

Curriculum Vitae

Personal information

First name / Surname	Simone Brogi		
Address	17, via Cialdini, 53021, Abbadia San Salvatore (Siena), Italia		
Telephone(s)	Home: +390577779568	Mobile: +393387982249	
E-mail	simone.brogi@unipi.it	simonebrogi1976@hotmail.com	simone.brogi@pec.it
	brogi32@unisi.it		
Web	http://www.simonebrogi1976.it		
Nationality	Italian		
Date of birth	13/09/1976		
Gender	male		

Work experience

Date	01/02/2019-to date
Occupation or position held	Senior Researcher (RTD_B L.240/2010 SSD: Pharmacology BIO/14)
Main activities and responsibilities	Head of <i>in silico</i> Pharmacology and Toxicology Unit.
Name and address of employer	University of Pisa – Dept. of Pharmacy Via Bonanno 6 – 56125 Pisa (Italy)
Type of business or sector	Pharmacology
Date	11/05/2018-31/01/2019
Occupation or position held	Research Fellow
Main activities and responsibilities	Responsible for the computational part of the project “Bioinformatics studies on innovative targets for developing new natural product-based drugs” with scientific advisor Prof. Ettore Novellino.
Name and address of employer	University of Naples “Federico II” – Dept. of Pharmacy Via D. Montesano 49 – 80131 Napoli (Italy)
Type of business or sector	Medicinal Chemistry
Date	01/06/2012-30/04/2018
Occupation or position held	Research Fellow
Main activities and responsibilities	Head of Molecular Modeling Unit at Department of Biotechnology, Chemistry and Pharmacy in the research group directed by Prof. Giuseppe Campiani
Name and address of employer	University of Siena –Dept. Biotechnology, Chemistry and Pharmacy Via A. Moro 2 – 53100 Siena (Italy)
Type of business or sector	Medicinal Chemistry
Date	01/04/2011-31/03/2012
Occupation or position held	Post-Doctoral Research Fellow
Main activities and responsibilities	Responsible of the Molecular Modeling Unit at Department of Pharmaceutical and Applied Chemistry in the research group directed by Prof. Giuseppe Campiani
Name and address of employer	University of Siena – Dept. Pharmaceutical and Applied Chemistry Via A. Moro 2 – 53100 Siena (Italy)
Type of business or sector	Medicinal Chemistry

Date	01/05/2011-31/06/2011
Occupation or position held	Internship (Drug Design Unit Medicinal Chemistry Department)
Name and address of employer	Siena Biotech S.p.A. Strada del Petriccio e Belriguardo 35 53100 Siena
Type of business or sector	Pharmaceutical Industry
Date	01/06/2006-01/11/2006
Occupation or position held	Pharmaceutical Sales Representative
Name and address of employer	Psoriasis Organization S.r.l. Zona industriale Settevene, Nepi (VT) (Italia)
Type of business or sector	Pharmaceutical Industry
Date	01/06/2006-01/11/2006
Education and training	
Date	01/10/2007-30/09/2010
Title of qualification awarded	Ph.D. in Pharmaceutical Sciences (XXIII Cycle)
Title of Ph.D. dissertation	Computational Approaches in Drug Discovery Advisor: Prof. Andrea Tafi
Principal subjects/occupational skills covered	Computational Chemistry, Drug Design, Drug Discovery, Molecular Modeling, Lead Discovery and Lead Optimization
Name and type of organisation providing education and training	University of Siena – Dept. Pharmaceutical and Applied Chemistry Via A. Moro 2 – 53100 Siena (Italy)
Date	20/01/2007-20/01/2008
Title of qualification awarded	M.Sc. (Second Level Master) in Drug Design and Synthesis
Principal subjects/occupational skills covered	Molecular Modeling, Advanced Chemical Synthesis, Drug Design, Drug Discovery
Name and type of organisation providing education and training	University of Siena – Dept. Pharmaceutical and Applied Chemistry Via A. Moro 2 – 53100 Siena (Italy)
Date	01/07/2006-20/07/2006
Title of qualification awarded	Professional Qualification in Biology
Principal subjects/occupational skills covered	Biological and Genetic Processes
Name and type of organisation providing education and training	University of Siena
Date	03/10/1996-28/09/2005
Title of qualification awarded	Master's Degree (Italian "Laurea") in Biological Sciences
Title of Thesis	Ricerca di modificatori della non-disgiunzione e drive meiotico nei maschi di <i>Drosophila Melanogaster</i> Advisor: Prof. Leonard Gilbert Robbins; Co-Advisor: Dr. Massimo Belloni.

Principal subjects/occupational skills covered	Genetic, Molecular Genetic, Molecular and Cellular Biology, Evolutionary Biology, Microbiology, Molecular Pathology, Biochemistry, Bioinformatics, Developmental Biology.
Name and type of organisation providing education and training	University of Siena
Level in national or international classification	"Dottore Magistrale" (5-years long Master's Degree) 109/110
Date	13/09/1991-04/07/1995
Title of qualification awarded	High School Diploma with Specialization in Chemistry
Principal subjects/occupational skills covered	Inorganic and Organic Chemistry, Microbiology, Biochemistry, Physical Chemistry
Name and type of organisation providing education and training	I.T.I.S. "A. Avogadro" Via case nuove, 53021 Abbadia San Salvatore (Italia)
Level in national or international classification	42/60
Personal skills and competences	
Mother tongue	Italian
Other language	English, French
Self-assessment	
European level (*)	
English	
French	
Social skills and competences	From 2009 to 2014 voluntary clowns for the non-governmental organization onlus V.I.P. "ViviamoInPositivo" in Siena http://www.vipsiena.it/ Operational Center: Via Cristalliera, 25 – 10139 Torino Legal Center: Via Pacchiotti, 79 - 10146 Torino Tel 011.198.36.557 CF: 97623990013 – PI: 08577420014 E-Mail: viviamoinpositivo@gmail.com Communication and interpersonal skills (acquired from the interaction with others throughout academic, professional and personal life) Optimal ability to speak in public (developed along the presentation of lectures and group works at the graduate studies) Good experience in working with a variety of different people and coping with different types of personalities. I also have good abilities in time management and scheduling skills.
Organisational skills and competences	Good experience in the management and targeting of research projects and layout of scientific publications acquired during my works in the laboratories of research

Technical skills and competences

Over 10 years of experience in applying the knowledge of molecular modeling to solve problems inherent to medicinal chemistry research.

