UNIVERSITÀ DEGLI STUDI DI MILANO

Curriculum vitae

AL MAGNIFICO RETTORE
DELL'UNIVERSITA' DEGLI STUDI DI MILANO **COD. ID: 6654**

Il sottoscritto chiede di essere ammesso a partecipare alla selezione pubblica, per titoli ed esami, per il conferimento di un assegno di ricerca presso il Dipartimento di _____**Dipartimento di Scienze Farmaceutiche**_____

Responsabile scientifico: _____**Prof. Sara Sattin** _____

[Nome e cognome]

CURRICULUM VITAE

Highly motivated and polyvalent scientist, expert in the field of Computer-Aided Drug Design (rational design, virtual screening, homology modeling, docking …) and in the application of classical and enhanced sampling Molecular Dynamics simulations. Good proficiency with bash and python. Interested in the development of methodologies for the molecular modeling and the use of Intelligence Artificial in the drug discovery field.
I also have expertise in organic chemistry synthesis and biochemical assays.

INFORMAZIONI PERSONALI

Cognome	FATIMA EZZAHRA
Nome	AGHARBAOUI

OCCUPAZIONE ATTUALE

Incarico	**Struttura**
Postdoctoral research fellow	University of Milan, Department of Chemistry

ISTRUZIONE E FORMAZIONE

Titolo	**Corso di studi**	**Università**	**anno conseguimento titolo**
Dottorato Di Ricerca	Pharmaceutical Sciences	University of Messina, Italy	2013-2015
Master	Artificial Intelligence and Bioinformatics	The National School of Applied Sciences of Tangier (ENSAT), University Abdelmalek Essadi, Morocco.	2008-2011
Master 1	Biotechnology	Faculty of Sciences Semlalia Marrakech, Cady Ayyad University, Morocco.	2007-2008
Bachelor	Life Sciences (Biology - Chemistry)	Faculty of Sciences Semlalia Marrakech, Cady Ayyad University, Morocco	2004-2007

Bachelor	Science and Art : Chemistry - Biology	University of Quebec at Montreal (UQAM), Montréal, Canada	2003-2004

LINGUE STRANIERE CONOSCIUTE

lingue	**livello di conoscenza**
Arabic	Mother tongue
English	Advanced
French	Advanced
Italian	Medium

PREMI, RICONOSCIMENTI E BORSE DI STUDIO

anno	**Descrizione premio**
2013-2015	Scholarship from the University of Messina, Italian Ministry for education University and Research (MIUR)
01/04/2015-30/09/2015	Scholarship from the Ohio State University. Sponsor Pr. Mamuka Kvaratskhelia
12/04/2015-30/09/2015	Scholarship from CIRAD (Centre for International Cooperation in Agronomic Research for Development), Montpellier, France

ATTIVITÀ DI FORMAZIONE O DI RICERCA

Anno	**ATTIVITÀ DI FORMAZIONE O DI RICERCA**
01/01/2023 – present	Postdoctoral research fellow at University of Milan, Department of Chemistry under supervision of Prof. Alessandro Contini Project: IRON homeostasis in Neuroferritinopathy: unravelling the molecular details of abnormal ferritin functionality (IRONYc) using classical and enhanced sampling molecular dynamics simulations. In silico design of natural and non-natural peptides to mimic the portion of the protein altered by the mutation(s): conformational space and interaction studies. Amber 22 package and Python scripts were used for the simulations and the results analysis.
01/07/2020 – 30/06/2022	Postdoctoral research fellow at University of Milan, Department of Chemistry under supervision of Prof. Dr Stefano Pieraccini Projects: 1. Member of the FetOpen project NOPEST (http://www.h2020nopest.org/) that explores

