Contribution ID: **25** Type: **Workshop/Tutorial Proposal**

Accelerated free energy calculations using open-source tools

We will use open-source free energy tools and the Galaxy Platform (BRIDGE) to calculate absolute and relative free energies of protein-ligand binding. Setting up free energy molecular simulations, using scripts, the Linux command line and using HPC resources can be complex. Further not all steps are repeatable. With the Galaxy Project platform, BRIDGE and Galaxy Comp Chem we aim to provide a web application to assist researchers in conducting repeatable computer simulations and analysis using curated workflows.

Supported Student

Primary authors: Prof. NAIDOO, Kevin J. (University of Cape Town); Dr BARNETT, Chris (University of Cape Town); SENAPATHI, Tharindu

Presenters: Prof. NAIDOO, Kevin J. (University of Cape Town); Dr BARNETT, Chris (University of Cape Town); SENAPATHI, Tharindu

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