

A large, stylized red halftone graphic of two men's faces, one slightly behind the other, occupies the left side of the slide. The halftone dots are of varying sizes, creating a textured effect.

**CERTΔINTY  
DISCOVERY**

CERTARA<sup>®</sup> |  Chemaxon

# **Aligning the early-stage discovery strategies across Chemaxon and Certara**

**David Lewis**

Certara

**Adrian Stevens**

Chemaxon



# Unifying the Discovery Portfolio

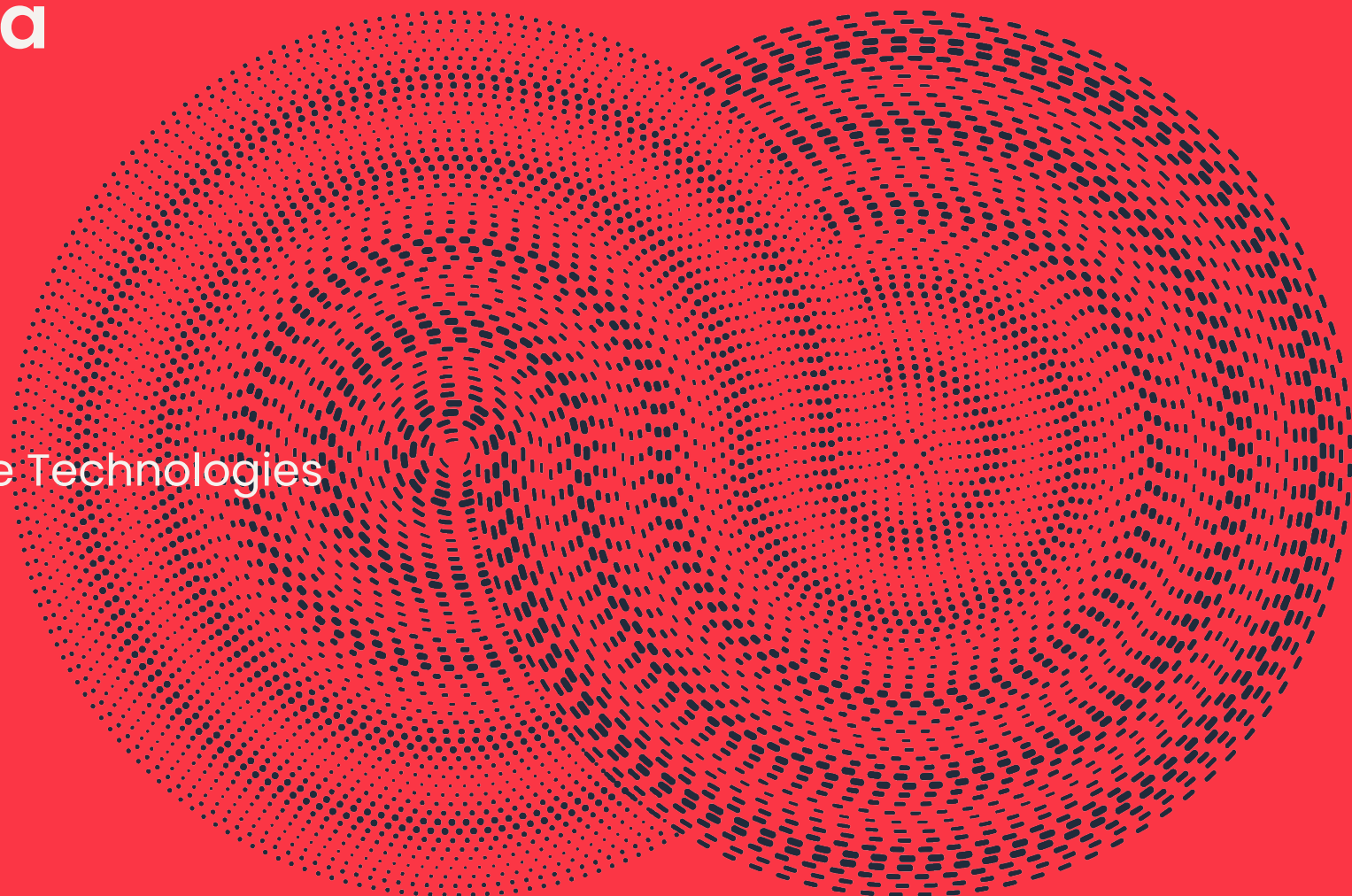
## Aligning the Early-Stage Discovery Software across Chemaxon and Certara

Adrian Stevens  
Chief Product Officer, Chemaxon

David Lewis  
Executive Director, Certara Predictive Technologies

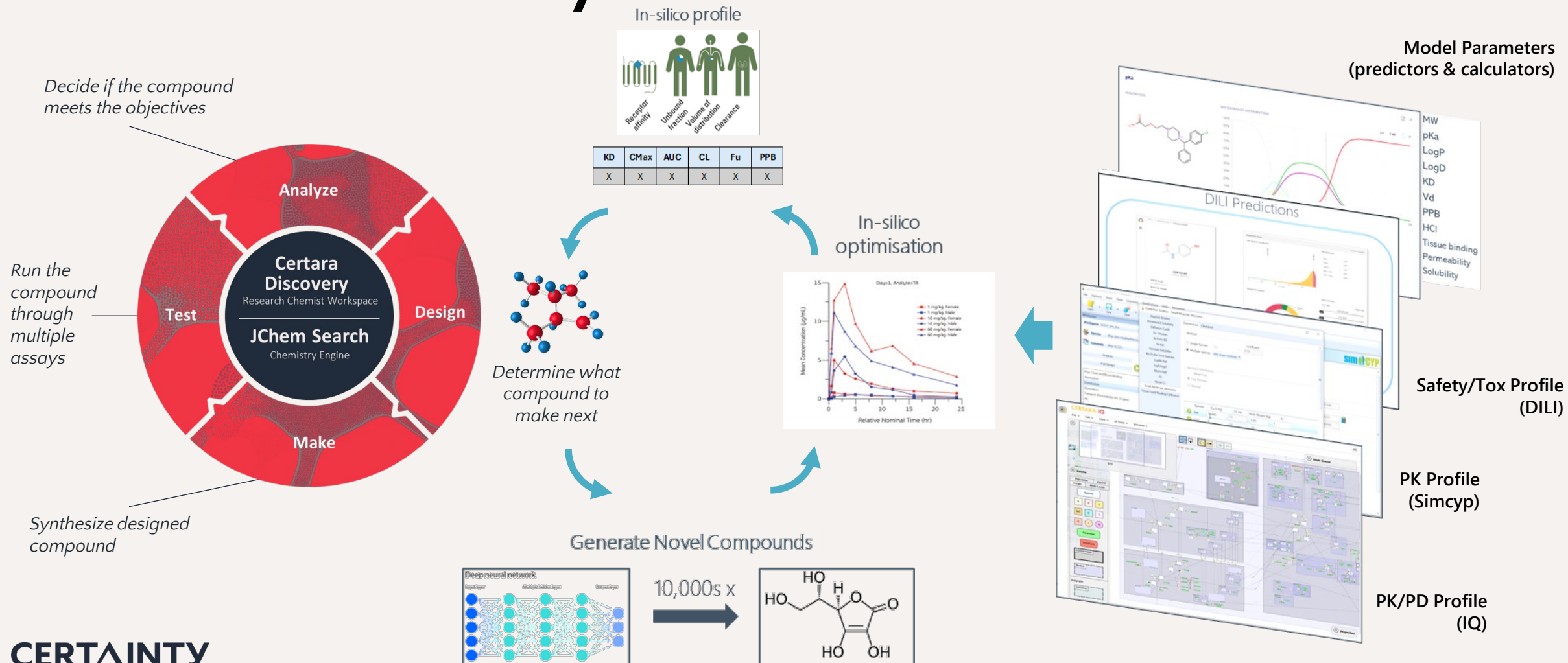
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# In-silico Models Can Enhance The Design Process in Discovery

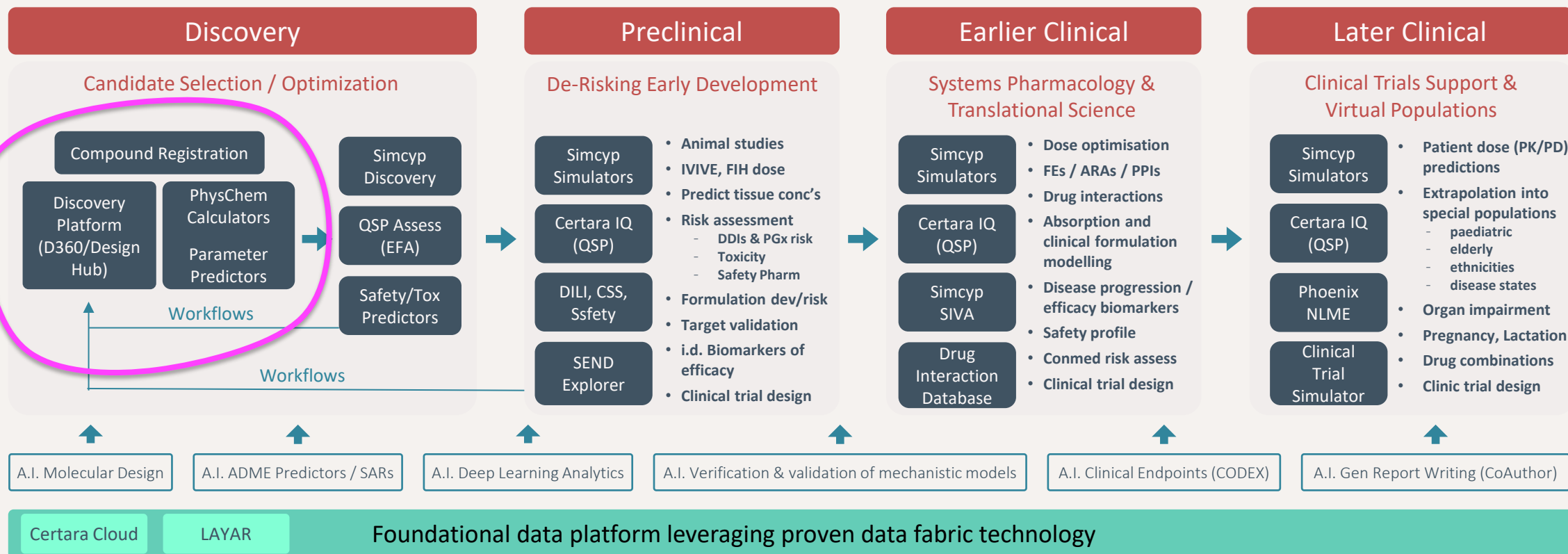


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# Certara MIDD Platform

Data Integration & Predictive Analytics Delivering Certainty Across Drug Development



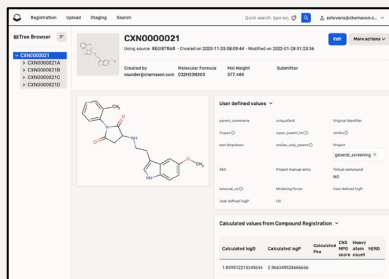
## "In-Silico Profile" concept

- Unique library of data which defines/characterizes a specific compound and provides input parameters for in-silico
- Compound Profile 'file' will expand and transform over time as experimental data is generated and accumulated
- Standardized data formats will allow predictive models to be run as automated workflows across large numbers of compounds and test scenarios.

