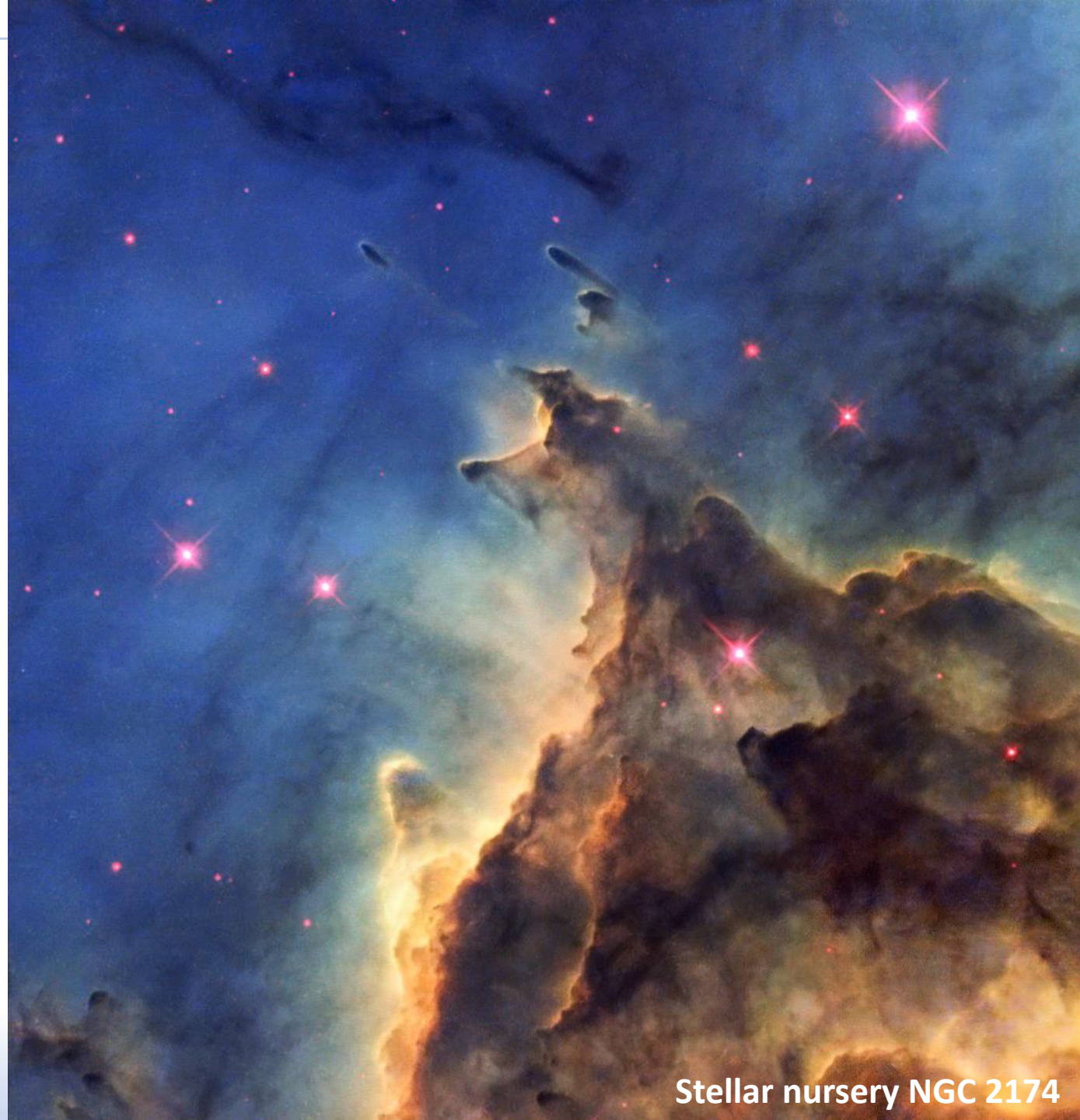


Looking Over the Horizon: Orion in 2021 (and beyond)

Matt Geballe
VP of Product
Spring miniCUP 2021

Agenda

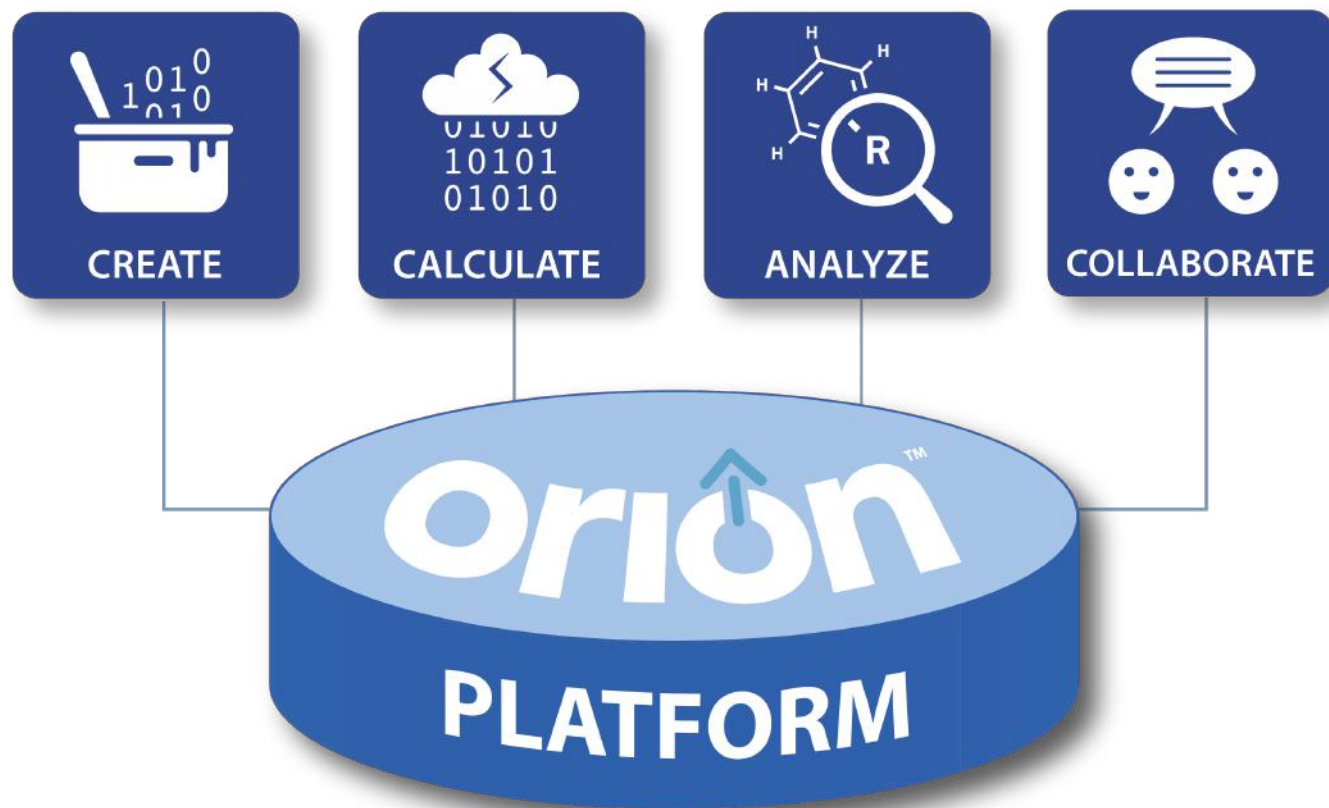
- What is Orion (in 2020)
- What's Coming in 2021.1
- Over the Horizon



Stellar nursery NGC 2174



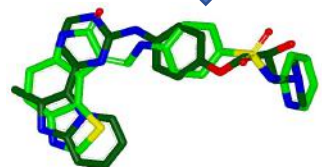
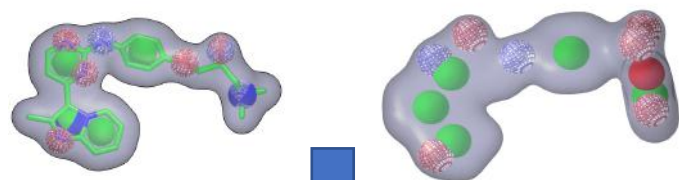
Cloud-Native Molecular Design



