Supplementary Information

for

Excitation wavelength dependent fluorescence anisotropy of 3-Hydroxyflavone: Revisiting the solvation processes and high-energy state excitation in ESIPT-active compounds.

Dzmitryi Ushakou [a,b], Marek Józefowicz [a]

[a] *Institute of Experimental Physics, Faculty of Mathematics, Physics and Informatics, University of Gdańsk, str. Wita Stwosza 57, 80-308 Gdańsk, Poland*
[b] *Institute of Exact and Technical Sciences, Pomeranian University in Słupsk, str. Arciszewskiego 22d, 76-200 Słupsk, Poland*

Table of contents

The ground state S_0

The parameters and the ground state optimized structures are obtained at B3LYP/cc-pVTZ level of theory (based on DFT) and the IEFPCM solvation model. The red balls represent oxygen atoms, the grey balls represent carbon atoms, and the white balls represent hydrogen atoms in the depicted optimized geometries.

Table SI.1. The parameters of 3HF molecule (conformer 1 and 2) dissolved in methanol.

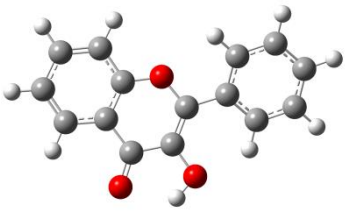
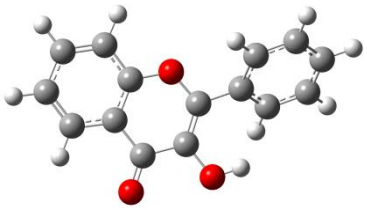
	Conformer 1 (the normal form)	**Conformer 2**
Total energy	-803.5872 hartrees; -21866.72 eV	-803.5778 hartrees; -21866.47 eV
Dipole moment	4.60 D	7.38 D
Structure		

Table SI.2. The parameters of 3HF-MeOH complex in methanol. The hydrogen binding occurs at the ESIPT site of 3HF.

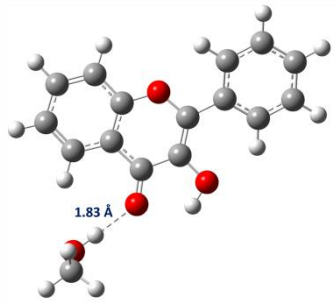
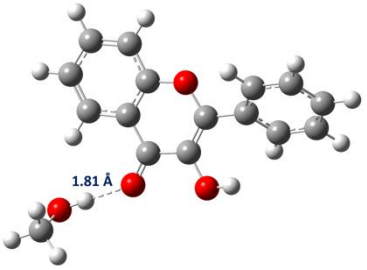
	Conformer 1 (the normal form)	**Conformer 2**
Total energy	-919.3727 hartrees; -25017.40 eV	-919.3637 hartees; -25017.16 eV
Dipole moment	6.28 D	9.76 D
Structure		

Table SI.3. The parameters of 3HF-MeOH complex in methanol. The hydrogen binding occurs at the non-ESIPT site of 3HF.

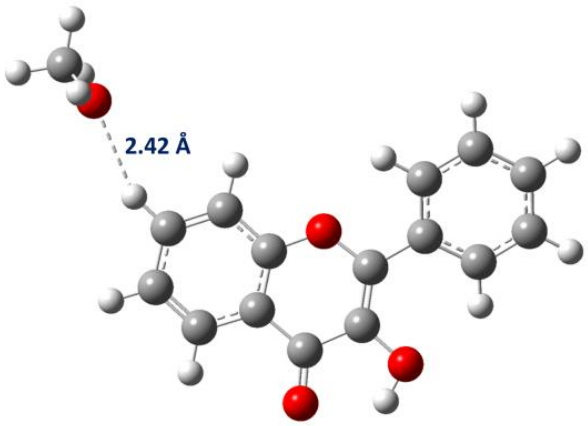
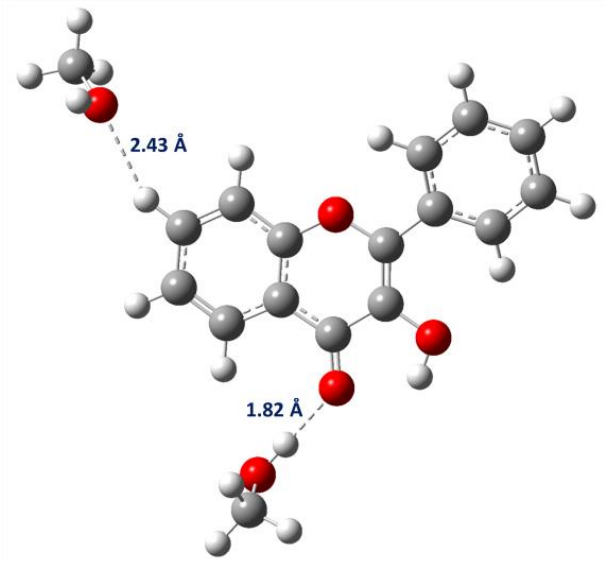
Total energy	-919.3662 hartrees -25017.23 eV
Dipole moment	6.75 D
Structure	

Table SI.4. The parameters of 3HF-$(MeOH)_2$ complex in methanol. The hydrogen bindings occur at the ESIPT and non-ESIPT sites of 3HF.

