Supplementary materials for:

The substituent effect on the radical scavenging activity of apigenin

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14 **Table S1.** The linear formulas related with the Hammett sigma constants and the BDE/IP/PA. In the

15 formulas, y represents the BDE/IP/PA, x represents the Hammett sigma constants

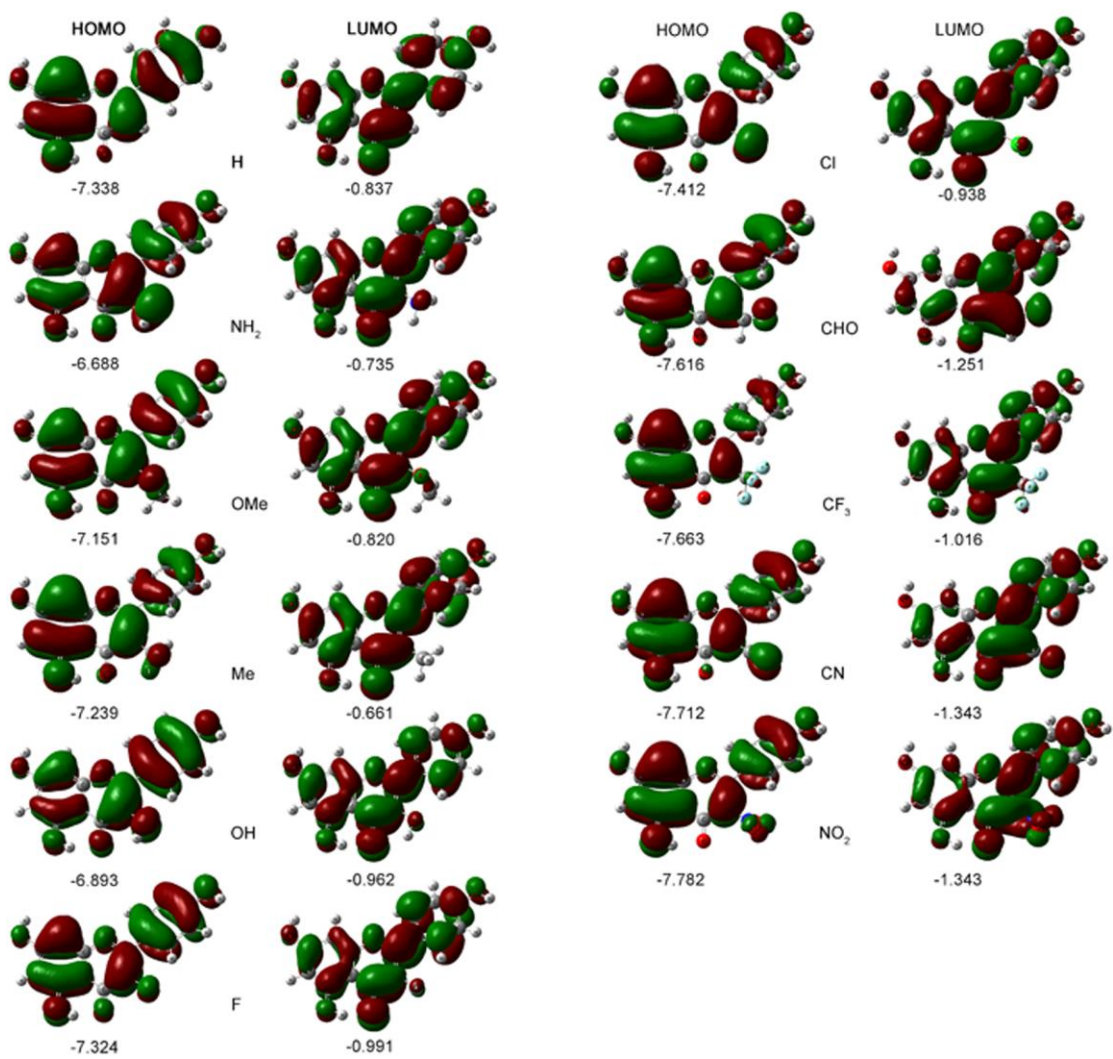|	gas	benzene	water
BDE(4′−OH) vs σ_P	y = 14.5x + 368.5	y = 15.7x + 372.0	y = 18.1x + 367.7
BDE(5−OH) vs σ_P	y = 7.4x + 431.0	y = 6.7x + 425.4	y = 8.1x + 391.0
BDE(7−OH) vs σ_m	y = 9.9x + 386.7	y = 13.2x + 390.1	y = 19.9x + 386.5
IP vs σ_P	y = 86.4x + 774.5	y = 84.3x + 666.6	y = 79.3x + 578.2
PA(4′−OH) vs σ_P	y = -30.0x + 1355.0	y = -21.4x + 400.4	y = -10.5x + 148.7
PA(5−OH) vs σ_m	y = -46.4x + 1446.1	y = -38.2x + 470.3	y = -19.0x + 162.4
PA(7−OH) vs σ_m	y = -46.9x + 1376.2	y = -37.9x + 411.7	y = -15.9x + 140.9

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Figure S1. The energies and distributions of HOMO and LUMO orbitals for the investigated compounds in the gas phase.

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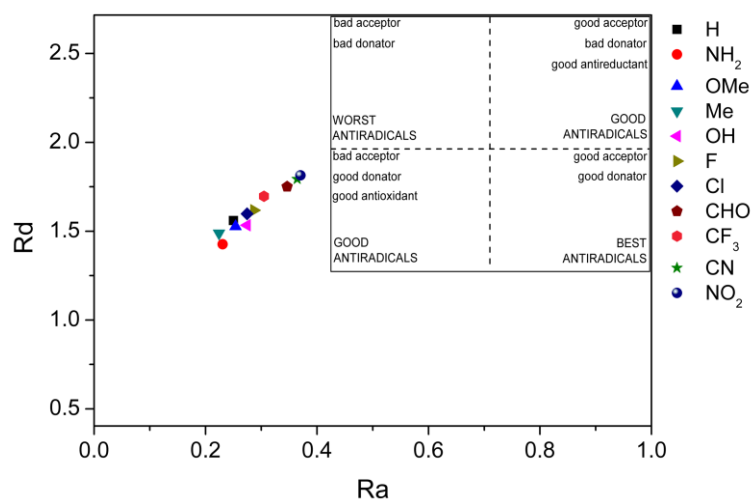
Figure S2. DAM for apigenin and its derivatives. The inset is definition of the four regions in DAM.

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