Joint Pharmacophoric Space through Geometric Features

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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,
Pharmacophoric, 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

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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