

PERSONAL INFORMATION

Eleonora Gianquinto

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Dept. of Drug Science and Technology

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Current position Non-tenure Track Research Associate

Ricercatore a tempo determinato di tipo A (RTDA)

University of Turin

Department of Drug Science and Technology

via Giuria 9, 10125, Turin, Italy

WORK EXPERIENCE

01/02/2023 – 31/05/2023 Fellowship

University of Turin

Department of Drug Science and Technology

via Giuria 9, 10125, Turin, Italy

Project title: “*In silico* analyses for the development of beta-lactamase inhibitors”

Supervisor Prof. F. Spyraakis, Molecular Modelling for Drug Design (M4D) Group

01/02/2022 – 31/01/2023 Post-doctoral Researcher

University of Turin

Department of Drug Science and Technology

via Giuria 9, 10125, Turin, Italy

Project title: *in silico* design of NLRP3 inflammasome inhibitors targeting neuroinflammation

Funding project: Protecting the brain from COVID-19-mediated neurodegeneration through inflammasome inhibition (BRAVE)

Principal Investigator Prof. F. Spyraakis, Molecular Modelling for Drug Design (M4D) Group

EDUCATION AND TRAINING

Oct. 2018 – May 2022 PhD in Pharmaceutical and Biomolecular Sciences

top grade

University of Turin

Department of Drug Science and Technology

via Giuria 9, 10125, Turin, Italy

Thesis Title: *In silico* approaches for the design of innovative agents against emerging infectious diseases.

Supervisor: Prof. Francesca Spyraakis

Reviewers: Prof. F. Javier Luque, Prof. Giulio Rastelli

June 2021 Pharmacist license

University of Turin
Department of Drug Science and Technology
via Giuria 9, 10125, Turin, Italy

June 2019 **Master Degree**

grade: 70/70 *summa cum laude*

University of Turin

Institution of Excellence and Higher Education for University Studies "Ferdinando Rossi"
(Scuola di Studi Superiori "Ferdinando Rossi" dell'Università di Torino, SSST)
via Verdi 8, 10124, Turin, Italy

Thesis Title: Digital sustainability: between disappointed expectations and disillusioned prospects

Supervisor: Prof. Matteo Baldoni

Oct 2013 - Oct 2018 **Master of Science in Industrial Pharmacy**

grade: 110/110 *summa cum laude*

University of Turin

Department of Drug Science and Technology
via Giuria 9, 10125, Turin, Italy

Thesis Title: Investigating and disrupting the interaction between hemoglobin and MRSA hemophores: *in silico* approaches to design novel antimicrobials.

Supervisor: Prof. Francesca Spyraakis,

Co-Supervisor: Prof. F. Javier Luque Garriga

TEACHING AND TUTORING
ACTIVITIES

Teaching activity

- 2023 **Lecturer (1 hour), course: Medicinal Chemistry II.**
Course held by Prof. Massimo Bertinaria and Prof. Clara Cena
University of Turin
Department of Drug Science and Technology, Turin.
Master of Science in Industrial Pharmacy
- 2023 **Lecturer (4 hours), course: Computer-Aided Drug Design.**
Course held by Prof. Francesca Spyraakis.
University of Turin
Department of Drug Science and Technology, Turin.
Master of Science in Pharmacy
- 2022 **Lab assistant (60 hours), course: Preparation of herbal medicinal products.**
Course held by Prof. Konstantin Chegaev.
University of Turin
Department of Drug Science and Technology, Savigliano.
Bachelor of Science in Herbal Techniques
- 2021 **Lab assistant, course: Computer-Aided Drug Design (CADD)**
Course held by Prof. Francesca Spyraakis
University of Turin
Department of Drug Science and Technology.
Master of Science in Industrial Pharmacy

2020 Lab assistant, course: Computer-Aided Drug Design (CADD)

Course held by Prof. Francesca Spyraakis
University of Turin
Department of Drug Science and Technology.
Master of Science in Industrial Pharmacy

2019 Lab assistant, course: Computer-Aided Drug Design (CADD)

Course held by Prof. Francesca Spyraakis
University of Turin
Department of Drug Science and Technology.
Master of Science in Industrial Pharmacy

Tutoring activity

Co-supervision of Master's theses

2022 – 2023 *In Silico* Approaches for Drug Repurposing and Novel Molecule Discovery Against NLRP3 Inflammasome by Luca Cortello. Master of Science in Pharmacy. University of Turin, A.Y.: 2022-2023

2022 – 2023 "Identification of SbnA inhibitors to fight antimicrobial resistance" by Lorenza Rinaldi. Master of Science in Chemistry, University of Turin, A.Y.: 2022-2023

2021 – 2022 "*In silico* methods applied to the development of novel molecules targeting the NLRP3 inflammasome." by Alessio Atzei. University of Turin, Department of Drug Science and Technology, Master of Science in Industrial Pharmacy, A.Y.: 2021-2022

Technical assistance to fellow students, PhD students, and Post-Doctoral researchers

2023 – present Postdoctoral project entitled "*In silico* design and synthesis of antimicrobials against Gram positive bacteria, with a focus on *Staphylococcus aureus* (PRIN 2020)" by Somayeh Asghapour. University of Turin, Department of Drug Science and Technology.

