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Poster Abstract – D.50

AN AB INITIO METHOD TO PREDICT MULTIPLE BINDING SITES ON A PROTEIN: AN APPLICATION ON TOMATO INHIBITOR-II

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One of the most interesting challenges in the analysis of protein structure data is to extract general information and/or specific peculiarities that could support knowledge increase and biotechnological applications.

We present here a new algorithm implemented to predict the binding sites of proteins when the experimentally determined coordinates of the three dimensional structures are available (Protein Data Bank). The proposed methodology is based on the presence of protein structural features that strongly influence the directionalities of the interaction.

We present the results of the application of the methodology to the analyses of the Tomato Inhibitor-II, a member of the multi-domain proteinase inhibitors which play critical roles in the defence of plants against predation by a wide range of pests.

The method is able to predict each of the binding sites of the protein and can be considered a reliable approach to support docking analyses and related applications when no experimental data on protein-ligand interactions are known.

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