.23132000	
O	2.05695800	-1.54439600	1.71262200	
H	2.94512000	-1.24637900	1.95755200	
Name				**1-C4'-OH-RAF (gas)**
Cartesian Coordinates				Frequency and Energy
O	0.45905900	0.94549100	0.04362600	Zero-point correction= 0.222765 (Hartree/Particle)
O	5.16858700	1.73447600	-0.00753400	Thermal correction to Energy= 0.239483

O	-4.29578200	2.53301600	0.26816200	Thermal correction to Enthalpy= 0.240427
O	-4.76201900	-2.10891600	-0.12289400	Thermal correction to Gibbs Free Energy= 0.176984
C	1.87464600	-0.76636900	-0.36719000	Sum of electronic and zero-point Energies= -915.814834
C	-0.27550100	-0.19362600	-0.16021300	Sum of electronic and thermal Energies= -915.798117
C	1.76569600	0.59816900	-0.07732900	Sum of electronic and thermal Enthalpies= -915.797173
C	-1.72521100	-0.05470400	-0.07650700	Sum of electronic and thermal Free Energies= -915.860615
C	0.53434800	-1.25935700	-0.41250400	
C	3.16400100	-1.33575400	-0.49146100	
C	2.84245400	1.45382500	0.05233100	
C	-2.53622800	-1.19053100	-0.13991600	
C	-2.29503200	1.21050400	0.06241100	
C	4.10993200	0.88620900	-0.12782000	
C	4.26894500	-0.46365700	-0.42481200	
C	-3.68153200	1.32852800	0.13385900	
C	-3.91746100	-1.04532100	-0.06882500	
C	-4.50052000	0.20973300	0.06744100	
H	0.22090500	-2.27224700	-0.60373900	
H	3.28942500	-2.32945200	-0.89595400	
H	2.73450200	2.50605000	0.27802200	
H	-2.09675100	-2.17726600	-0.23316700	
H	-1.66136800	2.08785200	0.11174200	
H	5.26572200	-0.86895900	-0.55914700	
H	-5.57596000	0.31129100	0.12459100	
H	5.99036200	1.24759800	-0.11240300	
H	-3.63747700	3.23165300	0.31186000	
H	-4.25914900	-2.92323300	-0.20737900	
O	3.27757600	-2.29886700	1.32758300	
H	3.17919600	-1.52078700	1.89724100	

Name				**1-C5'-OH-RAF (gas)**
Cartesian Coordinates				Frequency and Energy
O	0.35344600	0.83765900	-0.08273500	Zero-point correction= 0.223629 (Hartree/Particle)
O	5.08292700	1.48898400	-0.18113400	Thermal correction to Energy= 0.239925
O	-4.34929700	2.54757400	0.16011700	Thermal correction to Enthalpy= 0.240869
O	-4.94354400	-2.09533600	0.11248200	Thermal correction to Gibbs Free Energy= 0.178362
C	1.73711200	-0.93881600	-0.31231800	Sum of electronic and zero-point Energies= -915.819962
C	-0.40910100	-0.31058800	-0.13884100	Sum of electronic and thermal Energies= -915.803666
C	1.64602400	0.46367900	-0.18940400	Sum of electronic and thermal Enthalpies= -915.802722
C	-1.85395000	-0.12679200	-0.04192700	Sum of electronic and thermal Free Energies= -915.865229
C	0.37378100	-1.40712800	-0.28054900	
C	2.98863800	-1.51749000	-0.46283700	
C	2.73377800	1.32248500	-0.15615200	
C	-2.69521400	-1.24167800	-0.00856700	
C	-2.38787600	1.15974200	0.01543100	
C	3.97737100	0.72564600	-0.26967700	
C	4.12383400	-0.68950000	-0.42812900	
C	-3.76976600	1.32044300	0.10221400	
C	-4.07050400	-1.05428300	0.07627700	
C	-4.61828400	0.22271800	0.13261000	
H	0.03597900	-2.42738500	-0.35834700	
H	3.10650400	-2.58322700	-0.61189100	
H	2.63644800	2.38962500	-0.01287600	
H	-2.28444500	-2.24448700	-0.04296500	
H	-1.73159500	2.02122800	-0.00943100	
H	5.06528200	-1.06469500	-0.80466400	

