Molecular Biotechnology Programme
Uppsala University School of Engineering

UPTEC X 01 025	**Date of issue 2001-05**

Author

Gisela Larsson

Title (English)

Computational studies of early intermediates in the bacteriorhodopsin photocycle

Title (Swedish)

Abstract

We have performed molecular dynamics simulations of the ground-, K- and L-state structures of the bacteriorhodopsin proton pump-cycle, and mapped the hydrogen-bond networks. Our results suggest that the primary proton transfer event is direct and not water mediated.

Keywords

molecular dynamics simulation, proton transfer, bacteriorhodopsin

Supervisor

David van der Spoel
Uppsala University

Examiner

Janos Hajdu
Uppsala University

Project name	Sponsors
Language **English**	Security
ISSN 1401-2138	Classification
Supplementary bibliographical information	Pages **29**

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