UNIVERSITÀ DEGLI STUDI DI MILANO

Curriculum vitae

AL MAGNIFICO RETTORE
DELL'UNIVERSITA' DEGLI STUDI DI MILANO **COD. ID: 4428**

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 ___ **SCIENZE CHIMICHE** ____

Responsabile scientifico: _ Prof. Pieraccini _____

Fatima Ezzahra AGHARBAOUI

CURRICULUM VITAE

INFORMAZIONI PERSONALI

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

OCCUPAZIONE ATTUALE

Incarico	Struttura
Posdoctoral research Fellow	University of Malaya, department of chemistry, Faculty of Sciences, Drug Discovery and Development Research Group, Kuala Lumpur, Malaysia.

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: Drug Discovery and Development Research Group, Chemistry department, Faculty of Sciences, University of Malaya. Kuala Lumpur, Malaysia.

Supervisor: Prof. Dr. Noorsaadah Binti Abd Rahman, Vice Deputy Chancellor of research.
Subjects:

1. Development of peptidomimetics inhibitors of dengue 2 virus envelope protein: Computational, synthetic and biological approaches.
   a. Rational design,
   b. Docking and Molecular dynamics studies.
2. Discovery, development and synthesis of novel scaffold of leucine-rich repeat kinase 2 (LRRK2) inhibitors for Parkinson's disease (PD).
   a. Creation and validation of LRRK2 protein homology model
   b. Docking studies of a small library of compounds
   c. Molecular dynamics simulations
   d. Biological evaluation and SAR studies.

3. 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.
4. Computational studies, synthesis and biological evaluation of novel chikungunya virus inhibitors (flavonoids based scaffold).
   a. Rational design,
   b. Docking and Molecular dynamics studies.

01/04/2016-30/07/2018: Collaboration with my PhD research group, 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: Monforte AM, et al. Bioorg Med Chem. 2018 Feb 1;26(3):661-674. Ferro S, et al. Bioorg Med Chem. 2017 Jul 15;25(14):3861-3870).

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 computational, synthesis and the evaluation of the designed compounds). This study permitted the discovery of a new promising scaffold with a multimodal mechanism of action for the inhibition of HIV-1 integrase-LEDGF/p75 interaction (Agharbaoui, F.E, et al. Eur J Med Chem, 2016. 123: p. 673-683).

- 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).

ATTIVITÀ PROGETTUALE

Anno	Progetto
2018-present	1. Development of peptidomimetics as inhibitors of dengue 2 virus envelope protein: Computational, synthetic and biological approaches. 2. Discovery, development and synthesis of novel scaffold of leucine-rich repeat kinase 2 (LRRK2) inhibitors for Parkinson's disease (PD). 3. Discovery, optimization and synthesis of novel antimalarials able to inhibit Plasmepsin V activity and block parasites growth of P. falciparum and P. vivax. 4. Computational studies, synthesis and biological evaluation of novel chikungunya virus inhibitors (flavonoids based scaffold).
2013-2015	HIV-1 key enzymes inhibitors: 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	Innovative approaches for identification of antiviral agents summer school.	Pula, Sardinia,

October 2014	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.	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 computational chemistry

- **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, …

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

- Handle multiple projects simultaneously due to organization and problem solving abilities.
- Strong motivation and ability to adapt to change and easily apply new skills.
- 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: ____04/12/2019_____, _____

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