ChemAxon

MARVIN LIVE

András Strácz

Budapest Annual Meeting

2016

Ecosystem

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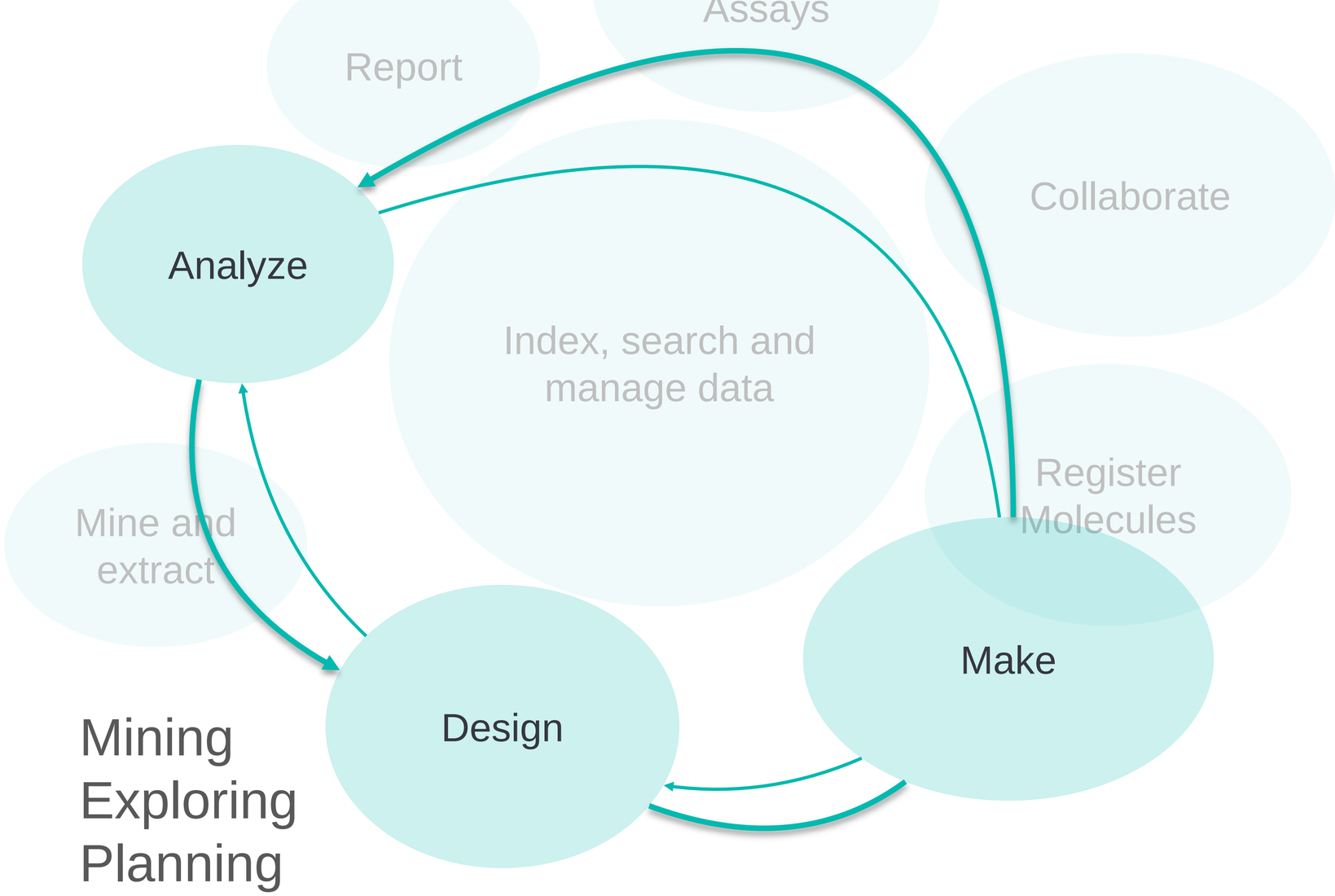
Assays
Report
Collaborate
Analyze
Index, search and
manage data
Register
Molecules
Mine and
extract
Make
Design
Mining
Exploring
Planning

