ChemAxon

Norbert Sas

Consultancy

Consultancy at ChemAxon











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taking care of:

- architect solutions
- integration
- migration
- customization / extension

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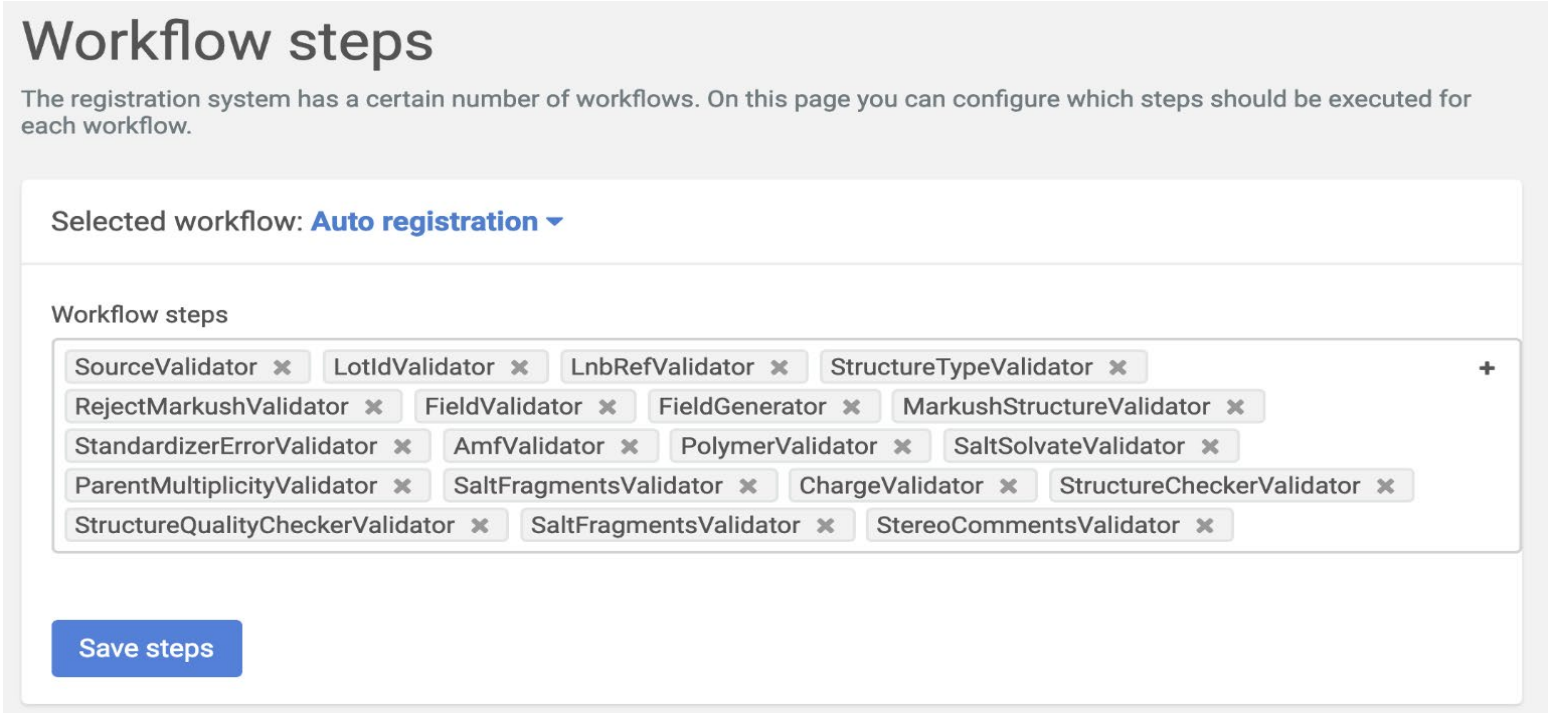
Customizing Compound Registration workflows



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Custom ID generator

Single compound CXN-1234

Custom ID generator

Single compound	CXN-1234
Single compound + salt/solvent	CXN-S-1234

Custom ID generator

Single compound	CXN-1234
Single compound + salt/solvent	CXN-S-1234
Polymer	CXN-P-1234

Custom ID generator

Single compound	CXN-1234
Single compound + salt/solvent	CXN-S-1234
Polymer	CXN-P-1234
Mixture	CXN-M-1234

Custom ID generator

Single compound	CXN-1234
Single compound + salt/solvent	CXN-S-1234
Polymer	CXN-P-1234
Mixture	CXN-M-1234
Formulation	CXN-F-1234

Custom ID generator

Single compound	CXN-1234
Single compound + salt/solvent	CXN-S-1234
Polymer	CXN-P-1234
Mixture	CXN-M-1234
Formulation	CXN-F-1234
No structure	CXN-NS-1234

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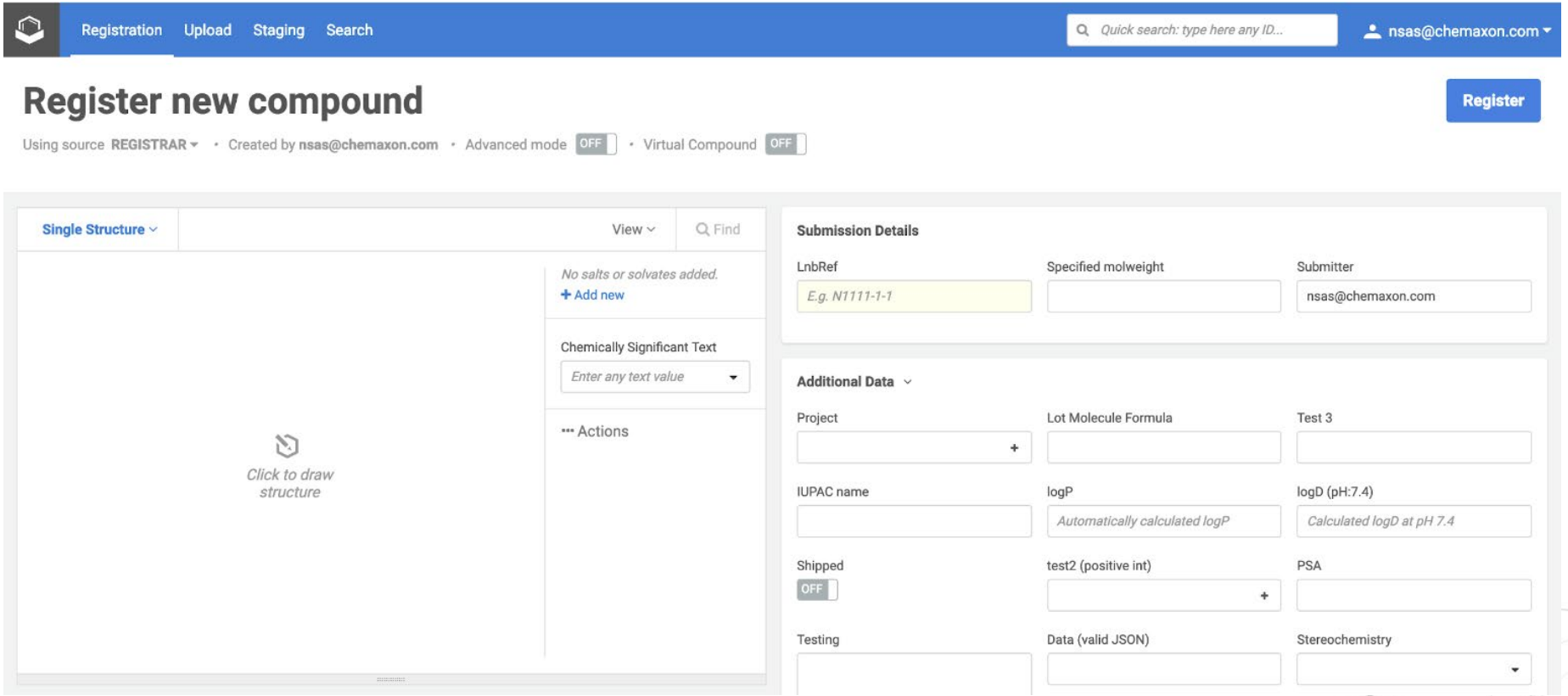
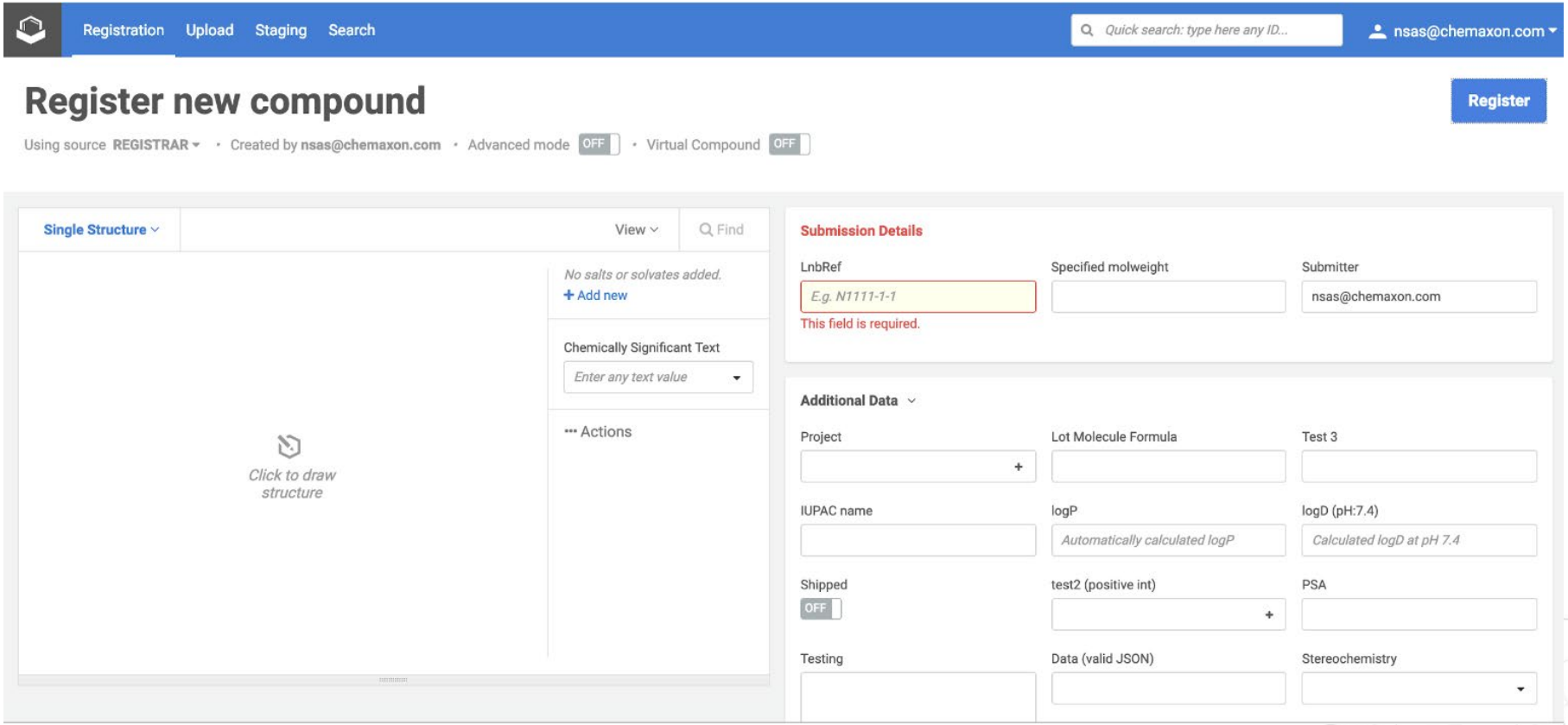
Custom Field Validator



