



## PERSONAL INFORMATION

## Rino Ragno



 Dep. Of Pharmaceutical Chemistry and Technology, Sapienza University - p.le A.Moro, 5 00185 Roma, Italia

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 Skype contact: rino.ragno

Sex Male | Nationality Italian

## POSITION

## Associate Professor

## BIOSKETCH

Rino Ragno is an associate professor at the Pharmacy and Medicine Faculty, Sapienza University of Rome where is in charge to teach medicinal chemistry at bachelor, master and PhD level. Since 1999, he started a new med chem design lab ([www.rcmd.it](http://www.rcmd.it)) with the aim to apply computational methodologies in the field of medicinal chemistry.

He published 139 international papers and presented more than 140 posters/oral communications at international meetings.

In 2005 he was awarded by the Italian Chemical Society - Italian division of medicinal chemistry for its research in medicinal chemistry.

Since 2017 he is enabled by Italian Government to be eligible as full professor in medicinal chemistry

Since 2015 he is in charge of leading the Sapienza MOOC Team to produce new MOOCs from Sapienza.

The main fields of the research are:

- Computational Medicinal Chemistry;
- Development of new QSAR and 3-D QSAR methods;
- Extraction, analysis and biological activity of essential oils;
- Development of scientific web sites ([www.3d-qsar.com](http://www.3d-qsar.com) and [eo.3d-qsar.com](http://eo.3d-qsar.com)).
- Drug Design through computational techniques: machine learning, molecular docking
- Virtual Screenings to select new potential bioactive compounds

## WORK EXPERIENCE

December 2010 - Present

## Associate Professor

Dept. Drug Chemistry and Technology - Sapienza University of Rome (Piazzale Aldo Moro, 5 00185 Roma – [www.uniroma1.it](http://www.uniroma1.it))

- Teacher of Medicinal Chemistry courses at Bachelor, Master and PhD Degree Level at Sapienza Rome University
- Component of the Pharmaceutical Science PhD Program Committee
- Component of the Pharmacy and Medicine Web Committee
- Vice-President of Sapienza University Editorial Web Committee
- Reference for Sapienza MOOC activities

March 2017

Business or sector Medicinal Chemistry (CHIM08)

## Enabled to Full Professorship for Medicinal Chemistry Research and Teaching.

ASN results 2016-2018. Academic Recruitment Field: Medicinal, Toxicological and Nutritional Chemistry and Applied Technologies (03/D1), Academic Discipline: Pharmaceutical Chemistry CHIM/08

May 2016 - Present

## President of Alchemical Dynamics a University Start Up

[www.alchemicaldynamics.com](http://www.alchemicaldynamics.com)

- November 2000 – December 2010 **Assistant Professor**  
Dept. Drug Chemistry and Technology - Sapienza University of Rome (Piazzale Aldo Moro, 5 00185 Roma – www.uniroma1.it)
- October 1990 – November 2000 **Assistant Professor**  
Dept. Drug Chemistry and Technology - Sapienza University of Rome (Piazzale Aldo Moro, 5 00185 Roma – www.uniroma1.it)
- March 1996 – March 1998 **Post-Doc**  
Center for Molecular Design - Washington University of St Louis - directed by prof. Garland R. Marshall.
- January 1999 - **Rome Center for Molecular Design Coordinator**  
Dept. Drug Chemistry and Technology - Sapienza University of Rome (Piazzale Aldo Moro, 5 00185 Roma – www.uniroma1.it)
- Sep 2009, Sep 2011, Sep 2014 **Visiting Professor**  
Laboratoire d'Ingénierie Moléculaire et Biochimie Pharmacologique chaired by Professeur Gilbert KIRSCH – Ex Université Paul Verlaine Metz - UMR CNRS 7565 SRSMC Université de Lorraine (France)

## EDUCATION AND TRAINING

- Nov 1990 – Feb 1992 **Master Degree in Pharmacy** Master  
Sapienza University of Rome (Piazzale Aldo Moro, 5 00185 Roma – www.uniroma1.it)  
▪ Experimental Thesis in Synthesis of antifungal compounds
- December 1991 **Pharmacist State Abilitation** Master  
Sapienza University of Rome (Piazzale Aldo Moro, 5 00185 Roma – www.uniroma1.it)
- Nov 1985 – Nov 1989 **Master Degree in Medicinal Chemistry** Bachelor + Master  
Sapienza University of Rome (Piazzale Aldo Moro, 5 00185 Roma – www.uniroma1.it)  
▪ Experimental Thesis in Synthesis of antiviral compounds
- Sep 1980 – June 1985 **Chemistry high School** High School  
ITIS GL Bernini Roma

