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

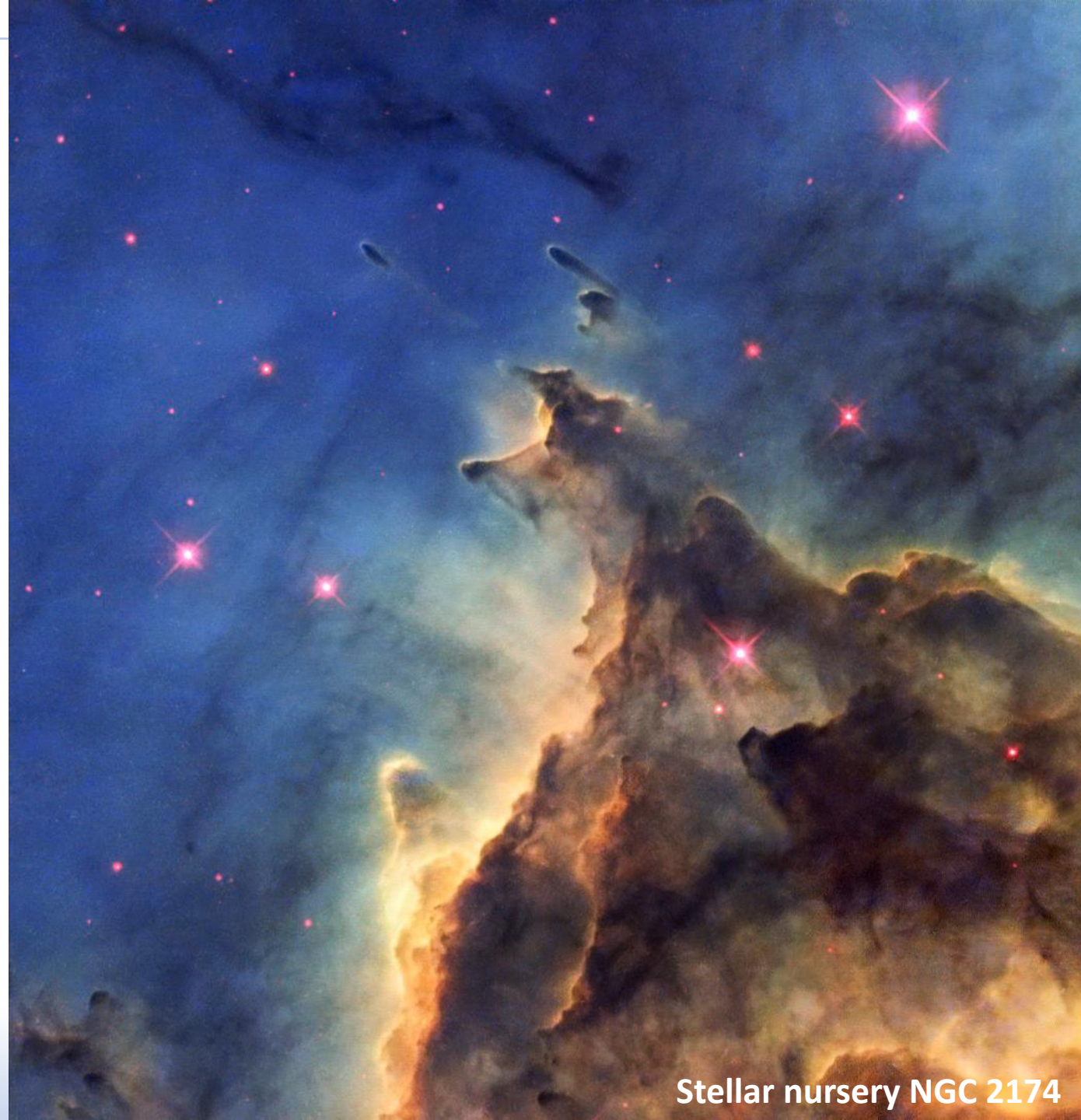
Matt Geballe
VP of Product

Spring miniCUP 2021

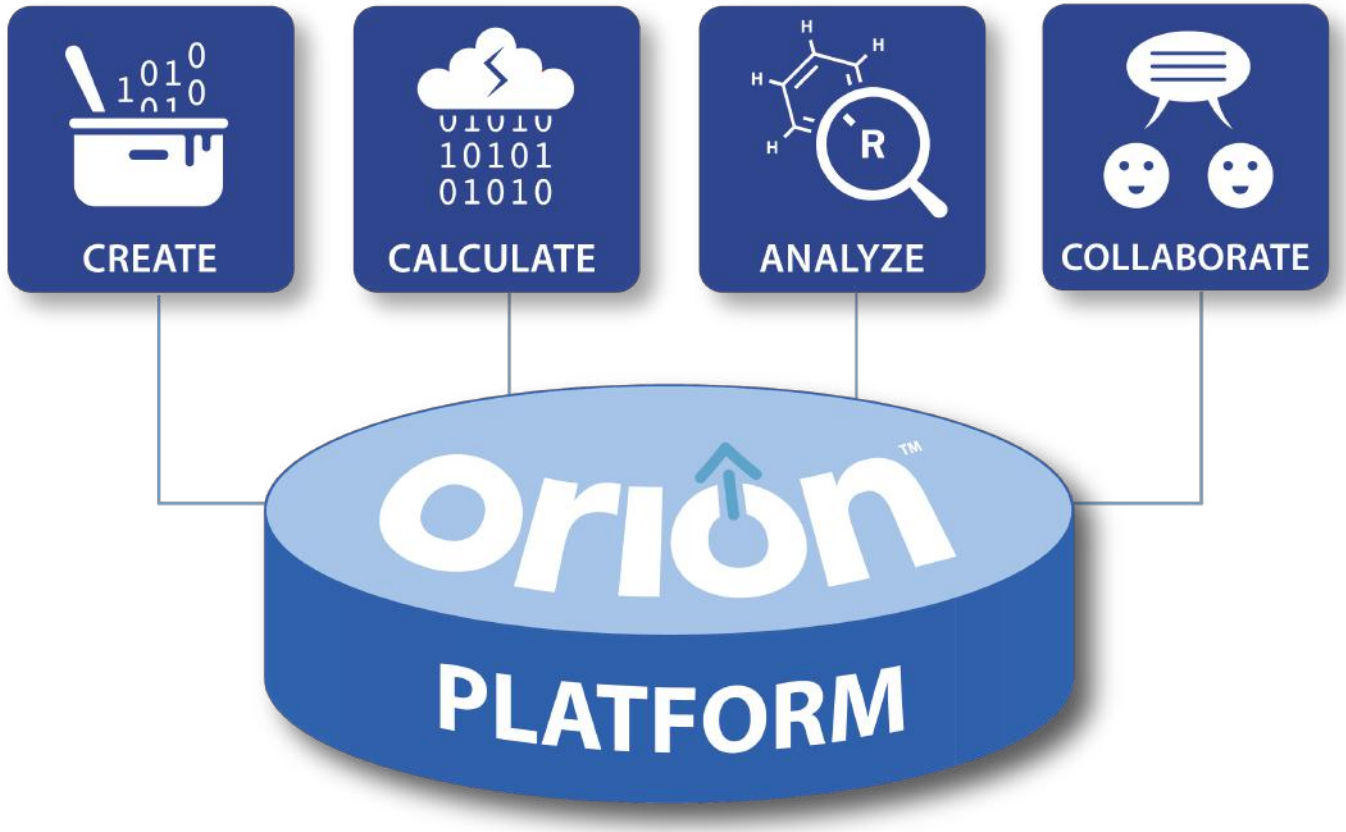
OpenEye SCIENTIFIC

Agenda

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


Stellar nursery NGC 2174

orion™ Cloud-Native Molecular Design



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Well-known for VS Calculations at Scale

Billions

FastROCS on Enamine Real

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

Docking Enamine Real

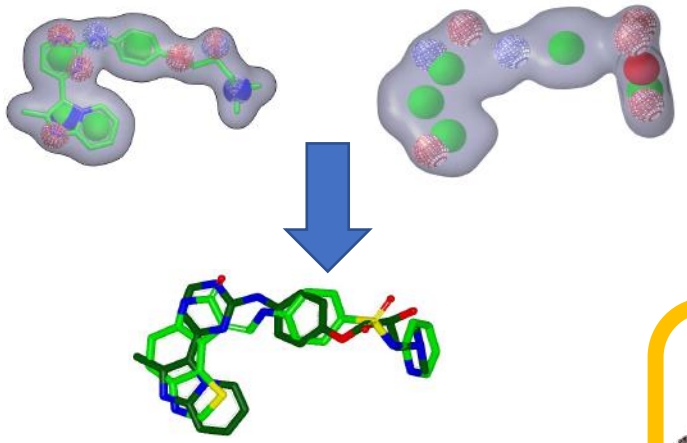
- Structure Based
- Search 2.5B
  - Time: ~24 Hours
  - Cost : **$10k – $30k**

Enamine

药明康德 WuXi AppTec

mcule
MORE THAN MOLECULES

Other Commercial or Internal DBs

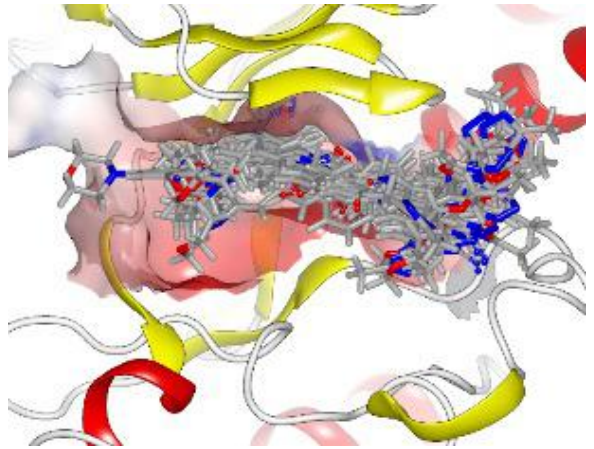


3D Tanimoto Similarity

~100

aws EC2

~10000



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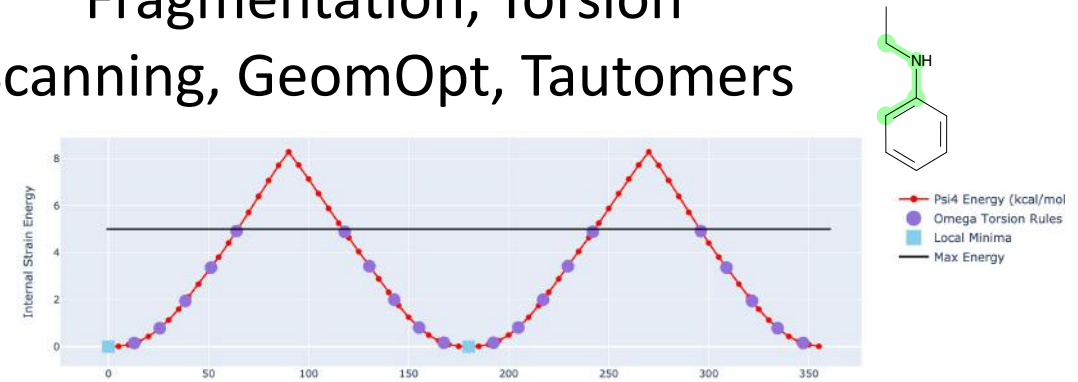
Not just Virtual Screening

