Società Chimica Italiana
Divisione di Chimica Farmaceutica

NMMC

BOOK OF ABSTRACTS

XXVII National Meeting on Medicinal Chemistry

UNIVERSITÀ DEGLI STUDI DI BARI ALDO MORO

7N 15P 6C 9F 14

14th Young Medicinal Chemists' Symposium
Nuove Prospettive in Chimica Farmaceutica

Palazzo Del Prete, Piazza Cesare Battisti
Università degli Studi di Bari Aldo Moro
September 11-14, 2022

WELCOME MESSAGE

The Scientific and Organizing Committees are pleased to welcome you in Bari for attending the 27th National Meeting in Medicinal Chemistry (NMMC27), organized by the *Medicinal Chemistry Division of the Italian Chemical Society* (DCF-SCI) and sponsored by the *European Federation of Medicinal Chemistry and Chemical Biology* (EFMC). Bari is a beautiful seaside town, rich in churches, palaces, piazzas, theatres and restaurants, with a special charm throughout the year.

NMMC27, jointly with the 14th Young Medicinal Chemists Symposium "Nuove Prospettive in Chimica Farmaceutica" (NPCF14), will give you the opportunity to share views about the challenges around the corner, as well as medicinal chemistry hot topics. After two years of virtual meetings, the 2022 edition of the NMMC/NPCF symposium will be a presential event, although restricted to fully vaccinated individuals.

The meeting will cover advances in drug discovery in major therapeutic areas, including the treatment of bacterial and viral infections, with a particular focus on the emerging COVID-19 pandemics, but also neurodegenerative and cardiovascular diseases, rare diseases, and cancer. In five scientific sessions, artificial intelligence and machine learning techniques as applied to drug discovery, the so-called "new modalities in medicinal chemistry" and the most recent advances in sustainable, chemical and biophysical technologies will be also featured. More importantly, participants will have the chance to establish and strengthen collaborative networks, a key option for successful research.

The meeting starts on September 11th with the Opening Ceremony and continues at the Aula Aldo Moro (Palazzo Del Prete, Piazza Cesare Battisti) from 12 to 14 September 2022. The scientific program will include five plenary and ten keynote lectures, as well as numerous oral and poster presentations. We actively encourage the participation of young scientists through dedicated grants and reduced registration fees.

More than 250 delegates from academia and industry are expected. Upon application, more than forty grants for young people, covering full registration fees and suitable accommodations, have been provided by DCF-SCI and other Institutional Sponsors.

Welcome in Bari!

Prof. Gianluca Sbardella	Prof. Maria Laura Bolognesi	Prof. Cosimo D. Altomare
Scientific Committee Chair	*President DCF-SCI*	*Local Organizing Committee Chair*

Scientific committee

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Department of Pharmacy – Pharmaceutical Sciences
University of Bari Aldo Moro

EFMC

European Federation
for Medicinal Chemistry
and Chemical Biology

EFMC is an independent association founded in 1969, representing 30 societies from 26 European countries, and more than **9000 scientists**. It's main objective is to **advance the science of medicinal chemistry and chemical biology.**

Upcoming Events

EFMC-YSN MedChemBioOnline

Webinars mixing science, soft-skills training
& round table discussions
www.efmc.info/efmc-ysn-medchembioonline

17th EFMC Short Course on Medicinal Chemistry

Oegstgeest, The Netherlands | April 23-26, 2023

EFMC-ASMC'25
IX International Symposium on Advances in Synthetic and Medicinal Chemistry

Zagreb, Croatia | September 3-7, 2023

EFMC-YMCS 2023
10th EFMC Young Medicinal Chemists' Symposium

Zagreb, Croatia | September 7-8, 2023

EFMC-ISCB 2023
International Symposium on Chemical Biology

Basel, Switzerland | November 16-18, 2023

Awards

— The Nauta Pharmacochemistry Award for Medicinal Chemistry and Chemical Biology
— The "UCB-Ehrlich Award for Excellence in Medicinal Chemistry"
— Prous Institute - Overton and Meyer Award for New Technologies in Drug Discovery
Visit **www.efmc.info/awards** for more information

Prizes

— EFMC Prizes for Young Medicinal Chemists in Industry & Academia
Visit **www.efmc.info/prizes** for more information