## PERSONAL SKILLS

Mother tongue(s) Italian

Other language(s)

	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken interaction	Spoken production	
English	C1	C1	C1	C1	C1

Levels: A1/2: Basic user - B1/2: Independent user - C1/2 Proficient user  
Common European Framework of Reference for Languages

- Communication skills**
- Good communication skills gained through my experience as teacher at University and several International Congresses
- Organisational / managerial skills**
- Leadership (currently responsible for a team of more than 10 people)
- Job-related skills**
- Good command of quality control processes (currently responsible of a computational lab)
- Computer skills**
- Good command of Microsoft Office™ tools
  - MS Windows Operating System
  - MacOSX Operating System
  - Linux Operating System
  - HTML, C, bash, python programmer
  - Web Master (Drupal, Django, Joomla!)

- Other skills
- Medicinal Chemist
  - Drug Design
  - Molecular Modeling
  - E-learning (Moodle, Coursera, MOOC)
- Driving licence
- A + B + C

ADDITIONAL INFORMATION  
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**N References**

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- 2 Coluccia, A.; Passacantilli, S.; Famigliani, V.; Sabatino, M.; Patsilnakos, A.; **Ragno, R.**; Mazzoccoli, C.; Sisinni, L.; Okuno, A.; Takikawa, O.; Silvestri, R.; La Regina, G., New Inhibitors of Indoleamine 2,3-Dioxygenase 1: Molecular Modeling Studies, Synthesis, and Biological Evaluation. *J Med Chem* **2016**, *59*, 9760-9773.
- 3 Bozovic, M.; Garzoli, S.; Sabatino, M.; Pepi, F.; Baldisserotto, A.; Andreotti, E.; Romagnoli, C.; Mai, A.; Manfredini, S.; **Ragno, R.**, Essential Oil Extraction, Chemical Analysis and Anti-Candida Activity of *Calamintha nepeta* (L.) Savi subsp. *glandulosa* (Req.) Ball-New Approaches. *Molecules* **2017**, *22*
- 4 Mollica, A.; Pelliccia, S.; Famigliani, V.; Stefanucci, A.; Macedonio, G.; Chiavaroli, A.; Orlando, G.; Brunetti, L.; Ferrante, C.; Pieretti, S.; Novellino, E.; Benyhe, S.; Zador, F.; Erdei, A.; Szucs, E.; Samavati, R.; Dvrorskó, S.; Tomboly, C.; **Ragno, R.**; Patsilnakos, A.; Silvestri, R., Exploring the first Rimonabant analog-opioid peptide hybrid compound, as bivalent ligand for CB1 and opioid receptors. *J Enzyme Inhib Med Chem* **2017**, *32*, 444-451.
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- 6 Mijat Božović and **Rino Ragno** *Calamintha nepeta* (L.) Savi and its Main Essential Oil Constituent Pulegone: Biological Activities and Chemistry. *Molecules*. **2017** Feb 14;22(2). pii: E290. doi: 10.3390/molecules22020290
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- 8 Milan Mladenovic, Alexandros Patsilnakos, Adele Pirolli, Manuela Sabatino, and **Rino Ragno**. Understanding the Molecular Determinant of Reversible Human Monoamine Oxidase B Inhibitors Containing 2H-chromen-2-One Core: Structure-Based and Ligand-Based Derived 3-D QSAR Predictive Models. *J. Chem. Inf. Model.*, (2017). DOI: 10.1021/acs.jcim.6b00608. Publication Date (Web): March 14, 201
- 9 Clemens Zwergel, PhD; Brigitte Czepukojc.; Emilie Evain-Bana, Zhanjie Xu, Giulia Stazi, Mattia Mori, Alexandros Patsilnakos, Antonello Mai, Bruno Botta, **Rino Ragno**, Denyse Bagrel, Gilbert Kirsch, Peter Meiser, Claus Jacob, Mathias Montenarh, Sergio Valente. Novel Coumarin- and Quinolinone-Based Polycycles as Cell Division Cycle 25-A and -C Phosphatases Inhibitors Induce Proliferation Arrest and Apoptosis in Cancer Cells. *European Journal of Medicinal Chemistry*, **2017**
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- 57** Rinaldi, F.; Oliva, A.; Sabatino, M.; Imbriano, A.; Hanieh, P.N.; Garzoli, S.; Mastroianni, C.M.; De Angelis, M.; Miele, M.C.; Arnaut, M.; Di Timoteo, F.; Marianecchi, C.; **Ragno, R.**; Carafa, M. Antimicrobial Essential Oil Formulation: Chitosan Coated Nanoemulsions for Nose to Brain Delivery. *Pharmaceutics* **2020**, *12*, 678.
