STEFANO DI STEFANO
Curriculum Vitae

Part I – General Information

Full Name	Stefano Di Stefano
Date of Birth	07 / 01 / 1972
Place of Birth	Roma
Citizenship	Italiana
E-mail	stefano.distefano@uniroma1.it
Spoken Languages	Italian, English

Part II – Education

Type	Year	Institution	Notes (Degree, Experience,…)
Maturità Scientifica High School (5 years)	1990	L.S. “C. Cavour" di Roma	Full marks (60 / 60)
Laurea in Chimica (Master in Chemistry)	1997	Università di Roma La Sapienza	Full marks (110/110 e Lode)
Qualification for the Chemist profession	1997		
Ranked 1° at the competition for the admission to the PhD in Chemical Sciences, cycle XIII (1997-2000) at Università di Roma “La Sapienza”	1997-2000	Università di Roma La Sapienza	
PhD in Chemical Sciences	1/12/ 2000	Università di Roma La Sapienza	PhD thesis title: *Supramolecular Catalysts for Amide and Ester Cleavage*

Part III – Appointments

III A – Academic Appointments

Start	End	Institution	Position
2001	2005	Università di Roma La Sapienza	Holder of one-year scientific collaboration contracts
2005	2006	Università di Roma La Sapienza	Winner of one-year University grant (scholarship)
2006	2007	Università di Roma La Sapienza	Holder of a 6 months scientific collaboration contract
2006		Università di Roma La Sapienza	Ranked 1° at the competition for 2 positions of "Ricercatore Universitario" in Organic Chemistry (CHIM 06) held on 5, 6 e 7 December 2006.
2007	2010	Università di Roma La Sapienza	Ricercatore Universitario
2010	2019	Università di Roma La Sapienza	Ricercatore Universitario Confermato
2017	2023		Qualified for the role of "Professore di II fascia" for the "Settore Concorsuale 03/C1, SSD CHIM/06", Organic Chemistry (Associate Professor).
2018		Università di Roma La Sapienza	Winner of a permanent position of "Professore Associato" of Organic Chemistry (CHIM/06), 4 June 2018.
2019	2022	Università di Roma La Sapienza	"Professore Associato" of Organic Chemistry (CHIM/06).
2020	2029		Qualified for the role of "Professore di I fascia" for the "Settore Concorsuale 03/C1, SSD CHIM/06", Organic Chemistry (Full Professor).
2022		Università di Roma La Sapienza	Winner of a permanent position of "Professore Ordinario" (Full Professor) of Organic Chemistry (CHIM/06), 7 February 2022.
2022	**currently**	**Università di Roma La Sapienza**	**"Professore Ordinario" (Full Professor) of Organic Chemistry (CHIM/06).**

III B – Other Academic Appointments

Start	End	Institution	Position
March 2000	April 2000	Universidad Autonoma de Madrid, Spain (laboratories of Prof. Javier de Mendoza)	PhD visiting student (mission funded by CNR in the frame of "Short Term Mobility" program and by COST D11 as a "Short Term Mission" in the frame of a European Project on Supramolecular Chemistry)
October 2002		Albrecht-Christian Universität di Kiel, Germany (laboratories of Prof. Ulrich Lüning)	Visiting scientist (mission funded by COST D11 as a "Short Term Mission" in the frame of a European Project on Supramolecular Chemistry)

2005	2006	Dipartimento di Chimica, Facoltà SS.MM.FF.NN, Università di Roma "La Sapienza"	Winner of a university grant (scholarship) for the assistance to the students of Organic Chemistry
July 2016	July 2016	European Synchrotron Radiation Facility (ESRF) di Grenoble, France	Visiting Scientist. Execution of the Project: "Structure and reactivity of non-heme high valent iron peroxo complexes"
February 2018	February 2018	European Synchrotron Radiation Facility (ESRF) di Grenoble, France	Visiting Scientist. Execution of the Project: "Following the ms timescale evolution of redox processes in iron catalysts by simultaneous X-ray and UV/Vis absorption spectroscopy"

III C – Other non-Academic Appointments

Start	End	Institution	Position
December 2000	June 2001	Merck Sharp & Dohme	Clinical Monitor (activity in the field of clinical research, phase IV)
2004	2005	CHEMI spa	Scientific Advisor (a program concerning sulfated polysaccharides. In particular I was employed in the identification of unknown molecular species through HPLC/HRMS-ESI and HPLC/MS/MS-ESI analyses).
2006	2006	Istituto Biochimico Italiano (IBI)	Scientific Advisor (a program concerning the identification of unknown molecular species through HPLC/MS-ESI analysis).
2010	2011	EDISES (publishing house)	Translator from English to Italian of chapters 24, 25 e 26 of the Book "Organic Chemistry" by P. Y. Bruice (2010).
2017	2019	Beaumont Italia s.r.l.	Scientific Advisor (a program concerning the study of organic anticorrosive agents for cooling systems. I was employed in ^{1}H-NMR and ESI-Mass spectroscopy based investigations).

Part IV – Teaching experience

IV A – Lectures and Courses in Academic Institutions

Year	Institution	Lecture/Course
Academic years: 2005/2006, 2006/2007, 2007/2008, 2008/2009	"Prima Facoltà" of "Medicina e Chirurgia", Università di Roma La Sapienza	"Chimica degli Alimenti" for "Dietista" Bechelor (2 cfu for academic years 2005/2006, 2006/2007, 2007/2008, and 3 cfu for academic year 2008/2009)
Academic year: 2006/2007	Faculty of Science, Università di Roma Tor Vergata	"Chimica Organica" for the Bechelor degree in "Ecologia" (5 cfu)
Academic years: 2009/2010, 2010/2011, 2011/2012	Faculty of Science, Università di Roma La Sapienza	"Chimica Organica" for the Bechelor degree in "Scienze Naturali" (6 cfu)
Academic year: 2016/2017	PhD in Chemical Sciences, Università di Roma La Sapienza	"Chimica Supramolecolare" (6 cfu) for the sudents of the PhD school in Chemical Sciences
Academic years: 2012/2013, 2013/2014, 2014/2015, 2015/2016, 2016/2017, 2017/2018, 2018/2019, 2019/2020, 2020/2021 2021/2022 2022/2023 2023/2024	Faculty of Science, Università di Roma La Sapienza	"Chimica Organica IV" (9 cfu) for the Master degree in "Chimica"
Academic year: 2018/2019, 2019/2020, 2020/2021 2021/2022	Faculty of Science, Università di Roma La Sapienza	"Chimica Organica II con Laboratorio" (9 cfu) for the Bachelor degree in "Chimica"
Academic year: 2021/2022 2022/2023 2023/2024	Faculty of Science, Università di Roma La Sapienza	"Chimica Organica II" (6 cfu) for the Bachelor degree in "Scienze Chimiche"

IV B – Supervisor of Master Thesis Works carried out at Università di Roma La Sapienza

Acad. Year	Title of the **Chemistry master thesis works**	Student
2009/2010	*Studio di Sistemi di Macrociclizzazione sotto Controllo Termodinamico*	Josè Augusto Berrocal
2009/2010	*Sviluppo di nano particelle funzionalizzate con metallo-catalizzatori*	Maria Luisa Aufiero
2010 / 2011	*La Transamminazione: un versatile strumento di scambio e riconoscimento molecolare?*	Maria Ciaccia
2010 / 2011	*Studi dinamici combinatori basati sull'inversione di solfossidi*	Leonardo Maugeri
2010 / 2011	*Sintesi di derivati calix[4]arenici bifunzionali. Reattività intramolecolare di funzioni in posizione 1,3-distale*	Marzia Galli
2011 / 2012	*Studio degli effetti elettronici e strutturali nell'ossidazione di composti alifatici da parte di complessi non-eme del ferro*	Giorgio Olivo
2012 / 2013	*Studio delle reazioni di transimminazione e metatesi di immine su substrati aromatici*	Silvia Pilati
2012 / 2013	*Sintesi di unità monomeriche per polimerizzazioni supramolecolari*	Federica Laurenzi
2013 / 2014	*Progettazione e sintesi di complessi non-eme del ferro e del manganese per l'ossidazione di legami C-H non attivati*	Teresina Ambrosio
2014 / 2015	*Meccanismo d'azione di complessi imminici del ferro non eme*	Martina Nardi
2014 / 2015	*Sintesi e studio del funzionamento di un legante amminico con siti di riconoscimento per la complessazione del ferro (II)*	Giulio Farinelli
2014 / 2015	*Sintesi di unità monomeriche cicliche per l'ottenimento di aggregati supramolecolari*	Simone Albano
2014 / 2015	*Formazione statistica di catenani in processi di ciclooligomerizzazione*	Francesca Manni
2014 / 2015	*Sintesi di Complessi Tetra e Pentadentati del Ferro per Studi di Reattività e Attività Catalitica in Reazioni di Ossidazione*	Valeria Dantignana
2015 / 2016	*Un carburante per il funzionamento autonomo di macchine molecolari*	Chiara Biagini
2015 / 2016	*Riconoscimento chirale nella transimminazione di derivati diimminici di calix[4]areni con ammine chirali*	Valentina Armiento
2015 / 2016	*Utilizzo di un complesso imminico del Fe(II) come catalizzatore dell'ossidazione ecosostenibile della funzione alcolica*	Simone Giosia
2015 / 2016	*Studio dell'effetto della concatenazione nella formazione di un gel supramolecolare*	Alessio Fantozzi
2015 / 2016	*Sintesi di carburanti chimici per lo studio di movimenti molecolari*	Rachele Caruso
2016 / 2017	*Un complesso imminico del ferro, generato in situ da precursori commerciali, catalizza l'ossidazione di legami C-H aromatici*	Giorgio Capocasa
2017 / 2018	*Rilascio fotoindotto di un carburante chimico per macchine molecolari acido-base*	Flaminia Di Pietri
2017/2018	*Sintesi parziale di un catalizzatore supramolecolari per C-H ossidazioni e dei relativi substrati amminici insature*	Simone Restante

