

The Importance of Maintaining IP Integrity in Collaborative Design

Jonathan Buttrick, PhD
Application Scientist

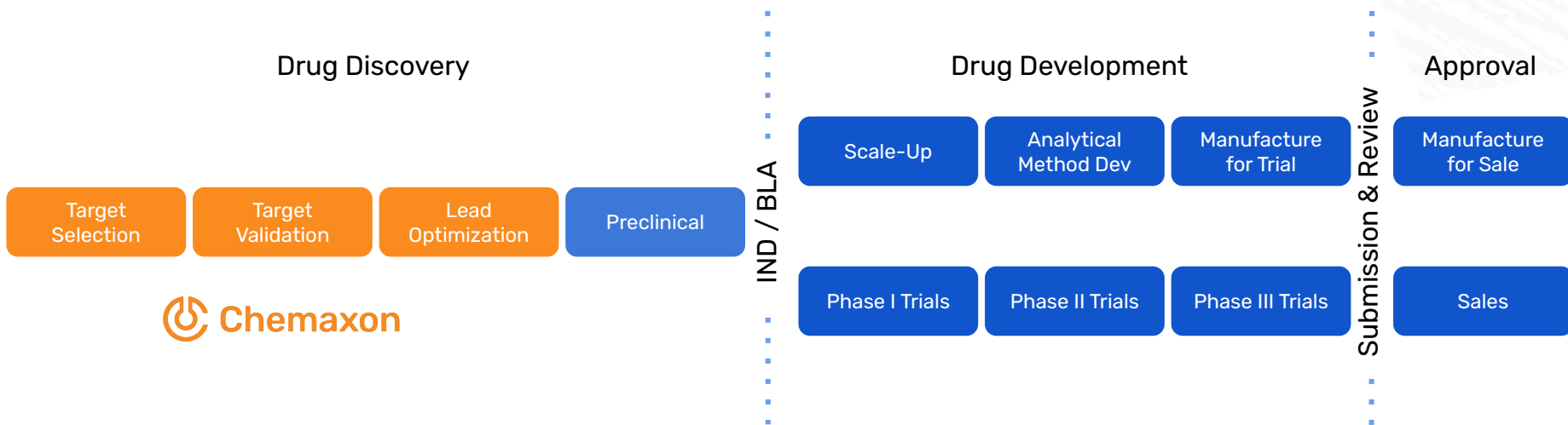


Who is Chemaxon?

- ~1 000 000 users
- ~600 active organizations
- ~500 000 users in academia/education
- >130 countries
- ~14,000 active licenses



