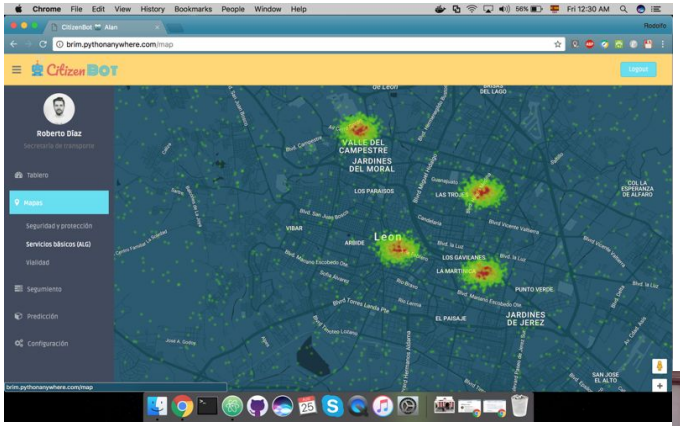
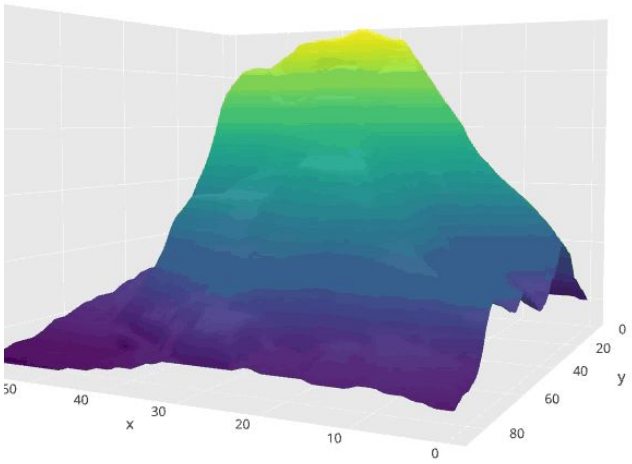
De visualización de moléculas, bots y más. 🤖

Rodolfo Ferro Pérez

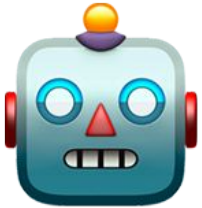
Rodo (no el reno)

Entre otras cosas...


Chrome File Edit View History Bookmarks People Window Help
brim.pythonanywhere.com/map
CitizenBOT
Logout
Roberto Díaz
Tablero
Mapas
Seguridad y protección
Servicios básicos (ALG)
Vialidad
Seguimiento
Predicción
Configuración
VALLE DEL CAMPESTRE
JARDINES DEL MORAL
LOS PARAÍSOS
LAS TROJES
COL LA ESPERANZA DE ALFARO
VIBAR
ARBIDE
León
LOS GAVILANES
LA MARTINICA
PUNTO VERDE
EL PAISAJE
JARDINES DE JEREZ
SAN JOSE EL ALTO


50
40
30
20
10
0
x
0
20
40
60
80
y

future·lab



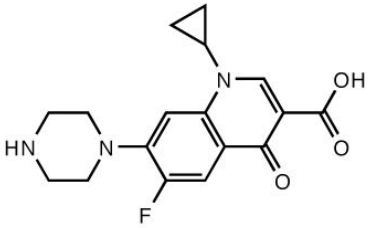

SUNSHINE
NEW YORK CITY
EST. 2009

SMILES

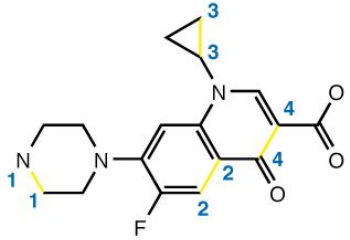
SMILES

(Simplified Molecular Input Line Entry System)

