

## ELECTRONIC SUPPLEMENTARY INFORMATION

### Impact of the phenolic O–H vs C-ring C–H bond cleavage on the antioxidant potency of dihydrokaempferol

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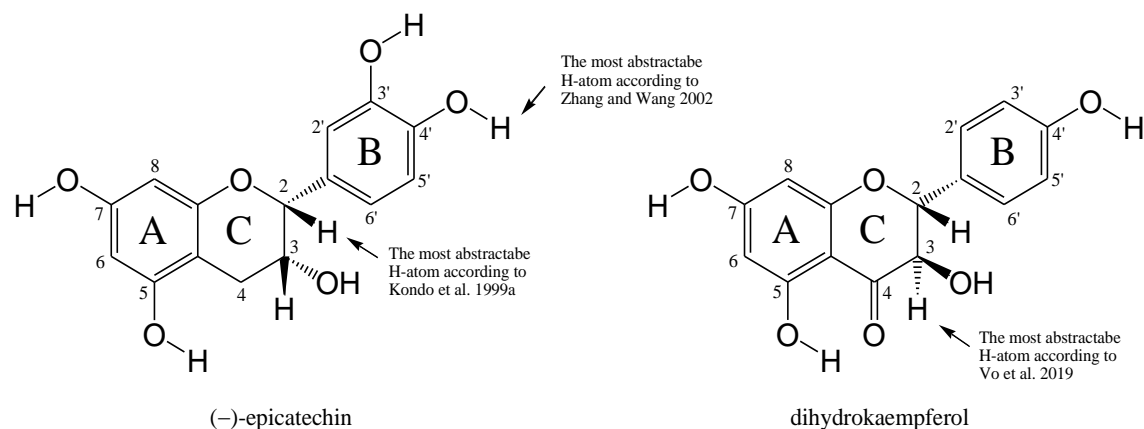
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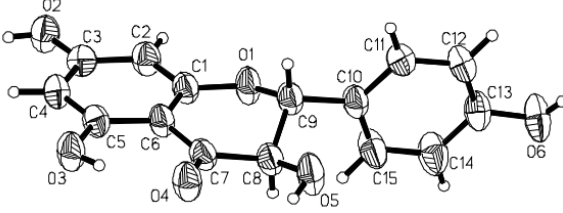
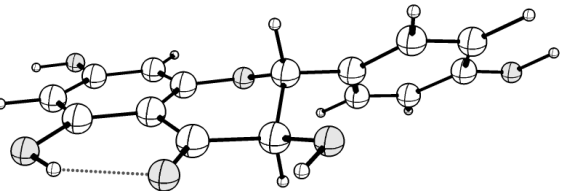
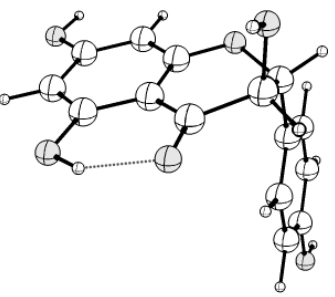
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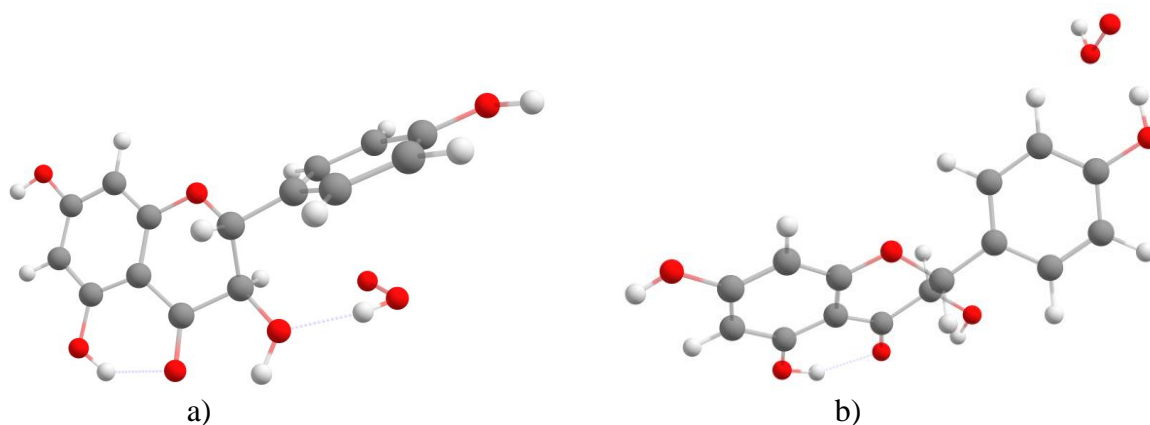
*\*corresponding author*



