Developing new science and technologies that aid future drug discovery needs

Adrian Stevens

Chemaxon

Chief Product Officer

Developing New Science and Technologies

How to Help Future Drug Discovery Needs?
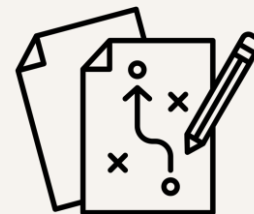
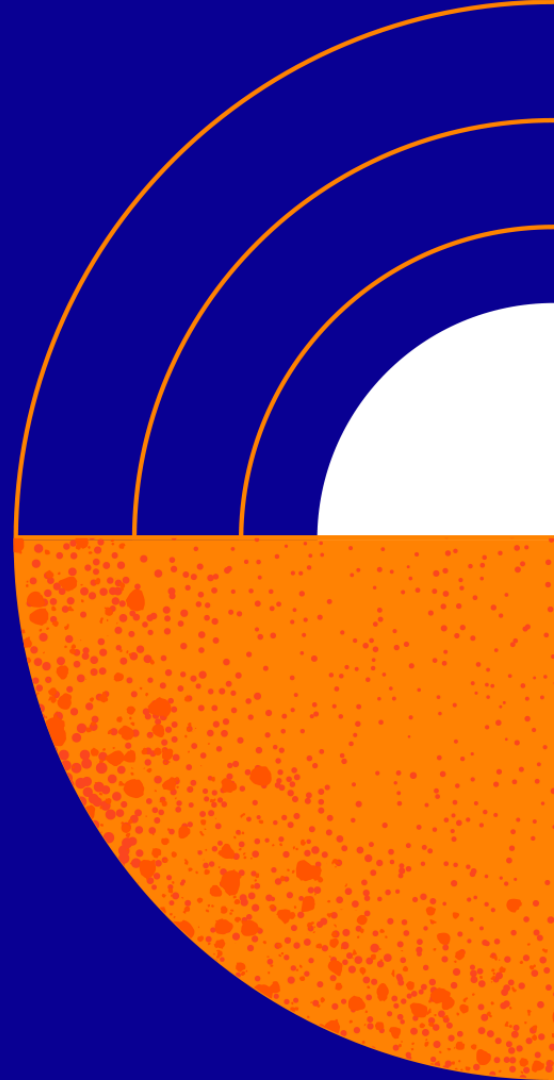Dr Adrian Stevens
Chief Product Officer
Chemaxon Ltd
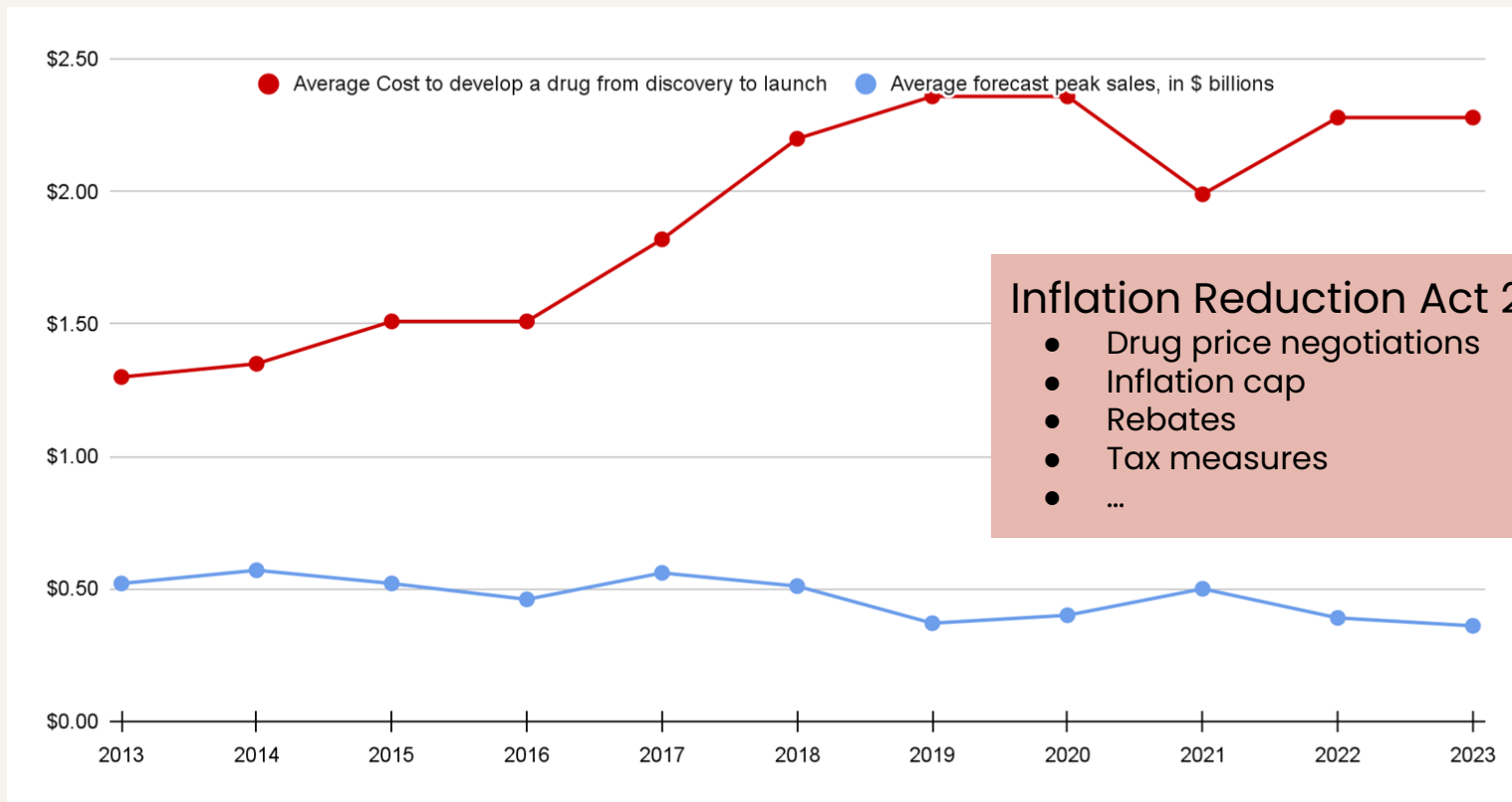
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Agenda

Industry Challenges

Chemaxon's Plan

New Technologies

Define the problem

Chemaxon

Increasing Costs, Declining Rewards

Average Cost to develop a drug from discovery to launch ● Average forecast peak sales, in $ billions

Inflation Reduction Act 2022
- Drug price negotiations
- Inflation cap
- Rebates
- Tax measures
- ...