Classic Floes

Replicating familiar OpenEye Apps

QM Floes

Fragmentation, Torsion Scanning, GeomOpt, Tautomers



Generative Floes

MMPs, 2D fragment replacement, transform extraction

orion™

MD Floes

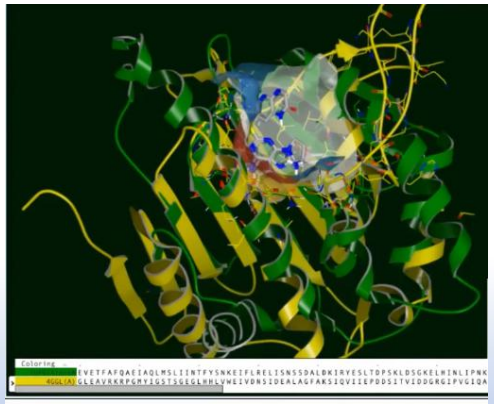
“Standard” MD, Solvate System, P-L MD and Analysis

ChemInfo Floes

Fingerprints, Filtering, Clustering, Bemis-Murcko

BioModeler Floes

Protein Prep and Modification, Loop Modeling, SiteHopper



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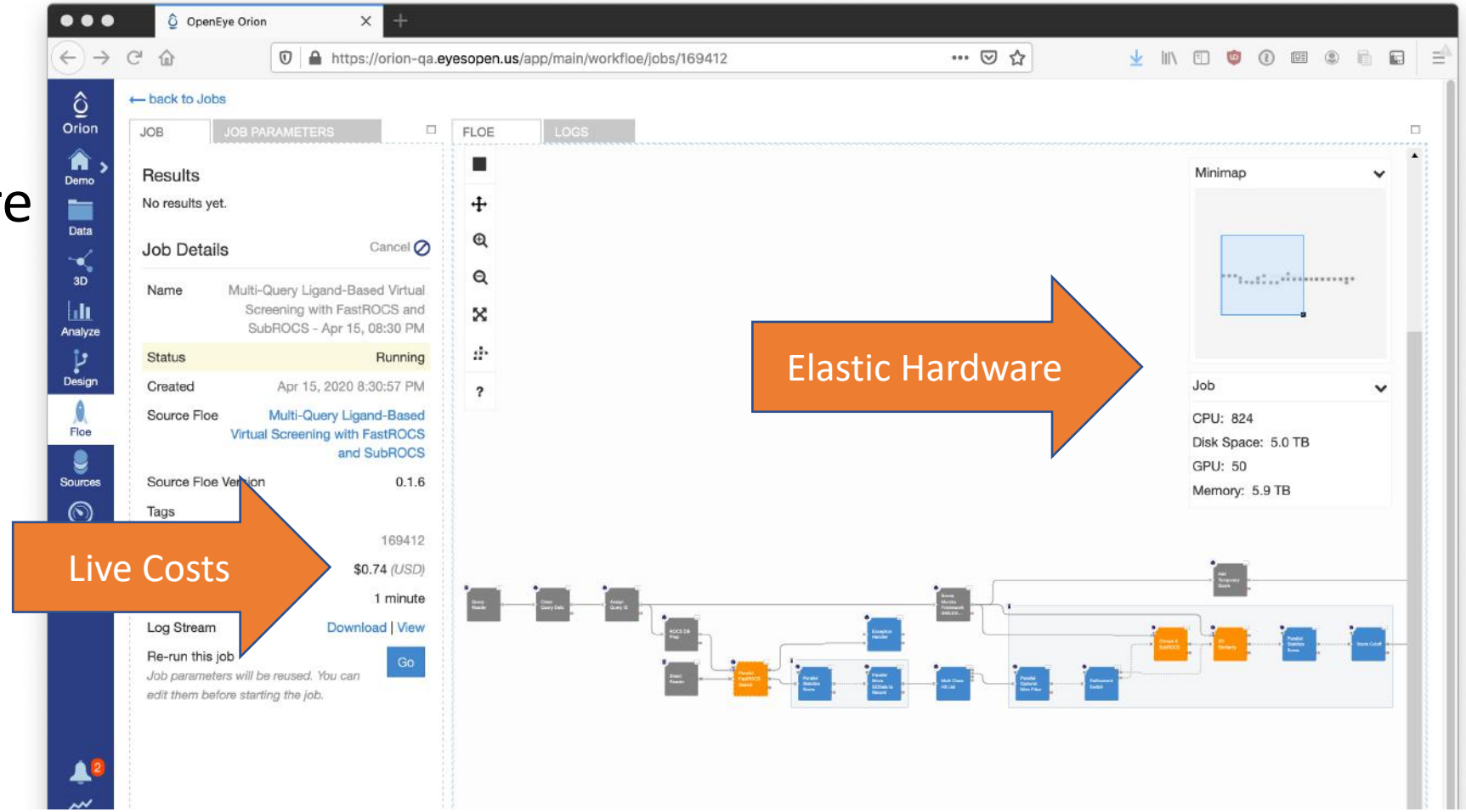
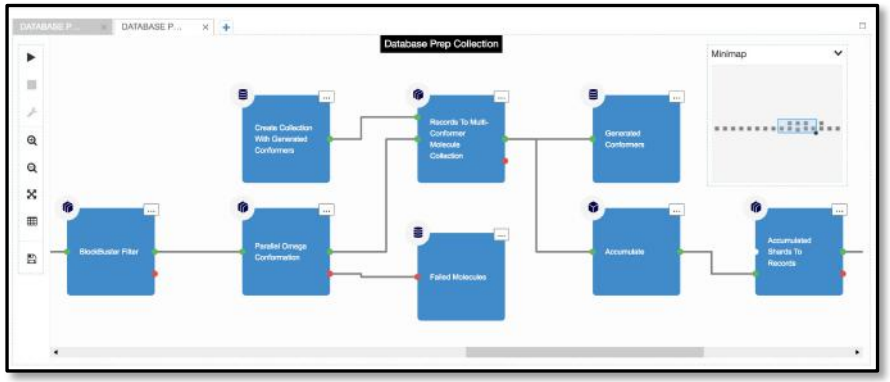
Orion Orchestrates Compute Resources

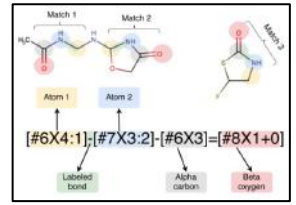
- Workflow paradigm (cubes and floes)
- Powerful, cost-aware scheduling
  - Parallelization
  - Fault tolerance
  - Cycles
  - Per-cube hardware requirements
    - Metrics
  - On-demand & Spot
- Project & User Cost Accounting



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*





PSI4

OpenMM

SciPy

matplotlib

scikit learn

biopython

PyTorch

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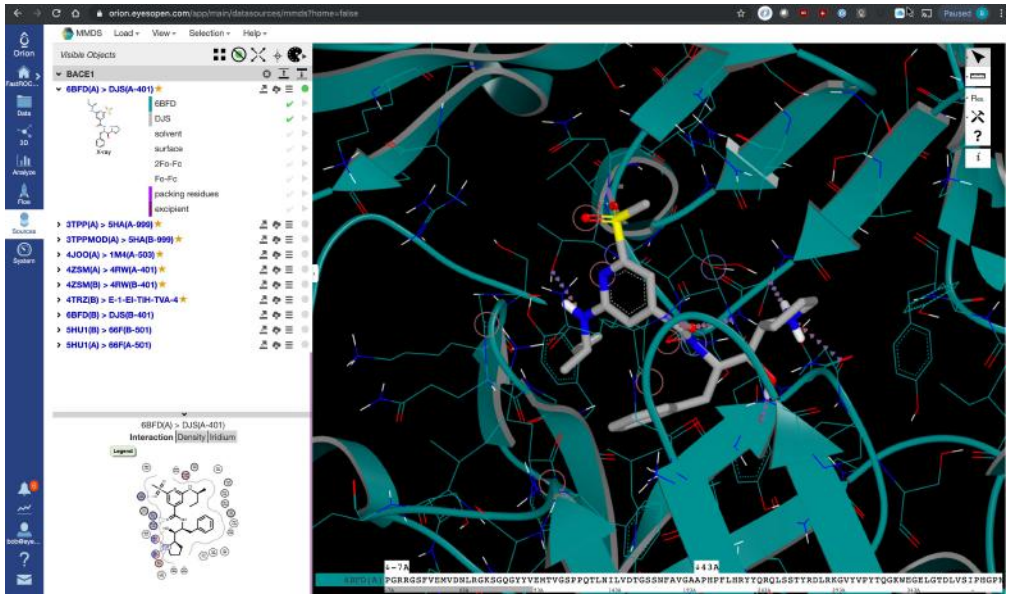
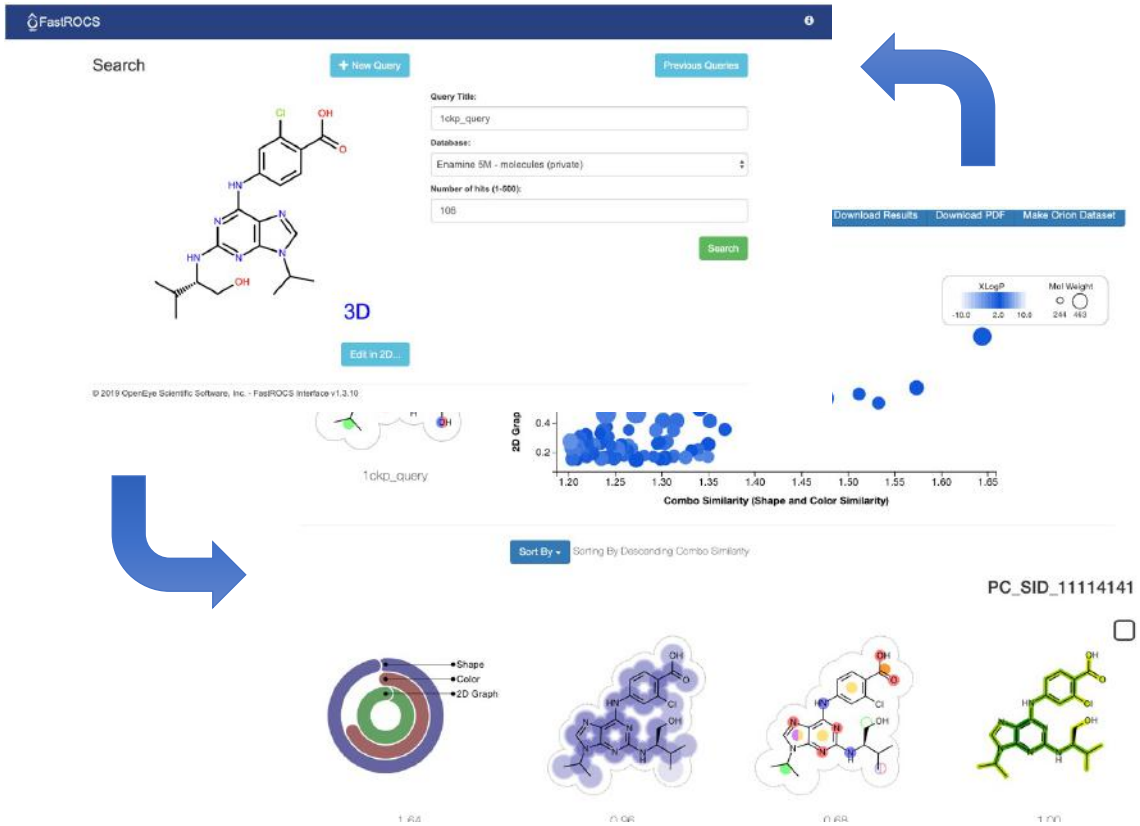
Interactive Search and Exploration