Well-known for VS Calculations at Scale

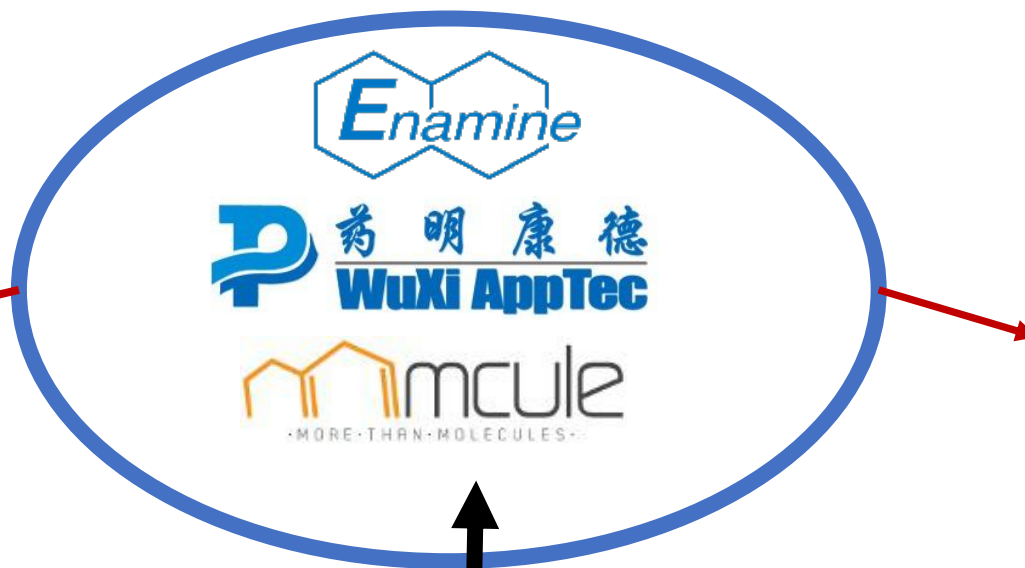
FastROCS on Enamine Real

- 3D Ligand Based
- Search 2.5B
 - Time: ~ 30min
 - Cost: **\$50-\$200**



3D Tanimoto
Similarity

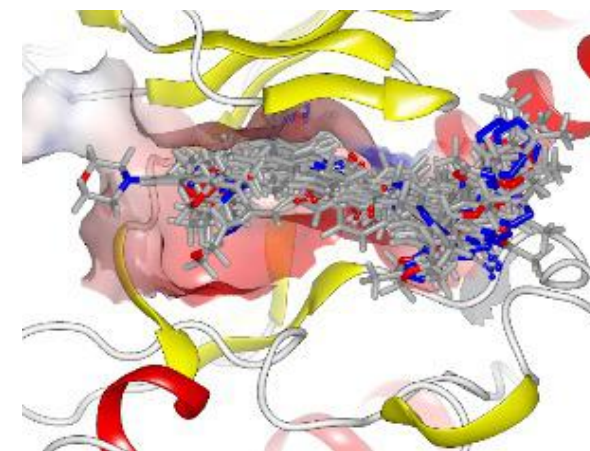
Billions



Other Commercial or Internal DBs

Docking Enamine Real

- Structure Based
- Search 2.5B
 - Time: ~24 Hours
 - Cost : **\$10k – \$30k**



Not just Virtual Screening

Classic Floes

Replicating familiar
OpenEye Apps

Generative Floes

MMPs, 2D fragment
replacement, transform
extraction

ChemInfo Floes

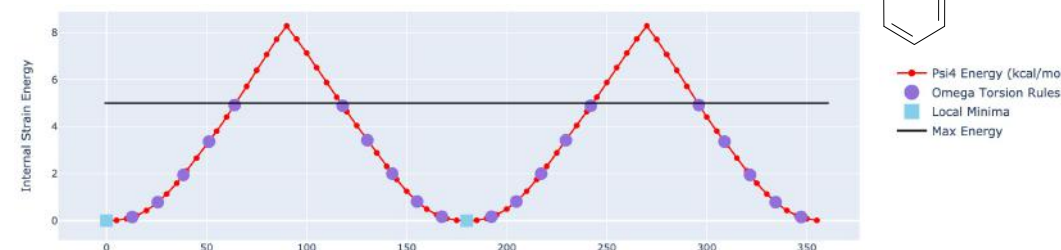
Fingerprints, Filtering,
Clustering, Bemis-Murcko

BioModeler Floes

Protein Prep and
Modification, Loop
Modeling, SiteHopper

QM Floes

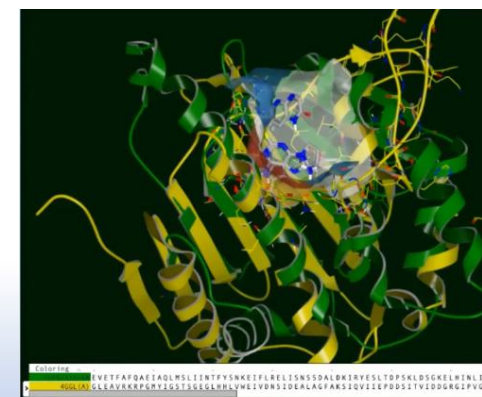
Fragmentation, Torsion
Scanning, GeomOpt, Tautomers



orionTM

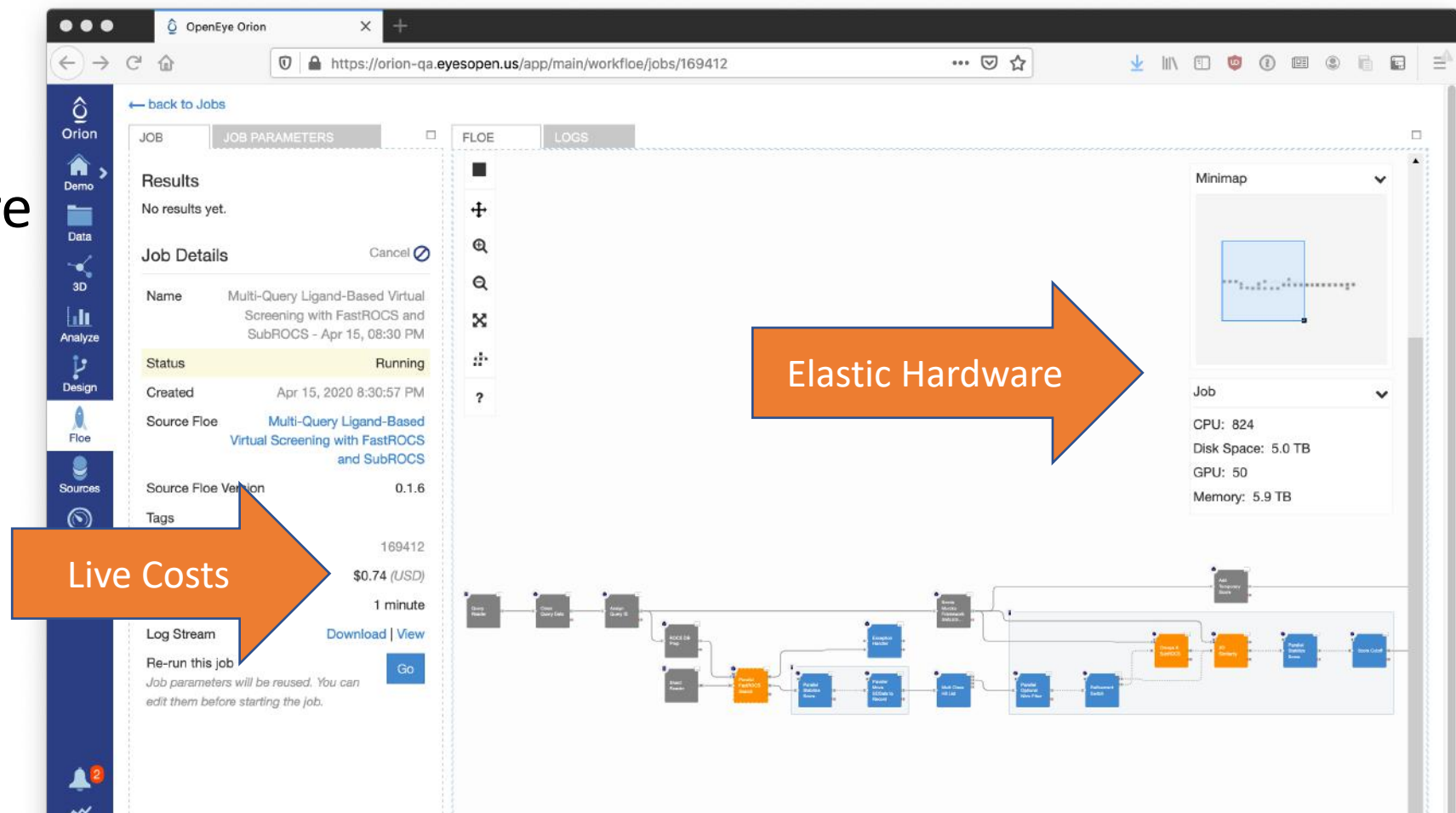
MD Floes

“Standard” MD, Solvate
System, P-L MD and
Analysis



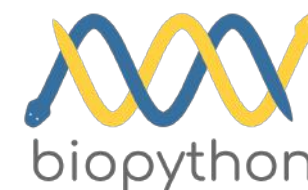
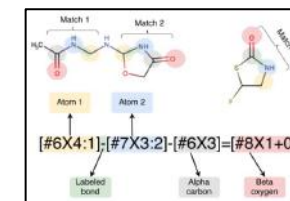
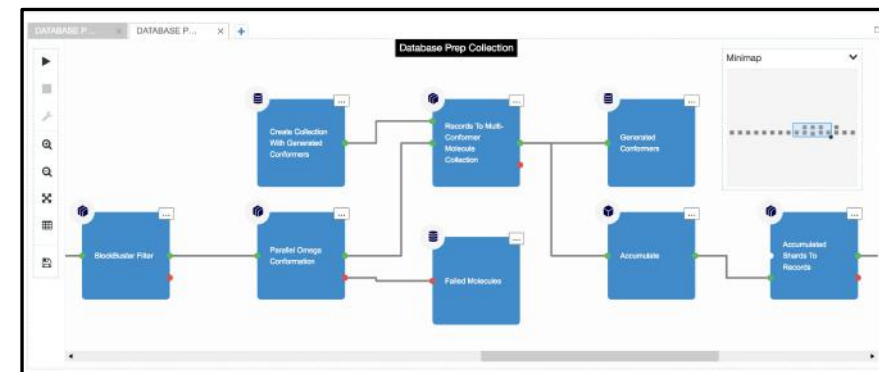
Orion Orchestrates Compute Resources