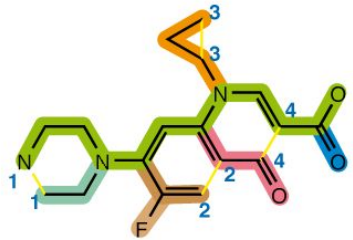
A



B



C



D

N1CCN(CC1)C(C(F)=C2)=CC(=C2C4=O)N(C3CC3)C=C4C(=O)O

Fuente: https://es.wikipedia.org/wiki/SMILES

Referencia: http://www.daylight.com/smiles/

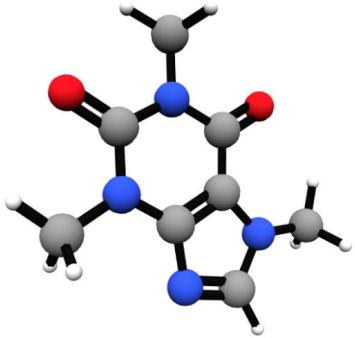
Gracias, University of Cambridge.

http://opsin.ch.cam.ac.uk


python

imolecule

An embeddable webGL molecule viewer and file format converter.



View the Project on GitHub
patrickfuller/imolecule

Download **ZIP File** | Download **TAR Ball** | View **Blender Tool**

This project is maintained by patrickfuller

Hosted on GitHub Pages — Theme by orderedlist

Examples

- IPython notebook
- metal-organic frameworks

IPython

The IPython notebook is an open-source tool poised to replace MATLAB in many applications. As a scientist of sorts, I'm all about it. Therefore, I made handles to use imolecule with the notebook. Install through pip:

```
pip install imolecule
```

Open a new notebook and test the setup by typing:

```
import imolecule
imolecule.draw("CC1(C(N2C(S1)C(C2=O)NC(=O)CC3=CC=CC=C3)C(=O)O)C")
```

into a notebook cell. This should convert, optimize and draw the specified SMILES structure (in this case, penicillin) into the notebook.

Note that this requires Open Babel to function. If you do not have Open Babel, see below for installation details.

The drawer can handle any format specified here, and can be set up to better handle different use cases. Check out the docstrings associated with the IPython interface for more.

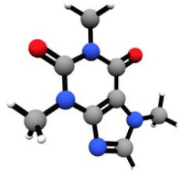
Server

If you want to run the file format converter on your own computer, install the library with:


I've made a robot that screams!
AAAAAAAAAA
WHY?
AAAA
AAA

Telegram

Don't have **Telegram** yet? Try it now! >



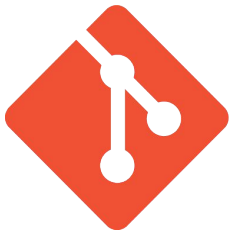
ChemDrawBot

@ChemDrawBot

SEND MESSAGE

OPEN IN WEB

https://t.me/ChemDrawBot



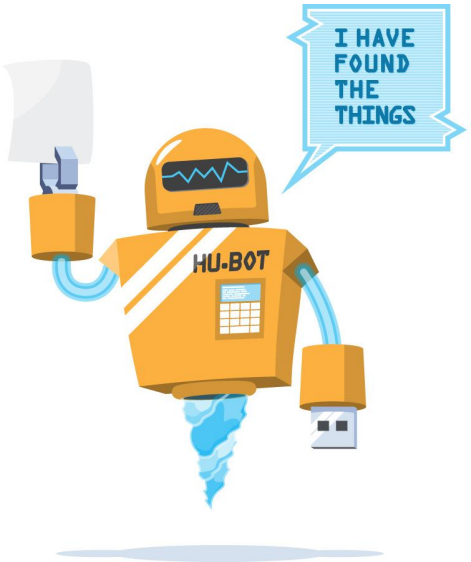
git

GitHub

Repositorios y control de versiones

Git es una herramienta que te permite tener un control de versiones en desarrollos.

GitHub por su parte, es una plataforma que te permite desplegar tus versiones en la nube.



ELECTRON

axosoft GitKraken

GraphQL

ATOM


TELMEX
hub //
PythonDayMéxico
2017
10 de junio
@TelmexHub
python SOFTWARE FOUNDATION
toptal
WIZELINE
Perengo BETA
Experis
Microsoft
SG


HACKATON
CFOX
$150,000
Centro Fox
1er
PROYECTO
CITIZEN BOT
CIENTO CINCUENTA MIL PESOS 00/100 MN


IBM

https://github.com/RodolfoFerro/SemanaIQ2017

future·lab

GitHub
Campus Experts

A nombre de *future·lab*:

¡Gracias!