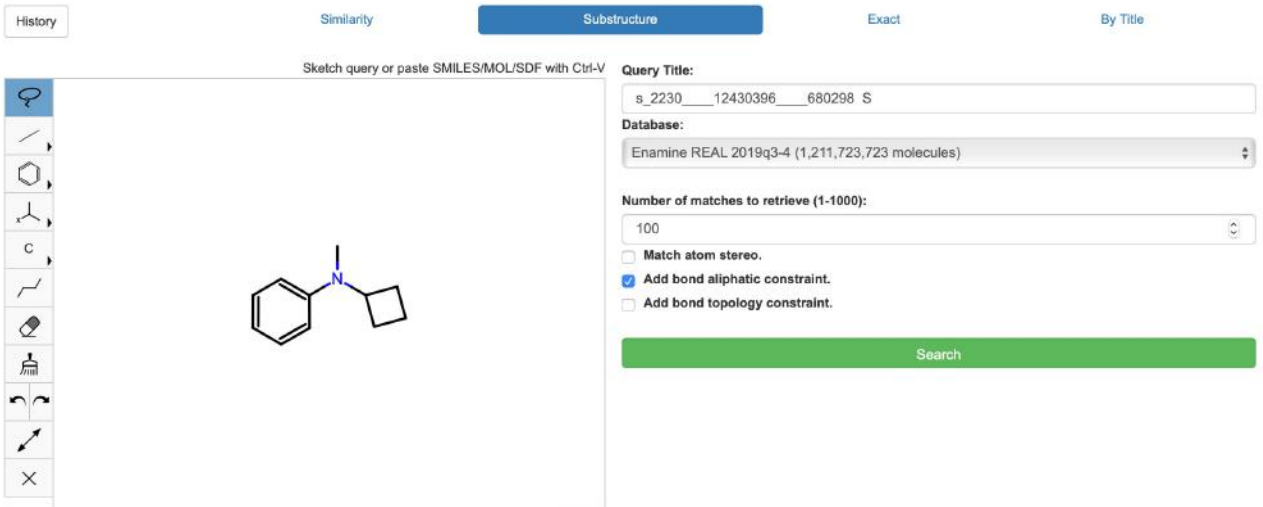
MMDS



FastROCS



MaaS



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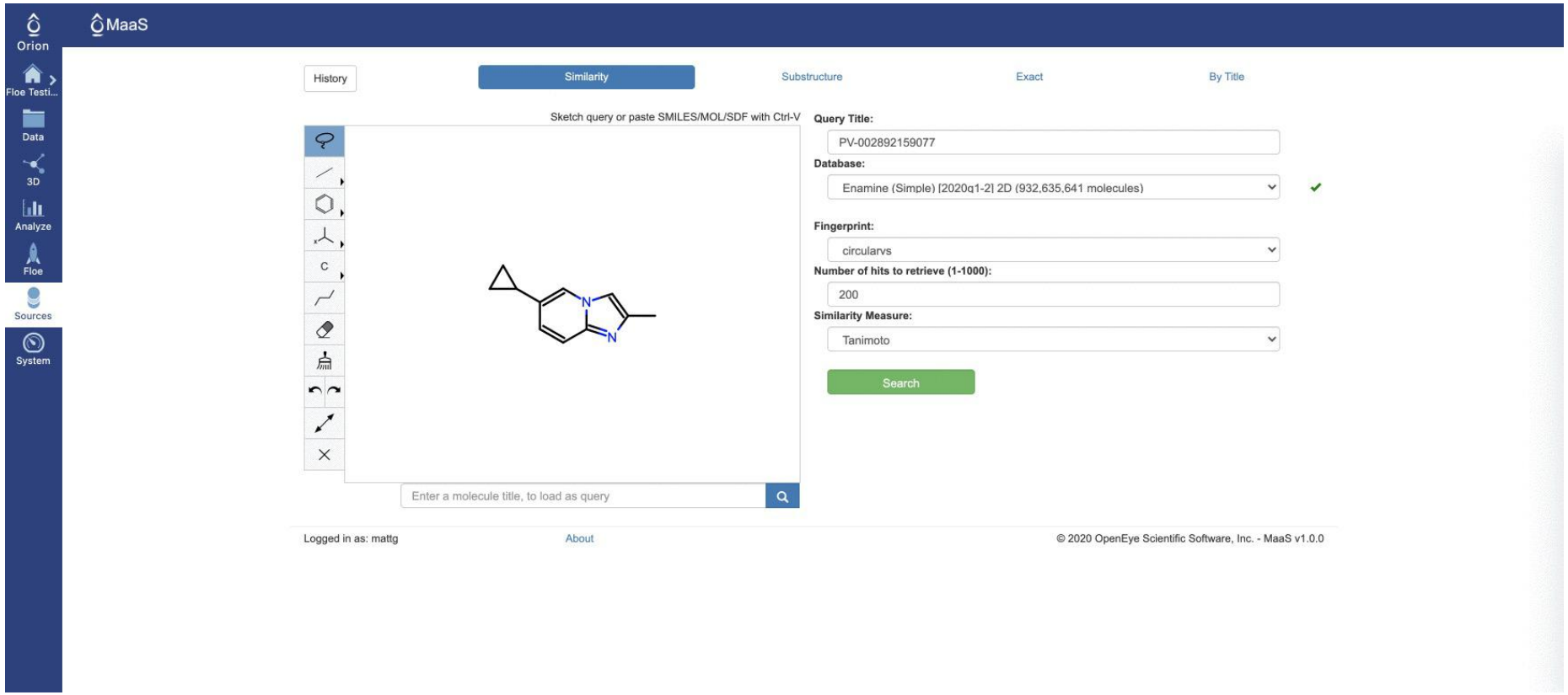
Search Billions in Seconds with MaaS

