Electronic Supplementary Information

Piceatannol, a better peroxyl radical scavenger than Resveratrol.

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Table 1S Data used for pKas Caulculations using isodesmic (reference pKa) method

Sudied molecule	**RESVERATROL**		Studied molecule	**PICEATANNOL**
Reference molecule	Phenol		Reference	Catechol
Reference`s pKa	10.09		Reference`s pKa	9.25
Model	HA+Ref- --> A- + Href		Model	HA+Ref- --> A- + Href
	G			G
Resveratrol	-766.34818	HA	Piceatannol	-841.591445
Base 4b	-765.889865	A-	Base 4b	-841.139903
Fenol	-307.451232	Href	Catechol	-382.694961
Base fenol	-306.990902	Ref-	Base Catechol	-382.240404
ΔG (Hartrees)	-0.002015		ΔG (Hartrees)	-0.003015
ΔG (Cal/mol K)	-1264.430635		ΔG (Cal/mol K)	-1891.939635
RTln(10)	1363.282967		RTln(10)	1363.282967
pKa	**9.16**		**pKa**	**7.86**

Table 2S: Gibbs free energies of reaction (ΔG^0, kcal/mol) for *trans*-piceatannol via RAF mechanism in water.

Position	ΔG^0	Position	ΔG^0	Position	ΔG^0
Neutral *trans*-piceatannol					
α	-2.16	1A	20.98	1B	17.62
β	-4.04	2A or 6A	8.15	2B	12.27
		3A or 5A	14.34	3B	11.09
		4A	7.72	4B	5.44
				5B	15.94
				6B	8.33
Anionic *trans*-piceatannol					
α	-3.52	1A	21.22	1B	14.06
β	-2.11	2A or 6A	7.30	2B	13.49
		3A or 5A	14.36	3B	5.68
		4A	7.51	4B	5.98
				5B	9.52
				6B	5.01

Table 3S. Gibbs free energies of activation ($\Delta G^{0\neq}$, kcal/mol); reaction path degeneracy (σ); and rate constants (k, $M^{-1}s^{-1}$) at room temperature for *trans*-piceatannol via RAF mechanism in water.

Position	$\Delta G^{0\neq}$	sigma	k
α (neutral)	12.99	2	3.69E+03
β (neutral)	13.56	2	1.41E+03
α (anion)	8.80	2	4.40E+06
β (anion)	11.98	2	2.04E+04

Table 4S. Transmission coefficients (κ) and reaction paths degeneracies (σ) used in the calculations of the HT rate constants for the reactions of stilbenes with OOH radical in water.

	κ	σ
Resveratrol (neutral)		
position 3a or 5a	1493.6	2
position 4b	1328.4	1
Piceatannol (neutral)		
position 3a or 5a	1350.0	2
position 3b	168.6	1
position 4b	52.2	1
Resveratrol (anion)		
position 3a or 5a	603.0	2
Piceatannol (anion)		
position 3a or 5a	3855.4	2

Table 5S. Transmission coefficients (κ) and reaction paths degeneracies (σ) used in the calculations of the HT rate constants for the reactions of stilbenes with OOH radical in pentylethanoate.

	kappa	sigma
Resveratrol (neutral)		
position 3a o 5a	111.4	2
position 4b	58.8	1
Piceatannol (neutral)		
position 3a o 5a	76.1	2
position 3b	20.0	1
position 4b	10.8	1

Table 6S. Reorganization energies (λ, kcal/mol) for the studied SET reactions.

Reaction with OOH	
Resveratrol (neutral)	16.44
Piceatannol (neutral)	16.00
Resveratrol (anion)	14.69
Piceatannol (anion)	14.55
Antioxidant regeneration with $O_2^{\bullet-}$	
Resveratrol	17.01
Piceatannol	18.76

Table 7S. Vertical energies (kcal/mol) for the studied SET reactions

SET reaction of antioxidants		
Hidroperoxyl radical	+e	-94.67
Resveratrol (neutral)	-e	133.16
Piceatannol (neutral)	-e	132.90
Resveratrol (anion)	-e	110.30
Piceatannol (anion)	-e	109.60
SET regeneration of antioxidants		
Superoxide	-e	103.88
Resveratrol (radical)	+e	-103.18
Piceatannol (radical)	+e	-100.86

Cartesian coordinates of the HT transition structures in the *trans*-resveratrol oxidation by •OOH radicals in water.

HT-3A/HT-5A

C	5.01665400	0.86689100	0.61176500
C	3.65935200	1.14528800	0.55567800
C	2.74615000	0.23694900	0.00788500
C	4.59692500	-1.26409100	-0.44143800
C	5.48343200	-0.34172400	0.11063400
C	1.32613100	0.60093900	-0.01239700
C	-1.10151800	0.20481700	-0.43748800
C	0.31664200	-0.17369300	-0.43058800
C	-2.04524200	-0.76446700	-0.75394200
H	-1.74694900	-1.77601600	-0.99458100
C	-3.41907900	-0.44658700	-0.76042600
C	-3.85411600	0.85245000	-0.44074400
C	-2.90708800	1.81001000	-0.13386500
H	1.11709200	1.59622100	0.36465600
H	5.71552200	1.57436800	1.03669900
H	3.29512500	2.08734800	0.94569200
H	4.97487200	-2.20116300	-0.83068900
H	0.51299900	-1.17834000	-0.78657300
H	-4.90902200	1.08854600	-0.44702400
O	-3.35008500	3.06820700	0.16533800
H	-2.60374800	3.64453600	0.36677400
O	-4.31070400	-1.37904500	-1.08513700
H	-4.65142800	-1.87314000	-0.13976100
O	6.83115000	-0.58683400	0.17727600
H	7.02575100	-1.44227700	-0.22251400
C	-1.54481300	1.50211100	-0.13286400
H	-0.84212600	2.28951800	0.10443200
C	3.24394600	-0.97307300	-0.49219500
H	2.57517200	-1.70115600	-0.93037600
O	-4.79358400	-2.21031400	1.07396000
O	-3.79821200	-1.51360700	1.67854700
H	-4.19603900	-0.67063300	1.95330800

Zero-point correction= 0.241150 (Hartree/Particle)
Thermal correction to Energy= 0.258779
Thermal correction to Enthalpy= 0.259723
Thermal correction to Gibbs Free Energy= 0.192910
Sum of electronic and zero-point Energies= -917.208680
Sum of electronic and thermal Energies= -917.191051
Sum of electronic and thermal Enthalpies= -917.190107
Sum of electronic and thermal Free Energies= -917.256920

HT-4B

C	3.24845200	-1.35441700	-0.46634500
C	1.89421600	-1.15375100	-0.34469300
C	1.34254200	0.13996800	-0.45952500
C	3.56865100	1.02997700	-0.83354400
C	4.10697700	-0.26510300	-0.71779500
C	-0.08005400	0.41931100	-0.33519100
C	-2.47824400	-0.22137700	-0.03672600
C	-1.04579100	-0.50019000	-0.16513200
C	-3.33822000	-1.31534400	0.07284000
H	-2.95027900	-2.32481700	0.06140300
C	-4.70740000	-1.10743800	0.19633800
C	-5.23956100	0.17282600	0.21566000
C	-4.36985500	1.25558400	0.10866400
H	-0.34199300	1.46883400	-0.39720100
H	3.67893700	-2.34231700	-0.37463200
H	1.25506400	-2.00321600	-0.15066400
H	4.23787200	1.85807500	-1.02547200
H	-0.78846100	-1.55141900	-0.12003000
H	-6.30514900	0.33397100	0.31348100
O	-4.93624200	2.50458300	0.13695800
H	-4.24922000	3.17660800	0.05831000
O	-5.50599500	-2.21716400	0.29893100
H	-6.42872800	-1.95107700	0.38231500
O	5.41972900	-0.47144100	-0.88136600
H	5.92702000	-0.22272900	0.03353400
C	-3.00145100	1.07854100	-0.01755600
H	-2.36364700	1.94877000	-0.09290700
C	2.21005700	1.22043000	-0.70208300
H	1.79516700	2.21616700	-0.78861500
O	6.20088300	0.10418500	1.30751700
O	4.95926000	0.29908400	1.80383400
H	4.77043000	1.24507900	1.68400200

Zero-point correction= 0.240830 (Hartree/Particle)
Thermal correction to Energy= 0.258641
Thermal correction to Enthalpy= 0.259585
Thermal correction to Gibbs Free Energy= 0.192387
Sum of electronic and zero-point Energies= -917.213681
Sum of electronic and thermal Energies= -917.195869
Sum of electronic and thermal Enthalpies= -917.194925
Sum of electronic and thermal Free Energies= -917.262123

Cartesian coordinates of the HT transition structures in the *trans*-resveratrol oxidation by •OOH radicals in pentylethanoate.

HT-3A/HT-5A

C	5.05265400	0.87057700	0.57164500
C	3.69774100	1.15578100	0.52265600
C	2.77006300	0.23771900	0.01732300
C	4.60715700	-1.28635900	-0.40917700
C	5.50952300	-0.35604400	0.10438800
C	1.35180700	0.60815200	-0.00009900
C	-1.08557400	0.19998400	-0.39059100
C	0.33187100	-0.17916500	-0.36404000
C	-2.02265400	-0.77142600	-0.71703200
H	-1.72065200	-1.78531300	-0.94169600
C	-3.39792400	-0.45754500	-0.76674500
C	-3.83609900	0.84797300	-0.46816600
C	-2.89752300	1.80886200	-0.14017000
H	1.15295500	1.62359700	0.32536800
H	5.76184100	1.58557300	0.96532100
H	3.34696000	2.11311800	0.88767700
H	4.96688200	-2.23985700	-0.77744600
H	0.52332800	-1.20136700	-0.66822500
H	-4.88877200	1.09024300	-0.51739600
O	-3.34775300	3.05970700	0.13882900
H	-2.60661800	3.64375000	0.32917100
O	-4.27029100	-1.38206700	-1.11295700
H	-4.68803400	-1.85265900	-0.16879700
O	6.84547200	-0.60131400	0.16597600
H	7.03383200	-1.47615300	-0.18816400
C	-1.53662900	1.49883200	-0.10369300
H	-0.83367300	2.28349600	0.14517900
C	3.25575000	-0.98821000	-0.45239300
H	2.57845500	-1.72403300	-0.86346600
O	-4.93294800	-2.13990900	1.01391800
O	-3.93437100	-1.50497500	1.68294500
H	-4.30834900	-0.64671300	1.93934300

Zero-point correction= 0.241216 (Hartree/Particle)
Thermal correction to Energy= 0.259025
Thermal correction to Enthalpy= 0.259969
Thermal correction to Gibbs Free Energy= 0.192621
Sum of electronic and zero-point Energies= -917.201255
Sum of electronic and thermal Energies= -917.183446
Sum of electronic and thermal Enthalpies= -917.182502
Sum of electronic and thermal Free Energies= -917.249850

HT-4B

C	3.26525800	-0.97600600	-1.03014400
C	1.90646100	-0.83953800	-0.87929800
C	1.34729300	0.36628600	-0.40881200
C	3.57726800	1.31499800	-0.27450100
C	4.12992600	0.10014800	-0.73227700
C	-0.08183700	0.56417300	-0.21622400
C	-2.46388400	-0.19563100	-0.11481500
C	-1.02430400	-0.38929500	-0.30691200
C	-3.26293700	-1.33595900	-0.04042500
H	-2.82838600	-2.32293500	-0.12044500
C	-4.63539500	-1.20972200	0.15139600
C	-5.22706900	0.03987800	0.25834700
C	-4.42158400	1.17345000	0.17191000
H	-0.36880300	1.57673000	0.04292000
H	3.70082000	-1.89934800	-1.38690900
H	1.26524300	-1.67208100	-1.13130100
H	4.24454500	2.14074000	-0.06275200
H	-0.73372500	-1.41126100	-0.51946800
H	-6.29431900	0.15067700	0.40155100
O	-5.05118300	2.37515100	0.27224300
H	-4.40857100	3.08691100	0.19141100
O	-5.36227600	-2.35597700	0.22682800
H	-6.29240900	-2.14651200	0.35813600
O	5.43337700	-0.01805200	-0.92166700
H	5.91726000	-0.19628400	0.04133300
C	-3.05158100	1.07258600	-0.01255300
H	-2.45791800	1.97401600	-0.08955900
C	2.21377600	1.43652200	-0.11831400
H	1.79323700	2.37020200	0.23271500
O	6.13439600	-0.42396500	1.31140000
O	4.87953700	-0.65094900	1.76933100
H	4.56387000	0.20812500	2.09302700

Zero-point correction= 0.241394 (Hartree/Particle)
Thermal correction to Energy= 0.259187
Thermal correction to Enthalpy= 0.260131
Thermal correction to Gibbs Free Energy= 0.192417
Sum of electronic and zero-point Energies= -917.205753
Sum of electronic and thermal Energies= -917.187959
Sum of electronic and thermal Enthalpies= -917.187015
Sum of electronic and thermal Free Energies= -917.254730

Cartesian coordinates of the HT transition structures in the *trans*-piceatannol oxidation by •OOH radicals in water.

