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DockingPie

A Consensus Docking plugin for PyMOL

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What?

- A Graphical User Interface for Smina, Vina, RxDock and ADFR
- An environment for Consensus Docking analyses

The increased popularity of docking has resulted in the development of different docking algorithms and scoring functions. Nonetheless, it is unlikely that a single approach outperforms the others in terms of reproducibility and precision. In this ground, consensus docking techniques are taking hold. We have developed DockingPie, a **plugin** of the popular molecular graphics viewer **PyMOL** (Schrödinger LLC) that offers a versatile and user-friendly graphical user interface for assisting molecular and consensus docking analyses. At the current, and first release, the implemented docking programs are **Smina**, **Autodock Vina**, **RxDock** and **ADFR [1-5]**. Providing an easy interface to four docking programs, DockingPie is particularly suited as a platform to carry out **consensus docking** analyses.

Where?

Scan the QR-code for the GitHub page

Published on *Bioinformatics, OUP*
Serena Rosignoli and Alessandro Paiardini, DockingPie: a consensus docking plugin for PyMOL, *Bioinformatics*, 2022.

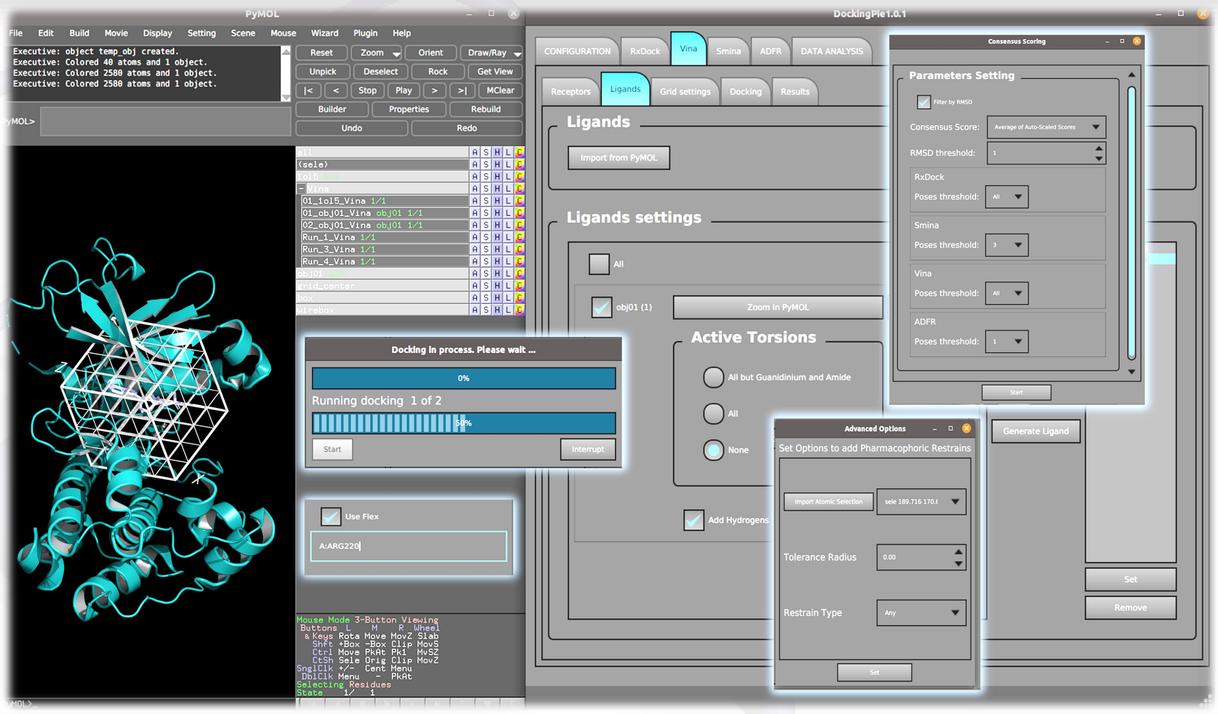
Available on GitHub
The source-code, instructions, tutorials and videos can be found in its GitHub page (remember to browse to the Wiki section!).

Why?

Implementation
- Cross-Platform (macOS, Windows and Ubuntu Linux)
- Easy to install
- Active support from the Developers
- All-in-One Environment

Didactic purposes
- Currently the tool of choice in our Departments
- Successfully used in International Summer/Winter Schools
- Appreciated by the students

Not a Bioinformatician?
- Avoid struggles with command-line implementations
- Exploit DockingPie to learn the cornerstones of Molecular Docking



Who?

<u>YOU!</u>
Interested in working on the development of DockingPie?

Such opportunity will bring you to the knowledge of **OOP in Python**, **GUI development**, **Molecular Docking tools.**

<u>Contact us</u> for further details.
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When?

2021
- Beta-version presented for the MSc thesis discussion

2022
- Published on *Bioinformatics, OUP*
- Presented at the CIVIS Summer School in Bioinformatics

a.a.2022/2023
- Adopted as the method of choice for 3 courses at Sapienza University

Ongoing
- Addition of molecular docking tools
- Optimization of the consensus docking procedure

... and so more

[1] Ruiz-Carmona, S. et al. (2014) rDock: a fast, versatile and open source program for docking ligands to proteins and nucleic acids. PLoS computational biology.
[2] Trott, O. et al. (2010) AutoDock Vina: improving the speed and accuracy of docking with a new scoring function, efficient optimization and multithreading, Journal of Computational Chemistry
[3] Koes, D. R. et al. (2013) Lessons learned in empirical scoring with smina from the CSAR 2011 benchmarking exercise. Journal of chemical information and modelling
[4] Ravindranath, P.A. et al. (2015) AutoDockFR: Advances in Protein-Ligand Docking with Explicitly Specified Binding Site Flexibility. PLoS Comput Biol.
[5] Morris, G. M. et al. (2009). AutoDock4 and AutoDockTools4: Automated docking with selective receptor flexibility. Journal of Computational Chemistry

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