

CBI 学会 2017 年大会 ランチョンセミナー

日時：10月5日(木) 12:00~13:30

会場：タワーホール船堀 401 会議室

主催：オープンアイ・ジャパン株式会社

“The Cloud is the only place for Computational Chemistry”

Gregory L Warren, Anthony Nicholls, A. Geoffrey Skillman

Many parts of the computer-aided drug discovery (CADD) process are a perfect match for the Cloud. The first is the increasing requirement for large “on demand” compute resources. This is because CADD calculations are becoming increasingly complex and are being applied to larger and larger datasets. Second, modelers interact with both biological data and the chemists creating compounds.

Communication and data sharing between these separate groups can be difficult.

Last, computational chemists frequently need to test or develop new and better CADD methods, which requires appropriate validation datasets, resources for testing and analysis methods. The Cloud can solve all these problems. This presentation will show how the new OpenEye cloud platform, Orion, provides rapidly scalable compute resources, easy to use yet secure communication and data sharing between groups, and a workflow approach that allows for rapid development, testing and deployment of new computational methods.

OpenEye Scientific Software Inc. 及びオープンアイ・ジャパン株式会社について

米国サンタフェに本社を置くオープンアイ・サイエンティフィックソフトウェア社は 1997 年から分子モデリング、ケモインフォマティクス分野のソフトウェアを製薬業界に提供しています。創業以来一貫して、新規科学に基づく斬新なソフトウェア、及び効率的な研究環境の提供を使命としてきました。事業方針の中核を為すものは次の三つです。

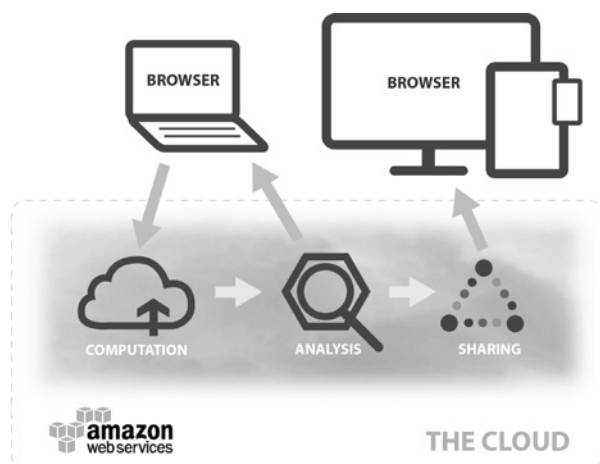
- 1) 分子形状と静電ポテンシャルに基づいた分子特性の記述
- 2) 二次元/三次元ハイスループット・モデリング用のプラットフォーム非依存プログラム開発
- 3) 辻褃合わせではなく厳密性に重きを置く研究姿勢。

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A Cloud Native Platform for Computer-Aided Drug Design

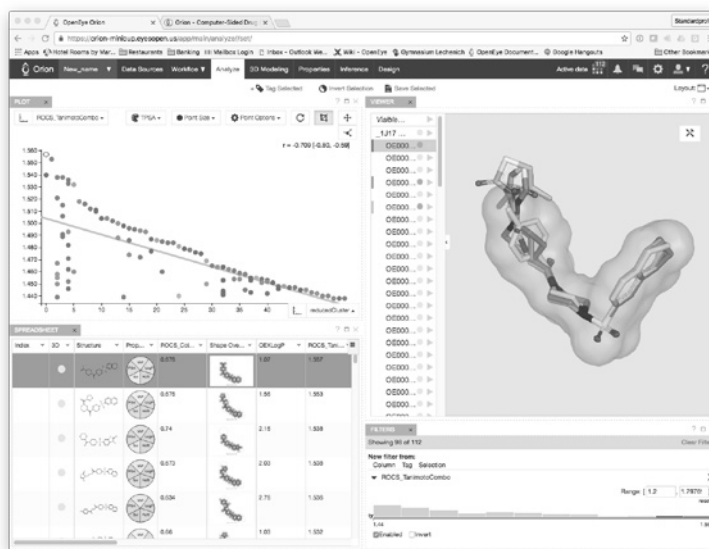
Orion is our reimagining of computational drug discovery and design powered by the cloud. It includes all of OpenEye's software, extensive tools for data visualization and communication, useful data sources and task-oriented workflows, all in a robust, scalable, cloud environment. Orion is a 'cloud native' platform in that all elements of Orion reside on, Amazon Web Services (AWS):



- Easy, scalable, maintenance-free
- Access to hundreds, thousands, or even tens of thousands of CPUs
- Unlimited storage and archiving via reliable networks
- World-class data-security. Access directly through the customer's relationship with AWS, or indirectly through OpenEye

Features

- Scalable environment via Amazon Web Services (AWS)
- Access to ALL OpenEye computational software and toolkits
- Results sharing via chat and text-like environment with access privileges
- Easily handles large-scale computation including data analysis and file handling
- Seamless access to third party code



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