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

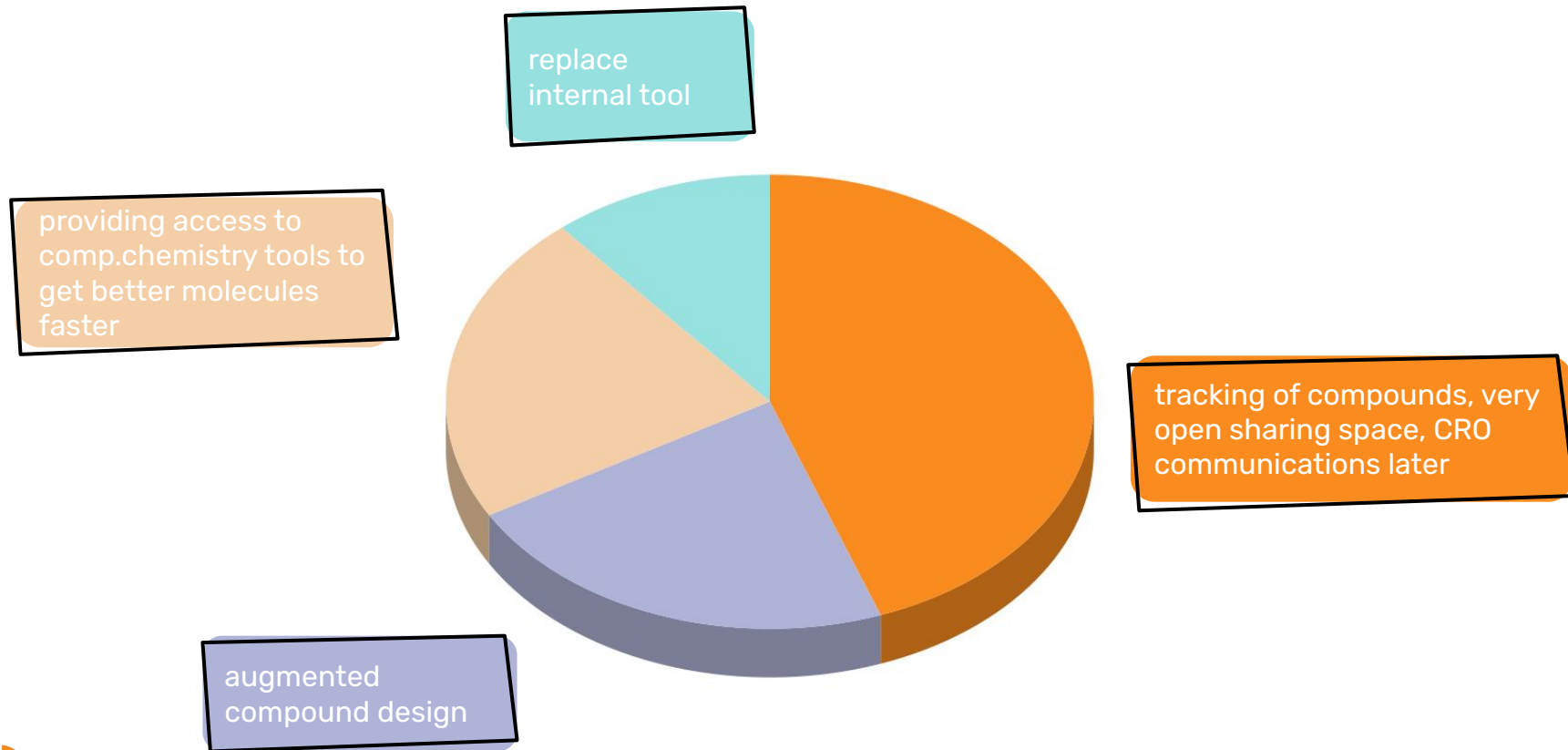


What drives our strategic direction?

- Customer Feedback
- Market Research
- Chemical Innovation



User motivations case study



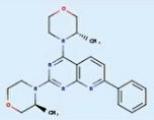
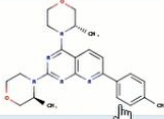
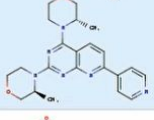
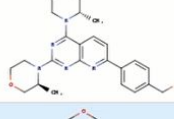
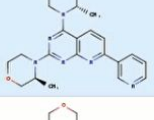
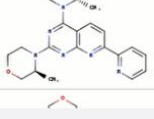
The background is a solid teal color with a subtle pattern of small white speckles. In the top right corner, there is a white line-art graphic consisting of several overlapping, curved shapes. In the bottom left corner, there is a white line-art graphic of a jagged, irregular shape with several small white dashes extending from its left side.

What is Design Hub?

Augmented design and prioritization

DDR
DDR1 Inhibitors > Increasing solubility by decreasing LogP + New

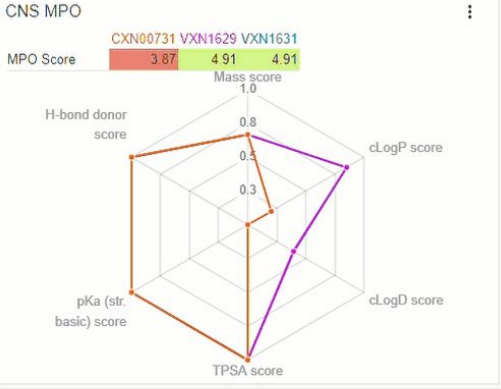
Showing 7 compounds 3 selected Search... Jonathan But...

