

Welcome! The OpenEye webinar will start shortly

Make sure you're ready to attend the webinar:

- Check your system:
<https://support.goto.com/webinar/system-check-attendee-av>
- Troubleshoot any connection problems:
<https://support.goto.com/webinar/help/i-cant-join-my-session>
- Mute or minimize other programs so you can focus on the presentation
- Have a program open to take notes, if helpful

Orion 2020.2 Update

Matt Geballe
VP of Product

September 17, 2020

Agenda

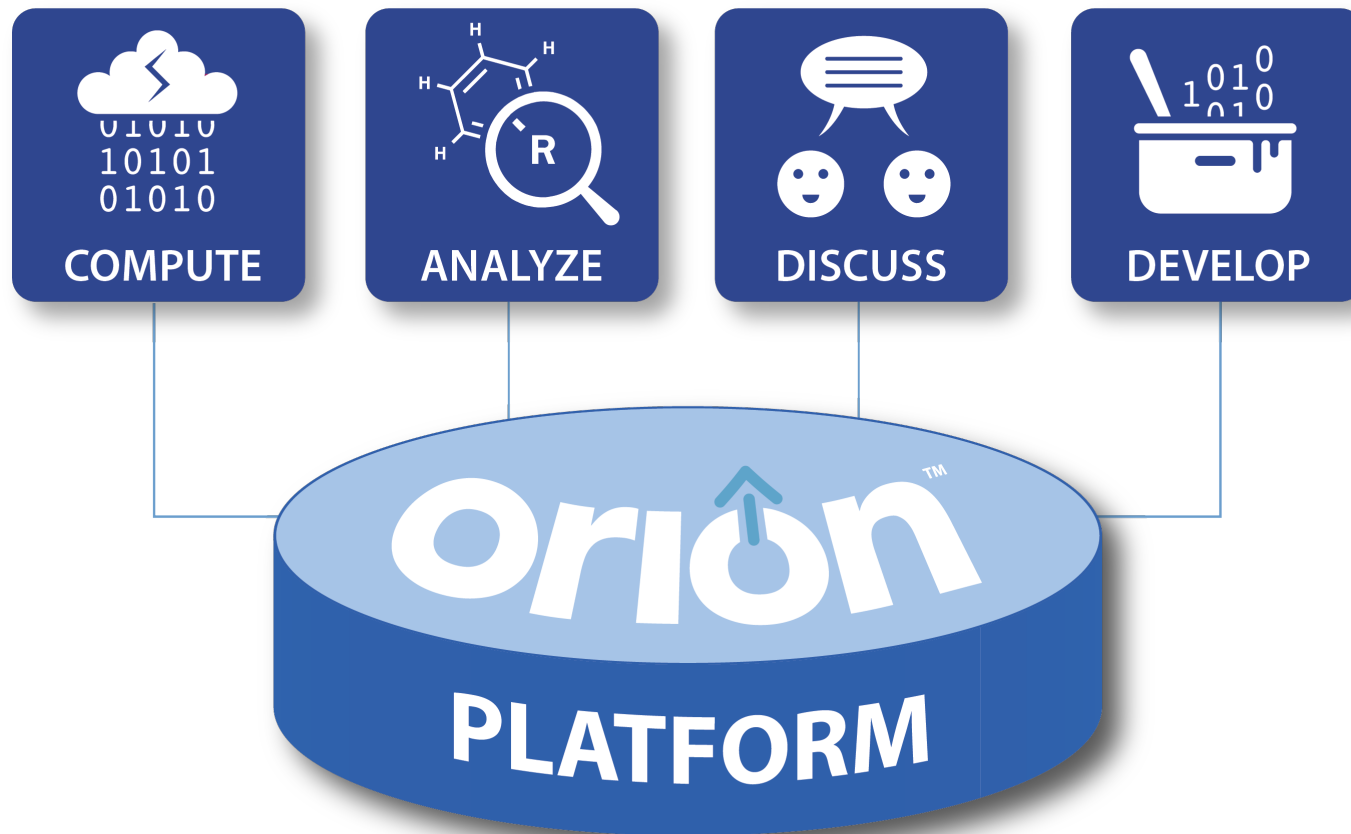
- Orion Intro
- Updates for Users
- Updates for Programmers
- Updates for Admins/IT
- Future Plans



Stellar nursery NGC 2174



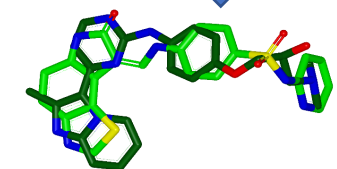
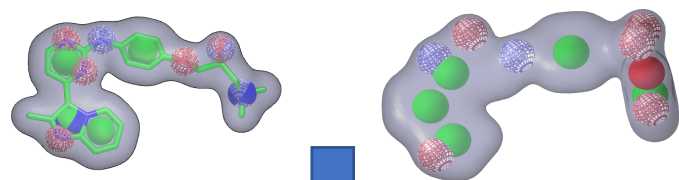
Cloud-Native Molecular Design



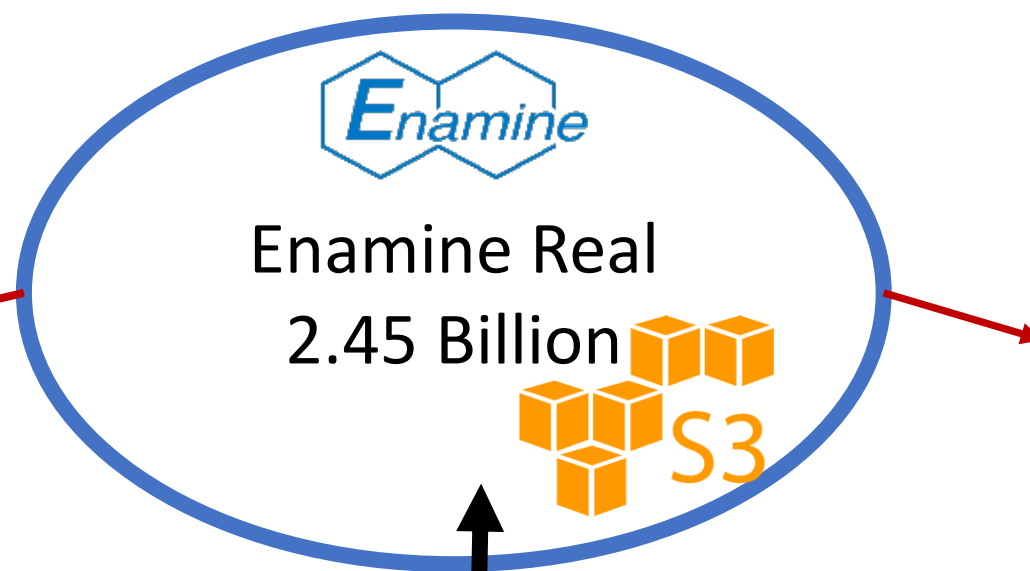
Large-Scale Virt. Screens require a Platform

