

Supplementary Materials: The Antioxidant Activity of Quercetin in Water Solution

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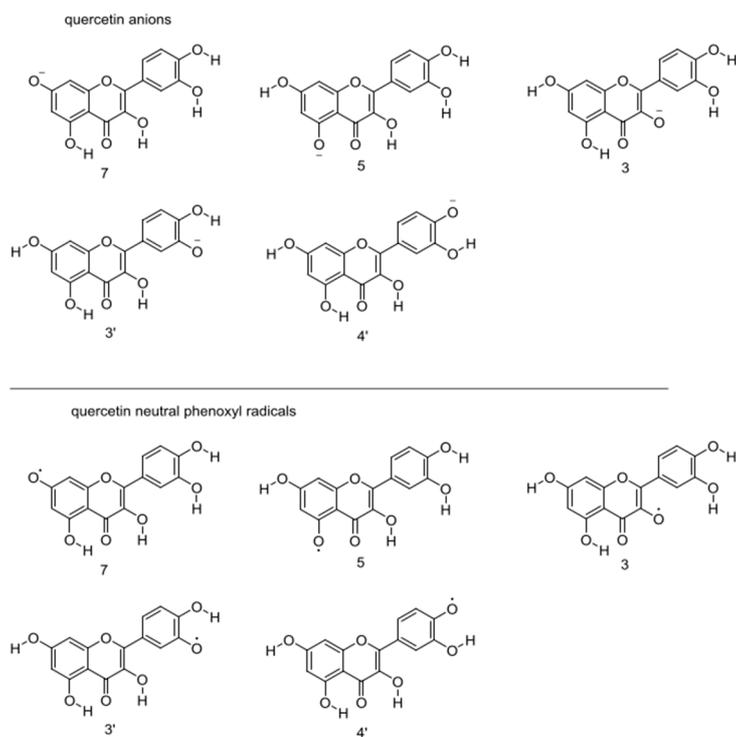


Figure S1. Structures of the anions and of the neutral phenoxyl radicals of quercetin.

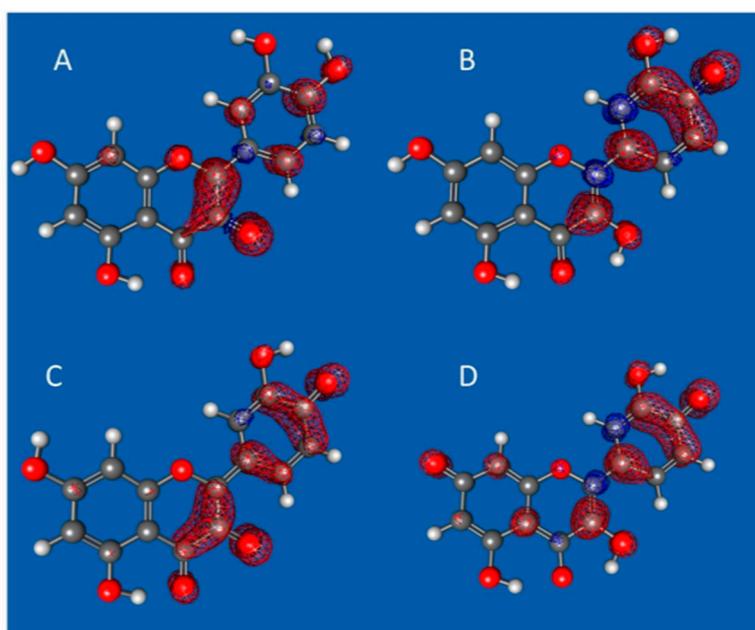


Figure S2. Spin distribution of quercetin radicals. Neutral radicals (A) 3-OH and (B) 4'-OH, and radical anions (C) 3,4' and (D) 7,4' of quercetin.

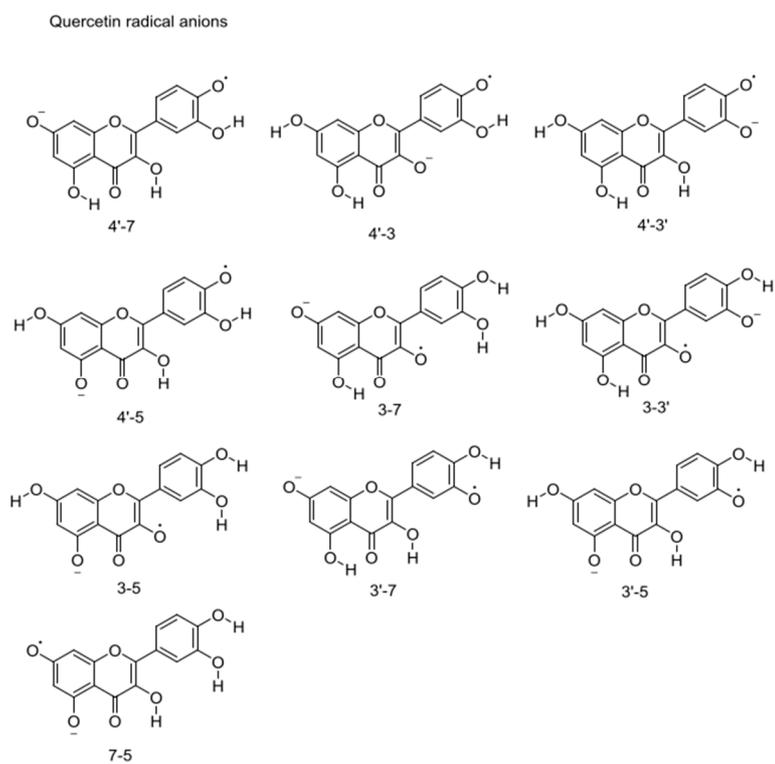


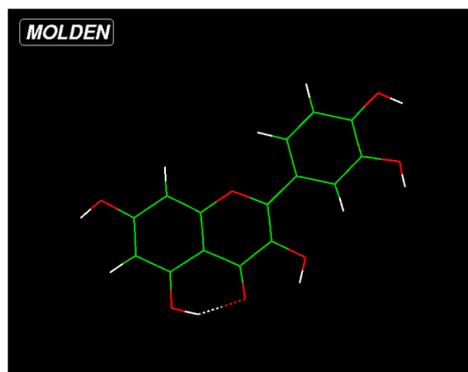
Figure S3. Structures of the radical anions of quercetin.

Appendix A. Details on quanto-mechanical calculations

Cartesian atomic coordinates, thermal correction to Enthalpy, thermal correction to Gibbs Free Energy, single point electronic energies in the gas phase, total free energy in solution with all non-electrostatic terms, excitation energies, and oscillator strengths (all energies are in Hartrees).

Appendix A1. Quercetin

B3LYP/6-31+g(d,p) gas phase



Coordinates:

```
C,0,-0.0078071959,-0.2910001478,0.0354204811 \ C ,0,0.0063972896,-
0.1101873431,1.4145395653 \ C,0,1.2030198006,0.0584779642,2.137511677 \ C,0,2.4376714705,0.0426733
324,1.4284629163 \ C,0,2.441209 877,-0.1370469386,0.0492697546 \ C,0,1.2215243701,-0.3013335742,-
0.62916 0678 \ O,0,-1.1931496794,-0.1008115556,2.0576005531 \ C,0,-
1.3105990374,0.0692129039,3.4167369365 \ C,0,-0.1733487801,0.2375716181,4.1656273012 \
C,0,1.1424756376,0.2401385033,3.5587304268 \ C,0,-2.7042012003,0.040993469 7,3.8640567551 \ C,0,-
3.0437489202,0.197720567,5.2269802045 \ C,0,-4.3718383627,0.1668026031,5.6224199363 \ C,0,-
5.4032197343,-0.0194259845,4.6861 938121 \ C,0,-5.0754268878,-0.1747024843,3.339981163 \ C,0,-
3.7450301314,- 0.1453112871,2.9317396581 \ O,0,-6.7047624162,-0.049130089,5.0783051859 \ O,0,-
4.7921091481,0.3109369843,6.9272628041 \ O,0,-0.1798179732,0.413225 3216,5.5150626314 \
O,0,2.154612756,0.3996030163,4.2990336765 \ O,0,3.5984 954905,0.2005342064,2.0856698183 \
O,0,1.1798805265,-0.4800373784,-1.979 0484292 \ H,0,-0.9351572163,-0.4195183347,-
0.508055014 \ H,0,3.3886270904, -0.147364379,-0.4809468675 \
H,0,0.766864687,0.5031308769,5.753382007 \ H,0,3.3859573833,0.3127867801,3.0472672791 \
H,0,2.0743226,-0.4722815034,- 2.345509958 \ H,0,-3.5110738982,-0.2676976015,1.8823005101 \ H,0,-
5.876333 0998,-0.3180964542,2.6223148804 \ H,0,-2.267990637,0.3426561172,5.968440 0827 \ H,0,-
6.7439808571,0.0738401339,6.0395107583 \ H,0,-4.0375103265,0.4347725366,7.5171893773
```

Thermal correction to Enthalpy= 0.244747

Thermal correction to Gibbs Free Energy= 0.179105

Lowest Frequency: 19.3458 cm⁻¹

B3LYP TD(nstates=10) /6-311+g(d,p)

HF=-1104.5156848

Excitation energies and oscillator strengths:

Excited State	1:	Singlet-A	3.2984 eV	375.89 nm	f=0.4668
Excited State	2:	Singlet-A	3.7065 eV	334.50 nm	f=0.0875
Excited State	3:	Singlet-A	4.1529 eV	298.55 nm	f=0.0569
Excited State	4:	Singlet-A	4.2495 eV	291.76 nm	f=0.0145
Excited State	5:	Singlet-A	4.4283 eV	279.98 nm	f=0.0000
Excited State	6:	Singlet-A	4.5696 eV	271.32 nm	f=0.0721
Excited State	7:	Singlet-A	4.7582 eV	260.57 nm	f=0.0010
Excited State	8:	Singlet-A	4.7810 eV	259.33 nm	f=0.0859
Excited State	9:	Singlet-A	4.8587 eV	255.18 nm	f=0.2427
Excited State	10:	Singlet-A	4.9676 eV	249.58 nm	f=0.0514

B3LYP TD(nstates=10) /6-311+g(d,p) scrf=(pcm,solvent=water)

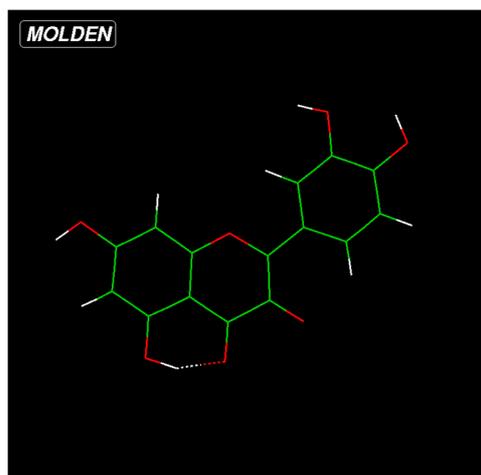
Total free energy in solution: with all non-electrostatic terms

(a.u.) = -1104.538472

Excited State	1:	Singlet-A	3.1891 eV	388.78 nm	f=0.5963
Excited State	2:	Singlet-A	3.6238 eV	342.14 nm	f=0.0443
Excited State	3:	Singlet-A	4.0581 eV	305.52 nm	f=0.1013
Excited State	4:	Singlet-A	4.2127 eV	294.31 nm	f=0.0334
Excited State	5:	Singlet-A	4.5203 eV	274.29 nm	f=0.0000
Excited State	6:	Singlet-A	4.5319 eV	273.58 nm	f=0.1161
Excited State	7:	Singlet-A	4.7547 eV	260.76 nm	f=0.1081
Excited State	8:	Singlet-A	4.8235 eV	257.04 nm	f=0.2781
Excited State	9:	Singlet-A	4.9521 eV	250.37 nm	f=0.0648
Excited State	10:	Singlet-A	5.0066 eV	247.64 nm	f=0.0561

Appendix A2. Quercetin anion 3-OH

B3LYP/6-31+g(d,p) gas phase



Coordinates:

```
C,0,0.0131867979,0.0000236305,-0.0027265828 \ C,0,0.010961563,0.0000635511,1.4031508721 \
C,0,1.2026364,0.0001749924,2.1513754718 \ C,0,2.4441800041,0.0000581137,1.4429794258 \ C,0,2.460183
4784,0.0000603272,0.0492112974 \ C,0,1.2403140518,0.0000566433,-0.6515908374 \ O,0,-
1.175282915,0.0000522071,2.0230766642 \ C,0,-1.2930821963,-0.0000070669,3.4203708848 \ C,0,-
0.162603546,-0.0000114215,4.2811745853 \ C,0,1.1714608723,0.0005603602,3.5995087251 \ C,0,-
2.6863314895,0.0000592124,3.8263481115 \ C,0,-3.7232232363,0.0000994583,2.8576392 \ C,0,-
5.0570592603,0.0001336243,3.2399875534 \ C,0,-5.4284402633,0.0001394423,4.5884326722 \ C,0,-
4.4223297703,0.0001010799,5.5529967748 \ C,0,-3.0753437983,0.0000612135,5.1908939955 \ O,0,-
6.759949381,0.0001746694,4.9565133319 \ O,0,-6.1107645389,0.0001672702,2.3267990346 \ O,0,-
0.2203459536,0.000459893,5.5434407633 \ O,0,2.2488069637,0.0003227239,4.2581479034 \ O,0,3.5939027
972,-0.0001917672,2.1350504829 \ O,0,1.2255526147,0.000177665,-2.0319066158 \ H,0,-0.9156524318,-
0.0000144712,-0.5601278375 \ H,0,3.4139972465,-0.0000013919,-0.4719993364 \ H,0,3.302004331,-
0.0006360679,3.1156235194 \ H,0,2.1372504459,0.0000191068,-2.3498394684 \ H,0,-
2.2921896271,0.0000214799,5.9383421861 \ H,0,-4.7086397312,0.0000993899,6.6011673253 \ H,0,-
3.4721748378,0.0000952527,1.8010933778 \ H,0,-5.7494848782,0.0001606306,1.4319653031 \ H,0,-
7.2848663356,0.0001947088,4.1431852818
```

Thermal correction to Enthalpy= 0.229758

Thermal correction to Gibbs Free Energy= 0.164168

Lowest freq: 32.0787 cm⁻¹

B3LYP TD(nstates=12) /6-311+g(d,p)

HF=-1103.969728

Excited State	1:	Singlet-A	2.5533 eV	485.58 nm	f=0.3648
Excited State	2:	Singlet-A	2.6696 eV	464.43 nm	f=0.0003
Excited State	3:	Singlet-A	2.8624 eV	433.15 nm	f=0.0000