Custom Field Validator



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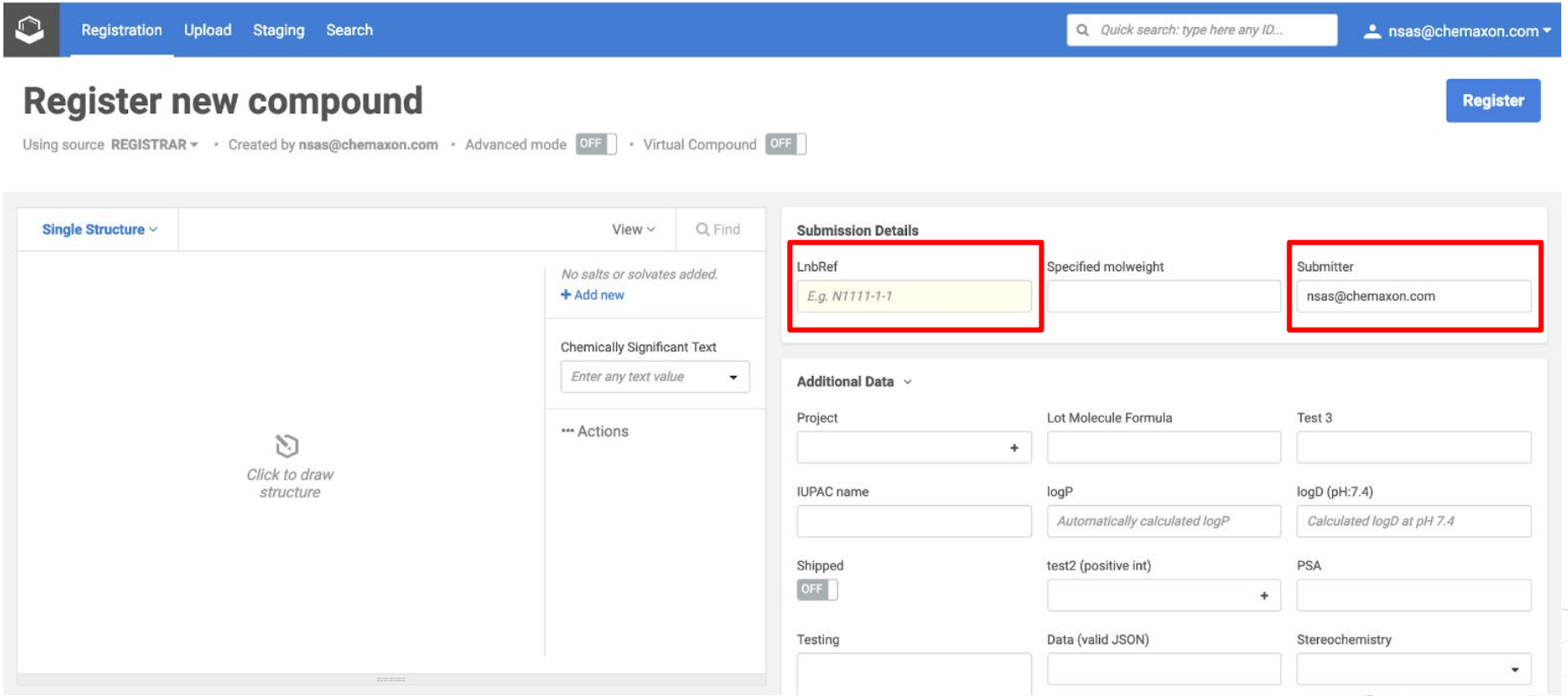