FastROCS on Enamine Real

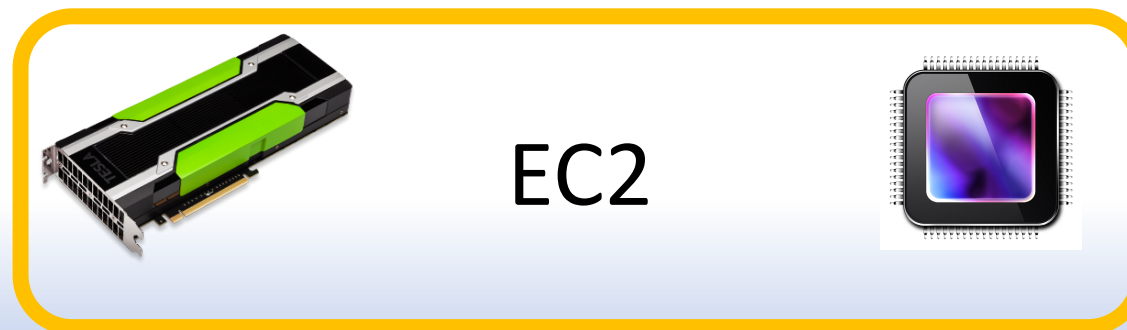
- 3D Ligand Based
- Runtime ~ 30min
- Cost: **\$50-\$200**



3D Tanimoto
Similarity

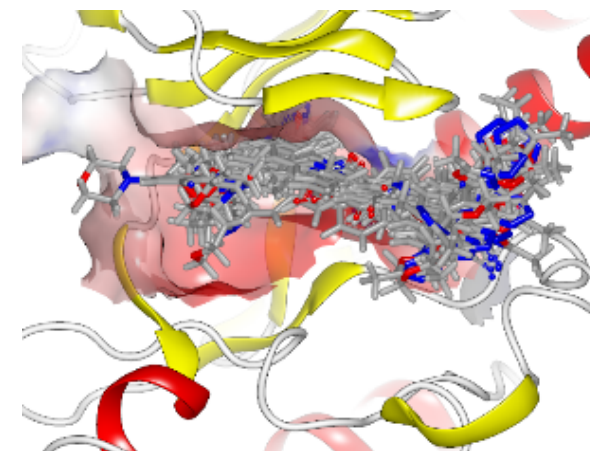


Other Commercial or Internal DBs



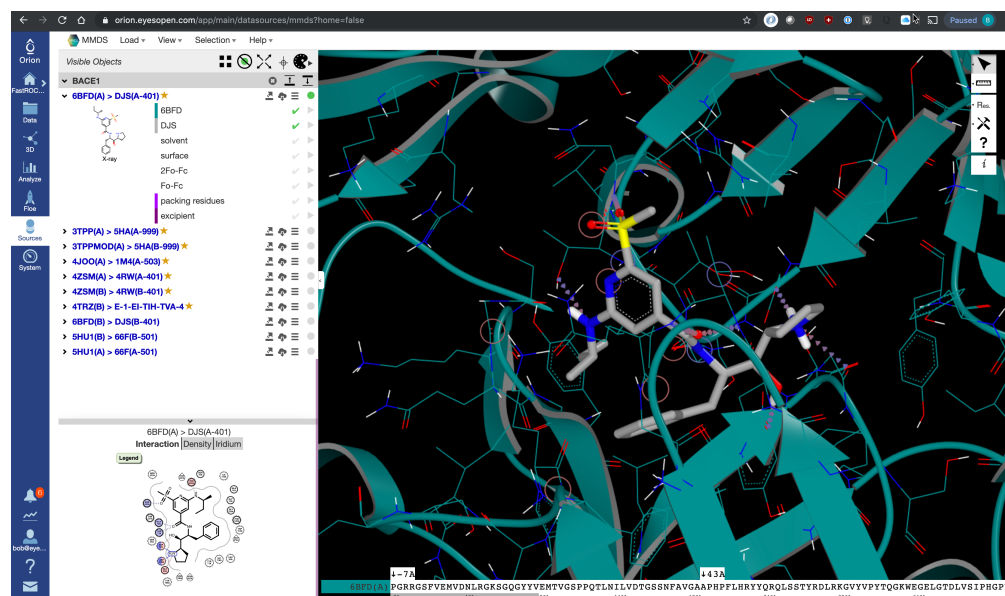
Docking Enamine Real

- Structure Based
- Runtime ~24 Hours
- Cost : **\$10k – \$30k**



Interactive Search and Exploration

MMDS



MaaS

History

Similarity Substructure Exact By Title

Sketch query or paste SMILES/MOL/SDF with Ctrl-V

Query Title: s_2230 12430396 680298 S

Database: Enamine REAL 2019q3-4 (1,211,723,723 molecules)

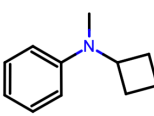
Number of matches to retrieve (1-1000): 100

☐ Match atom stereo.