Registered	Molecule	cLogP	FSP3	H-bond acceptors	H-bond donors	Mass	pKa (str. basic)	Solubility	TPSA	MPO Score
<input checked="" type="checkbox"/>	 CXN00731	4.6	0.43	7	0	405.5	4.75	0	63.61	3.87
<input type="checkbox"/>	 VXN1628	5.07	0.46	7	0	419.53	4.75	0	63.61	3.57
<input checked="" type="checkbox"/>	 VXN1629	3.29	0.45	8	0	406.49	4.84	0.01	76.5	4.91
<input type="checkbox"/>	 VXN1630	3.77	0.46	8	1	435.53	4.75	0	83.84	4.06
<input checked="" type="checkbox"/>	 VXN1631	3.29	0.45	8	0	406.49	4.87	0.01	76.5	4.91
<input type="checkbox"/>	 VXN1632	3.69	0.45	8	0	406.49	4.8	0.01	76.5	4.52

CNS MPO

CXN00731 VXN1629 VXN1631

MPO Score 3.87 4.91 4.91



RDock

CXN00731 VXN1629 VXN1631

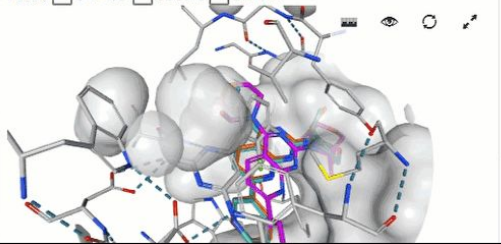
Pose 1 -19.5932 7.41086 -23.6353

Pose 2 -18.1251 25.2526 -20.0526

Pose 3 3.44312 29.4059 -18.988

Pose 4 27.3869 29.5811 8.86619

Pose 5 34.7452 32.8875 20.1044



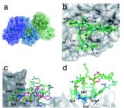
Augmented design and prioritization

PROJECT DATA **HYPOTHESIS** DESIGN SET COMPOUND KANBAN + New Search... Jonathan But...

My projects (6) Assigned to me Created by me Sort by

AVCP > ☆ AVCP for SARS-COVID

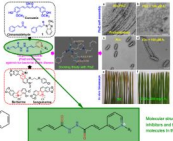
Antiviral cyclic peptides targeting the main protease of SARS-CoV-2



Priority: High Author: Armando Pardillo
 Status: Ready for review Date created: 24th May 2023
 Assignee: Tim Parrott Date modified: 2nd Nov 2023
 Tags:

Most recent design sets
 AA6
 Status: Ready for review
 Priority: -
 Assignee: Armando Pardillo

