

Supporting information for

**Rate constants for H-Atom abstraction by HOO• from
H-donor compounds of Antioxidant Relevance**

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Table of Contents

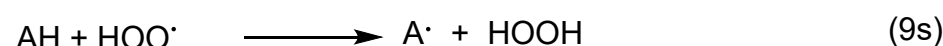
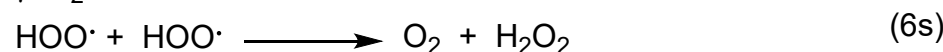
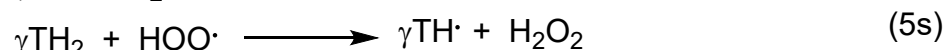
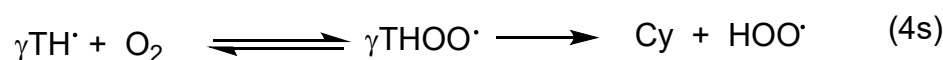
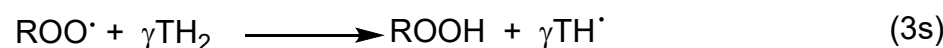
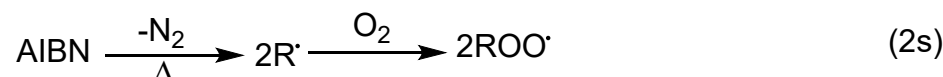
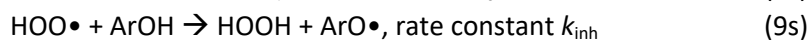
p. 3S.....	Antioxidants in acetonitrile at 37 °C
p. 3S.....	Apolar Solvents
p. 4S.....	Polar Solvents and Calculations
p. 5S.....	Calculations of the Rate Constant for PMHC as an example
p. 7S.....	Inhibition Rate Constants k_9 in Acetonitrile at 37 °C
p. 11S.....	NMR Data
p. 12S.....	Table 4S with the initial rates
p. 13S.....	HAT/PCET published papers

1s. Antioxidants in acetonitrile at 37 °C

Phenolic antioxidants (ArOH) exert their full action in apolar media. In polar media, i.e., solvents (S) with the ability to form H-bonding to phenols, ArOH---S, they have a lower ability to capture free radicals.

Organic matter (γ -terpinene, γ TH₂, in our case) is subject to a process of peroxidation caused by the air oxygen which forms terpenyl peroxy radicals, THOO• and then HOO•, see the paper.

These species self-quench to non-radical products or are quenched by ArOH



AH = 1 - 16

Scheme 1s. Autoxidation of γ -terpinene (γ -TH₂) to *p*-cymene (Cy) and H₂O₂. The reaction steps are numbered with an “s” because these reactions are reported in the current Supporting Information file. The rate constant k_9 (see step 9s) is reported in the old literature as k_{inh} . We prefer to keep the same nomenclature, therefore instead of talking about k_9 we called it k_{inh} .

2s. Apolar Solvents

In *apolar* solvents, the main quenching reactions are reactions 9s and 10s only, because the self-quenching of two HOO• is negligible because the concentration of HOO• in inhibited peroxidation is very low. The steady-state concentration of HOO• is given by eq. 12s,

$$nk_{\text{inh}} [\text{ArOH}] [\text{HOO}\bullet] = R_i \quad (12s)$$

$$[\text{HOO}\bullet] = R_i / nk_{\text{inh}}[\text{ArOH}] \quad (13s)$$

where R_i is the rate of initiation and n the number of HOO• captured by one molecule of ArOH (typically 2.0). Equation 12s expresses the condition for having steady state for HOO•,

rate of formation of HOO• = rate of quenching of HOO• by ArOH

The rate-law for the inhibited peroxidation is then

$$R_p = k_5 [\gamma\text{TH}_2][\text{HOO}\bullet] = k_5[\gamma\text{TH}_2] R_i / nk_{inh} [\text{ArOH}] \quad (14s)$$

k_5 is the propagation rate constant, R_p the rate of peroxidation.

3s. Polar solvents and Calculations

In *polar* solvents (e.g. acetonitrile), the quenching reactions are now reactions 6s, 9s, 10s (reaction 11s is negligible since ArO• has a low concentration). Reaction 6s must be included, this time, because the HOO• concentration is higher, and this is because the quenching reaction 10s is slow. Again, we must equal R_i to the sum of reactions 6s and 9s (eq. 10s is included through the n value since it is a fast process while reaction 6s is the slow step)

$$R_i = 2k_6 [\text{HOO}\bullet]^2 + nk_{inh}[\text{ArOH}] [\text{HOO}\bullet] \quad (15s)$$

Equation 15s is a second-degree equation with one variable (HOO•)

$$2k_6 [\text{HOO}\bullet]^2 + \alpha[\text{HOO}\bullet] - R_i = 0 \quad (16s)$$

$\alpha = nk_9[\text{ArOH}]_0$ k_9 is called k_{inh} in the paper

The solution to eq. 16s is given by $[\text{HOO}\bullet] = (-\alpha + (\alpha^2 + 8 R_i k_6)^{0.5}) / 4k_6$

Then the peroxidation rate in the presence of inhibitors is calculated

$$R_p = k_5 [\gamma\text{TH}_2][\text{HOO}\bullet] = k_5 [\text{TH}_2] (-\alpha + (\alpha^2 + 8 R_i k_6)^{0.5}) / 4k_6 \quad (17s)$$

In the *absence* of inhibitors, the peroxidation rate is indicated with R_0 and its value is given by

$$R_0 = k_5[\text{TH}_2] R_i^{0.5} / (2k_6)^{0.5} \quad (18s)$$

Therefore, $R_0/R_p = (8 k_6 \times R_i)^{0.5} / (-\alpha + (\alpha^2 + 8 k_6 R_i)^{0.5}) \quad (19s)$

And $R_p/R_0 = (-\alpha + (\alpha^2 + 8 k_6 R_i)^{0.5}) / (8 k_6 R_i)^{0.5} \quad (20s)$

Now, $R_0/R_p - R_p/R_0 =$

$$= (8 k_6 R_i)^{0.5} / (-\alpha + (\alpha^2 + 8 k_6 R_i)^{0.5}) - (-\alpha + (\alpha^2 + 8 k_6 R_i)^{0.5}) / (8 k_6 R_i)^{0.5} \quad (21s)$$

$$= (8 k_6 R_i - (-\alpha + (\alpha^2 + 8 k_6 R_i)^{0.5})^2 / ((8 k_6 R_i)^{0.5} (-\alpha + (\alpha^2 + 8 k_6 R_i)^{0.5}))) \quad (22s)$$

$$= (2 \alpha (\alpha^2 + 8 k_6 R_i)^{0.5} - 2 \alpha^2) / (8 k_6 R_i)^{0.5} (-\alpha + (\alpha^2 + 8 k_6 R_i)^{0.5}) \quad (23s)$$

$$= \alpha ((\alpha^2 + 8 k_6 R_i)^{0.5} - \alpha) / ((2 k_6 R_i)^{0.5} (-\alpha + (\alpha^2 + 8 k_6 R_i)^{0.5})) \quad (24s)$$

$$= \alpha / (2 k_6 R_i)^{0.5} = \quad (25s)$$

$$= nk_{inh}[ArOH]_0 / (2k_6 \times Ri)^{0.5} \quad (26s)$$

Let's pose $\Gamma_{inh} = R_0/R_p - R_p/R_0 =$

$$= nk_{inh} [ArOH]_0 / (2k_6 Ri)^{0.5} \quad (27s)$$

Then

$$nk_{inh} = \Gamma_{inh} (2k_6 Ri)^{0.5} / [ArOH]_0 \quad (28s)$$

4s. Calculations of the Rate Constant relative to PMHC as an example

We must first determine the initial rate of peroxidation with and without antioxidant

$$Rp = \frac{\Delta[Cy]_{inh}}{\Delta t}$$

where $\Delta[Cy]_{inh}$ is the increase in [Cy] in the first 150 – 250 min of kinetics and in the *presence* of antioxidant. In the absence of antioxidant,

$$Rp0 = \frac{\Delta[Cy]_0}{\Delta t}$$

where $\Delta[Cy]_0$ is the increase in the Cy concentration in the first 100 – 150 min. The average of R_p^0 was calculated to be $10.1 \times 10^{-6} \pm 4.0 \times 10^{-6}$ M/s. The standard acetonitrile solution used in the experiments was 0.945 M in γTH_2 , 6.0×10^{-2} M in AIBN and 6.54×10^{-2} M in mesitylene used as an internal standard.

The term $(2k_6 Ri)^{1/2} = (2k_6 \times 2ek_d \times [AIBN])^{1/2}$

[AIBN] = 6.0×10^{-2} M in all experiments, $2ek_d$ in acetonitrile at 37 °C is about $1.0 \times 10^{-6} s^{-1}$. Therefore, $Ri = 2ek_d[AIBN] = 6.0 \times 10^{-8}$ M/s. The rate constant $2k_6$ is $8.2 \times 10^7 M^{-1}s^{-1}$ in acetonitrile at 50 °C and probably $4.1 \times 10^7 M^{-1}s^{-1}$ at 37 °C (reaction rates double for every 10 degrees rise in temperature). Thus $(Ri \times 2k_6)^{1/2}$ is about 1.6 and the calculation of nk_9 has been done with this number

$$\begin{aligned} nk_{inh} &= \Gamma_{inh} (2k_6 Ri)^{0.5} / [ArOH]_0 \\ &= 1.6 \Gamma_{inh} / [ArOH]_0 \end{aligned}$$

Example: **PMHC** (2,2,5,7,8-pentamethyl-6-chromanol)

A solution containing 6.0×10^{-2} M AIBN, 0.946 M (purified) γTH_2 and 6.54×10^{-2} M mesitylene was prepared in acetonitrile. PMHC was added at a final concentration of 9.74×10^{-5} M, 1.95×10^{-4} M, 3.9×10^{-4} M and 5.85×10^{-4} M. Three aliquots of 400 μ L of the first solution ([PMHC] = 9.74×10^{-5} M)

were added to three vials of 5.2 mL. The vials were kept open to the air for 20 min, thereafter they were capped and placed in a shaker at 37 °C with or without shaking. At given time intervals, aliquots of the above solution (2 - 3 μ L) were withdrawn with a syringe and immediately diluted with acetonitrile 1:50 v/v, then, 1 μ L of the final solution was injected in a HP5890A GC-MS instrument. The area of the peak of Cy was divided by the area of the mesitylene peak and the ratios A₁, A₂ and A₃ are reported in Table 1. These operations were repeated for each [PMHC].