Excited State	4:	Singlet-A	2.9316 eV	422.92 nm	f=0.0001
Excited State	5:	Singlet-A	3.2691 eV	379.26 nm	f=0.0108
Excited State	6:	Singlet-A	3.5032 eV	353.92 nm	f=0.0001
Excited State	7:	Singlet-A	3.5235 eV	351.87 nm	f=0.0726
Excited State	8:	Singlet-A	3.8672 eV	320.60 nm	f=0.0442
Excited State	9:	Singlet-A	3.8778 eV	319.73 nm	f=0.0000
Excited State	10:	Singlet-A	3.9512 eV	313.79 nm	f=0.0003
Excited State	11:	Singlet-A	4.0596 eV	305.41 nm	f=0.0000
Excited State	12:	Singlet-A	4.0715 eV	304.51 nm	f=0.0020

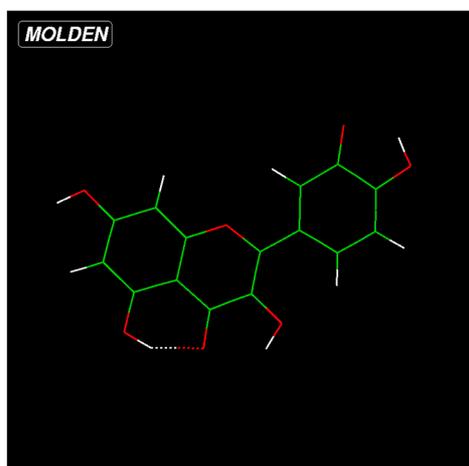
B3LYP TD(nstates=12) /6-311+g(d,p) scrf=(pcm,solvent=water)

Total free energy in solution: with all non-electrostatic terms (a.u.) = -1104.060891

Excited State	1:	Singlet-A	2.6905 eV	460.83 nm	f=0.5259
Excited State	2:	Singlet-A	3.4480 eV	359.59 nm	f=0.0001
Excited State	3:	Singlet-A	3.7648 eV	329.32 nm	f=0.0016
Excited State	4:	Singlet-A	3.8019 eV	326.12 nm	f=0.0343
Excited State	5:	Singlet-A	3.9544 eV	313.53 nm	f=0.0716
Excited State	6:	Singlet-A	4.0894 eV	303.19 nm	f=0.0003
Excited State	7:	Singlet-A	4.1462 eV	299.03 nm	f=0.0143
Excited State	8:	Singlet-A	4.2248 eV	293.47 nm	f=0.1529
Excited State	9:	Singlet-A	4.3166 eV	287.23 nm	f=0.0000
Excited State	10:	Singlet-A	4.4461 eV	278.86 nm	f=0.1150
Excited State	11:	Singlet-A	4.5422 eV	272.96 nm	f=0.0000
Excited State	12:	Singlet-A	4.5843 eV	270.45 nm	f=0.0024

Appendix A3. Quercetin anion 3'-OH

B3LYP/6-31+g(d,p) gas phase



Coordinates:

```
C,0,-0.0206146779,0.0822931545,0.0113391735 \ C,0,-0.0121614738,0.0303429173,1.4080353232 \
C,0,1.1814629241,-0.0224817552,2.1436394868 \ C,0,2.4181149159,-
0.0231353673,1.4474470991 \ C,0,2.4299380824,0.0281869349,0.0553137672 \ C,0,1.2102427036,0.080124
1495,-0.6415225135 \ C,0,1.1108449736,-0.0743085248,3.5809788705 \ C,0,-0.1851608055,-
0.0686467127,4.1757959699 \ C,0,-1.3506396393,-0.0155385328,3.4171573702 \ O,0,-
1.2077362758,0.0323762583,2.0431934939 \ C,0,-2.7368999414,-0.0013406381,3.8342703831 \ C,0,-
3.0712218159,-0.0451652256,5.2114922483 \ C,0,-4.4148126328,-0.0308100027,5.6032997769 \ C,0,-
5.4114180745,0.026189291,4.6394944024 \ C,0,-5.1312099455,0.0728198467,3.2156818644 \ C,0,-
3.7703087577,0.057082116,2.8549683899 \ O,0,-6.1622615412,0.1242405763,2.441879986 \ O,0,-
6.732972036,0.0439918427,4.9208736876 \ O,0,2.1550610524,-0.1243108899,4.3213728124 \ O,0,-
0.1863309303,-0.1193791534,5.5432491594 \ O,0,3.5752523683,-
0.0734021323,2.137623278 \ O,0,1.1864960017,0.1315108566,-2.0143969915 \ H,0,-
0.9511153555,0.1226780955,-0.5408270467 \ H,0,3.381392325,0.0272788285,-
0.4694440548 \ H,0,0.7645794967,-0.1482383634,5.7729372311 \ H,0,3.3187912628,-
0.1036271566,3.1056752771 \ H,0,2.0926595307,0.1244788684,-2.3482465767 \ H,0,-2.2964310704,-
0.0895474384,5.9619780037 \ H,0,-4.6835589279,-0.0640295356,6.6562901995 \ H,0,-
3.5253775223,0.091008246,1.8006887895 \ H,0,-7.1017649577,0.0859459237,3.9901684622
```

Thermal correction to Enthalpy= 0.230739

Thermal correction to Gibbs Free Energy= 0.164478

Lowest freq: 3.8592 cm⁻¹

B3LYP TD(nstates=12) /6-311+g(d,p)

HF=-1103.985417

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 1.8633 eV 665.39 nm f=0.1248

Excited State 2: Singlet-A 2.7082 eV 457.82 nm f=0.0000

Excited State	3:	Singlet-A	2.7317 eV	453.87 nm	f=0.0002
Excited State	4:	Singlet-A	3.0308 eV	409.07 nm	f=0.0000
Excited State	5:	Singlet-A	3.1312 eV	395.96 nm	f=0.4551
Excited State	6:	Singlet-A	3.2826 eV	377.70 nm	f=0.1053
Excited State	7:	Singlet-A	3.4707 eV	357.23 nm	f=0.0006
Excited State	8:	Singlet-A	3.8840 eV	319.22 nm	f=0.0001
Excited State	9:	Singlet-A	3.9049 eV	317.51 nm	f=0.0018
Excited State	10:	Singlet-A	3.9293 eV	315.54 nm	f=0.0014
Excited State	11:	Singlet-A	3.9687 eV	312.40 nm	f=0.0000
Excited State	12:	Singlet-A	4.0352 eV	307.26 nm	f=0.0413

B3LYP TD(nstates=12) /6-311+g(d,p) scrf=(pcm,solvent=water)

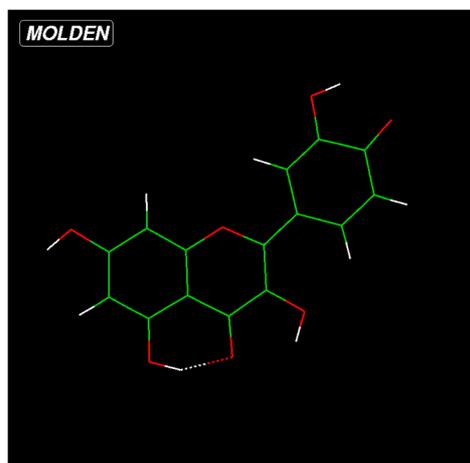
Total free energy in solution: with all non-electrostatic terms

(a.u.) = -1104.062933

Excited State	1:	Singlet-A	2.4962 eV	496.70 nm	f=0.3070
Excited State	3:	Singlet-A	3.7005 eV	335.05 nm	f=0.0905
Excited State	4:	Singlet-A	3.7450 eV	331.06 nm	f=0.0003
Excited State	5:	Singlet-A	3.9940 eV	310.43 nm	f=0.0000
Excited State	6:	Singlet-A	4.1959 eV	295.49 nm	f=0.0498
Excited State	7:	Singlet-A	4.2936 eV	288.77 nm	f=0.0464
Excited State	8:	Singlet-A	4.3045 eV	288.03 nm	f=0.0009
Excited State	9:	Singlet-A	4.5282 eV	273.81 nm	f=0.0000
Excited State	10:	Singlet-A	4.5471 eV	272.66 nm	f=0.0567
Excited State	11:	Singlet-A	4.5743 eV	271.05 nm	f=0.0000
Excited State	12:	Singlet-A	4.6961 eV	264.01 nm	f=0.1417

Appendix A4. Quercetin anion 4'-OH

B3LYP/6-31+g(d,p) gas phase



Coordinates:

```
C,0,0.0153326944,-0.0008669633,-0.0203593888\C,0,0.0070812045,-
0.0003153334,1.3773023165\C,0,1.1909509824,0.00027001,2.1279141938\C,0,2.4343655938,0.00029086
98,1.4475849615\C,0,2.4642323331,-0.0002415826,0.0526008216\C,0,1.2543782389,-0.0008128757, -
0.6594374299\C,0,1.1058808781,0.0008536841,3.5698856883\C,0,-
0.187096276,0.0007855866,4.1471026205\C,0,-1.355256542,0.0001803988,3.3771552454\O,0,-
1.1994334405,-0.0003502669,1.9978936059\C,0,-2.7249623935,0.0000185596,3.7828410366\C,0,-
3.1087339273,0.0005038115,5.1559787405\C,0,-4.4374306083,0.0003439876,5.5393666615\C,0,-
5.4994749576,-0.0003234332,4.580002121\C,0,-5.0830766207,-0.0008020402,3.1830747833\C,0,-
3.770428871,-0.0006449702,2.7975320645\O,0,-6.1200359853,-0.0014279226,2.2929621773\O,0,-
6.7470168445,-0.0004874115,4.8288941261\O,0,2.1519602766,0.0014987772,4.3176702533\O,0,-
0.213170659,0.0013549255,5.5193123546\O,0,3.5829898656,0.0008026916,2.1539646226\O,0,1.2449379
475,-0.0013555979,-2.0355967146\H,0,-0.9081556941,-0.0013123641,-0.5858008495\H,0,3.4227700616,-
0.0002191626,-
0.4593091847\H,0,0.7342398542,0.0016769215,5.7638854239\H,0,3.3085706171,0.0010374073,3.121106
4632\H,0,2.1555819002,-0.001260084,-2.3569408242\H,0,-
2.3398966622,0.0010127576,5.916620925\H,0,-4.707043599,0.0007285016,6.5922538284\H,0,-
3.5283099267,-0.0010290213,1.7414429389\H,0,-6.9021870492,-0.0013774248,2.8925547595
```

Thermal correction to Enthalpy= 0.231069

Thermal correction to Gibbs Free Energy= 0.166319

Lowest freq: 24.0923

B3LYP TD(nstates=12) /6-311+g(d,p)

HF=-1103.9961136

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.6857 eV 461.65 nm f=0.6648

Excited State 2: Singlet-A 3.0232 eV 410.11 nm f=0.0000

Excited State	3:	Singlet-A	3.1858 eV	389.18 nm	f=0.1009
Excited State	4:	Singlet-A	3.5566 eV	348.60 nm	f=0.0732
Excited State	5:	Singlet-A	3.5722 eV	347.08 nm	f=0.0000
Excited State	6:	Singlet-A	3.6815 eV	336.78 nm	f=0.1199
Excited State	7:	Singlet-A	3.7569 eV	330.02 nm	f=0.0004
Excited State	8:	Singlet-A	3.9975 eV	310.15 nm	f=0.0082
Excited State	9:	Singlet-A	4.0991 eV	302.47 nm	f=0.0000
Excited State	10:	Singlet-A	4.2516 eV	291.62 nm	f=0.0001
Excited State	11:	Singlet-A	4.3484 eV	285.12 nm	f=0.0000
Excited State	12:	Singlet-A	4.4383 eV	279.35 nm	f=0.0003

B3LYP TD(nstates=12) /6-311+g(d,p) scrf=(pcm,solvent=water)

Total free energy in solution: with all non-electrostatic terms

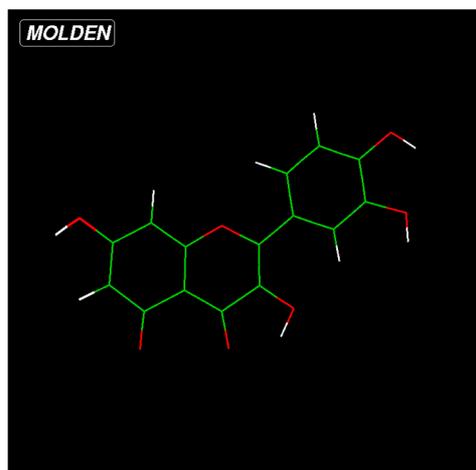
(a.u.) = -1104.068424

Excitation energies and oscillator strengths:

Excited State	1:	Singlet-A	2.7581 eV	449.53 nm	f=0.9346
Excited State	2:	Singlet-A	3.6115 eV	343.30 nm	f=0.0056
Excited State	3:	Singlet-A	3.7921 eV	326.95 nm	f=0.0762
Excited State	4:	Singlet-A	3.8549 eV	321.63 nm	f=0.0051
Excited State	5:	Singlet-A	4.0713 eV	304.53 nm	f=0.0000
Excited State	6:	Singlet-A	4.2221 eV	293.65 nm	f=0.0401
Excited State	7:	Singlet-A	4.2788 eV	289.76 nm	f=0.0003
Excited State	8:	Singlet-A	4.3816 eV	282.96 nm	f=0.0646
Excited State	9:	Singlet-A	4.4822 eV	276.62 nm	f=0.1234
Excited State	10:	Singlet-A	4.5057 eV	275.17 nm	f=0.0000
Excited State	11:	Singlet-A	4.6235 eV	268.16 nm	f=0.0000
Excited State	12:	Singlet-A	4.6434 eV	267.01 nm	f=0.0035

