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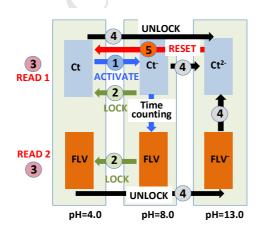
#### ACCEPTED MANUSCRIPT

# On the Multistate of 2'-hydroxyflavylium-Flavanone System. Illustrating the Concept of a Timer with Reset at the Molecular Level.

Stoyanka Slavcheva, <sup>1</sup> Johan Mendoza, <sup>2</sup> Stanislav Stanimirov, <sup>1</sup> Ivan Petkov, <sup>1</sup> Nuno Basílio, <sup>2</sup> Fernando Pina, <sup>2\*</sup> Vesselin Petrov <sup>3\*</sup>

#### **Abstract**

The multistate of species regarding 2'-hydroxyflavylium derivatives have a peculiar behavior due to the formation in moderately basic solutions of a flavanone from the mono-ionized *trans*-chalcone. The firmly established theory to account for the thermodynamics and kinetics of the flavylium based multistate of species in acidic medium was extended to the basic medium. The key experimental procedure to carry out this study is a sequence of reverse pH jumps from all pH range to a final pH sufficiently acid to have flavylium cation as the sole species. The reverse pH jumps can be performed from the equilibrium and pseudo-equilibrium. Acidification of the flavanone to pH=1 does not give back flavylium cation. In contrast, the di-ionized species *trans*-chalcone is obtained in a very fast process from the flavanone at pH>12. A cycle constituted by a sequence of pH jumps illustrates the concept of a timer at the molecular level with reset capacity.



The multistate based on 2'-hydroxyflavylium are related to a flavanone and permit to carry out a cycle that illustrates the concept of a timer at the molecular level.

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