Table 1s. Ratios of the peak area for pCy divided by the peak area of mesitylene.

[PMHC] = 9.74x10 ⁻⁵ M	Time/min	A1	A2	A3
	0	1.45	1.43	1.47
	114	1.92	1.95	1.955
	160	2.149	2.274	2.31
	255	2.84	3.16	3.14

$$\text{Initial rate, } R_{p1} = (1.92-1.45) \times 6.54 \times 10^{-2} / (60 \times 114) = 4.49 \times 10^{-6} \text{ M/s}$$

$$R_{p2} = (1.95-1.43) \times 6.54 \times 10^{-2} / (60 \times 114) = 4.97 \times 10^{-6} \text{ M/s}$$

$$R_{p3} = (1.955-1.47) \times 6.54 \times 10^{-2} / (60 \times 114) = 4.64 \times 10^{-6} \text{ M/s}$$

where 6.54x10⁻² M is the concentration of mesitylene. R_p⁰ was determined from kinetics without PMHC. The average value was 10.1x10⁻⁶ \pm 4.0x10⁻⁶ M/s, see **Table 4s**. In the presence of PMHC, R_p < 10.1x10⁻⁶ M/s. Now, it is possible to calculate the rate constants nk_g.

$$\Gamma_{inh-1} = R_p^0 / R_p^{inh} - R_p^{inh} / R_p^0 = 10.1/4.49 - 4.49/10.1 = 1.805$$

$$nk_{inh-1} = 1.805 \times 1.6 / 9.74 \times 10^{-5} = \mathbf{3.0 \times 10^4 \text{ M}^{-1} \text{s}^{-1}}$$

$$\Gamma_{inh-2} = R_p^0 / R_p^{inh} - R_p^{inh} / R_p^0 = 10.1/4.97 - 4.97/10.1 = 1.540$$

$$nk_{inh-2} = 1.540 \times 1.6 / 9.74 \times 10^{-5} = \mathbf{2.5 \times 10^4 \text{ M}^{-1} \text{s}^{-1}}$$

$$\Gamma_{inh-3} = R_p^0 / R_p^{inh} - R_p^{inh} / R_p^0 = 10.1/4.64 - 4.64/10.1 = 1.717$$

$$nk_{inh-3} = 1.717 \times 1.6 / 9.74 \times 10^{-5} = \mathbf{2.8 \times 10^4 \text{ M}^{-1} \text{s}^{-1}}$$

Table 2s. Ratios of the peak area for pCy divided by the peak area of mesitylene.

[PMHC] = 1.95x10 ⁻⁴ M	Time/min	A1	A2	A3
	0	1.35	1.40	1.39
	93	1.51	1.525	1.50
	178	1.659	1.71	1.72
	272	2.268	2.29	2.27

$$R_{p1} = (1.51-1.35) \times 6.54 \times 10^{-2} / (60 \times 93) = 1.9 \times 10^{-6} \text{ M/s}$$

$$R_{p2} = (1.525-1.40) \times 6.54 \times 10^{-2} / (60 \times 93) = 1.52 \times 10^{-6} \text{ M/s}$$

$$R_{p3} = (1.50-1.39) \times 6.54 \times 10^{-2} / (60 \times 93) = 1.29 \times 10^{-6} \text{ M/s}$$

$$\Gamma_{inh-1} = R_p^0 / R_{inh}^p - R_{inh}^p / R_p^0 = 10.1/1.9 - 1.9/10.1 = 5.128$$

$$nk_{inh-1} = 5.128 \times 1.6 / 1.95 \times 10^{-4} = \mathbf{4.2 \times 10^4 \text{ M}^{-1}\text{s}^{-1}}$$

$$\Gamma_{inh-2} = R_p^0 / R_{inh}^p - R_{inh}^p / R_p^0 = 10.1/1.52 - 1.52/10.1 = 6.494$$

$$nk_{inh-2} = 6.494 \times 1.6 / 1.95 \times 10^{-4} = \mathbf{5.3 \times 10^4 \text{ M}^{-1}\text{s}^{-1}}$$

$$\Gamma_{inh-3} = R_p^0 / R_{inh}^p - R_{inh}^p / R_p^0 = 10.1/1.29 - 1.29/10.1 = 7.702$$

$$nk_{inh-3} = 7.702 \times 1.6 / 1.95 \times 10^{-4} = \mathbf{6.3 \times 10^4 \text{ M}^{-1}\text{s}^{-1}}$$

1. Inhibition Rate Constants nk_{inh} in Acetonitrile at 37 °C

Table 3s. Rate constants of PMHC as a function of [PMHC]. Initial rates.

[PMHC]	$nk_{inh}/10^4 \text{ M}^{-1}\text{s}^{-1}$	Initial Rate M/s
9.74×10^{-5}	3.0	4.49×10^{-6}
"	2.5	4.97×10^{-6}
"	2.8	4.64×10^{-6}
1.95×10^{-4}	4.2	1.90×10^{-6}
"	5.3	1.52×10^{-6}
"	6.3	1.29×10^{-6}
3.9×10^{-4}	3.1	1.31×10^{-6}
"	3.8	1.07×10^{-6}
"	3.1	1.31×10^{-6}
5.85×10^{-4}	2.7	1.0×10^{-6}
"	3.0	0.91×10^{-6}
	Average $\mathbf{3.6 \pm 1.2}$	

4-Methylcatechol

[4MeCat] / mM	Initial Rate $\times 10^6 \text{ M/s}$	nk_{inh} , rate constants / $\text{M}^{-1}\text{s}^{-1}$
9.62×10^{-2}	3.5 ± 0.5	4.2×10^4
0.162	1.56 ± 0.5	6.2×10^4
0.206	1.03 ± 0.5	7.5×10^4
0.326	0.55 ± 0.5	9.0×10^4
		Average $\mathbf{7 \times 10^4 \pm 2 \times 10^4}$

Quercetin

[quercetin] / mM	Initial Rate $\times 10^6 \text{ M/s}$	nk_{inh} , rate constants / $\text{M}^{-1}\text{s}^{-1}$
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8.91E-02	7 ± 0.7	1.3×10^4
1.71E-01	4 ± 0.7	2.0×10^4
2.40E-01	2.4 ± 0.7	4.0×10^4
3.43E-01	1.2 ± 0.7	3.9×10^4
5.14E-01	0.49 ± 0.20	6.4×10^4
		Average $3.5 \times 10^4 \pm 2.0 \times 10^4$

Catechol

[catechol] / mM	Initial Rate x 10^6 M/s	nk_{inh} , rate constants / $M^{-1}s^{-1}$
1.06E-01	6 ± 0.8	1.6×10^4
2.07E-01	3.3 ± 0.8	2.1×10^4
3.38E-01	2.6 ± 0.8	1.7×10^4
5.80E-01	2.14 ± 0.8	1.2×10^4
		Average $1.7 \times 10^4 \pm 0.4 \times 10^4$

Caffeic acid

[caffeic acid] / mM	Initial Rate x 10^6 M/s	nk_g , rate constants / $M^{-1}s^{-1}$
1.19E-01	7 ± 0.7	1.0×10^4
2.39E-01	4.5 ± 0.7	3.8×10^4
4.77E-01	2.5 ± 0.7	1.3×10^4
5.97E-01	2.1 ± 0.7	1.2×10^4
7.16E-01	1.9 ± 0.7	1.1×10^4
		Average $1.15 \times 10^4 \pm 0.13 \times 10^4$

di-Hydrocaffeic acid

[di-hydrocaffeic acid] / mM	Initial Rate x 10^6 M/s	nk_g , rate constants / $M^{-1}s^{-1}$
0.120	4.52 ± 0.4	2.4×10^4
0.48	2.5 ± 0.4	1.3×10^4
0.721	2.3 ± 0.4	0.92×10^4
		Average $1.5 \times 10^4 \pm 0.8 \times 10^4$

Ascorbyl palmitate

[ascorbyl palmitate] / mM	Initial Rate x 10^6 M/s	nk_{inh} , rate constants / $M^{-1}s^{-1}$
0.418	0.4 ± 0.3	10.0×10^4
0.224	1.0 ± 0.7	7.1×10^4
0.596	0.2 ± 0.1	13.6×10^4
0.294	0.8 ± 0.7	6.8×10^4
0.0735	2.5 ± 0.7	8.3×10^4
		Average $9.2 \times 10^4 \pm 2.5 \times 10^4$

Luteolin

[luteolin] / mM	Initial Rate x 10 ⁶ M/s	nk _g , rate constants /M ⁻¹ s ⁻¹
0.0916	6.4 ± 0.3	1.6 x10 ⁴
0.174	6.3 ± 0.3	0.90x10 ⁴
0.521	1.9 ± 0.3	1.6x10 ⁴
		Average 1.4x10 ⁴ ± 0.2 x10 ⁴

6-Methoxyluteolin (nepetin)

[6-methoxyluteolin] / mM	Initial Rate x 10 ⁶ M/s	nk _g , rate constants /M ⁻¹ s ⁻¹
0.0556	6.3 ± 0.3	2.8 x10 ⁴
0.156	3.7 ± 0.3	2.4 x10 ⁴
0.487	1.3 ± 0.3	2.5 x10 ⁴
		Average 2.6x10 ⁴ ± 0.3 x10 ⁴