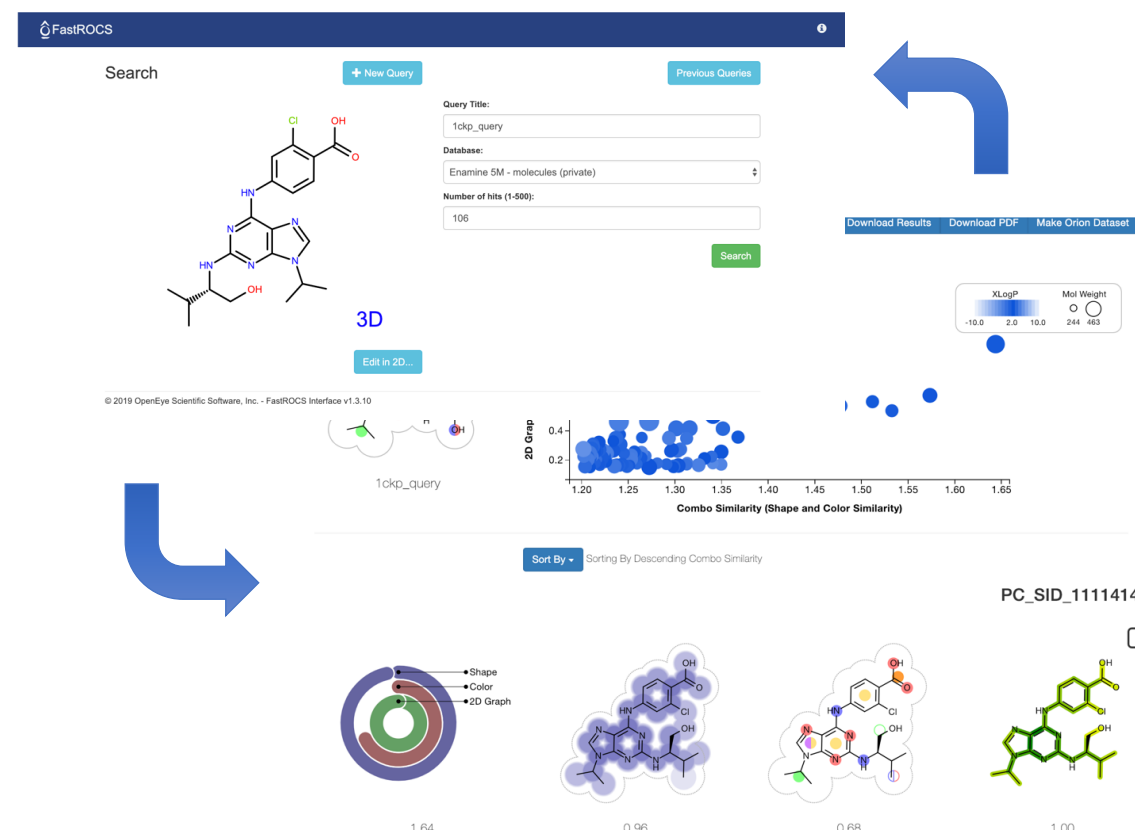
☒ Add bond aliphatic constraint.

☐ Add bond topology constraint.

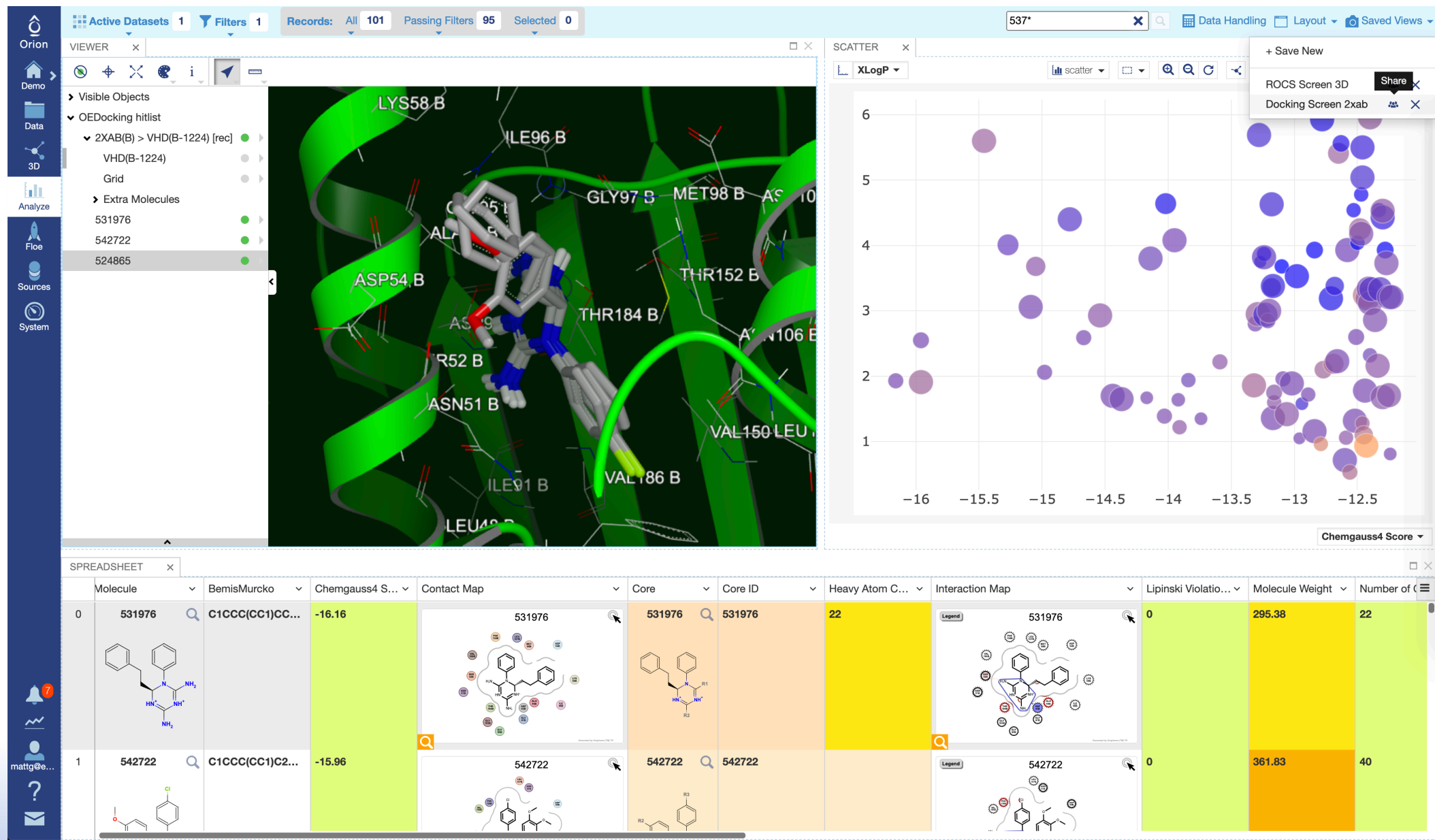
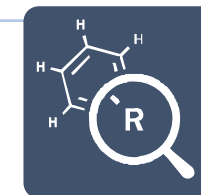
Search



