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Mr. Rogers Algorithm for Protein Pathway Discovery

Two related technologies, a pipeline for generating a custom PathFX algorithm and a new algorithm named Mr. Rogers, are used to identify protein pathways around drug targets. The PathFX customization expands use of the published PathFX algorithm beyond publicly available data to identify solutions to specific disease areas using inhouse experimental data. By identifying experimental data relevant to a disease of interest, this implementation will yield a custom version of PathFX. The custom PathFX enables analysis of gene-phenotype association tables, gene/protein interaction tables, and drug-protein binding tables, and these results assist in discovering novel drug candidates based on their pathways. The Mr. Rogers algorithm is a depth-first search which returns a set of paths and intermediate paths of protein-protein interaction and is used in the custom PathFX pipeline. Inputting a single or multiple seed protein(s) into the generated custom PathFX returns the interaction pathways surrounding the seed, which helps to identify the drug-target pathways.

Stage of Research

Prototype

Applications

- Drug discovery
- Therapeutics and therapeutic pathways
- Biological network discovery
- Pharmacodynamic pathways
- Bioengineering

Advantages

- Data-specific PathFX implementations
- User-defined scoring criteria for network and pathway identification

Publications

Wilson et al. Plos Computational Biology (2018) <u>"PathFX provides mechanistic insights into drug efficacy and safety for regulatory review and therapeutic development"</u>

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