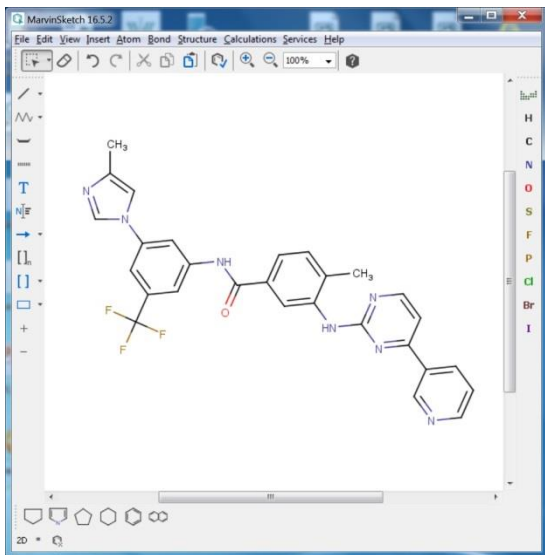


CALCULATOR PLUGINS

Dániel Szisz
Budapest Annual Meeting
2016

What questions can You answer with them ?



- Elemental Analysis
- pK_a, microspheres
- logP, logD, HLB
- Solubility (logS)
- CNMR & HNMR spectra
- Isomers, tautomers
- HBDA
- *and many more ...*

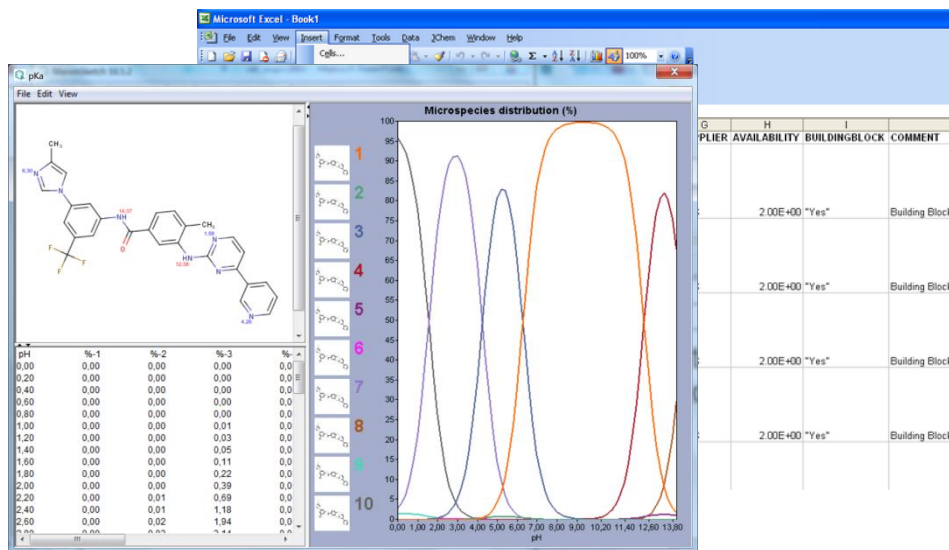
Will my drug be ionized at blood pH?

Will my drug have optimal lipophilicity?

Will my drug be soluble in water?

High-quality physico-chemical predictions for pre-clinical drug design

How can You use them ?



„1-click” plugins in MarvinSketch

Storing & calculating properties in Excel

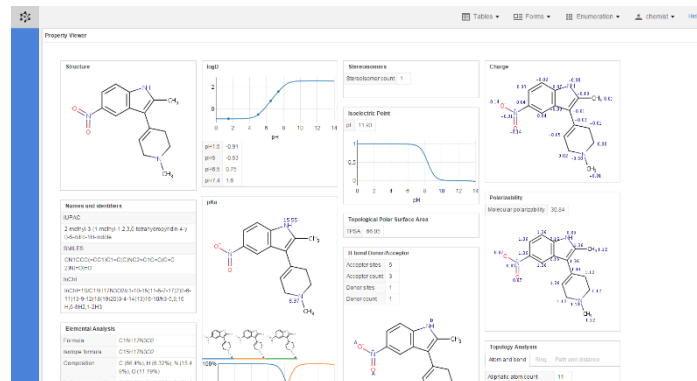
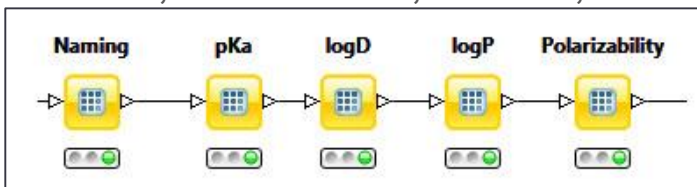
How can You use them?

```
cxcalc pka sildenafil
```

```
id apKa1 apKa2 bpKa1 bpKa2
```

```
atoms
```

```
1 7,63 5,98 -1,08 12,30,5
```



Fully customizable command line interface

Property calculation in Plexus Design and Instant JChem

Calculator nodes in KNIME and Pipeline Pilot

Reference for the Calculators

An analysis of the attrition of drug candidates from four major pharmaceutical companies (2015)