Total energy	-1035.1517 hartrees -28167.91 eV
Dipole moment	8.10 D
Structure	

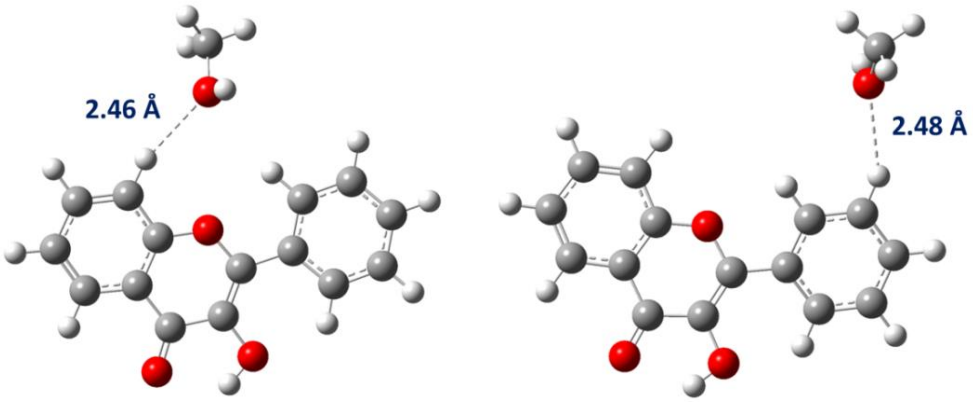


Fig. SI.1. The optimized geometries of some possible structures of 3HF-MeOH complexes (in the ground state) bonded at non-ESIPT site of 3HF.

The excited state S_1 (the first singlet state)

The parameters and the excited state S_1 optimized structures are obtained at B3LYP/cc-pVTZ level of theory (based on TD-DFT) and the IEFPCM solvation model. The red balls represent oxygen atoms, the grey balls represent carbon atoms, and the white balls represent hydrogen atoms in the depicted optimized geometries.

Table SI.5. The parameters of the excited state S_1 of 3HF (normal form) in methanol.

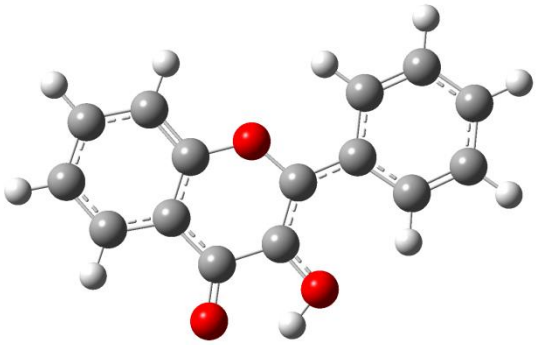
Total energy	-803.4711 hartrees -21863.56 eV
Dipole moment	5.08 D
Molar volume	168.4 cm^3/mol
Structure	

Table SI.6. The parameters of the excited state S_1 of 3HF-MeOH complex in methanol. The hydrogen binding occurs at the ESIPT site of 3HF.

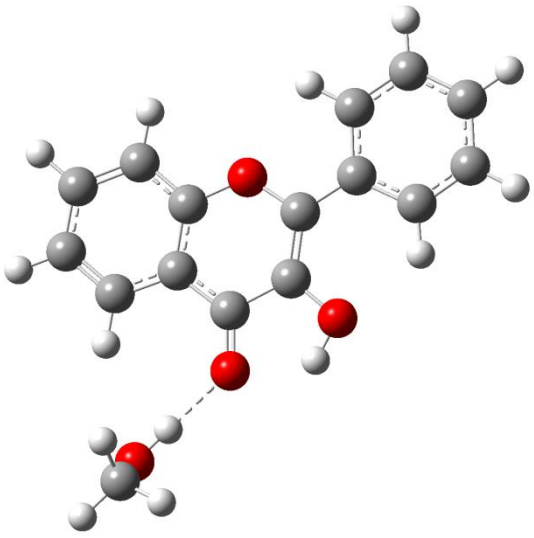
Total energy	-919.2578 hartrees -25014.28 eV
Dipole moment	7.79 D
Molar volume	200.1 cm^3/mol
Structure	

Table SI.7. The parameters of the excited state S_1 of 3HF-MeOH complex in methanol. The hydrogen binding occurs at the non-ESIPT site of 3HF.

