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Molecular Big Data, Computing, and Atomic-Level Simulation for Drug Discovery and Biology

Guest Editor:

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Message from the Guest Editor

Current development of machine learning algorithms and data technology make drug discovery and biology gain new challenges and opportunities to solve a scientific big problem. In particular, diverse unstructured data (e.g., real world data) as well as public databases are considerable to improve the applicability domain and predictive power in molecular simulations. In the same way we can find a shortcut to reach the summit of a mountain through searching uncertain different paths, a scientific big problem can be solved through investigating different methodologies of diverse research area (at a glance, unrelated). This issue covers recent diverse and novel approaches of atomic-level simulations using algorithms and data technologies. In this issue, unconventional or unexpected methods are recommended to suggest innovative prediction of atomic level molecular mechanics or biological activity. However, the prediction can also be conducted by current major methods (e.g., molecular dynamics simulations, docking simulations, QSAR, pharmacophore modeling) using well-encoded unique data.

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Message from the Editor-in-Chief

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