

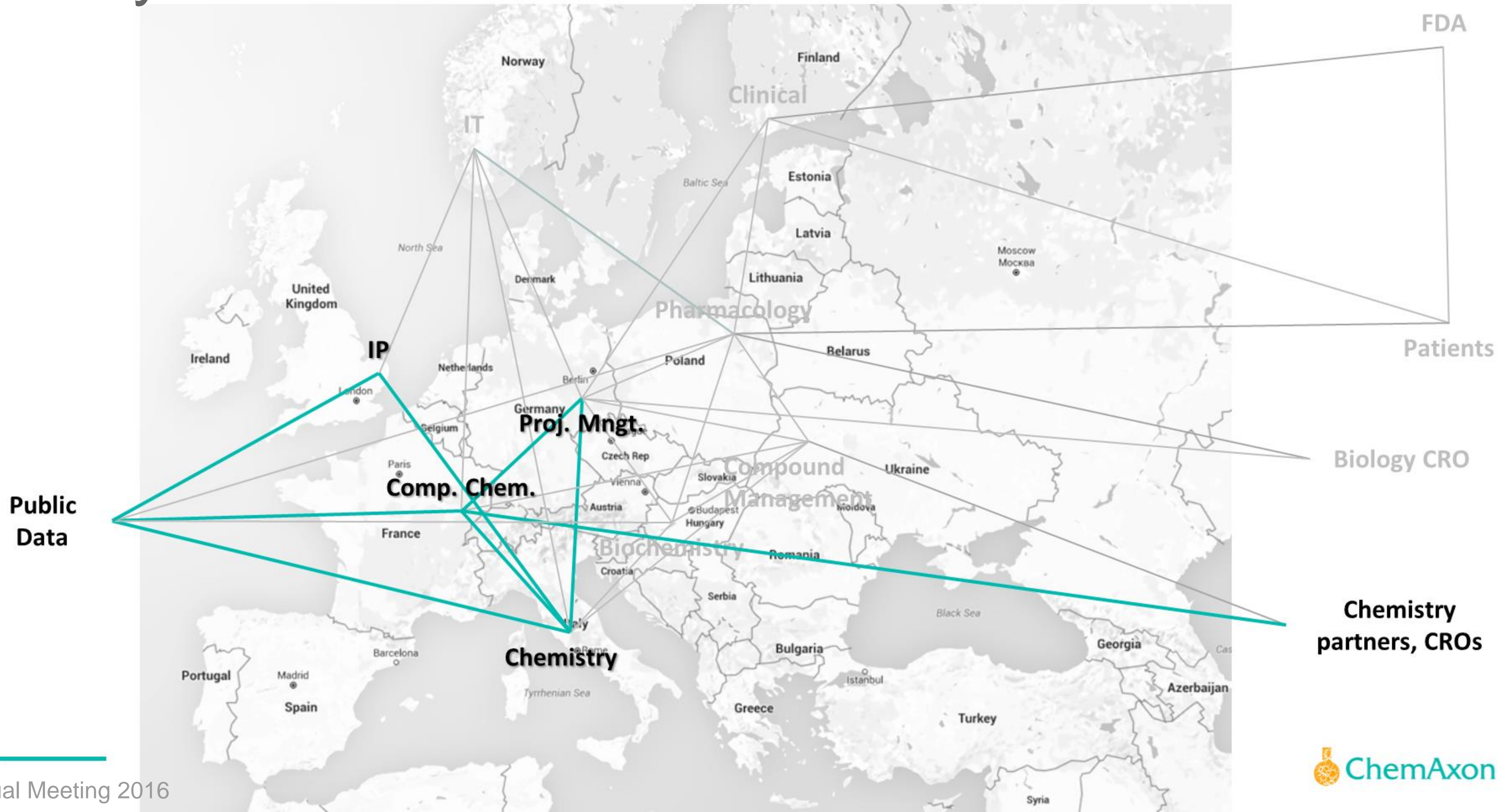
 MARVIN LIVE

