Conformational preference of flavonols and its effect on the chemical properties involved in radical scavenging activity

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Table S1. The Gibbs energies and dihedral angles of C3-C2-C1'-C2' after the geometry optimization using DFT in gas phase for each conformer. Values of G^o and $\omega_{C3\text{-}C2\text{-}C1'\text{-}C2}$ are shown in a.u. and degree, respectively.

	Myricetin		Quercetin		Kaempferol	
Conf. index	G^o	$\omega_{C3\text{-}C2\text{-}C1'\text{-}C2}$	G^o	$\omega_{C3\text{-}C2\text{-}C1'\text{-}C2}$	G^o	$\omega_{C3\text{-}C2\text{-}C1'\text{-}C2}$
i	-1179.141206 [a]	0.1	-1103.918622	-3.8	-1028.694043	-10.9
ii	-1179.139359 [b]	11.1	-1103.917549 [d]	171.8	-1028.694246	9.4
iii	-1179.140819 [c]	0.0	-1103.916189	167.6	-1028.693322	13.2
iv	-1179.138633	-13.3	-1103.918066	4.9	-1028.693422	13.9
v	-1179.141212 [a]	0.0	-1103.916343	168.1	-1028.681395	42.5
vi	-1179.139347 [b]	-10.9	-1103.917595 [d]	-172.0	-1028.681421	-41.3
vii	-1179.140809 [c]	0.0	-1103.919201	-1.2	-1028.680530	43.3
viii	-1179.139347 [b]	-10.9	-1103.904703	139.6	-1028.677158	9.3
ix	-1179.133063	13.9	-1103.904691	41.7	-1028.676955	8.5
x	-1179.127419	-41.2	-1103.911769	0.5	-1028.677241	-5.1
xi	-1179.127093	40.6	-1103.904202	138.3	-1028.676329	5.0
xii	-1179.126584	40.8	-1103.910301	170.0	-1028.676153	0.0
xiii	-1179.124135	0.0	-1103.902388	-0.1	-1028.691212	0.0
xiv	-1179.135137	-0.1	-1103.909479	167.7	-1028.679585	0.0
xv	-1179.135372	-0.1	-1103.901001	0.0	-	-
xvi	-1179.123018	0.1	-1103.899990	170.0	-	-
xvii	-1179.131112	0.0	-1103.897821	179.5	-	-
xviii	-1179.122280	-11.2	-1103.900187	180.0	-	-
xix	-1179.121734	-8.1	-1103.914025	180.0	-	-
xx	-1179.120947	40.7	-1103.901657	0.0	-	-
xxi	-1179.124134	-0.1	-1103.889105	180.0	-	-
xxii	-1179.117371	-10.3	-1103.890822	180.0	-	-
xxiii	-1179.116014	-9.5	-1103.897452	180.0	-	-
xxiv	-1179.119621	0.0	-	-	-	-
xxv	-1179.108097	0.0	-	-	-	-

[a] The optimized structures were identical to each other. [b] The optimized structures were identical to each other. [c] The optimized structures were identical to each other. [d] The optimized structures were identical to each other.

Table S2. The Gibbs energies and dihedral angles of C3-C2-C1'-C2' after the geometry optimization using DFT in water solvent for each conformer. Values of G^o and $\omega_{C3\text{-}C2\text{-}C1'\text{-}C2}$ are shown in a.u. and degree, respectively.