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



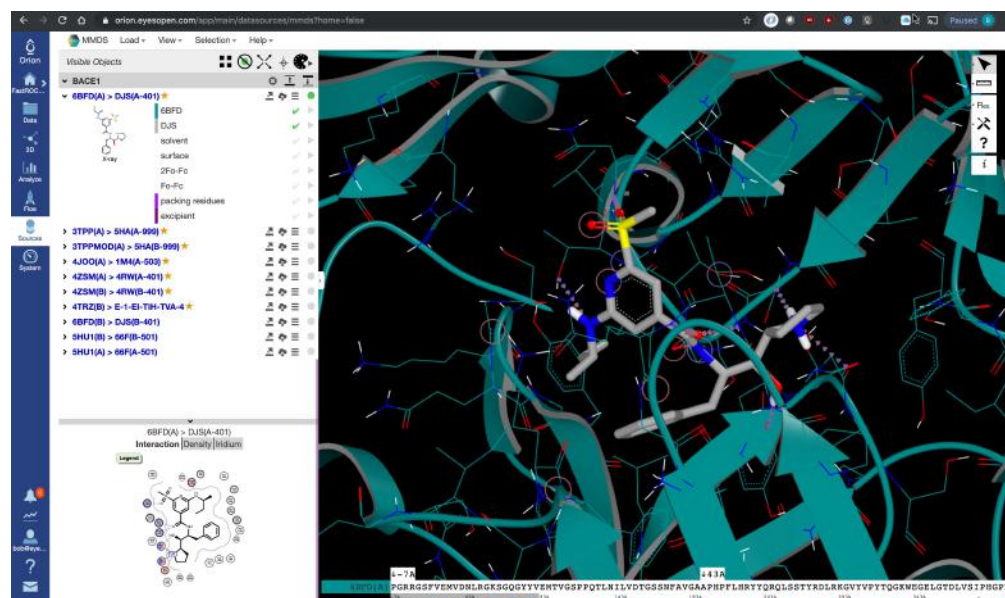
Open Programming Platform

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

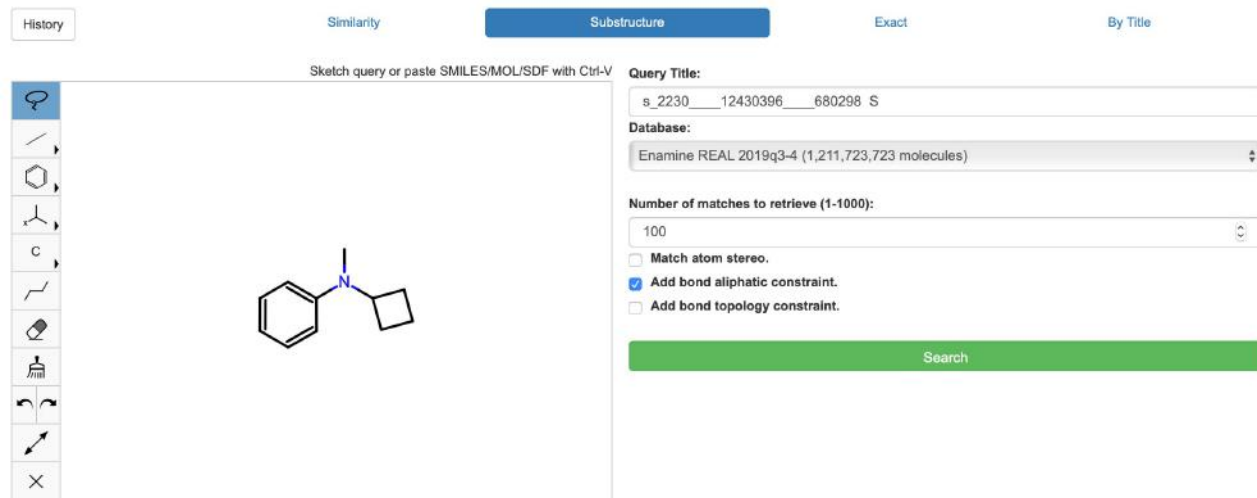


Interactive Search and Exploration

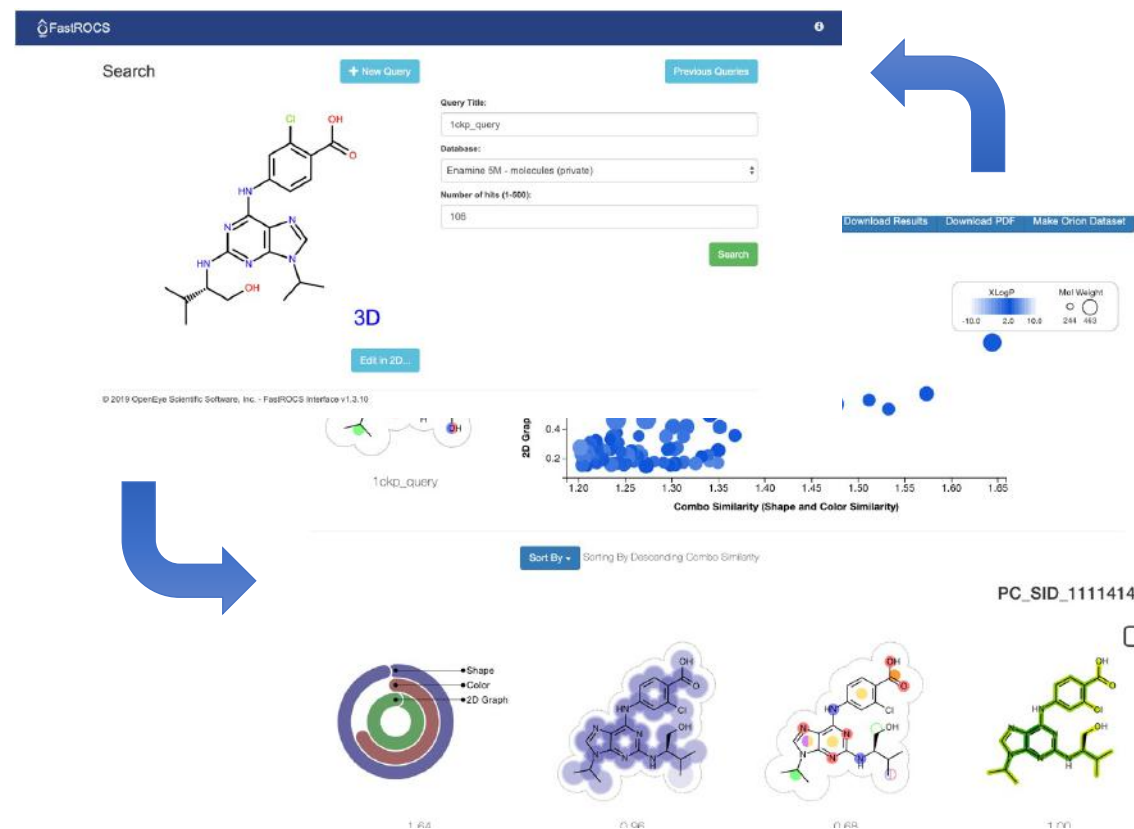
MMDS



MaaS



FastROCS



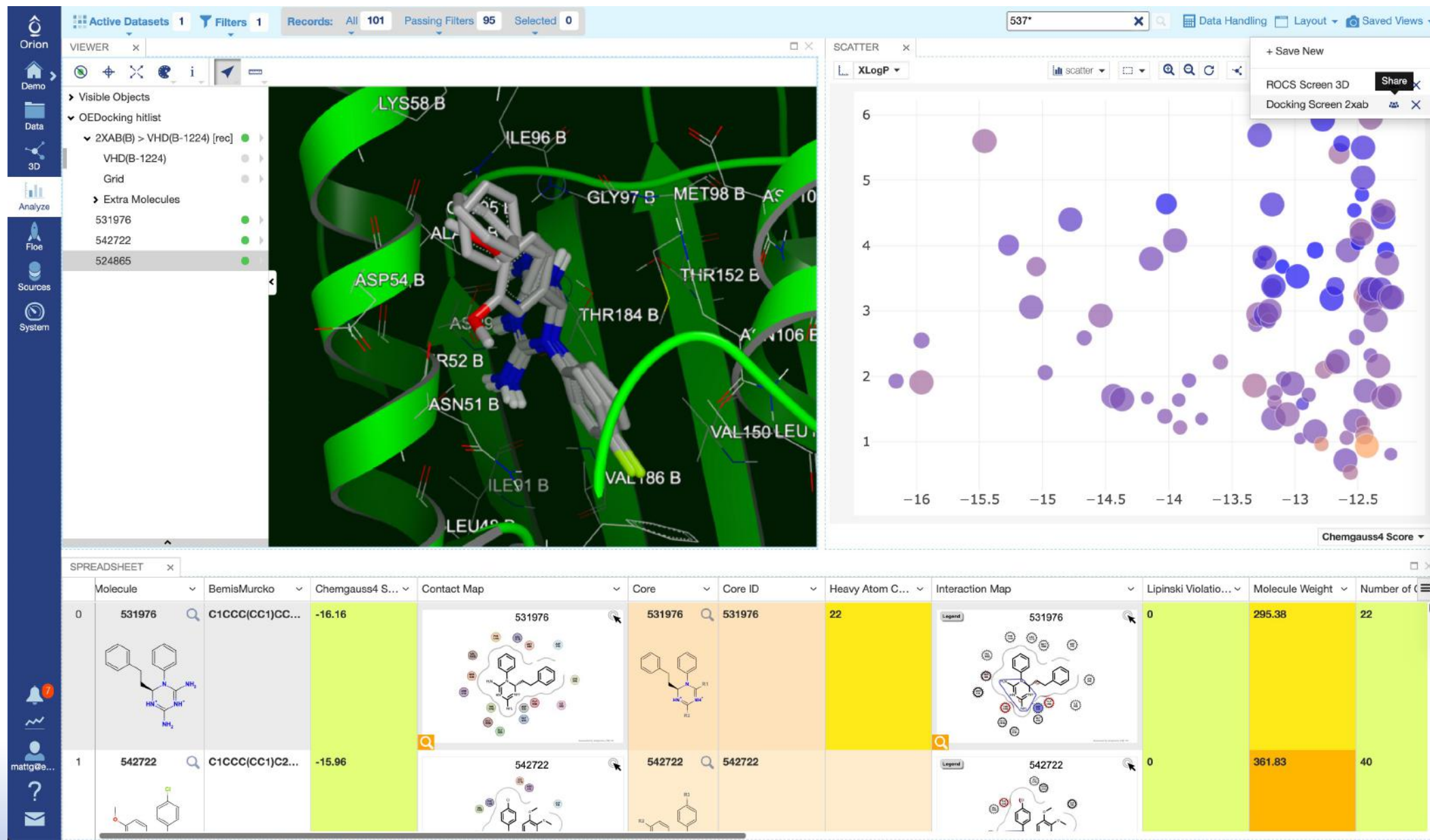
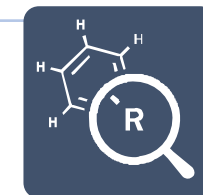
Search Billions in Seconds with MaaS

- Blazing fast 2D, Substructure, Exact Structure, Title search

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

Exploration, Screening, Hit Expansion, and more...

Integrated Analysis and 3D



Data Storage: Cloud-Scale and Integrated

- Project-centric Data Organization
 - Flexible collaboration
 - Critical data shared across entire org
