Curriculum Vitae

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

Full Professor

BIOSKETCH

Rino Ragno is a full 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.
In 1989 he finished the 5-year thesis in Pharmaceutical Chemistry and Technology at Sapienza University of Rome. Since 1990 he is enrolled in Sapienza University of Rome. In 1996-1998 he spent two years at the Center for Molecular Design lab directed by prof Garland Marshal ad Washington University of St. Louis (MO - USA). Since 1999, he started a new med chem design lab (www.rcmd.it) with the aim to apply computational methodologies in the field of medicinal chemistry. In 2005 he was awarded by the Italian Chemical Society - Italian division of medicinal chemistry for its research in medicinal chemistry.
From 2000 to 2010 he was an assisant professorand form 2010 20 2022 associate professor at Sapienza University of Rome.
Since 2015 he is in charge of leading the Sapienza MOOC Team to produce new MOOCs from Sapienza.
He published 162 international papers (156 listed in scopus.com) and presented more than 160 posters/oral communications at international meetings.
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, db.3d-qsar.com and www.ai4essoil.com).
- Drug Design through computational techniques: machine learning, molecular docking
- Virtual Screening to select new potential bioactive compounds
- Application of machine learning algorithms for the design of new bioactive molecules
- Application of machine learning algorithms for analysis of complex mixtures and correlation with their biological activity

WORK EXPERIENCE

March 2022 - Present

Full Professor

Dept. Drug Chemistry and Technology - Sapienza University of Rome (Piazzale Aldo Moro, 5 00185 Roma – www.uniroma1.it) - Academic Recruitment Field: Medicinal, Toxicological and Nutritional Chemistry and Applied Technologies (03/D1), Academic Discipline: Pharmaceutical Chemistry CHIM/08

- 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 Farmacy and Medicine Web Committee
- Vice-President of Sapienza University Editorial Web Committee
- Reference for Sapienza MOOC activities

Business or sector Medicinal Chemistry (CHIM08)

December 2010 - March 2022 **Associate Professor**

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

May 2016 - 2020 **President of Alchemical Dynamics a University Sturt Up**

www.alchemical dynamics.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 – Rank 110/110 cum laude

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 – Rank 110/110 cum laude

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 programming
- Web Master (Drupal, Django, Joomla!)
- Machine learning modeling

Other skills
- Medicinal Chemist
- Drug Design
- Molecular Modeling
- Extraction of Natural Compounds
- E-learning (Moodle, Coursera, MOOC)

Driving licence
- A + B + C

ADDITIONAL INFORMATION
Follow

Publications of last 5 years

N	References
1	Diego Muñoz-Torrero, Arduino A. Mangoni, Hong Liu, Christopher Hulme, Jarkko Rautio, Rafik Karaman, Maria Emília de Sousa, Katalin Prokai-Tatrai, Jean-Marc Sabatier, Carlo Siciliano, F. Javier Luque, George Kokotos, **Rino Ragno**, Simona Collina, Catherine Guillou, Michael Gütschow and Luigi A. Agrofoglio. *Molecules* **2018**, 23(1), 65; doi:10.3390/molecules23010065
2	Manuela Sabatino, Dante Rotili, Alexandros Patsilinakos, Mariantonietta Forgione, Daniela Tomaselli, Fréderic Alby, Paola B. Arimondo, Antonello Mai, **Rino Ragno**. *J Comput Aided Mol Des* (**2018**). https://doi.org/10.1007/s10822-018-0096-z
3	Alessandra Masci, Simone Carradori, Maria Antonietta Casadei, Patrizia Paolicelli, Stefania Petralito, **Rino Ragno**, Stefania Cesa. Lycium barbarum polysaccharides: Extraction, purification, structural characterisation and evidence about hypoglycaemic and hypolipidaemic effects. A review. *Food Chemistry* (**2018**)
4	L. Antonini, S. Garzoli, A. Ricci, A. Troiani, C. Salvitti, P. Giacomello, **R. Ragno**, A. Patsilinakos, B.Di Rienzo and F. Pepi. Ab-initio and experimental study of pentose sugar dehydration mechanism in the gas phase. Carbohydrate Research 458-459 (**2018**) 19-28
5	Marco Artini, Alexandros Patsilinakos, Rosanna Papa, Mijat Božović, Manuela Sabatino, Stefania Garzoli, Gianluca Vrenna, Marco Tilotta, Federico Pepi, **Rino Ragno** and Laura Selan. Antimicrobial and antibiofilm activity and machine learning classification analysis of essential oils from different Mediterranean plants against Pseudomonas aeruginosa. *Molecules* (**2018**)
6	Dr. Vincenzo Carafa, Angela Nebbioso, Francesca Cuomo, Dr. Dante Rotili, Dr. Gilda Cobellis, Dr. Paola Bontempo, Dr. Baldi Alfonso, Dr. Enrico P Spugnini, Dr. Gennaro Citro, Dr. Angela Chambery, Dr. Rosita Russo, Dr. Menotti Ruvo, Dr. Paolo Ciana, Dr. Luca Maravigna, Dr. Jani Shaik, Dr. Enrico Radaelli, Dr. Pasqualino De Antonellis, Dr. Domenico Tarantino, Dr. Adele Pirolli, **Dr. Rino Ragno**, Dr. Massimo Zollo, Dr. Hendrik G. Stunnenberg, Dr. Antonello Mai. RIP1-HAT1-SirT complex identification and targeting in treatment and prevention of cancer. *Clinical Cancer Research* MS# CCR-17-3081R (**2018**)