Source: Deloitte, '**Measuring the return from pharmaceutical innovation – 14th edition**, analysis 2024

Islands of Data - Disconnected Silos

GO FAIR

Island of Data
Disconnected data silos

Chemical synthesis

Assay measurements

LIMS systems

Documents, files

Different:
Standards
Quality
Databases
Semantics

Establishment of Complex Drug Modalities

Small molecules

Modified peptides
emphasis on synthetically produced peptides
RNA therapeutics
ADCs

Peptides
Vaccines
Biosimilars
Antibodies
Therapeutic proteins
Cell therapies
Gene therapies
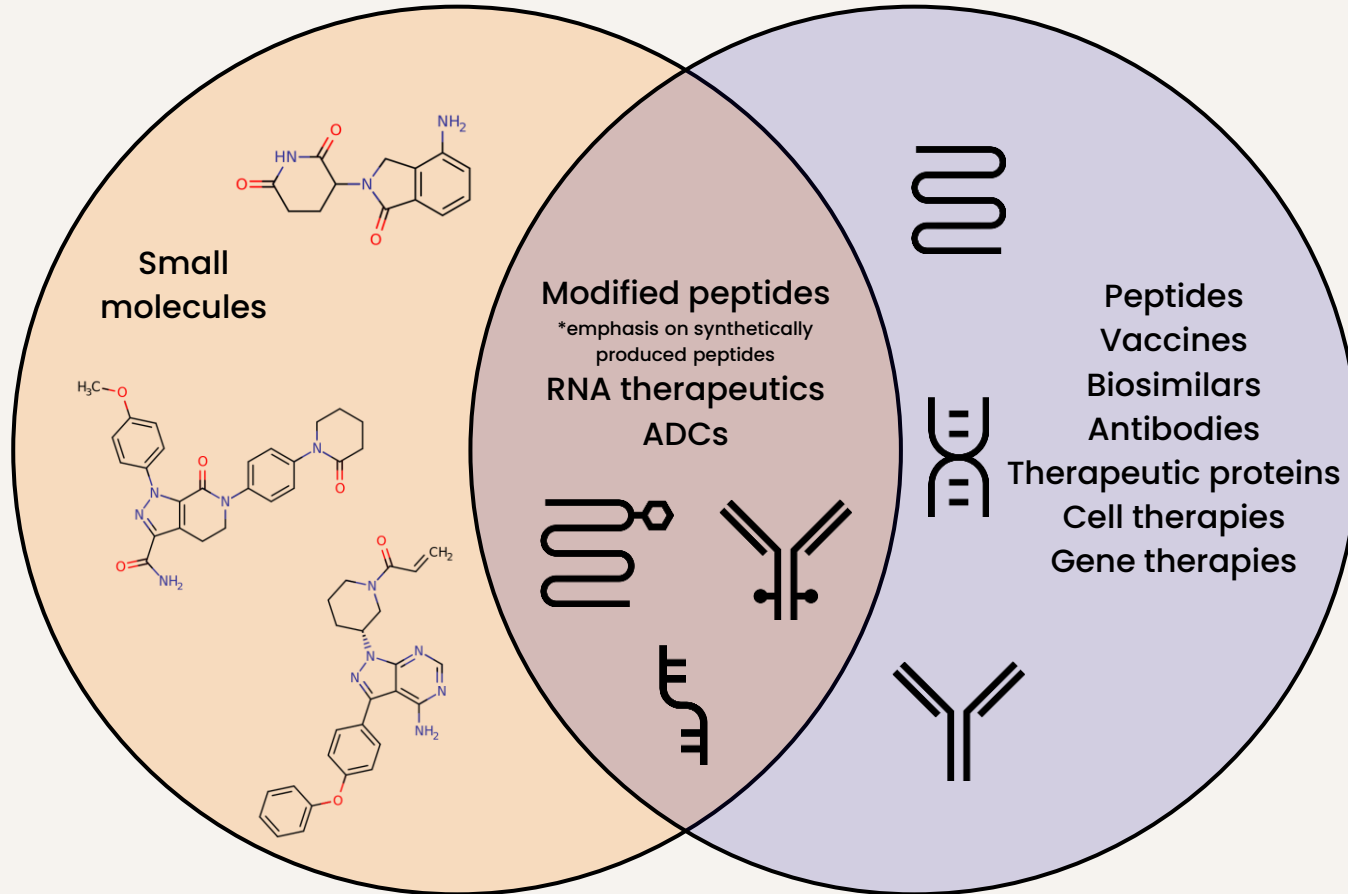
How does Chemaxon plan to help?
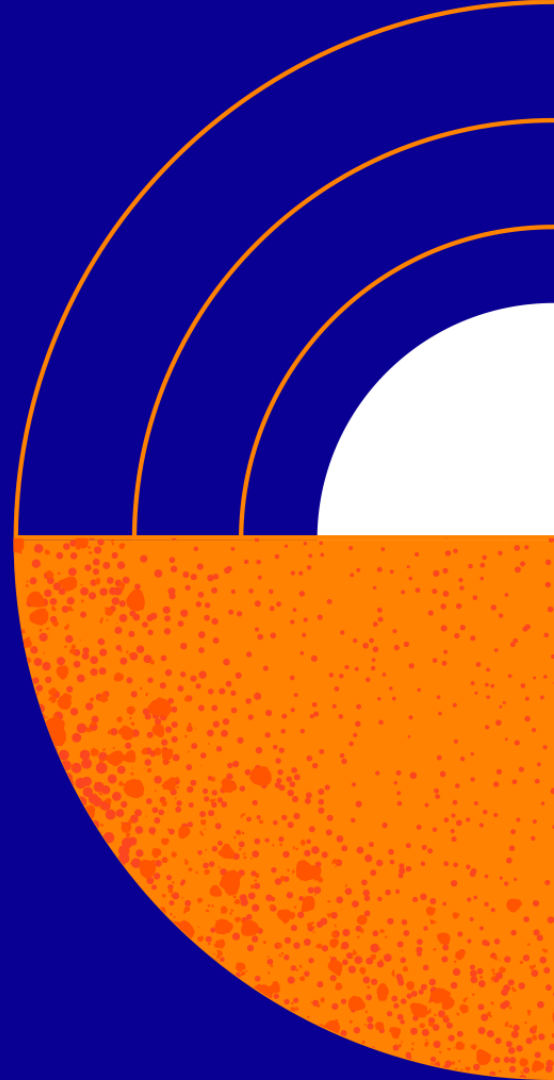
Chemaxon Core Science
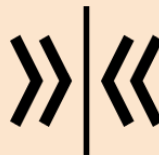
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Will now be a part of

