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The use of structural modelling to infer structure and function in biocontrol agents

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Abstract:

Homology modelling can provide important insights into the structures of proteins when a related protein structure has already been solved. However, for many proteins, including a number of invertebrate-active toxins and accessory proteins, no such templates exist. In these cases, techniques of *ab initio*, template-independent modelling can be employed to generate models that may give insight into structure and function. In this overview, examples of both the problems and the potential benefits of *ab initio* techniques are illustrated. Consistent modelling results may indicate useful approximations to actual protein structures and can thus allow the generation of hypotheses regarding activity that can be tested experimentally.

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