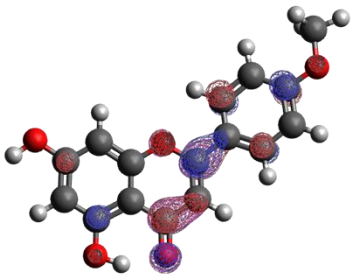
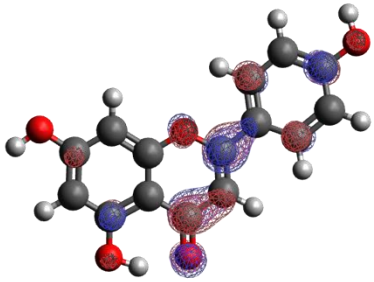
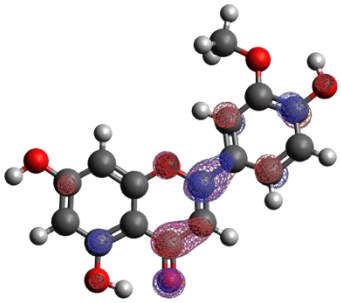
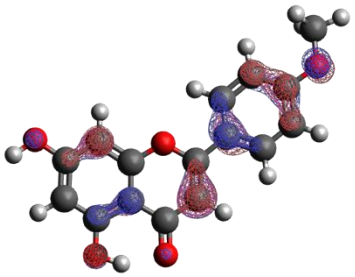
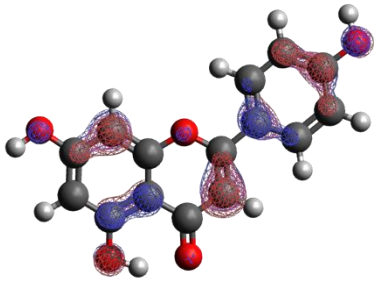
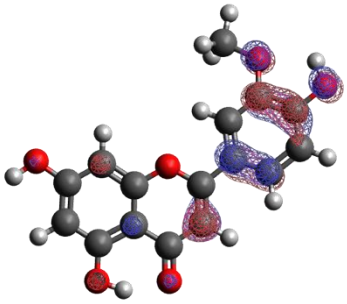
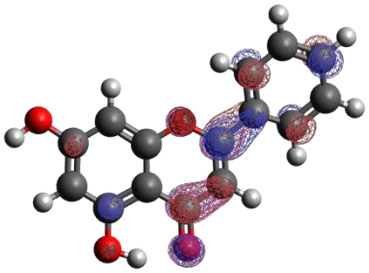
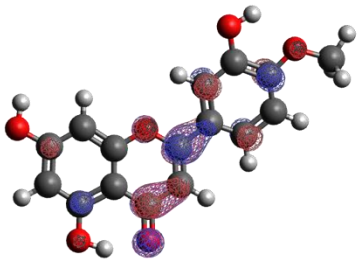
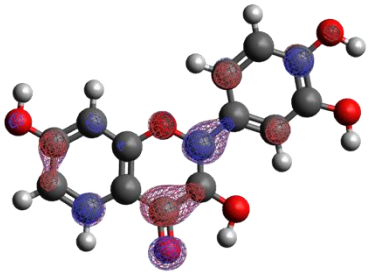
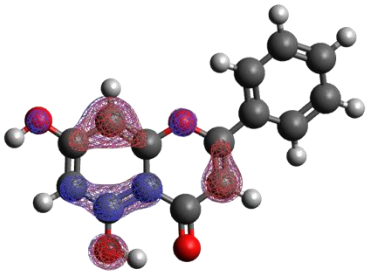
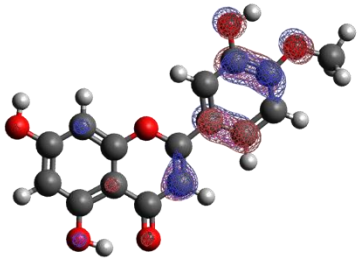
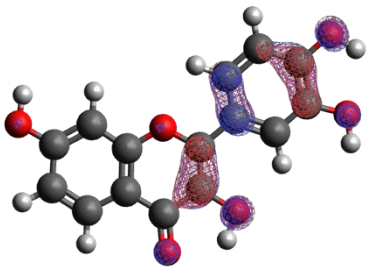
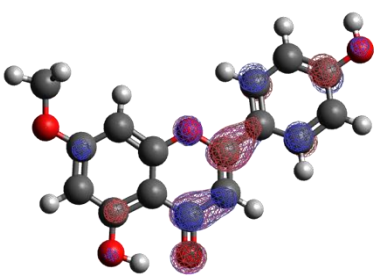
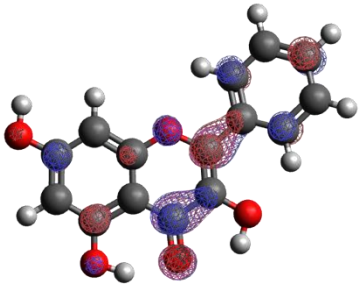
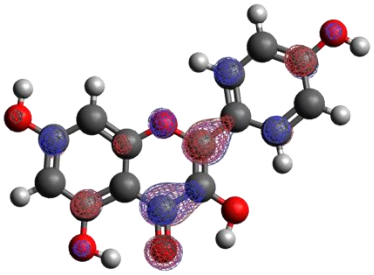
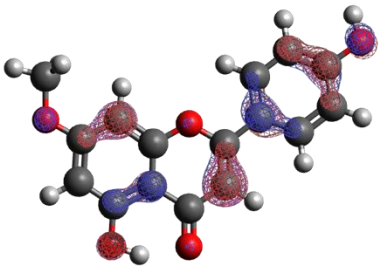
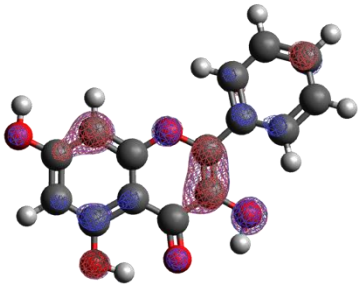
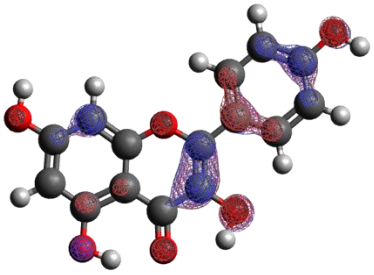
antioxidants