CERTARA®

Chemaxon and Certara Portfolio Overlap

Chemaxon Strengths

Certara Strengths
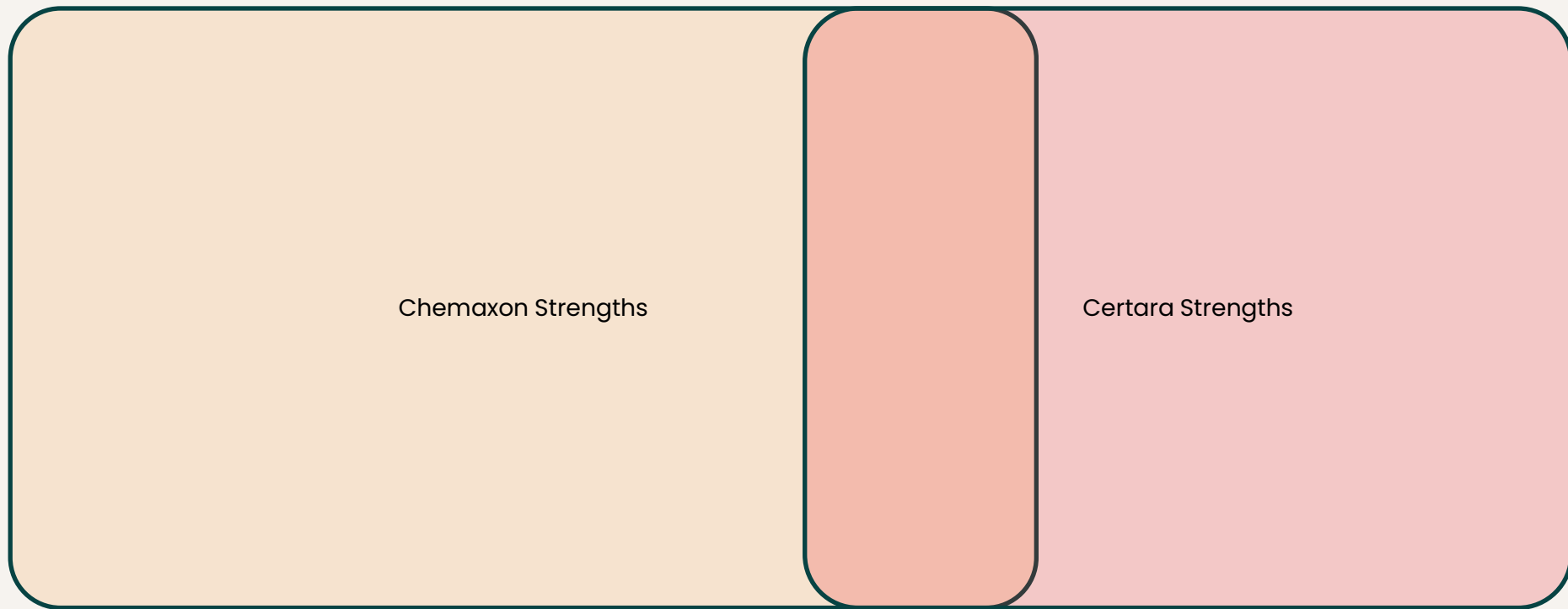
Lead Identification

Lead Optimization

Pre-Clinical

Chemaxon Applications

Design Hub

Chemaxon Tools

Search
Calculators
Predictors
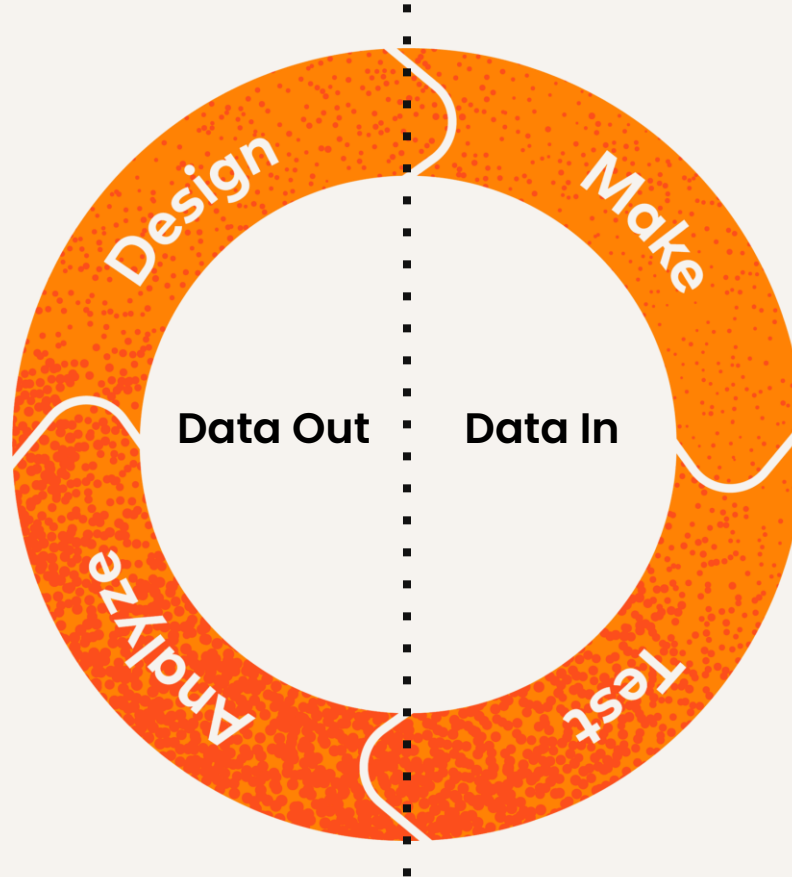Enumeration
Drawing
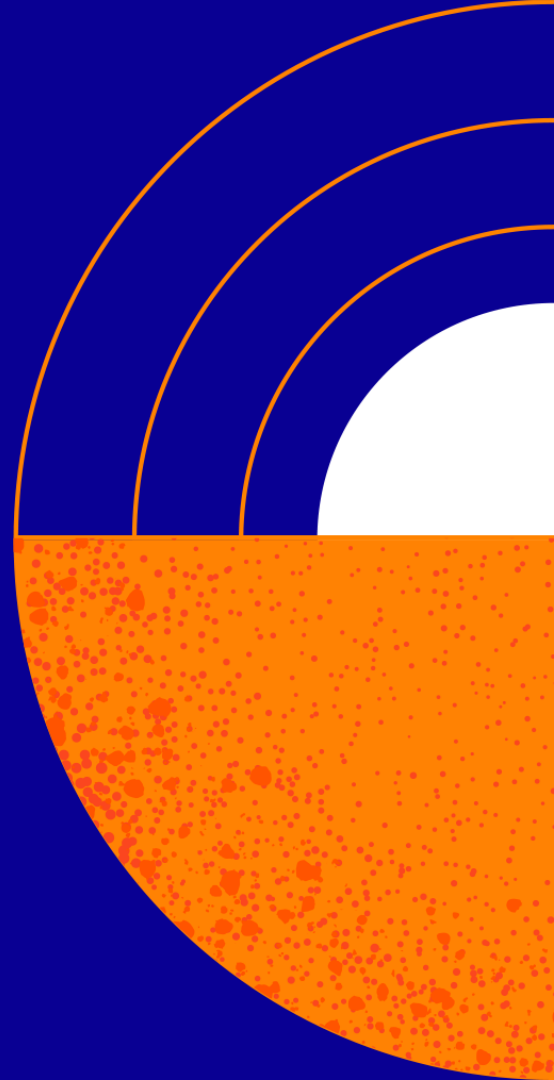Compound Registration