EFMC-YSN

The Young Scientists Network

Building a strong network at an early stage in your career is crucial!
The aim of the EFMC-YSN is to **inspire, connect** and **provide opportunities** to medicinal chemists and chemical biologists in their Early Career.
Visit **www.efmc.info/ysn** for more information

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SCIENTIFIC PROGRAM

Sunday, September 11th, 2022	
14.30-17.00	**REGISTRATION**
	Aldo Moro Hall
17.00-17.45	**OPENING CEREMONY** **Stefano Bronzini** – Rector of the University of Bari Aldo Moro **Antonio F. Uricchio** – President of ANVUR **Francesco Leonetti** – Head of the Department of Pharmacy-Pharmaceutical Sciences **Luigi D'Ambrosio Lettieri** – Vice-president of F.O.F.I. **Regional Political Authorities** **Gianluca Sbardella** – Chair of the Meeting **Maria Laura Bolognesi** – President of the Medicinal Chemistry Division **Cosimo D. Altomare** – Chair of the Local Organizing Committee
17.45-18.15	**Medicinal Chemistry Division of the Italian Chemical Society's Awards** **Francesco Merlino**, *University of Naples Federico II, Italy* **Laura Scalvini**, *University of Parma, Italy* **Best Doctoral Thesis Awards** Design and Synthesis of new PET radiotracers in drug discovery **Marco Maspero**, *University of Milan, Italy* Design and synthesis of (pro)electrophilic compounds for investigating the multifactorial nature of neurodegenerative diseases: focus on inflammation-driven events **Filippo Basagni**, *University of Bologna, Italy*
18.15-18.45	**Musajo Medal of the Medicinal Chemistry Division of the Italian Chemical Society** Recipient: **Gabriele Costantino**, *University of Parma, Italy*
	Chair: Maria Laura Bolognesi – President of the Medicinal Chemistry Division
18.45-19.45	**PL1:** Exploring molecular promiscuity through activity data analysis and explainable artificial intelligence **Jürgen Bajorath**, *University of Bonn, Germany*
20.00	**WELCOME BUFFET**

Monday, September 12th, 2022			
	Aldo Moro Hall		
	Chair: **Cosimo D. Altomare**		
9.00-9.50	**PL2**: Going with the flow - the use of continuous processing for synthesizing Active Pharmaceutical Ingredients **C. Oliver Kappe,** *University of Graz, Austria*		
	Aldo Moro Hall		**Vincenzo Starace Hall**
	Chairs: **Vincenza Andrisano**, **Orazio Nicolotti**		Chairs: **Violetta Cecchetti, Stefano Alcaro**
10.00-10.30	**KN1:** Computational approaches to the design of covalent drugs **Marco Mor,** *University of Parma, Italy* ***ChemMedChem Lecture***		**KN2:** Unleashing the potential of Translocator Protein as a therapeutic and diagnostic target: a successful MedChem tale **Sabrina Taliani**, *University of Pisa, Italy*
10.30-10.50	**OC1:** SQM-Score: Universal Quantum-Mechanical Scoring Function for Structure-based Drug Design **Adam Pecina**, *Czech Academy of Sciences Prague, Czech Republic*		**OC2:** Functionalized 6*H*-dibenzo[c,e]thiazine 5,5-dioxides are potent suppressors of the toxicity mediated by the cellular prion protein **Giuseppe Manfroni,** *University of Perugia, Italy*
10.50-11.00	**FC1:** Machine learning applied to early prediction of drug metabolism **Marta Lettieri**, *S-IN Soluzioni Informatiche srl, Vicenza, Italy*		**FC2:** Extra virgin olive oil extracts enriched in secoiridoids induce an anti-inflammatory profile in PBMCs from obese children **Stefania De Santis,** *University of Bari, Italy*
11.00-11.20	**COFFEE BREAK**		
11.20-11.40	**OC3:** The 3D-QSAR.COM portal as tool to develop predictive ligand-based and structure-based models for SARS-CoV-2 main protease inhibitors **Rino Ragno**, *Sapienza University of Rome, Italy*		**OC6:** Discovery of orexant and anorexant agents with indazole scaffold endowed with peripheral antiedema activity **Adriano Mollica**, *University of Chieti-Pescara G. D'Annunzio, Italy*
11.40-12.00	**OC4:** Development of a LC-MS platform for monoclonal antibody characterization to assist the production of a rituximab biosimilar from plants **Francesca Rinaldi**, *University of Pavia, Italy*		**OC7:** New class of potential antidiabesity agents targeting DPPIV and CAs enzymes **Laura Fumagalli**, *University of Milan, Italy*
12.00-12.20	**OC5:** A proof-of-concept of the analgesic effect of non-psychotropic *Cannabis sativa l.* and its main components on peripheral neuropathy **Federica Pellati**, *University of Modena and Reggio-Emilia, Italy*		**OC8:** Towards the characterization of corrector ARN23765 mechanism of action via photo-affinity labeling (PAL) approach **Francesco Saccoliti**, *Italian Institute of Technology, Genoa, Italy*
12.30-14.00	**LUNCH**		
14.00-15.30	**POSTER SESSION & COMMERCIAL EXHIBITION**		

