The Importance of Maintaining IP Integrity in Collaborative Design

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Application Scientist

Chemaxon

Who is Chemaxon?

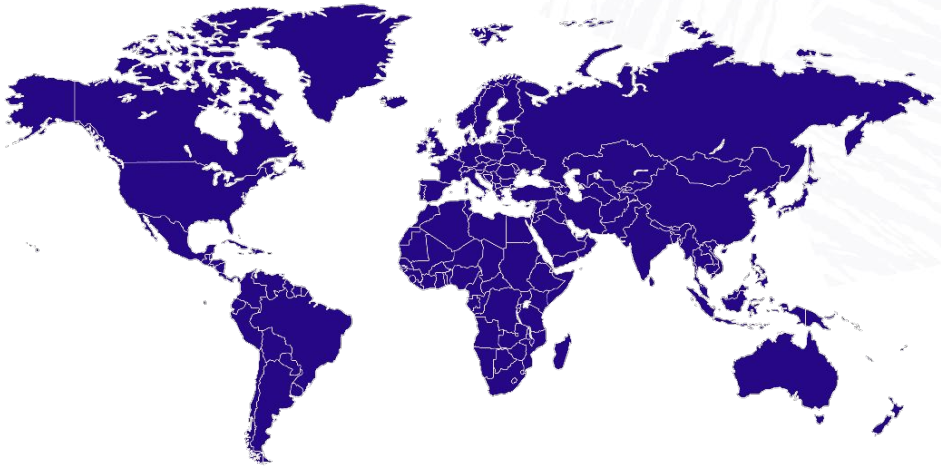
~1 000 000 users

~600 active organizations

~500 000 users in academia/education

>130 countries

~14,000 active licenses



NOVARTIS

Bristol-Myers Squibb

Johnson&Johnson

AMGEN

Lilly

Boehringer Ingelheim

BAYER

SANOFI

Roche

abbvie

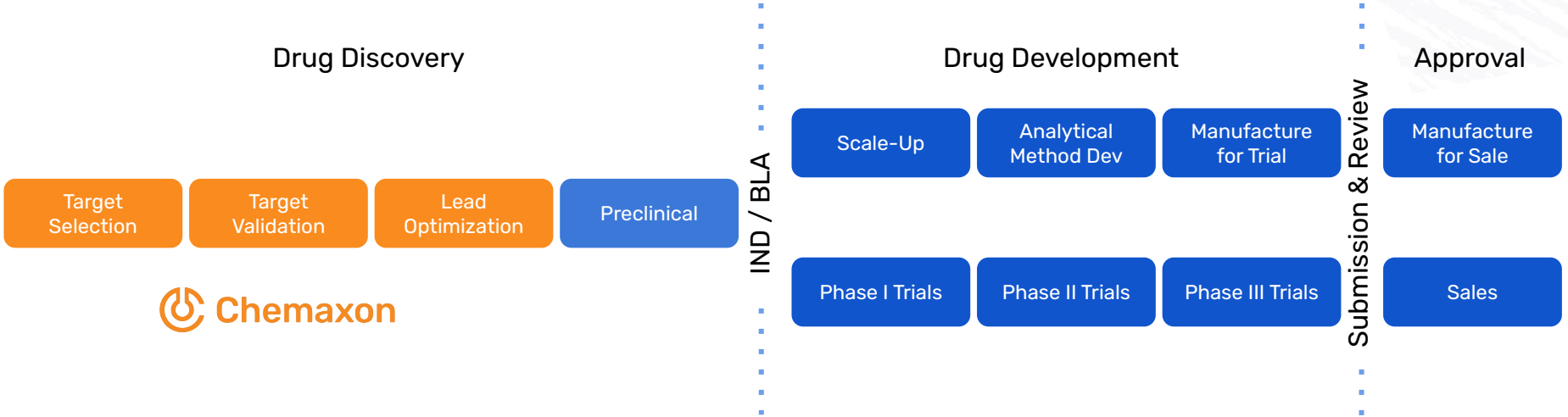
Takeda

MERCK

gsk GlaxoSmithKline

ucb

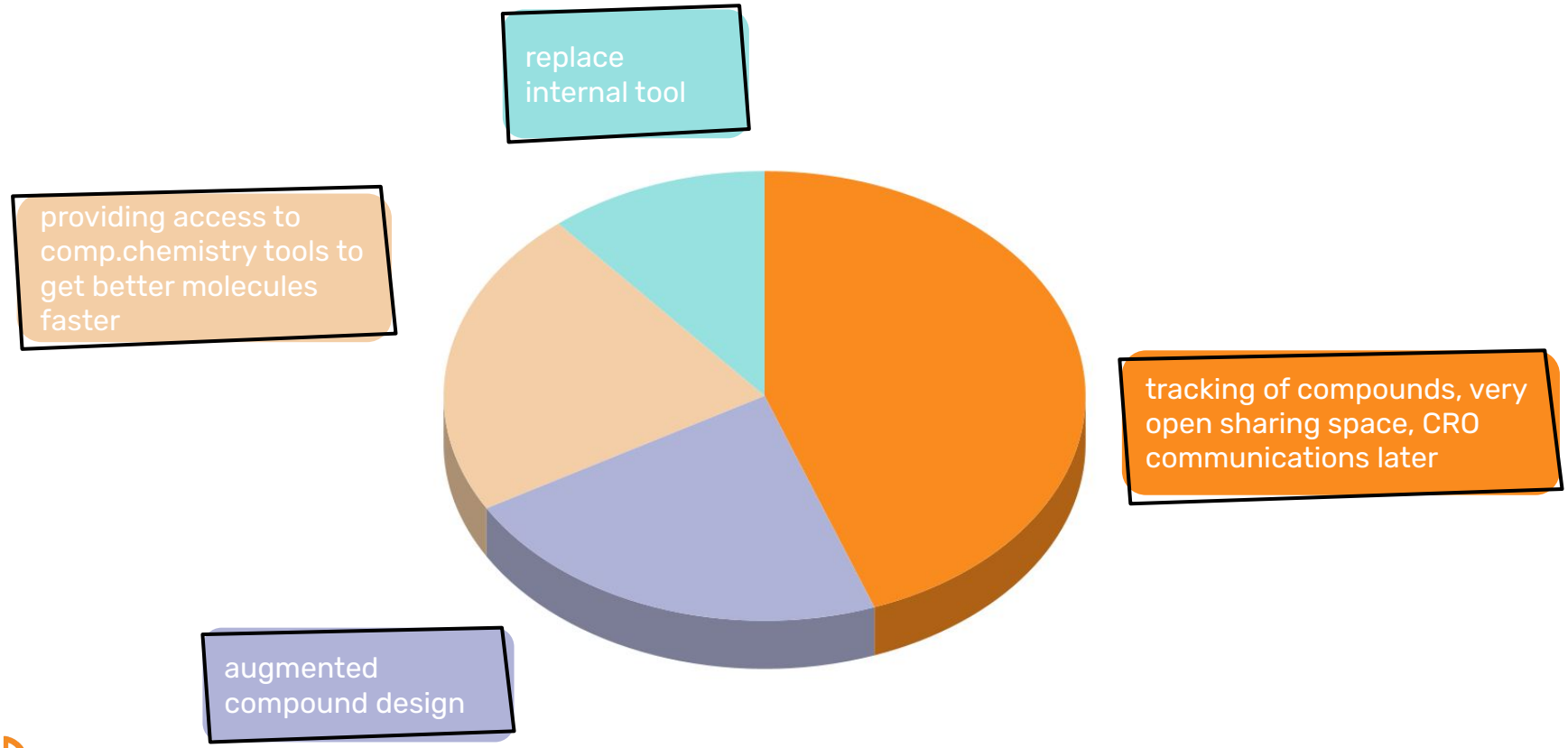
Where does Chemaxon fit in the stages of pharmaceutical drug development?