2018/2019	*Studi di applicabilità di fuel decarbossilativi i sistemi complessi*	Flavia Cenesi
2018/2019	*Sintesi di un catalizzatore supramolecolare autoassemblante*	Federico Frateloreto
2018/2019	*Catalizzatore supramolecolare auto-assemblante per ossidazioni selettive di composti aromatici*	Marika Di Berto Mancini
2018/2019	*Sintesi e studio di componenti per una macchina molecolare con movimento autonomo*	Valerio Cataldi
2018/2019	*Studio sul rilascio controllato di fuel chimico per il funzionamento autonomo di switch acido-base*	Daniele Del Giudice
2018/2019	*Inibitori Fotomodulabili per un Catalizzatore Supramolecolare*	Luis Claudio Pantaleone
2018/2019	*Studio sull'induzione temporanea di chiralità su bifenili*	Gabriele Cianfoni
2019/2020	*Controllo della conformazione della struttura calix[4]arenica mediante fuels chimici*	Emanuele Spatola
2019/2020	*Studio di un organocatalizzatore supramolecolare per la funzionalizzazione di idrocarburi e sintesi di un suo modello*	Michela Guida
2019/2020	*Studio degli effetti dell'ingombro sterico sulla reattività di un catalizzatore a base di ferro non-eme attivo nelle C-H ossidazioni*	Karim Abdel Hady
2020/2021	*pH controllabile nel tempo: la decarbossilazione dell'acido nitroacetico permette l'ascesa del pH ad un valore definito*	Matteo Valentini
2020/2021	*Metodi catalitici per epossidazioni di alcheni e idrossilazioni di legami C-H alifatici*	Roberto Taberini
2020/2021	*Sintesi di un complesso penta-coordinato del ferro non-eme decorato con un etere corona*	Alessandro Fagnano
2020/2021	*Sintesi di substrati bifenilici e controllo della loro conformazione mediante l'uso di fuel chimici*	Aurora Murru
2021/2022	*Chimica dinamica covalente dissipativa basata su reazioni di transimminazione*	Gabriele Melchiorre
2021/2022	*Studio sistematico della decarbossilazione dell'acido 2-ciano-2-fenilpropanoico promossa da ammine*	Chiara Mentesana
2021/2022	*Reazioni di ciclizzazione in ambiente confinato*	Alessandra Procopio
2021/2022	*Sintesi e caratterizzazione di un catalizzatore a base di ferro non-eme per reazioni selettive di ossidazione di legami C-H*	Roberta Paoloni
2021/2022	*Studio sul controllo temporale dell'attività catalitica di un calix[4]arene mediante l'uso di un fuel chimico.*	Benedetta Malvagna
2022/2023	*Traslocazione di ioni tra eteri corona indotta da stimolo chimico e radiativo*	Matteo Conti
2022/2023	*Applicazioni della Chimica dissipativa di Immine*	Francesco Ranieri
2022/2023	*Chimica dinamica covalente dissipativa applicata all'assemblaggio transiente di nanoparticelle d'oro*	Giulia Ziaco
2022/2023	*Reazioni di transimminazione in sistemi polimerici guidati dal fuel*	Aurora Patrizi
2023/2024	*Trasduzione del segnale che permette il controllo temporale del potenziale di una cella a concentrazione guidata dalla decarbossilazione di un acido carbossilico attivato*	Stefania Correale Cavallari
2023/2024	*Studio di fattibilità per la sintesi one-pot di un Rotaxano.*	Alessandra Parisella

IV C – Supervisor of **PhD thesis works** in Chemical Sciences carried out at Università di Roma La Sapienza

Cycle	Title of the PhD thesis works	Student
XXVI	*Quantitative features of intramolecular reactions*	Josè Augusto Berrocal
XXVII	*Mechanisms and Applications of Imine Chemistry*	Maria Ciaccia
XXVIII	*Nonheme iron complexes as catalysts for non-activated C-H oxidation reactions*	Giorgio Olivo
XXXI	*On Some Adventure in the Field of Supramolecular Chemistry*	Simone Albano
XXXII	*Decarboxylative Fuels for the Operation of Molecular Machines*	Chiara Biagini
XXXIII	*A Supramolecular Approach to Hydrocarbon Functionalization*	Giorgio Capocasa
XXXV	*Activated Carboxylic Acids for the Operation of pH-Responsive Supramolecular Systems*	Daniele Del Giudice
XXXV	*Supramolecular Systems Involving Transition Metals: Catalysis and Translocation*	Federico Frateloreto
XXXVI	*A Diversified Journey Through Typical and New Supramolecular Scaffolds: Calixarenes, Cyclodextrins and Cryptands*	Emanuele Spatola
XXXVII	Currently ongoing	Matteo Valentini
XXXVII	Currently ongoing	Alessandro Fagnano
XXXVIII	Currently ongoing	Gabriele Melchiorre
XXXIX	Currently ongoing	Francesco Ranieri

IV D – Supervisor of **Post Doc Positions** at Università di Roma La Sapienza

2019/2020	*Sintesi e Studio di catalizzatori supramolecolari per le C-H ossidazioni*	Carla Sappino
2021	*Catalizzatori supramolecolari per C-H attivazione*	Giorgio Olivo
2023/2024	*Sistemi redox dissipativi* (Currently ongoing)	Giorgio Capocasa
2024	*Dissipative Systems Driven by the Decarboxylation of Fuel Acids* (Currently ongoing)	Martina De Angelis

Part V - Awards and Honors

V A Awards and Honors for **Research**

Year	Title
2020	National Scientific Research Prize assigned by the *Società Chimica Italiana* (*Italian Chemical Society*), Division of Organic Chemistry. The Prize is called "**PREMIO ALLA RICERCA SCIENTIFICA IN CHIMICA ORGANICA NEI SUOI ASPETTI METODOLOGICI**". It is a Prize assigned every year to a researcher who has distinguished her/himself in the field of physical organic chemistry. The motivation is the following: "PER L'ORIGINALITA' E LA VERSATILITA' DEI SUOI CONTRIBUTI ALLA CHIMICA SUPRAMOLECOLARE CHE VANNO DALLO STUDIO DEI CARBURANTI ARTIFICIALI PER IL MOVIMENTO DI MACCHINE MOLECOLARI, ALLA CHIMICA DINAMICA COMBINATORIA E ALLA CATALISI A BASE DI COMPLESSI DI FE A MN PER L'OSSIDAZIONE DI SUBSTRATI ORGANICI" (For the originality and versatility of his contributions, which range from the studies on chemical fuels for the motions of molecular machines to dynamic combinatorial chemistry and to the catalysis of organic compound oxidations based on Fe and Mn complexes).

V B Awards and Honors for **Teaching**

Year	Title
2014	Award for the teaching of Chimica Organica IV: on 19 November 2014 I was the recipient of a prize for "**INSEGNAMENTO UNIVERSITARIO ECCELLENTE**" which is assigned by the Dean of the Faculty of Science of University of Rome "La Sapienza" for the teachings given during the previous academic year. The prize is assigned to the 5% of the teachers of the Faculty who distinguished in the teaching. It is assigned every year and this was the first edition.
2017	Award for the teaching of Chimica Organica IV: on 29 March 2017 I was the recipient of a prize for "**INSEGNAMENTO UNIVERSITARIO ECCELLENTE**" which is assigned by the Dean of the Faculty of Science of University of Rome "La Sapienza" for the teachings given during the previous academic year. The prize is assigned to the 5% of the teachers of the Faculty who distinguished in the teaching. It is assigned every year and this was the third edition.
2018	Award for the teaching of Chimica Organica IV: on 13 December 2018 I was the recipient of a prize for "**INSEGNAMENTO UNIVERSITARIO ECCELLENTE**" which is assigned by the Dean of the Faculty of Science of University of Rome "La Sapienza" for the teachings given during the previous academic year. The prize is assigned to the 5% of the teachers of the Faculty who distinguished in the teaching. It is assigned every year and this was the fifth edition.
2021	On 25 May 2021 I was the recipient of a prize for "**INSEGNAMENTO UNIVERSITARIO ECCELLENTE**" which is assigned by the Dean of the Faculty of Science of University of Rome "La Sapienza" for the teachings given during the previous academic year (Chimica Organica II e Chimica Organiva IV). In this case I was within the three most appreciated teachers of the Faculty of Science and the first most appreciated in the Chemistry Department. The prize is assigned every year and this was the seventh edition.

V C Editorial Merit Notes

Year	Title
2017	The following article has been labeled as **HOT ARTICLE** by the Editor "Direct Hydroxylation of Benzene and Aromatics with H_2O_2 Catalyzed by a Self-Assembled Iron Complex: Evidence for a Metal-based Mechanism", G. Capocasa, G. Olivo, A. Barbieri, O. Lanzalunga, S. Di Stefano*, *Cat. Sci. & Techn.*, **2017**, *7*, 5677–5686.
2018	The following article belongs to the **EDITOR'S CHOICE COLLECTION** of *Chem. Sci.* "Variations in the Fuel Structure Control the Rate of the Back and Forth Motions of a Chemically Fuelled Molecular Switch", C. Biagini, S. Albano, R. Caruso, L. Mandolini, J. A. Berrocal, S. Di Stefano*, *Chem. Sci.* **2018**, *9*, 181-188.
2018	The following article has been labeled as **HOT PAPER** by the Editor "Photoinduced Release of a Chemical Fuel for Acid-Base Operated Molecular Machines", C. Biagini, F. Di Pietri, L. Mandolini, O. Lanzalunga, S. Di Stefano*, *Chem. Eur. J.*, **2018**, *24*, 10122-10127. Furthermore the article has been **spotlighted** in *Angew. Chem. Int. Ed.*, **2018**, *57*, 10006-10009.
2019	The following article has been labeled as **HOT PAPER** by the Editor "Dissipative Catalysis with a Molecular Machine" C. Biagini, S. D. P. Fielden, D. A. Leigh*, F. Schaufelberger, S. Di Stefano, D. Thomas, *Angew. Chem. Int. Ed.*, **2019**, *58*, 9876-9880. Furthermore the paper received the ***First Cover*** in *Angew. Chem. Int. Ed.*, and resulted to be in the ***Top Downloaded list of 2018-2019***.
2019	The following article has been labeled as **HOT ARTICLE** by the Editor "The Canonical Behavior of the Entropic Component of Thermodynamic Effective Molarity. An Attempt at Unifying Covalent and Noncovalent Cyclizations" S. Di Stefano*, L. Mandolini*, *Phys. Chem. Chem. Phys.*, **2019**, 21, 955-987.
2020	The following article has been labeled as **VERY IMPORTANT PAPER** (**VIP**) by the Editor "Supramolecular Catalysts Featuring Crown Ethers as Recognition Units" S. Di Stefano*, G. Capocasa, L. Mandolini*, *Eur. J. Org. Chem.*, **2020**, 3340–3350.
2020	The following article has been included in the **HOT ARTICLE COLLECTION** by the Editor "Controlling the Liberation Rate of the In Situ Release of a Chemical Fuel for the Operationally Autonomous Motions of Molecular Machines" C. Biagini, G. Capocasa, D. Del Giudice, V. Cataldi, L. Mandolini, S. Di Stefano*, *Org. Biomol. Chem.*, **2020**, *18*, 3867-3873.
2020	The following article has been labeled as **VERY IMPORTANT PAPER** (**VIP**) by the Editor "Predictable selectivity in remote C-H Oxidation of steroids: analysis of substrate binding mode" G. Olivo*, G. Capocasa, B. Ticconi, O. Lanzalunga, S. Di Stefano*, M. Costas*, *Angew. Chem. Int. Ed.*, **2020**, 59, 12703–12708.
2022	The following article has been included in the **HOT ARTICLE COLLECTION** by the Editor "Dissipative Control of the Fluorescence of a 1,3-Dipyrenyl Calix[4]arene in the Cone Conformation" E. Spatola, F. Rispoli, D. Del Giudice, R. Cacciapaglia, A. Casnati, L. Marchiò, L. Baldini*, S. Di Stefano*, *Org. Biomol. Chem.*, **2022,** *20*, 132–138.
2022	The following article has been labeled as **HOT PAPER** by the Editor "Dissipative Dynamic Covalent Chemistry (DDCvC) Based on the Transimination Reaction", D. Del Giudice, M. Valentini, G. Melchiorre, E. Spatola, S. Di Stefano*, *Chem. Eur. J.*, **2022**, *28*, e202200685.
2022	The following article has been labeled as **VERY IMPORTANT PAPER** (**VIP**) by the Editor "Chemical Tools for the Temporal Control of Water Solution pH and Applications in Dissipative Systems" D. Del Giudice, F. Frateloreto, C. Sappino, S. Di Stefano*, *Eur. J. Org. Chem.* **2022**, e202200407.
2022	The following article has been labeled as **VERY IMPORTANT PAPER** (**VIP**) by the Editor "Dissipative Dynamic Libraries (DDL) and Dissipative Dynamic Combinatorial Chemistry (DDCC)" D. Del Giudice, E. Spatola, M. Valentini, G. Ercolani,* S. Di Stefano*, *ChemSystemsChem* **2022**, e20220002.