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



Exploration, Screening, Hit Expansion, and more…

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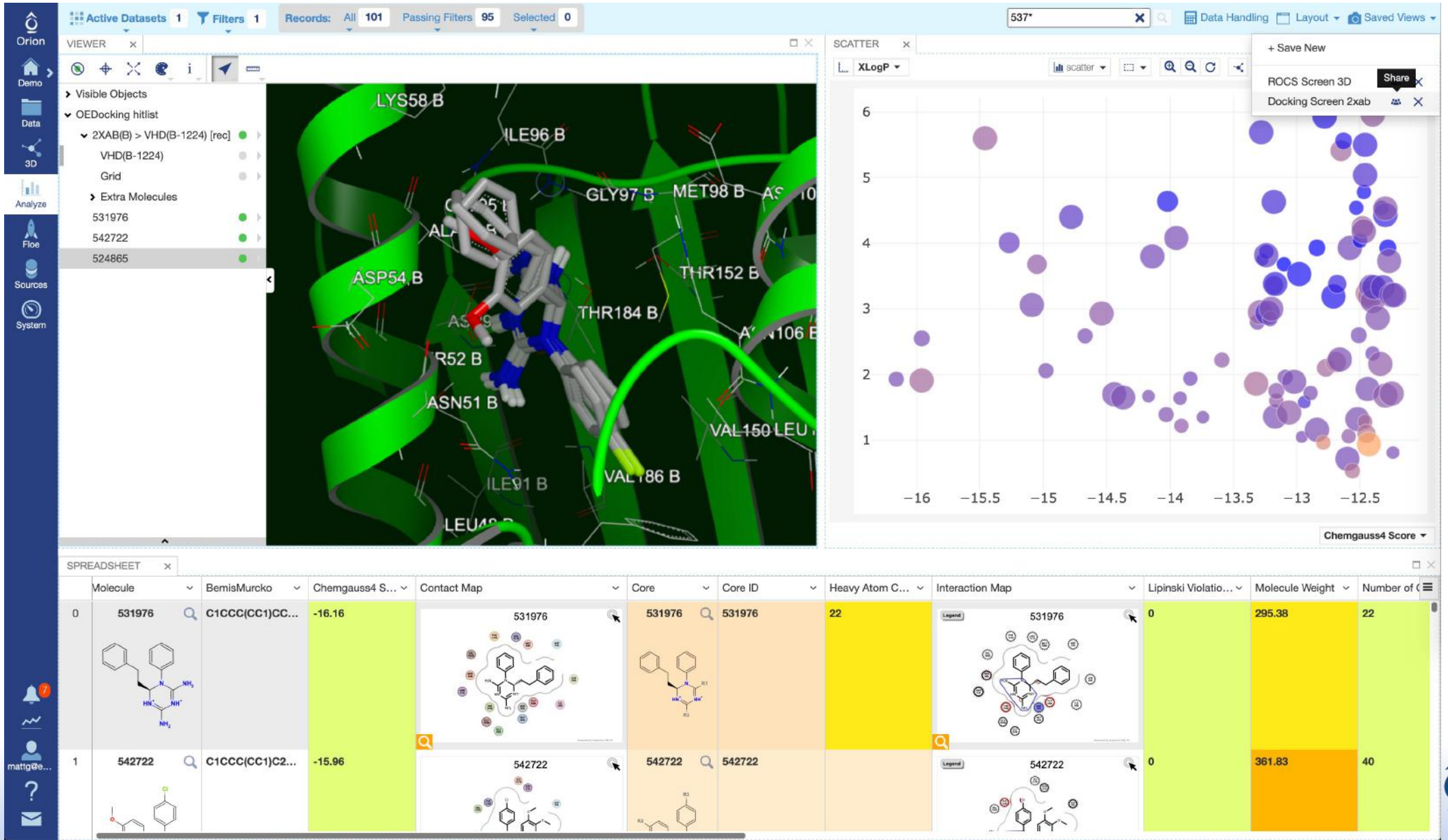
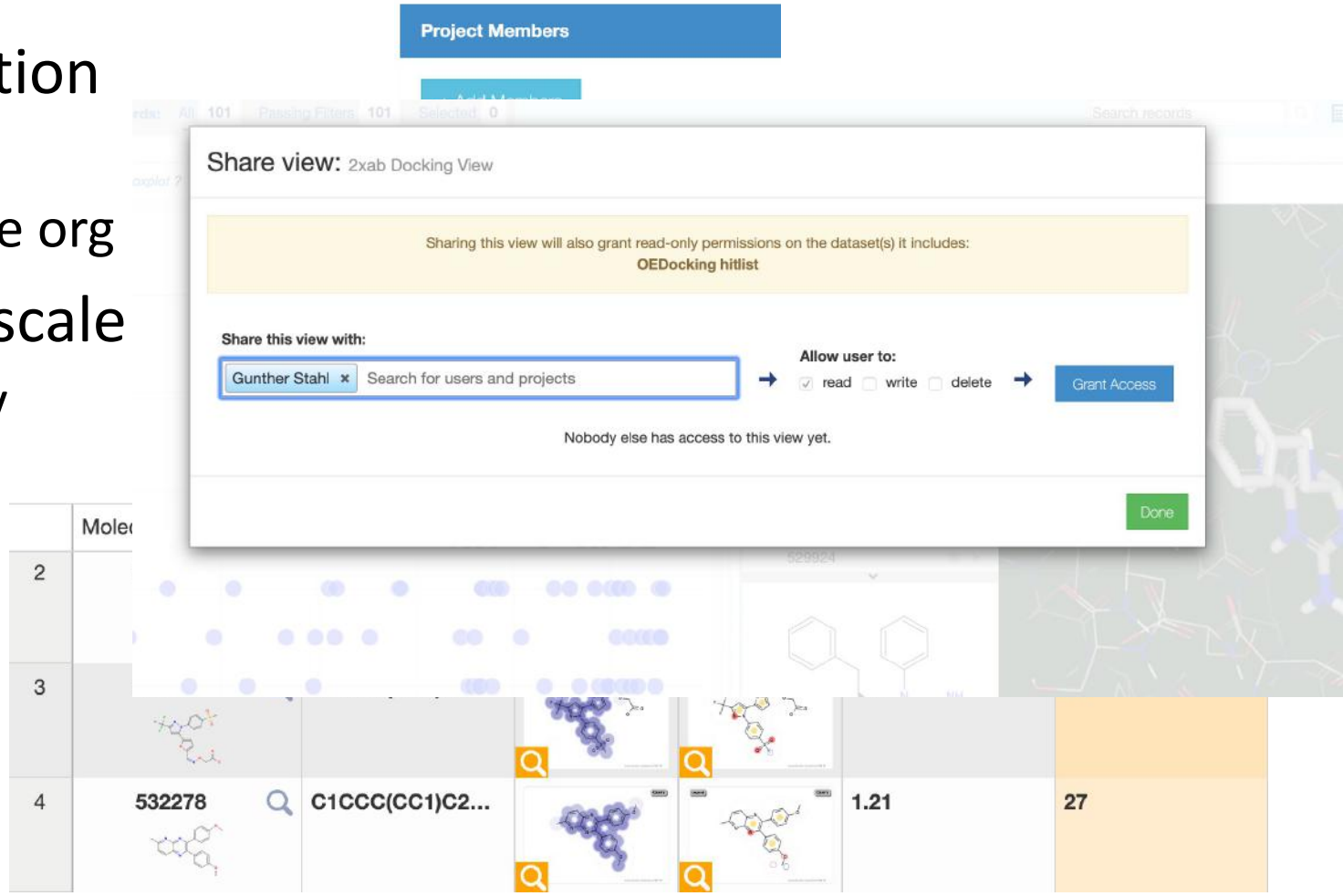
Integrated Analysis and 3D



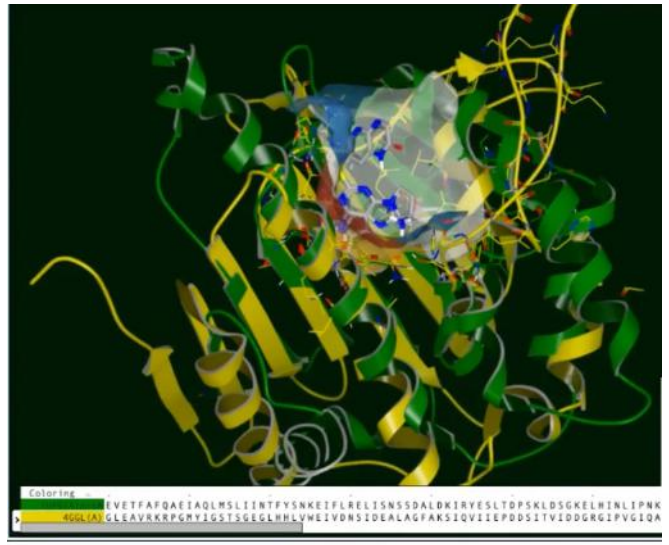
Data Storage: Cloud-Scale and Integrated

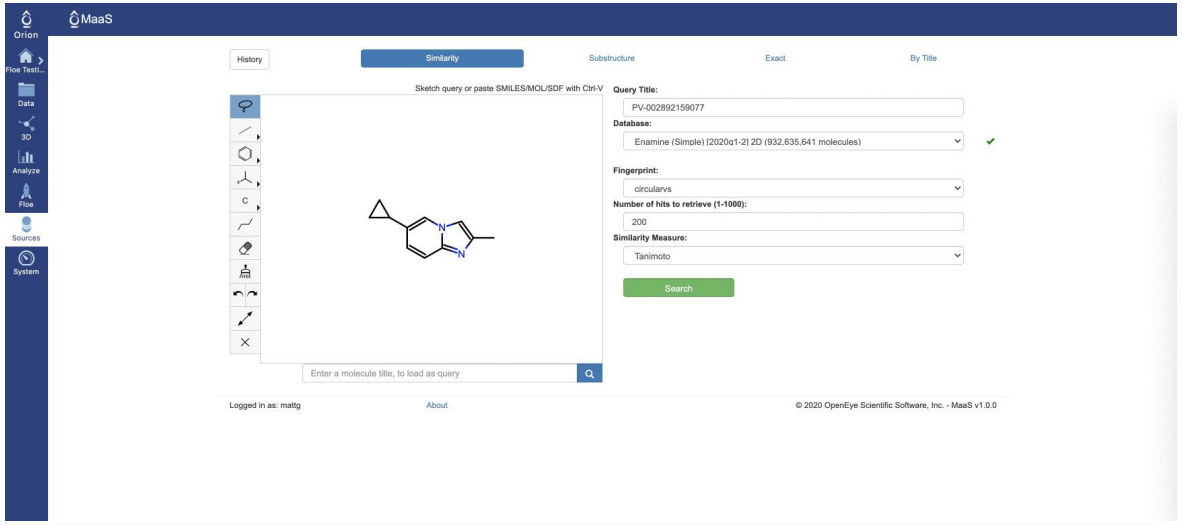
- Project-centric Data Organization
  - Flexible collaboration
  - Critical data shared across entire org
- Storage models designed for scale
  - Interactive analysis to massively parallel I/O
- Generic data container
  - C++ implementation
  - Uses beyond molecules
  - **Integrated into Orion UI**