Strong organizational skills.

Excellent communication skills (both written and oral) and attention to details.

Proven ability to handle multiple projects simultaneously.

Proven experience in document generation, including writing, experimental methods, methods validation and computational reports, documents for patents and proposal submissions, and manuscripts for scientific journals.

Expertise in "*in-silico*" drug discovery and optimization.

Superb understanding of computational approaches used in medicinal chemistry research.

Strong familiarity with mathematical modelling.

Expertise in the retrieval and analysis of relevant literature, and proficiency in presenting a case.

90 published articles in scientific journals with relevant impact factor (*h-index* = 23). Two book chapters, one ebook and one patent.

Excellent Knowledge in molecular biology, molecular genetics and biochemistry.

Sound knowledge of various computational methodologies: pharmacophore modeling, virtual screening, High throughput Docking (HTD), molecular docking, homology modeling, 3D-QSAR and 3D-QSSR models, molecular dynamics, QM/MM calculations, *in-silico* prediction of ADME+T properties.

Expertise in GPU calculation by means of CUDA technology applied to Molecular Dynamics software.

National Scientific Habilitation (ASN 2016) as Associate Professor in Medicinal, Toxicological and Nutritional Chemistry and Applied Technologies (03/D1) – Medicinal Chemistry (SSD CHIM08) (2017-2023).

Academic and Teaching Activity

From February 2019

Teaching activity at University of Pisa ([Unimap Simone Brogi](http://www.unimap.unipi.it))

-**Farmacologia Generale (Cod. 031EE)** per Laurea Magistrale Ciclo Unico 5 anni in Farmacia (2019-to date)

-**Metodi Alternativi alla Sperimentazione Animale in Campo preclinico (Cod. 005EC)** per Laurea Magistrale Ciclo Unico 5 anni in Farmacia (2019-to date)

-**Farmacologia, Farmacoterapia e Tossicologia (Cod. 023EE)** per Laurea Magistrale Ciclo Unico 5 anni in Chimica e Tecnologia Farmaceutiche (2019)

-**Farmacognosia e Tossicologia (Modulo dell'insegnamento Farmacologia, Farmacoterapia, Farmacognosia e Tossicologia Cod. 464EE)** per Laurea Magistrale Ciclo Unico 5 anni in Chimica e Tecnologia Farmaceutiche (2020-to date)

-**Nutraceutica e Nutrigenomica (Cod. 003EG)** per Corso di Laurea Magistrale in Scienze Della Nutrizione Umana (2019-todate)

-**Capacità Informatiche (CdS F0-SP4)** per Scuola di Specializzazione in Farmacia Ospedaliera (2019-to date)

-**In silico approaches in Pharmacology and Toxicology** per Scuola di dottorato in "SCIENZA DEL FARMACO E DELLE SOSTANZE BIOATTIVE" (2019)

January 2021

Thesis relator in the thesis entitled "CoVid-19 e potenziali approcci di "drug repurposing". Area of Expertise: Pharmacology. Candidate: Rachele Sorce.

January 2021

Thesis co-relator in the thesis entitled "Screening di nuovi modulatori dell'enzima SIRT1". Area of Expertise: Pharmacology. Candidate: Rita Garreffa.

September 2020

Thesis relator in the thesis entitled "Utilizzo di Farmaci in Gravidanza, Stato dell'Arte e Nuove Prospettive". Area of Expertise: Pharmacology. Candidate: Giada Dello Sbarba.

July 2020

Thesis relator in the thesis entitled "Attuali approcci nutraceutici per il potenziale trattamento del morbo di Alzheimer". Area of Expertise: Pharmacology. Candidate: Carlotta Ferrari.

May 2020

Thesis relator in the thesis entitled "Il solfuro di idrogeno nelle patologie oftalmiche: ruolo fisiopatologico e nuove prospettive terapeutiche". Area of Expertise: Pharmacology. Candidate: Mariella Speranza.

April 2020

Thesis relator in the thesis entitled "Sigaretta elettronica: davvero così innocua". Area of Expertise: Toxicology/pharmacology. Candidate: Eleonora Barbieri.

March 2020

Thesis relator in the thesis entitled "Regime Dietetico ed efficacia dei nutraceutici nel trattamento delle problematiche psicofisiche della donna in menopausa". Area of Expertise: Nutrition/Nutraceuticals. Candidate: Simona Alfa Sciacca.

July 2019

Thesis relator in the thesis entitled "Valutazione amperometrica del rilascio di H₂S e determinazione *in silico* delle proprietà chimico-fisiche di una serie di isotiocianati di sintesi". Area of Expertise: Pharmacology. Candidate: Cecilia Orlandini.

July 2018

Thesis correlator in the thesis entitled: "Progettazione *in silico* di nuovi potenziali inibitori Mcl-1 come agenti antitumorali" Relator: Prof. Stefania Butini. Area of Expertise: Medicinal Chemistry, Molecular Modeling. Candidate: Emanuele Ancora.

January 2018

Teaching activity at University of Siena within the course "Medicinal Chemistry and Toxicology II" ("Chimica Farmaceutica e Tossicologica II") held by Professor Maurizio Anzini. The teaching activity, for the degree course in Pharmacy (LM-13), consisted in a cycle of lessons and esercitations in "Computational Approaches in Medicinal Chemistry" (8 hours).

From October 2016

Advisor of PhD student Giulia Chemi (XXXII Cycle of Doctoral School in Chemical and Pharmaceutical Sciences, University of Siena) for the computational studies within her PhD training. Research Project: "Computer-Aided Drug Discovery Methodologies for the Identification and Optimization of Bioactive Compounds". Tutor Prof. Sandra Gemma. Area of Expertise: Drug Discovery, Molecular Modeling.

May 2016 - October 2016

Advisor of research fellow Giulia Chemi (University of Siena). Research Project "Progettazione razionale di potenziali molecole biologicamente attive e selettive verso l'enzima del sistema endocannabinoide FAAH": Area of Expertise: Drug Discovery, Molecular Modeling.