	new solutions to counteract oomycete infections in commercial crops. The project aims to develop an environmentally friendly approach for crop protection as an alternative to conventional chemical pesticides. PCA technics were used for the classification ad selection of the potential active peptides. cMD, aMD and Metadynamics simulations methods were used for the optimization and investigation of the peptides/peptidomimetics structural and conformational properties in different solvents. Gromcas 2016.5 package, Amber, PCA technique and Python scripts were used for the simulations and the results analysis. The obtained results were very promising and are going to be patented. 2. Antimicrobial YeaZ-based peptides: identification and supramolecular aggregation studies. The lead peptide was obtained using SASA analysis and computational alanine scan. Rational design of the obtained peptide to improve its stability was performed. The designed peptides conformational properties and the nucleation of the aggregation processes were investigated using molecular Dynamics and Metadynamics simulations in different solvents and in the presence of LPS lipid-A bilayers. Gromcas 2016.5 and Python scripts were used for the simulations and the results analysis.
10/08/2018 – 07/03/2020	Postdoctoral research fellow at the University of Malaya, Drug Discovery and Development Research Group, department of chemistry, Faculty of Sciences, Kuala Lumpur, Malaysia. Supervisor: Prof. Dr. Noorsaadah Binti Abd Rahman. Projects: 1. Discovery, development and synthesis of novel scaffold of leucine-rich repeat kinase 2 (LRRK2) inhibitors for Parkinson's disease (PD). a. Preparation and validation of LRRK2 protein homology model b. Docking studies of a small library of compounds c. Molecular dynamics simulations d. Chemical Synthesis of designed compounds e. Biological evaluation and SAR studies. 2. Discovery, optimization and synthesis of novel antimalarials able to inhibit Plasmepsin V activity and block parasites growth of P. falciparum and P. vivax. a. Pharmacophore-based virtual screening strategy of natural products database, b. Docking and molecular dynamics simulations studies, c. Biological evaluation of the best hit and SAR. 3. Computational studies, synthesis and biological evaluation of novel chikungunya virus inhibitors (flavonoids based scaffold). a. Rational design, b. Docking and Molecular dynamics studies. c. Chemical Synthesis of designed compounds 4. Development of peptide inhibitors of dengue 2 virus envelope protein: Computational, synthetic and biological approaches. a. Rational design, b. Docking and Molecular dynamics studies. c. Biological evaluation of the synthetized compounds. 5. Spiro-oxindole construction of a double penta-hexa fusedring system: Approach towards collective synthesis of mitraphylline and its related isomers via aza-Diels-Alder reaction.
01/04/2016-30/07/2018	Collaboration with my PhD research team, particularly Prof. Stefania Ferro and Prof. Laura De Luca, from the University of Messina, for the optimization of N1-aryl-benzimidazoles as non-nucleoside reverse transcriptase inhibitors active against wild-type and mutant HIV-1 strains: Computational studies and chemical synthesis (2 papers have been published).
01/01/2013 – 31/12/2015	Ph.D. Student in Pharmaceutical Sciences (Computational and Medicinal chemistry), at the University of Messina, department of Chemical, Biological, Pharmaceutical and Environmental Sciences under supervision of Prof. Laura De Luca, Associate Professor in Medicinal Chemistry. Subject: HIV-1 key enzymes: rational design, computational and synthetic approaches. 1. Rational design, docking studies, molecular dynamics simulations and hydrogen bond

	analysis for both Integrase-LEDGF-p/75 interaction inhibitors (LEDGINIs) and non-nucleoside reverse transcriptase inhibitors (NNRTIs). 2. Synthesis of the designed compounds and chemical characterization using NMR (1H and 13C), IR and Mass spectroscopy. 3. Biochemical and antiretroviral assays at Ohio State University, Columbus, Ohio, USA.
01/04/2015-30/09/2015	Visiting Scholar in the laboratories of Prof. Mamuka Kvaratskhelia and Prof. James Fuchs at College of Pharmacy, Ohio State University, USA. (I worked simultaneously on both the synthesis and the evaluation of the designed compounds). Subject: Discovery and development of a new class of LEDGINs. 1. Rational design and computational studies. 2. Synthesis of the designed compounds and chemical identification using NMR and Mass spectroscopy. 3. Biochemical assays using HTRF assays to determinate the IC50 for LEDGF/p75 dependent activity and Binding activity then 3'processing and strand transfer assays. SPR and western Blot were used to evaluate the binding of the potential inhibitors. 4. Crystallography of the best compounds with Integrase in order to determinate their binding position. 5. Antiviral and cytotoxicity assays.
12/04/2010 – 30/09/2010	Internship at CIRAD (Centre for International Cooperation in Agronomic Research for Development) within the Joint Research Unit, Data Integration Team, Montpellier, France. Subject: Design and development of a new generation of deductive database dedicated to the study of structure-function relationships of proteins: a pilot study with the superfamily nsLTP (Non Specific Lipid Transfer Protein) plant.