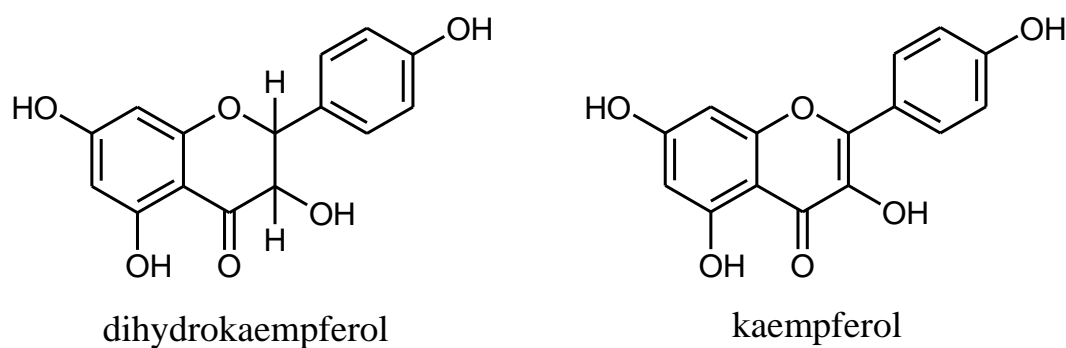
**Fig. S1** Proposed preferred sites for the hydrogen atom abstraction for (-)-epicatechin and dihydrokaempferol.

**Table S1.** Dihydrokaempferol structure.

	dihedral angle	
 <p>experimental structure in methanol<sup>26</sup></p>	C8 C9 C10 C15	52.8°
	C8 C9 C10 C11	-122.4°
	O5 C8 C9 C10	60.4°
	O1 C9 C10 C15	-65.8°
 <p>calculated in gas-phase – this work E(RM062X) = -1030.07613233 a.u.</p>	C8 C9 C10 C15	-82.9°
	C8 C9 C10 C11	94.2°
	O5 C8 C9 C10	60.4°
	O1 C9 C10 C15	156.5°
 <p>structure by Vo et al. in gas-phase<sup>11</sup> E(RM062X) = -1030.06838504 a.u.</p>	C8 C9 C10 C15	3.2°
	C8 C9 C10 C11	-177.7°
	O5 C8 C9 C10	170.4°
	O1 C9 C10 C15	-121.7°



**Fig. S2** Hydrogen bonding in: a) C3-H...<sup>•</sup>OOH RC, b) C4'-OH...<sup>•</sup>OOH RC related to Fig. 2.



**Fig. S3** Structure of dihydrokaempferol and kaempferol.

**Table S2.** The QTAIM properties (in a.u.) of the transferred hydrogen specie in RC, TS, and PC for reaction of dihydrokaempferol C4'-OH site with <sup>•</sup>OOH.

QTAIM property	RC	transoid TS above B ring PCET	transoid TS below B ring PCET	cisoid TS above B ring PCET/HAT	cisoid TS below B ring PCET/HAT	PC
density (H)	0.382	0.379	0.380	0.397	0.401	0.364
charge $q(\text{H})$	0.618	0.621	0.620	0.603	0.599	0.636
volume $V(\text{H})$	13.43	8.662	8.632	9.273	9.373	11.33
dipole moment $d(\text{H})$	0.131	0.015	0.014	0.022	0.021	0.118

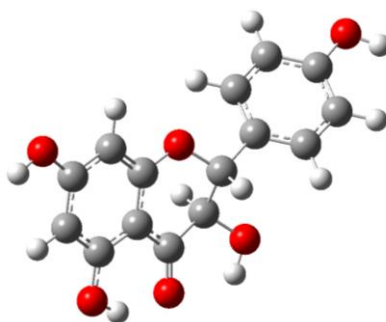
**Table S3.** Published  $pK_a$  values (and order of acidity) for kaempferol

$pK_{a1}$	$pK_{a2}$	$pK_{a3}$	reference
7.49 (7-OH)	9.12 (4'-OH)	10.90 (3-OH)	i
7.49 (7-OH)	7.96 (4'-OH)	11.05 (5-OH)	ii
7.05 (7-OH)	9.04 (4'-OH)	11.04 (5-OH)	iii
8.20 (7-OH)	9.50 (4'-OH)	10.50 (3-OH)	iv

## References

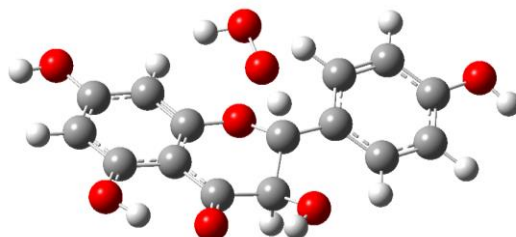
- i. R. Alvarez-Diduk, M. T. Ramirez-Silva, A. Galano and A. Merkoci, *J. Phys. Chem. B*, 2013, **117**, 12347–12359.
- ii. I. Matei, C. Tablet, S. Ionescu and M. Hillebrand, *Rev. Roum. Chim.*, 2014, **59**, 401–405.
- iii. J. M. Herrero-Martinez, M. Sanmartin, M. Roses, E. Bosch and C. Rafols, *Electrophoresis*, 2005, **26**, 1886–1895.
- iv. N. A. Tyukavkina and N. N. Pogodaeva, *Khim. Prirodn. Soedin.*, 1975, **11**, 708–711.