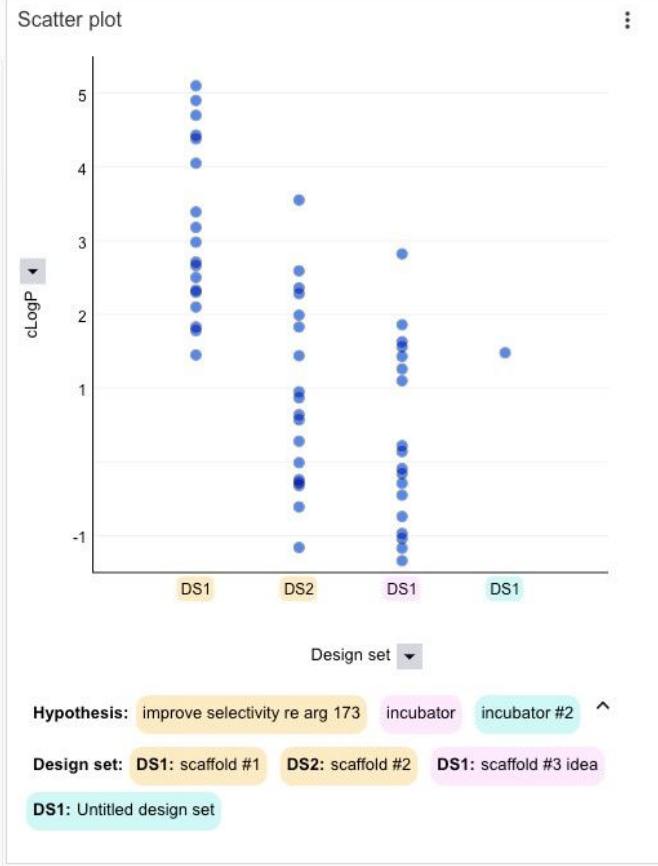
EX-1 > ☆ Protein-Z Inhibitor



Xanthomonas oryzae pv. oryzae (Xoo) is an offensive phytopathogen that can invade a wide range of plant hosts to develop bacterial diseases, including the well-known rice bacterial leaf blight. However, few agrochemicals have been identified to effectively prevent and eliminate Xoo-induced diseases. Thus,...

Priority: High Author: Khoa Le
 Status: In progress Date created: 16th Mar 2023
 Assignee: Khoa Le Date modified: 31st Oct 2023
 Tags: Inhibitors Xoo XooFisZ

Most recent design sets
 Assay_Data_import
 Status: Ready for review
 Priority: -
 Assignee: Khoa Le



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

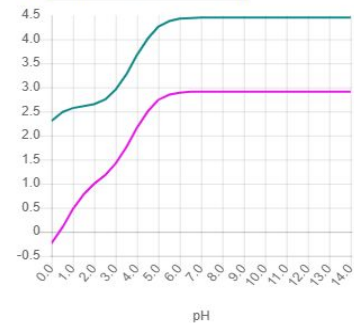
hERG

	Current	Pinned
Class	SAFE	SAFE

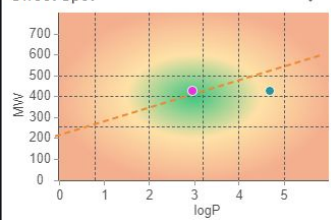
▶ See applicability domain...

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

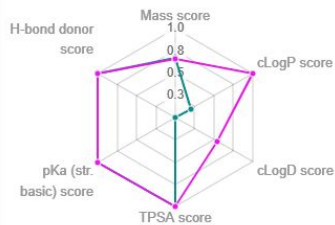


Sweet Spot

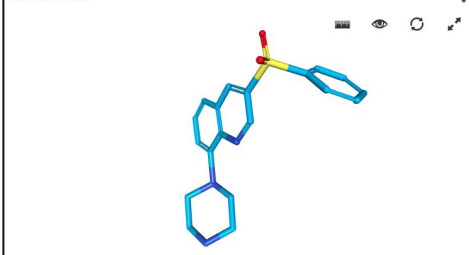


CNS MPO

MPO Score	Current	CXN00731
	5.2	3.87

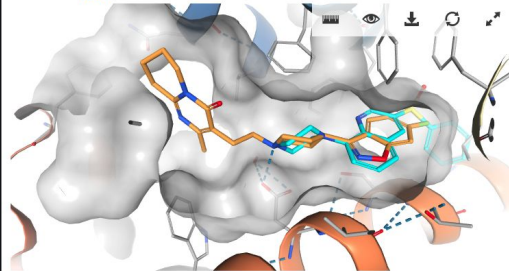


Conformers



Alignment (PDB)

Reference: 6A93 - 8NU.



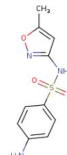
Structural Alerts

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

Showing page 1 of 2. [Prev](#) [Next](#)

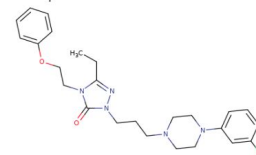
Rule: True anilines (Ph-NH2)

Example: Sulfamethoxazole



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

Example: Nefazodone



Toxpredict

Structural Alert for *S. typhimurium* mutagenicity

No alerts for *S. typhimurium* mutagenicity

Potential *S. typhimurium* TA100 mutagen based on QSAR

Unlikely to be a *S. typhimurium* TA100 mutagen based on QSAR

For a better assessment a QSAR calculation could be applied.