Monday, September 12th, 2022

	Aldo Moro Hall		Vincenzo Starace Hall
	Chair: **Gabriele Costantino**, **Giovanni Lentini**		Chair: **Maria Laura Bolognesi**, **Roberto Di Santo**
15.30-16.00	**KN3:** Synthetic lethality for next generation precision oncology **Andrea Cavalli,** *University of Bologna, Italy*		**KN4:** A nature inspired approach to develop covalent enzyme inhibitors with anti-infective and anticancer activity **Paola Conti**, *University of Milan, Italy*
16.00-16.20	**OC9:** New nicotinamide mimic scaffold allowed nanomolar inhibition of human PARP enzymes **Oriana Tabarrini**, *University of Perugia, Italy*		**OC11:** Broad spectrum metallo β-lactamases inhibitors: new tools against clinically-relevant carbapenemases **Loretta Lazzarato**, *University of Turin, Italy*
16.20-16.40	**OC10:** Spindlin-1 degraders: stairway to heaven (?) **Monica Viviano,** *University of Salerno, Italy*		**OC12:** Novel dipeptide nitriles as antitrypanosomal agents targeting rhodesain of *Trypanosoma brucei rhodesiense*: development and combination studies **Roberta Ettari**, *University of Messina, Italy*
16.40-17.00	**COFFEE BREAK**		
17.00-17.20	**OC13:** TRPM8 ion channel: new target in the treatment of castration-resistant prostate cancer (CRPC) **Veronica Di Sarno,** *University of Salerno, Italy*		**OC15:** The PADAM oxidation route for the synthesis of SARS-CoV-2 main protease inhibitors **Sveva Pelliccia**, *University of Naples Federico II, Italy*
17.20-17.40	**OC14:** Challenge transability of "in vitro" to "in vivo": gene-expression biomarkers and fluorescent image-guided surgery probes identification for ovarian cancer **Antonio Scilimati**, *University of Bari, Italy*		**OC16:** Discovery of diketo acid derivatives targeting the SARS-CoV-2 NSP13 helicase **Valentina Madia**, *Sapienza University of Rome, Italy*
17.40-17.50	**FC3:** Combining mass spectrometry and nuclear magnetic resonance for the study of ligand:G-quadruplex interaction **Erika Oselladore**, *University of Brescia, Italy*		**OC17:** An integrated medicinal chemistry workflow for the development of new peptides as SARS-CoV-2 MPro covalent inhibitors **Simona Musella,** *University of Salerno, Italy*
17.50-18.00	**FC4:** Carbazole derivatives as multi-target agents in breast cancer treatment **Jessica Ceramella**, *University of Calabria, Italy*		
18.00-19:00	**NETWORKING**		
	Tavola rotonda ***Malattia di Lafora: dalla ricerca di farmaci ai diritti dei pazienti*** ***Per una stretta cooperazione tra ricerca e assistenza*** **G. d'Orsi, T. Bressanello, G. Annichiarico, A. Liantonio, G. Costantino, C. Altomare**		**Workshop** **Why was my paper rejected? Optimizing manuscripts for successful submission and publication** **David Peralta**, Editor-in-Chief ChemMedChem, Wiley-VCH
19:30	**CONCERT OF CORUS HARMONIA – BASILICA DI S. NICOLA**		

