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Drug repositioning system using the power of network analysis and machine learning to predict new indications for the approved drugs "Drug repositioning and rate the level of the drug similarity"

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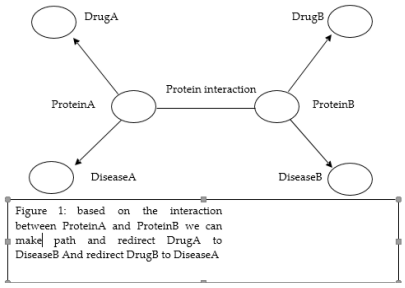
Drug discovery is a lengthy process, taking on average 12 years for the drugs to reach the market –but as Sir James Black OM once said, "the best way to discover a new drug is to start with the old one". As result, this will drive to Drug repositioning concept. Drug Repurposing and repositioning is finding a new clinical use for an approved drug. There are many factors that can be used to predict new target disease. i.e. protein-protein interaction, chemical structure, gene expression and functional genomics, Phenotype and side effect, genetic variation and Machine learning. Protein-protein interaction (PPI) is Physical contacts with molecular docking between proteins that occur in a cell or in a living organism *in vivo*. There are Two Alternative Approaches PPI "Binary: yeast two-hybrid (Y2H) and co-complex: (TAP-MS)". Drug Repositioning System, is a system built based on protein-protein Binary interaction to predict new targets for the approved drugs. The system curates the data sets for human PPI, Drugs and diseases from well-known online sources (PPI from HRPD, drugs from DrugBank, Diseases from DisGeNET), Drug Repositioning System relates the 3 data sets based on genes name. Drug Repositioning System consisting of two interfaces: backend system where the curated data sets stored based on rational database and frontend web interface where the end users can use many search engines to search inside the system for diseases, genes and drugs to predict and find new targets for the approved drugs based on protein interactions, from the web interface the user can make analysis based on his search result and build network between the genes, diseases and drugs and generate statistics to be able to answer his question. There are many questions that can be answered by Drug Repositioning System and generate statistics: for example the main question is can we find new indications for existing approved drugs. Drug similarity: from the Drug Repositioning System we can measure the percentage of drugs similarity between any pair genes interaction based on the number of shared drugs between them to rate the level of drug repositioning strength and then use the ROC (Receiver Operating characteristic Curve) analysis.



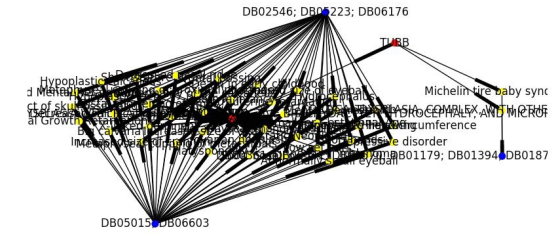


Figure 2: in the left side of the picture, it's clear that there are two groups of drugs target numerous diseases related to HDAC6 gene and also on the right side we will find one group of drugs targets two groups of disease that are related to TUBB gene while there link between TUBB and HDAC6 indicates the interaction between them. As result we can make drug repositioning between the two genes.

Biography

Sherief El Rweney has over 13 years experience in computer science systems and information technology, he has done Master's degree at Royal Holloway University of London in Computer Science, Data Analysis, Machine Learning and Bioinformatics. The merging between his experience in bioinformatics and machine learning study motivated him to build the Drug Repositioning System based on protein interaction where can be used to predict new indication for the approved drugs and help drugs scientists to go easy through their drug discovery research. He is aiming to develop the Drug Repositioning System by merging many other factors beside the protein interaction to strength the predication of the drugs repositioning.

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