



**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



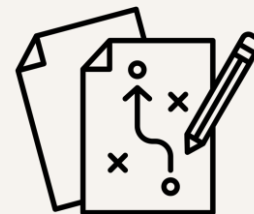
Agenda



Industry Challenges

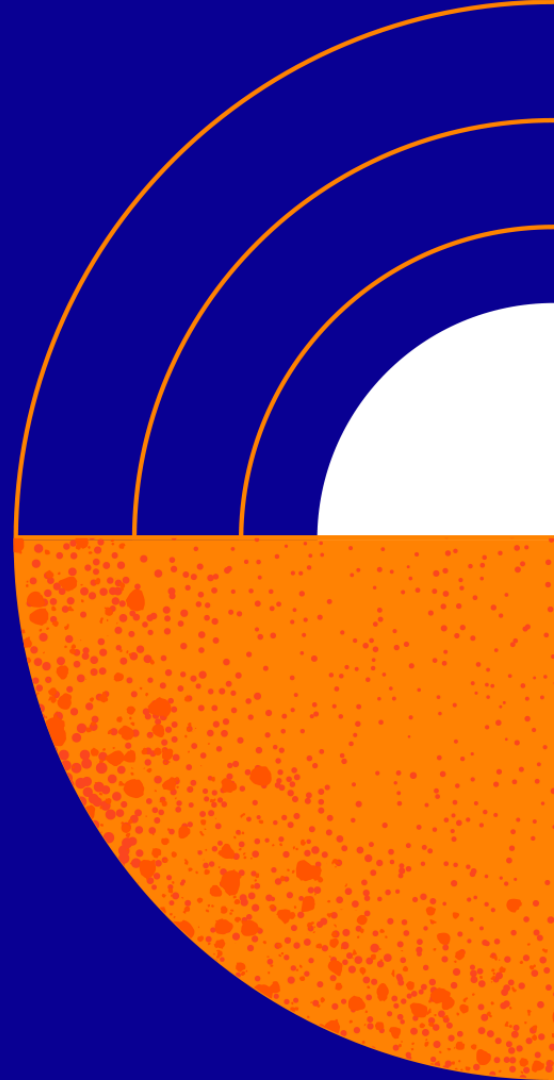


Chemaxon's Plan

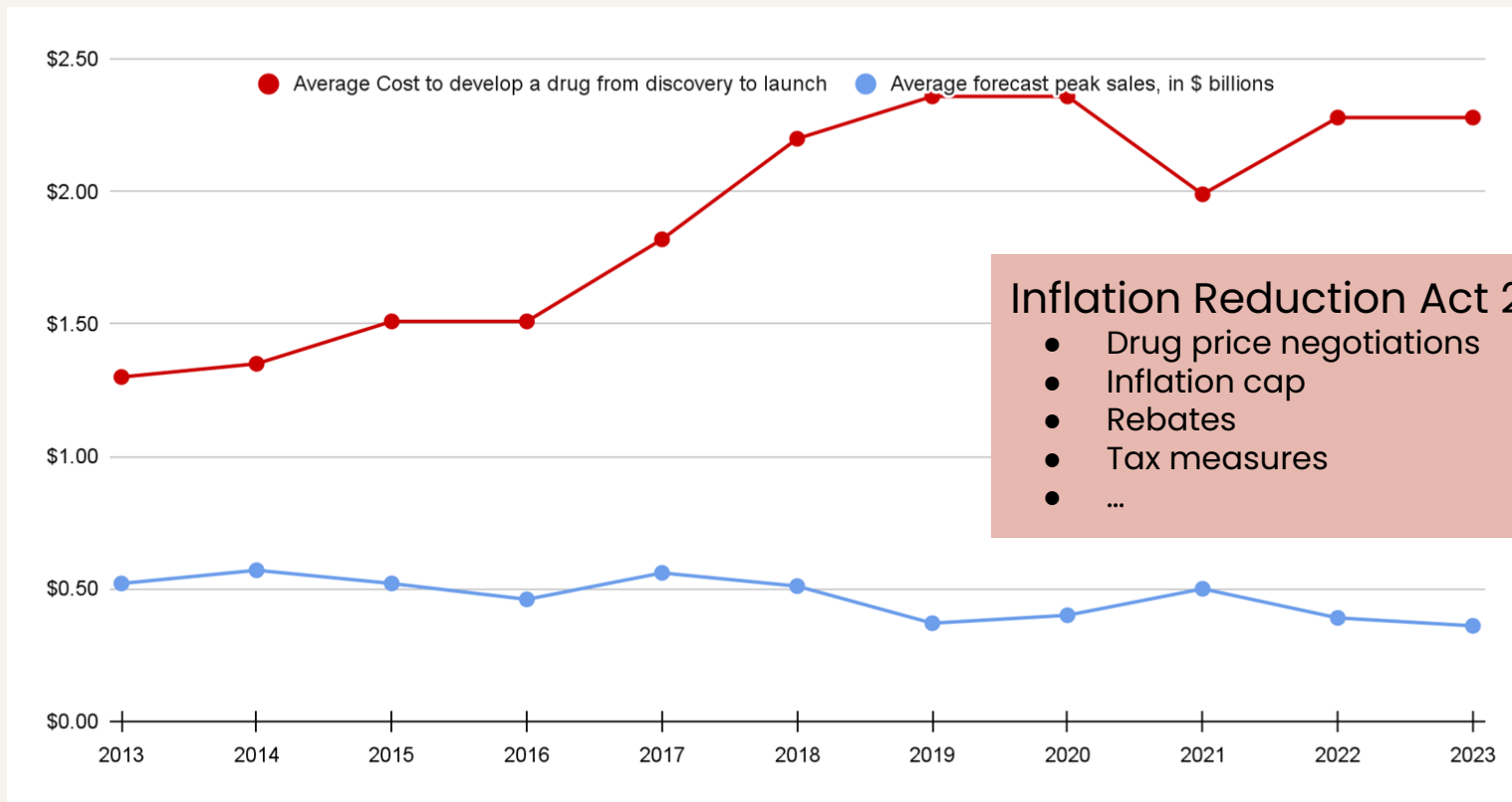


New Technologies

Define the problem



Increasing Costs, Declining Rewards



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

