Cheminformatics and Network science applied with high content screening data

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For over a decade, computational chemical biology has contributed to a wide array of scientific tasks from analytical chemistry and biochemistry to pharmacology and toxicology. With the increasing availability of data from the"omics" technologies, we start to be able to profile chemical effect, not only at the molecular level, but also at more complex layers (cells, tissues, organs) allowing a better understanding of the mechanism of action underlying complex diseases.

Recently, phenotypic drug discovery has re-emerged as promising approaches in the identification and development of novel and safe drugs. Although, phenotypic screening does not rely on knowledge of specific drug targets, combination of chemical biology data with network sciences and cheminformatics give the opportunity to suggest therapeutic targets and mechanisms of actions induced by drugs and associated with an observable phenotype.

In our laboratory, we have developed a system pharmacology network integrating chemicals-proteins/genes-pathway-disease relationships and high content imaging-based high-throughput phenotypic profiling assays.

First, I will present the implementation of this system pharmacology network and then I will go through different examples showing how such analysis might be of interest in the study of chemical action across multiple scales of complexity from molecular and cellular to phenotypes and diseases.