[P47] Validation of Pythia's target prediction

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Determining the main molecular target of biological active compounds is a key step in drug discovery. Determination of off-targets is essential to enhance compounds selectivity and reduce drug secondary effect. Recently we developed Pythia, a *in silico* tool that combine molecular similarity and experimental biological activities to determine the main biological target for active compounds. Moreover it can be used to find off-targets for drug candidates for which secondary effects need to be mitigated.
Results showed that Pythia is able to early recover in the top 20 positions most of known therapeutic and off-targets for most approved drugs, Investigational New Drugs (IND) and preclinical drug candidates.