

# Introducing Marvin Live

András Strácz, Iván Solt

ChemAxon

# Common Problems

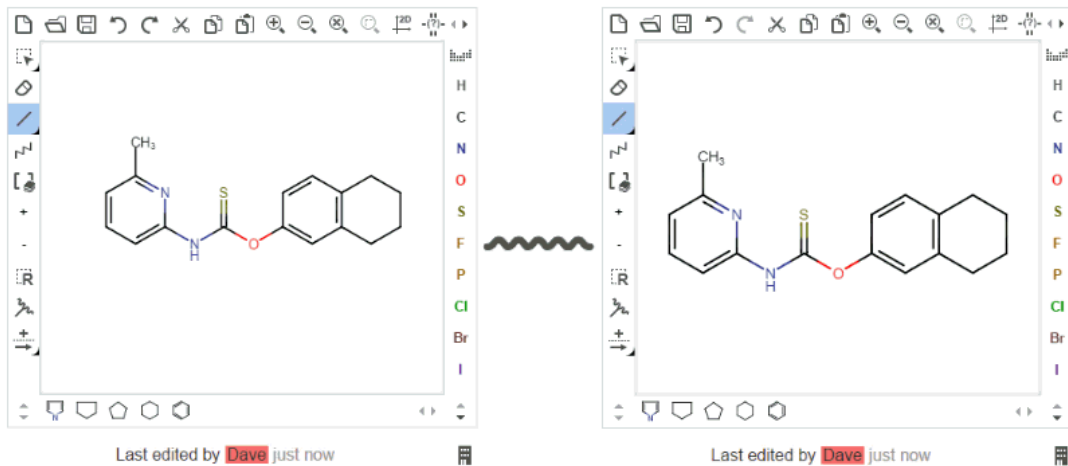
- hard to work collaboratively on chemical structures
- meetings are difficult to organize and prepare for
- relevant data isn't available on-the-fly
- capturing ideas is cumbersome



# Marvin Live

A virtual research meeting room

# Shared chemistry editor



**design** and **review** structures with your **team** members; **fast**, **self-updating**, powered by **Marvin JS**

# Meeting assistant

## real time feedback

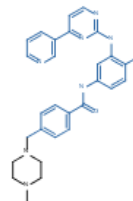
- connect to external services
- display information
- predictions, searches, references

### Calculated Properties

Mass: 395.46  
cLogP: 5.10  
pKa: 13.18  
pKb: 4.27  
FSP3: 0.08  
Solubility: -6.43 logS

### DrugBank analogs

SUBSTRUCTURE matches in Drugbank: 1



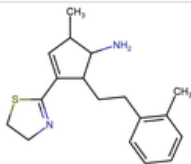
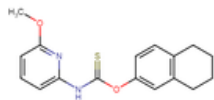
ID: [DB00619](#)

### ChEMBL data

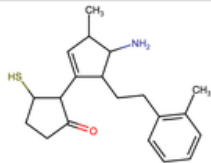
Duplicate matches in ChEMBL: 1

- ID: [CHEMBL20867](#)

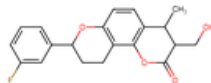
# Meeting assistant



review tox + literature



review tox



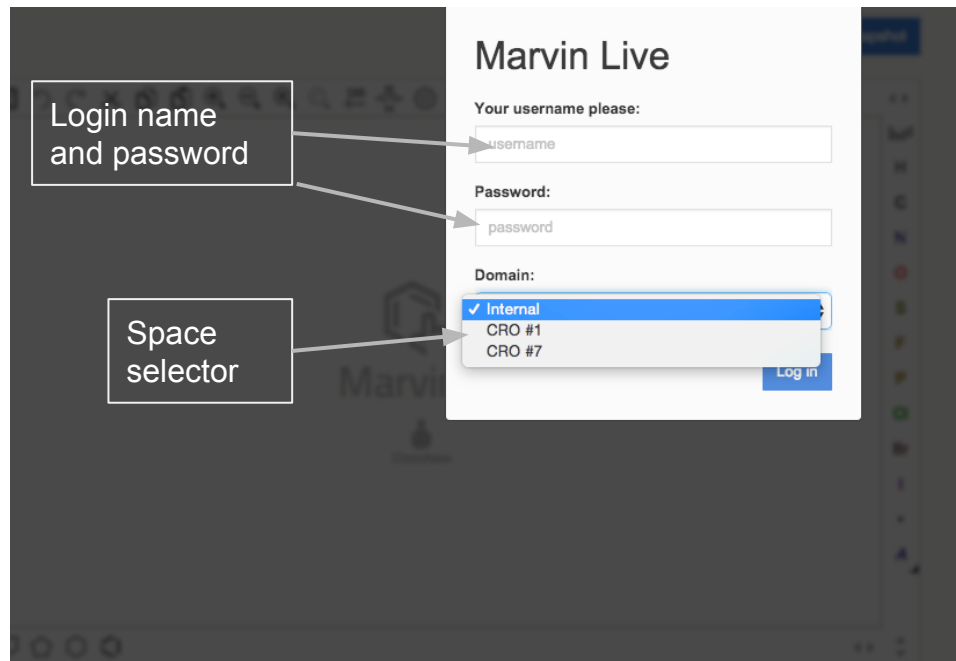
## meeting reports

- saving **important structures**
- for presentations (MS Office)
- for databases/ELN (SDF)
- customizable

# Meeting assistant

## meeting room **service**

- rooms, no scheduling
- separate spaces
  - authorization, history
  - e.g: internal vs external
- authentication (LDAP, AD, SAML)



# Technology

- NodeJS server
- IE9 or newer supported
- customization with JavaScript plugins
- low bandwidth requirement
- default chemical file formats (MRV, SDF) can be extended with JChem Web Services



**DEMO**

# Marvin Live: new possibilities

- work with off-site people on molecules
- 1-click meeting reports
- meeting service
  - track entire project
  - personal idea repository
  - ad-hoc meetings

[chemaxon.com/contact-us/](https://chemaxon.com/contact-us/)