## Cartesian coordinates of dihydrokaempferol in gas-phase



6	2.080838000	0.497040000	-0.057832000
6	1.476492000	-0.776174000	0.051368000
6	1.258053000	1.666618000	-0.243376000
6	3.494232000	0.583668000	-0.047246000
8	0.131714000	-0.916931000	0.060687000
6	2.236306000	-1.925049000	0.137847000
6	-0.230040000	1.418768000	-0.422492000
8	1.681253000	2.819203000	-0.276400000
6	4.264849000	-0.566942000	0.038121000
8	4.116868000	1.760632000	-0.135794000
6	-0.647154000	0.222949000	0.437508000
6	3.627361000	-1.803431000	0.122196000
8	-0.968029000	2.547372000	-0.060688000
6	-2.102815000	-0.119145000	0.272437000
8	4.328138000	-2.953481000	0.209173000
6	-2.520871000	-1.085352000	-0.641950000
6	-3.059465000	0.581221000	1.001061000
6	-3.870120000	-1.351917000	-0.822887000
6	-4.412800000	0.325778000	0.822513000
6	-4.818630000	-0.643188000	-0.091274000
8	-6.128954000	-0.942315000	-0.309157000
1	1.768435000	-2.894658000	0.232823000
1	-0.393496000	1.149815000	-1.479182000
1	5.344655000	-0.479657000	0.037792000
1	3.445538000	2.468189000	-0.184896000
1	-0.431281000	0.465021000	1.486589000
1	-0.376579000	3.307301000	-0.147880000
1	5.271767000	-2.768109000	0.204404000
1	-1.782756000	-1.642462000	-1.205738000
1	-2.745628000	1.346363000	1.701949000
1	-4.207914000	-2.104996000	-1.523852000
1	-5.152152000	0.878825000	1.393087000
1	-6.685939000	-0.390542000	0.246364000

Cartesian coordinates of TS dihydrokaempferol C2-H...OOH  
 imaginary frequency =  $-1910.28 \text{ cm}^{-1}$



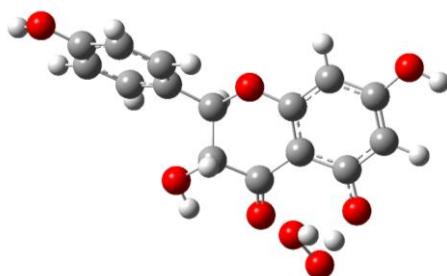
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6	1.329056000	1.805876000	-0.208872000
6	3.491191000	0.560852000	-0.174096000
8	0.051985000	-0.684501000	-0.570315000
6	2.081435000	-1.838642000	-0.587043000
6	-0.167311000	1.724907000	-0.493565000
8	1.815659000	2.899109000	0.056987000
6	4.186246000	-0.636673000	-0.288664000
8	4.187137000	1.678270000	0.033120000
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6	3.477155000	-1.816417000	-0.499436000
8	-0.827052000	2.787260000	0.127465000
6	-2.142230000	0.066990000	-0.139178000
8	4.099328000	-3.007602000	-0.611824000
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6	-4.452441000	0.692992000	-0.474972000
6	-4.844460000	-0.628588000	-0.280137000
8	-6.142112000	-1.023721000	-0.340851000
1	1.551093000	-2.768936000	-0.736110000
1	5.266394000	-0.627341000	-0.205315000
1	3.566752000	2.425492000	0.128451000
1	-0.418097000	0.333080000	1.231314000
1	-0.155661000	3.454716000	0.328316000
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1	-2.822099000	2.074133000	-0.534264000
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1	-6.707974000	-0.265766000	-0.510987000
8	0.192632000	-1.344314000	2.281237000
1	1.090660000	-1.522336000	1.962939000
8	0.118001000	0.029051000	2.322354000
1	-0.281250000	1.776662000	-1.591937000

Cartesian coordinates of TS dihydrokaempferol C3-H...OOH  
 imaginary frequency  $-1965.40\text{ cm}^{-1}$