FastROCS



Integrated Analysis and 3D



Data Storage: General, Flexible, Integrated

- Project-centric
 - Flexible access permissions
- Sharing is fundamental
 - Cornerstone of Orion's design
- Storage models designed for scale
- Generic data container
 - C++ implementation
 - Uses beyond molecules
 - **Integrated into Orion UI**

Project Members

Share view: 2xab Docking View

Sharing this view will also grant read-only permissions on the dataset(s) it includes:
OEDocking hitlist

Share this view with:

Gunther Stahl x Search for users and projects

Allow user to:

☒ read ☐ write ☐ delete

Grant Access

Nobody else has access to this view yet.

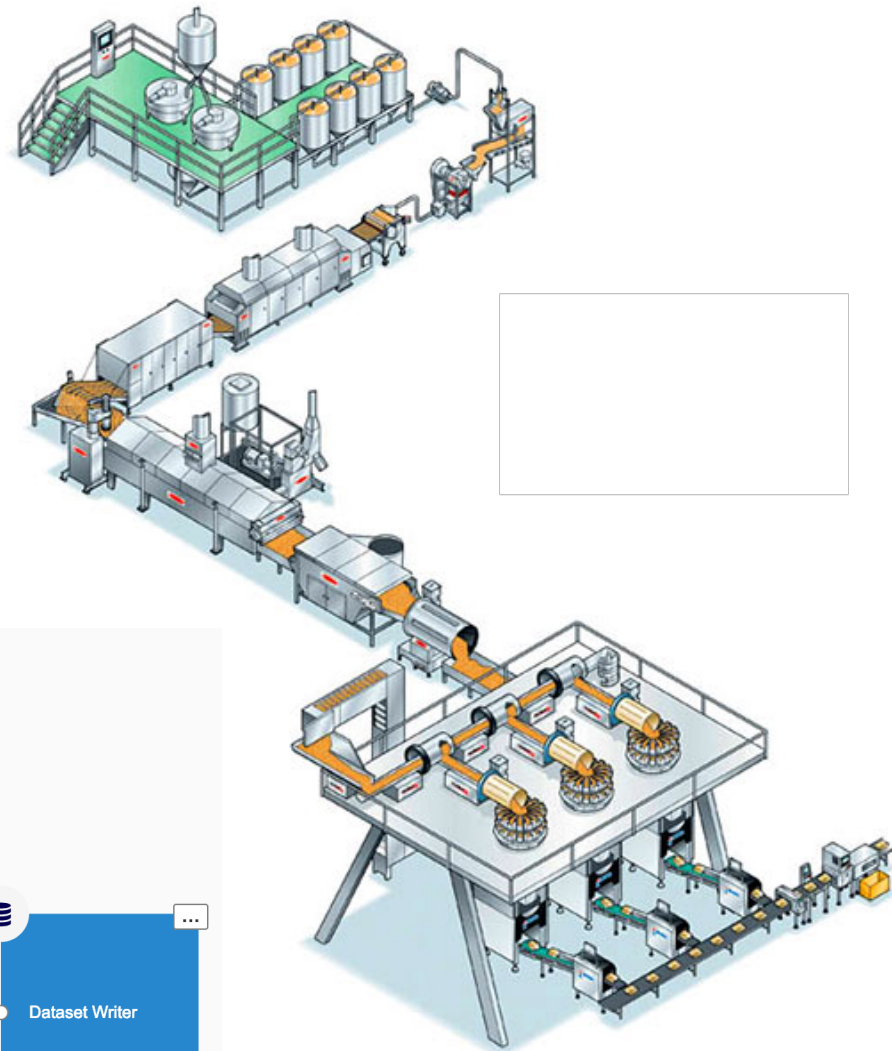
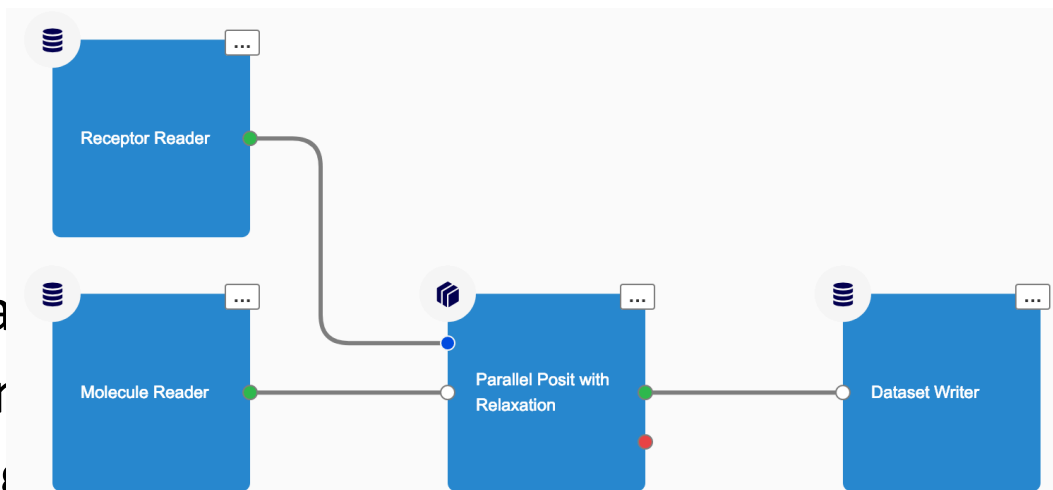
Done