- Storage models designed for scale
 - Interactive analysis to massively parallel I/O
- 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

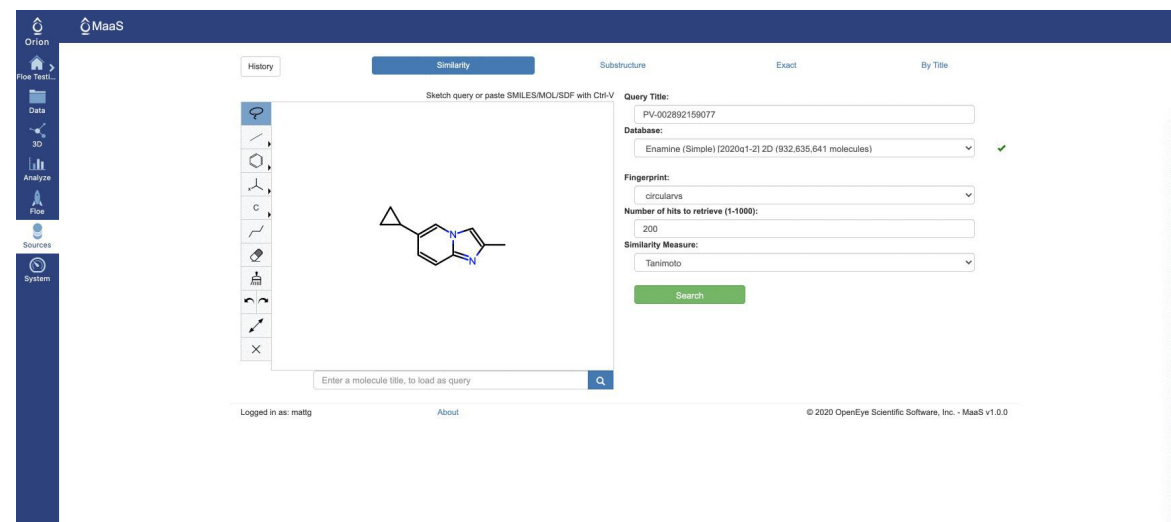
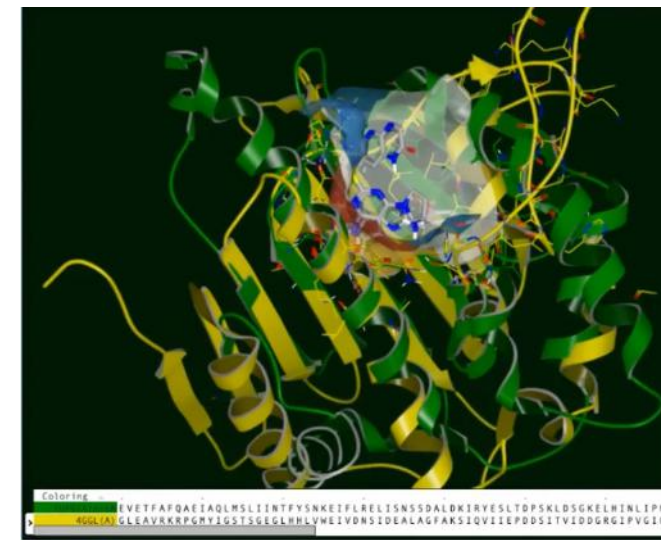
Nobody else has access to this view yet.

Done

	Mole
2	
3	
4	532278 <chem>C1CCC(CC1)C2...</chem> 1.21 27

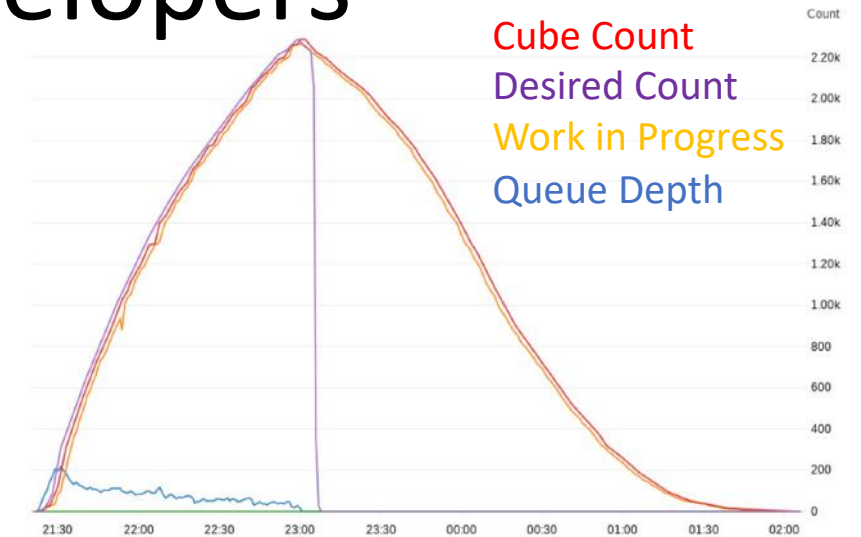
2020 Major Features – Users

- **New and Improved Floes and Floe Packages**
 - BioModeling, Loop Modeling, ChemInfo, Generative Floes, Large-Scale Floes, FastFred GigaDocking, New Collections
 - Documentation & Tutorials
- Externalized Vendor Collections (📁 storage costs)
- **Molecules-as-a-Service**
- DesignUnit Visualization
- **Interactive Binding Site Interactions**
- Better extrapolated cost estimates
- Integrated Floes on Analyze Page