6	-2.236327000	0.429961000	-0.180538000
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6	0.097375000	1.269817000	-0.252407000
8	-1.730504000	2.749231000	-0.278634000
6	-4.455473000	-0.527598000	0.083318000
8	-4.202296000	1.794072000	-0.040306000
6	0.451946000	-0.076092000	-0.865790000
6	-3.877848000	-1.795161000	0.087108000
8	0.879466000	2.281258000	-0.723444000
6	1.898821000	-0.430695000	-0.634161000
8	-4.625703000	-2.911217000	0.215429000
6	2.281851000	-1.209715000	0.459289000
6	2.880386000	0.098812000	-1.465340000
6	3.624779000	-1.444577000	0.722767000
6	4.227056000	-0.132138000	-1.211015000
6	4.600985000	-0.904245000	-0.113889000
8	5.898503000	-1.169622000	0.190034000
1	-2.081251000	-2.981761000	-0.061595000
1	-5.524545000	-0.385923000	0.187410000
1	-3.503065000	2.470762000	-0.128080000
1	0.245548000	-0.026010000	-1.945537000
1	0.390607000	3.107610000	-0.585652000
1	-5.554183000	-2.678684000	0.307679000
1	1.523456000	-1.622039000	1.112665000
1	2.595141000	0.715421000	-2.310347000
1	3.934660000	-2.050002000	1.565692000
1	4.984506000	0.288089000	-1.864695000
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8	2.150274000	1.632184000	1.941554000
1	2.736533000	0.921627000	1.629582000
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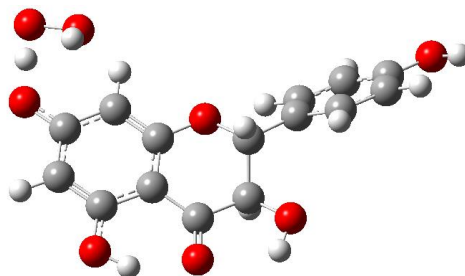
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6	3.214192000	-0.010228000	-0.395261000
8	-0.292440000	1.135097000	-0.155917000
6	1.695912000	2.332853000	-0.099711000
6	-0.415369000	-1.274729000	-0.058163000
8	1.507216000	-2.410682000	-0.846551000
6	3.849778000	1.242951000	-0.258649000
8	3.955342000	-1.062249000	-0.543901000
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6	3.091321000	2.393259000	-0.126863000
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6	-2.467254000	0.179496000	-0.316106000
8	3.641139000	3.622932000	-0.012494000
6	-2.870661000	0.955109000	0.770087000
6	-3.432570000	-0.483241000	-1.068480000
6	-4.213723000	1.073801000	1.096760000
6	-4.778630000	-0.376033000	-0.745501000
6	-5.170301000	0.405519000	0.338567000
8	-6.474449000	0.555745000	0.700429000
1	1.110994000	3.238118000	-0.004529000
1	4.933200000	1.263405000	-0.273579000
1	3.697081000	-1.919133000	0.233756000
1	-0.883400000	-0.037054000	-1.746253000
1	-0.451471000	-3.057175000	-0.738792000
1	4.599336000	3.564752000	-0.070700000
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1	-3.129101000	-1.102046000	-1.904996000
1	-4.538836000	1.680650000	1.932586000
1	-5.524293000	-0.898455000	-1.336350000
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8	2.526704000	-1.789360000	1.857091000
1	2.909064000	-1.387802000	2.650662000
8	3.578914000	-2.446082000	1.283338000
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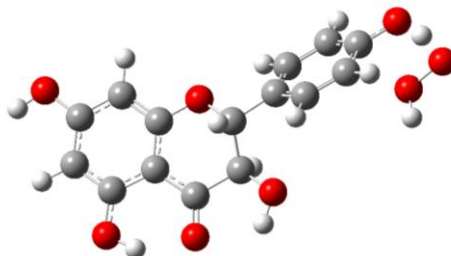


Cartesian coordinates of TS dihydrokaempferol 7-OH...•OOH  
 imaginary frequency =  $-2267.49 \text{ cm}^{-1}$



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6	2.961680000	1.493395000	-0.207586000
8	-0.140940000	-0.528655000	-0.304676000
6	2.088606000	-1.160537000	-0.599688000
6	-0.884699000	1.759331000	-0.183637000
8	0.802335000	3.372971000	0.245050000
6	3.894114000	0.509173000	-0.446796000
8	3.380314000	2.748855000	-0.020292000
6	-1.048607000	0.344144000	0.375879000
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6	-2.444230000	-0.184607000	0.194529000
8	4.345905000	-1.743222000	-0.921968000
6	-2.798959000	-0.902193000	-0.947842000
6	-3.417515000	0.094380000	1.147968000
6	-4.101646000	-1.339226000	-1.132286000
6	-4.726704000	-0.333667000	0.969608000
6	-5.068989000	-1.052490000	-0.172897000
8	-6.330884000	-1.505679000	-0.403485000
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1	-1.081839000	1.718908000	-1.268100000
1	4.948773000	0.744844000	-0.485079000
1	2.612844000	3.323467000	0.150219000
1	-0.786186000	0.363596000	1.442209000
1	-1.307242000	3.484045000	0.539182000
1	4.272380000	-2.646118000	-0.139068000
1	-2.044973000	-1.132757000	-1.690850000
1	-3.156026000	0.663922000	2.032724000
1	-4.387898000	-1.905516000	-2.009739000
1	-5.480003000	-0.112637000	1.719074000
1	-6.910731000	-1.240471000	0.315292000
8	4.209991000	-3.259417000	0.847158000
8	3.097398000	-2.769493000	1.468125000
1	3.446550000	-2.318666000	2.251349000

Cartesian coordinates of TS dihydrokaempferol 4'-OH...OOH cisoid below B-ring  
 imaginary frequency =  $-2081.62 \text{ cm}^{-1}$



