



A CHEMO-CENTRIC VIEW OF HUMAN HEALTH AND DISEASE

PROJECT DESCRIPTION

Recent advances in text-mining techniques and subsequent curation efforts are committed to compiling direct human response data from the knowledge accumulated through the years. We have recently profited from this enterprise to revisit the classical structure-activity relationship notion, this time for a vast and diverse list of human diseases. In this study, we considered thousands of chemicals and analyzed their relationship with respect to a comprehensive collection of adverse and beneficial clinical outcomes.

Our study included molecules related to the etiology of 934 health threatening conditions and others used to treat 835 diseases. We first identified chemical moieties that could be independently associated with each phenotypic effect, which we use to build accurate predictors for approximately 400 clinical phenotypes. Among fragment–disease relationships, we found many privileged and liable structures that could inform the drug discovery process, although not all disease classes are equally suitable for a chemo-centric view. Finally, we connected two diseases if they relate to a similar chemistry.

The resulting networks of human conditions are able to predict disease comorbidities, as well as identifying potential drug side effects and opportunities for drug repositioning, and show a remarkable coincidence with clinical observations. Moreover, the derived chemo-centric maps are of singular interest for drug development, since they are directly based on effector compounds. Our analysis is the most exhaustive study to date of the spectrum of effects that small molecules have on our health, and it sheds light on the chemical basis of human diseases.

More information available on:

“A chemo-centric view of human health and disease” [Nat Commun, 5 5676 \(2014\)](#)

COLLABORATION OPPORTUNITY

Results from the project are available for out-licensing. In addition, collaborations applying this algorithm and methodology to different therapeutic areas are also envisioned.



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