(+)-Catechin hydrate • H₂O. We determined via NMR that in our sample the water content was 6 mol H₂O per mol of catechin, i.e. (+)-catechin • 6H₂O

[catechin] / mM	Initial Rate x 10 ⁶ M/s	nk _{inh} , rate constants /M ⁻¹ s ⁻¹
0.166	4.3 ± 0.5	1.9 x10 ⁴
0.066	3.6 ± 0.5	5.9 x10 ⁴
0.400	2.9 ± 0.5	1.3 x10 ⁴
0.249	2.9 ± 0.5	2.1x10 ⁴
0.125	4.4 ± 0.5	2.4x10 ⁴
		Average 2.7x10 ⁴ ± 0.4 x10 ⁴

Protocatechuic acid

[protocatechuic acid] / mM	Initial Rate x 10 ⁶ M/s	nk _{inh} , rate constants /M ⁻¹ s ⁻¹
0.345	9.6 ± 0.9	0.5x10 ³
0.645	5.35 ± 0.8	3.4 x10 ³
0.115	9.3 ± 0.8	2.3 x10 ³
		Average 2.8x10 ³ ± 0.8 x10 ³

3-Hydroxyflavone

[3-hydroxyflavone] / mM	Initial Rate x 10 ⁶ M/s	Nk _{inh} , rate constants /M ⁻¹ s ⁻¹
0.354	6.3 ± 0.5	4.4 x10 ³
0.637	7.8 ± 0.5	1.3 x10 ³
		Average 2.9x10 ³ ± 1.0 x10 ³

Galangin

[galangin] / mM	Initial Rate x 10 ⁶ M/s	nk _{inh} , rate constants /M ⁻¹ s ⁻¹
0.115	9.6± 0.5	1.4 x10 ³

0.604	8.1 ± 0.5	1.2×10^3
		Average $1.3 \times 10^3 \pm 0.1 \times 10^3$

4-Methoxyphenol

[4-methoxyphenol] / mM	Initial Rate x 10^6 M/s	nk_{inh} , rate constants / $M^{-1}s^{-1}$
0.0958	7.5 ± 0.7	1.0×10^4
0.383	6.0 ± 0.7	4.6×10^3
0.192	4.0 ± 0.7	1.8×10^4
		Average $1.1 \times 10^4 \pm 0.6 \times 10^4$

Phenol

[phenol] / mM	Initial Rate x 10^6 M/s	nk_{inh} , rate constants / $M^{-1}s^{-1}$
0.720	8.0 ± 0.8	1.0×10^3
0.720	7.9 ± 0.8	1.1×10^3
1.077	7.1 ± 0.8	1.1×10^3
		Average $1.1 \times 10^3 \pm 0.1 \times 10^3$

Pinobanksin

[pinobanksin] / mM	Initial Rate x 10^6 M/s	nk_{inh} , rate constants / $M^{-1}s^{-1}$
0.1113	no effect	---
0.223	9.8 – 10.1	$\leq 10^2$

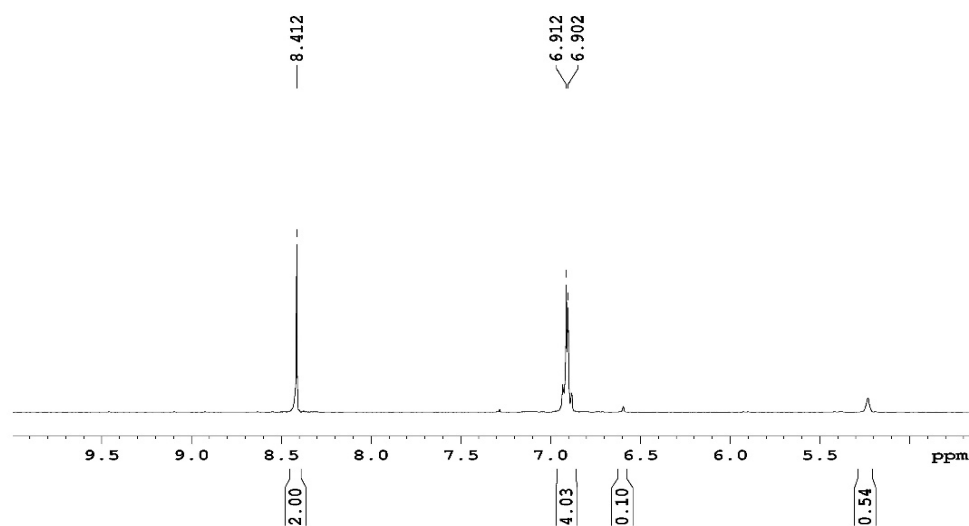
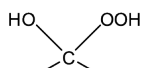


Figure 1s. ^1H NMR of the solution of $\gamma\text{-TH}_2$ (0.898 M) + AIBN ($6.00 \times 10^{-2}\text{ M}$) + mesitylene ($2.18 \times 10^{-2}\text{ M}$) in acetonitrile after 24 hours of reaction at $37\text{ }^\circ\text{C}$. The spectrum was done by mixing $50\text{ }\mu\text{L}$ of the final solution to $500\text{ }\mu\text{L}$ of CDCl_3 . The singlet at 8.41 ppm was due to HOOH while the aromatic moiety of *p*-cymene gave rise to the multiplet at 6.91 ppm . The broad signal at 5.25 ppm was assigned to the protons of the residual $\gamma\text{-TH}_2$. Finally, the peak at 6.6 ppm was due to mesitylene (the internal standard). The peaks of Cy and HOOH were in the area ratio of $4:2$ corresponding to a molar ratio of $1:1$.

The final products of reaction 1 were identified by NMR to be H_2O_2 and Cy in $1:1$ mole ratio. The proton signal of H_2O_2 (in $\text{CDCl}_3 + \text{CH}_3\text{CN}$ $10:1$ v/v) appeared, rather variably, at a chemical shift of *ca.* 8.41 ppm as a sharp singlet that disappeared after treatment with D_2O or methanol- d_4 . Occasionally, a weaker singlet, shifted by $\pm 0.02\text{ ppm}$ from the H_2O_2 main peak, was observed. Most likely, this peak was generated by the mono-deuterated form, HOOD .¹ Addition of a genuine sample of H_2O_2 increased the area of the main peak and hence confirmed the presence of H_2O_2 in the reaction mixture. The aromatic signals of Cy appeared at *ca.* 6.91 ppm . The area of the Cy peak was in a $2:1$ ratio with that of H_2O_2 i.e., in a molar ratio of $1:1$ as dictated by reaction 1. The presence of Cy was confirmed by comparing the spectrum of the mixture with that of an authentic sample of Cy.

In acetone- d_6 , the proton spectrum of H_2O_2 showed one singlet at ca. 9.50 ppm due to H_2O_2 and two more peaks at 10.09 ppm and 5.04 ppm both growing over time at the expense of H_2O_2 . These two peaks disappeared after treatment with heavy water, D_2O . The carbon spectrum showed the presence of a peak at 101.05 ppm which disappeared in the DEPT-135 spectrum, proof that this resonance was generated by a quaternary C atom. When we changed the solvent to acetonitrile- d_3 , CH_3OH (external lock with D_2O in a coaxial insert) or chloroform- d_1 , all these peaks, except for the H_2O_2 signal, did not appear. Hence, we think that these resonances are due to 2-



hydroperoxypropan-2-ol- d_6 produced by the reaction of H_2O_2 with $(CD_3)_2CO$.² As a further proof, the spectra of H_2O_2 in a mix $(CH_3)_2CO/(CD_3)_2CO$ 3:1 v/v showed an additional proton peak at 1.33 ppm for the methyl groups in $(CH_3)_2C(OOH)(OH)$ and the corresponding carbon peak at 24.8 ppm. Finally, we observed that reaction 1 was faster in acetone than in other solvents, most likely because of the presence of this hydroperoxide.

(1) Double Water Peaks in Deuterated NMR Solvents (Sigma-Aldrich)

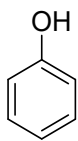
https://www.sigmaaldrich.com/content/dam/sigma-aldrich/docs/Aldrich/General_Information/double_water_peaks.pdf

(2) Sauer, M. C. V.; Edwards, J. O. *J. Phys. Chem.* **1971**, 75, 3004-3011.

Table 4s. Initial rates in the absence of inhibitor R_p^0 (in 10^{-5} M/s units) measured in vials of 5.2 ml containing aliquots of the standard solution at 37 °C. The average value was calculated using the data 5.2/200+400+600+800+shaken 5.2/200 yielding 1.01 ± 0.4 .

mL vial volume/ μ L solution								
5.2/200	5.2/400	5.2/600	5.2/800	18.0/720	18.0/1650		shaken/40.0/650	shaken/5.2/200
0.99 \pm 0.08	1.82 \pm 0.10	0.42 \pm 0.09	0.84 \pm 0.07	2.63 \pm 0.20	0.56 \pm 0.06		1.07 \pm 0.05	1.49 \pm 0.08
0.92 \pm 0.05	1.71 \pm 0.12	0.76 \pm 0.06	0.57 \pm 0.08	2.53 \pm 0.06	0.13 \pm 0.07		2.06 \pm 0.05	1.19 \pm 0.10
1.17 \pm 0.1	1.96 \pm 0.10	0.77 \pm 0.06	1.01 \pm 0.06	2.73 \pm 0.12	0.42 \pm 0.08		2.09 \pm 0.05	1.27 \pm 0.06
1.03 \pm 0.03	0.43 \pm 0.10		0.37 \pm 0.02	2.80 \pm 0.05	0.62 \pm 0.07		1.53 \pm 0.03	1.20 \pm 0.10
0.99 \pm 0.05	0.38 \pm 0.08		0.63 \pm 0.03				1.85 \pm 0.02	0.39 \pm 0.09
1.14 \pm 0.04	0.35 \pm 0.08		0.49 \pm 0.03					
1.04 \pm 0.08	1.05 \pm 0.05							
1.31 \pm 0.07	1.10 \pm 0.15							
1.11 \pm 0.10	1.41 \pm 0.16							
1.22 \pm 0.10	1.61 \pm 0.07							
1.15 \pm 0.04								
1.12 \pm 0.08								
0.99 \pm 0.05								
averages								
1.091	1.182	0.65	0.65	2.67	0.43		1.72	1.11
\pm 0.109	\pm 0.62	\pm 0.20	\pm 0.24	\pm 0.12	\pm 0.22		\pm 0.43	\pm 0.42

