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A drug discovery pipeline integrating the processing and analysis of NMR spectra and the identification of lead compounds.

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In this work we present a web service that allows users to execute the full workflow that enables a Nuclear Magnetic Resonance (NMR)-based drug discovery pipeline. NMR spectroscopy has been widely used in the early steps of drug discovery. It is especially suited to the structure-based approach in lead design and is the most powerful method for studies of structure, dynamics, and the interactions of molecules in solution. The NMR-based drug discovery pipeline starts with the acquisition of 2D 1H-15N heteronuclear single quantum correlation (HSQC) spectra on the free protein target, followed by the acquisition of the same experiments for the protein in the presence of different ligands. The changes in the chemical environment of the protein nuclei near the drug binding site induce detectable chemical shift perturbations (CSPs). The measurement of CSPs indicates whether a binding event has occurred at all and, if yes, can provide information on the ligand affinity for the target. Here we have developed a workflow that take as input a HSQC peak assignment of the free protein and a series of raw experimental HSQC data for the screening of a library of candidate ligands. The spectra are automatically processed and assigned; this data is then evaluated to identify the peaks shifted due to the presence of the ligand. This workflow is made available via a web user-friendly interface that is publicly available. The workflow was developed as a Nextflow pipeline and all software was translated to Docker Images. For the front-end and back-end services we have used respectively JavaScript React JS framework and Java Spring Boot framework.

Any relevant links

Topic

EOSC Compute Platform

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