H	-5.68951000	0.35713600	0.19998400	
H	5.75146700	0.94807800	0.26635700	
H	-3.67350900	3.22997300	0.12705100	
H	-4.46522800	-2.92710200	0.06349400	
O	5.13254400	-0.83976300	1.36356800	
H	4.38493700	-0.78271700	1.97610600	
Name				**1-C5'-OH-RAF (water)**
Cartesian Coordinates				Frequency and Energy
O	0.39640000	0.84876700	-0.13983200	Zero-point correction= 0.222123 (Hartree/Particle)
O	5.12168800	1.46176900	-0.37389800	Thermal correction to Energy= 0.238612
O	-4.31806900	2.56198600	0.27409500	Thermal correction to Enthalpy= 0.239556
O	-4.90902300	-2.09520500	-0.00921500	Thermal correction to Gibbs Free Energy= 0.177185
C	1.75867800	-0.95529300	-0.29762900	Sum of electronic and zero-point Energies= -915.857636
C	-0.38038800	-0.30220100	-0.15538400	Sum of electronic and thermal Energies= -915.841148
C	1.68927500	0.45174000	-0.22749500	Sum of electronic and thermal Enthalpies= -915.840203
C	-1.82443100	-0.10882400	-0.06273100	Sum of electronic and thermal Free Energies= -915.902575
C	0.39129600	-1.40995200	-0.25003300	
C	3.00382500	-1.55695700	-0.39849100	
C	2.78340200	1.29726500	-0.25018800	
C	-2.66489400	-1.22609200	-0.08974600	
C	-2.35559200	1.17672400	0.05650300	
C	4.02020100	0.67361600	-0.34384000	
C	4.14454400	-0.74294000	-0.37837600	
C	-3.73732100	1.32922000	0.15162400	
C	-4.03799500	-1.04007600	0.00759400	
C	-4.58908000	0.23226700	0.12801600	
H	0.04331800	-2.43045600	-0.27893300	
H	3.10922600	-2.63246200	-0.46710000	
H	2.69318800	2.37447000	-0.20169000	
H	-2.26462900	-2.22911500	-0.18473700	
H	-1.71434900	2.04939000	0.07956300	
H	5.12240500	-1.16701600	-0.57056000	
H	-5.66136800	0.36443000	0.20474400	
H	5.91922400	0.91574800	-0.39363000	
H	-3.63725800	3.24647100	0.29779800	
H	-4.41737300	-2.92378800	-0.07809100	
O	4.68538400	-0.77172400	1.77465200	
H	3.78745300	-0.52340100	2.04727400	
Name				**1-C5'-OH-RAF (pentyl ethanoate)**
Cartesian Coordinates				Frequency and Energy
O	0.36250600	0.83498000	-0.14475200	Zero-point correction= 0.223184 (Hartree/Particle)
O	5.08842200	1.46578600	-0.32120700	Thermal correction to Energy= 0.239525
O	-4.33489100	2.55285800	0.24756300	Thermal correction to Enthalpy= 0.240469
O	-4.94197500	-2.08541700	0.01142800	Thermal correction to Gibbs Free Energy= 0.178239
C	1.73755900	-0.95867100	-0.25307000	Sum of electronic and zero-point Energies= -915.846647
C	-0.40456700	-0.31262100	-0.12588500	Sum of electronic and thermal Energies= -915.830306
C	1.65284600	0.44952100	-0.22513300	Sum of electronic and thermal Enthalpies= -915.829362
C	-1.84988200	-0.12112700	-0.04027700	Sum of electronic and thermal Free Energies= -915.891592
C	0.37286600	-1.41998600	-0.18995300	
C	2.98682400	-1.55198300	-0.35879400	
C	2.74304300	1.30529600	-0.25672100	
C	-2.69395700	-1.23510500	-0.05878100	
C	-2.37901000	1.16576100	0.06090100	
C	3.98356000	0.69468300	-0.33067900	

C	4.12457100	-0.72755400	-0.37738700
C	-3.76139800	1.32693600	0.14562100
C	-4.06907100	-1.04563200	0.02602800
C	-4.61421500	0.23092400	0.12915300
H	0.03090100	-2.44264900	-0.18897500
H	3.10011200	-2.62663300	-0.42995700
H	2.64580200	2.38134300	-0.19878400
H	-2.28841300	-2.23742100	-0.14124900
H	-1.72601000	2.03026400	0.07386200
H	5.07146900	-1.13701700	-0.70363600
H	-5.68652800	0.36669100	0.19415400
H	5.79752800	0.94703400	0.08632400
H	-3.65263800	3.23417000	0.24947500
H	-4.46032800	-2.91702600	-0.06438400
O	5.06445700	-0.74715800	1.48446500
H	4.28494500	-0.56978200	2.03306100