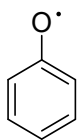
B3LYP/6-31+g(d,p) SRCF=(PCM, solvent =acetonitrile) optimized structures and energies



Sum of electronic and thermal Enthalpies: -307.389836

0 1

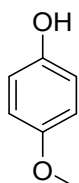
C	0.00000000	0.94034500	0.00000000
C	1.21954500	0.25282800	0.00000000
C	1.22276100	-1.14384200	0.00000000
C	0.02053400	-1.86102500	0.00000000
C	-1.19174000	-1.16367100	0.00000000
C	-1.20929700	0.23439900	0.00000000
H	2.14769200	0.81581900	0.00000000
H	2.17186400	-1.67225900	0.00000000
H	0.02872700	-2.94642800	0.00000000
H	-2.13318800	-1.70550200	0.00000000
H	-2.15369100	0.77268600	0.00000000
O	0.05143300	2.31251500	0.00000000
H	-0.84368300	2.68135200	0.00000000



Sum of electronic and thermal Enthalpies: -306.760624

0 2

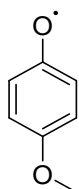
C	1.24263100	0.29089100	0.00000000
C	0.00000000	1.04421500	0.00000000
C	-1.24271500	0.29086100	0.00000000
C	-1.22825500	-1.08778900	0.00000000
C	0.00002600	-1.78644600	0.00000000
C	1.22824300	-1.08784600	0.00000000
O	0.00004400	2.30913600	0.00000000
H	-2.17160200	0.85269800	0.00000000
H	-2.16007400	-1.64481500	0.00000000
H	0.00004100	-2.87185300	0.00000000
H	2.16004800	-1.64489900	0.00000000
H	2.17165700	0.85246700	0.00000000



Sum of electronic and thermal Enthalpies: -421.883095

0 1

C	0.44358700	1.79936100	0.00000000
C	1.52916200	0.91323100	0.00000000
C	1.30743500	-0.46047200	0.00000000
C	0.00000000	-0.97256700	0.00000000
C	-1.08365300	-0.08805300	0.00000000
C	-0.85696100	1.29606100	0.00000000
H	2.54048100	1.30776500	0.00000000
H	2.14378200	-1.15256700	0.00000000
O	-0.11001300	-2.34162100	0.00000000
H	-2.10488400	-0.44919900	0.00000000
H	-1.70600700	1.97475300	0.00000000
O	0.72565400	3.14809700	0.00000000
H	-0.09558600	3.65971800	0.00000000
C	-1.41827700	-2.91344300	0.00000000
H	-1.27152400	-3.99373000	0.00000000
H	-1.97957000	-2.62162600	0.89540000
H	-1.97957000	-2.62162600	-0.89540000

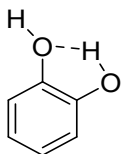


Sum of electronic and thermal Enthalpies: -421.263950

0 2

C	0.87729000	-1.34402300	0.00000000
C	-0.46310000	-1.89794200	0.00000000
C	-1.56162500	-0.94687200	0.00000000
C	-1.33166000	0.40366200	0.00000000
C	0.00000000	0.90677100	0.00000000
C	1.10183800	0.01533200	0.00000000
O	-0.66460100	-3.14765200	0.00000000
O	0.10796800	2.24606300	0.00000000
C	1.40935400	2.86110900	0.00000000
H	-2.57240000	-1.34268500	0.00000000
H	-2.14855800	1.11844200	0.00000000
H	2.11666200	0.39414000	0.00000000
H	1.70918900	-2.04149800	0.00000000
H	1.22074700	3.93332600	0.00000000

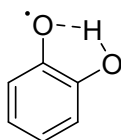
H	1.96741700	2.58137900	0.89789900
H	1.96741700	2.58137900	-0.89789900



Sum of electronic and thermal Enthalpies: -382.612745

0 1

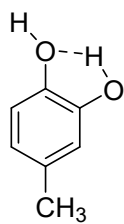
C	1.38414300	0.70023100	0.00000000
C	0.00000000	0.86255900	0.00000000
C	-0.84506100	-0.26077100	0.00000000
C	-0.29534800	-1.54147400	0.00000000
C	1.09494000	-1.70574800	0.00000000
C	1.93377500	-0.58825000	0.00000000
O	-0.64365400	2.07908700	0.00000000
O	-2.20710100	-0.10570900	0.00000000
H	-0.96316500	-2.39750100	0.00000000
H	1.51604800	-2.70622100	0.00000000
H	3.01235400	-0.70967000	0.00000000
H	2.02718900	1.57661100	0.00000000
H	-0.00774300	2.80802300	0.00000000
H	-2.41334400	0.84246000	0.00000000



Sum of electronic and thermal Enthalpies: -381.994869

0 2

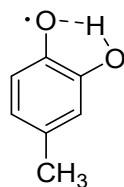
C	1.00648300	-1.71727400	0.00000000
C	-0.35793200	-1.55629000	0.00000000
C	-0.93046700	-0.23259400	0.00000000
C	0.00000000	0.90266800	0.00000000
C	1.37985700	0.71489400	0.00000000
C	1.87572700	-0.58725200	0.00000000
O	-2.16910900	0.01999500	0.00000000
O	-0.54566800	2.12436200	0.00000000
H	2.04381200	1.57288900	0.00000000
H	2.94917700	-0.74664900	0.00000000
H	1.43825000	-2.71301900	0.00000000
H	-1.03736200	-2.40257400	0.00000000
H	-1.51767900	1.98957800	0.00000000



Sum of electronic and thermal Enthalpies: -421.903823

0 1

C	1.15696000	1.08942300	0.00000000
C	1.18255100	-0.31659500	0.00000000
C	0.00000000	-1.05124600	0.00000000
C	-1.24404100	-0.39750800	0.00000000
C	-1.28167800	0.99302900	0.00000000
C	-0.08903500	1.72830900	0.00000000
O	-0.06090700	-2.42682500	0.00000000
O	-2.41329400	-1.11736600	0.00000000
H	-2.24554300	1.49305800	0.00000000
H	-0.13671400	2.81359700	0.00000000
C	2.44872300	1.87556200	0.00000000
H	2.13406900	-0.84438100	0.00000000
H	0.82596100	-2.81317900	0.00000000
H	-2.19604600	-2.06285400	0.00000000
H	2.25439800	2.95170600	0.00000000
H	3.05830100	1.64487500	0.88155100
H	3.05830100	1.64487500	-0.88155100

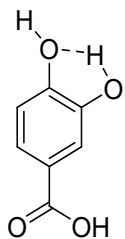


Sum of electronic and thermal Enthalpies: -421.290101

0 2

C	0.13349400	-1.69997200	0.00000000
C	-1.13305600	-1.03705600	0.00000000
C	-1.17985600	0.36636300	0.00000000
C	0.00000000	1.09331700	0.00000000
C	1.31132500	0.43803100	0.00000000
C	1.31719600	-1.00176500	0.00000000
C	-2.40911600	-1.83363400	0.00000000
O	0.00281200	2.43520500	0.00000000
O	2.34306300	1.17042200	0.00000000
H	2.27814600	-1.50634400	0.00000000
H	0.14890500	-2.78582900	0.00000000
H	-2.13186000	0.88877900	0.00000000
H	0.94661500	2.70299100	0.00000000
H	-2.21400400	-2.90826800	0.00000000

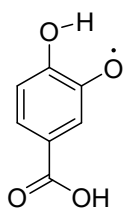
H	-3.01736400	-1.59402600	0.88020700
H	-3.01736400	-1.59402600	-0.88020700



Sum of electronic and thermal Enthalpies: -571.189004

0 1

C	0.00000000	0.91863800	0.00000000
C	0.99344500	-0.07874600	0.00000000
C	0.63031100	-1.41663200	0.00000000
C	-0.73200900	-1.78069900	0.00000000
C	-1.71697800	-0.79231600	0.00000000
C	-1.35528700	0.55368800	0.00000000
O	1.50889800	-2.47048500	0.00000000
O	-1.09364200	-3.09149200	0.00000000
H	-2.75987400	-1.09127700	0.00000000
H	-2.12318100	1.31740500	0.00000000
C	0.43563000	2.33074000	0.00000000
H	2.04014200	0.20868700	0.00000000
H	2.42728500	-2.16573700	0.00000000
H	-0.29368400	-3.64246400	0.00000000
O	-0.59246200	3.21331200	0.00000000
O	1.60112900	2.70569100	0.00000000
H	-0.21275100	4.10914400	0.00000000

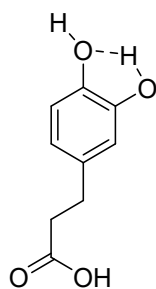


Sum of electronic and thermal Enthalpies: -570.565870

0 2

C	0.00000000	0.87838900	0.00000000
C	1.04599600	-0.02252900	0.00000000
C	0.78632000	-1.43744200	0.00000000
C	-0.61654400	-1.86513300	0.00000000
C	-1.65708700	-0.93876600	0.00000000
C	-1.35123200	0.41711000	0.00000000
O	1.68046700	-2.32974500	0.00000000
O	-0.84599700	-3.17723900	0.00000000
H	-2.68649400	-1.27999400	0.00000000
H	-2.15479800	1.14354100	0.00000000

