Python in a Drug Discovery Environment

Andrew Dalke
Bioreason, Inc.
309 Johnson St.
Santa Fe, NM, 87501
dalke@bioreason.com

Abstract

Bioreason, Inc. develops data mining tools for drug discovery based on high throughput screening. Our software uses Python to combine existing and novel data mining techniques with chemical information and molecular modeling. It will automate the experimental analysis and present the results and reasoning to the pharmaceutical chemist in an interactive environment; enabling the chemist to concentrate on chemistry rather than software mechanics.

Python has proven capable for algorithm development, file parsing, and other standard programming tasks that could have been done in any language. It has been especially useful as an (understandable!) interactive development language, an interface wrapper for both C APIs and stand-alone executables, a cross-platform GUI display and a COM client. This poster will present how these different aspects have been important for our work and our end-users.

Availability

Nearly all of the computational chemistry software will be made available on the Python Starship. This is the non-proprietary "glue" logic we use to embed code that was not originally designed to be embedded. We hope the contribution will help advance our field and the use of Python in chemistry. The name and URL of the software has yet to be determined by the time this abstract was submitted.