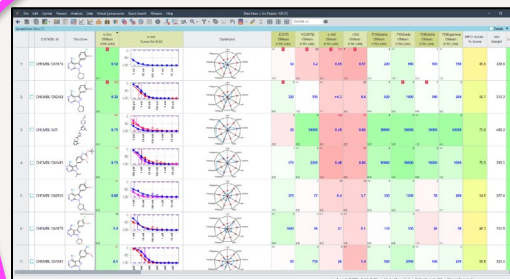


# Aligning the Discovery Portfolio

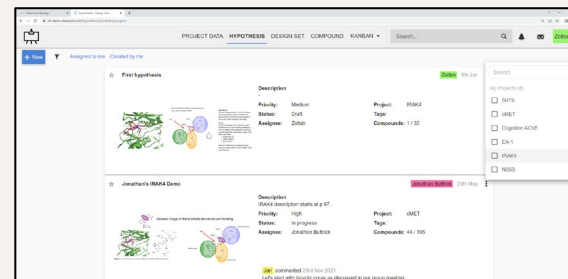
Starting with D360 and Design Hub



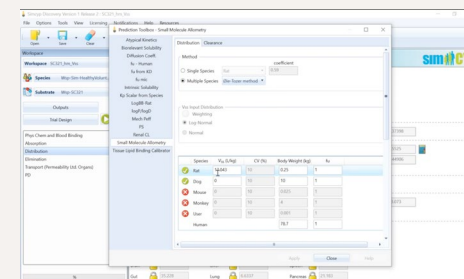
Compound Registration



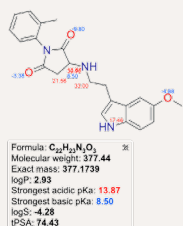
D360



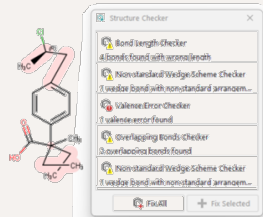
Design Hub



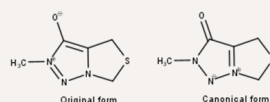
Simcyp Discovery



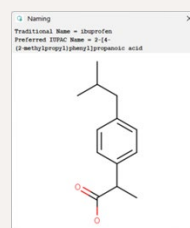
Calculators



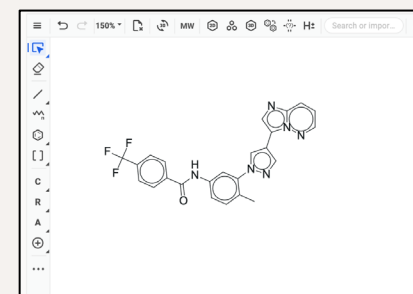
Structure Validation



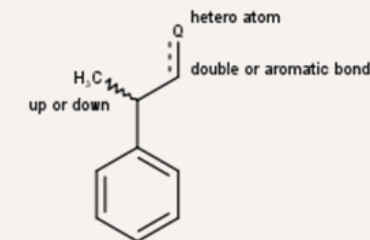
Tautomer handling



IUPAC Naming



Marvin



JChem Search

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Chemistry Toolkits



# Key Areas of Product Development

Combining the Discovery capabilities of Certara and Chemaxon

## Improved cross-modality support

- Small molecules, peptides, oligos, Ab, ADC, ....
- Working groups set up to develop analysis best practises

## Improved consistency in substance representation

- Consistent chemistry representation
- Consistent representation for other modalities (HELM, BILN)

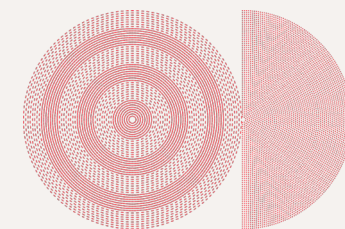
## Improved access to Certara CPT science

- Inclusion of SimCyp PK prediction technologies
- Secondary Intelligence, DILI, ...

## Transition towards product convergence in Discovery

- Improve user workflow my connecting Analyze-Design-Make
- An open web-based application within the MIDD platform with data orchestration layer

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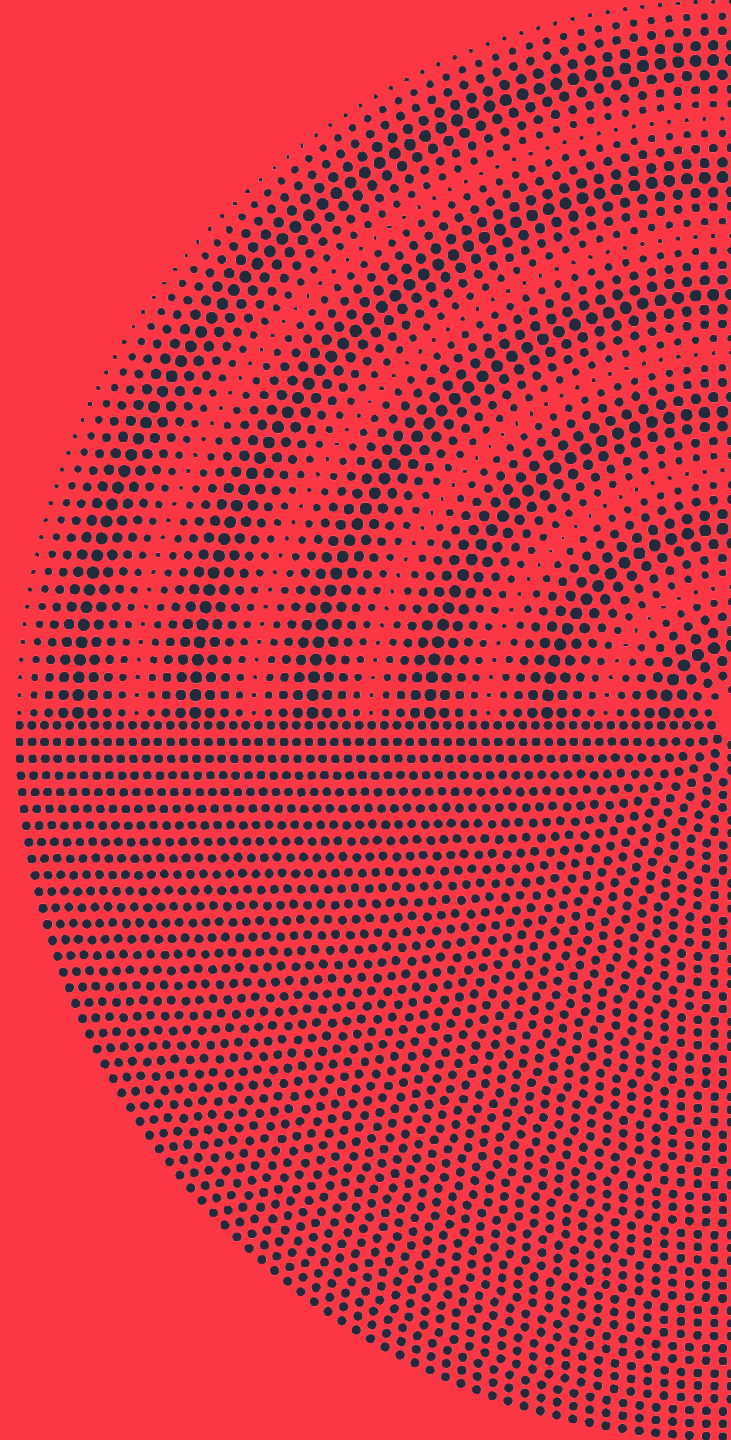




# Near-term: Cross-Application Consistency

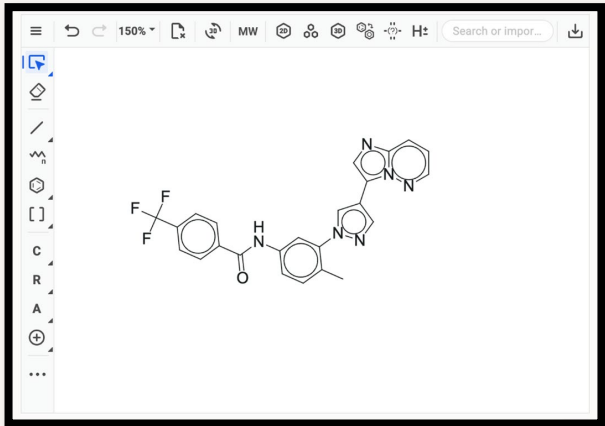
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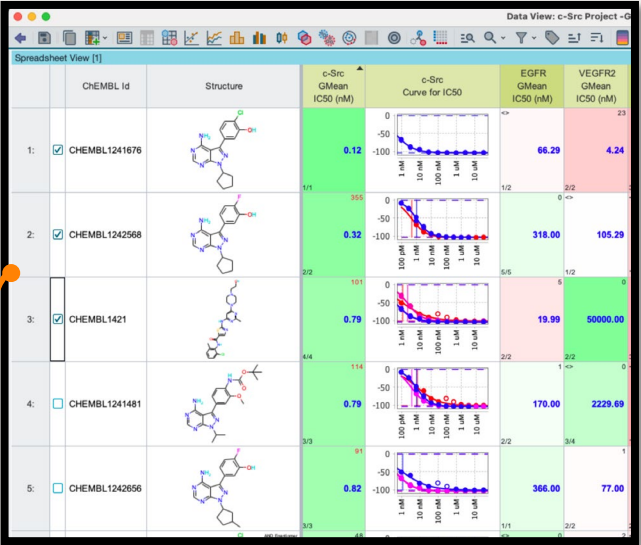
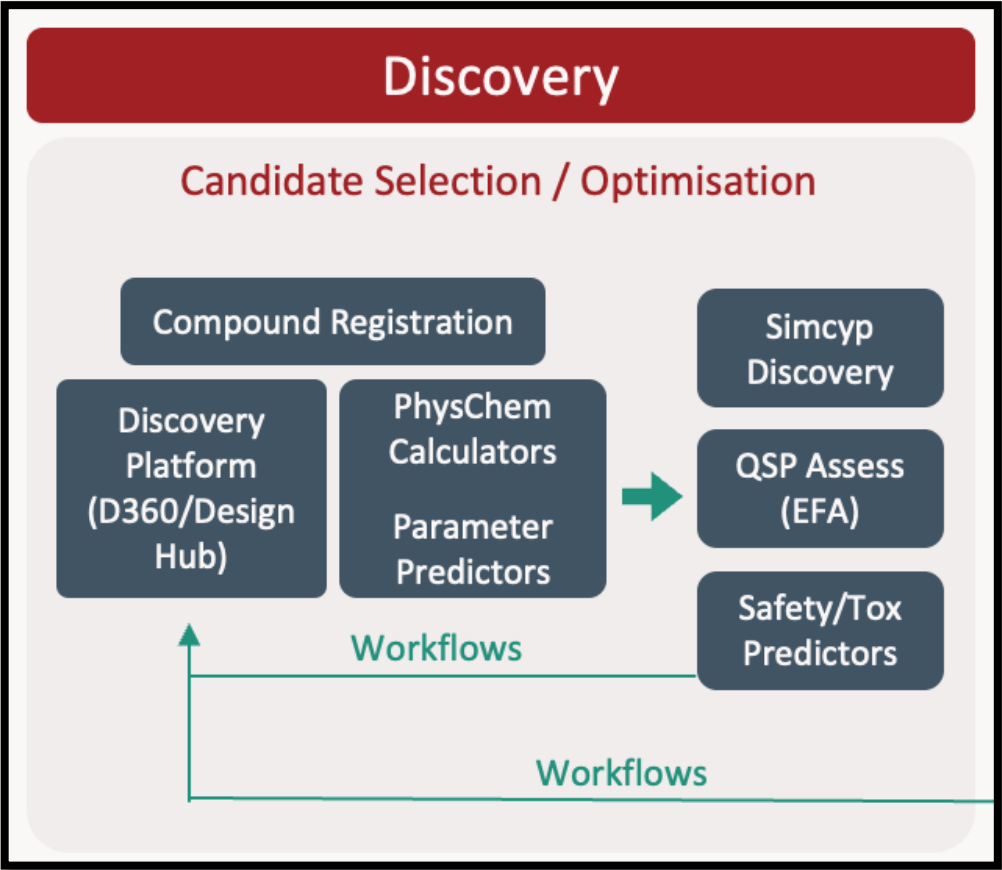