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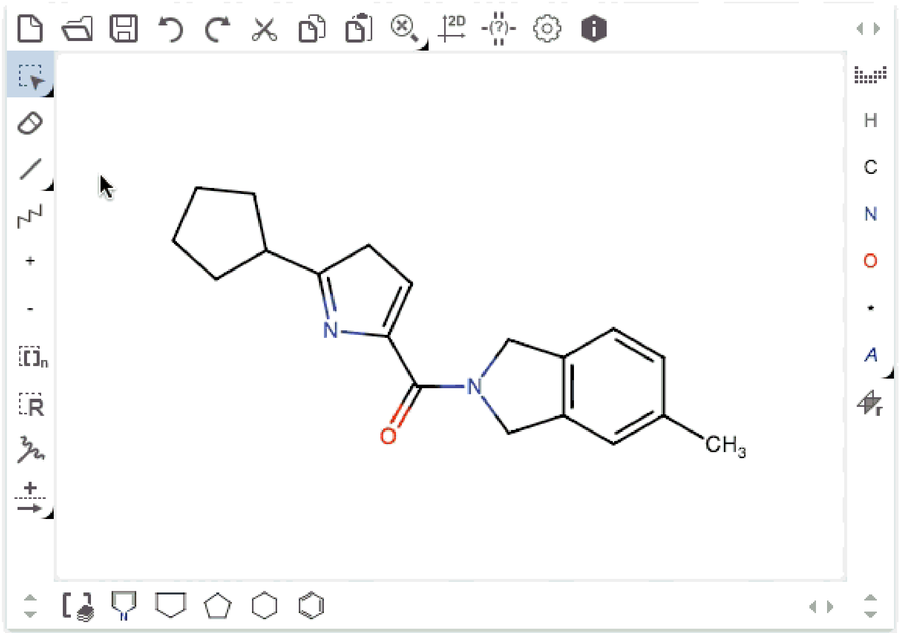
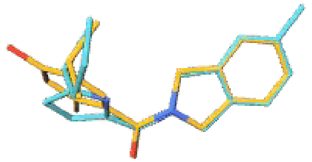
MOLECULE DESIGN & COLLABORATION

Video

Bring in all the data



Alignment (preview)



Calculated Properties

- ▼ **Mass**: 294.4
- ▼ **cLogP**: 3.38
- ▼ **TPSA**: 32.67 Å²
- ▲ **pKa (str. acidic)**: 11.42
- ▲ **pKa (str. basic)**: 3.98
- **Solubility**: logS
- ▼ **H-bond acceptors**: 2
- ▼ **H-bond donors**: 0

Compound registry

Substructure matches: 16

- ACME56
- ACME69
- ACME1002
- ACME1432
- ACME1433

Over 60 plugins, and counting…

Mining

SciFinder
Reaxys
ChEMBL
SureChEMBL
Corporate assay DB
Legislations
Registration

Exploring

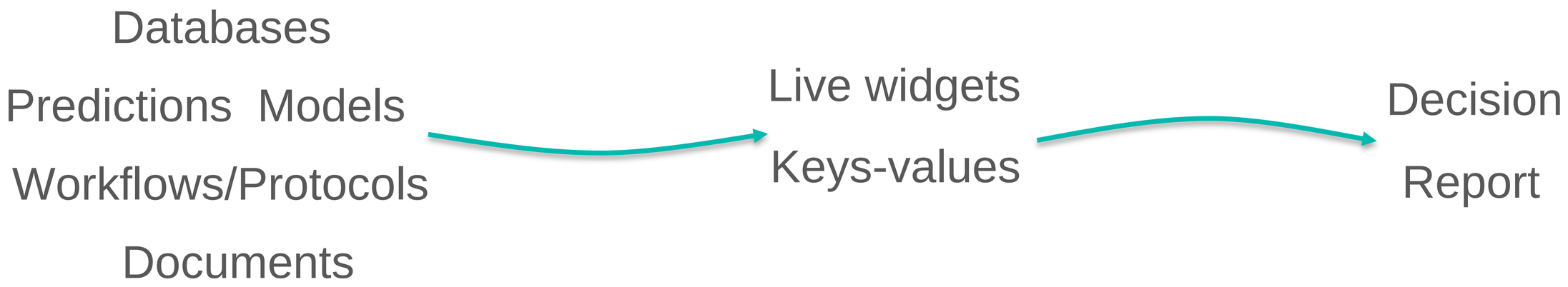
Med. chem. descriptors
Predictive models
Conformations
Overlays
Similarities
KNIME Workflows
PP protocols