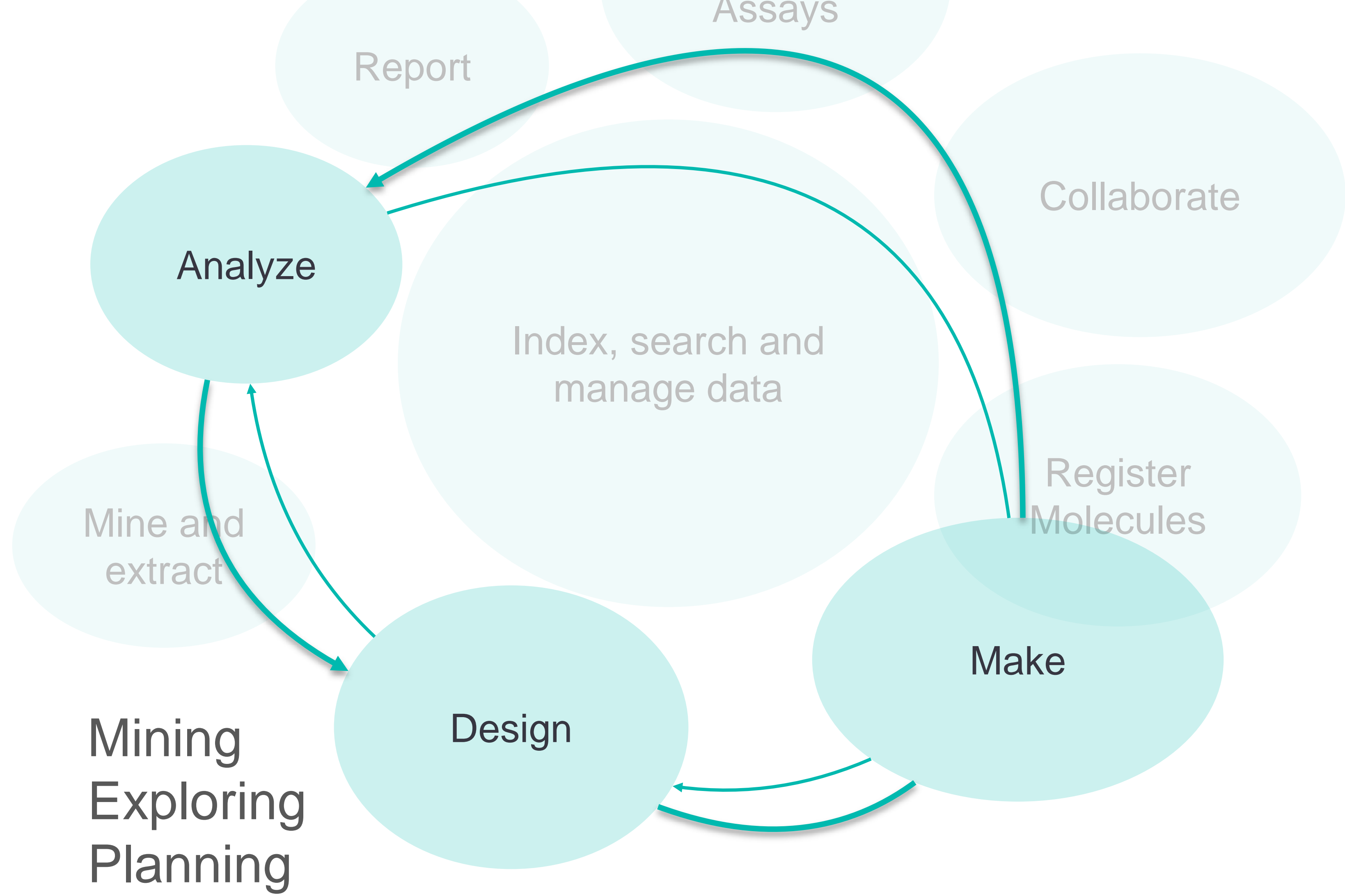
András Strácz
Budapest Annual Meeting
2016


