TO MAGNIFICO RETTORE OF UNIVERSITA' DEGLI STUDI DI MILANO **ID CODE 5728**

I the undersigned asks to participate in the public selection, for qualifications and examinations, for the awarding of a type B fellowship at **Dipartimento di Scienze Farmaceutiche**

Scientist- in - charge: **Prof. Giulio Vistoli**

CASSIANO LANGINI

CURRICULUM VITAE

PERSONAL INFORMATION

Surname	Langini
Name	Cassiano

PRESENT OCCUPATION

Appointment	**Structure**
Postdoctoral researcher	Department of Biochemistry, University of Zurich, Zurich (CH)

EDUCATION AND TRAINING

Degree	**Course of studies**	**Lab/University**	**year of achievement of the degree**
Bachelor of Science	Engineering Physics (L-9)	Politecnico di Milano	2012
Master of Science	Engineering Physics (LM-44)	Politecnico di Milano	2015
PhD	Biomolecular Structure and Mechanism	University of Zurich (CH)	2021
Other Experience			
Intern	Department of Biochemistry	University of Zurich (CH)	Sep-Dec 2015
Postdoctoral researcher	Department of Biochemistry	University of Zurich (CH)	2022 - present

FOREIGN LANGUAGES

Language	**Level of knowledge**	**Certifications (score, year)**
Italian	First language	
English	Professional working proficiency (C1)	IELTS (8.0/9.0, 2013) TOEFL iBT (106/120, 2012)

German	Elementary proficiency (B1/B2)	

AWARDS, ACKNOWLEDGEMENTS, SCHOLARSHIPS

Year	Description of award
2018	Best poster award, first place, at the PASC (Platform for Advanced Scientific Computing) 2018 conference in Basel (CH) Poster title: "The bromodomain-peptide (un)binding network"
2011-2013	Resident student at Collegio di Milano, a multidisciplinary campus of excellence providing a cultural program and extracurricular activities to qualified university students.
2009	Premio per la Fisica "Valerio Filippini", 2nd place Physics competition for high school final-year students, awarding a scholarship

TRAINING OR RESEARCH ACTIVITY

Period	Description of activity
2022-present	**Postdoctoral researcher, group of Prof. Amedeo Caflisch, Department of Biochemistry, University of Zurich (CH):** • Analysis of molecular dynamics (MD) simulation trajectories using several statistical and unsupervised learning methods, including clustering of conformations, dimensionality reduction, Markov state models, transition path theory, pathway decomposition, reaction coordinates. Specific focus on applying these methods to adaptive sampling simulation protocols. • Energy estimation to determine the most favorable conformation of Vamifeport in complex with ferroportin, between two possible alternatives compatible with the Cryo-EM structure (collaboration with CSL Vifor and Prof. Raimund Dutzler at the University of Zurich). • Part of the development team of a new web-based molecular modeling platform (involving multiple technologies, including a Javascript front-end, a C++ back-end, a PostgreSQL database, several Python and bash scripts for deploying calculations to a Slurm queuing system). More specifically, I have worked on the docking modules, and on enabling chemical substructure search on the SQL database. • Implementation of graph neural networks for prediction of molecular properties (partial charges), protein-ligand binding affinity, and ranking of poses, to be integrated in a general docking workflow and fine-tuned on specific targets of interest (epitranscriptomic targets) via transfer learning.
2015 - 2021	**Research assistant (intern and PhD student), group of Prof. Amedeo Caflisch, Department of Biochemistry, University of Zurich (CH):** Title of the PhD dissertation: "Computational Studies of Bromodomains and Their Interactions with Natural and Synthetic Ligands" • MD simulations of bromodomains binding to their natural ligands (acetylated lysine-containing peptides derived from histone tails). • Validation of an adaptive MD simulation protocol, which is able to focus the sampling enhancement on specific degrees of freedom of the system under study. • MD simulation comparison of the bromodomain of ATAD2 with and without a disulfide bridge connecting two helices of the fold (collaboration with Prof. Karen Glass at the Albany College of Pharmacy).