Planning

Reactions
Inventory
Supplier catalogs
Export to ELN
Export to Registration

code examples published under MIT license on docs.chemaxon.com

Integrated data driven approach



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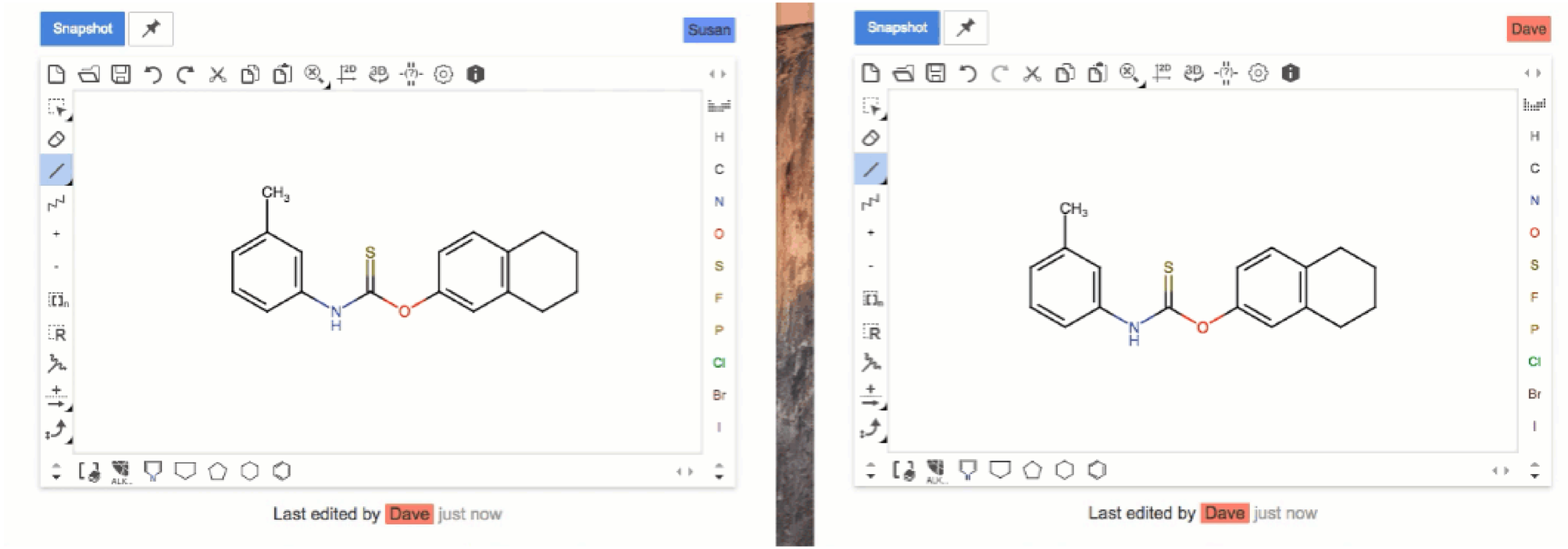
COLLABORATION

