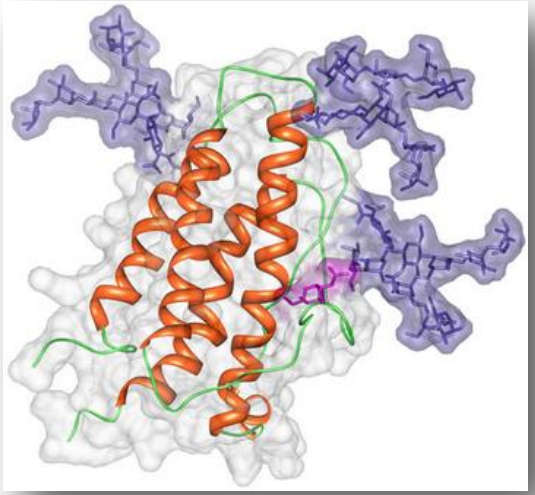
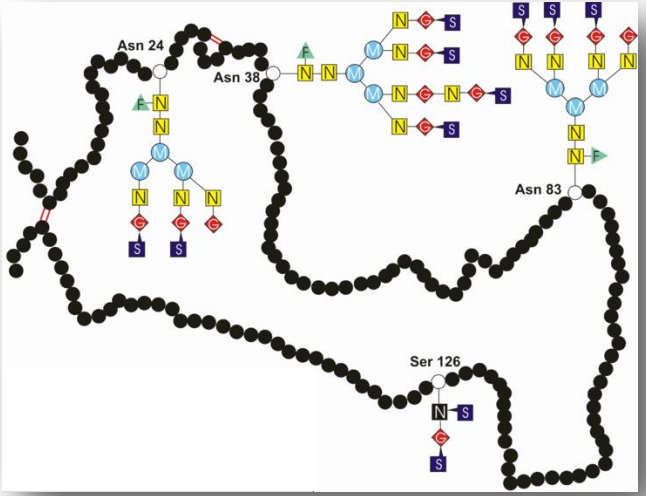
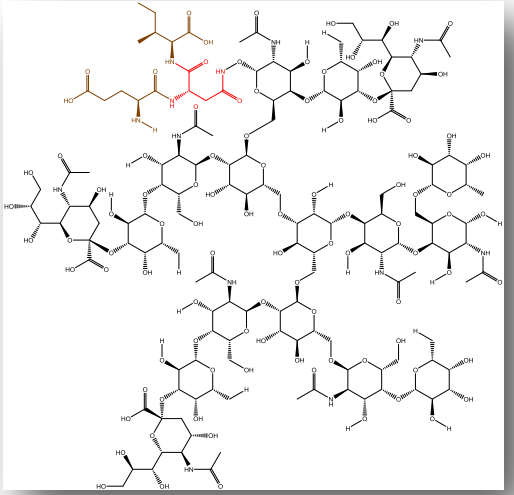
Erythropoietin (EPO)







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SLNENITVPD TKVNFYAWKR MEVGQQAVEV WQGLALLSEA VLRGQALLVN SSQPWEPLQL
HVDKAVSGLR SLTTLLRALG AQKEAISPPD AASAAPLRTI TADTFRKLFR VYSNFLRGKL
KLYTGEACRT GDR