MDPI

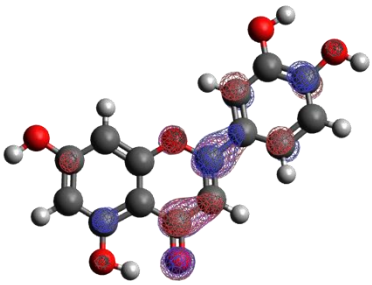
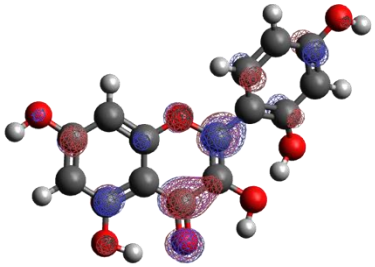
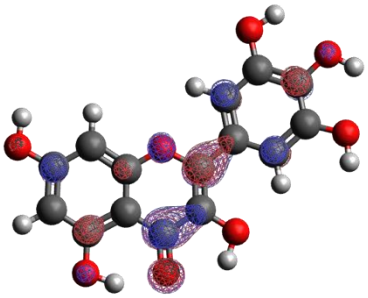
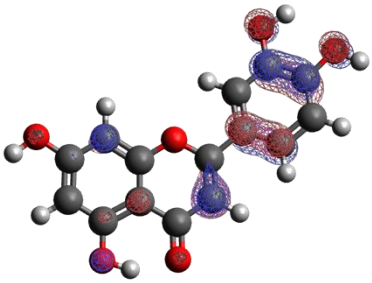
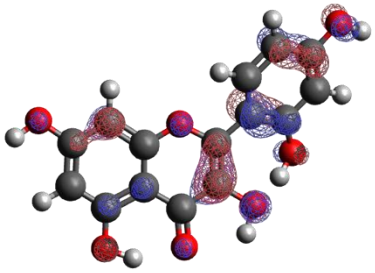
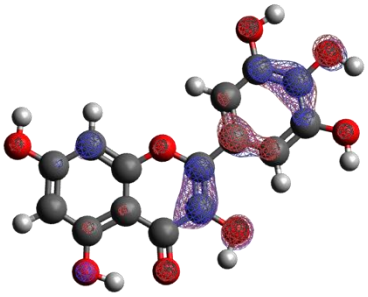
Supplementary Materials