Name			**1-C6'-OH-RAF (gas)**
Cartesian Coordinates			Frequency and Energy
O	0.43975500	0.70425400	-0.15265900
O	5.24175800	0.99041100	-0.60394500
O	-4.18411100	2.64948100	-0.12209500
O	-4.98367200	-1.94612100	0.26094200
C	1.72963700	-1.15709800	-0.19228400
C	-0.37282500	-0.39232100	-0.10067500
C	1.72030700	0.24629300	-0.20899700
C	-1.80836600	-0.13766000	-0.04101600
C	0.35565700	-1.54542700	-0.11952300
C	2.96567300	-1.83267100	-0.26359200
C	2.85317000	1.02317500	-0.29773200
C	-2.69839600	-1.20708100	0.08585600
C	-2.28457800	1.17101900	-0.11187500
C	4.08863700	0.33512600	-0.29230300
C	4.11691200	-1.09066400	-0.32937300
C	-3.65822700	1.39917300	-0.05700900
C	-4.06466000	-0.95277800	0.13755800
C	-4.55476400	0.34658800	0.06681400
H	-0.03797800	-2.54833700	-0.09478200
H	3.00351800	-2.91477000	-0.27199200
H	2.82621000	2.10379700	-0.34009600
H	-2.33282700	-2.22578900	0.14860800
H	-1.58954400	1.99619500	-0.20989700
H	5.09247200	-1.55582900	-0.38257800
H	-5.61943000	0.53348800	0.10899600
H	5.45108100	1.56118800	0.14675200
H	-3.47931600	3.29715300	-0.20743300
H	-4.54313900	-2.79893000	0.30225600
O	4.40022500	0.70788700	1.73531300
H	3.58824700	0.47048900	2.20463600

Thermal correction to Energy= 0.238997
Thermal correction to Enthalpy= 0.239941
Thermal correction to Gibbs Free Energy= 0.176205
Sum of electronic and zero-point Energies= -915.817086
Sum of electronic and thermal Energies= -915.800299
Sum of electronic and thermal Enthalpies= -915.799355
Sum of electronic and thermal Free Energies= -915.863091

Name			**1-C7'-OH-RAF (gas)**
Cartesian Coordinates			Frequency and Energy
O	0.53508200	0.56869300	-0.32075500
O	5.28619400	0.87286700	-0.60503600
O	-4.02741400	2.66195100	-0.09294500
O	-4.96188000	-1.92537300	0.04323000

Thermal correction to Energy= 0.239799
Thermal correction to Enthalpy= 0.240743
Thermal correction to Gibbs Free Energy= 0.177867

C	1.79795500	-1.24810900	0.09148300
C	-0.30065100	-0.48109200	-0.03004500
C	1.79495700	0.10050100	-0.24747700
C	-1.73192000	-0.19165400	-0.03988400
C	0.41152000	-1.60764500	0.22941600
C	3.03044500	-1.91073100	0.20812700
C	2.95048800	0.87594300	-0.42328400
C	-2.65359800	-1.24022100	-0.00302000
C	-2.17087700	1.13070600	-0.07538300
C	4.16015100	0.15369500	-0.36577700
C	4.19864900	-1.20301500	-0.02210100
C	-3.53916200	1.39412500	-0.06489400
C	-4.01397400	-0.95036000	0.00919100
C	-4.46792200	0.36320100	-0.02227100
H	0.00737000	-2.56777200	0.50568000
H	3.07450500	-2.96008900	0.47216800
H	2.91853600	1.85739500	-0.87349100
H	-2.31533600	-2.27053000	0.00108300
H	-1.45040900	1.93969300	-0.09895300
H	5.15907700	-1.70133600	0.05561800
H	-5.52814800	0.57759000	-0.01469700
H	6.06270600	0.31504900	-0.50308100
H	-3.29980300	3.28965800	-0.10492800
H	-4.54112300	-2.78867000	0.06671300
O	3.06059900	1.71769900	1.43340900
H	3.97561100	2.03024900	1.36617900