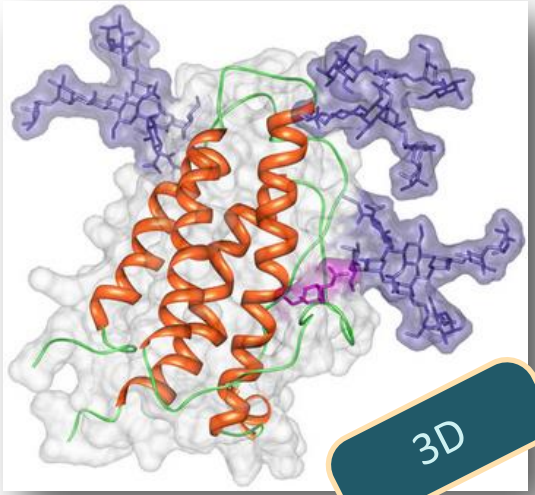
ChemAxon

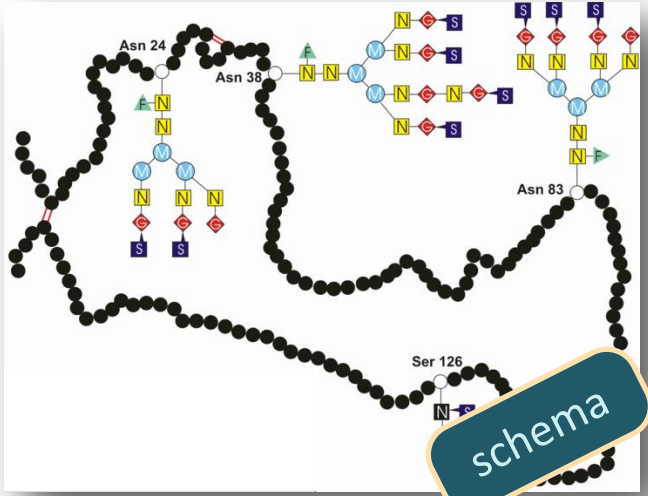
Connecting dots…

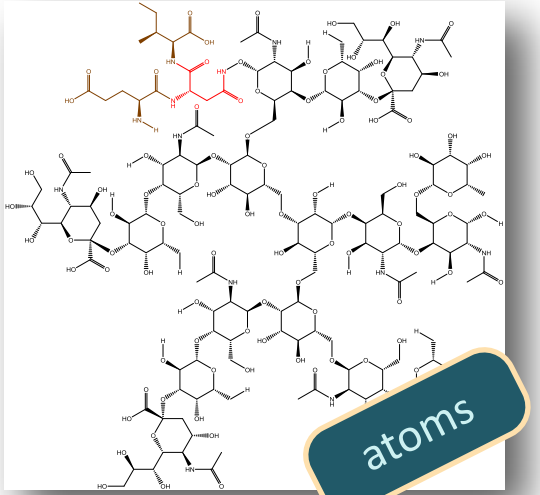
Bio-molecule registration using HELM and ChemAxon tools

Roland Knispel

Erythropoietin (EPO)