—



Ecosystem



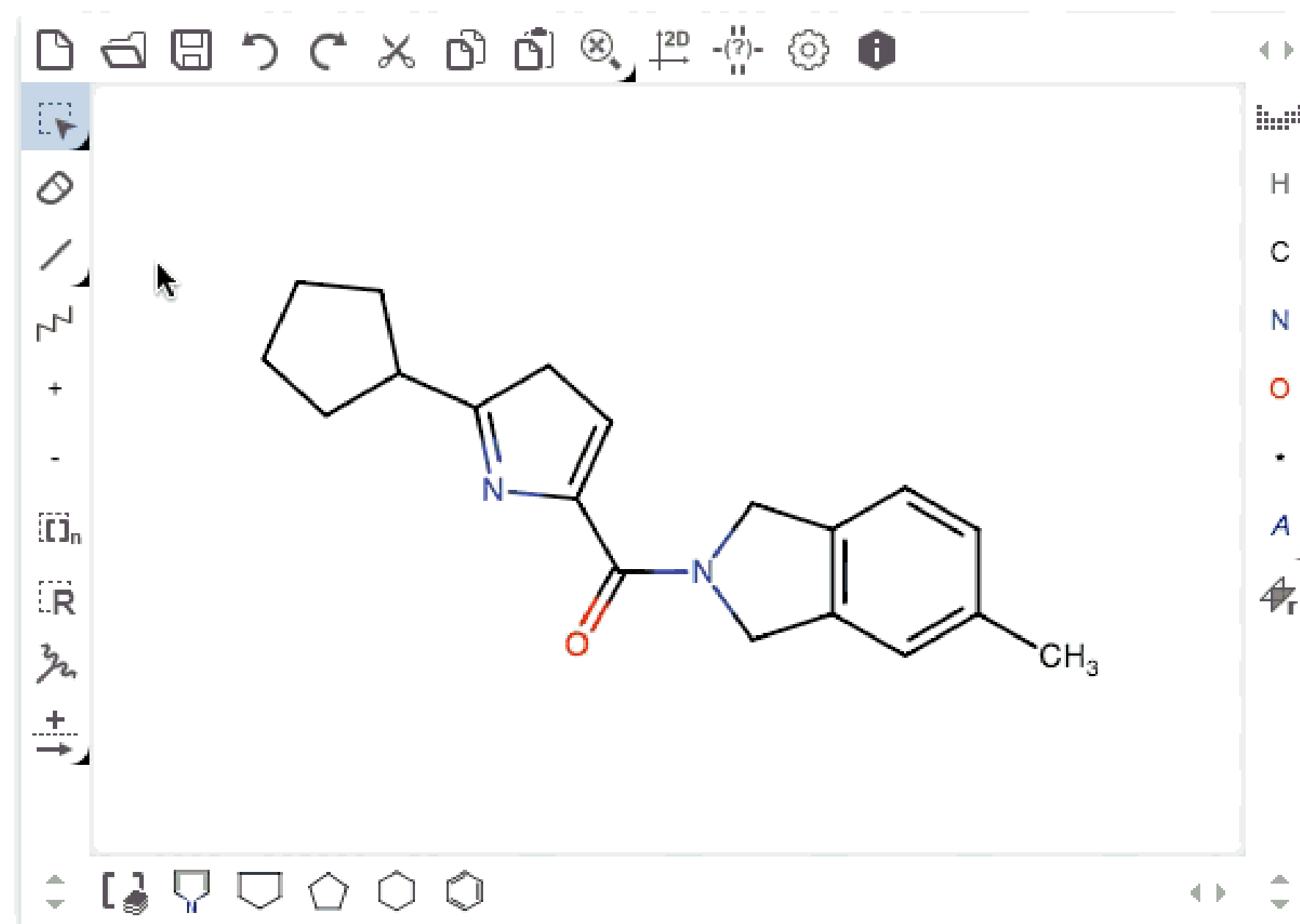




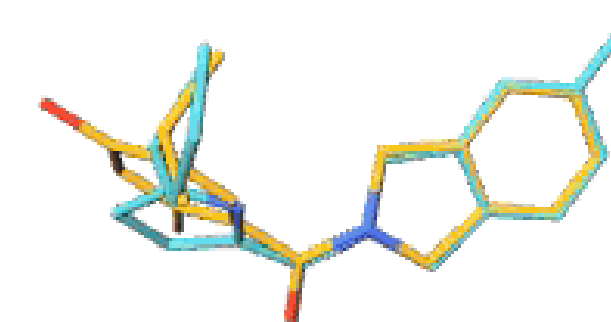
MOLECULE DESIGN & COLLABORATION

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

