Joint Pharmacophoric Space through Geometric Features

Tech ID: 29289 / UC Case 2011-077-0

BRIEF DESCRIPTION

Pharmacophore analysis through examination of Joint Pharmacophore Space of chemical compounds, targets, and chemical/biological properties.

BACKGROUND

Despite steady and significant increases in R&D spending, an increase in the number of new drug applications and approvals has not been seen. Current target-driven approaches to drug discovery limit focus to a single target and have phenotypic effects such as toxicity and low efficacy that are discovered too late in the discovery process. As a result, current interest is shifting towards evaluating biological properties at the onset and attempting to gain a global understanding of the binding activity between compounds and targets. There have been a number of attempts to understand the relationship between drug chemical structures and target proteins, including pharmacophore based screening. A key weakness of existing pharmacophore based technologies is its ability to analyze compounds only on target-by target basis, aimed at extracting and optimizing a specific pharmacophore. Often, multiple pharmacophoric targets need to be analyzed in the search for drugs against diseases such as cancer or AIDS.

DESCRIPTION

Researchers at the University of California, Santa Barbara have proposed a novel method for pharmacophore analysis by examining the *Joint Pharmacophore Space* (JPS) of chemical compounds, targets, and chemical/biological properties. The underlying geometry of the pharmacophores is responsible for binding between compounds and targets as well as properties of compounds such as Blood Brain Barrier (BBB) permeability. The use of geometric pharmacophoric features allows for the consideration of different conformations of compounds and isolation of the geometry of important pharmacophoric points in these conformations. The benefits of such joint pharmacophore analysis include increased sensitivity and specificity of results, flexibility in posing queries, scaffold hopping, and early *in silico* prediction and pruning of compounds with undesirable properties.

ADVANTAGES

- Increased sensitivity and specificity of results
- Improved beginning investigation point for medicinal chemists

APPLICATIONS

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OTHER INFORMATION

KEYWORDS

indpharma, Pharma, Pharmacaphoric, Chemical Properties, Drug Applications, Drug Design, Blood Brain Barrier, Silico Prediction, Drug Discovery, Molecular Classification, Cancer, Aids, Drug

CATEGORIZED AS

- **Biotechnology**
  - Health
  - Other
- **Medical**
  - Delivery Systems
  - New Chemical Entities, Drug Leads
  - Research Tools
- **Research Tools**
  - Bioinformatics

RELATED CASES

2011-077-0

- Drug design and discovery
- Molecular classification

PATENT STATUS

Country	Type	Number	Dated	Case
United States Of America	Issued Patent	9,218,460	12/22/2015	2011-077

ADDITIONAL TECHNOLOGIES BY THESE INVENTORS

- Closure-Tree: An Index Structure for Graph Queries
- Mind Reader: Reconstructing Complex Images From Brain Activities
- A Video Fingerprinting Method For Duplicate Detection

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