Islands of Data – Disconnected Silos



Chemical synthesis



Assay measurements

Island of Data
Disconnected data silos



Different:
Standards
Quality
Databases
Semantics

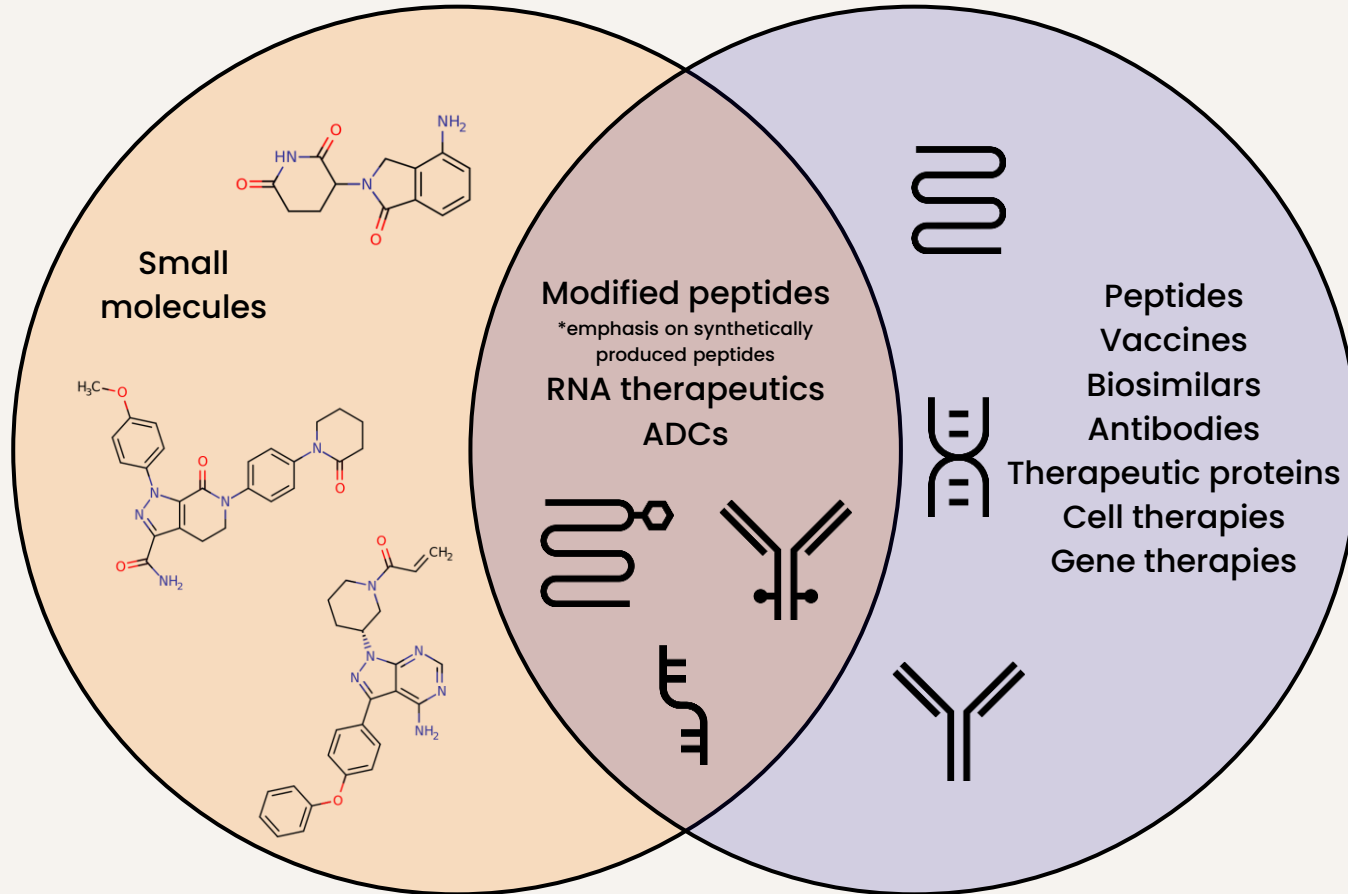


LIMS systems

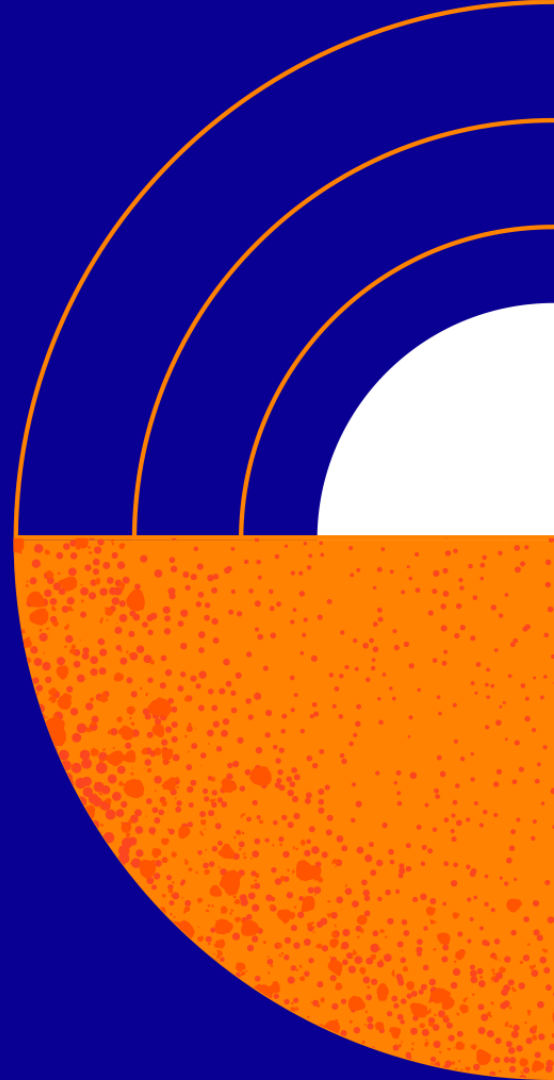


Documents, files

Establishment of Complex Drug Modalities



How does Chemaxon plan to help?