ATTIVITÀ PROGETTUALE

Anno	**Progetto**
2013-2015	HIV-1 key enzymes: rational design, computational and synthetic approaches.
01/04/2015 - 30/09/2015	Discovery and development of a new class of LEDGF/p75 Integrase Inhibitors.
12/04/2010 – 30/09/2010	Design and development of a new generation of deductive database dedicated to the study of structure-function relationships of proteins: a pilot study with the superfamily nsLTP (Non Specific Lipid Transfer Protein) plant.enzymes

CONGRESSI, CONVEGNI E SEMINARI

Data	**Titolo**	**Sede**
2-3 December 2015	Convegno Congiunto Delle Sezioni Calabria E Sicilia 2015. Società Chimica Italiana Natural Product-based inhibitors of HIV-1 IN-LEDGF/p75 interaction: computational and synthetic approaches. F.E. Agharbaoui, S. Ferro, R. Gitto, A. Hoyte, M. Kvaratskhelia, L. De Luca., Oral Presentation.	Catanzaro Italy
28th September – 3rd October 2014	Innovative approaches for identification of antiviral agents summer school. F.E. Agharbaoui, L. De Luca, S. Ferro, G. Lo Surdo, F. Morreale, Z. Debyser, R. Gitto; From natural products to HIV-1 IN/LEDGF interaction inhibitors: computational and synthetic approaches. Oral Presentation.	Pula, Sardinia, Italy
9-11 June 2014	NPCF 8 From Natural Products to potential drugs: a new hope in the antiviral	Parma Italy

	research. S. Ferro, L. De Luca, F.E. Agharbaoui, G. Lo Surdo, F. Morreale, Z.Debyser and R. Gitto	
2-3 December 2013	Convegno Congiunto Delle Sezioni Calabria E Sicilia 2013. Società Chimica Italiana. Lavendustin B and analogues as new promising molecules for inhibition of the interaction between HIV-1 IN and LEDGF. F.E. Agharbaoui, F. Morreale, S.Ferro, R. Gitto, Z. Debyser,b A. Chimirri, L. De Luca. Oral Presentation.	Catania Italy

PUBBLICAZIONI

1. Fasola E, Alboreggia G, Pieraccini S, Oliva F, **Agharbaoui FE,** Bollati M, Bertoni G, Recchia S, Marelli M, Piarulli U, Pellegrino S, Gazzola S. Conformational switch and multiple supramolecular structures of a newly identified self-assembling protein-mimetic peptide from Pseudomonas aeruginosa YeaZ protein. Front Chem. 2022 Dec.
2. Arumugam, A.C, **Agharbaoui, F.E,** Khazali, A.S., Yusof, R., Abd Rahman N., Ahmad Fuaad A.A.H., Computational-aided design: minimal peptide sequence to block dengue virus transmission into cells. J Biomol Struct Dyn. 2020 Dec 31:1-10. doi: 10.1080/07391102.2020.1866074. **(Co-first author)**
3. Lani, R., **Agharbaoui, F.E.,** Hassandarvish, P., Teoh, B.T, Sam, S.S, Zandi, K., Abd Rahman, N., AbuBakar, S., In silico studies of fisetin and silymarin as novel chikungunya virus nonstructural proteins inhibitors. Future virology vol. 16, no. 3, 2021, Short Communication. **(Co-first author)**
4. Monforte, A.M., Luca, L.D., Buemi, M.R**., Agharbaoui, F.E.,** Pannecouque, C., Ferro, S., Structural optimization of N1-aryl-benzimidazoles for the discovery of new non-nucleoside reverse transcriptase inhibitors active against wild-type and mutant HIV-1 strains. Bioorg Med Chem, 2018. 26(3): p. 661-674.
5. Ferro, S., Buemi, M.R., Luca, L.D., **Agharbaoui, F.E.,** Pannecouque, C., Monforte, A-M., Searching for novel N1-substituted benzimidazol-2-ones as non-nucleoside HIV-1 RT inhibitors, Bioorg Med Chem, 2017. 25(14):3861-3870.
6. **Agharbaoui, F.E.,** Hoyte A. C., Ferro S., Gitto R., Buemi M.R., Fuchs J.R., Kvaratskhelia M., De Luca L., Computational and synthetic approaches for developing Lavendustin B derivatives as allosteric inhibitors of HIV-1 integrase. Eur J Med Chem, 2016. 123: p. 673-683.
7. De Luca, L**., Agharbaoui, F.E.,** Gitto R., Christ F., Debyser Z., and Ferro S., Rational Design, Synthesis and Evaluation of Coumarin Derivatives as Protein-protein Interaction Inhibitors. Mol Inform, 2016. 35(8-9): p. 460-73. (Co-first author)
8. Ferro, S., De Luca, L., **Agharbaoui, F.E.,** Christ F., Debyser Z., Gitto R., Optimization of rhodanine scaffold for the development of protein-protein interaction inhibitors. Bioorg Med Chem, 2015. 23(13): p. 3208-14.