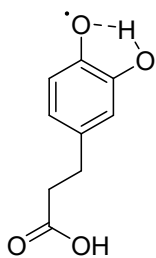
C	0.32039300	2.33328500	0.00000000
H	2.07621700	0.31540500	0.00000000
H	0.03159000	-3.61642800	0.00000000
O	-0.77862700	3.11575100	0.00000000
O	1.45120000	2.79160900	0.00000000
H	-0.48993300	4.04498700	0.00000000



Sum of electronic and thermal Enthalpies: -649.761437

0 1

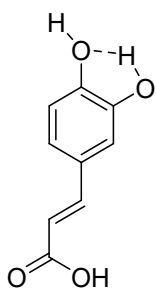
C	-0.15287900	-0.28845300	-0.48329600
C	-0.93578400	0.87560100	-0.40512300
C	-2.28677100	0.80301900	-0.07317100
C	-2.88786400	-0.43926200	0.18827100
C	-2.12119700	-1.59890600	0.111108100
C	-0.76438500	-1.52176200	-0.22290100
O	-3.12468600	1.89105000	0.01867300
O	-4.21900800	-0.51819000	0.51042100
H	-2.59439800	-2.55607800	0.30785600
H	-0.18088300	-2.43628700	-0.28422000
C	1.32305500	-0.20002800	-0.81506500
H	-0.49088700	1.84732600	-0.60952200
H	-2.65170800	2.71121300	-0.17979600
H	-4.59304400	0.37699100	0.51188300
H	1.64364200	-1.11894400	-1.31620300
H	1.50016900	0.62094400	-1.51759600
C	2.18966500	0.01617000	0.43577300
C	3.66778200	0.10785200	0.14007800
H	1.90046700	0.93500100	0.96040300
H	2.04552000	-0.79648700	1.15795800
O	4.39418700	0.28220400	1.26789300
O	4.18662700	0.03938100	-0.96016100
H	5.33444300	0.33537500	1.02074500



Sum of electronic and thermal Enthalpies: -649.145630

0 2

C	-0.19939600	-0.09791400	-0.49262000
C	-1.02971100	1.01128700	-0.29496900
C	-2.36848600	0.81875900	0.02353400
C	-2.94456600	-0.52229200	0.15723100
C	-2.05644100	-1.63632900	-0.05775400
C	-0.73776700	-1.41924200	-0.36991800
O	-3.20059900	1.85001700	0.22034300
O	-4.17230000	-0.61583100	0.44579400
H	-2.46512000	-2.63789600	0.03009200
H	-0.07782200	-2.26607700	-0.53637900
C	1.26375100	0.08581100	-0.81250300
H	-0.64125000	2.02076100	-0.38942100
H	-4.07595500	1.45713600	0.42584900
H	1.57158600	-0.65073300	-1.56235300
H	1.42885200	1.07651700	-1.24490200
C	2.14822900	-0.07474500	0.43692500
C	3.62176700	0.08210900	0.14055800
H	1.88139200	0.66155500	1.20398000
H	2.00686200	-1.05770900	0.90128700
O	4.37004200	-0.05727700	1.25668500
O	4.11291200	0.30563000	-0.95095500
H	5.30672000	0.05146600	1.01400000

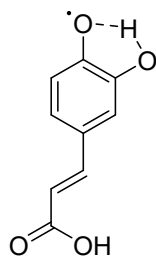


Sum of electronic and thermal Enthalpies: -648.563853

0 1

C	-0.88547500	-1.64821500	-0.00001800
C	-0.10566200	-0.47584700	-0.00001400
C	-0.76729600	0.77399600	0.00002400
C	-2.15129200	0.83308500	0.00001100
C	-2.91926300	-0.35202800	-0.00001000

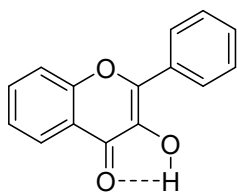
C	-2.27862600	-1.58908900	-0.00003000
C	1.34506800	-0.60353300	0.00000600
C	2.26696300	0.38640700	-0.00003100
C	3.69854300	0.07373800	0.00000600
O	4.20740400	-1.04209400	0.00009500
O	-2.88714000	1.99089600	0.00003800
O	-4.27880700	-0.29116800	-0.00002700
O	4.45957600	1.20021800	-0.00007100
H	-2.87867100	-2.49307900	-0.00004100
H	-0.39373700	-2.61619800	-0.00003100
H	-0.20129400	1.70060800	0.00003000
H	-2.31657500	2.77237000	0.00002500
H	-4.55506900	0.63992200	0.00015200
H	1.72298800	-1.62463900	0.00004300
H	2.00257500	1.43815000	-0.00007600
H	5.39376500	0.92898100	-0.00003800



Sum of electronic and thermal Enthalpies: -647.946192

0 2

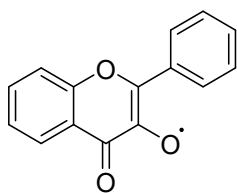
C	0.94591500	1.65057800	0.00025600
C	0.15122200	0.45074000	-0.00006200
C	0.79234900	-0.80923100	-0.00027000
C	2.16964600	-0.87121900	-0.00010500
C	3.00396300	0.34369200	0.00012100
C	2.31299900	1.61237100	0.00038800
C	-1.28756000	0.60213600	-0.00022200
C	-2.21150700	-0.39158400	0.00007600
C	-3.65008400	-0.07438400	-0.00006400
O	-4.14129700	1.04597500	-0.00077500
O	2.82531300	-2.03969200	-0.00026600
O	4.25239500	0.20387900	0.00005600
O	-4.40606800	-1.19722900	0.00077300
H	2.91106400	2.51752000	0.00065100
H	0.43165700	2.60691800	0.00045000
H	0.22426400	-1.73252600	-0.00053700
H	3.78098400	-1.82051300	-0.00026700
H	-1.66121200	1.62374400	-0.00045800
H	-1.94814600	-1.44317400	0.00048600
H	-5.34302200	-0.93401700	0.00066200



Sum of electronic and thermal Enthalpies: -803.125400

0 1

O	0.81812200	-0.50606000	0.00000000
C	0.33485500	-1.77776600	0.00000000
C	-1.04437700	-2.04513800	0.00000000
C	-1.96368500	-0.91939700	0.00000000
C	-1.35999100	0.40552100	0.00000000
C	0.00000000	0.59222100	0.00000000
O	-3.21179300	-1.00609900	0.00000000
O	-2.25114600	1.43062600	0.00000000
C	0.75786200	1.85223000	0.00000000
C	1.27989600	-2.81340500	0.00000000
C	0.83041200	-4.12626800	0.00000000
C	-0.54980500	-4.41887700	0.00000000
C	-1.47566400	-3.38896400	0.00000000
H	2.33709600	-2.57128200	0.00000000
H	1.55320700	-4.93607400	0.00000000
H	-0.88240900	-5.45168000	0.00000000
H	-2.54180800	-3.58895000	0.00000000
H	-3.12814800	0.98967600	0.00000000
C	2.16961700	1.81626700	0.00000000
C	2.91195600	2.99555500	0.00000000
C	2.26801300	4.23738500	0.00000000
C	0.87134600	4.28570900	0.00000000
C	0.11844500	3.11073500	0.00000000
H	2.68360900	0.86312200	0.00000000
H	3.99656300	2.94335800	0.00000000
H	2.84832200	5.15514200	0.00000000
H	0.35942800	5.24337300	0.00000000
H	-0.96059600	3.17071000	0.00000000

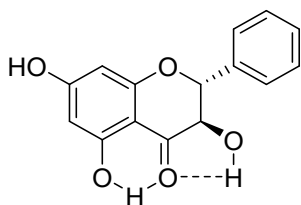


Sum of electronic and thermal Enthalpies: -802.498975

0 2

O	0.75094600	-0.49997300	0.00000000
C	0.22910700	-1.76846200	0.00000000

C	-1.15239000	-2.00085000	0.00000000
C	-2.07280800	-0.86147000	0.00000000
C	-1.44584400	0.52325400	0.00000000
C	0.00000000	0.62099000	0.00000000
O	-3.29823600	-0.98027600	0.00000000
O	-2.19217200	1.52512000	0.00000000
C	0.79845300	1.83577400	0.00000000
C	1.15481400	-2.81462900	0.00000000
C	0.68063700	-4.12266400	0.00000000
C	-0.70139400	-4.38640000	0.00000000
C	-1.60706300	-3.33491000	0.00000000
H	2.21600100	-2.59181000	0.00000000
H	1.38885500	-4.94499700	0.00000000
H	-1.05676100	-5.41142400	0.00000000
H	-2.67678800	-3.51395800	0.00000000
C	2.21433100	1.73583400	0.00000000
C	3.00637600	2.87762400	0.00000000
C	2.41561200	4.14806500	0.00000000
C	1.02144600	4.26305400	0.00000000
C	0.21525100	3.12761000	0.00000000
H	2.68417100	0.76044200	0.00000000
H	4.08739900	2.77933600	0.00000000
H	3.03721900	5.03823200	0.00000000
H	0.55704700	5.24426100	0.00000000
H	-0.86059900	3.22403300	0.00000000

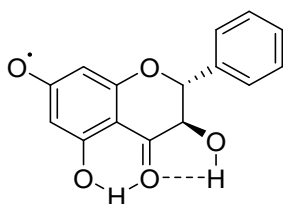


Sum of electronic and thermal Enthalpies: -954.760668

0 1

O	0.00000000	0.88792300	0.00000000
C	1.27783100	0.42391000	0.00000000
C	1.53003500	-0.96208300	0.00000000
C	0.42583500	-1.87322800	0.00000000
C	-0.90551600	-1.29684000	0.00000000
C	-1.09665300	0.06188700	0.00000000
O	0.54666700	-3.13433300	0.00000000
O	-1.92475600	-2.19549500	0.00000000
C	-2.35895600	0.81465900	0.00000000
C	2.30152900	1.36545400	0.00000000
C	3.61752400	0.89353800	0.00000000
C	3.91998000	-0.48123000	0.00000000

