ConTour: Data-Driven Exploration of Multi-Relational Datasets for Drug Discovery

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Abstract

Large scale data analysis is nowadays a crucial part of drug discovery. Multiple interrelated datasets need to be investigated to evaluate potentially effective yet safe drugs. ConTour is a visual analysis system for the interactive exploration of these complex datasets. It employs several intuitive interaction techniques to reveal relationships between data items and provides analytical methods to judge the quality of these relationships. Diverse filters can be used to reduce the data space and advanced visualizations of data items at different levels of detail provide the analyst with enough information to make profound decisions during the data exploration.

Goals

- Identify a drug's mechanism of action.
- Identify the biological process that a drug modulates.
- Identify new drugs for specific therapeutic indications.



Learn about ConTour: http://contour.caleydo.org Contact: partl@icg.tugraz.at

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Selection and Highlighting () intersection mode: union mode: Selecting individual items identifies related items by highlighting and reordering.

Enrichment Score $|K_i \cap K_j|/|K_j|$ $s_{i,j}(K) = K_i \bigcap K_j$ $|K_i|/|K|$ k4 Describes how specific two different types items are related considering a third type.

