



**Molecular Biotechnology Programme
Uppsala University School of Engineering**

UPTEC X 01 013	Date of issue 2001-02	
Author Katarina Jansson		
Title (English) A pilot study for virtual screening: finding inhibitors of hen egg-white lysozyme		
Title (Swedish)		
Abstract Virtual screening (VS) is a computer-based method to search for new drugs or protein ligands. In this work some of the VS methods available and computer programs for this purpose have been tested. Hen egg-white lysozyme (HEWL) was chosen as the model receptor system and the molecule database chosen for screening was the Available Chemical Directory (ACD) database. An iterative protocol using docking simulations combined with diversity and similarity selections, and a flexible search where the database was explored using a query defined by interaction properties gave promising results. The hits obtained by both methods cluster in a small area of the descriptor-space defined by the molecular distribution of hydrophobicity and partial charges. This could be interpreted as the discovery of a new "activity island" for inhibitors of lysozyme and probably even other glycosyl hydrolases.		
Keywords Virtual screening, molecular modelling, docking, diversity selection, similarity selection, flexible query search, lysozyme, inhibitor		
Supervisors Dr. Enrique Carredano Polymer and Surface Chemistry, Amersham Pharmacia Biotech		
Examiner Dr. Gerard Kleywegt Dept. of Cell and Molecular Biology, Uppsala University		
Project name	Sponsors	
Language English	Security	
ISSN 1401-2138	Classification	
Supplementary bibliographical information	Pages 46	
Biology Education Centre Box 592 S-75124 Uppsala	Biomedical Center Tel +46 (0)18 4710000	Husargatan 3 Uppsala Fax +46 (0)18 555217