	Myricetin		Quercetin		Kaempferol	
Conf. index	G^o	$\omega_{C3\text{-}C2\text{-}C1'\text{-}C2}$	G^o	$\omega_{C3\text{-}C2\text{-}C1'\text{-}C2}$	G^o	$\omega_{C3\text{-}C2\text{-}C1'\text{-}C2}$
i	-1179.175764	27.0	-1103.950163	-27.8	-1028.722257	-29.5
ii	-1179.175238	26.6	-1103.948744 [a]	153.5	-1028.722241	31.0
iii	-1179.176521	27.0	-1103.948951	151.5	-1028.721852	29.9
iv	-1179.175851	-25.4	-1103.949448	26.6	-1028.721931	30.6
v	-1179.171763	27.9	-1103.948907	152.8	-1028.718234	43.5
vi	-1179.172057	28.9	-1103.948729 [a]	153.5	-1028.718523	-42.4
vii	-1179.172056	-28.3	-1103.942633	28.2	-1028.718073	43.1
viii	-1179.168647	28.9	-1103.945780	137.9	-1028.713509	28.1
ix	-1179.168687	28.8	-1103.944940	43.2	-1028.713593	29.6
x	-1179.172109	-43.0	-1103.947884	27.4	-1028.713567	-28.3
xi	-1179.171116	42.2	-1103.946045	137.7	-1028.713628	29.8
xii	-1179.171544	42.3	-1103.947952	153.0	-1028.713046	0.0
xiii	-1179.170092	-26.1	-1103.939833	24.7	-1028.721474	0.0
xiv	-1179.174676	25.7	-1103.948073	152.3	-1028.713322	0.0
xv	-1179.170875	-26.1	-1103.939815	25.6	-1028.713172	0.0
xvi	-1179.169735	26.1	-1103.939927	152.7	-	-
xvii	-1179.175505	25.4	-1103.940001	153.3	-	-
xviii	-1179.169511	-25.1	-1103.939831	180.0	-	-
xix	-1179.169049	-25.7	-1103.945667	180.0	-	-
xx	-1179.170523	43.9	-1103.939787	0.0	-	-
xxi	-1179.166739	-27.1	-1103.935442	180.0	-	-
xxii	-1179.163008	-28.0	-1103.939073	180.0	-	-
xxiii	-1179.166033	-28.2	-1103.939846	180.0	-	-
xxiv	-1179.165956	0.0	-	-	-	-
xxv	-1179.161311	0.0	-	-	-	-

[a] The optimized structures were identical to each other.

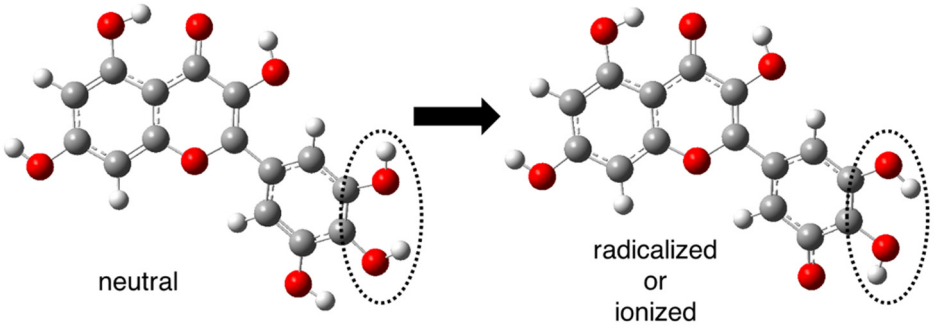

Figure S1. Change of orientation of hydrogen atoms upon radicalization or ionization as exemplified by the first conformer of myricetin.

Table S3. Dihedral angles of C3-C2-C1'-C2' of the neutral molecule and radical cation after the geometry optimization in water solvent. Values of $\omega_{C3\text{-}C2\text{-}C1'\text{-}C2}$ are shown in degree.

Conf. index	Myricetin		Quercetin		Kaempferol	
	Neutral	Radical cation	Neutral	Radical cation	Neutral	Radical cation
w-1	27.0	7.0	-27.9	-7.9	-29.4	-7.2
w-2	-25.4	-13.7	26.5	2.1	31.0	10.0
w-3	27.0	8.1	151.4	167.8	30.7	10.2
w-4	25.4	6.3	152.9	166.4	29.8	11.6
w-5	26.6	14.3	153.4	166.9	-	-
w-6	25.7	6.5	152.3	167.2	-	-
w-7	-	-	153.0	167.6	-	-
w-8	-	-	27.4	9.2	-	-