What drives our strategic direction?

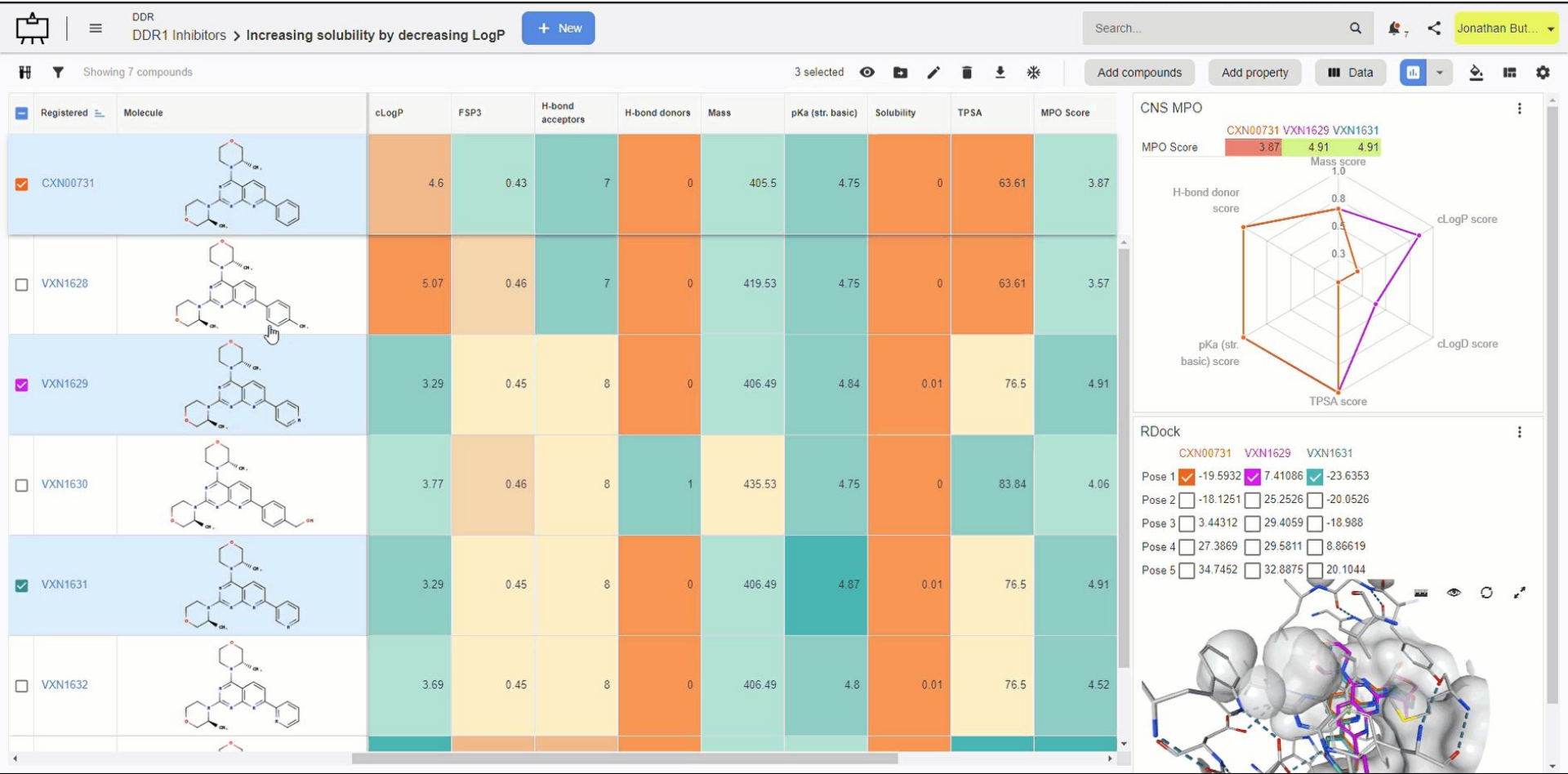
- Customer Feedback
- Market Research
- Chemical Innovation