HT-3A/HT-5A

C	-3.79268300	-0.39150800	-0.71399100
C	-2.43497200	-0.76950600	-0.70503800
C	-1.44314600	0.16878200	-0.43574900
C	-1.82425400	1.49132800	-0.17550400
C	-3.17324200	1.85965200	-0.17789900
C	-4.16598900	0.93756600	-0.44192000
H	-2.18404800	-1.80160500	-0.90974700
H	-1.09260900	2.25947000	0.03021300
H	-5.21133300	1.21696900	-0.44917500
C	-0.04425400	-0.27707200	-0.43470000
H	0.09357100	-1.31634900	-0.70962900
C	1.01453800	0.47912500	-0.11885200
H	0.86881400	1.51325500	0.17340900
C	2.41523200	0.04126200	-0.11389100
C	3.38339900	0.95242000	0.32357800
C	2.83013300	-1.23076600	-0.52292400
C	4.72217600	0.60648300	0.35847800
H	3.09549100	1.94567600	0.64403100
C	4.17260500	-1.57816200	-0.48771500
H	2.11352800	-1.95848100	-0.87575800
C	5.12144400	-0.66556800	-0.04883500
H	4.49979900	-2.56068100	-0.80471900
O	5.64356700	1.52488600	0.79555700
H	6.52512100	1.13359500	0.75802300
O	6.46411800	-0.93429400	0.01191300
H	6.63490000	-1.83109200	-0.29845200
O	-4.72769100	-1.29545200	-0.99681000
H	-5.02211200	-1.79838100	-0.04523300
O	-3.44827100	3.17065900	0.09123200
H	-4.40091500	3.32011200	0.07246200
O	-5.12062100	-2.14324100	1.17645900
O	-4.08106300	-1.47716000	1.73915000
H	-4.44644100	-0.62989400	2.04435400

Zero-point correction= 0.245155 (Hartree/Particle)
Thermal correction to Energy= 0.264027
Thermal correction to Enthalpy= 0.264971
Thermal correction to Gibbs Free Energy= 0.195923
Sum of electronic and zero-point Energies= -992.451208
Sum of electronic and thermal Energies= -992.432336
Sum of electronic and thermal Enthalpies= -992.431392
Sum of electronic and thermal Free Energies= -992.500440

HT-3B

C	-4.47094600	1.33300400	-0.21074300
C	-3.12251400	1.03566800	-0.33055700
C	-2.68069900	-0.26619000	-0.06221700
C	-3.60305100	-1.24411400	0.31287100
C	-4.94949600	-0.91606000	0.42867100
C	-5.40104000	0.36920600	0.17019300
H	-2.43973800	1.81461200	-0.64214700
H	-3.28100600	-2.25583600	0.51929700
H	-6.44949600	0.62311700	0.25641300
C	-1.27005700	-0.66271400	-0.15919900
H	-1.09275300	-1.72548600	-0.04251400
C	-0.23859200	0.17019300	-0.35276600
H	-0.41613700	1.23611400	-0.43869000
C	1.17037900	-0.21773800	-0.44090400
C	2.12908300	0.78021800	-0.52235800
C	1.59906200	-1.56766200	-0.44337100
C	3.48890100	0.46473100	-0.59956900
H	1.84453700	1.82448100	-0.52410600
C	2.93338300	-1.90145800	-0.52161700
H	0.87166700	-2.36476700	-0.38727800
C	3.89076300	-0.89163500	-0.60246700
H	3.25491400	-2.93341900	-0.52615700
O	4.43868900	1.40504000	-0.70106200
H	4.85991500	1.56392600	0.27340400
O	5.19825100	-1.20660200	-0.67427700
H	5.71280200	-0.39043000	-0.76676300
O	-4.95771800	2.59049000	-0.46659500
H	-4.23621600	3.17326400	-0.73022900
O	-5.81087500	-1.91427800	0.80775200
H	-6.71130500	-1.57194900	0.84456600
O	5.15839700	1.44222400	1.59010900
O	4.27985400	0.48813300	1.96859800
H	4.77897900	-0.34638400	1.97220400

Zero-point correction= 0.246328 (Hartree/Particle)
Thermal correction to Energy= 0.264833
Thermal correction to Enthalpy= 0.265777
Thermal correction to Gibbs Free Energy= 0.197472
Sum of electronic and zero-point Energies= -992.458584
Sum of electronic and thermal Energies= -992.440078
Sum of electronic and thermal Enthalpies= -992.439134
Sum of electronic and thermal Free Energies= -992.507439

HT-4B

C	-4.55807700	1.30086400	0.17721500
C	-3.19596200	1.06908700	0.07521800
C	-2.73128500	-0.24896500	-0.02306000
C	-3.64213600	-1.30604700	-0.00844800
C	-5.00393500	-1.04365700	0.09641900
C	-5.47867700	0.25589000	0.19049300
H	-2.51812700	1.91186700	0.07679300
H	-3.30034000	-2.32958100	-0.08161300
H	-6.53837700	0.46022600	0.27180800
C	-1.30818400	-0.58317900	-0.14355700
H	-1.09589200	-1.64557000	-0.15051300
C	-0.30555800	0.30179400	-0.25311100
H	-0.52383000	1.36308200	-0.26632100
C	1.11136100	-0.02971200	-0.37456100
C	2.00931200	1.02123100	-0.57319600
C	1.60382800	-1.35250300	-0.29473400
C	3.36483800	0.76946200	-0.69537900
H	1.65527300	2.04178800	-0.63525200
C	2.95049100	-1.60422500	-0.40320400
H	0.92563100	-2.17793300	-0.13669600
C	3.85553600	-0.55159700	-0.60563800
H	3.34194800	-2.61019900	-0.33652500
O	4.22887700	1.79640800	-0.88070900
H	5.12066200	1.43720700	-0.99700000
O	5.17404400	-0.75857300	-0.74868900
H	5.65617600	-0.52996400	0.16906800
O	-5.06744100	2.57130600	0.27211500
H	-4.34955800	3.21359500	0.22682900
O	-5.85198700	-2.12134700	0.10280600
H	-6.76579600	-1.82248200	0.17222400
O	5.88126100	-0.12224200	1.47006400
O	4.62262200	0.09089000	1.89725700
H	4.46391800	1.04577500	1.79770400

Zero-point correction= 0.245886 (Hartree/Particle)
Thermal correction to Energy= 0.264520
Thermal correction to Enthalpy= 0.265464
Thermal correction to Gibbs Free Energy= 0.197321
Sum of electronic and zero-point Energies= -992.460586
Sum of electronic and thermal Energies= -992.441953
Sum of electronic and thermal Enthalpies= -992.441009
Sum of electronic and thermal Free Energies= -992.509152

Cartesian coordinates of the HT transition structures in the *trans*-piceatannol oxidation by •OOH radicals in pentylethanoate.

HT-3A/HT-5A

C	-3.81432500	-0.12585700	-0.76133300
C	-2.47383700	-0.56513200	-0.70418000
C	-1.47426000	0.26549200	-0.19500800
C	-1.82903500	1.53009700	0.27345400
C	-3.16055600	1.96729700	0.21359700
C	-4.15671600	1.15547100	-0.28793400
H	-2.23920500	-1.55205400	-1.07772700
H	-1.09637400	2.19645300	0.70648800
H	-5.18969700	1.47628700	-0.33306900
C	-0.09321300	-0.23346500	-0.16968000
H	0.00753600	-1.30290400	-0.31318500
C	0.99647800	0.52933000	-0.02542400
H	0.88229000	1.60497400	0.05441000
C	2.38507500	0.05626400	0.00635800
C	3.40684500	1.00972100	-0.07093600
C	2.73255500	-1.29327900	0.11363100
C	4.73648800	0.62969300	-0.05688500
H	3.16997600	2.06324100	-0.14746900
C	4.06600100	-1.67818400	0.12747000
H	1.96917800	-2.05329800	0.19933900
C	5.06649700	-0.72266400	0.04018200
H	4.33344100	-2.72459200	0.21306800
O	5.71332400	1.57057500	-0.13451400
H	6.56962900	1.12803100	-0.11127600
O	6.40407300	-1.00078900	0.05061000
H	6.55479100	-1.94891600	0.11767500
O	-4.74663400	-0.91087300	-1.26133700
H	-4.94908800	-1.75458000	-0.54462900
O	-3.40463800	3.21395100	0.68898600
H	-4.34058700	3.42314800	0.60124100
O	-5.04566800	-2.47302000	0.48007800
O	-3.89988300	-2.17271300	1.15060100
H	-4.16446000	-1.52153300	1.81987000

Zero-point correction= 0.245182 (Hartree/Particle)
Thermal correction to Energy= 0.264334
Thermal correction to Enthalpy= 0.265278
Thermal correction to Gibbs Free Energy= 0.194467
Sum of electronic and zero-point Energies= -992.441775
Sum of electronic and thermal Energies= -992.422624
Sum of electronic and thermal Enthalpies= -992.421680
Sum of electronic and thermal Free Energies= -992.492491

HT-3B

C	-4.41189700	1.40764900	-0.10279300
C	-3.06560300	1.07782300	-0.10787400
C	-2.68395400	-0.26304000	0.02934700
C	-3.66234500	-1.24481100	0.17745600
C	-5.00823000	-0.89064400	0.17596200
C	-5.39764400	0.43304900	0.03686200
H	-2.32831600	1.86321100	-0.20732500
H	-3.39079400	-2.28563900	0.28774500
H	-6.44111000	0.72114900	0.03924900
C	-1.28039500	-0.69491700	0.02774400
H	-1.13572900	-1.74388700	0.25850500
C	-0.22219500	0.07868800	-0.24582500
H	-0.37281000	1.11995300	-0.50714500
C	1.17919400	-0.34747200	-0.25284500
C	2.14271200	0.54585100	-0.69384400
C	1.59597000	-1.63051300	0.17613900
C	3.49393600	0.18537900	-0.72632300
H	1.86941500	1.54078900	-1.02132400
C	2.92132400	-2.01024800	0.14981000
H	0.86571700	-2.33937900	0.53924300
C	3.88014100	-1.10996100	-0.30755000
H	3.23018200	-2.99357600	0.47590500
O	4.45715300	0.99624300	-1.15904100
H	4.80377500	1.59204000	-0.32198100
O	5.17777200	-1.44945500	-0.34031100
H	5.65814100	-0.72923100	-0.77611300
O	-4.83955200	2.69343000	-0.22858400
H	-4.08151900	3.28056100	-0.31090300
O	-5.91553000	-1.89425800	0.31667000
H	-6.80731700	-1.53276500	0.30298500
O	5.12897300	1.95158800	0.91642000
O	4.29073400	1.17938700	1.64676700
H	4.84788300	0.47029700	2.00818500

Zero-point correction= 0.246951 (Hartree/Particle)
Thermal correction to Energy= 0.265596
Thermal correction to Enthalpy= 0.266540
Thermal correction to Gibbs Free Energy= 0.197766
Sum of electronic and zero-point Energies= -992.448244
Sum of electronic and thermal Energies= -992.429599
Sum of electronic and thermal Enthalpies= -992.428655
Sum of electronic and thermal Free Energies= -992.497429

HT-4B

C	-4.57687500	1.25347300	0.33450600
C	-3.21011800	1.04077000	0.24325200
C	-2.73022400	-0.25210500	-0.00416500
C	-3.62967600	-1.30828500	-0.14023400
C	-4.99766700	-1.07007000	-0.04816700
C	-5.48461500	0.20683900	0.18803900
H	-2.53222900	1.87246200	0.38345200
H	-3.27891300	-2.31430900	-0.32529700
H	-6.54666500	0.40188100	0.26629600
C	-1.30020600	-0.55565600	-0.12546600
H	-1.06284200	-1.61272600	-0.12723900
C	-0.31813300	0.34855000	-0.25668000
H	-0.56637000	1.40260700	-0.30046700
C	1.10661700	0.05210600	-0.37864300
C	1.97416300	1.11945600	-0.62893500
C	1.63542900	-1.25176900	-0.25252700
C	3.33393000	0.89930500	-0.75659000
H	1.59138800	2.12601000	-0.73357200
C	2.98586000	-1.47403700	-0.37583400
H	0.98202400	-2.08692400	-0.04792400
C	3.86103900	-0.40486000	-0.62469000
H	3.40370800	-2.46676600	-0.27516900
O	4.17248300	1.92398100	-1.00228100
H	5.05567000	1.55120300	-1.13781200
O	5.17599900	-0.55503900	-0.78904100
H	5.64524500	-0.63192600	0.16692900
O	-5.10109400	2.48501900	0.57809000
H	-4.39173400	3.13023400	0.65904800
O	-5.82725500	-2.13682800	-0.19735800
H	-6.74313600	-1.85387900	-0.11195400
O	5.90929200	-0.43881500	1.48582100
O	4.66540100	-0.25797800	1.97520200
H	4.58808800	0.69712100	2.13704400

Zero-point correction= 0.246808 (Hartree/Particle)
Thermal correction to Energy= 0.265581
Thermal correction to Enthalpy= 0.266525
Thermal correction to Gibbs Free Energy= 0.197163
Sum of electronic and zero-point Energies= -992.450127
Sum of electronic and thermal Energies= -992.431354
Sum of electronic and thermal Enthalpies= -992.430410
Sum of electronic and thermal Free Energies= -992.499771

Cartesian coordinates of the RAF products in the *trans*-piceatannol oxidation by •OOH radicals in water.

α

C	-3.79673600	1.31992300	0.02945900
C	-2.46345700	1.00395500	0.25958700
C	-2.01092100	-0.28083800	-0.03856700
C	-2.88115500	-1.22939800	-0.56351600
C	-4.21039200	-0.88546500	-0.78865400
C	-4.68165600	0.38597800	-0.49682100
H	-1.80187000	1.75464000	0.67069400
H	-2.54010400	-2.22851700	-0.79918100
H	-5.71614600	0.65127600	-0.67335100
C	-0.58742800	-0.69743500	0.24384600
H	-0.39658600	-1.64871700	-0.25783600
C	0.43667700	0.31317800	-0.13597200
H	0.11151600	1.30421300	-0.41523800
C	1.82391600	0.04216200	-0.14724600
C	2.72423900	1.07196000	-0.52298000
C	2.36644000	-1.21879700	0.19891600
C	4.07996600	0.85160500	-0.54965800
H	2.34529900	2.04827600	-0.79591700
C	3.73338200	-1.43087700	0.16849200
H	1.71667500	-2.03015500	0.49150200
C	4.59567900	-0.40600500	-0.20145500
H	4.15007900	-2.39477800	0.43230100
O	4.92702900	1.86661300	-0.91856500
H	5.83627700	1.54255100	-0.90355200
O	5.95595200	-0.53405600	-0.25500000
H	6.22135200	-1.42644000	-0.00300700
O	-4.30267000	2.56480000	0.30805400
H	-3.60837800	3.12785900	0.66995900
O	-5.03438400	-1.85073200	-1.30845300
H	-5.92758800	-1.50048300	-1.40186000
O	-0.45220900	-1.11967600	1.63750700
O	-0.53764000	0.01027800	2.49197700
H	0.38953700	0.26278500	2.60873900

Zero-point correction= 0.251436 (Hartree/Particle)
Thermal correction to Energy= 0.270163
Thermal correction to Enthalpy= 0.271107
Thermal correction to Gibbs Free Energy= 0.202945
Sum of electronic and zero-point Energies= -992.484719
Sum of electronic and thermal Energies= -992.465993
Sum of electronic and thermal Enthalpies= -992.465048
Sum of electronic and thermal Free Energies= -992.533210