Lead Identification

Lead Optimization

Pre-Clinical

Future: Chemaxon and Certara Combined

Quantitative Systems Pharmacology

Design Hub

Pirana

Phoenix

Chemaxon Tools

Search
Calculators
Predictors
Enumeration
Drawing
Compound Registration

Integral Data Repository

D360

Simcyp Discovery Simulator

Certara.AI

Lead Identification

Lead Optimization

Pre-Clinical

Data In *vs* Data Out

Design

Make

Data Out

Data In

Analyze
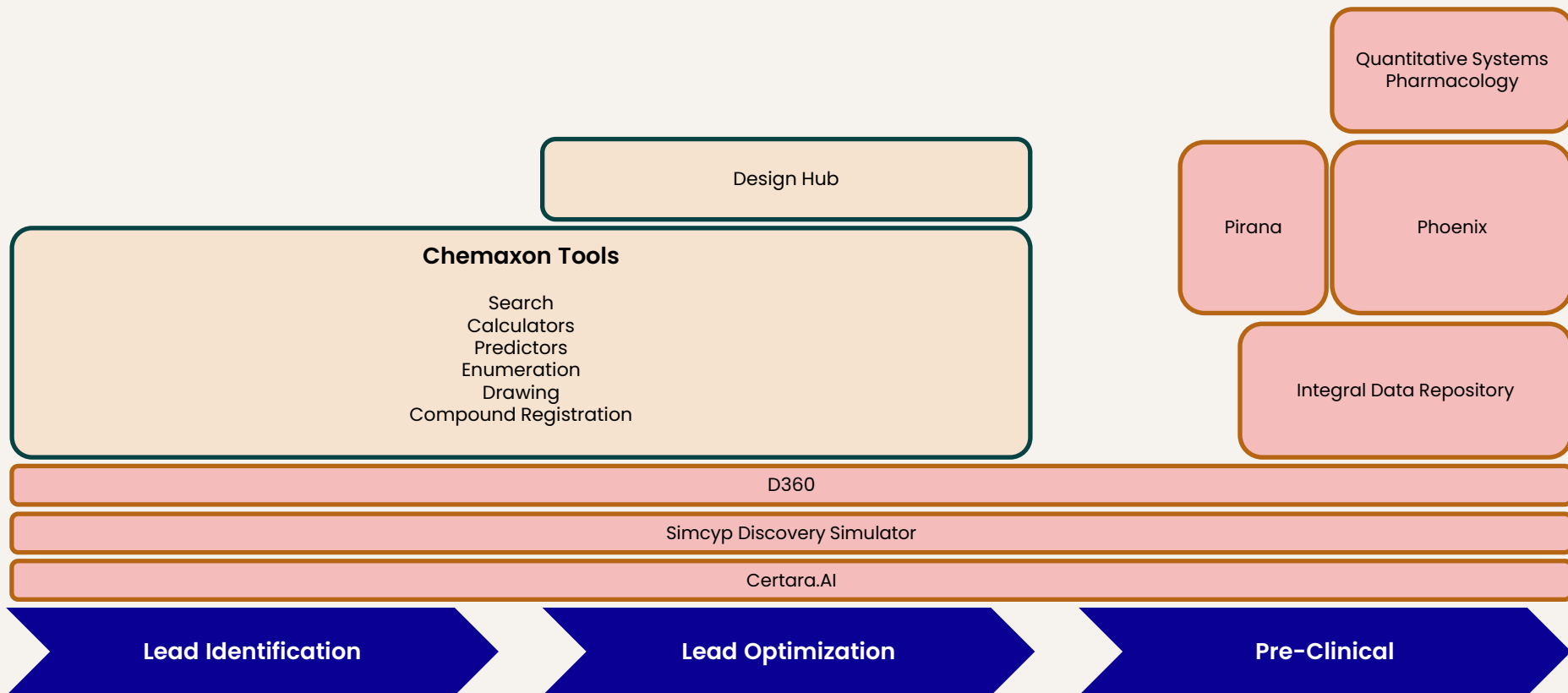
Test

How we are thinking we can help...

Chemaxon

Cheaper, Better, Faster...
Improving DMTA Decision Support

Building intelligent features...

Libraries →

← ML

↑ Search

Expand Access to Our Science

Accelerates our ability to:

- Enhance algorithms
- Develop new science features
- Deploy faster computations

Future: native C and Python API

Microservices

Jupyter Knime Etc…
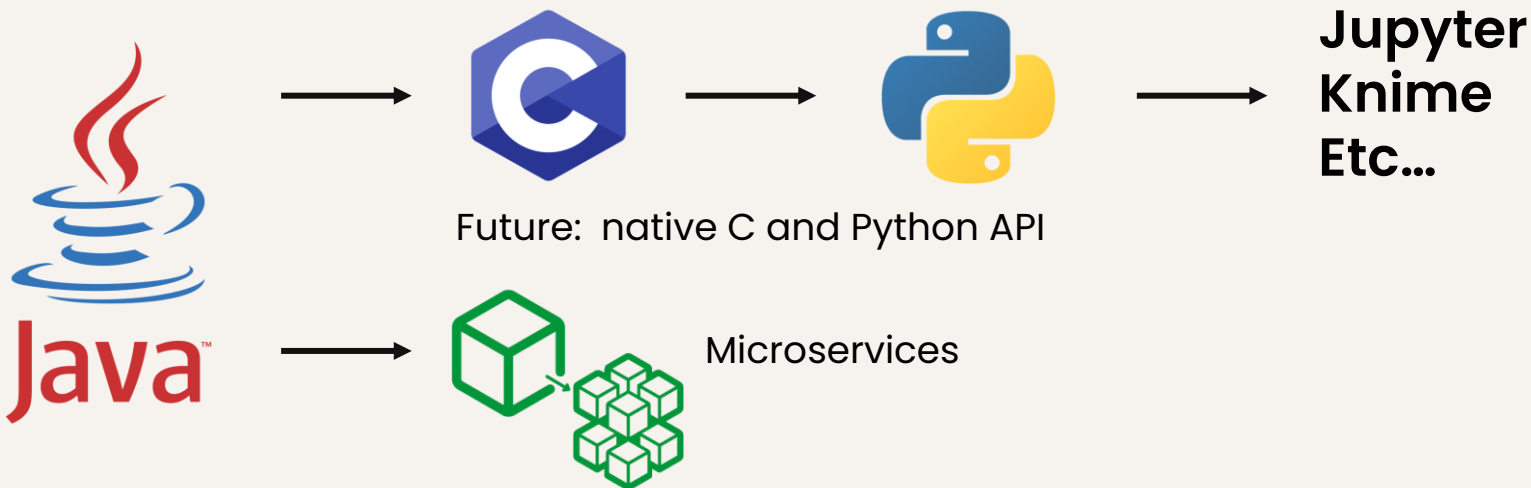
Going Beyond Chemical Search

Scalable Search
(1 data source)
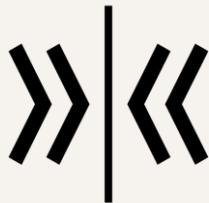
Federated Search
(multiple data sources)
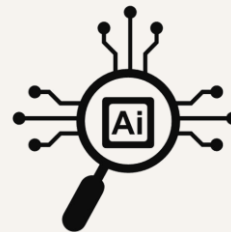
AI Search
(learning from data)