User motivations case study

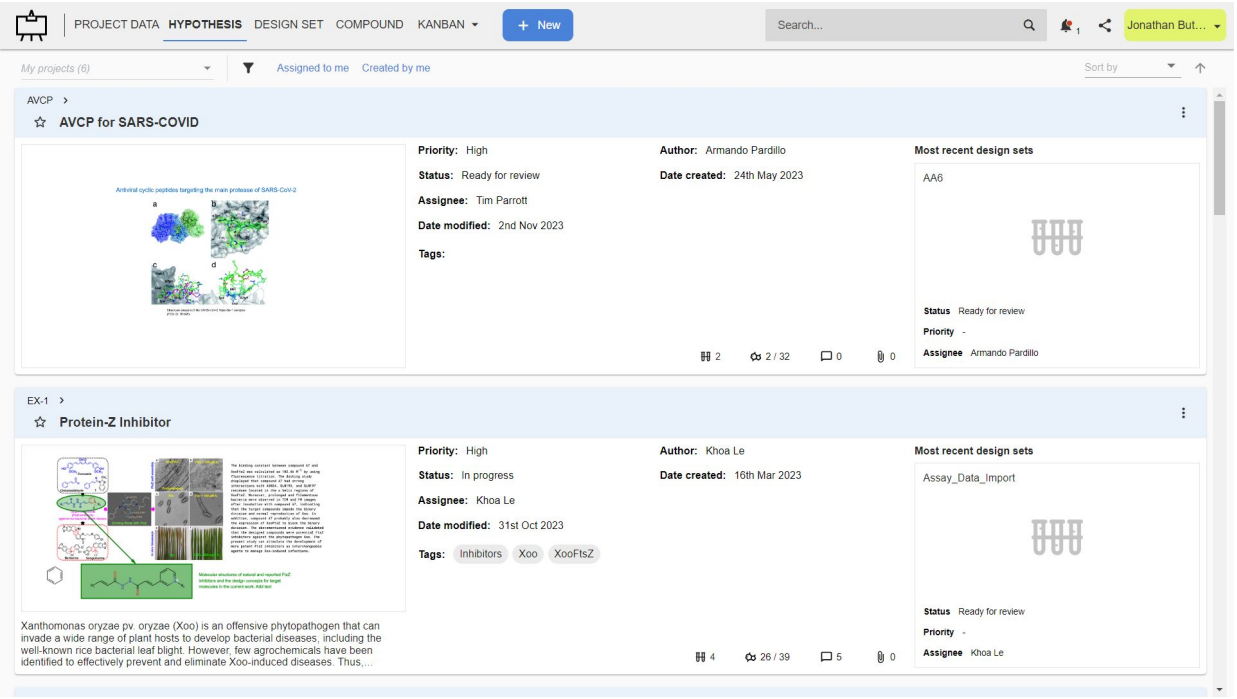


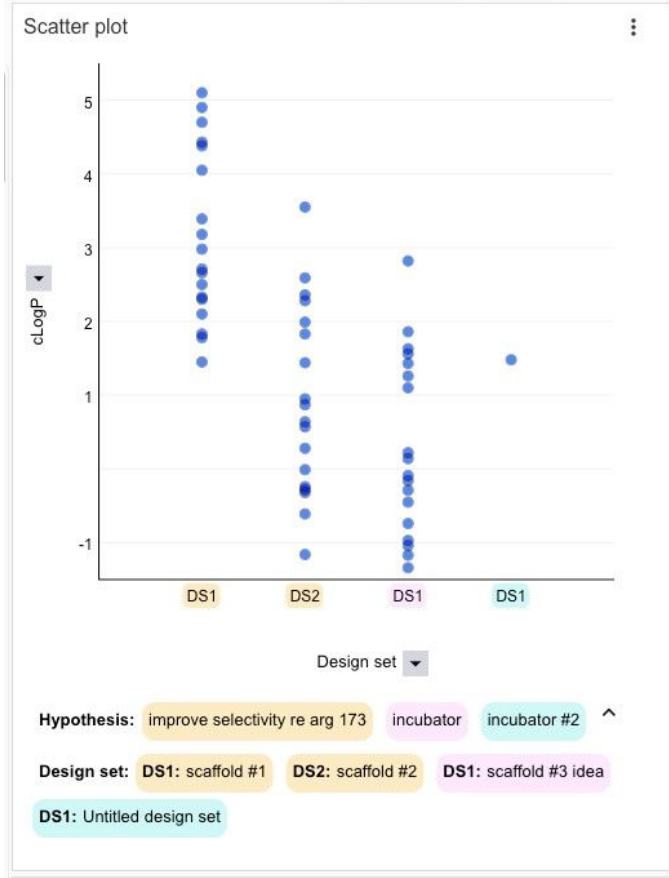
What is Design Hub?

Augmented design and prioritization



Augmented design and prioritization





Democratize access to tools

Calculated Properties

	Current	Pinned
▲ Mass	407.48	405.5
▼ cLogP	2.87	4.6
▲ TPSA (Å²)	89.39	63.61
pKa (str. acidic)		
▼ pKa (str. basic)	4.71	4.75
▲ FSP3	0.48	0.43
▲ Solubility (mM)	0.01	0
▲ H-bond acceptors	9	7
H-bond donors	0	0

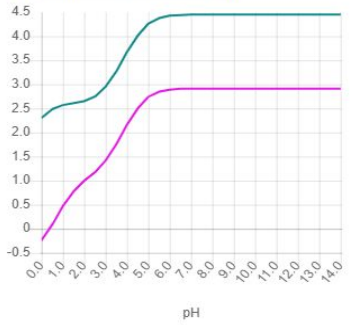
hERG

	Current	Pinned
Class	SAFE	SAFE

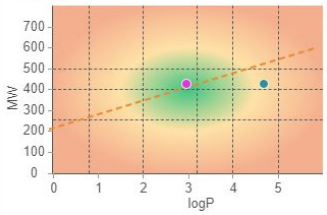
› See applicability domain...

cLogD

	Current	CXN00731
▼ pH1.5	0.79	2.61
▼ pH5	2.74	4.26
▼ pH6.5	2.91	4.44
▼ pH7.4	2.91	4.45

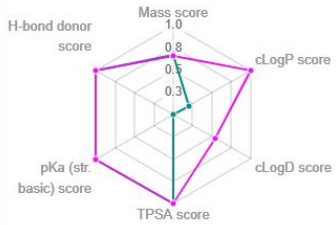


Sweet Spot

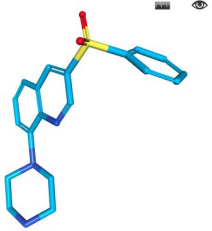


CNS MPO

	Current	CXN00731
MPO Score	5.2	3.87

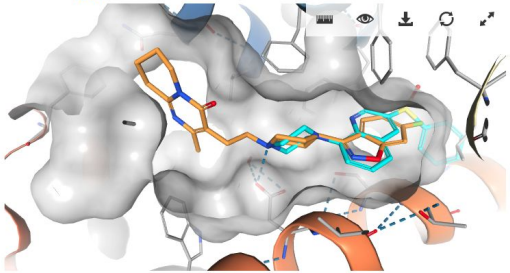


Conformers



Alignment (PDB)

Reference: 6A93 - 8NU.



