Sara Fortuna www.sarafortuna.eu — sara.fortuna@uniud.it — fortuna.sara@gmail.com

EDUCATION

Sept. 2010 Doctor of Philosophy in Chemistry, The University of Warwick, UK
Equipollenza: riconosciuto equipollente al titolo di Dottore di Ricerca ai sensi del DPR 11 luglio 1980, n. 382 con decreto MIUR, Prot.n.0000506 - 14/03/2017

Nov. 2006 Diploma di Laurea in Chimica (5 years Chemistry degree), University of Trieste, IT

HABILITATIONS (ITALIAN ASN)

Full Professor (ASN fascia I)
Biophysics (02/D1 - FISICA APPLICATA, DIDATTICA E STORIA DELLA FISICA)
Biochemistry (05/E1 - BIOCHIMICA GENERALE)

Professor (ASN fascia II)
Theoretical Physics - Soft Matter (02/B2 - FISICA TEORICA DELLA MATERIA)
Physical Chemistry (03/A2 - MODELLI E METODOLOGIE PER LE SCIENZE CHIMICHE)
Chemistry (03/B1 - FONDAMENTI DELLE SCIENZE CHIMICHE E SISTEMI INORGANICI)
Chemical Technologies (03/B2 - FONDAMENTI CHIMICI DELLE TECNOLOGIE)

POSITIONS

Nov. 2023 - Nov. 2024 Consultant for peptides and antibodies software development (Product Manager)
Cresset, Cambridge, UK

Nov. 2021 - Nov. 2023 Research Collaborator and Project PI
Istituto Italiano di Tecnologia (IIT), Genova, IT
Project: **Computational design of theragnostic nanobodies: targeting missense mutants in metastatic breast cancer cells**
Funding: AIRC - Italian Association for Cancer Research (2021-2025 PI: S. Fortuna)

Nov. 2018 - Ott. 2021 Researcher/Assistant Professor
Dept. of Chemical and Pharmaceutical Sciences (DSCF), University of Trieste, IT

Nov. 2017 - Nov. 2018 Postdoctoral Researcher and Junior PI
Dept. of Chemical and Pharmaceutical Sciences (DSCF), University of Trieste, IT
Project: **Computational design of customised nanobodies for oncology applications: prognostic candidates for HER2 as first case**
Funding: AIRC - Italian Association for Cancer Research (2017-2020 PI: S. Fortuna)

Apr. 2016 - Sep. 2017 Talents3 fellow
University of Nova Gorica, Slovenia & SISSA, Trieste, IT
Group: Prof. Ario de Marco and Prof. Alessandro Laio
Project: **Computational design of customised nanobodies for biotechnological applications: the optimisation of stable humanised, high affinity therapeutic candidates for HER2 as first test case**
Funding: Area Science Park, IT, European Social Fund - 2014/2020 Regional Operative Programme (proposal NB4HER2, 2016-2017 PI: S. Fortuna)

Nov. 2013 - Mar. 2016 Postdoctoral Researcher and Coordinator of the MoNaLiSA Theory Group
Department of Medical and Biological Sciences, University of Udine, IT
Group: Prof. Giacinto Scoles
Project: **Multiscale Modelling for the development of novel peptide-based nanodevices**
Funding: 7FP, Ideas, ERC Advanced Grant: Molecular Nanotechnology For Life Science Application: QUantitative Interactomics for Diagnostics, Proteomics and QUantitative Oncology, (Quidroquo) (proposal n. 269025, 2011-2016 PI: G. Scoles)

