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Advances in Structure-Based Drug Design of Venom Peptides

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Message from the Guest Editors

Structure-based drug design has become the dominant paradigm for small-molecules. However, its impact on venom peptide therapeutic efforts, while still considerable, has been more limited because of the challenges of obtaining structures of these peptides in complex with their targets, as well as the difficulty of simulating them. Emerging technologies such as cryo-electron microscopy (cryo-EM) for structure determination, graphical processor units (GPUs) for molecular simulation, and free energy methods for potency prediction have the potential to remove these roadblocks. In this Special Issue, our aim is to collect the latest advances in structure-based drug design for venom peptides utilizing these technologies and others. We welcome experimental, theoretical, computational, and interdisciplinary contributions from both academic and industry practitioners.

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