Appendix A5. Quercetin anion 5-OH

B3LYP/6-31+g(d,p) gas phase



Coordinates:

```
C,0,0.0070082759,0.0000005073,-0.0122822893 \ C,0,0.0043355042,0.0000007195,1.3974073583 \
C,0,1.2502801368,0.0000010043,2.0613686278 \ C,0,2.432346031,0.0000012414,1.3347077248 \ C,0,2.4269
183142,0.0000010882,-0.0658399755 \ C,0,1.2031352917,0.0000006851,-0.7308845027 \ C,0,-
1.2570171304,0.0000006111,2.1447449839 \ O,0,-2.3629601802,0.0000000588,1.3268972682 \ C,0,-
3.6471363269,0.0000000077,1.8281324578 \ C,0,-3.9115247395,0.000000492,3.2271956704 \ C,0,-
2.7920518417,0.0000010801,4.116719814 \ C,0,-1.4452126261,0.0000010756,3.488783016 \ C,0,-
5.3229650941,0.0000003528,3.6887335676 \ C,0,-6.3168064862,-0.0000004681,2.6337983933 \ C,0,-
5.9743079475,-0.0000008881,1.2986178931 \ C,0,-4.6375247523,-0.0000006332,0.8563231461 \ O,0,-
5.647376921,0.0000004574,4.8975761211 \ O,0,-6.9370820103,-0.0000015968,0.3024245507 \ O,0,-
0.4538011345,0.0000016954,4.4171616818 \ O,0,-2.7613462749,0.0000011661,5.3734435248 \
O,0,3.6891135208,0.0000014594,1.924343639 \ O,0,3.6052140474,0.0000013477,-0.7740016406 \ H,0,-
4.3909124227,-0.0000009872,-0.1977499343 \ H,0,-7.3590771376,-0.0000007137,2.9477999836 \ H,0,-
1.0108663025,0.0000021027,5.2511118245 \ H,0,-7.8029395594,-0.0000017148,0.7309884926 \ H,0,-
0.9372595584,0.0000002438,-0.5419793036 \ H,0,1.1996740055,0.0000005964,-1.8167188629 \
H,0,1.2791174855,0.0000010498,3.1454839716 \ H,0,4.3328760566,0.0000021259,-0.1345999328 \
H,0,3.5914981053,0.0000040841,2.8849904464
```

Thermal correction to Enthalpy= 0.230403

Thermal correction to Gibbs Free Energy= 0.164233

Lowest freq: 28.5721 cm⁻¹

B3LYP TD(nstates=12) /6-311+g(d,p)

HF=-1103.9633303

Excitation energies and oscillator strengths:

Excited State	1:	Singlet-A	2.4681 eV	502.35 nm	f=0.1015
Excited State	2:	Singlet-A	2.8648 eV	432.78 nm	f=0.0000
Excited State	3:	Singlet-A	2.9066 eV	426.55 nm	f=0.0000

Excited State	4:	Singlet-A	3.1020 eV	399.70 nm	f=0.0087
Excited State	5:	Singlet-A	3.4641 eV	357.91 nm	f=0.0003
Excited State	6:	Singlet-A	3.5946 eV	344.92 nm	f=0.0000
Excited State	7:	Singlet-A	3.7094 eV	334.24 nm	f=0.0005
Excited State	8:	Singlet-A	3.7614 eV	329.62 nm	f=0.1275
Excited State	9:	Singlet-A	3.7702 eV	328.86 nm	f=0.0007
Excited State	10:	Singlet-A	3.8203 eV	324.54 nm	f=0.0000
Excited State	11:	Singlet-A	3.9247 eV	315.91 nm	f=0.3601
Excited State	12:	Singlet-A	3.9550 eV	313.49 nm	f=0.0009

B3LYP TD(nstates=12) /6-311+g(d,p) scrf=(pcm,solvent=water)

Total free energy in solution: with all non-electrostatic terms

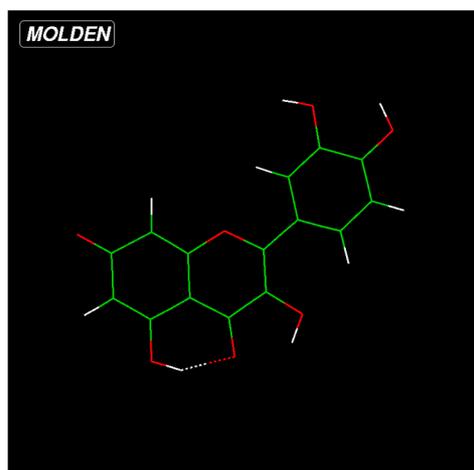
(a.u.) = -1104.056683

Excitation energies and oscillator strengths:

Excited State	1:	Singlet-A	2.8656 eV	432.66 nm	f=0.2346
Excited State	2:	Singlet-A	3.6346 eV	341.12 nm	f=0.0000
Excited State	3:	Singlet-A	3.7434 eV	331.21 nm	f=0.4524
Excited State	4:	Singlet-A	3.9455 eV	314.24 nm	f=0.0194
Excited State	5:	Singlet-A	4.1921 eV	295.76 nm	f=0.0000
Excited State	6:	Singlet-A	4.4140 eV	280.89 nm	f=0.0160
Excited State	7:	Singlet-A	4.4508 eV	278.57 nm	f=0.0001
Excited State	8:	Singlet-A	4.4771 eV	276.93 nm	f=0.2863
Excited State	9:	Singlet-A	4.6839 eV	264.70 nm	f=0.0002
Excited State	10:	Singlet-A	4.7288 eV	262.19 nm	f=0.0453
Excited State	11:	Singlet-A	4.7683 eV	260.02 nm	f=0.0000
Excited State	12:	Singlet-A	4.8819 eV	253.97 nm	f=0.0000

Appendix A6. Quercetin anion 7-OH

B3LYP/6-31+g(d,p) gas phase



Coordinates:

```
C,0,0.0147492405,-0.0173296013,-0.0556273427\C,0,-0.0223486398,-
0.0021387864,1.3545089644\C,0,1.2068771912,0.0113673486,2.0486823243\C,0,2.4098620535,0.009655
4718,1.358136114\C,0,2.4388280722,-0.0054691175,-0.0423685303\C,0,1.2319900081,-0.0188843639,-
0.7379894346\C,0,-1.2749328702,0.0001184616,2.116737957\O,0,-
1.0590777719,0.0160714034,3.4774797323\C,0,-2.0915176204,0.0211119909,4.3981538263\C,0,-
3.4427404264,0.0094126579,3.9310908858\C,0,-3.7065682032,-0.0069713616,2.5511866601\C,0,-
2.5539864066,-0.0112551897,1.6468301276\C,0,-4.4823548263,0.0152708526,4.9294005825\C,0,-
4.177844572,0.0313749414,6.2653067123\C,0,-2.8012992145,0.0433479655,6.7470823741\C,0,-
1.7629378867,0.0372626734,5.7276476334\O,0,-5.7799448363,0.0043335094,4.5080580278\O,0,-
2.5269067326,0.0581484597,7.9752741818\O,0,-2.8958396868,-0.0273622346,0.3278622472\O,0,-
4.8636332361,-0.0186597375,1.9981643354\O,0,3.650407333,0.0224005212,1.9776443387\
O,0,3.6328555396,-0.0070910222,-0.7207530491\H,0,-0.7260048129,0.045806132,6.0459547233\H,0,-
4.973248137,0.035581006,7.0036495854\H,0,-3.8822178449,-0.0316678798,0.373467569\H,0,-
5.7648366191,-0.0064008626,3.5203051246\H,0,-0.9106053731,-0.02789775,-0.6148720144\
H,0,1.2573213084,-0.0305905926,-1.8233765669\H,0,1.2039237126,0.0231817621,3.1338907031\
H,0,4.3458643475,0.0035078203,-0.0650108772\H,0,3.5342358582,0.032327257,2.9361430314
```

Thermal correction to Enthalpy= 0.231289

Thermal correction to Gibbs Free Energy= 0.165862

Lowest freq: 24.2265 cm⁻¹

B3LYP TD(nstates=12) /6-311+g(d,p)

HF=-1103.9866386

Excitation energies and oscillator strengths:

Excited State	1:	Singlet-A	2.5961 eV	477.58 nm	f=0.2410
Excited State	2:	Singlet-A	3.0237 eV	410.04 nm	f=0.0000
Excited State	3:	Singlet-A	3.0710 eV	403.73 nm	f=0.0000

Excited State	4:	Singlet-A	3.2034 eV	387.04 nm	f=0.0226
Excited State	5:	Singlet-A	3.3339 eV	371.89 nm	f=0.0064
Excited State	6:	Singlet-A	3.8239 eV	324.23 nm	f=0.0004
Excited State	7:	Singlet-A	3.8425 eV	322.67 nm	f=0.0000
Excited State	8:	Singlet-A	3.9005 eV	317.87 nm	f=0.0003
Excited State	9:	Singlet-A	3.9639 eV	312.78 nm	f=0.3151
Excited State	10:	Singlet-A	3.9876 eV	310.93 nm	f=0.0001
Excited State	11:	Singlet-A	4.1239 eV	300.65 nm	f=0.0163
Excited State	12:	Singlet-A	4.1785 eV	296.72 nm	f=0.0000

B3LYP TD(nstates=12) /6-311+g(d,p) scrf=(pcm,solvent=water)

Total free energy in solution: with all non-electrostatic terms

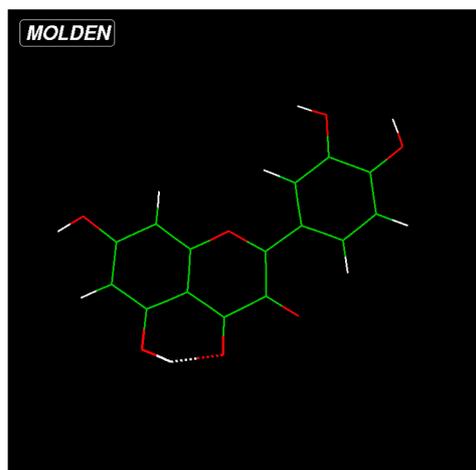
(a.u.) = -1104.065982

Excitation energies and oscillator strengths:

Excited State	1:	Singlet-A	2.9687 eV	417.64 nm	f=0.4815
Excited State	2:	Singlet-A	3.7208 eV	333.22 nm	f=0.0653
Excited State	3:	Singlet-A	3.8406 eV	322.83 nm	f=0.2465
Excited State	4:	Singlet-A	3.9650 eV	312.69 nm	f=0.0000
Excited State	5:	Singlet-A	4.1957 eV	295.50 nm	f=0.0221
Excited State	6:	Singlet-A	4.4278 eV	280.01 nm	f=0.0087
Excited State	7:	Singlet-A	4.5948 eV	269.84 nm	f=0.3865
Excited State	8:	Singlet-A	4.6033 eV	269.34 nm	f=0.0008
Excited State	9:	Singlet-A	4.7162 eV	262.89 nm	f=0.0000
Excited State	10:	Singlet-A	4.7673 eV	260.07 nm	f=0.0105
Excited State	11:	Singlet-A	4.8212 eV	257.16 nm	f=0.0005
Excited State	12:	Singlet-A	4.8861 eV	253.75 nm	f=0.0107

Appendix A7. Quercetin radical 3-OH

B3LYP/6-31+g(d,p) gas phase



Coordinates:

```
C,0,0.0022645505,-0.0121847062,0.0168201966 \ C,0,0.002905019,0.0012461642,1.4393750599 \
C,0,1.2541423258,0.0166486978,2.1081728467 \ C,0,2.4423182665,0.0184926785,1.3889763055 \ C,0,2.428
8157968,0.0052142902,-0.0068439213 \ C,0,1.1902548713,-0.0101832531,-0.6848271011 \ C,0,-
1.2536371148,-0.0011661434,2.1486139635 \ C,0,-1.438252584,0.0109055973,3.5874392409 \ C,0,-
2.8621038168,0.0055856891,4.1073232348 \ C,0,-3.9208958446,-0.0111532808,3.1264544891 \ C,0,-
3.6279382111,-0.0218920999,1.7512074544 \ O,0,-2.3320369908,-0.0167110367,1.3122801431 \ C,0,-
5.2927634622,-0.0173080809,3.5189128327 \ C,0,-6.3003116601,-0.0335305361,2.552640384 \ C,0,-
5.9508931091,-0.0436719743,1.1979608616 \ C,0,-4.6127311872,-0.0380415945,0.775662585 \ O,0,-
5.6223817543,-0.0076000703,4.8136728284 \ O,0,-6.8903997788,-0.0595713946,0.2141193903 \ O,0,-
3.0844504587,0.0154506353,5.3306031747 \ O,0,-0.4920410014,0.025157112,4.3931753556 \
O,0,3.5932994619,0.0071571577,-0.6969765376 \ O,0,1.2906133063,-0.0224189915,-2.0576079894 \ H,0,-
4.3661035187,-0.0461087989,-0.2783710106 \ H,0,-7.337724674,-0.0379700698,2.872530788 \ H,0,-
4.7688918017,0.0033292578,5.3319465829 \ H,0,-7.7779931766,-0.0623523032,0.5976870281 \
H,0,1.2725176918,0.0269713624,3.1883756711 \ H,0,3.3996494738,0.0302653555,1.8989631933 \ H,0,-
0.9387746628,-0.0241053051,-0.5219402709 \ H,0,0.4168059286,-0.0326776514,-2.4687317584 \
H,0,3.3985772657,-0.003241257,-1.6476225956
```

Thermal correction to Enthalpy= 0.231720

Thermal correction to Gibbs Free Energy= 0.165424

Lowest freq: 26.8366 cm⁻¹

B3LYP TD(nstates=10) /6-311+g(d,p)

HF=-1103.872719

Excited State 1: ?Spin -A 1.4680 eV 844.58 nm f=0.0000

Excited State 2: ?Spin -A 2.0289 eV 611.10 nm f=0.0465

Excited State 3: ?Spin -A 2.2711 eV 545.92 nm f=0.0467

Excited State	4:	?Spin -A	2.4399 eV	508.16 nm	f=0.0141
Excited State	5:	?Spin -A	2.6188 eV	473.44 nm	f=0.2419
Excited State	6:	?Spin -A	2.8032 eV	442.30 nm	f=0.0910
Excited State	7:	?Spin -A	2.8048 eV	442.04 nm	f=0.0000
Excited State	8:	?Spin -A	3.2760 eV	378.46 nm	f=0.0000
Excited State	9:	?Spin -A	3.3354 eV	371.72 nm	f=0.0126
Excited State	10:	?Spin -A	3.5145 eV	352.78 nm	f=0.0115

B3LYP TD(nstates=10) /6-311+g(d,p) scrf=(pcm,solvent=water)

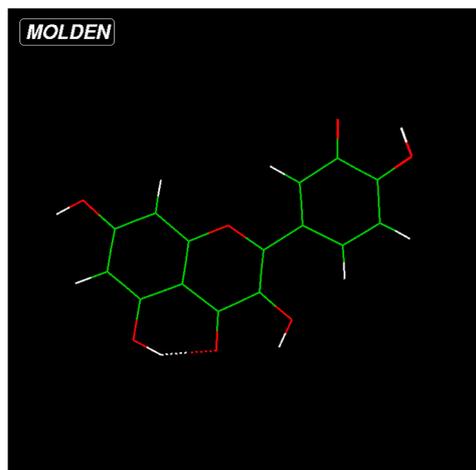
Total free energy in solution: with all non-electrostatic terms

