MS02-P06 | FRAGMENT SCREENING PROJECT MANAGEMENT WEB APPLICATION - FRAGMAX

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Fragment screening as a tool for drug discovery has been extensively explored by industry and academia. In this method, small molecules are used to probe protein surface and pockets, identifying weak binders that can be developed into hits. While fast data collection is now widely available in modern photon sources, it generates a few terabytes of data within a single data collection, hindering data manipulation. At MAX IV, we are developing an OS-independent Web Application focused on Fragment Screening project management that gathers information from target and fragment library from ISPyB and present users with full data collection reports. The web-app provides data processing (XDSAPP, autoPROC, XIA2/Dials and XIA2/XDS), refinement (BUSTER, FSPiepeline, Dimple) and ligand fitting (RhoFit, Phenix LigFit) from a simple and intuitive interface relying on MAX IV HPC, requiring minimal resource on user's computer for displaying a WebGL application. This tool allows 1-click automatic data analysis as well as advanced parameters input, with several pipelines to choose including Pipedream (Global Phasing) and PanDDA, and electron density visualisation through UglyMOL. In our current stage of development, we ran three commissioning projects whereas one using a custom fragment library. More information about FragMAX and our web-app is available at BioMAX webpage.