10^{9-11}

Chemical space

Structured   **Unstructured**

LLM +
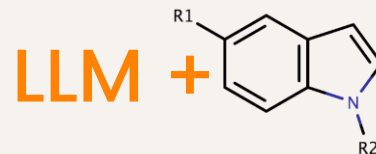
Summarise SAR

Integration of the 50B Search in Design Hub

Automated ML on Data Columns within Design Hub

Improving Efficiency: Better Workflow Experiences
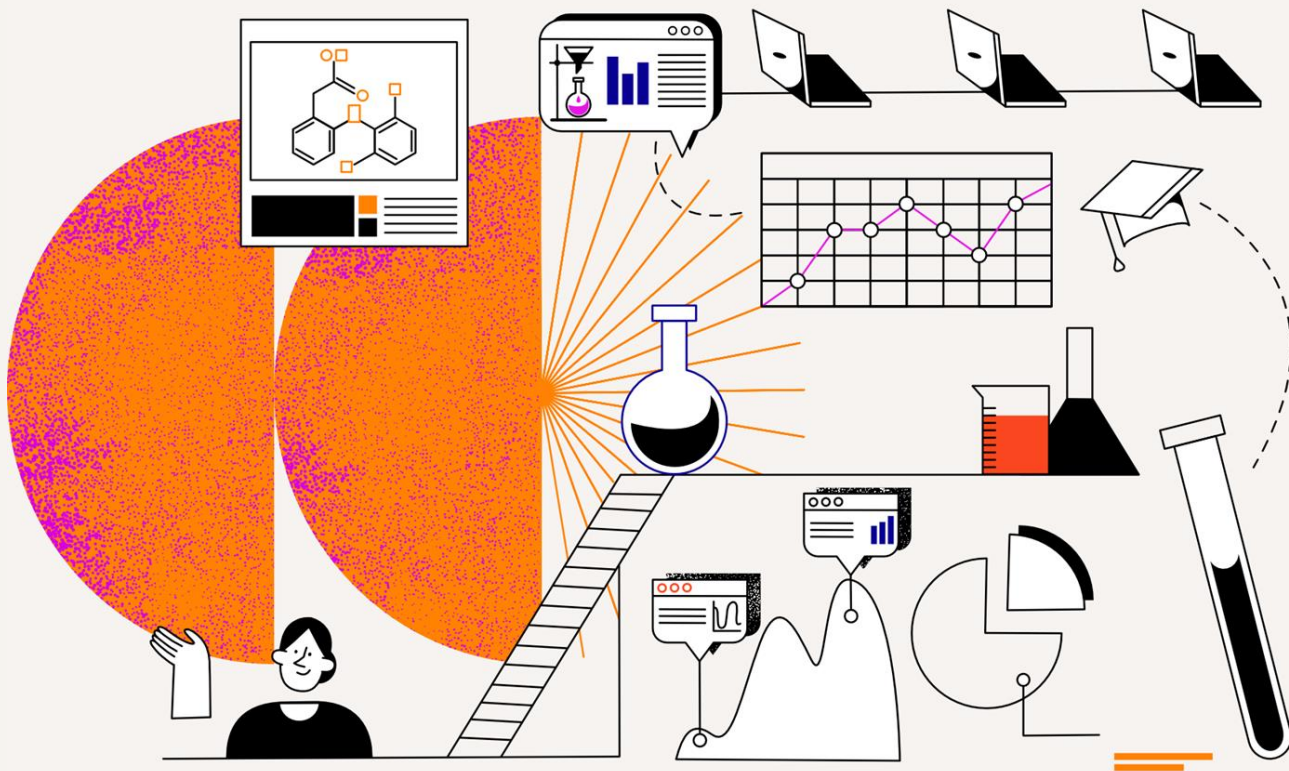
Improving User Workflows: Connecting Apps

From D360...

...to Design Hub

Example: Pulling Data from D360 into Design Hub

Supporting Complex Modalities

Small molecules

Modified peptides
*emphasis on synthetically produced peptides
RNA therapeutics
ADCs