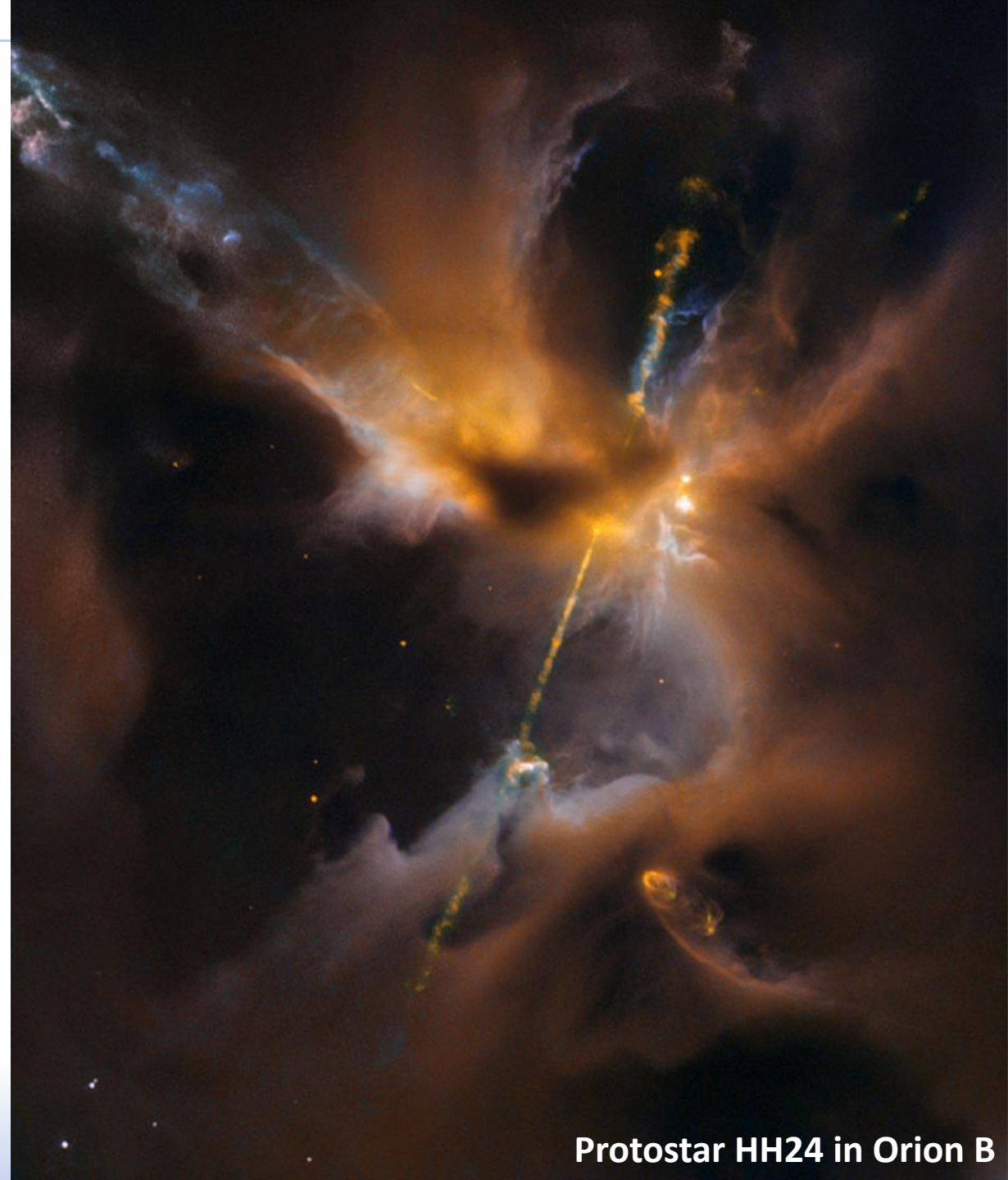
2020 Major Features – Floe Developers

- **Cube Metrics**
- Disk Quotas
- Better CUDA and GPU support
- improved flexibility in instance selection
- Standard Scaling Groups
- **Performance Improvements:** scale up/down, setup/teardown
- Cubes to append records to datasets and update records in-place
- **Control order of Promoted Parameters in UI**
- **OERecord into C++ Toolkits**



Agenda

- What is Orion (in 2020)
- **Coming Soon in 2021.1**
- Over the Horizon



Protostar HH24 in Orion B

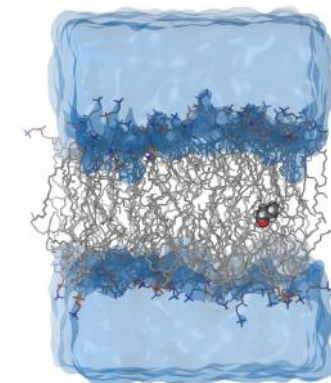
Orion 2021.1

- Largest update in several years
 - Hope to have it in your hands in June

- **Data Organization and Management**

- 3D Modeling Data
- Project Data

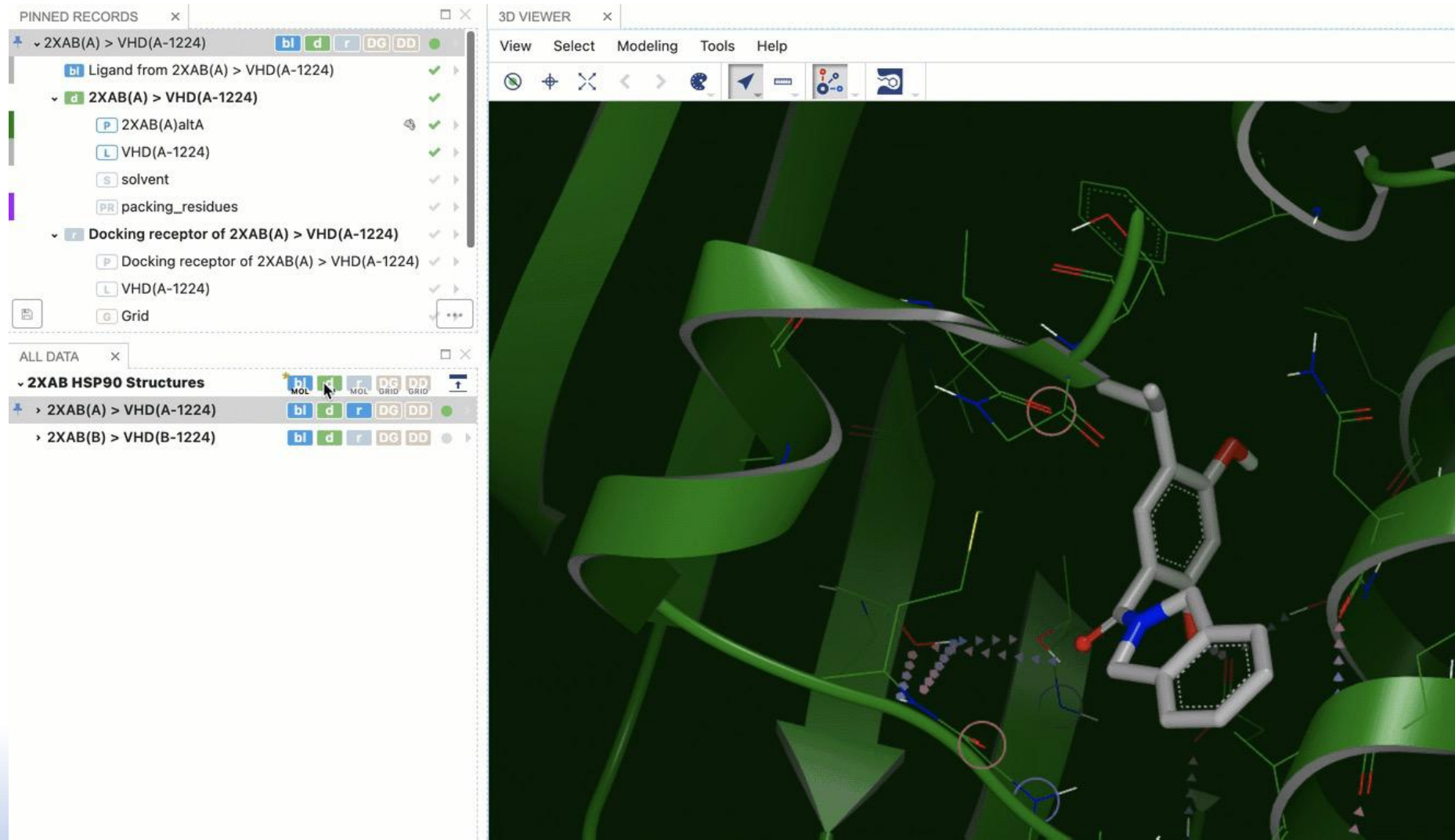
- Exciting new Science
 - Relative Binding Free Energy predictions with NES
 - WestPA Permeability model



- Cost Alert Thresholds
- Parameter Grouping and Organization
- Protein Editing
- Collaborative Discussion Boards
- and much more...