Error when applying the decision tree

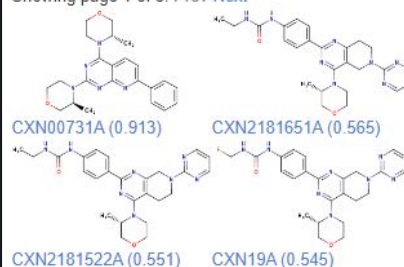
[Learn more...](#)

NO	NO
YES	YES
NO	NO
NO	NO
NO	NO
NO	NO

Compound Registration

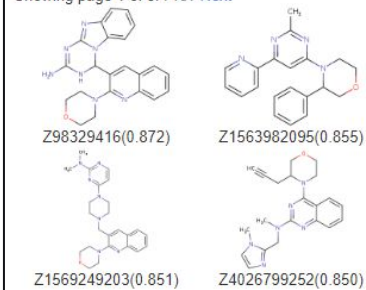
Matches: 20

Showing page 1 of 5. [Prev](#) [Next](#)



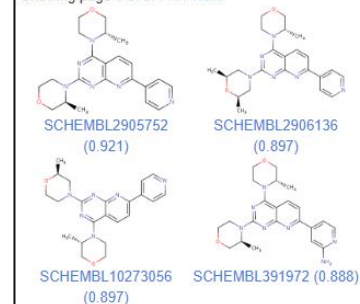
Enamine 1212

Showing page 1 of 5. [Prev](#) [Next](#)



SureChEMBL

Showing page 1 of 5. [Prev](#) [Next](#)



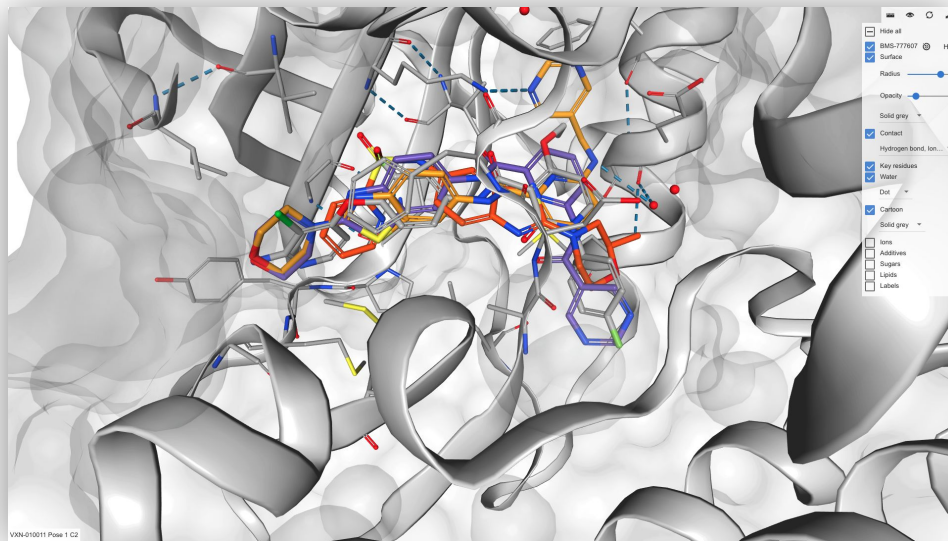
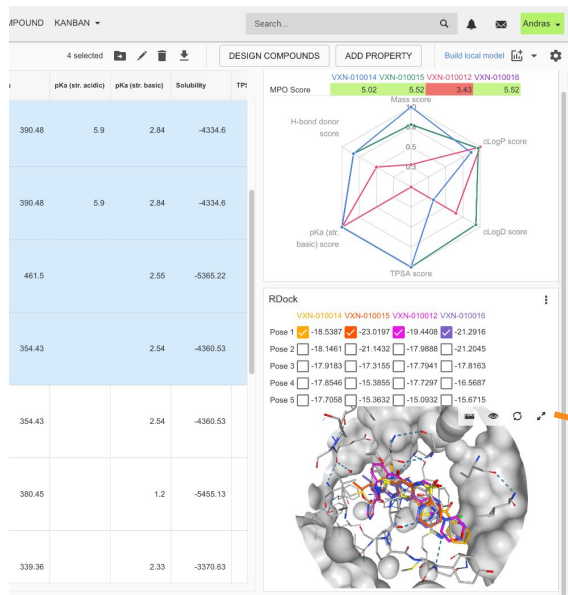
Patent search