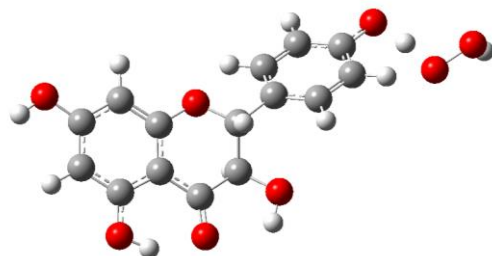
6	2.673170000	0.511018000	-0.081253000
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6	4.077262000	0.631217000	-0.224043000
8	0.776943000	-0.952905000	0.203535000
6	2.898241000	-1.911920000	0.015178000
6	0.317761000	1.383991000	-0.166542000
8	2.199345000	2.828854000	-0.176682000
6	4.875426000	-0.503164000	-0.263464000
8	4.662899000	1.823992000	-0.341465000
6	0.029068000	0.155811000	0.703009000
6	4.277234000	-1.756664000	-0.150492000
8	-0.408862000	2.482379000	0.294199000
6	-1.429981000	-0.204996000	0.689249000
8	5.004943000	-2.891187000	-0.178550000
6	-1.930938000	-1.116625000	-0.242280000
6	-2.300661000	0.434105000	1.583704000
6	-3.285377000	-1.393624000	-0.283784000
6	-3.653327000	0.172163000	1.547986000
6	-4.172813000	-0.758080000	0.616657000
8	-5.456425000	-1.026121000	0.603791000
1	2.463486000	-2.894937000	0.128416000
1	0.053103000	1.129866000	-1.206095000
1	5.946515000	-0.389709000	-0.380376000
1	3.979476000	2.519141000	-0.292255000
1	0.354664000	0.373772000	1.728773000
1	0.157972000	3.258732000	0.185820000
1	5.938781000	-2.685451000	-0.281162000
1	-1.250938000	-1.611025000	-0.924744000
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1	-4.346189000	0.650244000	2.229770000
1	-5.927384000	-0.643143000	-0.367170000
8	-6.179650000	0.021491000	-1.358649000
8	-4.945396000	0.317031000	-1.853735000
1	-4.793348000	1.238812000	-1.595106000

Cartesian coordinates of TS dihydrokaempferol 4'-OH...OOH cisoid above B-ring  
 imaginary frequency =  $-2187.47 \text{ cm}^{-1}$



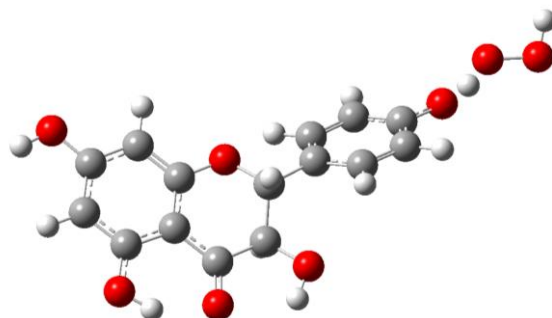
6	2.768369000	-0.359100000	0.011005000
6	1.951758000	0.794332000	0.015432000
6	2.167127000	-1.662874000	0.136855000
6	4.174273000	-0.197099000	-0.045106000
8	0.601283000	0.697659000	0.056352000
6	2.496762000	2.060677000	-0.004627000
6	0.666970000	-1.691533000	0.384047000
8	2.779392000	-2.724763000	0.071977000
6	4.731278000	1.073632000	-0.063403000
8	4.993504000	-1.249467000	-0.063889000
6	0.016787000	-0.530248000	-0.375994000
6	3.888484000	2.182943000	-0.035128000
8	0.117944000	-2.905121000	-0.031067000
6	-1.468128000	-0.459423000	-0.142426000
8	4.374772000	3.440371000	-0.051791000
6	-2.010805000	0.453670000	0.762800000
6	-2.308564000	-1.355822000	-0.822710000
6	-3.375303000	0.478083000	0.993595000
6	-3.668895000	-1.335267000	-0.608683000
6	-4.230676000	-0.422435000	0.316337000
8	-5.521876000	-0.432334000	0.540061000
1	1.866441000	2.938639000	-0.009028000
1	0.508214000	-1.521645000	1.461470000
1	5.809145000	1.176430000	-0.098235000
1	4.460122000	-2.066777000	-0.048644000
1	0.221978000	-0.664958000	-1.446829000
1	0.834483000	-3.554829000	-0.021806000
1	5.336031000	3.426253000	-0.079203000
1	-1.359047000	1.149856000	1.274236000
1	-1.874053000	-2.071202000	-1.511023000
1	-3.816158000	1.182543000	1.688233000
1	-4.337420000	-2.016227000	-1.121104000
1	-5.980889000	0.583711000	0.298413000
8	-6.254794000	1.647077000	-0.244156000
8	-5.030986000	2.176120000	-0.531139000
1	-4.939399000	2.064661000	-1.489221000

Cartesian coordinates of TS dihydrokaempferol 4'-OH...OOH transoid below B-ring  
 imaginary frequency =  $-2739.89 \text{ cm}^{-1}$