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- 58** Boriero, Diana, Carcereri de Prati, Alessandra; Antonini, Lorenzo; **Ragno, Rino**, Shoji, Kazuo, MARIOTTO, Sofia Giovanna, Butturini, Elena. The anti-STAT1 polyphenol myricetin inhibits M1 microglia activation and counteracts neuronal death. *FEBS 2020*
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- 59** Marta Di Martile, Stefania Garzoli, **Rino Ragno** and Donatella Del Bufalo. Essential oils and their main chemical components: 3 the past 20 years of preclinical studies in melanoma. *Cancers* **2020**.
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- 60** Rosanna Papa, Stefania Garzoli, Gianluca Vrenna, Manuela Sabatino, Filippo Sapienza, Michela Relucenti, Orlando Donfrancesco, Ersilia Vita Fiscarelli, Marco Artini, Laura Selan, **Rino Ragno**. Essential Oils Biofilm Modulation Activity, Chemical and Machine Learning Analysis. Application on *Staphylococcus aureus* Isolates from Cystic Fibrosis Patients. *Int J Mol Sci*, **2020** Dec 4;21(23):9258. doi: 10.3390/ijms21239258
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- 61** Di Martile M., Garzoli, Sabatino M., Valentini E., D'Aguzzo S., **Ragno R.**, Del Bufalo D. Antitumor effect of Melaleuca alternifolia essential oil and its main component terpinen-4-ol in combination with target therapy in melanoma models. *Cell Death Discovery*, Volume 7, Issue 1 June **2021** Article number 127
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- 62** Boriero D., Carcereri de Prati A., Antonini L., **Ragno R.**, Sohji K., Mariotto S.a, Butturini E. The anti-STAT1 polyphenol myricetin inhibits M1 microglia activation and counteracts neuronal death. *FEBS Journal* Volume 288, Issue 7, Pages 2347 – 2359 April **2021**
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- 63** Mihovic N., Tomasevic N., Matic S., Mitrovic M.M., Kostic D.A., Sabatino M., Antonini L., Ragno R., Mladenovic M. Human Estrogen Receptor  $\alpha$  Antagonists. Part 1: 3-D QSAR-Driven Rational Design of Innovative Coumarin-Related Antiestrogens as Breast Cancer Suppressants through Structure-Based and Ligand-Based Studies. *Journal of Chemical Information and Modeling*. **2021**. 61, 10,
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- 64** Vrenna G., Artini M., Ragno R., Relucenti M., Fiscarelli E.V., Assanti V.T.G., Papa R., Selan L. Anti-virulence properties of coridothymus capitatus essential oil against pseudomonas aeruginosa clinical isolates from cystic fibrosis patients. *Microorganisms*. **2021**. 9, 11.
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- 65** Paglia G., Antonini L., Cervoni L., Ragno R., Sabatino M., Minacori M., Rubini E., Altieri F. A comparative analysis of punicalagin interaction with PDIA1 and PDIA3 by biochemical and computational approaches. *Biomedicines*. **2021**. 9, 11.
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- 66** Kurtanovic N., Tomasevic N., Matic S., Mitrovic M.M., Kostic D.A., Sabatino M., Antonini L., Ragno R., Mladenovic M. Human estrogen receptor  $\alpha$  antagonists, part 2: Synthesis driven by rational design, in vitro antiproliferative, and in vivo anticancer evaluation of innovative coumarin-related antiestrogens as breast cancer suppressants. *European Journal of Medicinal Chemistry*. **2022**. 227
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- 67** Elisabetta Valentini, Simona D'Aguzzo, Marta Di Martile, Camilla Montesano, Virginia Ferraresi, Alexandros Patsilinos, Manuela Sabatino, Lorenzo Antonini,