Tuesday, September 13th, 2022

	Aldo Moro Hall		
	Chair: **Nicola A. Colabufo**		
9.00-9.50	**PL3**: Innovative strategies to target non-coding RNAs with synthetic ligands **Maria Duca**, *Université Côte d'Azur Nice, France*		
	Aldo Moro Hall		**Vincenzo Starace Hall**
	Chairs: **Patrizia Diana**, **Francesco Leonetti**		Chairs: **Enza Lacivita**, **Tiziano Bandiera**
10.00-10.30	**KN5:** Targeting dopamine D4 receptor as a thrilling challenge to explore new therapeutic opportunities **Fabio Del Bello**, *University of Camerino, Italy*		**KN6:** Identification of ARN21641, an orally available and CNS penetrant Acid Ceramidase inhibitor with target engagement in mouse models of Gaucher and Krabbe diseases **Rita Scarpelli**, *Italian Institute of Technology, Genoa, Italy*
10.30-10.50	**OC18:** Development of novel enzyme inhibitors of the endocannabinoids' catabolism for the treatment of epilepsy and neuroinflammatory conditions **Stefania Butini**, *University of Siena, Italy*		**OC19:** Hijacking the folding process for targeted protein degradation **Andrea Astolfi**, *University of Perugia, Italy*
10.50-11.00	**FC5:** Targeting the mycobactin biosynthesis pathway in *M. tuberculosis*: a step towards the improvement of the anti-virulence activity of MbtI inhibitors **Matteo Mori**, *University of Milan, Italy*		**FC6:** Development of hydrogen sulfide-releasing hybrids as novel multitarget drugs **Angela Corvino**, *University of Naples Federico II, Italy*
11.00-11.20	**COFFEE BREAK**		
11.20-11.40	**OC20**: The pivotal role of pyrrolidine ring as multitarget scaffold in neurodegenerative diseases **Antonio Carrieri**, *University of Bari, Italy*		**OC23:** Nucleic acid aptamers: potential therapeutic agents for cancer and neurodegenerative disorders **Jussara Amato**, *University of Naples Federico II, Italy*
11.40-12.00	**OC21:** Pursuing the complexity of bipolar disorder: rational design and optimization of first-in-class D3R/GSK-3β modulators towards an in vivo proof of concept **Rita M.C. Di Martino**, *Italian Institute of Technology, Genoa, Italy*		**OC24:** Combining quantum mechanics and machine learning in the search of the bioactive conformation of drug-like compounds **Antonio Viayna**, *University of Barcelona, Spain*
12.00-12.20	**OC22:** S.M.A.R.T. steroids: synthesis and structure-activity relationship study towards allosteric modulators of *N*-methyl-D-aspartate receptors **Eva Kudova**, *Czech Academy of Sciences Prague, Czech Republic*		**OC25:** Challenging bioisosteric switch in AChE-MAO B dual-targeting hit optimization **Leonardo Pisani**, *University of Bari, Italy*
12.30-14.00	**LUNCH**		
14.00-15.30	**POSTER SESSION & COMMERCIAL EXHIBITION**		

Tuesday, September 13th, 2022			
	Aldo Moro Hall		**Vincenzo Starace Hall**
	Chair: **Giannamaria Annunziato**, **Laura Scalvini**		Chair: **Isabella Romeo**, **Francesco Merlino**
15.30-16.00	**KN7:** From the catalytic mechanism to the enzyme substrate selectivity: a study on *N*-acylethanolamine acid amidase **Laura Scalvini,** *University of Parma, Italy*		**KN8:** From natural resource to preclinical candidate: our experience with the temporin-derived peptide antimicrobial agents **Francesco Merlino**, *University of Naples Federico II, Italy*
16.00-16.10	**FC7:** Discovery of 2-(4-hydroxy-3,5-dimethylphenyl)-*N*-(pyridin-2-yl)-1*H*-benzo[*d*]imidazole-6-sulfonamide as BET inhibitor with selectivity for the first bromodomain **Alessandra Cipriano**, *University of Salerno, Italy*		**FC11:** Tetrahydropyran and cyclohexane linked novel bacterial topoisomerase inhibitors with improved balanced antibacterial activity and safety profile **Maja Kokot**, *National Institute of Chemistry, Ljubljana, Slovenia*
16.10-16.20	**FC8:** First-in-class selective inhibitors of the histone acetyltransferase KAT8 **Francesco Fiorentino**, *Sapienza University of Rome, Italy*		**FC12:** Miconazole-like scaffold is a promising lead for developing *Naegleria fowleri*-specific brain permeable CYP51 inhibitors **Valeria Tudino**, *University of Rome Tor Vergata, Italy*
16.20-16.30	**FC9:** Design, synthesis, and biological evaluation of new hybrid MOR agonist/HDACi compounds: an innovative approach for persistent pain management **Giuliana Costanzo**, *University of Catania, Italy*		**FC13:** Structural modifications of triazine-based compounds for high-efficiency PDK inhibition **Camilla Pecoraro**, *University of Palermo, Italy*
16.30-16.40	**FC10:** Visible-light photocatalytic activity of isocyanides: from the proof-of-concept to the synthetic application in Ugi-like chemistry **Camilla Russo**, *University of Naples Federico II, Italy*		**FC14:** In silico assisted discovery of dual 5-LOX/sHE inhibitors: in vitro characterization and in vivo anti-inflammatory properties **Tania Ciaglia**, *University of Salerno, Italy*
16.40-17.00	**COFFEE BREAK**		
17.00-17.30	**In memoriam of Prof. Vincenzo Tortorella (1932-2022)** **Celebration of retired colleagues**		
17.30-19.30	**DCF-SCI GENERAL MEETING (ASSEMBLEA DELLA DIVISIONE DI CHIMICA FARMACEUTICA)**		
20.30	**SOCIAL DINNER AT RISTORANTE ZONNO (Lungomare di Bari)**		

