

**Table S1.** Relevant geometrical parameters of flavone and 7(OH)flavone in gas and solution phase calculated at B3LYP/6-311+G(2d,p) theoretical level. Interatomic distances,  $r$ , in Å; bond angles and dihedral angles,  $A$  and  $\omega$ , in degrees.

	Flavone		7(OH)Flavone				
	$r$ (C <sub>4</sub> =O)	$\omega$ (O <sub>1</sub> C <sub>2</sub> C <sub>1</sub> C <sub>2</sub> )	$r$ (C <sub>4</sub> =O)	$\omega$ (O <sub>1</sub> C <sub>2</sub> C <sub>1</sub> C <sub>2</sub> )	$r$ (C <sub>7</sub> -O)	$r$ (O-H)	$A$ (C <sub>7</sub> OH)
gas	1.226	20.9	1.228	21.7	1.363	0.964	109.8
Cy	1.231	21.4	1.233	22.1	1.360	0.970	110.5
<i>n</i> -Hp	1.231	21.5	1.232	22.2	1.360	0.970	110.5
CCl <sub>4</sub>	1.232	21.4	1.233	22.0	1.360	0.971	110.6
ACN	1.240	20.4	1.242	21.8	1.354	0.985	111.3
DMSO	1.240	20.8	1.242	22.1	1.354	0.985	111.3
CHCl <sub>3</sub>	1.236	21.3	1.238	22.2	1.357	0.977	111.0
EtOH	1.240	20.8	1.242	22.0	1.355	0.984	111.2
MeOH	1.240	20.7	1.242	21.6	1.355	0.985	111.2

**Figure S1.** Computer Visualization of the Molecular Orbitals Involved in the Electronic Transitions of Flavone in Different Solvents Calculated with the TD-B3LYP/6-311+G(2d,p) Method and the IEF-PCM Model.

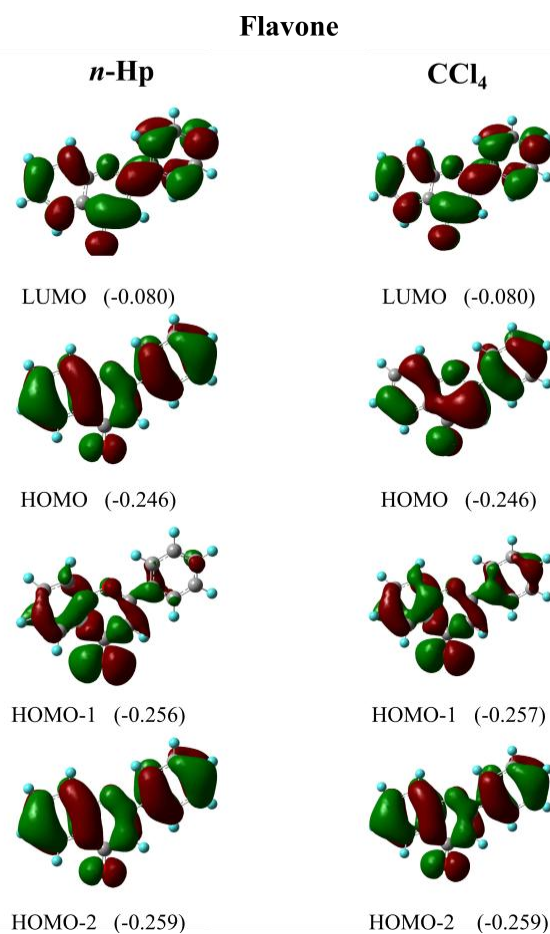
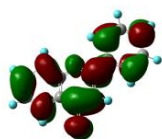
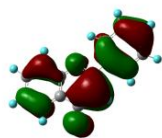


Figure S1. Cont.