	Molec				
2					
3					
4	532278	C1CCC(CC1)C2...		1.21	27



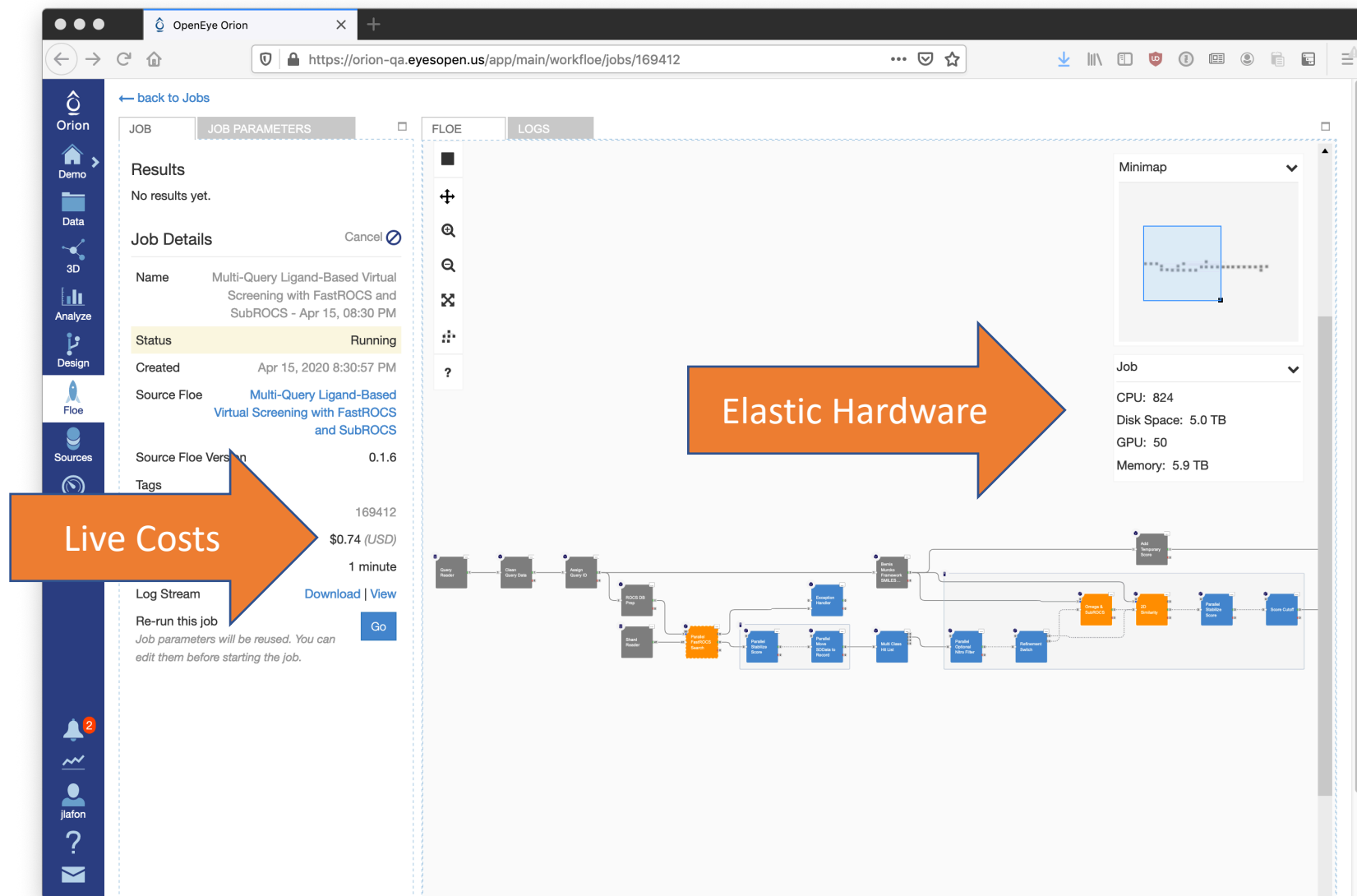
Flow-Based Programming

- Independent units of work (Cube)
 - Data flows through
- Assemble units for a specific task
 - (Floe)
- Good fit for
 - Inherent parallelism
 - Independent tasks
 - Ease of prototyping



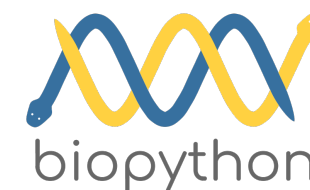
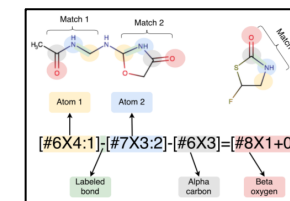
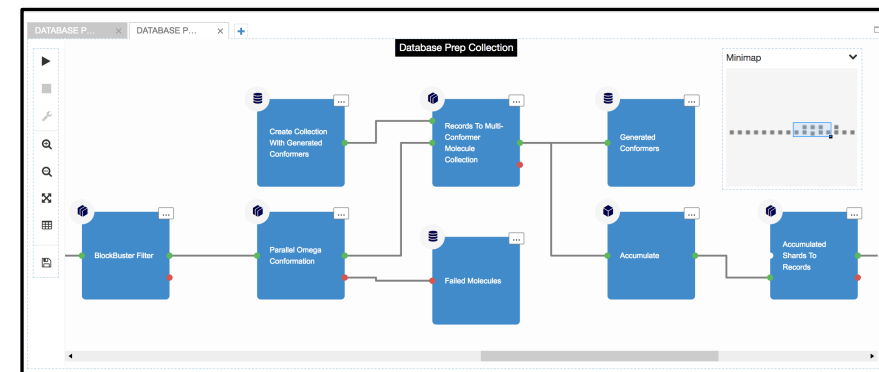
Running Floes in Orion

- Workflow paradigm (cubes and floes)
- Powerful, cost-aware scheduling
 - Cycles
 - Per-cube hardware requirements
 - On-demand & Spot
- Project & User Cost Accounting