- ✗ 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



PROJECT DATA HYPOTHESIS DESIGN SET COMPOUND **KANBAN**

Search...



Andras Stracz

Assigned to me Created by me


Compounds + New

ABC-1

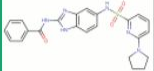
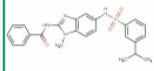
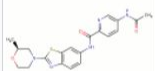

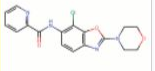
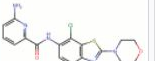
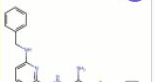
× Clear filters

▼ Molecule within the selected projects

SUBSTRUCTURE SIMILARITY EXACT



▼

	Draft	Ready for review	For Synthesis	In Synthesis	Synthesis Completed	In shipment	Cancelled	On hold
Andras Stracz					<p>CXN06836A AS</p>  <p>13th Apr combine properties of CXN06836 and CXN06837 / References</p>	<p>CXN06837A AS</p>  <p>13th Apr combine properties of CXN06836 and CXN06837 / References</p>		
Bilal Nizami		<p>VXN2196 BN</p>  <p>8th Apr combine properties of CXN06836 and CXN06837 / Morpholine- Amide analogues</p>						
CRO 1			<p>VXN1970 C1</p>  <p>5th Apr combine properties of CXN06836 and CXN06837 / Morpholine- Amide analogues</p>	<p>VXN1974 C1</p>  <p>5th Apr combine properties of CXN06836 and CXN06837 / Morpholine- Amide analogues</p>				
			<p>VXN1973 C1</p> 	<p>VXN1971 C1</p> 				

Compound details

Hypothesis

combine properties of CXN06836 and CXN06837 Select one or mor...