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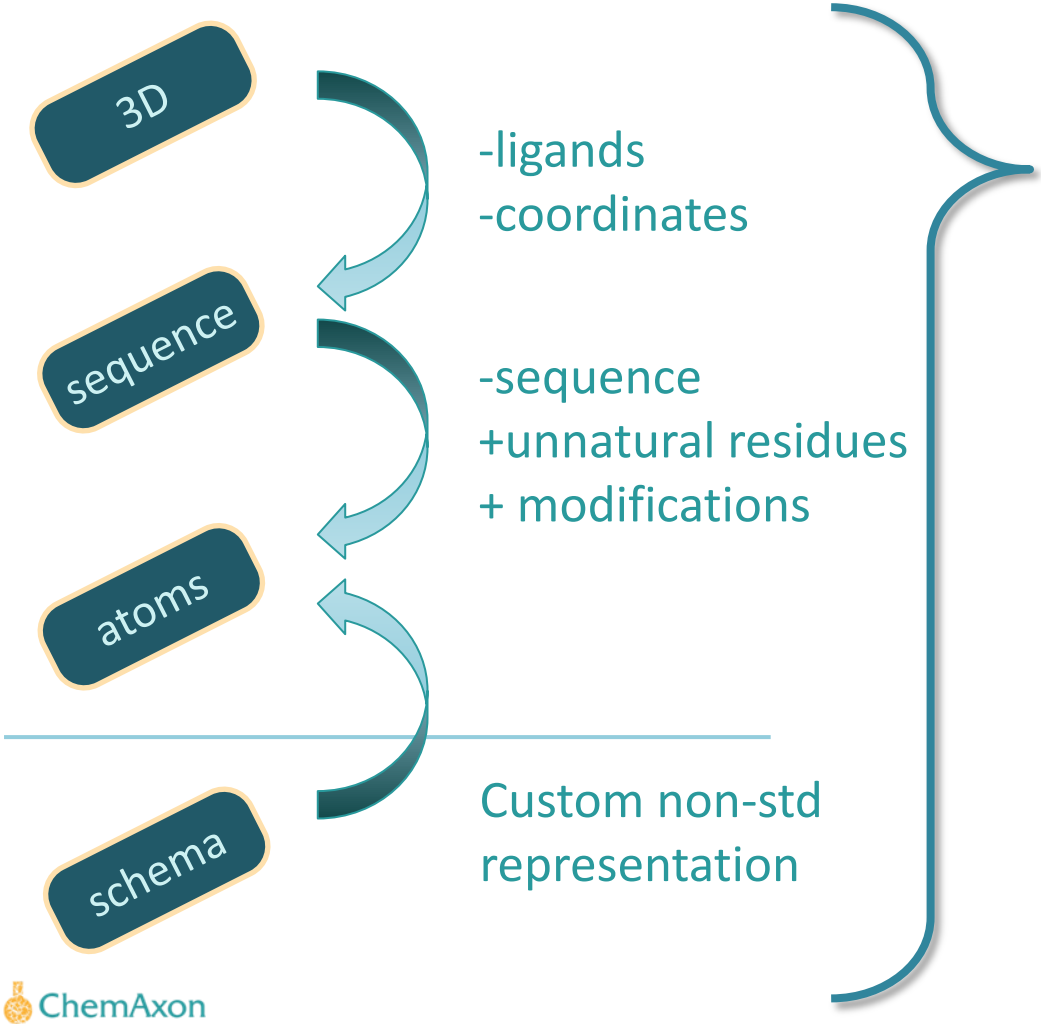
KLYTGEACRT GDR