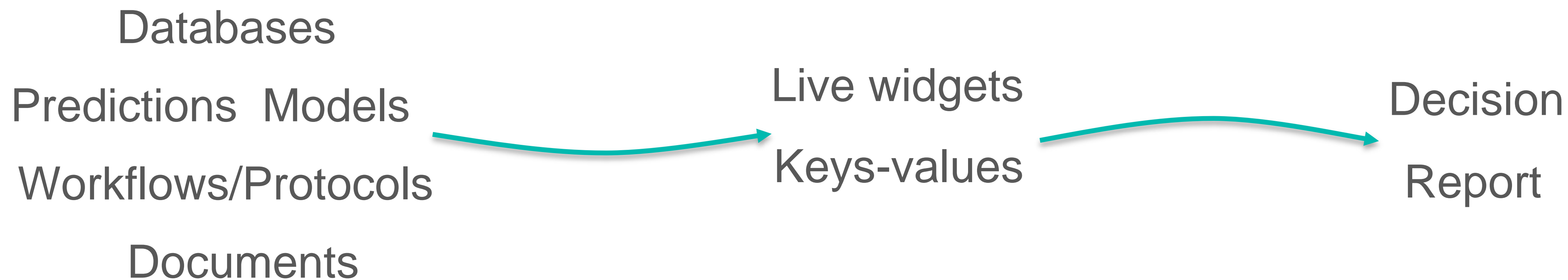
Inventory

Supplier catalogs

Export to ELN

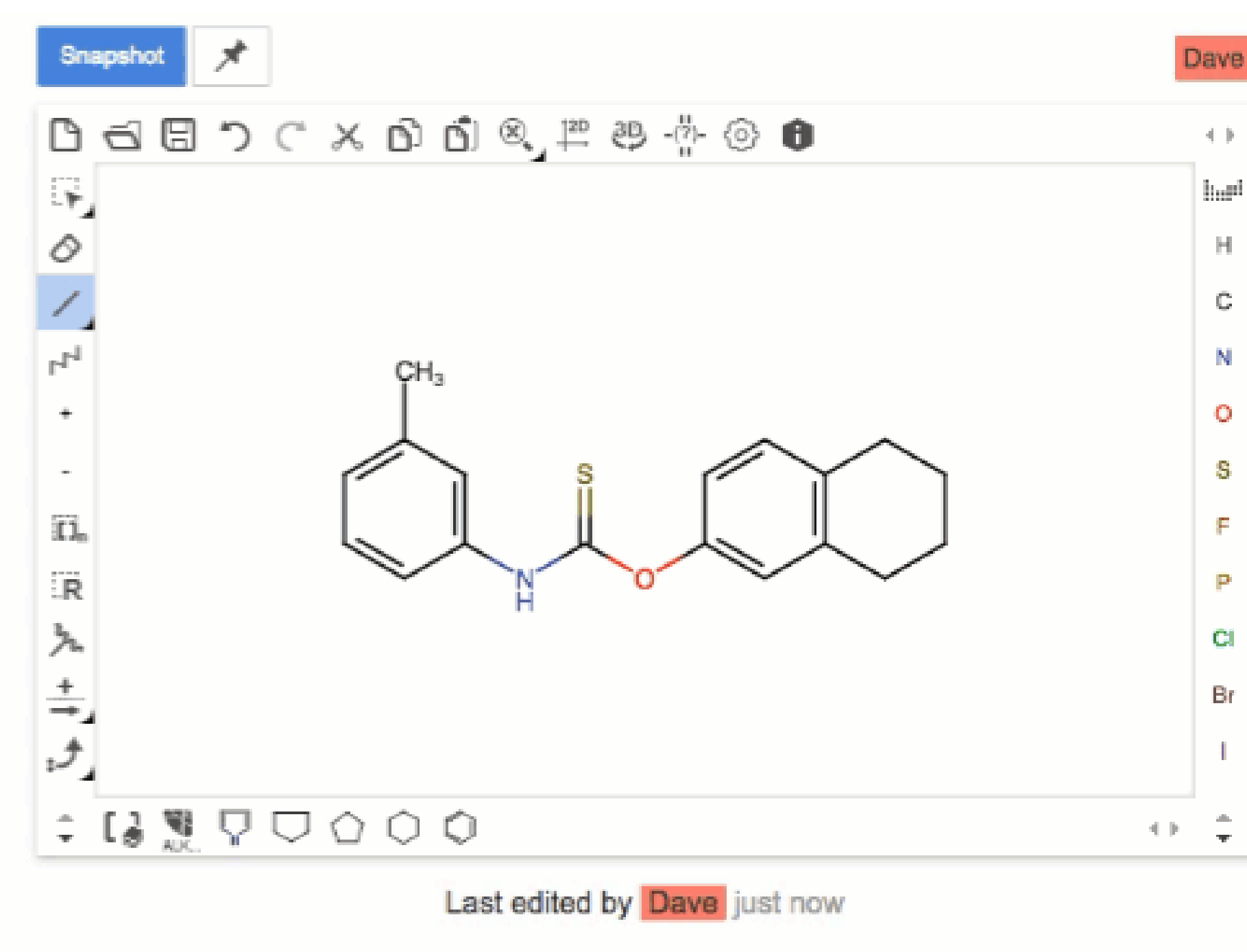