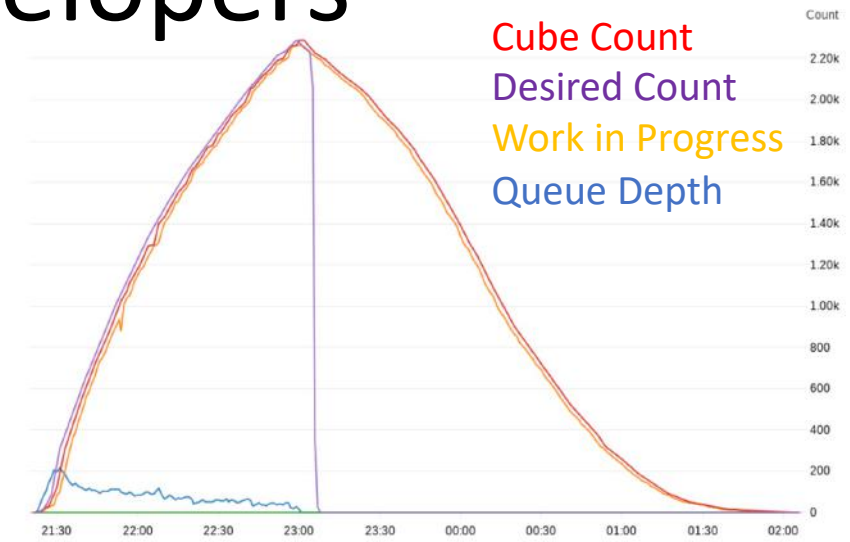
2020 Major Features – Users

- **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**

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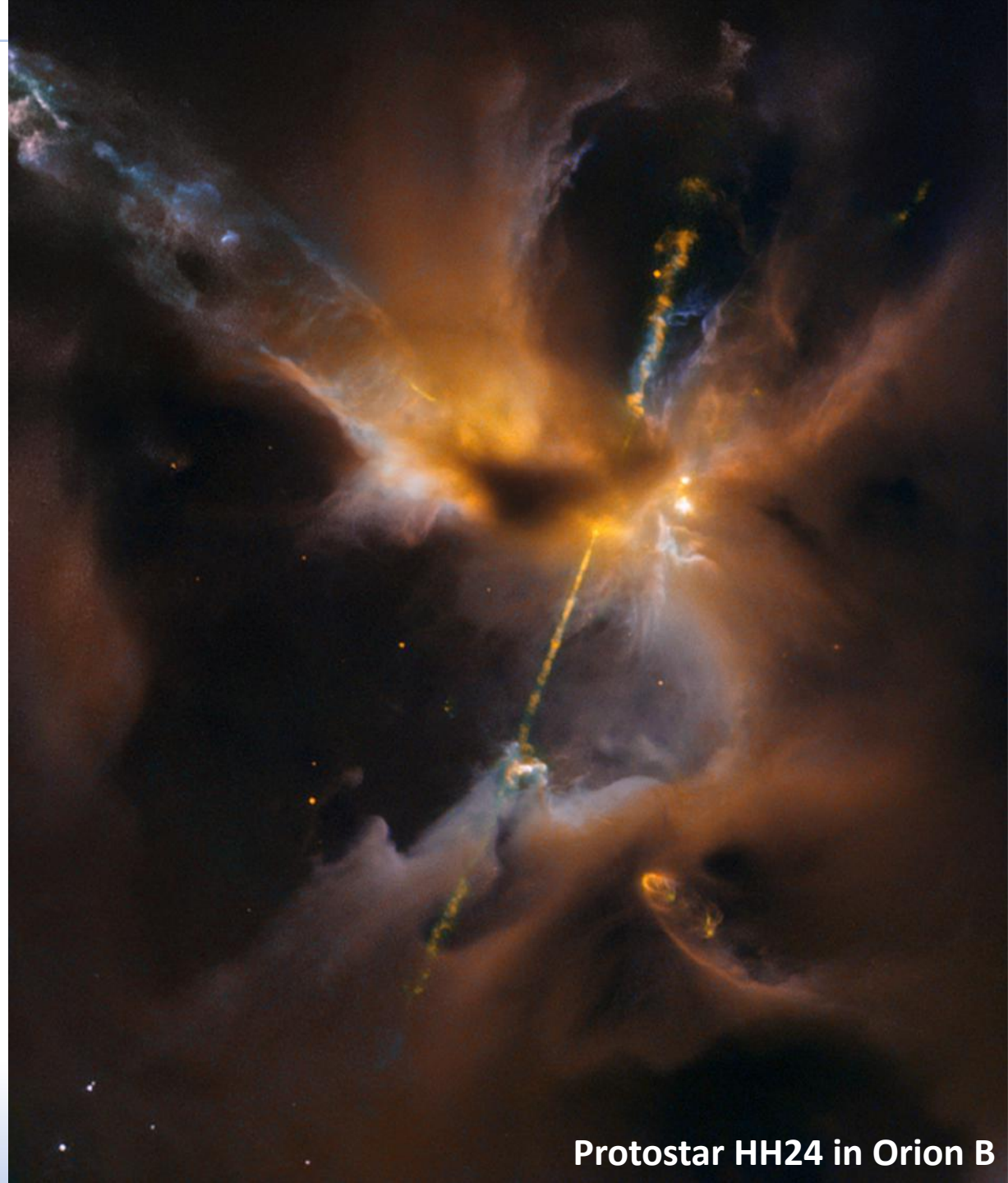
- **Coming Soon in 2021.1**
- Over the Horizon



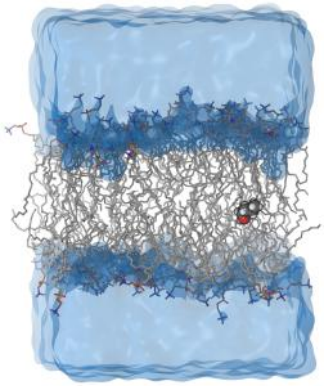
Protostar HH24 in Orion B

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…

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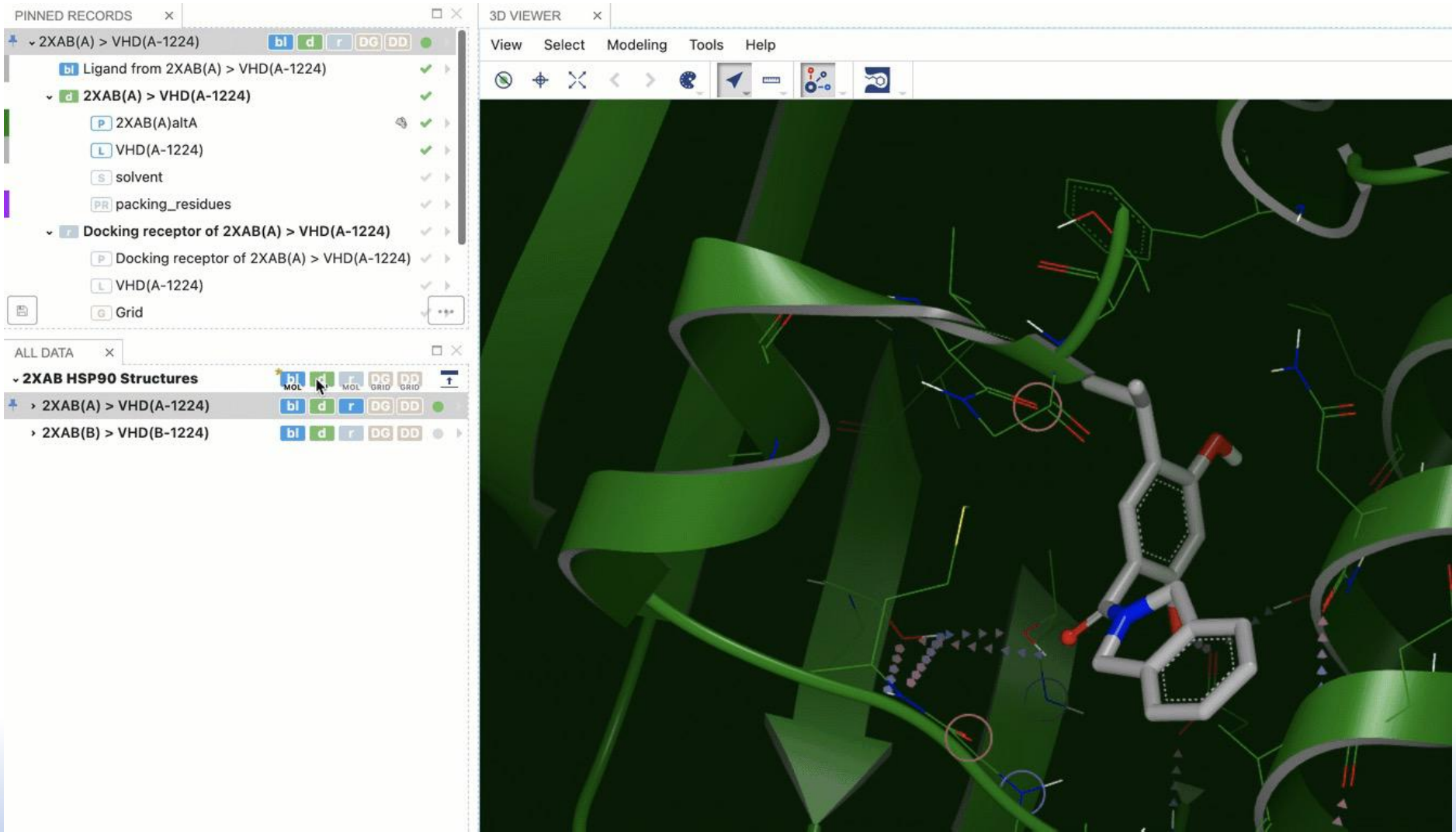
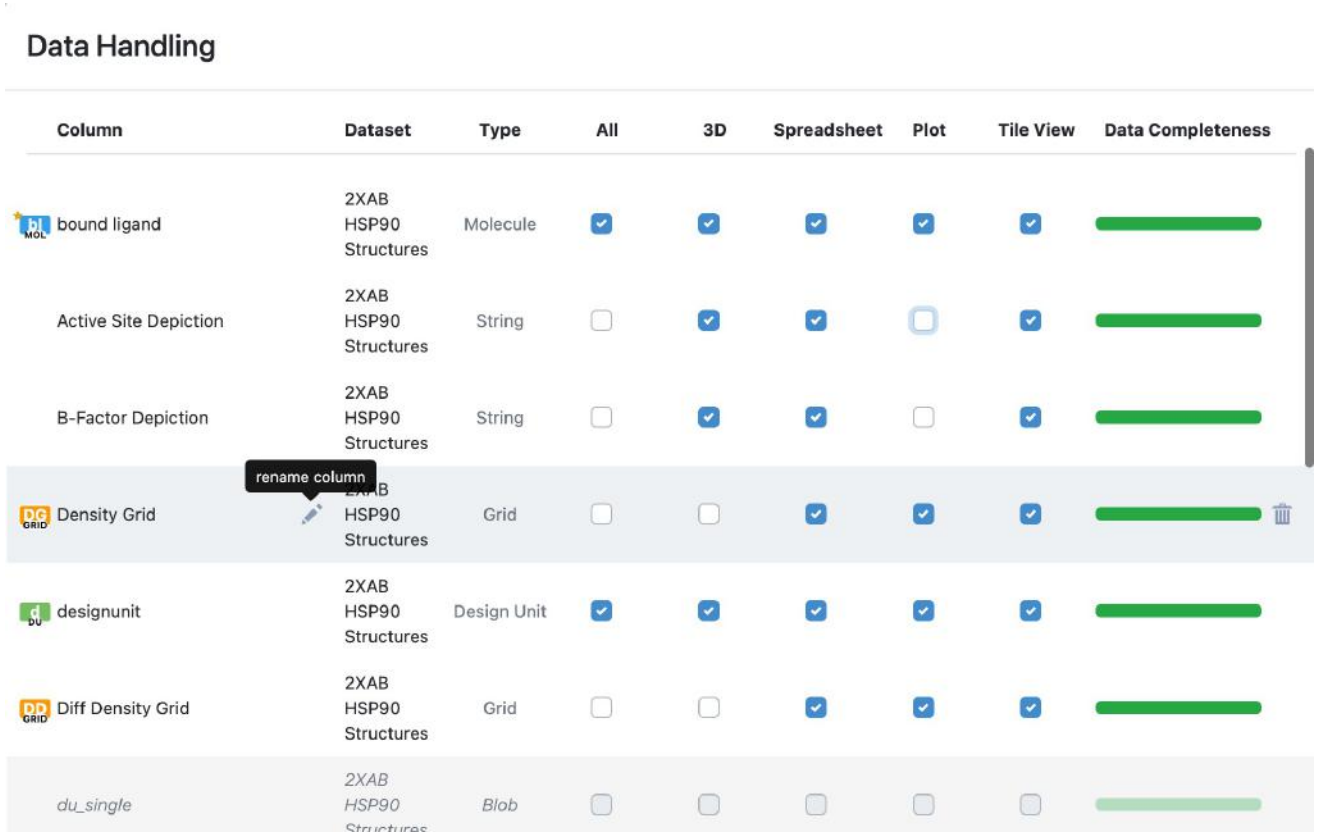
Managing Data in 3D Modeling

