RDKit

- http://www.rdkit.org/
- Getting Started with the RDKit in Python — The RDKit 2020.09.1 documentation
- Depict a compound as an image | Chemistry Toolkit Rosetta Wiki | Fandom
- Jupyter & RDKit
    - Getting Started with RDKit and Jupyter | Depth-First
    - http://davies-lee.com/index.php/2018/10/06/rdkit-in-jupyter-notebooks/
- ChemSpider | Search and share chemistry site reprenant de nombreuses informations sur des molécules
- ...

Exemples d'utilisation

test-rdkit.py

```
# from http://ctr.wikia.com/wiki/Depict_a_compound_as_an_image
from rdkit.Chem import AllChem
from rdkit.Chem import Draw

smiles = "CN1C=NC2=C1C(=O)N(C(=O)N2C)C"
mol = AllChem.MolFromSmiles(smiles)

# technically this step isn't required since the drawing code
# will automatically add a 2D conformation to a molecule that has
# no conformation information, I'm including it to show how to
# generate 2D coords with the RDKit:
AllChem.Compute2DCoords(mol)

Draw.MolToFile(mol,"caffeine.png",size=(200,250))
```