C	2.88374200	-1.40492100	0.00000000
H	2.08823300	2.42715200	0.00000000
O	4.60018100	1.83310600	0.00000000
H	4.94889600	-0.82624700	0.00000000
O	3.15923900	-2.72592700	0.00000000
C	-2.32945400	2.22653600	0.00000000
C	-3.51240700	2.96300800	0.00000000
C	-4.75101400	2.31304900	0.00000000
C	-4.79280800	0.91611200	0.00000000
C	-3.61441000	0.16890100	0.00000000
H	-1.37881100	2.74498000	0.00000000
H	-3.46550400	4.04782800	0.00000000
H	-5.67158400	2.88887300	0.00000000
H	-5.74806100	0.39976800	0.00000000
H	-3.66956700	-0.91038100	0.00000000
H	5.47414100	1.41557900	0.00000000
H	2.29249300	-3.20803800	0.00000000
H	-1.49241700	-3.07422900	0.00000000

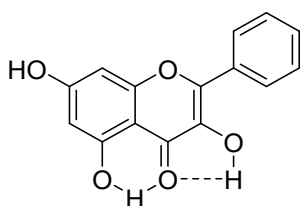


Sum of electronic and thermal Enthalpies: -954.119187

0 2

O	0.00000000	0.90812100	0.00000000
C	1.29262400	0.47983800	0.00000000
C	1.59691800	-0.89431400	0.00000000
C	0.52267300	-1.84179500	0.00000000
C	-0.82108800	-1.30455500	0.00000000
C	-1.06402700	0.06038200	0.00000000
O	0.67546400	-3.09830000	0.00000000
O	-1.80487500	-2.22208600	0.00000000
C	-2.34877500	0.76070600	0.00000000
C	2.28141200	1.44833400	0.00000000
C	3.68284000	1.03899200	0.00000000
C	3.99024900	-0.37378700	0.00000000
C	2.98706000	-1.30724300	0.00000000
H	2.03843300	2.50431800	0.00000000
O	4.58223300	1.92143100	0.00000000
H	5.03027800	-0.67918500	0.00000000
O	3.26716400	-2.62556300	0.00000000
C	-2.36690900	2.17473600	0.00000000
C	-3.57394100	2.86703600	0.00000000

C	-4.78810100	2.17066100	0.00000000
C	-4.78297600	0.77289300	0.00000000
C	-3.58051700	0.06780400	0.00000000
H	-1.43527600	2.72639900	0.00000000
H	-3.56757700	3.95246700	0.00000000
H	-5.72840400	2.71337400	0.00000000
H	-5.71982400	0.22464300	0.00000000
H	-3.59881800	-1.01232200	0.00000000
H	2.40941300	-3.12325700	0.00000000
H	-1.35275900	-3.09338700	0.00000000

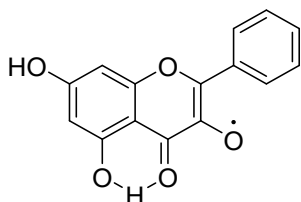


Sum of electronic and thermal Enthalpies: -953.582895

0 1

C	-3.37710300	-0.17030400	1.26037500
C	-2.47345400	-0.24148500	0.19325300
C	-2.92855800	-0.67292100	-1.06212800
C	-4.26675700	-1.02712200	-1.24353600
C	-5.16659500	-0.94705500	-0.17421800
C	-4.71979900	-0.51681200	1.07781800
C	-1.03238100	0.15695700	0.40007800
O	-0.19943600	-0.95800100	-0.02657300
C	1.14945000	-0.78113900	0.00005500
C	1.72180000	0.52004900	-0.03072600
C	0.87721000	1.67030900	-0.16262000
C	-0.60889500	1.41104900	-0.38173500
C	3.14239700	0.63935800	0.01646900
C	3.94921700	-0.49323000	0.05663000
C	3.34020800	-1.75615300	0.05980000
C	1.94460900	-1.91524600	0.04019800
O	1.28529300	2.85143100	-0.13481000
O	-1.37846100	2.52281800	0.02282700
O	4.07113800	-2.89760900	0.09910900
O	3.72229900	1.85469000	0.00468300
H	1.50234500	-2.90349100	0.07178900
H	5.02856500	-0.38689900	0.08271000
H	-2.23668900	-0.74255500	-1.89639900
H	-4.60760500	-1.36438500	-2.21795100
H	-6.20774900	-1.22085900	-0.31731200
H	-5.41090400	-0.45530200	1.91317400
H	-3.03175900	0.15767000	2.23704000

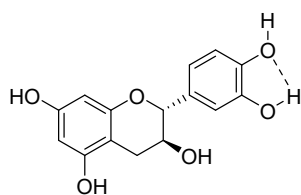
H	5.01924900	-2.69962400	0.12285400
H	3.00155400	2.53160300	-0.02803500
H	-0.78180600	3.29215500	0.00386900
H	-0.84573700	0.33129400	1.46729400
H	-0.74421100	1.21623500	-1.45919300



Sum of electronic and thermal Enthalpies: -1031.153668

0 2

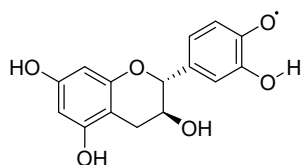
C	-3.34381500	-0.14110800	1.26779300
C	-2.44865900	-0.22247200	0.19434200
C	-2.91694000	-0.64090400	-1.06044700
C	-4.26168200	-0.97256600	-1.23499200
C	-5.15346100	-0.88251100	-0.15977400
C	-4.69276300	-0.46518200	1.09155500
C	-1.00068100	0.14992600	0.39618400
O	-0.18725900	-0.97546700	-0.04120400
C	1.16513200	-0.83887000	-0.00192700
C	1.77627400	0.45695700	-0.03763900
C	0.92727500	1.63163200	-0.16219100
C	-0.55561100	1.39155800	-0.39595500
C	3.20441100	0.57846100	0.02341800
C	3.99193600	-0.55583100	0.06208800
C	3.38055700	-1.86965700	0.06195000
C	1.93368200	-1.97827100	0.03965300
O	1.35882300	2.79380600	-0.10273600
O	-1.31973000	2.51281300	-0.02181300
O	4.09798800	-2.90693900	0.09722800
O	3.79356900	1.78943400	0.02299600
H	1.47942400	-2.96154800	0.06538100
H	5.07272800	-0.48182200	0.09286600
H	-2.23163700	-0.71883700	-1.89937600
H	-4.61374100	-1.30015600	-2.20862800
H	-6.19971400	-1.13872800	-0.29780400
H	-5.37787000	-0.39633500	1.93116400
H	-2.98742800	0.17691100	2.24370600
H	3.09112000	2.47992800	0.00039400
H	-0.73374300	3.28846400	-0.05798400
H	-0.80748200	0.32001500	1.46244200
H	-0.67271400	1.17596400	-1.47227600



Sum of electronic and thermal Enthalpies: -1031.153668

0 1

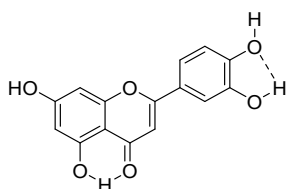
C	-2.73659300	0.15760000	1.03444200
C	-1.77094700	0.02599200	0.02679100
C	-2.16021500	-0.45739700	-1.22924100
C	-3.49089900	-0.80052800	-1.47842900
C	-4.44973300	-0.65868900	-0.47622700
C	-4.06647700	-0.17508400	0.78488100
C	-0.33907200	0.41530600	0.30470700
O	0.48741100	-0.73634400	0.00398700
C	1.85032700	-0.57573100	0.04704100
C	2.45033800	0.69325700	-0.00967800
C	1.60940900	1.94601700	-0.12901300
C	0.16400900	1.61908000	-0.51843800
C	3.85525000	0.73342200	0.03374100
C	4.63216600	-0.42563200	0.10613200
C	3.98978900	-1.66624700	0.14206500
C	2.59778600	-1.75465600	0.11911300
O	-0.68538200	2.75461700	-0.38078100
O	4.68878000	-2.84427400	0.21163600
O	4.54572000	1.91824300	0.00232900
H	2.09936000	-2.71621300	0.15969400
H	5.71426700	-0.34450400	0.13238300
H	-1.42500200	-0.57809500	-2.01825100
H	-3.79794900	-1.17891600	-2.44843100
O	-5.75251300	-0.99506600	-0.72880700
O	-5.08022600	-0.07572600	1.70880800
H	-2.45444700	0.52245500	2.01922000
H	5.64020500	-2.66807200	0.22558400
H	3.94054700	2.67160500	-0.03586500
H	-0.62675400	3.09145900	0.52567000
H	-0.22501100	0.64823800	1.37350300
H	0.11424200	1.35047200	-1.57846200
H	1.59467500	2.49574500	0.82473900
H	2.01722400	2.63115700	-0.88345700
H	-6.27847700	-0.83459500	0.07070000
H	-4.75402100	0.27739700	2.54825600



