PERSONAL INFORMATION

Francesca Spyrakis

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Sex Female | Place and date of birth 17/06/1977 | Nationality Italian

CURRENT POSITION
MARCH 2022 - PRESENT

Full Professor in Medicinal Chemistry (CHIM/08) at the University of Turin (Department of Drug Science and Technology)

WORK EXPERIENCE

October 2016 - present

Associate Professor in Medicinal Chemistry

University of Turin, Department of Drug Science and Technology

Teaching assignments

- 2016/2017 – present. “Analysis of Medicinal products”, Pharmacy degree, University of Turin.
- 2016/2017 – present. “Advanced Medicinal Chemistry”, Industrial Pharmacy degree, University of Turin.
- 2017/2018 – present. “Computer-aided Drug Design”, Pharmacy degree, University of Turin.
- 2017/2018, 2021/2022. “Drug Design”, PhD in Pharmaceutical and Biomolecular Sciences, University of Turin.
- 2017/2018 – 2018/2019. “Specific training on Health and Safety for workers”, Pharmacy and Industrial Pharmacy degrees, University of Turin.
- 2021/2022 – present. “Molecular basis of Drug Action”, Hospital Phramacy School, University of Turin.
- 2022/2023. “Medicinal and Toxicological Chemistry 1”, Pharmacy degree, University of Turin.

Institutional positions

- 2017/2018 – present. Member of the International Committee of the Department of Drug Science and Technology, University of Turin.
- 2018/2019 – 2020/2021. Member of the Department of Drug Science and Technology junta, University of Turin.
- 2019/2020 – 2021/2022. Member of the Public Engagement Committee of the Department of Drug Science and Technology, University of Turin.
- 2021/2022 – 2023/2024: Member of the Research Committee of the Department of Drug Science and Technology, University of Turin.

Competition selection boards

- Febbraio 2023 - member of the competition selection board for a full professor position in Medicinal Chemistry (03/D1). Department of Pharmacy, University of Pisa
- Febbraio 2023 - member of the competition selection board for a full professor position in Medicinal Chemistry (03/D1). Department of Pharmaceutical Sciences, University of Piemonte Orientale.
- October 2022 - member of the competition selection board for a full professor position in Medicinal Chemistry (03/D1). Department of Drug Science and Technology, University of Turin.
- October 2022 - member of the competition selection board for an associate professor position in Medicinal Chemistry (03/D1). Department of Pharmaceutical Sciences, University

of Piemonte Orientale.

- July 2022 - member of the competition selection board for a temporary research (RTDB) position in Medicinal Chemistry (03/D1). Department of Drug Science and Technology, University of Turin.
- November 2021 - member of the competition selection board for a temporary research (RTDA) position in Medicinal Chemistry (03/D1). Department of Pharmaceutical Sciences, University of Perugia.
- January 2021 - member of the competition selection board for an associate professor position in Medicinal Chemistry (03/D1). Department of Drug Science and Technology, University of Turin.
- July 2020 - member of the competition selection board for an associate professor position in Medicinal Chemistry (03/D1). Department of Drug Science and Technology, University of Turin.
- June 2020 - member of the competition selection board for a temporary research (RTDA) position in Medicinal Chemistry (03/D1). Department of Chemistry and Pharmacy, University of Sassari.
- September 2019 – member of the competition selection board for an associate professor position in Medicinal Chemistry (03/D1). Department of Drug Science and Technology, University of Turin.
- February 2017 – member of the competition selection board for a PostDoc position. Department of Drug Science and Technology, University of Turin.

PhD committees

- 2018. Candidate: Constantì Seira Castàn. Thesis title: “Simulaciòn molecular aplicada a inhibidores de 11 β hydroxiesteroide deshidrogenasa tipo 1 y efecto de temperatura en Citoglobina”. Universitat de Barcelona, Facultat de Farmacia i Ciences de l’Alimentaciò, Departament de Nutriciò, Ciences de l’Alimentaciò i Gastronomia, Program de Doctorat en RecErca, Desenvolupament i Control de Medicaments. Universitat de Barcelona. July 8th 2018, Barcelona, Spain.
- 2018. Candidate: Alessandro Giraudo. Thesis title: “Development of innovative GABAA receptor ligands using a bioisosteric approach”. Pharmaceutical and Biomolecular Sciences, University of Turin. April 6th 2018, Torino.
- 2014. Candidate: Inger Lyndin. Thesis title: “Mitogen-activated protein kinase-activated protein kinase; structure, function and inhibition”. Department of Medical Biology, Medical Pharmacology and Toxicology. Faculty of Health Science. The Arctic University. September 26th 2014, Trømso, Norway.

PhD thesis Reviewer

- 2019. Candidate: Bertazzo Martina. Thesis title: “Dynamic docking, path analysis and free energy computation in protein-ligand binding”. PhD in Biotehcnological and Pharmaceutical Sciences, University of Bologna, cicle XXXII. December 2019.
- 2019. Candidate: Nicolò Milani. Thesis title: “Sustainable solvents as media for the synthesis of target heterocyclic compounds”. PhD in Chemistry, University of Perugia, cicle XXXI. June 2019.
- 2019. Candidate: Stefano Di Bona. Thesis title: “identification quantification and metabolic characterization of xenobiotics in complex matrices using experimental and computational methods”. PhD in Chemistry, University of Perugia, cicle XXXI. June 2019.
- 2019. Candidate: Dorothea Gobbo. Thesis title: “Free energy and kinetics in protein-ligand binding: experimental measurements and computational estimates”. PhD in Biotehcnological and Pharmaceutical Sciences, University of Bologna, cicle XXXI. January 2019.
- 2017. Candidate: Martina Ceccarelli. Thesis title: “The importance of physicochemical and ADMET related properties assessment through the study of drug-induced Phospholipidosis and Aldehyde Oxidase metabolism.” PhD in Biotechnology, University of Perugia, cicle XXIX. June 2017.

Tutorig activities for PhD thesis, PostDoc, Research Fellowships and master degree thesis

- Tutor for a PhD student in Pharmaceutical and Biomolecular Sciences, for the project “Identification of low environmental impact molecules to counteract antimicrobial resistance through *in silico* methodologies”, cicle XXXVII, University of Turin, 2023-2025 (PNRR action, fellowship co-financed by Solvay Polymers)
- Tutor for a PhD student in Pharmaceutical and Biomolecular Sciences, for the project

"Identification of low environmental impact molecules to counteract antimicrobial resistance through *in silico* methodologies", cicle XXXVII, University of Turin, 2022-2024 (PON action)

- Tutor for a PhD student in Pharmaceutical and Biomolecular Sciences, for the project "Discovery of new carbapenemase inhibitors by means of innovative in silico methodologies", cicle XXXIX, University of Turin, 2018-2021.
- Tutor for a PhD student in Pharmaceutical and Biomolecular Sciences, for the project "Nuclear receptors: structural and dynamic relationships analysis by innovative *in silico* methodologies", cicle XXXIII, University of Turin, 2017-2020. (PhD fellowship supported by Molecular Discovery Ltd).

- Tutor for a 2-years PostDoc position funded by the project ERASE (PRIN2020). Title of the project: "In silico design of new antimicrobials to starve Staphylococcus aureus". Department of Drug Science and Technology, University of Turin. September 2023-August 2025.
- Tutor for a 1-years PostDoc position funded by the project BRAVE (call H2020-SGA-FETFLAG-HBP-2019). Title of the project: "In silico design of inflammasome interferents to prevent neurodegeneration". Department of Drug Science and Technology, University of Turin. February 2022-January 2024.
- Tutor for a 1-year research fellowship within the research funded project NEWAIMS for "Identification of new antimicrobials through *in silico* simulations". Department of Drug Science and Technology, University of Turin. February 2019-January 2020.
- Tutor for a 1-year PostDoc position co-supported by the project NEWAIMS and the interdepartmental centre BIOPHARMANET-TEC of the University of Parma. Title of the project: "Expression and purification of proteins of biomedical and study of their ligand interaction". Department of Drug Science and Technology, University of Turin. April 2018-March 2019.
- Tutor for eight master degree thesis in Industrial Pharmacy, Pharmacy, Chemistry, University of Turin, 2018-2022.
- Tutor for one master degree thesis in Scuola di Studi Superiori "Ferdinando Rossi" University of Turin, 2017.
- Co-tutor for one master degree thesis in Chemistry, Department of Chemistry, Biology and Biotechnology, University of Perugia, 2015.
- Co-tutor for six master degree theses in Industrial Pharmacy (Faculty of Pharmacy), two master degree theses in Physics, and one in Biology, (Faculty of Sciences), University of Parma, 2004-2013.
- Co-tutor for a PhD thesis in Biochemical Sciences, University of Turin, 2008-2010.
- Co-tutor for a research fellowship on the project "Evaluation of protein-protein interactions through the HINT force field", 2009, Department of Biochemistry and Molecular Biology, University of Parma, 2009.
- Opponent member for master degree theses in Industrial Pharmacy, University of Turin 2016-present.

January 2015 – January 2016

Postdoc in medicinal chemistry (CHIM/08)

University of Modena and Reggio Emilia, Department of Life Sciences.

Project title: "Design of folate-dependent enzyme inhibitors and off-target identification through pocket-based analyses". (FP7 NMTrypI, new medicines for trypanosomatidic infections; Grant agreement no: 603240).

January 2013 – January 2015

Postdoc in medicinal chemistry (CHIM/08)

University of Modena and Reggio Emilia, Department of Life Sciences.

Project title: "Design of enzyme inhibitors involved in hyperproliferative diseases". (FP7 OPTObacteria; Grant agreement no: 286998).

November 2008 – January 2013

Postdoc in general chemistry (CHIM/03)

University of Parma, Department of General Chemistry.

Project title: "Molecular engineering of biological receptors for the identification of novel drugs and food pollutants".

September 2007 – August 2008

Fellowship

National Institute for Biostructures and Biosystems, Department of General Chemistry, University of Parma.

Project title: “Investigation of protein-ligand, protein-protein and protein-nucleic acid interactions through innovative computational methods”.

February 2008 – April 2008

Fellowship

HPC-Europe Transnational Access. University of Barcelona, Department of Physical Chemistry.

Project title: “Ligand migration in non-symbiotic *Arabidopsis thaliana* hemoglobins”.

June 2007 – August 2007

Fellowship

University of Parma, Department of Biochemistry and Molecular Biology.

Project title: “Computational design of PLP-dependent enzyme inhibitors”.

January 2007 – March 2007

Fellowship

University of Parma, Department of Biochemistry and Molecular Biology.

Project title: “Biophysical and biochemical characterization of human hemoglobin tby means of genetic and chemical methods”.

EDUCATION & TRAINING

March 16th 2007

PhD in Biochemistry and Molecular Biology

Mark: excellent

University of Parma. Dissertation thesis: “The HINT force field: development of novel approaches for investigating biomolecular interactions”.

April 29th 2003

Master Degree in Pharmaceutical Chemistry and Technology

Mark: 110/110 laude

University of Parma. Dissertation thesis: “Computational analysis of water role in protein-ligand interaction”.

PERSONAL SKILLS

Mother tongue: Italian

Other language(s)

	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken interaction	Spoken production	
English	C1/2 Proficient user	C1/2 Proficient user	C1/2 Proficient user	C1/2 Proficient user	C1/2 Proficient user
Spanish	C1/2 Proficient user	C1/2 Proficient user	C1/2 Proficient user	B1/2 Independent user	B1/2 Independent user

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

Communication and job skills

- Good scientific communication testified by more than 80 publications in relevant international scientific journals, numerous communications to congresses (78) and several lectures to international meetings (16).
- Good ability to network with other scientists at national and international level.

Organisational/managerial skills

Good ability in managing projects and research groups (as a supervisor of laboratory activities, graduate and doctorate thesis and lecturer).
Good organizing skills for national and international workshops, meetings, Summer Schools.

Principal collaborations:

- Prof. Rebecca Wade: Identification of inflammasome inhibitors and new antivirals through *in silico* methodologies. Molecular and Cellular Modeling Group, Heidelberg Institute for Theoretical Studies (HITS), Schloss-Wolfsbrunnenweg 35, Heidelberg, 69118, Germany.
- Proff. Paolo Carloni, Giulia Rossetti: Identification of inflammasome inhibitors and new antivirals through *in silico* methodologies. Julich Supercomputing Center (JSC), Institute for Neuroscience and Medicine (INM-9), Forschungszentrum Julich, Julich, Germany.

- Prof. Giorgio Colombo: Study of dynamics and network interplay within inflammasome proteins. Department of Chemistry, University of Pavia. Italy.
- Prof. Gabriele Cruciani: Development of virtual screening methodologies. Department of Chemistry, Biology and Biotechnologies, University of Perugia, Perugia, Italy; Molecular Discovery Ltd, UK.
- Dr. Sergio Decherchi, Prof. Andrea Cavalli: Cross relationship analyses among kinase superfamily. Italian Italiano di Tecnologia.
- Proff. Barbara Campanini, Stefano Bettati, Luca Ronda: Research of new antimicrobials to target S. aureus. Department of Food and Drug and of Medicine and Surgery, University of Parma, Parma, Italy.
- Proff. Donatella Tondi, Maria Paola Costi: Development of new beta-lactamase inhibitors. Department of Life Science. University of Modena and Reggio Emilia, Modena, Italy.
- Prof. F. Javier Luque: Molecular dynamic simulations of different members of the globin family. Departament de Fisicoquimica and Institut de Biomedicina, University of Barcelona, Spain.
- Prof. Glen. E. Kellogg: Development of scoring functions for protein-ligand interaction. Department of Medicinal Chemistry and Institute for Structural Biology and Drug Discovery, VCU, Richmond, Virginia, USA.
- Dr. Stefano Lorenzetti: Studio di interferenti endocrini. Istituto Superiore di Sanità. È attualmente in atto una convenzione con ISS.

Organization of meeting and conferences:

- 2021 Member of the scientific and organizing committee of “Computationally Driven Drug Discovery”, virtual edition, June 24th.
- 2019 Member of the scientific committee of “12th European Workshop on Drug Design”, Siena, 19-24 May.
- 2019 Member of the scientific and organizing committee of “Computationally Driven Drug Discovery”, Rome, 28-29 March.
- 2016 Member of the organizing committee of: “Summer school on: *In silico/in vitro* Approaches for Food Science”, EFSA, Parma, 9 September.
- 2012 Member of the organizing committee of: “From Structural Genomics to Drug Discovery – Nuclear Receptors: from in silico modelling to in vivo experiments”, Parma, 21 September.
- 2012 Member of the organizing committee of: “XVIIth International Conference on Oxygen Binding and Sensing Proteins”, Parma, 29 Agosto 1 September.
- 2009 Member of the organizing committee of: “XII Symposium on Blood Substitutes”, Parma, 25-28 August.
- 2007 Member of the organizing committee of: “From Structural Genomics to Drug Discovery - Modeling the Flexibility”, Parma, 20-21 September.
- 2006 Member of the organizing committee of: “International Visions on Blood Substitutes”, Parma, 17-20 September.
- 2004 Member of the organizing committee of: “From Structural Genomics to Drug Discovery”, Parma, 27-28 September.

Professional skills

The scientific activity of Dr. Spyrakis is mainly based on the development and application of computational methods for the identification of protein ligands, with particular attention to the development of antimicrobials active towards Gram-positives and Gram-negatives.
During the years, different research lines have been carried out: i) development and application of the force field HINT (Hydropathic INTeractions), based on experimental $LogP_{o/w}$ values and able of quantitatively estimating the enthalpic and entropic contribution to the free energy of binding in the formation of biological ineractions. Particular attention has been paied to the role played by water molecules and by active site ionization state during the formation pf protein-ligand, protein-protein and protein-nucleic acid complexes. ii) Identification of new inhibitors for PLP-dipendent enzymes, β-lactamases and carbapenemases, and endocrine disruptors through virtual screening, molecular docking and scoring approaches. iii) Analysis of the dynamics and of the migration of small ligands in proteins belonging to the globin family, by means of Molecular Dynamics integrated with laser flash photolysis. iv) Development of new strategies for the implementation of protein flexibility in virtual screening. v) Investigation and inhibition of iron acquisition by *Staphylococcus aureus*, as an innovative way to fight bacteria growth and antimicrobial resistance.