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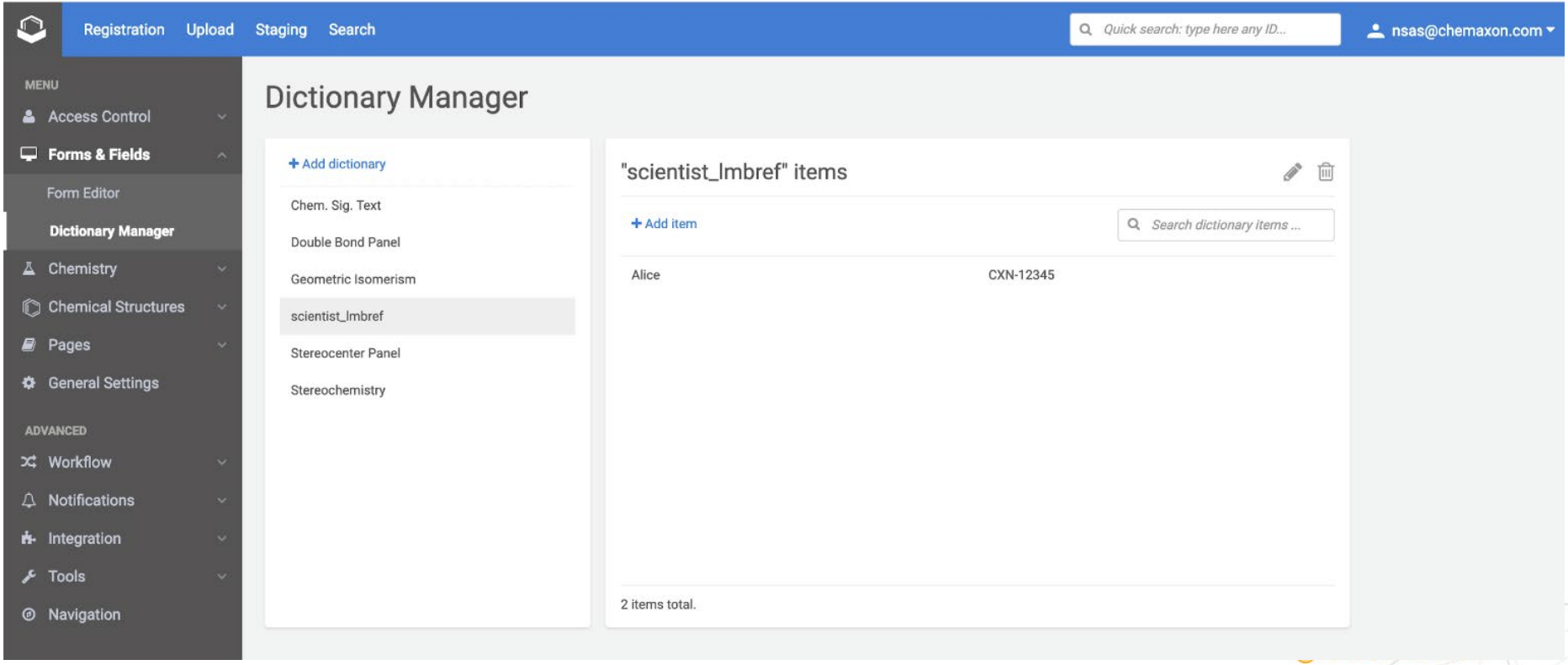
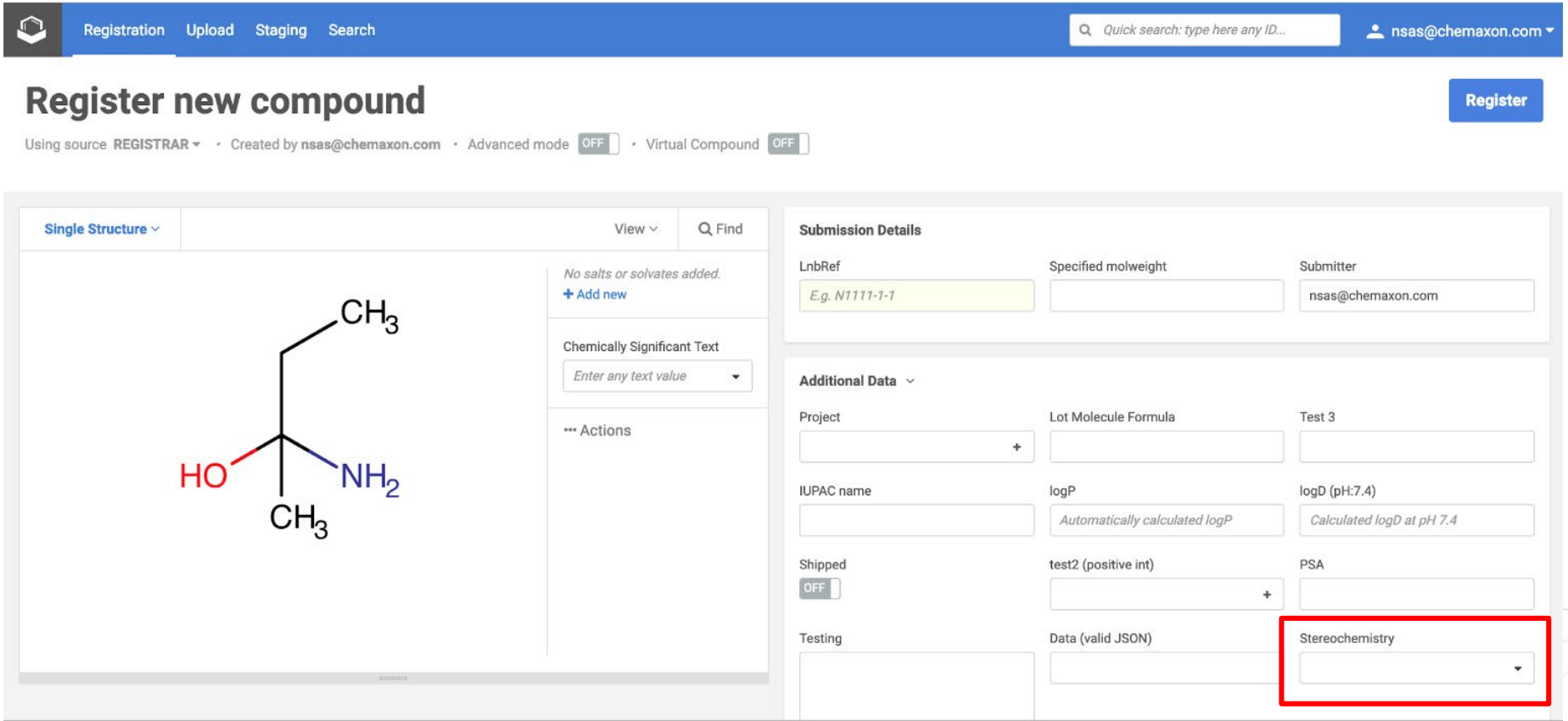
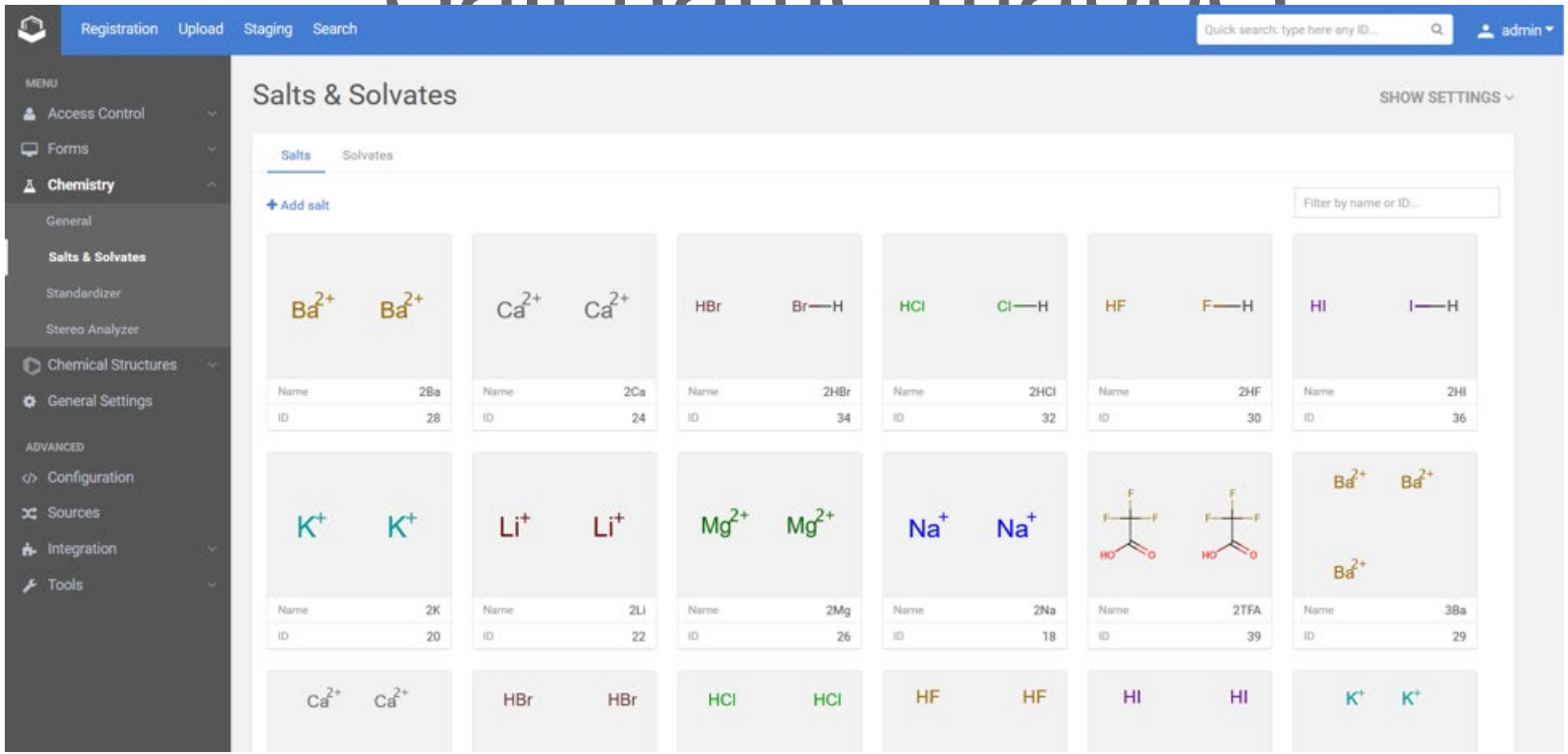


