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Databases and Bioinformatics Tools

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A. Surface representation of HIV-1 protease with a color scale from 1 (blue) to 7 (red) indicating variable and conserved regions.

B. Surface representation of HIV-1 protease with the active site highlighted in red.

C. Ribbon diagram of HIV-1 protease with specific residues highlighted: ARG372, ARG292, ARG119, ARG132, and GLU276.

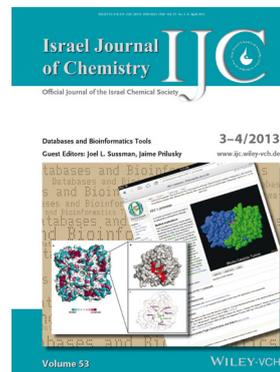
Proteopedia Screenshot: The screenshot shows the article "HIV-1 protease" on the Proteopedia website. It includes a 3D molecular model of the enzyme, a "Medical Implications" section, and a "Blocks Catalytic Tunnel" section. The article text mentions that there is currently no cure or vaccine against HIV, but researchers have discovered treatments that can halt and even reverse the progression of AIDS. It also notes that the first understanding of the structure of HIV-1 was approved by the FDA for the drug Saquinavir (Invirase).

Cover Picture

Gershon Celniker, Guy Nimrod, Haim Ashkenazy, Fabian Glaser, Eric Martz, Itay Mayrose, Tal Pupko, and Nir Ben-Tal*

Robert M. Hanson, Jaime Prilusky, Zhou Renjian, Takanori Nakane, and Joel L. Sussman*

The cover shows on the left a ConSurf analysis of the influenza neuraminidase protein. The 3D tetramer colored by conservation grades is shown in (A) with maroon indicating the most conserved amino acids, and close-up views (B,C) are shown of one of the conserved regions with the anti-flu drug, oseltamivir (tamiflu) bound; see Celniker et al. for details, page 199. On the right is a page from Proteopedia as viewed on an iPad, via the JSmol viewer, showing a complex of HIV-Protease and Saquinavir (Invirase), the first protease inhibitor approved by the FDA for the treatment of HIV; see Hanson et al. for details, page 207.



Databases and Bioinformatics Tools

Bioinformatics is a field at the crossroads of Chemistry and Biology encompassing databases and computational tools for the analysis of biological processes. With the enormous increase in speed of both genome sequencing and determination of 3D structures of biological macromolecules, this area has become incredibly important as a discipline that is able to discover key information and ideas from this astonishing large amount of data. This special issue of the *Israel Journal of Chemistry* is focused on this field, with ten papers discussing widely different aspects. The papers range from analysis of plant breeding (Ophir), mass-spectrometry (Linial), analysis of effect of single-base effects on nucleosomes (Trifonov) and on their mutations as to their effect on protein function (Unger), protein-protein interactions (Wolfson), tools for prediction of metal bindings in proteins (Edelman), predicting function from either structure (Kosloff) or via evolutionary tools (Ben-Tal), new ways to visualize 3D structures of biomacromolecules (Hanson & Prilusky) to an overview of synergistic data tools for examining biological activity (Lancet). These articles are from scientists in Israel where bioinformatics is a key area of research, but has also involved a great deal of interaction between Israeli scientists and those from around the world as can be seen in several of the papers where the authors are from Europe, USA, Japan and China. Bioinformatics is a field that has no borders. The tools described here are

being used both by students and scientists throughout the world and students and scientists from these different countries are also actively contributing data and methods. As the generation of new data continues to explode it is likely that databases and bioinformatics tools will play an ever-increasing role in our attempt to understand the chemical basis of the molecules of life.



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