ALTRE INFORMAZIONI

Skills in Chemistry and computational chemistry

- **Enhanced Sampling Methods:** aMD, GaMD, Pep-GaMD, PPI-GAMD, LiGaMD, LiGaMD2, REMD...
- **Computational Chemistry:** Structure based virtual screening, Docking, Molecular dynamics simulations, enhanced sampling molecular dynamics, Drug binding analysis, Homology modeling…
- **Modeling and Computational chemistry tools:** Gromacs, Amber, MOE, Autodock, Discovery Studio, Maestro, LigandScout, CHARMm, GOLD, LigPlus, Pymol, Chimera, QSAR, Modeller, Plumed, ADME properties prediction, ...

Skills in Informatics / Bioinformatics

- **Operating Systems**: Linux (Ubuntu), Windows.
- **Languages**: Python, Bash, PERL, HTML, SQL, R…
- **Bioinformatics software:** Blast, ARPanno, EMBOSS, Fasta, GCG, ClustalX, ClustalW, Jalview, LEON, GCK, SRS, valid SeqMerge, GOanno, NetLogo, Prolog, R/Bioconductor ...
- **Statistics and Biostatistics:** MATLAB, SPSS, Origin

- **Office:** Word, Excel, PowerPoint.

Skills in Chemistry

- **Chemistry:** Synthetic routes design, Multi-step Organic synthesis, Peptide synthesis, Purification and Characterization techniques, Multi-nuclear NMR spectroscopy, Mass spectrometry, Microwave synthesis, Solvent purification systems, HPLC, Gas chromatography, FT-IR spectroscopy, Fluorescence and UV-Vis spectroscopy, structure elucidation, elemental analysis, UV melting...
- **Chemistry Tools:** SciFinder, ISIS Draw; Chem office, MestRenova, ACDLabs,...

Personal Skills

- Strong motivation and ability to adapt to change and easily apply new skills.
- Highly organized, attentive to detail, conscientious, and reliable team player.
- Self-driven, proactive, with creative problem-solving skills and forward-thinking attitude.
- Excellent oral and written communication and presentation skills: to share complex ideas and results with non-experts.

Le dichiarazioni rese nel presente curriculum sono da ritenersi rilasciate ai sensi degli artt. 46 e 47 del DPR n. 445/2000.

Il presente curriculum, non contiene dati sensibili e dati giudiziari di cui all'art. 4, comma 1, lettere d) ed e) del D.Lgs. 30.6.2003 n. 196.

RICORDIAMO che **i curricula SARANNO RESI PUBBLICI sul sito di Ateneo** e pertanto si prega di non inserire dati sensibili e personali. Il presente modello è già precostruito per soddisfare la necessità di pubblicazione senza dati sensibili.

Si prega pertanto di **NON FIRMARE** il presente modello.

Luogo e data: ___**Milano**__ , __**27/05/2024**_____