Wednesday September 14th, 2022

	Aldo Moro Hall		
	Chair: **Marcello Leopoldo**		
9.00-9.50	**PL4**: Targeting chemokine receptor CCR2 - From insurmountable antagonists to affinity-based probes **Laura Heitman**, *Leiden University, The Netherlands*		
	Aldo Moro Hall		**Vincenzo Starace Hall**
	Chairs: **Marco Catto**, **Marcello Leopoldo**		Chairs: **Gianluca Sbardella**, **Cosimo D. Altomare**
10.00-10.30	**KN9:** Development and hands-on application of PyRMD: a new AI-powered virtual screening tool **Sandro Cosconati,** *Luigi Vanvitelli University, Naples, Italy*		**KN10:** The discovery of potent and selective agonists of human transient receptor potential Cation Channel Subfamily M member 5: from HTS to early hit validation **Alessio Barilli**, *Aptuit, an Evotec Company, Verona, Italy*
10.30-10.50	**OC26:** exploring CCRL2 Chemerin binding using accelerated molecular dynamics **Antonio Coluccia**, *Sapienza University of Rome, Italy*		**OC28:** The first in vivo proof-of-concept for the efficacy of selective HDAC6 inhibition in cystic fibrosis: anti-inflammatory profile, effects on bacterial load, formulation and biodistribution studies **Margherita Brindisi**, *University of Naples Federico II, Italy*
10.50-11.10	**OC27:** Functionalized ligands targeting G protein-coupled adenosine receptors **Stephanie Federico,** *University of Trieste, Italy*		**OC29:** New insights in the development of cannabinoid receptor subtype 2 (CB2R) ligands **Marialessandra Contino,** *University of Bari, Italy*
11.10-11.30	**COFFEE BREAK**		
11.30-11.50	**OC30:** Optimizing the choice of 3D query structures in ligand-based virtual screenings with PharmScreen® **Giorgia Zaetta,** *Parc Científic de Barcelona, Spain*		**OC32:** Novel cyclic uPA-derived decapeptides reduce in vivo lung dissemination and re-educate CAF phenotype by acting through integrin αvβ5 **Alfonso Carotenuto**, *University of Naples Federico II, Italy*
11.50-12.10	**OC31:** A computational grid-based analysis to map drug-like peptide binding pockets of peptide-protein interactions systems **Daniela Trisciuzzi,** *University of Bari, Italy*		**OC33:** Screening of amino-acid-anthraquinone click chemistry conjugates targeting human telomeric G-quadruplexes **Giovanni Ribaudo,** *University of Brescia, Italy*
	Aldo Moro Hall		
	Chair: **Gianluca Sbardella**		
12.10-13.10	**PL5**: COVID-19 pandemic: what we learnt in antiviral drug discovery, successes, and failures **Vincenzo Summa,** *University of Naples Federico II, Italy*		
13.10-13.30	**CLOSING REMARKS and POSTER PRIZES**		
13.30	**LUNCH**		

PO-032

IPEROXO/DEQUALINIUM AND W84/DEQUALINIUM HYBRID LIGANDS: SYNTHESIS, PHARMACOLOGICAL AND COMPUTATIONAL INVESTIGATION AT M_2 mAChRs

