Jessica Lombino

Contact

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Languages

Italian (native)
English (fluent)
French (basic)

Research interests

Medicinal chemist with drug design and computational chemistry expertise acquired during my PhD focused on the design and synthesis of novel inhibitors of epigenetic oncology-related therapeutic targets.

Work Experiences

October 2021 – Present **Postdoctoral researcher in Medicinal Chemistry**

University of Catania, Department of Drug and Health Sciences.
Group Leader: Prof. Emanuele Amata

Education

November 2017 – May 2021 **PhD in molecular and biomolecular sciences**
(with the additional label of Doctor Europaeus)

Industrial PhD in a collaboration between University of Palermo and Fondazione Ri.MED.
Company supervisor: Dr. Alessandro Padova. Academic supervisor: Prof. Patrizia Diana

Dissertation title: *"Rational design and synthesis of novel inhibitors of epigenetic target involved in cancer"*

May 2019 – December 2019 **PhD visiting scientist**
University of Vienna, Austria. Supervisor: Prof. Vittorio Pace

Project Title: *"New landscape in halogen-guided homologation chemistry of imine surrogates"*

July 2017 **Pharmacist License**

March 2017 **Master's Degree. Pharmacy and industrial pharmacy, Faculty of Pharmacy**
University of Palermo, Italy. Final mark: 110/110 *cum laude*

Thesis title: "*Synthesis of 5-phenoxyacetoamido-1H-pyrazole-4-carboxamide with potential biological activity"*

Conference attendance and Poster presentations

- **1-5 July 2018** *ESMEC European School of Medicinal Chemistry*. Urbino, Italy
- **17-20 July 2018** *MedChemSicily 2018*
- **26-28 September 2018:** *18th Annual European Schrodinger User Meeting*. Rome, Italy
- **19-24 May 2019** *XII European Workshop in Drug Design*. Siena, Italy.
- **11-13 July 2019** *XI Young Investigators Workshop* Vienna, Austria.

Skills

- Synthetic organic and medicinal chemistry, including purification and characterization of products.
- Computer Aided Drug Design: molecular modeling, drug design, docking, Pharmacophore modeling, molecular dynamics.
- Use of analytical instrumentation for compound identification
- Design and carry out scientific experiments safely and accurately
- Excellent written communication and report writing
- Work collaboratively within a multidisciplinary team
- Problem-solving skills to develop new and improved scientific solutions
- Plan and manage my own work effectively
- Flexibility

IT Skills

- Schrodinger suite: Maestro (Glide, Desmond, Prime) and Canvas
- LigandScout software
- Microsoft Office suite
- MestReNova software
- Operative system: Windows, IOS, Linux.

Publications

- *An overview of recent Molecular Dynamics applications as medicinal chemistry tool for undruggable sites challenge.*
  U. Perricone, M.R. Gulotta, **J. Lombino,** B. Parrino, S. Cascioferro, P. Diana, G. Cirrincione, A. Padova *MedChemComm* **9**, 920–936 (2018).

- *In Silico Insights towards the Identification of NLRP3 Druggable Hot Spots.*
  N. Mekni, M. De Rosa, C. Cipollina, M.R. Gulotta, G. De Simone, **J. Lombino**, A. Padova, U. Perricone. *International Journal of Molecular Sciences* **20**, 4974 (2019).

- *A New Family of Jumonji C Domain-Containing KDM Inhibitors Inspired by Natural Product Purpurogallin.*
  J.A Souto, F. Sarno, A. Nebbioso, C. Papulino, R. Alvarez, **J. Lombino**, U. Perricone, A. Padova, L. Altucci, A. de Lera. *Frontiers in Chemistry* **8**, 1–20 (2020).

- *Dynamic-shared pharmacophore approach as tool to design new allosteric PRC inhibitors, targeting EED binding pocket.*
  J. Lombino, M.R Gulotta, G. De Simone, N. Mekni, M. De Rosa, D. Carbone, B. Parrino, S.M Cascioferro, P. Diana, A. Padova, U. Perricone *Molecular Informatics* (2020). doi:10.1002/minf.202000148

- *Targeting SARS-CoV-2 RBD Interface: a Supervised Computational Data-Driven Approach to Identify Potential Modulators.*
  M.R Gulotta*, **J. Lombino*,** U. Perricone, G. De Simone, N. Mekni, M. De Rosa, P. Diana, A. Padova. *ChemMedChem* **15**, 1921–1931 (2020). *equal contribution

- *Halogen-Imparted Reactivity in Lithium Carbenoid Mediated Homologations of Imine Surrogates: Direct Assembly of bis-Trifluoromethyl-β-Diketiminates and the Dual Role of LiCH2I*
  L. Ielo, L. Castoldi, S. Touqeer, **J. Lombino**, A. Roller, C. Prandi, W. Holzer, V. Pace *Angewandte Chemie* **132**, 21038–21043 (2020).