# Near-term Goals

Greater consistency of entity and data handling

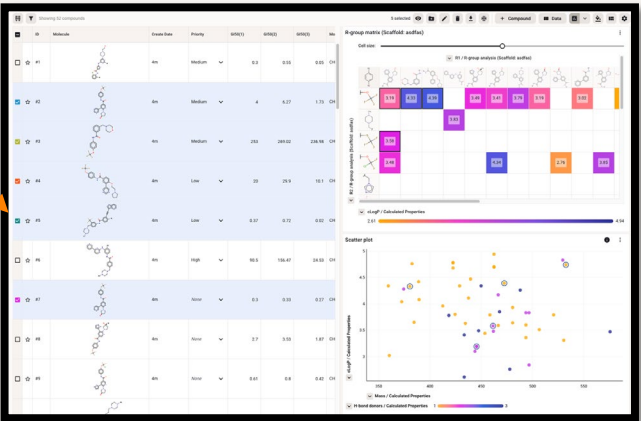


Standardized drawing



	CHEMBL Id	Structure	c-Src GMean IC50 (nM)	c-Src Curve for IC50	EGFR GMean IC50 (nM)	VEGFR2 GMean IC50 (nM)
1:	<input checked="" type="checkbox"/> CHEMBL1241676		0.12		66.29	4.24
2:	<input checked="" type="checkbox"/> CHEMBL1242568		0.32		318.00	105.29
3:	<input checked="" type="checkbox"/> CHEMBL1421		0.79		19.99	50000.00
4:	<input type="checkbox"/> CHEMBL1241481		0.79		170.00	2229.69
5:	<input type="checkbox"/> CHEMBL1242656		0.82		366.00	77.00

Improved data synch





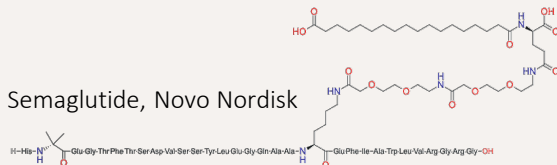
# Marvin – An Awesome Drawing Product!

Expand on supported modalities

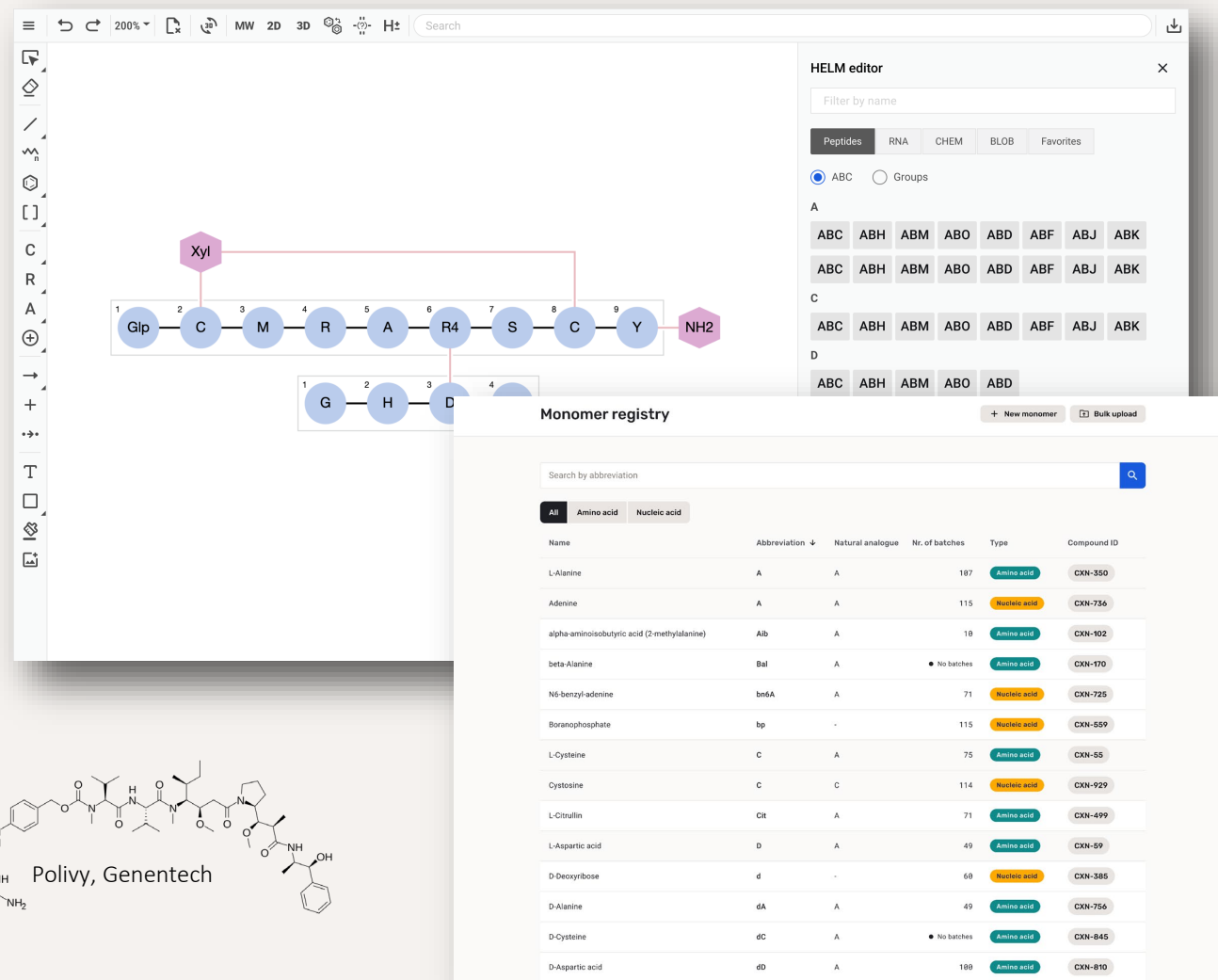
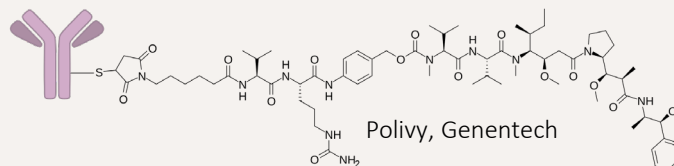
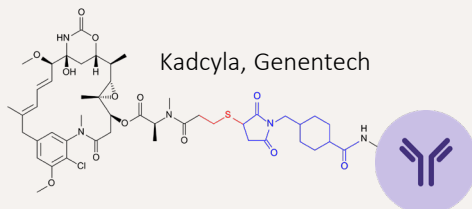
## Coming soon:

- Export CDXML
- Monomer library
- Support HELM

Semaglutide, Novo Nordisk



Kadcyla, Genentech



The screenshot displays the Marvin software interface. The main window shows a chemical structure being edited in the HELM editor, which includes a monomer library and a search bar. The Monomer registry is open, showing a table of monomers with columns for Name, Abbreviation, Natural analogue, Nr. of batches, Type, and Compound ID.

Name	Abbreviation	Natural analogue	Nr. of batches	Type	Compound ID
L-Alanine	A	A	187	Amino acid	CXN-350
Adenine	A	A	115	Nucleic acid	CXN-736
alpha-aminobutyric acid (2-methylalanine)	Alb	A	18	Amino acid	CXN-102
beta-Alanine	Bal	A	No batches	Amino acid	CXN-170
N6-benzyl-adenine	bn6A	A	71	Nucleic acid	CXN-725
Borophosphate	bp	-	115	Nucleic acid	CXN-559
L-Cysteine	C	A	75	Amino acid	CXN-55
Cytosine	C	C	114	Nucleic acid	CXN-929
L-Citrullin	Cit	A	71	Amino acid	CXN-499
L-Aspartic acid	D	A	49	Amino acid	CXN-59
D-Deoxyribose	d	-	68	Nucleic acid	CXN-385
D-Alanine	dA	A	49	Amino acid	CXN-756
D-Cysteine	dC	A	No batches	Amino acid	CXN-845
D-Aspartic acid	dD	A	188	Amino acid	CXN-810

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# Cross-Platform Drawing Standard