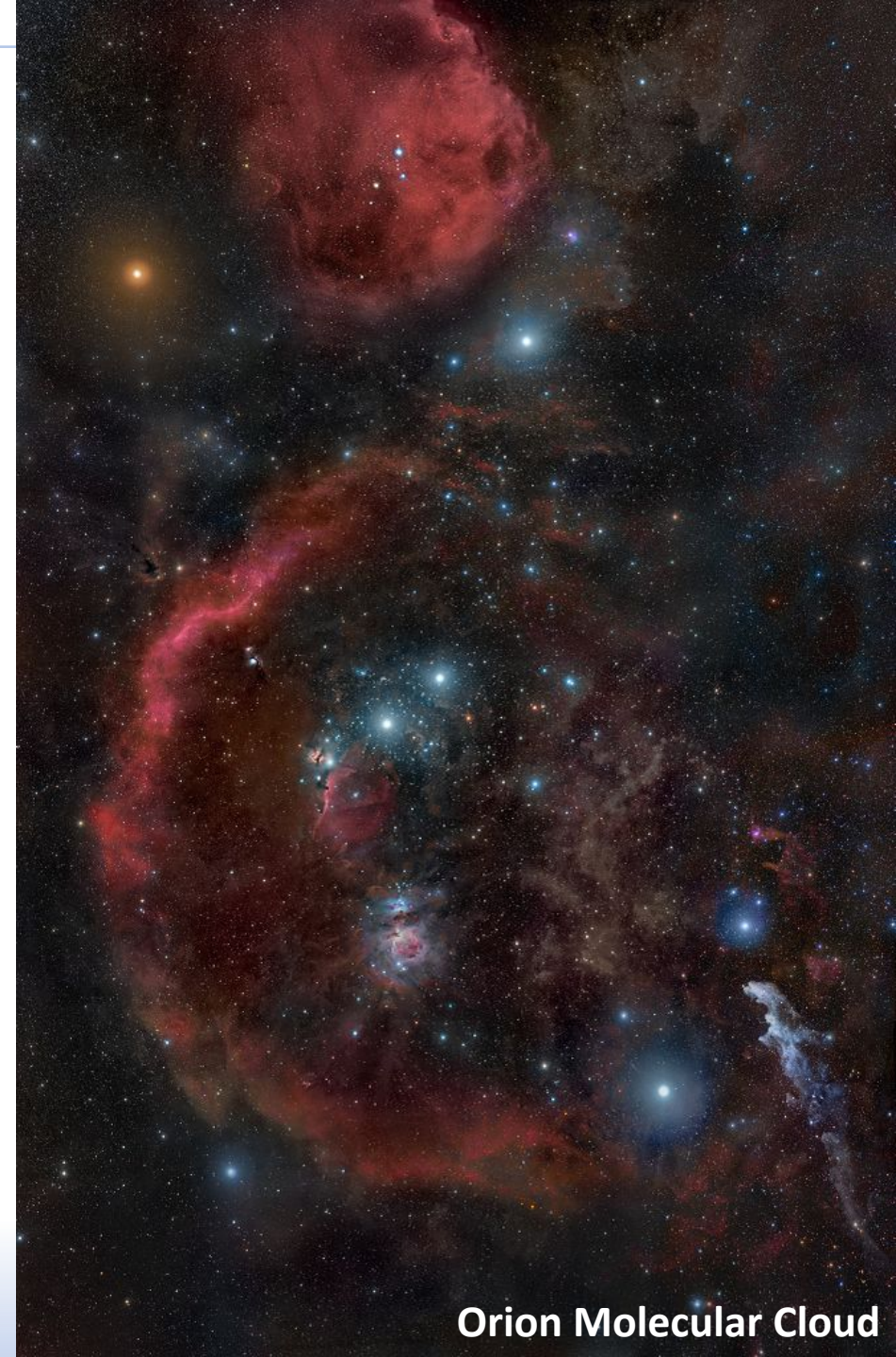
Open Programming Platform

- Python to its core
 - Cubes are Python
 - Floes assembled in Python or UI
- Compiled binaries
- Third-party libraries
 - PSI4, OpenMM, GROMACS, etc
 - Scientific Python ecosystem
 - Commercial Code*



Agenda

- Orion Intro
- Updates for Users
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Orion Molecular Cloud

Search Billions in Seconds with MaaS

- Molecules-as-a-Service available in Orion
- Blazing fast 2D, Substructure, Exact Structure search

Search Billions in Seconds with MaaS

- Molecules-as-a-Service available in Orion
- Blazing fast 2D, Substructure, Exact Structure search

The screenshot displays the Orion MaaS web interface. On the left is a dark blue sidebar with navigation icons for Orion, Home, Data, 3D, Analyze, Floe, Sources, and System. The main content area has a top navigation bar with 'MaaS' and tabs for 'History', 'Similarity' (selected), 'Substructure', 'Exact', and 'By Title'. Below the tabs, a central workspace shows a chemical structure of a quinoline derivative with a cyclopropyl group. To the right of the workspace is a search configuration panel with fields for 'Query Title' (PV-002892159077), 'Database' (Enamine (Simple) [2020q1-2] 2D (932,635,641 molecules)), 'Fingerprint' (circularvs), 'Number of hits to retrieve (1-1000)' (200), and 'Similarity Measure' (Tanimoto). A green 'Search' button is at the bottom of this panel. At the bottom of the interface, it shows 'Logged in as: matlg', an 'About' link, and a copyright notice: '© 2020 OpenEye Scientific Software, Inc. - MaaS v1.0.0'.

