



UPPSALA
UNIVERSITET

Molecular Biotechnology Programme

Uppsala University School of Engineering

UPTEC X 08 054	Date of issue 2009-01
Author	Magnus Gäredal
Title (English)	Novel inhibitors to novel targets in infectious diseases through structure-based virtual screening
Title (Swedish)	
Abstract	<p>An approach using structure-based virtual screening to identify potential inhibitors for <i>Plasmodium falciparum</i> spermidine synthetase (<i>Pf</i>-SRM) and <i>Mycobacterium tuberculosis</i> 1-deoxy-d-xylulose 5-phosphate reductoisomerase (<i>Mt</i>-DXR) was developed. Starting from a database of 2.6 million compounds and applying this strategy, 26 and 30 potential inhibitors to <i>Mt</i>-DXR and <i>Pf</i>-SRM were suggested.</p>
Keywords	
Supervisors	Micael Jacobsson, iNovacia AB
Scientific reviewer	Anders Karlén, Uppsala University
Project name	Sponsors
Language	Security
English	
ISSN 1401-2138	Classification
Supplementary bibliographical information	Pages
	40
Department of medical Chemistry Box 574 S-75123 Uppsala	Biomedical Center Tel +46 (0)18 4710000
	Husargatan 3 Uppsala Fax +46 (0)18 555217