2022 – present PhD thesis entitled "*In silico* prediction of bioaccumulation, toxicity and biodegradability of PFAS." by Gioele A. Tiburtini. University of Turin, Department of Drug Science and Technology, Doctoral School in Pharmaceutical and Biomolecular Sciences

2022 – 2023 Research fellowship entitled "Computational approaches for the discovery of novel carbapenemase inhibitors" by Laura Bertarini. University of Turin, Department of Drug Science and Technology

2021 – present PhD thesis entitled "Identification of low environmental impact molecules to counteract antimicrobial resistance through *in silico* methodologies." by Matteo Bersani. University of Turin, Department of Drug Science and Technology, Doctoral School in Pharmaceutical and Biomolecular Sciences

2019 – 2020 Research fellowship entitled "Computational methods for the development of novel antimicrobials" by Sandra Kovachka. University of Turin, Department of Drug Science and Technology

INSTITUTIONAL ASSIGNMENTS

2023 – present Member of the Teaching Committee

2023 – present Member of the Departmental Academic Council

Representation of postdoctoral fellows and temporary affiliates

Department of Drug Science and Technology, University of Turin

2022 – 2023 Member of the Teaching Committee
2022 – 2023 Postdoctoral fellows' representative the Departmental Academic Council

Representation of PhD students Department of Drug Science and Technology, University of Turin
2018 – 2022 Member of the Research Funding Committee
2018 – 2022 PhD students' representative the Departmental Academic Council

Representation of students Department of Drug Science and Technology, University of Turin
2014 – 2018 Students' representative in the Departmental Academic Council

LANGUAGE SKILLS

Mother tongue Italian

Other languages

	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken interaction	Spoken production	
English	C2	C2	C1	C1	C1
Global IELTS score: 8.0 (assessed on 16/05/2019)					

Levels: A1 and A2: Basic user – B1 and B2: Independent user – C1 and C2: Proficient user
[Common European Framework of Reference for Languages](#)

Driver License B1

GRANTS AND PRIZES

presenting author

2022 Best poster prize

XXVI National Meeting on Medicinal Chemistry (NMMC), Bari, Sept. 11th-14th 2022.

F. Spyraakis, 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 *Staphylococcus aureus* resistance" in XXVI National Meeting on Medicinal Chemistry (NMMC), Bari, Sept. 11th-14th 2022. *Poster presentation*.

2021 Best poster prize

CECAM workshop: "Quantifying Protein Dynamics and Allosteric regulation in the cell with emerging technologies", Lausanne, 15-17/09/2021.

E. Gianquinto, F. Marchesani, I. Autiero, A. Michielon, B. Campanini, S. Faggiano, S. Bettati, Andrea Mozzarelli, Stefano Bruno, Francesca Spyraakis: "An allosteric interplay among glycine, ATP and S-nitrosylation modulating serine racemase activity" in Quantifying Protein Dynamics and Allosteric regulation in the cell with emerging technologies: From Cryo-EM and NMR to Multiscale Simulations, Networks and Machine Learning hosted by CECAM, 15-17/09/2021, Lausanne.

2021 EFMC grant

EFMC International Symposium on Medicinal Chemistry (EFMC-ISMC 2021) e a 7th EFMC Young Medicinal Chemist Symposium (EFMC-YMCS 2021), 29/08/2021 e 9-10/09/2021

2021 Best poster prize

European School of Medicinal Chemistry (ESMEC), virtual event, 28/06/2021-01/07/2021.

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. Spyraakis: “*in silico*-guided discovery of inhibitors with cross-class activity on clinically relevant carbapenemases” in ESMEC school 2021, virtual event, 28/06/2021.

2021 Best poster prize

BioExcel Summer School, virtual event, 4-11/06/2021.

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. Spyraakis: “An *in silico* pipeline identifies inhibitors with cross-class activity on clinically relevant serine- and metallo-beta-lactamases” in Bioexcel Summer School, virtual event, 04-11/06/2021.

2021 NPCF13 fellowship

13th Young Medicinal Chemist Symposium (NPCF), virtual event.

2020 HPC-Europa3 fellowship

Borsa HPC-Europa3 per un periodo di visita (13 mesi) al centro di calcolo EPCC (Edinburgh). Mobilità convertita in 4 mesi di visita virtuale causa pandemia di COVID-19.

2020 Winner of Erasmus Traineeship mobility

Erasmus Traineeship (three months) at University College of London (UCL). Mobility was cancelled due to COVID-19 pandemic.

2020 Prize for the best Master's thesis in Industrial Pharmacy - A.Y. 2017/18

University of Turin

2019 Best poster prize

12th Workshop on Drug Design, Certosa di Pontignano, Siena (Italy).

E. Gianquinto, O. De Bei, M. Marchetti, L. Lazzarato, S. Guglielmo, R. Fruttero, S. Bettati, L. Ronda, B. Campanini, F.J. Luque, F. Spyraakis: “Structural and Dynamic characterization 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, 19-24/05/2019.

2017 Winner of "Cecilia Gilardi" Fellowship

"Cecilia Gilardi" fellow for research activity in Computer-Aided Drug Design (CADD) at University of Barcelona. Fondazione "Cecilia Gilardi", Turin, Italy.

2017 Winner of Erasmus+ Fellowship

Erasmus+ student (four months) at the University of Barcelona, for completing the Master's Thesis in Industrial Pharmacy.