Structural Alerts

The following structural alerts were found in your idea, please consider possible toxic effects:

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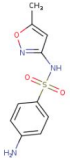
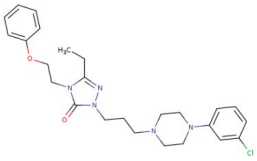
Rule: True anilines (Ph-NH2)
Example: Sulfamethoxazole



Rule: 4-H-Benzene-N-C (not acyl)
Example: Nefazodone



Toxpredict

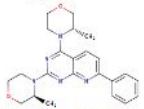
Structural Alert for S. typhimurium mutagenicity	NO
No alerts for S. typhimurium mutagenicity	YES
Potential S. typhimurium TA100 mutagen based on QSAR	NO
Unlikely to be a S. typhimurium TA100 mutagen based on QSAR	NO
For a better assessment a QSAR calculation could be applied.	NO
Error when applying the decision tree	NO

Learn more...

Compound Registration

Matches: 20

Showing page 1 of 5. Prev Next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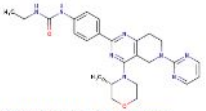
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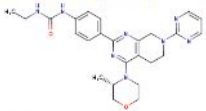
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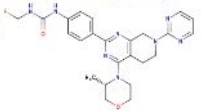
CXN19A (0.545)

Enamine 1212

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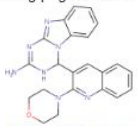
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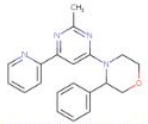
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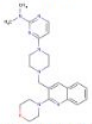
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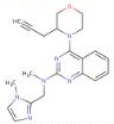
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SureChEMBL

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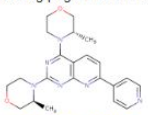
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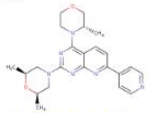
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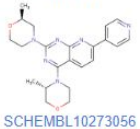
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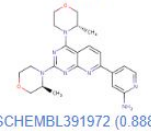
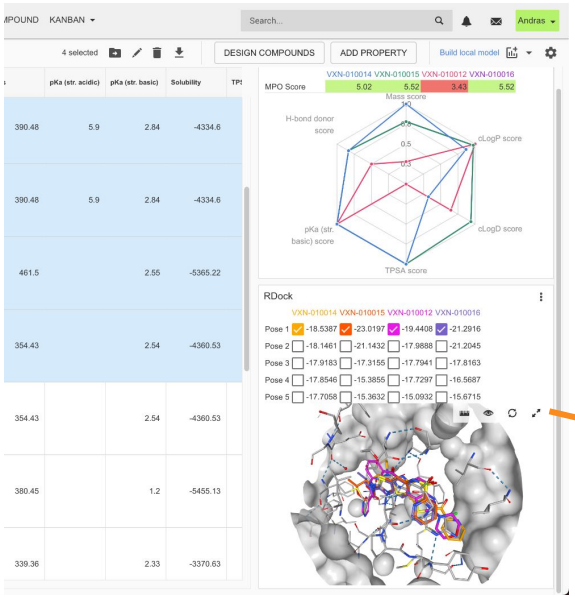

SCHEMBL391972 (0.888)

Patent search

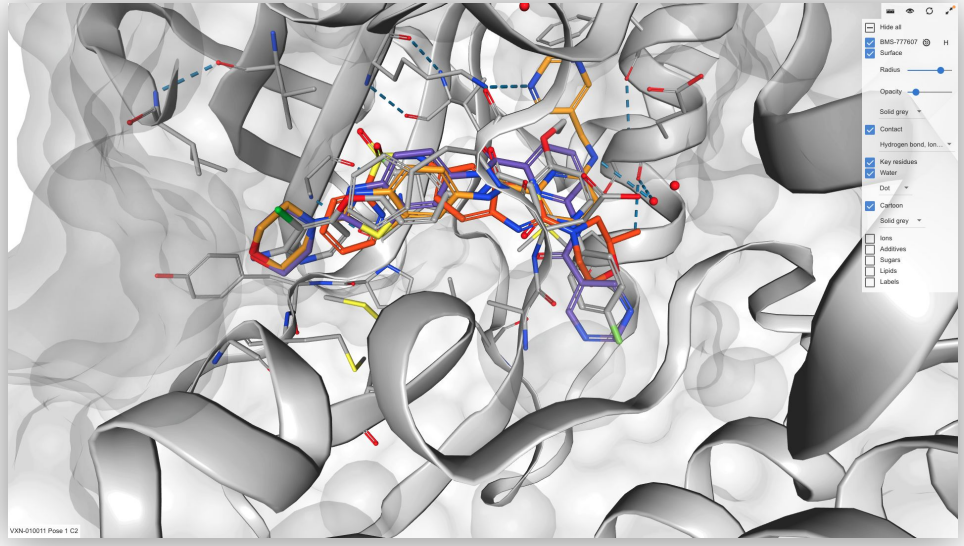
- ✕ US6267958B1
- ✕ US6331415B1
- ✕ US7527791B2
- ✓ US4933294A
- ✕ US7521541B2