Sum of electronic and zero-point Energies= -915.814110
Sum of electronic and thermal Energies= -915.797549
Sum of electronic and thermal Enthalpies= -915.796605
Sum of electronic and thermal Free Energies= -915.859482

Name			**1-C8'-OH-RAF (gas)**
Cartesian Coordinates			Frequency and Energy
O	0.59768000	0.70415800	-0.26365100
O	5.34049000	1.08893400	-0.72600600
O	-4.05172400	2.58703300	0.00473400
O	-4.78008300	-2.03310200	-0.22640500
C	1.91503500	-1.10179100	0.14023600
C	-0.19172700	-0.38413200	-0.03091600
C	1.88121000	0.31075400	-0.05235200
C	-1.63181300	-0.16034900	-0.06816000
C	0.55074400	-1.50399400	0.20738800
C	3.15860600	-1.74223300	0.17663600
C	3.01438600	1.04530800	-0.45809500
C	-2.50418900	-1.24927200	-0.13915300
C	-2.12744800	1.14178100	-0.02433500
C	4.21558600	0.37992100	-0.42468500
C	4.29117300	-0.99782700	-0.08961000
C	-3.50555100	1.34420900	-0.04281400
C	-3.87554700	-1.02001400	-0.15578500
C	-4.38616200	0.27249300	-0.10868800
H	0.16585200	-2.48643100	0.42586600
H	3.23394600	-2.80440900	0.37251500
H	2.95435300	2.09630100	-0.70339700
H	-2.11889800	-2.26115500	-0.19741600
H	-1.44132300	1.97769500	0.04151000
H	5.26560400	-1.47589200	-0.07135300
H	-5.45489000	0.43964100	-0.12295000
H	6.10124300	0.50342600	-0.75218700

Zero-point correction= 0.222692 (Hartree/Particle)
Thermal correction to Energy= 0.239265
Thermal correction to Enthalpy= 0.240209
Thermal correction to Gibbs Free Energy= 0.177791
Sum of electronic and zero-point Energies= -915.810846
Sum of electronic and thermal Energies= -915.794273
Sum of electronic and thermal Enthalpies= -915.793329
Sum of electronic and thermal Free Energies= -915.855746

H	-3.35503800	3.24604200	0.06819600	
H	-4.32383900	-2.87837900	-0.24298400	
O	1.82637000	0.79643600	1.88574600	
H	2.68531700	0.48638500	2.20885700	
Name				**1-O6'-OH-FHT (gas)**
Cartesian Coordinates				Frequency and Energy
O	-0.48787000	0.51869300	-0.22081400	Zero-point correction= 0.220414 (Hartree/Particle)
O	-5.28479600	0.55313900	-0.33307000	Thermal correction to Energy= 0.236800
O	4.00625900	2.74156200	-0.21934200	Thermal correction to Enthalpy= 0.237744
O	5.08458000	-1.78842000	0.25166700	Thermal correction to Gibbs Free Energy= 0.174426
C	-1.67863300	-1.37977700	0.02575000	Sum of electronic and zero-point Energies= -915.819953
C	0.38270700	-0.51343500	-0.02933800	Sum of electronic and thermal Energies= -915.803567
C	-1.74022700	-0.00193000	-0.18226700	Sum of electronic and thermal Enthalpies= -915.802623
C	1.80206100	-0.17683300	-0.01747200	Sum of electronic and thermal Free Energies= -915.865940
C	-0.28863900	-1.69334100	0.12284400	
C	-2.88644300	-2.12129200	0.04267800	
C	-2.91507000	0.70902800	-0.37805600	
C	2.75619700	-1.18922100	0.11252100	
C	2.19831800	1.15520900	-0.13240400	
C	-4.11644300	-0.04883100	-0.28989500	
C	-4.07631300	-1.46209900	-0.11812500	
C	3.55671800	1.46494700	-0.11321800	
C	4.10586900	-0.85358900	0.12886000	
C	4.51646600	0.47009300	0.01706100	
H	0.15392400	-2.66285900	0.28320500	
H	-2.86779600	-3.19435600	0.19071600	
H	-2.92094100	1.74042900	-0.69751300	
H	2.45346700	-2.22694300	0.19592500	
H	1.45382600	1.93581700	-0.23259900	
H	-5.02457300	-1.98238300	-0.08146300	
H	5.56883100	0.72021500	0.03051900	
H	-5.09022500	1.46065200	0.11745900	
H	3.26293100	3.34523900	-0.30153600	
H	4.69622300	-2.66469400	0.31757400	
O	-4.22732400	2.38143700	0.92137500	
H	-4.11186100	2.12401300	1.84554500	
Name				**1-O6'-OH-FHT (water)**
Cartesian Coordinates				Frequency and Energy
O	-0.48787000	0.51869300	-0.22081400	Zero-point correction= 0.219152 (Hartree/Particle)
O	-5.28479600	0.55313900	-0.33307000	Thermal correction to Energy= 0.233658
O	4.00625900	2.74156200	-0.21934200	Thermal correction to Enthalpy= 0.234602
O	5.08458000	-1.78842000	0.25166700	Thermal correction to Gibbs Free Energy= 0.177115
C	-1.67863300	-1.37977700	0.02575000	Sum of electronic and zero-point Energies= -915.860742
C	0.38270700	-0.51343500	-0.02933800	Sum of electronic and thermal Energies= -915.846236
C	-1.74022700	-0.00193000	-0.18226700	Sum of electronic and thermal Enthalpies= -915.845292
C	1.80206100	-0.17683300	-0.01747200	Sum of electronic and thermal Free Energies= -915.902778
C	-0.28863900	-1.69334100	0.12284400	
C	-2.88644300	-2.12129200	0.04267800	
C	-2.91507000	0.70902800	-0.37805600	
C	2.75619700	-1.18922100	0.11252100	
C	2.19831800	1.15520900	-0.13240400	
C	-4.11644300	-0.04883100	-0.28989500	
C	-4.07631300	-1.46209900	-0.11812500	
C	3.55671800	1.46494700	-0.11321800	