To reach the aforementioned aims, specific expertise in *in silico* screening, molecular docking, scoring and molecular dynamics has been acquired.

Computer skills: OS: iOS, Windows, Linux. Molecular modeling programs: Pymol, VMD, Sybyl. Scoring e docking: GRID, HINT, Autodock, GOLD, FlexX. Homology modelling programs: Modeller, TASSER, Swiss-model. Amber, NAMD and Gromacs for Molecular Dynamics simulations. FLAP for Virtual Screening.

Driving license: B

ITALIAN PROFESSORSHIP QUALIFICATION

ASN 2016-2018

ASN for Full Professor in:

- **03/D1, Medicinal, toxicological and nutritional chemistry and applied technologies**

ASN 2012

ASN for Associate Professor in:

- **03/B1, Principles of Chemistry and Inorganic Systems**
- **03/D1, Medicinal, toxicological and nutritional chemistry and applied technologies**
- **05/E1, General Biochemistry.**

PUBLICATIONS

Bibliometrics: number of publications: 104, H-index: 29, citations: 2534 (Scopus)

ORCID: http://orcid.org/0000-0002-4016-227X

*Corresponding author
#Co-first author

- C. Pozzi, A. Vanet, V. Francesconi, L. Tagliazucchi, G. Tassone, A. Venturelli, **F. Spyrakis**, M. Mazzorana, M.P. Costi, M. Tonelli: "Antitarget, anti-SARS-CoV-2 leads, drugs, and the drug discovery-genetics alliance perspective" *J. Med. Chem*. 2023, 66, 3664-3703, doi: 10.1021/acs.jmedchem.2c01229.
- P.J. de Vink, A.A. Koops, G. D'Arrigo, G. Cruciani, **F. Spyrakis***, L. Brunsveld: "Cooperativity as quantification and optimization paradigm for nuclear receptor modulators" Chem. Sci. 2022, 13, 2744-2752, doi: 10.1039/d1sc06426f.
- E. Gianquinto, F. Sodano, B. Rolando, M. Kostrzewa, M. Allarà, A.M. Mahmoud, K. Poulami, **F. Spyrakis**, A. Ligresti, K. Chegaev: "N-[1,3-Dialkyl(aryl)-2-oxoinidazolidin-4-ylidene]-aryl(alkyl)sulphonamides as novel selective human cannabinoid type 2 receptor (hCB2R) ligands: insight into the mechanism of receptor activation/deactivation" *Molecules* 2022, 27, 8152, doi:10.3390/molecules27238152.
- E. Marini, M. Marino, G. Gionfriddo, F. Maione, M. Pandini, D. Oddo, M. Giorgis, B. Rolando, F. Blua, S. gastaldi, S. Marchiò, S. Kovachka, **F. Spyrakis**, E. Gianquinto, F. Di Nicolantonio, M. Bertinaria: "Investigation into the use of encorafenib to develop potential PROTACs directed against $BRAF^{V600E}$ protein" *Molecules* 2022, 27, 8513, doi: 10.3390/molecules27238513.
- I. Andreana, E. Gazzano, E. Gianquinto, G. Piatti, V. Bincoletto, D. Kryza, G. Lollo, **F. Spyrakis**, C. Riganti, S. Arpicco, B. Stella: "Selective delivery of pentamidine toward cancer cells by self-assembled nanoparticles" Int. J. Pharm 2022, 625, 122102, doi: 10.1016/j.ijpharm.2022.122102.
- E. Dahdouh, L. Allander, L. Falgenhauer, B.I. Iorga, S. Lorenzetti, I. Marcos-Alcalde, N.I. Martin, L. Martinez-Martinez, J. Mingorance, T. Naas, J.E. Rubin, **F. Spyrakis**, T. Tangden, P. Gomez-Puertas: "Computational modeling and design of new inhibitors of carbapenemase: a discussion from the EPIC alliance network" IJMS 2022, 23, 9746, doi: 10.3390/ijms23179746.
- G. D'Arrigo, I. Autiero, E. Gianquinto, L. Siragusa, M. Baroni, G. Cruciani, **F. Spyrakis***: "Exploring ligand binding domain dynamics in the NRs superfamily" IJMS 2022, 23, 8732, doi: 10.3390/ijms23158732.
- A.C. Pippione, Z. Kilic-Kurt, S. Kovachka, S. Sainas, B. Rolando, E. Denasio, K. Pors, S. Adinolfi, D. Zonari, R. Bagnati, M.L. Lolli, **F.Spyrakis***, S. Oliaro-Bosso, D. Boschi: "New

aldo-keto reductase 1C3 (AKR1C3) inhibitors based on the hydroxytriazole scaffold" E. J. Med. Chem. 2022, 237, 114366, doi: 10.1016/j.ejmech.2022.114366.

- S. Bruno, M. Bersani, S. Astore, G. Chiabotto, A. Barge, A. Binello, **F. Spyrakis**: "Lack of interaction of the fluorosurfactant C6O4 with human ren al tran sporters: in vitro/in silico analysis" Toxicology 2022, 476, 153257, doi: 10.1016/j.tox.2022.153257.
- V. Fiorilli, M. Forgia, A. de Saint Germain, G. D'Arrigo, D. Cornu, P. Le Bris, S. Al-Babili, F. Cardinale, C. Prandi, **F. Spyrakis**, F.-D. Boyer, M. Turina, L. Lanfranco: "A structural homologue of the plant receptor D14 mediates responses to strigolactones in the fungal phytopathogen Cryphonectria parasitica" New Phytologist 2022, 234, 1003-1017, doi: 10.1111/nph.18013.
- O. De Bei, M. Marchetti, L. Ronda, E. gianquinto, L. Lazzarato, D.Y. Chigadze, S.W. Hardwick, L.R. Cooper, **F. Spyrakis**, B.F. Luisi, B. Campanini, S. Bettati: "Cryo-EM structures of staphylococcal IsdB bound to human hemoglobin reveal the process of heme extraction" PNAS 2022, 119, e2116708119, doi: 10.1073/pnas.2116708119.
- M. Marengo, D. Pezzilli, E. Gianquinto, A. Fissore, S. Oliaro-Bosso, B. Sgorbini, **F. Spyrakis***, A. Salvatore: "Evaluation of porcine and *Aspergillus oryzae* a-amylase as possible model for the human enzyme" processes 2022, 10, 780, doi: 10.3390/pr10040780.
- M. Santucci, R. Luciani, E. Gianquinto, C. Pozzi, F. Di Pisa, L. Dello Iacono, G. Lan di, L. Tagliazucchi, S. Mangani, **F. Spyrakis**, M.P. Costi: "Repurposing the trypanosomatidic gsk kinetobox for the inhibition of parasitic pteridine and dihydrofolate reductases" pharmaceuticals 2021, 14, 1246, doi: 10.3390/ph14121246.
- V. Dell'Oste, **F. Spyrakis***, C. Prandi: "Strigolactones, from plants to human health: achievements and challenges" *Molecules* 2021, 26(15), 4579, doi: 10.3390/molecules26154579.
- S. Gastaldi, V. Boscaro, E. Gianquinto, C.F. Sandall, M. Giorgis, E. Marini, F. Blua, M. Gallicchio, **F. Spyrakis**, J.A. Macdonald, M. Bertinaria: "Chemical modulation of the 1-(piperidin-4-yl)-1,3-dihydro-2h-benzo[d]imidazole-2-one scaffold as a novel NLRP3 inhibitor" *Molecules* 2021, 26(13), 3975, doi: 10.3390/molecules26133975.
- F. Marchesani, E. Gianquinto, I Autiero, A. Michielon, B. campanini, S. Faggiano, S. Bettati, A. Mozzarelli, **F. Spyrakis***, S. Bruno: "The allosteric interplay between S-nitrosylation and glycine binding controls the activity of human serine racemase" *FEBS J*. 2021, 288(9), 3034, doi: 10.1111/febs.15645.
- J. Gossen, S. Albani, A. Hanke, B.P. Joseph, C. Bergh, M. Kuzikov, E. Costanzi, C. Manelfi, P. Storici, P Gribbon, A.R. Beccari, C. talarico, **F. Spyrakis**, E. Lindahl, A. Zaliani, P. Carloni, R.C. wade, F. Musiani, D.B. Kokh, G. Rossetti: "A blueprint for high affinity SARS-CoV-2 Mpro inhibitors from activity-based compound library screening guided by analysis of protein dynamics" *ACS Pharmacology and Translational Science* 2021, 4(3), 1079, doi: 10.1021/acsptsci.0c00215.
- C. Parisi, M. Failla, A. Fraix, L. Menilli, F. Moret, E. Reddi, B. Rolando, **F. Spyrakis**, L. Lazzarato, R. Fruttero, A. Gasco, S. Sortino: "A generator of peroxynitrite activable with red light" *Chemical Science*, 2021, 12(13), 4740, doi: 10.1039/d0sc06970a.
- G. Marverti, C. Marracini, A. Martello, D. D'Arca, S. Pacifico, R. Guerrini, **F. Spyrakis**, G. Gozzi, A. Lauriola, M. Santucci, G. Cannazza, L. Tagliazucchi, A.S. Cazzato, L. Losi, S. ferrari, G. Ponterini, M.P. Costi: "Folic acid-peptide conjugates combine selective cancer cell internalization with thymidylate synthase dimer interface targeting" *J. Med Chem*. 2021, 64(6), 3204, doi: 10.1021/acs.jmedchem.0c02107.
- G. D'Arrigo, E. Gianquinto, G. Rossetti, G. Cruciani, S. Lorenzetti, **F. Spyrakis***: "Binding of androgen- and estrogen-like flavonoids to their cognate (non)nuclear receptors: a comparison by computational prediction" *Molecules*, 2021, 26(6), doi: 10.3390/molecules26061613.
- E. Gianquinto, D. Tondi, G. D'Arrigo, L. Lazzarato, **F. Spyrakis***: "Can we exploit β-lactamases intrinsic dynamics for designing more effective inhibitors?" *Antibiotics* 2020, 9, 833, doi: 10.2290/antibiotics9110833.
- L. Ronda, A. Tonelli, E. Sogne, I. Autiero, **F. Spyrakis**, S. Pellegrino, G. Abbiati, E. Maffioli, C. Schulte, R. Piano, P. Cozzini, A. Mozzarelli, S. Bettati, F. Clerici, P. Milani. C. Lenardi, G. Tedeschi, M.L. Gelmi: "Rational design of a user-friendly aptamer/peptide-based evice for the detection of *Staphylococcus aureus*" *Sensors* 2020, 20, 4977, doi:10.3390/s20174977.
- **F. Spyrakis**, M. Santucci, L. Maso, S. Cross, E. Gianquinto, F. Sannio, F. Verdirosa, F. De Luca, J-D. Docquier, L. Cendron, D. Tondi, A. Venturelli, G. Cruciani, M.P. Costi: "Virtual screening identifies broad-spectrum beta-lactamase inhibitors with activity on clinically relevant serine- and metallo-carbapenemases" *Scientific Reports*, 2020, 10, 12763, doi: 10.1038/s41598-020-69431-y.
- J.T. Duskey, I. Ottonelli, F. Da Ros, A. Vilella, M. Zoli, S. Kovachka, **F. Spyrakis**, M.A.

Vandelli, G. Tosi, B. Ruozi: "Novel peptide-conjugated nanomedicines for brain targeting: in vivo evidences" *Nanomedicine*, 2020, 28, 102226, doi: 10.1016/j.nano.2020.102226.

- C. Parisi, A. Fraix, S. Guglielmo, **F. Spyrakis**, B. Rolando, L. Lazzarato, R. Fruttero, A. Gasco, S. Sortino: "DNA-targeted NO release photoregulated by green light" *Chemistry – A European Journal*, 2020, 26, 13627, doi: 10.1002/chem.202001538.
- A. Fraix, C. Parisi, M. Failla, K. Chegaev, **F. Spyrakis**, L. Lazzarato, R. Fruttero, A. Gasco, S. Sortino: "NO release regulated by doxorubicin as the green light-harvesting antenna" *Chem. Commun.*, 2020, 56, 6332-6335, doi: 10.1039/d0cc02512g. *Journal cover*.
- M. Biolatti, M. Blangetti, G. D'Arrigo, **F. Spyrakis**, P. Cappello, C. Albano, P. Ravanini, S. Landolfo, M. De Andrea, C. Prandi, V. Dell'Oste: "Strigolactone analogs are promising antiviral agents for the treatment of human cytomegalovirus infection" *Microorganisms*, 2020 8, 703, doi: 10.3390/microorganisms8050703.
- M. Marchetti, O. De Bei, S. Bettai, B. Campanini. S. Kovachka, E. Gianquinto. **F. Spyrakis**, L. Ronda: "Iron metabolism at the interface between host and pathogen: from nutritional immunity to antibacterial development" *Int. J. Mol. Sci.*, 2020, 21, 2145, doi: 10.3390/ijms21062145.
- P. Linciano, E. Gianquinto, M. Montanari, L. Maso, P. Bellio, E. Cebriàn-Sastre, G. Celenza, J. Blàzquez, L. Cendron, **F. Spyrakis***, D. Tondi: "4-Amine-1,2,4-triazole-3-thione as a promising scaffold for the inhibition of serine and metallo-beta-lactamases" *Pharmaceuticals*, 2020, 13, 52, doi: 10.3390/ph13030052.
- T. Ferrante, S. Adinolfi, G. D'Arrigo, D. Poirier, M. Daga, M.L. Lolli, G. Balliano, **F. Spyrakis**, S. Oliaro-Bosso: "Multiple catalytic activities of human 17beta-hydroxysteroid dehidrogenase type 7 respond differently to inhibitors" *Biochimie*, 2020, 170, 106-117, doi: 10.1016/j.biochi.2019.12.012.
- M. Celegato, L. Messa, L. Goracci, B. Mercorelli, C. Bertagnin, **F. Spyrakis**, I. Suarez, A. Cousidi-Siah, G. Travé, L. Banks, G. Cruciani, G. Palù, A. Loregian: "A novel small-molecule inhibitor of the human papillomavirus E6-p53 interaction that reactivates p53 function and blocks cancer cells growth" *Cancer Lett.*, 2020, 470, 115-125, doi: 10.1016/j.canlet.2019.10.046.
- P. Bellio, A. Mancini, L. Di Pietro, S. Cracchiolo, N. Franceschini, S. Reale, F. de Angelis, M. Perilli, G. Amicosante, **F. Spyrakis**, D. Tondi, L. Cendron, G. Celenza: "Inhibition of the transcriptional repressor LexA: withstanding drug resistance by inhibiting the bacterial mechanisms of adaptation to antimicrobials" *Life Science*, 2020, 241, 117116, doi: 10.1016/j.lfs.2019.117116.
- E. Gianquinto, I. Moscetti, O. De Bei, B. Campanini, M. Marchetti, F.J. Luque, S. Cannistraro, L. Ronda, A.R. Bizzarri, F. **Spyrakis*,** S. Bettati: "Interaction of human hemoglobin and semi-hemoglobins with the *Staphylococcus Aureus* hemophore IsdB: a kinetic and mechanistic insight" *Scientific Reports*, 2019, 9, 18629, doi: 10.1038/s41598-019-54970-w.
- C. Estarellas, S. Scaffidi, G. Saladino, **F. Spyrakis**, L. Franzoni, C. Galdeano, A. Bidon-Chanal, F.L. Gervasio, F.J. Luque: "Modulating ligand dissociation through methyl isomerism in accessory sites: binding of retinol to cellular carriers" *J. Phys. Chem. Lett.*, 2019, 10, 7333-7339, doi: 10.1021/acs.jpclett.9b02861.
- F. Sodano, L. Lazzarato, B. Rolando, **F. Spyrakis**, C. De Caro, S. Magliocca, D. Marabello, K. Chegaev, E. Gazzano, C. Riganti, A. Calignano, R. Russo, M.G. Rimoli: "Paracetamol-galactose conjugate: a novel prodrug for an old analgesic drug" Mol. Pharm., 2019, 16, 4181-4189, doi: 10.1021/acs.molpharmaceutic.9b00508.
- S. Sortino, C. Parisi, M. Failla, A. Fraix, B. Rolando, E. Gianquinto, **F. Spyrakis**, E. Gazzano, C. riganti, L. Lazzarato, R. Fruttero, A. Gasco: "Fluorescent nitric oxide photodonors based on BODIPY and rhodamine antennae" *Chemistry*, 2019, 25, 11080-11084. doi: 10.1002/chem.201902062.
- **F. Spyrakis***, P. Bellio, A. Quotadamo, P. Linciano, P. Benedetti, G. D'Arrigo, M. Baroni, L. Cendron, G. Celenza, D. Tondi: "First virtual screening and experiment validation of inhibitors targeting GES-5 carbapenemase" *Journal of Computer-aided Molecular Design*, 2019, 33(2), 295-305. doi: 10.1007/s10822-018-0182-2.
- S. Sciabola, P. Benedetti, G. D'Arrigo, R. Torella, M. Baroni, G. Cruciani, **F. Spyrakis***: "Discovering new casein kinase 1d inhibitors with an innovative MD-enabled virtual screening workflow" *ACS Med. Chem. Letters*, 2018, 10(4), 487.492. doi: 10.1021/acsmedchemlett.8b00523.
- P. Linciano, L. Cendron, E. Gianquinto, **F. Spyrakis**, D. Tondi: "Ten years with New Delhi metallo beta-lactamase-1" *ACS Infectious Diseases*, 2019, 5(1), 9-34. Doi: 10.1021/acsinfecdis.8b00247.
- F. Sodano, B. Rolando, **F. Spyrakis**, M. Failla, L. Lazzarato, E. Gazzano, C. Riganti, R. Fruttero, A. Gasco, S. Sortino: "Tuning the hydrophobicity of a mitochondria-targeted NO

