SUPPLEMENTARY INFORMATION

Quercetin and its analogues: Optical and acido-basic properties

Michal Biler[a,b,#,*], David Biedermann[c], Kateřina Valentová[c], Vladimír Křen[c], Martin Kubala[a,*]

[a] *Department of Biophysics, Centre of the Region Haná for Biotechnological and Agricultural Research, Palacký University, Šlechtitelů 27, 783 71, Olomouc, Czech Republic*

[b] *INSERM UMR-S850, Univ. Limoges, School of Pharmacy, University de Limoges, 2 rue du Dr. Marcland, 87 025 Limoges, France*

[c] *Institute of Microbiology, Laboratory of Biotransformation, Czech Academy of Sciences, Vídeňská 1083, Prague, 142 20, Czech Republic*

[#] *Present address: Division of Theoretical Chemistry and Biology, Royal Institute of Technology. Roslagstullsbacken 15, S-106 91 Stockholm, Sweden*

*Correspondence: martin.kubala@upol.cz, michal.biler@seznam.cz

Figures

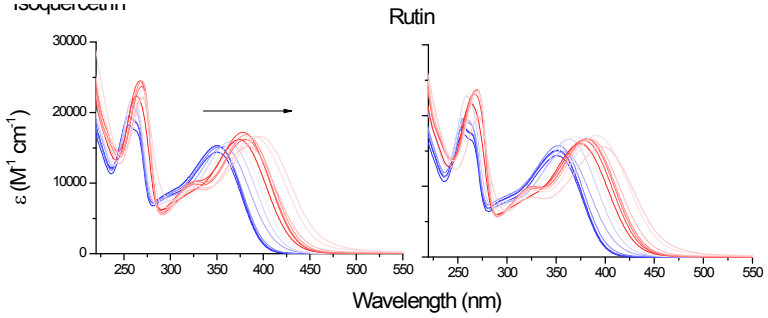

Figure S1– pH dependence of absorption spectra of isoquercitrin and rutin. Spectra are colored in rainbow colors (blue → light blue → red → light red) for pH 1.9, 2.9, 4.0, 5.0, 5.9, 6.4, 6.9, 7.4, 8.1, 9.1, 10.0, 10.5, 11.1, 11.9.

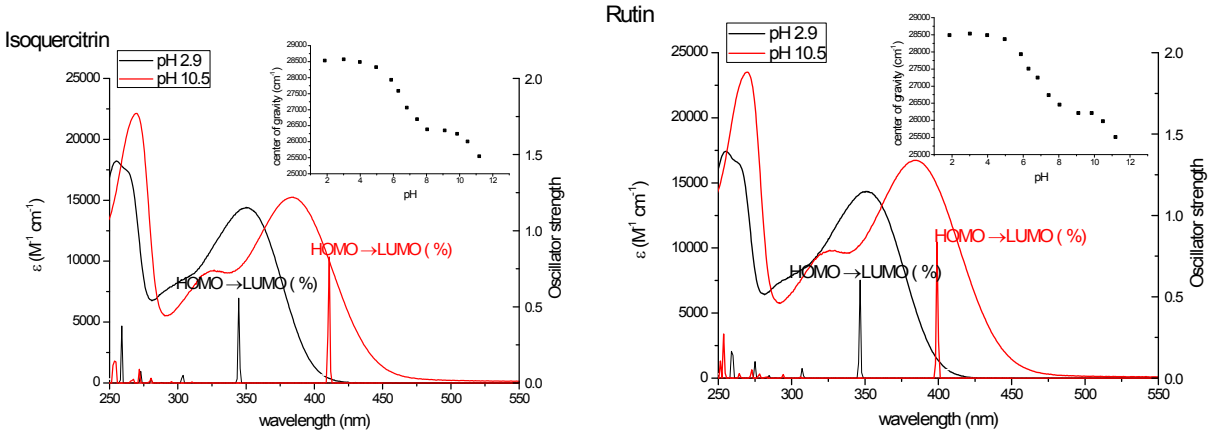

Figure S2– Superimposed theoretical and experimental spectra of isoquercitrin and rutin. Insets: Shift of center of gravity *vs.* pH.