Peptides
Vaccines
Biosimilars
Antibodies
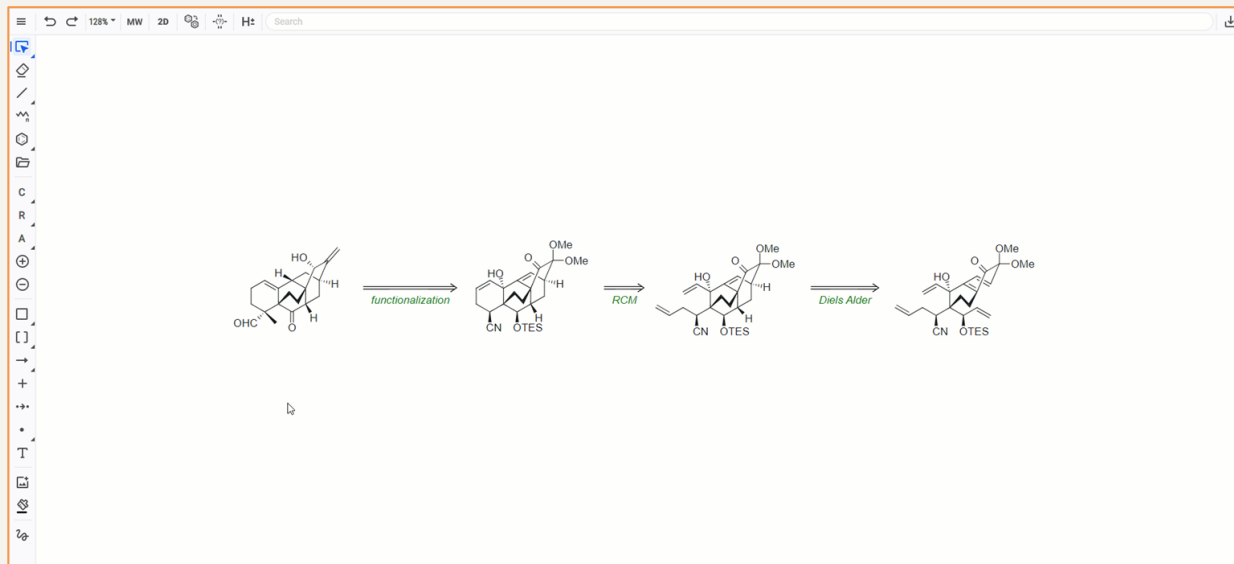Therapeutic proteins
Cell therapies
Gene therapies