Managing Data in 3D Modeling






- Badging for visual information and control



Managing Data in 3D Modeling

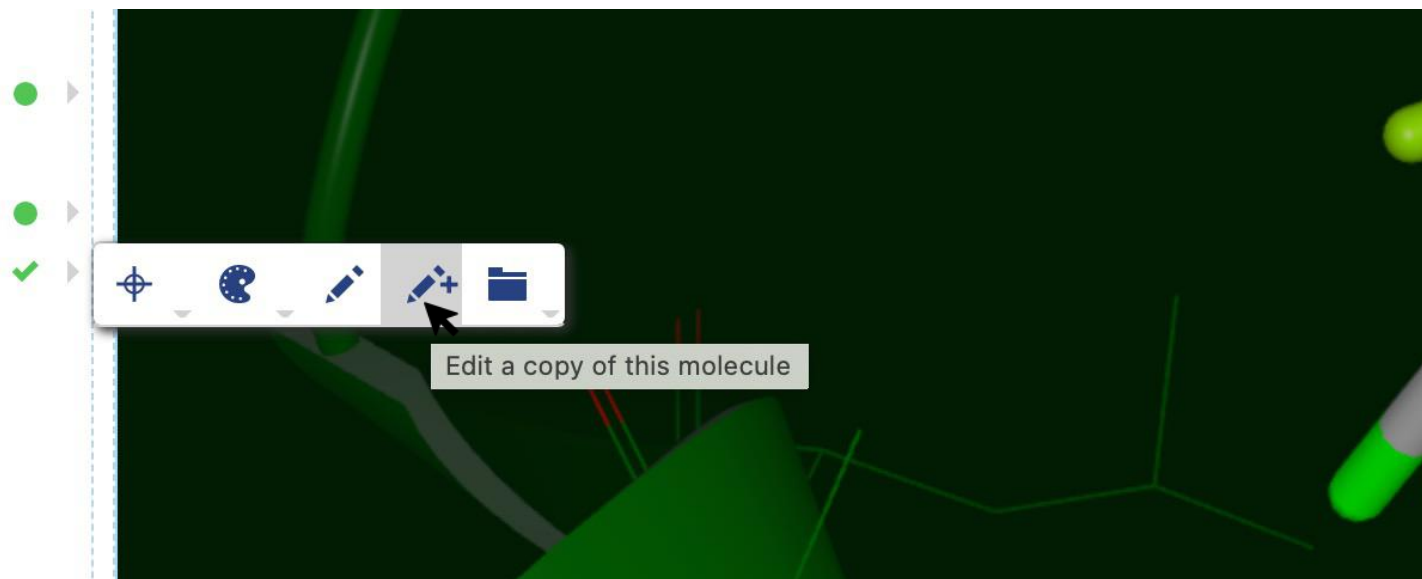
- Badging for visual information and control
- Controls over visibility

Data Handling

Column	Dataset	Type	All	3D	Spreadsheet	Plot	Tile View	Data Completeness
 bound ligand	2XAB HSP90 Structures	Molecule	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<div><div></div></div>
Active Site Depiction	2XAB HSP90 Structures	String	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<div><div></div></div>
B-Factor Depiction	2XAB HSP90 Structures	String	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<div><div></div></div>
 Density Grid	2XAB HSP90 Structures	Grid	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<div><div></div></div> 
 designunit	2XAB HSP90 Structures	Design Unit	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<div><div></div></div>
 Diff Density Grid	2XAB HSP90 Structures	Grid	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<div><div></div></div>
du_single	2XAB HSP90 Structures	Blob	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<div><div></div></div>

Managing Data in 3D Modeling

- Badging for visual information and control
- Controls over visibility
- Easier editing and saving



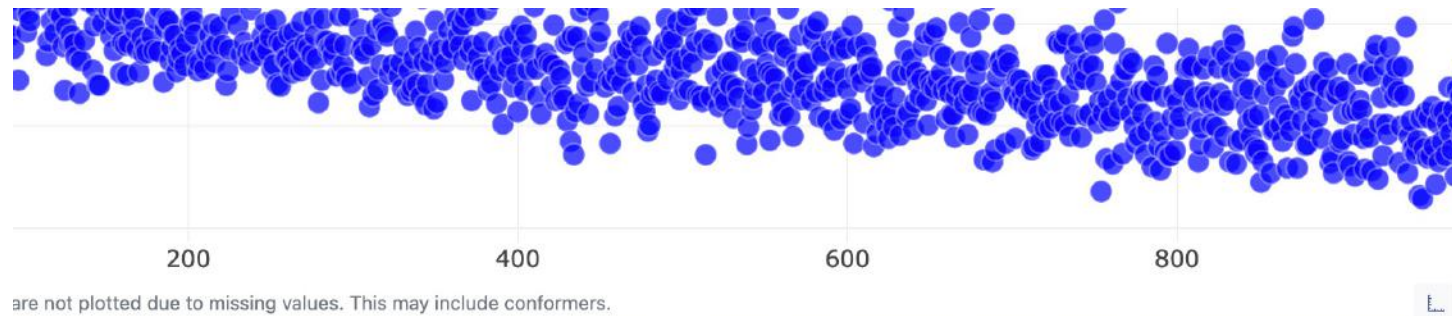
Managing Data in 3D Modeling

- Badging for visual information and control

- Controls over visibility

- Easier editing and saving

- Use Fields as Record Titles



Column Options ▾ Views:

ie URL ▾	Heavy Atom Co... ▾	idnumber ▾	Molecule Weight ▾	Shape Tanimoto ▾	Tanimoto Combo ▾	TPSA ▾	TPSA (Calculat... ▾
www.e...			442.41	0.83	1.38	76.15	
www.e...			401.52	0.81	1.38	66.84	
www.e...			386.44	0.689	1.35	84.94	
www.e...			409.52	0.799	1.35	83.91	

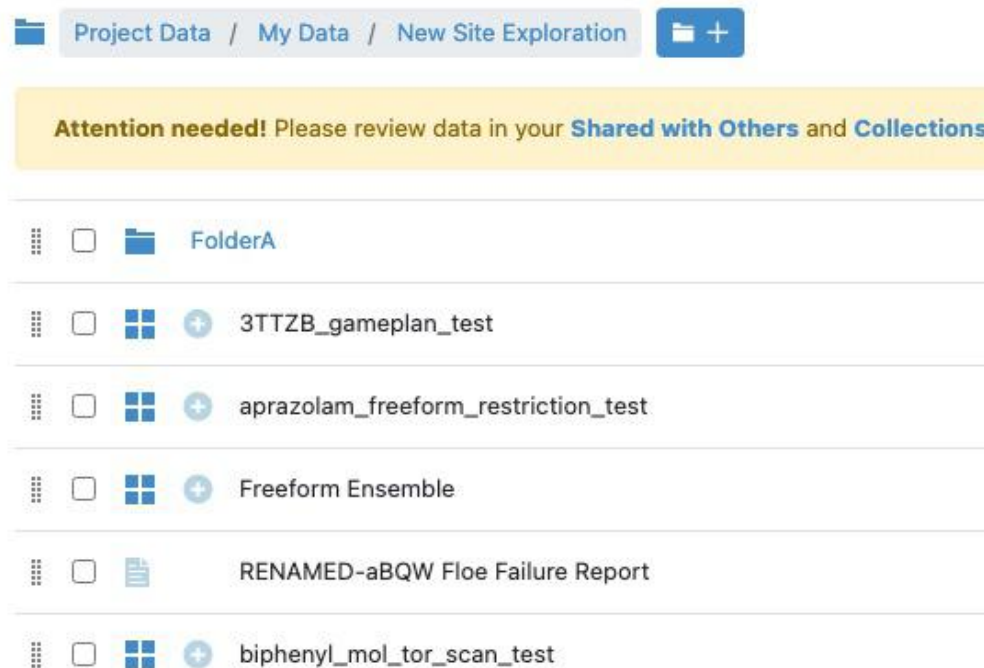
Context menu for 'idnumber' column:

- Sort Ascending
- Sort Descending
- Hide Column
- Delete Column
- Rename Column
- Click to set as record title
- Pin Left
- Pin Right

New Orion Data Organization

New Orion Data Organization:

- **Better** organization for **more** data via **familiar** concepts



Flat structure

All new data into same place

Separate View of Datasets/Files/Collections

Shared access via individual sharing



Multi-level organization with drag & drop

Control location of upload and floe output

Combined View

Location dictates shared access

Location Controls Data Access



Org Data



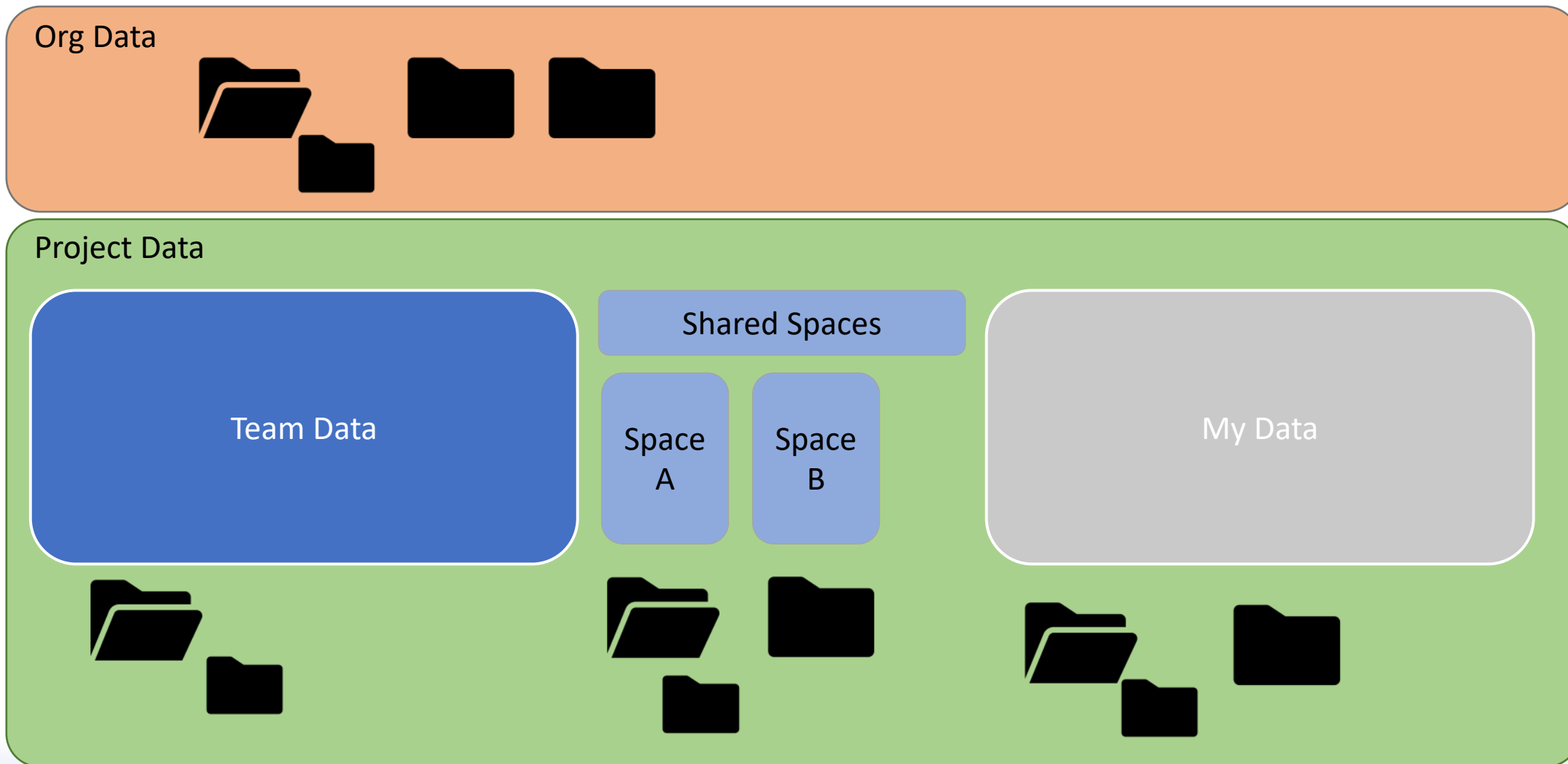
Project Data

Team Data

My Data



Location Controls Data Access



Good Migrations

- No loss of data access
- No change in underlying data resource IDs
- No required work in cubes or floes to support

- Additional features
 - Handling name collisions
 - Orion Client support
 - Favorite Folders
 - Location-based Search



A screenshot of the OpenEye Scientific data management interface. On the left is a sidebar with navigation options: '+ Add Data', 'Active Datasets', 'Project Data' (selected), 'Organization Data', 'Trash', 'Shared with Others', 'Shared with Me', 'Collections', 'Favorite Folders' (with sub-items 'jobs', 'Current Best', and 'Protein Structures'). The main area features a search bar with 'Conf' entered, a 'Project Data' filter, and a yellow warning banner: 'Attention needed! Please review data in your Shared with Others and Collections folder'. Below, search results for 'Conf' are shown, including 'BFS analogs Enamine BestConf' and 'EMol 5k Omega Conformers'.

Agenda

- What is Orion (in 2020)
- Coming Soon in 2021.1
- **Orion Over the Horizon**



M42 Orion Nebula

The Long Arc of OpenEye

OpenEye
Scientific
Software

...just like Mom used to make.



circa 1999

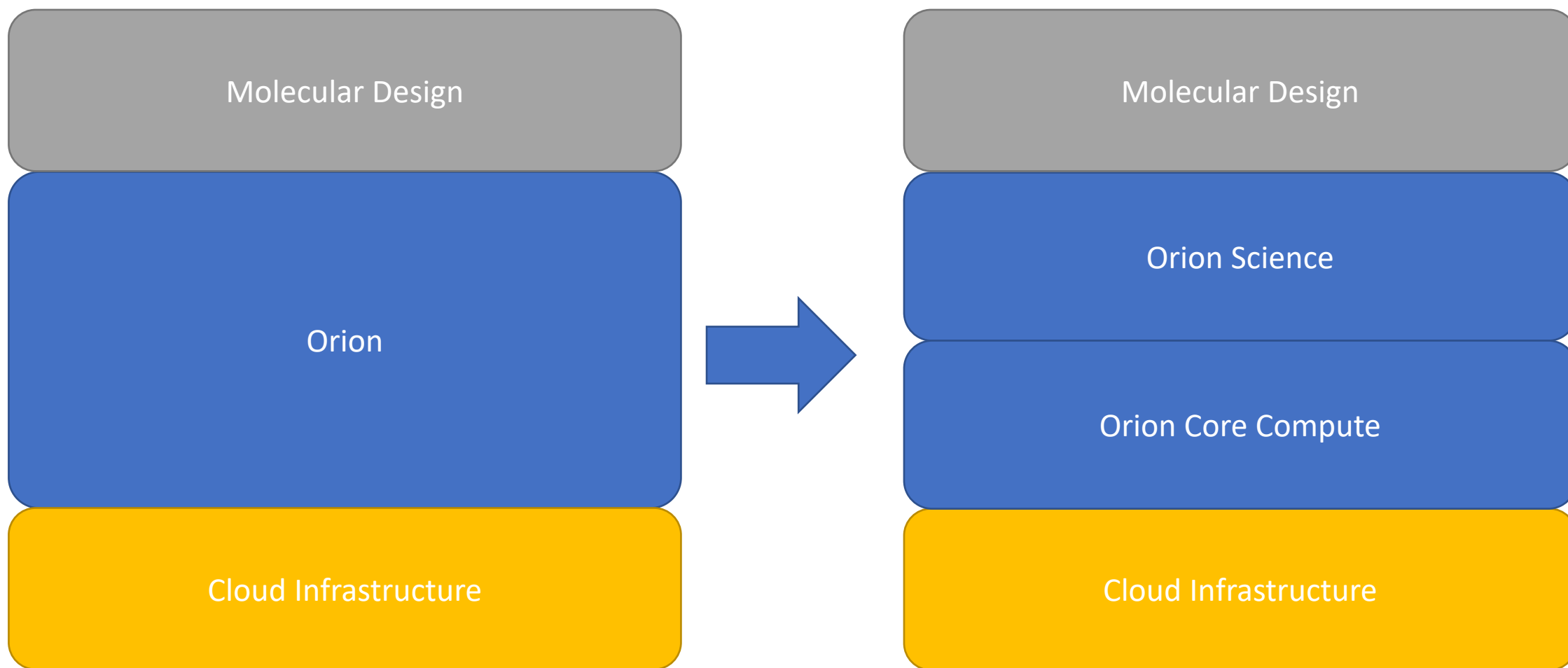
“we provide tools that vastly increase the scale of operation of computational chemistry in drug design.”