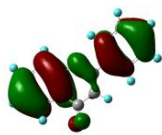
ACN



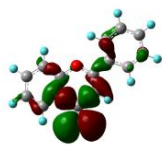
LUMO (-0.083)



HOMO (-0.248)

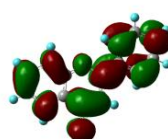


HOMO-1 (-0.257)

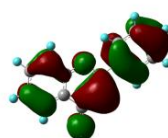


HOMO-2 (-0.266)

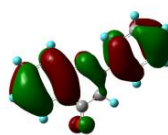
DMSO



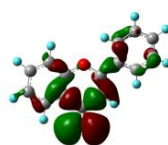
LUMO (-0.083)



HOMO (-0.248)

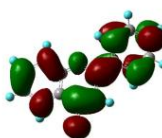


HOMO-1 (-0.257)

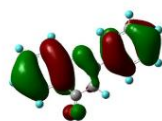


HOMO-2 (-0.266)

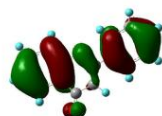
EtOH



LUMO (-0.082)



HOMO (-0.248)

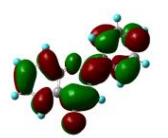


HOMO-1 (-0.257)

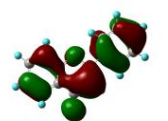


HOMO-2 (-0.266)

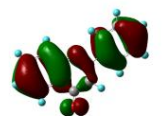
CHCl<sub>3</sub>



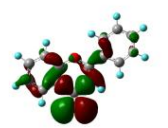
LUMO (-0.081)



HOMO (-0.247)