December 2015 - April 2016

Advisor of research fellow Giulia Chemi (University of Siena). Research Project "Identificazione di composti biologicamente attivi attraverso metodiche computazionali": Area of Expertise: Drug Discovery, Molecular Modeling.

April 2016

Thesis correlator in the thesis entitled: "Studi di modellistica molecolare per l'identificazione di potenziali inibitori dell'enzima acetilcolinesterasi umana" Relator: Prof. Giuseppe Campiani. Area of Expertise: Drug Discovery, Molecular Modeling. Candidate: Cesare Turchi.

December 2015

Thesis correlator in the thesis entitled: "Progettazione razionale *in silico* di ligandi selettivi per il recettore serotoninergico 5-HT₇" Relator: Prof. Giuseppe Campiani. Area of Expertise: Drug Discovery, Molecular Modeling. Candidate: Filippo Minnella.

October 2015-June 2016

Advisor for the computational studies of PhD student Hajar Sirous-Najafabadi from Isfahan University (Iran) during her part of research at University of Siena. Research Project: "Design, synthesis and biological evaluation of novel chemical agents against HIV-1 integrase acting as metal chelating agents". Area of Expertise: Drug discovery, Computer-aided drug discovery, Molecular Modeling

April 2015

Thesis correlator in the thesis entitled: "Sviluppo ed applicazione di un protocollo computazionale per l'analisi e la predizione dell'attività antiprionica" Relator: Prof. Giuseppe Campiani. Area of Expertise: Drug Discovery, Molecular Modeling. Candidate: Giulia Chemi.

April 2015

Thesis correlator in the thesis entitled: "Identificazione di ligandi selettivi per il recettore ionotropico glutammatergico GluK3 attraverso l'utilizzo di metodologie computazionali innovative" Relator: Prof. Giuseppe Campiani. Area of Expertise: Medicinal Chemistry, Molecular Modeling. Candidate: Michele D'Elia.

December 2014-September 2016

Administrator of the official Facebook page of the Department of Biotechnology, Chemistry and Pharmacy (University of Siena) <https://www.facebook.com/DptBCP>

June 2014-July 2016

Elected representative of Research Fellows (Assegnisti di Ricerca) at Department of Biotechnology, Chemistry and Pharmacy Committee, University of Siena.

Awards

April 2018

Outstanding reviewer

Computational Biology and Chemistry (Elsevier)

[Reviewer recognition page](#)

October 2017

Outstanding reviewer

European Journal of Medicinal Chemistry (Elsevier)

[Reviewer recognition page](#)

September 2015

The scientific poster "Design and synthesis of novel PfSUB1 inhibitors"

Gloria Alfano, **Simone Brogi**, Margherita Brindisi, Michael J. Blackman, Stefania Butini, Sandra Gemma; XXIII NMMC & 9th NPCF - September 6-9 2015, Salerno (Italy) has been awarded as best poster from StepBio srl

April 2015

Outstanding reviewer

Journal of Molecular Graphics and Modelling (Elsevier)

[Reviewer recognition page](#)

July 2014

The article "Rational design of the first difluorostatone-based PfSUB1 inhibitors, *Bioorg. Med. Chem. Lett.* **2014**, 24(15), 3582-3586" has been highlighted as a Feature Article on the Malaria Nexus website (<http://www.malarianexus.com/>). Malaria Nexus is Elsevier's Global Malaria Resource: A major hub for scientists working in all aspects of malaria research

Bibliometric Parameters (BP)

BP of the total number of publications

Number of publications: 94 (90 peer-reviewed articles, one patent, two book chapters and one eBook)

90 papers *h index* (Scopus/Google Scholar) 23/25

Number of citations (Scopus/Google Scholar) 1404/1683

First author: 19; Senior author: 7; Corresponding author: 14

National Scientific Habilitation (ASN 2016) as Associate Professor in Medicinal, Toxicological and Nutritional Chemistry and Applied Technologies (03/D1) – Medicinal Chemistry (SSD CHIM08) (2017-2023)

Fund Raising on Competitive Basis and Research Cooperation

Funded Project

2016	Multi-target inhibitors against metalloproteases for developing effective anti- <i>Mycobacterium</i> drugs
	GA2016_087R
Role	Principal Investigator (PI) (£ 21,000)
Funder	BSAC - British Society for Antimicrobial Chemotherapy

2020	Agenti innovativi e nanosistemi per target molecolari nell'ambito dell'oncologia di precisione
	PRA_2020_58
Role	Research Unit Coordinator (75.460,33 Euros)
Funder	University of Pisa "PRA: bando progetti di ricerca di Ateneo 2020-2021"

Contract of Collaboration

2016 – 2020 - Targeting *eIF4F* complex for developing innovative anticancer agents -

The contract was established among:

- University of Strasbourg "Laboratoire d'Innovation Thérapeutique UMR7200" (Dr Laurent Desaubry)
- Gustave Roussy cancer center (Dr Stephan Vagner and Dr Caroline Robert)
- University of Siena "Department of Biotechnology, Chemistry and Pharmacy" (Dr **Simone Brogi**)

