Drug Target Discovery Using Open PHACTS

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Abstract:

Translational research is a rapidly maturing research area in the medical field. With the advent of omics technologies scientists have access to vast amounts of data, ranging from transcriptomics, to proteomics and metabolomics, of the phenotype under study. However, to process and mine this data with the aim to find drug therapies that can be quickly used for the treatment of patients remains a critical challenge. In this work we focus our efforts on linking drugs to their protein targets and identifying influenced molecular pathways and biological processes relevant to a disease of interest. We used OpenPHACTS resources to identify drug targets and linked them to biological databases to acquire valuable information of these targets. Specifically, we developed a Taverna Workbench workflow that 1) converts a generic drug or compound name to a URI using a conjuction of the Chemspider Web services and the OpenPHACTS API, 2) retrieves information about compound targets from OpenPHACTS and filters out anything that is not a single protein (other target types such as cell lines was not the target of our study), 3) retrieves information about target pathway descriptions from OpenPHACTS. We applied our pipeline on proven drugs used in Polycystic Kidney Disease treatment to identify the genes and pathways targeted by these drugs. Identifying new drugs that target the same genes and pathways, we managed to repurpose several drugs for PKD treatment.