photodonor" ChemMedChem, 2018, 13(12), 1238-1245. doi:10.1002/cmdc.201800088.

- T. Djikic, Y. Martì, **F. Spyrakis**, T. Lau, P. Benedetti, G. Davey, P. Schloss, K. Yelekci: "Human dopamine transporter: the first implementation of a combined in silico/in vitro approach revealing the substrate and inhibitor specificities" *J. of Biomolecular Structure and Dynamics*, 2018, 1-16. doi: 10.1038/s41598-017-17399-7.
- G. Cruciani, N. Milani, P. Benedetti, S. Lepri, L. Cesarini, M. Baroni, **F. Spyrakis**, S. Tortorella, E. Mosconi, L. Goracci: "From experiments to a fast easy-to-use computational methodology to predict human aldehyde oxidase selectivity and metabolic reactions" *J. Med Chem*., 2018, 61(1), 360-371. doi: 10.1021/acsjmedchem.7b01552.
- **F. Spyrakis**, G. Celenza, F. Marcoccia, M. Santucci, S. Cross, P. Bellio, L. Cendron, M. Perilli, D. Tondi: "Structure-based virtual screening for the discovery of novel inhibitors of New Dehli Metallo-beta-lactamase-1 (NDM-1)" *ACS Med. Chem. Letters*, 2018, 9, 45-50. doi: 10.1021/acsmedchemlett.7b00428.
- E. Sanchez, E. Artuso, C. Lombardi, I. Visentin, B. Lace, W. Saeed, M.L. Lolli, P. Koubari, Z. Ali, **F. Spyrakis**, P. Cubas, F. Cardinale, C. Prandi: "Structure-activity relationships of strigolactones via a novel, quantitative in planta bioassay" J. Exp. Bot. 2018, 69, 2333-2343. doi: 10.1093/jxb/ery092.
- M. Santucci[#], **F. Spyrakis**[#], S. Cross, A. Quotadamo, D. Farina, D. Tondi, F. De Luca, J-D. Docquier, a. I. Prieto, C. Ibacache, J. Blàzquez, A. Venturelli, G. Cruciani, M. P. Costi: "Computational and biological profile of boronic acids for the detection of bacterial serine- and metallo-beta-lactamases *Sci. Rep*., 2017, 7(1), 17716. doi: 10.1038/s41598-017-17399-7.
- S. Zuppolini, G. Quero, M. Consales, L. Diodato, P. Vaiano, A. Venturelli, M. Santucci, **F. Spyrakis**, M.P. Costi, M. Giordano, A. Cutolo, A. Cusano, A. Borriello: "Label-free fiber optic optrode for the detection of drug resistant bacteria" *Biomedical Optics Express*, 2017, 8(11), 5191-5205. doi: 10.1364/BOE.8.005191.
- J. Panecka-Hofman, I. Pöhner, **F. Spyrakis**, T. Zeppelin, F. Di Pisa, L. Dello Iacono, A. Bonucci, A. Quotadamo, A. Venturelli, S. Mangani, M.P. Costi, R.C. Wade: "Comparative mapping of on-targets and off-targets for the discovery of anti-trypanosomatid folate pathway inhibitors" *BBA General Subjects*, 2017, 1861, 3215-3230. doi: 10.1016/j.bbagen.2017.09.012
- C. Lombardi, E. Artuso, E. Grandi, M. Lolli, **F. Spyrakis**, E. Priola, C. Prandi: "Recent advances in the synthesis of analogues of phytohormones strigolactones with ring-closing metathesis as a key step". *Org Biomol Chem*, 2017, 15, 8218-8231. doi: 10.1039/c7ob01917c
- **F. Spyrakis**, M.H. Ahmed, A.S. Bayden, P. Cozzini, A. Mozzarelli, G.E. Kellogg: "The role of water in the protein matrix: a largely untapped resource for drug discovery." *J Med Chem*, 2017, 60, 6781-6827; doi: 10.1021/acs.jmedchem.7b00057.
- L. Siragusa, R. Luciani, C. Borsari, S. Ferrari, M.P. Costi, G. Cruciani, **F. Spyrakis***: "Comparing drugs image and repurposing drugs with BioGPS and FLAP dock: the thymidylate synthase case." *ChemMedChem.*, 2016, 11, 1653-1666; doi: 10.1002/cmdc.201600121.
- R. Benoni, T.A. Pertinhez, **F. Spyrakis**, S. Davalli, S. Pellegrino, G. Paredi, S. Bettati, B. Campanini, A. Mozzarelli: "Structural insight into the interaction of O-acetylserine sulfhydrylase with competitive, peptidic inhibitors by Saturation Transfer Difference-NMR." *FEBS Lett*, 2016, 590, 943-953; doi: 10.1002/1873-3468.12126.
- **F. Spyrakis**, P. Cozzini, G.E. Kellogg: "Applying computational scoring functions to assess biomolecular interactions in food science: applications to the estrogen receptors." Nuclear Receptor Research, 2016, 3, ID: 101202; doi: 10.11131/2016/101202.
- G. Quero, S. Zuppolini, M. Consales, L. Diodato, P. Vaiano, A. Venturelli, M. Santucci, **F. Spyrakis**, M.P. Costi, M. Giordano, A. Borriello, A. Cutolo, A. Cusano: Long period fiber grating working in reflection mode as valuable biosensing platform for the detection of drug resistant bacteria." *Sensors and Actuators B*, 2016, 230, 510-520; doi: 10.1016/j.snb.2016.02.086.
- D. Tondi, S. Cross, A. Venturelli, M.P. Costi, G. Cruciani, **F. Spyrakis***: "Decoding the structural basis for carbapenem hydrolysis by class A beta-lactamases: fishing for a pharmacophore". *Current Drug Targets*, 2015, 17, 983-1005.
- **F. Spyrakis***: "From extended spectrum beta-lactamases to carbapenemases: the never ending challenge against Gram-negative bacteria". *Current Drug Targets*, 2015, 17, 972-973.
- **F. Spyrakis***, P. Benedetti, S. Decherchi, W. Rocchia, A. Cavalli, S. Alcaro, F. Ortuso, M. Baroni, G. Cruciani: "A pipeline to enhance ligand virtual screening: integrating Molecular Dynamics and FLAP". *J. Comput. Inf. Model*., 2015, 55, 2256-2274; doi: 10.1021/acs.jcim.5b00169 *(paper and journal cover)*.

- L. Dellafiora, M. Marchetti, **F. Spyrakis**, V. Orlandi, B. Campanini, G. Cruciani, P. Cozzini, A. Mozzarelli: "Expanding the chimical space of human serine racemase inhibitors". *Bioorg Med Chem Lett*, 2015, 25, 4297-4303; doi: 10.1016/j.bmcl.2015.07.081.
- **F. Spyrakis**, C. Cavasotto: "Open challenges in structure-based virtual screening: state-of-the-art, pitfalls and perspectives". *Archives Biochem. Biophys*., 2015, 583, 105-119; doi: 10.1016/j.abb.2015.08.002.
- L. Siragusa, **F. Spyrakis**, L. Goracci, S. Cross, G. Cruciani: "BioGPS: the Music for Chemo- and Bioinformatics Walzer". *Molecular Informatics*, 2014, 33, 446-453; doi: 10.1002/minf.201400028.
- T. Ginex, **F. Spyrakis**, P. Cozzini: "FADB: a food additive molecular database for *in silico* screening in food toxicology". *Food Additives & Contaminants: Part A Chem. Anal. Control Expo. Risk Assess.*, 2014, 31, 792-798; doi: 10.1080/19440049.2014.888784.
- **F. Spyrakis**, B. Cellini, S. Bruno, P. Benedetti, E. Carosati, G. Cruciani, F. Micheli, A. Felici, G.E. Kellogg, P. Cozzini, C. Borri Voltattorni, A. Mozzarelli: "Targeting cystalysin, a key enzyme for the treatment of adult periodontitis". *Chem. Med. Chem.*, 2014, 9, 1501-1511; doi: 10.1002/cmdc.201300527.
- D. Farina[#], **F. Spyrakis[#]**, A. Venturelli, S. Cross, D. Tondi, M.P. Costi: "The inhibition of extended spectrum beta-lactamases: hits and leads". *Curr. Med. Chem.*, 2014, 21, 1405-34; doi: 10.2174/09298673113206660323.
- **F. Spyrakis**, R. Singh, P. Cozzini, B. Campanini, E. Salsi, P. Felici, S. Raboni, P. Benedetti, G. Cruciani, G.E. Kellogg, P.F. Cook, A. Mozzarelli: "Isozyme-specific ligands for O-acetylserine sulfhydrylase, a novel antibiotic target". *PLoS ONE*, 2013, 8(10), e77558; doi: 10.1371/journal.pone.0077558.
- M.H. Ahmed, M. Habtemariam, M.K. Safo, J.N. Scarsdale, **F. Spyrakis**, P. Cozzini, A. Mozzarelli, G.E. Kellogg: "Unintended consequences? Water molecules at biological and crystallographic protein-protein interfaces". *Comput. Biol. Chem.*, 2013, 47C, 126-141; doi: 10.1016/j.compbiolchem.2013.08.009.
- S. Abbruzzetti, **F. Spyrakis**, A. Bidon-Chanal, J. Luque, C. Viappiani: "Ligand migration through hemeprotein cavities: insights from laser flash photolysis and molecular dynamics simulations". *Phys. Chem. Chem. Phys.*, 2013, 15, 10686-10701; doi: 10.1039/c3cp51149a.
- **F. Spyrakis***, F. Lucas, A. Bidon-Chanal, C. Viappiani, V. Guallar, F.J. Luque: "Comparative analysis of inner cavities and ligand migration in non-symbiotic AHb1 and AHb2". *BBA Proteins and Proteomics*, 2013, 1834 (9), 1957-1967; doi: 10.1016/j.bbapap.2013.04.003.
- B. Campanini, **F. Spyrakis**, A. Peracchi, A. Mozzarelli: "Serine racemase: a key player in neuron activity and in neuropathologies". *Frontiers in Bioscience (Landmark Ed)*, 2013, 18, 1112-1128; doi: 10.2741/4167.
- M. Gabba[#], S. Abbruzzetti[#], **F. Spyrakis[#]**, F. Forti, S. Bruno, A. Mozzarelli, F.J. Luque, C. Viappiani, P. Cozzini, M. Nardini, F. Germani, M. Bolognesi, L. Moens, S. Dewilde: "CO rebinding kinetics and molecular dynamics simulations highlight dynamic regulation of internal cavities in human cytoglobin". *PLoS ONE*, 2013, 8(1), e49770; doi: 10.1371/journal.pone.0049770.
- **F. Spyrakis**, L. Dellafiora, C. Da, G.E. Kellogg, P. Cozzini: "Correct protonation state and relevant waters = better computational simulations?" *Curr. Pharm. Des.*, 2013, 19 (23), 4291-4309; doi: 10.2174/1381612811319230011.
- **F. Spyrakis**, P. Felici, A.S. Bayden, E. Salsi, R. Miggiano, G.E. Kellogg, P. Cozzini, P.F. Cook, A. Mozzarelli, B. Campanini: "Fine tuning of the active site modulates specificity in the interaction of *O*-acetylserine sulfhydrylase isozymes with serine acetyl transferase". *BBA Proteins and Proteomics*, 2013, 1834(1), 169-181; doi: 10.1016/j.bbapap.2012.09.009.
- R. Singh. **F. Spyrakis**, P. Cozzini, A. Paiardini, S. Pascarella, A. Mozzarelli: "Chemogenomics of pyridoxal 5'-phosphate dependent enzymes". *J. Enzyme Inhib. Med. Chem.*, 2013, 28(1), 183-194; doi: 10.3109/14756366.2011.643305.
- A. Dal Palú, **F. Spyrakis**, P. Cozzini: "A new approach for investigating protein flexibility based on Constraint Logic Programming. The first application in the case of estrogen receptor". *Eur. J. Med. Chem.*, 2012, 49, 127-140; doi: 10.1016/j.ejmech.2012.01.003.
- M.H. Ahmed, **F. Spyrakis**, P. Cozzini, P.K. Tripathi, A. Mozzarelli, J.N. Scarsdale, M.A: Safo, G.E. Kellogg: "Bound water at protein-protein interfaces: partners, roles and hydrophobic bubbles as a conserved motif". *PLOS One*, 2011, e24712; doi: 10.1371/journal.pone.0024712.
- S. Abbruzzetti, S. Faggiano, **F. Spyrakis**, S. Bruno, A. Mozzarelli, A. Astegno, P. Dominici, C. Viappiani: "Oxygen and nitric oxide rebinding kinetics in non-symbiotic hemoglobin AHb1 from *Arabidopsis thaliana*". *IUBMB Life*, 2011, 63, 1094-1100; doi: 10.1002/iub.546.
- A. Mozzarelli, S. Bettati, B. Campanini, E. Salsi, S. Raboni, R. Singh, **F. Spyrakis**, V.P. Kumar, P.F. Cook: "The multifaceted pyridoxal 5'-phosphate-dependent O-acetylserine sulfhydrilase". *BBA Proteins and Proteomics*, 2011, 1814, 1497-1510; doi:

