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Computational chemistry and computer-aided drug discovery: Part II

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The special focus issue on computational chemistry and computer-aided drug discovery contains a variety of contributions describing advances in computational medicinal chemistry including new concepts, computational methods, infrastructures and applications. The special focus issue is published in two parts and Part II is described herein.

To avoid redundancies in introducing the special focus issue, the interested reader is referred to the editorial conceptualizing this issue and calling for contributions [1] as well as the recent introduction of Part I [2].

As pointed out in the introduction of Part I, several publications in this special issue address emerging trends in medicinal chemistry such as the quest for integration of computational methods and experimental efforts or increasing orientation toward data-driven science. This also applies to Part II that contains contributions focusing on ‘big data’ and data visualization including a panel interview on big data challenges.

In addition, Part II of the special focus issue particularly emphasizes advanced computational approaches with relevance for virtual compound screening, activity prediction and drug design. For example, the use of computational solvent mapping for the identification and chemical characterization of ligand binding sites in target proteins is reported. Furthermore, different computational descriptors and

representations were explored to assess the similarity of ligand binding sites in various proteins. In another study, a machine learning approach was applied to automate the generation, evaluation and application of models for quantitative structure–activity relationship analysis, a mainstay in computational medicinal chemistry to predict compound activities. Furthermore, in a prospective virtual screening application, structure- and ligand-based methods, including pharmacophore and quantitative structure–activity relationship models, were used in concert in the search for new kinase inhibitors that were confirmed experimentally. Finally, in another contribution, computational methods for modeling and sampling of alternative protein conformations were reviewed. These approaches take protein dynamics into account and yield conformational ensembles of target proteins with often altered binding site feature that can be further explored in drug design.

Taken together, papers in Parts I and II of the special focus issue, originating from both academia and the pharmaceutical industry, cover a wide spectrum of computational methods for medicinal chemistry and drug discovery, including a number of new developments, and also highlight emerging trends. This outcome was envisioned and hoped for when planning the special issue. Many thanks to our authors who have made this project a success.

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