Research Activity

Dr Brogi is a Senior Researcher at the Department of Pharmacy at University of Pisa, Italy. Dr Brogi is the head of *in silico* Pharmacology and Toxicology Unit in the research group directed by Prof. Vincenzo Calderone. The scientific production of Dr Brogi consists of **90 papers** published on international journals (first publication year 2009), one patent, two book chapters and one eBook. Dr Brogi research activity has been mainly focused on computational approaches in drug discovery with particular attention to lead optimization in terms of pharmacokinetics properties and metabolic stability. Research activities focusing on the discovery and optimization of small-molecules as potential antalgic agents, antitumor compounds, and also with therapeutic potential for the treatment of neurodegenerative, cardiovascular, and parasitic diseases. These interests include target selection and the rational design of innovative drugs, the application and validation of novel computational strategies, and the study of important structure-function relationships. On 31 July 2017 Dr Brogi obtained the Italian National Scientific Habilitation (ASN 2016) as Associate Professor in Medicinal, Toxicological and Nutritional Chemistry and Applied Technologies (03/D1; SSD CHIM08). Dr Brogi operates as reviewer for the Journal of Medicinal Chemistry, European Journal of Medicinal Chemistry, British Journal of Pharmacology, Drug Discovery Today, Scientific Reports, Journal of Enzyme Inhibition and Medicinal Chemistry, Antibiotics, Biomolecules, Journal of Cheminformatics, ChemMedChem, Journal of Advanced Research, Pharmacological Reports, Journal of Agricultural and Food Chemistry, Bioorganic & Medicinal Chemistry Letters, Computers in Biology and Medicine, Fundamental & Clinical Pharmacology, Future Medicinal Chemistry, Nanomaterials, PLoS One, Journal of Computer-Aided Molecular Design, Expert Opinion on Drug Discovery, International Journal of Environmental Research and Public Health, Journal of Molecular Graphics and Modelling, Molecules, International Journal of Molecular Sciences, Nutrients, Diagnostics, Mathematics, Applied Sciences, Frontiers in Pharmacology, Frontiers in Chemistry, Frontiers in Genetics, Frontiers in Microbiology, Frontiers in Immunology, Frontiers in Neuroscience, Frontiers in Medicine, Frontiers in Molecular Biosciences, Frontiers in Physiology, Frontiers in Plant Science, Frontiers Cell and Developmental Biology, Journal of Natural Products, Journal of Theoretical Biology, Computational Biology and Chemistry, Chemical Biology & Drug Design, Food Chemistry, BMC Pharmacology & Toxicology, European Journal of Plant Pathology, Mini-review in Medicinal Chemistry, Current Medicinal Chemistry, Current Drug Targets, Current Topics in Medicinal Chemistry, Current Pharmaceutical Design, Medicinal Chemistry, Medicinal Chemistry Research, RSC Advances, Journal of Chemistry, ChemistrySelect, Journal of Drug Research and Development, Journal of Systems Biology Research, Informatics in Medicine Unlocked (IMU), Scientia Pharmaceutica, Journal of Forensic Research and Analysis, International Journal of Biopharmaceutical Sciences, Modern Approaches in Drug Designing, Virology & Immunology Journal, and Interdisciplinary Sciences: Computational Life Sciences.

From November 2015 Dr Brogi is Associate Editor of "BMC Pharmacology & Toxicology" (IF 2.103).

From June 2016 Dr Brogi is a member of the Editorial Board of "Journal of Drug Research and Development".

From September 2016 Dr Brogi is Associate Editor of "Frontiers in Chemistry" (IF 3.782).

From October 2016 Dr Brogi is a member of the Editorial Board of "Pharmacology, Drug Development & Therapeutics (PDDT)".

From March 2017 Dr Brogi is a member of the Editorial Board of "NESSA Journal of Pharmacy and Pharmacology (NJPP)".

From May 2017 Dr Brogi is a member of the Editorial Board of "Journal of Addiction Therapy".

From July 2017 Dr Brogi is a member of the Editorial Board of "International Journal of Biopharmaceutical Sciences (IJBS)".

From September 2017 Dr Brogi is a member of the Editorial Board of "EC Microbiology".

From September 2017 Dr Brogi is Associate Editor of "Modern Approaches in Drug Designing (MADD)".

From October 2017 Dr Brogi is Associate Editor of "Virology & Immunology Journal (VIJ)".

From September 2017 Dr Brogi is a member of the Editorial Board of "International Journal of Innovative Studies in Medical Sciences (IJISMS)".

On June 2018 Dr Brogi has been selected as Guest Editor of Molecules (IF 3.060) to edit the Special Issue "Computational Approaches for Drug Discovery".

On October 2018 Dr Brogi has been selected as Referee for the Ministry of Education, University and Research (MIUR) PRIN 2017 (Projects of National Interest) program.

From November 2018 Dr Brogi is a member of the Editorial Board of "The Open Medicinal Chemistry Journal".

On February 2019 Dr Brogi has been selected as Topic Editor of Frontiers in Chemistry (IF 3.782) to edit the Research Topic "In Silico Methods for Drug Design and Discovery".

From July 2019 Dr Brogi is a member of the Editorial Board of Computation.

On April 2020 Dr Brogi has been selected as Guest Editor of Computation to edit the Special Issue "Computation to Fight SARS-CoV-2 (CoVid-19)".

On May 2020 Dr Brogi has been selected as Referee for the Academy of Finland for the call "Special funding for research into COVID-19 vaccines and pharmaceutical development Academy of Finland, Helsinki (Finland).

On September 2020 Dr Brogi has been selected as Referee from the "Ministero dell'Università e della Ricerca Italiano (MUR)" for the evaluation of the projects "Fondo Integrativo Speciale per la Ricerca (FISR) Covid-19".

On September 2020 Dr Brogi has been selected as European commission expert for the evaluation of the 2020 Marie Skłodowska-Curie Individual Fellowships (IF).

Publications

Patents:

1] PROKINETICIN 1 RECEPTOR AGONISTS AND THEIR USES

Laurent Désaubry, Günsel Canan Desaubry, Mounia Boulberdaa, Michel Kindo, Andrea Tafi, **Simone Brogi**, Kyoji Urayama, Nigel Riberio Pub. No.: WO/2012/084999 International Application No.: PCT/EP2011/073474 <http://patentscope.wipo.int/search/en/WO2012084999>

Peer-reviewed scientific articles:

2] ROLE OF HYDROGEN SULFIDE IN ENDOTHELIAL DYSFUNCTION: PATHOPHYSIOLOGY AND THERAPEUTIC APPROACHES

Valentina Citi, Alma Martelli, Era Gorica, **Simone Brogi**, Lara Testai, Vincenzo Calderone *J. Adv. Res.* **2021**, 27, 99-113 [DOI: 10.1016/j.jare.2020.05.015](https://doi.org/10.1016/j.jare.2020.05.015)

3] STRUCTURE-ACTIVITY RELATIONSHIPS STUDY OF ISOTHIOCYANATES FOR H₂S RELEASING PROPERTIES: 3-PYRIDYL-ISOTHIOCYANATE AS A NEW PROMISING CARDIOPROTECTIVE AGENT

