sdf2ppt: Creating Powerpoints from SDFiles

Daniel Kuhn
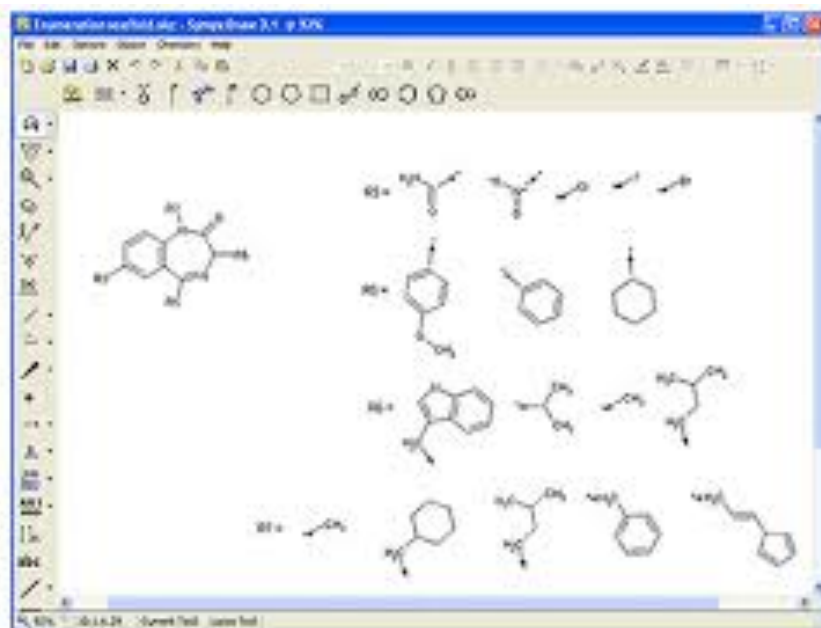
RDKit UGM 2014

Global Computational Chemistry

How do you discuss compound ideas with your chemist?
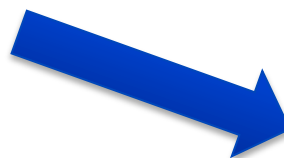
"Could you model these compounds?"

How to track the discussion and prioritization of the compounds?
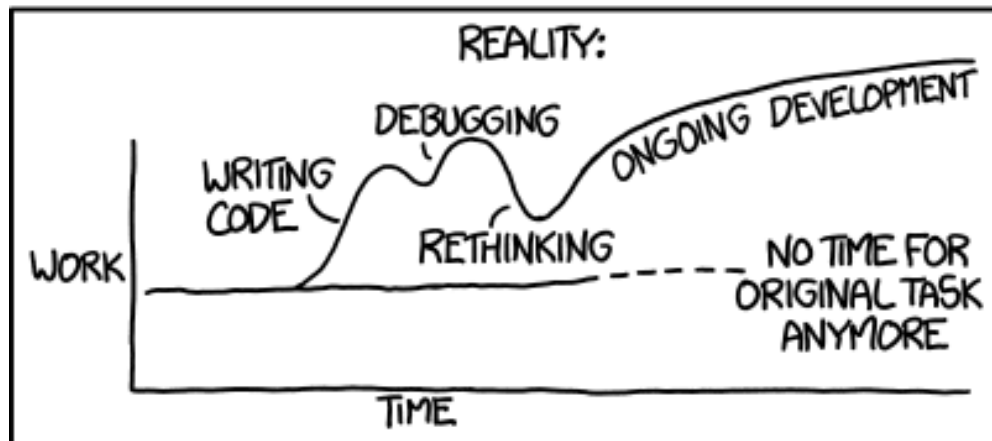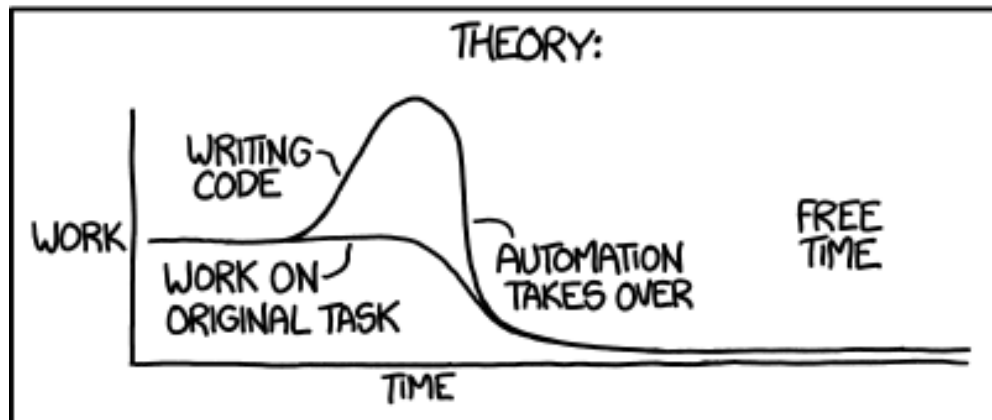
HTML table (PP)
→ Not interactive