10.1016/j.bbapap.2011.04.011

- **F. Spyrakis**, F.J. Luque, C. Viappiani: "Structural analysis in nonsymbiotic hemoglobins: what can we learn from inner cavities?". *Plant Science*, 2011, 181, 8-13; doi: 10.1016/j.plantsci.2011.03.021.
- **F. Spyrakis**, S. Bruno, A. Bidon-Chanal, F.J. Luque, S. Abbruzzetti, C. Viappiani, P. Dominici, A. Mozzarelli: "Oxygen binding to *Arabidopsis thaliana* AHb2 non-symbiotic hemoglobin: evidence for a role in oxygen transport". *IUBMB Life*, 2011, 63, 355-362; doi: 10.1002/iub.470.
- **F. Spyrakis**, S. Faggiano, S. Abbruzzetti, P. Dominici, E. Cacciatore, A. Astegno, E. Droghetti, A. Feis, G. Smulevich, S. Bruno, A. Mozzarelli, P. Cozzini, C. Viappiani, A. Bidon-Chanal, F.J. Luque: "Histidine E7 dynamics modulates ligand exchange between distal pocket and solvent in AHb1 from *Arabidopsis thaliana*". *J. Phys. Chem. B*, 2011, 115, 4138-4146; doi: 10.1021/jp110816h.
- **F. Spyrakis**, A. Sarkar, P. Cozzini, G.E. Kellogg: "Applying induced fit in drug discovery: square pegs and round holes?" *Curr. Top. Med. Chem.*, 2011, 11, 131-132; doi: 10.2174/156802611794863553.
- **F. Spyrakis***, A. Bidon-Chanal, X. Barril, F.J. Luque: "Protein flexibility and ligand recognition: challenges for molecular modeling". *Curr. Top. Med. Chem.*, 2011, 11, 192-210; doi: 10.2174/156802611794863571.
- N.K. Bisht, S. Abbruzzetti, S. Uppal, S. Bruno, **F. Spyrakis**, A. Mozzarelli, C. Viappiani, S. Kundu. "Ligand migration and hexacoordination in type 1 non-symbiotic rice hemoglobin". *BBA Proteins and Proteomics*, 2011, 1814, 1042-1053; doi: 10.1016/j.bbapap.2010.09.016.
- E. Salsi, A. Bayden, **F. Spyrakis**, A. Amadasi, B. Campanini, S. Bettati, T. Dodatko, P. Cozzini, G.E. Kellogg, P. Cook, S. Roderick, A. Mozzarelli: "Design of *O*-acetylserine sulfhydrylase inhibitors by mimicking Nature". *J. Med. Chem.*, 2010, 53, 345-356; doi: 10.1021/jm901325e.
- S. Faggiano, S. Abbruzzetti, **F. Spyrakis**, E. Grandi, C. Viappiani, S. Bruno, A. Mozzarelli, P. Cozzini, A. Astegno, P. Dominici, S. Brogioni, A. Feis, G. Smulevich, O. Carrillo, P. Schmidtke, A. Bidon-Chanal, F.J. Luque: "Structural plasticity and functional implications of internal cavities in distal mutants of type 1 non-symbiotic hemoglobin AHb1 from *Arabidopsis thaliana*". *J. Phys. Chem. B,* 2009, 113, 16028-16038; doi: 10.1021/jp9074477.
- S. Abbruzzetti, S. Faggiano, S. Bruno, **F. Spyrakis**, A. Mozzarelli, S. Dewilde, L. Moens, C. Viappiani: "Ligand migration through the internal hydrophobic cavities in human neuroglobin". *Proc. Natl. Acad. Sci. U.S.A.*, 2009, 106, 18984-18989; doi: 10.1073/pnas.0905433106.
- **F. Spyrakis**, P. Cozzini: "How computational methods try to disclose the estrogen receptor secrecy - Modelling the flexibility". *Curr. Med. Chem.*, 2009, 16, 2987-3027; doi: 10.2174/092986709788803123.
- R. Ponassi, B. Biasotti, V. Tomati, S. Bruno, A. Poggi, D. Malacarne, G. Cimoli, A. Salis, S. Pozzi, M. Miglino, G. Damonte, P. Cozzini, **F. Spyrakis**, B. Campanini, L. Bagnasco, N. Castagnino, L. Tortolina, A. Mumot, F. Frassoni, A Daga, M. Cilli, F. Piccardi, I. Monfardini, M. Perugini, G. Zoppoli, C. D'Arrigo, R. Pesenti, S. Parodi: "A novel Bim-BH3-derived Bcl-XL inhibitor: biochemical characterization, in vitro, in vivo and ex-vivo anti-leukemic activity". *Cell Cycle*, 2008, 7, 3211-3224; doi: 10.4161/cc.7.20.6830.
- P. Cozzini, G.E. Kellogg, **F. Spyrakis**, D.J. Abraham, G. Costantino, A. Emerson, F. Fanelli, H. Gohlke, L.A. Kuhn, G.M. Morris, M. Orozco, T.A. Perthinez, M. Rizzi and C. Sotriffer: "Target flexibility: an emerging consideration in drug discovery and design". *J. Med Chem. Perspective*, 2008, 51, 6237-6255; doi: 10.1021/jm800562d.
- A. Marabotti[#], **F. Spyrakis**[#], A. Facchiano, P. Cozzini, S. Alberti, G.E. Kellogg, A. Mozzarelli: "Energy-based prediction of amino acid-nucleotide base recognition". *J. Comput. Chem.*, 2008, 29, 1955-1969; doi: 10.1002/jcc.20954.
- A. Amadasi, A. Surface, **F. Spyrakis**, P. Cozzini, A. Mozzarelli and G.E. Kellogg: "Robust classification of relevant water molecules in putative protein binding sites". *J. Med. Chem.*, 2008, 51, 1063-1067; doi: 10.1021/jm701023h.
- O.A. Gani, O.A. Adekoya, L. Giurato, **F. Spyrakis**, P. Cozzini, S. Guccione, J.-O. Winberg and I. Sylte: "Theoretical calculations of the catalytic triad in short chain alcohol dehydrogenases/reductases". *Biophys. J.*, 2008, 94, 1412-1427; doi: 10.1529/biophysj.107.111096.
- S. Abbruzzetti, E. Grandi, S. Bruno, S. Faggiano, **F. Spyrakis**, A. Mozzarelli, E. Cacciatori, P. Dominici and C. Viappiani: "Ligand migration in nonsymbiotic hemoglobin AHb1 from *Arabidopsis thaliana*". *J. Phys. Chem.* B, 2007, 111, 12582-12590; doi: 10.1021/jp074954o.
- A. Tripathi, M. Fornabaio, **F. Spyrakis**, A. Mozzarelli, P. Cozzini, A. Mozzarelli: "Complexity in modeling and understanding protonation states: computational titration of HIV-1 protease inhibitor complexes". *Chem. Biodivers.*, 2007, 4, 2564-2577; doi: 10.1002/cbdv.200790210.

- S. Bruno, S. Faggiano, **F. Spyrakis**, A. Mozzarelli, E. Cacciatori, P. Dominici, E. Grandi, S. Abbruzzetti, C. Viappiani: "Different roles of protein dynamics and ligand migration in non-symbiotic hemoglobins AHb1 and AHb2 from *Arabidopsis thaliana*". *Gene,* 2007, 398, 224-233; doi: 10.1016/j.gene.2007.02.042.
- **F. Spyrakis**, A. Amadasi, M. Fornabaio, D.J. Abraham, A. Mozzarelli, G.E. Kellogg and P. Cozzini: "The consequences of scoring docked ligand conformations using free energy correlations". *Eur. J. Med. Chem.,* 2007, 42, 921-933; doi: 10.1016/j.ejmech.2006.12.037.
- S. Bruno, S. Faggiano, **F. Spyrakis**, A. Mozzarelli, S. Abbruzzetti, E. Grandi, C. Viappiani, A. Feis, S. Mackowiak, G. Smulevich, E. Cacciatori, P. Dominici: "The reactivity with CO of AHb1 and AHb2 from *Arabidopsis thaliana* is controlled by the distal His E7 and internal hydrophobic cavities". *J. Am. Chem. Soc.,* 2007, 129, 2880-2889; doi: 10.1021/ja066638d.
- **F. Spyrakis**, P. Cozzini, C. Bertoli, A. Marabotti, G.E. Kellogg and A. Mozzarelli: "Energetics of the protein-DNA-water interactions". *BMC Structural Biology*, 2007, 7, 4; doi: 10.1186/1472-6807-7-4.
- **F. Spyrakis**, S. Raboni, P. Cozzini, S. Bettati and A. Mozzarelli: "Allosteric communication between alpha and beta subunits of tryptophan synthase: modelling the open-closed transition of the alpha subunit". *BBA Proteins and Proteomics*, 2006, 1764 (6), 1102-1109; doi: 10.1016/j.bbapap.2006.03.005.
- A. Amadasi, **F. Spyrakis**, P. Cozzini, D.J. Abraham, G.K. Kellogg and A. Mozzarelli: "Mapping the energetics of water-protein and water-ligand interactions with the "natural" HINT forcefield: predictive tools for characterizing the roles of water in biomolecules". *J. Mol. Biol.*, 2006, 358 (1), 289-309; doi: 10.1016/j.jmb.2006.01.053.
- G.E. Kellogg, M. Fornabaio, D.L. Chen, D.J. Abraham, **F. Spyrakis**, P. Cozzini and A. Mozzarelli: "Tools for building a comprehensive modeling system for virtual screening under real biological conditions". *J. Mol. Graph. Model.*, 2006, 24 (6), 434-439; doi: 10.1016/j.jmgm.2005.09.001.
- S. Sottini, S. Abbruzzetti, **F. Spyrakis**, S. Bettati, L. Ronda, A. Mozzarelli and C. Viappiani: "Geminate rebinding in R state hemoglobin: kinetic and computational evidence for multiple hydrophobic pockets". *J. Am. Chem. Soc.,* 2005, 127 (49), 17427-17432; doi: 10.1021/ja056101k.
- P. Cozzini, M. Fornabaio, A. Mozzarelli, **F. Spyrakis**, D.J. Abraham, and G.E. Kellogg. "Water: How to evaluate its contribution in protein-ligand interactions". *Int. J. Quant. Chem.,* 2006, 106 (3), 647-651; doi: 10.1002/qua.20812.
- **F. Spyrakis**, M. Fornabaio, P. Cozzini, A. Mozzarelli, D.J. Abraham, G.E. Kellogg "Computational titration analysis of a multiprotic HIV-1 protease-ligand complex". *J. Am Chem. Soc.,* 2004, 126, 11764-11765; doi: 10.1021/ja0465754.
- M. Fornabaio, **F. Spyrakis**, A. Mozzarelli, P. Cozzini, D.J. Abraham and G.E. Kellogg "Simple, intuitive calculations of free energy of binding for protein-ligand complexes. 3 Including the free energy contribution of structural water molecules in HIV-1 Protease". J *Med. Chem.*, 2004, 47, 4507-4516; doi: 10.1021/jm030596b.
- G.E. Kellogg. M. Fornabaio, **F. Spyrakis**, A. Lodola, P. Cozzini, A. Mozzarelli and D.J. Abraham. "Getting it right. Modeling of pH, solvent and "nearly" everything else in virtual screening of biological targets". *J. Mol. Graph. Model.,* 2004, 22, 479-486; doi: 10.1016/j.jmgm.2004.03.008.

Book chapters

- Autori vari: Chimica farmaceutica di Graham Patrick, a cura di Gabriele Costantino e Gianluca Sbardella, 2022. Personal contributions to chapters "Strategie per l'identificazione di hit", "Agenti antibatterici", "Farmaci antinfiammatori non steroidei". EdiSES, in press
- **F. Spyrakis**, A. Sarkar, G.E. Kellogg: "Docking and Scoring in Drug Discovery" in *Burger's Medicinal Chemistry and Drug Discovery*, 8th edition, edited by Prof. D.J. Abraham and Kent Stewart, 2021. Wiley-VCH, New York
- M.H. Ahmed, A. Amadasi, A.S. Bayden, D.J. Cashman, P. Cozzini, C. Da, D.L. Chen, M. Fornabaio, V.N. Koparde, A. Mozzarelli, H.I. Parikh, A. Sarkar, J.N. Scarsdale, **F. Spyrakis**, J.A. Surface, A. Tripathi, S.A. Zaidi, G.E. Kellogg: "Understanding water and its many roles in biological structure: some ways to exploit a resource for drug discovery" in *Methods in Pharmacology and Toxicology*, 2015. ISSN: 1557-2153. Humana Press, Springer, New York, USA.
- **F. Spyrakis**, C. Cavasotto: "Incorporating protein flexibility in structure-based drug design" in *From Medicinal Chemistry to Food Science: A Transfer of In Silico Methods Applications*, edited by Prof. P. Cozzini, 2015, Chapter 7, 131-156, in press; ISBN 978-1-63483-587-9. Nova Science Publishers, New York, USA.
- P. Cozzini, L. Dellafiora, T. Ginex, **F. Spyrakis**: "How protein flexibility can influence

docking/scoring simulations" in *In Silico Drug Discovery and Design: Theory, Methods, Challenges and Applications*, edited by Prof. C. Cavasotto, 2015, Chapter 16, 411-440; ISBN: 978-1-4822-1783-4.
CRC Press, Boca Raton, USA.

- **F. Spyrakis***, X. Barril, F.J. Luque: "Molecular Dynamics: a tool to understand nuclear receptors" in *Computational Approaches to Nuclear Receptors*, edited by Proff. P. Cozzini and G.E. Kellogg, 2012, Chapter 3, 40-59; ISBN: 978-1-84973-364-9.
RSC Publishing, London, UK.
- **F. Spyrakis***, P. Cozzini, G.E. Kellogg: "Molecular descriptors for database mining. Translating empirical chemistry into mathematics: tools for QSAR and *in silico* screening based on the hydrophobicity of small molecules" in *Physico-Chemical and Computational Approaches to drug Discovery*, edited by Proff. F.J. Luque and X. Barril, 2012, Chapter 5, 128-150; ISBN: 978-1-84973-353-3.
RSC Publishing, London, UK.
- **F. Spyrakis**, L. Giurato, S. Guccione and P. Cozzini: "Structural data: the basis for molecular modelling" Practice III.1, Chapter III Molecular Modeling, in *Practical studies for medicinal chemistry*, edited by Proff. A. Monge and C.R. Ganellin. On-line IUPAC edition (www.iupac.org/home/publications/cd/practical-studies-for-medicinal-chemistry.html), 2007. Printed edition Universidad Nacional de Rio Cuarto, Rio Cuarto, Argentina, 2011.
- P. Cozzini and **F. Spyrakis**: "Hydrophobicity in drug design" Practice I.12, Chapter I. Physicochemical Properties, in *Practical studies for medicinal chemistry*, edited by Proff. A. Monge and C.R. Ganellin. On-line IUPAC edition (www.iupac.org/home/publications/cd/practical-studies-for-medicinal-chemistry.html), 2007. Printed edition Universidad Nacional de Rio Cuarto, Rio Cuarto, Argentina, 2011.
- S. Raboni, R. Contestabile, **F. Spyrakis**, B. Campanini, A. Amadasi, S. Bettati, A. Peracchi and A. Mozzarelli: "Pyridoxal 5'-phosphate-dependent enzymes: catalysis, conformation and genomics" in *Comprehensive Natural Products Chemistry II*, edited by Proff. L. Mander and H.-W. Liu, 2010, 7, 253-350; ISBN: 978-0-08-045381-1.
Elsevier, Oxford, United Kingdom
- **F. Spyrakis**, P. Cozzini, G.E. Kellogg: "Docking and Scoring in Drug Discovery" in *Burger's Medicinal Chemistry and Drug Discovery*, 7th edition, edited by Prof. D.J. Abraham, 2010, pp 601-684; ISBN: 9780471266945; doi: 10.1002/0471266949.
Wiley-VCH, New York.
- **F. Spyrakis**, G.E. Kellogg, A. Amadasi and P. Cozzini. "Scoring functions for virtual screening" in *Frontiers in Drug Design and Discovery*, edited by A. Rahman, G.W. Caldwell, M.I. Choudhary and M.R. Player, 2007, 3, 317-379; ISBN: 978-90-77527-11-5; ISSN: 1574-0889/07; doi: 10.2174/97816080520111070301.
Bentham Science Publishers Ltd, Hilversum, the Netherlands.