Chemaxon Core Science



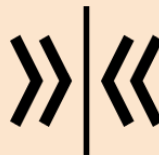
Analysis &
Design



Drawing



Calculators



Standardization



Compliance



Search



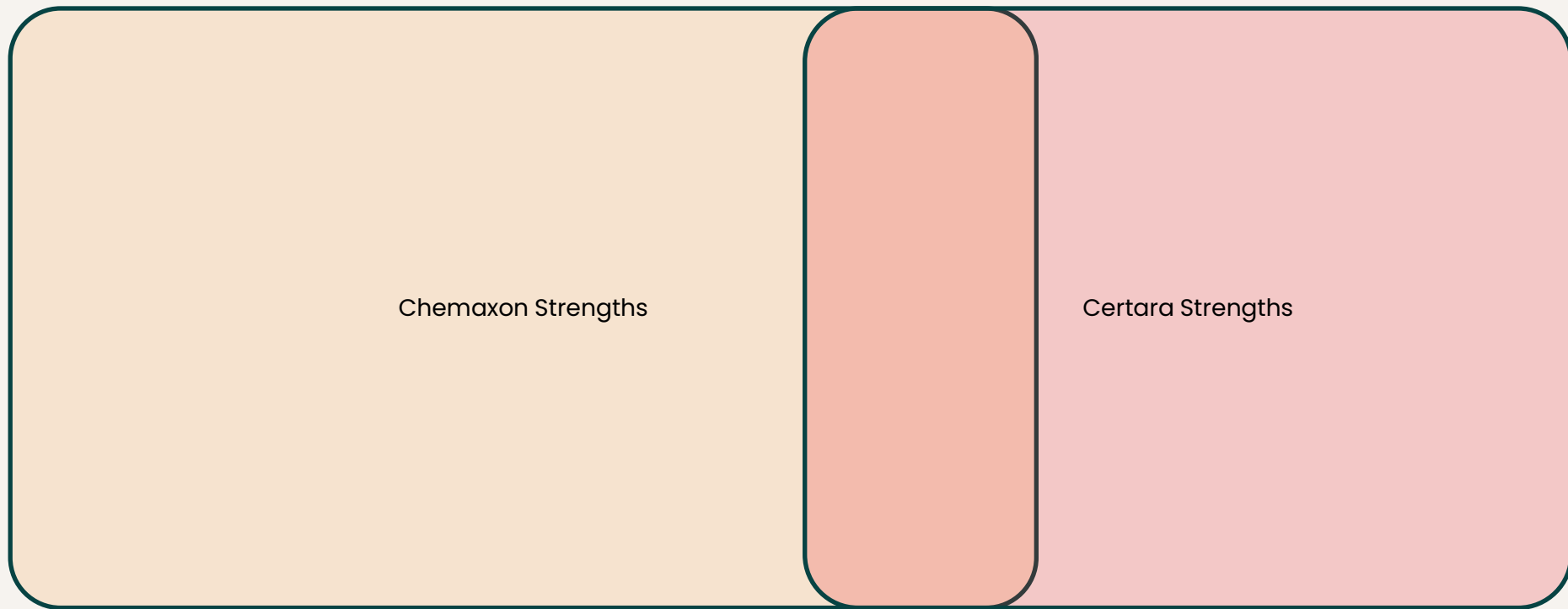
Registration



Will now be a part of



Chemaxon and Certara Portfolio Overlap



Lead Identification

Lead Optimization

Pre-Clinical

Chemaxon Applications



Design Hub

Chemaxon Tools

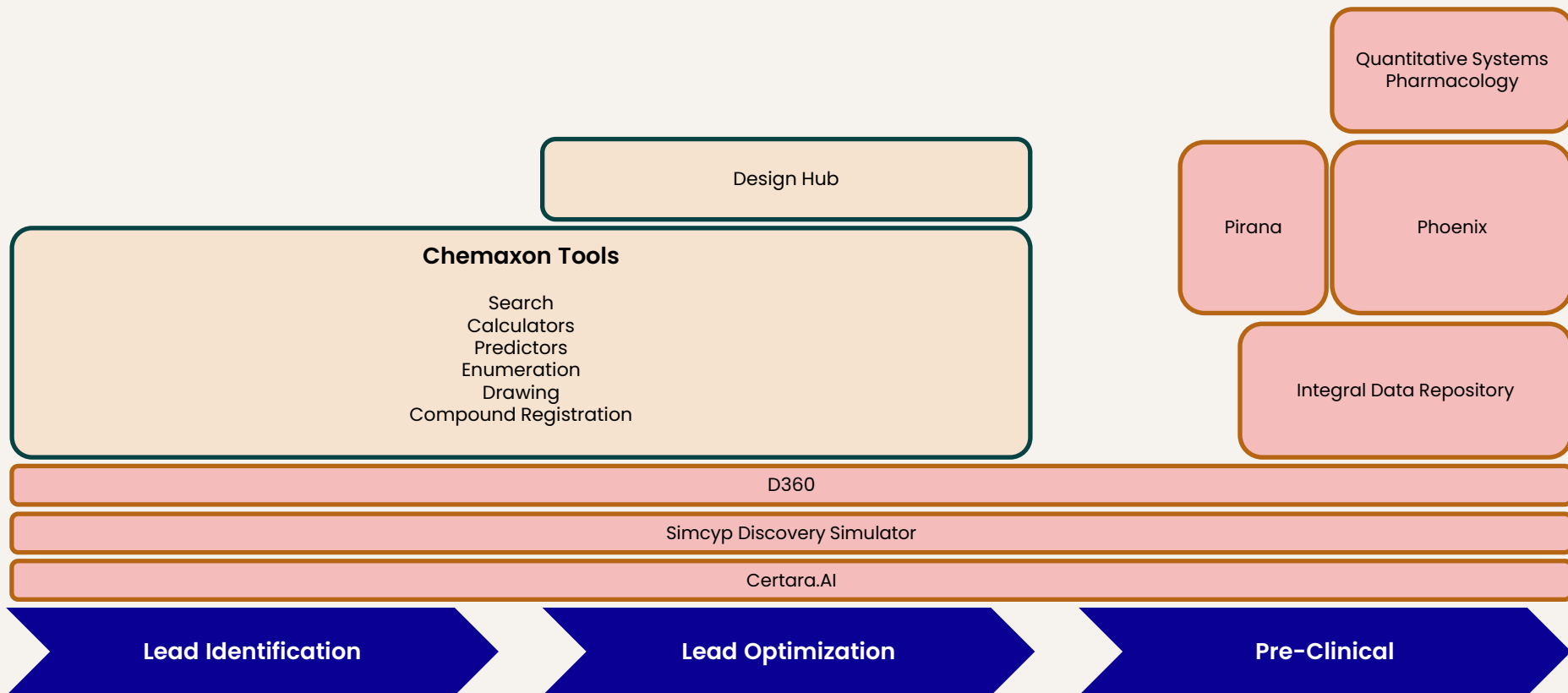
Search
Calculators
Predictors
Enumeration
Drawing
Compound Registration