Increase utilization of best prioritization tools

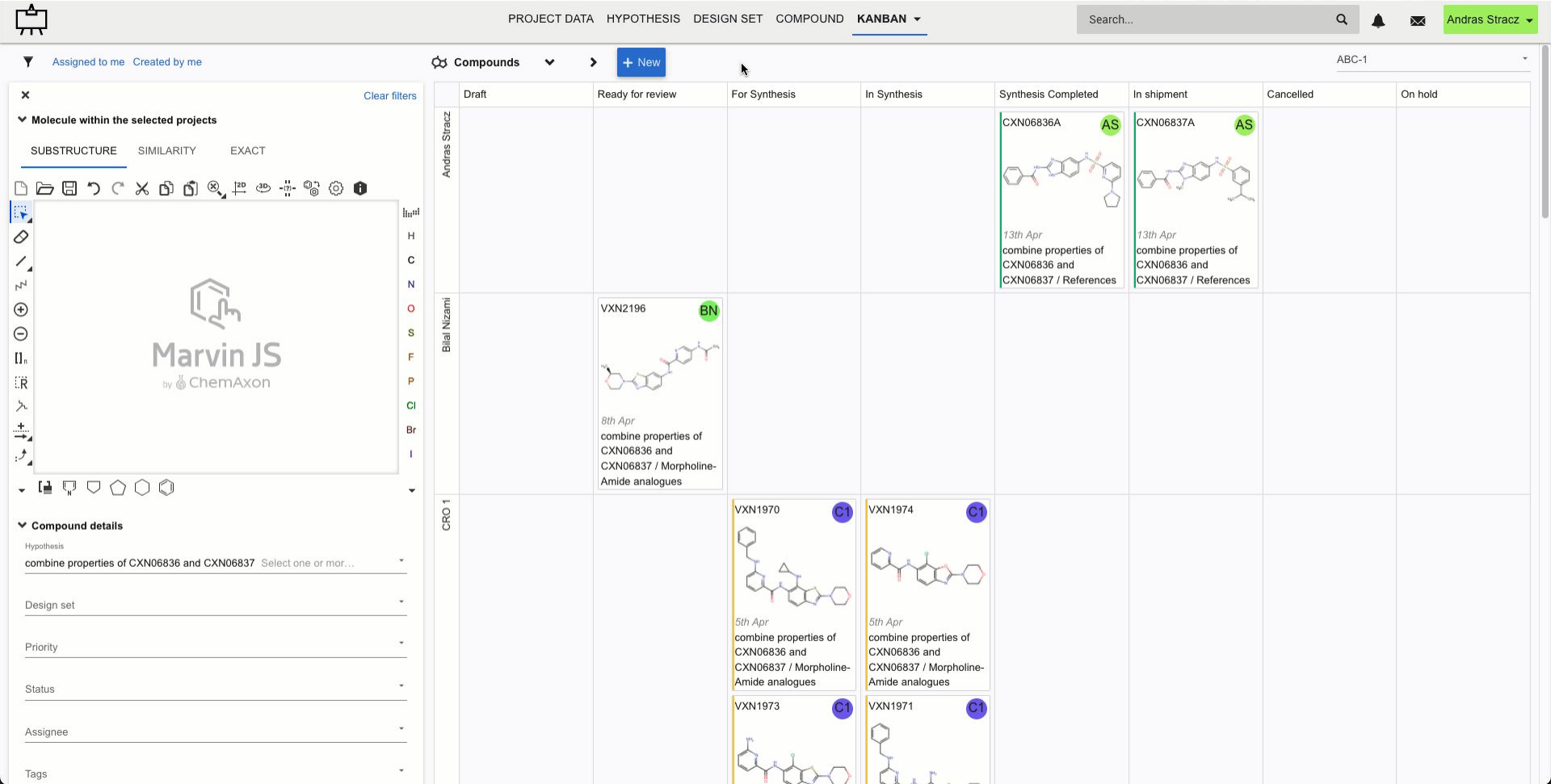


integrations to commercial, in-house, and open source tools, set up project specific models and grids to the entire team

