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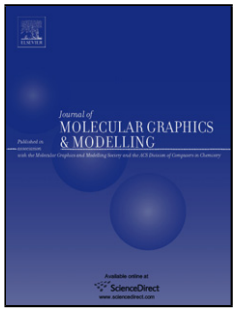

Title: First Universal Pharmacophore Model for hERG1 K^+ Channel Activators

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First Universal Pharmacophore Model for hERG1 K^+ Channel Activators

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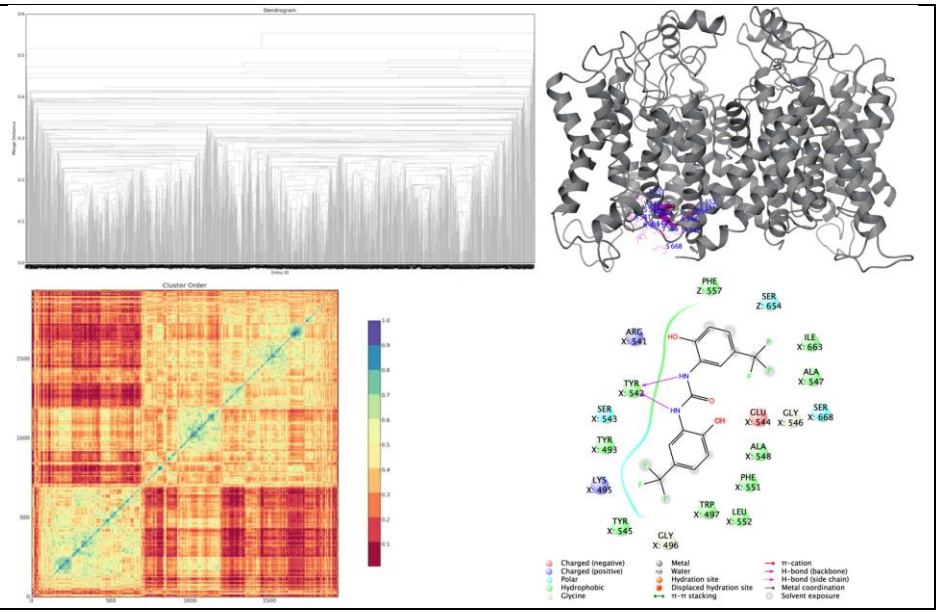
Graphical Abstract

First Universal Pharmacophore Model for hERG1 K^+ Channel Activators Serdar Durdagi, Ismail Erol, Ramin Ekhteiari Salmas, Matthew Patterson, and Sergei Y. Noskov	

Highlights

- The first universal pharmacophore model for hERG1 K^+ 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^+ 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^+