Oct. 2012 - Sep. 2013	Postdoctoral Researcher Department of Medical and Biological Sciences, University of Udine, IT *Group:* Prof. Giacinto Scoles *Project:* **Molecular Simulations for Nanomedicine** *Funding:* AIRC 5x1000 Special program 2011: Application of advanced Nanotechnology in the development of Cancer Diagnostics tools (Rif. 12214, 2012-2014, PI: G. Toffoli, Co-PI: G. Scoles)
Oct. 2010 - Sept. 2012	Postdoctoral Researcher CNR-IOM and Sissa, Trieste, IT *Project:* **Computational microscopy and spectroscopy of metal-supported organometallic nanostructures** *Funding:* PRIN - MIUR, IT: Controlling the structure and function of metallorganic nanostructures on metal surfaces (2010-2013, PI: M.G. Betti, Co-PI: S. Fabris)
Mar. 2007 - Jul. 2010	Graduate Student (Supervisor: Prof. A. Troisi), Department of Chemistry and Centre for Scientific Computing, University of Warwick, UK *Project:* **Modelling Techniques for the study of Molecular Self-Organisation** *Funding:* The Leverhulme Trust: Agent Based Modeling of molecular self-organization (2007-2010, PI:A.Troisi)

MEMBERSHIPS

Committee Member of the IOP Liquids and Complex Fluids Group (2015-2019)
Associate Member of the Institute of Physics (IOP, 2008-)
Associate Member of the Royal Society of Chemistry (RSC, 2008-)
Member of the European Physical Society (EPS, 2017-)
Member of the Biochemical Society (2017-)

ORGANISATION OF SCIENTIFIC MEETINGS

2017	Organiser IOP Workshop: **Self-Assembly, Recognition and Applications (SARA) 2017** 14 Dec.2017, Lincoln, UK
2016	Organiser IOP Workshop: **Self-Assembly, Recognition and Applications (SARA) 2016** 9 Dec.2016, Edimburgh, UK

PEER REVIEW

PRIZES — IOP Liquids and Complex Fluids Group

JOURNALS — J. Chem. Theory Comput., J. Phys. Chem. B/C/Lett, ACS Chem. Neurosci., ACS Comb. Sci., J. Chem Inf. Model. (ACS), Surf. Sci., J. Mol. Struct. (Elsevier), J. Biomol. Struct. Dyn. , Free Radic. Res. (Taylor & Francis), Microb. Cell. Fact. (BioMed Central), Int. J. Mol. Sci. (MDPI), Sci. Rep. (Springer Nature).

GRANTS — I am scientific referee for the following National Science Councils:

- National Research Foundation of South Africa (NRF, 2015-2017)
- Irish Research Council (2017-)
- National Science Center, Poland (Narodowe Centrum Nauki, NCN, 2019-)
- Ministry of Education, University, and Research, Italy (MIUR, 2019 -)

Funding Record

Research Grants as PI

2021-2024 **Investigator Grant (IG), Italian Association for Cancer Research - AIRC (IT)**
Computational design of theragnostic nanobodies: targeting missense mutants in metastatic breast cancer cells (**PI**; 409,000€; 5 years)

2021-2022 **Annual Open Grant, Alternatives Research & Development Foundation - ARDF (US)**
De-novo engineered antibody fragments: validation of the first in-silico pipeline for antibody discovery (**PI**; 40,000$; 1 year)

2019-2020 **Annual Open Grant, Alternatives Research & Development Foundation - ARDF (US)**
In silico design of customised high-affinity antibody fragments (**PI**; 39,980$; 1 year)

2017-2020 **My First Airc Grant (MFAG), Italian Association for Cancer Research - AIRC (IT)**
Computational design of customised nanobodies for oncology applications: prognostic candidates for HER2 as first case (**PI**; 225,000€; 3 years)

2017 **Research Fund, The Royal Society of Chemistry (UK)**
Computational design of bidentate binders of increased affinity and selectivity (**PI**; £2,800; 1 year)

2016-2017 **Talents3 Research Fellowship, European Social Fund - 2014/2020 Regional Operative Programme**
Computational design of customised nanobodies for biotechnological applications: the optimisation of stable, humanised, high affinity therapeutic candidates for HER2 as first test case (**PI**; 52,380€; 18 months)

