



Roberta Astolfi

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WORK EXPERIENCE

 **UNIVERSITÉ CLAUDE BERNARD LYON 1 – LYON, FRANCE**

VISITING RESEARCHER – 01/09/2025 – CURRENT

Synthesis of new molecules active against DYRK1A

 **SAPIENZA, UNIVERSITY OF ROME – ROME, ITALY**

PHD STUDENT IN PHARMACEUTICAL SCIENCES – 01/11/2023 – CURRENT

- Design of Machine Learning Models for Prediction of Essential Oil Activity
- Study of Machine Learning Models through Analysis of Feature Importance and Partial Dependence
- 3D-QSAR and Drug Design
- Chemometrics

 **SAPIENZA, UNIVERSITY OF ROME – ROME, ITALY**

TUTORING FELLOWSHIP AT "ADVANCED TRAINING COURSE IN BIOINFORMATICS" – 04/2024 – 09/2024

- Support for attending students
- Support in handling python scripts, R or use of the bash shell
- Support in lectures based on Drug Design, 3D QSAR, Ligand Based and Structure Based approaches and Docking

 **SAPIENZA, UNIVERSITY OF ROME – ROME, ITALY**

TUTORING FELLOWSHIP "ORIENTAMENTO NEXT GENERATION" – 02/2024 – 07/2024

- Coordination Sapienza/Contracted school
- Coordination of teachers within each orientation course
- Keeping of students' attendance records
- Distance tutoring of students who have attended courses

 **SAPIENZA, UNIVERSITY OF ROME – ROME, ITALY**

FELLOWSHIP IN MEDICINAL CHEMISTRY – 02/2023 – 11/2023

Application of Machine Learning Methods to Develop Quantitative Composition-Activity Relationship Models for Complex Blends (Essential Oils)

 **DEPARTMENT OF DRUG CHEMISTRY AND TECHNOLOGY OF SAPIENZA, UNIVERSITY OF ROME – ROME, ITALY**

COLLABORATION FELLOWSHIP – 01/2022 – 01/2023

- Management and maintenance of the e-learning platform for the Faculty of Pharmacy

 **FARMACIA DEGLI ESTENSI – ROME, ITALY**

TRAINING INTERNSHIP – 10/2021 – 04/2022

EDUCATION AND TRAINING

21/07/2024 – 27/07/2024 Tübingen, Germany

SUMMER SCHOOL DRUG DESIGN AND DISCOVERY - 2024 University Eberhard Karls, Universität Tübingen

16/11/2023 Rome, Italy

STATE EXAM FOR THE PROFESSION OF PHARMACIST Sapienza, University of Rome

- Design of Machine Learning Models
- Microbiological Laboratory Analysis (MIC and MBC)
- Use of online databases: *AI4EssOil*

Address Piazzale Aldo Moro 5, 00185, Rome, Italy | **Field of study** Medicinal Chemistry | **Final grade** 110/110 cum Laude |

Thesis Application of Machine Learning algorithms to essential oils and their chemical compositions, to develop quantitative composition-activity relationship classification (QCAR) models. Predictive analysis and validation.

- Basic techniques for Steam Distillation
- Extraction and separation of essential oils and hydrolates
- Microbiological Laboratory Analysis (MIC and MBC)

Address Piazzale Aldo Moro 5, 00185, Rome, Italy | **Field of study** Medicinal Chemistry | **Final grade** 110/110 cum Laude |

Thesis Thymus vulgaris: extraction of essential oils and hydrolates for the evaluation of antibacterial activity against Acinetobacter baumannii

Address Via del Forte Braschi 99, 00167, Rome, Italy

● **LANGUAGE SKILLS**

Mother tongue(s): **ITALIANO**

Other language(s):

	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken production	Spoken interaction	
ENGLISH	B2	B2	B2	B2	B2

Levels: A1 and A2: Basic user; B1 and B2: Independent user; C1 and C2: Proficient user

● **SKILLS**

R | Bash | Python | Windows | MacOS | Linux

● **PUBLICATIONS**

2025
[Discovery of First-in-Class Carbonic Anhydrase/Histone Deacetylase Dual Inhibitors with Antiproliferative Activity in Cancer Cells](#)

Bozdag Murat, Mroweh Nabil, Raucci Alessia, Angeli Andrea, Peppicelli Silvia, Biagioni Alessio, Calorini Lido, Trisciunglio Daniela, Ragno Rino, Astolfi Roberta, Giuliani Lidia, Zwergel Clemens, Valente Sergio, Andreucci Elena, Carta Fabrizio, Mai Antonello, Supuran Claudiu T. - 20 Oct 2025

ACS Publications

2025
[Identification of D-Fructose Dehydration Products by Infrared Multi-Photon Dissociation Mass Spectrometry: The Spectral Signature of an Elusive 5-Hydroxymethylfurfural Isomer](#)

Fraschetti Caterina, Aschi Massimiliano, Ricci Andreina, Astolfi Roberta, Filippi Antonello

Publisher: ChemistryOpen

2025
[1,2,4-Oxadiazoles in medicinal chemistry: trends of the last years](#)

Cherkasova Anastasia, Astolfi Roberta, Nawrozki Maxim, Gladkikh Boris, Proia Eleonora, Giuliani Lidia, Rotili Dante, Ragno Rino - 5 Jul 2025

Journal Name: European Journal of Medicinal Chemistry

Ragno Alessio, Astolfi Roberta, Proietti Michela

Journal Name: Springer International Publishing

2025
Essential Oils as Antimicrobials against *Acinetobacter baumannii*: Experimental and Literature Data to Define Predictive Quantitative Composition-Activity Relationship Models Using Machine Learning Algorithms