2024	The following article has been labeled as **HOT PAPER** by the Editor "Signal Transduction Allows Temporal Control of the Potential of a Concentration Cell Driven by the Decarboxylation of an Activated Carboxylic Acid" G. Capocasa*, F. Frateloreto, S. Correale Cavallari, M. Valentini, O. Lanzalunga, S. Di Stefano*, *Chem. Eur. J.*, **2024**, *30*, e202303897.
2024	The following article has been labeled as **HOT PAPER** by the Editor "Proximity Effects on the Reactivity of a Nonheme Iron (IV) Oxo Complex in C-H Oxidation" A. Fagnano, F. Frateloreto, R. Paoloni, C. Sappino, O. Lanzalunga, M. Costas*, S. Di Stefano*, G. Olivo*, *Angew. Chem. Int. Ed.*, **2024**, *63*, e202401694.

Part VI - Funding Information

VI A grants as **Principal Investigator**

Year	Title	Program	Grant value
2008	*"Il ruolo del solvente nella struttura e reattività di sistemi dinamici: teoria ed esperimenti*"	"Bando per Finanziamento di Ateneo Federato di Scienza e Tecnologia, per giovani ricercatori AST 2008, La Sapienza"	10,000 euro
2009	*"Solfossidi in chimica dinamica combinatoria: studi sperimentali e teorici*"	"Bando per Finanziamento di Ateneo Federato di Scienza e Tecnologia, AST 2009, La Sapienza"	6,070 euro
2010	*"Utilizzo della reazione di metatesi per la verifica della teoria sugli equilibri anello-anello*"	"Bando Finanziamento Universitario 2010, La Sapienza"	15,000 euro
2011	*"Formazione di basi di Schiff come strumento per il riconoscimento del substrato da parte di catalizzatori supramolecolari basati sulla struttura calixarenica*"	"Bando Finanziamento Universitario 2011, La Sapienza"	8,000 euro
2012	*"Reazioni di Transimminazione e di Metatesi di Immine in Soventi non Acquosi*"	"Bando Finanziamento Universitario 2012, La Sapienza"	2,000 euro
2014	*"Sudio di Materiali Polimerici Basati su Interazioni Covalenti e Supramolecolari tra Strutture Molecolari Cicliche Interbloccate (Catenani e Rotassani) e non*"	"Bando Finanziamento Universitario 2014, La Sapienza"	5,000 euro
2017	--------	"Finanziamento annuale individuale delle attività base di ricerca", grant from MIUR	3,000 euro
2017-2018	*"NMR and ESI TOF analysis of surfactant samples"*	Advisor for Beaumont Italia srl "Contoterzi" contract	15,000 euro
2018	*"Non-heme iron and manganese supramolecular catalysts for the oxidation of aliphatic and aromatic C-H bonds"*	"Grande Progetto Universitario" in the frame of "Bando Ricerca Scientifica - Anno 2018, La Sapienza", DR n.1349/2018 prot. n.43892 del 24/05/2018	54,800 euro
2019	*"Controllo del Movimento Autonomo di Macchine Molecolari Acido-Base"*	"Bando Finanziamento Universitario 2019, La Sapienza" protocollo n. RP11916B45B22987	4,000 euro
2020	*"Macchine Molecolari Basate sulla Struttura Calix[4]arenica"*	"Bando Finanziamento Universitario 2020, La Sapienza" n. protocollo RM12017293222D84	15,000 euro
2022	"*ORIONE (laboratORIO analisi Nmr per struttura e purEzza campioni)*"	Modernization of a NMR Bruker 400 MHz instrument. 376.800.22 euro	376,800 euro

2022	*"Dissipative Systems Driven by the Decarboxylation of Fuel Acids"*	"Progetti di Ricerca Grandi - Progetti Grandi" in the frame of "Bando Ricerca 2022 - Anno 2022, La Sapienza", prot. RG1221815C85AF91.	70,890 euro
2023	*"Chemically-Driven Autonomous Molecular Machines and Other Dissipative Systems"*	PRIN 2022 (Research Project of National Interest), Local PI, 2 years duration	215,560 euro (Local 107,780 euro)
2024	*"A Molecular Pump Driven by an Activated Carboxylic Acid"*	"Progetti di Ricerca (Piccoli e medi in the frame of "Bando Ricerca 2023-Anno 2023, La Sapienza", prot. RP123188D319A51F.	4,000 euro

VI B grants as **Investigator**

Year	Title	Program	position
1999	*"Dispositivi Supramolecolari*"	"PRIN 1999" protocol. 9903032124_008	As a PhD student
2006	*"Materiali Molecolari per Sensing e Catalisi*"	"PRIN 2006" protocol 2006034123_002	As a university scholarship holder
2007	"*Materiali Molecolari e Supramolecolari per Sensing e Catalisi*"	"Bando Ricerca Scientifica - Anno 2007 La Sapienza", project C26A0798ZX	As "Ricercatore Universitario"
2008	"*Materiali Molecolari e Supramolecolari per Sensing e Catalisi*"	"Bando Ricerca Scientifica - Anno 2008 La Sapienza", project C26A08WZ52	As "Ricercatore Universitario"
2008	"*Materiali Molecolari e Supramolecolari per Sensing e Catalisi*"	"PRIN 2008", protocol 2008HZJW2L_005	As "Ricercatore Universitario"
2009	*"Materiali Molecolari e Supramolecolari per Sensing e Catalisi*"	"Bando Ricerca Scientifica - Anno 2009, La Sapienza", project C26A092JAL	As "Ricercatore Universitario"
2011	*"Tecnologie supramolecolari integrate per il trattamento dell'informazione chimica: dispositivi e materiali molecolari avanzati (InfoChem)*"	"PRIN 2010-2011" protocol 2010CX2TLM_007	As "Ricercatore Universitario"
2015	"*Hydrogen Peroxide Activation by Non-Heme Iron Complexes: A Route for Sustainable and Selective Oxidation Processes*"	"Grande Progetto Universitario" in the frame of "Bando Ricerca Scientifica - Anno 2015, La Sapienza", project C26H159F5B, 30,000 euro	As "Ricercatore Universitario"
2016	"*Processi Ossidativi Catalizzati da Complessi di Ferro-noneme*"	"Bando Ricerca Scientifica - Anno 2016, La Sapienza" project RM116154C2F23F40	As "Ricercatore Universitario"
2017	"*Non-heme iron complexes as efficient and versatile catalysts of oxidative processes*"	"Grande Progetto Universitario" in the frame of "Bando Ricerca Scientifica - Anno 2017, La Sapienza", DR n. 2936/2017, 35,000 euro	As "Ricercatore Universitario"
2021	"*New Supramolecular Catalysts for Selective C-H Bond Functionalization by Hydrogen Atom Transfer (HAT) Based Oxidative Process*"	"Grande Progetto Universitario" nell'ambito del "Bando Ricerca Scientifica - Anno 2021, La Sapienza", protocollo RG12117A5D586DA9, 73.787 euro	As an Associate Professor

Part VII – Organization Activities and Other Institutional Roles

Period	Role
From 27 / 10 /2017	**Member of the PhD Board of the PhD School in Chemical Sciences of the University of Rome La Sapienza**
From September to October 2015	Member of the Commission for the admission to the PhD in Chemical Sciences for the 31st cycle at the University of Rome La Sapienza
From 17 / 10 /2017 to 31 /10 /2018	Member of the Commission for assignment of rooms and laboratories to Researchers and Professors of the Chemistry Department of University of Rome La Sapienza (Commissione Spazi)
From 26 / 10 /2017	Member of the Commission "Commissione Strutture Didattiche e Scientifiche" of the Faculty of Science of University of Rome La Sapienza
From 04 / 04 /2019	**President** of the Commission of the Library Organization of Chemistry Department of University of Rome La Sapienza (**Commissione Biblioteca**)
From 25 / 11 /2019	**President** of the Commission "**Commissione Strutture Didattiche e Scientifiche**" of the Faculty of Science of University of Rome La Sapienza. This Commission administrates the funding for different activities held in the Departments of the Faculty, from the scholarships for Bachelor, Master and PhD students, to funds for educational laboratories. The Commission manages around 500,000 Euros per year.
From 03/09/2021 to 15/10/2021	Member of the Commission for the selection of an Associate Professor in Organic Chemistry (Settore Concorsuale 03/C1 – SSD CHIM/06) at Chemistry Department, University of Rome La Sapienza
23 / 02 /2022	President of the National Commission evaluating of the Defense of three candidates of the PhD in Chemical Science (cycle XXXIV) of University of Rome Tor Vergata
13 / 07 /2022	Member of the Commission evaluating of the Defense of the candidate Eduard Masferrer Rius of University of Utrecht (The Netherlands)
From 11/08/2022 to 11/08/2022	Member of the Commission for the selection of an Assistant Professor (RTDA) in Organic Chemistry (Settore Concorsuale 03/C1 – SSD CHIM/06) at Chemical and life Science and Environmental Sustainability Department, University of Parma.
From 03 / 05 / 2023	Deputy President of PhD Board of the PhD School in Chemical Sciences of the University of Rome La Sapienza
From 28/07/2023 to 26/09/2023	President of the Commission for the selection of a CNR Researcher at ISB (Institute of Biological System) – Sezione Secondaria Meccanismi di Rezione, Chemistry Department, University of Rome La Sapienza"
From 26/09/2023 to 15/12/2023	Member of the Commission for the selection of an Associate Professor in Organic Chemistry (Settore Concorsuale 03/C1 – SSD CHIM/06) at "Dipartimento di Scienze e Tecnologie Chimiche dell'Università degli Studi di Roma Tor Vergata"
From 08/01/2024 to 26/03/2024	President of the Commission for the selection of an Assistant Professor (RTT) in Organic Chemistry (Settore Concorsuale 03/C1 – SSD CHIM/06) at Chemistry Department, University of Rome La Sapienza.

