Overview

Combining Graphical User Interfaces and HPC

*LigandScout* Remote enables the seamless integration of high-performance computing (HPC) resources into the *LigandScout* desktop application. By handling necessary data conversion and network communication transparently to the user, this approach evades any HPC usability barriers.

Motivation

HPC clusters play a major role in scientific research. However, working with these clusters is often cumbersome, especially for researchers without a formal background in computer science.

It requires preparation and transfer of the input data, manual gathering of results, and command-line expertise. Current approaches for improving accessibility to remote HPC clusters are focused on providing web-based graphical front-ends that allow jobs to be submitted to the distributed resource management system running on the cluster. This comes with significant usability...
benefits over command-line usage but does not circumvent the need for manual handling of the input and output files.

### Reference

**LigandScout Remote: A New User-Friendly Interface for HPC and Cloud Resources**

Thomas Kainrad, Sascha Hunold, Thomas Seidel, and Thierry Langer

*Journal of Chemical Information and Modeling* Article ASAP

DOI: [https://www.doi.org/10.1021/acs.jcim.8b00716](https://www.doi.org/10.1021/acs.jcim.8b00716)

### About this Documentation

This documentation explains how to install and configure the *LigandScout* Server application (*iserver*) on physical HPC clusters and Amazon Web Services (AWS) cloud clusters.

For usage instructions of *LigandScout Remote* within the *LigandScout* desktop application, you can refer to Chapter 10 of the regular *LigandScout* user manual. It can be accessed from within *LigandScout* under **Help -> LigandScout Help**.