Journal of Chemical Information and Modeling

Astolfi Roberta, Oliva Alessandra, Raffo Antonio, Sapienza Filippo, Ragno Alessio, Proia Eleonora, Mastroianni Claudio M, Luceri Cristina, Bozovic Mijat, Mladenovic Milan, Papa Rosanna, Bottoni Patrizia, Mazzinelli Elena, Nocca Giuseppina, Ragno Rino

2024
New methodological approaches applied to Cencelle (Tarquinia, VT)

Annoscia Giorgia Maria, Astolfi Roberta, Bellini Ilaria, Cavallero Serena, Chiovoloni Claudia, D'Amelio Stefano, Di Fazio Melania, Gabrielli Simona, Moschetto Francesco, Perugini Eleonora, Pombi Marco, Ragno Alessio, Ragno Rino, Rondón Silvia, Sapienza Filippo

SPOLIA

2023
Chemical Composition and Anti-Candida Activity of *Mentha suaveolens* Ehrh. Essential Oils Obtained by Different Distillation Processes

Tadić Vanja, Mijat Božović, Filippo Sapienza, Roberta Astolfi, Milan Mladenović, Maria Cristina Zaka, Fabiana Del Bove, Francesca Borzacchi, Caterina Frascchetti, Caterina Rossi, Silvia Vertuani, Anna Baldisserotto, Stefano Manfredini, Rino Ragno - 4 Oct 2023

MDPI - Molecules

2023
In Vitro Antioxidant and In Vivo Antigenotoxic Features of a Series of 61 Essential Oils and Quantitative Composition-Activity Relationships Modeled through Machine Learning Algorithms

Mladenović Milan, Roberta Astolfi, Nevena Tomašević, Sanja Matić, Mijat Božović, Filippo Sapienza, Rino Ragno - 29 Sep 2023

MDPI - Antioxidants

2023
Effect of Different Soil Treatments on Production and Chemical Composition of Essential Oils Extracted from *Foeniculum vulgare* Mill., *Origanum vulgare* L. and *Thymus vulgaris* L.

Raffo Antonio, Sapienza Umberto Filippo, Astolfi Roberta, Lombardi Gabriele, Frascchetti Caterina, Bozovic Mijat, Artini Marco, Papa Rosanna, Trecca Marika, Fiorentino Simona, Vecchiarelli Valerio, Papalini Claudia, Selan Laura, Ragno Rino - 31 Jul 2023

MDPI - Plants

2023
In Vivo Antiphytoviral and Aphid Repellency Activity of Essential Oils and Hydrosols from *Mentha suaveolens* and *Foeniculum vulgare* to Control Zucchini Yellow Mosaic Virus and Its Vector *Aphis gossypii*

Taglienti Anna, Donati Livia, Dragone Immacolata, Ferretti Luca, Gentili Andrea, Araniti Fabrizio, Sapienza Filippo, Astolfi Roberta, Fiorentino Simona, Vecchiarelli Valerio, Papalini Claudia, Ragno Rino, Bertin Sabrina - 28 Feb 2023

MDPI - Plants

● **DRIVING LICENCE**

Driving Licence: B

● **CONFERENCES AND SEMINARS**

06/12/2024 Viterbo
Valorizzazione della filiera di specie aromatiche e officinali nel Lazio - Progetto VOLA

Oral Presentation

22/09/2024 – 26/09/2024 Barcelona, Spain
24th EuroQSAR 2024

- **Poster Presentation** - "QCAR through machine learning algorithm. Application to essential oils tested as acetylcholinesterase inhibitors."

08/09/2024 – 11/09/2024 Balatonalmádi, Hungary
ISEO Internation Congress 2024

- **Oral Presentation** - "QCAR through machine learning algorithm. Application to essential oils tested as acetylcholinesterase inhibitors."

- **Poster Presentation** - "AI4EssOil: Revolutionizing Essential Oil Insights Through Artificial Intelligence"

05/09/2024 – 06/09/2024 Rome, Italy
EFMC-YMCS 2024

- **Poster Presentation** - "QCAR through machine learning algorithm. Application to essential oils tested as acetylcholinesterase inhibitors."

01/09/2024 – 05/09/2024 Rome, Italy
EFMC-ISMIC 2024

- **Poster Presentation** - "QCAR through machine learning algorithm. Application to essential oils tested as acetylcholinesterase inhibitors."

17/06/2024 – 19/06/2024 Sapienza, University of Rome
MedChem2024 - XIII Meeting Paul Ehrlich Euro-PhD Network & COST action

- **Oral Presentation** - "QCAR through machine learning algorithm. Application to essential oils tested as acetylcholinesterase inhibitors."

13/09/2023 – 16/09/2023 Milazzo, Sicily
ISEO International Congress 2023

- **Poster Presentation** - "Application of Machine Learning algorithms to essential oils to develop quantitative composition-activity relationships (QCAR) classification models."

30/06/2023 – 01/07/2023 Sapienza, University of Rome
SIROE National Congress 2023

- **Oral Presentation** - "Application of Machine Learning algorithms to essential oils to develop quantitative composition-activity relationships (QCAR) classification models."

● **HONOURS AND AWARDS**

11/2024
Research Initiation Grant 2024/2025 – Sapienza, University of Rome

26/09/2024
HITS Fellowship – 24th EuroQSAR 2024

11/09/2024
Young Scientists IFEAT Fellowship – ISEO International Congress 2024

16/09/2023
Young Scientists IFEAT Fellowship – ISEO International Congress 2023

Curriculum destinato al fine della pubblicazione

Rome , 10/11/2025



Roberta Astolfi