Part VIII – Reviewer Activity

I have carried out a reviewing activity for the following publishing houses (*The journals for which I carried out the reviewing activity are in brackets*):
-**AAAS** (*Science, Science Advances*)
-***Nature Publishing group*** (*Nature Chemistry, Nature Reviews Chemistry, Nature Synthesis, Chemistry Communications*)
-***Royal Society of Chemistry*** (*Chem. Soc. Rev., Chem. Sci., Chem. Comm., Org. Biomol. Chem., Cat. Sci. & Techn., Dalton Trans., New J. Chem., Green Chemistry, React. Chem. & Eng., Phys. Chem. Chem. Phys., Polym. Chem., Org. Chem. Front.*)
-***American Chemical Society*** (*J. Am. Chem. Soc., J. Org. Chem., Macromolecules, ACS Catalysis, ACS Macro, Inorg. Chem., Crystal Growth & Design, Ind. Eng. Chem. Res., ACS Org. & Inorg. Au*)
-***Wiley*** (*Angew. Chem. Int. Ed., Chem. Eur. J., Chem. Asian J., Asian J. Org. Chem., Eur. J. Org. Chem., Israel J. Chem.; J. Polym. Sci. part A, ChemistrySelect, Adv. Opt. Mater., ChemSystemsChem*)
-***Elsevier*** (*Coord. Chem. Rev., Tetrahedron Lett., J. Molec. Catal. A, Material Today Communications, Polyhedron*)
-***Springer*** (*Res. Chem. Int.*)
-***MDPI*** (*Molecules, Symmetry*)

I have carried out reviewing activity for
i) ANVUR,
ii) Dutch Research Council (Paesi Bassi),
iii) National Science Centre (Polonia)
iv) Frontier Research in Chemistry (FRC) Foundation (Francia, Università di Strasburgo).
v) Swiss National Science Foundation (SNSF). ETH Zürich–ETHZ.
vi) Università degli Studi di Parma
vii) Office of Basic Energy Sciences (BES) within the Department of Energy Office of Science (PAMS), Ohio, USA.
viii) ERC foundation (evaluation of *ERC consolidator*)
ix) Swiss National Science Foundation (SNSF). AMBIZIONE

In 2022 I was included in the top 10% *Angew Chem Int. Ed.* list of best quality Reviewers

Part IX – Research Activities

Keywords	Brief description of past and current research interests.
Supramolecular Chemistry Organic Chemistry Supramolecular Catalysis Reaction Mechanisms Molecular Recognition Intramolecular Reactivity Effective Molarities	My research activity has mostly concerned Supramolecular Chemistry in its Organic and Physical Organic implications. My interest was firstly focused on the synthesis and mechanistic characterization of supramolecular catalysts able to efficiently and selectively catalyze the solvolysis of esters and amides in a bio-mimetic fashion. In such catalysts an active site and a recognition site cooperate in order to accelerate the reaction of the desired substrate. We focused on the importance of the geometrical complementarity between the substrate and the supramolecular catalyst which guided us to realize prototypes of photo-modulated catalysts and of an artificial acetylcholinesterase. Furthermore, comparison of intra-complex reactivity with the intermolecular reactivity in supramolecular systems has been a lietmotiv during all my studies on supramolecular catalysis. In particular, we have shown that the concept of effective molarity (EM) can be used for the evaluation of the efficiency of a great number of supramolecular catalysts.
Dynamic Combinatorial Chemistry Jacobson-Stockmayer Theory Organic Chemistry Imine Chemistry Olefin metathesis Acetal Exchange Catenane Polycatenanes	Another topic of my research has been Dynamic Combinatorial Chemistry (DCC). This relatively recent branch of chemistry studies systems under thermodynamic equilibrium and the effects on their composition due to the addition of molecular entities called “templates”. In particular my investigation was focused first on the theoretical features of such systems (which are based on the Jacobson-Stockmayer theory since, most of the times, the systems involved in DCC are ring-chain systems) and secondly on the application of the theoretical results to real equilibrium systems that I realized through reversible reactions such as acetal exchange, olefin metathesis and imine metathesis. In the case of imine metathesis new fundamental mechanistic results were found in the course of the study. During the olefin metathesis investigation, a polymeric material, which resulted to be one of the first main-chain polycatenanes mainly consisting of interlocked cyclic molecules, has been obtained. Currently, I am working to the experimental verification of our recent re-formulation of the Jacobson Stockmayer theory, which includes interlocked cyclic molecules (catenanes).
Chemical Fuels Molecular Machine Host-Guest Chemistry Catalysis Smart Materials Dynamic Libraries	I developed a series of chemical fuels capable of driving the operation of dissipative systems (molecular machines, host-guest systems, dynamic libraries, catalysts, smart materials). The fuels are activated carboxylic acids that, after giving the proton to the dissipative system, which pass from a state A to a state B, decarboxylates to give carbanionic species. The latter are strong base able to take back the proton from the protonated system, which in turn goes back to state A. In practice, there is no need to add any chemical counter-stimulus to complete the A→B→A cycle. The chemical structures and the amount of the added fuel can be varied in order to have a control over time on the system structure and properties.

Non Heme Iron Catalyst
Organic Chemistry
Reaction Mechanisms
C-H Activation
Supramolecular Catalysis

The previous studies I carried out on imine chemistry have been of inspiration for the one-pot synthesis of a non-heme iron (II) complex which is an efficient catalyst for the oxidation of aliphatic and aromatic C–H bonds by H_2O_2. Such catalyst is prepared from cheap and commercially available precursors, just before use. It presents peculiar properties among which the ability of oxidizing aromatic substrates is probably the most intriguing. Mechanistic studies demonstrated that it works with a metal based mechanism. Moreover, I developed a supramolecular catalyst based on White's tetracoordinated iron (II) or manganese (II) complex, which efficiently oxidizes selected methylenic positions of long primary amines due to the presence of crown ethers in the catalyst backbone that allow the substrate recognition. We recently used this catalyst to selectively oxidize substrates of biological interest such as derivatives of cholesterol. Moreover the catalyst has been demonstrated to act as an artificial enzyme, which selectively catalyzes the reaction of its substrate, even in the presence of other intrinsically more reactive compounds that are left untouched or nearly so. Research on non-heme iron and manganese catalysts is currently one of the main topics in my lab.

Part X– DIRECTION to the activities of a research group characterized by international and national collaboration.

XI A **Direction and co-direction** (corresponding author/s is/are asterisked) at **international** level

Collaboration with the group of Prof. E. W. Meijer, Institute for Complex Molecular Systems, University of Eindhoven (The Netherlands):

1) "*Copper(I)-Induced Amplification of a [2]catenane in a Virtual Dynamic Library of Macrocyclic Alkenes*" J. A. Berrocal, M. M. L. Nieuwenhuizen, L. Mandolini, E. W. Meijer, S. Di Stefano*, *Org. Biomol. Chem.*, **2014**, *12*, 6167-6174.
2) "*Ring-opening Metathesis Polymerization of a Diolefinic [2]-Catenane-copper(I) Complex: An Easy Route to Polycatenanes*"J. A. Berrocal, L. M. Pitet, M. M. L. Nieuwenhuizen, L. Mandolini, E. W. Meijer*, S. Di Stefano*, *Macromolecules*, **2015**, *48*, 1358-1363.

Collaboration with the group of Prof C. A. Hunter del Department of Chemistry della University of Sheffield (United Kingdom) and the group of Prof. L. Baldini of Università di Parma (Italia):

1) "*Applications of Dynamic Combinatorial Chemistry for the Determination of Effective Molarity*" M. Ciaccia, I. Tosi, L. Baldini, R. Cacciapaglia, L. Mandolini, S. Di Stefano*, C. A. Hunter*, *Chem. Sci.*, **2015**, *6*, 144–151.

Collaboration with the group of Prof M. Costas of the Departament de Química i Institut de Química Computacional i Catalisi (IQCC), Facultat de Ciències, Universitat de Girona (Spain):

1) "*C-H Bond Oxidation Catalyzed by an Imine Based Iron Complex: A Mechanistic Insight*" G. Olivo, M. Nardi, D. Vìdal-Sanchez, A. Barbieri, A. Lapi, L. Gómez, O. Lanzalunga, M. Costas*, S. Di Stefano*, *Inorg. Chem.*, **2015**, *54*, 10141−10152.
2) "*Supramolecular Recognition Allows Remote, Site-Selective C-H Oxidation of Methylenic Sites in Linear Amines*" G. Olivo*, G. Farinelli, A. Barbieri, O. Lanzalunga, S. Di Stefano*, M. Costas*, *Angew. Chem. Int. Ed.* **2017**, *56*, 16347 –16351.
3) "*Enzyme-like Substrate-Selectivity in C-H Oxidation Enabled by Recognition*" G. Olivo*, G. Capocasa, O. Lanzalunga, S. Di Stefano*, M. Costas*, *Chem. Comm.*, **2019**, *55*, 917-920.
4) "*Predictable selectivity in remote C-H Oxidation of steroids: analysis of substrate binding mode*" G. Olivo*, G. Capocasa, B. Ticconi, O. Lanzalunga, S. Di Stefano*, M. Costas*, *Angew. Chem. Int. Ed.*, *Angew. Chem. Int. Ed.* **2020**, *59*, 12703 –12708. (*Very Important Paper*, *VIP*)
5) "*Proximity Effects on the Reactivity of a Nonheme Iron (IV) Oxo Complex in C-H Oxidation*" A. Fagnano, F. Frateloreto, R. Paoloni, C. Sappino, O. Lanzalunga, M. Costas*, S. Di Stefano*, G. Olivo* *Angew. Chem. Int. Ed.*, **2024**, *63*, e202401694.

Collaboration with the group of Doctor Sakura Pascarelli and of Doctor Theyencheri Narayanan of European Synchrotron Radiation Facility, Grenoble (Fr):

1) "*Following a Chemical Reaction on the Millisecond Time Scale by Simultaneous X‑ray and UV/Vis Spectroscopy"* G. Olivo, A. Barbieri, V. Dantignana, F. Sessa, V. Migliorati, M. Monte, S. Pascarelli, T. Narayanan, O. Lanzalunga*, S. Di Stefano*, P. D'Angelo*, *J. Phys. Chem. Lett.* **2017**, *8*, 2958−2963.
2) "*Coupled X-Ray Absorption/ UV-Vis Monitoring of Fast Oxidation Reactions Involving a Non-Heme Iron Oxo Complex*" G. Capocasa, F. Sessa, F. Tavani, G. Olivo, M. Monte, S. Pascarelli, O. Lanzalunga*, S. Di Stefano*, P. D'Angelo*, *J. Am. Chem. Soc.* **2019**, *141*, 2299−2304.