Oral presentations

- F. Spyrakis, E. Gianquinto, M. Bersani, M. Failla, L. Bertarini, F. Vascon, F. Sannio, F. Verdirosa, F. De Luca, M.P. Costi, G. Cruciani, J.-D. Docquier, L. Cendron, D. Tondi, L. Lazzarato: "Prospecting for broad-spectrum b-lactamase inhibitors targeting clinically-relevant carbapenemases" in Protein 2022, Pisa, May 18th-20th, 2022. Invited oral communication.
- F. Spyrakis: "Metodi computazionali per l'identificazione di potenziali inibitori di SARS-CoV-2" in IPAM2021, Convegno annuale IPAM (Italian Platform on Alternative Methods) – webinar day, December 3rd, 2021. Invited oral communication.
- F. Spyrakis, D. Tondi, E. Gianquinto, M.C. Failla, L. Lazzarato, P. Linciano, M. Santucci, L. Maso, S. Cross, F. Sannio, F. Verdirosa, F. De Luca, J.-D. Docquier, L. Cendron, A. Venturelli, G. Cruciani, M.P. Costi: "Identification of carbapenemase broad-spectrum inhibitors through in silico methodologies" in XXVII Congresso Nazionale della Società Chimica Italiana, virtual edition, September 14th-23rd, 2021. Oral communication.
- F. Spyrakis: "S-nitrosylation and glycine control the activity of human serine racemase through an allosteric interplay" in ACS FALL 2021, virtual edition, August 22nd-26th 2021. Oral communication.
- F. Spyrakis, M. Santucci, L. Maso, S. Cross, E. Gianquinto, L. Lazzarato, F. Sannio, F. Verdirosa, F. De Luca, J.-D. Docquier, L. Cendron, D. Tondi, A. Venturelli, G. Cruciani, M.P. Costi: "Identification of carbapenemase broad-spectrum inhibitors through in silico screening" in IC2AR 2021, 4th International Caparica Congress in Antibiotic Resistance, virtual edition June 13th-17th, 2021. Invited oral communication.
- F. Spyrakis, E. Gianquinto, O. De Bei, M Marchetti, L. Lazzarato, F.J. Luque, I. Moscetti, A. Bizzarri, S. Cannistraro, M. Levantino, B. Campanini, L. Ronda, S. Bettati: "Novel strategies to fight resistant Staphylococcus aureus: structural, dynamic and kinetic characterization of the S. aureus IsdB and human haemoglobin interaction" in 3rd International Conference on

Pharmacy and Pharmaceutical Sciences, Rome, Italy, July 22nd-24th, 2019. Invited keynote presentation.

- E. Gianquinto, O. De Bei, M Marchetti, L. Lazzarato, S. Guglielmo, R. Fruttero, S. Bettati, L. Ronda, B. Campanini, J.F. Luque, F. Spyrakis: "Novel strategies to iron-starve Staphylococcus aureus: structural and dynamic characterization of the hemophore-Hb interaction" in XXVI National Meeting in Medicinal Chemistry. Milan, Italy, July 16th-19th 2019. Oral presentation.
- F. Spyrakis: "Computational methods for antibiotic discovery" in OUTREACH FINAL Conference ITN MSCA "INTEGRATE" Interdisciplinary Training Network for Validation of Gram-negative Antibacterial Targets. Parma, Italy, November 21st-23rd, 2018. Invited oral presentation
- F. Spyrakis: "Structure-based drug design: sometimes x-ray crystallography is not enough" in Giornate del CrisDi, The role of crystallography in drug science and biology, Department of Drug Science and Technology, University of Turin, Italy, March 5th, 2018. Invited oral communication.
- F. Spyrakis, S. Sciabola, P. Benedetti, M. Baroni, G. Cruciani: "Integrating Molecular Dynamics and Molecular Interaction Fields in virtual screening: the case of casein kinase 1d" in 5th CDDD meeting, IFOM, Milan, Italy, November 16th-17th, 2017. Oral communication.
- F. Spyrakis, S. Sciabola, P. Benedetti, M. Baroni, G. Cruciani: "Discovering new kinase 1d inhibitors with innovative MD-integrated virtual screening" in XXVI Congresso Nazionale della Società Chimica Italiana, Paestum, Salerno, Italy, September 10th-14th, 2017. Oral communication.
- F. Spyrakis: "Screening, docking, scoring and other computational methods: in In silico methods for food safety, EFSA, Parma, Italy, June 13th-15th, 2017, Invited oral communication.
- F. Spyrakis: "Computational techniques for EDC's identification in food" in In silico/in Vitro Approaches for Food Science, EFSA, Parma, Italy, September 9th, 2016, Invited oral communication.
- F. Spyrakis, P. Benedetti, S. Decherchi, W. rocchia, A. Cavalli, M. Baroni: "Integrating molecular dynamics and molecular interactio fields: a way to enhance structure-based virtual screening" in 21st EuroQSAR, Where Molecular Simulations Meet Drug Discovery, Verona, Italy, September 4th-8th, 2016, Oral communication.
- F. Spyrakis, S. Cross, G. Cruciani, M. Santucci, D. Farina, A. Venturelli, J. Blazquez, M.P. Costi. "New ligands for targeting extended spectrum β-lactamases" in Winter Modeling 2014, Modena, Italy, March 13-14, 2014. Oral presentation.
- F. Spyrakis, S. Abbruzzetti, M. Gabba, C. Viappiani, A. Mozzarelli, S. Bruno, F. Forti, A. Bidon-Chanal, F.J. Luque. "The hydrophobic breathing of cytoglobin" in Ninth Triennal Congress of the WORLD ASSOCIATION OF THEORETICAL AND COMPUTATIONAL CHEMISST WATOC 2011, Santiago de Compostela, Spain, July 17-22, 2011. Oral presentation.
- A. Mozzarelli, F. Spyrakis, P. Cozzini. "Development of enzyme inhibitors by experimental and computational tools" in 10th ULLA Summer School, Parma, Italy, July 2-8, 2011. Invited Lecture.
- S. Bruno and F. Spyrakis. "Plant hemoglobins: structural plasticity and ligand migration" in XVIth International Conference on Oxygen Binding and Sensing Proteins, Antwerp, Belgium, August 22-26, 2010. Invited oral presentation.
- F. Spyrakis, S. Faggiano, S. Abbruzzetti, E. Grandi, C. Viappiani, S. Bruno, A. Mozzarelli, P. Cozzini, A. Astegno, P. Dominici, S. Brogioni, A. Feis, G. Smulevich, O. Carrillo, P. Schmidtke, A. Bidon-Chanal, F. J. Luque. "Structural plasticity and ligand migration in wild type and distal mutants of non-symbiotic hemoglobins from Arabidopsis thaliana" in Proteine 2010, Parma, Italy, April 8-10, 2010. Poster session and oral presentation.
- F. Spyrakis, A. Marabotti, A. Facchiano, P. Cozzini, S. Alberti, G.E. Kellogg, D.J. Abraham, A. Mozzarelli. "Investigating the energetic principles that govern the amino acid-nucleotide base recognition process in protein-DNA complexes" in Computer Aided Drug Design GRC conference. Tilton, New Hampshire, USA, July 29-August 3, 2007. Poster session and selected oral presentation.
- P. Cozzini and F. Spyrakis: "Docking and Scoring" in the International Workshop: Introduction to Molecular Modelling. Tromso, Norway, December 12-13, 2005. Invited Lecture.
- F. Spyrakis, P. Cozzini, A. Amadasi, A. Mozzarelli, M. Fornabaio, G.E. Kellogg and D.J. Abraham: "Structural data: the milestone for reliable computational predictions and simulations" in Evolving Methods in Macromolecular Crystallography the 37th crystallographic meeting at Erice, Erice, Sicily, Italy, May 12-22 , 2005. Oral communication and Poster session.

Communications

- P. Otero, C. Perez-garcia, C. Hurtado, F. Spyrakis, G. Caron, S. Visentin, C. Bertea, R. davies, P. Gharanei, M. Babba, E. Alonso, M.P. Ramos-Alvarez: "Collaborative online international learning (COIL) program: your career opportunity worldwide. Learning from the experience and personal view of professionals in the sector" in Annual Conference of the European Association of Faculties of Pharmacy (EAFP), Malta, May 11th 2022. **Oral communication.**
- O. De Bei, M. Marchetti, L. Ronda, E. Gianquinto, M. Levantino, L. Lazzarato, D.Y. Chirgadze, S.W. Hardwick, L.R. Cooper, M. Cozzi, S. Faggiano, F. Spyrakis, B.F. Luisi, B. Campanini, S. Bettati: "understanding iron hijacking by Staphylococcus aureus: a structural and mechanistic insight into the interaction of IsdB hemophore with human hemoglobin" in The Biochemistry Global Summit, Lisbon, Portugal, July 9th-14th 2022. **Poster presentation.**
- O. De Bei, E. Gianquinto, D.Y. Chirgadze, S.W. Hardwick, L. Cooper, M. Marchetti, F. Spyrakis, S. Bettati, L. Ronda, B.F. Luisi, B. Campanini: "Cryo-EM reveals how hemophore binding to Hb prompts heme removal: a structural and mechanistic insight into the function of IsdB from S. aureus" in SIB 2021, virtual event, September 23rd-24th 2021. **Poster presentation and selected short talk.**
- E. Gianquinto, M. Santucci, L. Maso, S. Cross, F. Sannio, F. Verdirosa, F. de Luca, J.-D Doquier, L. Cendron, D. Tondi, A. Venturelli, G. Cruciani, M.P. Costi, F. Spyrakis: "An in silico pipeline identifies inhibitors with cross-class activity on clinically relevant serine- and metallo-beta-lactamases" in Bioexcel Student Webinar: Summer School 2021 Edition, virtual event, September 21st 2021. **Oral communication.**
- E. Gianquinto, F. Marchesani, I. Autiero, A. Michielon, B. Campanini, S. Gaggiano, S. Bettati, A. Mozzarelli, S: Bruno, F. Spyrakis: "ATP, S-nitrosylation and glycine: a three-way regulation mechanism modulating the activity of serine racemase" in EFMC-YSMC, virtual event, September 9th-10th 2021. **Poster presentation.**
- E. Gianquinto, M. Santucci, L. Maso, S. Cross, F. Sannio, F. Verdirosa, F. de Luca, J.-D. Doquier, L. Cendron, D. Tondi, A. Venturelli, G. Cruciani, M.P. Costi, F. Spyrakis: "An in silico pipeline identifies inhibitors with cross-class activity on clinically relevant serine- and metallo-beta-lactamases" in EFMC-ISMC, virtual event, August 29th-September 2nd 2021. **Poster presentation.**
- A.C. Pippione, Z. Kilic-Kurt, S. Sainas, B. Rolando, S. Kovachka, F. Spyrakis, A. Buschini, S. Montalbano, S. Oliaro Bosso, D. Boschi, M.L. Lolli: "Multiple-targeting ligands against prostate cancer: effect on both AKR1C3 enzyme and androgen receptor" in EFMC-ISMC, virtual event, August 29th-September 2nd 2021. **Poster presentation.**
- M. Cozzi, R. Giaccari, O. de Bei, E. Gianquinto, S. Kovachka, M. Marchetti, L. Ronda, B. Campanini, L. Lazzarato, F. Spyrakis, S. Bettati: "An ELISA and STD-NMR combined approach to evaluate disruptors of the interaction between human haemoglobin and the bacterial hemophore IsdB" in ULLA Summer School, virtual event, July 6th-8th 2021.
- E. Gianquinto, M. Santucci, L. Maso, S. Cross, F. Sannio, F. Verdirosa, F. de Luca, J.-D. Doquier, L. Cendron, D. Tondi, A. Venturelli, G. Cruciani, M.P. Costi, F. Spyrakis: "In silico-guided discovery of inhibitors with cross-class activity on clinically relevant carbapenemases" in ESMEC school 2021, virtual event, June 28th-July 1st 2021. **Poster presentation and award winner.**
- E. Gianquinto, M. Santucci, L. Maso, S. Cross, F. Sannio, F. Verdirosa, F. de Luca, J.-D. Doquier, L. Cendron, D. Tondi, A. Venturelli, G. Cruciani, M.P. Costi, F. Spyrakis: "Virtual screening identifies cross-class inhibitors of clinically relevant carbapenemases" in CDDD 7th edition, virtual event, June 25th 2021. **Oral communication.**
- G. D'Arrigo, I. Autiero, F. falchi, G. cruciani, F. Spyrakis: "From the derection of cross-correlations till the identification of alternative sruggable pockets in Nuclear Receptors" in CDDD 7th edition, virtual event, June 25th 2021. **Oral communication.**
- A.C. Pippione, Z. Kilic-Kurt, S. Sainas, B. Rolando, S. Kovachka, F. Spyrakis, A. Buschini, S. Montalbano, S. Oliaro Bosso, D. Boschi, M.L. Lolli: "Multiple-targeting ligands against prostate cancer: effect on both AKR1C3 enzyme and androgen receptor" in 13th International Symposium on Pharmaceutical Sciences, Turkey, virtual event. June 22nd-25th 2021. **Oral communication.**
- E. Gianquinto, M. Santucci, L. Maso, S. Cross, F. Sannio, F. Verdirosa, F. de Luca, J.-D. Doquier, L. Cendron, D. Tondi, A. Venturelli, G. Cruciani, M.P. Costi, F. Spyrakis: "An in silico pipeline identifies inhibitors with cross-class activity on clinically relevant serine- and metallo-beta-lactamases" in Bioexcel Summer School, virtual event, June 4th-11th 2021. **Poster presentation and award winner.**
- F. Spyrakis, E. Gianquinto, F. Marchesani, I. Autiero, A. Michielon, B. Campanini, S. Faggiano, S. Bettati, A. Mozzarelli, S. Bruno: "SS-nitrosylation and glycine control the activity of human serine racemase through an allosteric interplay" in Web Pro – Proteins

on the Web 2021, virtual event, May 20th-21st 2021. **Poster presentation and award winner.**