Structure Based Field Validation



Salt name mapper



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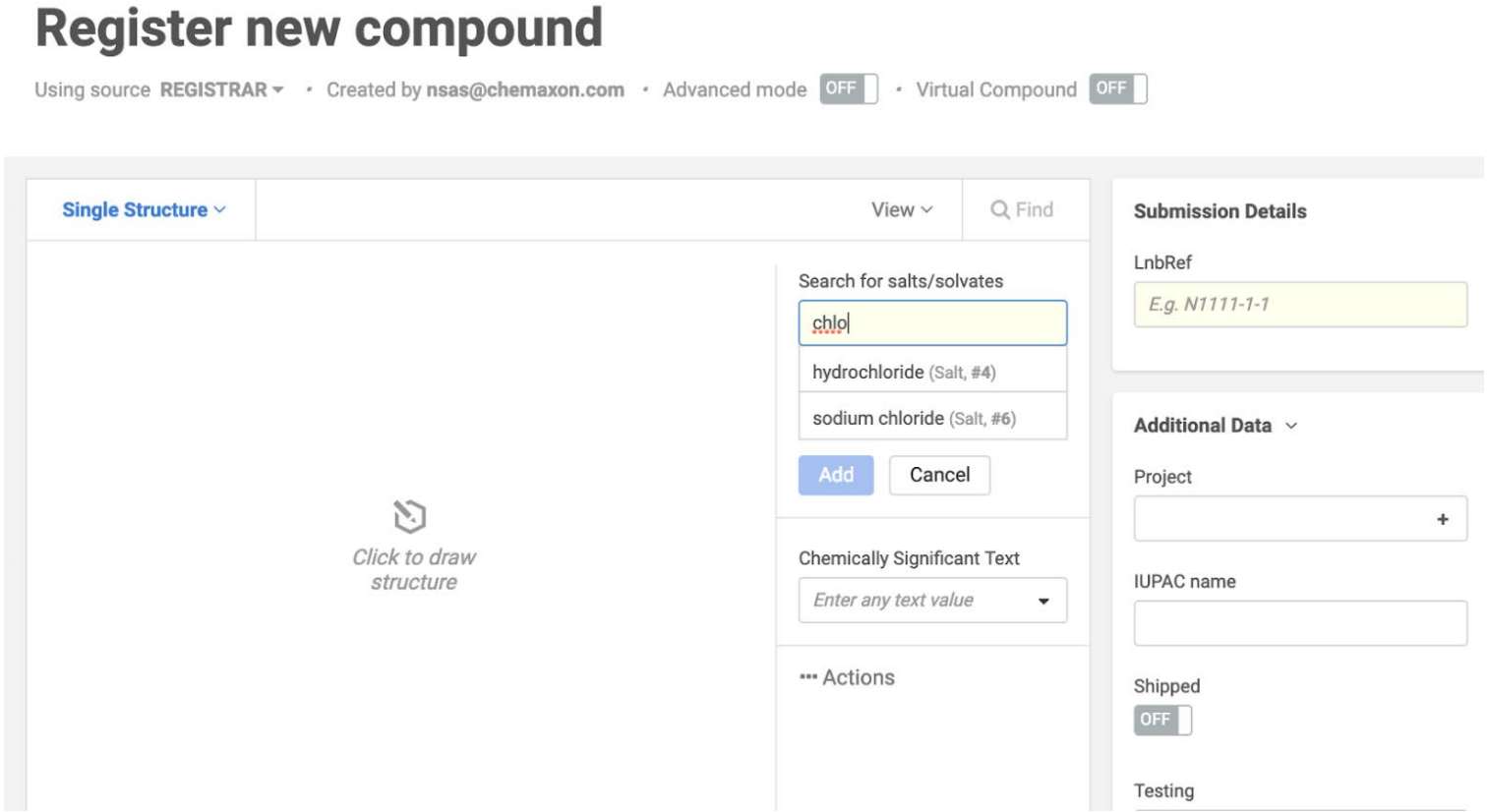
Salt name mapper



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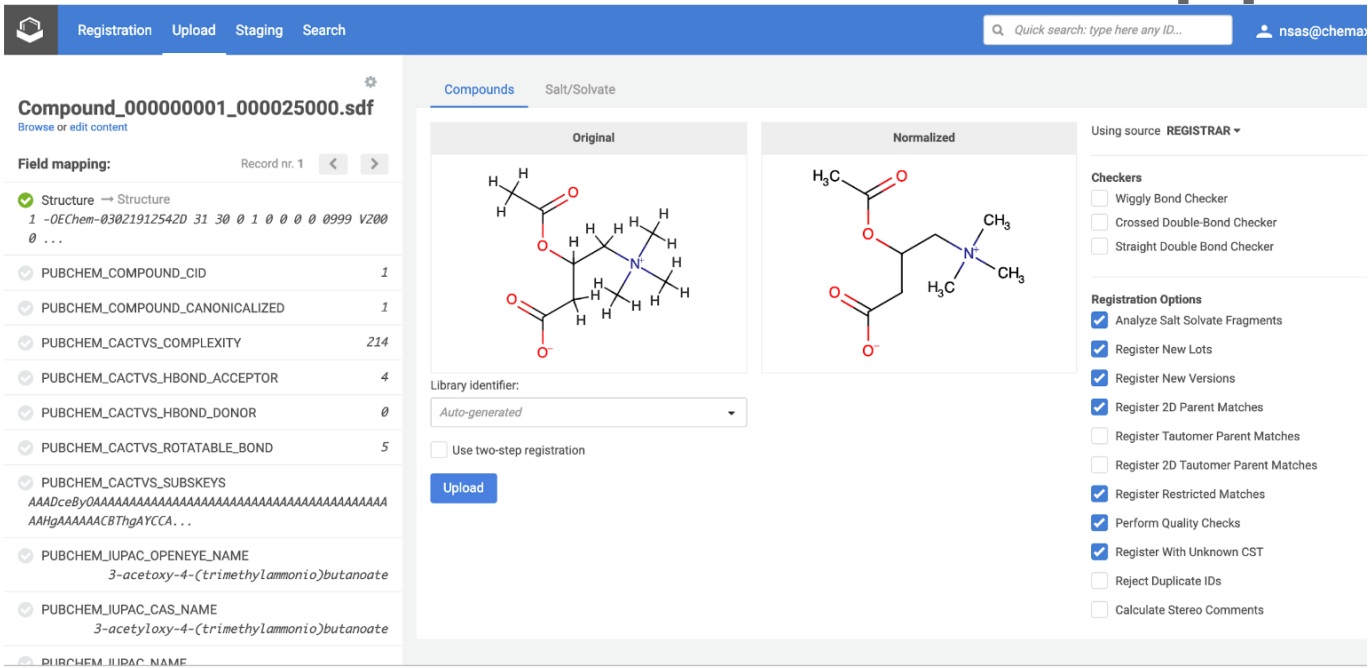
Salt name mapper



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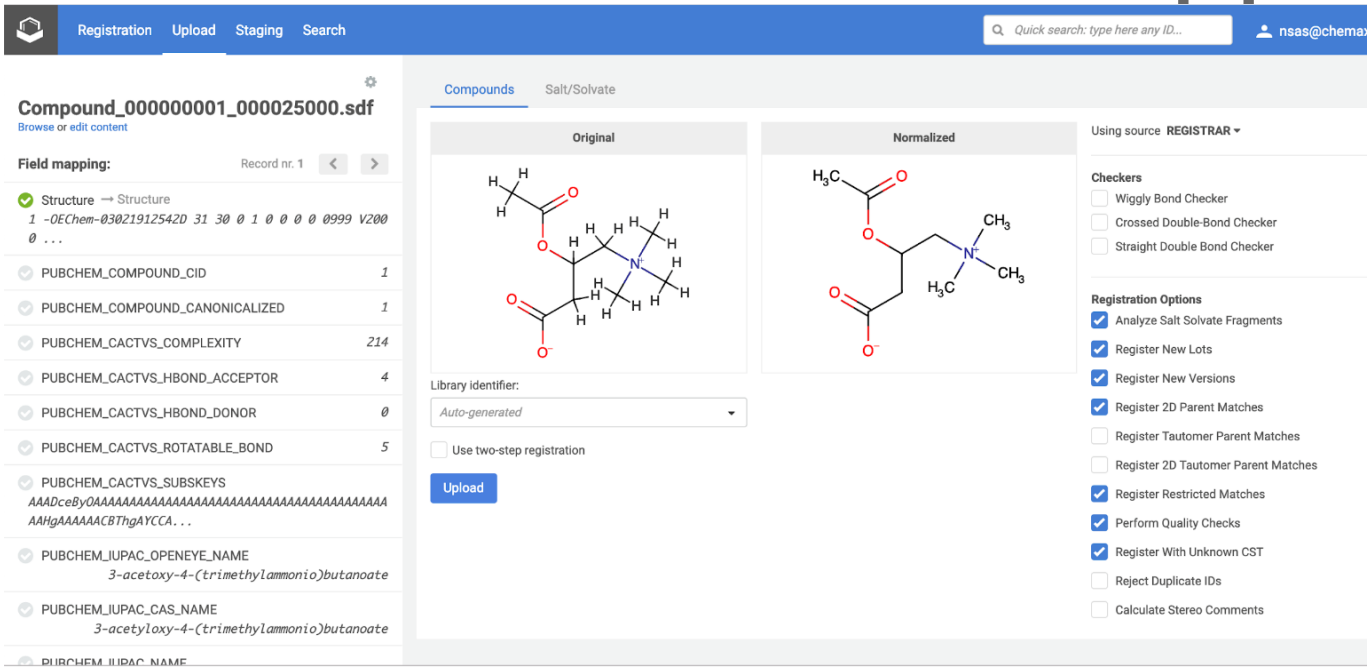
Salt name mapper



