CBI 学会 2022 年大会（2 日目）スポンサードセッション
日時：10 月 26 日（水）15:30-17:00

Structure-Based Lead Optimization in Orion®

– Progressively Improving Estimates of Binding Affinity –

OpenEye, Cadence Molecular Sciences

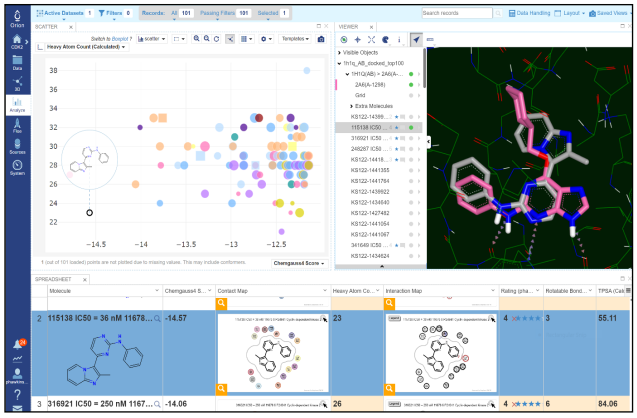
Lead optimization happens in cycles, beginning with the core of the lead and generating a great many candidate analogs based on R-group substitution. In the end, only a few of these candidates will be synthesized to be assayed. Using computational methods to reduce the great many candidates to the few involves progressive stages of refinement aimed at rejecting a majority of worse candidates from the previous stage. As the stages progress, the set of remaining candidates becomes smaller and of higher quality, requiring a gradually improving estimate of binding affinity. We will look at this process in the context of the protein structure-based approach. All steps in this process will be performed seamlessly in Orion while taking advantage of massive parallelism in the Cloud. We will present the sequential stages of a cycle of lead optimization, beginning with generative modeling and progressing through to relative binding free energies. More detail will be given on the use of the relatively new Non-Equilibrium Switching (NES) method for relative binding free energies.

お問い合わせ先：oe_japan@eyesopen.com
https://www.eyesopen.inc/orion

Trusted OpenEye Science

Orion® delivers the OpenEye computational tools scientists have trusted for more than twenty years in an integrated web platform backed by the computer power of Amazon Web Services.

- Run ligand-based or structure-based virtual screenings, molecular dynamics (MD) simulations, free energy predictions, quantum mechanics calculations, sequence analysis, and more from just a web browser
- Perform ultra-fast 2D and 3D search of over 4 billion stereo-enumerated commercially available molecules and 40 billion conformers
- Integrate third-party or in-house tools
- Collaborate with colleagues without file transfers and formatting



The Orion platform provides all the tools and data needed to allow calculation, analysis, collaboration, and decision-making in one environment.

Orion Platform

The Orion Platform Provides:

- An integrated web-based environment to design, calculate, view, and analyze all your computation and modeling projects, in real-time
- Freedom to program your own calculations that use diverse hardware
- Connectivity to Orion's flexible storage system, including large-scale distributed I/O
- Automatic parallelization to optimize your workflows
- A single platform for your data and applications, eliminating the need for data transfer and app switching and letting you collaborate with your team in real-time

Orion Science Suites

OpenEye is renowned for its chemical modeling applications and toolkits. All of its science has been through rigorous validations and peer-reviews. Running these trusted solutions on AWS means you can now solve modeling questions that were previously impossible due to compute-time or hardware limitations.

Small Molecule Discovery Suite

Structure- and Ligand-based Design

The Small Molecule Discovery Suite in Orion® provides a complete range of easy-to-use ligand- and structure-based modeling workflows for all your therapeutic project needs, such as increasing the hit rate of your virtual screen, optimizing affinity of lead candidates, and predicting off-target effects. *Learn more at: https://www.eyesopen.com/orion/small-molecule-discovery-suite*

For more information on Orion and additional science suites,
please visit our website at **www.openeye.inc/orion**
or contact us at o**e_japan@eyesopen.com**

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