TRAINING AND RESEARCH ACTIVITIES IN INTERNATIONAL INSTITUTIONS

19/11/2023 – 01/12/2023

Erasmus+ Staff Training

University of Geneva, Switzerland

– Sampling Water Interfaces through Scaled Hamiltonians Expanded (SWISH-X) simulation for the detection of cryptic pockets at the protein-protein interface

Host Prof. F.L. Gervasio, Protein Dynamics Group, University of Geneva, Switzerland

30/03/2021 – 30/03/2022

HPC-Europa3 mobility

Virtual visit, due to COVID-19 restrictions

- HPC MD (High Performance Computing molecular dynamics) applied to tyrosine kinase inhibitors binding to SARS-CoV-2 Mpro
- HPC MD performance optimization on GPU nodes (Cirrus supercomputer)
- HPC MD performance optimization on CPU nodes (Archer2 supercomputer)

Host Edinburgh Parallel Computing Centre (EPCC), Edinburgh, UK

01/09/2021 – 31/10/2022 Research activity abroad

University of Geneva, Switzerland

- Sampling Water Interfaces through Scaled Hamiltonians (SWISH) simulations for repurposing tyrosine kinase inhibitors on SARS-CoV-2 Mpro
- Sampling Water Interfaces through Scaled Hamiltonians (SWISH) simulations for detecting cryptic pockets in proteins

Host Prof. F.L. Gervasio, Protein Dynamics Group, University of Geneva, Switzerland

01/06/2018 – 30/09/2018 Erasmus+ student

University of Barcelona, Spain

- Extended molecular dynamics of protein-protein complexes
- Assessing protein-protein binding energies through computational methods

Host Prof. F.J. Luque, Computational Biology and Drug Design Group, University of Barcelona, Spain

SCIENTIFIC ACTIVITY

General description

I obtained my PhD and later a postdoctoral research fellowship in the Molecular Modelling for Drug Design laboratory (M4D, PI: Prof. F. Spyraakis) at the Department of Drug Science and Technology at the University of Turin. The M4D research group has specific expertise in rational drug design, particularly in *in silico* screening, molecular docking, scoring, and molecular dynamics. My scientific activity is mainly based on the development and application of computational methods for identifying ligands for protein targets, in collaboration with experimental groups specialized in synthetic and analytical chemistry at the Department of Drug Science and Technology (University of Turin). My research focuses on the design and identification of antimicrobials against Gram-positive and Gram-negative bacteria and inflammasome inhibitors. The results obtained from various research projects are supported by the publication of numerous articles in internationally recognized scientific journals.

Main research activities and projects

1. Identification of small molecules capable of inhibiting the hydrolytic activity of beta-lactamases and carbapenemases.

Project description. This research activity aims to identify novel ligands of beta-lactamases expressed by Gram-negative bacteria as possible diagnostic tools and as hit compounds for the development of inhibitors capable of combating bacterial resistance. The research was supported by several grants, including the CRT Foundation Grant 2nd Round 2019 RF. 2019.2258 (Project REARM, Project Title Funding Entity: "REARM, antimicrobial resistance: new strategies to combat it"), and is currently underway to identify broad-spectrum carbapenemase inhibitors, in collaboration with Professors Maria Paola Costi and Donatella Tondi from the University of Modena and Reggio Emilia and Prof. Jean-Denis Docquier from the University of Siena. The combination of computational analyses with binding assays *in vitro* and microbiological assays led to the identification of new inhibitors active at low micromolar level.

Activity performed. Identification of potential beta-lactamase inhibitors by computational virtual screening studies and molecular docking

Project-related publications 4 (refs. (2), (4), (6), (7) in Publications section)

2. Identification of NLRP3 inflammasome inhibitors

Project description. Development of a three-dimensional model of the NLRP3 protein, a major component of the human inflammasome, and *in silico* studies for the identification and development of molecules capable of interfering with inflammasome activation processes. The project "BRAVE" (Call H2020-SGA-FETFLAG-HBP-2019. Framework Partnership Agreement (FPA) No: 650003 - Specific Agreement Number: 945539 - HBP SGA3) has recently been approved for funding in the Human Brain Project call "Impact of COVID-19 on brain and mental health," and involving national and international partners, in particular Prof. R. Wade (HITS Institute, Heidelberg, Germany), Profs. P. Carloni and G. Rossetti (Forschungszentrum Jülich, Jülich, Germany), G. Colombo (University of Pavia, Pavia, Italy). The aim of this research project is to identify small molecules that can counteract COVID-19-induced neuroinflammatory processes and subsequent neurodegeneration.

Activity performed. Identification of potential NLRP3 inhibitors by virtual screening, docking and molecular dynamics simulations.

Number of publications related to the project 3 (ref. (10, 19, 21) in Publications section)

3. Design of selective human cannabinoid receptor type 2 (hCBR2) antagonists with analgesic, anti-inflammatory, and anticancer activity

Project description. Human cannabinoid type 1 and type 2 receptors (hCBR1 and hCBR2, respectively) are essential factors in restoring homeostasis following injury. hCBR2 is mainly expressed peripherally, while hCBR1 is predominantly expressed in the central nervous system and is involved in cognitive processes, memory and motor control. Accordingly, this research project aims to design selective antagonists of hCBR2, which have a safer therapeutic profile than nonselective antagonists, for analgesic, anti-inflammatory, and anticancer purposes. This aim is pursued by combining the synthesis of potential hCBR2 antagonists (Prof. K. Chegaev, University of Turin, Italy) with *in silico* molecular docking studies rationalizing the potential agonist/antagonist activity of candidate compounds. Finally, the library of compounds selected as potential hCBR2 selective antagonists is tested *in vitro* (Dr. A. Ligresti, CNR, Italy) to confirm selective antagonism on hCBR2.

Activity performed. Construction of a molecular docking model *in silico* that rationalizes the agonist/antagonist activity of compounds on hCBR2.

Number of publications related to the project 1 (ref. (18) in Publications section)

4. Study of the impact of orthosteric and allosteric ligands on the conformational balance of the PLP-dependent enzyme human serine racemase.