Valentina Citi, Angela Corvino, Ferdinando Fiorino, Francesco Frecentese, Elisa Magli, Elisa Perissutti, Vincenzo Santagada, **Simone Brogi**, Lorenzo Flori, Era Gorica, Lara Testai, Alma Martelli, Vincenzo Calderone, Giuseppe Caliendo, Beatrice Severino *J. Adv. Res.* **2021**, 27, 41-53 [DOI: 10.1016/j.jare.2020.02.017](https://doi.org/10.1016/j.jare.2020.02.017)

4] NOVEL QUINOLONE-BASED POTENT AND SELECTIVE HDAC6 INHIBITORS: SYNTHESIS, MOLECULAR MODELLING STUDIES AND BIOLOGICAL INVESTIGATION

Nicola Relitti, A. Prasanth Saraswati, Giulia Chemi, Margherita Brindisi, **Simone Brogi**, Daniel Herp, Karin Schmidtkunz, Fulvio Saccoccia, Giovina Ruberti, Cristina Ulivieri, Francesca Vanni, Federica Sarno, Lucia Altucci, Stefania Lamponi, Manfred Jung, Sandra Gemma, Stefania Butini, Giuseppe Campiani *Eur. J. Med. Chem.* **2020**, Accepted [DOI: 10.1016/j.ejmech.2020.112998](https://doi.org/10.1016/j.ejmech.2020.112998)

5] CINNAMIDES TARGET *Leishmania amazonensis* ARGINASE SELECTIVELY

Edson Roberto da Silva, Júlio Abel Alfredo dos Santos Simone Come, **Simone Brogi**,* Vincenzo Calderone, Giulia Chemi, Giuseppe Campiani, Trícia Maria Ferreira de Sousa Oliveira, Thanh-Nhat Pham, Marc Pudlo, Corine Girard, Claudia do Carmo Maquiaveli *Molecules* **2020**, 25(22), 5271 [DOI: 10.3390/molecules24173061](https://doi.org/10.3390/molecules24173061)
*corresponding author

6] DEVELOPMENT OF IN VITRO CORNEAL MODELS: OPPORTUNITY FOR PHARMACOLOGICAL TESTING

Valentina Citi, Eugenia Piragine, **Simone Brogi**,* Sara Ottino, Vincenzo Calderone *Methods Protoc.* **2020**, 3(4), 74 [DOI: 10.3390/mps3040074](https://doi.org/10.3390/mps3040074) *corresponding author

7] SPIROINDOLINE-CAPPED SELECTIVE HDAC6 INHIBITORS: DESIGN, SYNTHESIS, STRUCTURAL ANALYSIS AND BIOLOGICAL EVALUATION

A. Prasanth Saraswati, Nicola Relitti, Margherita Brindisi, Jeremy D. Osko, Giulia Chemi, Stefano Federico, Alessandro Grillo, **Simone Brogi**, Niamh H. McCabe, Richard C. Turkington, Ola Ibrahim, Jeffrey O'Sullivan, Stefania Lamponi, Magda Ghanim, Vincent P. Kelly, Daniela Zisterer, Rebecca Amet, Patricia Hannon, Francesca Vanni, Cristina Ulivieri, Daniel Herp, Federica Sarno, Antonella Di Costanzo, Fulvio Saccoccia, Giovina Ruberti, Manfred Jung, Lucia Altucci, Sandra Gemma, Stefania Butini, David W. Christianson, Giuseppe Campiani *ACS Med. Chem. Lett.* **2020**, 11 (11), 2268-2276 [DOI: 10.1021/acsmmedchemlett.0c00395](https://doi.org/10.1021/acsmmedchemlett.0c00395)

8] ROLE OF HYDROGEN SULFIDE IN CARDIOVASCULAR AGEING

Lara Testai, Valentina Citi, Alma Martelli, **Simone Brogi**, Vincenzo Calderone *Pharmacol. Res.* **2020**, 160, 105125 [DOI: 10.1016/j.phrs.2020.105125](https://doi.org/10.1016/j.phrs.2020.105125)

9] AMYLOID β FIBRILS DISRUPTION BY OLEUROPEIN AGLYCONE: LONG-TIME MOLECULAR DYNAMICS SIMULATION TO GAIN INSIGHT INTO THE MECHANISM OF ACTION OF THIS POLYPHENOL FROM EXTRA VIRGIN OLIVE OIL

Simone Brogi,* Hajar Sirous, Vincenzo Calderone, Giulia Chemi *Food Funct.* **2020**, 11, 8122-8132 [DOI: 10.1039/D0FO01511C](https://doi.org/10.1039/D0FO01511C) *corresponding author

10] ANTI-INFLAMMATORY AND ANTIVIRAL ROLES OF HYDROGEN SULFIDE: RATIONALE FOR CONSIDERING H₂S-DONORS IN COVID-19 THERAPY

Valentina Citi, Alma Martelli, Vincenzo Brancaleone, Simone Brogi, Gabriel Gojon, Rosangela Montanaro, Guillermo Morales, Lara Testai, Vincenzo Calderone *Br. J. Pharmacol.* **2020**, 177(21), 4931-4941 [DOI: 10.1111/bph.15230](https://doi.org/10.1111/bph.15230)

11] MICRORNA-BASED MULTITARGET APPROACH FOR ALZHEIMER'S DISEASE: DISCOVERY OF FIRST-IN-CLASS DUAL INHIBITOR OF ACETYLCHOLINESTERASE AND MICRORNA-15B BIOGENESIS

Moustafa T. Gabr, **Simone Brogi** *J. Med. Chem.* **2020**, 63(17), 9695-9704 [DOI: 10.1021/acs.jmedchem.0c00756](https://doi.org/10.1021/acs.jmedchem.0c00756)

12] EDITORIAL: *IN SILICO* METHODS FOR DRUG DESIGN AND DISCOVERY

Simone Brogi,* Teodorico Castro Ramalho, Kamil Kuca, José L. Medina-Franco, Marian Valko *Front. Chem.* **2020**, 8, 612 [DOI: 10.3389/fchem.2020.00612](https://doi.org/10.3389/fchem.2020.00612) *corresponding author