Working with colleagues…

on molecules



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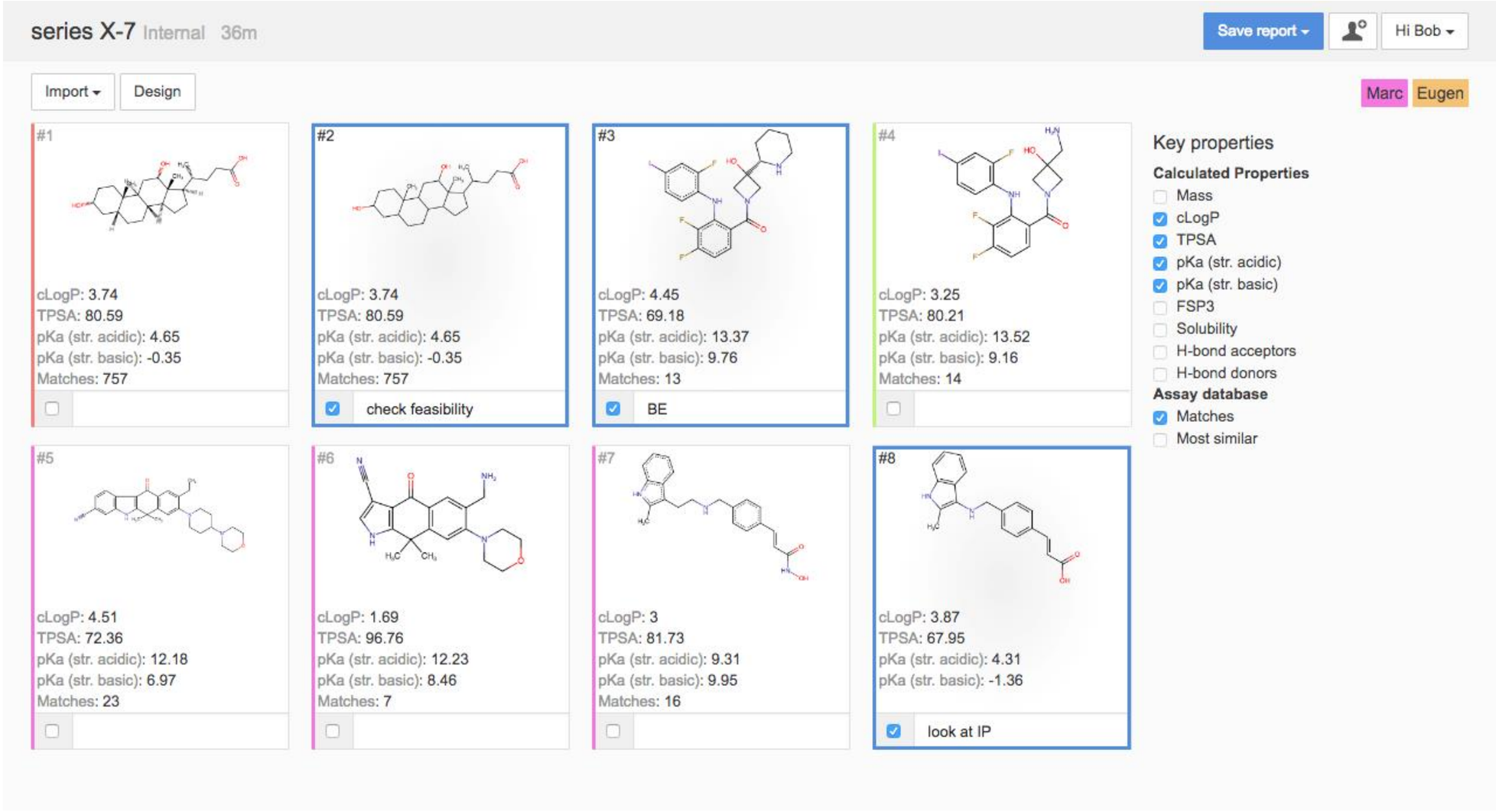
Working with colleagues…

on molecules
on series



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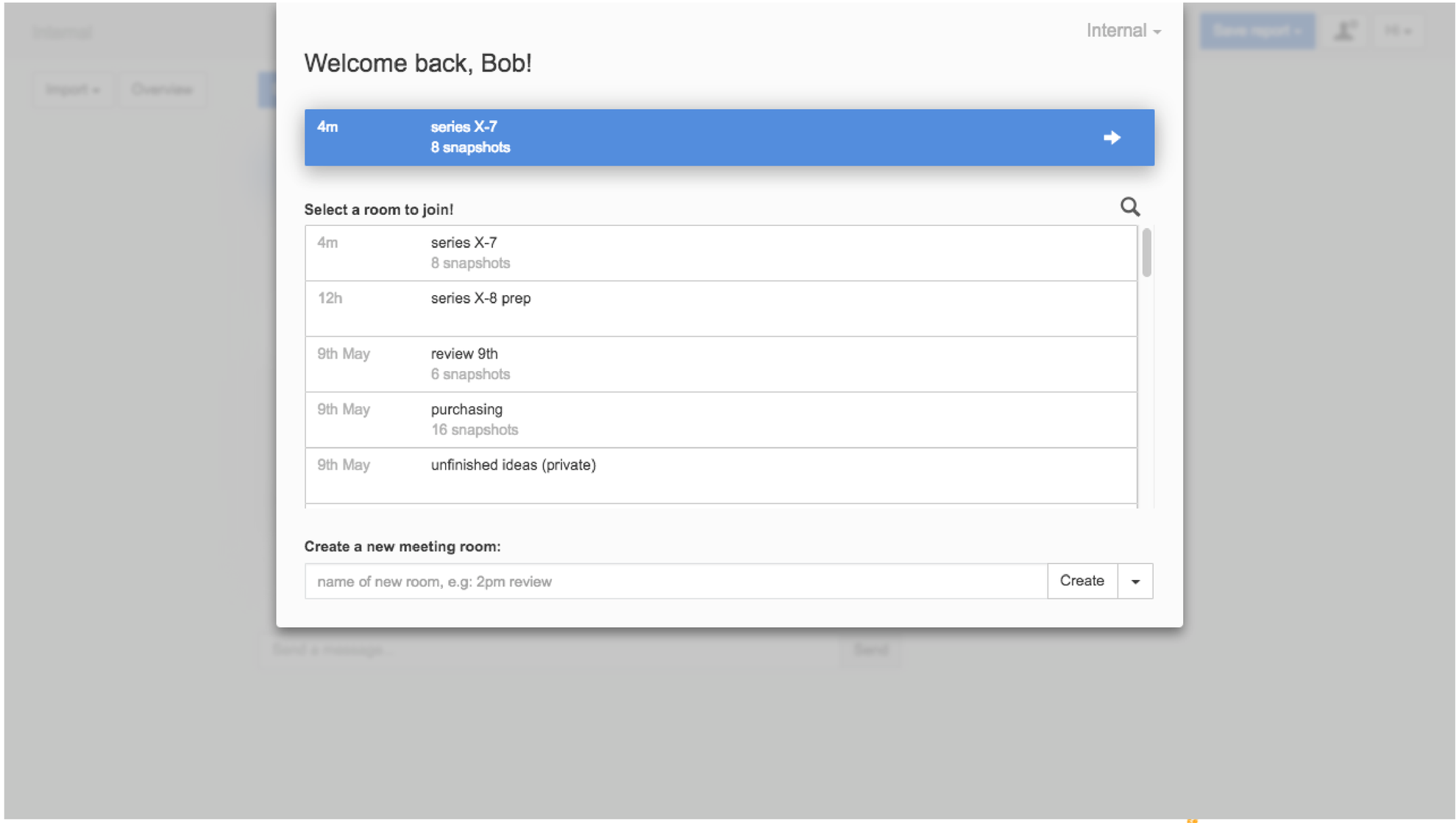
Working with colleagues…

