Computational studies of snake venom toxins

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Most snake venom toxins are proteins, and participate to envenomation through a diverse array of bioactivities, such as bleeding, inflammation, and pain, cytotoxic, cardiotoxic or neurotoxic effects. The venom of a single snake species contains hundreds of toxins, and the venoms of the 725 species of venomous snakes represent a large pool of potentially bioactive proteins. Despite considerable discovery efforts, most of the snake venom toxins are still uncharacterized. Modern bioinformatics tools have been recently developed to mine snake venoms, helping focus experimental research on the most potentially interesting toxins. Some computational techniques predict toxin molecular targets, and the binding mode to these targets. This review gives an overview of current knowledge on the ~2200 sequences, and more than 400 three-dimensional structures of snake toxins deposited in public repositories, as well as of molecular modeling studies of the interaction between these toxins and their molecular targets. We also describe how modern bioinformatics have been used to study the snake venom protein phospholipase A2, the small basic myotoxin Crotamine, and the three-finger peptide Mambalgin.

Databases

Molecular dynamics simulations

Molecular modeling

Proteomics

Snake peptides

complementary DNA

crotamine

epidermal growth factor receptor

metalloproteinase

peptide

phospholipase A2

serine proteinase

snake venom

toxin

vasculotropin

snake venom

binding affinity

cell specificity

computer simulation

crystal structure

disulfide bond

envenomation

expressed sequence tag

molecular dynamics

molecular model

next generation sequencing

nonhuman

nuclear magnetic resonance imaging

protein family

protein motif

proteomics

Review

sequence analysis

sequence homology

structural bioinformatics

structure activity relation

transcriptomics

ultra performance liquid chromatography

X ray crystallography

animal

biology

chemistry

human

Animals

Computational Biology

Humans

Snake Venoms