Research Grants as Co-PI, WP Leader, or Team Member

2022-2026 **Marie Skłodowska-Curie Innovative Training Networks (MSCA-ITN-2021), Horizon 2020, European Commission**
STOP SPREAD BAD BUGS: novel antimicrobial approaches to combat multidrug resistance in bacteria
(workgroup leader, 130,000€; project: 4,028,713.19€; 4 years)

2021-2023 **PRIN 2020 (Under 40), The Ministry of Education, University and Research, MIUR, Italy**
Targeting baCteriAl cell eNvelope of Nocosomial paThogens to ESKAPE resistance
(Team Member; Unit PI: Rita De Zorzi, University of Trieste, 114,000€; PI: F. Squeglia; project: 489,928€; 3 years)

2021-2023 **Marie Skłodowska-Curie Individual Fellowships (MSCA-IF-2020), Horizon 2020, European Commission**
Sustainable route for circularity of renewable polyesters (RenEcoPol)
(Team Member; Beneficiary: Anamaria Todea, University of Trieste; Supervisor: Lucia Gardossi; 2 years)

2020-2024 **Marie Skłodowska-Curie Innovative Training Networks (MSCA-ITN-EID-2020), Horizon 2020, European Commission**
Heterogenous biocatalytic reaction cascades training network (INTERfaces)
(Team Member; local PI: Lucia Gardossi, University of Trieste; project: 3,709,260€; 4 years)

Other Funding, Awards, and Prizes

Feb. 2020	University Research Fund for Young Researchers (FRA, 1 year, 3.000), 2020-2021
Jun. 2016	The Royal Society of Chemistry: Small Grant for Scientific Activities (£732)
Apr. 2016	ERASMUS+ (600€)
Mar. 2016	The Royal Society of Edinburgh and Accademia Nazionale dei Lincei (1,000€)
Jun. 2014	The Royal Society of Edinburgh and Accademia Nazionale dei Lincei (1,600€)
Oct. 2012	SISSA young scientists competition (10,000€)
Jun. 2011	SISSA young scientists competition (6,000€)
Jul. 2009	RSC travel bursaries for conferences attendance (IUPAC conference, £95 and Faraday Discussion, £150)
Jul. 2006	University of Illinois travel bursary (700€) for Summer School attendance

Computational Grants as PI

Since 2010 I have been awarded CPU/GPU time with continuity by CINECA (the Italian supercomputing centre for scientific research) and from PRACE (Partnership for Advanced Computing in Europe)