All Chemaxon applications standardized on Marvin

## Consistent drawing application

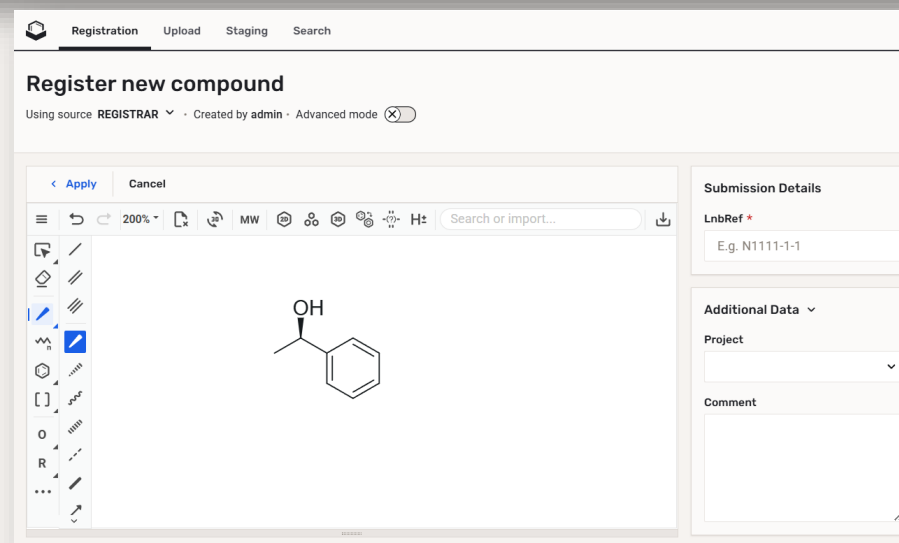
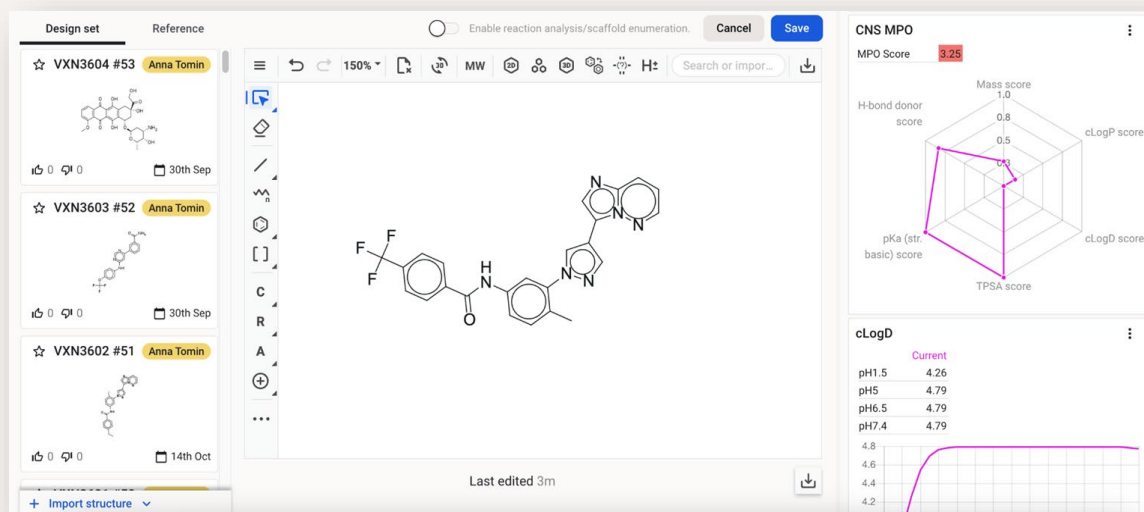
- 2025: Design Hub, Compound Registration, Compliance Checker
- Early 2026: D360

Design Hub

## Expansion of modality support

- 2025: Peptides, Oligonucleotides, Oligosaccharides
- 2026: Monomer library, HELM notation support, registration of peptides, oligonucleotides, followed by the handling of conjugates

Compound Registration



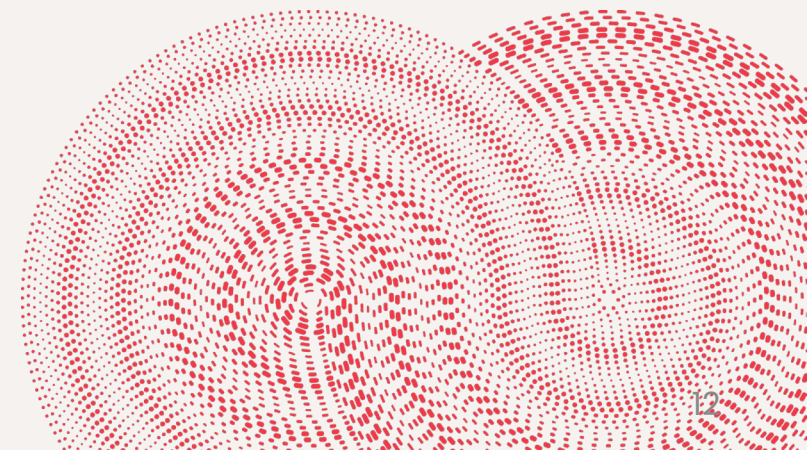


## 2025 Highlights

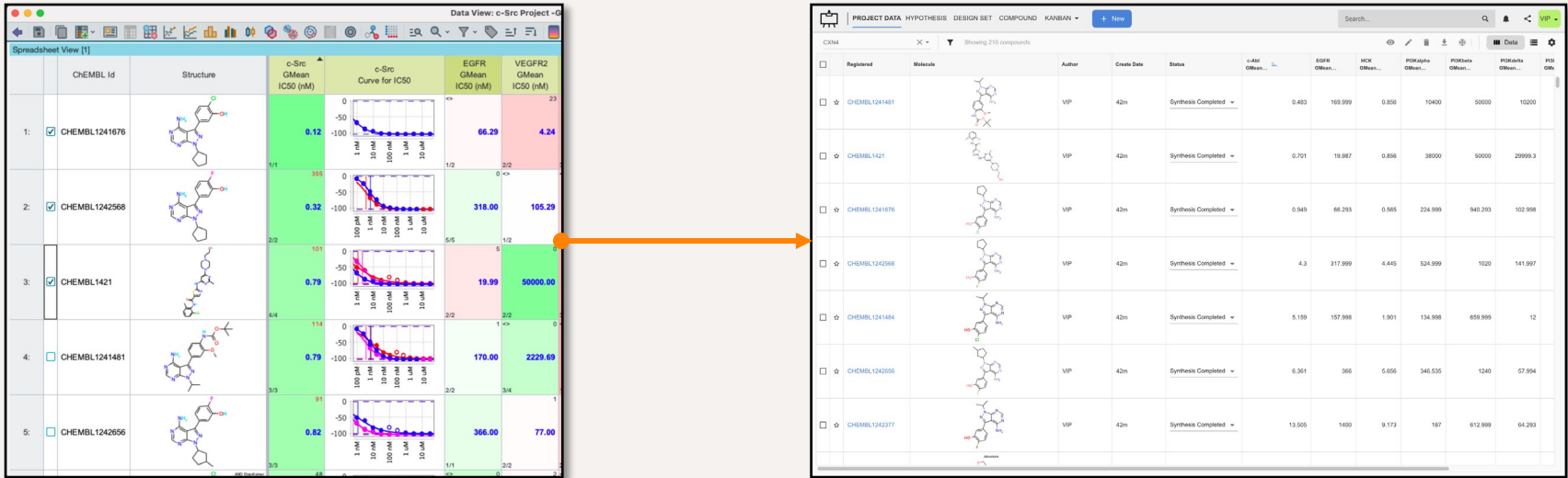
- Matched Pair Searching
- SAR Matrix
- Enhanced support for external collaborations
- Registry workflow improvements

## Next: Near-term Plans

- Improved data synchronization with D360
- Complete the migration to (new) Marvin
- Image support for spreadsheet view



# Next: Improved D360 Data Synchronization



**Schedule import**

+ Create new schedule | Scheduled imports (4)

Project:

Data set:

Schedule \*

☐ One time

☒ Recurring

Schedule frequency:

Start date:

End date:

**Schedule import**

+ Create new schedule | Scheduled imports (4)

Project:

Data set:

Schedule \*

☐ One time

☒ Recurring

Schedule frequency:

Start date:

End date:

**Schedule import**

+ Create new schedule | Scheduled imports (5)

Project: Project A, Data set: Data set A

Next import scheduled: 2025.06.23. 13:11

Weekly

# Next: Improved D360 Data Synchronization

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# Next: Marvin!

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# Next: Include Simcyp Results

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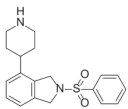

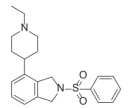
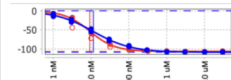

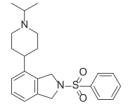
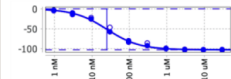

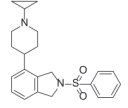
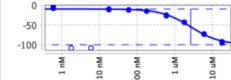
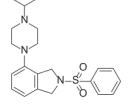
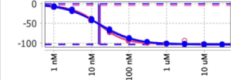
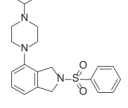
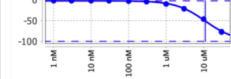
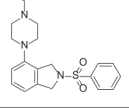
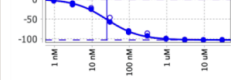
# Next: Image in Spreadsheet

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Project data Hypothesis Design set Compound Kanban ▾ + New

My projects (2) ▾ Showing 23 compounds

👁️ 📁 ✎ 🗑️ ⬇️ ✨ Data 📊 ▾ 📄 📋 ⚙️

<input type="checkbox"/>	Registered	Molecule	c-Src Overlay Curve for IC50	Hypothesis, Design set	Author	Cr
<input type="checkbox"/>	★ CXN3452			<a href="#">My second hypothesis</a> <a href="#">My second design set</a>	John Chemist	11
<input type="checkbox"/>	★ VXN0242			<a href="#">My first hypothesis</a> <a href="#">My first design set</a>	John Chemist	11
<input type="checkbox"/>	★ 			<a href="#">My second hypothesis</a> <a href="#">My second design set</a>	John Chemist	11
<input type="checkbox"/>	★ 			<a href="#">My first hypothesis</a> <a href="#">My first design set</a>	John Chemist	11
<input type="checkbox"/>	★ CXN3452			<a href="#">My first hypothesis</a> <a href="#">My first design set</a>	John Chemist	11
<input type="checkbox"/>	★ VXN8245			<a href="#">My first hypothesis</a> <a href="#">My first design set</a>	John Chemist	11
<input type="checkbox"/>	★ VXN8246			<a href="#">My first hypothesis</a> <a href="#">My first design set</a>	John Chemist	11

### Manage data columns

- > Compound details
- > Additional fields
- > Structure check
- > Novelty and analog
- > Phys-Chem calculated data
- > ADMET calculated data
- > Other properties
- ▼ Imported data
  - ☒ Imported data
    - ☒ c-Src Overlay Curve for IC50

[Change column order](#) [Import data from file](#)



# D360: Recent Highlights and Plans

## 2025 Highlights (D360 25.0 & 25.5)

### Other modalities: Enhancement of sequence alignment

- Alignment of sequence subsets
- Manual sequence editing
- Undo and realignment

### Data visualization

- Dynamic data subset viewers
- Chart error bars
- Overlaid dose-response curves from different assays

### Workflow:

- Active filter gadget display
- Contains constraints with multiple values
- Elimination of blocking progress dialogs
- Improved spreadsheet row/column navigation