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Sergio Valente, Antonello Mai, Gianni Colotti, Rino Ragno, Daniela Trisciuglio, Donatella Del Bufalo. Targeting the anti-apoptotic Bcl-2 family proteins: machine learning virtual screening and biological evaluation of new small molecules. *Theranostics* 2021; doi:10.7150/thno.64233; accepted

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Oral Presentations at Conferences  
(Last 5 Years)

1. XXIII National Meeting on Medicinal Chemistry. Salerno 2015
2. IV Congresso Nazionale dell'Associazione Scientifica S.I.R.O.E. Roma, 25-26 novembre 2016
3. Giornata Formativa SIROE sugli Oli Essenziali. Sapienza, Roma 8 settembre 2017
4. NanoInnovation 2018 Conference & Exhibition Rome, 11-14 September
5. The 22nd European Symposium on Quantitative Structure-Activity Relationships EuroQSAR 2018 September 2018 16 – 20 Thessaloniki, Greece
6. 2nd Molecules Medicinal Chemistry Symposium (MMCS): Facing Novel Challenges in Drug Discovery, Barcelona, Spain, 15–17 May 2019
7. 2nd Global Summit on Dermatology and Cosmetology Edinburgh, Scotland September 09-10, 2019
8. COST CM1406 Epigenetic Chemical Biology Scientific Workshop, 18-20 February 2019 Campus de Gambelas, University of Algarve, Faro, Portugal
9. Repositioning Natural Products in Drug Discover, FRIDAY, JANUARY 17th, 2020. University of Modena and Reggio Emilia
10. Invited for the plenary lecture at the 57th Meeting of the Serbian Chemical Society (scheduled for October 02-03. 2020 and postponed to June 18-19 2021 as an online meeting)

ERASMUS Teaching Mobility

- ✓ 2016: Laboratoire d'Ingénierie Moléculaire et Biochimie Pharmacologique – Ex Université Paul Verlaine Metz - UMR CNRS 7565 SRSMC Université de Lorraine (France)
- ✓ 2017: Laboratoire d'Ingénierie Moléculaire et Biochimie Pharmacologique – Ex Université Paul Verlaine Metz - UMR CNRS 7565 SRSMC Université de Lorraine (France)
- ✓ 2018: Laboratoire d'Ingénierie Moléculaire et Biochimie Pharmacologique – Ex Université Paul Verlaine Metz - UMR CNRS 7565 SRSMC Université de Lorraine (France)
- ✓ 2019: Laboratoire d'Ingénierie Moléculaire et Biochimie Pharmacologique – Ex Université Paul Verlaine Metz - UMR CNRS 7565 SRSMC Université de Lorraine (France)
- ✓ 2019: University of Barcelona (ES) – Pharmacy Faculty
- ✓ 2019: King's College of London (UK) – Pharmacy Faculty
- ✓ 2019: University of Motenegro (MN) – Science Faculty
- ✓ 2020: University of East Anglia (UK) – Pharmacy Faculty

Honours and awards

- 2005: Italian Division of Medicinal Chemistry Award for the Research in Medicinal Chemistry

Last Grants

- Italian Minister of Education: PRIN 2017 (141.100 euro/three years 2019-2022) Class IIa HDACs as therapeutic targets in human diseases: new roles and new selective inhibitors.
- European commission: Modernizing and Enhancing Indian E Learning Educational Strategies "MIELES". (573708-EPP-1-2016-1ES-EPPKA2-CBHE-JP) (45915 euro/three years 2017-2020)
- Ricerche di Ateneo 2018: 12000 euro/year
- Ricerche di Ateneo 2019: 14.500 euro/year
- Ricerche di Ateneo 2020: 13.000 euro/year