β

C	-3.96219200	0.88713500	-0.59407100
C	-2.61050300	0.85357900	-0.30592000
C	-2.02567300	-0.35758100	0.13240200
C	-2.83830300	-1.50455500	0.26728400
C	-4.18635000	-1.43167200	-0.03219800
C	-4.76827900	-0.24397700	-0.46504800
H	-2.02423200	1.75694500	-0.40851400
H	-2.40990900	-2.43953900	0.60130100
H	-5.82373900	-0.19227500	-0.69818700
C	-0.64830000	-0.46673300	0.44504900
H	-0.28103600	-1.41362500	0.81468400
C	0.32328900	0.65524000	0.32278600
H	0.08788100	1.29770300	-0.52630900
C	1.74790400	0.17586800	0.21280400
C	2.46362600	0.40227900	-0.95939800
C	2.35120800	-0.49538900	1.27340800
C	3.76724300	-0.05076200	-1.07631600
H	2.01426100	0.93115900	-1.79033000
C	3.66303500	-0.94041500	1.16154200
H	1.80080900	-0.66996000	2.18868400
C	4.36873600	-0.72212400	-0.01212300
H	4.14816000	-1.46129700	1.97752000
O	4.45981500	0.17262900	-2.23897800
H	5.34797600	-0.19593600	-2.15110400
O	5.66376700	-1.12821000	-0.21192500
H	6.00092600	-1.56804700	0.57693000
O	-4.58480500	2.03408400	-1.01874900
H	-3.94316000	2.75111300	-1.07624000
O	-4.93246000	-2.57473400	0.11035700
H	-5.84922400	-2.39628100	-0.12679900
O	0.13532500	1.44922700	1.52740400
O	0.91864300	2.63072300	1.40989600
H	1.77635600	2.36493400	1.77313700

Zero-point correction= 0.250929 (Hartree/Particle)
Thermal correction to Energy= 0.269964
Thermal correction to Enthalpy= 0.270908
Thermal correction to Gibbs Free Energy= 0.201595
Sum of electronic and zero-point Energies= -992.486875
Sum of electronic and thermal Energies= -992.467841
Sum of electronic and thermal Enthalpies= -992.466897
Sum of electronic and thermal Free Energies= -992.536209

1A

C	3.20827000	1.63939300	-0.17771400
C	2.27563000	0.96010600	-0.88380500
C	1.95870100	-0.46260600	-0.57558600
C	2.72216200	-1.02306800	0.57984200
C	3.64071900	-0.28044500	1.25584500
C	3.91575300	1.05337400	0.90385500
H	1.75324000	1.43067500	-1.70619100
H	2.51474700	-2.04006900	0.88228900
H	4.65165000	1.63281800	1.44321400
C	0.48970100	-0.73352500	-0.36160200
H	0.24191200	-1.78148800	-0.24438500
C	-0.44731600	0.21203100	-0.27325100
H	-0.16655500	1.25249900	-0.39452500
C	-1.87946800	-0.01896200	-0.03024500
C	-2.75612800	1.05795800	-0.19893700
C	-2.40314300	-1.25685800	0.35328900
C	-4.11748900	0.90127800	-0.00889700
H	-2.38028000	2.03046900	-0.49073400
C	-3.76796600	-1.41363600	0.54905000
H	-1.75189300	-2.10464600	0.51123400
C	-4.62841200	-0.34076600	0.36628800
H	-4.17843900	-2.36957700	0.84907300
O	-4.95251900	1.97475400	-0.19253700
H	-5.86357400	1.69772900	-0.03408200
O	-5.98719100	-0.41299400	0.53823700
H	-6.24563000	-1.30896700	0.78441300
O	3.53802700	2.94600700	-0.43797000
H	3.01424700	3.27203200	-1.17929000
O	4.30129400	-0.86366300	2.31219900
H	4.90920300	-0.23073400	2.71049400
O	2.38385600	-1.14632000	-1.82701400
O	2.12507400	-2.54153800	-1.73126800
H	2.96694300	-2.89635900	-1.41348200

Zero-point correction= 0.250027 (Hartree/Particle)
Thermal correction to Energy= 0.268920
Thermal correction to Enthalpy= 0.269864
Thermal correction to Gibbs Free Energy= 0.201938
Sum of electronic and zero-point Energies= -992.448238
Sum of electronic and thermal Energies= -992.429345
Sum of electronic and thermal Enthalpies= -992.428401
Sum of electronic and thermal Free Energies= -992.496326

2A

C	-3.40233600	1.89935200	-0.03935500
C	-2.06698000	1.56625800	0.00880900
C	-1.65355200	0.23841500	-0.14200900
C	-2.67356400	-0.85608400	-0.23496800
C	-4.07863300	-0.37150000	-0.37061600
C	-4.42555800	0.92209300	-0.24697300
H	-1.34032500	2.36068800	0.12131800
H	-2.43120200	-1.56911700	-1.02533000
H	-5.45963200	1.23533600	-0.31133000
C	-0.29204400	-0.19111800	-0.18259400
H	-0.15096100	-1.24781400	-0.38286900
C	0.80170600	0.59432800	0.00932300
H	0.66783200	1.64451400	0.24104200
C	2.18989400	0.15661800	-0.05993100
C	3.19324600	1.09597000	0.22443200
C	2.57874400	-1.14755800	-0.39886400
C	4.52970300	0.74809000	0.17698900
H	2.92987700	2.11245500	0.48820400
C	3.92047600	-1.49506800	-0.44647500
H	1.83948000	-1.90013700	-0.63175700
C	4.89944700	-0.55424200	-0.15953700
H	4.22200500	-2.50135600	-0.70945100
O	5.48473800	1.69281900	0.46043100
H	6.35792200	1.28585300	0.39950400
O	6.24474500	-0.81941700	-0.18659500
H	6.39454400	-1.74139600	-0.42535300
O	-3.84613700	3.18379300	0.08114200
H	-3.09723500	3.78152900	0.19475000
O	-4.96122300	-1.38926100	-0.56347700
H	-5.86624300	-1.05102300	-0.56775300
O	-2.56828000	-1.61330100	1.02035600
O	-3.00601700	-2.95083200	0.80982300
H	-3.97196600	-2.87326300	0.80621100

Zero-point correction= 0.251567 (Hartree/Particle)
Thermal correction to Energy= 0.270353
Thermal correction to Enthalpy= 0.271298
Thermal correction to Gibbs Free Energy= 0.203268
Sum of electronic and zero-point Energies= -992.466214
Sum of electronic and thermal Energies= -992.447428
Sum of electronic and thermal Enthalpies= -992.446483
Sum of electronic and thermal Free Energies= -992.514513

3A

C	-3.23444400	1.83866800	-0.09893500
C	-1.86577900	1.46954400	-0.09609400
C	-1.49344200	0.10006700	-0.18463400
C	-2.46319200	-0.85823100	-0.25483900
C	-3.91618500	-0.53475600	-0.17333000
C	-4.22699200	0.91913000	-0.14526400
H	-1.12186300	2.25198800	-0.05574800
H	-2.20391000	-1.90306700	-0.34890400
H	-5.26868300	1.21101400	-0.15490200
C	-0.08749100	-0.32444600	-0.22002900
H	0.05258700	-1.38602200	-0.38877000
C	0.97515500	0.47083300	-0.04512400
H	0.83383800	1.52821500	0.14885300
C	2.37989900	0.04292000	-0.07219500
C	3.36069200	0.98965300	0.24519000
C	2.78515200	-1.25540100	-0.39924400
C	4.70225100	0.65192800	0.24430300
H	3.08081300	2.00389400	0.50052300
C	4.13044100	-1.59452000	-0.40054400
H	2.05822300	-2.01154900	-0.65861800
C	5.09185300	-0.64631300	-0.08139000
H	4.44832200	-2.59794900	-0.65485800
O	5.63790800	1.60415000	0.56275800
H	6.51642600	1.20526300	0.53447500
O	6.43869200	-0.90265100	-0.06418200
H	6.60311800	-1.81926200	-0.31405400
O	-3.57975900	3.16771400	-0.06365900
H	-2.78748700	3.71612200	-0.06797600
O	-4.57277400	-1.21388000	-1.22070000
H	-5.49331100	-0.92069200	-1.25184800
O	-4.46789500	-1.00832300	1.09085500
O	-4.27132500	-2.41136500	1.20546300
H	-5.02436300	-2.77755700	0.72032300

Zero-point correction= 0.250937 (Hartree/Particle)
Thermal correction to Energy= 0.269882
Thermal correction to Enthalpy= 0.270826
Thermal correction to Gibbs Free Energy= 0.202807
Sum of electronic and zero-point Energies= -992.458783
Sum of electronic and thermal Energies= -992.439838
Sum of electronic and thermal Enthalpies= -992.438894
Sum of electronic and thermal Free Energies= -992.506913

4A

C	3.15833200	-1.09033600	-0.30414300
C	1.82703700	-0.90752600	-0.22761000
C	1.27143500	0.41485600	-0.14126600
C	2.17202400	1.52549400	-0.10805200
C	3.50880200	1.35414400	-0.16684400
C	4.15511300	0.01788300	-0.28796900
H	1.18372000	-1.77758900	-0.23986300
H	1.77252100	2.52953300	-0.04300200
H	4.80941700	-0.02003500	-1.16439700
C	-0.12281900	0.67202400	-0.08434700
H	-0.39066000	1.72052400	-0.02535900
C	-1.11860600	-0.26335300	-0.09807500
H	-0.86328500	-1.31435400	-0.14950800
C	-2.54464900	0.01685700	-0.04024700
C	-3.43206100	-1.07156000	-0.01513900
C	-3.08344900	1.31219000	-0.00534500
C	-4.79797500	-0.87657000	0.05053400
H	-3.05286900	-2.08517000	-0.04284600
C	-4.45499100	1.50558100	0.05879100
H	-2.43976400	2.17947100	-0.02826300
C	-5.31707600	0.41841600	0.09016600
H	-4.87146800	2.50478000	0.08755900
O	-5.63534800	-1.96393400	0.07969700
H	-6.54900300	-1.65576800	0.12513200
O	-6.68287500	0.52415800	0.16050500
H	-6.94609500	1.45161100	0.17978800
O	3.77463000	-2.30661300	-0.37758900
H	3.12240900	-3.01678600	-0.32269100
O	4.35216900	2.43125200	-0.16128200
H	5.25977500	2.13259500	-0.02605600
O	5.03324200	-0.11967000	0.86803200
O	6.14107800	-0.93805000	0.52446300
H	5.77543800	-1.83455200	0.57618100

Zero-point correction= 0.251653 (Hartree/Particle)
Thermal correction to Energy= 0.270560
Thermal correction to Enthalpy= 0.271504
Thermal correction to Gibbs Free Energy= 0.203103
Sum of electronic and zero-point Energies= -992.468921
Sum of electronic and thermal Energies= -992.450015
Sum of electronic and thermal Enthalpies= -992.449071
Sum of electronic and thermal Free Energies= -992.517471

5A

C	3.58985800	0.74961700	0.35677200
C	2.12094500	0.49798000	0.45707300
C	1.55580500	-0.69404400	0.07850400
C	2.38813300	-1.75633700	-0.33005900
C	3.80386400	-1.59944800	-0.34958800
C	4.40193100	-0.43733100	-0.01296700
H	1.52134500	1.30685800	0.85172800
H	1.96560000	-2.70889400	-0.61549200
H	5.47800600	-0.32455000	-0.01343700
C	0.10303200	-0.92681600	0.10642200
H	-0.19880800	-1.96726000	0.14422700
C	-0.81745300	0.04307700	0.04888300
H	-0.49476800	1.07312400	-0.06303600
C	-2.27222300	-0.14881800	0.08737100
C	-3.08954000	0.93260000	-0.26074300
C	-2.87629700	-1.35451000	0.45739700
C	-4.46728600	0.80979700	-0.26046900
H	-2.65157900	1.88190500	-0.54210200
C	-4.25848300	-1.47753900	0.45994900
H	-2.27555400	-2.20120900	0.75795800
C	-5.05672600	-0.40205800	0.09858600
H	-4.73236400	-2.40728500	0.74926000
O	-5.24127900	1.88718800	-0.61219000
H	-6.17313600	1.64121700	-0.55474000
O	-6.42726500	-0.44321500	0.07657300
H	-6.73607900	-1.31930500	0.33498200
O	4.10193100	1.30197800	1.54811700
H	3.55212600	2.05806300	1.79221600
O	4.50249400	-2.71954200	-0.71737500
H	5.44916300	-2.53323500	-0.70644500
O	3.85247300	1.69001100	-0.72979000
O	3.22970700	2.93291800	-0.42084300
H	2.39821100	2.88884300	-0.91384000

Zero-point correction= 0.250878 (Hartree/Particle)
Thermal correction to Energy= 0.269631
Thermal correction to Enthalpy= 0.270575
Thermal correction to Gibbs Free Energy= 0.202931
Sum of electronic and zero-point Energies= -992.458309
Sum of electronic and thermal Energies= -992.439555
Sum of electronic and thermal Enthalpies= -992.438611
Sum of electronic and thermal Free Energies= -992.506255

6A

C	-3.73314500	0.82191200	-0.39723200
C	-2.25789400	0.71090600	-0.18761400
C	-1.77101700	-0.69059100	0.00909500
C	-2.68086400	-1.73734600	0.11735500
C	-4.04000500	-1.52430900	-0.02639400
C	-4.57123600	-0.23039700	-0.30209100
H	-1.72280000	1.20704300	-1.00303100
H	-2.32136000	-2.74471400	0.28356800
H	-5.63733400	-0.09829600	-0.43785000
C	-0.36433600	-0.93852400	0.06591300
H	-0.08827900	-1.97783200	0.20424400
C	0.60754500	0.00177300	-0.05174000
H	0.33076300	1.04339900	-0.16951200
C	2.04530000	-0.24788100	-0.02917000
C	2.90685100	0.85233200	-0.15189200
C	2.61173200	-1.52331300	0.10253000
C	4.27893800	0.68703700	-0.14695800
H	2.50445400	1.85206000	-0.25578600
C	3.98909900	-1.68768800	0.10852300
H	1.98547600	-2.39857200	0.19768400
C	4.82715200	-0.58901100	-0.01841500
H	4.42790000	-2.67275500	0.20774000
O	5.09320600	1.78511500	-0.27233500
H	6.01412300	1.49581000	-0.26049000
O	6.19714100	-0.66654100	-0.02931300
H	6.47893700	-1.58663000	0.03063400
O	-4.21707700	2.06388400	-0.68223500
H	-3.52946400	2.72422300	-0.51266600
O	-4.87736100	-2.59709100	0.08537000
H	-5.79109200	-2.32021700	-0.04920000
O	-1.89855300	1.45294900	1.02884700
O	-1.89130300	2.84361100	0.72131900
H	-0.98846600	2.99165800	0.39998700

