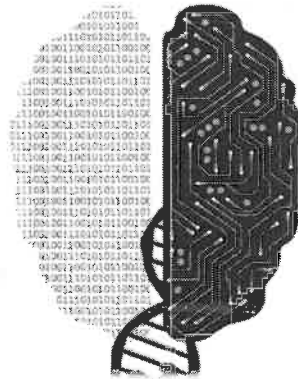# BIOINFORMATICS OPEN DAYS

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Book of Abstracts

VScore: a software for management of large scale virtual screening projects in computer clusters

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Virtual screening (VS) of large compound databases using docking tools present several challenges for the average user and currently the use of High Processing Computer (HPC) clusters is mandatory. The availability of software tools with the ability to perform all the necessary VS tasks, ranging from compound and protein structure preparation, cluster job submitting to results management and analysis is a requisite for successful VS projects. We have developed VScore (Virtual Screening core), a ready-to-use automated software tool with a graphical user interface that can manage large scale VS projects, using AutoDock4 and/or AutoDock Vina as docking tools. VScore handles information in a dedicated database, implemented in MySQL making data management of large libraries of chemical compounds easier. This database structure makes possible several advanced features that set VScore apart including: one time protein/ligand preparation step, comparative docking using multiple structures from the same protein targets or even structures of different protein

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