

~~Marvin Cast.~~  
~~Marvin for Meetings.~~  
~~Marvin Sessions.~~  
  
Marvin Live.






Browser

← → 🔍 http://


Title





H  
B  
C  
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A  
R  
u  
X

Leave meeting   Add property   Snapshot   Save report

Calculated property >  
Ligand binding  
Pubchem

Anne 9:31  


Bob 9:42  


Anne 9:45  


I increasingly feel  
 Comment Alice

Would you like to reshape your business future? If yes, you must need Enterprise Resource Planning. Well planned ERP solutions drive growth and add value to your organization.

Jirajs 9:32  
 Repurpose real-time platforms networkeffects implement markets, cultivate monetize value social real-time customized 24/765 res-capable benchmark robust.

Doug 9:31  
 Eyeballs Cluetron generate, communities, reinvent seize. Syndicate, engage extensible, reintermediate synergies engage, user-centric webservices.

Bob 9:29  
 Everyone joined, let's get this party started!

Alice 9:25  
 Good morning!

- Save report
- Take snapshot
- Review snapshot
- Leave meeting

Browser

Mobile app

Product

Would you like to reshape your business future? If yes, you must need Enterprise Resource Planning. Well planned ERP solutions drive growth and add value to your organization.

Jirajs 9:32  
 Repurpose real-time platforms networkeffects implement markets, cultivate monetize value social real-time customized 24/765 res-capable benchmark robust.

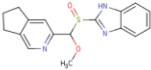
Doug 9:31  
 Eyeballs Cluetron generate, communities, reinvent seize. Syndicate, engage extensible, reintermediate synergies engage, user-centric webservices.

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 Good morning!

Add a comment

TV / Receiver app





By Charlie at 9:48


9:46 - 25 minutes

Product

5 joined


Anne 9:31  


Bob 9:42  


Anne 9:45  


Doug 9:32  
 Repurpose real-time platforms networkeffects implement markets, cultivate monetize value social real-time customized 24/765 res-capable benchmark robust.

Doug 9:31  
 Eyeballs Cluetron generate, communities, reinvent seize. Syndicate, engage extensible, reintermediate synergies engage, user-centric webservices.

logD  


Google

4:28

# Marvin for meetings



Hello! What's your name?

Andris

New meeting or joining one?

3pm review

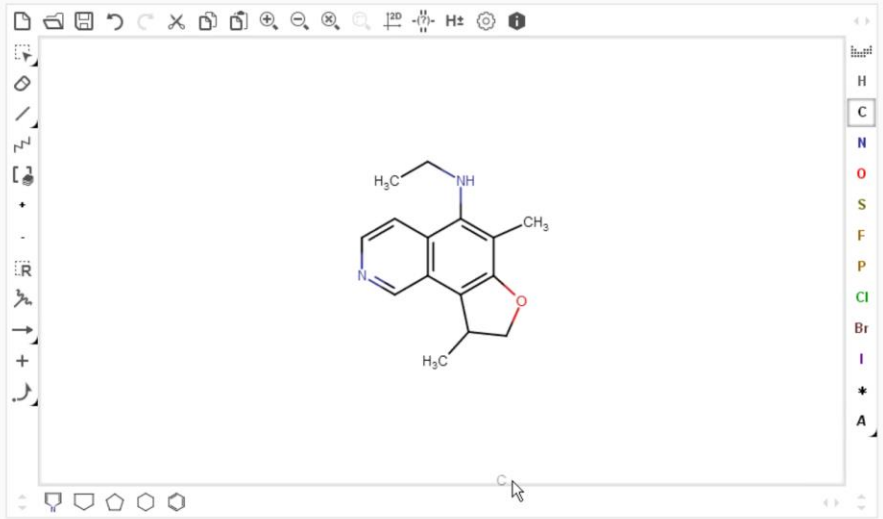
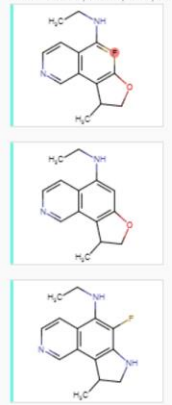
asd (0)

# 11am review 6m

With: Jesse, Keith, Mic, Richard

Load Snapshot

Add property Save report



By Andris just now

### Calculated Properties

Mass: 242.32  
 cLogP: 2.34  
 pKa: -  
 pKb: 6.59  
 FSP3: 0.40  
 Solubility: -3.31 logS

### DrugBank analogs

SUBSTRUCTURE matches in Drugbank: 0

### Novelty check

Drugbank: 0  
 ChEMBL: -  
 PubChem: -

### Pubchem compounds

Substructure matches: 0

### ChEMBL data

matches: 0

Richard 5m  
I n eed to stop deleting

Richard 4m  
the eraser is dangerous

Jesse 4m  
Dan didn't like may Flourine...

Richard 4m  
he prefers pentane

Send a message ...

Send ■ Andris

Import Overview

Snapshot

Thumbnail gallery showing chemical structures #9 to #13.

Chemical structure editor with tools and a central canvas showing a chemical structure.

Last edited by Ivan 1m

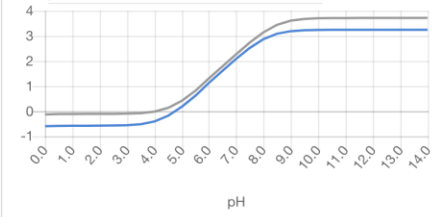
Add property

### Calculated Properties

	Current	Pinned
Mass	371.5	385.53
cLogP	3.24	3.71
TPSA (Å²)	45.06	45.06
pKa (str. acidic)		
pKa (str. basic)	8.14	8.44
FSP3	0.4	0.43
Solubility (mM)	0.22	0.09
H-bond acceptors	4	4
H-bond donors	0	0

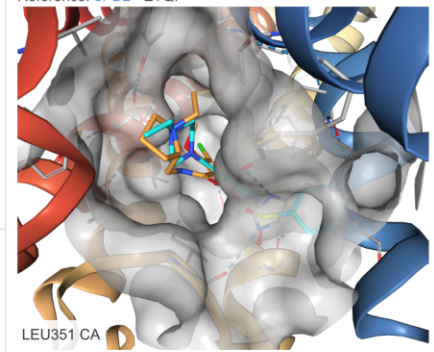
### cLogD

	Current	Pinned
pH1.5	-0.5775	-0.1093
pH5	0.1854	0.4229
pH6.5	1.5965	1.7728
pH7.4	2.4314	2.6349



### Alignment (PDB)

Reference: 3PBL - ETQ.



### ChEMBL Activity

Matches: 77

Showing page 1 of 10. Prev Next

Activity list showing CHEMBL 1699209 (Sim: 0.90) and CHEMBL 1446832 (Sim: 0.89) with their respective chemical structures.

Comments