C	4.10586900	-0.85358900	0.12886000
C	4.51646600	0.47009300	0.01706100
H	0.15392400	-2.66285900	0.28320500
H	-2.86779600	-3.19435600	0.19071600
H	-2.92094100	1.74042900	-0.69751300
H	2.45346700	-2.22694300	0.19592500
H	1.45382600	1.93581700	-0.23259900
H	-5.02457300	-1.98238300	-0.08146300
H	5.56883100	0.72021500	0.03051900
H	-5.09022500	1.46065200	0.11745900
H	3.26293100	3.34523900	-0.30153600
H	4.69622300	-2.66469400	0.31757400
O	-4.24076884	2.35819177	0.90542582
H	-4.12530584	2.10076777	1.82959582

Name			**1-O6'-OH-FHT (pentyl ethanoate)**
Cartesian Coordinates			Frequency and Energy
O	-0.49461300	0.54173200	-0.22215700
O	-5.28900100	0.60647600	-0.33911400
O	4.02912300	2.71778900	-0.26188500
O	5.05057300	-1.81744000	0.29832900
C	-1.69336200	-1.35304300	-0.00052500
C	0.37061100	-0.49737500	-0.03826400
C	-1.74756900	0.02616800	-0.19302600
C	1.79334600	-0.17087000	-0.02049500
C	-0.30532200	-1.67626100	0.09817000
C	-2.90309600	-2.09222400	-0.00111800
C	-2.92174200	0.74380300	-0.38390300
C	2.73305800	-1.19384800	0.13524700
C	2.20469800	1.15557500	-0.15685800
C	-4.12391600	-0.01698300	-0.31130400
C	-4.09309100	-1.42766700	-0.15955900
C	3.56697000	1.44870200	-0.13511800
C	4.08666200	-0.87286300	0.15235600
C	4.51459100	0.44444000	0.01846300
H	0.13301700	-2.65067900	0.24553000
H	-2.88707900	-3.16706900	0.13550400
H	-2.92144200	1.76599400	-0.73208400
H	2.41833400	-2.22650700	0.23983400
H	1.47732900	1.94966700	-0.27684300
H	-5.03975200	-1.95241800	-0.13031700
H	5.57087400	0.68216500	0.03369900
H	-5.07520300	1.47044900	0.16460900
H	3.28894500	3.32831800	-0.35803300
H	4.64644400	-2.68867400	0.38239600
O	-4.10999800	2.26705200	1.06673400
H	-3.99115700	1.85855700	1.93605400