7	Mijat Božović, Stefania Garzoli, Anna Baldisserotto, Elisa Andreotti, Federico Pepi, Stefania Cesa, Silvia Vertuani, Stefano Manfredini and **Rino Ragno**. Melissa officinalis L. subsp. altissima (Sibth. & Sm.) Arcang. Essential Oil: Chemical Composition and2 Preliminary Antimicrobial Investigation of Samples Obtained at Different Harvestin2g Periods and by Fractionated Extractions. *Industrial Crops and Products* (**20182**)
8	Alexandros Patsilinakosa, **Rino Ragno**, Simone Carradori, Stefania Petralito,2 Stefania Cesa. Carotenoid content of Goji berries: CIELAB, HPLC-DAD analyses and quantitative correlation. *Food Chemistry* (**2018**)
9	Mijat Božović, Stefania Garzoli, Anna Baldisserotto, Elisa Andreotti, Stefania Cesa, Federico Pepi, Silvia Vertuani, Stefano Manfredini & **Rino Ragno**. Variation in Essential Oil Content and Composition of Ridolfia segetum Moris based on 30-hour Prolonged Fractionated Extraction Procedure. (ID: 1561688 DOI:10.1080/14786419.2018.1561688). Journal: Natural Product Research (**2019**)
10	Arduino A Mangoni, Catherine Guillou, Jean Jacques Vanden Eynde, Christopher Hulme, Josef Jampilek, Wei Li, Katalin Prokai-Tatrai, Jarkko Rautio, Simona Collina, Tiziano Tuccinardi, Maria Emília de Sousa, Jean-Marc Sabatier, Stefania Galdiero, Rafik Karaman, George Kokotos, Giangiacomo Torri, F. Javier Luque, M. Helena Vasconcelos, Dimitra Hadjipavlou-Litina, Carlo Siciliano, Michael Gütschow, **Rino Ragno**, Paula A. C. Gomes and Diego Muñoz-Torrero. Breakthroughs in Medicinal Chemistry: New Targets and Mechanisms, New Drugs, New Hopes–4. Molecules **2019**, 24, 130; doi:10.3390/molecules24010130
11	Nawrozkij Maxim, Forgione Mariantonietta, Yablokov Alexandre, Lucidi Alessia, Tomaselli Daniela, Patsilinakos Alexandros, Panella Cristina, Hailu Gebremedhin, Kirillov Ivan, Badia Roger, Riveira Muñoz Eva, Crespan Emmanuele, Armijos-Rivera Jorge, Cirilli Roberto, **Ragno Rino**, Este Jose, Maga Giovanni, Mai Antonello, Rotili Dante. Effect of α-Methoxy Substitution on the anti-HIV Activity of Dihydropyrimidin-4(3H)-ones". J. Med. Chem (**2019**)
12	G. Stazi, C. Battistelli, V. Piano, R. Mazzone, B. Marrocco, S. Marchese, S.M. Louie, C. Zwergel, L. Antonini, A. Patsilinakos, **R. Ragno**, M. Viviano, G. Sbardella, A. Ciogli, G. Fabrizi, R. Cirilli, R. Strippoli, A. Marchetti, M. Tripodi, D.K. Nomura, A. Mattevi, A. Mai, S. Valente, Development of alkyl glycerone phosphate synthase inhibitors: Structure-activity relationship and effects on ether lipids and epithelial-mesenchymal transition in cancer cells, European Journal of Medicinal Chemistry (**2019**), doi: https://doi.org/10.1016/j.ejmech.2018.11.050
13	Alessandra Oliva, Stefania Garzoli, Massimiliano De Angelis, Carolina Marzuillo, Vincenzo Vullo, Claudio M. Mastroianni and **Rino Ragno**. In-Vitro Evaluation of Different Antimicrobial Combinations with and without Colistin Against Carbapenem-Resistant Acinetobacter Baumannii. Molecules **2019**, 24(5), 886; https://doi.org/10.3390/molecules24050886
14	Alexandros Patsilinakos, Marco Artini, Rosanna Papa, Manuela Sabatino, Mijat Božović, Stefania Garzoli, Gianluca Vrenna, Raissa Buzzi, Stefano Manfredini, Laura Selan and **Rino Ragno**. Machine Learning Analyses on Data including Essential Oil Chemical Composition and In VitroExperimental Antibiofilm Activities against Staphylococcus Species. Molecules **2019**, 24(5), 890; https://doi.org/10.3390/molecules24050890
15	Mangoni, A.A., Eynde, J.J.V., Jampilek, J., Hadjipavlou-Litina, D., Liu, H.f, Reynisson, J., Sousa, M.E., Gomes, P.A.C., Prokai-Tatrai, K., Tuccinardi, T., Sabatier, J.-M., Luque, F.J., Rautio, J., Karaman, R., Vasconcelos, M.H., Gemma, S., Galdiero, S., Hulme, C., Collina, S., Gütschow, M., Kokotos, G., Siciliano, C., Capasso, R., Agrofoglio, L.A., **Ragno, R.**, Muñoz-Torrero, D. Breakthroughs in medicinal chemistry: New targets and mechanisms, New Drugs, New Hopes-5. *Molecules* **2019**, 24(13), 2415. DOI: 10.3390/molecules24132415