Project description. The research targets the enzyme PLP-dependent human serine racemase (hSR), a potential target for neurodegenerative and cognitive diseases, which catalyzes the biosynthesis of D-serine, an obligatory co-agonist of NMDA receptors. hSR is modulated by several organic and inorganic ligands (e.g., magnesium, ATP, PLP, glycine, nitric oxide), which orthosterically and allosterically modify its conformation and consequently its activity. This project aims to study the effect of ligands on the conformation and activity of the hSR enzyme, integrating the limited structural data in the literature with site-directed mutagenesis experiments, mass and fluorescence spectroscopy (Prof. S. Bruno, University of Parma), and molecular dynamics simulations, in order to enrich the structural information available for the design of hSR inhibitors.

Activity performed. Molecular dynamics replications of hSR bound to different modulators, such as NO, glycine, ATP and PLP. Identification of key residues for allosteric communication in nitrosylated hSR.

Number of publications related to the project 1 (ref. (9) in Publications section)

5. **Identification of small molecules interfering with the interaction between bacterial hemophores and human hemoglobin: an approach to hinder the iron acquisition process in *Staphylococcus aureus*.**

Project description. The research, initially funded by the Compagnia San Paolo through the NEWAIMS project, aims to identify possible interferents of the interaction between hemophores of *S. aureus* and human hemoglobin, a mechanism that allows the supply of iron by the bacterium, and is therefore critical for its virulence. The current project aims to identify new antimicrobials and is in line with World Health Organization directives that there is an urgent need for the development of new antibiotics. The research has led to the identification *in silico* of the first possible interferents and the study of the hemophore-hemoglobin recognition process through the integration of molecular dynamics techniques, virtual screening and molecular docking. The results of computational simulations (in collaboration with Prof. F.J. Luque, University of Barcelona, Spain), in combination with in-solution and plate biochemical assays (Professors S. Bettati, B. Campanini, and L. Ronda, University of Parma, Italy), of spiking by SPR (Prof. S. Cannistraro, University of Tuscia-Viterbo, Italy) and of WAXS at the synchrotron (Prof. M. Levantino, ESRF Grenoble, France), have allowed to rationalize from a mechanistic point of view the interaction of the two macromolecules and the process of heme extraction, as well as to evaluate the activity of possible interferents. The identified molecules will be implemented, optimized and tested on *S. aureus* strains as part of the "ERASE" project, recently approved for funding from the PRIN2020 call.

Activity performed. Identification of potential inhibitors of hemophore-hemoglobin interaction by screening large virtual libraries and molecular docking. Characterization of protein-protein interactions at the hemophore-hemoglobin interface by molecular dynamics simulations. Simulation of heme extraction using enhanced molecular dynamics methods, in collaboration with Dr. D. Gobbo (University of Geneva, Switzerland) and Dr. S. Decherchi (IIT Genoa, Italy).

Number of publications related to the project 3 (ref. (14), (5), (3) in Publications section)

Peer-review activity

- Peer-reviewer for Journal of Chemical Information and Modelling (JCIM), ACS publications
- Peer-reviewer for Frontiers in Molecular Bioscience, Frontiers
- Peer-reviewer for Scientific Reports, Nature Journals

NATIONAL AND INTERNATIONAL COLLABORATIONS

The scientific production and activities reported in the present document highlight national and international collaborations with relevant scientists in the fields of pharmaceutical chemistry, computational chemistry, and biochemistry:

- 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-Wolfsbrunnengasse 35, Heidelberg, 69118, Germany.
- Proff. Paolo Carloni, Giulia Rossetti: Identification of inflammasome inhibitors and new antivirals through *in silico methodologies*. Jülich Supercomputing Center (JSC), Institute for Neuroscience and Medicine (INM-9), Forschungszentrum Jülich, Jülich, 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: Heme transfer simulations between hemoglobin and staphylococcal IsdB. Italian Istituto di Tecnologia, Genova, Italy.
- 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.

- Prof. Stefano Bruno: Characterization of PLP-dependent serine racemase enzyme. Department of Food, 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 staphylococcal IsdB-hemoglobin complexes. Department of Nutrition, Food Sciences and Gastronomy, University of Barcelona, Barcelona, Spain.
- Prof. Francesco Luigi Gervasio: Hamiltonian replica exchange simulations of protein-protein complexes. Department of Pharmacy, University of Geneva, Geneva, Switzerland.

PUBLICATIONS

Metrics

23 Publications

255 Citations by 263 documents

H-index 8

Journal impact factor (JIF) according to JCR 2023 (Updated 12th December 2023)

co-first author, † corresponding author

23. Borsatto, A., **Gianquinto, E.**, Rizzi, V., Gervasio, F.L. SWISH-X, an expanded approach to detect cryptic pockets in proteins and at protein-protein interfaces (2023) *BioRxiv*, DOI:10.1101/2023.11.03.565527
22. Bersani M, Failla M, Vascon F, Gianquinto E, Bertarini L, Baroni M, Cruciani G, Verdirosa F, Sannio F, Docquier JD, Cendron L., Spyrakis, F., Lazzarato, L., Tondi, D. Structure-Based Optimization of 1, 2, 4-Triazole-3-Thione Derivatives: Improving Inhibition of NDM-/VIM-Type Metallo-beta-Lactamases and Synergistic Activity on Resistant Bacteria. (2023) *Pharmaceuticals*, 16(12), art.no. 1682. DOI: 10.3390/ph16121682 OPEN ACCESS: All Open Access, Gold, Green JIF: 4.6, cited: 0
21. Gastaldi, S., Rocca, C., **Gianquinto, E.**, Granieri, M.C., Boscaro, V., Blua, F., Rolando, B., Marini, E., Gallicchio, M., De Bartolo, A., Romeo, N., Mazza, R., Fedele, F., Pagliaro, P., Penna, C., Spyrakis, F., Bertinaria, M., Angelone, T. Discovery of a novel 1,3,4-oxadiazol-2-one-based NLRP3 inhibitor as a pharmacological agent to mitigate cardiac and metabolic complications in an experimental model of diet-induced metaflammation (2023) *European Journal of Medicinal Chemistry*, 257, (115542), JIF: 6.7, cited: 2