Lead Identification

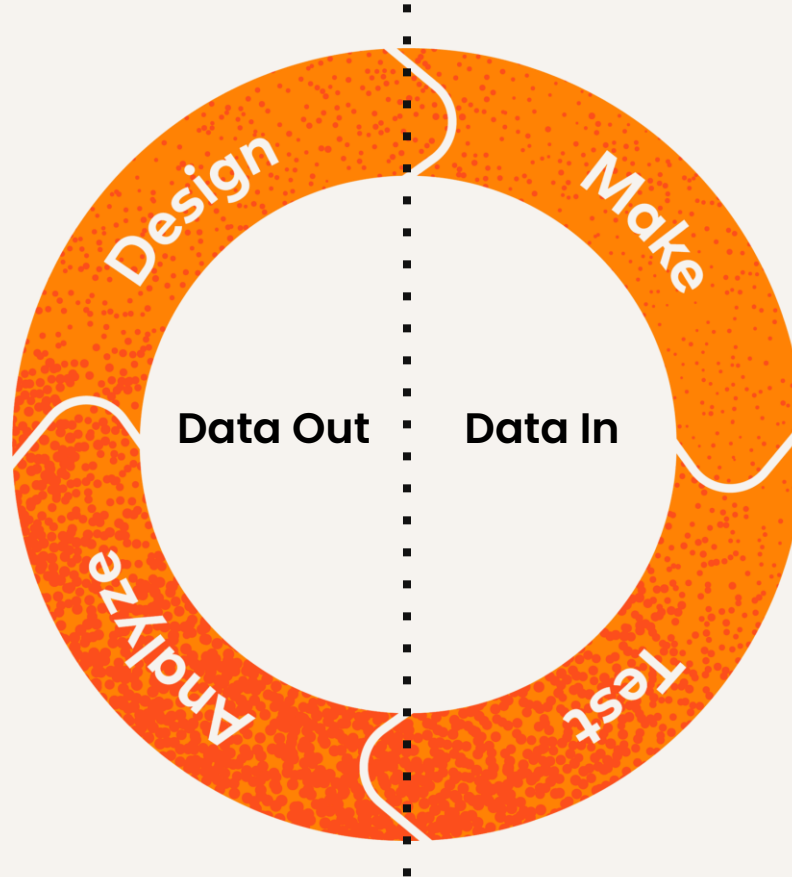
Lead Optimization

Pre-Clinical

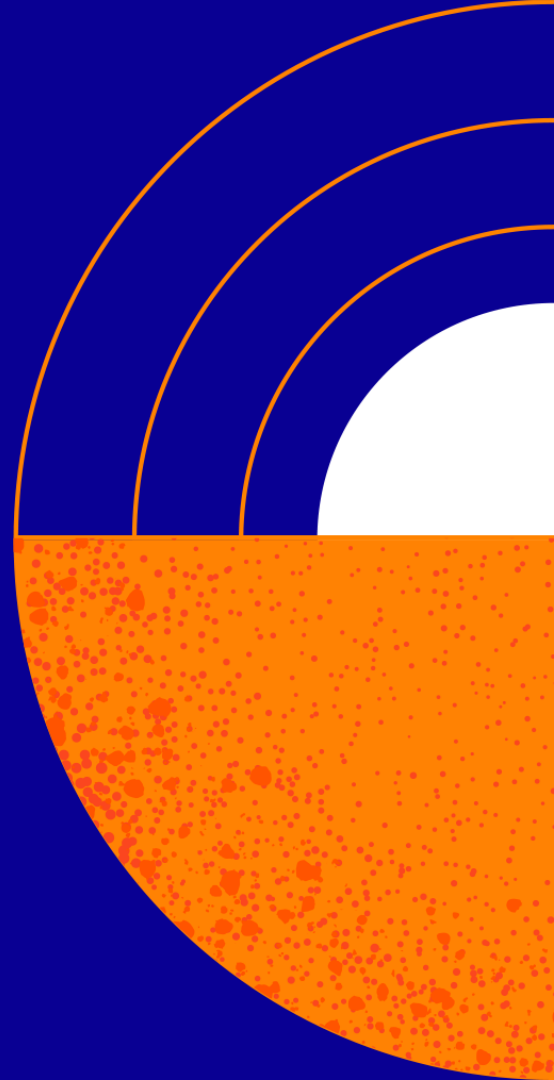
Future: Chemaxon and Certara Combined



Data In vs Data Out



How we are thinking we can help...



Cheaper, Better, Faster...

Improving DMTA Decision Support



Libraries



Building
intelligent
features...



ML



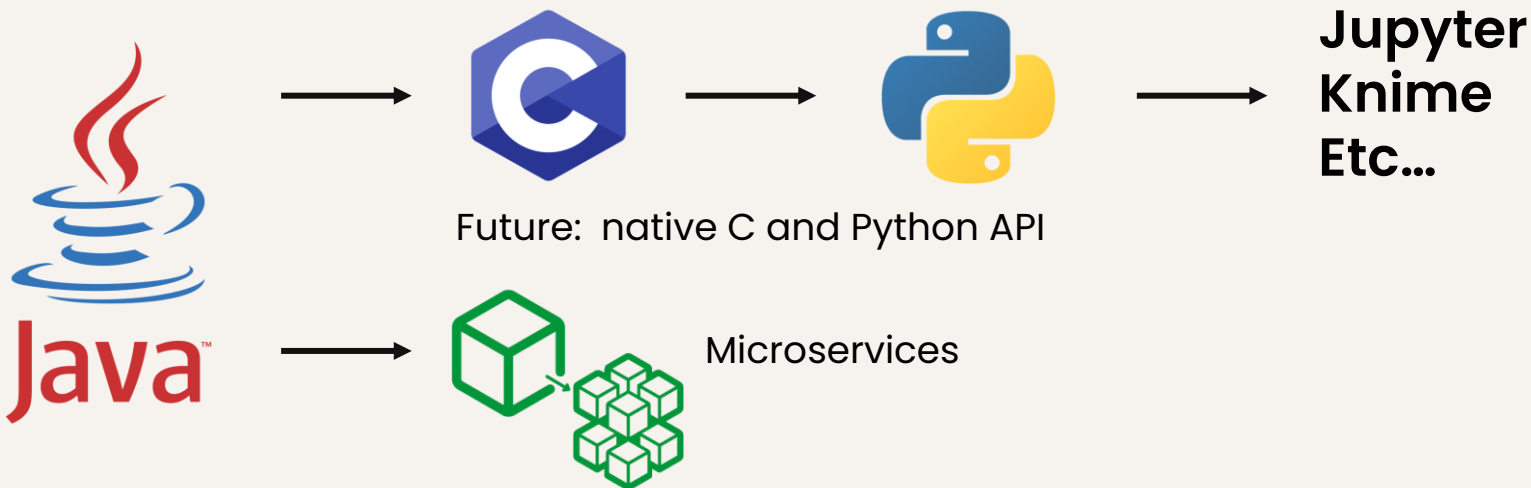
Search

Expand Access to Our Science



Accelerates our ability to:

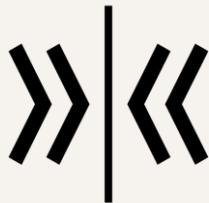
- Enhance algorithms
- Develop new science features
- Deploy faster computations



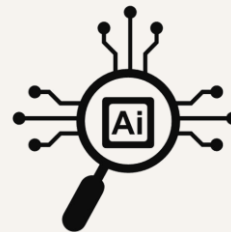
Going Beyond Chemical Search



Scalable Search
(1 data source)



Federated Search
(multiple data sources)



AI Search
(learning from data)

10^9-11

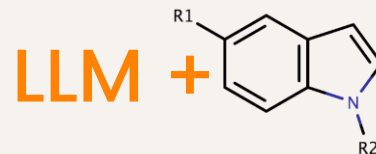
Chemical space



Structured



Unstructured



Summarise SAR

Integration of the 50B Search in Design Hub



The screenshot displays the Design Hub interface for a project titled "P1 improve selectivity with arg173 > route #1". The interface includes a top navigation bar with a search field, a user profile for "Jonathan But...", and tabs for "DESIGN SET" and "REFERENCE". A "Save" button and an "Import" button are visible, along with a toggle for "Enable reaction analysis/scaffold enumeration".