BYOL model for docking engine



Compound tracking

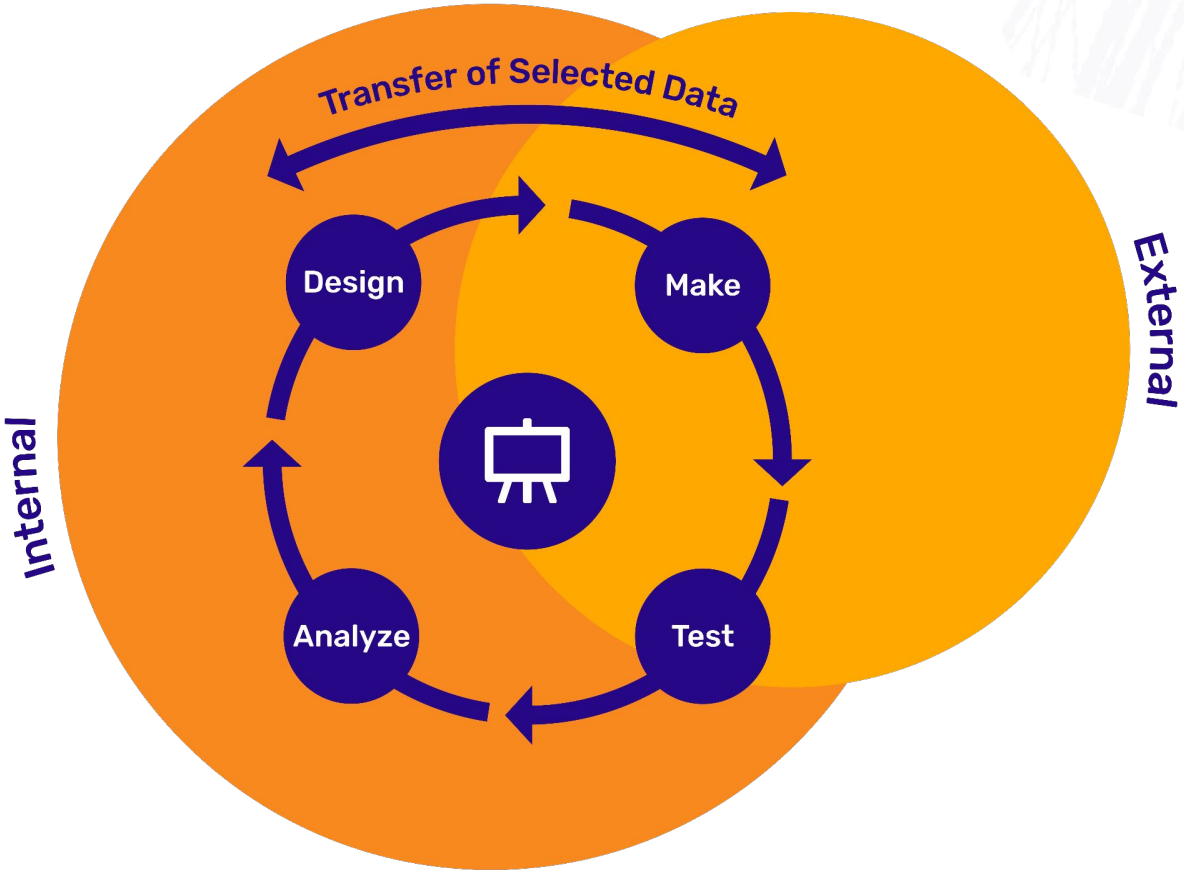


Collaboration in Modern Drug Discovery

20 years ago

Pharma

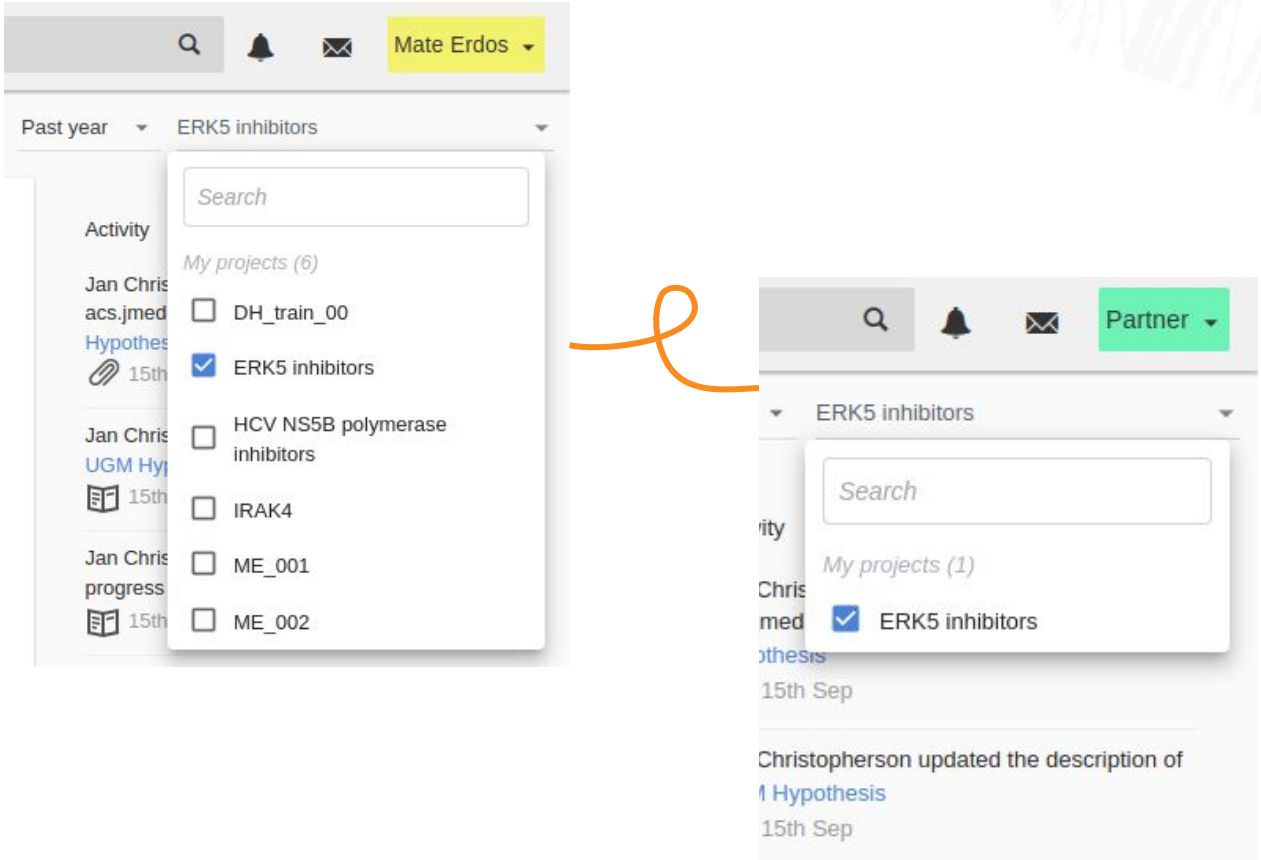
Now

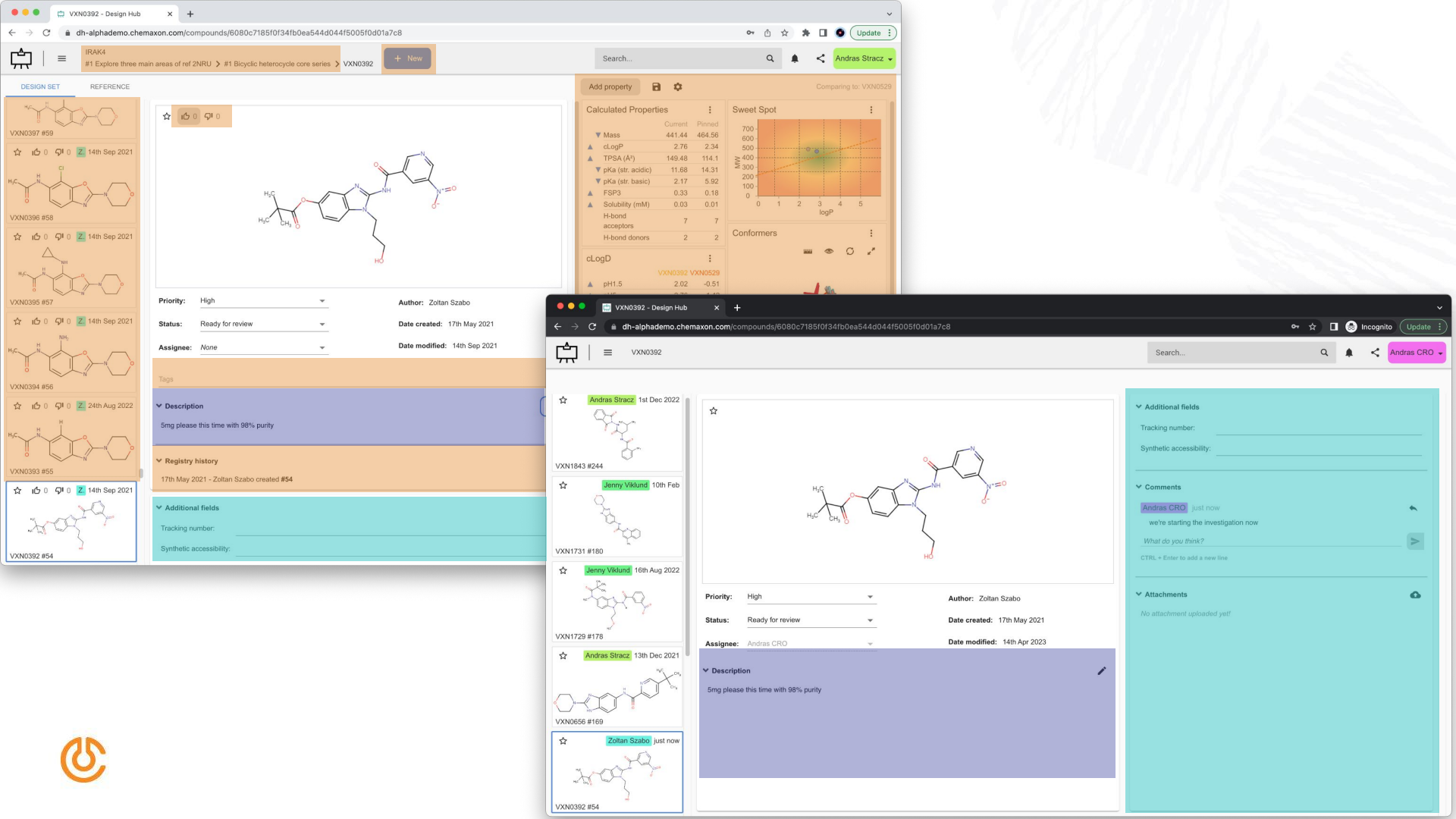

Transfer of Selected Data
Design
Make
Analyze
Test
Internal
External

Role based access control - Default profiles

		Admin	Team admin	User	External	CRO
Manage users		•				
View content	w/ project membership		•	•	•	
	w/o project membership		•	•		
	When assigned		•	•	•	•
	When not assigned		•	•	•	
	Hypotheses / design sets / compounds		H DS C	H DS C	H DS C	C
Create content			•	•	•	
Communication	Internal comments and files		•	•	•	
	Public comments, and files		•	•	•	•
View metadata	Substance IDs		•	•	•	
	Phys-chem properties		•	•	•	
	Custom data fields		•	•	?	?

Selectively shared projects




VXN0392 - Design Hub
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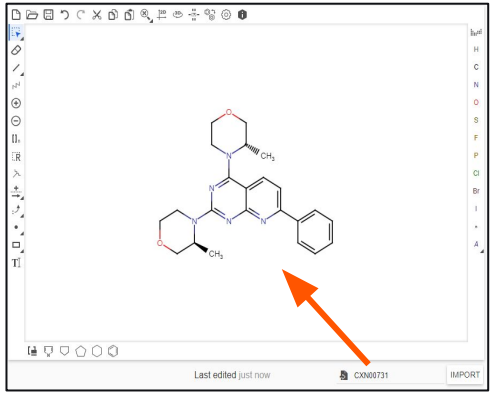
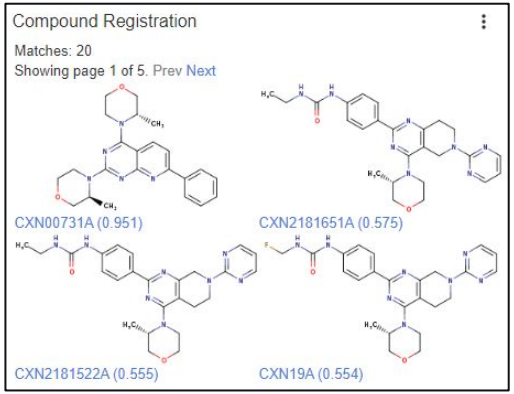
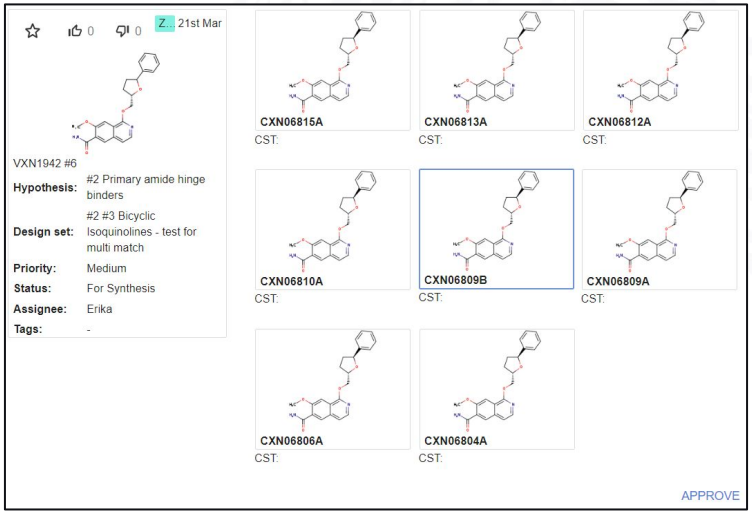
Update
IRAK4
#1 Explore three main areas of ref 2NRU
#1 Bicyclic heterocycle core series
VXN0392
New
Search...
Andras Stracz
DESIGN SET
REFERENCE
Add property
Comparing to: VXN0529
Calculated Properties
Current
Pinned
Mass 441.44 464.56
cLogP 2.76 2.34
TPSA (Å²) 149.48 114.1
pKa (str. acidic) 11.68 14.31