><*SaltName*>

HCl

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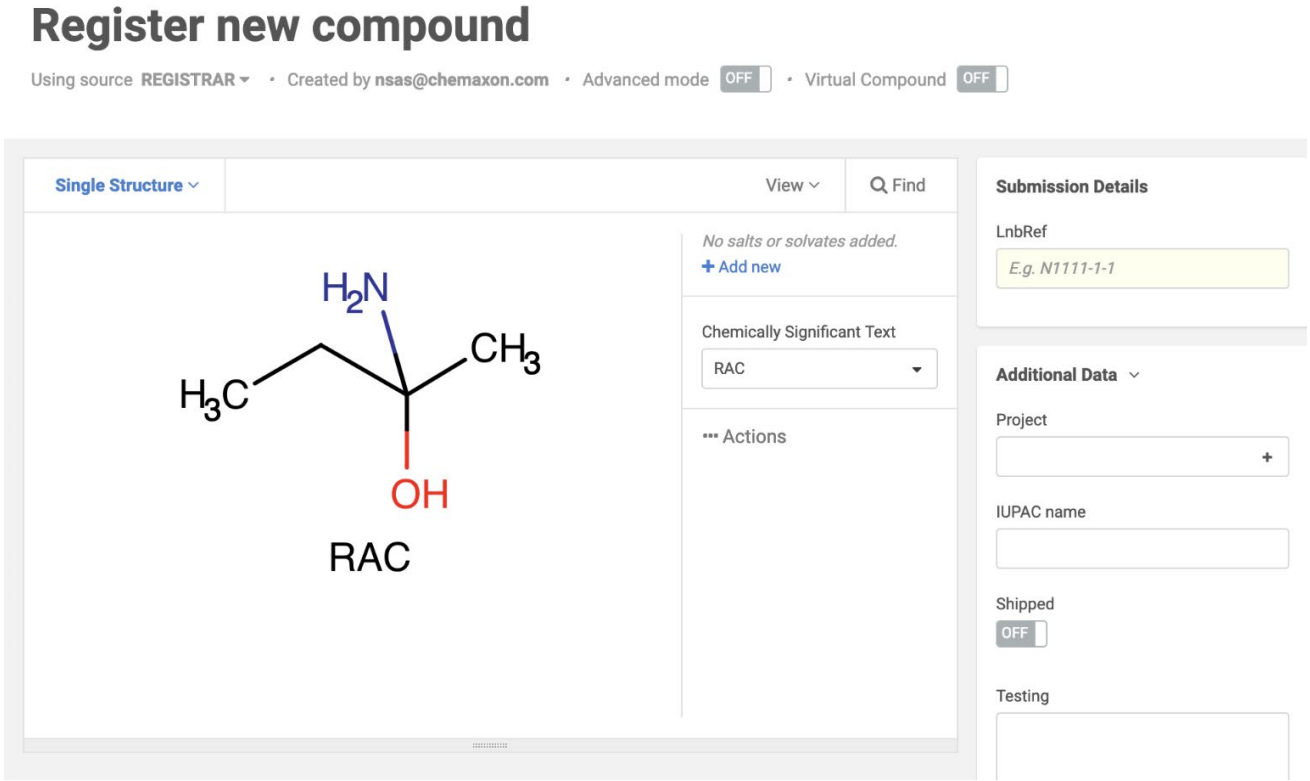
StereoCommentCSTGenerator



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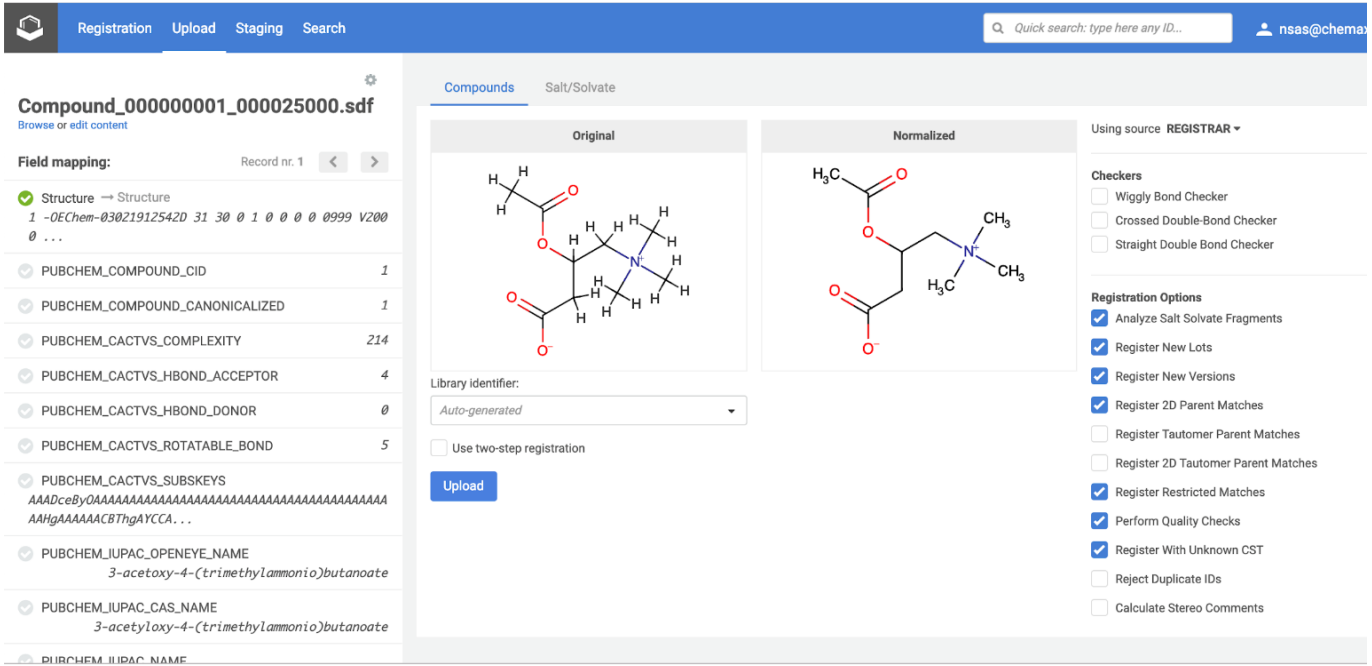
StereoCommentCSTGenerator



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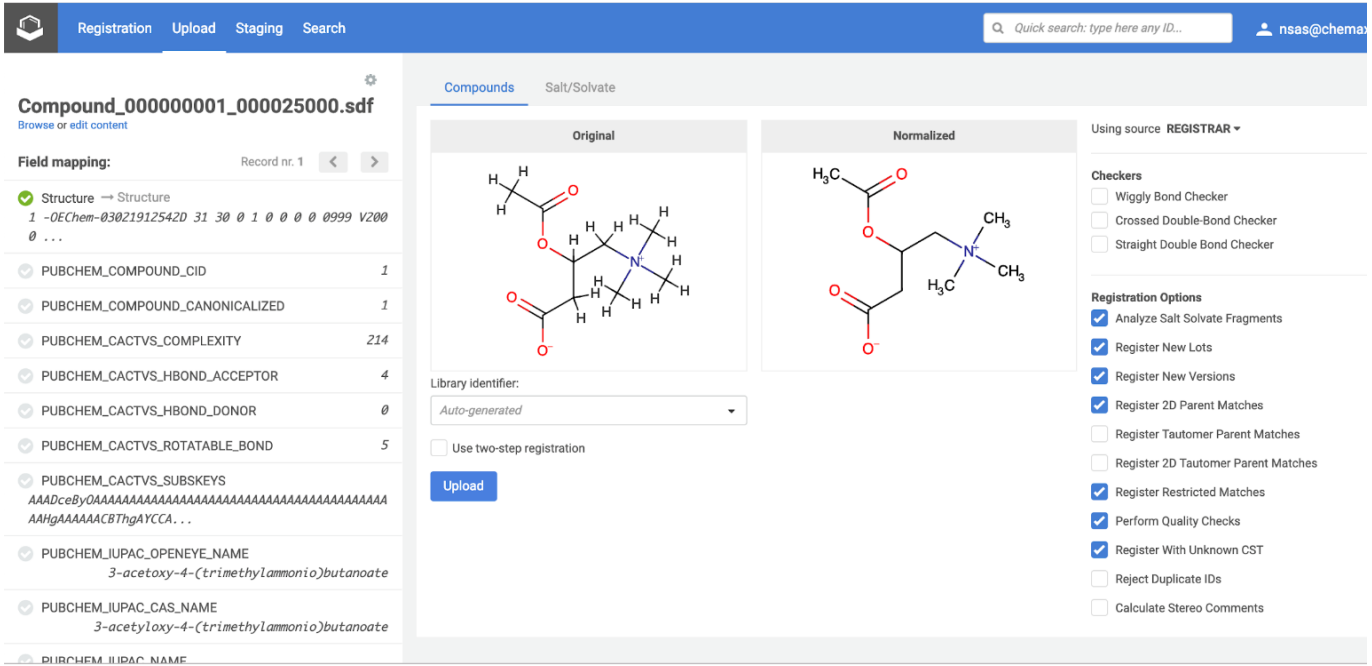
StereoCommentCSTGenerator