Sum of electronic and thermal Enthalpies: -1030.536076

0 2

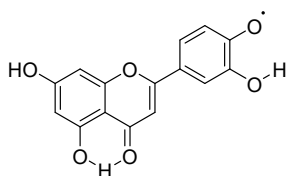
C	-2.79877200	0.30509700	1.01400100
C	-1.80506000	-0.02018700	0.09021000
C	-2.13275200	-0.72804900	-1.10919800
C	-3.42306300	-1.10033100	-1.38757400
C	-4.48715200	-0.78113100	-0.46874600
C	-4.11596600	-0.05649200	0.75084500
C	-0.37771500	0.40035700	0.34616900
O	0.45276700	-0.74674200	0.09025900
C	1.81645500	-0.56445300	0.09513900
C	2.39255700	0.70966500	-0.02812100
C	1.52662700	1.94183300	-0.17919700
C	0.08492600	1.57025500	-0.54296400
C	3.79748700	0.77231800	-0.01496300
C	4.59241300	-0.37174700	0.08947300
C	3.97094500	-1.61924500	0.19183300
C	2.58007300	-1.72902600	0.20179100
O	-0.81379300	2.65206200	-0.31553900
O	4.68909300	-2.78221300	0.29766700
O	4.46940600	1.96375900	-0.10938900
H	2.09671800	-2.69452500	0.29492700
H	5.67334400	-0.27367000	0.09148900
H	-1.33587300	-0.97860300	-1.80137200
H	-3.67832700	-1.63896600	-2.29437900
O	-5.70355600	-1.07887800	-0.63456600
O	-5.10634300	0.23318100	1.60244900
H	-2.56037400	0.83612400	1.92994800
H	5.63791600	-2.59172100	0.29013900
H	3.85389300	2.70858900	-0.14808000
H	-0.57198400	3.38697500	-0.89654400
H	-0.26525700	0.69598400	1.39751600
H	0.03334400	1.24457600	-1.59091900
H	1.49760200	2.52577700	0.75142900
H	1.91875300	2.60292300	-0.96401700
H	-5.92637300	-0.12599800	1.20063100



Sum of electronic and thermal Enthalpies: -1028.812150

0 1

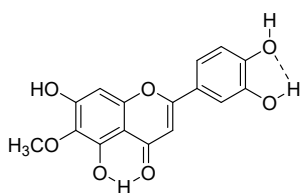
O	0.40327200	-0.74919800	0.00000000
C	-0.50219400	-1.77628200	0.00000000
C	-1.88274800	-1.50711200	0.00000000
C	-2.35097400	-0.13502800	0.00000000
C	-1.32785800	0.87737800	0.00000000
C	0.00000000	0.55187800	0.00000000
O	-3.58640600	0.14005900	0.00000000
C	1.13454000	1.48560900	0.00000000
C	0.01183900	-3.06659000	0.00000000
C	-0.90042200	-4.12818300	0.00000000
C	-2.28832300	-3.91581300	0.00000000
C	-2.77780200	-2.61243600	0.00000000
H	1.07973300	-3.24662800	0.00000000
O	-0.37190900	-5.38206900	0.00000000
H	-2.98260600	-4.75026800	0.00000000
O	-4.10791400	-2.39415900	0.00000000
C	2.45694400	1.00676400	0.00000000
C	3.53492800	1.89055700	0.00000000
C	3.31418400	3.26615100	0.00000000
C	1.99242900	3.75632600	0.00000000
C	0.91815000	2.88058000	0.00000000
H	2.64679400	-0.05886100	0.00000000
H	4.55525600	1.52169100	0.00000000
O	4.37021700	4.12352400	0.00000000
O	1.88454400	5.12336300	0.00000000
H	-0.08486400	3.29262100	0.00000000
H	-1.07473800	-6.04819500	0.00000000
H	-4.22535600	-1.39988800	0.00000000
H	4.03977600	5.03677900	0.00000000
H	0.95901300	5.40585700	0.00000000
H	-1.64359700	1.91195100	0.00000000



Sum of electronic and thermal Enthalpies: -1028.192342

0 2

O	0.45446800	-0.68978600	0.00000000
C	-0.41208400	-1.75018700	0.00000000
C	-1.80410500	-1.53278000	0.00000000
C	-2.32646400	-0.18379900	0.00000000
C	-1.33877500	0.87199300	0.00000000
C	0.00000000	0.59351600	0.00000000
O	-3.56624800	0.05309400	0.00000000
C	1.08799700	1.57438100	0.00000000
C	0.14982700	-3.01863100	0.00000000
C	-0.72223900	-4.11449200	0.00000000
C	-2.11755200	-3.95516300	0.00000000
C	-2.65709800	-2.67281000	0.00000000
H	1.22362100	-3.15846900	0.00000000
O	-0.14760500	-5.34537800	0.00000000
H	-2.77851500	-4.81588600	0.00000000
O	-3.99365300	-2.50785100	0.00000000
C	2.45111800	1.11953600	0.00000000
C	3.49820400	2.00059400	0.00000000
C	3.26028300	3.42399100	0.00000000
C	1.85589400	3.85927900	0.00000000
C	0.81023800	2.95462500	0.00000000
H	2.64540000	0.05474800	0.00000000
H	4.52710100	1.65668300	0.00000000
O	4.15537300	4.30674000	0.00000000
O	1.63870000	5.17927300	0.00000000
H	-0.20309300	3.33637100	0.00000000
H	-0.82382700	-6.03889300	0.00000000
H	-4.15679000	-1.52239000	0.00000000
H	2.52171700	5.60590200	0.00000000
H	-1.69536800	1.89289200	0.00000000

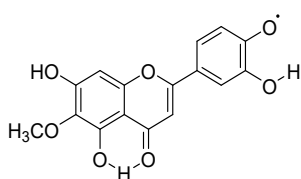


Sum of electronic and thermal Enthalpies: -1143.297935

0 1

C	-3.61385400	0.21802700	0.00000000
C	-2.35281600	0.84870100	0.00000000
C	-2.29657200	2.25366500	0.00000000
C	-3.46827100	3.01093000	0.00000000
C	-4.70922700	2.37759200	0.00000000
C	-4.77877300	0.97042500	0.00000000
C	-1.11706800	0.05123000	0.00000000

O	0.00000000	0.82417100	0.00000000
C	1.25174200	0.26582400	0.00000000
C	1.41948100	-1.12900900	0.00000000
C	0.24626700	-1.98401500	0.00000000
C	-1.02546900	-1.31294700	0.00000000
C	2.73725300	-1.67539300	0.00000000
C	3.83586100	-0.81190100	0.00000000
C	3.60923100	0.58711100	0.00000000
C	2.33119200	1.14009200	0.00000000
O	0.34575900	-3.24753600	0.00000000
O	4.68001800	1.42030500	0.00000000
O	2.89352200	-3.01920800	0.00000000
O	-5.91509000	3.02001600	0.00000000
O	-5.98910700	0.33551100	0.00000000
H	2.19173700	2.21411200	0.00000000
O	5.17157300	-1.12354400	0.00000000
H	-1.33997200	2.76013500	0.00000000
H	-3.41650100	4.09609700	0.00000000
H	-3.71344600	-0.86081900	0.00000000
H	5.48587000	0.87392200	0.00000000
H	1.96327700	-3.39860200	0.00000000
H	-5.80378500	3.98151800	0.00000000
H	-6.69590600	1.00035200	0.00000000
H	-1.91616800	-1.92639000	0.00000000
C	5.65682200	-2.47906300	0.00000000
H	6.74274000	-2.38368300	0.00000000
H	5.32697800	-3.01098300	0.89400400
H	5.32697800	-3.01098300	-0.89400400

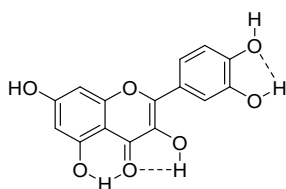


Sum of electronic and thermal Enthalpies: -1142.678393

0 2

C	-3.63571500	0.42087800	0.00000000
C	-2.34605400	0.98542900	0.00000000
C	-2.19099000	2.41389700	0.00000000
C	-3.27431700	3.25010600	0.00000000
C	-4.61454900	2.71534200	0.00000000
C	-4.74161800	1.25085400	0.00000000
C	-1.15711500	0.13039300	0.00000000
O	0.00000000	0.84133300	0.00000000
C	1.21745500	0.21320800	0.00000000
C	1.30714400	-1.19158400	0.00000000

C	0.09212000	-1.98129100	0.00000000
C	-1.14498100	-1.23757000	0.00000000
C	2.59324600	-1.81023200	0.00000000
C	3.73731300	-1.00882400	0.00000000
C	3.58814700	0.40197200	0.00000000
C	2.34266500	1.02541200	0.00000000
O	0.11225100	-3.24533700	0.00000000
O	4.70109600	1.17332700	0.00000000
O	2.67786600	-3.15975400	0.00000000
O	-5.66767000	3.40266400	0.00000000
O	-5.98585200	0.75854500	0.00000000
H	2.26335900	2.10540800	0.00000000
O	5.05185800	-1.39195700	0.00000000
H	-1.19157500	2.82958000	0.00000000
H	-3.15684800	4.32860200	0.00000000
H	-3.79282800	-0.65063100	0.00000000
H	5.47718200	0.58503500	0.00000000
H	1.73326200	-3.49387600	0.00000000
H	-6.58983300	1.53122500	0.00000000
H	-2.06739900	-1.80175900	0.00000000
C	5.46631800	-2.77176800	0.00000000
H	6.55552500	-2.73195900	0.00000000
H	5.10918200	-3.28476700	0.89435800
H	5.10918200	-3.28476700	-0.89435800

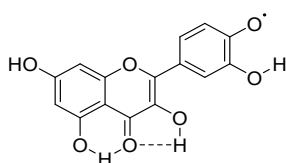


Sum of electronic and thermal Enthalpies: -1104.031250

0 1

C	-0.64524600	2.91809700	0.00000000
C	-1.00796000	1.55290800	0.00000000
C	-2.37823800	1.21925700	0.00000000
C	-3.35342400	2.21436100	0.00000000
C	-2.98353300	3.55878800	0.00000000
C	-1.62112100	3.90599900	0.00000000
C	0.00000000	0.48829400	0.00000000
O	-0.56542500	-0.76220200	0.00000000
C	0.16797900	-1.90760100	0.00000000
C	1.57473800	-1.84964200	0.00000000
C	2.22168600	-0.57120800	0.00000000
C	1.36899100	0.59858300	0.00000000
C	2.30320000	-3.07273300	0.00000000
C	1.62981900	-4.28719900	0.00000000