20. Schimunek, J., Seidl, P., Elez, K., Hempel, T., Le, T., Noé, F., Olsson, S., Raich, L., Winter, R., Gokcan, H., Gusev, F., Gutkin, E.M., Isayev, O., Kurnikova, M.G., Narangoda, C.H., Zubatyuk, R., Bosko, I.P., Furs, K.V., Karpenko, A.D., Kornoushenko, Y.V., Shuldau, M., Yushkevich, A., Benabderrahmane, M.B., Bousquet-Melou, P., Bureau, R., Charton, B., Cirou, B.C., Gil, G., Allen, W.J., Sirimulla, S., Watowich, S., Antonopoulos, N.A., Epitropakis, N.E., Krasoulis, A.K., Pitsikalis, V.P., Theodorakis, S.T., Kozlovskii, I., Maliutin, A., Medvedev, A., Popov, P., Zaretskii, M., Eghbal-Zadeh, H., Halmich, C., Hochreiter, S., Mayr, A., Ruch, P., Widrich, M., Berenger, F., Kumar, A., Yamanishi, Y., Zhang, K.Y.J., Bengio, E., Bengio, Y., Jain, M., Korablyov, M., Liu, C., Marcou, G., Glaab, E., Barnsley, K., Iyengar, S. M., Ondrechen, Mary Jo, Haupt, V.J., Kaiser, F., Schroeder, M., Pugliese, L., Albani, S., Athanasiou, C., Beccari, A., Carloni, P., D'Arrigo, G., **Gianquinto, E.**, Goßen, J., Hanke, A., Joseph, B.P., Kokh, D.B., Kovachka, S., Manelfi, C., Mukherjee, G., Muñoz-Chicharro, A., Musiani, F., Nunes-Alves, A., Paiardi, G., Rossetti, G., Sadiq, S.K., Spyraakis, F., Talarico, C., Tsengenesis, A., Wade, R.C., Copeland, C., Gaiser, J., Olson, D.R., Roy, A., Venkatraman, V., Wheeler, T.J., Arthanari, H., Blaschitz, K., Cesugli, M., Durmaz, V., Fackeldey, K., Fischer, P.D., Gorgulla, C., Gruber, C., Gruber, K., Hetmann, M., Kinney, J.E., Padmanabha Das, K.M., Pandita, S., Singh, A., Steinkellner, G., Tesseyre, G., Wagner, G., Wang, Z., Yust, R.J., Druzhilovskiy, D.S., Filimonov, D.A., Pogodin, P.V., Poroikov, V., Rudik, A.V., Stolbov, L.A., Veselovsky, A.V., De Rosa, M., De Simone, G., Gulotta, M.R., Lombino, J., Mekni, N., Perricone, U., Casini, A., Embree, A., Gordon, D.B., Lei, D., Pratt, K., Voigt, C.A., Chen, K., Jacob, Y., Krischuns, T., Lafaye, P., Zettor, A., Rodríguez, M.L., White, K.M., Fearon, D., Von Delft, F., Walsh, M.A., Horvath, D., Brooks, C.L., Falsafi, B., Ford, B., García-Sastre, A., Yip Lee, S. A community effort in (SARS)-CoV-2 drug discovery (2023) *Molecular Informatics*. DOI: 10.1002/minf.202300262 JIF: 3.6, cited: 0
19. Casali, E., Serapian, S.A., **Gianquinto, E.**, Castelli, M., Bertinaria, M., Spyraakis, F. and Colombo, G. NLRP3 monomer functional dynamics: From the effects of allosteric binding to implications for drug design (2023) *International Journal of Biological Macromolecules*, 246, (125609), JIF: 8.2, cited: 1
18. **Gianquinto, E.**, Sodano, F., Rolando, B., Kostrzewa, M., Allarà, M., Mahmoud, A. M., Kumar, P., Spyraakis, F., Ligresti, A., Chegaev, K. N-[1,3-Dialkyl(aryl)-2-oxoimidazolidin-4-ylidene]-aryl(alkyl)sulphonamides as Novel Selective Human Cannabinoid Type 2 Receptor (CB2R) Ligands; Insights into the Mechanism of Receptor Activation/Deactivation (2022) *Molecules*, 27(23), art. no. 8152. DOI: 10.3390/molecules27238152 OPEN ACCESS: All Open Access, Gold, Green JIF: 4.6, cited: 1
17. Marini, E., Marino, M., Gionfriddo, G., Maione, F., Pandini, M., Oddo, D., Giorgis, M., Rolando, B., Blua, F., Gastaldi, S., Marchiò, S., Kovachka, S., Spyraakis, F., **Gianquinto, E.**, Di Nicolantonio, F., Bertinaria, M. Investigation into the Use of Encorafenib to Develop Potential PROTACs Directed against BRAFV600E Protein (2022) *Molecules*, 27(23), art. no. 8513. DOI: 10.3390/molecules27238152 OPEN ACCESS: All Open Access, Gold, Green JIF: 4.6, cited: 3
16. Andreana, I., Gazzano, E., **Gianquinto, E.**, Piatti, G., Bincoletto, V., Kryza, D., Lollo, G., Spyraakis, F., Riganti, C., Arpicco, S., Stella, B. Selective delivery of pentamidine toward cancer cells by self-assembled nanoparticles (2022) *Int. J. Pharm.* 625, art. no. 122102. DOI: 10.1016/j.ijpharm.2022.122102 JIF: 5.8, cited: 1
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CONTRIBUTIONS TO CONFERENCES