## Next: Near-term Plans (D360 26.0 & 26.5)

### Antibodies and ADCs

- Display of sequence annotation
- Improved ADC data configuration capabilities

### Design of Peptides

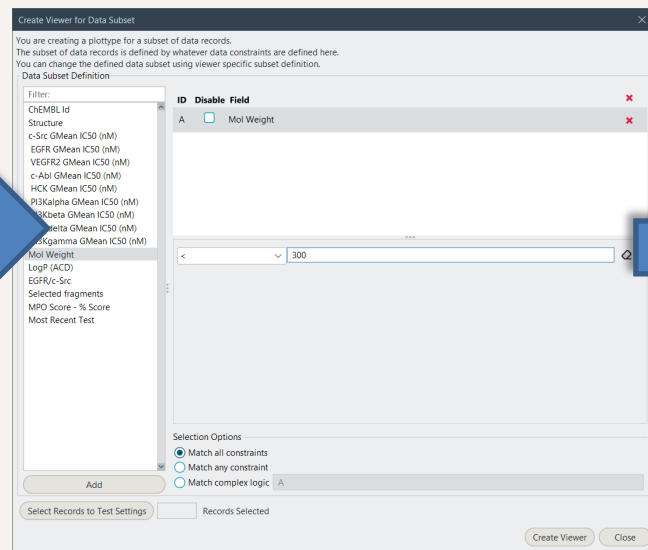
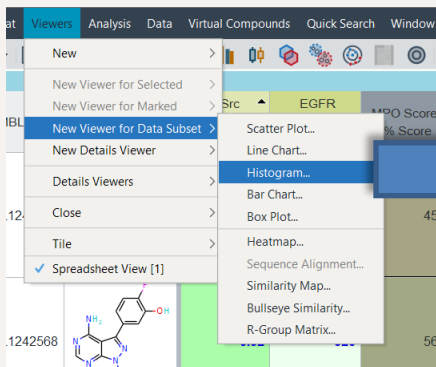
- Design of peptides in context of sequence alignment
- Capture of Design Peptides
- Use of external reference sequence

### Workflow

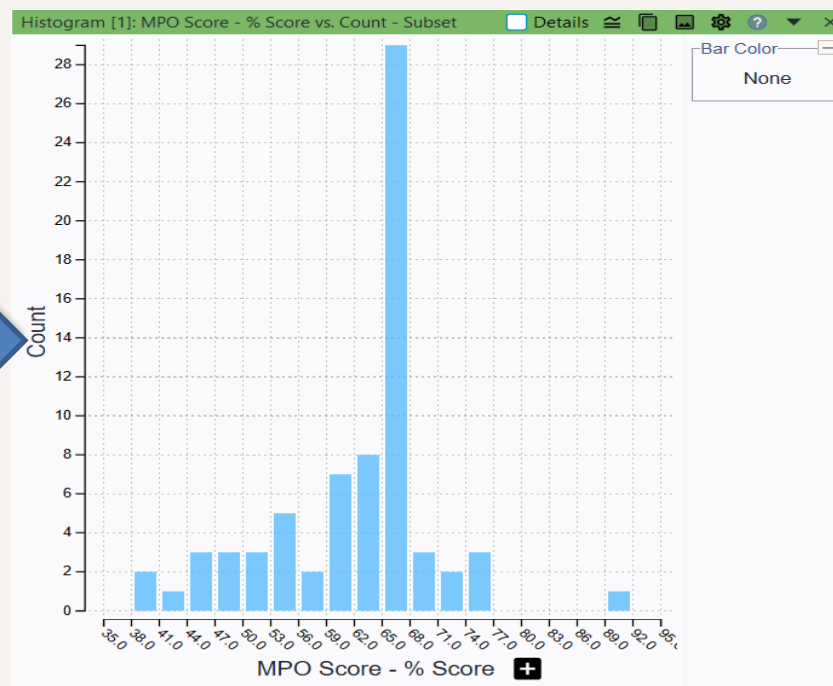
- Integration of Marvin
- Dynamic data series
- Integration of Secondary Intelligence

# Highlights – Data Visualization

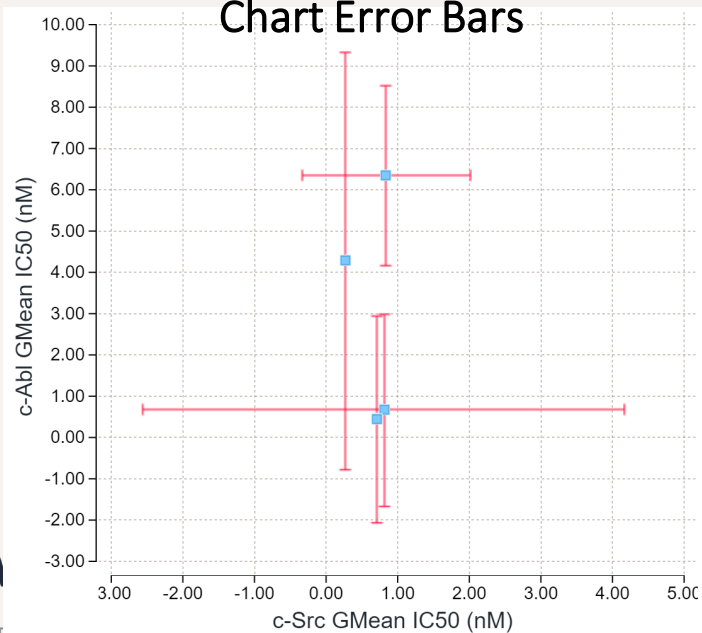
## Data Subset Viewers



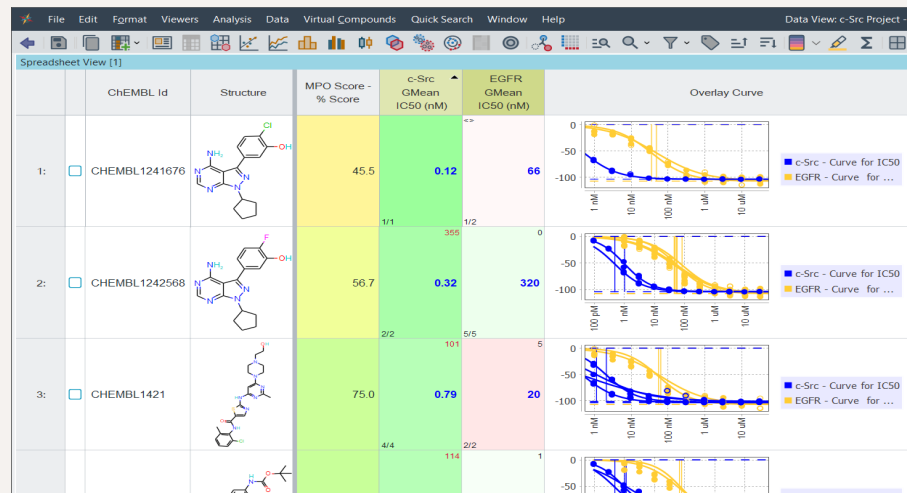
## Data Subset Histogram



## Chart Error Bars



## Overlaid Dose-Response Curves for Different Assays



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# Highlights – Sequence Alignment

## Manual Sequence Alignment Editing

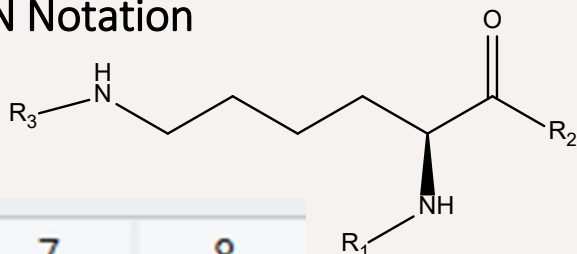
Reference CHEMBL402482 Alignment: Identity Matrix - All

Sequence Alignment: Main

ALT+→  
To move selected monomers

CTRL+Z  
To undo edit

## Use of BILN Notation



	6	7	8
	G	K <sub>1</sub>	S
	G	K <sub>3</sub>	S

## Realign Sequences

### Aligned to Reference 1

	1	2	3	4	5	6	7	8	9
CHEMBL402482	I	L	W	Q	V	P	F	S	V
CHEMBL412034	I	L	F	Q	V	P	F	S	V
CHEMBL426344	I	L	D	Q	V	P	F	S	V
CHEMBL440266	I	L	Y	Q	V	P	F	S	V
CHEMBL437514	I	L	M	Q	V	P	F	S	V
CHEMBL263685	I	L	A	Q	V	P	F	S	V
CHEMBL263600	I	L	S	Q	V	P	F	S	V
CHEMBL36217	I	L	T	W	Q	V	P	F	S

### Aligned to Reference 2

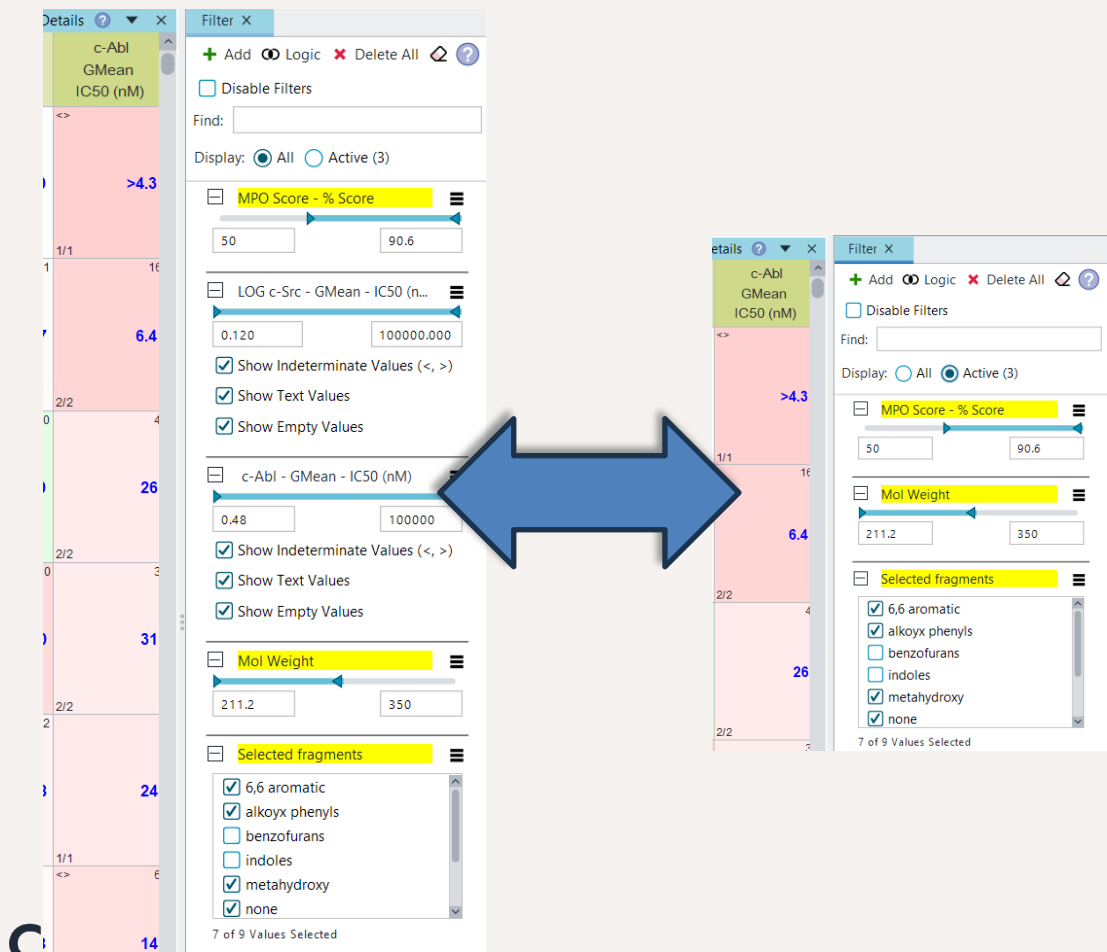
	1	2	3	4	5	6	7	8	9
CHEMBL402482	I	L	W	Q	V	P	F	S	V
CHEMBL412034	I	L	F	Q	V	P	F	S	V
CHEMBL440266	I	L	Y	Q	V	P	F	S	V
CHEMBL437514	I	L	M	Q	V	P	F	S	V
CHEMBL263685	I	L	A	Q	V	P	F	S	V
CHEMBL263600	I	L	S	Q	V	P	F	S	V
CHEMBL36217	I	L	T	W	Q	V	P	F	S