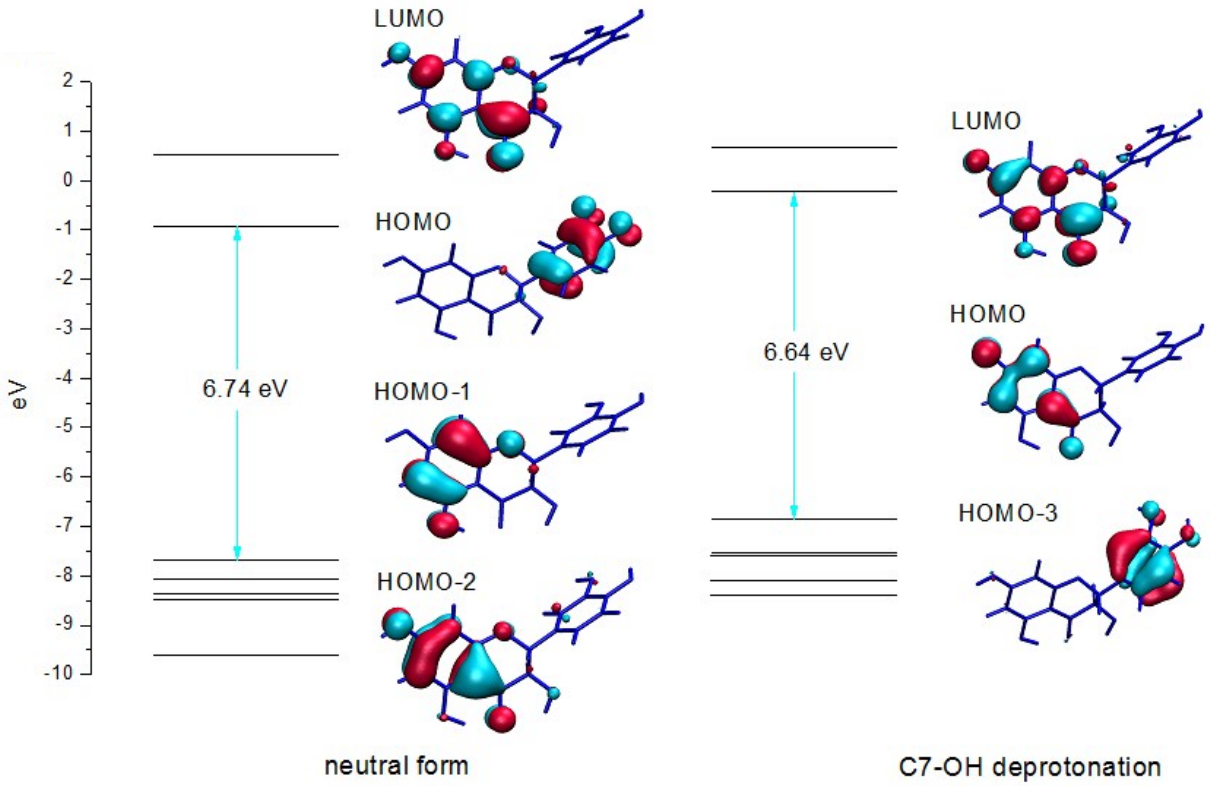

Figure S3 – MO diagram of the neutral and deprotonated form of taxifolin.