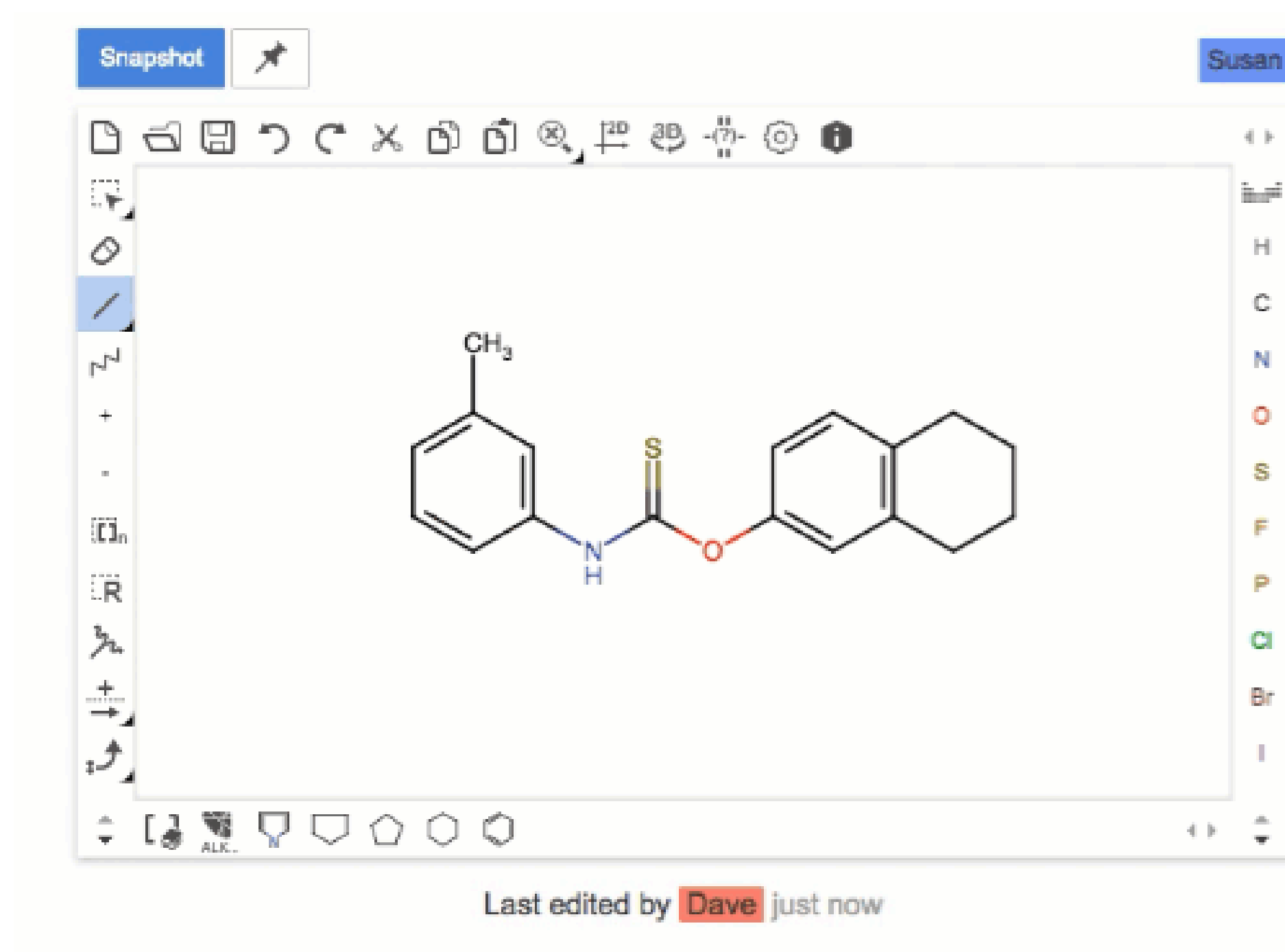
Export to Registration

Integrated data driven approach



COLLABORATION

Working with colleagues... on molecules



Working with colleagues...

