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COMPUTATIONAL MODELING OF THE TAUTOMERIC INTERCONVERSIONS OF THE QUERCETIN MOLECULE

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Quercetin molecule (3, 3′, 4′, 5, 7-pentahydroxyflvanone, $C_{15}H_{10}O_7$) is an important flavonoid compound, which is found in many foods and plants, and is known to act as a natural drug molecule with a wide range of treatment properties, like an anti-oxidant, anti-toxic etc. Notably, that in the composition of the biologically-active compounds in natural conditions quercetin shows quite effective treatment properties, while in the extracted state this molecule shows more effective mechanism of action, however already with toxicological manifestations.

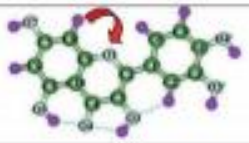
So, at the analysis of the pharmacological properties of the quercetin molecule it should be taking into account its possibility to acquire different tautomeric forms, ranging greatly by their energies.

In this study we revealed and investigated the possible pathways of the tautomeric transformations of the quercetin molecule, which potentially influence on its pharmacological and clinical effectivity (Scheme 1). Also, it was revealed that single proton transfer can induce cascade tautomeric reactions in the quercetin molecule.

These transformations of the quercetin molecule are accompanied by the rearrangement (breakage and formation) of the intramolecular H-bonds, changes of their geometry and dipole moment (value and direction).

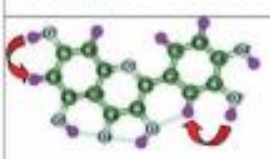
Obtained results can be useful for the formulation of the general rules of the formation and importance of tautomeric states, which can be applied to different heterocyclic molecules with potential biological or pharmaceutical activity.

Transition of the proton atom to the neighboring oxygen atom O1

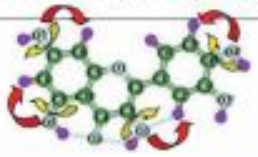


(1)

Transition of the proton atom from the O7H/O3'H hydoxyl groups to the neighboring C6/C2' carbon atoms (2) and from the O7H/O5H/O3H/O4'H hydoxyl groups to the C8/C6/C2'/C5' carbon atoms, preceded by the rotations of the hydroxyl groups around the C7O7/C5O5/C3O3/C4'O4' axis by 180 degree (3)

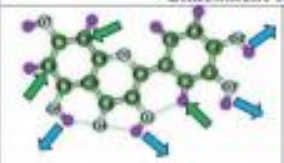


(2)

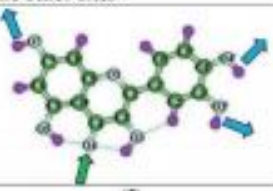


(3)

Transition of the proton atom by its splitting from one sites and attachment to the other sites



(4)



(5)

Scheme 1. Schematic representations of the possible mechanisms of the proton mobility inside the quercetin molecule, causing different tautomeric forms. Red arrows denote the directions of the intramolecular proton transfer, yellow – rotations o the hydroxyl groups by 180 degree, blue – sites of the proton splitting and green – sites of the proton attachment.