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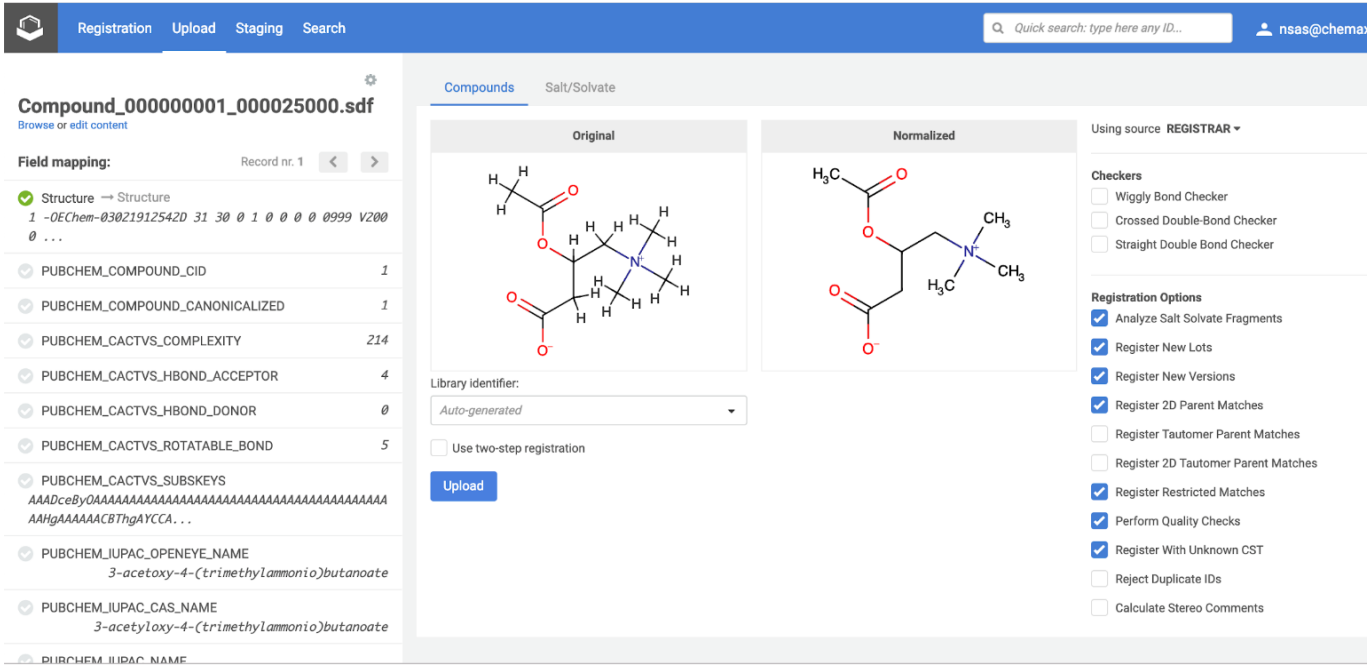
StereoCommentCSTGenerator




```
M  SED  1 Rac
```

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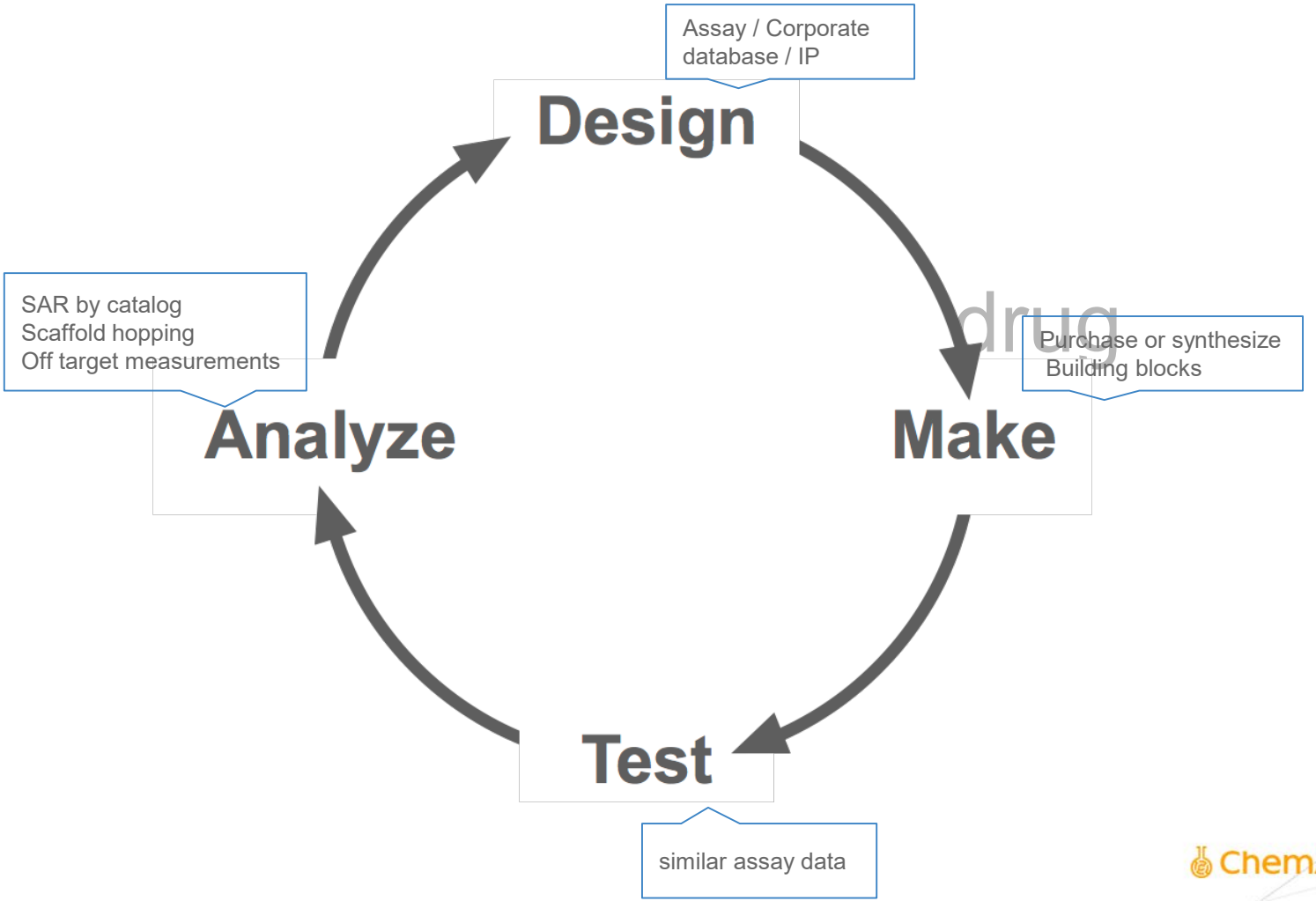
Haystack Project


Assay / Corporate database / IP
Design
drug
Purchase or synthesize Building blocks
Make
Test
similar assay data
Analyze
SAR by catalog
Scaffold hopping
Off target measurements

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Goal

Quickly explore your chemical space

Indexing arbitrary amount of data and running substructure and similarity search.

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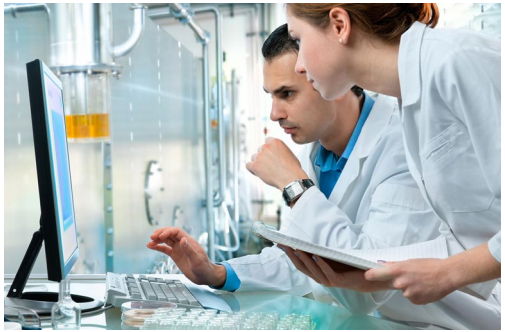
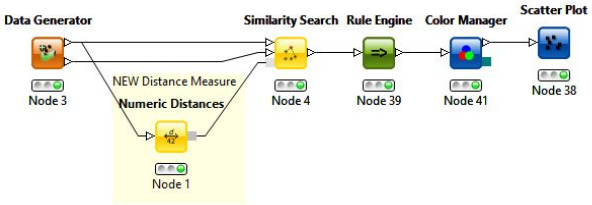
Typical workflows

