

# Chemoinformatic Python tools used in French academic laboratories

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Since its first release in 1991 by Guido van Rossum, Python has become a gold reference in programming languages. Since 2003 it was consistently ranked in the top ten most popular languages [1]. As of September 2019 it is the third most popular language after Java and C.

The Python's large standard library [2] is suited for many tasks such as connecting to relational databases, driving scientific computing, creating graphical user interfaces, etc. Besides those built-in libraries, the Python Package Index [3], the official repository for third-party Python software, contains around 200,000 projects with a wide range of functionality. Thus many specialized libraries have been developed and some of them specifically oriented towards cheminformatics will be presented. We will discuss data acquisition, and how to treat them as chemical objects, their use in machine learning and deep learning models, their analysis and finally their visualization.

We will also briefly describe the Anaconda platform [4], aimed at simplifying the use of Python and dedicated to data science and machine learning package management and deployment on Windows, Linux and MacOS systems.

Next, we will highlight Jupyter notebooks [5], a web-based interactive computational environment for creating documents based on an ordered list of input/output cells which can contain code, text, equations, plots and rich media, resulting in a user-friendly tool for reporting.

Finally, we will walk through Python tools already used in several French academic laboratories.

## Bibliography :

[1] <https://www.tiobe.com/tiobe-index>

[2] <https://docs.python.org/3/library>

[3] <https://pypi.org>

[4] <https://www.anaconda.com/distribution/>

[5] <https://jupyter.org/>