13] THE IONOTROPIC GLUTAMATE RECEPTOR GLUA2 IN COMPLEX WITH BICYCLIC PYRIMIDINEDIONE-BASED COMPOUNDS: WHEN SMALL COMPOUND MODIFICATIONS HAVE DISTINCT EFFECTS ON BINDING INTERACTIONS

Karla Frydenvang, Darryl S. Pickering, Giridhar U. Kshirsagar, Giulia Chemi, Sandra Gemma, Desiree Sprogøe, Anne Mette Kærn, **Simone Brogi**,* Giuseppe Campiani, Stefania Butini, Jette Sandholm Kastrup *ACS Chem. Neurosci.* **2020**, 11(12), 1791–1800 [DOI: 10.1021/acschemneuro.0c00195](https://doi.org/10.1021/acschemneuro.0c00195) *corresponding author

14] OFF-TARGET ACE2 LIGANDS: POSSIBLE THERAPEUTIC OPTION FOR CoVID-19?

Simone Brogi, Vincenzo Calderone *Br. J. Clin. Pharmacol.* **2020**, 86(6), 1178-1179 [DOI: 10.1111/bcp.14343](https://doi.org/10.1111/bcp.14343)

15] DESIGN, SYNTHESIS AND BIOLOGICAL EVALUATION OF 7-SUBSTITUTED 4-PHENYL-6H-IMIDAZO[1,5-A]THIENO[3,2-F][1,4]DIAZEPINES AS SAFE ANXIOLYTIC AGENTS

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Abstracts at Scientific Conferences (Posters and Oral Presentations)

Oral presentations:

Oleuropein aglycone as a potent anti-amyloidogenic drug: a computational analysis
Simone Brogi
5th International Conference on Central Nervous System Disorders and Therapeutics
10-11 December 2020, Amsterdam, Netherlands, virtual conference due to COVID-19 lockdown worldwide

Invited Lecture "Natural Products as Source of Potential Anti-Alzheimer Drugs: the Case of Oleuropein Aglycone"
27th November 2020, Department of Chemistry of the University of Santo Tomas, Manila (Philippines)

MICROSECOND MOLECULAR DYNAMICS SIMULATION FOR INVESTIGATING THE MECHANISM OF ACTION OF OLEUROPEIN AGLYCONE AS AMYLOID β FIBRILS DISRUPTOR
Simone Brogi, Vincenzo Calderone
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Simone Brogi
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Amyloid Beta Fibrils Disruption by Oleuropein Aglycone: Investigation of the Mechanism of Action of this Polyphenol from Extra Virgin Olive Oil
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Oleuropein aglycone as amyloid β fibrils disruptor: Insight into the mechanism of action of this polyphenol from extra virgin olive oil

Simone Brogi

2nd Edition of International Nutrition Research meeting

September 10-11, 2020, Orlando, Florida, U.S.A., virtual conference due to COVID-19 lockdown worldwide

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Computational tool for predicting drug-induced liver toxicity (DILT)

Simone Brogi, Valentina Citi, Vincenzo Calderone

39th meeting of the Italian Society of Pharmacology (SIF - SOCIETÀ ITALIANA DI FARMACOLOGIA)

20th-23th November 2019, Florence, Italy

https://congresso.sifweb.org/docs/sif_cong39_programma_congresso_completo.pdf

Combination of *in silico* Approaches to Identify Fluorescent Probes Preventing PrP^{Sc} Replication in Prion Diseases

31st Molecular Modeling Workshop 2017, March 27th-29th 2017, Erlangen, Germany [https://mmws2017.mgms-](https://mmws2017.mgms-ds.de/docs/MMWS2017_final2-www_100dpi_complete.pdf)

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Molecular Modeling in Regenerative Medicine

VIII meeting "Nuove Prospettive in Chimica Farmaceutica" NPCF8 9th-11th June 2014 Parma, Italy

Human Prokineticin Receptor 1: Homology Modeling and High Throughput Docking approach to select first non-peptidic ligands

Meeting at Prestwick Chemicals 3rd April 2013 Prestwick Chemicals, Strasbourg, France

Computational Approaches in Drug Discovery

V giornata della Scuola di Dottorato in Scienze farmaceutiche-Sez. Scienze Farmaceutiche

6th October 2010 Certosa di Pontignano, Siena, Italy

Scientific Posters:

Identification of *Schistosoma mansoni* Histone Deacetylase 8 (*SmHDAC8*) Inhibitors Through Virtual Screening

Giulia Chemi, **Simone Brogi**, Margherita Brindisi, Stefania Butini, Sandra Gemma, Giuseppe Campiani

"European School of Medicinal Chemistry ESMEC, XXXIX Advanced Course of Medicinal Chemistry and Seminar for PhD students", June 30-July 4 2019, Urbino, Italy

P-2.48 Discovery of iminobenzimidazole derivatives as novel cytotoxic agents

Nora Chouha, Hassan Hammoud, **Simone Brogi**, Giuseppe Campiani, Caroline Welsch, Caroline Robert, Stéphan Vagner, Thierry Cresteil, Embarek Bentouhami, Laurent Désaubry

19th Tetrahedron Symposium 26-29 June 2018 | Riva del Garda, Lake Garda, Italy [-link-](#)

Mcl-1 Inhibitors in the Treatment of Oral Squamous Cell Carcinoma

Akella Prasanth Saraswati, **Simone Brogi**, Giulia Chemi, Margherita Brindisi, Sandra Gemma, Daniela Zisterer, Stefania Butini, Giuseppe Campiani

"European School of Medicinal Chemistry ESMEC, XXXVIII Advanced Course of Medicinal Chemistry and Seminar for PhD students", 1-5 July 2018, Urbino, Italy

Development of Novel Compounds for Improving the Sensitivity of Oral Squamous Cell Carcinoma to Chemotherapy

Tuhina Khan, Margherita Brindisi, Stefano Federico, Gloria Alfano, Giulia Chemi, **Simone Brogi**, Daniela M. Zisterer, Cristina Ulivieri, Sandra Gemma, Stefania Butini, Giuseppe Campiani

"European School of Medicinal Chemistry ESMEC, XXXVIII Advanced Course of Medicinal Chemistry and Seminar for PhD students", 1-5 July 2018, Urbino, Italy