on molecules
on series
on a project



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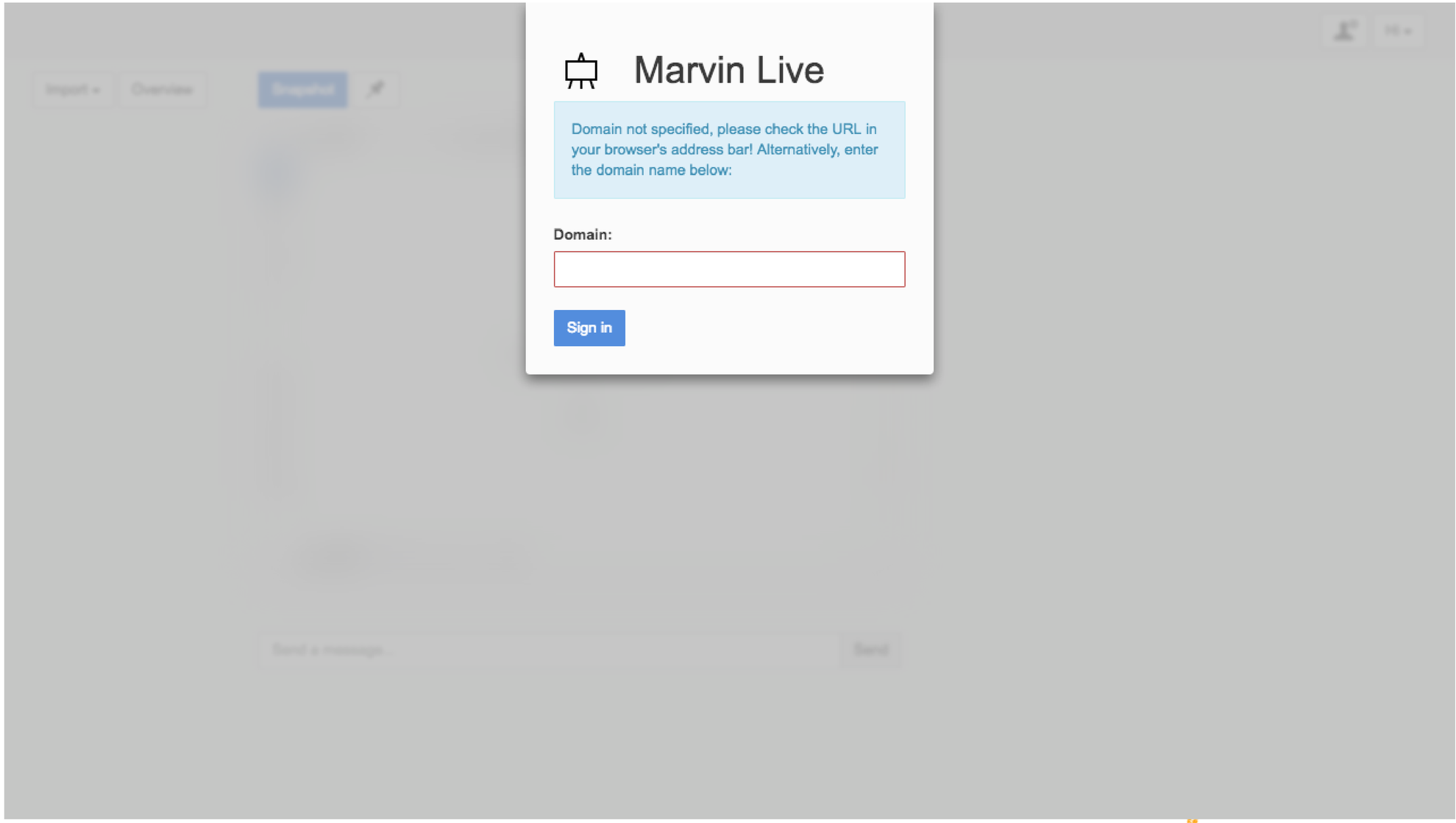
Working with colleagues…