Apr. 2020 - Apr. 2021	CINECA-ISCRA Class B proposal (576,000 GPU hours on M100@CINECA) **Computational design of highly specific nanobodies for HER2 isoforms recognition**
Nov. 2019 - Ago. 2020	CINECA-ISCRA Class C proposal (36,000 GPU hours on Marconi@CINECA) **Targeting the sigma-1 receptor with diazepanic scaffold based molecules**
May. 2019 - Feb. 2020	CINECA-ISCRA Class C proposal (33,600 GPU hours on Marconi@CINECA) **Computational design of peptides for capturing beta-2-microglobulin**
Jul. 2018 - Apr. 2019	CINECA-ISCRA Class C proposal (40,000 GPU hours on Marconi@CINECA) **Ex-novo optimisation of antibodies fragments**
Feb. 2018 - May 2019	CINECA-ISCRA Class B proposal (480,000 GPU hours on Marconi@CINECA) **Computational design of customised nanobodies for HER2 recognition**
Nov. 2017 - Aug. 2018	CINECA-ISCRA Class C proposal (40,000 GPU hours on Marconi@CINECA) **Computational design of peptides for lysozyme recognition**
May. 2017 - Feb. 2018	CINECA-ISCRA Class C proposal (38,400 GPU hours on Marconi@CINECA) **Scoring functions assessment for nanobodies screening**
Jul. 2016 - Apr. 2017	CINECA-ISCRA Class C proposal (50,000 GPU hours on Marconi@CINECA) **Predicting the properties of peptoids by molecular dynamics simulations**
Nov. 2015 - Dec. 2015	PRACE Preparatory Access (5000 MIC hours on Marenostrum, Spain + 50000 GPU hours on Curie, France) **Effect of humanizing mutations on natural nanobodies for the development novel therapeutic agents**
Aug. 2015 - May 2016	CINECA-ISCRA Class C proposal (100,800 GPU hours on Galileo@CINECA) **Effect of humanising mutations on natural nanobodies for the development novel therapeutic agents**
Sep. 2014 - Jul. 2015	CINECA-ISCRA Class C proposal (48,000 GPU hours on Eurora@CINECA) **Identification of chemokine receptor/ligand binding configurations for the development enhanced binders for biomolecular recognition**
Jul. 2013 - Apr. 2014	CINECA-ISCRA Class C proposal (1,000,000 CPU hours on Fermi@CINECA) **Scoring functions Assessment for the development of new peptide-based nanodevices**
Oct. 2012 - Oct. 2013	CINECA-ISCRA Class B proposal (3,609,600 CPU hours on Fermi@CINECA) The GW method for the accurate simulation of the photoemission spectra of metal supported metal-phthalocyanine self-assemblies
Oct. 2012 - Jul. 2013	CINECA-ISCRA Class C proposal (1,998,850 CPU hours on Fermi@CINECA) Self-assembled monolayers for the decoupling of molecules from their metallic substrate
Dec. 2011- Dec. 2012	CINECA-ISCRA Class B proposal (161,280 CPU hourss on SP6@CINECA): Molecule-substrate interplay and spectroscopic properties of metal-supported metal-phthalocyanine
Sep. 2011 - Jun. 2012	CINECA-ISCRA Class C proposal (20,000 CPU hours on SP6@CINECA) DFT methods for the study of metal phthalocyanine
Dec. 2010 - Sep. 2011	CINECA-ISCRA Class C proposal (20,000 CPU hours on SP6@CINECA) Metalphthalocyanine self-assemblies on metallic surfaces

Teaching and Supervising

Teaching Appointments

2019 - 2021 — Assistant Professor, Department of Chemical and Pharmaceutical Sciences, University of Trieste, IT, for the following courses:

2020/2021

• *Drug Analysis* (Analisi dei Medicinali)
Pharmacy (5 years degree), third year students, summer term, 128 hrs.

• *Molecular Modelling for Life Sciences*
PhD School in Chemistry, winter term, 16 hrs.

• *Molecular Modelling for Life Sciences*
Seminar Series for the Marie Skłodowska-Curie Innovative Training Network PhD students, winter term, 16 hrs.

2019/2020

• *Drug Analysis - module* (Analisi dei Medicinali - modulo)
Pharmacy (5 years degree), third year students, summer term, 60 hrs.

• *Molecular Modelling* (Principi di Modellazione Molecolare)
Pharmaceutical Chemistry and Technology (CTF, 5 years degree), fourth year strudents, summer term, 32 hrs.

2016 - 2017 — External Lecturer, Molecular Genetics and Biotechnology PhD, University of Nova Gorica, Slovenia:
• contributed lectures for the course *Basics in Molecular Biology and Biotechnology* (2hrs)

2014 - 2018 — Contract Professor of *Computer Science - Practical Applications* (Idoneità informatica pratica), Department of Chemical and Pharmaceutical Sciences, University of Trieste, IT, for the following degrees:
• Pharmacy (5 years), first year students, summer term, 88 hrs;
• Pharmaceutical Chemistry and Technology (CTF, 5 years), first year students, winter term, 48 hrs.