circa 2005

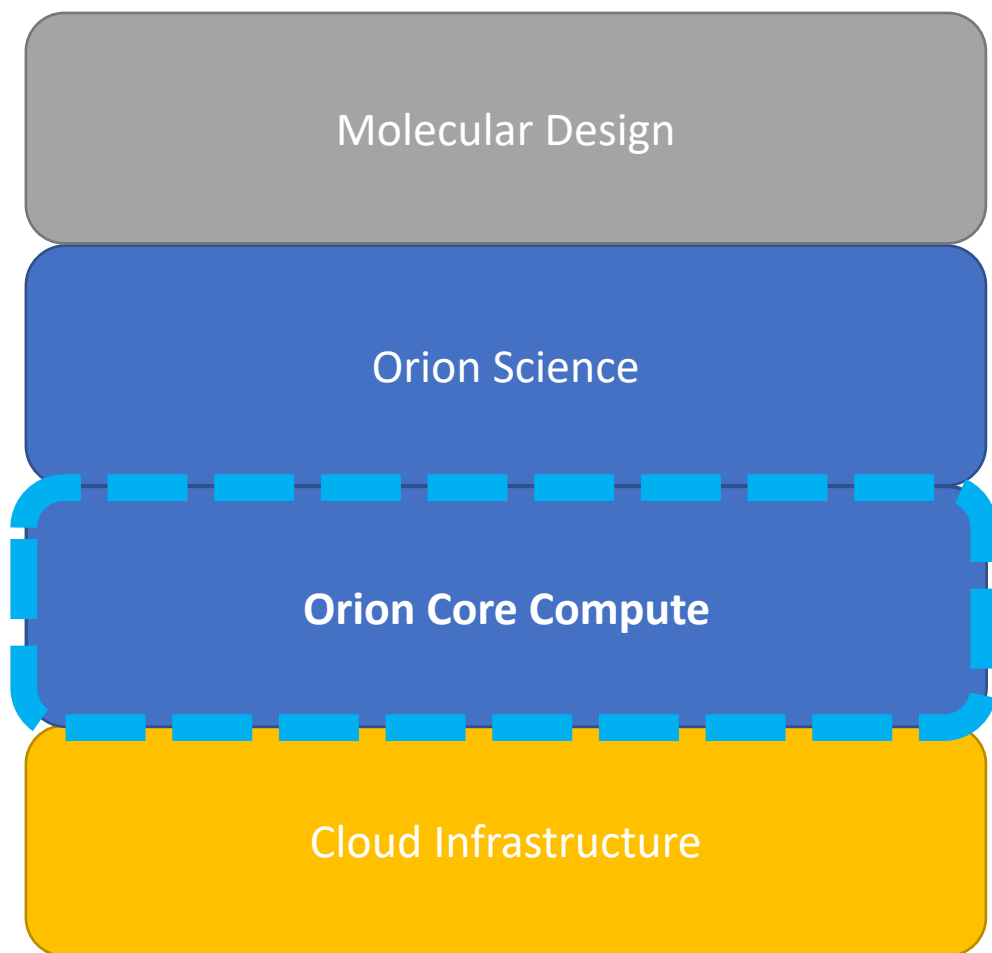
orion[↑]



Orion has Layers

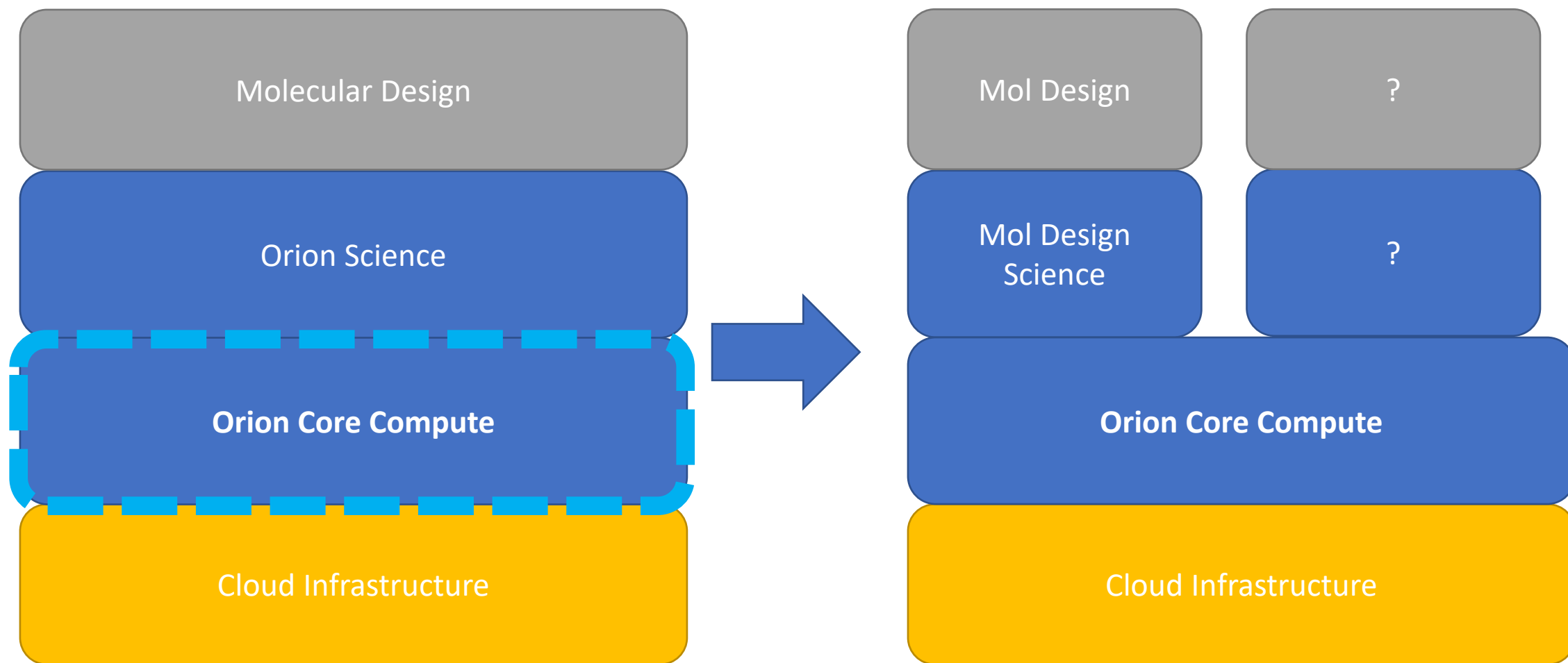


Prioritizing the Core



- Prioritize Core Compute Platform
 - Usability, Organization, Discovery
 - Data, Floes & Cubes, Versioning
 - Floe Developer and User Experience
 - Floe Customization, Floes of Floes, Complex Floe Launching UI
- Orion Infrastructure
 - Interactive compute, dynamic parallelism, direct Docker access

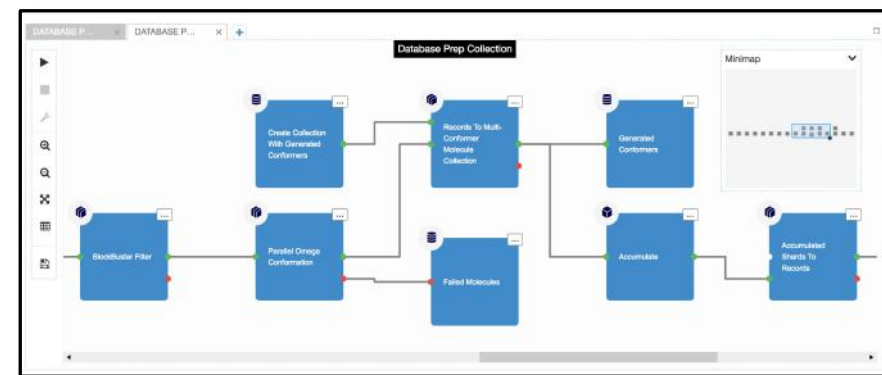
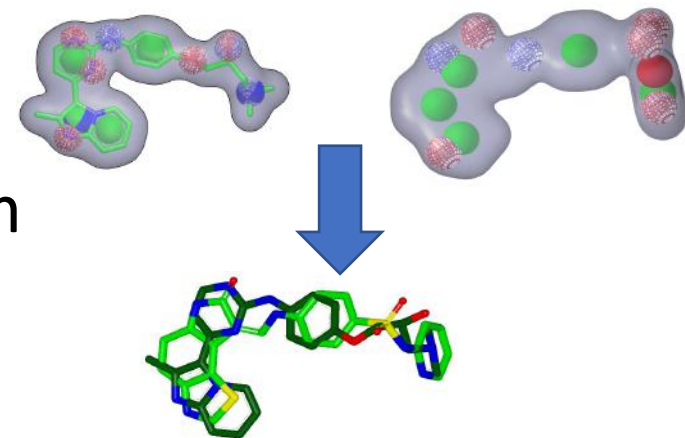
Enabling and Accelerating Science



Make Orion a better platform for scientific developers

Summary

- Orion is a powerful, unified molecular design platform
 - OpenEye calculations and much more
 - Large scale and small
- Orion is a Cloud-Native compute platform combining:
 - Large & diverse compute and storage resources
 - Open programming platform for reproducible calcs
- Major improvements in 2021.1 release
 - Data Management and Organization
- Focus on Core Compute Platform
 - Accelerate science by improving the platform for scientific developers



A full-page background image of a starry night sky with the Milky Way galaxy visible. In the bottom right corner, the dark silhouette of a person stands on a grassy hill, looking up at the stars.

Thank You

For more information, please contact:

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