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Classification of Ligands of Constitutive Androstane Receptor Using Structure-Based Analysis

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Constitutive Androsatane Receptor (CAR) is predominantly expressed in liver and performs an important role in regulating drug metabolism and transport. The relationship between a binding structure and physiological properties of ligands has not yet been elucidated due to hugeness and hydrophobicity of binding site. Here we build a novel model predicting the property of compounds based on their binding pose. The pharmacophores, complementary to the binding residues, were generated and the core hypotheses were selected. On the other hand, by using various algorithms, ligands interacting with CAR were docked into the binding site and the best pose was selected. The two structural model, pharmacophore and docking, were merged into a model and some points matched up to them were converted to a matrix. As each hypothesis was used as a descriptor, ligands were classified through decision tree and GA-kNN. These descriptors used to construct classification models were involving significant information of binding position of ligands. This model leads to a new approach that connects the receptor-ligand structure with the physiological property of ligands. The model is being more optimized, so it will be able to classify the CAR ligand-type of a compound and to predict its contribution to drug metabolism by regulating the transcriptional role of CAR.

Biography

Kyungro Lee is graduate school student of Yonsei University Department of biotechnology.