Special Issue

Calculations in Solution

Message from the Guest Editor

Many industrial processes, all the processes occurring within living organisms, and the processes occurring in the water bodies in our planet are all processes in which the relevant molecules are in solution. Solute molecules and solvent molecules interact, and these interactions cause changes in many properties of solute molecules, such as their conformational preferences, energetics, separation of the various types of energy levels and, therefore, electronic and IR spectra, NMR signals, the way in which molecules of different solutes interact with each other, etc. This Special Issue of *Computation* is devoted to the theoretical/computational study of molecules and molecular processes in solution. The scope of the Special Issue is broad, extending to all the aspects of these studies, from theoretical modeling to the study of specific molecules, classes of molecules or processes.

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