Collaboration with Dr. José Augusto Berrocal, Institute for Complex Molecular Systems, University of Eindhoven (The Netherlands):

1) "*A CuI-Based Metallo-Supramolecular Gellike Material Built from a Library of Oligomeric Ligands Featuring Exotopic 1,10-Phenanthroline Units*" J. A. Berrocal, S. Albano, L. Mandolini, S. Di Stefano*, *Eur. J. Org. Chem.*, **2015**, 7504–7510.
2) "*Coupling Decarboxylation of 2-Cyano-2-phenylpropanoic Acid to Large Amplitude Motions: a Convenient Fuel for an Acid-Base Operated Molecular Switch*" J. A. Berrocal, C. Biagini, L. Mandolini, S. Di Stefano*, *Angew. Chem. Int. Ed.*, **2016**, *55*, 6997 –7001.
3) "*Variations in the Fuel Structure Control the Rate of the Back and Forth Motions of a Chemically Fuelled Molecular Switch*" C. Biagini, S. Albano, R. Caruso, L. Mandolini, J. A. Berrocal, S. Di Stefano*, *Chem. Sci*. **2018**, *9*, 181-188.

Collaboration with Prof Andreas Walther, Life-Like Materials and Systems, Department of Chemistry, University of Mainz, (Germany):

1) "*Autonomous Soft Robots Empowered by Chemical Reaction Networks*" G. Fusi, D. Del Giudice, O. Skarsetz, S. Di Stefano,* Andreas Walther*, *Advanced Materials*, *Advanced Materials*, **2022**, 2209870. (IF = 32.09).

X B **Direction and co-direction** (corresponding author/s is/are asterisked) at **national** level

Collaboration with the groups of Prof A. Casnati, L. Baldini e F. Ugozzoli of Università di Parma (Italia):

1) *"A Highly Efficient Intramolecular Cannizzaro Reaction between 1,3-Distal Formyl Groups at the Upper Rim of a cone-Calix[4]arene*" M. Galli, J. A. Berrocal, S. Di Stefano*, R. Cacciapaglia, L. Mandolini, L. Baldini, A. Casnati, F. Ugozzoli, *Organic and Biomolecular Chemisty*, **2012**, *10*, 5109-5012.
2) "*One-Shot Preparation of an Inherently Chiral Trifunctional Calix[4]arene from an Easily Available Cone-Triformylcalix[4]arene*" M. Ciaccia, I. Tosi, R. Cacciapaglia, A. Casnati, L. Baldini*, S. Di Stefano*, *Org. Biomol. Chem.*, **2013**, *11*, 3642-2648.
3) "*Naphthalenophane Formaldehyde Acetals as Candidate Structures for the Generation of Dynamic Libraries via Transacetalation Processes*" A. Ruggi, R. Cacciapaglia*, S. Di Stefano*, E. Bodo, F. Ugozzoli, *Tetrahedron*, **2013**, *69*, 2767-2774.
4) "*Formation of Imidazo[1,5-a]pyridine Derivatives Due to the Action of Fe^{2+} on Dynamic Libraries of Imines*" S. Albano, G. Olivo, L. Mandolini, C. Massera, F. Ugozzoli, S. Di Stefano*, *J. Org. Chem.*, **2017**, *82*, 3820−3825.
5) "*Time Programmable Locking/Unlocking of the Calix[4]arene Scaffold by Means of Chemical Fuels* D. Del Giudice, E. Spatola, R. Cacciapaglia, A. Casnati, L. Baldini*, G. Ercolani*, S. Di Stefano*, *Chem. Eur. J.*, **2020**, *26*, 14954 – 14962.
6) "*Dissipative Control of the Fluorescence of a 1,3-Dipyrenyl Calix[4]arene in the Cone Conformation"*
   E. Spatola, F. Rispoli, D. Del Giudice, R. Cacciapaglia, A. Casnati, L. Marchiò, L. Baldini*, S. Di Stefano*, *Org. Biomol. Chem.*, **2022**, *20*, 132–138.

Collaboration with Prof G. Ercolani of Università di Roma Tor Vergata (Italia):

1) "*Combinatorial Macrocyclizations under Thermodynamic Control: the Two-monomer Case*" R. Cacciapaglia, **S**. Di Stefano*, G. Ercolani*, L. Mandolini*, *Macromolecules*, **2009**, *42*, 4077-4083.
2) "*Catenation Equilibria between Ring Oligomers and their Relation to Effective Molarities. Models from Theories and Simulations*" S. Di Stefano*, G. Ercolani*, *Macromolecular Theory and Simulations*, **2016**, *25*, 63–73.
3) "*Equilibrium Effective Molarity as a Key Concept in Ring-Chain Equilibria, Dynamic Combinatorial Chemistry, Cooperativity, and Self-Assembly*" S. Di Stefano*, G. Ercolani*, *Advances in Physical Organic Chemistry*, **2016**, volume *50*, 1-76.
4) "*Statistical Ring Catenation under Thermodynamic Control: Should the Jacobson−Stockmayer Cyclization Theory Take into Account Catenane Formation?*" S. Di Stefano*, G. Ercolani*, J. *Phys. Chem. B* **2017**, *121*, 649−656.
5) "*Time-programmable pH: Decarboxylation of Nitroacetic Acid Allows the Time-controlled Rising of pH to a Definite Value*" D. Del Giudice, E. Spatola, M. Valentini, C. Bombelli, G. Ercolani*, S. Di Stefano*, **2021**, *12*, 7460-7466.
6) *Dissipative Dynamic Libraries (DDLs) and Dissipative Dynamic Combinatorial Chemistry (DDCC)*" D. Del Giudice, E. Spatola, M. Valentini, G. Ercolani,* S. Di Stefano*, *ChemSystemsChem* **2022**, e202200023.

Collaboration with Profs. M. Lucarini ed E. Mezzina, Università di Bologna (Italia):

1) "*2-Cyano-2-phenylpropanoic Acid Triggers the Back and Forth Motions of an Acid–Base-Operated Paramagnetic Molecular Switch*"
   P. Franchi, C. Poderi, E. Mezzina, C. Biagini, S. Di Stefano*, M. Lucarini*, *J. Org. Chem.*, **2019**, *84*, 9364−9368.

Collaboration with Prof F. Ricci of Università di Roma Tor Vergata (Italia):

1) "*Dissipative operation of pH-responsive DNA-based nanodevices*"
D. Mariottini, D. Del Giudice, G. Ercolani, S. Di Stefano*, F. Ricci*, *Chem. Sci.*, **2021**, *12*, 11735-11739.

Part XI – PARTICIPATION to the activities of a research group characterized by international and national collaboration.

XII A **Participation** (corresponding author/s is/are asterisked) at **international** level

Collaboration with the group of Javier de Mendoza of Universidad Autonoma de Madrid (Spain):

1) "*Towards an Artificial Acetylcholinesterase*" F. Cuevas, S. Di Stefano, O. J. Magrans, P. Prados, J. de Mendoza*, L. Mandolini*, *Chem. Eur.J.*, **2000**, *6*, 3228-3234.
In this case the collaboration was in the frame of the COST D11 european program "Supramolecular Chemistry"
2) "*Zwitterion Receptors"* in *Encyclopedia of Supramolecular Chemistry* S. Di Stefano, L. Mandolini, P. Breccia, J. de Mendoza. J. R. Atwood & J. Steed editors, Marcel-Dekker Inc., New York, **2004**, 1639-1647. (no correspondent author appears)

Collaboration with the group of Prof. Ulrich Lüning of lnstitut fur Organische Chemie der Christian-Albrechts-Universitàt di Kiel (Germany):

1) "*Concave Reagents 40. The Cu(II) Complex of a Concave Reagent as a Selective Supramolecular Catalyst For Ester Methanolysis*" R. Cacciapaglia, S. Di Stefano, F. Fahrenkrug, U. Lüning*, L. Mandolini*, *J. Phys. Org. Chem.*, **2004**, *17*, 350-355.
In this case the collaboration was in the frame of the COST D11 european program "Supramolecular Chemistry"

Collaboration with the groups of Prof D. Reinhoudt della University of Twente Enschede (The Netherlands) and of Prof. Ungaro dell'Università di Parma (Italia):

1) "*Dinuclear Barium(II) Complexes Based on a Calix[4]arene Scaffold as Catalysts of Acyl Transfer*" R. Cacciapaglia, A. Casnati, S. Di Stefano, L. Mandolini*, D. Paolemili, D. N. Reinhoudt*, A. Sartori, and R. Ungaro*, *Chemistry a European Journal*, **2004**, *10*, 4336-4342.

Collaboration with the group of Prof L. Rodriguez of the Departament de Quimica Inorganica, Universitat de Barcelona (Spain)

1) "*Unusual reversible complexation between atropisomeric naphthalenophanes and molecular oxygen*" L. Rodríguez*, J. C. Lima, F. Pina, R. Cacciapaglia, S. Di Stefano, A. Ruggi, *J. Phys. Chem. A*, **2011**, *115*, 123-127

Collaboration with the group of Prof D. A Leigh of the School of Chemistry, University of Manchester (United Kingdom)

1) "*Dissipative Catalysis with a Molecular Machine*"
C. Biagini, S. D. P. Fielden, D. A. Leigh*, F. Schaufelberger, S. Di Stefano, D. Thomas, *Angew. Chem. Int. Ed.*, **2019**, *ASAP*

XII B **Participation** (corresponding author/s is/are asterisked) at **national** level

Collaboration with the group of Prof. F. Ugozzoli of Università di Parma (Italia):

1) "*Metathesis Reactions of Formaldehyde Acetals – Experimental and Computational Investigation of Isomeric Families of Cyclophanes under Dynamic Conditions*" R. Cacciapaglia, S. Di Stefano, L. Mandolini*, P. Mencarelli*, F. Ugozzoli*, *European Journal of Organic Chemistry*, **2008**, 186-195.

Collaboration with Prof. G. Ercolani of Università di Roma Tor Vergata (Italia):

1) "*Ring-Expanding Polymerization by Reversible Ring Fusion. A Fascinating Process Driven by Entropy*" G. Ercolani*, S. Di Stefano, *Journal of Physical Chemistry B*, **2008**, *112*, 4662-4665.

Part – XII Invited lectures held in Italian and Foreign Universities (*IC*), Invited lectures held at Congresses (*IL*), Oral Communications held at Congresses (*OL*), Flash Communication (*FC*) held at Congresses and Organization of congresses.