Modules taught:

academic year 2017/18 — *Practical Informatics (Idoneità informatica pratica)*, Pharmacy, summer term, 88 hrs.
Practical Informatics (Idoneità informatica pratica), CTF, winter term, 48 hrs.

academic year 2016/17 — *Practical Informatics (Idoneità informatica pratica)*, Pharmacy, summer term, 88 hrs.
Practical Informatics (Idoneità informatica pratica), CTF, winter term, 48 hrs.

academic year 2015/16 — *Practical Informatics (Idoneità informatica pratica)*, Pharmacy, summer term, 88 hrs.
Practical Informatics (Idoneità informatica pratica), CTF, winter term, 48 hrs.

academic year 2013/14 — *Practical Informatics (Idoneità informatica pratica)*, Pharmacy, summer term, 78 hrs.

2008 - 2010 — Laboratory Demonstrator for Undergraduate Students, Department of Chemistry, University of Warwick, UK:
• 1st year *Mathematics* (10hrs, 160 students);
• 2nd year *Statistical Mechanics Workshop* (6hrs, 100 students);
• 3rd year *Computational Chemistry Workshop* (2hrs, 100 students).

Mentoring and Supervising

• Federico Nolasco (PhD student, Nov.2021-Nov.2024)
Characterisation of antibody fragments
• Patricio German Barletta (ICTP-TRIL postdoctoral fellow, since Aug.2021-Aug.2023)
In silico design of customised high-affinity antibody fragments
• Marco De Conto (predoctoral, MSc Pharmaceutical Chemistry and Technology)
Computational design of biotheranostics
• Theo Battista (postdoctoral fellow, Jul.2021 - Jun. 2022)
Expression and purification of antibody fragments for oncology applications
• Nikola Minovski (postdoctoral fellow, Mar. 2020 - Feb. 2021)

In silico design of customised high-affinity antibody fragments
• Hendrik Vondracek (postdoctoral fellow, Nov. 2019 - Feb. 2021
Atomic Force Microscopy (AFM) and electrochemical measurements
• Barbara Medagli (postdoctoral fellow, Oct. 2017 - Sep. 2020)
Expression and purification of antibody fragments for oncology applications
• Luciana Gneo (postdoctoral fellow, Dec. 2017 - May 2019)
Characterisation of antibody fragments for oncology applications (AFM)
• Cedrix Dongmo (predoctoral ICTP-TRIL fellow, Jan. 2014 - Oct. 2014)
Molecular Dynamics simulations of biomolecules

THESIS (CO)SUPERVISOR

2022 • Marco De Conto (MSc Pharmaceutical Chemistry and Technology) University of Trieste, Trieste, Italy
Thesis: *In silico design of antibody fragments for (bio)molecular detection and theragnostic applications: the example of p53 reactivation*

2021 • Damiano Baroni (MSc Chemistry), University of Trieste, Trieste, Italy
Thesis: *Computational Methods for the rational mutagenesis of cutinaes*
• Sara Raso (MSc Medical and Pharmaceutical Biotechnologies)
Thesis: *Dall'ottimizzazione in silico alla provetta: produzione, caratterizzazione di nanobody e test preliminari su linee cellulari di carcinoma mammario Her2 positive come nuova prospettiva per il cancro al seno*

2017 • Katja Pracek (BSc Bioinformatics), University of Primorska, Koper, Slovenia
Thesis: *Homology modeling and molecular simulations of the camelid nanobodies as therapeutic tools in the treatment of sarcoma*

PHD THESIS EXTERNAL EXAMINER

2019 • Ornela Maloku, PhD program in Computer science, Mathematics and Physics, University of Udine, Italy

2018 • Nikhil Agrawal, School of Pharmacy and Pharmacology, University of KwaZulu-Natal, Durban, South Africa

Conferences Contributions: Oral

(16) *A computational protocol for the in silico maturation of antibody fragments*
European Biophysical Societies' Association Global Summit - EBSA 2023
Stockholm, Sweden (31 Jul. - 4 Aug. 2023)

(16) *Automatic screening of enzymes for synthesis and biodegradation of renewable polyesters*
COZYME - Computational Redesign of Enzymes Meeting - Fuengirola, Spain (March 20, 2023)

(14) *A Computational Protocol for the in Silico Maturation of Antibody Fragments*
CLINAM 12/2020 Conference and Exhibition: European & Global Summit for Cutting-Edge Medicine
Basel, Switzerland (25-28 Oct. 2020).