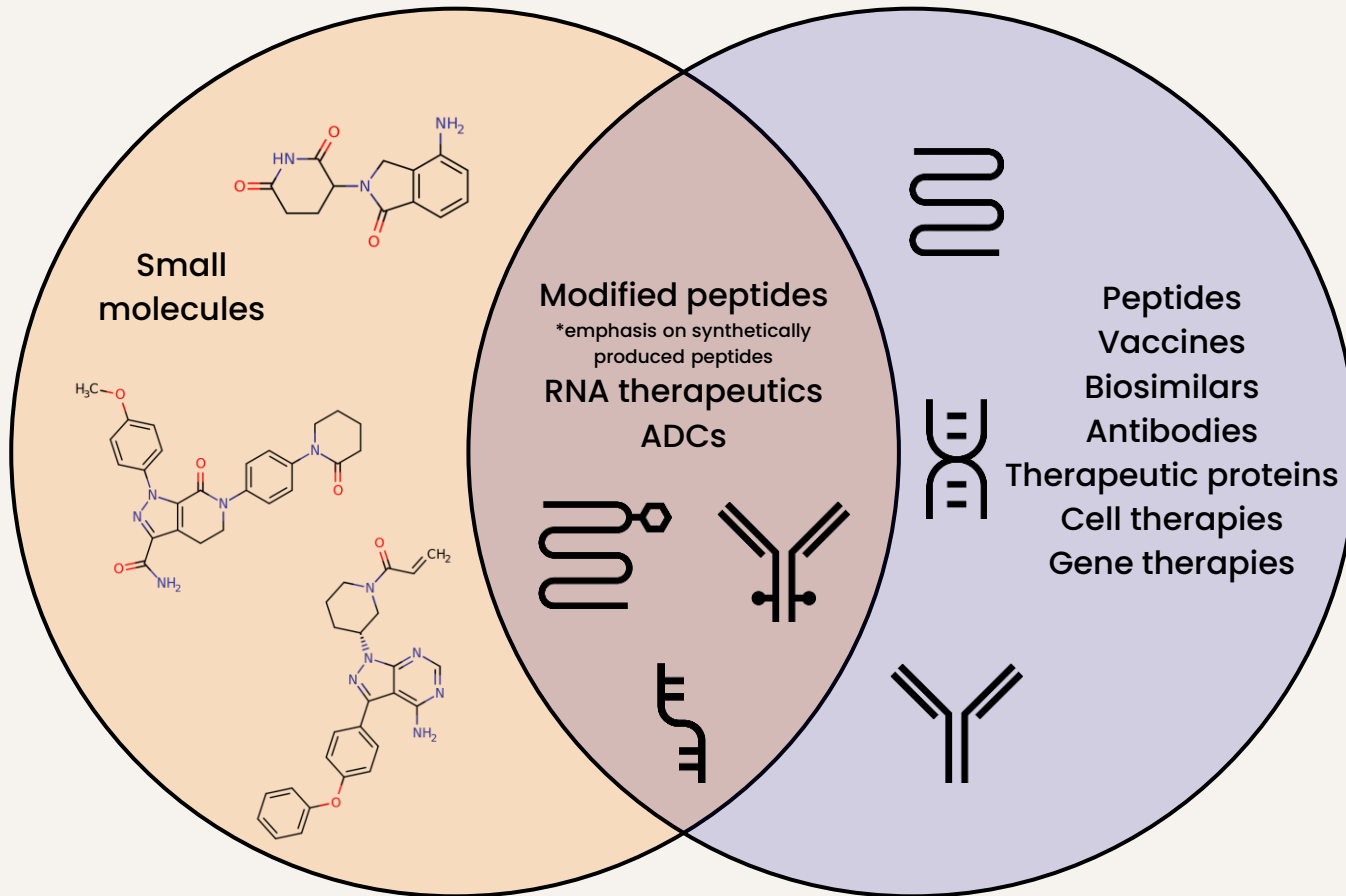
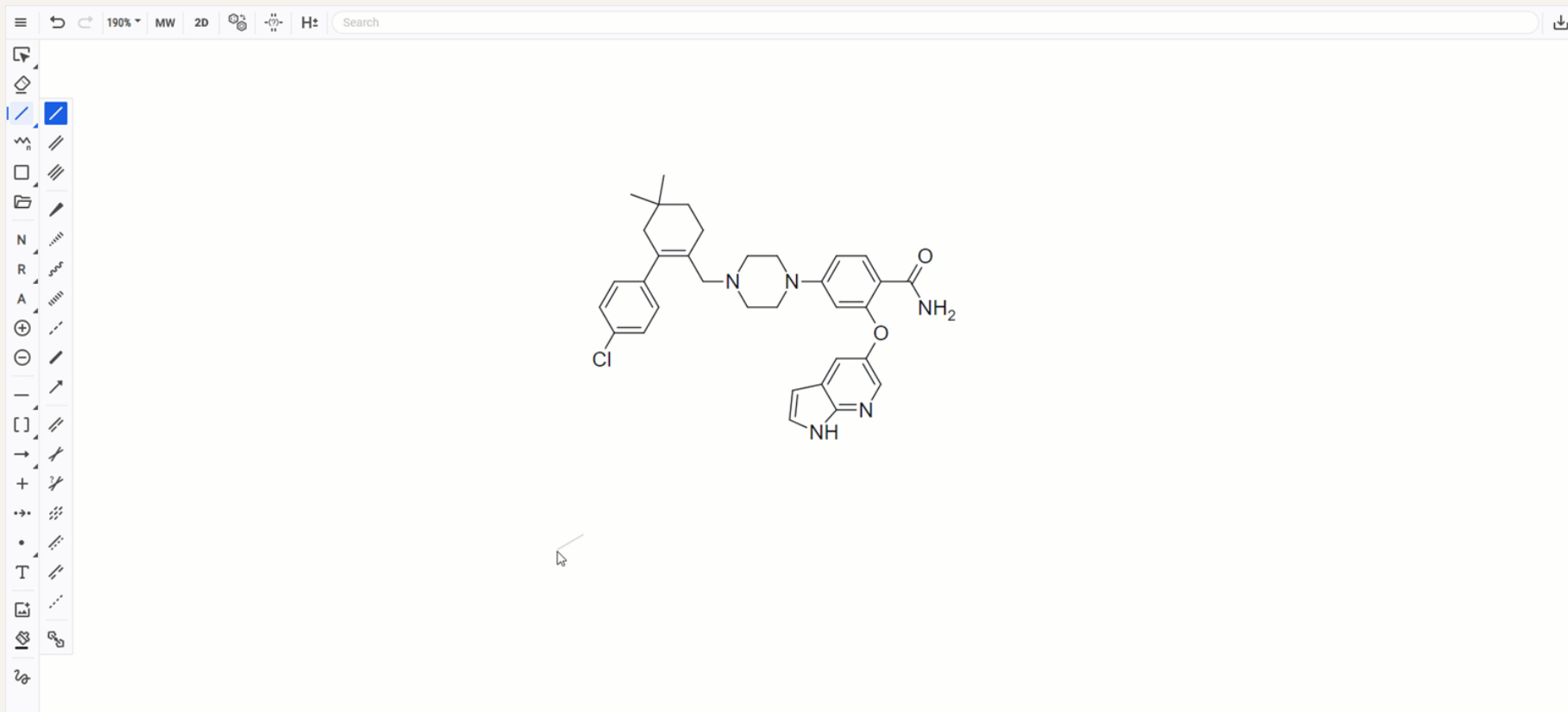# Sketch, Render, Publish Chemical Drawings