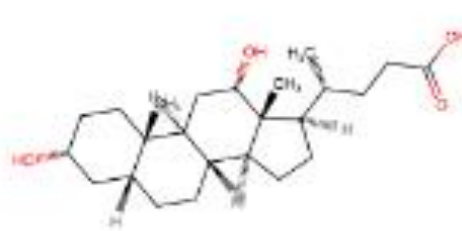
on molecules
on series

series X-7 Internal 36m Save report Hi Bob

Import Design

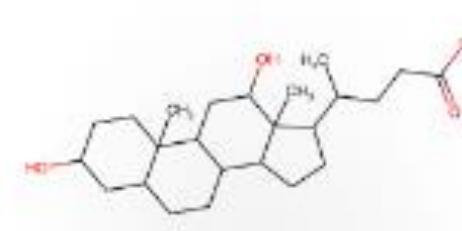
Marc Eugen

#1



cLogP: 3.74
TPSA: 80.59
pKa (str. acidic): 4.65
pKa (str. basic): -0.35
Matches: 757

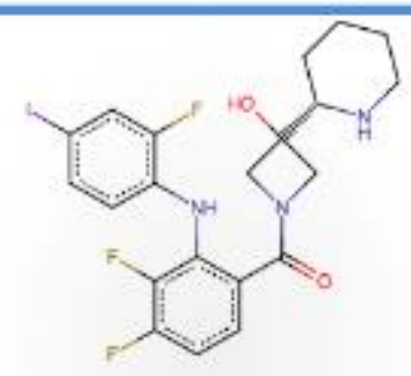
#2



cLogP: 3.74
TPSA: 80.59
pKa (str. acidic): 4.65
pKa (str. basic): -0.35
Matches: 757

 check feasibility


#3



cLogP: 4.45
TPSA: 69.18
pKa (str. acidic): 13.37
pKa (str. basic): 9.76
Matches: 13

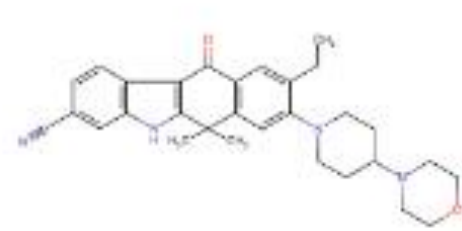
 BE

#4



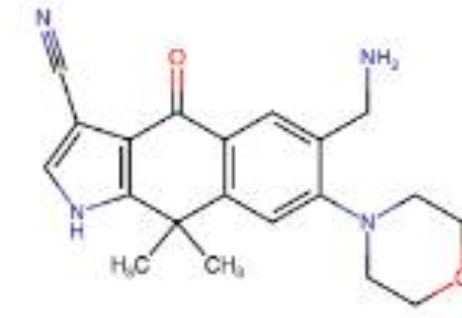
cLogP: 3.25
TPSA: 80.21
pKa (str. acidic): 13.52
pKa (str. basic): 9.16
Matches: 14

#5



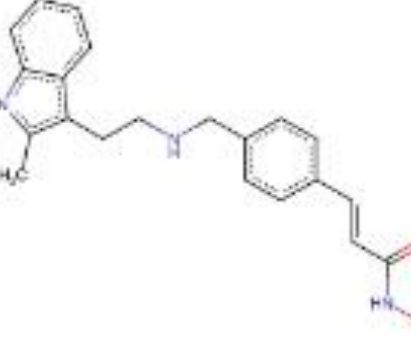
cLogP: 4.51
TPSA: 72.36
pKa (str. acidic): 12.18
pKa (str. basic): 6.97
Matches: 23

#6



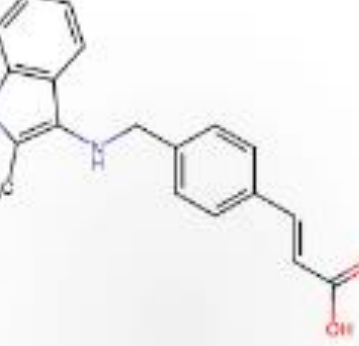
cLogP: 1.69
TPSA: 96.76
pKa (str. acidic): 12.23
pKa (str. basic): 8.46
Matches: 7