Prepared Vendor Collections






- Newly prepared databases for searching in 2D and 3D
 - MaaS: Enamine 2020q1-2, Mcule Ultimate, WuXi GalaXi (MW < 450)

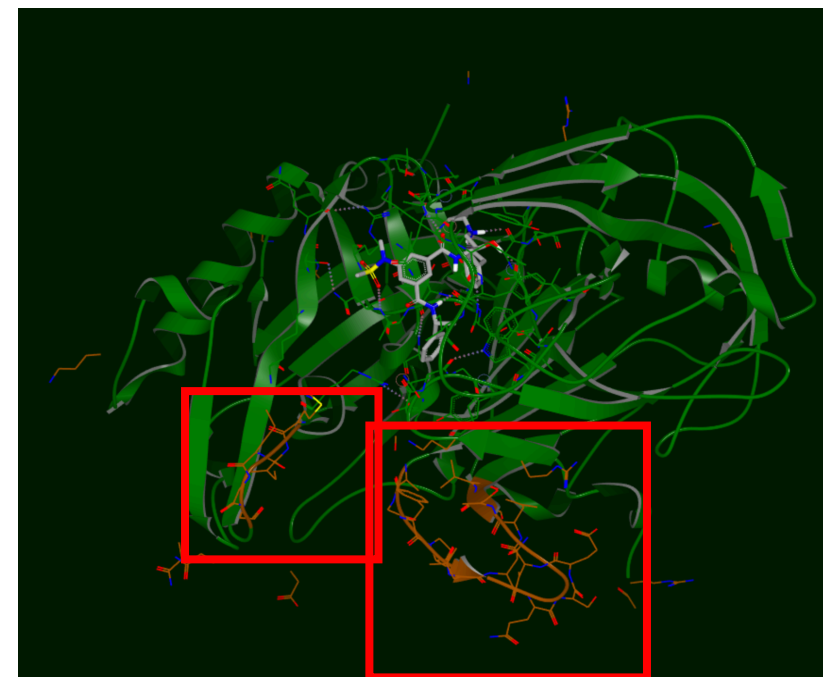
Collection	LBVS with FastROCS	Gigadock
Enamine Real (2.7B)		
Enamine Real "Simple" (1.8B)		Upon Request
Enamine Real "Hard" (968M)		Upon Request
Mcule Ultimate (159M)		Upon Request
WuXi GalaXi MW <= 500, nRotors <= 10 (1.1B)		Upon Request

- Also have 10M random subsets of each for Gigadock benchmarking

Improved Floes

- Merged “Giga Docking” floe with new Fast-FRED mode
 - Merged multiple DB prep floes into “Prepare Giga Collection”
- } Large Scale Floes
- Loop Modeling in Spruce Prep Floes
 - Ligand-centric STMD Analysis in MD Floes
 - New methods to generate reasonable analogs
 - Sprout, Trim
 - Join with Reagents

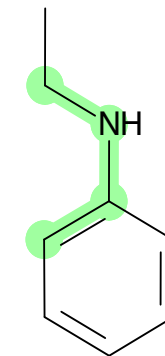
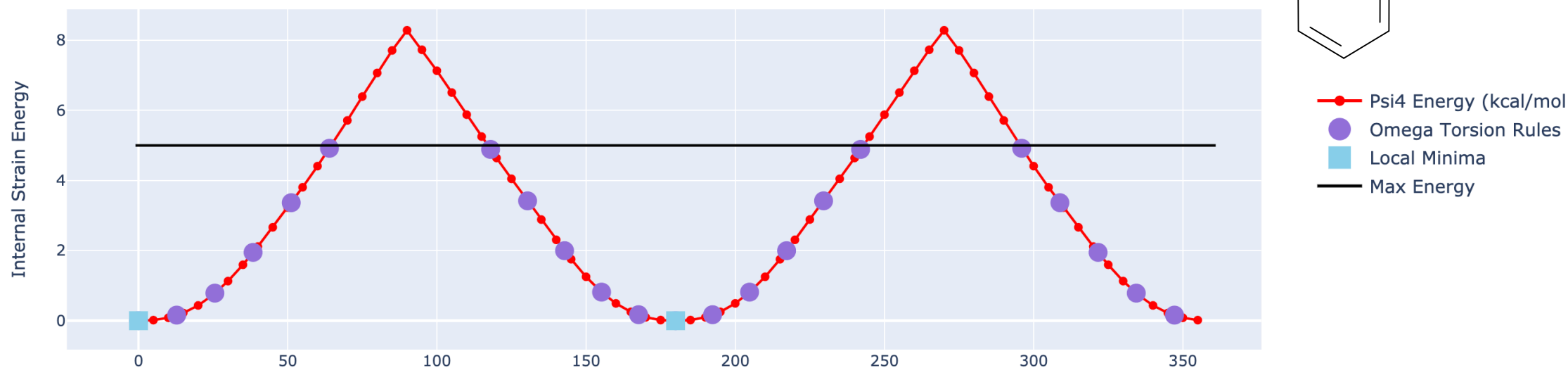
	Molecule	site_selection	generative_method	MedChemInterest	MolComplexity
0	51:GRAFT:lisinopril		Graft	1.34	0.78
1	52:GRAFT:lisinopril		Graft	1.35	0.739
2	28:GRAFT:lisinopril		Graft,MMP5sprout	1.37	0.671
3	16:GRAFT:lisinopril		Graft,MMP5sprout	1.37	0.67
4	339:lisinopriltopliss-17		Join	1.37	0.667