Realign  
sequences

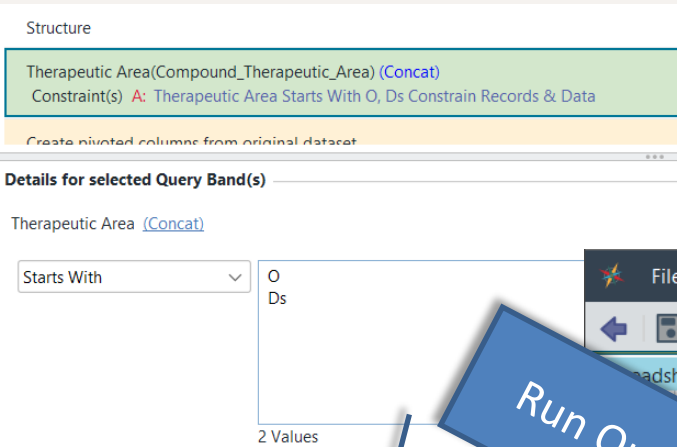


# Highlights – Workflow

## Active Filter Gadgets



## Multiple Text Operands



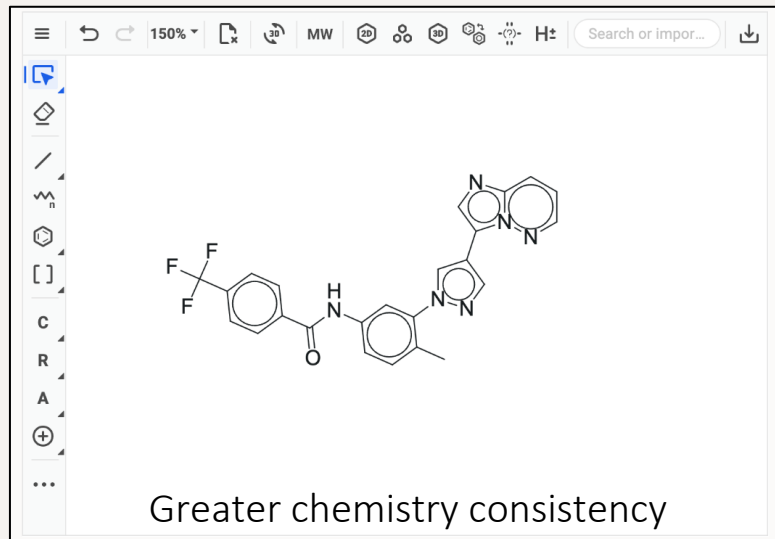
Run Query

“Starts With” text constraint operator constrained with 2 values

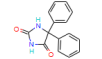
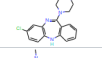
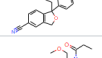
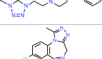
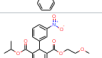
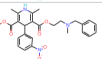
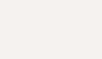
	EMBL Id	Structure	Concat Therapeutic Area
5:	<input type="checkbox"/> CHEMBL263076	<chem>Oc1cc(O)c2c(c1)c(=O)oc3cc(F)ccc32</chem>	Oncology
	<input type="checkbox"/> CHEMBL265773	<chem>COc1cc(OC)c2c(c1)c(=O)oc3cc(F)ccc32</chem>	Oncology
7:	<input type="checkbox"/> CHEMBL266223	<chem>Oc1cc(O)c2c(c1)c(=O)oc3cc(F)ccc32</chem>	Diabetes
8:	<input type="checkbox"/> CHEMBL266458	<chem>Oc1cc(O)c2c(c1)c(=O)oc3cc(F)ccc32</chem>	Diabetes

# Near Term Plans: Workflow

## Marvin as an Integrated Sketcher



## Secondary Intelligence Integration

	Sample Code	Structure	MACHR3 Secondary Intelligence	ADRA2A Secondary Intelligence	CBR2 Secondary Intelligence	DAT Secondary Intelligence	ACHE Secondary Intelligence	CAV1PT2 Secondary Intelligence
1:	<input type="checkbox"/> EX00000001		Inh: 31.0 % Ki: 15898.6 (nM)	Inh: 6.0 % Ki: 13333.3 (nM)	Inh: 60.0 % Ki: 4347.8 (nM)	Inh: 16.0 % Ki: 15882.4 (nM)	Inh: 4.0 % Ki: 30000.0 (nM)	Inh: 68.0 % Ki: 2443.4 (nM)
2:	<input type="checkbox"/> EX00000002		Inh: 40.0 % Ki: 10714.3 (nM)	Inh: 52.0 % Ki: 4102.6 (nM)	Inh: 49.0 % Ki: 6787.9 (nM)	Inh: 85.0 % Ki: 934.3 (nM)	Inh: 8.0 % Ki: 30000.0 (nM)	Inh: 84.0 % Ki: 989.0 (nM)
3:	<input type="checkbox"/> EX00000003		Inh: 7.0 % Ki: 21428.6 (nM)	Inh: 11.0 % Ki: 13333.3 (nM)	Inh: 47.0 % Ki: 7354.3 (nM)	Inh: 1.0 % Ki: 15882.4 (nM)	Inh: 7.0 % Ki: 30000.0 (nM)	Inh: 11.0 % Ki: 15576.9 (nM)
4:	<input type="checkbox"/> EX00000004		Inh: -3.0 % Ki: 21428.6 (nM)	Inh: -5.0 % Ki: 13333.3 (nM)	Inh: -13.0 % Ki: 19565.2 (nM)	Inh: 2.0 % Ki: 15882.4 (nM)	Inh: -3.0 % Ki: 30000.0 (nM)	Inh: 2.0 % Ki: 15576.9 (nM)
5:	<input type="checkbox"/> EX00000005		Inh: 55.0 % Ki: 5844.2 (nM)	Inh: 30.0 % Ki: 10370.4 (nM)	Inh: 74.0 % Ki: 2291.4 (nM)	Inh: 99.0 % Ki: 53.5 (nM)	Inh: 18.0 % Ki: 30000.0 (nM)	Inh: -24.0 % Ki: 15576.9 (nM)
6:	<input type="checkbox"/> EX00000006		Inh: -4.0 % Ki: 21428.6 (nM)	Inh: 6.0 % Ki: 13333.3 (nM)	Inh: -12.0 % Ki: 19565.2 (nM)	Inh: 1.0 % Ki: 15882.4 (nM)	Inh: 1.0 % Ki: 30000.0 (nM)	Inh: -2.0 % Ki: 15576.9 (nM)
7:	<input type="checkbox"/> EX00000007		Inh: 0.0 % Ki: 21428.6 (nM)	Inh: 7.0 % Ki: 13333.3 (nM)	Inh: -4.0 % Ki: 19565.2 (nM)	Inh: -10.0 % Ki: 15882.4 (nM)	Inh: -8.0 % Ki: 30000.0 (nM)	Inh: -7.0 % Ki: 15576.9 (nM)

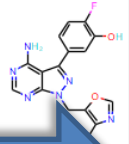
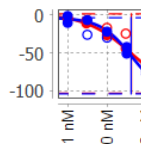
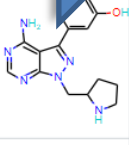
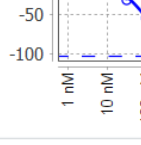

## Dynamic Data Subsets

Create an entry for each data series you wish to define. Each series must be provided with a name and definition in terms of data constraints. Any data records that match the data constraints for a series will be assigned to that series. The order of series definitions is important, any record matching more than one series will be assigned to the first matching series.

Series Rules	Count	Series Name
Logic: A AND B A) Inhibition of recombinant c-Src by radioactive phosphotransfer assay in presence of 10 uM ATP GMean IC50 (nM): Less than 100 B) Inhibition of recombinant c-Abl by radioactive phosphotransfer assay in presence of 10 uM ATP GMean IC50 (nM): Less than 100	63	Active c-Abl issue
Logic: A AND B A) Inhibition of recombinant c-Src by radioactive phosphotransfer assay in presence of 10 uM ATP GMean IC50 (nM): Less than 100 B) Inhibition of recombinant HCK by radioactive phosphotransfer assay in presence of 10 uM ATP GMean IC50 (nM): Less than 100	4	Active HCK issue
Logic: A AND B A) Inhibition of recombinant c-Src by radioactive phosphotransfer assay in presence of 10 uM ATP GMean IC50 (nM): Less than 100 B) Inhibition of recombinant EGFR by radioactive phosphotransfer assay in presence of 10 uM ATP GMean IC50 (nM): Less than 100	0	Active EGFR issue

Series Name for Non-Matching Records: \_\_\_\_\_

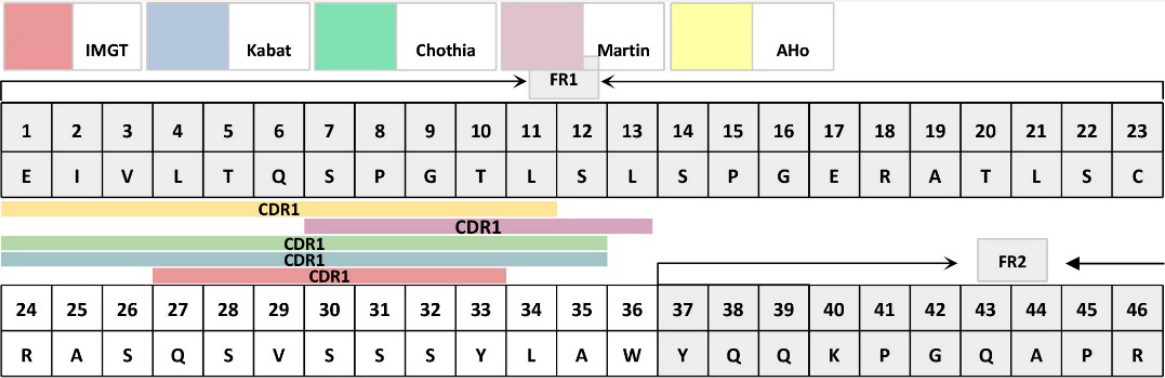
Data Series Column Name: Data Series

Spreadsheet: Spreadsheet Viewer					
	ChEMBL Id	Structure	Data Series	c-Src GMean IC50 (nM)	c-Src Curve for
1:	<input type="checkbox"/> CHEMBL1241482		Active c-Abl issue	41.99	
2:	<input type="checkbox"/> CHEMBL1241769		Active HCK issue	96.00	
				10	