	• Construction of a common unified structural representation from simulations of multiple bromodomains, in order to be able to analyze them within the same framework.
	• Implementation of transition path theory pathway decomposition in the CAMPARI software package (Fortran, https://campari.sourceforge.net/). Contributions to the corresponding R package (https://caflischlab.gitlab.io/CampaRi/).
	• Maintenance and performance improvement of the fragment docking software SEED (C/C++), including MPI parallelization, code speed-up, minimizers, online documentation (https://caflischlab-seed.readthedocs.io/), training of new users.
	• Assessment of SEED screening power on 15 target/library combinations and comparison to Glide (collaboration with Janssen and Prof. Hans de Winter at the University of Antwerp).
	• MD comparison of the structural properties of two microbial transglutaminases at different temperatures (collaboration with Dr. Angelo Facchiano at the Institute of Food Science in Avellino).
	
	Additional activities:
	
	• Mentoring of 1 Master and 2 visiting PhD students.
	• 300 hours of teaching duties, including:
	  ○ Teaching assistance for the lab practice of protein purification (1st year medical students).
	  ○ Teaching assistance for Protein Biophysics (code BCH304, 3rd/4th year biochemistry students): exercise sessions, writing of exam questions, exam correction.
	• Attended mandatory courses from the PhD program and additional university classes: Current Topics in Structural Biology (1 ECTS), Scientific Integrity, Scientific Writing (1 ECTS), Structural Biology Course (1 ECTS), Protein Biophysics (6 ECTS), Data Mining: Learning from Large Data Sets (4 ECTS, at ETH Zurich), Probabilistic Artificial Intelligence (8 ECTS, at ETH Zurich).
	• Participation in retreats organized by the PhD program and by the lab.

Apr 2019	**E-CAM Extended Software Development Workshop (ESDW), École Normale Supérieure, Lyon (FR)** Attendance of a workshop to learn best practices in software engineering for molecular simulation codes (documentation, testing, version control, continuous integration/delivery). • Development of the *pytbc* Python package (https://gitlab.com/clangi/pytbc), exposing bindings for selected clustering algorithms implemented in CAMPARI (Fortran).
Feb 2017	**Introduction to programming Pascal (P100) wih CUDA 8, Centro Svizzero di Calcolo Scientifico, Lugano (CH)** 3-day workshop on GPU programming with CUDA.
Apr 2014-Apr 2015	**Master student, group of Prof. Giacomo Ghiringhelli, Department of Physics, Politecnico di Milano** Title of the thesis: "Advances in the detection at the new XMCD and RIXS beamline of the ESRF" Supervisor: Prof. Giacomo Ghiringhelli. Grade: 110/110 cum Laude. • Enhancement of the resolution of a CCD detector through single-photon centroid reconstruction.

	• Experimental study of weak ferromagnetism in high-temperature superconductors using X-ray magnetic circular dichroism. The XMCD experiments were carried out at the beamline ID32 at the European Synchrotron Radiation Facility (ESRF) in Grenoble.
Aug - Dec 2013	**Erasmus student at the Technical University of Denmark, Lyngby (DK)** Coursework for 25 ECTS.
Jul 2012	**Bachelor student, Department of Physics, Politecnico di Milano** Title of the thesis: "Microfluorimetria risolta in tempo". Supervisor: Prof. Cosimo d'Andrea. Grade: 110/110 cum Laude. • Realization of an epi-illumination system by coupling a time-correlated single photon counting setup to an optical microscope.

CONGRESSES AND SEMINARS

Date	Title	Place
2020	NeurIPS (Conference on Neural Information Processing Systems). Participation as listener.	Online
2019	13th Symposium "Trends in Structural Biology". Short talk: "Is the mechanism of binding of histone tails conserved across the bromodomain family?" Authors: **C. Langini**	University of Zurich (CH)
2018	Artificial Intelligence in Chemical Research Participation as listener.	Syngenta Research Center, Stein (AG), CH
2018	PASC (Platform for Advanced Scientific Computing) 2018 Conference Poster: "The bromodomain-peptide (un)binding network" (Best poster award, first place). Authors: **C. Langini**, M. Bacci, A. Vitalis, A. Caflisch	Basel (CH)
2017	PASC (Platform for Advanced Scientific Computing) 2017 Conference Poster: "Focused diversification of biomolecules for drug discovery by Progress Index-guided sampling" Authors: **C. Langini**, M. Bacci, A. Caflisch, A. Vitalis.	Lugano (CH)

PUBLICATIONS

A full list of publications is available at: https://scholar.google.com/citations?user=MErdFgcAAAAJ&hl