16	Ilaria Marrocco, Fabio Altieri, Elisabetta Rubini, Giuliano Paglia, Silvia Chichiarelli, Flavia Giamogante, Alberto Macone, Giacomo Perugia, Fabio Massimo Magliocca, Aymone Gurtner, Bruno Maras, **Rino Ragno**, Alexandros Patsilinakos, Roberto Manganaro and Margherita Eufemi. Shmt2: A Stat3 Signaling New Player in Prostate Cancer Energy Metabolism. Cells **2019**, 8(9), 1048; https://doi.org/10.3390/cells8091048
17	**Rino Ragno**. www.3d-qsar.com. A Web Portal that Brings 3-D QSAR to All Electronic Devices. The Py-CoMFA Web Application as Tool to Build Models from Pre-Aligned Datasets. *Journal of Computer-Aided Molecular Design*, (**2019**) 33:855–864. https://doi.org/10.1007/s10822-019-00231-x
18	Giulia Stazi, Ludovica Taglieri, Alice Nicolai, Annalisa Romanelli, Rossella Fioravanti, Stefania Morrone, Manuela Sabatino, **Rino Ragno**, Samanta Taurone, Marcella Nebbioso, Raffaella Carletti, Marco Artico, Sergio Valente, Susanna Scarpa and Antonello Mai. Dissecting the role of novel EZH2 inhibitors in primary glioblastoma cell cultures: effects on proliferation, epithelial-mesenchymal transition, migration, and on the pro-inflammatory phenotype. Clinical Epigenetics volume 11, Article number: 173 (**2019**)
19	Stefania Garzoli, Lorenzo Antonini, Anna Troiani, Chiara Salvitti, Pierluigi Giacomello, Alexandros Patsilinakos, **Rino Ragno**, Federico Pepi. Gas-phase structures and thermochemical properties of protonated 5-HMF isomers. International Journal of Mass Spectrometry, **2020**, https://doi.org/10.1016/j.ijms.2019.116237
20	Nobile, V., Palumbo, F., Lanni, S., Ghisio, Vc, Vitali, A., Castagnola, M., Marzano, V., Maulucci, G., De Angelis, C., De Spirito, M., Pacini, L., D'Andrea, L., **Ragno, R**., Stazi, G., Valente, S., Mai, A., Chiurazzi, P., Genuardi, M., Neri, G., Tabolacci, E. Altered mitochondrial function in cells carrying a premutation or unmethylated full mutation of the FMR1 gene. Human Genetics, Volume 139, Issue 2, 1 February **2020**, Pages 227-245
21	Alessandra Oliva, Stefania Garzoli, Manuela Sabatino, Vanja Tadić , Silvia Costantini , **Rino Ragno** and Mijat Božović. Chemical Composition and Antimicrobial Activity of Essential Oil of Helichrysum italicum (Roth) G. Don fil. (Asteraceae) from Montenegro. Nat Prod Res. **2020** Feb;34(3):445-448. doi: 10.1080/14786419.2018.1538218
22	Vanden Eynde, J.J., Mangoni, A.A., Rautio, J., Leprince, J., Azuma, Y.-T., García-Sosa, A.T., Hulme, C., Jampilek, J., Karaman, R., Li, W., Gomes, P.A.C., Hadjipavlou-Litina, D., Capasso, R., Geronikaki, A., Cerchia, L., Sabatier, J.-M., **Ragno, R**., Tuccinardi, T., Trabocchi, A., Winum, J.-Y. Breakthroughs in medicinal chemistry: New targets and mechanisms, new drugs, new hopes-6. Molecules. Volume 25, Issue 1, **2020**, Article number 119
23	**Rino Ragno**, Rosanna Papa, Alexandros Patsilinakos, Gianluca Vrenna, Stefania Garzoli, Vanessa Tuccio, Ersilia Vita Fiscarelli, Laura Selan, and Marco Artini. Essential oils against bacterial isolates from cystic fibrosis patients by means of antimicrobial and unsupervised machine learning approaches. Sci Rep. **2020** Feb 14;10(1):2653. doi: 10.1038/s41598-020-59553-8.
24	Silvia Caroselli, Clemens Zwergel, Adele Pirolli, Manuela Sabatino, Zhanjie Xu, Gilbert Kirsch, Antonello Mai, Gianni Colotti, Fabio Altieri, Rita Canipari, Sergio Valente, **Rino Ragno**. Discovery of the First Human Arylsulfatase A Reversible Inhibitor Impairing Mouse Oocyte Fertilization, **2020**, https://doi.org/10.1021/acschembio.9b00999
25	Tanira Matutino Bastos, Milena Botelho Pereira Soares, Caio Haddad Franco, Laura Alcântara, Lorenzo Antonini, Manuela Sabatino, Nicola Mautone, Lucio Holanda FreitasJunior, Carolina Borsoi Moraes, **Rino Ragno**, Dante Rotili, Sergio Schenkman, Antonello Mai and Nilmar Silvio Moretti. Identification of Inhibitors to Trypanosoma cruzi Sirtuins Based on Compounds Developed to Human Enzymes. Int. J. Mol. Sci. **2020**, 21, 3659. DOI: https://doi.org/10.3390/ijms21103659