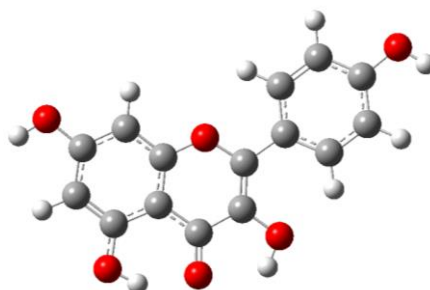
6	2.860178000	0.557420000	-0.065170000
6	2.329689000	-0.748289000	0.037810000
6	1.971087000	1.681211000	-0.221995000
6	4.266922000	0.721288000	-0.074825000
8	0.992653000	-0.962839000	0.062394000
6	3.149978000	-1.854688000	0.100710000
6	0.494130000	1.355678000	-0.381762000
8	2.326845000	2.855729000	-0.246711000
6	5.099946000	-0.386977000	-0.014681000
8	4.824067000	1.930407000	-0.158749000
6	0.161078000	0.124176000	0.468157000
6	4.532753000	-1.657254000	0.065468000
8	-0.298858000	2.434554000	0.009353000
6	-1.276028000	-0.293858000	0.319533000
8	5.294949000	-2.767849000	0.129640000
6	-1.638279000	-1.329646000	-0.551854000
6	-2.264230000	0.396675000	1.031067000
6	-2.965353000	-1.666686000	-0.718602000
6	-3.593826000	0.055857000	0.892775000
6	-3.968237000	-0.988907000	0.011416000
8	-5.218432000	-1.350486000	-0.119770000
1	2.737065000	-2.849349000	0.190948000
1	0.328460000	1.092499000	-1.439439000
1	6.173182000	-0.240344000	-0.029603000
1	4.117558000	2.603493000	-0.186691000
1	0.375671000	0.364692000	1.518078000
1	0.243539000	3.230156000	-0.080721000
1	6.227493000	-2.532914000	0.111981000
1	-0.866123000	-1.864710000	-1.089845000
1	-1.976398000	1.206938000	1.690345000
1	-3.273104000	-2.458542000	-1.390258000
1	-4.370347000	0.573475000	1.443404000
1	-5.885365000	-0.418193000	-0.121136000
8	-6.472441000	0.608489000	-0.359495000
8	-7.763084000	0.370763000	0.029058000
1	-8.276061000	0.546636000	-0.771119000

Cartesian coordinates of TS dihydrokaempferol 4'-OH...OOH transoid above B-ring  
 imaginary frequency =  $-2727.17 \text{ cm}^{-1}$



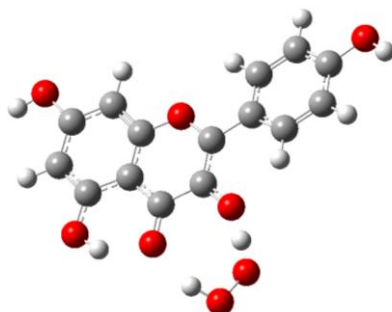
6	-2.904078000	0.447597000	-0.028854000
6	-2.239530000	-0.799348000	-0.009269000
6	-2.155221000	1.663319000	0.171585000
6	-4.311735000	0.464926000	-0.185816000
8	-0.892814000	-0.873941000	0.122027000
6	-2.933899000	-1.986284000	-0.108577000
6	-0.680666000	1.498030000	0.501712000
8	-2.626828000	2.794350000	0.101894000
6	-5.018790000	-0.724956000	-0.285092000
8	-4.992138000	1.611498000	-0.225566000
6	-0.139630000	0.279347000	-0.254025000
6	-4.324302000	-1.931828000	-0.238927000
8	0.040026000	2.639338000	0.150116000
6	1.310948000	0.027202000	0.049036000
8	-4.960524000	-3.116980000	-0.334012000
6	1.692703000	-0.898630000	1.029671000
6	2.285248000	0.770868000	-0.625866000
6	3.026658000	-1.093479000	1.319705000
6	3.622200000	0.609679000	-0.325959000
6	4.017097000	-0.332932000	0.656139000
8	5.276499000	-0.500200000	0.966343000
1	-2.416886000	-2.935235000	-0.103978000
1	-0.606501000	1.287038000	1.581259000
1	-6.095692000	-0.689865000	-0.398034000
1	-4.365262000	2.355541000	-0.148490000
1	-0.272460000	0.456028000	-1.329824000
1	-0.587744000	3.374904000	0.136282000
1	-5.906605000	-2.979449000	-0.438911000
1	0.931428000	-1.475532000	1.539570000
1	1.978875000	1.495478000	-1.371138000
1	3.351804000	-1.816719000	2.057380000
1	4.388764000	1.185358000	-0.830656000
1	5.904941000	-0.449892000	0.009843000
8	6.422541000	-0.627576000	-1.067842000
8	7.732387000	-0.266101000	-0.902070000
1	8.220123000	-1.051843000	-1.183208000