- Badging for visual information and control



Managing Data in 3D Modeling

- Badging for visual information and control
- Controls over visibility



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- Badging for visual information and control
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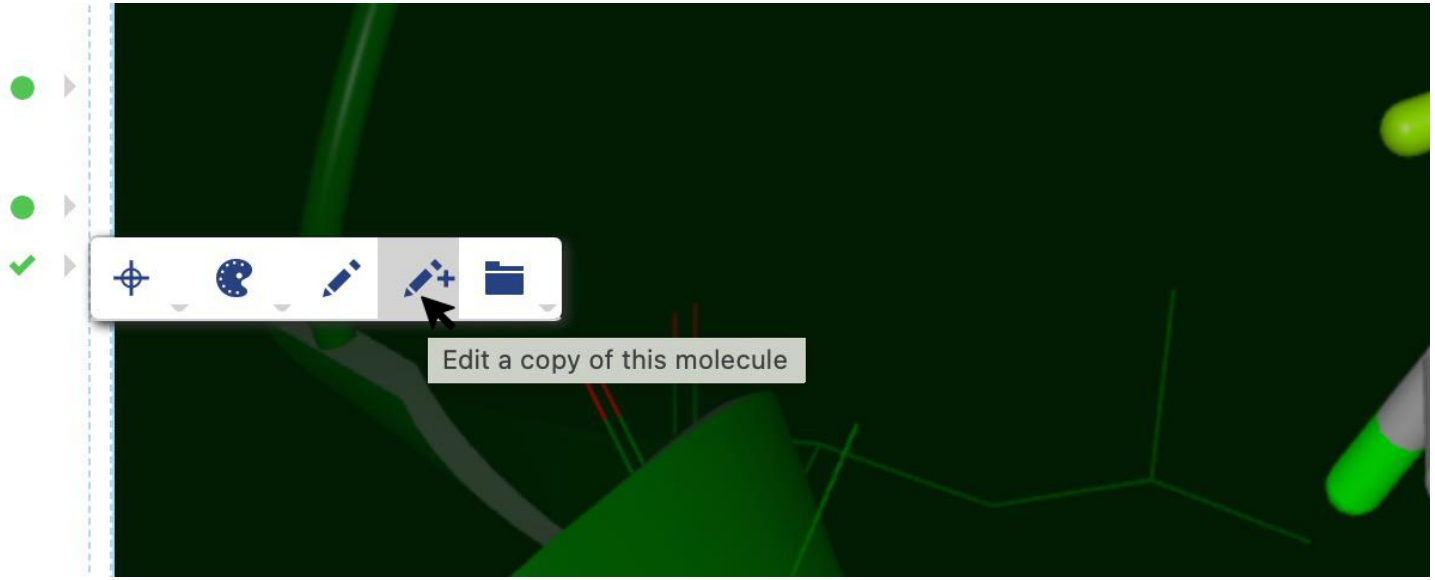
- Easier editing and saving



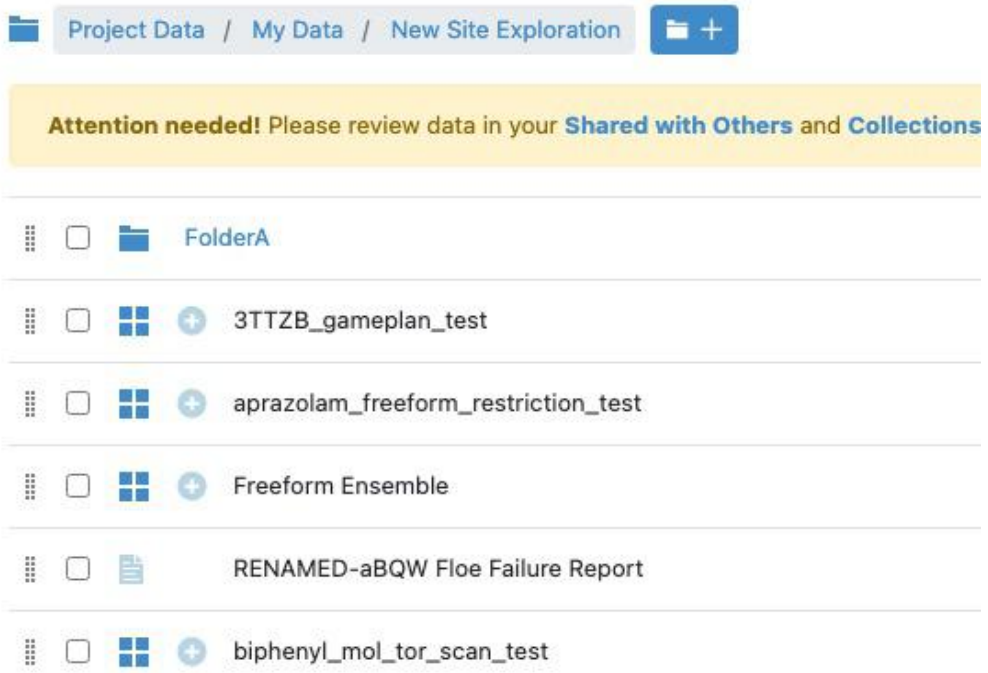
Managing Data in 3D Modeling

- Badging for visual information and control
- Controls over visibility
- Easier editing and saving
- Use Fields as Record Titles

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

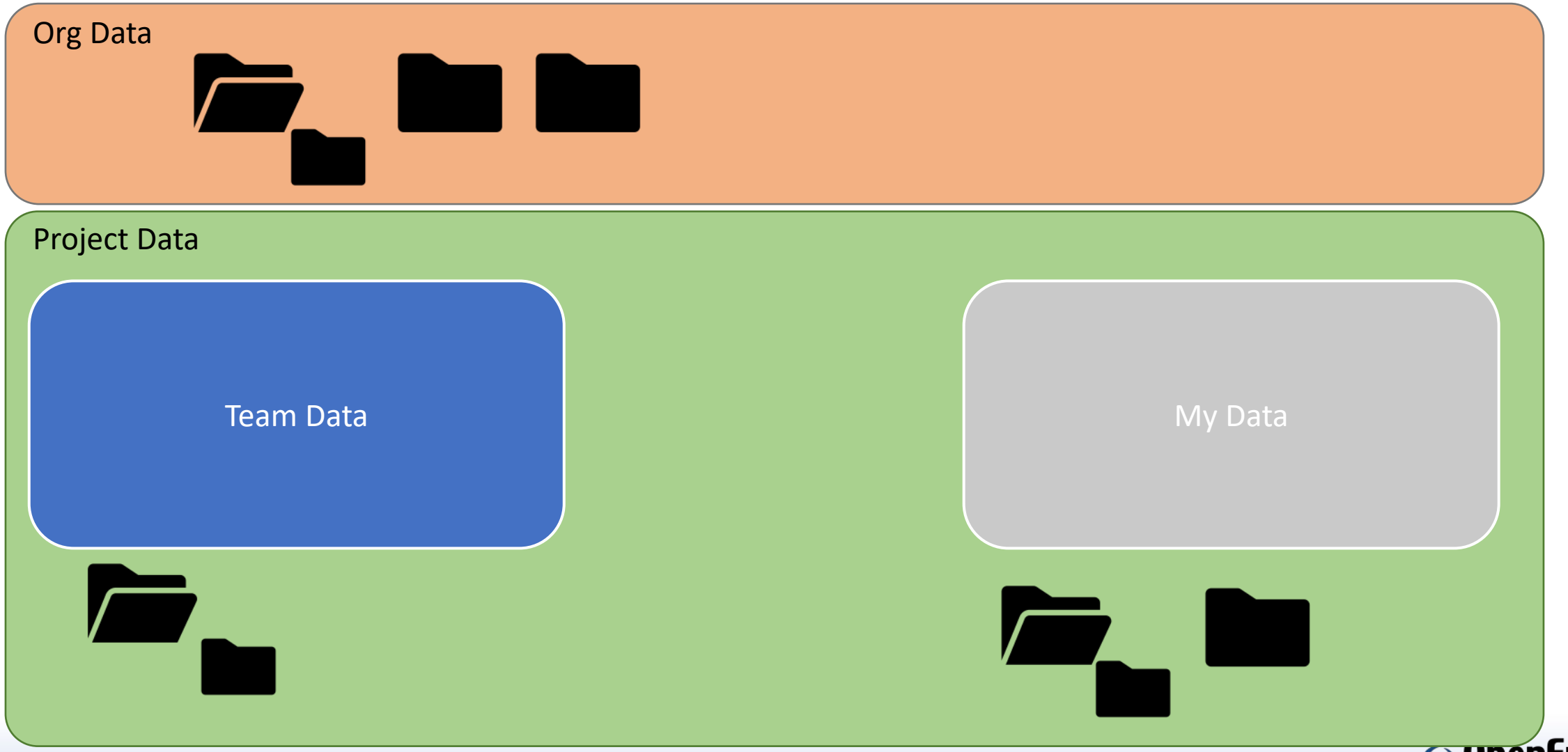
Multi-level organization with drag & drop