C	0.22233700	-4.29369000	0.00000000
C	-0.52634300	-3.11291600	0.00000000
O	3.48031100	-0.41552600	0.00000000
O	-0.48118100	-5.45771100	0.00000000
O	3.65293100	-3.05134200	0.00000000
O	-3.85840700	4.61074900	0.00000000
O	-1.23991500	5.22064100	0.00000000
H	-1.60895600	-3.13738400	0.00000000
H	2.19402300	-5.21406900	0.00000000
H	-2.68608400	0.18198400	0.00000000
H	-4.40565800	1.94416300	0.00000000
H	0.39180700	3.22211200	0.00000000
H	0.11556200	-6.22045000	0.00000000
H	3.93180400	-2.09914900	0.00000000
H	-4.77738200	4.30692300	0.00000000
H	-2.03303000	5.77955300	0.00000000
O	2.02023200	1.79331700	0.00000000
H	2.97224100	1.56511400	0.00000000

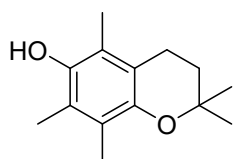


Sum of electronic and thermal Enthalpies: -1103.414263

0 2

C	-0.45926200	2.99271500	0.00000000
C	-0.91670400	1.65389500	0.00000000
C	-2.33458300	1.39345100	0.00000000
C	-3.25097300	2.40804900	0.00000000
C	-2.82472700	3.78648700	0.00000000
C	-1.37700400	4.02423600	0.00000000
C	0.00000000	0.53236000	0.00000000
O	-0.63962300	-0.68337600	0.00000000
C	0.02246600	-1.87163200	0.00000000
C	1.43314600	-1.90500200	0.00000000
C	2.16176600	-0.67649600	0.00000000
C	1.38178700	0.55443100	0.00000000
C	2.08209700	-3.17451400	0.00000000
C	1.33157400	-4.34172000	0.00000000
C	-0.07319600	-4.25643800	0.00000000
C	-0.74531500	-3.02841100	0.00000000
O	3.42270100	-0.58787500	0.00000000
O	-0.84965200	-5.36907900	0.00000000
O	3.42828500	-3.24318000	0.00000000
O	-3.59458500	4.78264400	0.00000000

O	-0.98568500	5.30851600	0.00000000
H	-1.82724300	-2.98465900	0.00000000
H	1.83389500	-5.30345500	0.00000000
H	-2.67526800	0.36628500	0.00000000
H	-4.31695400	2.20515300	0.00000000
H	0.59555900	3.22611700	0.00000000
H	-0.30571200	-6.17079500	0.00000000
H	3.77702600	-2.31669800	0.00000000
H	-1.80714800	5.84369800	0.00000000
O	2.10548800	1.69015900	0.00000000
H	3.04399500	1.40343400	0.00000000

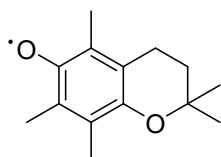


Sum of electronic and thermal Enthalpies: -695.731512

0 1

C	2.68810300	0.10094700	0.05878800
O	1.55528000	0.96752700	-0.23628300
C	0.27520200	0.45406500	-0.13194300
C	0.01594400	-0.92724700	-0.12469300
C	1.16793500	-1.91118400	-0.22362700
C	2.46854400	-1.23286600	-0.66432000
C	-1.31936200	-1.37099400	-0.02198900
C	-2.34965400	-0.41976900	0.02098100
C	-2.09636800	0.96076300	-0.01005000
C	-0.76344200	1.40420600	-0.06994300
C	-0.45262000	2.88379800	-0.08340200
C	-3.23745700	1.95214200	0.03302300
O	-3.67769700	-0.80912400	0.10391900
C	-1.67311900	-2.84263100	0.04300700
C	3.89923100	0.84269000	-0.50508000
C	2.81177000	-0.06009500	1.58104200
H	-0.79257400	-3.47213400	0.16788200
H	-2.33192000	-3.06094700	0.89387900
H	-2.18511700	-3.18552500	-0.86683400
H	-4.19879900	1.45311500	-0.09054700
H	-3.26272300	2.49367800	0.98772000
H	-3.13873800	2.70587400	-0.75578100
H	-3.74639900	-1.77097400	0.04862900
H	-1.02088600	3.41607100	0.68680500
H	0.60898500	3.06303300	0.08604800
H	-0.71831400	3.34083100	-1.04610800
H	2.43400800	-1.02919300	-1.74157800

H	3.32237100	-1.89551000	-0.48727500
H	0.92518400	-2.70523000	-0.93753500
H	1.31638900	-2.41200400	0.74304600
H	3.80026100	0.97808400	-1.58663700
H	3.99809400	1.82787600	-0.03826100
H	4.81417300	0.27511400	-0.30844300
H	3.65439200	-0.71539900	1.82574600
H	2.98545200	0.91406500	2.04855700
H	1.90725800	-0.49099300	2.01883900

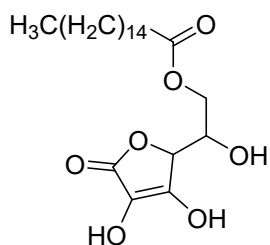


Sum of electronic and thermal Enthalpies: -695.121309

0 2

C	-2.65211500	-0.12885400	0.04434100
O	-1.45415200	-0.97094200	-0.12691400
C	-0.21591800	-0.43529900	-0.08605600
C	0.01521800	0.96595400	-0.08708400
C	-1.16202100	1.91307800	-0.17911300
C	-2.42075900	1.19992200	-0.67995000
C	1.31973900	1.42972600	-0.01197700
C	2.43586700	0.48746300	0.03132700
C	2.15186700	-0.95020500	-0.00274400
C	0.84476700	-1.39557500	-0.06018100
C	0.47316600	-2.85902900	-0.08750700
C	3.32545100	-1.89748000	0.03509100
O	3.62945000	0.90913600	0.09056800
C	1.62396200	2.90368500	0.01292500
C	-3.77556600	-0.93471800	-0.60296900
C	-2.88803700	0.03575200	1.55044100
H	1.02669300	3.42314200	0.77064100
H	2.68123100	3.06695800	0.22306900
H	1.39318000	3.37518700	-0.95167000
H	4.25632200	-1.33238400	0.08451000
H	3.27933300	-2.56211600	0.90559300
H	3.35659100	-2.53541600	-0.85588500
H	1.35435700	-3.49955300	-0.07350100
H	-0.15423700	-3.11974900	0.77206400
H	-0.11029800	-3.09838500	-0.98343800
H	-2.32672200	0.99414400	-1.75297600
H	-3.30082700	1.83731500	-0.54916600
H	-0.91928600	2.73910600	-0.85510300
H	-1.34716500	2.37383200	0.80057100

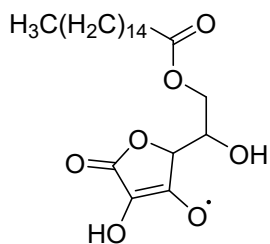
H	-3.58123100	-1.08464200	-1.66913300
H	-3.87394600	-1.91311100	-0.12316500
H	-4.72448700	-0.40077300	-0.49483700
H	-3.78276300	0.64251600	1.72217700
H	-3.03889600	-0.94202400	2.01695300
H	-2.04395700	0.52388100	2.04479900



Sum of electronic and thermal Enthalpies: -837.304830

0 1

C	2.16084500	0.85660100	0.19139200
C	3.00380200	-0.10427500	-0.23171800
C	2.36474200	-1.39631400	-0.01915400
O	1.12832800	-1.19522900	0.53426300
C	0.90148200	0.22325000	0.71925300
O	4.23765300	0.04833100	-0.77365400
O	2.80381900	-2.50433500	-0.27139900
C	-0.38353400	0.65791000	-0.02562900
C	-1.58719800	-0.11414100	0.48819500
O	-2.69351400	0.18344500	-0.39116400
C	-3.87756700	-0.39226000	-0.09519300
O	-4.03190500	-1.13875000	0.85689400
O	2.27057000	2.19771200	0.19385400
O	-0.62583800	2.04061800	0.20868800
C	-4.94880700	0.01569800	-1.07062700
H	0.78102300	0.40734200	1.79316000
H	-0.25417100	0.45676400	-1.09779400
H	4.60482200	-0.82869500	-0.97240500
H	-1.83730100	0.19707600	1.50670500
H	-1.39410300	-1.18858300	0.47594000
H	-5.15276500	1.08580200	-0.96282300
H	-4.61365900	-0.15486300	-2.09723700
H	0.09805400	2.56302300	-0.16849500
H	-5.85924200	-0.54981500	-0.87463500
H	3.11185200	2.47879500	-0.20137700



Sum of electronic and thermal Enthalpies: -836.688295

0 2

C	2.15089900	0.98463400	0.17185400
C	3.05635000	-0.05291400	-0.23007600
C	2.42404500	-1.35786100	-0.01799600
O	1.18506100	-1.16102000	0.50308800
C	0.91720400	0.25628200	0.71280700
O	4.25586400	0.11868900	-0.73990800
O	2.89414500	-2.45150700	-0.26287000
C	-0.37921600	0.68737200	-0.00711900
C	-1.56619700	-0.12659700	0.48012100
O	-2.68354800	0.19661900	-0.37481700
C	-3.85334800	-0.42095800	-0.10424100
O	-3.98355400	-1.22196400	0.80591600
O	2.27596800	2.20958800	0.08246700
O	-0.62759800	2.05618000	0.28524300
C	-4.93948200	0.01517800	-1.05020500
H	0.81911300	0.41957100	1.79102400
H	-0.25694500	0.53215400	-1.08865800
H	4.66579100	-0.74544200	-0.94152000
H	-1.81049700	0.13114500	1.51470400
H	-1.35697900	-1.19632600	0.41377700
H	-5.15642200	1.07670300	-0.89451000
H	-4.61190800	-0.10641300	-2.08627100
H	0.15564900	2.57636300	0.03857800
H	-5.84004800	-0.57124900	-0.87094900