Figures

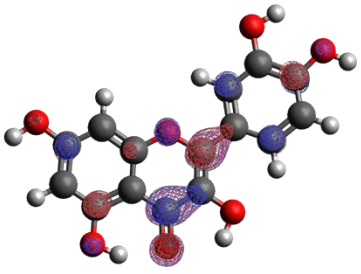
Acacetin	Apigenin	Chrysoeriol
		
		
Chrysine	**Diosmetin**	**Fisetin**
		
		
Genkwanin	**Galangin**	**Kaempferol**

Luteolin **Morin** **Myricetin**

Quercetin



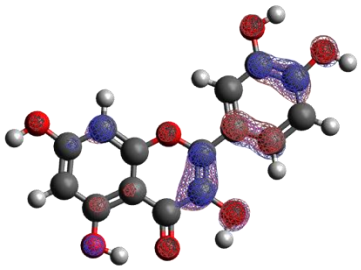


Figure 1. HOMOs (lower) and LUMOs (upper) visualization with isovalue 0.05

Acacetin C5	**Acacetin C7**	**Apigenin C4′**
Apigenin C5	**Apigenin C7**	**Chrysine C5**
Chrysine C7	**Chrysoeriol C4′**	**Chrysoeriol C5**
Chrysoeriol C7	**Diosmetin C3′**	**Disometin C5**
Diosmetin C7	**Fisetin C3**	**Fisetin C3′**
Fisetin C4′	**Fisetin C7**	**Genkwanin C4′**
Genkwanin C5′	**Galangin C3**	**Galangin C5**
Galangin C7	**Kaempferol C3**	**Kaempferol C4′**