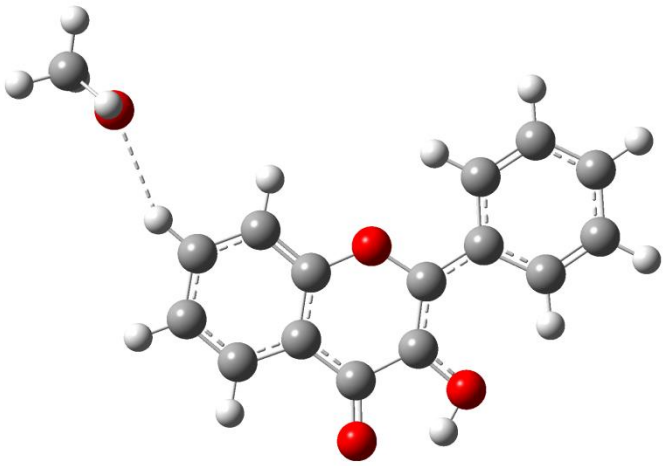
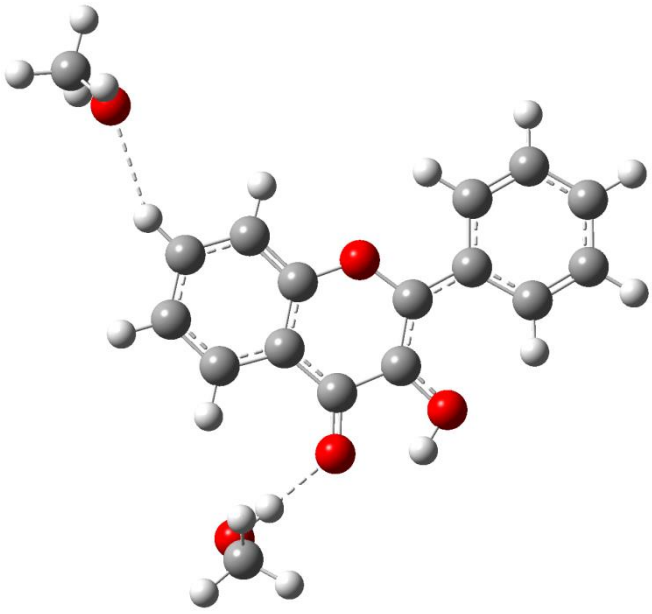
Total energy	-919.2499 hartrees -25014.06 eV
Dipole moment	6.04 D
Molar volume	197.8 cm^3/mol
Structure	

Table SI.8. The parameters of the excited state S_1 of 3HF-$(MeOH)_2$ complex in methanol. The hydrogen bindings occur at the ESIPT and non-ESIPT sites of 3HF.

Total energy	-1035.0367 hartrees -28164.78 eV
Dipole moment	8.65 D
Molar volume	232.1 cm^3/mol
Structure	

The excited state S_2 (the second singlet state)

The parameters and the second singlet excited state S_2 optimized structures are obtained at B3LYP/cc-pVTZ level of theory (based on TD-DFT) and the IEFPCM solvation model. The red balls represent oxygen atoms, the grey balls represent carbon atoms, and the white balls represent hydrogen atoms in the depicted optimized geometries.

Table SI.9. The parameters of the second singlet excited state S_2 of 3HF (normal form) in methanol.

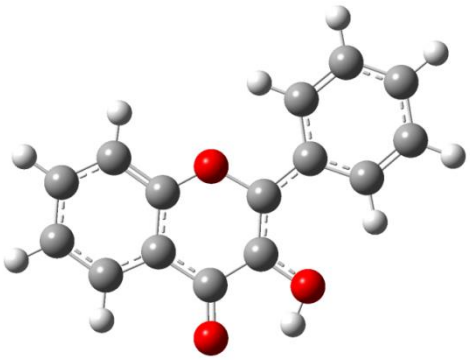
Total energy	-803.4476 hartrees -21862.92 eV
Dipole moment	8.68 D
Molar volume	169.1 cm^3/mol
Structure	

Table SI.10. The parameters of the second singlet excited state S_2 of 3HF-MeOH complex in methanol. The hydrogen binding occurs at the ESIPT site of 3HF.

Total energy	-919.2357 hartrees -25013.68 eV
Dipole moment	8.77 D
Molar volume	199.5 cm^3/mol
Structure