UNIVERSITÀ DEGLI STUDI DI MILANO

TO MAGNIFICO RETTORE OF UNIVERSITA' DEGLI STUDI DI MILANO   **ID CODE   6763**

I the undersigned asks to participate in the public selection, for qualifications and examinations, for the awarding of a type B fellowship at **Di**partimento di Chimica

Scientist- in – charge: **Prof. Stefano Pieraccini**

[Name and surname]

CURRICULUM VITAE
PERSONAL INFORMATION

Surname	GAO
Name	Xinyue

PRESENT OCCUPATION

Appointment	Structure
Master Student	

EDUCATION AND TRAINING

Degree	Course of studies	University	year of achievement of the degree
Degreen	Chemistry	University Paris Saclay	2022
Specialization	Chemical engineering and processing	University of Lorraine	2021
Master	Erasmus Mundus Joint Master, Chemoinformatics+	University of Strasbourg, University of Milano, University Paris Cite	2024

FOREIGN LANGUAGES

Languages	level of knowledge
English	C1
French	C1
Chinese	C2
Italian	A2

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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

AWARDS, ACKNOWLEDGEMENTS, SCHOLARSHIPS

Year	Description of award
2024	Kaggle Silver Medalist - NeurIPS 2024. Awarded a Silver Medal for placing 88th out of 1946 teams in the NeurIPS 2024 "Predict New Medicines with BELKA" competition. Recognized for outstanding performance in developing predictive models for drug discovery.
2022	Erasmus Mundus Joint Master's Degree (EMJMD) Scholarship in program Chemoinformaticsplus

TRAINING OR RESEARCH ACTIVITY

description of activity
After having two-year technical degree in Chemical engineering, obtained Bachelor diplome in Chemistry. Then got involved in Erasmus mundus joint master program, with a collaborative training among University of Strasbourg, University of Milano and University Paris Cite. Major in In Silico Drug Design. Key projects: Protein pocket analysis: Biostatistics and Introduction to Multivariate data analysis (R). Exploration of proteins' structures: Compare the sequences of the two proteases, analyze their overall structural folds, characterize their inhibitor binding pockets, and determine the impact of HIV-1/2 mutations (R). Homology modeling: Explore the family of alpha B crystallin and its homologs through bioinformatics analysis and homology modeling in order to better understand their structures, functions, and disease-associated mutations (R, Modeller, Data mining in UniProt, PDB). Dynamic analysis: Assessing the conformations flexibility, stability and to gain insights into its functional mechanisms by Molecular dynamics for Bcl-xL (Gromacs, PLIP). Ligand preparation: Data mining for creating and clustering RDkit descriptors of ligand(KNIME, Python Jupyter Notebook) Analysis of information in Drug Design: Discovery on supervised methods in machine learning to figure out the descriptors calculated for Bcl-xL dataset (R, Python, neural networks). Structure based high-throughput screening application: Identified two novel micromolar inhibitors of the Bcl-xL protein through robust structure-based molecular modeling, expanding potential therapeutic targeting opportunities of this anti-apoptotic protein implicated in cancer (AutoDock Vina, Bash, Python Jupyter Notebook).

PROJECT ACTIVITY

Year	Project
2024	Visiting student in University of Vienna. Participate in construction of a metabolic dataset, involving the collection, cleaning, and organization of large-scale biological data to ensure high quality and consistency.
2024	Visiting student in Hongkong Baptist University. Develop a large language model interface to facilitate communication and task delegation among specialized LLM across biology, chemistry, and materials science, streamlining complex, interdisciplinary problemsolving.
2024	Intern in NOVA Lisbon University of Science and Technology. Obtained molecular representations of chemical reactions using heteroencoders deep neural networks and explore the difference in latent space vectors between reactants and products as descriptors of reactions.

| 2021 | Intern in Huazhong University of Science and Technology. Conducted research on organometallic framework materials and successfully developed and analyzed two copper-based materials for the quantitative detection of ascorbic acid in human sweat. |

OWNERSHIP OF PATENTS

Patents
Gardenia Glycosides Anti-itch Lotion and Preparation Method

CONGRESSES AND SEMINARS

Date	Title	Place
09/07/2024	2024 Summer school on AI in Biology and Genetics	Paris, France
06/07/2024	Oxford Machine Learning Summer school 2024	Oxford, United Kindom
24/06/2024	9th Strasbourg Summer school in Chemoinformatics	Strasbroug, France
12/05/2023	Oxford Machine Learning Summer school 2023	On line
26/06/2023	Symposium Summer School Chemoinformatics+ & Scientific Conference	Paris, France
04/07/2022	Summer School of Chemistry & Physics	Orsay, France

PUBLICATIONS

Articles in reviews
Exploring molecular heteroencoders with latent space arithmetic:atomic descriptors and molecular operators, Gao, X.; Baimacheva, N.; Aires-de-Sousa, J. Molecules 2024, 29, 3969.

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: Paris, 30/08/2024