Zero-point correction= 0.220737 (Hartree/Particle)
Thermal correction to Energy= 0.236933
Thermal correction to Enthalpy= 0.237878
Thermal correction to Gibbs Free Energy= 0.175601
Sum of electronic and zero-point Energies= -915.846163
Sum of electronic and thermal Energies= -915.829967
Sum of electronic and thermal Enthalpies= -915.829022
Sum of electronic and thermal Free Energies= -915.891299

Name			**1-O6'-OOH-FHT (gas)**
Cartesian Coordinates			Frequency and Energy
O	0.00387300	0.74540100	-0.25215800
O	-4.72438400	1.11749400	-0.79597900
O	4.63410000	2.64424800	0.10012200
O	5.36943000	-1.96593900	0.42553400
C	-1.28990300	-1.10533400	-0.44866000
C	0.80629300	-0.35996200	-0.20017100

Zero-point correction= 0.223270 (Hartree/Particle)
Thermal correction to Energy= 0.240866
Thermal correction to Enthalpy= 0.241810
Thermal correction to Gibbs Free Energy= 0.174705
Sum of electronic and zero-point Energies= -990.965254
Sum of electronic and thermal Energies= -990.947658

C	-1.27368300	0.30253900	-0.40017800	Sum of electronic and thermal Enthalpies= -990.946714
C	2.23524400	-0.12064800	-0.03948000	Sum of electronic and thermal Free Energies= -991.013820
C	0.07433600	-1.50575400	-0.31778100	
C	-2.52174100	-1.76845100	-0.60008100	
C	-2.39713000	1.08912900	-0.48080100	
C	3.10617500	-1.20185100	0.11996100	
C	2.72527500	1.18518900	-0.04723200	
C	-3.62496500	0.41488500	-0.65143900	
C	-3.66459900	-1.01350600	-0.69940700	
C	4.09421600	1.39856100	0.10135300	
C	4.46813700	-0.96211900	0.26546300	
C	4.97185100	0.33419500	0.25756600	
H	0.46160300	-2.51142800	-0.31731800	
H	-2.56674800	-2.84978400	-0.63402500	
H	-2.37099400	2.16980300	-0.44207500	
H	2.72822200	-2.21778700	0.13714300	
H	2.04463200	2.01880600	-0.17120600	
H	-4.63677500	-1.47791200	-0.81000900	
H	6.03309300	0.50971400	0.37272900	
H	-5.46978700	0.83235000	-0.02688400	
H	3.94237800	3.30139500	-0.01494000	
H	4.92184100	-2.81605600	0.41544900	
H	-4.71774600	0.31036500	2.38316500	
O	-6.02204900	0.53599800	1.07989000	
O	-5.08931500	-0.25104100	1.68675300	

Name				**1-O6'-OOH-FHT (water)**
Cartesian Coordinates				Frequency and Energy
O	0.00387300	0.74540100	-0.25215800	Zero-point correction= 0.222136 (Hartree/Particle)
O	-4.72438400	1.11749400	-0.79597900	Thermal correction to Energy= 0.237598
O	4.63410000	2.64424800	0.10012200	Thermal correction to Enthalpy= 0.238542
O	5.36943000	-1.96593900	0.42553400	Thermal correction to Gibbs Free Energy= 0.176818
C	-1.28990300	-1.10533400	-0.44866000	Sum of electronic and zero-point Energies= -991.005752
C	0.80629300	-0.35996200	-0.20017100	Sum of electronic and thermal Energies= -990.990290
C	-1.27368300	0.30253900	-0.40017800	Sum of electronic and thermal Enthalpies= -990.989346
C	2.23524400	-0.12064800	-0.03948000	Sum of electronic and thermal Free Energies= -991.051071
C	0.07433600	-1.50575400	-0.31778100	
C	-2.52174100	-1.76845100	-0.60008100	
C	-2.39713000	1.08912900	-0.48080100	
C	3.10617500	-1.20185100	0.11996100	
C	2.72527500	1.18518900	-0.04723200	
C	-3.62496500	0.41488500	-0.65143900	
C	-3.66459900	-1.01350600	-0.69940700	
C	4.09421600	1.39856100	0.10135300	
C	4.46813700	-0.96211900	0.26546300	
C	4.97185100	0.33419500	0.25756600	
H	0.46160300	-2.51142800	-0.31731800	
H	-2.56674800	-2.84978400	-0.63402500	
H	-2.37099400	2.16980300	-0.44207500	
H	2.72822200	-2.21778700	0.13714300	
H	2.04463200	2.01880600	-0.17120600	
H	-4.63677500	-1.47791200	-0.81000900	
H	6.03309300	0.50971400	0.37272900	
H	-5.46978700	0.83235000	-0.02688400	
H	3.94237800	3.30139500	-0.01494000	