(13) *Computational design of peptide based architectures for biomarker recognition*
CLINAM 9/2016 Conference and Exhibition: European & Global Summit for Cutting-Edge Medicine
Basel, Switzerland (26-29 Jun. 2016).

(12) *Self-organisation of surface adsorbed molecular monolayers: does the surface matter?*
Nanomaterials for Technology Workshop - Department of Chemical and Process Engineering, University of Strathclyde, Glasgow, UK (20-21 Jun. 2016).

(11) *Computational design of peptide-based architectures for protein recognition*
IOP Conference: The Physics of Soft and Biological Matter 2016
Cambridge, UK (6-8 Apr. 2016).

(10) *Computationally engineered binders for protein recognition*
Workshop in honor of Giacinto Scoles: From Intermolecular Forces to Frontiers in Nanoscience and Nanomedicine - ICTP, Trieste, Italy (21-22 Jan. 2016).

(9) *Computational design of peptide based binders for biomarker recognition*
EMBO Workshop: Advances in Protein-Protein Interaction Analysis Modulation
Hyères, France (9-12 Sep. 2014).

(8) *Structure of self-assembled iron-phthalocyanines on the Au(110) surface through STM imaging and DFT calculations*
Science through Scanning Probe Microscopy - Bologna, Italy (12-13 Dec. 2013).

(7) *Structure and electronic properties of self-assembled transition metal phthalocyanines (M=Fe,Co,Ni,Cu,Zn) on the Au(110) surface*
CMD-24, ECOSS-29, ECSCD-11, CMMP-12
Edinburgh International Conference Centre, Edimburgh, UK (3-7 September 2012).

(6) *Self-organisation of surface adsorbed molecular monolayers: an agent-based view*
Thomas Young Centre workshop: Thermodynamics and Kinetics of Surfaces and Interfaces from Simulations - University College London, UK (22-24 Jun. 2011).

(5) *Agent Based modelling of realistic molecules*
ECCS'10 European Conference on Complex Systems - Lisbon, Portugal (13-17 Sep. 2010).

(4) *Monte Carlo simulation of polydisperse spheres on a spherical droplet*
CCP5 Workshop: Particle Adsorption at Soft Interfaces
University of Warwick, UK (8 Jul. 2010).

(3) *Agent Based algorithm for the study of molecular self-organisation*
European Conference on Complex Systems
University of Warwick, UK, (21-25 Sep. 2009).

(2) *Agent Based modelling for molecular self-organisation*
European Dynamics Days 2009
Göttingen, Germany (31 Aug. - 4 Sep. 2009).

(1) *Agent Based algorithm for the study of molecular self-organisation*
EPSRC Network Mathematical Challenges of Molecular Dynamics
University of Bath, UK (13-15 Jul. 2009).