1 *"Scissione di Ammidi Attivate: Catalisi da complessi Mono e Bimetallici"* R. Cacciapaglia, S. Di Stefano, L. Mandolini. COFEM '97 Giornate di Chimica Organica Fisica e Meccanicistica 11-14 June 1997 Folgaria (TN). (***OL***)

2 "*Towards An Acetylcholinesterase Mimic*" F. Cuevas, S. Di Stefano, L. Mandolini, J. de Mendoza, P. Prados. 4° Congresso Nazionale di Chimica Supramolecolare 5-8 September 1999, Catania. (***OL***)

3 *"Catalizzatori Supramolecolari"* S. Di Stefano. 25° Corso Estivo di Sintesi Organica "A. Corbella", 12-16 June 2000, Gargnano (Bs). (***OL***)

4 *"Towards An Artificial Acetylcholinesterase"* S. Di Stefano. European Research Conference on "Supramolecular Chemistry", 31 August-5 September 2000, Urbino. (***OL***)

5 *"Catalizzatori Supramolecolari Fotomodulabili"* R. Cacciapaglia, S. Di Stefano, L. Mandolini. 3° SAYCS Sigma-Aldrich Young Chemists Symposium, Riccione, 19-21 May 2003. (***OL***)

6 *"Effective Molarities in Supramolecular Catalysis"* R. Cacciapaglia, S. Di Stefano, L. Mandolini. 6° Congresso Nazionale di Chimica Supramolecolare 7-10 September 2003, Urbino. (***OL***)

7 *"The Dynamic Covalent Chemistry of Macrocyiclic Formals"* R. Cacciapaglia, S. Di Stefano, L. Mandolini, Working Group 0004-04 COST D31, 11-13 April 2005, Bonn. (***OL***)

8 *"Dynamic Covalent Chemistry of Macrocyiclic Formals"* R. Cacciapaglia, S. Di Stefano, L. Mandolini, ESOR 10, 10th European Symposium on Organic Reactivity, 25-30 July 2005, Roma. (***OL***)

9 *"Meccanismo di Fusione e Fissione di Anello per la Reazione di Metatesi di Acetali Macrociclici della Formaldeide (Una Classica Dicotomia S_N2/S_N1)"* R. Cacciapaglia, S. Di Stefano, L. Mandolini, COFEM 2006, Giornate di Chimica Organica Fisica e Meccanicistica, Catania, 21-23 September 2006. (***OL***)

10 *Macrocyclization under Thermodynamic Control: Theory and Experiments"* R. Cacciapaglia, S. Di Stefano, G. Ercolani, L. Mandolini, Working Group 0004-04 COST D31, 25-27 May 2008, Enschede (NE). (***OL***)

11 *"Macrociclizzazioni sotto Controllo Termodinamico: Teoria ed Esperimenti"* R. Cacciapaglia, S. Di Stefano, G. Ercolani, L. Mandolini, COFEM '08 Giornate di Chimica Organica Fisica e Meccanicistica 24-26 September 2008 Sestri Levante (La Spezia). (***IL***)

12 "*Theorethical and Experimental Features of Macrocyclization Equilibria*" S. Di Stefano, Seminario di Dipartimento, Istituto Ciamician, Alma Mater Università di Bologna, 26 January 2011, Bologna. (***IC***)

13 *"A Very Fast Hydride Transfer at the Upper Rim of a Calix[4]arene. Proximity of 1,3 Distal Groups"* S. Di Stefano, L. Baldini, R. Cacciapaglia, A. Casnati, L. Mandolini, Calix 11, 11th International Conference on Calixarenes, 26-29 June 2011, Tarragona (Spain). (***FP***)

14 "*From Ring-Chain Equilibria to Dynamic Combinatorial Chemistry"* S. Di Stefano, 10° Congresso Nazionale di Chimica Supramolecolare 25-28 settembre 2011, Perugia. (***IL***)

15 "*Ring-Chain Equilibria and Dynamic Libraries"* S. Di Stefano, Department Lecture, Department of Chemical Engineering and Chemistry, Eindhoven University of Technology, Eindhoven (The Netherlands), 23 April 2013. (***IC***)

16 "*Effective Molarity (EM) and Critical Monomer Concentration (CC) in the Description of Dynamic Libraries of Cyclic Compounds*" S. Di Stefano, Department Lecture, Department of Chemistry, The University of Sheffield, Sheffield (England), 11 June 2014. (***IC***)

17 "*Theoretical Aspects of Ring-Chain Equilibria and Implications for Real Dynamic Libraries*" S. Di Stefano, Faculty Lecture, Department of Chemistry, The University of Girona, Girona (Spagna), 12 March 2015. (***IC***)

18 "*Aspetti Teorici della Chimica Dinamica Combinatoria ed Applicazioni Sperimentali: dal Riconoscimento ai Materiali Supramolecolari*" S. Di Stefano, Seminario di Istituto, IMC Istituto di Metodologie Chimiche, Montelibretti (Roma), 19 March 2015. (***IL***)

19 "*A Chemical Fuel for an Acid-Based Operated Molecular Switch*" J. A. Berrocal, C. Biagini, L. Mandolini, S. Di Stefano, XXXVII Convegno Nazionale della Divisione di Chimica Organica, Mestre 18-22 September 2016. (***OL***)

20 "*Controlling the Rate of Cyclic Motions of a Molecular Switch by a Fine Tuning of the Fuel Molecular Structure*" S. Di Stefano, C. Biagini, S. Albano, 13° Congresso Nazionale di Chimica Supramolecolare 18-21 June 2017, Santa Margherita di Pula (CA). (***OL***)

21 "*Chemical Fuels for Acid-base Operated Molecular Machines*" S. Di Stefano, Scientific Seminar, CLAN (Center for Light Activated Nanostructures) ISOF-CNR, Bologna 22 January 2018. (***IC***)

22 "*Controlling the Motions of Acid-base Operated Molecular Machines*" S. Di Stefano, F. Di Pietri, S. Albano, L. Mandolini, O. Lanzalunga, C. Biagini, XXXVIII Convegno Nazionale della Divisione di Chimica Organica, Milano 09-13 September 2018. (***OL***)

23 "*How to make Autonomous the Motions of a Chemically Fuelled Molecular Machine*", C. Biagini, G. Capocasa, V. Cataldi, D. Del Giudice, L. Mandolini, S. Di Stefano, XXXIX Convegno Nazionale della Divisione di Chimica Organica, Torino 08-12 September 2019. (***OL***)

24 "*Exploring different features of supramolecular chemistry*", S. Di Stefano, Cerimonia di Conferimento Premi e Medaglie della Divisione di Chimica Organica 2020, Roma, 25 giugno 2021. (***IL***)

25 *"Dissipative Systems Driven by the Decarboxylation of Carboxylic Acids"* ArtMoMa (Artificial Molecular Machines" Workshop 2023 (Spring School), Bologna 17-19 April 2023. (***IL***)

26 *"Dissipative systems driven by the decarboxylation of activated carboxylic acids"* Systems Chemistry in Italy (Emerging Properties from Complex Chemical Systems), Roma, 25 September 2023. (***IL***)

Organizer as **Chairperson** of the congress "CHIMICA SUPRAMOLECOLARE: GIORNATA DEI DOTTORANDI" hold at CNR (Rome Central Builing, Piazzale Aldo Moro, 7) on 24 and 25 May 2018. During the congress 41 presentations were given as Invited Lectures, Oral Presentation and Flash Presentations. The congress was in the frame of the Italian Supramolecular Chemistry Group and of Società Chimica Italiana.

Member of the Organizing Committee of XLI Convegno della Divisione di Chimica Organica della Società Chimica Italiana (XLI Conference of Organic Division of Italian Chemical Society) held in Rome from 10 to

14 September 2023. The conference was attended by 450 participants and included lectures by speakers of foreign institutions.

Furthermore the results of my research work have been presented by me with poster presentations, and by my co-workers with poster and oral presentation in additional about 150 communications held at national and international congresses from 1997 to 2023.

Part – XIII Other information

I have attended the following national and international chemistry schools:
1) Corso Nazionale di Introduzione alla Fotochimica, 14-17 settembre 1998, Bologna.
2) Postgraduate Winter School on Organic Reactivity - Wisor VIII, 8-16 gennaio 1999, Bressanone (Bz).
3) 25° Corso Estivo di Sintesi Organica "A. Corbella", 12-16 giugno 2000, Gargnano (Bs).

I have completed the military service working as a volunteer fireman in the Corpo Nazionale dei Vigili del Fuoco (01/09/1997-31/08/1998). I carried out the service at "Ispettorato per l' Organizzazione Centrale e Periferica", Ministero dell' Interno.

Part – XIV Complete list of Publications. The IF is related to the year of publication (for the most recent publications, if not yet available, the IF of the previous year of the publication year is used)

1) "Catalysis of Anilide Ethanolysis by Barium- and Strontium-Ethoxide Pairs and Their Complexes with 18-Crown-6"
R. Cacciapaglia, S. Di Stefano, E. Kelderman, L. Mandolini, F. Spadola, *J. Org. Chem.*, **1998**, *63*, 6476-6479. (IF 3.50)

2) "Supramolecular Catalysis of Ester and Amide Cleavage by a Dinuclear Barium(II) Complex"
R. Cacciapaglia, S. Di Stefano, E. Kelderman, L. Mandolini, *Angew. Chem. Int. Ed.*, **1999**, *38*, 348-351. (IF 8.00)

3) "Towards an Artificial Acetylcholinesterase"
F. Cuevas, S. Di Stefano, O. J. Magrans, P. Prados, J. de Mendoza, L. Mandolini, *Chem. Eur. J.*, **2000**, *6*, 3228-3234. (IF 4.70)

4) "A Dinuclear Strontium(II) Complex as Substrate Selective Catalyst of Ester Cleavage"
R. Cacciapaglia, S. Di Stefano, L. Mandolini, *J. Org. Chem.*, **2001**, *66*, 5926-5928. (IF 3.28)

5) "Size Selective Catalysis of Ester and Anilide Cleavage by the Dinuclear Barium (II) Complexes of *Cis*- and *Trans*-Stilbeno-bis-18-Crown-6"
R. Cacciapaglia, S. Di Stefano, L. Mandolini, *J. Org. Chem.*, **2002**, *67*, 521-525. (IF 3.22)

6) "6-exo-Hydroxybicyclo[2.2.2]octan-2-ones from the Corresponding Acetates by Methanolysis in the Presence of CH_3ONa / $La(OTf)_3$"
S. Di Stefano, F. Leonelli, B. Garofalo, L. Mandolini, R. Marini Bettolo, L. M. Migneco, *Org. Lett.*, **2002**, *4*, 2783-2785. (IF 3.72)

7) "The Bis-Barium Complex of a Butterfly Crown Ether as a Phototunable Supramolecular Catalyst"
R. Cacciapaglia, S. Di Stefano, L. Mandolini, *J. Am. Chem. Soc.*, **2003**, *125*, 2224-2227. (IF 6.52)

8) "Effective Molarities in Supramolecular Catalysis of Two Substrate Reactions"
R. Cacciapaglia, S. Di Stefano, L. Mandolini, *Acc. Chem. Res.*, **2004**, *37*, 113122. (IF 13.15)

9) "Concave Reagents 40[#]. The Cu(II) Complex of a Concave Reagent as a Selective Supramolecular Catalyst For Ester Methanolysis"
R. Cacciapaglia, S. Di Stefano, F. Fahrenkrug, U. Lüning, L. Mandolini, *J. Phys. Org. Chem.*, **2004**, *17*, 350-355. (IF 1.21)

10) "Zwitterion Receptors" in Encyclopedia of Supramolecular Chemistry
S. Di Stefano, L. Mandolini, P. Breccia, J. de Mendoza.
J. R. Atwood & J. Steed editors, Marcel-Dekker Inc., New York, **2004**, 1639-1647 (Questa pubblicazione non è indicizzata né in Scopus né in Web of Science).