On the left, a chemical structure is shown with the identifier "VXN00000002 #1". The central workspace features the "Marvin JS by Chemaxon" logo. The right sidebar contains a vertical list of chemical elements: H, C, N, O, S, F, P, Cl, Br, I, and A. Below this list, a message states: "There is no selected data to show. Let's add your first property, or create or select a template to use." A "Add property" button is located above this message.

At the bottom of the workspace, it indicates "Last edited 10m".

Automated ML on Data Columns within Design Hub



combine properties of CXN06836 and CXN06837

PROJECT DATA HYPOTHESIS **DESIGN SET** COMPOUND KANBAN

Showing 17 compounds 4 selected

DESIGN COMPOUNDS ADD PROPERTY Build local model

ID	Registered	Molecule	Priority	Votes	cLogP	Mass	pKa (str. basic)	TPSA	MPO Score	Score	HERG-22051902
<input checked="" type="checkbox"/> ☆ #9	VXN-010011		None	👍 0 👎 0	2.76	447.52	2.66	105.16	3.95	-20.4898	
<input type="checkbox"/> ☆ #16	VXN-010018		None	👍 0 👎 0	2.59	411.48	2.54	96.45	4.62	-19.6503	
<input checked="" type="checkbox"/> ☆ #10	VXN-010012		None	👍 1 👎 0	2.47	461.5	2.55	122.23	3.43	-19.4408	
<input type="checkbox"/> ☆ #8	VXN-010010		None	👍 0 👎 0	3.28	389.86	2.69	93.37	4.38	-19.3684	
<input type="checkbox"/> ☆ #12	VXN-010014		None	👍 0 👎 0	3.26	354.43	2.54	67.35	5.02	-18.5387	
<input checked="" type="checkbox"/> ☆ #11	VXN-010013		None	👍 0 👎 0	3.26	354.43	2.54	67.35	5.02	-18.2004	
<input type="checkbox"/> ☆ #1	VXN-010003		None	👍 0 👎 0	1.61	339.36	2.33	106.51	4.95	-17.3837	

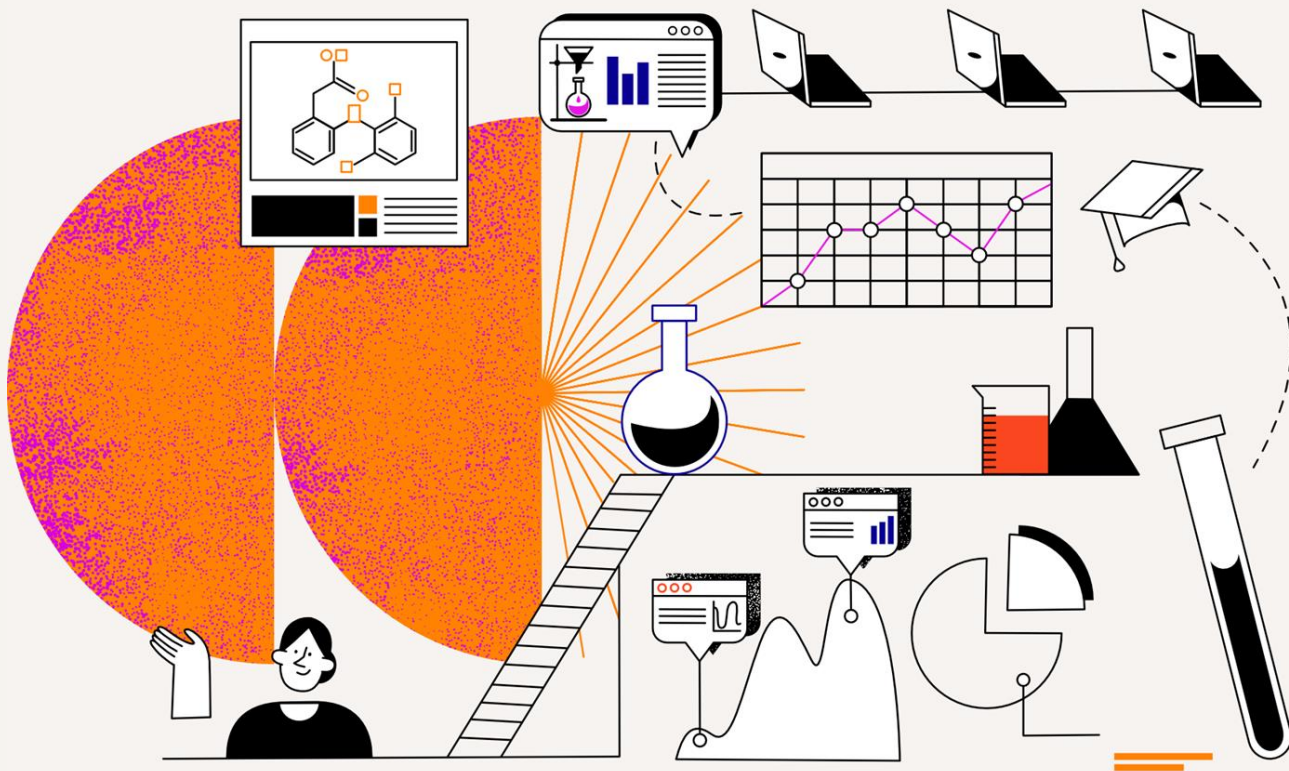
Scatter plot

CNS MPO

MPO Score: VXN-010011 (3.95), VXN-010013 (5.02), VXN-010015 (5.52), VXN-010012 (3.43)

RDock

Improving Efficiency: Better Workflow Experiences

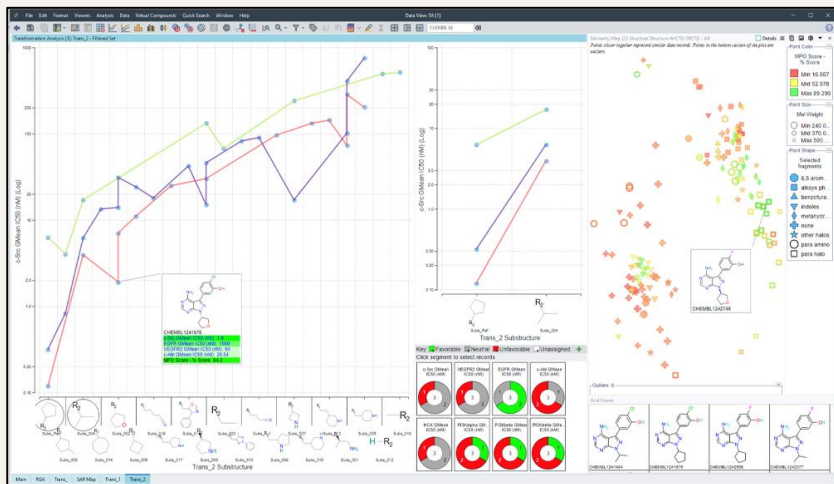


Improving User Workflows: Connecting Apps



From D360...