sequence

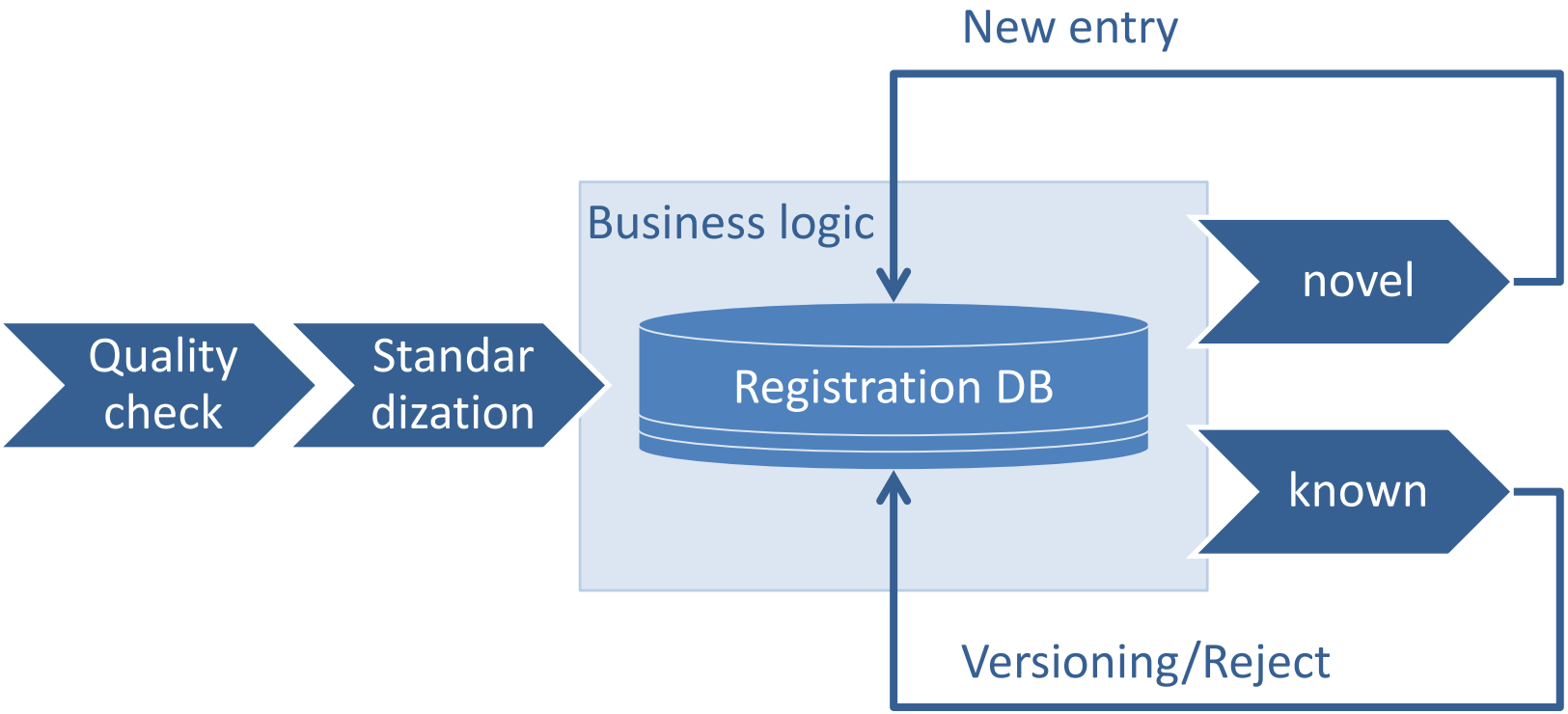
ChemAxon



Search