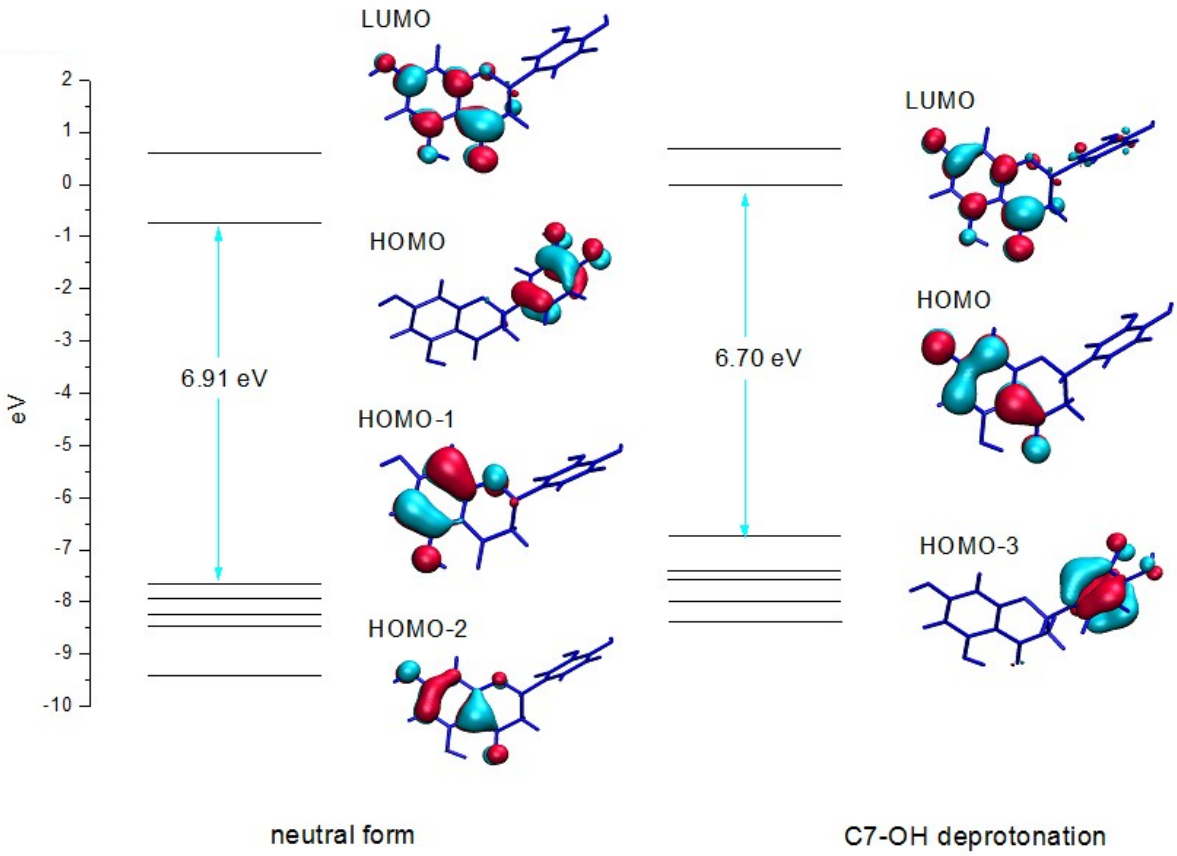

Figure S4 – MO diagram of the neutral and deprotonated form of eriodictyol.

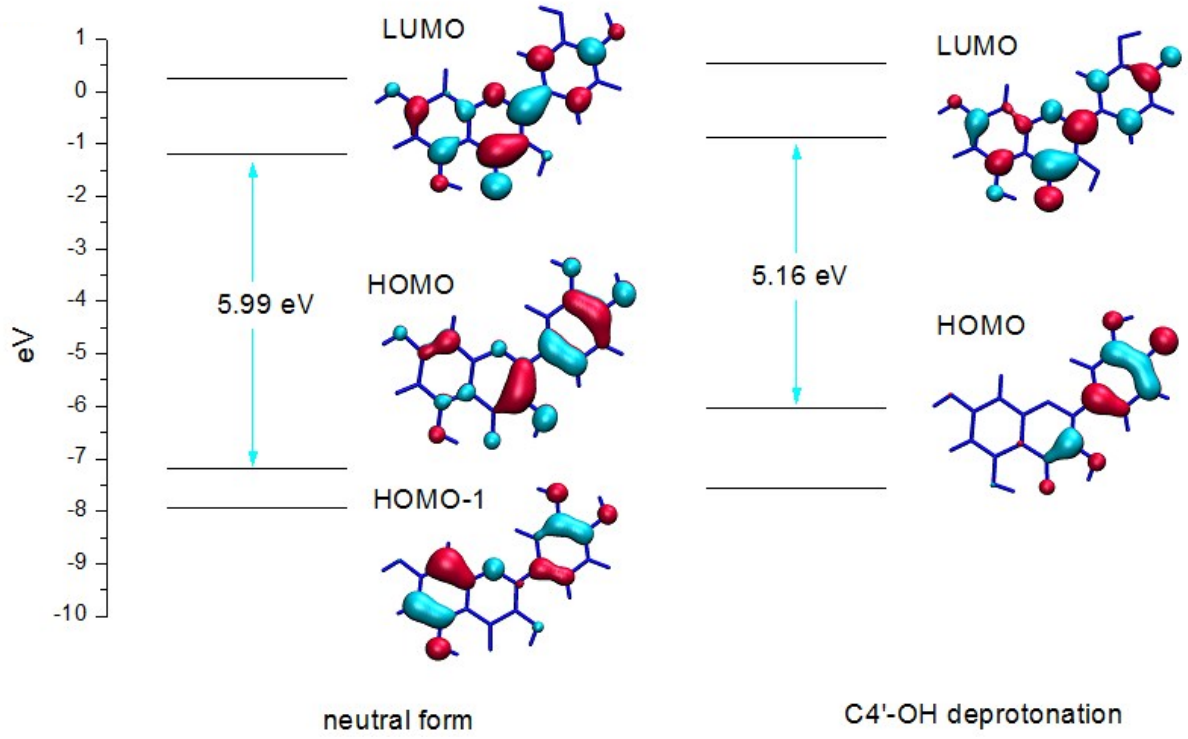

Figure S5 – MO diagram of the neutral and deprotonated form of quercetin.