Interactive search



VS

WorkFlow usage



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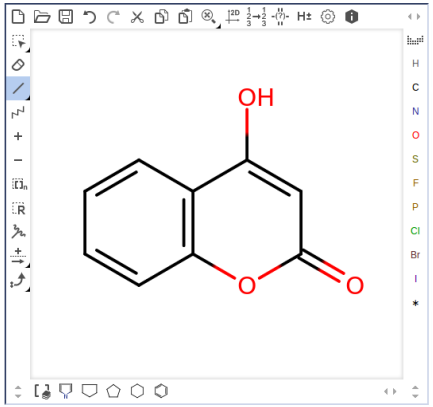
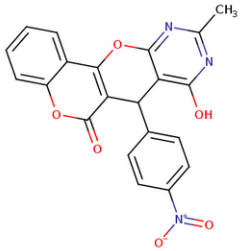
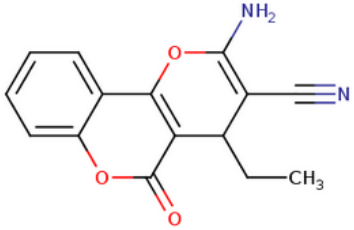
Relevance search

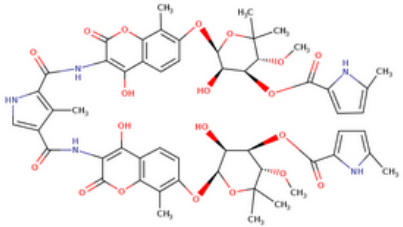
Unordered result

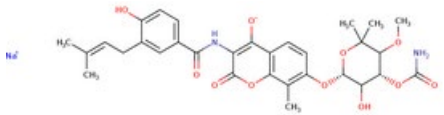


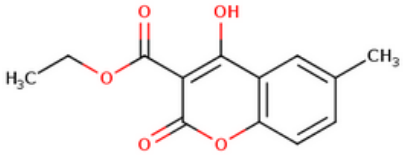
Hits :

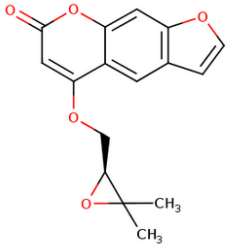












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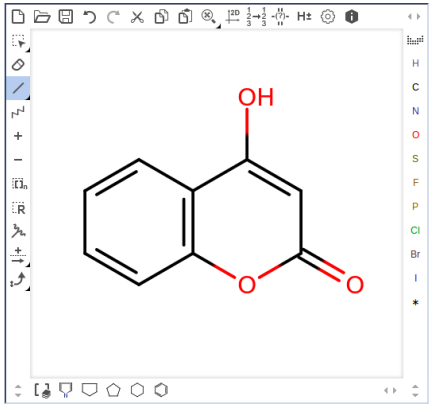
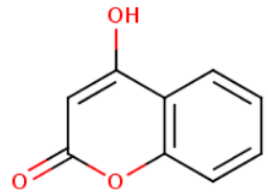
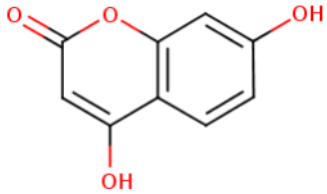
Relevance search

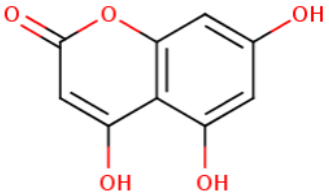
Order substructure search hits according to the relevance to the query structure.

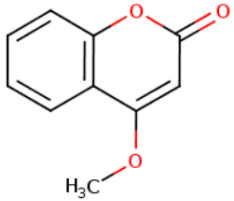


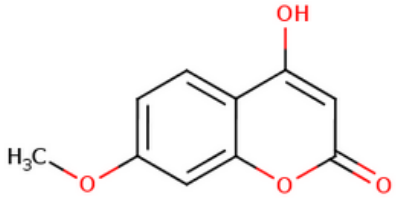
Hits :

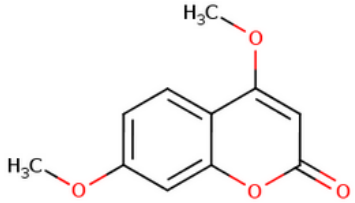












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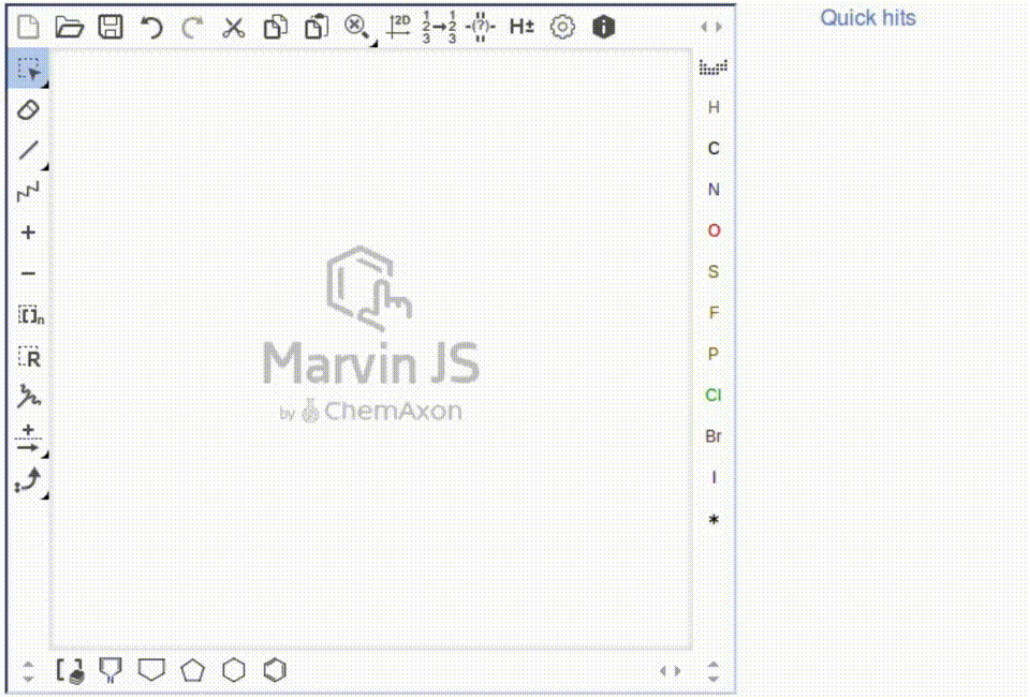
Hits as you draw



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Chemical space:

Current, partial solutions

Some searchable implementations for specific databases:

- eMolecules
- ChEMBL
- SureChEMBL
- ...

