Molecular Biotechnology Programme
Uppsala University School of Engineering

UPTEC X 02 022	**Date of issue 2000-05**

Author

Sinisa Bjelic

Title (English)

Computational study of P. falciparum plasmepsin II inhibitor binding

Title (Swedish)

Abstract

Prediction of free energy of binding for two inhibitors with four isomers each was performed against malaria parasite *Plasmodium falciparum* protease plasmepsin II by molecular dynamics simulations and linear interaction energy method. The binding energies were compared further for isomer dependent activity.

Keywords

Molecular dynamics, linear interaction energy method, malaria

Supervisors

Johan Åqvist
Uppsala Universitet

Examiner

Torsten Unge
Uppsala Universitet

Project name	Sponsors
Language **English**	Security
ISSN 1401-2138	Classification
Supplementary bibliographical information	Pages **30**

Biology Education Centre Biomedical Center Husargatan 3 Uppsala
Box 592 S-75124 Uppsala Tel +46 (0)18 4710000 Fax +46 (0)18 555217