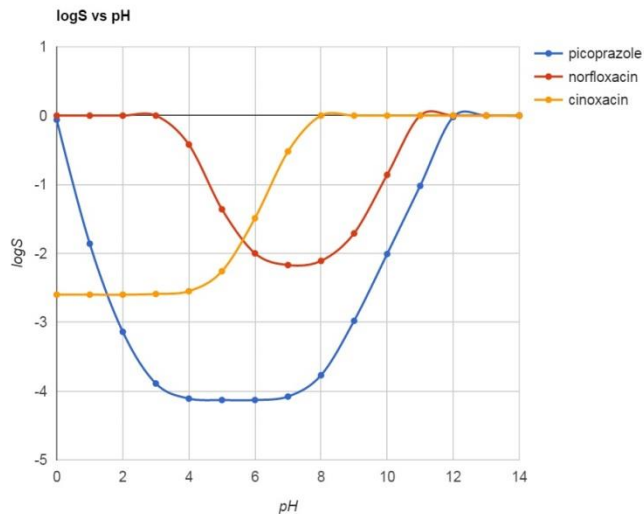
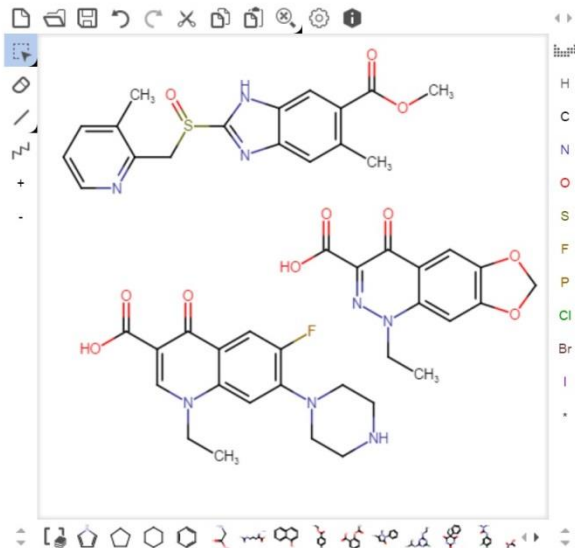
„The analysis reaffirms that control of physicochemical properties during compound optimization is beneficial in identifying compounds of candidate drug quality...”

„A set of physicochemical descriptors was independently calculated for these compounds by each company using ChemAxon 5.9 to provide a consistent set of descriptors...”



Around 500 citations from academia & research on Google Scholar since 2005

New features, developments



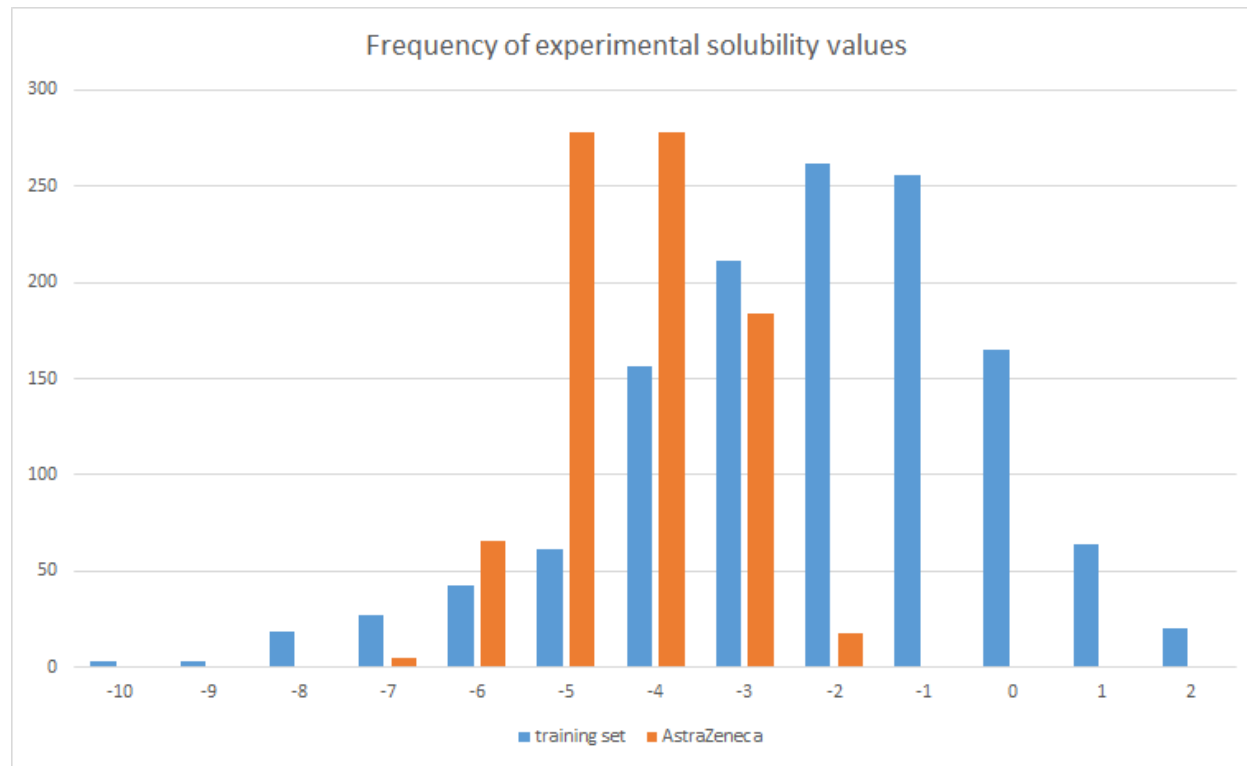
New demo site for the calculators

A nice web integration example of the calculators

Links: [Calculator demo pages](#), [Product page](#), [Documentation](#)

calculations-support@chemaxon.com

New features & developments



Solubility training
&
Prediction of error
for predicted value

Future plans & roadmap

- Developing further the solubility training
- PDB import module & electron density map visualization for ML
- pK_a prediction in dimethyl-sulfoxid (DMSO)
- Improving pK_a , logP/logD etc. calculations

Model improvements, developments based on Q3 achievements

2016 Q3

2016 Q4

THANK YOU !