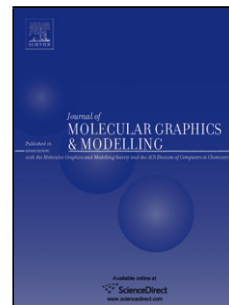


## Accepted Manuscript

Title: First Universal Pharmacophore Model for hERG1 K<sup>+</sup> Channel Activators

Authors: Serdar Durdagi, Ismail Erol, Ramin Ekhteiri Salmas, Matthew Patterson, Sergei Y. Noskov



PII: S1093-3263(17)30245-0  
DOI: <http://dx.doi.org/doi:10.1016/j.jmgm.2017.03.020>  
Reference: JMG 6881

To appear in: *Journal of Molecular Graphics and Modelling*

Received date: 19-8-2016  
Revised date: 28-3-2017  
Accepted date: 29-3-2017

Please cite this article as: Serdar Durdagi, Ismail Erol, Ramin Ekhteiri Salmas, Matthew Patterson, Sergei Y.Noskov, First Universal Pharmacophore Model for hERG1 K<sup>+</sup> Channel Activators, Journal of Molecular Graphics and Modelling <http://dx.doi.org/10.1016/j.jmgm.2017.03.020>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

# First Universal Pharmacophore Model for hERG1 K<sup>+</sup> Channel Activators

Serdar Durdagi<sup>a,\*</sup>, Ismail Erol<sup>a,b</sup>, Ramin Ekhteiri Salmas<sup>a</sup>, Matthew Patterson<sup>c</sup>, and Sergei Y. Noskov<sup>c,\*</sup>

<sup>a</sup>Computational Biology and Molecular Simulations Laboratory, Department of Biophysics,

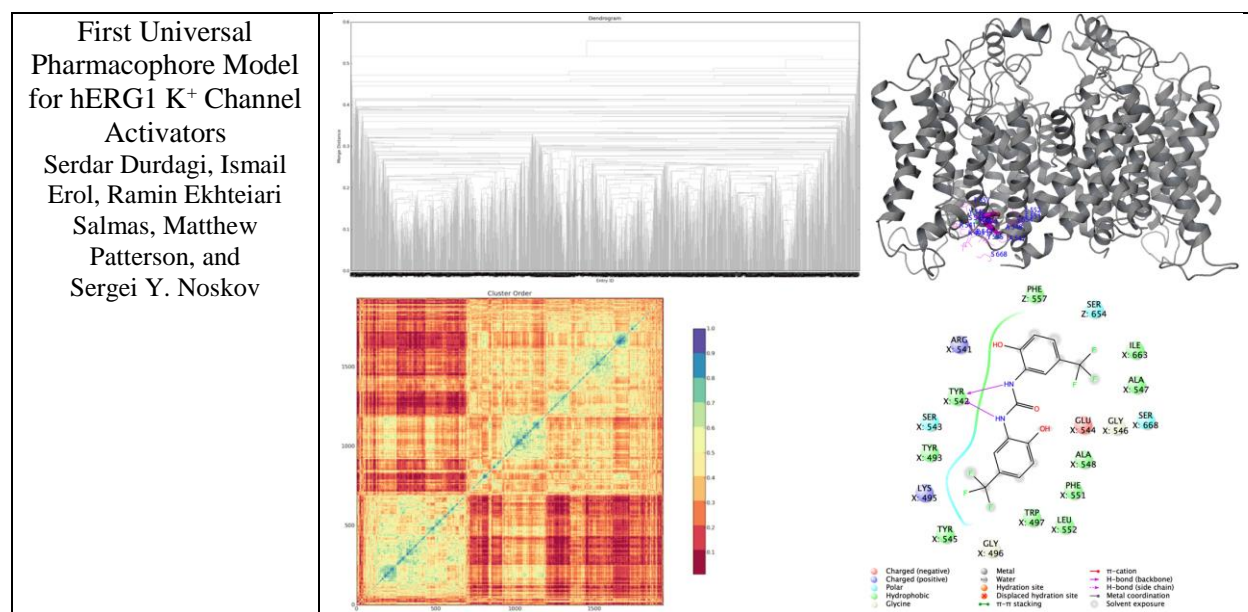
School of Medicine, Bahcesehir University, Istanbul, Turkey

<sup>b</sup>Department of Chemistry, Gebze Technical University, Kocaeli, Turkey

<sup>c</sup>Centre for Molecular Simulation, Department of Biological Sciences, University of Calgary,

Calgary, Alberta, Canada

## Graphical Abstract



## Highlights

- The first universal pharmacophore model for hERG1 K<sup>+</sup> channel activators
- was developed using PHASE
- A five-sited universal pharmacophore model (AAHRR) is successfully generated and validated with true unknowns for hERG1 channel openers
- The pharmacophore model was combined with the previously developed receptor-based model of hERG1 K<sup>+</sup> channel to develop and screen novel activators
- E-pharmacophore models (Structure-based pharmacophore models) were also derived for hERG activators

## Abstract

The intra-cavitary drug blockade of hERG1 channel has been extensively studied, both experimentally and theoretically. Structurally diverse ligands inadvertently block the hERG1 K<sup>+</sup>

Download English Version:

<https://daneshyari.com/en/article/4953104>

Download Persian Version:

<https://daneshyari.com/article/4953104>

[Daneshyari.com](https://daneshyari.com)