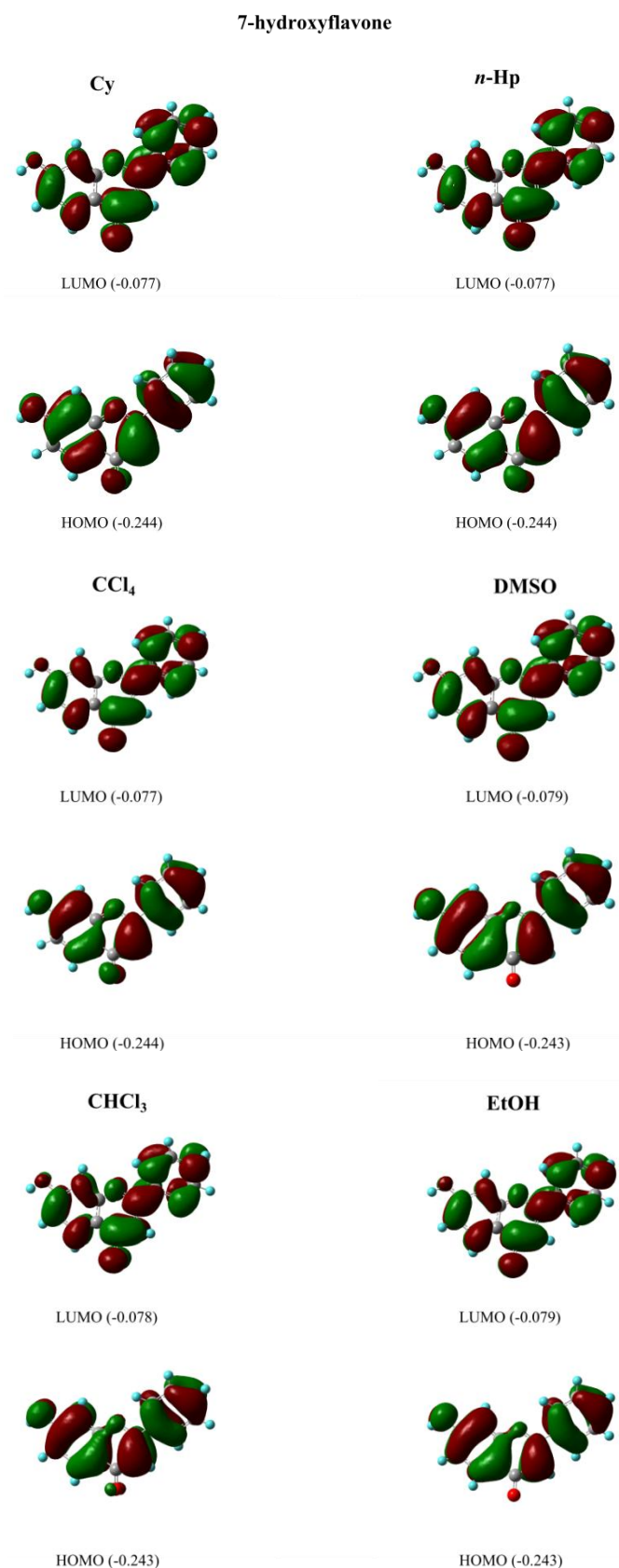


HOMO-1 (-0.258)



HOMO-2 (-0.262)

**Figure S2.** Computer Visualization of the Molecular Orbitals Involved in the Electronic Transitions of 7-hydroxyflavone in Different Solvents Calculated with the TD-B3LYP/6-311+G(2d,p) Method and the IEF-PCM Model.



**Figure S3.** Computer Visualization of the Molecular Orbitals Involved in the Electronic Transitions of Flavone in Different Solvents Calculated with the TD-PBE0/6-311+G(2d,2p) Method and the IEF-PCM Model.

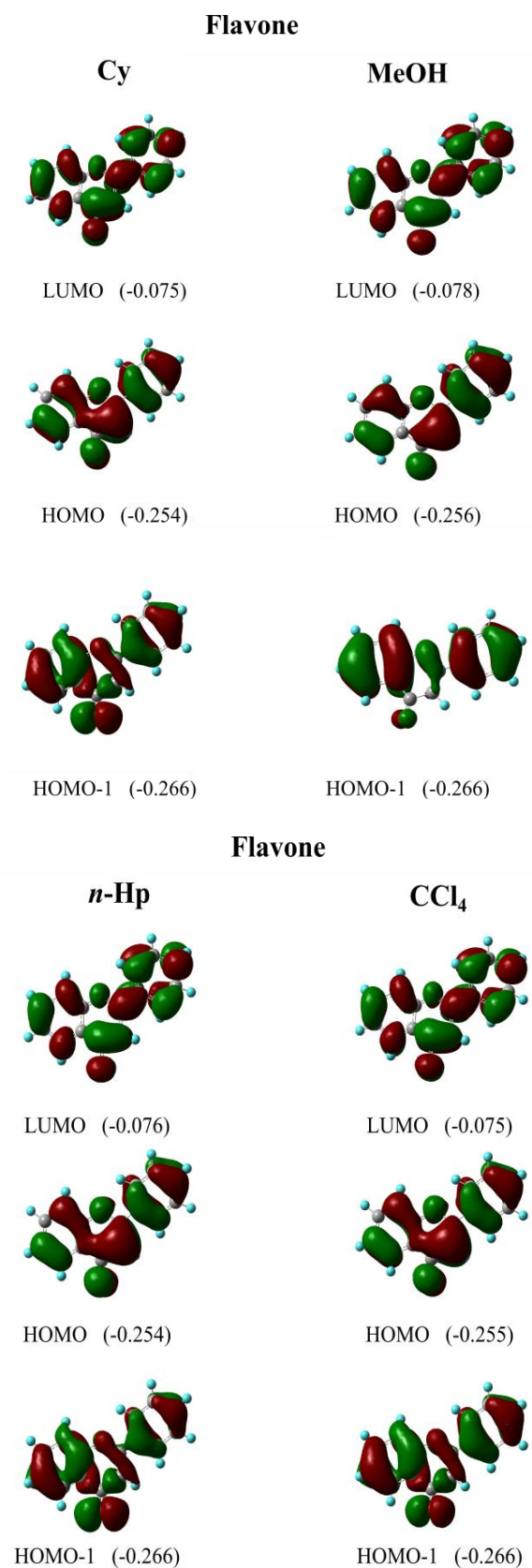
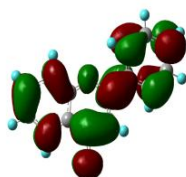
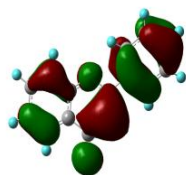


Figure S3. Cont.