## Cartesian coordinates of kaempferol in gas-phase



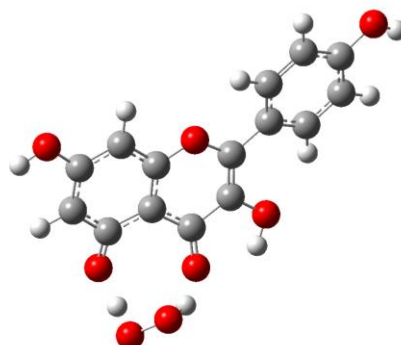
6	4.214370000	-0.686658000	0.016204000
6	3.518284000	0.509100000	-0.003041000
6	2.101073000	0.499267000	-0.002018000
6	1.437709000	-0.733760000	0.017020000
6	2.120345000	-1.939948000	0.035997000
6	3.508999000	-1.895041000	0.035207000
1	5.297742000	-0.664354000	0.015054000
6	1.329626000	1.711413000	-0.025195000
1	1.593632000	-2.883208000	0.052509000
6	-0.692929000	0.328992000	0.000104000
6	-0.114239000	1.558425000	-0.026508000
6	-2.123546000	0.007483000	0.000631000
6	-2.533754000	-1.326966000	-0.146210000
6	-3.107719000	0.992992000	0.152590000
6	-3.873132000	-1.668108000	-0.147313000
1	-1.790577000	-2.103844000	-0.262810000
6	-4.452192000	0.652478000	0.153271000
1	-2.825984000	2.028103000	0.272843000
6	-4.840319000	-0.675924000	0.002702000
1	-5.203235000	1.426758000	0.274090000
8	0.087713000	-0.790094000	0.019476000
8	1.814819000	2.855313000	-0.050830000
8	4.153278000	-3.083904000	0.054027000
1	5.104498000	-2.944838000	0.052752000
8	4.196428000	1.659083000	-0.022780000
1	3.554190000	2.397763000	-0.038960000
8	-0.815882000	2.713324000	-0.058585000
1	-0.147666000	3.418857000	-0.080169000
8	-6.140617000	-1.063897000	-0.005617000
1	-6.712059000	-0.300149000	0.111774000
1	-4.191917000	-2.696163000	-0.263252000

Cartesian coordinates of TS kaempferol 3-OH...OOH  
 imaginary frequency =  $-2975.04 \text{ cm}^{-1}$



6	2.585598000	-1.668835000	0.336651000
6	2.151351000	-0.406948000	-0.115707000
6	3.121468000	0.531807000	-0.505853000
6	4.468018000	0.219783000	-0.435761000
6	4.877356000	-1.030304000	0.026630000
6	3.926925000	-1.977364000	0.413558000
6	0.724186000	-0.126439000	-0.166271000
6	0.123948000	1.123851000	-0.332633000
6	-1.345616000	1.218657000	-0.309669000
6	-2.075505000	-0.013802000	-0.160287000
6	-1.380649000	-1.222004000	-0.024983000
8	-0.023664000	-1.241459000	-0.035907000
6	-3.494407000	-0.055907000	-0.140324000
6	-4.149494000	-1.269139000	0.003741000
6	-3.407993000	-2.444618000	0.132730000
6	-2.015276000	-2.440459000	0.121381000
8	-4.220374000	1.053961000	-0.261083000
8	-4.005156000	-3.646711000	0.274835000
8	-1.918854000	2.318855000	-0.413851000
8	0.813732000	2.205689000	-0.513904000
8	6.177910000	-1.385198000	0.119306000
1	2.814869000	1.500989000	-0.867887000
1	1.855677000	-2.406546000	0.641145000
1	5.206687000	0.951673000	-0.746136000
1	0.538704000	2.995843000	0.394427000
1	-1.455642000	-3.359324000	0.221370000
1	-5.232939000	-1.278532000	0.015202000
1	6.742439000	-0.661736000	-0.168350000
1	-3.608383000	1.813273000	-0.350146000
1	-4.961517000	-3.546129000	0.271505000
8	0.165607000	3.724339000	1.180798000
8	-0.682930000	4.523292000	0.490398000
1	4.265331000	-2.941598000	0.770812000
1	-1.274866000	3.880297000	0.034108000

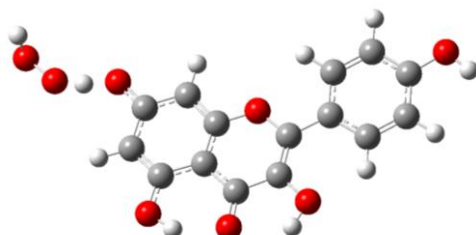
Cartesian coordinates of TS kaempferol 5-OH...OOH  
 imaginary frequency =  $-2138.07\text{cm}^{-1}$



6	3.109356000	1.148815000	0.447142000
6	2.550571000	-0.041129000	-0.045925000
6	3.413376000	-1.074204000	-0.432707000
6	4.786931000	-0.921910000	-0.323661000
6	5.324181000	0.262350000	0.175217000
6	4.477787000	1.301346000	0.560482000
6	1.096372000	-0.169802000	-0.149604000
6	0.369216000	-1.304700000	-0.335579000
6	-1.084461000	-1.289939000	-0.334425000
6	-1.711405000	0.009925000	-0.289830000
6	-0.890968000	1.123284000	-0.081244000
8	0.451634000	1.016368000	0.004903000
6	-3.126601000	0.242060000	-0.483376000
6	-3.619492000	1.556527000	-0.327081000
6	-2.765691000	2.616762000	-0.059323000
6	-1.391759000	2.416482000	0.050320000
8	-3.928857000	-0.679026000	-0.875105000
8	-3.203536000	3.886616000	0.086024000
8	-1.663371000	-2.389516000	-0.337437000
8	0.930365000	-2.524741000	-0.446302000
8	6.657957000	0.463066000	0.308297000
1	3.014058000	-1.998232000	-0.823499000
1	2.459662000	1.959342000	0.748815000
1	5.444030000	-1.729440000	-0.629835000
1	0.182312000	-3.146553000	-0.479318000
1	-0.722815000	3.247681000	0.226860000
1	-4.684634000	1.704410000	-0.464851000
1	7.140047000	-0.311967000	0.006733000
1	-4.240931000	-1.644316000	-0.072990000
1	-4.159650000	3.922479000	-0.011782000
8	-4.532652000	-2.212315000	0.806169000
8	-3.443561000	-2.185444000	1.617153000
1	4.912107000	2.214786000	0.946644000
1	-2.712493000	-2.473462000	1.021172000