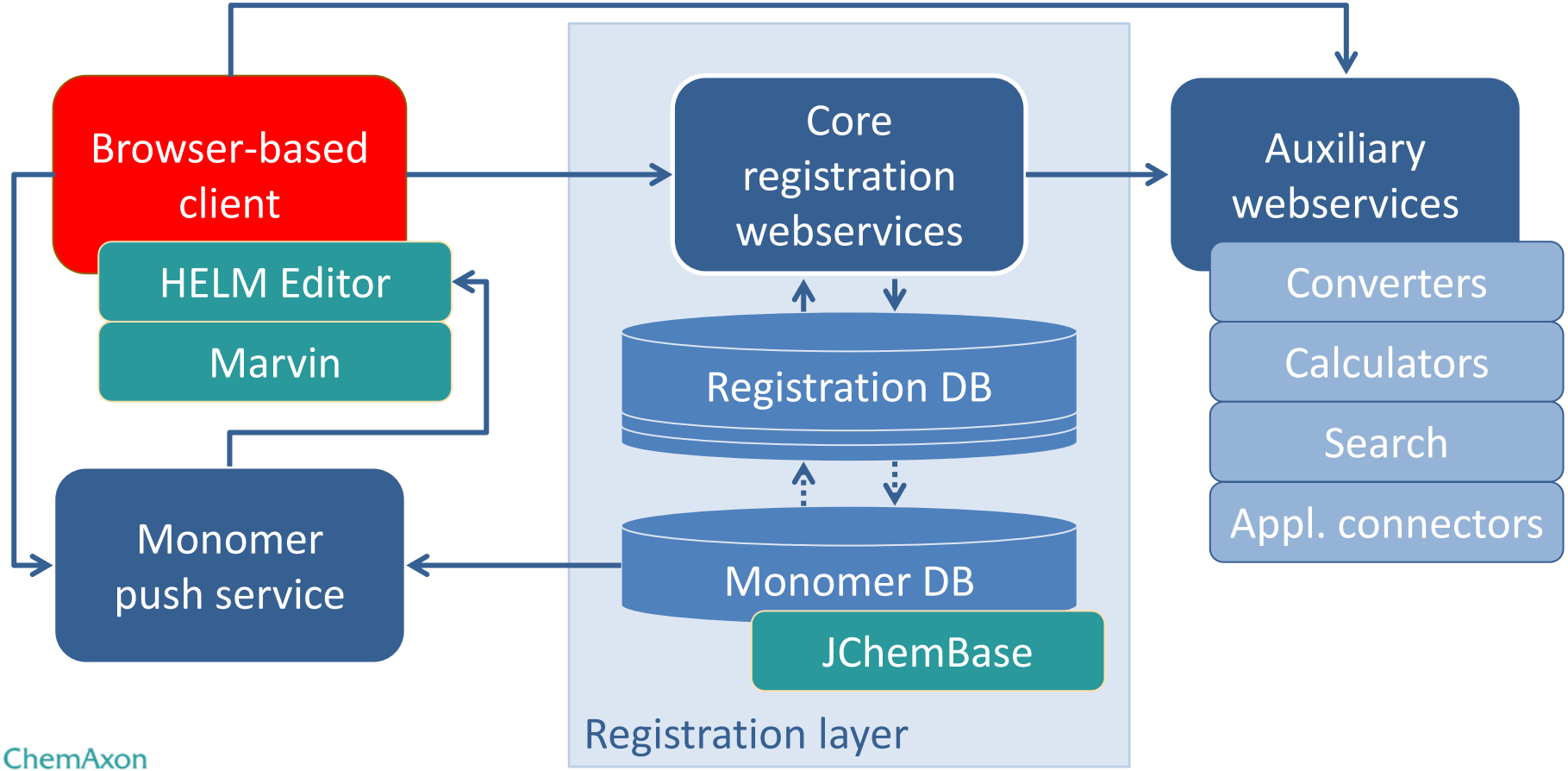
Consumers
DataMarts,
Data Analysis
applications