Conferences Organization/Scientific Committees

1. 22° National Meeting on Medicinal Chemistry. Scheduled for Roma 10-13 Settembre 2013 and postponed for COVID19 emergency to 16-18 February 2022 (<https://mmcs2022.sciforum.net/>)
2. Free Drupal Global Training Day - Venerdì 5 Febbraio 2016. Sapienza Università di Roma
3. Drupal Day 2017. 3-4 marzo 2017. Sapienza Università di Roma
4. Giornata Formativa SIROE sugli Oli Essenziali. Roma – Sapienza Università di Roma, 8 settembre 2017
5. Moodle MOOT Ita 2017. Roma – Sapienza Università di Roma, 28-30 settembre 2017
6. Member of CDA - SIROE

#### Textbooks or Book Chapters

1. Garland Marshall, Richard Head and Rino Ragno Affinity Prediction: The Sine Qua Non. Thermodynamics in Biology, Enrico di Cera, Editor, Oxford University Press. 87-111. 2000.
2. Rino Ragno. Tecniche di Screening per i nuovi farmaci. Alla ricerca del farmaco perduto, Carlo Tomino, Medi Service 2010, ISBN: 8890545925, ISBN-13: 9788890545924.
3. Ragno, R. Structure-Based Modeling of Histone Deacetylases Inhibitors. Epi-Informatics: Discovery and Development of Small Molecule Epigenetic Drugs and Probes. (2016) pp. 155-212. <https://www.scopus.com/inward/record.uri?eid=2-s2.0-84969722024&partnerID=40&md5=7e3020d6066e9a74a980146e42febd9f>
4. Milan Mladenović, Rino Ragno, Nevena Stanković, Nezirina Mihović, “RACIONALNI DIZAJN BIOAKTIVNIH JEDINJENjA: Od teorijskog do praktičnog pristupa”, (“RATIONAL DESIGN OF BIOACTIVE COMPOUNDS: From theoretical to practical approach”) ISBN: 978-86-6009-054-8

#### Patents

1. Mentha suaveolens essential oil and therapeutic activities thereof By Angiolella, Letizia; Ragno, Rino From Ital. (2013), IT 1398185 B1 20130214. | Language: Italian, Database: CAPLUS
2. Mentha suaveolens essential oil and therapeutic activities thereof By Angiolella, Letizia; Ragno, Rino From PCT Int. Appl. (2011), WO 2011092655 A2 20110804. | Language: English, Database: CAPLUS
3. Three-dimensional structure-based modeling predicting target selectivity in drug design By Ragno, Rino; Marshall, Garland R.; Ballante, Flavio From PCT Int. Appl. (2015), WO 2015002860 A1 20150108. | Language: English, Database: CAPLUS

#### Bibliometric Informations

1. Scopus (17/11/2021)
  - Total Papers 139
  - H-Index: 35
  - Total Citations: 3565

#### Journal Editing

1. Academic Editor for Molecules (<http://www.mdpi.com/journal/molecules>)
2. Academic Editor for International Journal of Molecular Science (<http://www.mdpi.com/journal/ijms>)

## Journal Reviewing

1. Reviewer for Medicinal Chemistry related journals
  - J. Med. Chem.
  - ACS Med. Chem. Lett.
  - European J. Med Chem.
  - Bioorg. Med. Chem.
  - Bioorg. Med. Chem. Lett.
  - Current Pharmaceutical Design
  - Medicinal Chemistry
  - Molecules
  - Journal of Pharmacy and Pharmacology
  - Medicinal Research Reviews
  - European Journal of Pharmaceutical Sciences
  - Journal Of Enzyme Inhibition And Medicinal Chemistry
  - Medicinal Research Reviews
  - Cancers
  - LETTERS IN DRUG DESIGN & DISCOVERY
  - CheMedChem
  - Medicinal Chemistry Communications
2. Reviewer for Chemical Informatic related journals
  - Journal of Chemical Information and Modeling
  - Bioinformatics
  - Journal of Molecular Graphics and Modelling
  - Molecular Informatics
  - Journal of Molecular Modeling
  - Journal of Computational Chemistry
  - Journal of Computer-Aided Molecular Design
  - PROTEINS: Structure, Function, and Bioinformatics
  - Chemical Biology & Drug Design
3. Reviewer for Natural Product related journals
  - Natural Product Research
4. General Biological and Chemistry related Journals
  - Nucleic Acids Research
  - The Journal of Physical Chemistry
  - FEBS Journal
  - Journal of the Taiwan Institute of Chemical Engineers