26	Maura Di Vito, Maria Grazia Bellardi, Maurizio Sanguinetti, Francesca Mondello, Antonietta Girolamo, Lorenzo Barbanti, Stefania Garzoli, Manuela Sabatino, **Rino Ragno**, Alberto Vitali, Ivana Palucci, Brunella Posteraro, Antonio Gasbarrini, Gian Maria Prati, Giovanni Aragona, Paola Mattarelli and Francesca Bugli. Potent in vitro activity of Citrus aurantium essential oil and Vitis vinifera hydrolate against gut yeast isolates from irritable bowel syndrome patients: the right mix for potential therapeutic use. Nutrients **2020**, 12, 1239; doi: https://doi.org/10.3390/nu12051329
27	Manuela Sabatino, Marco Fabiani, Mijat Bozovic, Stefania Garzoli, Lorenzo Antonini, Maria Elena Marcocci, Anna Teresa Palamara, Giovanna De Chiara, **Rino Ragno**. Experimental Data Based Machine Learning Classification Models with Predictive Ability to Select in-vitro Active Antiviral and Non–Toxic Essential Oils. Molecules **2020**, 25, 2452. DOI: https://doi.org/10.3390/molecules25102452
28	**Ragno, Rino**; Esposito, Valeria; Di Mario, Martina; Masiello, Stefano; Viscovo, Marco; Cramer, Richard. Teaching and Learning Computational Drug Design: Student Investigations of 3D Quantitative Structure–Activity Relationships through Web Applications. The Journal of Chemical Education, **2020**. DOI: 10.1021/acs.jchemed.0c00117
29	Michael Gütschow, Jean Jacques Vanden Eynde, Josef Jampílek, CongBao Kang, Arduino A. Mangoni, Paola Fossa, Rafik Karaman, Andrea Trabocchi, Peter J. H. Scott, Jóhannes Reynisson, Simona Rapposelli, Stefania Galdiero, Jean-Yves Winum, Chiara Brullo, Katalin Prokai-Tatrai, Arun K. Sharma, Matthieu Schapira, Yasu-Taka Azuma, Laura Cerchia, Mariana Spetea, Giangiacomo Torri, Simona Collina, Athina Geronikaki, Alfonso T. García-Sosa, Maria Helena Vasconcelos, Maria Emília Sousa, Ivan Kosalec, Tiziano Tuccinardi, Iola F. Duarte, Jorge A. R. Salvador, Massimo Bertinaria, Maurizio Pellecchia, Jussara Amato, Giulio Rastelli, Paula A. C. Gomes, Rita C. Guedes, Jean-Marc Sabatier, Ana Estévez-Braun, Bruno Pagano, Stefano Mangani, **Rino Ragno**, George Kokotos, Margherita Brindisi, Florenci V. González, Fernanda Borges, Mariarosaria Miloso, Jarkko Rautio and Diego Muñoz-Torrero. Breakthroughs in medicinal chemistry: New targets and mechanisms, new drugs, new hopes-7. Molecules. **2020**
30	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.; Marianecci, C.; **Ragno, R**.; Carafa, M. Antimicrobial Essential Oil Formulation: Chitosan Coated Nanoemulsions for Nose to Brain Delivery. Pharmaceutics **2020**, 12, 678.
31	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
32	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 ??????**.
33	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
34	Di Martile M., Garzoli, Sabatino M., Valentini E., D'Aguanno 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
35	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 JournalVolume 288, Issue 7, Pages 2347 – 2359 April **2021**