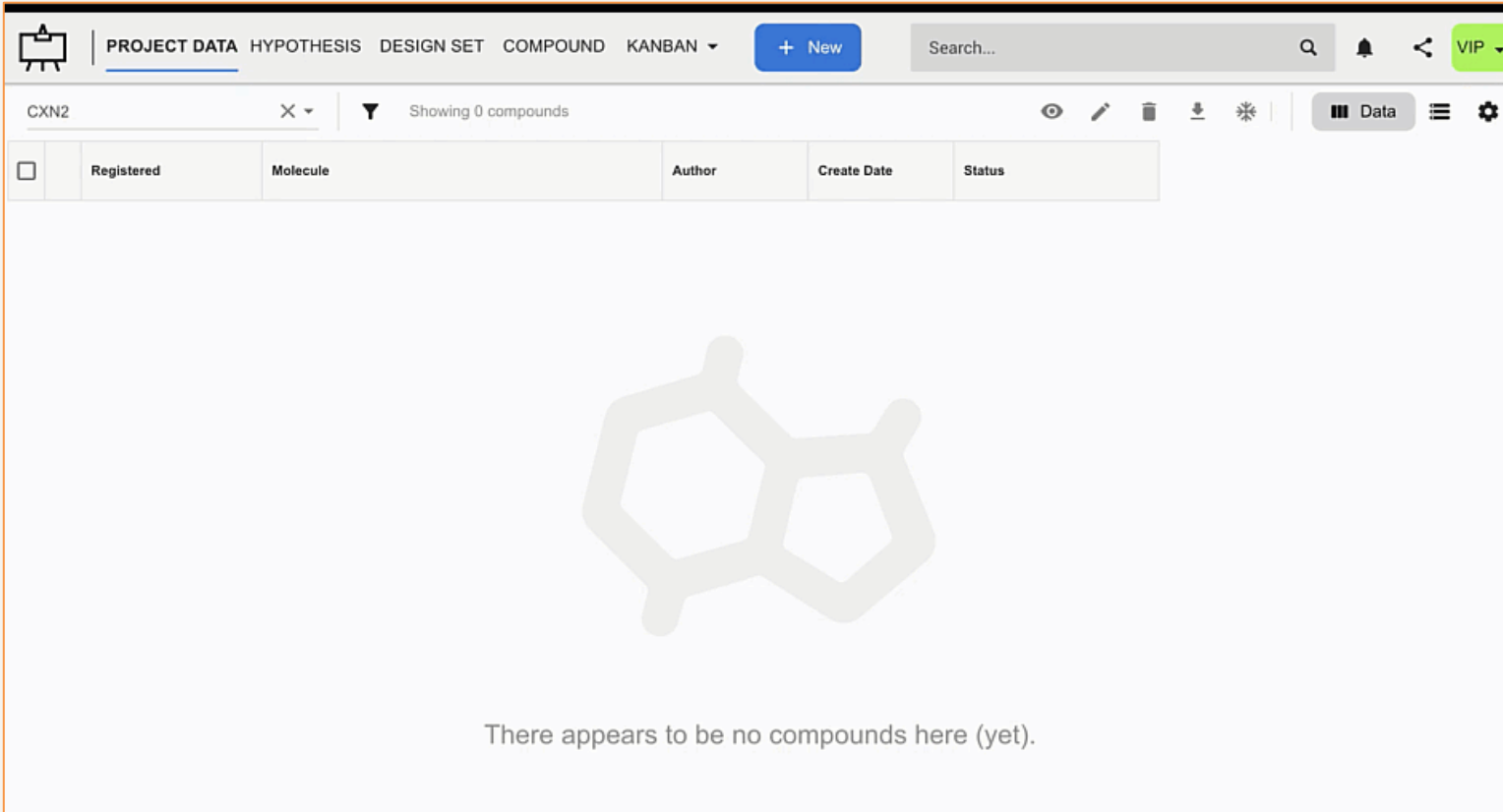
...to Design Hub



The screenshot shows the Design Hub software interface. It features a table of project data with columns for Author, Create Date, Status, and various performance metrics. The table is titled 'CXN2' and shows 210 compounds. The interface includes a menu bar at the top and a search bar.

Author	Create Date	Status	c-Abi GMean...	EGFR GMean...	HCK GMean...	P13Kalpha GMean...	P13Kbeta GMean...	P13Kdelta GMean...	P13Kgam GMean...	
VIP	12h	Synthesis Completed		0.483	169.999	0.856	10400	50000	10200	17
VIP	12h	Synthesis Completed		0.701	19.987	0.856	38000	50000	29999.3	t
VIP	12h	Synthesis Completed		0.949	66.293	0.565	224.999	940.293	102.996	14
VIP	12h	Synthesis Completed		4.3	317.999	4.445	524.999	1020	141.997	25

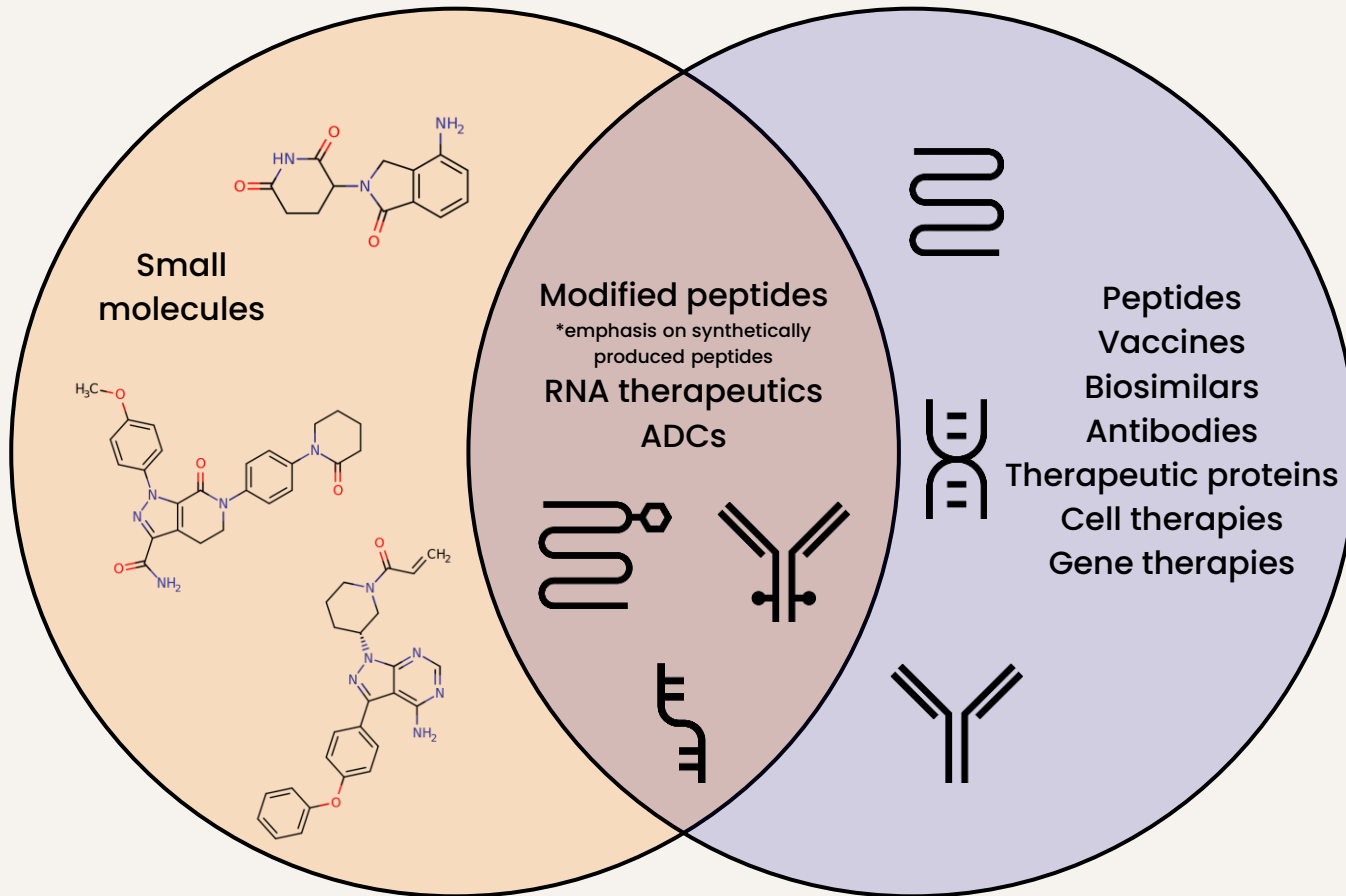
Example: Pulling Data from D360 into Design Hub