(a.u.) = -1103.902902

Excited State	1:	?Spin -A	1.7206 eV	720.57 nm	f=0.0000
Excited State	2:	?Spin -A	1.7599 eV	704.51 nm	f=0.0904
Excited State	3:	?Spin -A	2.0962 eV	591.46 nm	f=0.0441
Excited State	4:	?Spin -A	2.1795 eV	568.87 nm	f=0.0197
Excited State	5:	?Spin -A	2.4794 eV	500.06 nm	f=0.2632
Excited State	6:	?Spin -A	2.6003 eV	476.81 nm	f=0.1350
Excited State	7:	?Spin -A	3.0270 eV	409.60 nm	f=0.0000
Excited State	8:	?Spin -A	3.2402 eV	382.64 nm	f=0.0171
Excited State	9:	?Spin -A	3.4092 eV	363.67 nm	f=0.0110
Excited State	10:	?Spin -A	3.5579 eV	348.47 nm	f=0.0000

Appendix A8. Quercetin radical 3'-OH

B3LYP/6-31+g(d,p) gas phase



Coordinates:

```
C,0,-0.0002823267,0.0822717355,0.0023356495 \ C,0,0.000317777,0.0307703469,1.3909834114 \
C,0,1.1925579355,-0.0226210174,2.1412605207 \ C,0,2.4371136945,-0.0236052177,1.4472093477 \
C,0,2.4537628638,0.0275368655,0.058130848 \ C,0,1.2385875782,0.079734487,-
0.6463554621 \ C,0,1.1182821596,-0.0740085898,3.5694256587 \ C,0,-0.2119969597,-
0.0675077695,4.1636308966 \ C,0,-1.3396733059,-0.014489903,3.3855803047 \ O,0,-
1.2074449097,0.0334293064,2.0187320873 \ C,0,-2.746764078,0.0001393918,3.802992486 \ C,0,-
3.1044393973,-0.0437766307,5.194322019 \ C,0,-4.4291561688,-0.0309733426,5.613142311 \ C,0,-
5.4434548497,0.0259851214,4.6612933651 \ C,0,-5.1348215316,0.0724559377,3.2290811866 \ C,0,-
3.7516005788,0.0570380385,2.8471779276 \ O,0,-6.1062203061,0.1229988842,2.4258981277 \ O,0,-
6.7339445988,0.0414242249,4.9890723904 \ O,0,2.1178696724,-0.123927287,4.3372621764 \ O,0,-
0.2246163769,-0.11746132,5.5175751512 \ O,0,3.5937775029,-0.0736310969,2.1270198598 \
O,0,1.2095786776,0.1307152768,-2.0051678894 \ H,0,-0.9232852706,0.1229864853,-
0.5618368176 \ H,0,3.4076271169,0.0262784083,-0.4603564532 \ H,0,0.721952348,-
0.1472851867,5.7737182805 \ H,0,3.3786939779,-
0.1048192471,3.092464504 \ H,0,2.1080765495,0.1247368874,-2.3620105368 \ H,0,-2.3210074344,-
0.0880668558,5.9375873484 \ H,0,-4.6786202858,-0.0647522903,6.6683397862 \ H,0,-
3.5301016262,0.0915273471,1.7884799316 \ H,0,-7.2179285931,0.083483487,4.1334189056
```

Thermal correction to Enthalpy= 0.232352

Thermal correction to Gibbs Free Energy= 0.166151

Lowest freq: 7.9271 cm⁻¹

B3LYP TD(nstates=10) /6-311+g(d,p)

Excitation energies and oscillator strengths:

Excited State 1: ?Spin -A 1.4535 eV 852.98 nm f=0.0220

Excited State	2:	?Spin -A	1.7262 eV	718.24 nm	f=0.0000
Excited State	3:	?Spin -A	2.0860 eV	594.36 nm	f=0.0036
Excited State	4:	?Spin -A	2.4422 eV	507.68 nm	f=0.0270
Excited State	5:	?Spin -A	2.6265 eV	472.06 nm	f=0.0034
Excited State	6:	?Spin -A	2.8822 eV	430.17 nm	f=0.0146
Excited State	7:	?Spin -A	3.0836 eV	402.07 nm	f=0.1818
Excited State	8:	?Spin -A	3.2987 eV	375.85 nm	f=0.0441
Excited State	9:	?Spin -A	3.4409 eV	360.33 nm	f=0.0000
Excited State	10:	?Spin -A	3.4443 eV	359.97 nm	f=0.0430

B3LYP TD(nstates=10) /6-311+g(d,p) scrf=(pcm,solvent=water)

Total free energy in solution with all non-electrostatic terms

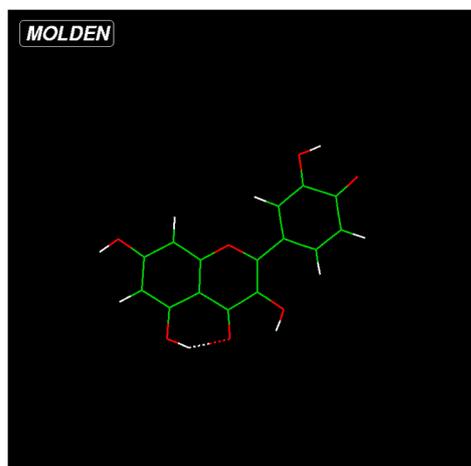
(a.u.) = -1103.898842

Excitation energies and oscillator strengths:

Excited State	1:	?Spin -A	1.2962 eV	956.48 nm	f=0.0357
Excited State	2:	?Spin -A	1.8981 eV	653.19 nm	f=0.0000
Excited State	3:	?Spin -A	1.9102 eV	649.08 nm	f=0.0075
Excited State	4:	?Spin -A	2.3564 eV	526.16 nm	f=0.0209
Excited State	5:	?Spin -A	2.4625 eV	503.50 nm	f=0.0131
Excited State	6:	?Spin -A	2.7187 eV	456.04 nm	f=0.0527
Excited State	7:	?Spin -A	3.0902 eV	401.21 nm	f=0.2634
Excited State	8:	?Spin -A	3.2873 eV	377.16 nm	f=0.0450
Excited State	9:	?Spin -A	3.3403 eV	371.18 nm	f=0.0000
Excited State	10:	?Spin -A	3.3933 eV	365.38 nm	f=0.0098

Appendix A9. Quercetin radical 4'-OH

B3LYP/6-31+g(d,p) gas phase



Coordinates:

```
C,0,0.0092101311,-0.0008555204,-0.0093248652\C,0,0.0024838779,-0.0002989597,1.3793654059\
C,0,1.1928589152,0.0002846902,2.1358058229\C,0,2.441185289,0.0003017259,1.4477186148\C,0,2.4643
922406,-0.0002517098,0.0577947066\C,0,1.2519255574,-0.0008219489,-0.6526420358\
C,0,1.1129243484,0.0008410215,3.563181981\C,0,-0.2200211872,0.0007662633,4.1536583581\C,0,-
1.3567408955,0.0001807087,3.3685383074\O,0,-1.2091132914,-0.0003369092,1.9993394622\C,0,-
2.7459269071,0.0000162718,3.7801686255\C,0,-3.1130305868,0.0005176952,5.1732079326\C,0,-
4.4246999737,0.0003674256,5.5635893811\C,0,-5.4898933404,-0.0003020351,4.5891247262\C,0,-
5.0855987032,-0.0008041164,3.174969328\C,0,-3.7599178335,-0.0006468783,2.7927340223\O,0,-
6.0826895661,-0.0014236827,2.2823653829\O,0,-6.7158820431,-0.0004854316,4.8513529602\
O,0,2.1076834463,0.0013865424,4.3392252315\O,0,-0.2328990055,0.0013052162,5.5018971009\
O,0,3.5947452168,0.0008484558,2.1336107047\O,0,1.2272093183,-0.0013738391,-2.0115957629\H,0,-
0.9109565851,-0.0013007338,-0.5795194215\H,0,3.4206865185,-0.0002335195,-
0.4560608911\H,0,0.7150071818,0.0016313896,5.7601445122\H,0,3.3775497367,0.0011857416,3.098699
5223\H,0,2.1267595723,-0.0013038059,-2.366083338\H,0,-2.3338269099,0.0010229061,5.9216983396\
H,0,-4.7028460706,0.0007455917,6.6123148121\H,0,-3.5107580543,-0.0010333619,1.739829707\H,0,-
6.9082580061,-0.0013967575,2.8143496621
```

Thermal correction to Enthalpy= 0.232345

Thermal correction to Gibbs Free Energy= 0.167690

Lowest freq: 21.0365 cm⁻¹

B3LYP TD(nstates=10) /6-311+g(d,p)

HF=-1103.8861223

Excitation energies and oscillator strengths:

Excited State 1: ?Spin -A 1.7086 eV 725.67 nm f=0.0486

Excited State 2: ?Spin -A 1.7913 eV 692.16 nm f=0.0000

Excited State	3:	?Spin -A	1.9384 eV	639.61 nm	f=0.0061
Excited State	4:	?Spin -A	2.4471 eV	506.65 nm	f=0.0331
Excited State	5:	?Spin -A	2.5715 eV	482.14 nm	f=0.0050
Excited State	6:	?Spin -A	2.9153 eV	425.29 nm	f=0.2909
Excited State	7:	?Spin -A	3.1749 eV	390.51 nm	f=0.2105
Excited State	8:	?Spin -A	3.2257 eV	384.36 nm	f=0.0000
Excited State	9:	?Spin -A	3.5639 eV	347.89 nm	f=0.0064
Excited State	10:	?Spin -A	3.6727 eV	337.59 nm	f=0.0019

B3LYP TD(nstates=10) /6-311+g(d,p) scrf=(pcm,solvent=water)

Total free energy in solution: with all non-electrostatic terms

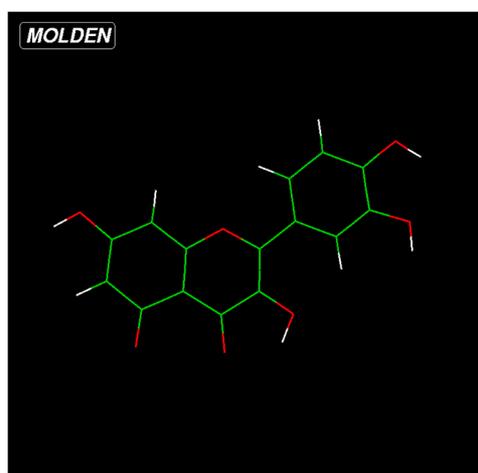
(a.u.) = -1103.903187

Excitation energies and oscillator strengths:

Excited State	1:	?Spin -A	1.5323 eV	809.14 nm	f=0.0854
Excited State	2:	?Spin -A	1.8552 eV	668.29 nm	f=0.0062
Excited State	3:	?Spin -A	2.0000 eV	619.92 nm	f=0.0000
Excited State	4:	?Spin -A	2.2522 eV	550.51 nm	f=0.0398
Excited State	5:	?Spin -A	2.4046 eV	515.61 nm	f=0.0011
Excited State	6:	?Spin -A	2.8077 eV	441.58 nm	f=0.3792
Excited State	7:	?Spin -A	3.1333 eV	395.69 nm	f=0.2278
Excited State	8:	?Spin -A	3.1348 eV	395.51 nm	f=0.0000
Excited State	9:	?Spin -A	3.5110 eV	353.13 nm	f=0.0042
Excited State	10:	?Spin -A	3.5818 eV	346.15 nm	f=0.0033

Appendix A10. Quercetin radical 5-OH

B3LYP/6-31+g(d,p) gas phase



Coordinates:

```
C,0,-0.0179676269,0.0000005829,0.006558922\C,0,-0.0002412969,0.0000006139,1.4165295601\
C,0,1.2512271688,0.0000005907,2.0739671946\C,0,2.424634518,0.0000009065,1.3369825476\C,0,2.3978
761406,0.0000009521,-0.0689474441\C,0,1.1665828435,0.0000007292,-0.7237402191\C,0,-
1.2513632181,0.0000005158,2.1711482375\O,0,-2.3640082591,-0.0000000898,1.3659417315\C,0,-
3.6240454314,-0.0000001595,1.8677237247\C,0,-3.8961573668,0.0000003205,3.2357639368\C,0,-
2.7764656015,0.0000009156,4.156870578\C,0,-1.4441669449,0.0000009922,3.5294056124\C,0,-
5.3121693111,0.0000002414,3.656656236\C,0,-6.3237688313,-0.0000003868,2.608803071\C,0,-
5.982951745,-0.0000008614,1.2693400575\C,0,-4.6310076365,-0.0000007558,0.8799224629\O,0,-
5.6584629862,0.0000006845,4.8522319123\O,0,-6.8937948881,-0.0000014484,0.2555225152\O,0,-
0.4403113656,0.0000016392,4.4270919978\O,0,-2.7996456911,0.0000013931,5.3985730853\
O,0,3.6854119834,0.000000543,1.8913056108\O,0,3.5503751316,0.0000012208,-0.7882735682\H,0,-
4.3593899237,-0.00000113,-0.1690355286\H,0,-7.3576649038,-0.0000004529,2.9418021641\H,0,-
0.922624878,0.0000018056,5.2929484592\H,0,-7.7926985172,-0.0000014914,0.6120138343\H,0,-
0.9633363503,0.0000005182,-0.5204643182\H,0,1.1541488382,0.0000008296,-1.8085469943\
H,0,1.2970407951,0.00000029,3.1560421263\H,0,4.3021893554,0.0000021791,-0.1753944278\
H,0,3.6361043276,0.0000065769,2.8559546381
```

Thermal correction to Enthalpy= 0.231008

Thermal correction to Gibbs Free Energy= 0.164050

Lowest freq: 22.2251 cm⁻¹

B3LYP TD(nstates=10) /6-311+g(d,p)

HF=-1103.8505164

Excitation energies and oscillator strengths:

Excited State 1: ?Spin -A 0.8972 eV 1381.97 nm f=0.0000

Excited State 2: ?Spin -A 1.1507 eV 1077.48 nm f=0.0865

Excited State	3:	?Spin -A	1.6404 eV	755.80 nm	f=0.0039
Excited State	4:	?Spin -A	2.0347 eV	609.35 nm	f=0.0080
Excited State	5:	?Spin -A	2.3408 eV	529.66 nm	f=0.0000
Excited State	6:	?Spin -A	2.4542 eV	505.19 nm	f=0.0011
Excited State	7:	?Spin -A	2.4671 eV	502.55 nm	f=0.0085
Excited State	8:	?Spin -A	3.1651 eV	391.73 nm	f=0.0165
Excited State	9:	?Spin -A	3.4936 eV	354.89 nm	f=0.0061
Excited State	10:	?Spin -A	3.5161 eV	352.62 nm	f=0.0000