36	Mihovic N., Tomasevic N., Matic S., Mitrovic M.M., Kostic D.A., Sabatino M., Antonini L., Ragno R., Mladenovic M. Human Estrogen Receptor α 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,
37	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.
38	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.
39	Kurtanovic N., Tomasevic N., Matic S., Mitrovic M.M., Kostic D.A., Sabatino M., Antonini L., Ragno R., Mladenovic M. Human estrogen receptor α 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
40	Elisabetta Valentini, Simona DAguanno, Marta Di Martile, Camilla Montesano, Virginia Ferraresi, Alexandros Patsilinakos, Manuela Sabatino, Lorenzo Antonini, Sergio Valente, Antonello Mai, Gianni Colotti, Rino Ragno, Daniela Trisciuoglio, Donatella Del Bufalo. Targeting the anti-apoptotic Bcl-2 family proteins: machine learning virtual screening and biological evaluation of new small molecules. Theranostics **2022**; 12(5):2427-2444. doi:10.7150/thno.64233
51	Martina Minisini, Eros Di Giorgio, Emanuela Kerschbamer, Emiliano Dalla, Massimo Faggiani, Elisa Franforte, Franz-Josef Meyer-Almes, **Rino Ragno**, Lorenzo Antonini, Antonello Mai, Francesco Fiorentino, Dante Rotili, Monica Chinellato, Stefano Perin, Laura Cendron, Christian X. Weichenberger, Alessandro Angelini and Claudio Brancolini. Transcriptomic and genomic studies classify NKL54 as a histone deacetylase inhibitor with indirect influence on MEF2-dependent transcription. Nucleic Acids Research, **2022** 1–21. https://doi.org/10.1093/nar/gkac081
52	Morroni, Jacopo, Leonardo Schirone, Valentina Valenti, Clemens Zwergel, Carles S. Riera, Sergio Valente, Daniele Vecchio, Sonia Schiavon, **Rino Ragno**, Antonello Mai, Sebastiano Sciarretta, Biliana Lozanoska-Ochser, and Marina Bouchè. "Inhibition of PKCθ Improves Dystrophic Heart Phenotype and Function in a Novel Model of DMD Cardiomyopathy" International Journal of Molecular Sciences **2022**, 23, no. 4: 2256. https://doi.org/10.3390/ijms23042256
53	Božović, M.; Garzoli, S.; Vujović, S.; Sapienza, F.; **Ragno, R**. Foeniculum vulgare Miller, a New Chemotype from Montenegro. Plants **2022**, 11, 42. https://doi.org/10.3390/plants11010042
54	Taglienti Anna, Donati Livia, Ferretti Luca, Tomassoli Laura, Sapienza Filippo, Sabatino Manuela, Di Massimo Gaia, Fiorentino Simona, Vecchiarelli Valerio, Nota Paolo, **Ragno Rino**. In vivo Antiphytoviral Activity of Essential Oils and Hydrosols From Origanum vulgare, Thymus vulgaris, and Rosmarinus officinalis to Control Zucchini Yellow Mosaic Virus and Tomato Leaf Curl New Delhi Virus in Cucurbita pepo L. **2022**. Frontiers in Microbiology, https://www.frontiersin.org/article/10.3389/fmicb.2022.840893
55	Artini, Marco, Rosanna Papa, Filippo Sapienza, Mijat Božović, Gianluca Vrenna, Vanessa Tuccio Guarna Assanti, Manuela Sabatino, Stefania Garzoli, Ersilia V. Fiscarelli, **Rino Ragno**, and Laura Selan. **2022**. "Essential Oils Biofilm Modulation Activity and Machine Learning Analysis on Pseudomonas aeruginosa Isolates from Cystic Fibrosis Patients" Microorganisms 10, no. 5: 887. https://doi.org/10.3390/microorganisms10050887
56	Kurtanović, Nezrina, Nevena Tomašević, Sanja Matić, Elenora Proia, Manuela Sabatino, Lorenzo Antonini, Milan Mladenović, and **Rino Ragno**. **2022**. "Human Estrogen Receptor Alpha Antagonists, Part 3: 3-D Pharmacophore and 3-D QSAR Guided Brefeldin A Hit-To-Lead Optimization toward New Breast Cancer Suppressants" Molecules 27, no. 9: 2823. https://doi.org/10.3390/molecules27092823