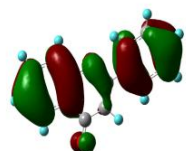
ACN



LUMO (-0.078)

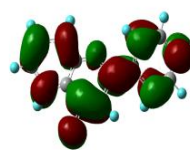


HOMO (-0.256)

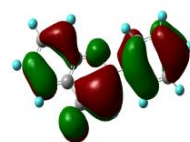


HOMO-1 (-0.266)

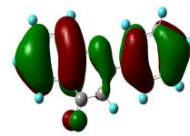
DMSO



LUMO (-0.078)

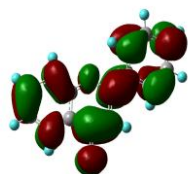


HOMO (-0.256)

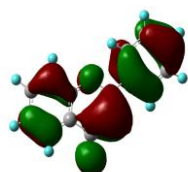


HOMO-1 (-0.266)

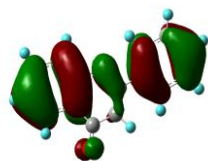
EtOH



LUMO (-0.078)

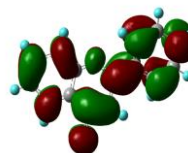


HOMO (-0.256)

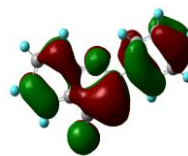


HOMO-1 (-0.266)

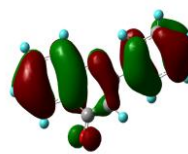
CHCl<sub>3</sub>



LUMO (-0.075)



HOMO (-0.255)



HOMO-1 (-0.266)

**Figure S4.** Computer Visualization of the Molecular Orbitals Involved in the Electronic Transitions of 7-hydroxyflavone in Different Solvents Calculated with the TD-PBE0/6-311+G(2d,2p) Method and the IEF-PCM Model.