Control location of upload and floe output

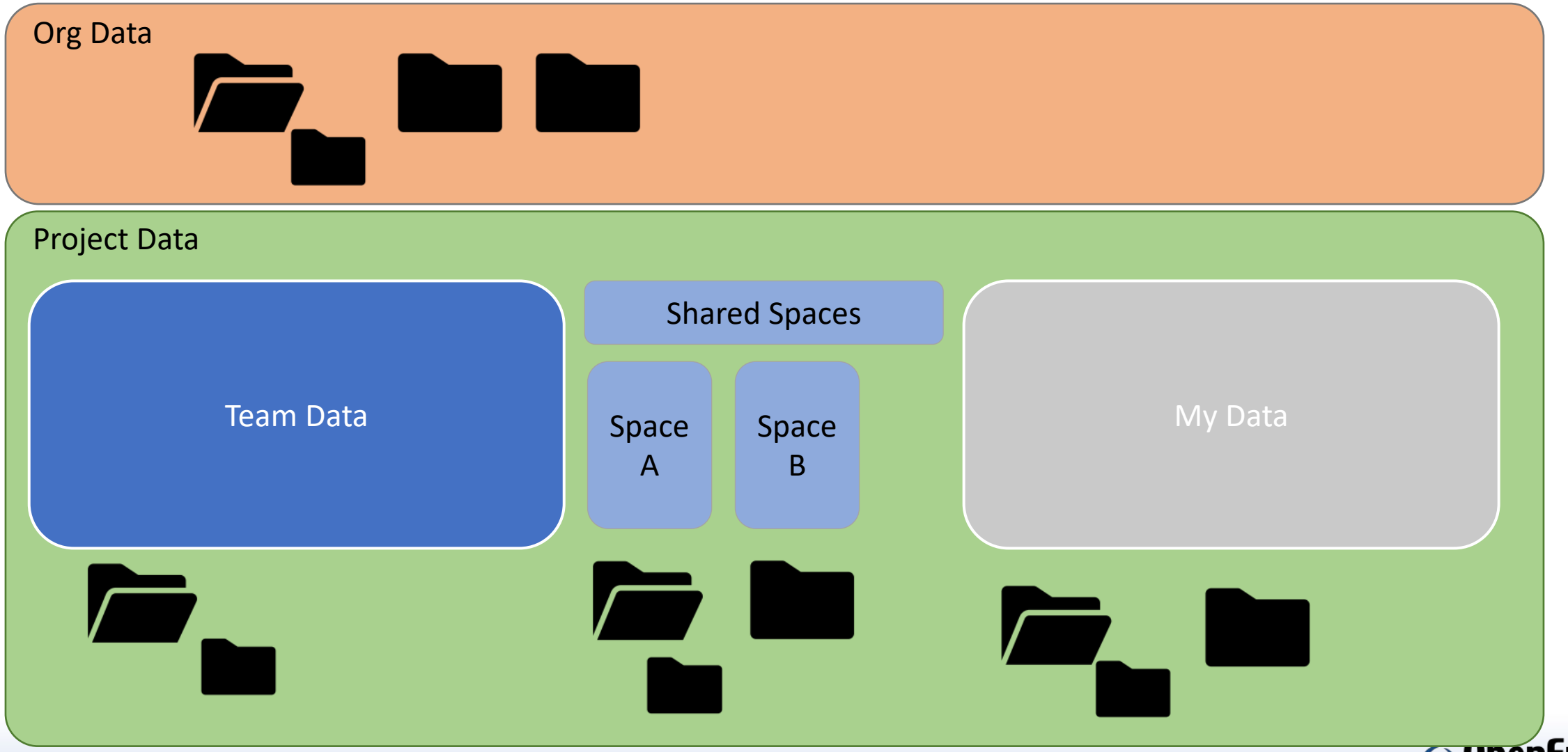
Combined View

Location dictates shared access

Location Controls Data Access



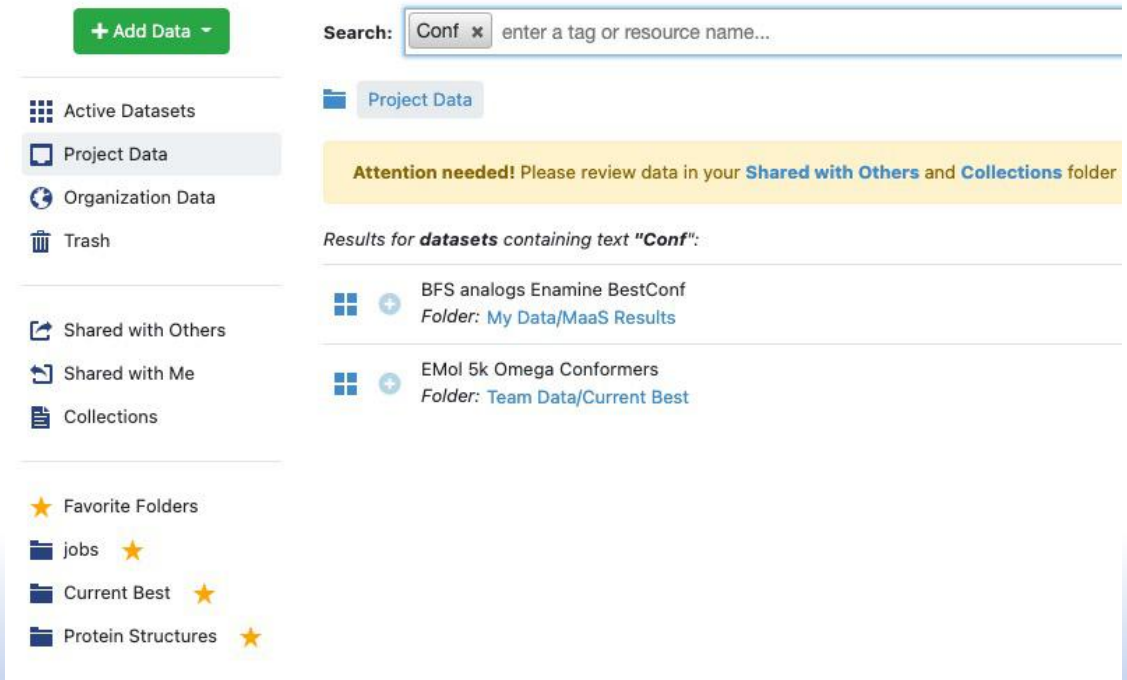
Location Controls Data Access



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



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- 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

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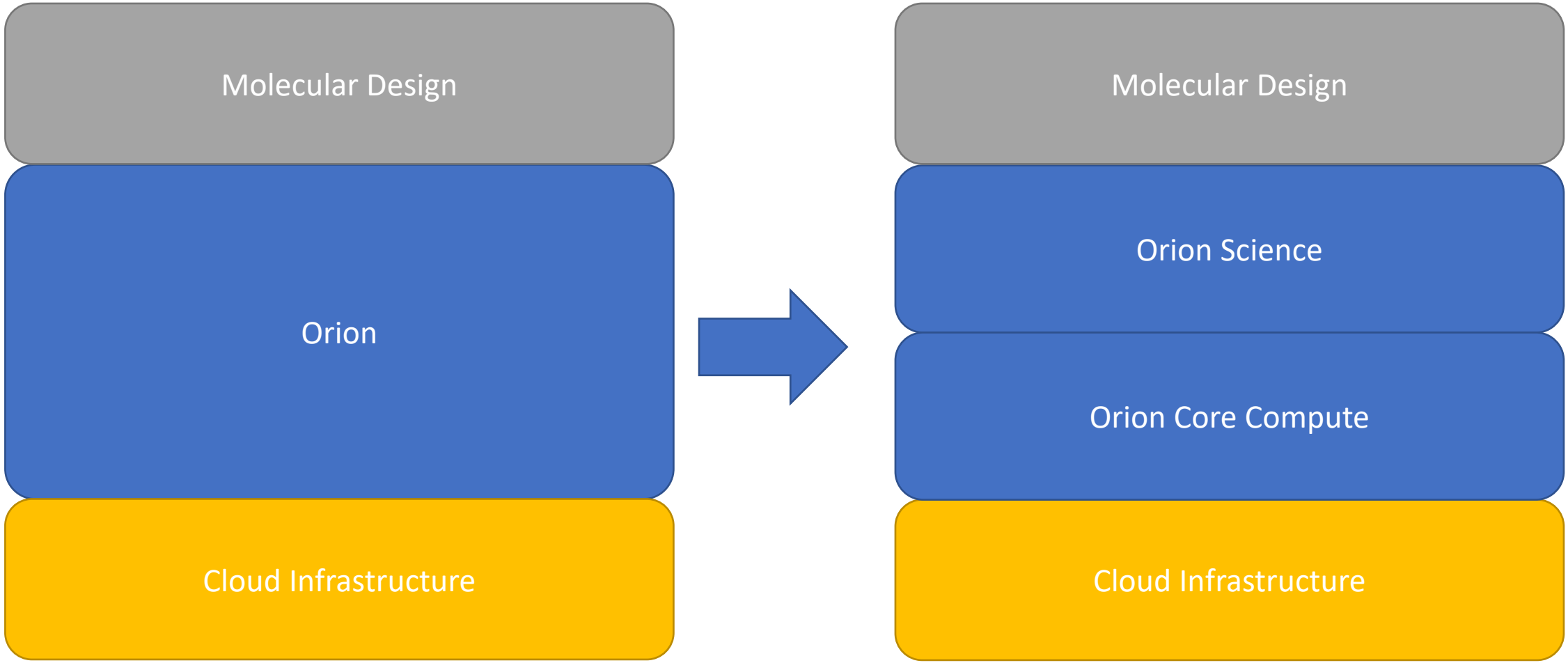
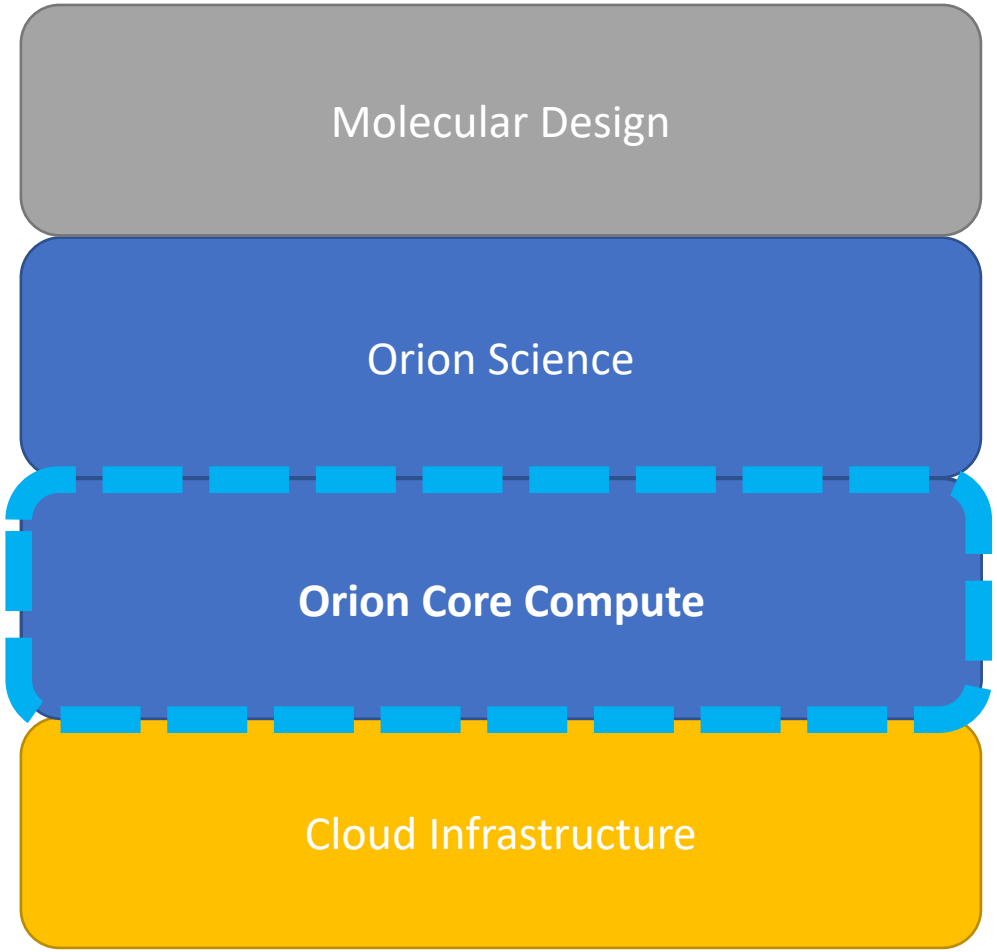
Orion has Layers