P-39. Reverse Virtual Screening Procedure for Identifying the Target of an Antiplasmodial Hit Compound

Simone Brogi, Giulia Chemi, Stefania Butini, Margherita Brindisi, Giuseppe Campiani, Sandra Gemma, Soon Goo Lee, Joseph Jez

11th International Conference on Chemical Structures May 27-31 2018, Noordwijkerhout, The Netherlands [DOI: 10.13140/RG.2.2.18825.54887](https://doi.org/10.13140/RG.2.2.18825.54887)

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P-13. Application of 3D-QSAR Methods in Drug Design & Discovery: Two Case Studies

Giulia Chemi, **Simone Brogi**, Margherita Brindisi, Stefania Butini, Sandra Gemma, Giuseppe Campiani
11th International Conference on Chemical Structures May 27-31 2018, Noordwijkerhout, The Netherlands [DOI: 10.13140/RG.2.2.24697.57448](https://doi.org/10.13140/RG.2.2.24697.57448)
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Computational studies of NBDHEX as *Giardia duodenalis* thioredoxin reductase (gTrxR) inhibitor
Giulia Chemi, **Simone Brogi**, Annarita Fiorillo, Stefania Butini, Marco Dalle, Andrea Ilari, Sandra Gemma, Giuseppe Campiani

OPENING OF THE EMORY@UNISI SUMMER SCHOOL + Department Biotechnology Chemistry
& Pharmacy Research Day; May 30th 2018; Aula 14 – Polo Scientifico S. Miniato, Siena, Italy
<https://www.dbcf.unisi.it/en/research/cooperation/emoryunisi-2018>

3D-QSAR methods in Drug Design & Discovery

Giulia Chemi, **Simone Brogi**, Margherita Brindisi, Stefania Butini, Sandra Gemma, Giuseppe Campiani
OPENING OF THE EMORY@UNISI SUMMER SCHOOL + Department Biotechnology Chemistry
& Pharmacy Research Day; May 30th 2018; Aula 14 – Polo Scientifico S. Miniato, Siena, Italy
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Synthèse et caractérisation de nouveaux dérivés d'iminobenzimidazoles pour leur cytotoxicité sur des cellules cancéreuses

Nora Chouha, Hassan Hammoud, Simone Brogi, Giuseppe Campiani, Caroline Welsch, Caroline Robert, Stéphan Vagner, Thierry Cresteil, Embarek Bentouhami, Laurent Désaubry
Cinquième Colloque International De Chimie, CIC-5; Batna (Algeria), 04-06 December 2018.

Virtual Screening and Biological Characterization of New Multi-Stage HDAC Inhibitors with Activity Against *Schistosoma mansoni*

Margherita Brindisi, Fulvio Saccoccia, Roberto Gimmelli, **Simone Brogi**, Alessandra Guidi, Sandra Gemma, Giuseppe Campiani, Giovina Ruberti
Malaria and Neglected Parasitic Diseases: Core Science and Perspectives
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3D-QSAR methods in Drug Design & Discovery

Giulia Chemi, **Simone Brogi**, Margherita Brindisi, Stefania Butini, Sandra Gemma, Giuseppe Campiani
Giornata della Scuola di Dottorato in Scienze chimiche e farmaceutiche 2017
1st December 2017 Università degli Studi di Siena, Siena, Italy

Computational studies of NBDHEX as *Giardia duodenalis* thioredoxin reductase (gTrxR) inhibitor

Giulia Chemi, **Simone Brogi**, Annarita Fiorillo, Stefania Butini, Marco Dalle, Andrea Ilari, Sandra Gemma, Giuseppe Campiani
31st Molecular Modeling Workshop 2017, March 27th-29th 2017, Erlangen, Germany
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13th Convention of Investigators in Cystic Fibrosis, Garda, Verona, Italy 26-28 November 2015
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Abstract 411: Discovery and Cardioprotective Effects of the First Non-peptide Agonists of Prokineticin Receptor-1
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Circ. Res. **2015**;117:A411
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Development of novel cyclic peptides as pro-apoptotic agents
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Design and synthesis of novel PFSUB1 inhibitors
Gloria Alfano, **Simone Brogi**, Margherita Brindisi, Michael J. Blackman, Stefania Butini, Sandra Gemma; XXIII NMMC & 9th NPCF - September 6-9 2015, Salerno (Italy)

Synthesis of novel fatty acid amide hydrolase inhibitors as potential therapeutic agents for epileptic disorders
Alessandro Grillo, **Simone Brogi**, Margherita Brindisi, Sandra Gemma, Mauro Maccarrone, Stefania Butini; XXIII NMMC & 9th NPCF - September 6-9 2015, Salerno (Italy)

Development of novel potential antimalarial agents characterized by an endoperoxide system
Luisa Di Cerbo, Margherita Brindisi, **Simone Brogi**, Stefania Butini, Donatella Taramelli, Sandra Gemma; XXIII NMMC & 9th NPCF - September 6-9 2015, Salerno (Italy)

MMV Malaria Box: Development of Novel Heterocyclic Compounds to Treat Parasitic Diseases Alessandra Vallone, Margherita Brindisi, Stefania Butini, **Simone Brogi**, Donatella Taramelli, Sandra Gemma; XXIII NMMC & 9th NPCF - September 6-9 2015, Salerno (Italy)

Design and synthesis of novel HDAC6 inhibitors
Caterina Cavella, Stefania Butini, Sandra Gemma, **Simone Brogi**, Lucia Altucci, Margherita Brindisi; XXIII NMMC & 9th NPCF - September 6-9 2015, Salerno (Italy)

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Nicola Relitti, Margherita Brindisi, **Simone Brogi**, Stefania Butini, Ettore Novellino, Andrea Ilari, Sandra Gemma; XXIII NMMC & 9th NPCF - September 6-9 2015, Salerno (Italy)

Pharmacophore Identification and Virtual Screening for MCF-7 cell line inhibitors
IV giornata della Scuola di Dottorato in Scienze Farmaceutiche-Sez. Scienze Farmaceutiche
4th November 2009 Certosa di Pontignano, Siena, Italy