57	Proia E, Ragno A, Antonini L, Sabatino M, Mladenovič M, Capobianco R, Ragno R. Ligand-based and structure-based studies to develop predictive models for SARS-CoV-2 main protease inhibitors through the 3d-qsar.com portal. J Comput Aided Mol Des. **2022** Jun 18:1–23. doi: 10.1007/s10822-022-00460-7. Epub ahead of print. PMID: 35716228; PMCID: PMC9206107.
58	Thalappil, Muhammed Ashiq, Elena Butturini, Alessandra Carcereri de Prati, Ilaria Bettin, Lorenzo Antonini, Filippo Umberto Sapienza, Stefania Garzoli, **Rino Ragno**, and Sofia Mariotto. **2022**. "Pinus mugo Essential Oil Impairs STAT3 Activation through Oxidative Stress and Induces Apoptosis in Prostate Cancer Cells" Molecules 27, no. 15: 4834. https://doi.org/10.3390/molecules27154834
59	**Rino Ragno**, Anna Minarini, Eleonora Proia, Antonini Lorenzo, Andrea Milelli, Vincenzo Tumiatti, Marco Fiore, Pasquale Fino, Lavinia Rutigliano, Rossella Fioravanti, Tomoaki Tahara, Elena Pacella, Antonio Greco, Gianluca Canettieri, Maria Luisa Di Paolo, and Enzo Agostinelli. Bovine Serum Amine Oxidase and Polyamine Analogues: Chemical Synthesis and Biological Evaluation Integrated with Molecular Docking and 3-D QSAR Studies. Journal of Chemical Information and Modeling. **2022**. Article ASAP. DOI: 10.1021/acs.jcim.2c00559
60	Vukić, Milena D., Nenad L. Vuković, Milan Mladenović, Nevena Tomašević, Sanja Matić, Snežana Stanić, Filippo Sapienza, **Rino Ragno**, Mijat Božović, and Miroslava Kačániová. **2022**. "Chemical Composition of Various *Nepeta cataria* Plant Organs' Methanol Extracts Associated with *In Vivo* Hepatoprotective and Antigenotoxic Features as well as Molecular Modeling Investigations" *Plants* 11, no. 16: 2114. https://doi.org/10.3390/plants11162114
61	Rossella Fioravanti, Eleonora Proia, Ivan N. Tyurenkov, Denis V. Kurkin, Dmitry A. Bakulin, Nikolay S. Kovalev, Dmitry S. Sheikin, Ivan A. Kirillov, Maxim B. Nawrozkij, Andrey A. Vernigora, Leila L. Brunilina, Francesco Fiorentino, Milan Mladenović, Dante Rotili, **Rino Ragno**, Pyrimidine thioethers: A novel class of antidepressant agents, endowed with anxiolytic, performance enhancing and nootropic activity, European Journal of Medicinal Chemistry, Volume 245, Part 2, **2023**, 114902, ISSN 0223-5234, https://doi.org/10.1016/j.ejmech.2022.114902
62	Božović M, Mladenović M, **Ragno R**. Editorial: Chemical composition and antimicrobial activity of essential oils. Front Pharmacol. **2023** Jan 13;14:1120756. doi: 10.3389/fphar.2023.1120756. PMID: 36713842; PMCID: PMC9880459.
63	Makhoba XH, **Ragno R**, Kaiser A, Agostinelli E. An Undefined Interaction between Polyamines and Heat Shock Proteins Leads to Cellular Protection in *Plasmodium falciparum* and Proliferating Cells in Various Organisms. Molecules. **2023** Feb 10;28(4):1686. doi: 10.3390/molecules28041686. PMID: 36838674; PMCID: PMC9958663.
64	Taglienti A, Donati L, Dragone I, Ferretti L, Gentili A, Araniti F, Sapienza F, Astolfi R, Fiorentino S, Vecchiarelli V, Papalini C, **Ragno R**, Bertin S. 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*. Plants (Basel). **2023** Feb 28;12(5):1078. doi: 10.3390/plants12051078. PMID: 36903936; PMCID: PMC10005592.
65	Schiavone V., Romasco T., Di Pietrantonio N., Garzoli S., Palmerini C., Di Tomo P., Pipino C., Mandatori D., Fioravanti R., Butturini E., Sabatino M., Baldassarre M.P.A., **Ragno R**., Pandolfi A., Di Pietro N.; Essential oils from mediterranean plants inhibit in vitro monocyte adhesion to endothelial cells from umbilical cords of females with gestational diabetes mellitus. International Journal of Molecular Sciences, **2023**, 24(8) doi:10.3390/ijms24087225
66	Giorgia Drudi Metalli and **Rino Ragno**. Oli Essenziali dalla preistoria al medio evo. Natural1 **2023**, Gen-Feb, pages 46-47.
67	Giorgia Drudi Metalli and **Rino Ragno**. Medicina e oli essenziali nell'Antico Egitto, nel vicino Oriente Antico e in Cina. Natural1 **2023**, March, pages 22-28.
68	Giorgia Drudi Metalli and **Rino Ragno**. Gli oli essenziali ai tempi delle antiche civiltà greca e romana. Natural1 **2023**, April, pages 32-38

