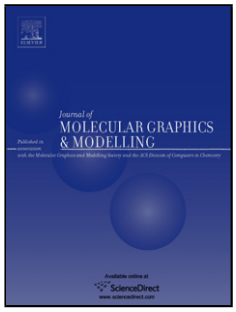

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Authors: Ali Hajiebrahimi, Younes Ghasemi, Amirhossein Sakhteman

PII: S1093-3263(17)30645-9
DOI: https://doi.org/10.1016/j.jmgm.2017.10.021
Reference: JMG 7060

To appear in: *Journal of Molecular Graphics and Modelling*

Received date: 21-8-2017
Revised date: 29-10-2017
Accepted date: 30-10-2017

Please cite this article as: Ali Hajiebrahimi, Younes Ghasemi, Amirhossein Sakhteman, FLIP: An assisting software in structure based drug design using fingerprint of protein-ligand interaction profiles, Journal of Molecular Graphics and Modelling https://doi.org/10.1016/j.jmgm.2017.10.021

FLIP: An assisting software in structure based drug design using fingerprint of protein-ligand interaction profiles

Ali Hajiebrahimi [1,2], Younes Ghasemi [1,2], Amirhossein Sakhteman *[3]

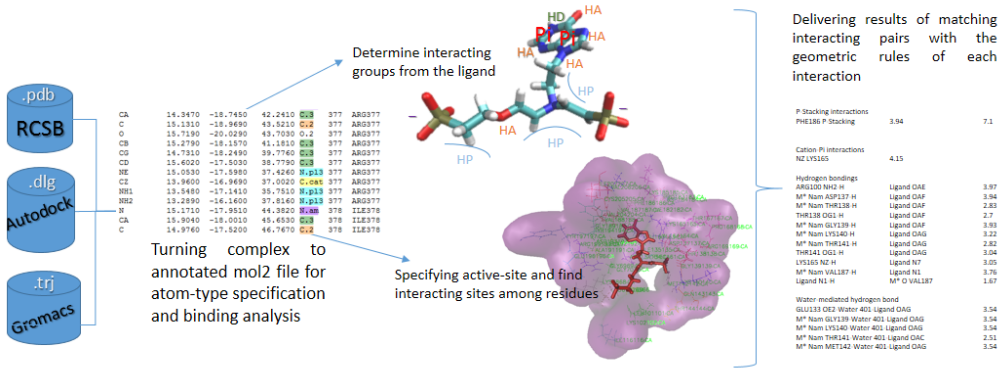
[1] Department of Pharmaceutical Biotechnology, School of Pharmacy, Shiraz University of Medical Sciences, Shiraz, Iran; hajiebrahimi@sums.ac.ir; ghasemiy@sums.ac.ir

[2] Pharmaceutical Sciences Research Center, Shiraz University of Medical Sciences, Shiraz, Iran; hajiebrahimi@sums.ac.ir; ghasemiy@sums.ac.ir

[3] Department of Medicinal Chemistry, School of Pharmacy, Shiraz University of Medical Sciences, Shiraz, Iran; asakhteman@sums.ac.ir

***** Correspondence: asakhteman@sums.ac.ir; Tel.: +98-713-242-4127

Graphical abstract



Highlights

- A novel application (FLIP) for generation of protein-ligand interaction profiles was developed
- The application was extensively validated for detection of different molecular interactions.
- Independent ring perception libraries were used to increase its efficiency and speed
- Tanimoto distance was implemented in the application to compare different docking fingerprints