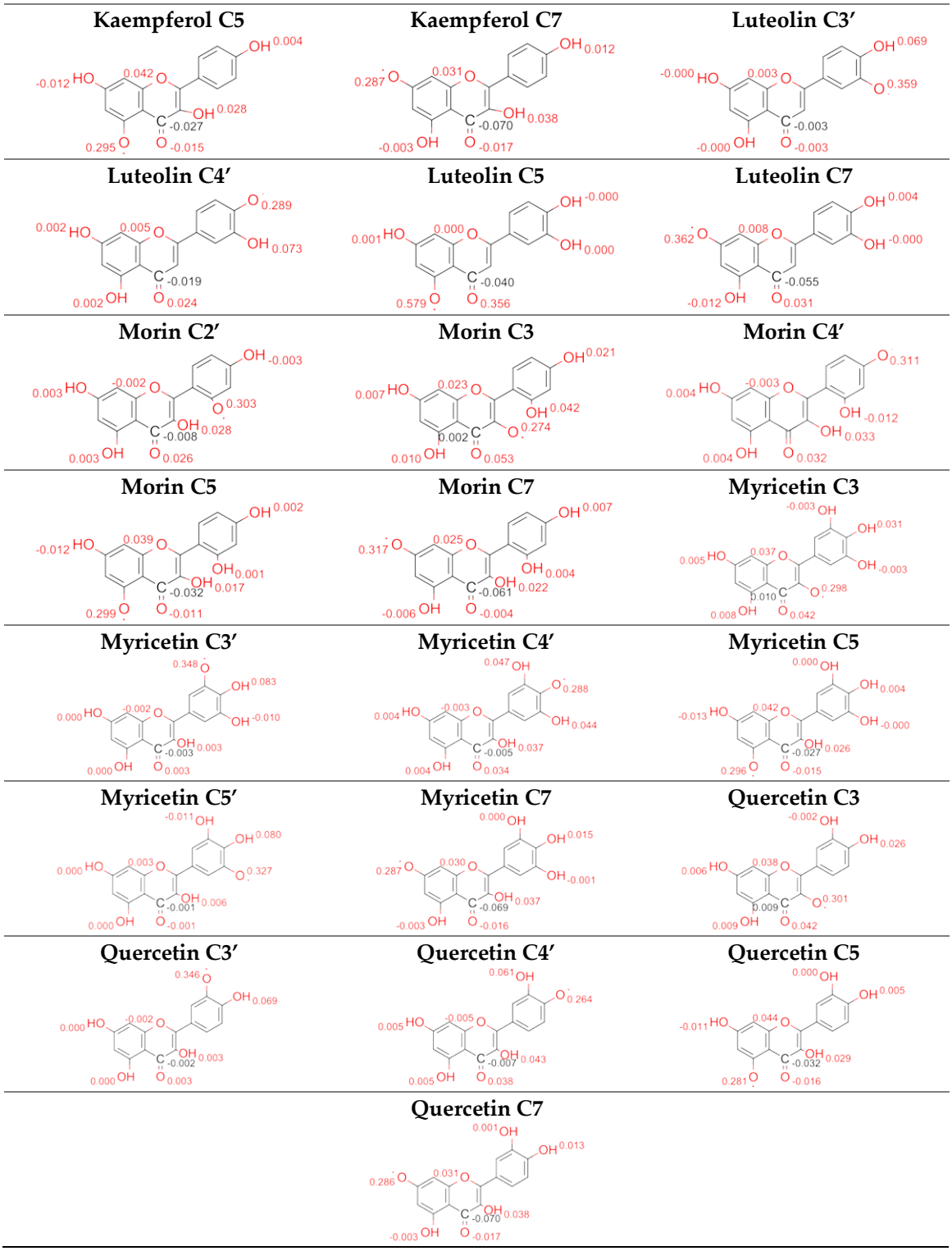


Figure 2. Radicals' Mulliken spin densities with hydrogen summed into heavy atoms