#7



cLogP: 3
TPSA: 81.73
pKa (str. acidic): 9.31
pKa (str. basic): 9.95
Matches: 16

#8



cLogP: 3.87
TPSA: 67.95
pKa (str. acidic): 4.31
pKa (str. basic): -1.36

 look at IP

Key properties

Calculated Properties

- Mass
- cLogP
- TPSA
- pKa (str. acidic)
- pKa (str. basic)
- FSP3
- Solubility
- H-bond acceptors
- H-bond donors

Assay database

- Matches
- Most similar

Working with colleagues...

on molecules
on series
on a project

Internal

Welcome back, Bob!

4m series X-7
8 snapshots

Select a room to join!

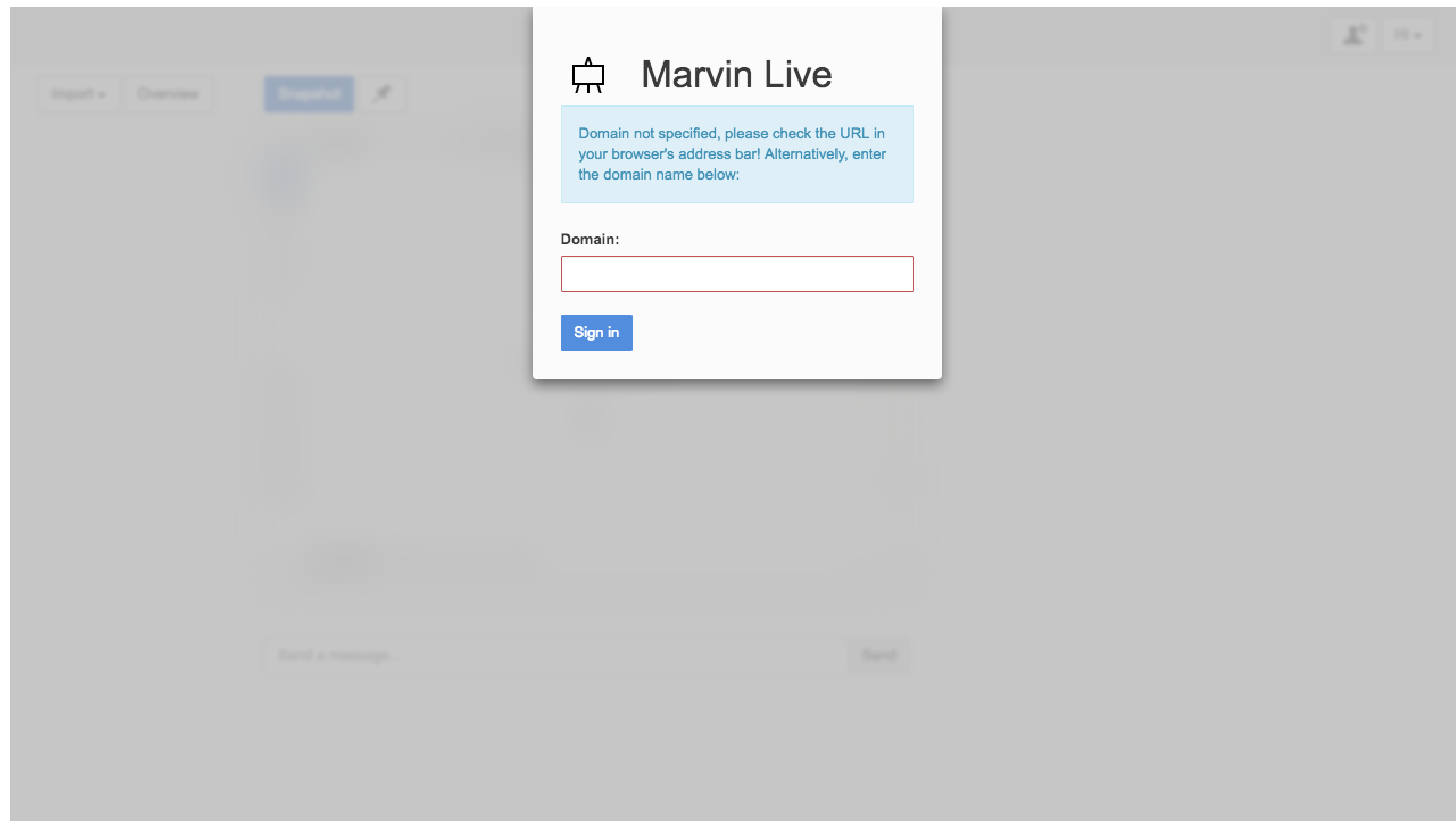
4m	series X-7 8 snapshots
12h	series X-8 prep
9th May	review 9th 6 snapshots
9th May	purchasing 16 snapshots
9th May	unfinished ideas (private)