Papotto, C.;[a] Matera, C.;[a] Brivio, N.;[a] Maspero, M.;[a] De Amici, M.;[a] Morando, S.;[b] Matucci, R.;[b] Vistoli, G.;[a] and Dallanoce, C.[a]

[a] *Department of Pharmaceutical Sciences, University of Milan, via L. Mangiagalli 25, 20133 Milano, Italy;*
[b] *Department of Neuroscience, Psychology, Drug Research and Child's Health, Section of Pharmacology and Toxicology, University of Florence, viale G. Pieraccini 6, 50139 Florence, Italy*

clelia.dallanoce@unimi.it

The use of bitopic ligands to study the properties of Muscarinic Acetylcholine Receptors (mAChRs) is a very active field of research.[1,2,3] In this regard, bipharmacophoric molecular probes were found to switch between two different binding orientations in the M_2 subtype, resulting in both active and inactive populations of receptors bound by a given ligand, a behavior that has been termed dynamic ligand binding.[2] Continuing our interest in this field, we focused our attention on the properties of Dequalinium chloride, a bis-pyridinium quaternary ammonium compound, which was recently reported to act as a potent muscarinic allosteric modulator, showing an overall selectivity towards the M_2 subtype.[4] Starting from this observation, we designed and synthesized two series of novel hybrid ligands incorporating in their molecular skeleton the allosteric moiety of Dequalinium (**Figure 1**). The first series is based on the combination of Dequalinium with the orthosteric superagonist Iperoxo and aimed at novel chemical probes interacting cooperatively with both the orthosteric and the allosteric binding site. In the second series, Dequalinium was hybridized with the allosteric modulator W-84, affording new putative allo/allosteric ligands.

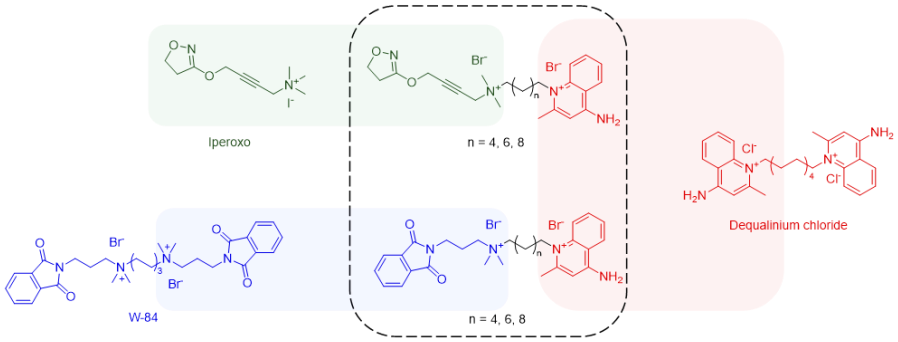

Figure 1: The new Dequalinium hybrid ligands.

In this study, the newly synthetized compounds have been characterized through competitive binding assays at the five mAChR subtypes. The activity on the allosteric site has been investigated by measuring the affinity ($logK_{occ}$) at the [^{3}H]-NMS-occupied muscarinic hM_2 subtype. Moreover, docking simulations have been performed to highlight the interactions within the ortho/allosteric binding pockets of the hM_2 crystal structure addressing the role of linker length. The synthetic approach and the details of the pharmacological and computational investigations will be illustrated and discussed.

References

1. Holze, J.; Bermudez, M.; Pfeil, E.M.; Matera, C.; Dallanoce, C.; De Amici, M. *et al. ACS Pharmacol. Transl. Sci.* **2020**, 3, 859–867.
2. Bock, A.; Bermudez, M.; Krebs, F.; Matera, C.; Chirinda, B.; Sydow, D.; Dallanoce, C. *et al. J. Biol. Chem.* **2016**, *291*, 16375.
3. Bock, A.; Merten, N.; Schrage, R.; Dallanoce C.; Bätz J.; Klöckner J.; Schmitz J.; Matera C. *et al. Nat. Commun.* **2012, *2*,** 1044.
4. Mazzolari, A.; Gervasoni, S.; Pedretti, A.; Fumagalli, L.; Matucci, R.; Vistoli, G. *Int. J. Mol. Sci.* **2020**, *21*, 5961.