APPLIED COMPUTATIONAL CHEMISTRY

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ABSTRACT

Computer bioengineering represents the application of engineering principles and methodologies in order to solve medical problems. The massive data obtained on the basis of various measurements on the human body at several levels from the molecular level to the population are modeled. With the advancement of new efficient algorithms and data processing protocols, new knowledge for clinical decision support can be extracted from these data.

The complexity of the challenges that computational chemistry methodologies are able to address is growing rapidly. Simulations are becoming increasingly accurate, while being able to access experimentally relevant timescales for large systems. Electronic structure methods are being used in new areas. Yet, there are many new, exciting challenges that computational chemists need to address that are critical to the future of the field such as maximizing how new computational architectures will impact the field, contributing to the development of these architectures, and utilizing data-driven and machine learning approaches towards scientific discovery. As well, addressing strongly correlated systems, predicting free energies and protein-ligand binding energies in biomolecules, and addressing chemistry at the interface are important areas that, in many ways, remain as some of the holy grails of computational chemistry, needing further developments.

The discussions will focus on the application of different methods of computational chemistry, such as DFT methods, molecular docking, molecular dynamics, QSAR, and others, in solving exact problems in various fields of chemistry. We will encourage cross-fertilization between different areas. The guiding principle of this meeting is to encourage a discussion of new unpublished results by gathering leading international scientists from the academic community and industry.

In this Mini-symposium, the following subjects are welcomed:

- Computer Applications in Chemistry
- Theoretical and Computational Chemistry
- Computer Application in Life Sciences
- Food Chemistry
- Medicinal Chemistry
- Drug design
- QSAR studies
- Characterization and Evaluation of Materials