pKa (str. basic) 2.17 5.92
FSP3 0.33 0.18
Solubility (mM) 0.03 0.01
H-bond acceptors 7 7
H-bond donors 2 2
Sweet Spot
MW
logP
Conformers
cLogD
VXN0392 VXN0529
pH1.5 2.02 -0.51
VXN0397 #59
VXN0396 #58
14th Sep 2021
VXN0395 #57
VXN0394 #56
VXN0393 #55
24th Aug 2022
VXN0392 #54
Priority: High
Status: Ready for review
Assignee: None
Author: Zoltan Szabo
Date created: 17th May 2021
Date modified: 14th Sep 2021
Tags
Description
5mg please this time with 98% purity
Registry history
17th May 2021 - Zoltan Szabo created #54
Additional fields
Tracking number:
Synthetic accessibility:
VXN0392 - Design Hub
dh-alphademo.chemaxon.com/compounds/6080c7185f0f34fb0ea544d044f5005f0d01a7c8
Incognito
Update
VXN0392
Search...
Andras CRO
Andras Stracz 1st Dec 2022
VXN1843 #244
Jenny Viklund 10th Feb
VXN1731 #180
Jenny Viklund 16th Aug 2022
VXN1729 #178
Andras Stracz 13th Dec 2021
VXN0656 #169
Zoltan Szabo just now
VXN0392 #54
Priority: High
Status: Ready for review
Assignee: Andras CRO
Author: Zoltan Szabo
Date created: 17th May 2021
Date modified: 14th Apr 2023
Description
5mg please this time with 98% purity
Additional fields
Tracking number:
Synthetic accessibility:
Comments
Andras CRO just now
we're starting the investigation now
What do you think?
CTRL + Enter to add a new line
Attachments
No attachment uploaded yet!