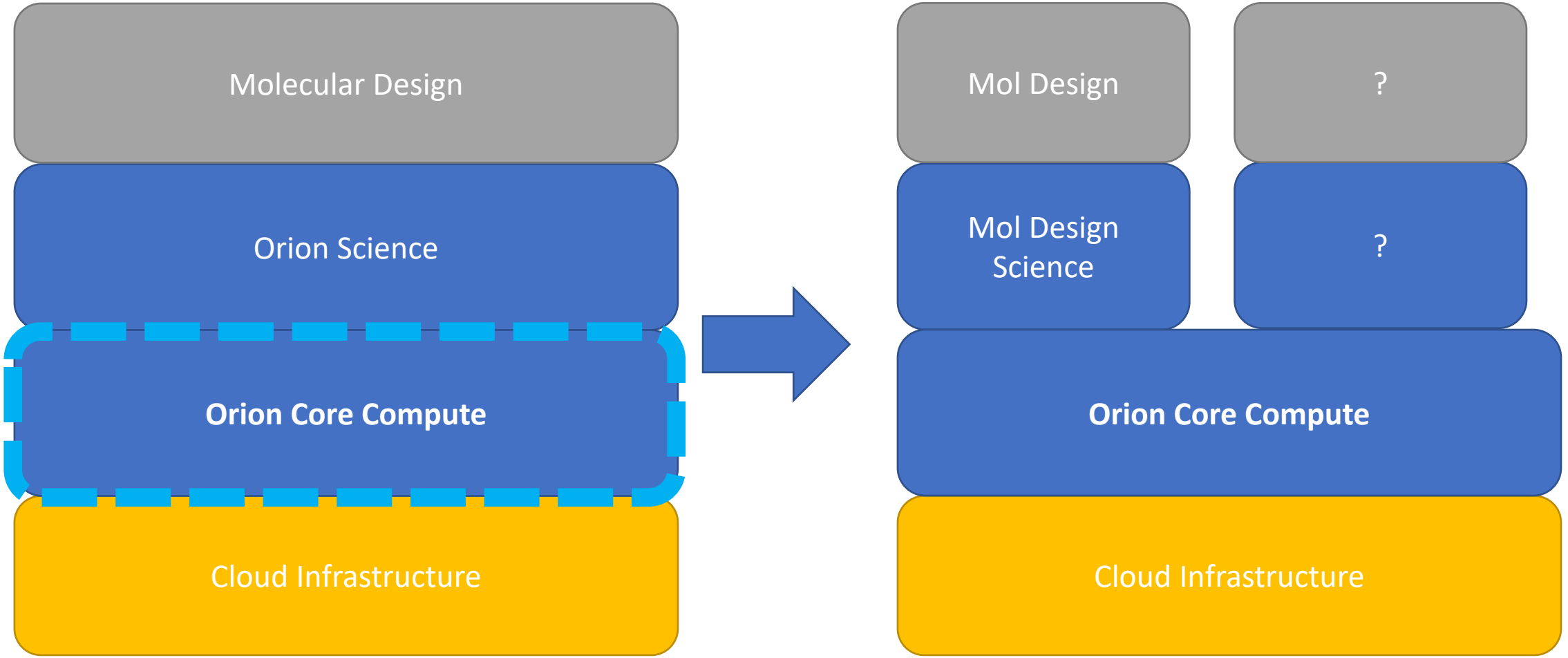


Prioritizing the Core



- 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

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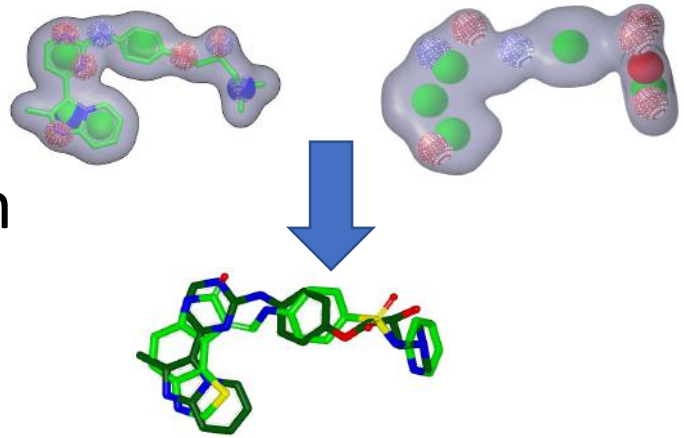
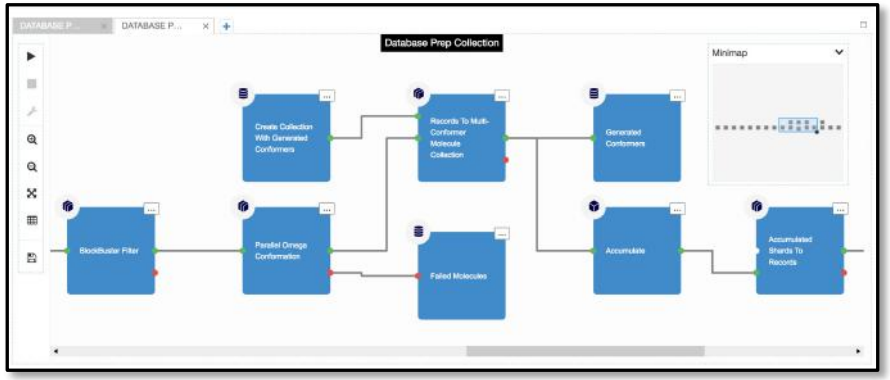
Summary



- 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



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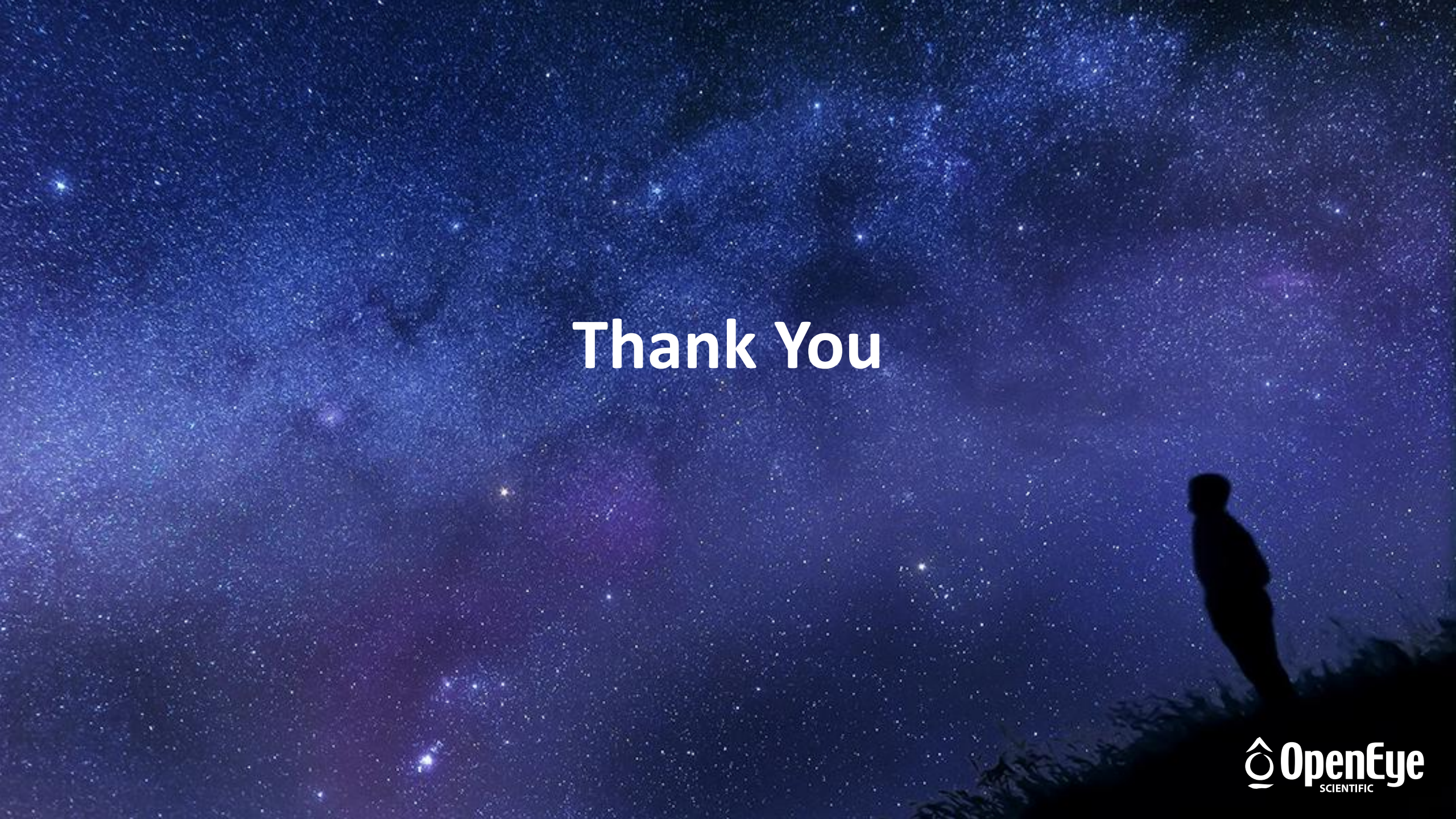
Thank You
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