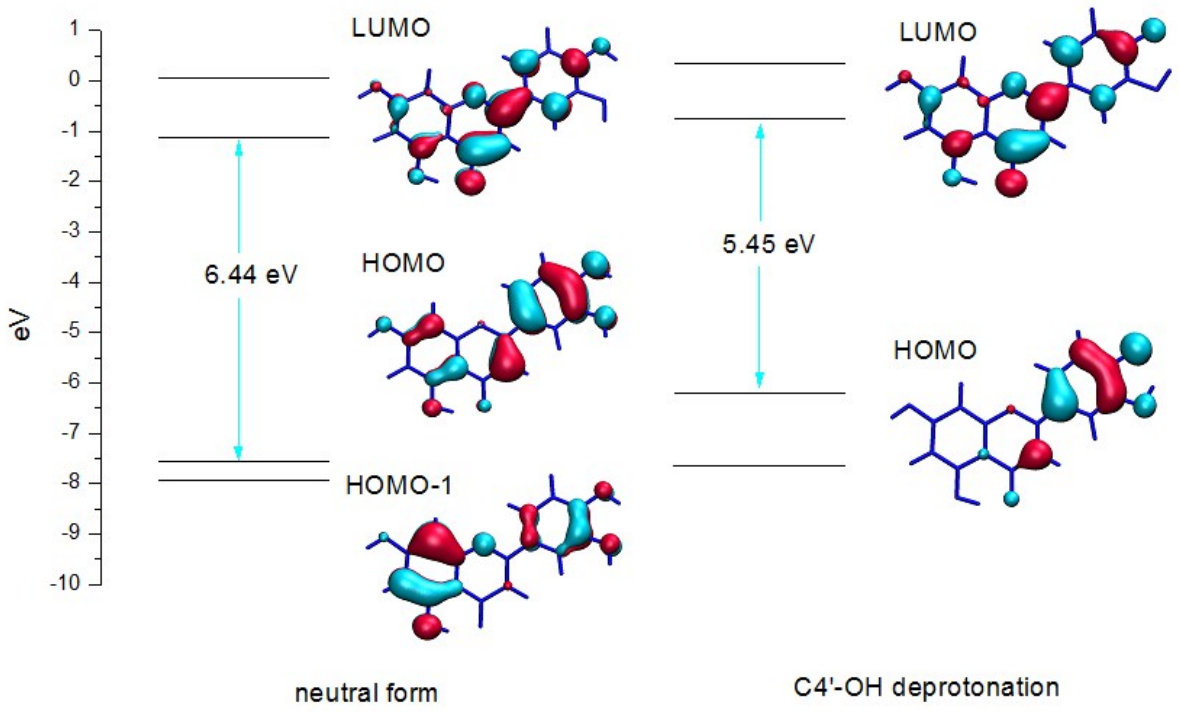

Figure S6 – MO diagram of the neutral and deprotonated form of luteolin.

