Molecular Biotechnology Programme

Uppsala University School of Engineering

UPPSALA UNIVERSITET

UPTEC X 06 011	Date of issue 2006-03

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Title (English)

hERG modelling using 3D-pharmacophores

Title (Swedish)

Abstract

Eleven pharmacophores for the cardiac K^+ channel hERG were developed using the modelling software Catalyst and evaluated with multivariate analysis. The pharmacophores will be used as visual feedback in drug design and as descriptors in predictive modelling. A pharmacophore-based automatic sorting scheme for hERG-compounds was generated and new approaches for classification modelling were explored.

Keywords

hERG, pharmacophores, exclusion volumes, structure-activity relationships, PLS-DA, descriptors

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Project name	Sponsors

Language **English**	Security

ISSN 1401-2138	Classification

Supplementary bibliographical information	Pages **40**