13.10.2022

Molecule Overviews

Display of molecules and their properties for communication purposes

Joos Kiener

RDKit UGM 2022

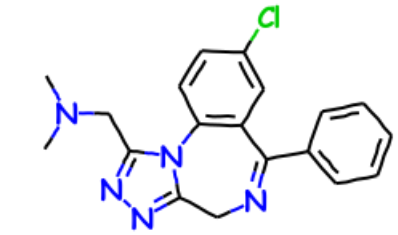
Givaudan

Human by nature

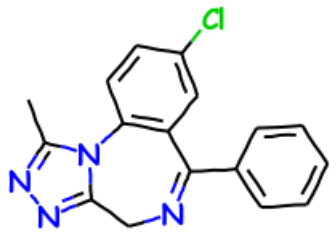
Slide Generator

Advanced MolsToGridImage

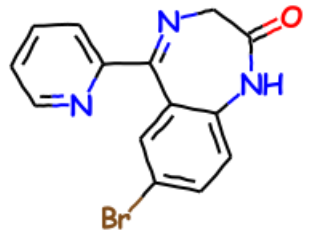
RDKit Slide Generator



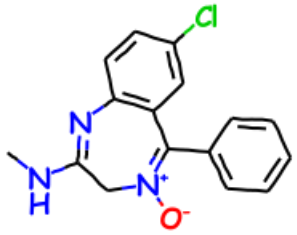
Adinazolam
6.87



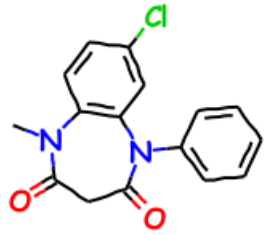
Alprazolam
7.7



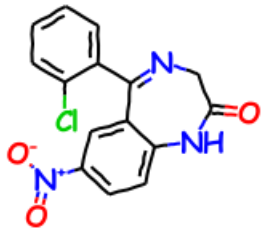
Bromazepam
7.74



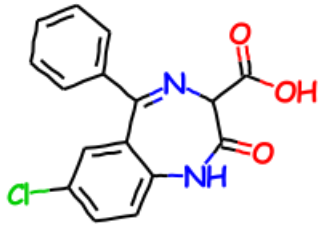
Chlordiazepoxide
6.45



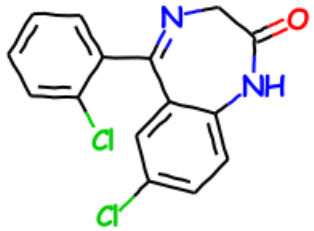
Clobazam
6.89



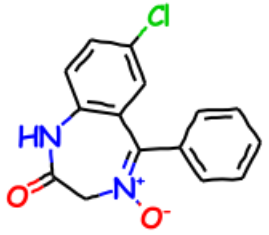
Clonazepam
8.74



Clorazepate
7.23



Delorazepam
8.74



Demoxepam
6.51

https://github.com/kienerj/molecule-slide-generator

RDKit Slide Generator
Options

- Dimensions of the image (width, height)
- Number of rows and columns (grid format)
- Each property can be displayed with or without its name
- Text can be colored separately for each molecule and each property
- Any true type font (.ttf) can be used for the atom labels and text
- Font size of atom labels and text
- Size of molecules (fixedBondLength drawing option)

RDKit Slide Generator
Features

- Molecules are automatically rescaled to RDKits default bond length
  - All molecules are the same size (= same bond length) regardless of input
  - Molecules too large will be “shrunk to fit”

- Output is a png image
  - Easy to work with (Office products, web mail, web sites,…)

- Data is stored in images metadata
  - Chemical structures and all properties
  - can be extracted again (manually or by provided helper class)

PyCDXML

Chemists love ChemDraw

PyCDXML
Python package for working with cdx and cdxml

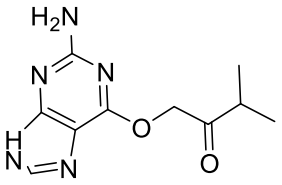
- Experimental!!! (do read the github readme)
- Pure Python, cross-platform (no need for ChemDraw installation)
- Convert between cdx and cdxml
- Change the visual style of cdxml files (bond length, atom label size,…)
- **RDKit Mol to cdxml**
- **Slide generator (cdxml as output)**

https://github.com/kienerj/pycdxml

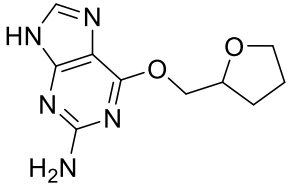
PyCDXML
Slide Generator end-to-end workflow