Corporate Compound Repository 1.5M – 3M

MolPort All Stock ~7M

Enamine REAL ~680M

ChEMBL 1.7M

SureChEMBL ~18M

BindingDB 651K

Namiki Shoji ~6M

Screening library 250k – 1M

PubChem Compounds ~95M

eMolecules ~18M

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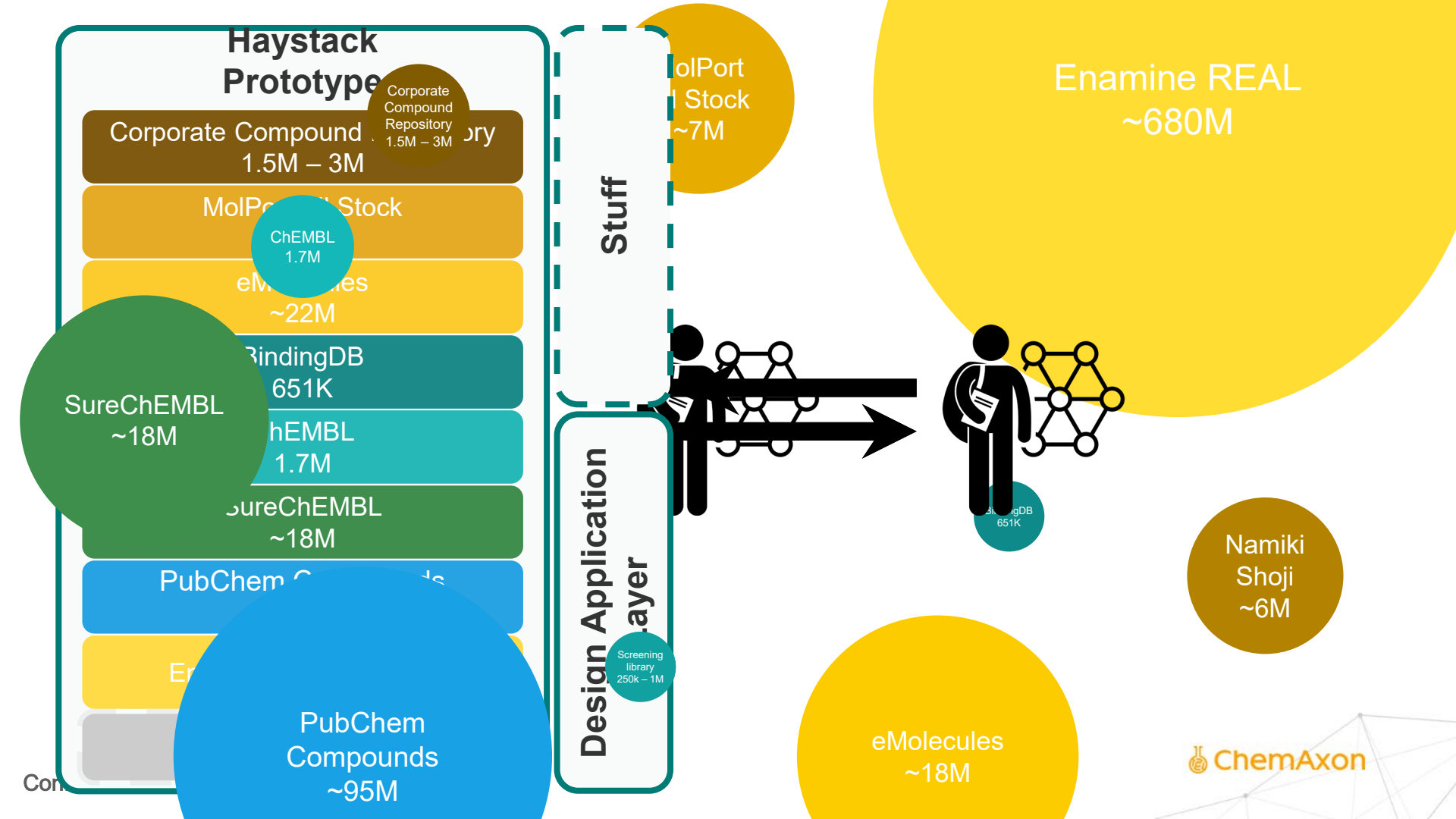
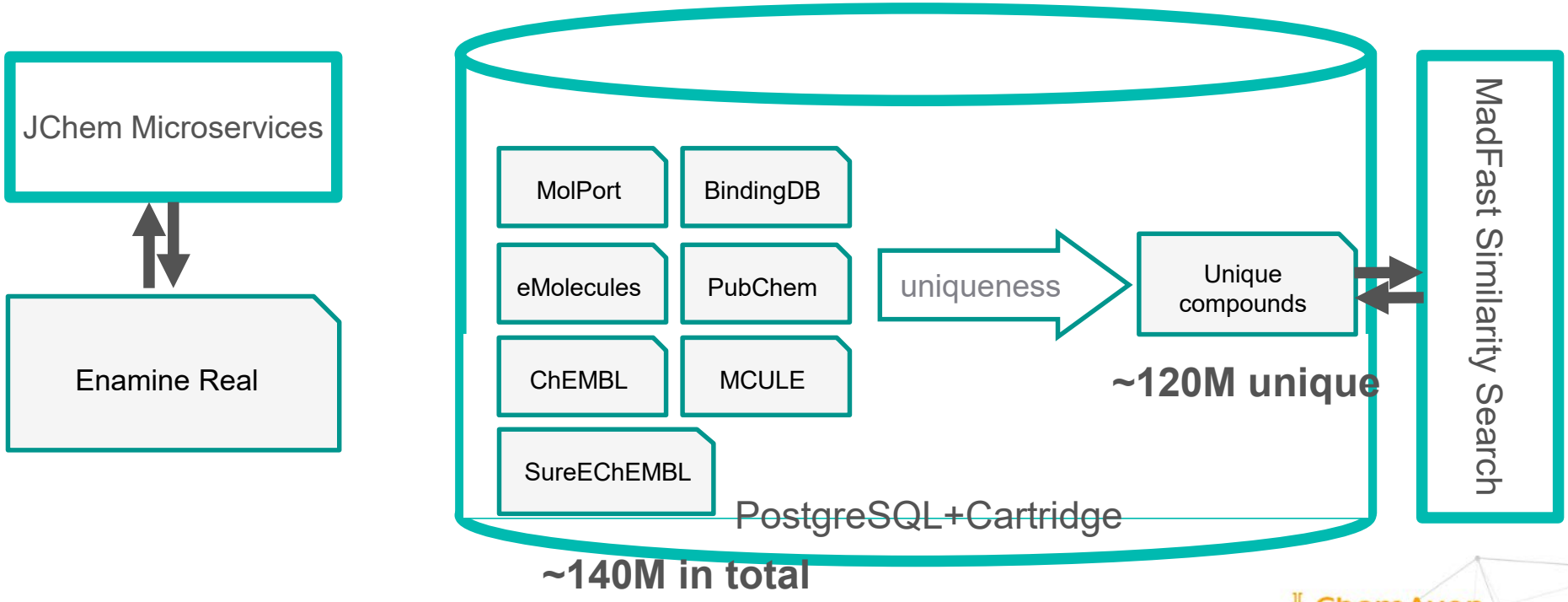
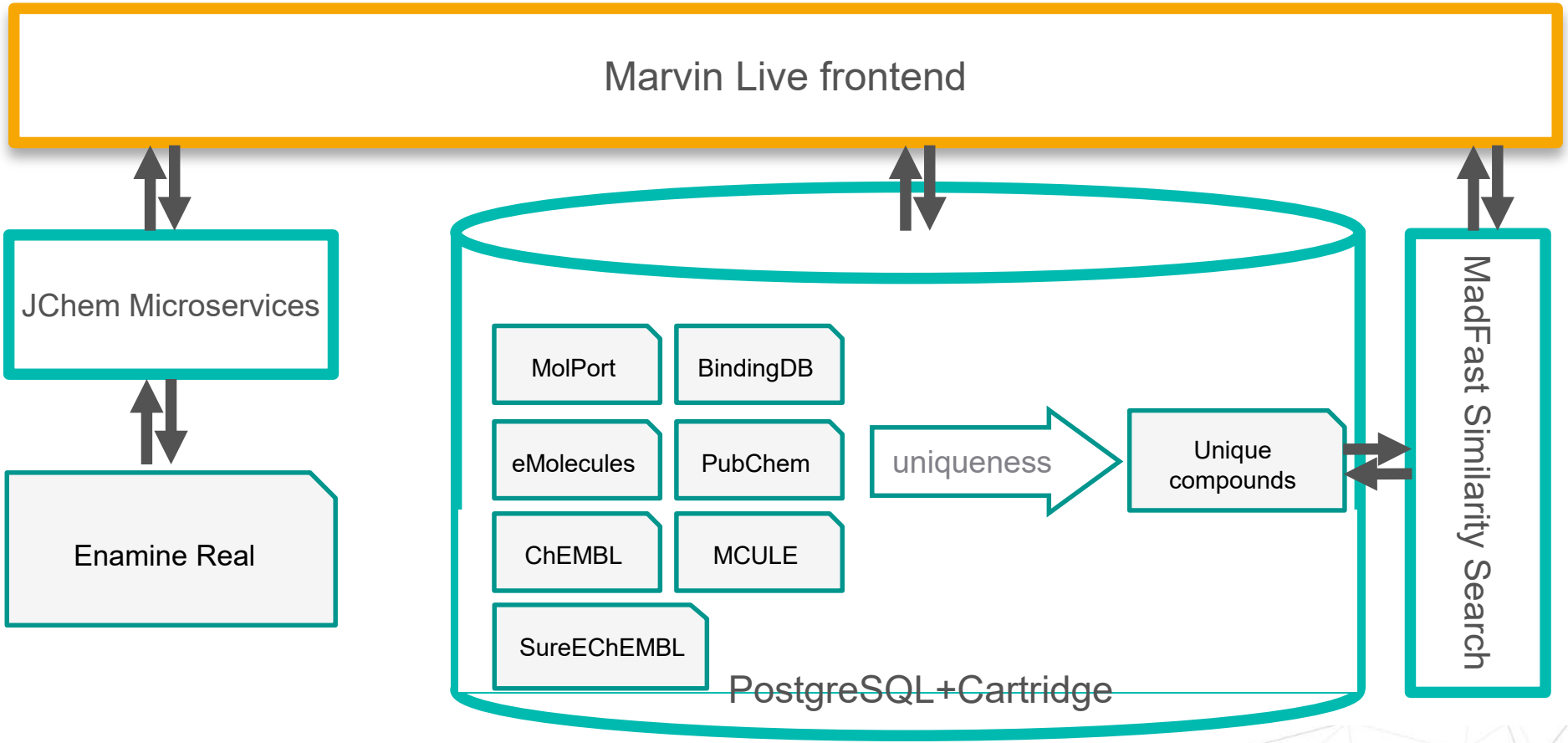

Haystack Prototype
Corporate Compound Repository 1.5M – 3M
Corporate Compound ory 1.5M – 3M
Mol Stock
ChEMBL 1.7M
~22M
BindingDB 651K
SureChEMBL ~18M
ChEMBL 1.7M
SureChEMBL ~18M
PubChem
Stuff
Design Application ayer
Screening library 250k – 1M
olPort Stock ~7M
Enamine REAL ~680M
BindingDB 651K
Namiki Shoji ~6M
eMolecules ~18M
PubChem Compounds ~95M
ChemAxon

The Haystack Database - prototype



The Haystack Database - prototype



DEMO

THANK YOU!

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