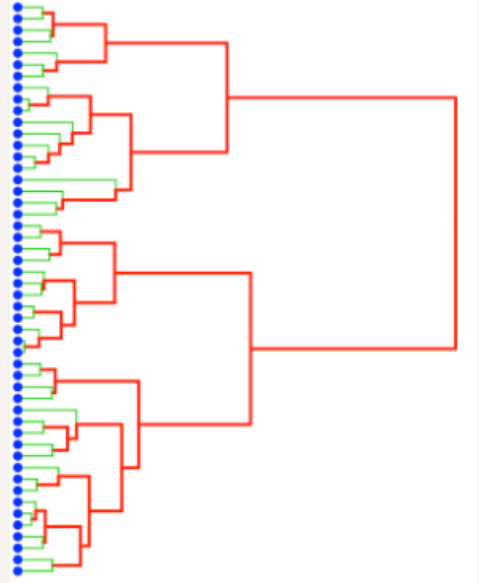
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# Near Term Plans: Antibody and ADC Representation

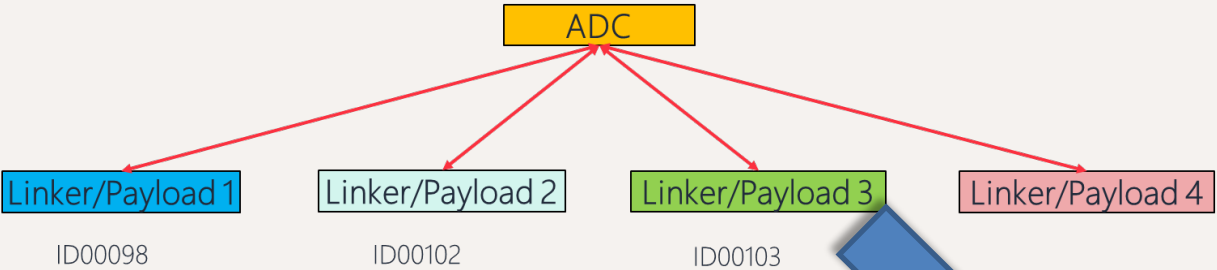
Antibody Sequence Feature Display



Antibody Sequence Relationship Display



Handling of Multiple Linker-Warheads



ADC ID	ADC Data	ADC Data	...	Data Target A ID1	Data Target A ID2	Data Target A ID3	Data Target B ID1	Data Target B ID2	Data Target B ID3	Data Target C ID1	Data Target C ID2	Data Target C ID3	Data Target D ID1	Data Target D ID2	Data Target D ID3
ID00256	123.6	0.63	1.5	...											
ID00986	160	>10	0.07	...											



# Near Term Plans: Peptide Design

Sequence Alignment: Reference CHEMBL402482 Alignment: Similarity Matrix - All

Sequence Alignment: Chain 1

	MHC class I BA (FLPSDYFPSV) GMean	Chain 1								
		1	2	3	4	5	6	7	8	9
<b>CHEMBL402482</b>	<b>1.698</b>	I	L	W	Q	V	P	F	S	V
CHEMBL412034	<b>2.000</b>	I	L	F	Q	V	P	F	S	V
CHEMBL410648	<b>2.198</b>	F	L	D	Q	V	P	F	S	V
CHEMBL415611	<b>2.301</b>	Y	L	D	Q	V	P	F	S	V
CHEMBL386178	<b>3.199</b>	Y	L	F	P	G	P	V	T	A
CHEMBL386299	<b>3.199</b>	Y	L	W	P	G	P	V	T	A
CHEMBL426344	<b>3.304</b>	I	L	D	Q	V	P	F	S	V
CHEMBL402481	<b>3.999</b>	N	M	V	P	F	F	P	P	V
CHEMBL122183	<b>4.295</b>	Y	L	M	P	G	P	V	T	A

\*\*\*

- Virtual Sequence Sandbox:

3 of 3 Sequences Displayed

	MHC class I BA (FLPSDYFPSV) GMean	1	2	3	4	5	6	7	8	9
tVP~00000003	<b>0.000</b>	I	L	W	Q	V	P	W	S	V
tVP~00000004	<b>0.000</b>	I	L	F	Q	V	P	F	S	V
tVP~00000005	<b>0.000</b>		L							

150 of 150 Sequences Displayed

Zoom

Unfilter All Copy Alignment Extract to

## Sequence Alignment

## Key Capabilities

- Add/Delete Sandbox sequences
- Edit Monomers
- Add/Remove Chains
- Copy/Paste of sequences/monomers
- Sequence Calculations
- Find/Replace motifs
- Enumerate (e.g. ALA scan)

## Workflow

- Create and evaluate new sequences in the Sandbox
- Promote to dataset for further analysis
- Capture in database as Design peptides
- Retrieve in regular D360 queries

## Sandbox Design Area

# Long-term: A Convergent User Experience

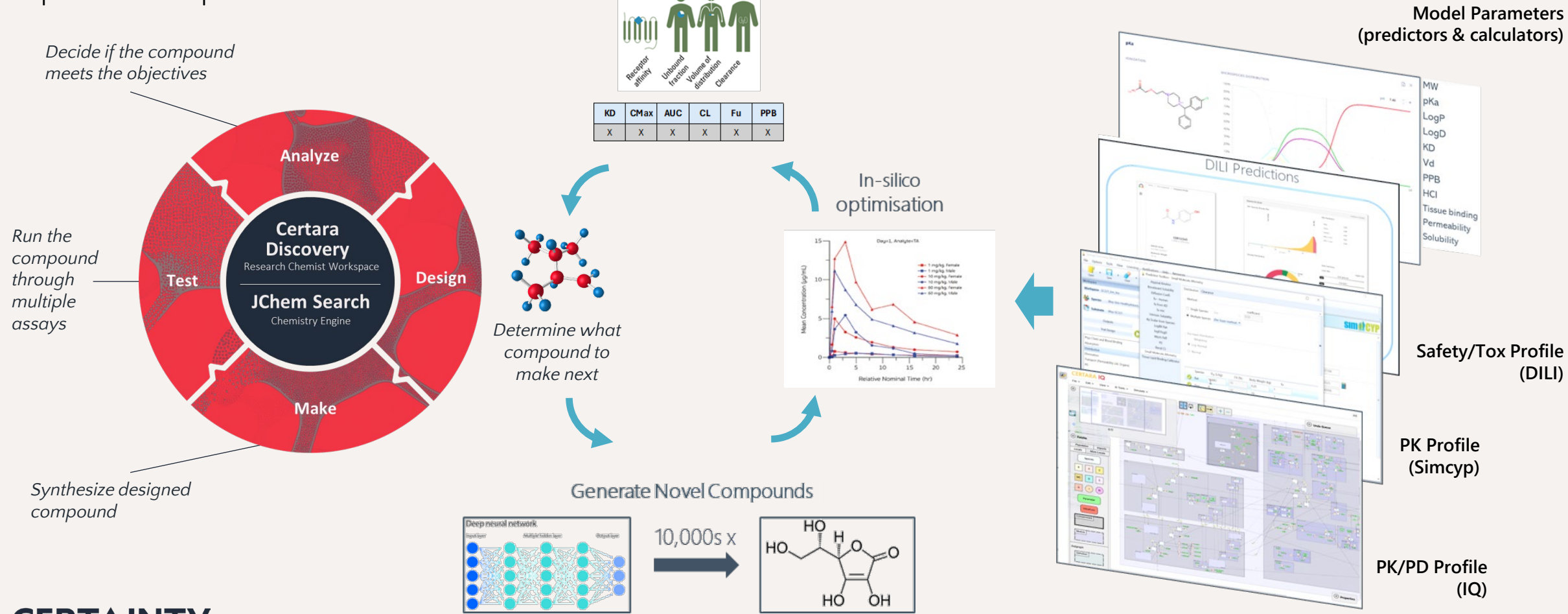
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# In-silico Models Can Enhance The Design Process in Discovery

## Multiparameter Optimization

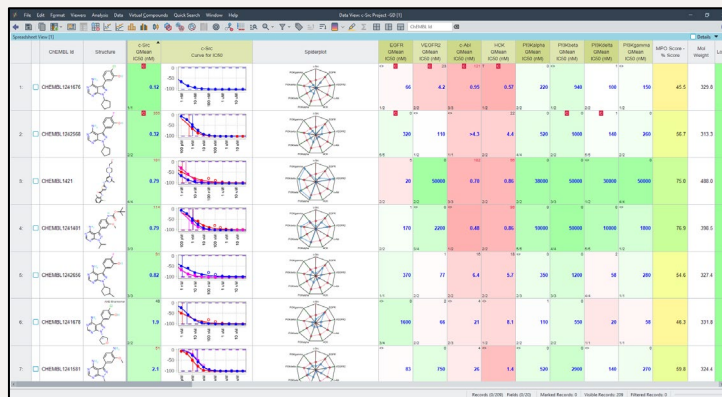


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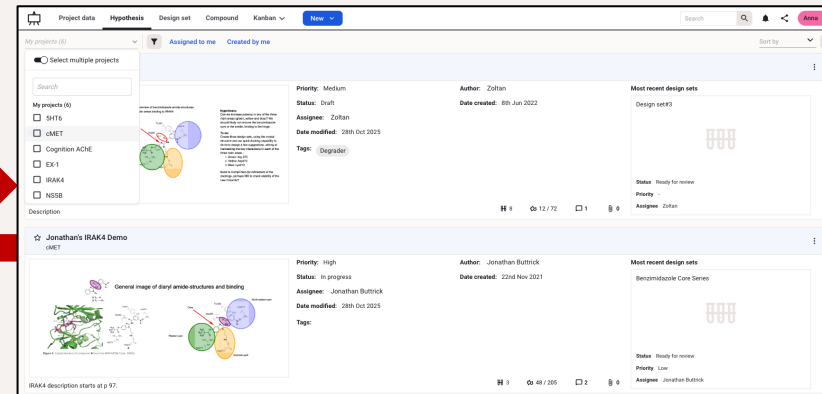
# Today: Different Applications & Data Sources

Trying to build workflows is time consuming

D360



Design Hub



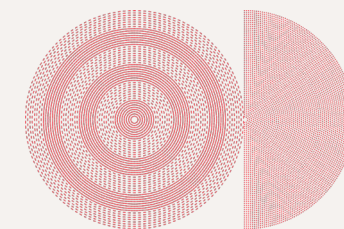
- Different data models
- Different back-end architectures
- Different user experiences



- Manual data exports and imports
- Manual data formatting & normalization
- Expertise required to run each application