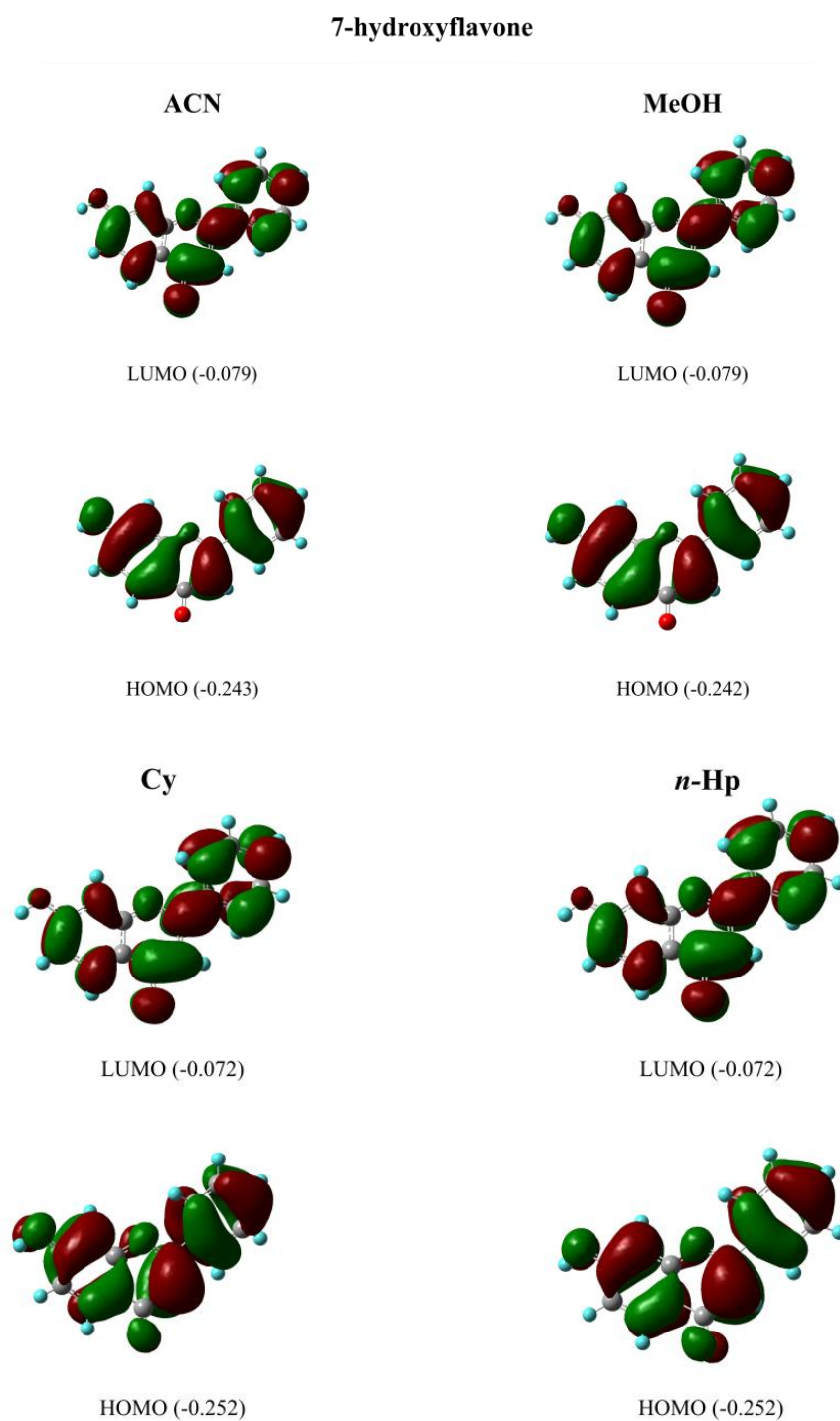
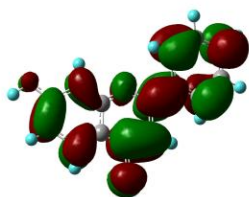


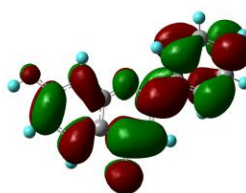
Figure S4. Cont.

**CCl<sub>4</sub>**

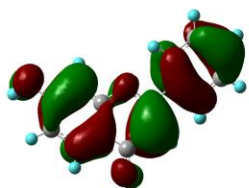


LUMO (-0.072)

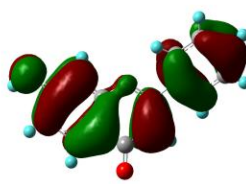
**DMSO**



LUMO (-0.075)

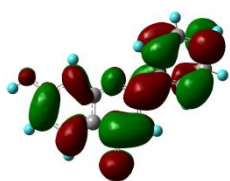


HOMO (-0.252)



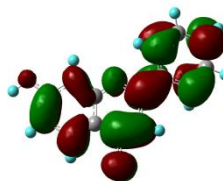
HOMO (-0.251)

**CHCl<sub>3</sub>**

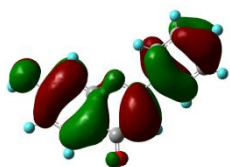


LUMO (-0.073)

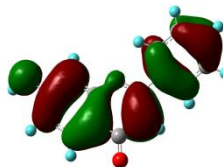
**EtOH**



LUMO (-0.074)



HOMO (-0.251)



HOMO (-0.251)