B3LYP TD(nstates=10) /6-311+g(d,p) scrf=(pcm,solvent=water)

Total free energy in solution: with all non-electrostatic terms

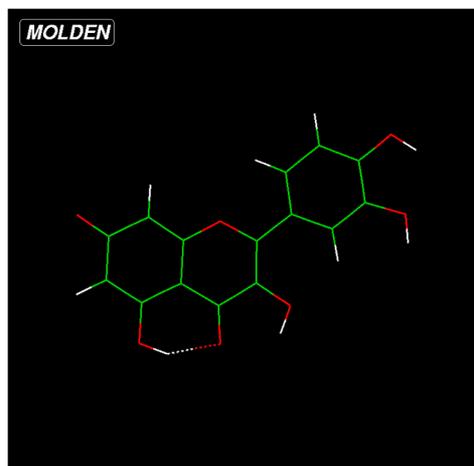
(a.u.) = -1103.883714

Excitation energies and oscillator strengths:

Excited State	1:	?Spin -A	1.0227 eV	1212.36 nm	f=0.1096
Excited State	2:	?Spin -A	1.2817 eV	967.37 nm	f=0.0000
Excited State	3:	?Spin -A	1.5531 eV	798.32 nm	f=0.0007
Excited State	4:	?Spin -A	1.8028 eV	687.75 nm	f=0.0127
Excited State	5:	?Spin -A	2.3143 eV	535.74 nm	f=0.0009
Excited State	6:	?Spin -A	2.4664 eV	502.69 nm	f=0.0123
Excited State	7:	?Spin -A	2.6778 eV	463.00 nm	f=0.0000
Excited State	8:	?Spin -A	3.0847 eV	401.93 nm	f=0.0266
Excited State	9:	?Spin -A	3.3649 eV	368.46 nm	f=0.2723
Excited State	10:	?Spin -A	3.4338 eV	361.07 nm	f=0.2349

Appendix A11. Quercetin radical 7-OH

B3LYP/6-31+g(d,p) gas phase



Coordinates:

```
C,0,0.0102158452,-0.0000000649,-0.0085169555 \ C,0,0.0052283676,0.0000003202,1.4034307547 \
C,0,1.2469781412,0.0000005327,2.0824972793 \ C,0,2.4311053901,0.0000009877,1.3652529478 \ C,0,2.425
7343345,0.000000785,-0.0425414786 \ C,0,1.2047195987,0.0000001435,-0.7187764697 \ C,0,-
1.2609098554,0.0000002698,2.1266857979 \ O,0,-2.3466767022,-0.0000002854,1.2984652978 \ C,0,-
3.6341189829,-0.00000036,1.7592818498 \ C,0,-3.9050407191,-0.0000000149,3.146448581 \ C,0,-
2.7993880776,0.0000005325,4.0645796554 \ C,0,-1.4718053836,0.0000007596,3.4917724966 \ C,0,-
5.2759950554,0.000000384,3.6022259877 \ C,0,-6.3032446174,-0.0000001204,2.6896093881 \ C,0,-
6.0317424915,-0.0000004758,1.266989722 \ C,0,-4.6450131629,-0.0000006371,0.819642309 \ O,0,-
5.531750896,-0.0000000559,4.9233566985 \ O,0,-6.9565276095,-0.0000006805,0.4146165914 \ O,0,-
0.4673947316,0.0000014759,4.3983255514 \ O,0,-2.9107998648,0.0000020488,5.3230116503 \
O,0,3.6834092921,0.0000007207,1.9351404204 \ O,0,3.5863633587,0.0000011809,-0.7414019553 \ H,0,-
4.4383336425,-0.0000008793,-0.2439377265 \ H,0,-7.3360734989,-0.0000001072,3.0173691475 \ H,0,-
0.9240699184,0.0000013155,5.2684029868 \ H,0,-4.6717146779,-0.0000006576,5.4092683471 \ H,0,-
0.9269975154,-0.0000003825,-0.549419782 \ H,0,1.2105073297,0.0000000376,-1.8034771602 \
H,0,1.2773485864,0.0000003302,3.1646167105 \ H,0,4.3306265541,0.0000024865,-
0.1187638906 \ H,0,3.6251923661,0.0000094019,2.8993367593
```

Thermal correction to Enthalpy= 0.231227

Thermal correction to Gibbs Free Energy= 0.165045

Lowest freq: 19.2127 cm⁻¹

B3LYP TD(nstates=10) /6-311+g(d,p)

HF=-1103.8638607

Excitation energies and oscillator strengths:

Excited State 1: ?Spin -A 0.8594 eV 1442.68 nm f=0.0000

Excited State	2:	?Spin -A	0.9985 eV	1241.73 nm	f=0.0296
Excited State	3:	?Spin -A	1.4043 eV	882.88 nm	f=0.0729
Excited State	4:	?Spin -A	2.1218 eV	584.33 nm	f=0.0001
Excited State	5:	?Spin -A	2.4581 eV	504.40 nm	f=0.0516
Excited State	6:	?Spin -A	2.5166 eV	492.67 nm	f=0.0045
Excited State	7:	?Spin -A	2.7110 eV	457.34 nm	f=0.0000
Excited State	8:	?Spin -A	3.1095 eV	398.73 nm	f=0.0246
Excited State	9:	?Spin -A	3.1393 eV	394.94 nm	f=0.0560
Excited State	10:	?Spin -A	3.3450 eV	370.65 nm	f=0.2186

B3LYP TD(nstates=10) /6-311+g(d,p) scrf=(pcm,solvent=water)

Total free energy in solution: with all non-electrostatic terms

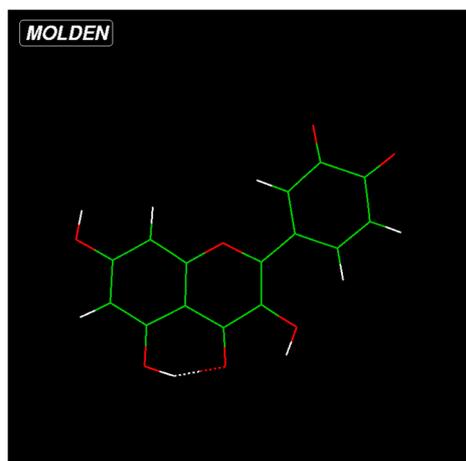
(a.u.) = -1103.884922

Excitation energies and oscillator strengths:

Excited State	1:	?Spin -A	0.9484 eV	1307.36 nm	f=0.0724
Excited State	2:	?Spin -A	1.1062 eV	1120.81 nm	f=0.0976
Excited State	3:	?Spin -A	1.2775 eV	970.50 nm	f=0.0000
Excited State	4:	?Spin -A	1.7217 eV	720.12 nm	f=0.0096
Excited State	5:	?Spin -A	2.2398 eV	553.56 nm	f=0.0126
Excited State	6:	?Spin -A	2.5197 eV	492.07 nm	f=0.0634
Excited State	7:	?Spin -A	2.6264 eV	472.07 nm	f=0.0000
Excited State	8:	?Spin -A	2.9876 eV	415.00 nm	f=0.0302
Excited State	9:	?Spin -A	3.1408 eV	394.75 nm	f=0.1121
Excited State	10:	?Spin -A	3.2341 eV	383.37 nm	f=0.2431

Appendix A12. Quercetin anion 3'-OH to 4'-OH

B3LYP/6-31+g(d,p) gas phase



Coordinates:

```
C,0,-0.0117431408,-0.0000487222,0.0053542299\C,0,-
0.0091392746,0.0000185989,1.4035331873\C,0,1.1832744519,0.0000398727,2.1392725666\C,0,2.421327
64,-0.0000026424,1.4405989568\C,0,2.4391152118,-0.0000747267,0.0481088008\C,0,1.2222124245,-
0.0000962196,-0.6485847204\O,0,-1.2097527278,0.000061097,2.0308632368\C,0,-
1.3536221205,0.0001171425,3.4094206165\C,0,-0.187827859,0.0001271574,4.1711151868\
C,0,1.1099561676,0.0000964462,3.5787513995\C,0,-2.7337823679,0.0001372286,3.8213514908\C,0,-
3.7627964155,0.0000200302,2.8683988261\C,0,-5.1588421419,0.0000374682,3.2057228967\C,0,-
5.521367539,0.000220832,4.6857234775\C,0,-4.4029902863,0.0003246987,5.6199319921\C,0,-
3.0963882986,0.0002873006,5.2224638569\O,0,-6.7030543314,0.0002424855,5.0687864524\O,0,-
6.0535717202,-0.000055804,2.3254719554\O,0,-0.1919521274,0.0001563773,5.539286636\
O,0,2.1507935157,0.0000724143,4.325033592\O,0,3.5767897035,0.0000346608,2.1353137891\O,0,1.302
4451473,-0.0001625569,-2.0197674171\H,0,-0.954003291,-0.000063897,-0.5333647168\
H,0,3.3789494489,-0.0001080336,-0.4910272067\H,0,0.759384302,0.0001574887,5.7715023424\
H,0,3.3226004228,0.0001196365,3.1025713165\H,0,0.4107723416,-0.0001715643,-2.3916728969\H,0,-
2.3109516544,0.0003769903,5.9661565366\H,0,-4.6591219246,0.0004426614,6.6768111006\H,0,-
3.5352082238,-0.0000950836,1.8088661602
```

Thermal correction to Enthalpy= 0.218600

Thermal correction to Gibbs Free Energy= 0.152517

Lowest freq: 16.8973 cm-1

B3LYP TD(nstates=10) /6-311+g(d,p)

HF=-1103.3600338

Excitation energies and oscillator strengths:

Excited State 1: ?Spin -A 1.3154 eV 942.56 nm f=0.0000

Excited State	2:	?Spin -A	1.6689 eV	742.91 nm	f=0.1236
Excited State	3:	?Spin -A	1.8870 eV	657.06 nm	f=0.1083
Excited State	4:	?Spin -A	2.2898 eV	541.46 nm	f=0.0000
Excited State	5:	?Spin -A	2.5623 eV	483.88 nm	f=0.0086
Excited State	6:	?Spin -A	2.6738 eV	463.70 nm	f=0.1056
Excited State	7:	?Spin -A	2.6763 eV	463.26 nm	f=0.0000
Excited State	8:	?Spin -A	2.7888 eV	444.57 nm	f=0.0000
Excited State	9:	?Spin -A	2.9975 eV	413.63 nm	f=0.0000
Excited State	10:	?Spin -A	3.0330 eV	408.79 nm	f=0.0029

B3LYP TD(nstates=10) /6-311+g(d,p) scrf=(pcm,solvent=water)

Total free energy in solution: with all non-electrostatic terms

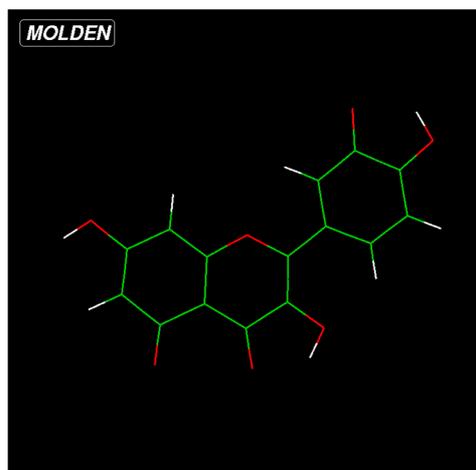
(a.u.) = -1103.439710

Excitation energies and oscillator strengths:

Excited State	1:	?Spin -A	1.6500 eV	751.44 nm	f=0.0000
Excited State	2:	?Spin -A	1.6761 eV	739.71 nm	f=0.0361
Excited State	3:	?Spin -A	1.9994 eV	620.11 nm	f=0.1574
Excited State	4:	?Spin -A	2.4191 eV	512.52 nm	f=0.1981
Excited State	5:	?Spin -A	2.6403 eV	469.58 nm	f=0.0000
Excited State	6:	?Spin -A	2.8533 eV	434.53 nm	f=0.0118
Excited State	7:	?Spin -A	3.0172 eV	410.92 nm	f=0.0486
Excited State	8:	?Spin -A	3.0760 eV	403.07 nm	f=0.0468
Excited State	9:	?Spin -A	3.3382 eV	371.42 nm	f=0.0480
Excited State	10:	?Spin -A	3.3643 eV	368.53 nm	f=0.0708

Appendix A13. Quercetin radical anion 3'-OH to 5-OH

B3LYP/6-31+g(d,p) gas phase



Coordinates:

```
C,0,0.0208938851,-0.0001060171,-0.0430109861 \ C,0,0.0094514269,0.0000646029,1.390987054 \
C,0,1.2202288494,0.0001037244,2.0915475122 \ C,0,2.4665182289,-0.0000225592,1.4067865238 \
C,0,2.419145524,-0.0001940979,-0.0562015584 \ C,0,1.2169924108,-0.0002335912,-0.7550739758 \ C,0,-
1.2588605554,0.0001959224,2.1097781269 \ O,0,-1.1006626403,0.0003601898,3.4723750692 \ C,0,-
2.1595974545,0.000503965,4.3460393632 \ C,0,-3.5064126447,0.0004915466,3.8997341503 \ C,0,-
3.742343601,0.0003255911,2.4904022516 \ C,0,-2.5388090599,0.000177698,1.6181489519 \ C,0,-
4.5912883941,0.0006510188,4.912268801 \ C,0,-4.1591196085,0.0008107497,6.2973232583 \ C,0,-
2.8276574293,0.0008120825,6.6473577726 \ C,0,-1.7954226841,0.0006588963,5.6852640223 \ O,0,-
5.803081932,0.0006516545,4.6086393089 \ O,0,-2.4144794427,0.0009627221,7.9637578521 \ O,0,-
2.8747029994,0.0000281162,0.3149188062 \ O,0,-4.8267049704,0.0002765161,1.858043574 \
O,0,3.6277986546,-0.000042311,1.9301032713 \ O,0,3.6205941127,-0.0003085444,-0.6542920232 \ H,0,-
0.7538972003,0.000662235,5.9802824 \ H,0,-4.9437459099,0.0009295373,7.0506383752 \ H,0,-
3.875730431,0.0000765126,0.394734349 \ H,0,-3.1994960197,0.0010604892,8.5270269675 \ H,0,-
0.918411435,-0.000135236,-0.5779088683 \ H,0,1.2195355454,-0.0003619641,-1.8409665199 \
H,0,1.2343816994,0.0002308291,3.173777685 \ H,0,4.2389487489,-0.0002372643,0.1210958482
```