Design set

Priority

Status

Assignee

Tags



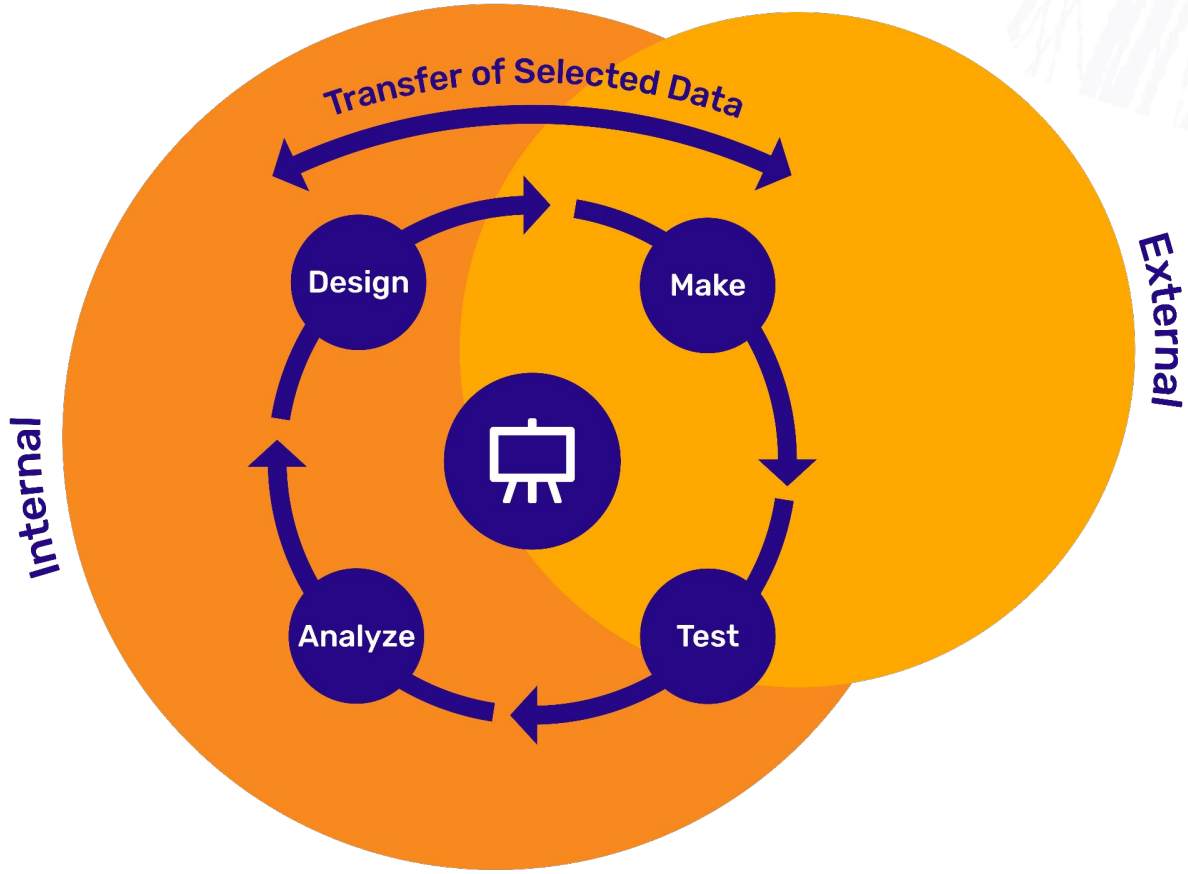
Collaboration in Modern Drug Discovery

20 years ago



Now





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 D S C	H D S C	H D S 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

Search

My projects (6)

- DH_train_00
- ERK5 inhibitors
- HCV NS5B polymerase inhibitors
- IRAK4
- ME_001
- ME_002

Activity

Jan Chris
acs.jmed
Hypothes
15th

Jan Chris
UGM Hy
15th

Jan Chris
progress
15th

Mate Erdos

Search

My projects (1)

- ERK5 inhibitors

Activity

Chris
med
Hypothes
15th Sep

Christopherson updated the description of
Hypothesis
15th Sep

Partner



VXN0392 - Design Hub

dh-alphademo.chemaxon.com/compounds/6080c7185f0f347be0ea544d044f5005f0d01a7c8

IRAK4
#1 Explore three main areas of ref 2NRU > #1 Bicyclic heterocycle core series > VXN0392

Search... Andras Stracz

DESIGN SET REFERENCE

VXN0397 #59
14th Sep 2021

VXN0396 #58
14th Sep 2021

VXN0395 #57
14th Sep 2021

VXN0394 #56
24th Aug 2022

VXN0393 #55
14th Sep 2021

VXN0392 #54

Calculated Properties

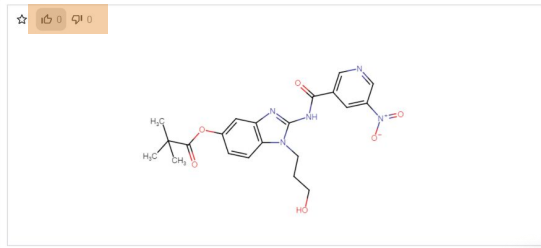
	Current	Pinned
Mass	441.44	464.56
cLogP	2.76	2.34
TPSA (Å²)	149.48	114.1
pKa (str. acidic)	11.68	14.31
pKa (str. basic)	2.17	5.92
FPS	0.33	0.18
Solubility (mM)	0.03	0.01
H-bond acceptors	7	7
H-bond donors	2	2