11) "Dinuclear Barium(II) Complexes Based on a Calix[4]arene Scaffold as Catalysts of Acyl Transfer"
R. Cacciapaglia, A. Casnati, S. Di Stefano, L. Mandolini, D. Paolemili, D. N. Reinhoudt, A. Sartori, and R. Ungaro, *Chem. Eur. J.* , **2004**, *10*, 4336-4342. (IF 4.52)

12) "Metathesis Reaction of Formaldeheyde Acetals: An Easy Entry into the Dynamic Covalent Chemistry of Cyclophane Formation"
R. Cacciapaglia, S. Di Stefano, L. Mandolini, *J. Am. Chem. Soc.*, **2005**, *127*, 13666-13671. (IF 7.42)

13) “Ring Fusion / Ring Fission Mechanism for the Metathesis Reaction of Macrocyclic Formaldehyde Acetals”
R. Cacciapaglia, S. Di Stefano, L. Mandolini, *Chem. Eur. J.*, **2006**, *12*, 8566-8570. (IF 5.02)

14) “Metathesis Reactions of Formaldehyde Acetals – Experimental and Computational Investigation of Isomeric Families of Cyclophanes under Dynamic Conditions”
R. Cacciapaglia, S. Di Stefano, L. Mandolini, P. Mencarelli, F. Ugozzoli, *Eur. J. Org. Chem.*, **2008**, 186-195. (IF 3.02)

15) “Catalysis of Acyl Transfer Processes by Crown-Ether Supported Alkaline-Earth Metal Ions”
R. Cacciapaglia, S. Di Stefano, L. Mandolini, in *Supramolecular Catalysis*, Piet W. N. M. van Leeuwen (Ed.), WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, **2008**.

16) “Ring-Expanding Polymerization by Reversible Ring Fusion. A Fascinating Process Driven by Entropy”
G. Ercolani, S. Di Stefano, *J. Phys. Chem. B*, **2008**, *112*, 4662-4665. (IF 4.19)

17) “On the ‘livingness’ of a dynamic library of cyclophane formaldehyde acetals incorporating calix[4]arene subunits”
R. Cacciapaglia, S. Di Stefano*, L. Mandolini, *J. Phys. Org. Chem.*, **2008**, *21*, 688-693. (IF 1.42)

18) “Combinatorial Macrocyclizations under Thermodynamic Control: the Two-monomer Case”
R. Cacciapaglia, S. Di Stefano*, G. Ercolani*, L. Mandolini*, *Macromolecules*, **2009**, *42*, 4077-4083. (IF 4.54)

19) “Reactivity Control by Calixarenes”
R. Cacciapaglia, S. Di Stefano, L. Mandolini, in *Molecular Encapsulation: Organic Reactions in Constrained Systems*, Udo Brinker J-L Mieusset (Eds.), WILEY and Sons Ltd, Chichester, West-Sussex (UK), **2010**, 201-224.)

20) “Electron transfer from wheel to axle in a rotaxane. A mass spectrometric investigation”
S. Pasquale, S. Di Stefano*, B. Masci*, *New J. Chem.*, **2010**, *34*, 426-431. (IF 2.63)

21) “Theorethical Features of Macrocyclization Equilibria and Their Application on Transacetalation Based Dynamic Libraries”
S. Di Stefano*, *J. Phys. Org. Chem.*, **2010**, *23*, 797-805. (IF 1.48)

22) “Photoinversion of Sulfoxides as a Source of Diversity in Dynamic Combinatorial Chemistry”
S. Di Stefano*, M. Mazzonna, E. Bodo, L. Mandolini, O. Lanzalunga*, *Org. Lett.*, **2011**, *13*, 142-145. (IF 5.86)

23) “Unusual reversible complexation between atropisomeric naphthalenophanes and molecular oxygen”
L. Rodríguez, J. C. Lima, F. Pina, R. Cacciapaglia, S. Di Stefano, A. Ruggi, *J. Phys. Chem. A*, **2011**, *115*, 123-127. (IF 2.95)

24) “A Well-Behaved Dynamic Library of Cyclophane Formaldehyde Acetals Incorporating Diphenylmethane Units”
J. A. Berrocal, R. Cacciapaglia, S. Di Stefano*, *Org. Biomol. Chem.*, **2011**, 9, 8190-8194. (IF 3.70)

25) “Target-Induced Amplification in a Dynamic Library of Macrocycles. A Quantitative Study”
J. A. Berrocal, R. Cacciapaglia, S. Di Stefano*, Luigi Mandolini, *New J. Chem.*, **2012**, *36*, 40-43. (IF 2.97)

26) “A Photodynamic Library of Tetrasulfinylcalix[4]arenes: the Sulfinyl Dance”
R. Cacciapaglia*, S. Di Stefano*, O. Lanzalunga, L. Maugeri, M. Mazzonna, *Eur. J. Org. Chem.*, **2012**, 1426-1430. (IF 3.34)

27) “A Highly Efficient Intramolecular Cannizzaro Reaction between 1,3-Distal Formyl Groups at the Upper Rim of a *cone*-Calix[4]arene”
M. Galli, J. A. Berrocal, S. Di Stefano*, R. Cacciapaglia, L. Mandolini, L. Baldini, A. Casnati, F. Ugozzoli, *Org. Biomol. Chem.*, **2012**, *10*, 5109-5012. (IF 3.57)

28) “Naphthalenophane Formaldehyde Acetals as Candidate Structures for the Generation of Dynamic Libraries via Transacetalation Processes”
A. Ruggi, R. Cacciapaglia*, S. Di Stefano*, E. Bodo, F. Ugozzoli, *Tetrahedron*, **2013**, *69*, 2767-2774. (IF 2.82)

29) “Fast Transimination in Organic Solvents in the Absence of Proton and Metal Catalysts. A Key to Imine Metathesis Catalyzed by Primary Amines under Mild Conditions”
M. Ciaccia, R. Cacciapaglia, P. Mencarelli, L. Mandolini, S. Di Stefano*, *Chem. Sci.*, **2013**, *4*, 2253–2261. (IF 8.60)

30) “One-Shot Preparation of an Inherently Chiral Trifunctional Calix[4]arene from an Easily Available Cone-Triformylcalix[4]arene”
M. Ciaccia, I. Tosi, R. Cacciapaglia, A. Casnati, L. Baldini*, S. Di Stefano*, *Org. Biomol. Chem.*, **2013**, *11*, 3642-2648. (IF 3.49)

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G. Olivo, O. Lanzalunga, L. Mandolini, S. Di Stefano*, *J. Org. Chem.*, **2013**, *78*, 11508−11512. (IF 4.64)

33) “Effective Catalysis of Imine Metathesis by means of Fast Transiminations between Aromatic-Aromatic or Aromatic-Aliphatic Amines”
M. Ciaccia, Silvia Pilati, R. Cacciapaglia, L. Mandolini, S. Di Stefano*, *Org. Biomol. Chem.*, **2014**, *12*, 3282-3287. (IF 3.56)

34) “Hydrocarbon Oxidation Catalyzed by a Cheap Nonheme Imine-based Iron(II) Complex”
G. Olivo, G. Arancio, L. Mandolini, O. Lanzalunga, S. Di Stefano*, *Cat. Sci. & Technol.*, **2014**, 4, 2900-2903. (IF 5.43)

35) “Copper(I)-Induced Amplification of a [2]catenane in a Virtual Dynamic Library of Macrocyclic Alkenes”
J. A. Berrocal, M. M. L. Nieuwenhuizen, L. Mandolini, E. W. Meijer*, S. Di Stefano*, *Org. Biomol. Chem.*, **2014**, *12*, 6167 - 6174. (IF 3.56)

36) “Supramolecular Control of Reactivity and Catalysis. Effective Molarities of Recognition-Mediated Bimolecular Reactions”
S. Di Stefano*, R. Cacciapaglia, L. Mandolini*, *Eur. J. Org. Chem.*, **2014**, 7304-7315. (IF 3.07)

37) “Applications of Dynamic Combinatorial Chemistry for the Determination of Effective Molarity”
M. Ciaccia, I. Tosi, L. Baldini, R. Cacciapaglia, L. Mandolini, S. Di Stefano*, C. A. Hunter*, *Chem. Sci.*, **2015**, *6*, 144–151. (IF 9.14)

38) “Mechanisms of Imine Exchange Reactions in Organic Solvents”
M. Ciaccia, S. Di Stefano*, *Org. Biomol. Chem.*, **2015**, *13*, 646–654. (IF 3.56)

39) "Isotope Effect Profiles in the *N*-demethylation of *N*,*N*-dimethylanilines. A Key to Determine the pK_a of Nonheme Fe(III)-OH Complexes"
A. Barbieri, M. De Gennaro, S. Di Stefano, O. Lanzalunga, A. Lapi, M. Mazzonna, G. Olivo, B. Ticconi, *Chem. Commun.*, **2015**, *51*, 5032-5035. (IF 6.57)

40) "Ring-opening Metathesis Polymerization of a Diolefinic [2]-Catenane-copper(I) Complex: An Easy Route to Polycatenanes"
J. A. Berrocal, L. M. Pitet, M. M. L. Nieuwenhuizen, L. Mandolini, E. W. Meijer*, S. Di Stefano*, *Macromolecules*, **2015**, *48*, 1358-1363. (IF 5.55)

41) "A CuI-Based Metallo-Supramolecular Gellike Material Built from a Library of Oligomeric Ligands Featuring Exotopic 1,10-Phenanthroline Units"
J. A. Berrocal, S. Albano, L. Mandolini, S. Di Stefano*, *Eur. J. Org. Chem.*, **2015**, 7504–7510. (IF 3.07)

42) "C-H Bond Oxidation Catalyzed by an Imine Based Iron Complex: A Mechanistic Insight"
G. Olivo, M. Nardi, D. Vìdal-Sanchez, A. Barbieri, A. Lapi, L. Gómez, O. Lanzalunga, M. Costas*, S. Di Stefano*, *Inorg. Chem.*, **2015**, *54*, 10141−10152. (IF 4.82)

43) "Catenation Equilibria between Ring Oligomers and their Relation to Effective Molarities. Models from Theories and Simulations"
S. Di Stefano*, G. Ercolani*, *Macromolecular Theory and Simulations*, **2016**, *25*, 63–73. (IF 1.72)

44) "Nonheme Imine-based Iron Complexes as Catalysts for Oxidative Processes"
G. Olivo, O. Lanzalunga, S. Di Stefano*, *Adv. Synth. & Cat.*, **2016**, *358*, 843-863. (IF 5.65)

45) "Oxidation of Aryl Diphenylmethyl Sulfides Promoted by a Non-Heme Iron(IV)-Oxo Complex: Evidence for Electron Transfer-Oxygen Transfer Mechanism"
A. Barbieri, R. De Carlo Chimienti, T. Del Giacco, S. Di Stefano, O. Lanzalunga, A. Lapi, M. Mazzonna, G. Olivo, M. Salamone, *J. Org. Chem.*, **2016**, *81*, 2513−2520. (IF 4.85)

46) "Coupling Decarboxylation of 2-Cyano-2-phenylpropanoic Acid to Large Amplitude Motions: a Convenient Fuel for an Acid-Base Operated Molecular Switch"
J. A. Berrocal, C. Biagini, L. Mandolini, S. Di Stefano*, *Angew. Chem. Int. Ed.*, **2016**, *55*, 6997 –7001. (IF 11.99)

47) "Equilibrium Effective Molarity as a Key Concept in Ring-Chain Equilibria, Dynamic Combinatorial Chemistry, Cooperativity, and Self-Assembly"
S. Di Stefano*, G. Ercolani*, *Adv. Phys. Org. Chem.*, **2016**, volume *50*, 1-76. (IF 0.75).