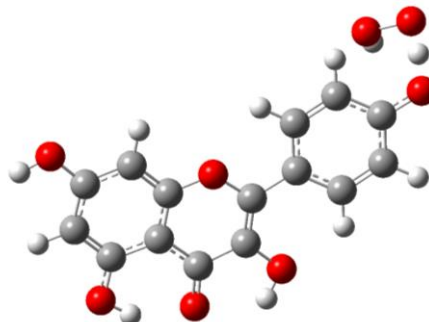


Cartesian coordinates of TS kaempferol 7-OH...OOH  
 imaginary frequency =  $-2807.24 \text{ cm}^{-1}$



6	-2.924265000	-1.616330000	0.044595000
6	-2.806727000	-0.216637000	0.014914000
6	-3.980094000	0.550442000	0.007814000
6	-5.222724000	-0.062876000	0.033812000
6	-5.319781000	-1.451770000	0.067768000
6	-4.161728000	-2.229035000	0.073024000
6	-1.477014000	0.394531000	-0.016040000
6	-1.161750000	1.716396000	0.098328000
6	0.212290000	2.173578000	0.053314000
6	1.221403000	1.158266000	-0.107176000
6	0.822702000	-0.182584000	-0.212925000
8	-0.486533000	-0.524700000	-0.169201000
6	2.611086000	1.480267000	-0.160918000
6	3.538532000	0.478831000	-0.334887000
6	3.111555000	-0.871224000	-0.429589000
6	1.739165000	-1.205961000	-0.350491000
8	3.017439000	2.748326000	-0.062238000
8	3.967100000	-1.830922000	-0.615494000
8	0.446017000	3.388465000	0.162597000
8	-2.083914000	2.686117000	0.263214000
8	-6.507033000	-2.103453000	0.096648000
1	-3.926028000	1.627991000	-0.019870000
1	-2.031646000	-2.226955000	0.047680000
1	-6.122489000	0.543998000	0.026648000
1	-1.580141000	3.515921000	0.322227000
1	1.430156000	-2.239971000	-0.413707000
1	4.592335000	0.718750000	-0.397283000
1	-7.231919000	-1.472276000	0.084311000
1	2.234943000	3.324596000	0.046270000
1	4.997228000	-1.623051000	-0.032563000
8	5.835827000	-1.512061000	0.748902000
8	6.778573000	-2.429957000	0.371315000
1	-4.255775000	-3.307247000	0.098946000
1	6.937606000	-2.931661000	1.182149000

Cartesian coordinates of TS kaempferol 4'-OH...OOH  
 imaginary frequency =  $-2271.83 \text{ cm}^{-1}$



6	-4.736005000	-1.037278000	0.120444000
6	-4.180704000	0.225457000	0.221612000
6	-2.778323000	0.390787000	0.089714000
6	-1.984437000	-0.741736000	-0.140846000
6	-2.526486000	-2.011775000	-0.244969000
6	-3.904816000	-2.138965000	-0.111267000
1	-5.808931000	-1.149874000	0.222668000
6	-2.153366000	1.677167000	0.188891000
1	-1.904031000	-2.876256000	-0.425970000
6	0.007015000	0.567852000	-0.186201000
6	-0.702769000	1.708420000	0.039711000
6	1.451413000	0.429119000	-0.347316000
6	2.011809000	-0.858587000	-0.454605000
6	2.306598000	1.553328000	-0.402798000
6	3.369072000	-1.027118000	-0.610341000
1	1.366995000	-1.725247000	-0.414014000
6	3.664169000	1.390046000	-0.546902000
1	1.894661000	2.548064000	-0.329981000
6	4.229597000	0.098217000	-0.667361000
1	4.331595000	2.241776000	-0.592588000
8	-0.643929000	-0.629691000	-0.272132000
8	-2.751325000	2.744890000	0.394615000
8	-4.407763000	-3.387361000	-0.218277000
1	-5.362525000	-3.373159000	-0.105280000
8	-4.978041000	1.272195000	0.443380000
1	-4.430345000	2.081049000	0.489874000
8	-0.148737000	2.928832000	0.151115000
1	-0.891024000	3.537113000	0.312794000
8	5.514919000	-0.033548000	-0.854012000
1	5.961324000	-0.753876000	-0.099289000
1	3.805607000	-2.015122000	-0.690149000
8	6.268574000	-1.323435000	0.950064000
8	5.078152000	-1.451361000	1.605444000
1	5.145290000	-0.828242000	2.343764000