Thermal correction to Enthalpy= 0.217911

Thermal correction to Gibbs Free Energy= 0.152097

lowest freq: 23.0434 cm⁻¹

B3LYP TD(nstates=10) /6-311+g(d,p)

HF=-1103.3432118

Excitation energies and oscillator strengths:

Excited State 1: ?Spin -A 0.6467 eV 1917.25 nm f=0.1066

Excited State 2: ?Spin -A 1.0852 eV 1142.54 nm f=0.0000

Excited State 3: ?Spin -A 1.3418 eV 924.05 nm f=0.0117

Excited State	4:	?Spin	-A	1.7802 eV	696.44 nm	f=0.0009
Excited State	5:	?Spin	-A	1.9172 eV	646.70 nm	f=0.0000
Excited State	6:	?Spin	-A	2.3808 eV	520.77 nm	f=0.0192
Excited State	7:	?Spin	-A	2.4136 eV	513.70 nm	f=0.0016
Excited State	8:	?Spin	-A	2.5906 eV	478.59 nm	f=0.0000
Excited State	9:	?Spin	-A	2.6746 eV	463.56 nm	f=0.1014
Excited State	10:	?Spin	-A	3.0289 eV	409.34 nm	f=0.0008

B3LYP TD(nstates=10) /6-311+g(d,p) scrf=(pcm,solvent=water)

Total free energy in solution: with all non-electrostatic terms

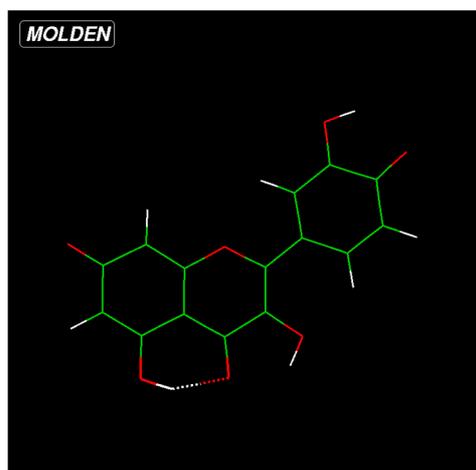
(a.u.) = -1103.420107

Excitation energies and oscillator strengths:

Excited State	1:	?Spin	-A	0.6982 eV	1775.88 nm	f=0.0971
Excited State	2:	?Spin	-A	1.3670 eV	906.96 nm	f=0.0128
Excited State	3:	?Spin	-A	1.7194 eV	721.07 nm	f=0.0000
Excited State	4:	?Spin	-A	1.9171 eV	646.73 nm	f=0.0059
Excited State	5:	?Spin	-A	2.0342 eV	609.50 nm	f=0.0000
Excited State	6:	?Spin	-A	2.2932 eV	540.66 nm	f=0.0098
Excited State	7:	?Spin	-A	2.3619 eV	524.94 nm	f=0.0661
Excited State	8:	?Spin	-A	2.7600 eV	449.22 nm	f=0.1276
Excited State	9:	?Spin	-A	3.0409 eV	407.72 nm	f=0.0098
Excited State	10:	?Spin	-A	3.0493 eV	406.60 nm	f=0.0000

Appendix A14. Quercetin radical anion 4'-OH to 7-OH

B3LYP/6-31+g(d,p) gas phase



Coordinates:

```
C,0,0.0192995846,-0.0008474387,-0.0137876706 \ C,0,0.0011761707,-0.0003154627,1.3546039336 \
C,0,1.194190604,0.000200514,2.1376332263 \ C,0,2.4593847742,0.0001455181,1.4412434222 \ C,0,2.50366
34568,-0.0003779673,0.0726191337 \ C,0,1.2890700691,-0.0009032606,-0.7319292228 \
C,0,1.1043848282,0.000756363,3.5437620118 \ C,0,-0.2271169172,0.0007351792,4.1254040618 \ C,0,-
1.3790241465,0.0002045104,3.3473047172 \ O,0,-1.226484487,-0.0002857727,1.9821612612 \ C,0,-
2.7497802402,0.0000347603,3.7719516145 \ C,0,-3.1111352043,0.0008041244,5.1601460352 \ C,0,-
4.42586368,0.0006759153,5.5606912679 \ C,0,-5.4991674914,-0.0002373841,4.6043435814 \ C,0,-
5.1043532429,-0.0010072391,3.1945766471 \ C,0,-3.7914192381,-0.0008688736,2.7964254148 \ O,0,-
6.1347654823,-0.0018703615,2.3161471337 \ O,0,-6.7333966567,-0.00042922,4.8765300535 \
O,0,2.090726131,0.0012306178,4.3639051968 \ O,0,-0.2188735353,0.0012359341,5.4760581591 \
O,0,3.6000415231,0.0006237961,2.1791256789 \ O,0,1.3271234365,-0.0013851414,-1.986816498 \ H,0,-
0.9004077124,-0.0012364953,-0.5873294984 \ H,0,3.4568236754,-0.0004136008,-0.4449105205 \
H,0,0.7504655324,0.0014884607,5.6780585637 \ H,0,3.3357105548,0.0009558376,3.1329694207 \ H,0,-
2.3280161122,0.001508053,5.9053614566 \ H,0,-4.6900212237,0.0012771501,6.6139887044 \ H,0,-
3.5498905332,-0.001454853,1.7410049909 \ H,0,-6.9294839526,-0.0017382333,2.8943638689
```

Thermal correction to Enthalpy= 0.218739

Thermal correction to Gibbs Free Energy= 0.153791

Lowest freq: 26.3164 cm⁻¹

B3LYP TD(nstates=10) /6-311+g(d,p)

HF=-1103.375027

Excitation energies and oscillator strengths:

Excited State 1: ?Spin -A 1.0299 eV 1203.86 nm f=0.1725

Excited State 2: ?Spin -A 1.3901 eV 891.92 nm f=0.0000

Excited State 3: ?Spin -A 1.3928 eV 890.16 nm f=0.0032

Excited State	4:	?Spin -A	2.0422 eV	607.11 nm	f=0.0093
Excited State	5:	?Spin -A	2.1371 eV	580.16 nm	f=0.0000
Excited State	6:	?Spin -A	2.3419 eV	529.42 nm	f=0.0038
Excited State	7:	?Spin -A	2.5871 eV	479.25 nm	f=0.0087
Excited State	8:	?Spin -A	2.7573 eV	449.66 nm	f=0.3798
Excited State	9:	?Spin -A	3.0730 eV	403.46 nm	f=0.0000
Excited State	10:	?Spin -A	3.1391 eV	394.96 nm	f=0.0031

B3LYP TD(nstates=10) /6-311+g(d,p) scrf=(pcm,solvent=water)

Total free energy in solution: with all non-electrostatic terms

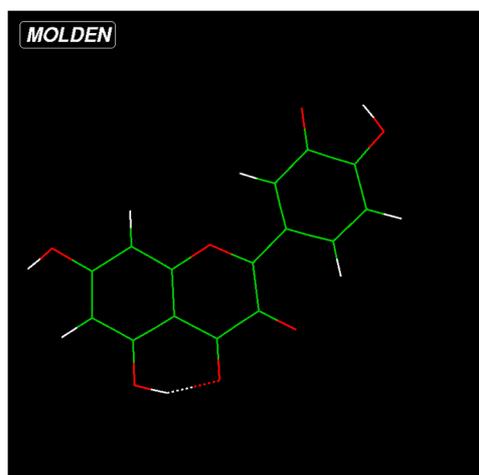
(a.u.) = -1103.435669

Excitation energies and oscillator strengths:

Excited State	1:	?Spin -A	1.1127 eV	1114.30 nm	f=0.1904
Excited State	2:	?Spin -A	1.5403 eV	804.95 nm	f=0.0112
Excited State	3:	?Spin -A	1.9033 eV	651.42 nm	f=0.0106
Excited State	4:	?Spin -A	2.0479 eV	605.43 nm	f=0.0000
Excited State	5:	?Spin -A	2.1573 eV	574.72 nm	f=0.0000
Excited State	6:	?Spin -A	2.3106 eV	536.59 nm	f=0.0052
Excited State	7:	?Spin -A	2.6403 eV	469.59 nm	f=0.3067
Excited State	8:	?Spin -A	2.8368 eV	437.05 nm	f=0.2001
Excited State	9:	?Spin -A	3.1093 eV	398.75 nm	f=0.0000
Excited State	10:	?Spin -A	3.1714 eV	390.94 nm	f=0.0116

Appendix A15. Quercetin radical anion 3'-OH to 3-OH

B3LYP/6-31+g(d,p) gas phase



Coordinates:

```
C,0,-0.0182599685,-0.0000016031,0.0129706061 \ C,0,-0.0158092435,-0.0000030758,1.4124094781 \
C,0,1.1771326706,-0.0000031446,2.1574842479 \ C,0,2.4173493605,0.0000026228,1.4508835193 \
C,0,2.431307694,0.0000080944,0.0575234078 \ C,0,1.2114375919,0.0000044103,-0.6398110731 \
C,0,1.1381162877,-0.000005075,3.6017502329 \ C,0,-0.2087437162,0.0000040549,4.2756956158 \ C,0,-
1.362699303,-0.0000013432,3.4110495067 \ O,0,-1.2104116801,-0.0000042531,2.0300678575 \ C,0,-
2.7498242863,-0.0000023705,3.7863530613 \ C,0,-3.108875201,0.0000020799,5.1815903488 \ C,0,-
4.4398219441,0.0000021716,5.5784184915 \ C,0,-5.436287178,-0.0000013031,4.6047583595 \ C,0,-
5.1357263832,-0.0000050072,3.1705741843 \ C,0,-3.7725520819,-0.0000055467,2.8088955003 \ O,0,-
6.1582563718,-0.0000083591,2.3993057495 \ O,0,-6.7484158037,-0.0000010309,4.8794689565 \
O,0,2.1970626564,0.0000242158,4.277621604 \ O,0,-0.2512017749,0.0000024675,5.5288233814 \
O,0,3.5707159573,0.000007595,2.1373781732 \ O,0,1.1880245838,0.0000088643,-2.0136115463 \ H,0,-
0.9484264696,-0.0000028676,-0.541388076 \ H,0,3.383926872,0.0000138504,-0.4650382603 \
H,0,3.2985031496,0.0000013648,3.1120499343 \ H,0,2.0952349862,0.0000137964,-2.3448891444 \ H,0,-
2.3112593628,0.0000053864,5.91188442 \ H,0,-4.7081560739,0.0000053028,6.6311204539 \ H,0,-
3.5279776629,-0.0000082845,1.7547254127 \ H,0,-7.129605635,-0.0000036127,3.9550961463
```

Thermal correction to Enthalpy= 0.217948

Thermal correction to Gibbs Free Energy= 0.152881

Lowest freq: 89.3482 cm⁻¹

B3LYP TD(nstates=10) /6-311+g(d,p)

HF=-1103.3600907

Excitation energies and oscillator strengths:

Excited State 1: ?Spin -A 0.9005 eV 1376.87 nm f=0.0543

Excited State 2: ?Spin -A 1.6931 eV 732.28 nm f=0.0000

Excited State 3: ?Spin -A 1.9754 eV 627.63 nm f=0.0640

Excited State	4:	?Spin	-A	2.1895 eV	566.27 nm	f=0.0000
Excited State	5:	?Spin	-A	2.2803 eV	543.72 nm	f=0.0089
Excited State	6:	?Spin	-A	2.5167 eV	492.64 nm	f=0.2773
Excited State	7:	?Spin	-A	2.8071 eV	441.68 nm	f=0.0402
Excited State	8:	?Spin	-A	2.8483 eV	435.30 nm	f=0.0120
Excited State	9:	?Spin	-A	3.0791 eV	402.67 nm	f=0.0014
Excited State	10:	?Spin	-A	3.0939 eV	400.73 nm	f=0.0000

B3LYP TD(nstates=10) /6-311+g(d,p) scrf=(pcm,solvent=water)

Total free energy in solution: with all non-electrostatic terms

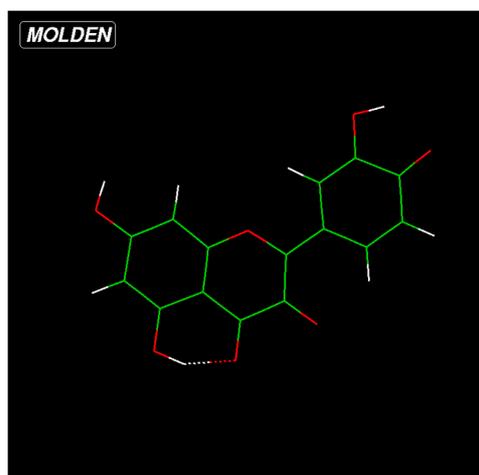
(a.u.) = -1103.435014

Excitation energies and oscillator strengths:

Excited State	1:	?Spin	-A	0.9464 eV	1310.02 nm	f=0.0844
Excited State	2:	?Spin	-A	1.8910 eV	655.65 nm	f=0.0000
Excited State	3:	?Spin	-A	2.0180 eV	614.38 nm	f=0.0023
Excited State	4:	?Spin	-A	2.2365 eV	554.36 nm	f=0.2622
Excited State	5:	?Spin	-A	2.4234 eV	511.61 nm	f=0.0336
Excited State	6:	?Spin	-A	2.4549 eV	505.06 nm	f=0.0000
Excited State	7:	?Spin	-A	2.5514 eV	485.95 nm	f=0.0750
Excited State	8:	?Spin	-A	2.6631 eV	465.57 nm	f=0.1069
Excited State	9:	?Spin	-A	3.0474 eV	406.86 nm	f=0.0316
Excited State	10:	?Spin	-A	3.1669 eV	391.50 nm	f=0.0000

