AL MAGNIFICO RETTORE
DELL'UNIVERSITA' DEGLI STUDI DI MILANO **COD. ID: 4372**

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 Chimica, responsabile scientifico il **Prof. Daniele Passarella**

Fatima Ezzahra AGHARBAOUI

CURRICULUM VITAE

I am active in lab designing synthetic routes, carrying out multi-step organic and peptides synthesis, purification, and analytical characterization. I have experience selecting and optimizing lead compounds through SAR for improved potency, selectivity, PK, and ADMET properties using synthetic and computational methods. I am also able to carry out biochemical assays.

INFORMAZIONI PERSONALI

Cognome	Fatima Ezzahra
Nome	AGHARBAOUI
Data Di Nascita	15/03/1985

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	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

10/08/2018 - present: Postdoctoral research fellow. at: Chemistry department, Faculty of Sciences, University of Malaya. Kuala Lumpur, Malaysia.

Subject:

1- Spiro-oxindole construction of a double penta-hexa fused-ring system: Approach towards collective synthesis of mitraphylline and its related isomers via aza-Diels-Alder reaction.

2- Discovery, optimization and synthesis of novel antimalarials able to inhibit Plasmepsin V activity and block parasites growth of P. falciparum and P. vivax and elucidation of their mechanism of action.

3- Development and synthesis of novel scaffold of leucine-rich repeat kinase 2 (LRRK2) inhibitors for Parkinson's disease.

4- Computational studies, synthesis and biological evaluation of novel chikungunya virus inhibitors.

5- Development of linear and cyclic peptidomimetics as inhibitors of dengue 2 virus envelope protein: Computational, synthetic and biological approaches.

01/04/2016-30/07/2018: Collaboration with Prof. Stefania Ferro and Prof. Laura De Luca from the university of Messina on the development of novel non-nucleoside reverse transcriptase inhibitors (Rational design, Computational studies and design of synthetic route). Two papers were recently published and others are going to be submitted soon.

01/01/2013 - 31/12/2015: Ph.D. Student in Pharmaceutical Sciences (Computational and Medicinal chemistry), at: University of Messina, department of Chemical, Biological, Pharmaceutical and Environmental Sciences.

- Supervisor: 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 IC_{50} 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.

01/07/2008 - 31/08/2008: Internship at INRA (National Institute of Agricultural Research), Rabat, Morocco.

- Subject: Study and Detection of genes resistant to drought in durum wheat using the technique of TILLING (Targeting Induced Local Lesions in Genomes).

01/07/2007 - 01/08/2007: Internship at the Laboratory of blood analysis at the provincial hospital in Beni Mellal

- Subject: Analysis of blood, semen and urine samples and microbiological test.

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.

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 research. S. Ferro, L. De Luca, F.E. Agharbaoui, G. Lo Surdo, F. Morreale, Z. Debyser and R. Gitto	Parma (Italy)
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

Articoli su riviste
P1. 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, 2017. In Press, https://doi.org/10.1016/j.bmc.2017.12.033
P2. 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.
P3. 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.
P4. 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)**
P5. 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

- **Chemistry :** Multi-step Organic synthesis, Solution and solid-phase peptide synthesis, Purification and Characterization techniques, Multi-nuclear NMR spectroscopy, Mass spectrometry, Microwave synthesis, Solvent purification systems, HPLC, LCMS, 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,
- **Computational Chemistry:** Structure based virtual screening, Docking, Molecular dynamics simulations, Drug binding analysis, Homology modeling…
- **Modeling and Computational chemistry tools :** Autodock, Discovery Studio, Maestro, Amber, LigandScout, CHARMm, GOLD, LigPlus, Pymol, Chimera, QSAR, Modeller, stochastic and continuous dynamical systems, neural networks, genetic algorithms, clustering…

Skills in Biology/Biochemistry

- **Cell Biology:** cell culture adherent, cryotheque management, optical microscopy.
- **Biochemistry:** extraction, synthesis, purification of peptides and proteins, protein assays, chromatography (TLC, GC, LC, HPLC), centrifugation and electrophoresis, HTRF assays, western Blot, SPR assays…
- **Genetic Engineering:** Extraction and analysis of nucleic acids (DNA and RNA) and protein electrophoresis, PCR…
- **Enzymology:** purification and determination of enzyme activity.
- **Microbiology :** culture, management, isolation, identification and determination of microorganisms. quantification by optical density measurement by spectrophotometry ...
- **Physical Chemistry:** UV-visible spectrophotometry, flow cytometry, solution preparation.
- **Materiel management:** preparation of culture media, reagents, equipment management to be sterilized, destruction of contaminated materials.

Skills in Informatics / Bioinformatics

- **Operating Systems :** Linux (Ubuntu), Windows (2008 server, XP, Vista, 7, 8, 10).
- **Languages :** C ++, PERL, LISP, HTML, SQL, Phyton…
- **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.

Personal Skills

- Strong motivation and ability to adapt to change and easily apply new skills.
- Handle multiple projects simultaneously due to organization and problem solving abilities.
- Strong Communication and teamwork skills.
- Ability to write scientific report and manuscript for publication.
- Ability to work independently as well as in a team environment.

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.

Luogo e data: _Kuala Lumpur, Malaysia__, __17/10/2019___

FIRMA _____

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