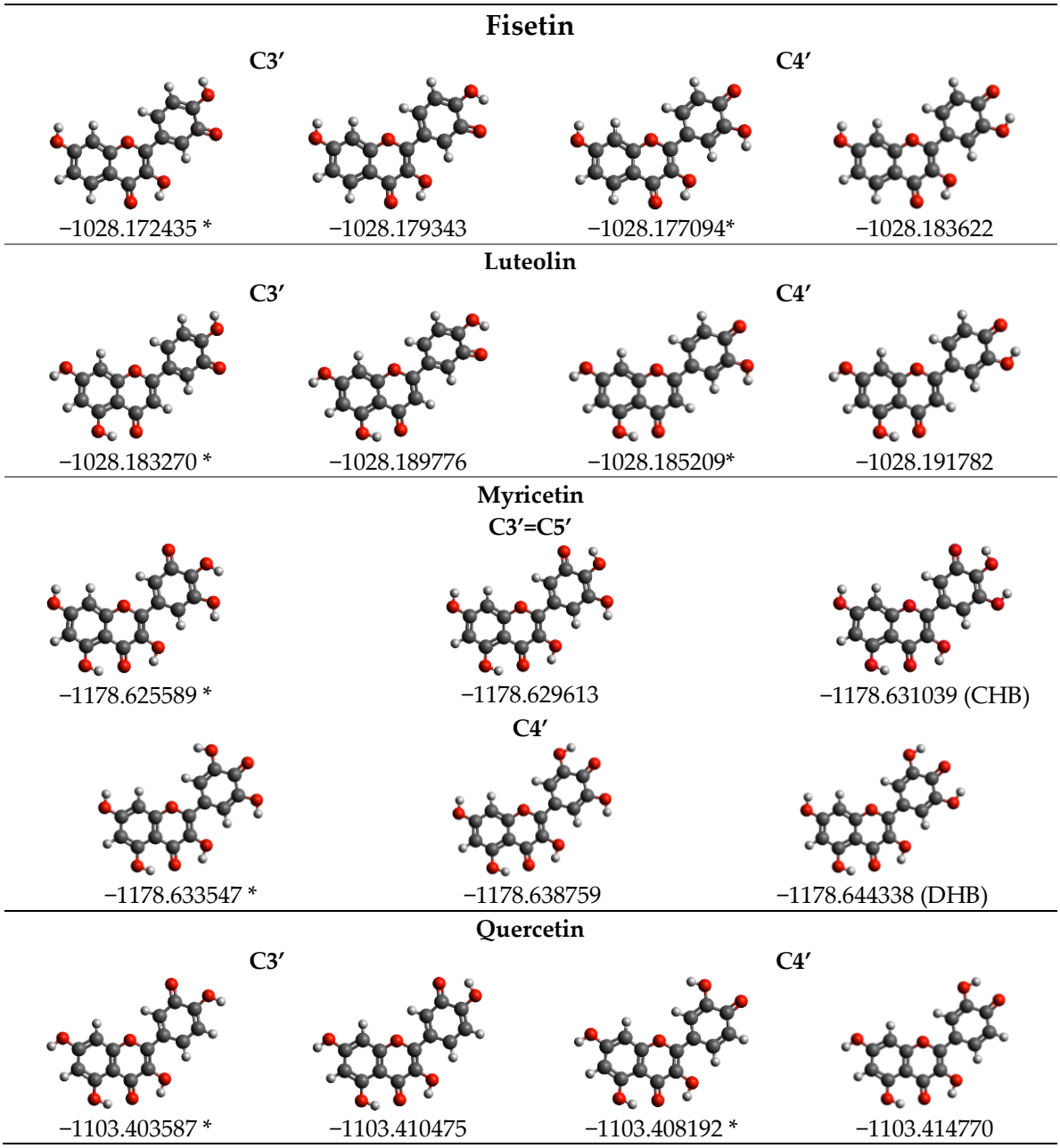
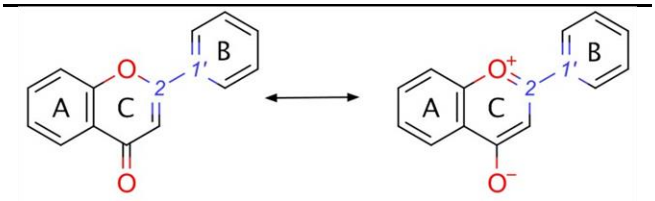


Figure 3. Enthalpies of flavonoids' radicals with and without hydrogen bond stabilization (isomer without H−bond is marked *) [a.u.]

Tables

Table 1. Enthalpies of the flavonoids' lowest energetic isomer at B3LYP/6−31+G(d,p) level of theory [a.u.]



	Flavonoid	Enthalpy
Flavones	Acacetin	−992.861147
	Apigenin	−953.589415
	Chrysin	−878.363148
	Chrysoeriol	−1068.084598
	Diosmetin	−1068.084312
	Genkwanin	−992.861115
	Luteolin	−1028.811831
Flavonols	Fisetin	−1028.799467
	Galangin	−953.582425
	Kaempferol	−1028.808400
	Morin	−1104.033327
	Myricetin	−1179.253341
	Quercetin	−1104.030864

Table 2. Enthalpies of unrelaxed and relaxed radicals of investigated compounds [a.u.]