69	Giorgia Drudi Metalli, Giorgia Annoscia and **Rino Ragno**. Gli oli essenziali nel Medioevo: i monasteri e gli orti ed erbari. Natural1 **2023**, July-August, pages 28-34
70	Elisabetta Valentini, Marta Di Martile, Matteo Brignone, Marica Di Caprio, Isabella Manni, Michela Chiappa, Ilaria Sergio, Martina Chiacchiarini, Chiara Bazzichetto, Fabiana Conciatori, Simona D'Aguanno, Carmen D'Angelo, **Rino Ragno**, Michelangelo Russillo, Gianni Colotti, Francesco Marchesi, Maria Laura Bellone, Fabrizio Dal Piaz, Maria Pia Felli, Giovanna Damia & Donatella Del Bufalo . Bcl-2 family inhibitors sensitize human cancer models to therapy. Cell Death Dis 14, 441 (**2023**). https://doi.org/10.1038/s41419-023-05963-1
71	Antonio Raffo, Filippo Umberto Sapienza, Roberta Astolfi, Gabriele Lombardi, Caterina Fraschetti, Mijat Božović, Marco Artini, Rosanna Papa, Marika Trecca, Simona Fiorentino, Valerio Vecchiarelli, Claudia Papalini, Laura Selan and **Rino Ragno**. 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. Plants **2023**, 12, 2835. https://doi.org/10.3390/plants12152835
72	Tomašević N, Vujović M, Kostić E, Ragavendran V, Arsić B, Matić SL, Božović M, Fioravanti R, Proia E, **Ragno R**, Mladenović M. Molecular Docking Assessment of Cathinones as 5-HT2AR Ligands: Developing of Predictive Structure-Based Bioactive Conformations and Three-Dimensional Structure-Activity Relationships Models for Future Recognition of Abuse Drugs. Molecules. **2023** Aug 24;28(17):6236. doi: 10.3390/molecules28176236. PMID: 37687065; PMCID: PMC10488745.
73	Makhoba XH, **Ragno R**, Kaiser A, Agostinelli E. An Undefined Interaction between Polyamines and Heat Shock Proteins Leads to Cellular Protection in Plasmodium falciparum and Proliferating Cells in Various Organisms. Molecules. **2023** Feb 10;28(4):1686. doi: 10.3390/molecules28041686. PMID: 36838674; PMCID: PMC9958663.
74	Mladenović, Milan, Roberta Astolfi, Nevena Tomašević, Sanja Matić, Mijat Božović, Filippo Sapienza, and **Rino Ragno**. **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" Antioxidants 12, no. 10: 1815. https://doi.org/10.3390/antiox12101815
75	Tadić, Vanja, Mijat Božović, Filippo Sapienza, Roberta Astolfi, Milan Mladenović, Maria Cristina Zaka, Fabiana Del Bove, Francesca Borzacchi, Caterina Fraschetti, Caterina Rossi, and et al, **Rino Ragno**. **2023**. "Chemical Composition and Anti-Candida Activity of Mentha suaveolens Ehrh. Essential Oils Obtained by Different Distillation Processes" Molecules 28, no. 19: 6934. https://doi.org/10.3390/molecules28196934
76	Deligianni E, Pizzi E, Kavelaki I, Siden-Kiamos I, Sapienza FU, Fioravanti R, Garzoli S, Pace T, Ponzi M, **Ragno R**, Currà C. Screening of the activity of sixty essential oils against plasmodium early mosquito stages in vitro and machine learning analysis reveals new putative inhibitors of malaria parasites. Int J Parasitol Drugs Drug Resist. **2023** Dec;23:87-93. doi: 10.1016/j.ijpddr.2023.11.002. Epub 2023 Nov 21. PMID: 38000094; PMCID: PMC10709126.