Sweet Spot

Conformers

cLogD

	VXN0392	VXN0529
pH1.5	2.02	-0.51



Priority: High
Author: Zoltan Szabo

Status: Ready for review
Date created: 17th May 2021

Assignee: None
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:

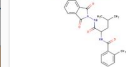
Synthetic accessibility:

VXN0392 - Design Hub

dh-alphademo.chemaxon.com/compounds/6080c7185f0f347be0ea544d044f5005f0d01a7c8

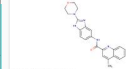
Search... Andras CRO

Andras Stracz 1st Dec 2022



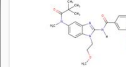
VXN1843 #244

Jenny Viklund 10th Feb



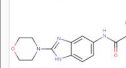
VXN1731 #180

Jenny Viklund 16th Aug 2022



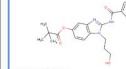
VXN1729 #176

Andras Stracz 13th Dec 2021



VXN0656 #169

Zoltan Szabo just now



VXN0392 #54

Chemical structure of VXN0392 #54.

Priority: High
Author: Zoltan Szabo

Status: Ready for review
Date created: 17th May 2021

Assignee: Andras CRO
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?

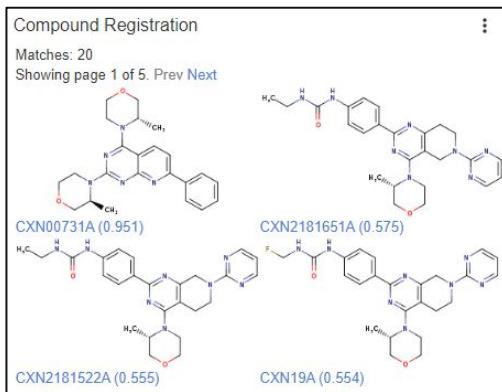
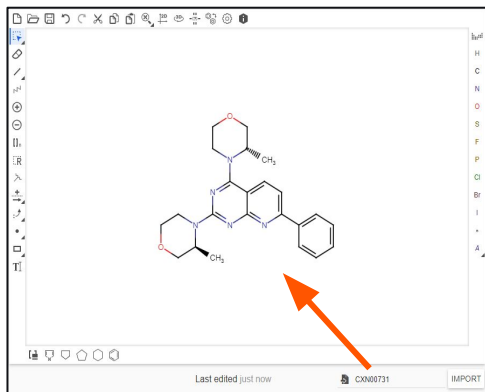
CTRL + Enter to add a new line

Attachments

No attachment uploaded yet



Integration with other vendors



A screenshot of a compound registration interface showing a grid of matches. The matches are:

- CXN06815A
- CXN06813A
- CXN06812A
- CXN06810A
- CXN06809B
- CXN06809A
- CXN06806A
- CXN06804A

Additional information:

- VXN1942 #6
- Hypothesis: #2 Primary amide hinge binders
- Design set: #2 #3 Bicyclic Isoquinolines - test for multi match
- Priority: Medium
- Status: For Synthesis
- Assignee: Erika
- Tags: -

APPROVE



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

P1
improve selectivity with arg173 > route #1

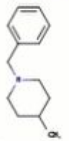
Search...

Jonathan But...

DESIGN SET REFERENCE Save Import Enable reaction analysis/scaffold enumeration. Add property

☆ 0 0 0 Andras... 27th Sep

VXN00000002 #1



Marvin JS
by Chemaxon

H
C
N
O
S
F
P
Cl
Br
I
*
A

There is no selected data to show.
Let's add your first property, or create or select a template to use.

Last edited 10m

Thank you

Jonathan Buttrick, PhD

jbuttrick@chemaxon.com

chemaxon.com/design-hub