The screenshot displays the Design Hub interface. At the top, there is a navigation bar with tabs for PROJECT DATA, HYPOTHESIS, DESIGN SET, COMPOUND, and KANBAN. A blue '+ New' button and a search bar are also present. Below the navigation bar, the current project is identified as 'CXN2'. A filter icon and the text 'Showing 0 compounds' are visible. The main content area features a table with the following columns: Registered, Molecule, Author, Create Date, and Status. The table is currently empty. A large, faint chemical structure is centered in the background. At the bottom of the page, a message reads: 'There appears to be no compounds here (yet).'

Registered	Molecule	Author	Create Date	Status
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Supporting Complex Modalities

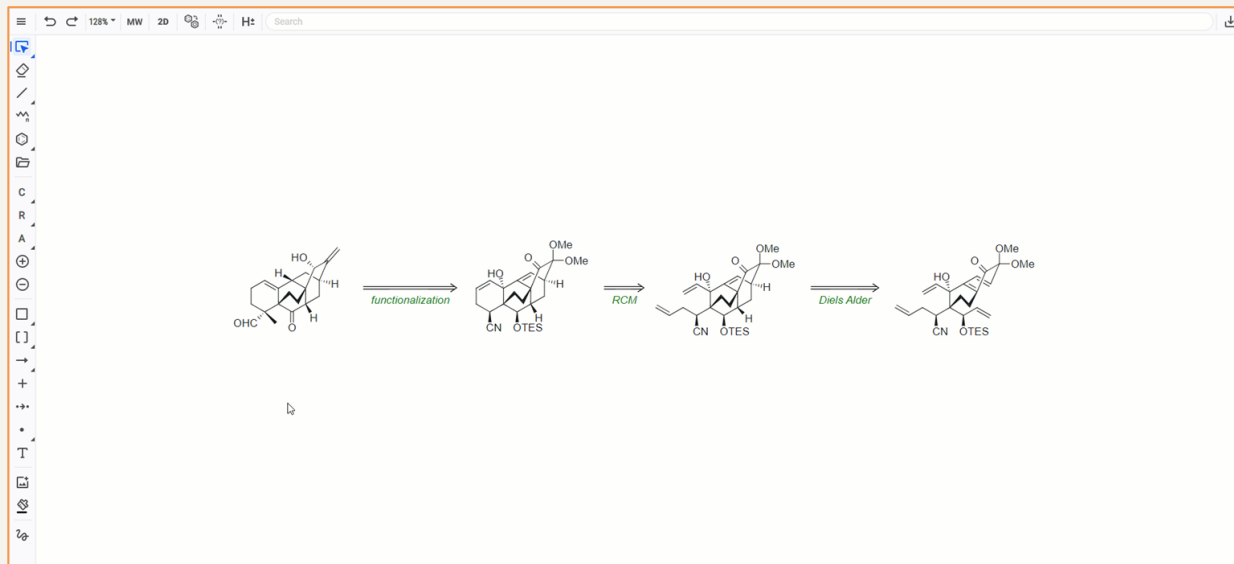


Sketch, Render, Publish Chemical Drawings

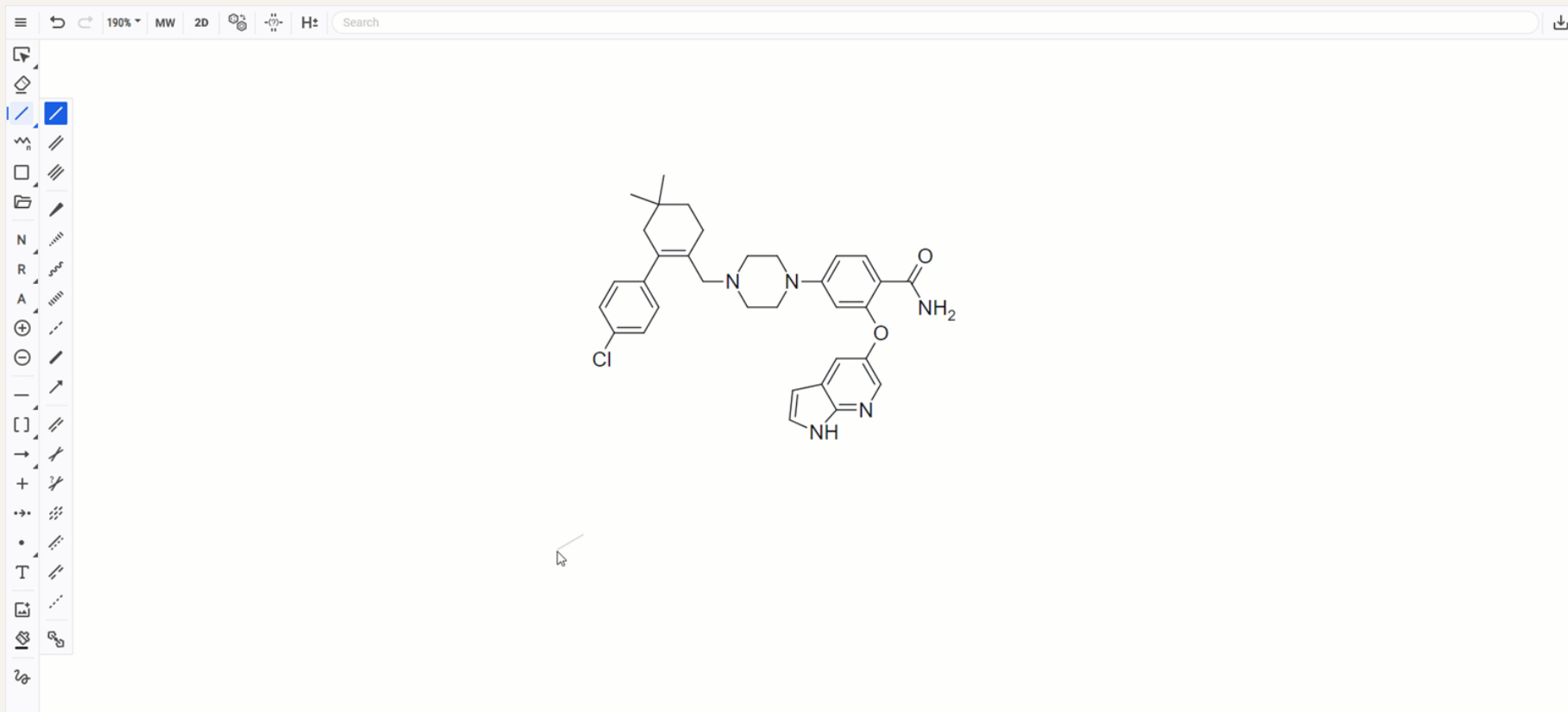


Marvin

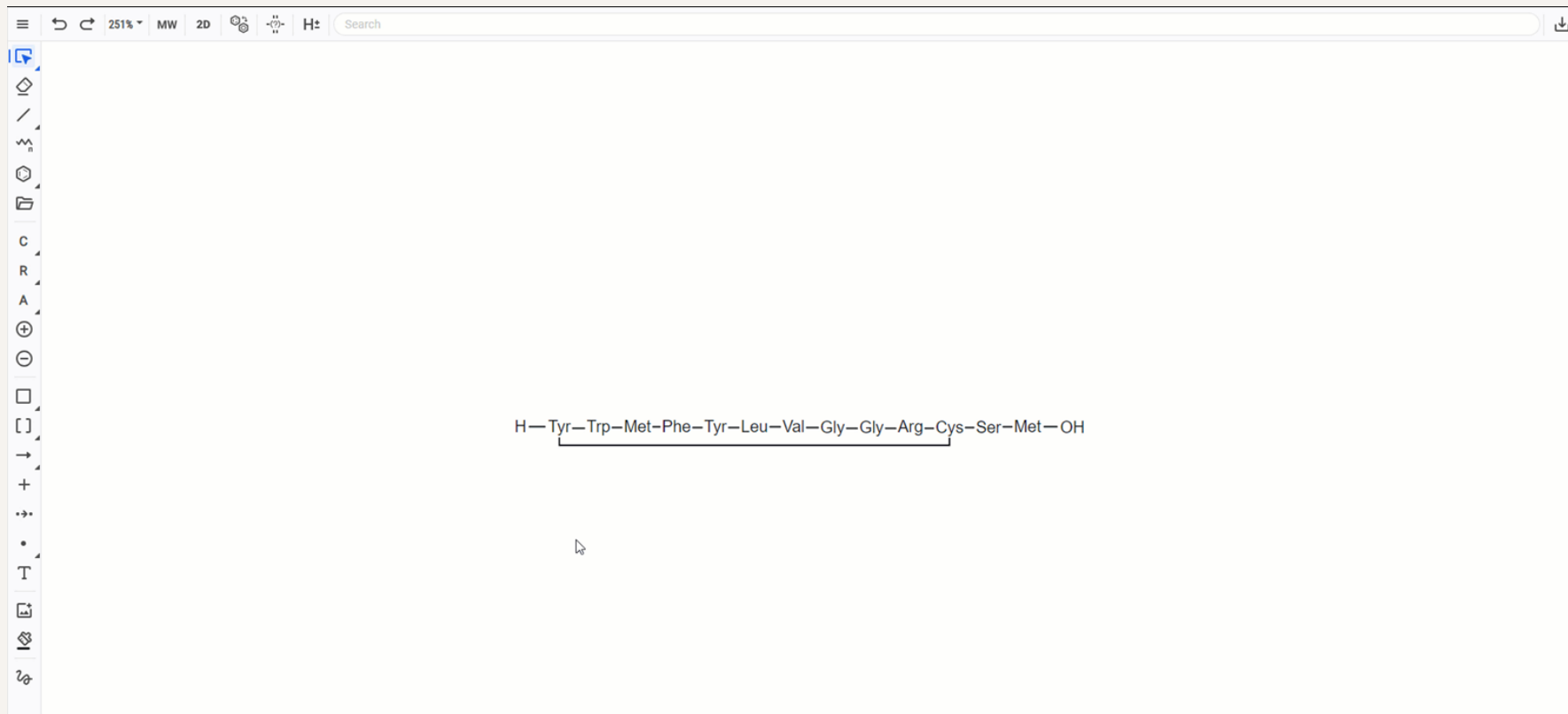
- Fast & intuitive drawing
- Complex images and biomolecules handled easily
- Integrates seamlessly with other tools
- Complies with EU accessibility reqs.



Calculating Properties as You Sketch



Handling Chemistry in Biologics



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



Acknowledgements

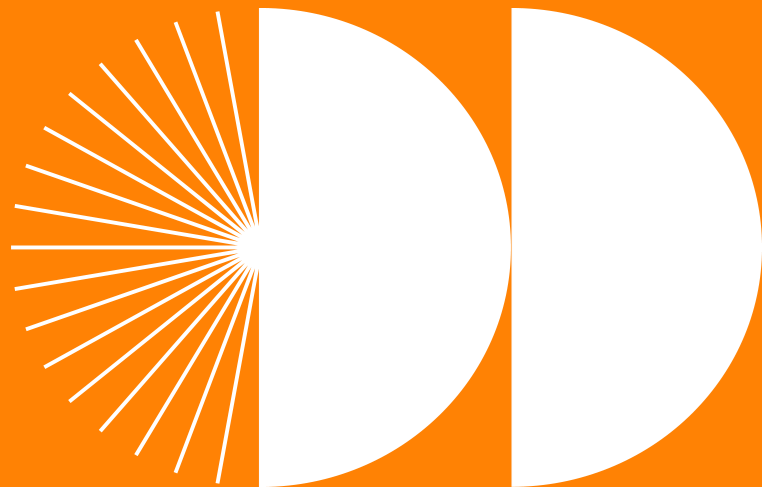
With thanks to the following for help!

- 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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and technologies that aid
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