

83. MODELLING THE STRUCTURE OF PROTEINS INVOLVED IN NEMATODE-PLANT INTERACTION

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In silico techniques were used to model the structure of a number of proteins involved in plant-nematode interaction in order either to assist the experimental work or to formulate hypotheses related to the structural basis of function in target proteins. To this end, probabilistic models of sequences with unassigned 3D structure were built by (remote) homology techniques and analysed according to the specific problem as in the following cases. Models of various nematode endoglucanase sequences were built starting from highly homologous endoglucanases from *E. chrysanthemi* and *Bacillus agaradherans*. These were used to raise the profile of variable regions. Results indicate that variations are mainly located in loops surrounding the Ca- and active sites, suggesting possible structural optimisation of the enzyme for various working conditions. Pectate lyase from *Globodera rostochiensis* was modeled starting from a highly homologous pectate lyase from *Bacillus* sp. strain2. The model was used to locate aminoacids involved in function. Results were subsequently confirmed by site-directed mutagenesis. The domains of a protein from *G. rostochiensis* shown to have expansin function were modeled by remote homology techniques starting from a xylan-binding domain and pollen allergen p1 from *Phleum pratense*. Analysis revealed high structural and functional similarities with plant expansins. A nematode calreticulin model was built from vertebrate templates. These were used to assess the exposure of a putative antigen that was further used to raise antibodies. These results suggest that modeling techniques could be useful in understanding function at molecular level in nematodes.

ORAL COMMUNICATION ABSTRACTS