Invited Seminars

(16) *Computational design of peptide-based architectures for protein recognition* - Department of Physics, University of Lisboa, Portugal (9 October 2019).
(15) *Computational design of peptide-based architectures for protein recognition* - Department of Computational Biochemistry and Drug Design, Kemijski intitut (KI) - National Institute of Chemistry, Ljubljana, Slovenia (21 May 2018).
(14) *Computational design of peptide-based architectures for protein recognition* - Department of Biological Sciences and Engineering, University of Nova Gorica, Vipava, Slovenia (16 May 2017).
(13) *Computational design of peptide-based architectures for protein recognition* - Faculty of Chemistry, University of Murcia, Spain (20 May 2016).
(12) *Computational design of peptide-based architectures for protein recognition* - Department of Chemistry University of Sheffield, Sheffield, UK (29 Apr. 2016).
(11) *Computational design of peptide-based architectures for protein recognition* - Department of Chemical and Process Engineering, University of Strathclyde, Glasgow, UK (2 Mar. 2016).
(10) *Computational design of peptide-based nano-devices* - MoNaLiSA Fourth Midsummer Meeting, ELETTRA Synchrotron Light Laboratory, Trieste, Italy (5 Jun. 2015).
(9) *Coupled binders for the development of novel nanodevices for protein recognition* - MoNaLiSA Third Midsummer Meeting, Department of Medical and Biological Sciences, University of Udine, Italy (11 Jul. 2014).
(8) *Estimating peptides-protein binding affinities for the development of new peptide-based nanodevices for protein recognition* - MoNaLiSA Second Midsummer Meeting, Department of Medical and Biological Sciences, University of Udine, Italy (26 Jul. 2013).
(7) *Auto-assemblamento molecolare tra laboratorio e calcolatore* (Molecular self-assembly through laboratory and computer), Department of Medical and Biological Sciences, University of Udine, Italy (7 Mar. 2013).
(6) *Modelling techniques for the study of self-organised surface adsorbed molecular monolayers* - Department of Information Sciences, Ochanomizu University, Tokyo, Japan (24 Jul. 2012).
(5) *Agent Based Modelling for the study of Molecular Self-Organisation* - Physics Department, University of Modena, Italy (19 May 2011).
(4) *Agent Based Modelling for the study of Molecular Self-Organisation* - ELETTRA Synchrotron Light Laboratory, Trieste, Italy (7 Apr. 2010).
(3) *Agent Based Modelling for the study of Molecular Self-Organisation* - Complexity Forum, Complexity Science Doctoral Training Centre, University of Warwick, UK (17 Feb. 2010).
(2) *An Agent-Based Model for Molecular Self-Organization* - CSC@Lunch Seminars, Centre for Scientific Computing, University of Warwick, UK (2 Feb. 2009).
(1) *Il caos quantistico nelle reazioni chimiche triatomiche* (Quantum Chaos in Triatomic Chemical Reactions) - Chemistry Department, University of Perugia, Italy (30 Jan. 2007).

REFEREED PAPERS IN JOURNALS:

1. S. La Manna, A. Cugudda, F.A. Mercurio, M. Leone, S. Fortuna, C. Di Natale, E.Lagreca, P.A. Netti, V. Panzetta, D. Marasco
PEGylated SOCS3 Mimetics Encapsulated into PLGA-NPs as Selective Inhibitors of JAK/STAT Pathway in TNBC Cell
Int. J. Nanomedicine, 2024, 19, 7237-7251.
2. G.P. Barletta, R. Tandiana, M. Soler, S. Fortuna*+, W. Rocchia
Locuaz: an in silico platform for protein binders optimization
Bioinformatics, 2024, 40 (8), btae492.
3. D. Zampieri, M. Romano, S. Fortuna, E. Amata, M. Dichiara, G. Cosentino, A. Marrazzo, M.G. Mamolo
Design, Synthesis, and Cytotoxic Assessment of New Haloperidol Analogues
Molecules, 2024, 29(11), 2697.
4. M. Iacomino, N. Houerbi, S. Fortuna, J. Howe, S. Li, G. Scorrano, A. Riva, K.-W. Cheng, M. Steiman, I. Peltekova, A. Yusuf, S. Baldassari, S. Tamburro, P. Scudieri, I. Musante, A. Di Ludovico, S. Guerrisi, G. Balagura, A. Corsello, S. Efthymiou, D. Murphy, P. Uva, A. Verrotti, C. Fiorillo, M. Delvecchio, A. Accogli, M. Elsabbagh, H. Houlden, S.W. Scherer, P. Striano, F. Zara, T.-F. Chou, V. Salpietro
Allelic heterogeneity and abnormal vesicle recycling in PLAA-related neurodevelopmental disorders
Front. Mol. Neurosci., 2024, 17, 1268013.
5. R. Tandiana, G.P. Barletta, M.A. Soler, S. Fortuna+, W. Rocchia
Computational Mutagenesis of Antibody Fragments: Disentangling Side Chains from G Predictions
J. Chem. Theory Comput., 2024, 20, 6, 26302642.
6. A.R. Buzatu, M.A. Soler, S. Fortuna, O. Ozkilinc, D.M. Dreavă, I. Bîtcan, V. Badea, P. Giannozzi, F. Fogolari, L. Gardossi, F. Peter, A. Todea, C.G. Boeriu
Reactive natural deep eutectic solvents increase selectivity and efficiency of lipase catalyzed esterification of carbohydrate polyols
Catal. Today, 2024, 426, 114373.
7. A.R. Buzatu, M.A. Soler, O. Ozkilinc, S. Fortuna, D.M. Dreavă, I. Bîtcan, P. Giannozzi, F. Fogolari, L. Gardossi, F. Peter, A. Todea, C.G. Boeriu
Lipase-catalysed esterification in a reactive natural deep eutectic solvent leads to lauroylcholine chloride rather than glucose ester
React. Chem. Eng., 2024, 9, 2623-2634.
8. G. Scorrano, G. DOnofrio, A. Accogli, M. Severino, R. Buchert, U. Kotzaeridou, G. Iapadre, G. Farello, M. Iacomino, F. Dono, L. Di Francesco, M.F. Fiorile, S. La Bella, A. Corsello, E. Caln, G. Di Rosa, E. Gitto, A. Verrotti, S. Fortuna, M.A. Soler, F. Chiarelli, B. Oehl-Jaschkowitz, T.B. Haack, F. Zara, P. Striano, V. Salpietro
A PAK1 mutational hotspot within the regulatory CRIPaK domain is associated with severe neurodevelopmental disorders in children
Pediatr. Neurol., 2023, 149, 84-92.
9. D. Zampieri, A. Calabretti, M. Romano, S. Fortuna, S. Collina, E. Amata, M. Dichiara, A. Marrazzo, M.G. Mamolo
Cytotoxicity profiles and neuroprotective properties of the novel ifenprodil analogues as sigma ligands
Molecules, 2023, 28(8), 3431.
10. M.A. Soler, N. Minovski, W. Rocchia, S. Fortuna*
Replica-exchange optimization of antibody fragments
Comput. Biol. Chem., 2023, 103, 107819.
11. A. Alsadig, B. Abbasgholi-NA, H. Vondracek, Ba. Medagli, S. Fortuna, P. Posocco, P. Parisse, H. Cabrera, L. Casalis
DNA-Directed Protein Anchoring on Oligo/Alkanethiol-Coated Gold Nanoparticles: A Versatile Platform for Biosensing Applications
Nanomaterials, 2023, 13(1), 78.

12. D. Zampieri, S. Fortuna, M. Romano, A. De Logu, G. Cabiddu, A. Sanna, M.G. Mamolo
Synthesis, Biological Evaluation and Computational Studies of New Hydrazide Derivatives Containing 1,3,4-Oxadiazole as Antitubercular Agents
Int. J. Mol. Sci., 2022, 23(23), 15295.

13. V. Salpietro, V. Galassi-Deforie, S. Efthymiou, E. OConnor, A. Marcé-Grau, R. Maroofian, P. Striano, F. Zara, M. Morrow, SYNAPS Study Group , A. Reich, A. Blevins, J. Sala-Coromina, A. Accogli, S. Fortuna, M. Alesandrini, P. Y. Billie Au, N. Shah Singhal, B. Cogne, B. Isidor, M. G. Hanna, A. Macaya, D. M. Kullmann, H. Houlden, R. Männikkö
De novo KCNA6 variants with attenuated KV1.6 channel deactivation in patients with epilepsy
Epilepsia, 2023, 64(2), 443-455.

14. A.L. Ferrara, M. Bova, A. Petraroli, D. Marasco, C. Payr, S. Fortuna, F. Palestra, R. Ciardi, G. Marone, G. Spadaro, G. Lambeau, S. Loffredo
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