Appendix A16. Quercetin radical anion 4'-OH to 3-OH

B3LYP/6-31+g(d,p) gas phase



Coordinates:

```
C,0,0.0022947557,-0.0000125581,-0.0083119787\C,0,0.0030805475,-0.0000005136,1.4289049999\
C,0,1.2749597088,0.0000082534,2.0990964467\C,0,2.4358680711,-0.0000028289,1.3770989989\
C,0,2.456589382,-0.0000263486,-0.0853641172\C,0,1.1734988585,-0.0000198678,-0.7298875635\C,0,-
1.2032962912,0.000008966,2.1779906587\O,0,-0.9699663399,0.0000144052,3.5492250275\C,0,-
1.9551115843,0.0000087977,4.469504702\C,0,-3.3042354779,-0.0000005056,4.0849662219\C,0,-
3.6657815029,-0.0000132213,2.6830949524\C,0,-2.561637532,0.0000030356,1.671211446\C,0,-
4.2999794574,-0.0000035445,5.1104802777\C,0,-3.9328368508,-0.0000144682,6.4548866632\C,0,-
2.571711501,-0.0000101734,6.7863197332\C,0,-1.5692250006,0.0000045827,5.8151104349\O,0,-
5.5971455987,0.0000172047,4.7663559714\O,0,-2.2648682864,-0.0000166739,8.1261064967\O,0,-
2.8490137602,-0.000056226,0.4501789392\O,0,-4.872914324,-0.0000569574,2.3286546775\
O,0,3.6674414805,-0.0000012768,1.9572024775\O,0,3.5846295544,0.0000030676,-0.6630366838\H,0,-
0.514608047,0.0000092057,6.0728161236\H,0,-4.6885800426,-0.0000182563,7.2312410623\H,0,-
5.6045240055,0.0000732707,3.7543451185\H,0,-1.304529407,-0.0000109523,8.2309252359\H,0,-
0.956464012,-0.0000115168,-0.5093656847\H,0,1.1564808653,-0.0000200849,-1.816235579\
H,0,1.3227126154,0.0000197837,3.1808600022\H,0,4.2725007545,-0.0000291147,1.1815410773
```

Thermal correction to Enthalpy= 0.218440

Thermal correction to Gibbs Free Energy= 0.153480

Lowest freq: 31.3014 cm⁻¹

B3LYP TD(nstates=10) /6-311+g(d,p)

HF=-1103.3734359

Excitation energies and oscillator strengths:

Excited State	1:	?Spin	-A	1.5523 eV	798.69 nm	f=0.0194
Excited State	2:	?Spin	-A	1.7863 eV	694.07 nm	f=0.0000
Excited State	3:	?Spin	-A	2.2246 eV	557.34 nm	f=0.3589

Excited State	4:	?Spin -A	2.4413 eV	507.87 nm	f=0.1597
Excited State	5:	?Spin -A	2.5111 eV	493.74 nm	f=0.0000
Excited State	6:	?Spin -A	2.8379 eV	436.89 nm	f=0.0177
Excited State	7:	?Spin -A	2.9633 eV	418.40 nm	f=0.0136
Excited State	8:	?Spin -A	3.0697 eV	403.90 nm	f=0.0000
Excited State	9:	?Spin -A	3.1379 eV	395.11 nm	f=0.0000
Excited State	10:	?Spin -A	3.1491 eV	393.72 nm	f=0.0050

B3LYP TD(nstates=10) /6-311+g(d,p) scrf=(pcm,solvent=water)

Total free energy in solution: with all non-electrostatic terms

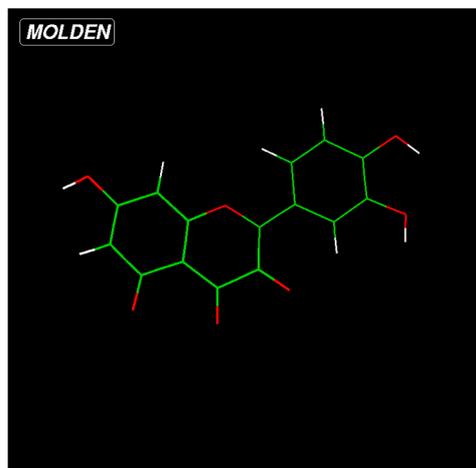
(a.u.) = -1103.446118

Excitation energies and oscillator strengths:

Excited State	1:	?Spin -A	1.5087 eV	821.81 nm	f=0.0725
Excited State	2:	?Spin -A	1.9994 eV	620.11 nm	f=0.0000
Excited State	3:	?Spin -A	2.2114 eV	560.66 nm	f=0.2336
Excited State	4:	?Spin -A	2.3055 eV	537.78 nm	f=0.3432
Excited State	5:	?Spin -A	2.5384 eV	488.44 nm	f=0.0465
Excited State	6:	?Spin -A	2.6256 eV	472.21 nm	f=0.0000
Excited State	7:	?Spin -A	2.6509 eV	467.71 nm	f=0.0095
Excited State	8:	?Spin -A	2.9760 eV	416.62 nm	f=0.0338
Excited State	9:	?Spin -A	3.2485 eV	381.67 nm	f=0.0000
Excited State	10:	?Spin -A	3.4719 eV	357.11 nm	f=0.0213

Appendix A17. Quercetin radical anion 3-OH to 5-OH

B3LYP/6-31+g(d,p) gas phase



Coordinates:

```
C,0,-0.024116405,0.0000003917,0.0026664697\ C,0,-0.0074560519,0.0000004835,1.4196278799\
C,0,1.2545985979,0.0000006036,2.0634738528\ C,0,2.4208776692,0.0000009864,1.3169641807\ C,0,2.393
2833229,0.000001066,-0.0849031624\ C,0,1.1579995173,0.0000006686,-0.732954355\ C,0,-
1.2493067258,0.0000003896,2.1749190521\ O,0,-2.3465240378,-0.000000291,1.3800251923\ C,0,-
3.6320360895,-0.0000002318,1.8773207318\ C,0,-3.9060008286,0.0000004645,3.2591191426\ C,0,-
2.806821887,0.0000011312,4.2120045652\ C,0,-1.3888744716,0.0000011016,3.6106542159\ C,0,-
5.3297971096,0.0000005111,3.6737566315\ C,0,-6.3103108991,-0.0000002054,2.5914459744\ C,0,-
5.9481624652,-0.000000894,1.2662184882\ C,0,-4.5945640466,-0.0000009275,0.8729793884\ O,0,-
5.7127891351,0.000001125,4.861680666\ O,0,-6.876228631,-0.0000015659,0.2401113656\ O,0,-
0.3974084805,0.000001768,4.3693219714\ O,0,-2.8999781375,0.0000017472,5.4383271086\
O,0,3.6870854008,0.0000009172,1.8832993445\ O,0,3.5580176045,0.000001543,-0.8102802756\ H,0,-
4.3092275952,-0.0000014625,-0.1714573963\ H,0,-7.355350526,-0.0000001659,2.894922122\ H,0,-
7.7579060813,-0.0000014967,0.6351053638\ H,0,-0.9744194016,0.0000002002,-0.516127538\
H,0,1.1386679788,0.0000007636,-1.8185777219\ H,0,1.2798144746,0.0000004575,3.1482016036\
H,0,4.2959077482,0.0000028062,-0.1820821995\ H,0,3.6044707868,0.0000060387,2.8457967402
```

Thermal correction to Enthalpy= 0.217771

Thermal correction to Gibbs Free Energy= 0.150310

Lowest freq: 28.9929 cm⁻¹

B3LYP TD(nstates=10) /6-311+g(d,p)

HF= -1103.3270752

Excitation energies and oscillator strengths:

Excited State 1: ?Spin -A 0.9320 eV 1330.24 nm f=0.0000

Excited State 2: ?Spin -A 1.0300 eV 1203.74 nm f=0.0956

Excited State 3: ?Spin -A 1.8050 eV 686.90 nm f=0.0000

Excited State	4:	?Spin -A	2.0130 eV	615.91 nm	f=0.0360
Excited State	5:	?Spin -A	2.3191 eV	534.62 nm	f=0.0000
Excited State	6:	?Spin -A	2.5807 eV	480.43 nm	f=0.0223
Excited State	7:	?Spin -A	2.5969 eV	477.43 nm	f=0.0000
Excited State	8:	?Spin -A	2.7060 eV	458.18 nm	f=0.0432
Excited State	9:	?Spin -A	2.8392 eV	436.68 nm	f=0.1231
Excited State	10:	?Spin -A	3.0045 eV	412.66 nm	f=0.0000

B3LYP TD(nstates=10) /6-311+g(d,p) scrf=(pcm,solvent=water)

Total free energy in solution: with all non-electrostatic terms

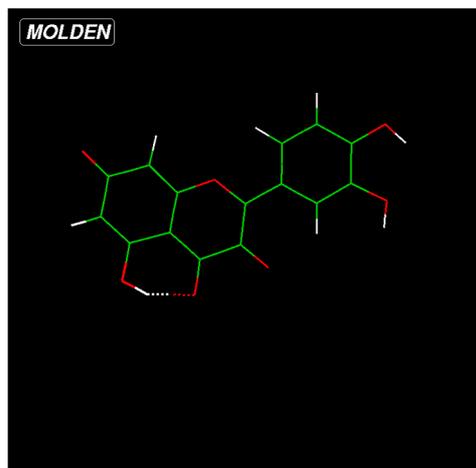
(a.u.) = -1103.426401

Excitation energies and oscillator strengths:

Excited State	1:	?Spin -A	1.2572 eV	986.18 nm	f=0.1444
Excited State	2:	?Spin -A	1.4598 eV	849.32 nm	f=0.0000
Excited State	3:	?Spin -A	1.9849 eV	624.63 nm	f=0.0255
Excited State	4:	?Spin -A	2.2664 eV	547.06 nm	f=0.0042
Excited State	5:	?Spin -A	2.2928 eV	540.74 nm	f=0.0000
Excited State	6:	?Spin -A	2.5754 eV	481.42 nm	f=0.1662
Excited State	7:	?Spin -A	2.7251 eV	454.97 nm	f=0.1277
Excited State	8:	?Spin -A	2.8842 eV	429.88 nm	f=0.0060
Excited State	9:	?Spin -A	2.9067 eV	426.54 nm	f=0.0000
Excited State	10:	?Spin -A	3.1158 eV	397.92 nm	f=0.0000

Appendix A18. Quercetin radical anion 3-OH to 7-OH

B3LYP/6-31+g(d,p) gas phase



Coordinates:

```
C,0,0.0047340414,0.0000010217,-0.0140597\C,0,-0.0038209355,0.0000008455,1.4028102137\
C,0,1.24553545,0.0000013017,2.0709478032\C,0,2.4253978283,0.000001886,1.3465674973\C,0,2.422887
6172,0.0000020694,-0.0559981323\C,0,1.1997579678,0.0000016169,-0.7273221201\C,0,-
1.2622473788,0.0000001671,2.1314686539\O,0,-2.340221986,-0.0000004516,1.3080141053\C,0,-
3.6363020749,-0.0000004443,1.7788448787\C,0,-3.8818950596,-0.000000274,3.1751594865\C,0,-
2.8221658711,-0.0000037468,4.1212911973\C,0,-1.414206225,-0.0000007007,3.5720564867\C,0,-
5.2737452966,0.0000005496,3.5878706531\C,0,-6.2949988313,-0.0000016177,2.6687319756\C,0,-
6.0382620491,-0.0000026605,1.2428436421\C,0,-4.6326853961,-0.0000014559,0.8360274855\O,0,-
5.5348984568,0.0000064795,4.9143594775\O,0,-6.9539065733,-0.0000041373,0.3810152864\O,0,-
0.4349193671,-0.0000007536,4.3487319468\O,0,-3.0002700175,-0.00000070708,5.3705010475\
O,0,3.6808192842,0.0000023932,1.9343415028\O,0,3.5988185954,0.0000026961,-0.7589330976\H,0,-
4.4000509198,-0.0000020893,-0.223120733\H,0,-7.3263490613,-0.000001188,3.0049908803\H,0,-
4.6436156654,0.00001453,5.3740297528\H,0,-0.9356363265,0.0000006662,-0.5502973359\
H,0,1.200675816,0.0000017553,-1.812938715\H,0,1.2512032332,0.0000012859,3.1557212171\
H,0,4.3265208453,0.0000029995,-0.1187703669\H,0,3.5837743409,0.000002643,2.8954682097
```

Thermal correction to Enthalpy= 0.218205

Thermal correction to Gibbs Free Energy= 0.152471

Lowest freq: 31.5131 cm⁻¹

B3LYP TD(nstates=10) /6-311+g(d,p)

HF= 1103.3565527

Excitation energies and oscillator strengths:

Excited State 1: ?Spin -A 0.9988 eV 1241.33 nm f=0.0482

Excited State 2: ?Spin -A 1.5386 eV 805.82 nm f=0.0000

Excited State 3: ?Spin -A 1.6979 eV 730.21 nm f=0.0000

Excited State	4:	?Spin -A	1.7226 eV	719.73 nm	f=0.0602
Excited State	5:	?Spin -A	2.4446 eV	507.17 nm	f=0.0015
Excited State	6:	?Spin -A	2.5245 eV	491.13 nm	f=0.0387
Excited State	7:	?Spin -A	2.7579 eV	449.56 nm	f=0.0000
Excited State	8:	?Spin -A	2.7890 eV	444.55 nm	f=0.2150
Excited State	9:	?Spin -A	3.1181 eV	397.63 nm	f=0.0460
Excited State	10:	?Spin -A	3.2235 eV	384.62 nm	f=0.0219

B3LYP TD(nstates=10) /6-311+g(d,p) scrf=(pcm,solvent=water)

Total free energy in solution: with all non-electrostatic terms

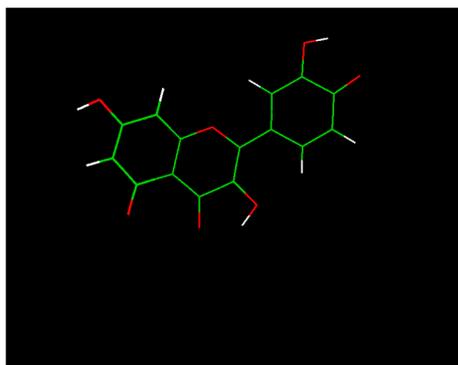
(a.u.) = -1103.437261

Excitation energies and oscillator strengths:

Excited State	1:	?Spin -A	1.3674 eV	906.75 nm	f=0.0784
Excited State	2:	?Spin -A	1.7975 eV	689.77 nm	f=0.0811
Excited State	3:	?Spin -A	1.8602 eV	666.50 nm	f=0.0000
Excited State	4:	?Spin -A	2.2014 eV	563.21 nm	f=0.0054
Excited State	5:	?Spin -A	2.2661 eV	547.13 nm	f=0.0000
Excited State	6:	?Spin -A	2.5030 eV	495.35 nm	f=0.1942
Excited State	7:	?Spin -A	2.6824 eV	462.21 nm	f=0.1871
Excited State	8:	?Spin -A	2.7929 eV	443.93 nm	f=0.0047
Excited State	9:	?Spin -A	3.0901 eV	401.22 nm	f=0.0000
Excited State	10:	?Spin -A	3.3356 eV	371.70 nm	f=0.0055