Zero-point correction= 0.251361 (Hartree/Particle)
Thermal correction to Energy= 0.270084
Thermal correction to Enthalpy= 0.271028
Thermal correction to Gibbs Free Energy= 0.203552
Sum of electronic and zero-point Energies= -992.468977
Sum of electronic and thermal Energies= -992.450255
Sum of electronic and thermal Enthalpies= -992.449311
Sum of electronic and thermal Free Energies= -992.516786

1B

C	4.04186200	0.91265200	0.58283600
C	2.68132700	0.94392900	0.31916000
C	2.05157900	-0.20844400	-0.16467000
C	2.79672400	-1.36817400	-0.37167900
C	4.16041300	-1.37208700	-0.09617800
C	4.79938100	-0.23807600	0.38057800
H	2.13223300	1.85949300	0.49404700
H	2.32499000	-2.26792600	-0.74291800
H	5.86005400	-0.24120800	0.59523800
C	0.61216600	-0.26097300	-0.47190500
H	0.25845400	-1.22599800	-0.81849700
C	-0.25188400	0.74657200	-0.34797600
H	0.05914300	1.71723700	0.01906000
C	-1.72945900	0.62768100	-0.62620100
C	-2.49079200	0.78404900	0.64960500
C	-2.10509000	-0.59050900	-1.40423100
C	-3.45978800	-0.08427900	1.01539600
H	-2.23178600	1.60508000	1.30421400
C	-3.09596600	-1.42931600	-1.00365900
H	-1.57062200	-0.76753400	-2.32644200
C	-3.78965300	-1.20379800	0.19710300
H	-3.36166400	-2.29539300	-1.59747800
O	-4.13089200	0.08608400	2.19850200
H	-4.77025100	-0.62895000	2.30824300
O	-4.77346500	-2.01394700	0.66099200
H	-4.91562700	-2.75781000	0.06179200
O	4.71027600	2.01366100	1.05740200
H	4.09454300	2.74803300	1.16219800
O	4.84258700	-2.54199200	-0.31587400
H	5.77082700	-2.43117400	-0.08037600
O	-2.10325200	1.71382000	-1.57743400
O	-1.83360400	2.98326800	-0.99482300
H	-2.66841100	3.20364100	-0.55829500

Zero-point correction= 0.250284 (Hartree/Particle)
Thermal correction to Energy= 0.269237
Thermal correction to Enthalpy= 0.270182
Thermal correction to Gibbs Free Energy= 0.201562
Sum of electronic and zero-point Energies= -992.452971
Sum of electronic and thermal Energies= -992.434017
Sum of electronic and thermal Enthalpies= -992.433073
Sum of electronic and thermal Free Energies= -992.501693

2B

C	-4.15525600	1.22587100	-0.38134400
C	-2.80735700	0.90759700	-0.35526400
C	-2.41530100	-0.39876300	-0.02657300
C	-3.39161100	-1.35626600	0.26498400
C	-4.73596700	-1.00588400	0.23401300
C	-5.13693200	0.28202900	-0.08895700
H	-2.08370900	1.67450700	-0.59520700
H	-3.11007600	-2.36911100	0.51957100
H	-6.18398500	0.55371500	-0.11658500
C	-1.01781600	-0.81906500	0.02470100
H	-0.86826100	-1.87160300	0.23315700
C	0.05748600	-0.01252900	-0.15230700
H	-0.09955600	1.04683300	-0.32289800
C	1.43006900	-0.42634100	-0.12738300
C	2.43609400	0.68888200	-0.15271500
C	1.86378100	-1.74604700	-0.05061600
C	3.84454300	0.23955700	-0.29486200
H	2.18965300	1.42891600	-0.91764100
C	3.20937400	-2.07365300	-0.07716300
H	1.13974200	-2.54672100	0.00230600
C	4.19761200	-1.06341300	-0.21727200
H	3.53006500	-3.10482000	-0.01709200
O	4.75171000	1.24882900	-0.44724100
H	5.64232500	0.87427900	-0.48968000
O	5.54187100	-1.36622000	-0.28661000
H	5.65594000	-2.30189300	-0.48652500
O	-4.59033600	2.48790300	-0.70002300
H	-3.83262600	3.05387800	-0.88654800
O	-5.65025900	-1.98427700	0.53310700
H	-6.54069500	-1.61627200	0.50576300
O	2.27047800	1.38451800	1.13023100
O	2.74887300	2.71738100	1.00742100
H	3.71017700	2.62137300	1.08084400

Zero-point correction= 0.251393 (Hartree/Particle)
Thermal correction to Energy= 0.270181
Thermal correction to Enthalpy= 0.271125
Thermal correction to Gibbs Free Energy= 0.203440
Sum of electronic and zero-point Energies= -992.462260
Sum of electronic and thermal Energies= -992.443472
Sum of electronic and thermal Enthalpies= -992.442528
Sum of electronic and thermal Free Energies= -992.510213

3B

C	-4.36312600	1.32362000	-0.27370200
C	-3.01185400	1.01517800	-0.29631800
C	-2.60295000	-0.29605100	-0.02244300
C	-3.55976000	-1.27132400	0.26024000
C	-4.90840600	-0.93200700	0.27992900
C	-5.32815100	0.36253300	0.01569000
H	-2.30038300	1.79410300	-0.53474000
H	-3.26376700	-2.29041500	0.46948300
H	-6.37779900	0.62559200	0.02711200
C	-1.19101200	-0.70651200	-0.02226000
H	-1.03479700	-1.77099100	0.10703600
C	-0.14267200	0.11567400	-0.14851700
H	-0.30330100	1.18275100	-0.25218000
C	1.27022200	-0.28647400	-0.14469000
C	2.21521400	0.69251900	-0.18719700
C	1.66753600	-1.66228700	-0.13098000
C	3.67347600	0.40578100	-0.13179000
H	1.93606100	1.73604300	-0.23056500
C	3.01826100	-2.01348100	-0.21487500
H	0.92750800	-2.44574500	-0.09973900
C	3.98735500	-1.05225700	-0.25640900
H	3.31132800	-3.05410200	-0.27416600
O	4.33352600	1.18474900	-1.09787800
H	5.26081400	0.91199300	-1.12880100
O	5.31221200	-1.28780200	-0.39949000
H	5.47570500	-2.23170400	-0.52456200
O	-4.81767300	2.59091300	-0.54022400
H	-4.07276100	3.16854600	-0.74190900
O	-5.80518300	-1.92967100	0.56752400
H	-6.70083800	-1.57358600	0.56034500
O	4.22815600	0.73574100	1.17803100
O	4.00526000	2.11034800	1.44940100
H	4.74704400	2.54380900	1.00369800

Zero-point correction= 0.251646 (Hartree/Particle)
Thermal correction to Energy= 0.270324
Thermal correction to Enthalpy= 0.271268
Thermal correction to Gibbs Free Energy= 0.203787
Sum of electronic and zero-point Energies= -992.464229
Sum of electronic and thermal Energies= -992.445552
Sum of electronic and thermal Enthalpies= -992.444607
Sum of electronic and thermal Free Energies= -992.512089

4B

C	-4.59690500	1.20141600	0.16900800
C	-3.22159400	1.05003400	0.09906600
C	-2.67775600	-0.23704300	-0.04030500
C	-3.53474700	-1.34124400	-0.10851200
C	-4.90944000	-1.15645100	-0.03841000
C	-5.45924300	0.10959300	0.10114300
H	-2.59521800	1.92998800	0.15342000
H	-3.13552100	-2.34058600	-0.21696500
H	-6.53050300	0.25160900	0.15783400
C	-1.24603000	-0.49213600	-0.12011100
H	-0.97904300	-1.53561200	-0.22332900
C	-0.26576700	0.45519400	-0.07558900
H	-0.54553200	1.49640000	0.03357700
C	1.13193600	0.21460200	-0.15612100
C	2.02290500	1.32727700	-0.09867900
C	1.70100500	-1.09814100	-0.33193600
C	3.36189900	1.16550500	-0.15208200
H	1.61952700	2.32969200	-0.03206300
C	3.02912100	-1.29704400	-0.37815700
H	1.04492200	-1.94899600	-0.44978600
C	4.00827300	-0.18470700	-0.19832800
H	3.44890800	-2.28226500	-0.53497100
O	4.20300400	2.23500900	-0.13199100
H	5.11156100	1.93744400	-0.27256800
O	4.99836900	-0.15994700	-1.19685300
H	5.43357800	-1.02248900	-1.21700700
O	-5.18093300	2.43574300	0.30888400
H	-4.49929800	3.11558400	0.35885900
O	-5.70154000	-2.27427300	-0.11128800
H	-6.62942700	-2.01944900	-0.05606800
O	4.66393400	-0.27883100	1.09609800
O	5.43389400	-1.47280300	1.12000500
H	4.86027200	-2.09163500	1.59430100

Zero-point correction= 0.251636 (Hartree/Particle)
Thermal correction to Energy= 0.270197
Thermal correction to Enthalpy= 0.271141
Thermal correction to Gibbs Free Energy= 0.203961
Sum of electronic and zero-point Energies= -992.473427
Sum of electronic and thermal Energies= -992.454866
Sum of electronic and thermal Enthalpies= -992.453922
Sum of electronic and thermal Free Energies= -992.521102

5B

C	-4.48373200	1.23403000	0.06759100
C	-3.10168300	1.14519000	0.01659200
C	-2.49773800	-0.11669100	-0.05164500
C	-3.29457300	-1.26167500	-0.07665200
C	-4.67957000	-1.14168800	-0.03311200
C	-5.29153500	0.09992900	0.04202200
H	-2.51581500	2.05430900	0.03445700
H	-2.84567000	-2.24430700	-0.13061800
H	-6.36890200	0.19297200	0.08325300
C	-1.04102300	-0.30365200	-0.09548500
H	-0.72310500	-1.33961700	-0.13119100
C	-0.12236400	0.66901500	-0.08769400
H	-0.42998500	1.70625400	-0.02438600
C	1.33461200	0.46206500	-0.14172100
C	2.15445400	1.59201200	0.13744900
C	1.91208200	-0.73265100	-0.47003600
C	3.54855100	1.50115300	0.06696500
H	1.70596300	2.54198700	0.39132000
C	3.38472400	-0.93236700	-0.44442300
H	1.31533100	-1.59246300	-0.73850900
C	4.15617600	0.31612200	-0.23960600
H	3.74159500	-1.45934100	-1.33367500
O	4.28622000	2.64215800	0.28672900
H	5.22596000	2.42409100	0.25625500
O	5.51365700	0.28396400	-0.34024600
H	5.82130600	-0.62324400	-0.45939900
O	-5.12468600	2.44531000	0.14559000
H	-4.47317600	3.15469200	0.18941100
O	-5.41372700	-2.30010200	-0.06318000
H	-6.35376800	-2.08995000	-0.03033600
O	3.78320500	-1.78864800	0.69035400
O	3.39225900	-3.12131700	0.39523500
H	2.53457200	-3.20105100	0.83609400

Zero-point correction= 0.250305 (Hartree/Particle)
Thermal correction to Energy= 0.269529
Thermal correction to Enthalpy= 0.270473
Thermal correction to Gibbs Free Energy= 0.201271
Sum of electronic and zero-point Energies= -992.455332
Sum of electronic and thermal Energies= -992.436108
Sum of electronic and thermal Enthalpies= -992.435164
Sum of electronic and thermal Free Energies= -992.504366

6B

C	-4.20174400	1.39714200	0.12525800
C	-2.82372100	1.25331200	0.11566800
C	-2.26560700	-0.01825300	-0.08788700
C	-3.11129700	-1.11639400	-0.27511000
C	-4.48915200	-0.94016500	-0.26194400
C	-5.05359000	0.31122100	-0.06276800
H	-2.20535100	2.12819600	0.26364200
H	-2.70177000	-2.10484600	-0.43367000
H	-6.12712400	0.44701400	-0.05397500
C	-0.82686100	-0.26039400	-0.11971300
H	-0.54528700	-1.29532700	-0.27306300
C	0.14067100	0.68277800	0.02303000
H	-0.13948200	1.71711500	0.18651300
C	1.54392500	0.43677000	-0.03502100
C	2.44504200	1.48799200	0.11894000
C	2.05664600	-0.96220900	-0.22194000
C	3.80334800	1.29514400	-0.00770600
H	2.07812500	2.48796700	0.31277500
C	3.51508000	-1.06222100	-0.50988800
H	1.47607200	-1.49478500	-0.97686800
C	4.32638100	-0.00374500	-0.35596400
H	3.92026900	-2.02366600	-0.79534300
O	4.65749800	2.33761700	0.15022800
H	5.56459200	2.03616400	0.00516600
O	5.68230500	-0.01677600	-0.53524800
H	5.98477700	-0.91124600	-0.73531200
O	-4.79804100	2.61826400	0.32043400
H	-4.12309000	3.29671900	0.43634800
O	-5.26897800	-2.05246800	-0.45643200
H	-6.20039600	-1.80552300	-0.43479500
O	1.74962800	-1.62931000	1.05283800
O	1.92887000	-3.02799600	0.87426000
H	1.05368500	-3.31829600	0.58021700

Zero-point correction= 0.251682 (Hartree/Particle)
Thermal correction to Energy= 0.270250
Thermal correction to Enthalpy= 0.271195
Thermal correction to Gibbs Free Energy= 0.204124
Sum of electronic and zero-point Energies= -992.468936
Sum of electronic and thermal Energies= -992.450368
Sum of electronic and thermal Enthalpies= -992.449423
Sum of electronic and thermal Free Energies= -992.516494

Cartesian coordinates of the HT transition-states in the *trans*-resveratrol oxidation by •OOH radicals in water (Anion)

