

Call for papers: Symposium on “Tautomers and biology,” American Chemical Society National Meeting, Boston, MA, USA, August 2010

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Introduction

Tautomerism is possible for approximately one quarter of biologically interesting small molecules such as xenobiotics, enzyme substrates or cofactors, and biological mediators. Tautomerism complicates investigations into enzyme mechanisms and structure-activity relationships as well as such simple calculations as pK_a , octanol–water log P , and molecular similarity. The objective of this symposium is to showcase the many facets of tautomerism. Examples of appropriate submissions would be observations of the form of a tautomeric molecule bound to a macromolecule, measurements and calculations of

tautomeric equilibrium constants in water and non-aqueous solvents, strategies to enumerate tautomers for applications such as molecular docking and pharmacophore perception, investigations of enzyme mechanisms that involve tautomerism, and challenges to data base and cheminformatic handling of tautomers. Deadline for submission of abstracts is March 30, 2010 and can be done at www.acs.org/meetings.

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