Articles in journals
1. Widmer, J., **Langini, C.**, Vitalis, A. and Caflisch, A., Optimized reaction coordinates for analysis of enhanced sampling. (under review at the *Journal of Chemical Physics*)
2. Lehmann, E.F., Liziczai, M., Drożdżyk, K., Altermatt, P., **Langini, C.**, Manolova, V., Sundstrom, H., Dürrenberger, F., Dutzler, R. and Manatschal, C., 2023. Structures of ferroportin in complex with its specific inhibitor vamifeport. *Elife*, *12*, p.e83053. https://doi.org/10.7554/eLife.83053
3. Giordano, D., **Langini, C.**, Caflisch, A., Marabotti, A. and Facchiano, A., 2022. Molecular dynamics analysis of the structural properties of the transglutaminases of Kutzneria albida and Streptomyces mobaraensis. *Computational and Structural Biotechnology Journal*, *20*, pp.3924-3934.

https://doi.org/10.1016/j.csbj.2022.07.024
4. Goossens, K., Wroblowski, B., **Langini, C.**, van Vlijmen, H., Caflisch, A. and De Winter, H., 2020. Assessment of the fragment docking program SEED. *Journal of chemical information and modeling*, *60*(10), pp.4881-4893. https://doi.org/10.1021/acs.jcim.0c00556
5. Amorese, A., **Langini, C.**, Dellea, G., Kummer, K., Brookes, N.B., Braicovich, L. and Ghiringhelli, G., 2019. Enhanced spatial resolution of commercial soft X-ray CCD detectors by single-photon centroid reconstruction. *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, *935*, pp.222-226. https://doi.org/10.1016/j.nima.2019.03.010
6. Amorese, A., **Langini, C.**, Dellea, G., Kummer, K., Brookes, N.B., Braicovich, L. and Ghiringhelli, G., 2019. Enhanced spatial resolution of commercial soft X-ray CCD detectors by single-photon centroid reconstruction: Technical Note. *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, *935*, pp.227-231. https://doi.org/10.1016/j.nima.2019.02.044
7. Gay, J.C., Eckenroth, B.E., Evans, C.M., **Langini, C.**, Carlson, S., Lloyd, J.T., Caflisch, A. and Glass, K.C., 2019. Disulfide bridge formation influences ligand recognition by the ATAD2 bromodomain. *Proteins: Structure, Function, and Bioinformatics*, *87*(2), pp.157-167. https://doi.org/10.1002/prot.25636
8. Bacci, M., **Langini, C.**, Vymětal, J., Caflisch, A. and Vitalis, A., 2017. Focused conformational sampling in proteins. *The Journal of chemical physics*, *147*(19), p.195102. https://doi.org/10.1063/1.4996879
9. **Langini, C.**, Caflisch, A. and Vitalis, A., 2017. The ATAD2 bromodomain binds different acetylation marks on the histone H4 in similar fuzzy complexes. *Journal of Biological Chemistry*, *292*(40), pp.16734-16745. https://doi.org/10.1074/jbc.M117.786350

COMPUTER SKILLS

Cheminformatics	RDKit, OpenBabel
MD and docking	GROMACS, CAMPARI, SEED, rDock
Molecular viewers	VMD, Pymol, ACGUI (not public yet, under active development)
ML/AI	PyTorch, deep graph library (DGL), scikit-learn
Others	SQL, MPI, git, CI/CD, Docker, Latex, Inkscape, Linux OS

Declarations given in the present curriculum must be considered released according to art. 46 and 47 of DPR n. 445/2000.

The present curriculum does not contain confidential and legal information according to art. 4, paragraph 1, points d) and e) of D.Lgs. 30.06.2003 n. 196.

Please note that CV WILL BE PUBLISHED on the University website and It is recommended that personal and sensitive data should not be included. This template is realized to satisfy the need of publication without personal and sensitive data.

Please DO NOT SIGN this form.

Place and date: Zurich, 02/05/2023

Università degli Studi di Milano – Direzione Trattamenti Economici e Lavoro Autonomo
Ufficio Contratti di formazione e Ricerca
Via Sant'Antonio 12 - 20122 Milano, Italia
assegni.ricerca@unimi.it DTELA_M_CVAssegniENG_rev. 00 del 02/09/2021