Oral Presentations at Conferences

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)
11. Oral presentation at XXVII edition of National Meeting in Medicinal Chemistry Bari 2022
12. Oral Presentation at the 53rd International Symposium on Essential Oils (ISEO 2023) Milazzo 2023
13. Oral Presentation at 2nd International Conference on Chemo and BioInformatics (ICCBIKG 2023) Kragujevac, September 28-29, 2023, Serbia

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: Uniersity of Motenegro (MN) – Science Faculty
- ✓ 2020: University of East Anglia (UK) – Pharmacy Faculty
- ✓ 2021: University of Athens (GR) – Pharmacy Faculty
- ✓ 2022: University of Bucarest (RO) – Pharmacy Faculty

Honours and awards

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

Last Grants

- ➢ Progetti di Ricerca e Sviluppo da realizzare nell'ambito degli Accordi di Innovazione ridefiniti nel DM 31 dicembre 2021 del Ministero per lo Sviluppo Economico e perfezionati nel DD del 18 marzo 2022, n.721. Ricerca per l'identificazione di nuovi approcci terapeutici nell'Oftalmologia con particolare riguardo alla "Innovazione nella terapia farmacologica della profilassi pre e post- operatoria della chirurgia oftalmologica". Finanziamento 378.000 Euro, 36 months
- ➢ 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 lndian 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
- ➢ Progetto di Ricerca e Sviluppo dal titolo "Innovazione nella Terapia Farmacologica e Clinica della Profilassi pre e post Operatoria della Chirurgia Oftalmologica" (numero posizione 139 - Progetto n. F/310139/01-02/X56) € 378000/three years

Conferences Organization/Scientific Committees

1. 7° Congresso Nazionale della Società Italian per la Ricerca sugli Oli Essenziali. Scheduled for June 2021 and postponed to June 30/July 1st 2023
2. 22° National Meeting on Medicinal Chemistry. Scheduled for Roma 10-13 Settembre 2021 and postponed for COVID19 emergency to July 2022 (https://mmcs2022.sciforum.net/)
3. Free Drupal Global Training Day - Venerdì 5 Febbraio 2016. Sapienza Università di Roma
4. Drupal Day 2017. 3-4 marzo 2017. Sapienza Università di Roma
5. Giornata Formativa SIROE sugli Oli Essenziali. Roma – Sapienza Università di Roma, 8 settembre 2017
6. Moodle MOOT Ita 2017. Roma – Sapienza Università di Roma, 28-30 settembre 2017
7. Member of CDA – SIROE
8. 3rd MMCS: "Shaping Medicinal Chemistry for the New Decade" 16–18 Feb 2022, Rome, Italy.
9. VII Congresso Nazionale della SIROE – Roma 2023

Textbooks or Book Chapters

1. Garland Marshall, Richard Head and Rino Ragno Affinity Prediction: The Sine Qua Non. Thermodinamics 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, Nezrina 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

Scopus (09/10/2023)

- Total Papers 164
- H-Index: 40
- Total Citations: 4711

Journal Editoring

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.
   - 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
   - ChemMedChem
   - 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
- FEBS Journal

Rome February 9th 2029

Rino Ragno