HT-3A/HT-5A

C	-4.69509600	-1.19467900	-0.20609400
C	-3.31632200	-1.18880100	-0.30329900
C	-2.56189300	-0.01481300	-0.14552300
C	-4.64798200	1.18128000	0.21174500
C	-5.42552600	-0.00532500	0.06186000
C	-1.11262600	-0.08966400	-0.24716700
C	1.21863400	0.78834600	-0.17978700
C	-0.23439400	0.91554300	-0.07534700
C	1.84937100	-0.38597400	-0.63383500
H	1.28709100	-1.23890500	-0.98129700
C	3.25766800	-0.46524800	-0.69060600
C	4.05469000	0.62315000	-0.31341700
C	3.42302300	1.77829000	0.09783400
H	-0.73573800	-1.08147500	-0.47643000
H	-5.24747600	-2.11828000	-0.33001100
H	-2.79486400	-2.11795900	-0.50531800
H	-5.17209200	2.10849300	0.41060700
H	-0.58694800	1.90782600	0.18114200
H	5.13298300	0.55141600	-0.35683200
O	4.11693500	2.89139200	0.46423200
H	5.06592100	2.73363400	0.38478300
O	3.82218100	-1.60153300	-1.09740000
H	3.59337900	-2.38178000	-0.35113600
O	-6.71834900	0.00589700	0.16703100
C	2.02130700	1.86656600	0.17092700
H	1.57841900	2.79380700	0.50982700
C	-3.27285300	1.17220200	0.11119200
H	-2.73727500	2.10563100	0.23290000
O	3.26496400	-3.02916100	0.72807000
O	2.32287900	-2.20574400	1.26782500
H	2.79971300	-1.63445200	1.89279400

Zero-point correction= 0.227907 (Hartree/Particle)
Thermal correction to Energy= 0.245074
Thermal correction to Enthalpy= 0.246019
Thermal correction to Gibbs Free Energy= 0.180127
Sum of electronic and zero-point Energies= -916.752098
Sum of electronic and thermal Energies= -916.734931
Sum of electronic and thermal Enthalpies= -916.733987
Sum of electronic and thermal Free Energies= -916.799878

Cartesian coordinates of the HT transition-states in the *trans*-piceatannol oxidation by •OOH radicals in water (Anion)

HT-3A/HT-5A

C	-3.49536400	0.55103400	-0.71331700
C	-2.09657800	0.43300100	-0.57537600
C	-1.52512200	-0.77925200	-0.16724600
C	-2.37790700	-1.85065900	0.09402300
C	-3.77034400	-1.72378900	-0.04531100
C	-4.34392400	-0.53634400	-0.43984600
H	-1.49777000	1.30354000	-0.80380400
H	-1.97538100	-2.80419200	0.40977500
H	-5.41515800	-0.42991600	-0.54575400
C	-0.08274400	-0.97834900	-0.00206900
H	0.19896800	-1.96518800	0.34645200
C	0.86224400	-0.05565200	-0.24810000
H	0.55878900	0.92709400	-0.59421300
C	2.30507500	-0.21600300	-0.09895700
C	3.12978600	0.89888900	-0.35352400
C	2.92236800	-1.41242200	0.28498700
C	4.49349500	0.80353900	-0.21788800
H	2.68925800	1.84199500	-0.65539600
C	4.30120400	-1.50203600	0.41993700
H	2.32393500	-2.29250400	0.48100300
C	5.14451600	-0.39802300	0.17725000
H	4.75958700	-2.43720200	0.71789100
O	5.31353000	1.88835800	-0.46058500
H	6.20948000	1.55116900	-0.29002500
O	6.44303300	-0.40416000	0.28728400
O	-4.01348700	1.70867600	-1.11482900
H	-3.92047700	2.43944900	-0.28173500
O	-4.50953000	-2.83450800	0.23710500
H	-5.44907800	-2.64282100	0.12999500
O	-3.74031800	2.99957200	0.85680600
O	-3.13138300	2.01061900	1.56243300
H	-2.17714700	2.15652700	1.45271300

Zero-point correction= 0.231975 (Hartree/Particle)
Thermal correction to Energy= 0.250280
Thermal correction to Enthalpy= 0.251224
Thermal correction to Gibbs Free Energy= 0.183101
Sum of electronic and zero-point Energies= -992.000054
Sum of electronic and thermal Energies= -991.981748
Sum of electronic and thermal Enthalpies= -991.980804
Sum of electronic and thermal Free Energies= -992.048928

Cartesian coordinates of the reagents in water

•OOH

O	0.05481200	-0.59559700	0.00000000
H	-0.87698800	-0.88325100	0.00000000
O	0.05481200	0.70600300	0.00000000

Zero-point correction= 0.014669 (Hartree/Particle)
Thermal correction to Energy= 0.017520
Thermal correction to Enthalpy= 0.018464
Thermal correction to Gibbs Free Energy= -0.007461
Sum of electronic and zero-point Energies= -150.923266
Sum of electronic and thermal Energies= -150.920415
Sum of electronic and thermal Enthalpies= -150.919471
Sum of electronic and thermal Free Energies= -150.945397

ΔE_{SET} (Hartree/Particle)
-0.150862042

$O_2^{-\cdot}$

O	0.00000000	0.00000000	0.65852600
O	0.00000000	0.00000000	-0.65852600

Zero-point correction= 0.002936 (Hartree/Particle)
Thermal correction to Energy= 0.005308
Thermal correction to Enthalpy= 0.006252
Thermal correction to Gibbs Free Energy= -0.016815
Sum of electronic and zero-point Energies= -150.484107
Sum of electronic and thermal Energies= -150.481735
Sum of electronic and thermal Enthalpies= -150.480790
Sum of electronic and thermal Free Energies= -150.503857

ΔE_{SET} (Hartree/Particle)
0.165536126

Resveratrol

C	3.63053300	1.22865200	-0.00009700
C	2.25391300	1.06916300	-0.00001600
C	1.71071900	-0.22246500	0.00003200
C	2.56528600	-1.32593000	0.00001200
C	3.94305000	-1.13590400	-0.00006400
C	4.49444600	0.13639400	-0.00012000
H	1.62483700	1.94893800	0.00000500
H	2.16689600	-2.33157900	0.00005000
H	5.56625000	0.28420400	-0.00018000
C	0.26437100	-0.48050500	0.00009300
H	-0.00372400	-1.53070800	0.00017500
C	-0.69566300	0.45337800	0.00003500
H	-0.42139900	1.50235400	-0.00005600
C	-2.14209900	0.21196600	0.00006700
C	-3.00175100	1.31669900	-0.00006900
C	-2.71716300	-1.06524700	0.00021300
C	-4.38013500	1.16528100	-0.00007800
H	-2.57881700	2.31349800	-0.00017800
C	-4.09250500	-1.23063000	0.00021100
H	-2.09206100	-1.94762100	0.00032600
C	-4.92447800	-0.11289200	0.00005600
H	-4.52822700	-2.22201700	0.00032100
O	-6.29236900	-0.22439600	0.00003100
H	-6.54738700	-1.15400300	0.00006000
O	4.21145900	2.47289700	-0.00015500
H	3.52730300	3.15255100	-0.00015500
O	4.73213500	-2.25883600	-0.00008100
H	5.66204500	-2.00536300	-0.00016600
H	-5.03665600	2.02467500	-0.00018900

Zero-point correction= 0.229626 (Hartree/Particle)
Thermal correction to Energy= 0.244516
Thermal correction to Enthalpy= 0.245461
Thermal correction to Gibbs Free Energy= 0.186003
Sum of electronic and zero-point Energies= -766.304556
Sum of electronic and thermal Energies= -766.289666
Sum of electronic and thermal Enthalpies= -766.288722
Sum of electronic and thermal Free Energies= -766.348180

ΔE_{SET} (Hartree/Particle)
0.212199083

Piceatannol

C	3.89658500	1.30029600	-0.03192600
C	2.53102100	1.06635200	-0.04161800
C	2.05844100	-0.25205800	-0.01030500
C	2.97088500	-1.30742800	0.02843600
C	4.33641400	-1.04298400	0.03838300
C	4.81804500	0.25707200	0.00639000
H	1.85548400	1.91027300	-0.07458100
H	2.62761800	-2.33285400	0.05364600
H	5.88069700	0.46180600	0.01343900
C	0.62771200	-0.58666700	-0.01568100
H	0.41550600	-1.64963400	-0.01901400
C	-0.38080600	0.29431400	-0.01060000
H	-0.16470900	1.35675200	0.00181100
C	-1.81186600	-0.03198000	-0.01439200
C	-2.72541500	1.02729200	0.03984900
C	-2.30728300	-1.33916000	-0.06968800
C	-4.08846700	0.79179600	0.04149700
H	-2.37557200	2.05090700	0.08369700
C	-3.67430900	-1.57540200	-0.06960000
H	-1.63435100	-2.18333300	-0.11495300
C	-4.56859000	-0.51576700	-0.01546300
H	-4.06220300	-2.58546000	-0.11329000
O	-4.95733500	1.85259400	0.09916100
H	-5.86261700	1.51737600	0.09769300
O	-5.93246200	-0.66280800	-0.01228900
H	-6.16964800	-1.59666100	-0.05402900
O	4.40690900	2.57453300	-0.06045300
H	3.68353400	3.21199000	-0.08032600
O	5.18441500	-2.12126700	0.08160800
H	6.09985000	-1.81963900	0.08999400

Zero-point correction= 0.233854 (Hartree/Particle)
Thermal correction to Energy= 0.249835
Thermal correction to Enthalpy= 0.250780
Thermal correction to Gibbs Free Energy= 0.189150
Sum of electronic and zero-point Energies= -841.546741
Sum of electronic and thermal Energies= -841.530759
Sum of electronic and thermal Enthalpies= -841.529815
Sum of electronic and thermal Free Energies= -841.591445

ΔE_{SET} (Hartree/Particle)
0.211784293

Anion of Resveratrol

C	3.57145500	1.23727600	-0.00015600
C	2.19645200	1.06562200	-0.00011000
C	1.66015400	-0.23058500	-0.00000800
C	2.52924200	-1.32501200	0.00005200
C	3.90445000	-1.12219900	0.00001100
C	4.44715300	0.15442300	-0.00009500
H	1.56113200	1.94092400	-0.00016000
H	2.14170700	-2.33496400	0.00013100
H	5.51764100	0.31106600	-0.00013300
C	0.21829000	-0.50093800	0.00003200
H	-0.04278100	-1.55316600	0.00009500
C	-0.75353500	0.42741000	-0.00000300
H	-0.47742000	1.47704700	-0.00005900
C	-2.19267400	0.19304100	0.00003000
C	-3.06213100	1.29489200	0.00001800
C	-2.78185900	-1.08387700	0.00007300
C	-4.43757800	1.14632600	0.00005300
H	-2.63712200	2.29276400	-0.00001700
C	-4.15222100	-1.24709700	0.00010700
H	-2.15497100	-1.96707700	0.00008000
C	-5.04580300	-0.13709600	0.00010100
H	-4.57973300	-2.24278600	0.00013900
O	-6.33570200	-0.29425900	0.00013600
O	4.13972000	2.48860800	-0.00026900
H	3.44762900	3.16009700	-0.00033300
O	4.70407800	-2.23917000	0.00007700
H	5.63138200	-1.97671800	0.00003300
H	-5.08059400	2.01828400	0.00004500

Zero-point correction= 0.216430 (Hartree/Particle)
Thermal correction to Energy= 0.230883
Thermal correction to Enthalpy= 0.231828
Thermal correction to Gibbs Free Energy= 0.173759
Sum of electronic and zero-point Energies= -765.847194
Sum of electronic and thermal Energies= -765.832740
Sum of electronic and thermal Enthalpies= -765.831796
Sum of electronic and thermal Free Energies= -765.889865

ΔE_{SET} (Hartree/Particle)
0.175773802

Anion of Piceatannol

C	-3.84011100	1.31315900	-0.00600800
C	-2.47773200	1.06278300	-0.00803700
C	-2.01745000	-0.26193100	-0.00233800
C	-2.94750900	-1.30475700	0.00483700
C	-4.30915800	-1.02330500	0.00689200
C	-4.77666300	0.28280600	0.00098600
H	-1.79355900	1.90036700	-0.01424500
H	-2.61882300	-2.33533600	0.00949600
H	-5.83653300	0.50125000	0.00253300
C	-0.59277400	-0.61359100	-0.00340100
H	-0.39112200	-1.67886500	-0.00540600
C	0.42872500	0.25848200	-0.00090200
H	0.21222300	1.32191100	0.00305000
C	1.85437800	-0.05959600	-0.00203500
C	2.77536700	1.00719100	0.00793100
C	2.36452600	-1.36278500	-0.01263500
C	4.12744200	0.76234800	0.00761100
H	2.42086800	2.03136200	0.01635800
C	3.73274600	-1.60315400	-0.01310600
H	1.68907000	-2.20836400	-0.02095700
C	4.67169900	-0.55151200	-0.00324200
H	4.10583100	-2.62011800	-0.02164300
O	5.03953500	1.80001700	0.01820400
H	5.90424400	1.35577200	0.01460500
O	5.96817900	-0.69602000	-0.00328100
O	-4.33317500	2.59569000	-0.01099800
H	-3.60036900	3.22246100	-0.01448700
O	-5.17080700	-2.09299800	0.01540600
H	-6.08260200	-1.78077900	0.01673900

Zero-point correction= 0.220862 (Hartree/Particle)
Thermal correction to Energy= 0.236284
Thermal correction to Enthalpy= 0.237228
Thermal correction to Gibbs Free Energy= 0.175577
Sum of electronic and zero-point Energies= -841.094618
Sum of electronic and thermal Energies= -841.079195
Sum of electronic and thermal Enthalpies= -841.078251
Sum of electronic and thermal Free Energies= -841.139903

ΔE_{SET} (Hartree/Particle)
0.174650871

Cartesian coordinates of the reagents in pentylethanoate.