Oral communications

5. **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. Spyraakis: "Virtual screening identifies cross-class inhibitors of clinically relevant carbapenemases" in CDDD 7th edition, virtual event, 25/07/2021.
4. **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. Spyraakis: "Virtual screening identifies cross-class inhibitors of clinically relevant serine- and metallo-beta-lactamases" in 13th Young Medicinal Chemist Symposium - Nuove Prospettive in Chimica Farmaceutica (NPCF13), virtual event, 26-29/04/2021.
3. **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. Spyraakis: "*in silico* identification of cross-class inhibitors against clinically relevant beta-lactamases" in EFMC-ISMC & EFMC-YMSC virtual poster session, 09/09/2020. *Slide & Talk Presentation*
2. **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. Spyraakis: "*in silico* identification of cross-class inhibitors against clinically relevant beta-lactamases" in AMYCBIO MED, virtual edition, 13-14/10/2020. *Slide & Talk Presentation*
1. **E. Gianquinto**, O. De Bei, M. Marchetti, L. Lazzarato, S. Guglielmo, R. Fruttero, S. Bettati, L. Ronda, B. Campanini, F.J. Luque, F. Spyraakis: "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, 28-29/03/2019.

Other contributions

presenting author

46. **E. Gianquinto**, S. Gastaldi, F. Blua, V. Boscaro, M. Bertinaria, F. Spyraakis: "Design, synthesis, and *in cellulo* evaluation of a novel 1,3,4-oxadiazol-2-one-based NLRP3 inhibitor" in SBDD, Sestri Levante, 2023. *Poster presentation*
45. **M. Bersani**, **E. Gianquinto**, M. Failla, L. Bertarini, F. Vascon, F. Sannio, F. Verdirosa, N. Beatrice, F. De Luca, M.P. Costi, G. Cruciani, J.D. Docquier, L. Cendron, D. Tondi, L. Lazzarato, F. Spyraakis: "*In Silico*-aided Optimization of Cross-class Beta-Lactamase Inhibitors Active against Clinically Relevant Carbapenemases" in ESMEC, Urbino, 2022. *Poster presentation*
44. **M. Marchetti**, O. De Bei, L. Ronda, **E. Gianquinto**, L. Lazzarato, D.Y. Chirgadze, S.W. Hardwick, L.R. Cooper, M. Cozzi, S. Faggiano, F. Spyraakis, B.F. Luisi, B. Campanini, S. Bettati: "Cryo-EM undiscovers structural and mechanistic details on iron hijacking by *Staphylococcus aureus*: an insight into the interaction of IsdB hemophore with human hemoglobin" in 108° Congresso Nazionale della Società Italiana di Fisica, Milano 2022. **Oral communication**
43. L. Ronda, O. De Bei, M. Marchetti, M. Levantino, **E. Gianquinto**, F. Spyraakis, B. Campanini, S. Bettati: "*Staphylococcus aureus* IsdB hemophore interaction with human hemoglobin: structural and functional insights" in 108° Congresso Nazionale della Società Italiana di Fisica, Milano, 2022. **Invited oral communication**
42. **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. Spyraakis, 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". IUBMB-FEBS-PABMB 2022 Congress, Lisbona, 2022. *Poster presentation*
41. **S. Bettati**, A.R. Bizzarri, P. Brear, S. Cannistraro, D.Y. Chirgadze, L.R. Cooper, M. Cozzi, O. De Bei, S. Faggiano, R. Giaccari, **E. Gianquinto**, S.W. Hardwick, S. Kovachka, L. Lazzarato, B.F. Luisi, M. Marchetti, L. Ronda, F. Spyraakis, B. Campanini: "Chasing new targets to fight antimicrobial resistance: interaction of the *Staphylococcus aureus* hemophore IsdB with human hemoglobin" in Proteine 2022, meeting of the Protein Group of the Italian Society of Biochemistry, Pisa, 2022. **Oral communication**
40. **Cozzi M**, De Bei O, Giaccari R, **E. Gianquinto**, Kovachka S, Campanini B, Faggiano S, Lazzarato L, Marchetti M, Ronda L, Spyraakis F, Bettati S. National Meeting of PhD students in Biochemistry "A. Castellani", Brallo di Pregola (2022). "Evaluation of disruptors of the protein-protein interaction between human hemoglobin and *S. aureus* hemophore IsdB by ELISA assay and STD-NMR". **Oral communication**
39. **O. De Bei**, S. Bettati, D.Y. Chirgadze, L. Cooper, M. Cozzi, S. Faggiano, **E. Gianquinto**, S. Guglielmo, S.W. Hardwick, L. Lazzarato, M. Levantino, B.F. Luisi, M. Marchetti, L. Ronda, F. Spyraakis, B. Campanini: "Structural and dynamic insights into complex formation between human hemoglobin and IsdB from *Staphylococcus aureus* by cryo-EM and solution X-ray scattering" in Proteine 2022, meeting of the Protein Group of the Italian Society of Biochemistry, Pisa, 2022. *Poster presentation*
38. S. Faggiano, M. Cozzi, R. Giaccari, O. De Bei, C. Compari, E. Fisicaro, **E. Gianquinto**, S. Kovachka, M. Marchetti, L. Ronda, B. Campanini, L. Lazzarato, F. Spyraakis, S. Bettati: "Evaluation of disruptors of the interaction between human hemoglobin and the *S. aureus* hemophore IsdB by ELISA assays, STD-NMR and ITC" in Proteine 2022, meeting of the Protein Group of the Italian Society of Biochemistry, Pisa, 2022. *Poster presentation*