CO-01-004: Discovery and Cardioprotective Effects of the First Non-Peptide Agonists of the G-Protein-Coupled Prokineticin Receptor-1
Adeline Gasser, **Simone Brogi**, Kyoji Urayama, Toshishide Nishi, Hitoshi Kurose, Andrea Tafi, Laurent Désaubry, Canan G. Nebigil *Acta Physiol.* Issue supplements S700 **2015**, 214, 5 DOI:10.1111/apha.12522
Special Issue: Abstracts of the 1st Congress of Physiology and Integrative Biology (CPBI) and 84th Congress of French Physiological Society (SFP), 4th-6th May 2015, Strasbourg, France

0365: Non-Peptidic Prokineticin Receptor 1 Agonist as a Novel Cardioprotective Therapeutic
Adeline Gasser, Toshishide Nishi, Thu Lan Nguyen, Kyoji Urayama, Hitoshi Kurose, Marine Charavin, **Simone Brogi**, Andrea Tafi, Laurent Désaubry, Canan Nebigil *Arch. Cardiovasc. Dis. Supplements* **2014**, 6, Supp. 1, 21-22
DOI: 10.1016/S1878-6480(14)71323-0
Printemps de la Cardiologie, 24th-25th April 2014 Strasbourg, France

Memberships

Targeting the *P. falciparum* erythrocyte life cycle for the development of novel antimalarials
CIRM (Consorzio Interuniversitario di Ricerche sulla Malaria) meeting 2013 Perugia, Italy

Targeting Heme Detoxification Process for the Development of Structurally Diverse Antimalarials: Focus on Novel Peroxides and Chloroquine/Clotrimazole Hybrids

COST annual meeting "New Drugs for Neglected Diseases" 2011 Università degli Studi di Modena e Reggio Emilia, Modena, Italy <http://www.cost-cm0801-2011.unimore.it/BOA.pdf>

Program PHASE in ligand-based pharmacophore model generation and 3D- database searching for MCF-7 cell line inhibitors

III meeting "Nuove Prospettive in Chimica Farmaceutica" February 2009 il Ciocco Castelvevchio Pascoli, Lucca, Italy <http://www.npcf3.farm.unipi.it/atti-del-meeting pg.71>
<http://www.farm.unipi.it/npcf3/poster/BrogiSimone.pdf>

Computational Approach to detect novel MCF-7 cell line inhibitors

III giornata della Scuola di Dottorato in Scienze Farmaceutiche-Sez. Scienze Farmaceutiche
22nd October 2008 Certosa di Pontignano, Siena, Italy <http://publicationlist.org/simonebrogi1976>

Associate Editor of BMC Pharmacology & Toxicology (IF 2.103) (2015 - to date)

Editorial Board Member of "BMC Pharmacology & Toxicology" Drug design, discovery and delivery section
<http://bmcparmacoltoxcol.biomedcentral.com/about/editorial-board>

Associate Editor of Frontiers in Chemistry (IF 3.782) (2016 - to date)

Editorial Board Member of "Frontiers in Chemistry" Medicinal and Pharmaceutical Chemistry section
<http://journal.frontiersin.org/journal/chemistry#editorial-board>

Associate Editor of Modern Approaches in Drug Designing (MADD) (2017-to date)

Editorial Board Member of "Modern Approaches in Drug Designing (MADD)"
<http://crimsonpublishers.com/madd/editorial-board.php>

Associate Editor of Virology & Immunology Journal (VIJ) (2017-to date)

Editorial Board Member of "Virology & Immunology Journal (VIJ)" <https://medwinpublishers.com/VIJ/editorial-board.php#>

Guest Editor of Molecules (IF 3.060) (June 2018)

Special Issue "Computational Approaches in Drug Discovery"
http://www.mdpi.com/journal/molecules/special_issues/Computational_Approaches_for_Drug_Discovery

Topic Editor of Frontiers in Chemistry (IF 3.782) (February 2019)

Research Topic "In Silico Methods for Drug Design and Discovery"
<https://www.frontiersin.org/research-topics/10032/in-silico-methods-for-drug-design-and-discovery>

Guest Editor of Computation (April 2020)

Special Issue "Computation to Fight SARS-CoV-2 (CoVid-19)"
https://www.mdpi.com/journal/computation/special_issues/computation_CoVid_19

Editorial Board Member of "Journal of Drug Research and Development" (2016 – to date)

<https://sciforschenonline.org/journals/drug/editorial-board.php>

Editorial Board Member of "Pharmacology, Drug Development & Therapeutics (PDDT)" (2016 - to date)

http://oatext.com/Pharmacology-Drug-Development-Therapeutics-PDDT.php#Editorial_Board

Editorial Board Member of "NESSA Journal of Pharmacy and Pharmacology (NJPP)" (2017 - to date)

<http://nessapublishers.com/view-board-member.php?id=248/Simone-Brogi#axzz4ebI9tS4h>

Editorial Board Member of "Journal of Addiction Therapy" (2017-to date)

<http://scifed.com/journal-of-addiction-therapy/editorial-board.php>

Editorial Board Member of "International Journal of Innovative Studies in Medical Sciences (IJISMS)" (2017-to date)

<http://ijisms.com/editorial-board/>

Editorial Board Member of "International Journal of Biopharmaceutical Sciences (IJBS)" (2017-to date)

<http://www.boffinaccess.com/journals/biopharmaceutical-sciences/editorial-board.php>

Editorial Board Member of "EC Microbiology" (2017-to date)

<https://www.econicon.com/microbiology-editorial-panel.php>

Editorial Board Member of "The Open Medicinal Chemistry Journal" (2018-to date)

<https://openmedicinalchemistryjournal.com/editorial-board.php>

Editorial Board Member of Computation (2019-to date)

<https://www.mdpi.com/journal/computation/editors>

Review Editor of Frontiers in Chemistry (2014 - 2016)

Editorial Board Member of "Frontiers in Chemistry" Medicinal and Pharmaceutical Chemistry section

<http://journal.frontiersin.org/journal/chemistry#editorial-board>

Italian Society of Pharmacology (S.I.F.)

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Washington, DC 20005-1020 USA

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91052 Erlangen, Germany

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