

Next-generation technologies in computational chemistry

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Abstract

Computational chemistry is becoming an essential element in the chemist's toolbox for rationally guiding experiments. The recent literature has many successful examples of bioactive molecules discovered using computational chemistry methods. As the compendium of chemical biological datasets available in publicly-accessible repositories is growing, there is a need for technologies that can generate, analyze, model, and screen extremely large amount of chemical data in order to identify the most promising compounds with the desired activities. In this presentation, we introduce three next-generation technologies that can:

- (i) Enumerate extremely large virtual libraries: we will introduce the PKS Enumerator technology that generate billions of macrolides with user-defined constraints. This research is relevant for the development of novel antibiotics;
- (ii) Screen very large libraries of virtual compounds using a GPU-accelerated cheminformatics platform: we will show how a GPU-powered ligand-based screening workflow can perform ultra-fast similarity searches among tens of billions of molecules;
- (iii) Use machine-learning techniques for analyzing molecular dynamics trajectories: we will discuss the rationale of examining both full-atom and coarse-grained molecular dynamics trajectories using machine-learning techniques, what additional knowledge can be extracted, and how next-generation QSAR models could benefit of such technology. A *proof-of-concept* case study will be presented.