•OOH

O	0.05495000	-0.59829000	0.00000000
H	-0.87920000	-0.87622900	0.00000000
O	0.05495000	0.70781800	0.00000000

Zero-point correction= 0.014503 (Hartree/Particle)
Thermal correction to Energy= 0.017355
Thermal correction to Enthalpy= 0.018299
Thermal correction to Gibbs Free Energy= -0.007637
Sum of electronic and zero-point Energies= -150.921088
Sum of electronic and thermal Energies= -150.918236
Sum of electronic and thermal Enthalpies= -150.917292
Sum of electronic and thermal Free Energies= -150.943228

ΔE_{SET} (Hartree/Particle)
-0.15426359

Resveratrol

C	3.63664100	1.22993600	-0.00012000
C	2.25957500	1.07095900	-0.00008100
C	1.71245500	-0.21927300	-0.00001000
C	2.56406000	-1.32350800	0.00002600
C	3.94343900	-1.13941800	-0.00001100
C	4.49513600	0.13288000	-0.00008300
H	1.62591200	1.94816300	-0.00010200
H	2.16601800	-2.32909000	0.00008100
H	5.56664800	0.28700800	-0.00010900
C	0.26563700	-0.47440500	0.00003400
H	-0.00290300	-1.52447900	0.00012200
C	-0.69771500	0.45519200	-0.00002800
H	-0.42366400	1.50422700	-0.00011500
C	-2.14404500	0.21389100	0.00001400
C	-3.00676200	1.31615000	-0.00003600
C	-2.71861900	-1.06235700	0.00010000
C	-4.38415700	1.16425800	0.00000200
H	-2.58609700	2.31403800	-0.00010600
C	-4.09349000	-1.22889700	0.00014000
H	-2.09214600	-1.94368000	0.00013700
C	-4.92999000	-0.11372300	0.00009300
H	-4.52134900	-2.22454400	0.00020500
O	-6.28588100	-0.22512300	0.00013700
H	-6.53698600	-1.15404900	0.00016800
O	4.22005100	2.46024100	-0.00019400
H	3.53962900	3.14057000	-0.00022700
O	4.72140800	-2.25567100	0.00002800
H	5.65049400	-2.00547100	-0.00002500
H	-5.04317400	2.02161400	-0.00003600

Zero-point correction= 0.229932 (Hartree/Particle)
Thermal correction to Energy= 0.244845
Thermal correction to Enthalpy= 0.245789
Thermal correction to Gibbs Free Energy= 0.187031
Sum of electronic and zero-point Energies= -766.298393
Sum of electronic and thermal Energies= -766.283480
Sum of electronic and thermal Enthalpies= -766.282536
Sum of electronic and thermal Free Energies= -766.341294

ΔE_{SET} (Hartree/Particle)
0.206050905

Piceatannol

C	3.89681400	1.29972000	-0.09146800
C	2.53210200	1.05987800	-0.12075400
C	2.05955800	-0.25581900	-0.02644900
C	2.97107700	-1.30477200	0.08584100
C	4.33718500	-1.04013400	0.11246900
C	4.81495100	0.25878400	0.02662200
H	1.85113400	1.89420700	-0.22531100
H	2.62983300	-2.32843200	0.15643500
H	5.87513200	0.47576800	0.04550200
C	0.62912900	-0.59120200	-0.04186700
H	0.41719800	-1.65407100	-0.06233500
C	-0.38126400	0.28603200	-0.01606300
H	-0.16293100	1.34697600	0.03296100
C	-1.81327000	-0.03543300	-0.03252900
C	-2.72212200	1.01740200	0.12560400
C	-2.31306300	-1.33013400	-0.20166300
C	-4.08608600	0.78928500	0.12162100
H	-2.36849700	2.03209200	0.25592600
C	-3.68141900	-1.56309700	-0.20493000
H	-1.64296600	-2.16645100	-0.33918200
C	-4.56774700	-0.50922900	-0.04444300
H	-4.06566600	-2.56762200	-0.33666200
O	-4.94886200	1.82741500	0.27740400
H	-5.84980900	1.48523100	0.25144000
O	-5.92868000	-0.63568900	-0.03919500
H	-6.18591000	-1.55510600	-0.15959700
O	4.40887700	2.55803100	-0.18075400
H	3.69115300	3.19388100	-0.26168400
O	5.17698300	-2.10517700	0.22436000
H	6.08971100	-1.80080400	0.23604600

Zero-point correction= 0.234053 (Hartree/Particle)
Thermal correction to Energy= 0.250187
Thermal correction to Enthalpy= 0.251131
Thermal correction to Gibbs Free Energy= 0.189781
Sum of electronic and zero-point Energies= -841.537951
Sum of electronic and thermal Energies= -841.521817
Sum of electronic and thermal Enthalpies= -841.520873
Sum of electronic and thermal Free Energies= -841.582223

ΔE_{SET} (Hartree/Particle)
0.149010609

Cartesian coordinates of the HT products in water.

HOOH

O	0.00000000	-0.71032100	-0.06901600
H	-0.70790200	-0.92610900	0.55212800
O	0.00000000	0.71032100	-0.06901600
H	0.70790200	0.92610900	0.55212800

Zero-point correction= 0.027011 (Hartree/Particle)
Thermal correction to Energy= 0.030242
Thermal correction to Enthalpy= 0.031187
Thermal correction to Gibbs Free Energy= 0.005391
Sum of electronic and zero-point Energies= -151.559264
Sum of electronic and thermal Energies= -151.556032
Sum of electronic and thermal Enthalpies= -151.555088
Sum of electronic and thermal Free Energies= -151.580884

Products for Resveratrol

3A/5A

C	3.70125100	1.18724000	-0.00008900
C	2.30280600	0.98811900	-0.00003900
C	1.74556900	-0.31409400	0.00000200
C	2.60117700	-1.39059900	-0.00000200
C	4.03756900	-1.21196600	-0.00005100
C	4.56378500	0.12900900	-0.00009600
H	1.66765000	1.86262800	-0.00002800
H	2.22482600	-2.40472000	0.00003200
H	5.63483600	0.27364200	-0.00013200
C	0.29831400	-0.54919600	0.00005100
H	0.01722400	-1.59554400	0.00013100
C	-0.64449700	0.40285000	-0.00000300
H	-0.35518100	1.44728200	-0.00009300
C	-2.09408600	0.19005900	0.00003700
C	-2.92849600	1.31406100	-0.00009400
C	-2.69528200	-1.07505000	0.00019600
C	-4.30938800	1.19299200	-0.00008000
H	-2.48278900	2.30082300	-0.00021300
C	-4.07356000	-1.21003300	0.00021600
H	-2.08891200	-1.97033700	0.00030500
C	-4.88054900	-0.07366800	0.00007200
H	-4.53151400	-2.19124500	0.00034000
O	-6.24902400	-0.15705300	0.00007400
H	-6.52076900	-1.08185800	0.00013300
O	4.21341300	2.45164300	-0.00012700
H	3.50325100	3.10489500	-0.00011800
O	4.80199700	-2.20584600	-0.00005800
H	-4.94740100	2.06614400	-0.00018500

Zero-point correction= 0.216646 (Hartree/Particle)
Thermal correction to Energy= 0.231191
Thermal correction to Enthalpy= 0.232135
Thermal correction to Gibbs Free Energy= 0.173077
Sum of electronic and zero-point Energies= -765.666224
Sum of electronic and thermal Energies= -765.651679
Sum of electronic and thermal Enthalpies= -765.650735
Sum of electronic and thermal Free Energies= -765.709794

4B

C	3.55047200	1.23547900	-0.00016800
C	2.17463000	1.07871900	-0.00010700
C	1.63439500	-0.21608100	0.00000700
C	2.48530400	-1.32511600	0.00007300
C	3.86197500	-1.13654100	0.00002600
C	4.40947600	0.13820400	-0.00009700
H	1.54532100	1.95784300	-0.00016200
H	2.08216800	-2.32859700	0.00016000
H	5.48146400	0.28559000	-0.00014600
C	0.20153600	-0.47493300	0.00004700
H	-0.06671900	-1.52309800	0.00010000
C	-0.77499800	0.47281900	0.00002200
H	-0.50082300	1.52028200	-0.00001700
C	-2.17728700	0.21418000	0.00004600
C	-3.06553000	1.33095400	0.00004700
C	-2.74116100	-1.09957200	0.00006300
C	-4.41439100	1.16842800	0.00006500
H	-2.63612300	2.32471800	0.00003500
C	-4.08522000	-1.28247900	0.00007800
H	-2.09244800	-1.96376400	0.00006000
C	-4.99943000	-0.15626800	0.00008000
H	-4.51784400	-2.27395800	0.00008800
O	-6.23918700	-0.32457400	0.00009100
O	4.13740300	2.47423800	-0.00030500
H	3.45858500	3.15941400	-0.00040100
O	4.65104800	-2.25663700	0.00009800
H	5.58142600	-2.00434800	0.00004400
H	-5.08774900	2.01494600	0.00006800

Zero-point correction= 0.217162 (Hartree/Particle)
Thermal correction to Energy= 0.231649
Thermal correction to Enthalpy= 0.232593
Thermal correction to Gibbs Free Energy= 0.174049
Sum of electronic and zero-point Energies= -765.676343
Sum of electronic and thermal Energies= -765.661856
Sum of electronic and thermal Enthalpies= -765.660912
Sum of electronic and thermal Free Energies= -765.719456

ΔE_{SET} (Hartree/Particle)
-0.164427178

Products for anionic Resveratrol

3A/5A

C	3.61694800	1.34537100	-0.00014200
C	2.20719600	1.15287500	-0.00011800
C	1.66433300	-0.11953200	-0.00003200
C	2.54066900	-1.25320700	0.00003000
C	3.92792400	-1.08758100	0.00000500
C	4.47129900	0.17090500	-0.00008100
H	1.58645800	2.03755700	-0.00016600
H	2.12706400	-2.25189900	0.00009800
H	5.54364500	0.31857300	-0.00010400
C	0.25624200	-0.43711700	0.00000400
H	0.01666500	-1.49268500	0.00006900
C	-0.74747800	0.48348000	-0.00003200
H	-0.48158700	1.53553900	-0.00009400
C	-2.15388200	0.22238600	0.00000800
C	-3.05194800	1.31490600	-0.00002500
C	-2.71543100	-1.07840400	0.00008700
C	-4.41314300	1.13798200	0.00002300
H	-2.64237200	2.31860100	-0.00008800
C	-4.07155800	-1.27088900	0.00013500
H	-2.06531000	-1.94380100	0.00011000
C	-4.99241400	-0.17003700	0.00011100
H	-4.48411900	-2.27214900	0.00019700
O	-6.25931600	-0.35292900	0.00016800
O	4.15154200	2.49384300	-0.00022000
O	4.68600000	-2.22923700	0.00006600
H	5.62260400	-1.99988100	0.00003900
H	-5.08139700	1.98990300	-0.00000100

Zero-point correction=	0.205536 (Hartree/Particle)
Thermal correction to Energy=	0.219565
Thermal correction to Enthalpy=	0.220509
Thermal correction to Gibbs Free Energy=	0.162675
Sum of electronic and zero-point Energies=	-765.205552
Sum of electronic and thermal Energies=	-765.191523
Sum of electronic and thermal Enthalpies=	-765.190579
Sum of electronic and thermal Free Energies=	-765.248413

Products for Piceatannol

3A/5A

C	3.97199100	1.26009900	0.00014200
C	2.58478100	0.99231900	0.00029700
C	2.09417100	-0.33563200	0.00007900
C	3.00259700	-1.36848800	-0.00019200
C	4.42847500	-1.11863200	-0.00026400
C	4.88657100	0.24668700	-0.00008000
H	1.90705700	1.83448600	0.00061100
H	2.67781300	-2.40025500	-0.00035300
H	5.94888600	0.44546800	-0.00014800
C	0.66091200	-0.64496100	0.00016900
H	0.43502300	-1.70457200	0.00027700
C	-0.33172000	0.25437200	0.00009700
H	-0.10229200	1.31362800	-0.00002100
C	-1.76676800	-0.04923300	0.00013500
C	-2.66246400	1.02660000	-0.00015200
C	-2.28162100	-1.34982300	0.00042900
C	-4.02888000	0.81337800	-0.00019300
H	-2.29586700	2.04523400	-0.00033900
C	-3.65198000	-1.56374800	0.00033200
H	-1.62214500	-2.20570100	0.00068800
C	-4.52919500	-0.48838300	0.00002500
H	-4.05580700	-2.56841700	0.00052100
O	-4.88014900	1.88928700	-0.00051800
H	-5.79106600	1.56980300	-0.00013600
O	-5.89415800	-0.61354900	-0.00026000
H	-6.14694300	-1.54427200	0.00151900
O	4.42087200	2.54805900	0.00026100
H	3.67869700	3.16437400	0.00038100
O	5.24161300	-2.07343400	-0.00047700

Zero-point correction= 0.221230 (Hartree/Particle)
Thermal correction to Energy= 0.236890
Thermal correction to Enthalpy= 0.237835
Thermal correction to Gibbs Free Energy= 0.176603
Sum of electronic and zero-point Energies= -840.908037
Sum of electronic and thermal Energies= -840.892376
Sum of electronic and thermal Enthalpies= -840.891432
Sum of electronic and thermal Free Energies= -840.952663

3B

C	-3.86174400	1.28844600	0.00004600
C	-2.49268600	1.07548100	0.00006900
C	-2.00305300	-0.23653900	0.00003300
C	-2.89687800	-1.30774900	-0.00002400
C	-4.26640500	-1.06446900	-0.00005200
C	-4.76582800	0.22918300	-0.00001000
H	-1.82943900	1.92951600	0.00012300
H	-2.53697500	-2.32767600	-0.00005300
H	-5.83151100	0.41756300	-0.00002000
C	-0.56862100	-0.55043400	0.00004900
H	-0.34567800	-1.61029700	0.00011700
C	0.42486900	0.34932600	-0.00002400
H	0.19568300	1.40825000	-0.00009900
C	1.85552100	0.04606200	-0.00001500
C	2.74863200	1.08687600	-0.00008600
C	2.34915300	-1.30270700	0.00006500
C	4.15957000	0.85515700	-0.00008500
H	2.40869900	2.11427700	-0.00014400
C	3.69573100	-1.58386600	0.00009000
H	1.65235400	-2.12703900	0.00011500
C	4.60466400	-0.53248200	0.00002700
H	4.05712100	-2.60228400	0.00015900
O	5.03290200	1.75735000	-0.00010500
O	5.91641600	-0.75173800	0.00005400
H	6.35819300	0.11652100	-0.00000900
O	-4.39260600	2.55350000	0.00006800
H	-3.68076500	3.20430100	0.00023300
O	-5.09765200	-2.15523300	-0.00011500
H	-6.01770800	-1.86788700	-0.00014800

