Andrea **Basciu**

Post-Doctoral Researcher in Computational Biophysics

linkedin.com/in/andrea-basciu/
a.basciu2@gmail.com

Professional Experience

Dec 2019 – Current | **Post-Doctoral Research fellow, Physics Department, University of Cagliari (Italy)**

- Development of computational protocols to improve the sampling of rare conformations of proteins and the predictive power of molecular docking and virtual screening
- Optimization of lead compounds to target serotonin receptors
- Computational studies on SARS-CoV-2 main-protease inhibitor drugs
- Computational investigation of the inhibition of bacterial multidrug efflux transporters
- Building machine learning pipelines to characterize protein properties (e.g. druggability, stability)

Teaching

2022 | **Lecturer, Physics Department, University of Cagliari (Italy)**

- Course : **Machine Learning Methods in Computational Biophysics** for graduate physics students.

2018-2022 | **Lecturer, BioExcel Summer School on Biomolecular Simulations,**

- Lectures on protein conformational dynamics;
- Hands-on tutorial on the EDES protocol to generate bound-like protein conformations (tutorial page)

2017 | **Teaching assistant, Physics Department, University of Cagliari (Italy)**

- Courses : **General Physics I** (12 CFU) and **Fundamentals of Computational Physics** (6 CFU) for undergraduate physics students.

Skills

Operative systems	Windows, Linux, Mac OS X and programs of the standard distributions.
Programming/Scripting/Text editing	Python, Linux shell (bash, csh), C/C++ (basic knowledge), Tcl, Emacs, MS Office
Data analysis	R, Mathematica, IgorPro, ROOT, xmgrace, gnuplot
Bioinformatics	DFT calculations tools (GAUSSIAN), Molecular dynamics packages (AMBER, GROMACS), docking and modelling tools such as : PLUMED, rDock, AutoDOCK (VINA), HADDOCK, VMD, Pymol, BLAST, MODELLER
Python libraries for Machine Learning	SciPy, Numpy, Pandas, Matplotlib, Scikit-learn and PyTorch

Education

Sep 2022 **Postgraduate specialization in Machine Learning and Big Data for Biomedical Research**,
University of Padua (Italy), Grade : Excellent,
Project : ML-based models to identify holo-like protein conformations from MD simulations,
Supervisors : Profs. Barbara Di Camillo, Carlo Ferrari

Feb 2020 **Philosophiæ Doctor (Ph.D.) in Physics**, with the *Doctor Europaeus* distinction, University of Cagliari (Italy),
Project : An enhanced sampling MD-based protocol to improve the predictive power of molecular docking,
Supervisors : Prof. Paolo Ruggerone, Dr. Attilio V. Vargiu

Mar 2016 **Master's degree (M.Sc.) in Physics**, University of Cagliari (Italy),
Thesis title : A protocol to improve the predictive power of molecular docking,
Supervisor : Dr. Attilio V. Vargiu, Grade : 110/110 *magna cum laude*

Projects

AndysRepo GitHub repository

https://andysrepo.github.io

AndysRepo is a repository where I collect and share the source codes written either for job or for fun. Codes will be mostly written in bash, python and C and they will usually address somehow maths-related questions, ranging from solving some physics problem to performing a certain statistical analysis on a set of data. Some other times the codes will regard something different, like simple computer games. Moreover, some codes also include interfacing with SQL databases and simple machine learning applications.

Publications

2022 **A. Basciu**, L. Callea, S. Motta, A.M.J.J. Bonvin, L. Bonati and A. V. Vargiu. **No dance, no partner! A tale of receptor flexibility in docking and virtual screening**. *Ann. Rep. in Med. Chem.*, 59 (**2022**)

2022 P. Cacciotto,**A. Basciu**, F. Oliva, G. Malloci, M. Zacharias, P. Ruggerone and A. V. Vargiu. **Molecular rationale for the impairment of the MexAB-OprM efflux pump by a single mutation in MexA**. *Comput. and Struct. Biotech. J.*, 20 (**2022**)

2020 **A. Basciu**, P. I. Koukos, G. Malloci, A.M.J.J. Bonvin and A. V. Vargiu. **Coupling enhanced sampling of the apo-receptor with template-based ligand conformers selection : Performance in pose prediction in the D3R Grand Challenge 4**. *J. of Computer-aided Drug Design*, 34 (**2020**)

2019 **A. Basciu**, G. Malloci, F. Pietrucci, A.M.J.J. Bonvin and A.V. Vargiu. **Holo-like and druggable protein conformations from enhanced-sampling of binding pocket shape**. *J. Chem. Inf. and Mod.*, 59 (**2019**)

2019 A. Atzori , G. Malloci, J.D. Prajapati, **A. Basciu**, A. Bosin, U. Kleinekathöfer, J. Dreier, A.V. Vargiu, P. Ruggerone. **Molecular Interactions of Cephalosporins with the Deep Binding Pocket of the RND Transporter AcrB**. *J. Phys. Chem. B*, 123 (**2019**)