

DevOps cloud-computing environment to perform virtual screening

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Failures in all phases of clinical trials have been increased the past decades. It is occurring despite improvements in all stages of the drug development pipeline. One of the key areas of improvement has been the virtual screening for drugs likely to fail clinical trials. The drug-likeness measures have been widely accepted as a useful guide to identification of promising molecules to be tested as drug candidates in the early stages of drug discovery. As consequence of virtual screening is the focus on efforts and resources on experiments with promising molecules. The virtual screening technique demands a dynamic and heterogeneous computational environments which can adapt itself according to each task. It is a challenge to drug discovery projects that have used for along the time. In order to attend this challenge is employed DevOps. It means the practice lays emphasis on the collaboration and communication between software developers and professionals while automating the process of software delivery and infrastructure changes. Resulting, DevOps aims at establishing a culture and environment where building, testing, and releasing software can happen rapidly, frequently, and more reliably. In this work is presented a DevOps strategy for virtual screening through docker and Galaxy project. Galaxy project is an open-source web-based platform what made easy the reproducible research and provides a good engine to make friendly interfaces to command line tools. Docker is an open-source platform which consists in docker container engine and docker hub. The docker container engine is responsible to create and manage isolated containers on top linux kernel with his technologies called namespaces and cgroups. The docker hub makes possible deploy and share our own images on docker environment with other people. We've implemented a docker image which has a galaxy platform instance with tools to perform virtual screening with autodock vina allowing system administrators deploy and increase resources on demand in cloud environments. Furthermore it allows the users have a user-friendly interface to autodock vina and track all steps made in your analysis. In some tests accomplished for us the time to get up the container working was on average 5 minutes, which is a good result compared to the 2 hours on average taken with the same tests performed manually.