	Flavonoids		Unrelaxed radical	Relaxed radical
Flavones	Acacetin	C5	−992,199222	−992,213026
		C7	−992,216822	−992,224983
	Apigenin	C4′	−952,947947	−952,958621
		C5	−952,930000	−952,941269
		C7	−952,944139	−952,952039
	Chrysin	C5	−877,701313	−877,715043
		C7	−877,716141	−877,725026
	Chrysoeriol	C4′	−1067,446832	−1067,459122
		C5	−1067,415336	−1067,419226
		C7	−1067,439373	−1067,447632
	Diosmetin	C3′	−1067,445198	−1067,456637
		C5	−1067,414907	−1067,418746
		C7	−1067,438585	−1067,447177
	Genkwanin	C4′	−992,220493	−992,230596
		C5	−992,199106	−992,212595
	Luteolin	C3′	−1028,172077	−1028,183270
		C4′	−1028,178156	−1028,191782
		C5	−1028,143630	−1028,146283
		C7	−1028,166412	−1028,174353
Flavonols	Fisetin	C3′	−1028,167323	−1028,179343
		C4′	−1028,164704	−1028,177094
		C3	−1028,162134	−1028,176690
		C7	−1028,156325	−1028,165763
	Galangin	C3	−952,944720	−952,958463

	C5	−952,926275	−952,939686
	C7	−952,937061	−952,946355
Kaempferol	C4′	−1028,171031	−1028,182027
	C3	−1028,173008	−1028,186897
	C5	−1028,152508	−1028,166096
	C7	−1028,165319	−1028,174020
Morin	C2′	−1103,385259	−1103,398629
	C4′	−1103,392680	−1103,402521
	C3	−1103,399249	−1103,419264
	C5	−1103,376267	−1103,390761
	C7	−1103,388420	−1103,396868
Myricetin	C3′	−1178,614708	−1178,625589
	C4′	−1178,625608	−1178,638759
	C5′	−1178,619670	−1178,631215
	C3	−1178,616992	−1178,631960
	C5	−1178,597496	−1178,611019
	C7	−1178,609123	−1178,618703
Quercetin	C3′	−1103,392412	−1103,403587
	C4′	−1103,401993	−1103,414770
	C3	−1103,395481	−1103,409514
	C5	−1103,375549	−1103,389360
	C7	−1103,387556	−1103,396441

Table 3. Radicals thermochemical values [a.u.]

Flavonoids	**Radical**	ε_0+H_{corr}	ε_0+G_{corr}
Luteolin	C3′	−1028.190	−1028.252
	TS	−1028.179	−1028.240
	C4′	−1028.192	−1028.255
Fisetin	C3′	−1028.179	−1028.243
	TS	−1028.170	−1028.232
	C4′	−1028.184	−1028.247
Myricetin	C3′=C5′	−1178.631	−1178.699
	TS	−1178.623	−1178.691
	C4′	−1178.643	−1178.711
Quercetin	C3′	−1103.410	−1103.477
	TS	−1103.401	−1103.466
	C4′	−1103.415	−1103.480

Table 4. Diradicals thermochemical values [a.u.] [ii].

Flavonoids		ε_0+H_{corr} [i]		ε_0+G_{corr}
Luteolin		−1027.514		−1027.574
		−1027.523	−1027.578 *(r)*	−1027.582
Fisetin		−1027.522		−1027.583
		−1027.545	−1027.570 *(r)*	−1027.604
Myricetin	*C3′–C4′*	−1177.982		−1178.046
		−1178.001	−1178.024 *(r)*	−1178.065
	C4′–C5′	−1177.993		−1178.057
		−1178.006	−1178.028 *(r)*	−1178.069
Quercetin		−1102.753		−1102.815
		−1102.776	−1102.801 *(r)*	−1102.839

[i] *(r)* marks for the relaxed forms of o−hydroquinone.

[ii] Underlined numbers stand for o−hydroquinone unrelaxed form.