H	4.92184100	-2.81605600	0.41544900	
H	-4.72137139	0.30874043	2.38840577	
O	-6.02567439	0.53437343	1.08513077	
O	-5.09294039	-0.25266557	1.69199377	
Name				**1-O6'-OOH-FHT (pentyl ethanoate)**
Cartesian Coordinates				Frequency and Energy
O	-0.04363200	0.69263900	-0.30948100	Zero-point correction= 0.223130 (Hartree/Particle)
O	-4.78026000	0.93356600	-0.90617200	Thermal correction to Energy= 0.240638
O	4.56259900	2.68168500	-0.05079200	Thermal correction to Enthalpy= 0.241582
O	5.35635000	-1.89460200	0.53537600	Thermal correction to Gibbs Free Energy= 0.175129
C	-1.29650900	-1.19207900	-0.40902600	Sum of electronic and zero-point Energies= -990.996663
C	0.77987600	-0.39155300	-0.19108000	Sum of electronic and thermal Energies= -990.979154
C	-1.30942600	0.21585500	-0.44058000	Sum of electronic and thermal Enthalpies= -990.978210
C	2.20418500	-0.11842000	-0.03914200	Sum of electronic and thermal Free Energies= -991.044663
C	0.07319300	-1.55835800	-0.24692800	
C	-2.51406700	-1.88927300	-0.53359600	
C	-2.44767400	0.97427700	-0.57890900	
C	3.08687400	-1.18008700	0.18080700	
C	2.67473400	1.19328600	-0.11747300	
C	-3.65782000	0.26379200	-0.71348400	
C	-3.67078800	-1.16329500	-0.68201200	
C	4.04081900	1.43164100	0.02090800	
C	4.44502700	-0.91307000	0.31758500	
C	4.93211900	0.38836800	0.23874400	
H	0.48290800	-2.55424400	-0.18619900	
H	-2.53510900	-2.97202900	-0.51047800	
H	-2.43850700	2.05669900	-0.60467200	
H	2.72177200	-2.19907900	0.25005100	
H	1.98959700	2.01538600	-0.28771600	
H	-4.63084500	-1.65662300	-0.78037200	
H	5.99167000	0.58459000	0.34646800	
H	-5.41873800	0.84114100	-0.02699600	
H	3.85892900	3.32266400	-0.20500100	
H	4.91528800	-2.75109800	0.57285100	
H	-4.32853700	0.79667900	2.27916500	
O	-5.84834200	0.75410500	1.20204200	
O	-4.82817600	0.10128300	1.81877800	

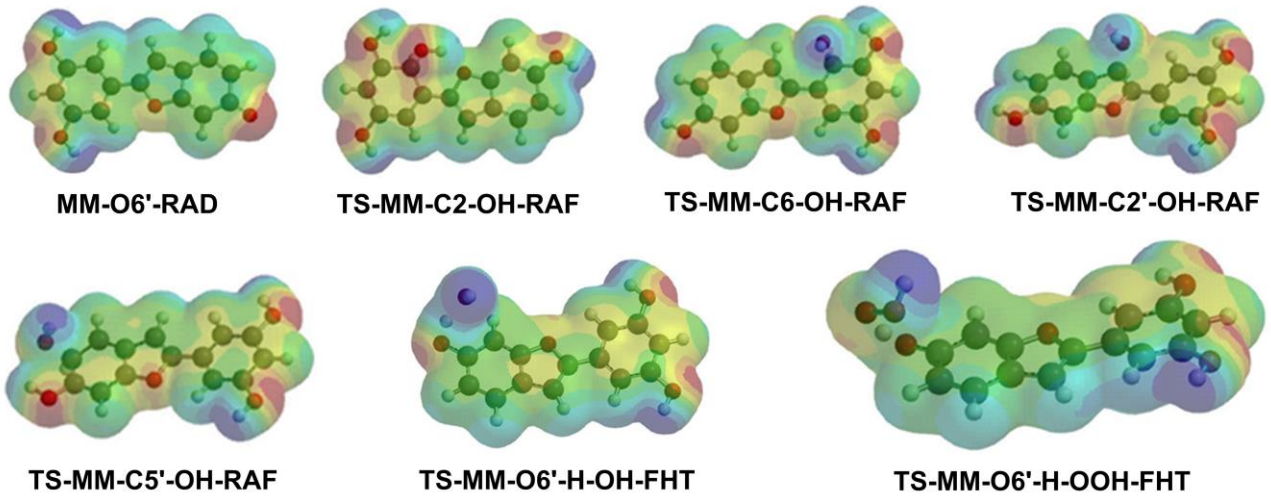

Figure S1: The density surface of the typical TSs and radicals according to FHT and RAF