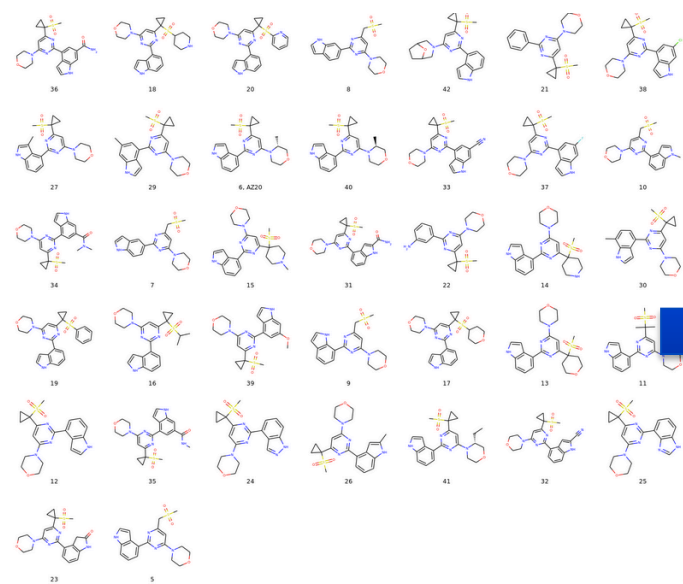Copy from Isis to PPT
→ Tedious
→ No info about cpd names

…

I should automate this!

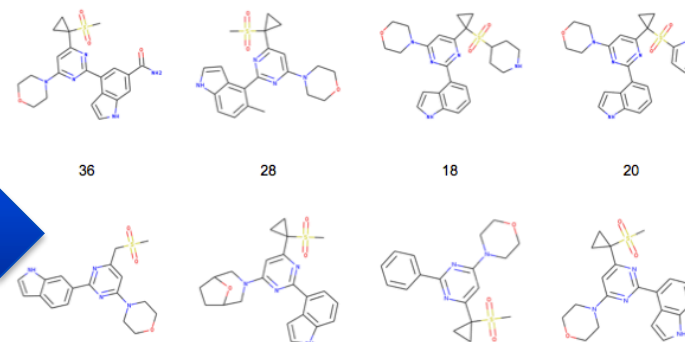http://xkcd.com/1319/

Wouldn't it be great …

sdf

Docking Results for atr_ligands.sdf 1/5

Quick search

Go

Enter search terms or a module, class or function name.

`pip install python-pptx`

python-pptx

Release v0.5.1 (*Installation*)

build passing

python-pptx is a Python library for creating and updating PowerPoint (.pptx) files.

A typical use would be generating a customized PowerPoint presentation from database content, downloadble by clicking a link in a web application. Several developers have used it to automate production of presentation-ready engineering status reports based on information held in their work management system. It could also be used for making bulk updates to a library of presentations or simply to automate the production of a slide or two that would be tedious to get right by hand.

More information is available in the python-pptx documentation.

Browse examples with screenshots to get a quick idea what you can do with python-pptx.

Feature Support

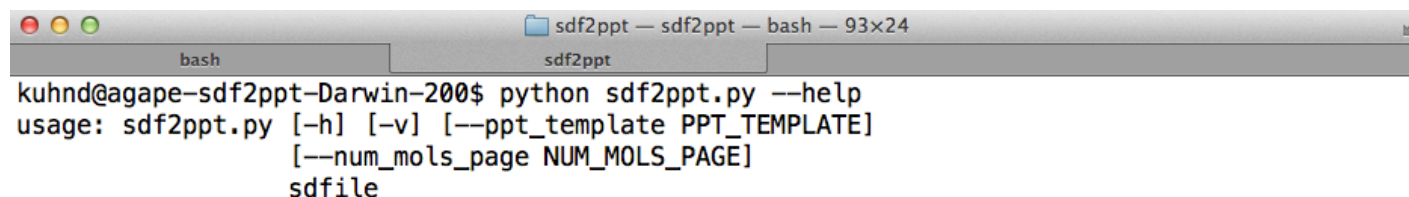`python-pptx` has the following capabilities, with many more on the roadmap:

- Round-trip any Open XML presentation (.pptx file) including all its elements
- Add slides
- Populate text placeholders, for example to create a bullet slide
- Add image to slide at arbitrary position and size
- Add textbox to a slide; manipulate text font size and bold
- Add table to a slide
- Add auto shapes (e.g. polygons, flowchart shapes, etc.) to a slide
- Add and manipulate column, bar, line, and pie charts
- Access and change core document properties such as title and subject

Additional capabilities are actively being developed and added on a release cadence of roughly once per month. If you find a feature you need that `python-pptx` doesn't yet have, reach out via the mailing list or issue tracker and we'll see if we can jump the queue for you to pop it in there :)

v: latest

sdf2ppt

Reads an SDFile and displays molecules as image grid in powerpoint/openoffice

Name of compounds are editable

```
kuhnd@agape-sdf2ppt-Darwin-200$ python sdf2ppt.py --help
usage: sdf2ppt.py [-h] [-v] [--ppt_template PPT_TEMPLATE]
                  [--num_mols_page NUM_MOLS_PAGE]
                  sdfile

sdf2ppt - Reads an SDFile and displays molecules as image grid in powerpoint/openoffice

#Contact: daniel.kuhn@merckgroup.com - 2014 - Merck Serono

positional arguments:
  sdfile                sdfile with ligands of interest

optional arguments:
  -h, --help            show this help message and exit
  -v, --verbose         Set verbosity level
  --ppt_template PPT_TEMPLATE, -p PPT_TEMPLATE
                        Powerpoint template file
  --num_mols_page NUM_MOLS_PAGE
                        Number of molecules per slide
kuhnd@agape-sdf2ppt-Darwin-201$
```
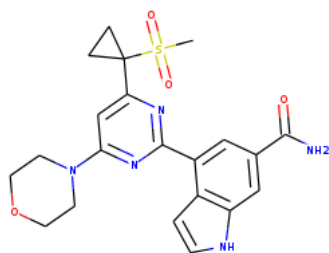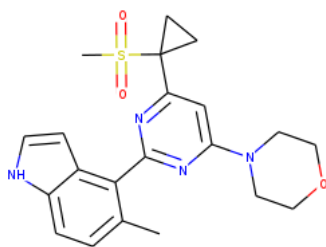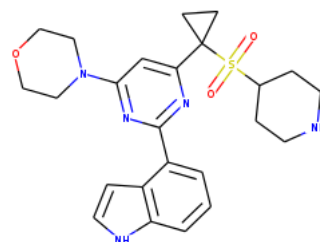
sdf2ppt on GitHub

Title of ppt

Daniel Kuhn

Docking Results for atr_ligands.sdf 1/5

36

28

18

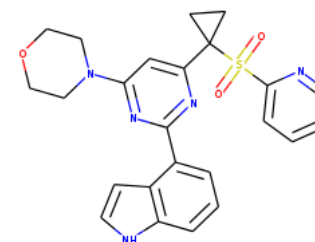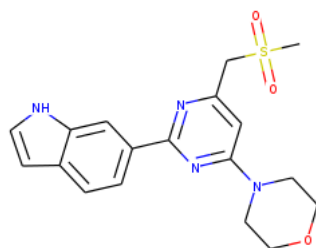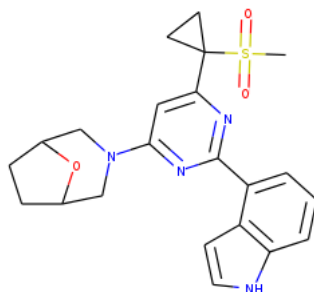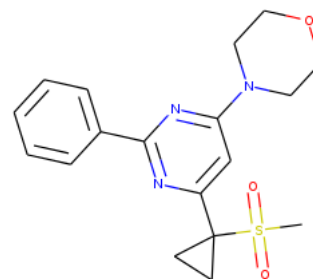20

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