The big problems don't go away by themselves

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In this issue Yvonne Martin provides us with a "Perspective" addressing an important and too often overlooked problem in chemistry, biology, and drug discovery, tautomerism. As she notes, the extent of this issue goes beyond common expectations. The phenomenon shines a bright light on the limitations of our methods of chemical structure representation and data basing. The problem is multifold. Many more molecules experience this phenomenon that one might expect. Also the magnitude of the apparent structural and electronic changes can be startling. Further, there are substantial effects of environment, whether solution, in a protein binding site, or in condensed phases. We can all be grateful to Yvonne for confronting this problem and forcing it to the forefront.

Consequently, Yvonne's Perspective serves to herald two special issues of JCAMD to be published next year.

Most direct to the effort, Yvonne is assembling an entire issue of "Perspectives" from notables in the field that will address the issue of tautomerism as totally as possible: the extent of the problem, experimental approaches, different methods of prediction, environmental effects, and others.

Additionally, JCAMD will publish the proceedings of OpenEye Scientific Software, Inc.'s SAMPL (Statistical Assessment of the Modeling of Proteins and Ligands) which is a blind assessment of contributed computational predictions of tautomers as well as vacuum-water transfer energies of small molecules. This is the third SAMPL, an annual event that brings together practitioners and developers of different theoretical methods. The Assessment—focused on science and what we need to do to improve as much as on what we can actually do now- is always illuminating.

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