Is it unique?


New entry
Business logic
Quality check
Standar dization
Registration DB
novel
known
Versioning/Reject

UGM

Registration toolkit architecture



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List of available webservices

HELM monomer registration

- Monomer Registration
- Monomer Updating
- Monomer Deletion
- GetByName
- GetByType
- GetAll

Macromolecule registration

- Macromolecule Registration
- Macromolecule Updating
- Macromolecule Deletion
- GetByCid
- GetAll

Conversion

- Sequence/FASTA -> HELM
- HELM -> Natural Analogue sequence
- HELM -> canonical HELM
- HELM <-> SMILES
- HELM <-> Mol

Search

- General search
- QueryBuilder with filter types:
  -Full sequence
  -Subsequence
  -Any unnatural residue
  -Any chemical modification
  -...

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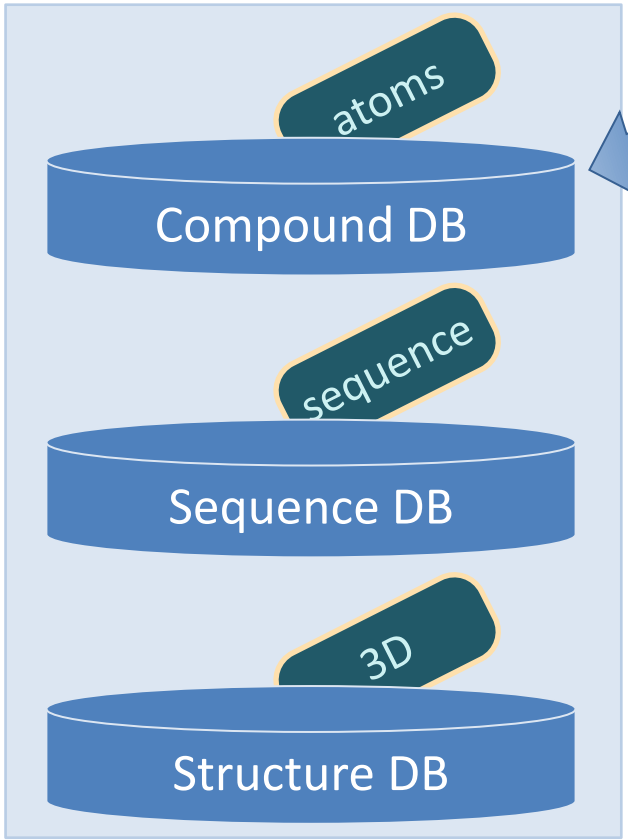
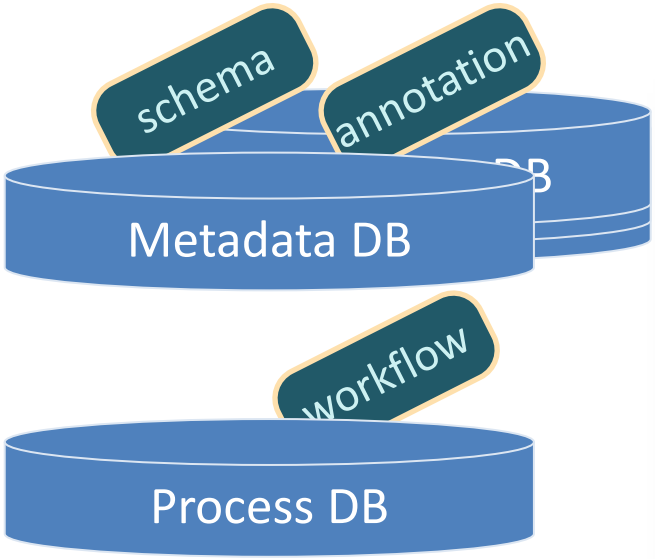
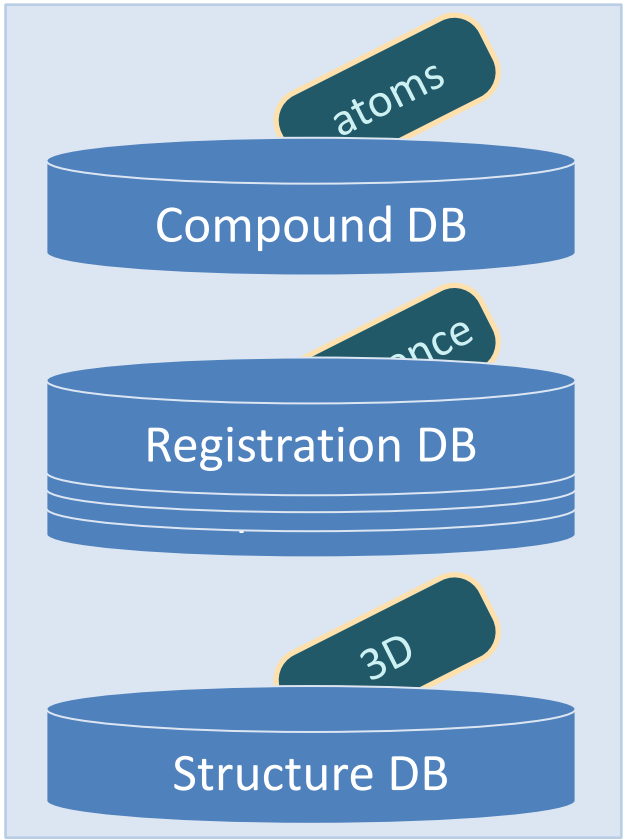
Why not re-use existing systems?






```
MGVHECPAWL WLLLSLLSLP LGLPVLGAPP RLI
RYLLEAKEAE NITTGCAEHC SLNENITVPD TK
MEVGQQAVEV WQGLALLSEA VLRGQALLVN S
HVDKAVSGLR SLTTLLRALG AQKEAISPPD A
TADTFRKLFR VYSNFLRGKL KLYTGEACRT GD
```