Marvin

- Fast & intuitive drawing
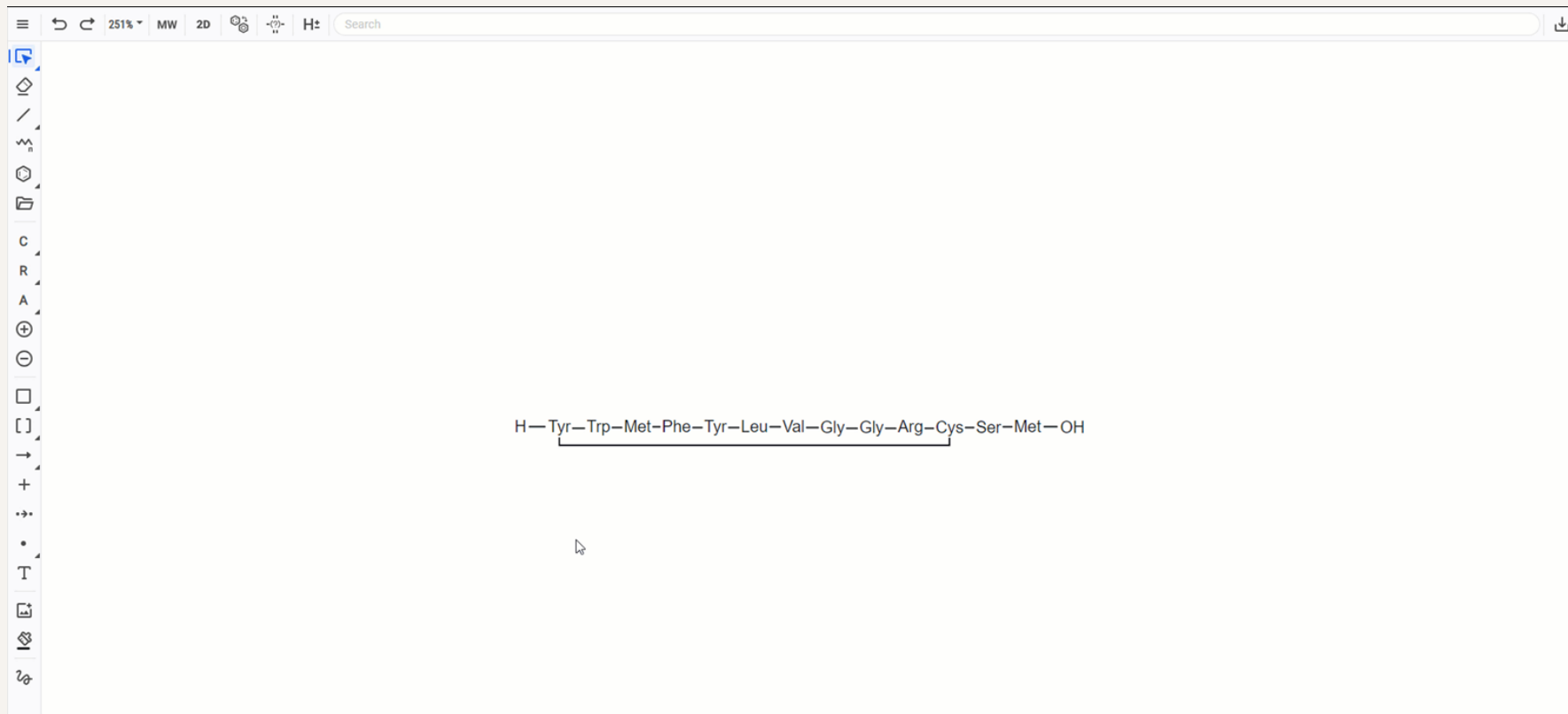
- Complex images and biomolecules handled easily

- Integrates seamlessly with other tools

- Complies with EU accessibility reqs.

Calculating Properties as You Sketch

Handling Chemistry in Biologics

H — Tyr — Trp — Met — Phe — Tyr — Leu — Val — Gly — Gly — Arg — Cys — Ser — Met — OH

These are *just* a few examples of capabilities that we have in active development or in planning
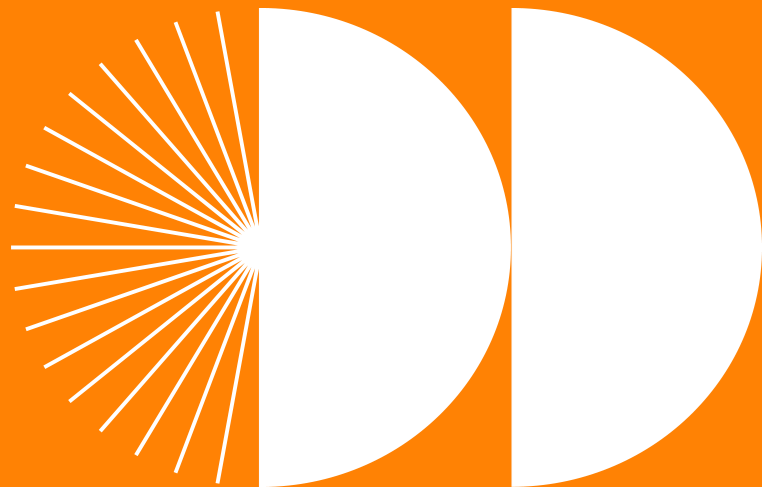
Acknowledgements

With thanks to the following for help!

- Roland, Balazs & the Chemlib Team
- Luca & the Marvin Team
- Ivan & the Representation Team
- Andras & the Design Hub Team
- Volfi & the Search Team
- Attila & Erneszt

- David & the Certara D360 Team!

And You, the audience,
for participating in this session!

Thank you!

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