48) "Alcohol Oxidation with H_2O_2 Catalyzed by a Cheap and Promptly Available Imine Based Iron Complex"
G. Olivo, S. Giosia, A. Barbieri, O. Lanzalunga, S. Di Stefano*, *Org. Biomol. Chem.*, **2016**, 14, 10630-10635. (IF 3.56)

49) "Electron Transfer Mechanism in the Oxidation of Aryl 1-Methyl-1-phenylethyl Sulfides Promoted by Nonheme Iron(IV)- Oxo Complexes: The Rate of the Oxygen Rebound Process"
A. Barbieri, T. Del Giacco, S. Di Stefano, O. Lanzalunga, A. Lapi, M. Mazzonna, G. Olivo, *J. Org. Chem.*, **2016**, *81*, 12382−12387. (IF 4.85)

50) "Role of Electron Transfer Processes in the Oxidation of Aryl Sulfides Catalysed by Nonheme Iron Complexes"
A. Barbieri, S. Di Stefano, O. Lanzalunga, A. Lapi, M. Mazzonna, G. Olivo, *Phosphorus, Sulfur and Silicon and the Related Elements*, **2017**, *112*, 241-244. (IF 0.67)

51) "Statistical Ring Catenation under Thermodynamic Control: Should the Jacobson−Stockmayer Cyclization Theory Take into Account Catenane Formation?"
S. Di Stefano*, G. Ercolani*, *J.Phys. Chem. B*, **2017**, *112*, 649-656. (IF 3.15)

52) "Influence of Topology on the Gelation Behavior of Coordination Polymers prepared via ROMP of Macrocyclic Olefins"
S. Albano, A. Fantozzi, J. A. Berrocal, S. Di Stefano*, *J. Poly. Sci., Part A: Polymer Chemistry*, **2017**, *55*, 1237–1242. (IF 2.59)

53) "Formation of Imidazo[1,5-a]pyridine Derivatives Due to the Action of Fe^{2+} on Dynamic Libraries of Imines"
S. Albano, G. Olivo, L. Mandolini, C. Massera, F. Ugozzoli, S. Di Stefano*, *J. Org. Chem.*, **2017**, *82*, 3820−3825. (IF 4.81)

54) "Following a Chemical Reaction in the ms Timescale by Simultaneous X-Ray and UV/Vis Spectroscopy"
G. Olivo, A. Barbieri, V. Dantignana, F. Sessa, V. Migliorati, M. Monte, S. Pascarelli, T. Narayanan, O. Lanzalunga*, S. Di Stefano*, P. D'Angelo*, *J. Phys. Chem. Lett.*, **2017**, *8*, 2958-2963. (IF 8.71)

55) "Supramolecular Recognition Allows Remote, Site-selective C-H Oxidation of Methylenic Sites in Linear Amines"
G. Olivo*, G. Farinelli, A. Barbieri, O. Lanzalunga, S. Di Stefano*, M. Costas*, *Angew. Chem. Int. Ed.*, **2017**, *56*, 16347 –16351. (IF = 12.10)

56) "Direct Hydroxylation of Benzene and Aromatics with H_2O_2 Catalyzed by a Self-Assembled Iron Complex: Evidence for a Metal-based Mechanism"
G. Capocasa, G. Olivo, A. Barbieri, O. Lanzalunga, S. Di Stefano*, *Cat. Sci. & Technol.*, **2017**, *7*, 5677–5686. (IF 5.37) **(*Hot Article*)**.

57) "Variations in the Fuel Structure Control the Rate of the Back and Forth Motions of a Chemically Fuelled Molecular Switch"
C. Biagini, S. Albano, R. Caruso, L. Mandolini, J. A. Berrocal, S. Di Stefano*, *Chem. Sci.* **2018**, *9*, 181-188. (IF = 9.56) (***Editor's Choice Collection***)

58) "Photoinduced Release of a Chemical Fuel for Acid-Base Operated Molecular Machines"
C. Biagini, F. Di Pietri, L. Mandolini, O. Lanzalunga, S. Di Stefano*, *Chem. Eur. J.*, **2018**, *24*, 10122-10127. (IF = 5.16) (***Hot Paper***, Spotlighted in *Angew. Chem. Int. Ed.*, **2018**, *57*, 10006-10009)

59) "Oxidative Functionalization of Aliphatic and Aromatic Amino Acid Derivatives with H_2O_2 Catalyzed by a Nonheme Imine Based Iron Complex"
B. Ticconi, A. Colcerasa, S. Di Stefano, O. Lanzalunga, A. Lapi, M. Mazzonna G. Olivo, *RSC Advances*, **2018**, *8*, 19144–19151. (IF = 3.05)

60) "Inherently Chiral Cone-calix[4]arenes via a Subsequent Upper Rim Ring-closing/opening Methodology"
J. A. Berrocal, M. B. Baker, L. Baldini, A. Casnati, S. Di Stefano, *Org. Biomol. Chem.*, **2018**, *16*, 7255-7264. (IF = 3.49)

61) "The Canonical Behavior of the Entropic Component of Thermodynamic Effective Molarity. An Attempt at Unifying Covalent and Noncovalent Cyclizations"
S. Di Stefano*, L. Mandolini*, *Phys. Chem. Chem. Phys.*, **2019**, *21*, 955-987. (IF = 3.43) (***Hot Article***).

62) "Enzyme-like Substrate-Selectivity in C-H Oxidation Enabled by Recognition"
G. Olivo*, G. Capocasa, O. Lanzalunga, S. Di Stefano*, M. Costas*, *Chem. Commun.*, **2019**, *55*, 917-920. (IF = 5.996)

63) “Coupled X-Ray Absorption/ UV-Vis Monitoring of Fast Oxidation Reactions Involving a Non-Heme Iron Oxo Complex”
G. Capocasa, F. Sessa, F. Tavani, G. Olivo, M. Monte, S. Pascarelli, O. Lanzalunga*, S. Di Stefano*, P. D'Angelo*, *J. Am. Chem. Soc.*, **2019**, *141*, 2299−2304. (IF = 14.61)

64) “Imine-based Iron and Manganese Complexes as Catalysts for Alkane Functionalization”
G. Olivo, O. Lanzalunga, S. Di Stefano, in *Alkane Functionalization*, Armando J. L Pombeiro, Maria de Fátima Costa Guedes da Silva (Eds.), John Wiley & Sons, Ltd., Hoboken (NJ), **2019**.

65) “Dissipative Catalysis with a Molecular Machine”
C. Biagini, S. D. P. Fielden, D. A. Leigh, F. Schaufelberger, S. Di Stefano, D. Thomas, *Angew. Chem. Int. Ed.*, **2019**, *58*, 9876-9880. (IF = 12.96) **(*Hot Paper, First Cover Angew. Chem. Int. Ed., Top Downloaded 2018-2019*)**

66) “2-Cyano-2-phenylpropanoic Acid Triggers the Back and Forth Motions of an Acid–Base-Operated Paramagnetic Molecular Switch”
P. Franchi, C. Poderi, E. Mezzina, C. Biagini, S. Di Stefano*, M. Lucarini*, *J. Org. Chem.*, **2019**, *84*, 9364−9368. (IF = 4.34)

67) “*N*-Hydroxyphthalimide: A Hydrogen Atom Transfer Mediator in Hydrocarbon Oxidations Promoted by Nonheme Iron(IV)−Oxo Complexes”
A. Barbieri, O. Lanzalunga, A. Lapi. S. Di Stefano, *J. Org. Chem.*, **2019**, *84*, 13549−13556. (IF = 4.34)

68) “The Hydrolysis of the Anhydride of 2-Cyano-2-phenylpropanoic Acid Triggers the Repeated Back and Forth Motions of an Acid- Base Operated Molecular Switch”
C. Biagini, G. Capocasa, V. Cataldi, D. Del Giudice, L. Mandolini, S. Di Stefano*, *Chem. Eur. J.*, **2019**, *25*, 15205 – 15211. (IF = 4.86)

69) “Abiotic Chemical Fuels for the Operation of Molecular Machines”
C. Biagini, S. Di Stefano*, *Angew. Chem. Int. Ed.*, **2020**, *59*, 8344 –8354. (IF = 15.34)

70) “Supramolecular Catalysts Featuring Crown Ethers as Recognition Units”
S. Di Stefano*, G. Capocasa, L. Mandolini*, *Eur. J. Org. Chem.*, **2020**, 3340–3350. (IF = 3.02) **(*Very Important Paper, VIP*)**

71) “Controlling the Liberation Rate of the In Situ Release of a Chemical Fuel for the Operationally Autonomous Motions of Molecular Machines”
C. Biagini, G. Capocasa, D. Del Giudice, V. Cataldi, L. Mandolini, S. Di Stefano*, *Org. Biomol. Chem.*, **2020**, *18*, 3867-3873. (IF = 3.88) (***Hot Article Collection***)

72) “Predictable Selectivity in Remote C-H Oxidation of Steroids: Analysis of Substrate Binding Mode”
G. Olivo*, G. Capocasa, B. Ticconi, O. Lanzalunga, S. Di Stefano*, M. Costas*, *Angew. Chem. Int. Ed.*, **2020**, 59, 12703–12708. (IF = 15.34) **(*Very Important Paper, VIP*)**

73) “Easy Synthesis of a Self-Assembled Imine-based Iron(II) Complex Endowed with Crown-ether Receptors”
G. Capocasa, M. Di Berto Mancini, F. Frateloreto, O. Lanzalunga, G. Olivo, S. Di Stefano*, *Eur. J. Org. Chem.*, **2020**, 3390–3397. (IF = 3.02)

74) “Direct Mechanistic Evidence for a Non-heme Complex Reaction Through a Multivariate XAS Analysis”
F. Tavani, A. Martini, G. Capocasa, S. Di Stefano, O. Lanzalunga, P. D'Angelo, *Inorg. Chem.*, **2020**, *59*, 14, 9979-9989. (IF = 5.17)

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