on molecules
on series
on a project
and partners



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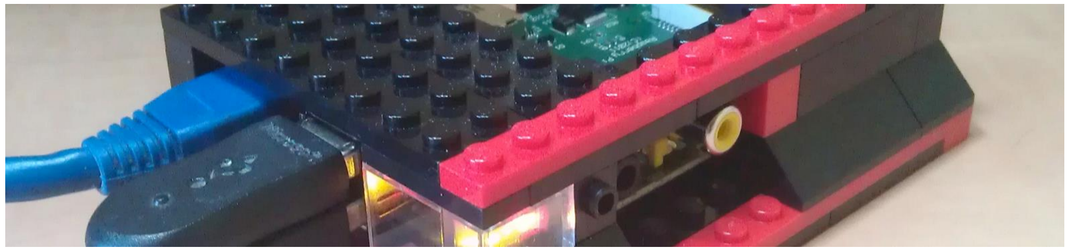
AVAILABILITY

Managed-hosted environment

- providers with SOC 2, single tenant setup
- customizations by ChemAxon
- flexible payment
- single support address

On-premise



- choose your own hardware, VM/container provided
- flexible setup
- annual license

NOW, IT’S YOUR TURN

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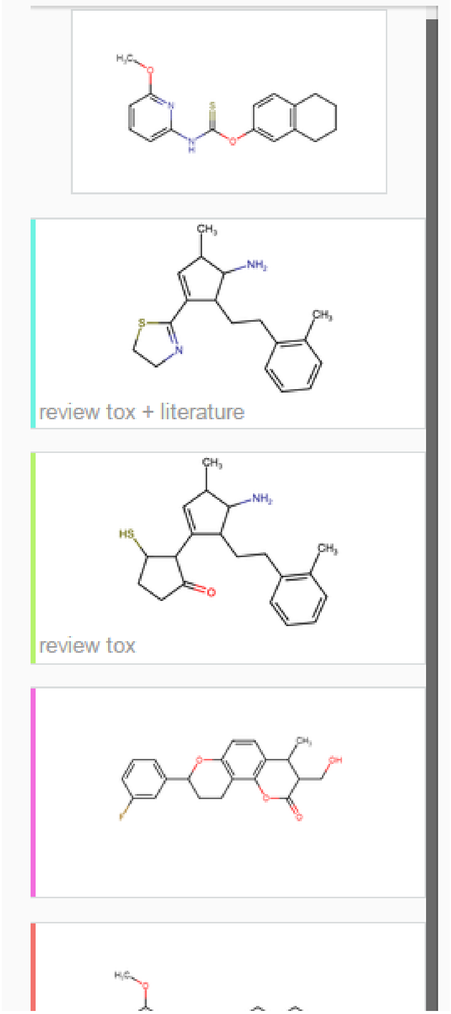
Roadmap

- more data providers, more examples, more use-cases
  - Plexus Assay
  - Plexus Inventory
- finer security controls
- improved 3D visualizations re: ligand-protein
- track compounds throughout the application

Reporting



- automatic capture (who, what, when)
- save important structures & metadata
  - for presentations
  - to desktop tools (SD file, SMILES)
  - to ELN, to registration, to other apps

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