Zero-point correction= 0.222018 (Hartree/Particle)
Thermal correction to Energy= 0.237422
Thermal correction to Enthalpy= 0.238366
Thermal correction to Gibbs Free Energy= 0.177777
Sum of electronic and zero-point Energies= -840.920272
Sum of electronic and thermal Energies= -840.904867
Sum of electronic and thermal Enthalpies= -840.903923
Sum of electronic and thermal Free Energies= -840.964512

4B

C	-3.82430200	1.30887900	-0.00000100
C	-2.45943700	1.07563500	0.00000600
C	-1.99073900	-0.24562000	0.00001000
C	-2.90162700	-1.30477100	-0.00000600
C	-4.26646300	-1.04037100	-0.00000900
C	-4.74358900	0.26227500	0.00000600
H	-1.78353000	1.91940400	0.00000400
H	-2.55647200	-2.32966600	-0.00002300
H	-5.80620300	0.46789300	0.00001000
C	-0.56943900	-0.58104000	0.00000900
H	-0.35869500	-1.64272900	-0.00002800
C	0.44833100	0.31183400	0.00004400
H	0.22865300	1.37236100	0.00007200
C	1.84817300	-0.01482300	0.00003700
C	2.77363200	1.04775700	0.00002400
C	2.33249700	-1.36366700	0.00003800
C	4.11758800	0.79015900	-0.00000600
H	2.42393600	2.07159700	0.00002900
C	3.66242000	-1.63467800	0.00001200
H	1.63033000	-2.18419100	0.00006700
C	4.63359100	-0.57223300	-0.00002500
H	4.03349300	-2.65036200	0.00002500
O	5.02538900	1.78275800	-0.00002400
H	5.90496000	1.36940900	-0.00004100
O	5.87234500	-0.75049900	-0.00004500
O	-4.33713900	2.58039800	-0.00003300
H	-3.61624400	3.22121600	0.00010500
O	-5.11475100	-2.11692500	-0.00000300
H	-6.03079300	-1.81680100	-0.00022100

Zero-point correction= 0.221848 (Hartree/Particle)
Thermal correction to Energy= 0.237196
Thermal correction to Enthalpy= 0.238140
Thermal correction to Gibbs Free Energy= 0.177520
Sum of electronic and zero-point Energies= -840.926072
Sum of electronic and thermal Energies= -840.910724
Sum of electronic and thermal Enthalpies= -840.909780
Sum of electronic and thermal Free Energies= -840.970400

ΔE_{SET} (Hartree/Particle)
-0.160723063

Products for anionic Piceatannol

3A/5A

C	3.88064900	1.41505700	-0.00015800
C	2.49510500	1.12260300	-0.00013700
C	2.02659800	-0.19408200	-0.00000500
C	2.92635700	-1.27023400	0.00011400
C	4.28851400	-0.99471800	0.00009300
C	4.76823700	0.30374800	-0.00004900
H	1.80788700	1.95786000	-0.00022200
H	2.57568100	-2.29303800	0.00022300
H	5.83736100	0.48456900	-0.00006200
C	0.60657400	-0.53284600	0.00002500
H	0.39932100	-1.59565600	0.00013200
C	-0.42305200	0.35007900	-0.00006500
H	-0.21230300	1.41254200	-0.00016800
C	-1.81616500	0.00643400	-0.00002300
C	-2.75876300	1.05660800	-0.00010800
C	-2.28538800	-1.34779500	0.00010600
C	-4.09792200	0.78146700	-0.00005500
H	-2.42252800	2.08504500	-0.00021500
C	-3.61241600	-1.63528100	0.00016500
H	-1.57402900	-2.16033300	0.00015900
C	-4.59692500	-0.58622600	0.00010200
H	-3.97022500	-2.65581100	0.00026600
O	-5.02103000	1.76298200	-0.00013900
H	-5.89388000	1.33580500	-0.00008000
O	-5.83482500	-0.78006600	0.00017000
O	4.33177200	2.63614800	-0.00028800
O	5.14735300	-2.07628700	0.00022400
H	6.05813300	-1.76208400	0.00021200

Zero-point correction= 0.208417 (Hartree/Particle)
Thermal correction to Energy= 0.223503
Thermal correction to Enthalpy= 0.224447
Thermal correction to Gibbs Free Energy= 0.164001
Sum of electronic and zero-point Energies= -840.469090
Sum of electronic and thermal Energies= -840.454003
Sum of electronic and thermal Enthalpies= -840.453059
Sum of electronic and thermal Free Energies= -840.513505

Cartesian coordinates of the HT products in pentylethanoate

HOOH

O	0.00000000	-0.71138400	-0.05935600
H	-0.77886300	-0.90955500	0.47484600
O	0.00000000	0.71138400	-0.05935600
H	0.77886300	0.90955500	0.47484600

Zero-point correction= 0.026972 (Hartree/Particle)
Thermal correction to Energy= 0.030186
Thermal correction to Enthalpy= 0.031130
Thermal correction to Gibbs Free Energy= 0.005368
Sum of electronic and zero-point Energies= -151.553001
Sum of electronic and thermal Energies= -151.549787
Sum of electronic and thermal Enthalpies= -151.548843
Sum of electronic and thermal Free Energies= -151.574605

Products for Resveratrol

3A/5A

C	3.70591500	1.18824500	-0.00013600
C	2.31098400	0.99183300	-0.00010800
C	1.74783300	-0.30691800	-0.00001100
C	2.59936500	-1.38773000	0.00006100
C	4.03895700	-1.22025000	0.00003800
C	4.56540000	0.12378100	-0.00006500
H	1.67090800	1.86366400	-0.00016100
H	2.22022500	-2.40074200	0.00013900
H	5.63672800	0.26593400	-0.00008500
C	0.29894100	-0.53748600	0.00002200
H	0.01610700	-1.58341900	0.00010200
C	-0.64790200	0.40957700	-0.00003500
H	-0.35958600	1.45452800	-0.00011000
C	-2.09743200	0.19486300	0.00000400
C	-2.93753500	1.31451400	-0.00002400
C	-2.69579900	-1.07033000	0.00006600
C	-4.31720200	1.18984800	0.00001600
H	-2.49727700	2.30392700	-0.00007600
C	-4.07334500	-1.20940000	0.00010700
H	-2.08703800	-1.96397500	0.00008400
C	-4.88772200	-0.07763700	0.00008400
H	-4.52105700	-2.19610000	0.00015500
O	-6.24445400	-0.16228800	0.00012600
H	-6.51470100	-1.08597600	0.00015400
O	4.22640400	2.44349700	-0.00023200
H	3.52084400	3.09798800	-0.00030000
O	4.79445900	-2.21036600	0.00010400
H	-4.95917400	2.05997000	-0.00000500

Zero-point correction= 0.216513 (Hartree/Particle)
Thermal correction to Energy= 0.231164
Thermal correction to Enthalpy= 0.232108
Thermal correction to Gibbs Free Energy= 0.173474
Sum of electronic and zero-point Energies= -765.660801
Sum of electronic and thermal Energies= -765.646149
Sum of electronic and thermal Enthalpies= -765.645205
Sum of electronic and thermal Free Energies= -765.703840

4B

C	3.55757500	1.23754800	-0.00013000
C	2.18138300	1.07825500	-0.00008600
C	1.63931000	-0.21592900	-0.00000900
C	2.49011600	-1.32290300	0.00002700
C	3.86872600	-1.13710200	-0.00001500
C	4.41446800	0.13800100	-0.00009100
H	1.54573100	1.95367200	-0.00011100
H	2.09084500	-2.32787900	0.00008600
H	5.48581800	0.29404500	-0.00012100
C	0.20380000	-0.47398100	0.00003700
H	-0.06426800	-1.52241900	0.00011200
C	-0.77460700	0.46676500	-0.00000800
H	-0.50016700	1.51441300	-0.00008300
C	-2.18232600	0.21191300	0.00003300
C	-3.06789500	1.32910000	-0.00002400
C	-2.74859900	-1.09973500	0.00012400
C	-4.41771200	1.17070000	0.00000500
H	-2.63717800	2.32271300	-0.00009100
C	-4.09284900	-1.28282800	0.00015500
H	-2.09845000	-1.96324600	0.00016800
C	-5.01442600	-0.15489400	0.00009600
H	-4.52804100	-2.27322800	0.00022300
O	-6.24174200	-0.31831300	0.00011900
O	4.14462000	2.46403800	-0.00021100
H	3.46918100	3.14964000	-0.00024700
O	4.64808800	-2.24997100	0.00002300
H	5.57770700	-2.00070700	-0.00002700
H	-5.09068700	2.01749300	-0.00003800

Zero-point correction= 0.217277 (Hartree/Particle)
Thermal correction to Energy= 0.231787
Thermal correction to Enthalpy= 0.232731
Thermal correction to Gibbs Free Energy= 0.174224
Sum of electronic and zero-point Energies= -765.670387
Sum of electronic and thermal Energies= -765.655878
Sum of electronic and thermal Enthalpies= -765.654934
Sum of electronic and thermal Free Energies= -765.713441

Products for Piceatannol

3A/5A

C	3.97885400	1.26109300	0.00014700
C	2.59431200	0.99848100	0.00023800
C	2.09599200	-0.32581400	0.00006400
C	2.99912800	-1.36418500	-0.00018500
C	4.42874500	-1.12791300	-0.00028800
C	4.88911400	0.23962300	-0.00011300
H	1.91282700	1.83877300	0.00046000
H	2.66956600	-2.39422400	-0.00032000
H	5.95225800	0.43396900	-0.00018300
C	0.66118000	-0.63150600	0.00013200
H	0.43448300	-1.69104000	0.00019600
C	-0.33578400	0.26173800	0.00007100
H	-0.10712600	1.32144200	-0.00004200
C	-1.77105900	-0.04409300	0.00009900
C	-2.66964600	1.02910700	-0.00020700
C	-2.28160500	-1.34551200	0.00040400
C	-4.03585300	0.81410400	-0.00021500
H	-2.30808100	2.04935300	-0.00042300
C	-3.65161100	-1.56519000	0.00036800
H	-1.61851800	-2.19834300	0.00065800
C	-4.52864300	-0.49116400	0.00006200
H	-4.04410500	-2.57498500	0.00057500
O	-4.88956300	1.87038900	-0.00049900
H	-5.79396400	1.53624300	-0.00019800
O	-5.88964000	-0.60371900	-0.00004900
H	-6.15618400	-1.52846700	0.00127700
O	4.43879600	2.53915500	0.00032500
H	3.70291300	3.15947600	0.00046800
O	5.23005600	-2.08142500	-0.00051800

Zero-point correction= 0.220748 (Hartree/Particle)
Thermal correction to Energy= 0.236746
Thermal correction to Enthalpy= 0.237690
Thermal correction to Gibbs Free Energy= 0.174623
Sum of electronic and zero-point Energies= -840.900146
Sum of electronic and thermal Energies= -840.884149
Sum of electronic and thermal Enthalpies= -840.883204
Sum of electronic and thermal Free Energies= -840.946272

3B

C	3.86820200	1.28853200	-0.05736100
C	2.49917800	1.07373300	-0.08869400
C	2.00631300	-0.23602400	-0.03125600
C	2.89697500	-1.30497500	0.04738000
C	4.26782600	-1.06539600	0.07816200
C	4.76680300	0.22730600	0.02897600
H	1.83173300	1.92185100	-0.16371100
H	2.53732000	-2.32385800	0.08976500
H	5.83096700	0.42442900	0.05324100
C	0.57103400	-0.54737500	-0.04919700
H	0.34633700	-1.60648400	-0.08323600
C	-0.42452200	0.34744400	-0.01083000
H	-0.19340500	1.40471800	0.04304200
C	-1.85748600	0.04681400	-0.01926100
C	-2.74896500	1.08320400	0.08993000
C	-2.35303800	-1.29398800	-0.13798800
C	-4.16319200	0.85164700	0.09167800
H	-2.40962400	2.10673500	0.18012800
C	-3.70145300	-1.57847100	-0.14213600
H	-1.65540500	-2.11277100	-0.22972200
C	-4.60800800	-0.53329500	-0.02925500
H	-4.06033100	-2.59413500	-0.23259300
O	-5.03890900	1.73474300	0.18931100
O	-5.91824200	-0.73244000	-0.02657400
H	-6.32173300	0.15133000	0.06171500
O	4.40348600	2.53818000	-0.11169800
H	3.69903000	3.19058500	-0.17662100
O	5.08751900	-2.14744400	0.15677800
H	6.00627000	-1.86164600	0.17456200

Zero-point correction= 0.222338 (Hartree/Particle)
Thermal correction to Energy= 0.237819
Thermal correction to Enthalpy= 0.238763
Thermal correction to Gibbs Free Energy= 0.177575
Sum of electronic and zero-point Energies= -840.914450
Sum of electronic and thermal Energies= -840.898969
Sum of electronic and thermal Enthalpies= -840.898025
Sum of electronic and thermal Free Energies= -840.959213

4B

C	3.83327000	1.30876900	-0.03507000
C	2.46764300	1.07617500	-0.05488000
C	1.99393100	-0.24307000	-0.02110300
C	2.90106600	-1.30198800	0.02853000
C	4.26800100	-1.04364200	0.04938300
C	4.74693800	0.25755900	0.01893100
H	1.78802800	1.91642400	-0.10090900
H	2.55580300	-2.32625400	0.05434900
H	5.80849400	0.46952300	0.03432900
C	0.57068200	-0.57537200	-0.03365000
H	0.35857700	-1.63670300	-0.05453200
C	-0.44821000	0.31241800	-0.00978200
H	-0.22582200	1.37204600	0.02512700
C	-1.85213900	-0.01035000	-0.01500900
C	-2.77489500	1.05098500	0.05143300
C	-2.33737100	-1.35683200	-0.08335200
C	-4.12018800	0.79288800	0.05149400
H	-2.42495300	2.07336300	0.10394000
C	-3.66664100	-1.63244500	-0.08517200
H	-1.63268800	-2.17377000	-0.13653500
C	-4.63999000	-0.57103900	-0.01712700
H	-4.03684300	-2.64719200	-0.13748400
O	-5.03381200	1.76402500	0.11322000
H	-5.89882700	1.31830700	0.09818600
O	-5.87217400	-0.73296000	-0.01359700
O	4.35219500	2.56530600	-0.06840500
H	3.63956200	3.21078200	-0.11027800
O	5.10347600	-2.11439600	0.09932700
H	6.01861500	-1.81666300	0.11168900

Zero-point correction= 0.222299 (Hartree/Particle)
Thermal correction to Energy= 0.237755
Thermal correction to Enthalpy= 0.238699
Thermal correction to Gibbs Free Energy= 0.177023
Sum of electronic and zero-point Energies= -840.919868
Sum of electronic and thermal Energies= -840.904412
Sum of electronic and thermal Enthalpies= -840.903468
Sum of electronic and thermal Free Energies= -840.965144

Cartesian coordinates of the SET products in water.