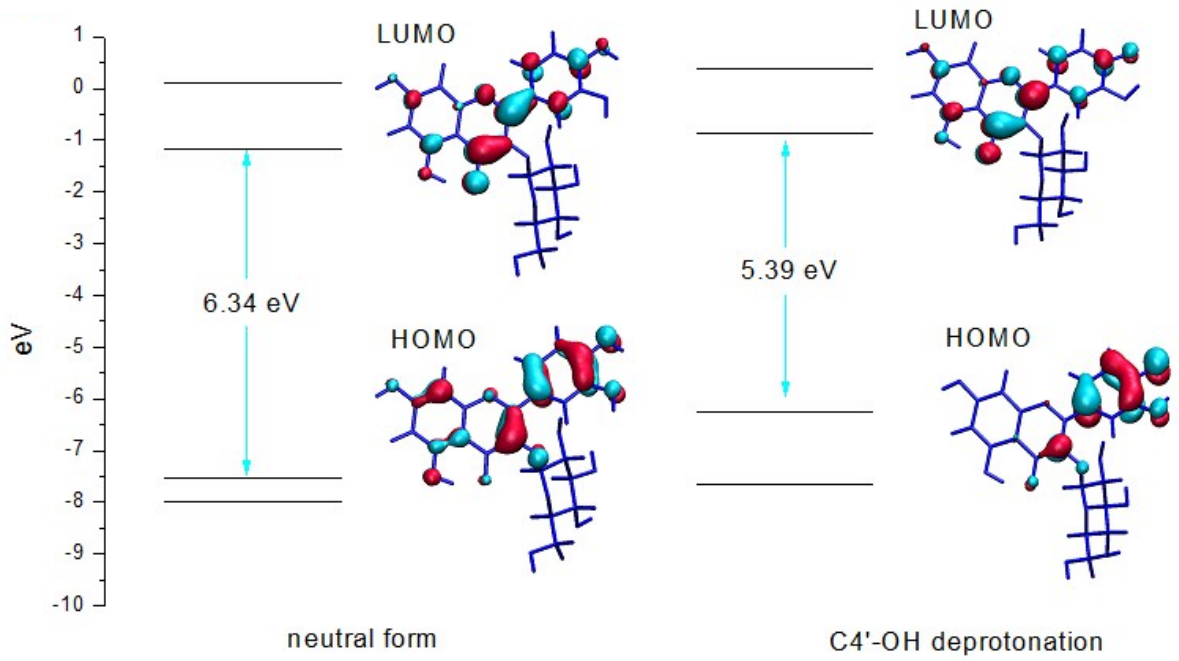

Figure S7 – MO diagram of the neutral and deprotonated form of isoquercitrin.

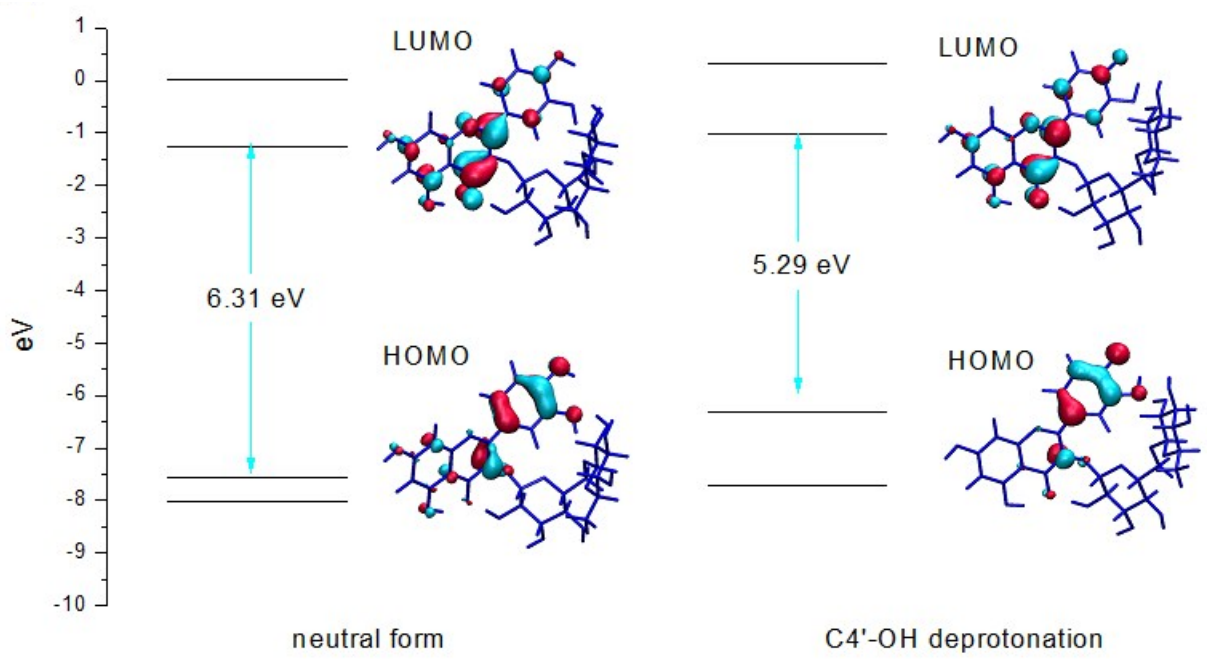

Figure S8 – MO diagram of the neutral and deprotonated form of rutin.