Create a new meeting room:

name of new room, e.g: 2pm review

Working with colleagues...

on molecules
on series
on a project
and partners



AVAILABILITY

Managed-hosted environment



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

On-premise



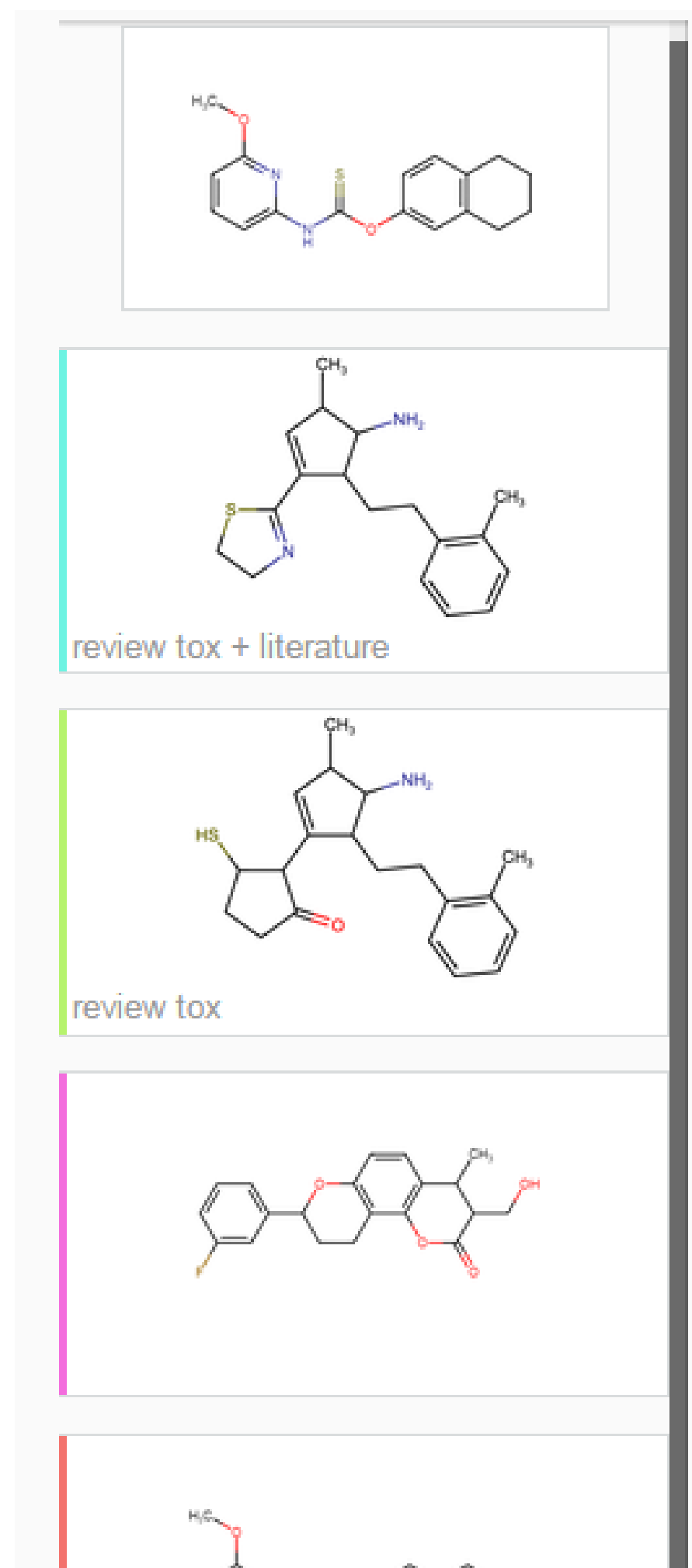
- choose your own hardware, VM/container provided
- flexible setup
- annual license

NOW, IT'S YOUR TURN

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