We want to make it more streamlined & technologically robust

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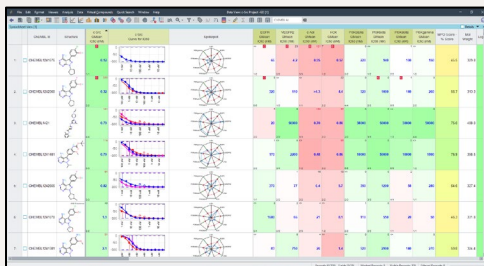




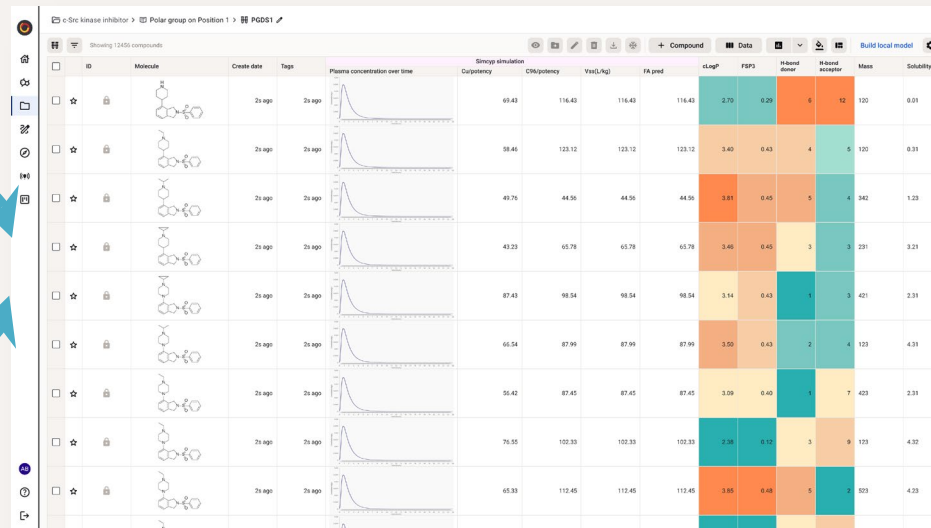
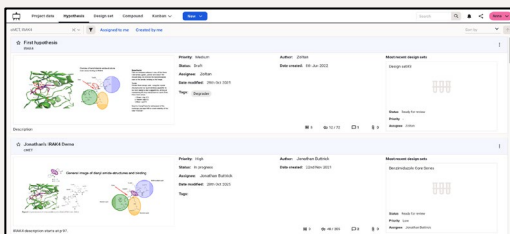
# Future: Integrated Design and Analysis Application

D360 and Design Hub converging into a single design and analysis application

D360



Design Hub



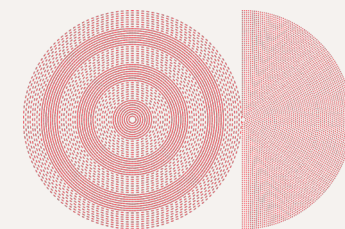
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- Applications converge into a single solution
- Single solution for workflow integration
- Common set of features

- No more ETL (export/import)
- Enabling Automation
- Business efficiency and Scaling

**CERTAINTY  
DISCOVERY**

Single holistic view of all your project data – Real, Design & Ideas



# Future: Integrated Design and Analysis Application

## Key Features and Benefits

### Web-based

- Offered either as a SaaS solution or self-hosted
- Team-based project data access

### Consistent chemistry model

- Using Marvin and Chemaxon toolkit (CCL)

### Improved workflow and data sharing

- Utilizing our data orchestration layer

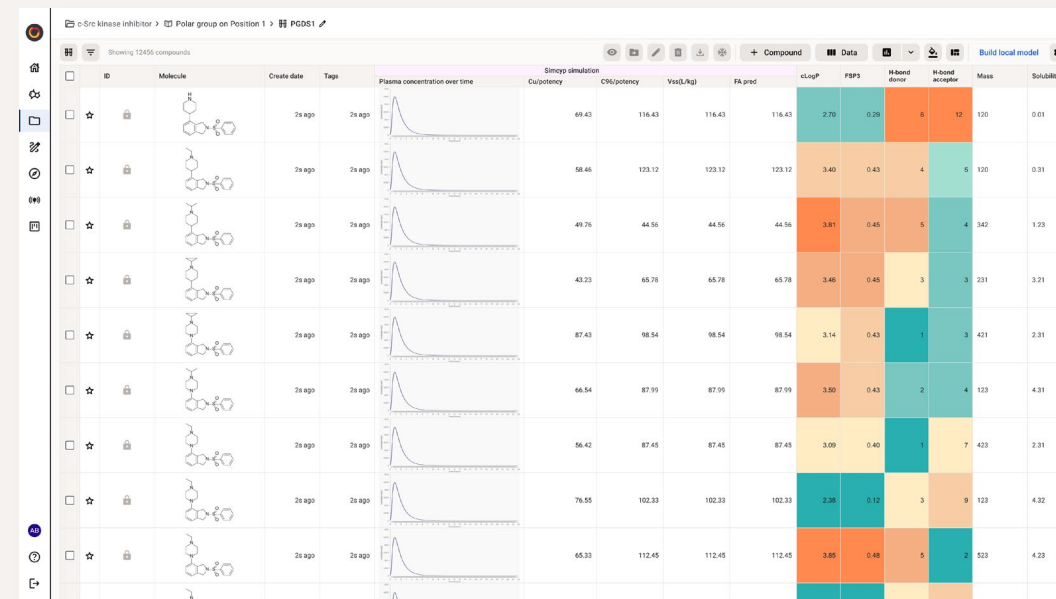
### Comprehensive access to AI services throughout

- Throughout aspects of Analysis, Design and Make

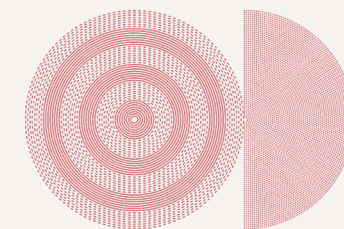
### Simplified deployment and set-up

- Improved connectivity to customer and third-party apps
- Reduce the time to Go-Live

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# Future: Integrated Design and Analysis Application

Certara Development Investment

## Focus will shift to the new software solution

- Ensure existing workflows from each product are preserved
- Combine the best features from each product
  - E.g., Web application, Query interface, Kanban board, Hypothesis capture
- Merge duplicate features between Design Hub and D360
  - E.g., SAR table, MMP Analysis, library enumeration

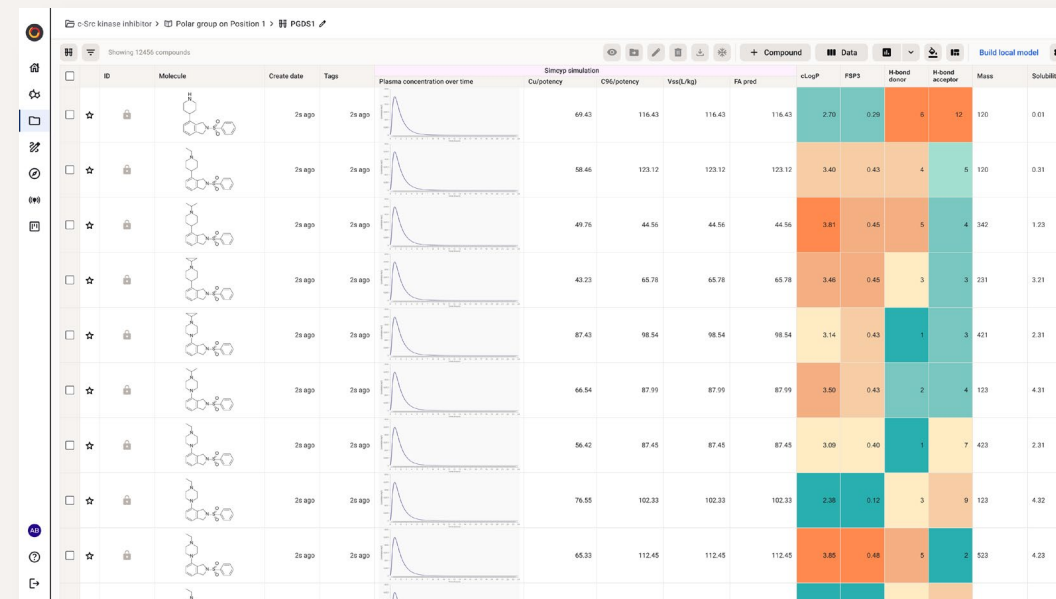
## Target 1<sup>st</sup> commercial release: Q4 2027

- Early access opportunity for interested customers

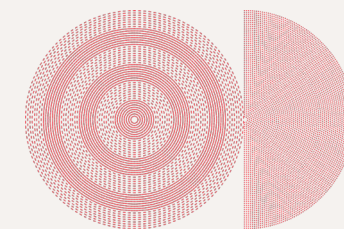
## Customers can continue to use our existing applications

- Continue to support and maintain D360 and Design Hub
  - Until the new solution reaches appropriate functional level
- Will formulate a transition plan
  - To support current customers of each product

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# Portfolio Timeline\*

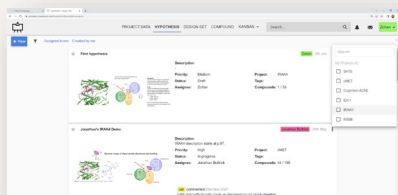
\* Disclaimer: As with all timelines, this is a plan, not a commitment!

2025

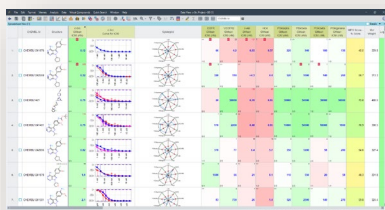
2026

2027

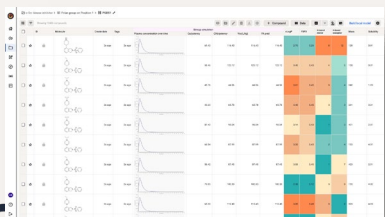
## Design Hub:



## D360



## Certara Discovery



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- Synch data with D360
- Marvin integration
- Image support for spreadsheet view

- Dynamic Data Subset viewers
- Manual sequence editing/undo
- Chart Error Bars
- Active Filter gadgets

- Support customer deployments
- Maintain product

- Peptide Design
- 2° Intelligence Integration
- Ab: Sequence features
- Marvin integration

- Maintenance & support only

- Other modality analytics

- First Alpha

- Beta testing

- First commercial release (V1.0)



# Acknowledgements

With grateful thanks to colleagues that have helped prepare this presentation

## With Special Thanks to

Rob Aspbury



Roland Knispel



Richard Jones



Csaba Peltz

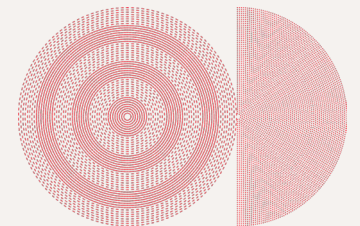


Andras Stracz

Luca Szabo



Anna Tomin



# Thank You!

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