- O. De Bei, E. Gianquinto, L. Ronda, S. Faggiano, M. Marchetti, M. Cozzi, R. Giaccari, B. Campanini, S. Bettati, L. Lazzarato, M. Failla, F. Spyrakis: "Identiifcation of PPI disrupters that bind human hemoglobin and block its interaction with bacterial hemophore IsdB" in Web Pro – Proteins on the Web 2021, virtual event, May 20th-21st 2021. **Oral communication.**
- D. Pezzilli, M. Marengo, S. Oliaro Bosso, F. Spyrakis, S. Adinolfi: "Evolutionary, structural and functional differences between alpha amylases" in Web Pro – Proteins on the Web 2021, virtual event, May 20th-21st 2021. **Poster presentation.**
- E. Gianquinto, O. De Bei, M. Marchetti, L. Lazzarato, M. Failla, S. Bettati, L. Ronda, B. Campanini, F. Spyrakis: "Novel targets for iron starving resistant Staphylococcus aureus: in silico characterization of the IsdB-human haemoglobin complex" in PDB50, virtual event, May 4th-5th 2021. **Poster presentation.**
- O. De Bei, M. Levantino, M. Marchetti, E. Gianquinto, F. Spyrakis, B. Campanini, S. Bettati, L. Ronda: "Hemoglobin binding and heme extraction by Staphylococcus aureus hemophore IsdB investigated with X-ray solution scattering" in PDB50, virtual event, May 4th-5th 2021. **Poster presentation.**
- O. De Bei, E. Gianquinto, D.Y. Chirgadze, S.W. Hardwick, L. Cooper, M. Marchetti, F. Spyrakis, S. Bettati, L. Ronda, B.F. Luisi, B. Campanini: "Cryo-EM reveals how hemophore binding to Hb prompts heme removal: a structural and mechanistic insight into the function of IsdB from S. aureus" in PDB50, virtual event, May 4th-5th 2021. **Poster presentation.**
- E. Gianquinto, M. Santucci, L. Maso, S. Cross, F. Sannio, F. Verdirosa, F. de Luca, J.-D. Doquier, L. Cendron, D. Tondi, A. Venturelli, G. Cruciani, M.P. Costi, F. Spyrakis: "Virtual screening identifies cross-class inhibitors of clinically relevant serine- and metallo-beta-lactamases" in 13th Young Medicinal Chemist Symposium – Nuove Prospettive in Chimica Farrnaceutica (NPCF13), virtual event, April 26th-29th 2021. **Oral communication.**
- I. Mannella, C. Vigato, R. Pasha, A.C. Pippione, A.C. Sainas, S. Oliaro Bosso, B. Rolando, S. Kovachka, F. Spyrakis, D. Boschi, M.L. Lolli: "New inhibitorsof aldo-keto reductase 1C3 (AKR1C3) based on benzoisoxazole scaffold and their potential application in cancer" in 13th Young Medicinal Chemist Symposium – Nuove Prospettive in Chimica Farrnaceutica (NPCF13), virtual event, April 26th-29th 2021. **Poster presentation.**
- A.C. Pippione, Z. Kilic-Kurt, S. Sainas, B. Rolando, S. Kovachka, F. Spyrakis, A. Buschini, S. Montalbano, S. Oliaro Bosso, D. Boschi, M.L. Lolli: "Multiple-targeting ligands against prostate cancer: effect on both AKR1C3 enzyme and androgen receptor" in 13th Young Medicinal Chemist Symposium – Nuove Prospettive in Chimica Farrnaceutica (NPCF13), virtual event, April 26th-29th 2021. **Poster presentation.**
- E. Gianquinto, M. Santucci, L. Maso, S. Cross, F. Sannio, F. Verdirosa, F. de Luca, J.-D. Doquier, L. Cendron, D. Tondi, A. Venturelli, G. Cruciani, M.P. Costi, F. Spyrakis: "In silico identification of cross-class inhibitors against clinically relevant beta-lactamases" in AMYC-BIOMED, virtual edition, October 13th-14th 2020. **Selected for slide & talk presentation.**
- M. Marchetti, O. De Bei, M. Levantino, O. Moscetti, E. Gianquinto, M. Cozzi, F. Spyrakis, A. Bizzarri, S. Cannistraro, B. Campanini, S. Bettati, L. Ronda: "Protein-protein interactions and bacterial virulence: a mechanistic insight into the interaction between IsdB, a Staphylococcus aureus hemophore, and human haemoglobin" in CVI Congress of the Italian Society of Physics, September 14th-18th 2020, Bologna, Italy. **Poster presentation.**
- E. Gianquinto, M. Santucci, L. Maso, S. Cross, F. Sannio, F. Verdirosa, F. de Luca, J.-D. Doquier, L. Cendron, D. Tondi, A. Venturelli, G. Cruciani, M.P. Costi, F. Spyrakis: "In silico identification of cross-class inhibitors against clinically relevant beta-lactamases" in EFMC-ISMC & EFMC-YMSC virtual poster session, September 9th 2020. **Poster presentation.**
- C. Vigato, A.C. Pippione, S. Kovachka, F. Spyrakis, M. Daga, S. Oliaro-Bosso, D. Boschi, L. Lolli: "Application of an in house bioisosteric approach to the design of innovative inhibitors of aldo-keto reductase 1C3 (AKR1C3) in Merck Young Chemists' Symposium 2019, November 25th-27th 2019, Rimini, Italy. **Poster presentation**.
- L. Ronda, S. Bettati, A. Bizzarri, B. Campanini, O. De Bei, E. Gianquinto, F.J. Luque, M. Marchetti, I. Moscetti, F. Spyrakis: "Staphylococcus aureus IsdB and human hemoglobin: a biophysical description of a protein-protein interaction" in FISMAT 2019 – Italian national Conference on Condensed Matter Physics, September 30th-October 4th 2019, Catania, Italy **Poster presentation.**
- I. Moscetti, S. Bettati, A. Bizzarri, B. Campanini, O. de Bei, E. Gianquinto, F.J. Luque, M.

Marchetti, F. Spyrakis, L. Rnda: "Kinetic and dynamic characterization of the interaction between Staphylococcus aureus and human haemoglobin" CV Congress of The Italian Society of Physics, September 23th-27th 2019, L'Aquila, Italy. **Poster presentation.**

- B. Campanini, O. De Bei, M. Marchetti, F. Spyrakis, E. Gianquinto, S. Cannistraro, I. Moscetti, A. Bizzarri, L. Ronda, M. Levantino, S. Bettati: "Heme extraction from hemoglobin: kinetic insight on the function of IsdB hemophore from Staphylococcus aureus" in SIB2019 60th congress, Lecce, Italy, September 18th-20th, 2019. **Poster presentation.**
- S. Oliaro-Bosso, S. Adinolfi, G. D'Arrigo, G. Balliano, D. Poirier, M. Daga, F. Spyrakis: "Multiple catalytic activities of human recombinant 17 β-hydroxisteroid dehydrogenase type 7 respond differently to inhibitors" in SIB2019 60th congress, Lecce, Italy, September 18th-20th, 2019. **Poster presentation.**
- M. Daga, D. Boschi, M.L. Lolli, F. Spyrakis, A.C. Pippione, S. Sainas, S. Kovachka, V. Boscaro, M. Gallicchio, G. Chiorino, S. Adinolfi, S. Oliaro-Bosso: "AKR1C3 inhibitors designed by a bioisosteric approach to hit prostate cancer" in SIB2019 60th congress, Lecce, Italy, September 18th-20th, 2019. **Poster presentation.**
- O. De Bei, F. Spyrakis, E. Gianquinto, B. Campanini, L. Ronda, S. Bettai, M. Marchetti, S. Cannistraro, I. Moscetti, A.R. Bizzarri, M. Levantino: "Complex between a S. aureus hemophore and human hemoglobin as a target for novel antimicrobial agents against MRSA" in ULLA Summer School. University of Helsinki, Helsinki, Finland, June 2019. **Poster presentation.**
- E. Gianquinto, O. De Bei, M. Marchetti, L. Lazzarato, S. Guglielmo, R. Fruttero, S. Bettati, L. Ronda, B. Campanini, F.J. Luque, F. Spyrakis: "Structural and Dynamic characetrization of the IsdB-human haemoglobin complex: towards a novel strategy for iron-starving resistant Staphylococcus aureus" in XII European Drug Design Workshop (EWDD). Certosa di Pontignano, Siena, Italy, May 19th-24th, 2019. **Poster presentation. Selected poster by WILEY editor.**
- G. D'Arrigo, L. Siragusa, M. Baroni, G. Cruciani, F. Spyrakis: "Exploring nuclear receptors flexibility through X-ray structure analysis" in XII European Drug Design Workshop (EWDD). Certosa di Pontignano, Siena, Italy, May 19th-24th, 2019. **Poster presentation.**
- G. D'Arrigo, L. Siragusa, M. Baroni, G. Cruciani, F. Spyrakis: "Investigation of nuclear receptor structural variability" in 6th CDDD Meeting. Università Cattolica del Sacro Cuore, Rome, Italy, March 28th-29th, 2019. **Oral communication.**
- E. Gianquinto, O. De Bei, M. Marchetti, L. Lazzarato, S. Guglielmo, R. Fruttero, S. Bettati, L. Ronda, B. Campanini, F.J. Luque, F. Spyrakis: "Investigating and disrupting the interaction between hemoglobin and MRSA hemophores: in silico approaches to design novel antimicrobials" in 6th CDDD Meeting. Università Cattolica del Sacro Cuore, Rome, Italy, March 28th-29th, 2019. **Oral communication.**
- F. Spyrakis, O. De Bei, M. Marchetti, E. Gianquinto, B. Campanini, L. Ronda, S. Bettati: "Development of a high throughput assay to identify inhibitors of S. aureus IsdB binding to human hemoglobin" in O_2BiP (XXth International Conference on Oxygen Binding and Sensing Proteins, Barcelona, Spain, September 3rd-6th, 2018. **Poster Presentation.**
- E. Gianquinto, S. Di Lella, L. Lazzarato, S. Guglielmo, R. Fruttero, O. De Bei, M. Marchetti, B. Campanini, L. Ronda, S. Bettati, F.J. Luque, F. Spyrakis: "Investigating and disrupting the interaction between hemoglobin and MRSA hemophores: in silico approaches to design novel antimicrobials" in O_2BiP (XXth International Conference on Oxygen Binding and Sensing Proteins, Barcelona, Spain, September 3rd-6th, 2018. **Poster Presentation.**
- F. Spyrakis, E. Gianquinto, S. Di Lella, L. Lazzarato, S. Guglielmo, R. Fruttero, O. De Bei, M. Marchetti, B. Campanini, L. Ronda, S. Bettati: "Investigating the interaction between human hemoglobin and S. aureus IsdB to design novel antimicrobials" in MedChemSicily2018 (Italian-Spanish-Portoguese Joint Meeting in Medicinal Chemistry), Palermo, Italy, July 17th-20th, 2018. **Poster Presentation.**
- F. Spyrakis, D. Tondi, G. Celenza, G. D'Arrigo, E. Gianquinto, M. Santucci, S. Cross, P. Bellio, L. Cendron, J.-D. Docquier, J. Blàzquez, A. Venturelli, G. Cruciani, M.P. Costi: "In silico/in vitro approaches for the identification of new carbapenemase inhibitors" in MedChemSicily2018 (Italian-Spanish-Portoguese Joint Meeting in Medicinal Chemistry), Palermo, Italy, July 17th-20th, 2018. **Poster Presentation.**
- G. D'Arrigo, L. Siragusa, G. Cruciani, F. Spyrakis: "Analysis of structural relationships among nuclear receptors by in silico methodologies" in European School of medicinal Chemistry ESMEC, Urbino, Italy, July 1st-5th, 2018. **Poster Presentation.**
- G. D'Arrigo, L. Siragusa, G. Cruciani, F. Spyrakis: "Exploring nuclear receptor variability with innovative computational tools" in IX Giornate Italo-Francesi di Chimica, Genova, Italy, April 16th-18th, 2018. **Poster Presentation.**
- M. Gallicchio, M.L. Lolli, F. Spyrakis, D. Bonanni, V. Boscaro: "Indomethacin inhibits proloferation in cells harbouring PIK3CA mutations" in 38° Congresso Nazionale SIF, Rimini,

Italy, October 25th-28th, 2017. **Poster session**.

- G. Celenza, D. Tondi, L. Cendron, F. Spyrakis, P. Bellio, A. Mancini, L. Di Pietro, M. Vicario, M. Perilli, G. Amicosante: "The SOS response in bacteria and the LexA transcriptional repressor: withstanding drug resistance by inhibiting the bacterial mechanisms of adaptation to antimicrobials" in IC2AR, II International Caparica Conference in Antibiotic Resistance, Caparica, Portugal, June 11th-15th, 2017. **Oral communication**.
- M.P. Costi, M. Santucci, F. Spyrakis, S. Cross, D. Farina, D. Tondi, A. Quotadamo, J.D. Docquier, F. Croce, A.I. Prieto, C. Ibacache, J. Blàzquez, A. Venturelli, G. Cruciani: "Multiligand approach to the identification of resistant strains overexpressing beta-lactamase" in IC2AR, II International Caparica Conference in Antibiotic Resistance, Caparica, Portugal, June 11th-15th, 2017. **Oral communication**.
- L. Cendron, F. Spyrakis, S. Cross, P. Bellio, M.G. Perrilli, G. celenza, D. Tondi: "Structure-based drug design: the discovery of novel inhibitors active against New Delhi Metallo-beta-lactamase 1" in 13th beta-lactamase meeting, L'Aquila, Italy, June 16th-19th, 2017, **Poster session.**
- D. Bonanni, F. Spyrakis, M. Lolli, D. Boschi: "Multi target strategy against Castrate Resistant Cancer (CPRC) using Molecular Interaction Fields analysis" in X EWDD, 10th European Workshop in Drug Design, Certosa di Pontignano, Siena, Italy, May 17th-22nd, 2017, **Poster session.**
- J. Panecka, I. Pohner, T. Zeppelin, F. Spyrakis, M.P. Costi, R.C. Wade: "Comparative mapping of on-targets and off-targets for the discovery of anti-trypanosomatid folate pathway inhibitors" in Drug Innovation in Academia, Helmholtz Drug Research, Heidelberg, Germany, December 8th-9th, 2016, **Poster session**.
- F. Spyrakis, P. Bellio, M. Vicario, L. Cendron, F. Marcoccia, M.G. Perrilli, G. Cruciani, M.P. Costi, G. Celenza, D. Tondi: "Designing novel inhibitors for carbapenemases: a multidisciplinary approach" in XXIV National Meeting in Medicinal Chemistry, Perugia, Italy, September 11th-14th, 2016, **Poster session**.
- J. Panecka, I. Pohner, T. Zeppelin, F.Spyrakis, M.P. Costi, R.C. Wade: "Comparative mapping of on-targets and off-targets for the discovery of anti-trypanosomatid folate pathway inhibitors" in 21st EuroQSAR, Where Molecular Simulations Meet Drug Discovery, Verona, Italy, September 4th-8th, 2016, **Poster session**.
- L. Di Pietro, P. Bellio, A. Mancini, D. Tondi, F. Spyrakis, L. Cendron, M. Nicoletti, M. piovano, M. Perilli, G. Celenza: "SOS response in bacteria: inhibitory activity of lichen secondary metabolites against RecA protein" in IV International Conference on Antimicrobial Research, Torremolinos, Malaga, Spain, June 29th – July 1st, 2016, **Poster session**.
- F. Spyrakis, P. Bellio, M. Vicario, L. Cendron, F. Marcoccia, G. Cruciani, M.P. Costi, M.G. Perilli, G. Celenza, D. Tondi: "Designing novel inhibitors for metallo beta-lactamases" in IV International Conference on Antimicrobial Research, Torremolinos, Malaga, Spain, June 29th – July 1st, 2016, **Poster session**.
- C. Estarellas, F. Spyrakis, L. Franzoni, F.J. Luque, A. Bidon-Chanal: "Protein flexibility and ligand binding affinity in CRBPS: How are thery related?" in 3rd NovAliX Conference Biophysics in Drug Discovery 2016, Strasbourg, France, June 7th-10th, 2016, **Poster session**.
- A. Quotadamo, F. Spyrakis, G. Marverti, A. Cordeiro de la Silva, A. Venturelli, M.P. Costi: "Targeting the folate transporters to transit anti-parasitic agents through the macrophage to Leishmania donovani intracellular target" in COST Action CM1307 meeting "Targeted chemotherapy towards diseases caused by endoparasites", Porto, Portugal, May 5th-6th, 2016, **Oral communication**.
- S. Davalli, R. Benoni, S. Bettati, B. Campanini, A. Mozzarelli, T.A. Pertinhez, A. Pezzotti, S. Pellegrino, F. Spyrakis. "The interaction of O-acetylserine sulshydrylase with peptides: structural insight by STD-NMR and dacking" in Small Molecule NMR Conference, Baveno, Italy, September 20th-23rd, 2015, **Poster session.**
- J. Panecka, I. Pöhner, T. Zeppelin, F. Spyrakis, M.P. Costi, R.C. Wade. "Comparative analysis of targets and off-targets for the discovery of anti-trypanosomatid folate pathway inhibitors" in X EWDD, 10th European Workshop in Drug Design, Certosa di Pontignano, Siena, Italy, May 17th-22nd, 2015. **Poster session.**
- M. Santucci, F. Spyrakis, N. Nalajala, A. Venturelli, S. Cross, J. Blazquez, A. Borriello, S. Zuppolini, M.P. Costi. "new ligands for beta-lactamases biosensing" in Giornata della Chimica dell'Emilia Romagna – XIV edizione, Parma, Italy, December 18, 2014. **Poster session.**
- C. Estarellas, F. Spyrakis, L. Franzoni, F.J. Luque, A. Bidon-Chanal. "Thermodynamics of ligand binding to retinol binding-protein types I and II" in Entropy in Biomolecular Systems, Vienna, Austria, May 14-17, 2014. **Invited oral presentation & poster session**.
- F. Spyrakis, S. Cross, G. Cruciani, M. Santucci, D. Farina, A. Venturelli, M.P. Costi. "New

ligands for detecting drug resistant bacteria" in 20th EuroQSAR, Understanding Chemical-Biological Interactions, St-Petersburg, Russia, August 31-September 4, 2014. **Poster session**.

