

A preliminary study on shifting from virtual machine to docker container for insilico drug discovery in the cloud

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Deskripsi Lengkap: <https://lib.ui.ac.id/detail?id=9999920532865&lokasi=lokal>

Abstrak

The rapid growth of information technology and internet access has moved many offline activities online. Cloud computing is an easy and inexpensive solution, as supported by virtualization servers that allow easier access to personal computing resources. Unfortunately, current virtualization technology has some major disadvantages that can lead to suboptimal server performance. As a result, some companies have begun to move from virtual machines to containers. While containers are not new technology, their use has increased recently due to the Docker container platform product. Docker's features can provide easier solutions. In this work, insilico drug discovery applications from molecular modelling to virtual screening were tested to run in Docker. The results are very promising, as Docker beat the virtual machine in most tests and reduced the performance gap that exists when using a virtual machine (VirtualBox). The virtual machine placed third in test performance, after the host itself and Docker.