OOH^-

O	0.05504300	-0.67656600	0.00000000
H	-0.88068800	-0.89743900	0.00000000
O	0.05504300	0.78874600	0.00000000

Zero-point correction= 0.013817 (Hartree/Particle)
Thermal correction to Energy= 0.016708
Thermal correction to Enthalpy= 0.017652
Thermal correction to Gibbs Free Energy= -0.007886
Sum of electronic and zero-point Energies= -151.092602
Sum of electronic and thermal Energies= -151.089710
Sum of electronic and thermal Enthalpies= -151.088766
Sum of electronic and thermal Free Energies= -151.114305

O_2

O	0.00000000	0.00000000	0.59248300
O	0.00000000	0.00000000	-0.59248300

Zero-point correction= 0.004044 (Hartree/Particle)
Thermal correction to Energy= 0.006406
Thermal correction to Enthalpy= 0.007350
Thermal correction to Gibbs Free Energy= -0.015888
Sum of electronic and zero-point Energies= -150.339507
Sum of electronic and thermal Energies= -150.337145
Sum of electronic and thermal Enthalpies= -150.336200
Sum of electronic and thermal Free Energies= -150.359439

Product from Resveratrol

C	3.89517600	-1.14190400	-0.00007300
C	2.52344600	-1.32328700	0.00007700
C	1.67699000	-0.20028500	0.00014100
C	2.21875900	1.09632300	0.00007800
C	3.59470900	1.24501600	-0.00006800
C	4.44112200	0.13816600	-0.00014500
H	2.10327100	-2.32057500	0.00013100
H	1.59842100	1.98009000	0.00012600
H	5.51573600	0.26787200	-0.00026900
C	0.26455900	-0.46009900	0.00023100
H	-0.00879600	-1.50600300	0.00025500
C	-0.72721000	0.49941600	0.00024800
H	-0.45143000	1.54572700	0.00023300
C	-2.11080000	0.22929300	0.00022600
C	-3.00302900	1.34079000	0.00015300
C	-2.66535600	-1.08625500	0.00021000
C	-4.35647100	1.16350400	-0.00001000
H	-2.58586900	2.33874700	0.00020500
C	-4.01504000	-1.27054200	0.00004900
H	-2.02109800	-1.95249500	0.00030000
C	-4.87194100	-0.14808000	-0.00011900
H	-4.45342800	-2.25807700	0.00000000
O	-6.17742300	-0.38730500	-0.00042100
H	-6.68571600	0.43623800	-0.00065700
O	4.76905400	-2.19158400	-0.00016500
H	4.28300100	-3.02490600	-0.00015300
O	4.09549700	2.51686800	-0.00014000
H	5.05982800	2.49550500	-0.00026700
H	-5.04043300	2.00171700	-0.00008900

Zero-point correction= 0.230064 (Hartree/Particle)
Thermal correction to Energy= 0.244817
Thermal correction to Enthalpy= 0.245762
Thermal correction to Gibbs Free Energy= 0.185966
Sum of electronic and zero-point Energies= -766.100040
Sum of electronic and thermal Energies= -766.085287
Sum of electronic and thermal Enthalpies= -766.084342
Sum of electronic and thermal Free Energies= -766.144138

Product from anionic Resveratrol

C	-3.55044600	1.23549700	0.00018800
C	-2.17460900	1.07872000	0.00012600
C	-1.63437500	-0.21609800	-0.00000500
C	-2.48534600	-1.32513400	-0.00009000
C	-3.86199300	-1.13654400	-0.00004700
C	-4.40945900	0.13823000	0.00009600
H	-1.54529900	1.95784000	0.00019700
H	-2.08216400	-2.32859600	-0.00018900
H	-5.48144500	0.28563800	0.00014800
C	-0.20162500	-0.47501300	-0.00004200
H	0.06668900	-1.52314900	-0.00008400
C	0.77507700	0.47277600	-0.00002800
H	0.50082300	1.52020600	-0.00000700
C	2.17720800	0.21412300	-0.00004800
C	3.06547800	1.33094800	-0.00008200
C	2.74121900	-1.09966900	-0.00002800
C	4.41431800	1.16847500	-0.00010200
H	2.63591300	2.32465700	-0.00009500
C	4.08524500	-1.28238300	-0.00004200
H	2.09256800	-1.96391300	0.00000400
C	4.99945300	-0.15614400	-0.00008200
H	4.51809600	-2.27372500	-0.00002200
O	6.23927600	-0.32462700	-0.00009700
O	-4.13736500	2.47424900	0.00034900
H	-3.45854800	3.15942700	0.00048500
O	-4.65111600	-2.25659700	-0.00013800
H	-5.58148600	-2.00428100	-0.00009400
H	5.08762600	2.01499100	-0.00013100

Zero-point correction= 0.217164 (Hartree/Particle)
Thermal correction to Energy= 0.231649
Thermal correction to Enthalpy= 0.232594
Thermal correction to Gibbs Free Energy= 0.174055
Sum of electronic and zero-point Energies= -765.676342
Sum of electronic and thermal Energies= -765.661856
Sum of electronic and thermal Enthalpies= -765.660912
Sum of electronic and thermal Free Energies= -765.719450

Product from Piceatannol

C	3.86095400	1.30532000	-0.01468200
C	2.49696600	1.08095400	-0.01145000
C	2.02535900	-0.24313300	0.00113300
C	2.92955700	-1.31341500	0.01118200
C	4.29343600	-1.05690100	0.00980100
C	4.77018500	0.24751400	-0.00463300
H	1.82468600	1.92696600	-0.02023300
H	2.57462300	-2.33462900	0.02142700
H	5.83390600	0.44840700	-0.00698000
C	0.62050400	-0.57335500	0.00326100
H	0.40153900	-1.63242400	0.00213500
C	-0.40782700	0.33542100	0.00862000
H	-0.18243000	1.39381400	0.01514000
C	-1.78565800	0.00537400	0.00761400
C	-2.71991900	1.06794100	0.02277400
C	-2.26548200	-1.34314200	-0.01203200
C	-4.06216100	0.81456200	0.01660800
H	-2.37437500	2.09243600	0.03935400
C	-3.60446900	-1.60277600	-0.02150300
H	-1.57462000	-2.17148200	-0.02192700
C	-4.51933900	-0.53721000	-0.01055200
H	-3.98795900	-2.61387500	-0.03956200
O	-4.95392000	1.82474000	0.03181700
H	-5.85723800	1.47923800	0.02609200
O	-5.83268200	-0.69320700	-0.02571500
H	-6.09552000	-1.62564600	-0.04932300
O	4.38798800	2.56693700	-0.02784600
H	3.67704400	3.21917200	-0.03341000
O	5.13762200	-2.13194800	0.02246200
H	6.05564400	-1.83707900	0.02470000

Zero-point correction= 0.234569 (Hartree/Particle)
Thermal correction to Energy= 0.250314
Thermal correction to Enthalpy= 0.251258
Thermal correction to Gibbs Free Energy= 0.189705
Sum of electronic and zero-point Energies= -841.342252
Sum of electronic and thermal Energies= -841.326507
Sum of electronic and thermal Enthalpies= -841.325563
Sum of electronic and thermal Free Energies= -841.387116

Product from anionic Piceatannol

C	-3.82431000	1.30886800	-0.00027700
C	-2.45944000	1.07563000	-0.00032300
C	-1.99072800	-0.24561300	-0.00008500
C	-2.90162200	-1.30476400	0.00019700
C	-4.26645700	-1.04037300	0.00026700
C	-4.74359900	0.26227100	-0.00001000
H	-1.78355200	1.91941600	-0.00056000
H	-2.55647900	-2.32966300	0.00040100
H	-5.80621400	0.46788000	0.00002500
C	-0.56942200	-0.58104800	-0.00011700
H	-0.35870500	-1.64274300	-0.00023200
C	0.44832300	0.31183400	0.00003900
H	0.22862000	1.37235800	0.00023500
C	1.84818900	-0.01478000	0.00001500
C	2.77362800	1.04776200	0.00039500
C	2.33249600	-1.36365600	-0.00040600
C	4.11761100	0.79013700	0.00034600
H	2.42401800	2.07163000	0.00075200
C	3.66240700	-1.63467100	-0.00051100
H	1.63030200	-2.18415600	-0.00066400
C	4.63360300	-0.57222600	-0.00018100
H	4.03350500	-2.65034500	-0.00086600
O	5.02534700	1.78278300	0.00076100
H	5.90494900	1.36951500	0.00064700
O	5.87234500	-0.75055400	-0.00037000
O	-4.33714200	2.58039400	-0.00050500
H	-3.61624600	3.22121000	-0.00060900
O	-5.11473600	-2.11693500	0.00059900
H	-6.03078200	-1.81681900	0.00090000

Zero-point correction= 0.221848 (Hartree/Particle)
Thermal correction to Energy= 0.237196
Thermal correction to Enthalpy= 0.238140
Thermal correction to Gibbs Free Energy= 0.177520
Sum of electronic and zero-point Energies= -840.926072
Sum of electronic and thermal Energies= -840.910724
Sum of electronic and thermal Enthalpies= -840.909780
Sum of electronic and thermal Free Energies= -840.970400

Cartesian coordinates of the SET products in pentylethanoate.

OOH^-

O	0.05522000	-0.68213900	0.00000000
H	-0.88352700	-0.87332300	0.00000000
O	0.05522000	0.79130500	0.00000000

Zero-point correction= 0.013666 (Hartree/Particle)
Thermal correction to Energy= 0.016565
Thermal correction to Enthalpy= 0.017510
Thermal correction to Gibbs Free Energy= -0.008051
Sum of electronic and zero-point Energies= -151.036482
Sum of electronic and thermal Energies= -151.033583
Sum of electronic and thermal Enthalpies= -151.032639
Sum of electronic and thermal Free Energies= -151.058199

Product from Resveratrol

C	3.90159700	-1.14681500	-0.00000600
C	2.53094500	-1.33427200	0.00000700
C	1.67839900	-0.21277400	0.00004500
C	2.21475700	1.08605400	0.00005100
C	3.59019800	1.24676300	0.00003000
C	4.43773600	0.14090300	0.00000100
H	2.11031400	-2.33222200	-0.00001300
H	1.59182000	1.96747900	0.00005100
H	5.51310300	0.26629500	-0.00003800
C	0.26899500	-0.47096800	0.00002900
H	-0.00964100	-1.51563600	0.00004000
C	-0.72380200	0.48876900	0.00002000
H	-0.44145300	1.53302500	-0.00000100
C	-2.11065000	0.23189100	-0.00002100
C	-2.99354600	1.35057600	-0.00005300
C	-2.67718800	-1.07613500	0.00001700
C	-4.34792600	1.18537700	-0.00007600
H	-2.56937800	2.34586400	-0.00008700
C	-4.03063500	-1.24983300	0.00003700
H	-2.04124200	-1.94903900	0.00007900
C	-4.87658200	-0.12000000	-0.00001200
H	-4.46305700	-2.24231600	0.00009100
O	-6.19712900	-0.23372500	0.00001700
H	-6.47321000	-1.16049000	0.00006900
O	4.78512000	-2.17145700	-0.00007400
H	4.32143500	-3.01561500	-0.00010100
O	4.07209600	2.51181900	0.00000400
H	5.03528900	2.50755100	0.00003900
H	-5.02846300	2.02480400	-0.00012100

Zero-point correction= 0.231640 (Hartree/Particle)
Thermal correction to Energy= 0.246014
Thermal correction to Enthalpy= 0.246958
Thermal correction to Gibbs Free Energy= 0.189684
Sum of electronic and zero-point Energies= -766.079700
Sum of electronic and thermal Energies= -766.065326
Sum of electronic and thermal Enthalpies= -766.064382
Sum of electronic and thermal Free Energies= -766.121656

Product from Piceatannol

C	3.86346400	1.31063200	0.00014100
C	2.50009700	1.08646700	0.00026100
C	2.02615700	-0.23999700	0.00012400
C	2.92961700	-1.31230400	-0.00011200
C	4.29490400	-1.06100700	-0.00023400
C	4.76846200	0.24482600	-0.00010500
H	1.82190100	1.92805900	0.00046000
H	2.57724700	-2.33421100	-0.00024000
H	5.83120300	0.45357500	-0.00020900
C	0.62765900	-0.57116100	0.00022600
H	0.40844100	-1.63023100	0.00030600
C	-0.40943700	0.33295200	0.00016700
H	-0.18343800	1.39132000	0.00010000
C	-1.78661600	0.00286000	0.00011500
C	-2.72127500	1.06567800	-0.00019500
C	-2.26722600	-1.34308400	0.00036300
C	-4.06450300	0.81335900	-0.00023800
H	-2.37950400	2.09142600	-0.00041600
C	-3.60985300	-1.60336100	0.00034000
H	-1.57780800	-2.17284100	0.00058300
C	-4.51693400	-0.53618400	0.00004300
H	-3.98106500	-2.62006100	0.00055000
O	-4.95223400	1.81696400	-0.00053700
H	-5.85466800	1.47262300	-0.00048600
O	-5.83812500	-0.67748900	-0.00000100
H	-6.11185800	-1.60564800	0.00020500
O	4.40113100	2.55332700	0.00030800
H	3.70577000	3.21960200	0.00005700
O	5.12567400	-2.12904800	-0.00047600
H	6.04510400	-1.84170000	-0.00064000

Zero-point correction= 0.235073 (Hartree/Particle)
Thermal correction to Energy= 0.250945
Thermal correction to Enthalpy= 0.251890
Thermal correction to Gibbs Free Energy= 0.189832
Sum of electronic and zero-point Energies= -841.318796
Sum of electronic and thermal Energies= -841.302923
Sum of electronic and thermal Enthalpies= -841.301979
Sum of electronic and thermal Free Energies= -841.364037