Integration with other vendors







CDD VAULT® Complexity Simplified

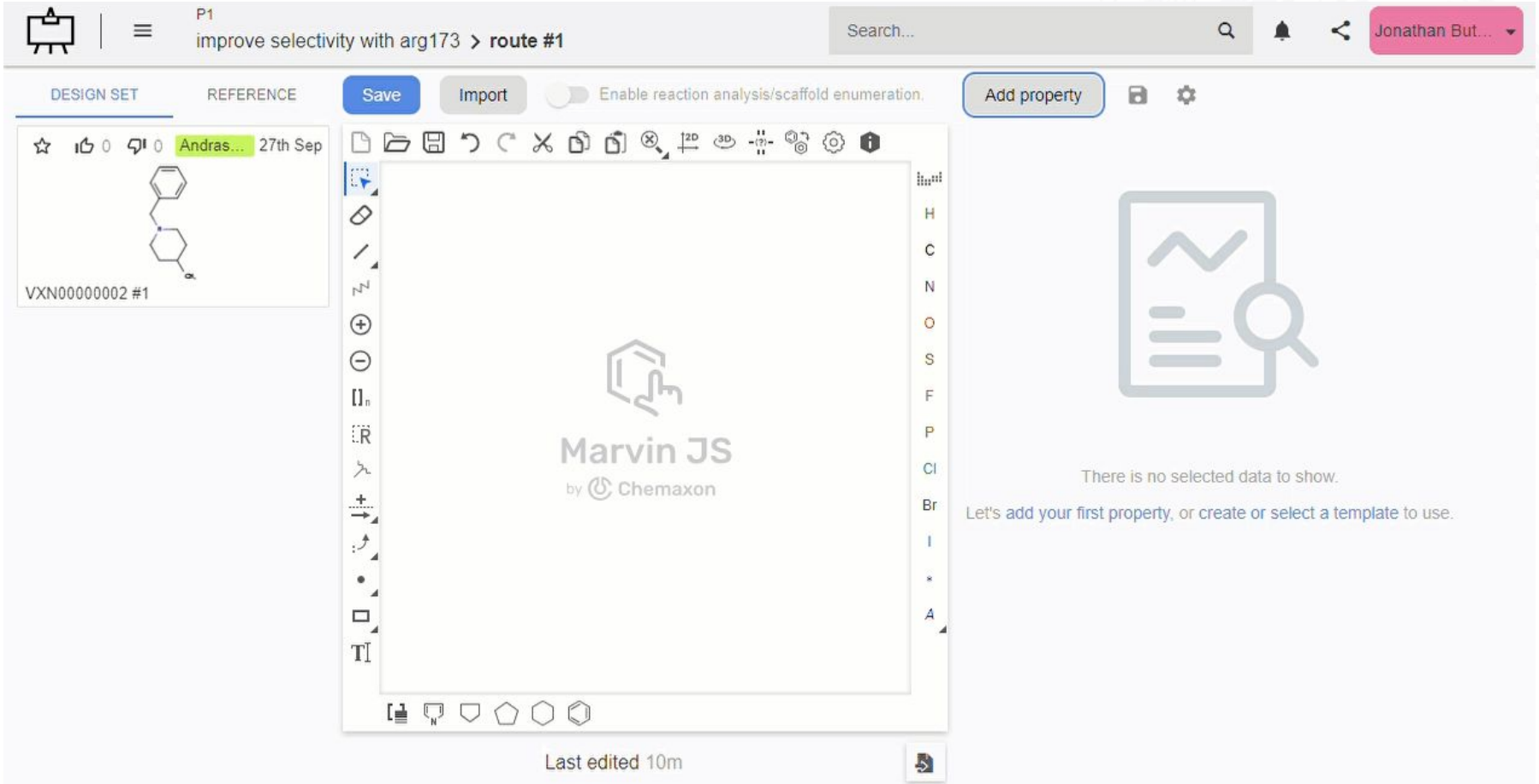
revvity signals

Dotmatics

Security with API usage

- API Keys
  - Not user specific
  - All or nothing data access
- Restrict API access by user role at the application level
  - Complex to set up
  - Hard to maintain
- Bearer Tokens
  - Each application handles its own permissions
  - Can be passed via API

Driving innovation - Searching 6 billion compounds



Thank you

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chemaxon.com/design-hub