References

1. M. G. Evans and M. Polanyi, *Trans. Faraday Soc.*, 1935, **31**, 875-894.
2. H. Eyring, *J. Chem. Phys.*, 1935, **3**, 107-115.
3. D. G. Truhlar, W. L. Hase and J. T. Hynes, *J. Phys. Chem.*, 1983, **87**, 2664-2682.
4. T. Furuncuoglu, I. Ugur, I. Degirmenci and V. Aviyente, *Macromolecules*, 2010, **43**, 1823-1835.
5. E. Vélez, J. Quijano, R. Notario, E. Pabón, J. Murillo, J. Leal, E. Zapata and G. Alarcón, *J. Phys. Org. Chem.*, 2009, **22**, 971-977.
6. E. Pollak and P. Pechukas, *J. Am. Chem. Soc.*, 1978, **100**, 2984-2991.
7. A. Fernández-Ramos, B. A. Ellingson, R. Meana-Pañeda, J. M. Marques and D. G. Truhlar, *Theor. Chem. Acc.*, 2007, **118**, 813-826.
8. C. Eckart, *Phy. Rev.*, 1930, **35**, 1303.
9. R. A. Marcus, *Annu. Rev. Phys. Chem.*, 1964, **15**, 155-196.
10. R. A. Marcus, *Rev. Mod. Phys.*, 1993, **65**, 599.
11. Y. Lu, A. Wang, P. Shi and H. Zhang, *PloS one*, 2017, **12**, e0169773.
12. Y. Lu, A. Wang, P. Shi, H. Zhang and Z. Li, *PloS one*, 2015, **10**, e0133259.
13. S. F. Nelsen, S. C. Blackstock and Y. Kim, *J. Am. Chem. Soc.*, 1987, **109**, 677-682.
14. S. F. Nelsen, M. N. Weaver, Y. Luo, J. R. Pladziewicz, L. K. Ausman, T. L. Jentzsch and J. J. O'Konek, *J. Phys. Chem. A*, 2006, **110**, 11665-11676.
15. A. Galano and J. R. Alvarez-Idaboy, *J. Comput. Chem.*, 2013, **34**, 2430-2445.
16. F. C. Collins and G. E. Kimball, *J. Colloid Sci.* , 1949, **4**, 425-437.
17. M. Von Smoluchowski, *Z. Phys. Chem*, 1917, **92**, 129-168.
18. D. G. Truhlar, *J. Chem. Educ.*, 1985, **62**, 104.
19. A. Einstein, *Ann. Phys.*, 1905, **17**, 549-560.
20. G. G. Stokes, *Mathematical and Physical Papers*, University Press, Cambridge, 1905.
21. A. Galano and J. Raúl Alvarez-Idaboy, *Int. J. Quantum Chem.*, 2019, **119**, e25665.
22. Q. V. Vo, T. V. Gon, M. V. Bay and A. Mechler, *J. Phys. Chem. B*, 2019, **123**, 10672-10679.
23. Q. V. Vo and A. Mechler, *J. Chem. Inf. Model.*, 2020, **60**, 316-321.
24. Y. Okuno, *Chem.: Eur. J.*, 1997, **3**, 212-218.
25. S. Benson, *The foundations of chemical kinetics:* , Malabar, Florida, 1982.
26. C. Iuga, J. R. Alvarez-Idaboy and A. Vivier-Bunge, *J. Phys. Chem. B*, 2011, **115**, 12234-12246.
27. J. R. Alvarez-Idaboy, L. Reyes and N. Mora-Diez, *Org. Biomol. Chem.*, 2007, **5**, 3682-3689.
28. T. H. Le, T. T. Tran and L. K. Huynh, *Chemom. Intell. Lab. Syst.*, 2018, **172**, 10-16.