PDB-ID: 3TPP. Modeled pieces in brown

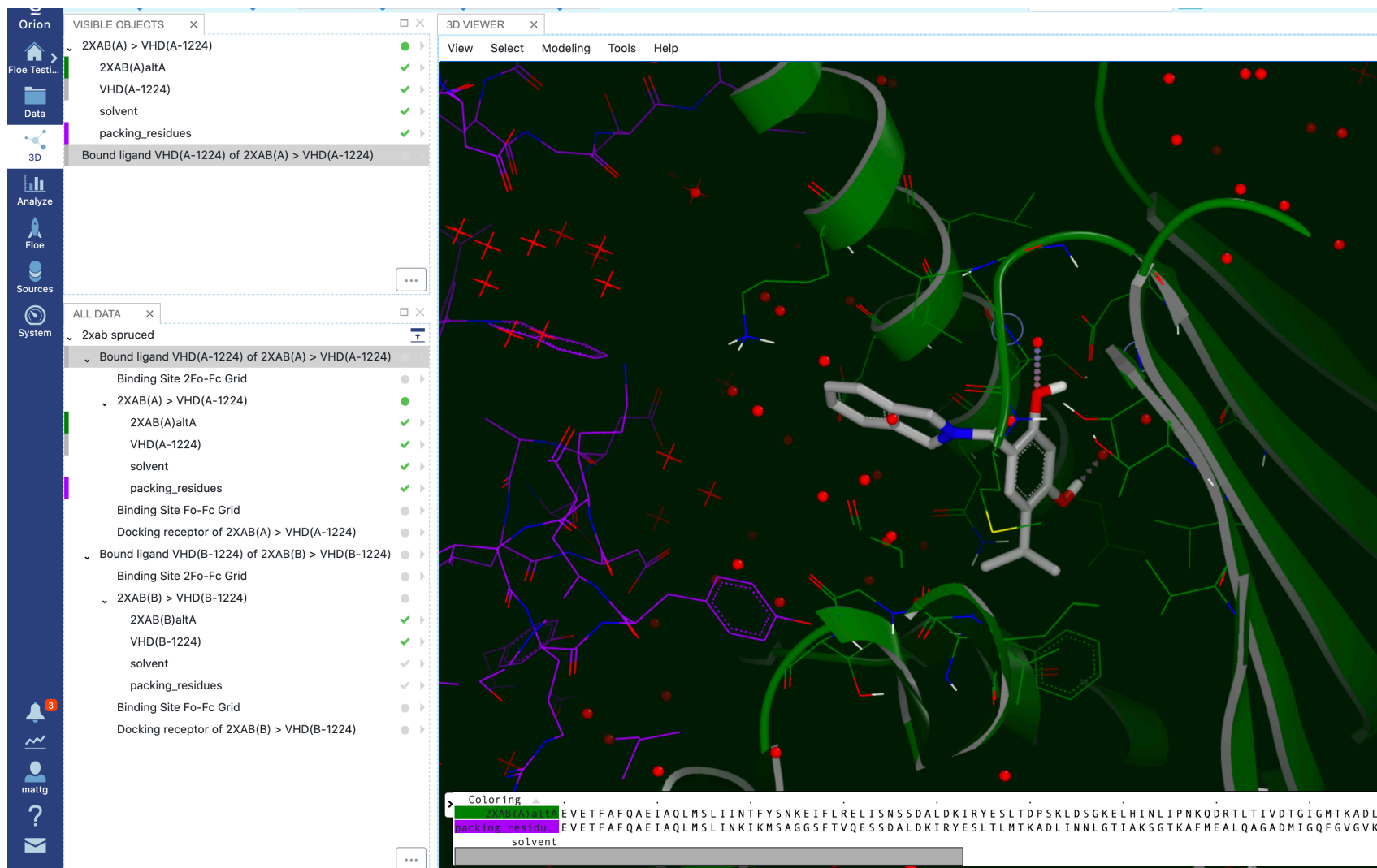
New Floes

- Automated Fragmentation and QM Torsion Scan
 - Generate custom torsion rules for conformer generation



- 2D Clustering using DBSCAN
- Build targeted libraries with simple reagent enumeration floe package

Visualization of Spruce Design Units



- Work with all separate components of a Spruce DU in Orion

And Much More

Parsley v1.2
in MD Floes

Curated Guide to
Pharmacology
data in MMDS

Selection tools in 3D
Modeling viewer

UI Refresh

Parallel cubes finish and
pass on work faster

Sped up job start-up
and teardown



Floe-Launching
Widget in Analyze

Floes to search
MaaS

Wildcard support
when filtering on text

ShapeQuery Support
in Classic ROCS

OpenFF 1.0 Support
in Classic Floes

Secondary list
in 3D Viewer

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M42 Orion Nebula

Platforms Progressing

OEToolkits v2020.1

OrionPlatform v3.0.1

Snowball v0.19.1

Python \geq v3.6

- C++ implementation of OERecords
 - Improved performance and memory management
 - Work with OERecords locally using just OEToolkits
 - Minimal code changes necessary
- New TK functionality in Snowball cubes
 - Loop Modeling in Spruce
- DUs have their own type: `Types.Chem.DesignUnit`
 - Updater floe in Classic Floes to enable in UI

Standard Scaling Groups

- Standard sets of EC2 instances configured
 - Provide standard ratios of RAM/CPU and Disk/CPU to target
 - Compute- and Memory-optimized hardware of various sizes

Instance Class	RAM/CPU	Disk/CPU (Spot)	Disk/CPU (Non-Spot)
Compute Optimized	2 GB	5 GB, 20 GB, 50 GB	20 GB, 50 GB
Memory Optimized	8 GB	10 GB, 50GB, 100GB	20 GB, 50GB, 100 GB, 200 GB

- Other instance types still configurable on managed service Orion

Performance Improvements

- Speed up Job start-up and tear-down
- Memory Usage
- Draining work from Parallel Cubes
- Parallel to Parallel connections

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Admin/IT Features

- User management for Admins
 - Unlock, activate/deactivate, role management
- Single Sign-On with a SAML Identity Provider
- User UI for Token Management



My Tokens

Tokens can be used to programmatically access Orion via OCLI.

Delete

+ Create Token

Description	Value	ID	Created
maas 🔗	21550	08/31/2020 @ 10:01 PM
orionclient token on pueo.local 🔗	19767	07/22/2020 @ 4:02 PM
fastrocs 🔗	5587	02/11/2019 @ 10:24 AM
orionclient token on shaka.local 🔗	989	10/31/2018 @ 12:43 AM



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Flame Nebula

Going Forward

- Orion Release Roadmap
 - 2020.1 – April
 - 2020.2 – August
 - 2020.3 – November 
 - 2021.1 – Feb 2021 
- Focus: Interactive Modeling
 - Bring calculations and results to users while retaining focus on the data
 - 3D Design
 - Generative Chemistry
 - Physics-based Molecular Properties
 - Cheminformatics & Clustering
 - Statistical Models



2020.3 Features

- Users
 - Floes that add new columns integrated into Analyze Page
 - Enhanced data organization within a Project
 - Floes for BFE via NES, Permeability via WESTPA, GPU Omega, and more
- Programmers
 - Controlling parameter ordering
 - Writing floes to update data on the Analyze page
 - More container OS options for cubes (Ubuntu18, Ubuntu20, AL2)
 - Require Python ≥ 3.7
- Admins/IT
 - Improved integrated service authentication

A person's silhouette is visible on the right side of the image, looking up at a vast, starry night sky. The Milky Way galaxy is visible as a bright, hazy band of light stretching across the sky. The text is centered in the upper half of the image.

Thank You

Questions?

Interested in an Orion Walkthrough?

Please email info@eyesopen.com