- Read sd-file with rdkit
- Convert rdkit molecule to cdxml
- Generate a cdxml file with molecules and properties nicley grouped and aligned
  - Can edit file in ChemDraw to fit needs exactly
- Properties stored as annotations and ChemDraw will export them into sd-file

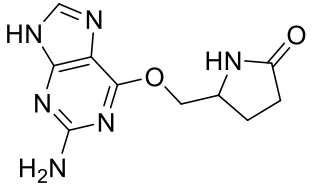
PyCDXMl – Slide Generator



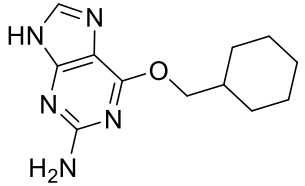
ZINC03814457
Energy: -78.6454



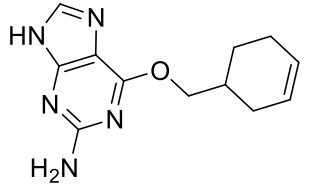
ZINC03814459
Energy: -67.4705



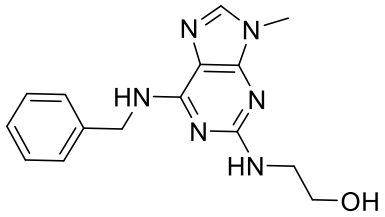
ZINC03814460
Energy: -89.4303



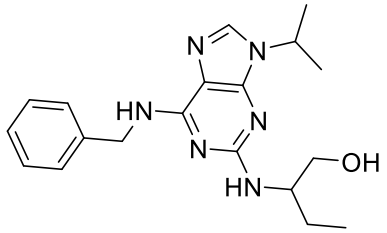
ZINC00023543
Energy: -70.2463



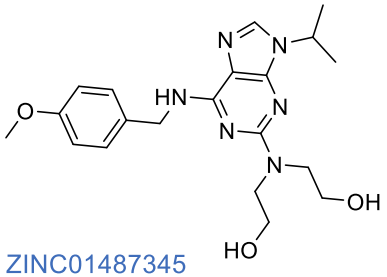
ZINC03814458
Energy: -72.9091



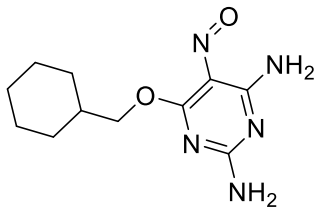
ZINC01641925
Energy: -42.2404



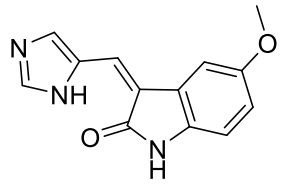
ZINC01649340
Energy: -33.4734



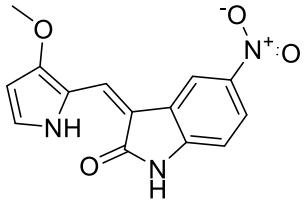
ZINC01487345
Energy: -23.1357



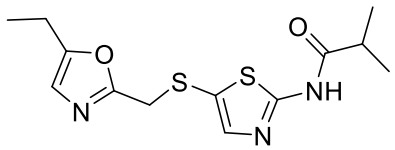
ZINC03814479
Energy: -112.542



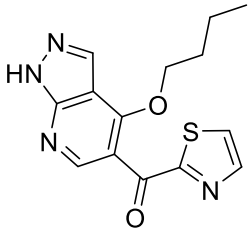
ZINC03814467
Energy: 15.8988



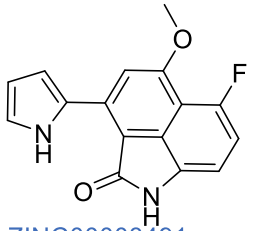
ZINC03814470
Energy: 18.0809



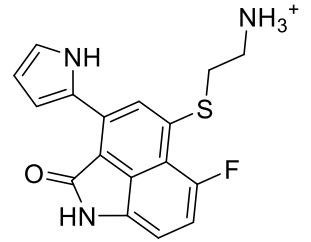
ZINC03814455
Energy: 0.133763



ZINC03814464
Energy: 0.565925



ZINC00003491
Energy: 46.1695



ZINC03814473
Energy: 49.1422

Follow us on social media

@givaudan

Givaudan

Human by nature