37. S. Bettati, A.R. Bizzarri, P. Brear, S. Cannistraro, B. Campanini, D.Y. Chirgadze, B. Citterio, L.R. Cooper, M. Cozzi, O. De Bei, S. Faggiano, E. Frangipani, R. Giaccari, **E. Gianquinto**, S.W. Hardwick, L. Lazzarato, G. Longo, B.F. Luisi, M. Marchetti, L. Ronda, F. Spyraakis: "A new target to fight *Staphylococcus aureus* infections: structural and mechanistic insight into the interaction of the IsdB hemophore with human hemoglobin, and preliminary inhibition studies" in Antimicrobial chemotherapy virtual conference 2022. *Poster presentation*
36. F. Spyraakis, 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 *Staphylococcus aureus* resistance" in XXVI National Meeting on Medicinal Chemistry (NMMC), Bari, Sept. 11th-14th 2022. *Poster presentation. Best poster prize winner.*
35. **E. Gianquinto**, E. Casali, S. Gastaldi, A. Atzei, I. Schimmenti, G. Rossetti, R.C. Wade, G. Colombo, M. Bertinaria, F. Spyraakis: "*in silico*-Assisted Design of NLRP3 Inflammasome Allosteric Inhibitors for Targeting Sars-Cov-2 Induced-Neuroinflammation" in EuroQSAR, Heidelberg, Sept 25th-30th 2022. *Poster presentation.*
34. **E. Gianquinto**, E. Casali, S. Gastaldi, A. Atzei, B. Canavera, G. Rossetti, R.C. Wade, G. Colombo, M. Bertinaria, F. Spyraakis: "Designing allosteric NLRP3 inflammasome inhibitors against neuroinflammation induced by COVID-19" in EFMC-YMCS, Nice, Sept 7th-11th, 2022. *Poster presentation.*
33. F. Blua, M. Marino, S. Gastaldi, F. Maione, **E. Gianquinto**, F. Di Nicolantonio, M. Bertinaria: "Design and Synthesis of encorafenib-based BRAF-V600E degraders" at MMCS 2022 - The 3rd Molecules Medicinal Chemistry Symposium, Rome, 27-29/07/2022. **Flash Communication.**
32. M. Cozzi, R. Giaccari, O. De Bei, **E. Gianquinto**, S. Kovachka, S. Faggiano, M. Marchetti, L. Ronda, B. Campanini, L. Lazzarato, F. Spyraakis, S. Bettati: "Identification of protein-protein interaction disruptors targeting human hemoglobin in complex with bacterial hemophore IsdB" in First Research Day of the Department of Medicine and Surgery, Castello di Rivalta (2021). **Oral communication.**
31. **E. Gianquinto**, F. Marchesani, I. Autiero, A. Michielon, B. Campanini, S. Faggiano, S. Bettati, Andrea Mozzarelli, Stefano Bruno, Francesca Spyraakis: "An allosteric interplay among glycine, ATP and S-nitrosylation modulating serine racemase activity" in Quantifying Protein Dynamics and Allosteric regulation in the cell with emerging technologies: From Cryo-EM and NMR to Multiscale Simulations, Networks and Machine Learning hosted by CECAM, September 15th-17th, 2021, Lausanne. *Poster presentation. Best poster prize winner.*
30. F. Spyraakis, 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.**
29. **E. Gianquinto**, M. Santucci, L. Maso, S. Cross, F. Sannio, F. Verdirosa, F. de Luca, J.-D. Docquier, L. Cendron, D. Tondi, A. Venturelli, G. Cruciani, M.P. Costi, F. Spyraakis: "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.*
28. **E. Gianquinto**, F. Marchesani, I. Autiero, A. Michielon, B. Campanini, S. Gaggiano, S. Bettati, A. Mozzarelli, S. Bruno, F. Spyraakis: "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.*

27. 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.**
26. **E. Gianquinto**, M. Santucci, L. Maso, S. Cross, F. Sannio, F. Verdirosa, F. de Luca, J.-D. Docquier, 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. Best poster prize winner.**
25. 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. **Poster presentation.**
24. M. Cozzi, R. Giaccari, O. De Bei, **E. Gianquinto**, S. Kovachka, S. Faggiano, M. Marchetti, L. Ronda, B. Campanini, L. Lazzarato, F. Spyrakis, S. Bettati: "Identification of PPI inhibitors that disrupt the interaction between human hemoglobin and the *S. aureus* hemophore IsdB" in European School of Medicinal Chemistry ESMEC, 2021. **Poster presentation.**
23. O. De Bei, **E. Gianquinto**, D.Y. Chirgadze, S.W. Hardwick SW, Cooper LR, Marchetti M, Spyrakis F, Bettati S, Ronda L, Luisi BF, Campanini B: "Cryo-EM reveals how hemophore binding to Hb prompts heme removal: a structural and mechanistic insight into the function of IsdB from *S. aureus*" 2021 Congress of the Italian Society of Biochemistry and Molecular Biology, 2021. **Oral communication**
22. **E. Gianquinto**, M. Santucci, L. Maso, S. Cross, F. Sannio, F. Verdirosa, F. de Luca, J.-D. Docquier, 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. Best poster prize winner.**
21. **E. Gianquinto**, M. Santucci, L. Maso, S. Cross, F. Sannio, F. Verdirosa, F. de Luca, J.-D. Docquier, 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 AMYCBIO MED, virtual edition, October 13th-14th 2020. **Poster presentation. Poster selected for slide & talk presentation.**
20. 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. Best poster prize winner.**
19. 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: "Identification 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.**
18. **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.**