- M. Santucci, A. Venturelli, F. Spyrakis, D. Farina, A. Cusano, A. Borriello, S. Zuppolini, L. Sansone, M.P. Costi "Ligands discovery: molecular tool for β-lactamases detection in biological matrix" in NPCF8: Nuove Prospettive in Chimica Farmaceutica, Parma, June 9-11, 2014. **Poster session**.
- F. Spyrakis, B. Cellini, S. Bruno, P. Benedetti, E. Carosati, G. Cruciani, F. Micheli, A. Felici, P. Cozzini, G.E. Kellogg, C. Borri Voltattorni, A. Mozzarelli. "Targeting Cystalysin, a virulence factor of Treponema Denticola-supported Periodontitis" in Proteine 2014, Padova, Italy, March 31-April 1, 2014. **Poster session.**
- B. Campanini, S. Bettati, F. Spyrakis, R. Benoni, M. Pieroni, G. Costantino, C. Pecchini, F. Zani, A. Mozzarelli. "Blocking cysteine biosynthesis in Salmonella typhimurium: the moonlighting enzyme CysK as a potential antibiotic target" in Metabolism Meets Virulence, 2nd International Symposium on Metabolism and Bacterial Pathogenesis, Osnabrück, Germany, April 6-9, 2014. **Poster session**.
- A. Mozzarelli, B. Campanini, F. Spyrakis, S. Bettati. "Sulfur assimilation pathways in bacteria: new avenues for antibiotics" in 38th Congress of the Federation of European Biochemical Society (FEBS), Saint Petersburg, Russia, July 6-11, 2013. **Oral presentation**.
- F. Spyrakis, M. Gabba, S. Abbruzzetti, F. Forti, S. Bruno, A. Mozzarelli, F.J. Luque, C. Viappiani, P. Cozzini, M. Nardini, F. Germani, M. Bolognesi, L. Moens, S. Dewilde. "The dynamic regulation of human cytoglobin" in XVIIth International Conference on Oxygen Binding and Sensing Proteins, Parma, Italy, August 29-September 1, 2012. **Poster session.**
- A. Oliveira, F. Spyrakis, F. Forti, F.J. Luque. "Functional implications of structural plasticity of internal cavities in globins" in XVIIth International Conference on Oxygen Binding and Sensing Proteins, Parma, Italy, August 29-September 1, 2012. **Oral presentation.**
- G.E. Kellogg, J.N. Scarsdale, V.N. Koparde, M.H. Ahmed, F. Spyrakis, P. Cozzini, A. Mozzarelli. "Structural Bioinformatics in 3D. Using Hydropathic Interactions for Protein Model Building, Analysis and Prediction" in ACS meeting, San Diego, March 25-29, 2012. **Oral presentation.**
- G.E. Kellogg, F. Spyrakis, P. Cozzini. "Practical thermodynamics: The success of QSAR and related tools in computational medicinal chemistry" in SERMACS, Richmond, October 26-29, 2011. **Oral presentation.**
- A. Mozzarelli, F. Spyrakis, P. Cozzini, and G. E. Kellogg. "HINT (Hydropathic Interactions): a "natural" force field linking computational and experimental biochemists" in New trends in computational chemistry for industry applications, Barcelona, Spain, May 26-27, 2011. **Oral presentation.**
- F. Spyrakis, L. Dellafiora, P. Cozzini, R. Singh, E. Salsi, P. Benedetti, G. Cruciani, E. Carosati, B. Campanini, B. Cellini, A. Mozzarelli. "Structure- and ligand-based virtual screening of PLP-dependent enzymes" in New trends in computational chemistry for industry applications, Barcelona, Spain, May 26-27, 2011. **Poster session**.
- F. Spyrakis, A. Feis, G. Smulevich, P. Dominici, S. Abbruzzetti, C. Viappiani, S. Faggiano, S. Bruno, A. Mozzarelli, P. Cozzini, A. Bidon-Chanal and F. Javier Luque. "Investigating the dynamics of the distal histidine in AHb1 hemoglobin from Arabidopsis thaliana, through a combined computational and experimental approach" in XVIth International Conference on Oxygen Binding and Sensing Proteins, Antwerp, Belgium, August 22-26, 2010. **Poster session.**
- M. Gabba, S. Bruno, A. Mozzarelli, S. Abbruzzetti, C. Viappiani, F. Spyrakis, P. Cozzini, L. Moens, S. Dewilde. "Ligand assisted conformational changes modulate ligand migration in human cytoglobin" in XVIth International Conference on Oxygen Binding and Sensing Proteins, Antwerp, Belgium, August 22-26, 2010. **Poster session.**
- E. Salsi, F. Spyrakis, A. Bayden, A. Amadasi, B. Campanini, S. Bettati, T. Dodatko, P. Cozzini, G.E. Kellogg, P.F Cook, S. L. Roderick and A. Mozzarelli. "Identification of inhibitors for bacterial O-acetylserine sulfhydrylase-A and –B isozymes via in silico screening of a biased pentapeptide library and in vitro validation" in Proteine 2010, Parma, Italy, April 8-10, 2010. **Poster session.**
- R. Singh, A. Paiardini, B. Campanini, F. Spyrakis, P. Cozzini, C. Giunta and A. Mozzarelli, "A chemogenomic approach for the development of specific ligands in PLP-dependent enzymes" in Proteine 2010, Parma, Italy, April 8-10, 2010. **Poster session.**
- F. Spyrakis, E. Salsi, A. Bayden, A. Amadasi, B. Campanini, S. Bettati, T. Dodatko, P. Cozzini, G.E. Kellogg, P.F Cook, S. L. Roderick and A. Mozzarelli. "Identification of inhibitors of O-acetylserine sulfhydrylase via virtual and experimental screening of a biased pentapeptide library" in Therapeutic Applications of Computational Biology and Chemistry 2010, Wellcome Trust Genome Campus, Hinxton, Cambridge, UK, March 1-3, 2010. **Poster**

session.

- F. Spyrakis, L. Goracci, F. Veneri, C. Dall'Asta, G. Ingletto, A. Mozzarelli, G. Cruciani, P. Benedetti and P. Cozzini. "Computational analysis for the identification of endocrine disruptors in food additives and contaminants" in Interferenti Endocrini: dai Biomarker alla Valutazione del Rischio: il Progetto Previeni, Istituto Superiore di Sanità, Roma, Italy, October 27, 2009. **Poster session.**
- F. Spyrakis, E. Salsi, A. Bayden, B. Campanini, S. Bettati, G.E: Kellogg, P.Cozzini, P.F. Cook, S.L. Roderick and A. Mozzarelli. "Design of O-acetylserine sulfhydrylase inhibitors by mimicking Nature" in 54th National Meeting of the Italian Society of Biochemistry and Molecular Biology (SIB), Catania, Italy, September 23-26, 2009. **Poster session.**
- S. Abbruzzetti, C. Viappiani, S. Bruno, S. Faggiano, A. Mozzarelli, F. Spyrakis, S. Dewilde and L. Moens. "Shining light on functional dynamics and ligand migration in human cytoglobin" in VII European Biophysics Congress, Genova, Italy, July 11-15, 2009. **Poster session**.
- A. Bayden, G.E. Kellogg, A. Amadasi, P. Cook, E. Salsi, B. Campanini, F. Spyrakis, P. Cozzini and A. Mozzarelli. "Modeling interactions of potential antibiotic targets OASS A and OASS B with inhibitory peptides" in Watts Research Symposium, Richmond, Virginia, October 30, 2008. **Poster session.**
- P. Cozzini, G. Ingletto, F. Spyrakis, C. Dall'Asta. "Ciclodestrine specializzate come chemosensori per la determinazione di xenoestrogeni e micotossine" in Interferenti Endocrini: Valutazione e Prevenzione dei Possibili Rischi per la Salute Umana. Istituto Superiore di Sanità, Roma, October 15, 2008. **Poster session.**
- P. Cozzini, A. Amadasi, F. Spyrakis, A. Mozzarelli, C. Meda, A. Maggi. "Additivi alimentari come xeno estrogeni: un approccio investigativo integrato in silico ed in vitro" in Interferenti Endocrini: Valutazione e Prevenzione dei Possibili Rischi per la Salute Umana. Istituto Superiore di Sanità, Roma, October 15, 2008. **Poster session.**
- S. Abbruzzetti, E. Grandi, C. Viappiani, S. Bruno, S. Faggiano, A. Mozzarelli, F. Spyrakis, A. Feis, G. Smulevich, P. Dominici. "Ligand migration and modulation by distal cavity residues in non-symbiotic hemoglobin AHb1 from Arabidopsis thaliana" in XVth International Conference on O2 Binding and Sensing Proteins, Aarhus, Denmark, August 17-21, 2008. **Oral presentation.**
- S. Abbruzzetti, C. Viappiani, S. Bruno, S. Faggiano, A. Mozzarelli, F. Spyrakis, S. Dewilde, L. Moens. "Ligand migration in human neuroglobin highlights a complex system of interconnected cavities" in XVth International Conference on O2 Binding and Sensing Proteins, Aarhus, Denmark, August 17-21, 2008. **Poster session.**
- S. Faggiano, S. Bruno, C. Viappiani, S. Abbruzzetti, E. Grandi, F. Spyrakis, P. Dominici, A. Mozzarelli. "Reactivity of Arabidopsis thaliana nonsymbiotic hemoglobin AHb1 with O2 and NO: insights for a NO dioxygenase activity" in XVth International Conference on O2 Binding and Sensing Proteins, Aarhus, Denmark, August 17-21, 2008. **Poster session.**
- F. Spyrakis, A. Marabotti, A. Facchiano, P. Cozzini, G.E. Kellogg, D.J. Abraham, A. Mozzarelli. "Energy-based code for preferential amino acid-base recognition" in From Molecules to Medicine: Integrating Crystallography in Drug Discovery, the 40th crystallographic meeting at Erice, Erice, Sicily, Italy, May 29-June 8, 2008. **Poster session.**
- F. Spyrakis, A. Marabotti, A. Facchiano, A. Mozzarelli, G.E. Kellogg, D.J. Abraham and P. Cozzini. "Energy-based principles to predict amino acid-nucleotide base specific recognition in protein-DNA complexes" in INBB Workshop "Biosensori per l'Ambiente e la Salute". Rome, Italy, October 9-10, 2007. **Poster session.**
- P. Cozzini, F. Spyrakis, A. Amadasi, A. Mozzarelli, G.E. Kellogg. "A fast empirical scoring method for docking and virtual screening" in 6th AFMC International Medicinal Chemistry Symposium, Istanbul, Turkey, July 8-11, 2007. **Oral communication.**
- A. Amadasi, F. Spyrakis, A. Mozzarelli, P. Cozzini. "Towards a virtual screening that includes protein flexibility: the case study of the estrogen receptor" in Gordon Research Conference on Computational Chemistry, Les Diablerets, Switzerland. October 8-13, 2006. **Poster session.**
- M. Fornabaio, F. Spyrakis, C. Calò, A. Amadasi, A. Tripathi, P. Cozzini, A. Mozzarelli, G.E. Kellogg: "Evaluating docking methods with a hydropathic scoring function" in American Chemical Society 232nd National Meeting & Exposition. San Francisco, CA, USA, September 10-14, 2006. **Poster session.**
- F. Spyrakis, S. Raboni, P. Cozzini, S. Bettati, A. Mozzarelli: "Allosteric communication between alpha and beta subunits of tryptophan synthase: modelling the open-closed transition of the alpha subunit" in International interdisciplinary conference on vitamins, coenzymes, and biofactors. Awaji, Japan, November 06-11, 2005. **Oral communication.**
- A. Amadasi, F. Spyrakis, P. Cozzini, A. Mozzarelli, D.J. Abraham, G.E. Kellogg: "Evaluation of the role played by water molecules in biomolecular recognition: a computational

approach" in Theoretical modelling of ligand binding and enzyme catalysis. FEBS advanced course. Tromso, Norway, October 16-21, 2005. **Poster session.**

- A. Marabotti, A. Facchiano, F. Spyrakis, P. Cozzini, G.E. Kellogg, D.J. Abraham and A. Mozzarelli: "Analysis of the interaction between proteins and DNA: finding recognition code" in "MGMS Annual International Meeting 2005 - Biomolecular Simulation". Dublin. Ireland, September 11-14, 2005. **Poster session.**
- G.E. Kellogg, M. Fornabaio, D.L. Chen, P. Cozzini, F. Spyrakis, A. Mozzarelli and D.J. Abraham: "Life, the universe and everything. Modeling binding with an empirical, solvation-based free energy paradigm" in Computer Aided Drug Design GRC conference. Tilton, New Hampshire, USA, July 31- August 5, 2005. **Poster session.**
- F. Spyrakis, P. Cozzini, A. Marabotti, G.E. Kellogg, D.J. Abraham and A. Mozzarelli: "A non Newtonian approach for the evaluation of protein-DNA binding free energy and molecular recognition" in Computer Aided Drug Design GRC conference. Tilton, New Hampshire, USA, July 31- August 5, 2005. **Poster session.**
- G.E. Kellogg, M. Fornabaio, P. Cozzini, A. Mozzarelli, F. Spyrakis and D.J. Abraham: "Understanding protein-ligand interactions and binding free energy with an empirical and solvation-based model" in 229th ACS National Meeting. San Diego CA, USA, March 13-17, 2005. **Oral communication.**
- F. Spyrakis, A. Amadasi, M. Fornabaio, P. Cozzini, G.E. Kellogg, D.J. Abraham and A. Mozzarelli: "Ranking the strength of interaction between water molecules and proteins using HINT, a "natural" force field" in VI Convegno Nazionale INBB. Napoli, Italy, November 4-6, 2004. **Poster session.**
- F. Spyrakis, L. Giurato, P. Cozzini, M. Modica, I. Sylte and S. Guccione: "5-HT$_{1A}$ receptor binding analysis of thienopyrimidinons partila agonists: a paradigm breaking study regarding the pharmacophoric leadership of the protonated piperazine ring in GPCR ligands" VI Convegno Nazionale INBB. Napoli, Italy, November 4-6, 2004. **Poster session.**
- P. Cozzini, M. Fornabaio, F. Spyrakis, G.E. Kellogg, D.J. Abraham and A. Mozzarelli: "Biomolecular association: from structural data to binding affinity prediction using HINT, a "natural" force field" in VI Convegno Nazionale INBB. Napoli, Italy, November 4-6, 2004. **Poster session.**
- M. Fornabaio, P. Cozzini, F. Spyrakis, A. Mozzarelli, D.J. Abraham and G.E. Kellogg: "Computational study of the role of bridging water molecules in the energetics of protein-ligand binding" in 228th ACS National Meeting. Philadelphia PA, USA, August 22-26, 2004. **Poster session.**
- K. Kristiansen, I. Sylte, R. Ciaccio, S. Forte, L. Giurato, P. Cozzini, F. Spyrakis and S. Guccione: "Molecular modelling of endothelin ET$_A$ and ET$_B$ receptor interactions" in XVIII'th International Symposium on Medicinal Chemistry. Copenhagen, Denmark & Malmö, Sweden, August 15-19, 2004. **Poster session.**
- P. Cozzini, M. Fornabaio, A. Mozzarelli, F. Spyrakis, D.J. Abraham and G.E. Kellogg "Water: How to evaluate its contribution in protein-ligand interactions" in EUCO CC5 Tolone, France, June 2004. **Oral communication.**
- F. Spyrakis, M. Fornabaio, P. Cozzini, A. Mozzarelli, G.E. Kellogg and D.J. Abraham: "Evaluation of the water contribution to the free energy of protein-ligand interaction" in Proteine 2004. Viterbo, Italy May 20-22, 2004. **Poster session.**
- P. Cozzini, M. Fornabaio, A. Mozzarelli, F. Spyrakis, G.E. Kellogg and D.J. Abraham "HIV-1 protease: a good system to evaluate protein-ligand interactions, water role and protonation state, using an empirical approach" in BITS 2004. Padova, Italy, March 26-27, 2004. **Poster session.**
- P. Cozzini, F. Spyrakis, M. Fornabaio, S. Forte, S. Guccione and L. Giurato: "The Significance of pH Effects in Protein-Ligand Interaction Models" in 2nd Workshop on "The state-of-art of Computational Chemistry in the University of Calabria and Basilicata". Catanzaro, Italy, February 5-6, 2004. **Poster session.**
- P. Cozzini, M. Fornabaio. F. Spyrakis, G.E. Kellogg, D.J. Abraham and A. Mozzarelli: "From LogP to computational titration: using a natural force field to predict binding affinity of protein-ligand complexes" in Computational Methods in Toxicology and Pharmacology Integrating Internet Resources, Thessaloniki, Greece, September 17-19, 2003. **Oral communication.**
- M. Fornabaio, P. Cozzini, F. Spyrakis, D.J. Abraham, G.E. Kellogg and A. Mozzarelli: "In silico Prediction of the free Energy of Protein-Ligand Binding" in INFMeeting, Genova, Italy, June 23-25, 2003. **Poster session.**