ChemAxon‘s Biomolecule toolkit

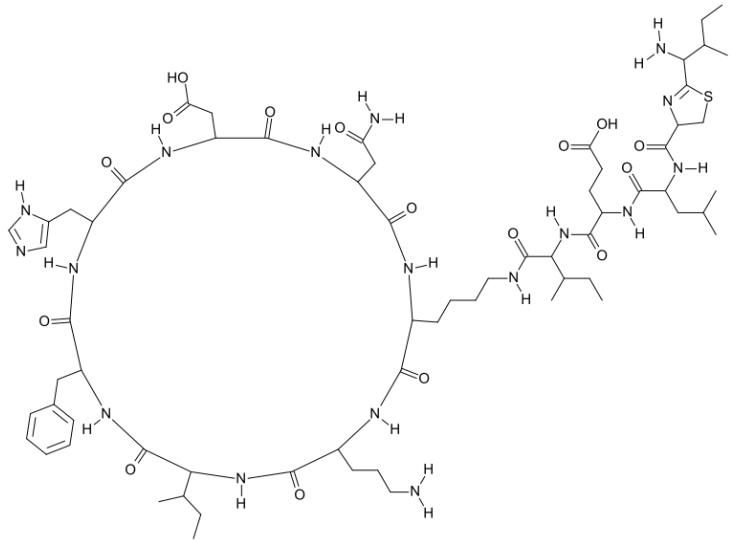


Canonical representation of small and large molecules

Registration of a chemically defined full IgG antibody in the „wink of an eye“ (100-400ms)

ChemAxon

Use case (Macrocyclic peptides)



Requirements:

- Registration of **sequence and chemical structure**
- **Unambiguous representation** of peptide sequence
- Ability to quickly **enumerate library** with residue replacements chosen from a large set of peptide building blocks

POC implemented with ChemAxon‘s Bio-molecule registration toolkit

Benefits

R&D IT
Research IT
Bioinformatics
Synthetic Biology
Biotherapeutics Development
Chemistry Informatics
Information Services

With this toolkit I can now:

- **Share** my molecules **unambiguously** internally and with external collaborators
- **Save time** on curating inconsistent representations received from collaborators
- **Save resources** on maintaining parallel systems for specimen registration
- **Remove bottlenecks** caused by legacy system limitations

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Edit biomolecule

Search biomolecules | Register biomolecules | Monomer manager

Query builder

Search

Clear query

	Match type	Sequence type	Sequence 1
Sequence 1	Subsequence	PEPTIDE	MTG

	Affects	Modification type
Modification 1	Sequence 1	Chemical

Search result

Quickfilter

CID	Name	Helm
CXN43	random peptide (Cys-Cys bridge)	PEPTIDE1{M.T.G.C.R.L.C.Y.W.E.C}$PEPTIDE1,PEPTIDE1,7:R3-4:R3$$$
CXN44	random peptide (Cys-Cys bridge)	PEPTIDE1{M.T.G.C.R.L.C.Y.W.E.C}$PEPTIDE1,PEPTIDE1,11:R3-4:R3$$$
CXN45	random peptide (Cys-Cys bridge)	PEPTIDE1{M.T.G.C.R.L.C.Y.W.E.C}$PEPTIDE1,PEPTIDE1,11:R3-7:R3$$$
CXN46	random peptide (Acetylation)	CHEM1{Ac}|PEPTIDE1{M.T.G.C.R.L.C.Y.W.E.C}$CHEM1,PEPTIDE1,1:R1-1:R1$$$

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Integration opportunities

SOAP and REST-ful WS toolkit

- Compound Registration
- JChem Base
- Plexus
- Instant JChem
- JChem for Office

+ 3rd party applications

Summary

- Template-based bio-molecule registration toolkit
- Fully compatible with the Open HELM standard for representing large molecules
- WS API for integration
- Shippable preview version

UGM

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How can we help you?

Explore our demo station