17. O. De Bei, **E. Gianquinto**, D.Y. Chirgadze, S.W. Hardwick, L.R. Cooper, M. Marchetti, F. Spyra-kis, 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: A special symposium celebrating the 50th anniversary of the PDB, 2021. *Poster presentation*.
16. 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*.
15. O. De Bei, **E. Gianquinto**, D.Y. Chirgadze, S.W. Hardwick, L. Cooper, M. Marchetti, F. Spyra-kis, 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*.
14. M. Marchetti, O. De Bei, M. Levantino, O. Moscetti, **E. Gianquinto**, M. Cozzi, F. Spyra-kis, 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*.
13. **E. Gianquinto**, M. Santucci, L. Maso, S. Cross, F. Sannio, F. Verdirosa, F. de Luca, J.-D. Do-quier, L. Cendron, D. Tondi, A. Venturelli, G. Cruciani, M.P. Costi, F. Spyra-kis: "*in silico* iden-tification of cross-class inhibitors against clinically relevant beta-lactamases" in EFMC-ISM-C & EFMC-YMSC virtual poster session, September 9th 2020. *Poster presentation*. **Poster selected for slide & talk presentation**.
12. L. Ronda, S. Bettati, A. Bizzarri, B. Campanini, O. De Bei, **E. Gianquinto**, F.J. Luque, M. Marchetti, I. Moscetti, F. Spyra-kis: "Staphylococcus aureus IsdB and human hemoglobin: a biophysical description of a protein-protein interaction" in FISMAT 2019 - Italian national Confe-rence on Condensed Matter Physics, September 30th-October 4th 2019, Catania, Italy. *Poster presentation*.
11. **E. Gianquinto**, O. De Bei, M. Marchetti, L. Lazzarato, S. Guglielmo, R. Fruttero, S. Bettati, L. Ronda, B. Campanini, J.F. Luque, F. Spyra-kis: "Novel strategies to iron-starve *Staphylococ-cus 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**.
10. **E. Gianquinto**, O. De Bei, M. Marchetti, L. Lazzarato, S. Guglielmo, R. Fruttero, S. Bettati, L. Ronda, B. Campanini, F.J. Luque, F. Spyra-kis: "Structural and Dynamic characetrization of the IsdB-human haemoglobin complex: towards a novel strategy for iron-starving resistant *Sta-phylococcus aureus*" in XII European Drug Design Workshop (EWDD). Certosa di Pontignano, Siena, Italy, May 19th-24th, 2019. *Poster presentation*. **Poster presentation. Selected poster by WILEY editor**.
9. F. Spyra-kis, **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**.
8. I. Moscetti, S. Bettati, A. Bizzarri, B. Campanini, O. de Bei, **E. Gianquinto**, F.J. Luque, M. Marchetti, F. Spyra-kis, L. Rnda: "Kinetic and dynamic characterization of the interaction bet-ween *Staphylococcus aureus* and human haemoglobin" CV Congress of The Italian Society of Physics, September 23th-27th 2019, L'Aquila, Italy. *Poster presentation*.

7. B. Campanini, O. De Bei, M. Marchetti, F. Spyraakis, **E. Gianquinto**, S. Cannistraro, I. Moschetti, 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*.
6. O. De Bei, F. Spyraakis, **E. Gianquinto**, B. Campanini, L. Ronda, S. Bettati, M. Marchetti, S. Cannistraro, I. Moschetti, 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, July 5th-19th 2019. *Poster presentation*.
5. L. Ronda, S. Bettati, A.R. Bizzarri, B. Campanini, S. Cannistraro, O. De Bei, **E. Gianquinto**, F.J. Luque, M. Marchetti, I. Moschetti, F. Spyraakis: "*Staphylococcus aureus* IsdB and human hemoglobin: a biophysical description of a protein-protein interaction" in Italian National Conference on the Physics of Matter, Catania, 2019. *Poster presentation*.
4. F. Spyraakis, 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 O2BiP (XXth International Conference on Oxygen Binding and Sensing Proteins), Barcelona, Spain, September 3rd-6th, 2018. *Poster presentation*.
3. F. Spyraakis, **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-Portuguese Joint Meeting in Medicinal Chemistry), Palermo, Italy, July 17th-20th, 2018. *Poster presentation*.
2. F. Spyraakis, D. Tondi, G. Celenza, G. D'Arrigo, **E. Gianquinto**, M. Santucci, S. Cross, P. Bellio, L. Cendron, J.-D. Docquier, J. Blázquez, A. Venturelli, G. Cruciani, M.P. Costi: "*in silico/in vitro* approaches for the identification of new carbapenemase inhibitors" in MedChemSicily2018 (Italian-Spanish-Portuguese Joint Meeting in Medicinal Chemistry), Palermo, Italy, July 17th-20th, 2018. *Poster presentation*.
1. **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. Spyraakis: "Investigating and disrupting the interaction between hemoglobin and MRSA hemophores: in silico approaches to design novel antimicrobials" in O2BiP (XXth International Conference on Oxygen Binding and Sensing Proteins), Barcelona, Spain, September 3rd-6th, 2018. *Poster presentation*.