Research projects

PI for international and national projects

- "Defeat antimicrobial resistance through iron starvation in *Staphylococcus aureus*" PRIN2020. Project granted by MUR. Total grant: 631.227 euros; grant to UNITO: 163.165 euros. **Local unit PI: Francesca Spyrakis**
- "BRAVE – Protecting the brain from COVID-19-mediated neurodegeneration through inflammasome inhibition". Call H2020-SGA-FETFLAG-HBP-2019. Framework Partnership Agreement (FPA) No: 650003 – Specific Agreement Number: 945539 – HBP SGA3. Project granted by EC. Total grant: 250.000 euros; grant to UNITO: 112.500 euros. **PI: Francesca Spyrakis.**
- Investigating Nuclear Receptors Dynamic cross-relationships". Iscra B project, Cineca, 2020. Total computational hours: 1.175.040. **PI: Francesca Spyrakis**
- NEWAIMS: New Antimicrobials to Starve Superbugs". Project granted by Compagnia San Paolo. 2017 – 2019. Total grant: 82.357 euros. **PI: Francesca Spyrakis.**
- "Investigation of nuclear receptors dynamic relationships". Iscra C project, Cineca, 2019. Total computational hours: 400.000. **PI: Francesca Spyrakis**
- "Unraveling the structure-dynamics-functions in newly discovered haemproteins: implications for novel biotechnological and biomedical applications." Beatriu de Pinós 2010. Fellowships for the recruitment and mobility of research personnel to the Catalan system of science and technology. Project granted by Generalität de Catalunya, Spain. Grant: 74.527 euros. **PI: Francesca Spyrakis.** I had to renounce because of maternity issues.

Scientific reference for company-financed researches

- Scientific reference for a PhD fellowship partially financed by per una convenzione di dottorato fra l'Università di Torino e l'azienda Solvay Polymers Spa. Project title: "In silico prediction of bioaccumulation and biodegradation of PFAS". Total grant: 30.000 euros.
- Scientific reference for a PhD fellowship totally financed by Molecular Discovery Ltd. Project title: "Nuclear receptors: structural and dynamic relationship analysis by innovative *in silico* methodologies". Total grant: 60.000 euros.

Participation to international and national research projects

- CN1 PNRR: ICSC, National Center HPC, Big Data e Quantum Computing, Spoke 8, In silico medicine and omics data. Project granted by PNRR. 2022-2025. Grant given to F. Spyrakis: 80.000 euros.
- "Processi sostenibili per la produzione di molecole ad attività antivirale a partire da biomasse residuali dell'industria agroalimentare piemontese". Project granted by Fondazione CRT 2023-2024. Total grant: 35.000 euro.
- "Alliance for the exploration of pipelines for inhibitors of carbapenemases – EPIC Alliance". Project granted by JPIAMR Network Plus 2020. 2020-2021. Total grant: 98.980 euro.
- "SMART - Strigolattoni: molecole antivirali naturali?" TOINPROVE. Project granted by MISE, 2021-2022.
- "New strategies to fight antimicrobial resistance". Project granted by Fondazione CRT 2019-2020. Total grant: 35.000 euros.
- "NACTUS: New weapons to fight castrate-resistant prostate cancer". Project granted by Fondazione CRT. 2018-2019. Total grant: 35.000 euros.
- "Investigating the heme extraction mechanism of hemophores with time-resolved WAXS". Progetto finanziato da ESRF (European Synchrotron Radiation Facility, 2018). Grant: beamline (5 days) + trip.
- "Towards an atlas of pockets on the kinome". Project granted by PRACE (Partnership for Advanced Computing in Europe, 2018-2019. Grant: 9.955.312 computation hours.
- "Role of class A carbapenemases in beta-lactam antibiotic resistance: from structural analysis to the development of new broad-spectrum inhibitors". Project granted by FAR2014, Fondo di Ateneo per la Ricerca, Università di Modena and Reggio Emilia. Total grant: 28.000 euros.
- "NMTrypI, new medicines for trypanosomatidic infections." Seventh Framework Programme. Grant agreement no: 603240, 2014-2016. Project granted by EC. Total grant: 7.609.868 euros. Grant to UNIMORE: 746.284 euros.
- "OPTObacteria, multianalyte automatic system for the detection of drug resistant bacteria." Seventh Framework Programme. Grant agreement no: 286998, 2012-2014. Project granted by EC. Total grant: 1.626.952 euros. Grant given to UNIMORE: 407.000

euros. Scientific manager assistant.

- "Role of hemoglobins in removing oxygen and nitrogen reactive species." Program of scientific and technological collaboration between Italy and Argentina. Project granted by Ministero Italiano degli Esteri, 2011-2013. Grant given to UNIPR: 30.000 euros.
- "Identification of cyclopropane fatty acid synthase inhibitors through computational analyses." Project granted by BICT s.r.l., 2010. Grant given to UNIPR: 21.000 euros.
- "Mapping ligand migration through hydrophobic cavities in non-symbiotic hemoglobins from Arabidopsis thaliana." Integrated Action Italy-Spain. Project granted by MIUR, 2010-2011. Grant given to UNIPR: 8.560 euros.
- "Biotechnological approach to hypo-oxygenation pathologies: hemoglobin-based blood substitutes." Project granted by Fondazione Cariparma, 2009-2011. Grant given to UNIPR: 54.000 euros.
- "Ligand-protein interaction evaluation by computational and experimental methods." International collaboration project with Virginia Commonwealth University, Richmond, Virginia, USA, and University of Oklahoma, Norman, Oklahoma, USA. Project granted by MIUR, 2006-2010. Grant given to UNIPR: 68.200 euro.
- "Analysis of the dynamic properties of the estrogen receptor and screening of food additives libraries for the identification of potential endocrine disruptors." Project granted by Regione Emilia-Romagna for food quality and safety (SITEIA-High technology laboratories), 2005-2010.
- "Identification of new hits for phosphodiesterase targets involved in COPD by a computational analysis with HINT, an experimental force field." Project granted by CHIESI Farmaceutici, 2005.
- "PLP-dependent enzymes. From genomics to the enzymatic regulation." Project granted by MIUR (COFIN 2005), 2005-2006. Grant given to UNIPR: 60.000 euro.
- Euroblood substitutes, genomics and blood substitutes for 21st century Europe." Six Framework Programme. Grant agreement no: 503023, 2004-2006. Project granted by EC. Total grant 2.655.091 euros. Grant given to UNIPR: 190.000 euros.

Periods abroad

- 2023 Teaching staff exchange within the Erasmus+ Programme. University of paris Saclay (1 week)
- 2023 Teaching staff exchange within the Erasmus+ Programme. University of West Timisoara (1 week)
- 2022 Teaching staff exchange within the Erasmus+ Programme. University of CEU San Pablo, Madrid (1 week).
- 2019 Visiting researcher at Virginia Commonwealth University (Prof. G.E. Kellogg, Medicinal Chemistry Department; 1 week).
- 2018 Teaching staff exchange within the Erasmus+ Programme. University of Barcelona (1 week).
- 2011 Visiting researcher at the lab of Professor Javier Luque, Department of Physical Chemistry, University of Barcelona (1 month).
- 2010 Visiting researcher at the lab of Professor Javier Luque, Department of Physical Chemistry, University of Barcelona (1 month).
- 2008 Fellowship financed by HPC-Europe Transnational Access, for the project "Ligand migration in non-symbiotic *Arabidopsis thaliana* hemoglobins", Department of Physical Chemistry, University of Barcelona (3 months).
- 2006 Visiting student at Virginia Commonwealth University (Proff. D.J. Abraham e G.E. Kellogg, Medicinal Chemistry Department; 3 months). Different periods were spent at VCU in the following years.

Invited seminars at foreigner institutions

- Computational methods for antibiotic discovery: targeting *Staphylococcus aureus* hemophores." February 15th 2019. Medicinal Chemistry Department, Virginia Commonwealth University, Richmond, Virginia, USA.
- "Nuclear receptors: structural and dynamic relationship analysis by innovative *in silico* methodologies." July 10th 2018. Campus de la Alimentaciòn de Torribera, Universitat de Barcelona. Barcelona. Spain.
- "*In silico* approaches for the identification of new carbapenemase inhibitors." July 11th 2018. Campus de la Alimentaciòn de Torribera, Universitat de Barcelona. Barcelona. Spain.

Honors and awards

- Best poster presented at: XXVII National Meeting in Medicinal Chemistry, September 11th-14th 2022, Bari, Italy. F. Spyrakis, A.R. Bizzarri, P. Brear, S. Cannistraro, D.Y. Chirgadze,

L.R. Cooper, M. Cozzi, O. De Bei, S. Faggiano, R. Giaccari, E. Gianquinto, D. Gobbo, S. Guglielmo, S.W. Hardwick, S. Kovachka, L. Lazzarato, B.F. Luisi, M. Marchetti, L. Ronda, B. Campanini, S. Decherchi, S. Bettati: "New targets and interferents to fight *Staphilococcus aureus* resistance*".*

- Best poster presented at: ESMEC school 2021, virtual event, June 28th-July 1st 2021. E. Gianquinto, M. Santucci, L. Maso, S. Cross, F. Sannio, F. Verdirosa, F. de Luca, J.-D. Doquier, L. Cendron, D. Tondi, A. Venturelli, G. Cruciani, M.P. Costi, F. Spyrakis: "*In silico*-guided discovery of inhibitors with cross-class activity on clinically relevant carbapenemases".
- Best poster presented at: Bioexcel Summer School, virtual event, June 4th-11th 2021.
  E. Gianquinto, M. Santucci, L. Maso, S. Cross, F. Sannio, F. Verdirosa, F. de Luca, J.-D. Doquier, L. Cendron, D. Tondi, A. Venturelli, G. Cruciani, M.P. Costi, F. Spyrakis: "An *in silico* pipeline identifies inhibitors with cross-class activity on clinically relevant serine- and metallo-beta-lactamases".
- Best poster presented at: Web Pro – Proteins on the Web 2021, virtual event, May 20th-21st 2021.
  F. Spyrakis, E. Gianquinto, F. Marchesani, I. Autiero, A. Michielon, B. Campanini, S. Faggiano, S. Bettati, A. Mozzarelli, S. Bruno: "SS-nitrosylation and glycine control the activity of human serine racemase through an allosteric interplay".
- Best poster presented at: XXII European Workshop on Drug Design, Certosa di Pontignano, Siena, May 19th-24th 2019.
  E. Gianquinto, O. De Bei, M. Marchetti, L. Lazzarato, S. Guglielmo, R. Fruttero, S. Bettati, L. Ronda, B. Campanini, F.J. Luque, F. Spyrakis: "Structural and Dynamic characetrization of the IsdB-human haemoglobin complex: towards a novel strategy for iron-starving resistant Staphylococcus aureus"

Membership in associations

- President of the local committee of the Italian Chemical Society for Piemonte-Valle d'Aosta, from 2023-2025.
- Member of the local committee of the Italian Chemical Society for Piemonte-Valle d'Aosta, from 2019-2022.
- Member of the Italian Chemical Society from 2017.
- Member of the American Chemical Society in 2018.

Editorial Activity

- Editor in Chief for the Biological Systems section of Processes, MDPI.
- Associate Editor per Biological Modeling and Simulation for Frontiers in Molecular Biosciences
- Associate Editor per *In silico* Methods and Artificial Intelligence for Frontiers in Drug Discovery
- Member of the Editorial Academic Panel for PLOS ONE.
- Member of the Editorial Board for Scientific Reports.
- Guest Editor for the special issue of Nuclear Receptor Research "Nuclear receptors: from drugs to food, from *in silico* to *in vivo* approaches" (2016). AgiAL Publishing House. Giza, Egypt.
- Guest Editor for the special issue of Current Drug Targets "From extended spectrum beta-lactamases to carbapenemases: the neverending challenge against Gram-negative bacteria" (2015). Bentham Science Publisher Ltd. Sharjah, United Arab Emirates.
- Guest Editor for volume 11 (issue 2) of Current Topics in Medicinal Chemistry "Applying Induced Fit in Drug Discovery: Square Pegs and Round Holes?" (2010). Bentham Science Publisher Ltd. Sharjah, United Arab Emirates.

Reviewing activity

Referee for Scientific Reports, ACS Medicinal Chemistry Letters, Journal of Medicinal Chemistry, European Journal of Medicinal Chemistry, PLOS Computational Biology, Journal of Cellular Biochemistry, Journal of Molecular Graphics and Modelling, International Journal of Molecular Sciences, Archives of Biochemistry and Biophysics, Journal of Alzheimer Disease, International Journal of Medicinal Chemistry, Acta Physica Polonica, Letters into

Drug Design and Discovery, Cell Biochemistry and Biophysics, Nuclear Receptor Research, Molecules.

Public Engagement

- "Quello che c'è nella compressa….mi fa effetto" di E. Ugazio, F. Spyrakis, F. Foglietta, L. Serpe, Dipartimento di Scienza e Tecnologia del Farmaco, Università di Torino. Seminario per le scuole superiori, Notte dei Ricercatori 2021, 21/22 Settembre 2021.
- Scrittura dei seguenti racconti della scienza per FRidA (Il forum della ricerca di Ateneo dell'Università di Torino):

"One health: una sfida multidisciplinare per il benessere in tutte le specie" di C. Prandi, V. Dell'Oste, F. Spyrakis. October 1st 2020.

"Herpesvirus e coronavirus: speciali ormoni delle piante possono aiutarci a combatterli" di C. Prandi, V. Dell'Oste, F. Spyrakis. October 1st 2020.

"Abili transformer. Il ruolo chiave degli strigolattoni contro il cancro" di C. Prandi, V. Dell'Oste, F. Spyrakis. October 1st 2020.

- Organization of the events *PHARMA MENTIS …in corpore sano.* Series of meeting on the role of graduate students in industry: the Department of Drug Science and Technology meets companies in the pharmaceutical and health products sector.

  June 21st 2019. "The role of graduate student in pharmaceutical companies". Department of Drug Science and Technology, University of Turin.

  October 18th 2019. "The University meets the pharmaceutical company". Department of Drug Science and Technology, University of Turin.

Turin, May 11rth, 2023