Appendix A19. Quercetin radical anion 5-OH to 4'-OH

B3LYP/6-31+g(d,p) gas phase



Coordinates:

C,0,0.0270913281,0.,-0.0461771015\ C,0,-0.005414375,0.,1.3866306569\
 C,0,1.2306419807,0.,2.0974881935\ C,0,2.4177812332,0.,1.4082878238\ C,0,2.4789247197,0.,-
 0.0535412097\ C,0,1.2159309596,0.,-0.7381551285\ C,0,-1.2462607324,0.,2.1112643741\ O,0,-
 1.093112621,0.,3.4748752222\ C,0,-2.1540408927,0.,4.3504680358\ C,0,-3.50270182,0.,3.9048396923\
 C,0,-3.7411470282,0.,2.4974512601\ C,0,-2.5411726172,0.,1.6254780944\ C,0,-
 4.5868815432,0.,4.9190452465\ C,0,-4.1540594678,0.,6.3042172484\ C,0,-
 2.8234935325,0.,6.6513418947\ C,0,-1.7904464582,0.,5.6864712535\ O,0,-
 5.7978928445,0.,4.6145960575\ O,0,-2.4055881737,0.,7.9658436934\ O,0,-
 2.8746279797,0.,0.3276695093\ O,0,-4.8255590658,0.,1.862190567\ O,0,3.6235466392,0.,2.0262902035\
 O,0,3.620577943,0.,-0.5998632612\ H,0,-0.7492753293,0.,5.9827932868\ H,0,-
 4.9378739039,0.,7.0582790309\ H,0,-3.8786808587,0.,0.4104160917\ H,0,-
 3.1885195545,0.,8.5320880998\ H,0,-0.9081515463,0.,-0.589321962\ H,0,1.231022674,0.,-
 1.8240116849\ H,0,1.2368726422,0.,3.1803517679\ H,0,4.2614791466,0.,1.2780051007

Thermal correction to Enthalpy= 0.218009

Thermal correction to Gibbs Free Energy= 0.152311

Lowest freq: 32.7474 cm⁻¹

B3LYP TD(nstates=10) /6-311+g(d,p)

HF=-1103.4455708

Excitation energies and oscillator strengths:

Excited State	1:	?Spin -A'	0.9041 eV	1371.40 nm	f=0.1487
Excited State	2:	?Spin -A''	1.7748 eV	698.58 nm	f=0.0000
Excited State	3:	?Spin -A'	1.8352 eV	675.57 nm	f=0.0245
Excited State	4:	?Spin -A'	1.9677 eV	630.11 nm	f=0.0078
Excited State	5:	?Spin -A'	2.1529 eV	575.90 nm	f=0.0279
Excited State	6:	?Spin -A''	2.1880 eV	566.67 nm	f=0.0000
Excited State	7:	?Spin -A'	2.5970 eV	477.42 nm	f=0.1583

Excited State	8:	?Spin -A'	2.7893 eV	444.49 nm	f=0.1584
Excited State	9:	?Spin -A''	3.0666 eV	404.30 nm	f=0.0000
Excited State	10:	?Spin -A'	3.3031 eV	375.36 nm	f=0.1524

B3LYP TD(nstates=10) /6-311+g(d,p) scrf=(pcm,solvent=water)

Total free energy in solution: with all non-electrostatic terms

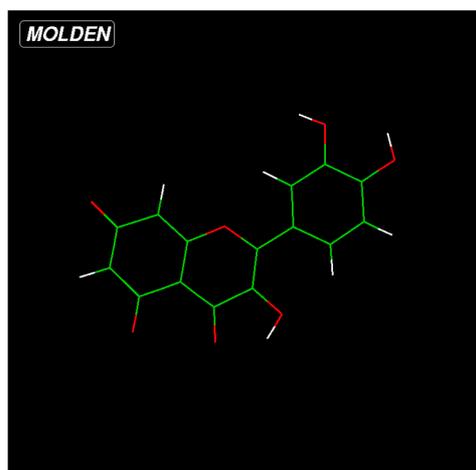
(a.u.) = -1103.427734

Excitation energies and oscillator strengths:

Excited State	1:	?Spin -A'	0.9041 eV	1371.40 nm	f=0.1487
Excited State	2:	?Spin -A''	1.7748 eV	698.58 nm	f=0.0000
Excited State	3:	?Spin -A'	1.8352 eV	675.57 nm	f=0.0245
Excited State	4:	?Spin -A'	1.9677 eV	630.11 nm	f=0.0078
Excited State	5:	?Spin -A'	2.1529 eV	575.90 nm	f=0.0279
Excited State	6:	?Spin -A''	2.1880 eV	566.67 nm	f=0.0000
Excited State	7:	?Spin -A'	2.5970 eV	477.42 nm	f=0.1583
Excited State	8:	?Spin -A'	2.7893 eV	444.49 nm	f=0.1584
Excited State	9:	?Spin -A''	3.0666 eV	404.30 nm	f=0.0000
Excited State	10:	?Spin -A'	3.3031 eV	375.36 nm	f=0.1524

Appendix A20. Quercetin radical anion 5-OH to 7-OH

B3LYP/6-31+g(d,p) gas phase



Coordinates:

```
C,0,0.0250590833,0.0000003435,-0.0577379875 \ C,0,-0.0177842372,0.0000003875,1.3515910926 \
C,0,1.2064268437,0.0000007167,2.0543110948 \ C,0,2.4130755342,0.0000012837,1.3708825976 \ C,0,2.448
3627139,0.000001348,-0.0304455674 \ C,0,1.2457149378,0.0000008161,-0.733423498 \ C,0,-
1.2760612124,0.0000000708,2.1046038325 \ O,0,-1.0795259239,0.0000005447,3.4608114083 \ C,0,-
2.1344793664,0.0000004078,4.3555595542 \ C,0,-3.4949518862,-0.0000001749,3.9364450356 \ C,0,-
3.7429432969,-0.0000009163,2.512487866 \ C,0,-2.5532889217,-0.0000006744,1.6309894881 \ C,0,-
4.596987471,0.000000065,4.9626942446 \ C,0,-4.1631157761,0.0000005365,6.325777901 \ C,0,-
2.806239384,0.0000010049,6.7219272831 \ C,0,-1.7679818355,0.0000009583,5.683294662 \ O,0,-
5.7988750667,-0.0000002961,4.6114750333 \ O,0,-2.409744811,0.0000014916,7.9361383602 \ O,0,-
2.8825482514,-0.0000013565,0.3177586676 \ O,0,-4.8356526748,-0.0000011101,1.9050790205 \
O,0,3.6506855933,0.0000014691,1.9941601731 \ O,0,3.6440242316,0.0000019212,-0.70163837 \ H,0,-
0.7272245637,0.0000013718,5.9856429842 \ H,0,-4.9256400192,0.0000006048,7.0976641431 \ H,0,-
3.877221399,-0.0000021942,0.3780523708 \ H,0,-0.8985687831,0.000000008,-0.6199873198 \
H,0,1.2774582778,0.0000009009,-1.818533644 \ H,0,1.1982949888,0.0000005216,3.1395713838 \
H,0,4.3554337958,0.0000030868,-0.0438989302 \ H,0,3.5341843734,0.0000056663,2.9526197113
```

Thermal correction to Enthalpy= 0.220461

Thermal correction to Gibbs Free Energy= 0.153307

Lowest freq: 22.5841 cm⁻¹

B3LYP TD(nstates=10) /6-311+g(d,p)

HF=-1103.3224478

Excitation energies and oscillator strengths:

Excited State	1:	?Spin	-A	0.2193 eV	5653.23 nm	f=0.0052
Excited State	2:	?Spin	-A	0.6815 eV	1819.40 nm	f=0.0000
Excited State	3:	?Spin	-A	1.1835 eV	1047.60 nm	f=0.0000

Excited State	4:	?Spin -A	1.8129 eV	683.92 nm	f=0.0357
Excited State	5:	?Spin -A	2.1115 eV	587.19 nm	f=0.0044
Excited State	6:	?Spin -A	2.5662 eV	483.15 nm	f=0.0089
Excited State	7:	?Spin -A	2.6220 eV	472.86 nm	f=0.0852
Excited State	8:	?Spin -A	2.6590 eV	466.27 nm	f=0.0000
Excited State	9:	?Spin -A	2.8097 eV	441.28 nm	f=0.1078
Excited State	10:	?Spin -A	2.9073 eV	426.46 nm	f=0.0000

B3LYP TD(nstates=10) /6-311+g(d,p) scrf=(pcm,solvent=water)

Total free energy in solution: with all non-electrostatic terms

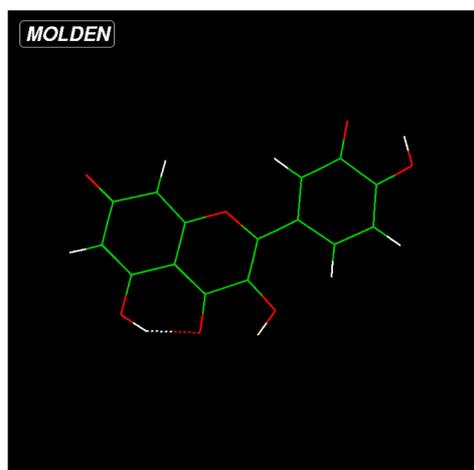
(a.u.) = -1103.412556

Excitation energies and oscillator strengths:

Excited State	1:	?Spin -A	0.4850 eV	2556.31 nm	f=0.0074
Excited State	2:	?Spin -A	1.1278 eV	1099.33 nm	f=0.0000
Excited State	3:	?Spin -A	1.3338 eV	929.54 nm	f=0.1212
Excited State	4:	?Spin -A	1.6334 eV	759.08 nm	f=0.0000
Excited State	5:	?Spin -A	2.0489 eV	605.12 nm	f=0.0008
Excited State	6:	?Spin -A	2.3325 eV	531.55 nm	f=0.0078
Excited State	7:	?Spin -A	2.6145 eV	474.23 nm	f=0.0328
Excited State	8:	?Spin -A	2.7707 eV	447.48 nm	f=0.0000
Excited State	9:	?Spin -A	2.8954 eV	428.21 nm	f=0.0097
Excited State	10:	?Spin -A	3.0732 eV	403.43 nm	f=0.0080

Appendix A21. Quercetin radical anion 3'-OH to 7-OH

B3LYP/6-31+g(d,p) gas phase



Coordinates:

```
C,0,0.00676412,0.,-0.0395134414 \ C,0,0.019059818,0.,1.3958684442
 \ C,0,1.2414033872,0.,2.0758843845 \ C,0,2.4755751401,0.,1.3688878847 \ C,0,2.4032741152,0.,-
0.0938885621 \ C,0,1.1889485446,0.,-0.7723633914 \ C,0,-1.2353622022,0.,2.1384113738 \ O,0,-
1.046590892,0.,3.4971393508 \ C,0,-2.0851427001,0.,4.403879016 \ C,0,-
3.4319517079,0.,3.9310674699 \ C,0,-3.6822798828,0.,2.5464973732 \ C,0,-
2.5251042034,0.,1.656685413 \ C,0,-4.4904276717,0.,4.9133374473 \ C,0,-4.202276383,0.,6.2517198169 \
C,0,-2.8292570615,0.,6.740630086 \ C,0,-1.771549897,0.,5.7371178709 \ O,0,-
5.7770571391,0.,4.47347475 \ O,0,-2.5647605341,0.,7.9683990721 \ O,0,-2.8670690699,0.,0.3453143226 \
O,0,-4.8345538287,0.,1.9860936469 \ O,0,3.6448128067,0.,1.8706567792 \ O,0,3.5921553022,0.,-
0.7123529864 \ H,0,-0.7400436514,0.,6.0700654955 \ H,0,-5.0024278666,0.,6.9840628478 \ H,0,-
3.8554871352,0.,0.3887553077 \ H,0,-5.7507694691,0.,3.4848984321 \ H,0,-0.9398985437,0.,-
0.5602302402 \ H,0,1.1726451999,0.,-1.8580158882 \ H,0,1.274344384,0.,3.1575741259 \
H,0,4.2257890167,0.,0.0508484937
```

Thermal correction to Enthalpy= 0.218604

Thermal correction to Gibbs Free Energy= 0.153584

Lowest freq: 19.4202 cm⁻¹

B3LYP TD(nstates=10) /6-311+g(d,p)

HF=-1103.3649958

Excitation energies and oscillator strengths:

Excited State	1:	?Spin -A'	0.7111 eV	1743.44 nm	f=0.1070
Excited State	2:	?Spin -A''	1.2168 eV	1018.92 nm	f=0.0000
Excited State	3:	?Spin -A'	1.2227 eV	1013.98 nm	f=0.0039
Excited State	4:	?Spin -A'	1.6339 eV	758.81 nm	f=0.0180
Excited State	5:	?Spin -A''	1.9005 eV	652.37 nm	f=0.0000

Excited State	6:	?Spin -A'	2.2346 eV	554.83 nm	f=0.0160
Excited State	7:	?Spin -A'	2.5002 eV	495.89 nm	f=0.0021
Excited State	8:	?Spin -A'	2.6796 eV	462.70 nm	f=0.1789
Excited State	9:	?Spin -A'	2.8681 eV	432.28 nm	f=0.0559
Excited State	10:	?Spin -A''	2.9952 eV	413.94 nm	f=0.0000

B3LYP TD(nstates=10) /6-311+g(d,p) scrf=(pcm,solvent=water)

Total free energy in solution: with all non-electrostatic terms

(a.u.) = -1103.428206

Excitation energies and oscillator strengths:

Excited State	1:	?Spin -A'	0.8415 eV	1473.29 nm	f=0.0945
Excited State	2:	?Spin -A'	1.4793 eV	838.14 nm	f=0.0160
Excited State	3:	?Spin -A'	1.6750 eV	740.21 nm	f=0.0111
Excited State	4:	?Spin -A''	2.0129 eV	615.96 nm	f=0.0000
Excited State	5:	?Spin -A''	2.0214 eV	613.35 nm	f=0.0000
Excited State	6:	?Spin -A'	2.3127 eV	536.10 nm	f=0.0417
Excited State	7:	?Spin -A'	2.4909 eV	497.75 nm	f=0.0411
Excited State	8:	?Spin -A'	2.8365 eV	437.11 nm	f=0.1928
Excited State	9:	?Spin -A'	2.9580 eV	419.15 nm	f=0.1178
Excited State	10:	?Spin -A''	3.1384 eV	395.06 nm	f=0.0000