



**33<sup>rd</sup> GP<sub>2</sub>A Annual Medicinal Chemistry Conference,  
XIV<sup>th</sup> Paul Ehrlich MedChem Euro-PhD Network Meeting  
& COST Action One Health drugs against parasitic vector borne diseases  
in Europe and beyond (OneHealth*drugs*)**

**Nantes Université - France**

**11<sup>th</sup> – 13<sup>th</sup> June 2025**

**PROGRAMME**

**SPONSORS**



<b>Wednesday 11<sup>th</sup> June 2025</b>	
<i>Venue: Amphi Virginie Ferré, School of Pharmacy NU</i>	
10:00 – 12:00	<b>Workshop:</b> Artificial intelligence in drug discovery: a new era of molecular design <b>Dr. Dylan Sérillon</b> , WhiteLab Genomics, Paris, France
13:00 – 17:00	Registration open
<b>Session 1 - Session chair</b>	
<b>Prof. Pascal Marchand</b> , Vice-Dean for Research, School of Pharmacy, Nantes Université, France	
14:00 – 14:20	Opening of the conference <b>Assoc. Prof. Florence McCarthy</b> , University College, Cork, Ireland Chair of the GP <sub>2</sub> A Committee <b>Prof. Fernanda Borges</b> , University of Porto, Portugal Coordinator of the Paul Ehrlich MedChem Euro-PhD Network <b>Prof. Maria Paola Costi</b> , University of Modena and Reggio Emilia, Italy Chair of the COST Action OneHealth <i>drugs</i>
14:20 – 14:55	<b>KN1:</b> Discovery and structure-activity relationships of cyclic antimicrobial peptides <b>Dr. Rachael Dickman</b> , University College London, UK
14:55 – 15:10	<b>OC1:</b> Evaluation of SQ109 and Bedaquiline efficacy against <i>Mycobacterium abscessus</i> using transposon mutagenesis under host-like conditions <b>Benedetta Salvucci</b> , Sapienza University of Rome, Italy
15:10 – 15:25	<b>OC2:</b> Synthesis and optimization of novel peptidomimetics derivatives inhibiting the efflux pumps of <i>Pseudomonas aeruginosa</i> <b>Mélanie Sébastien</b> , Université Paris Cité, France
15:25 – 16:00	Coffee Break, Sponsor Exhibitions and Poster Viewing
<b>Session 2 - Session chair</b>	
<b>Assoc. Prof. Vânia M. Moreira</b> , University of Coimbra, Portugal	
16:00 – 16:35	<b>KN2:</b> Discoveries in natural products chemistry from renewable biomass: addressing synthetic and therapeutic challenges, abietanes' story <b>Dr. Miguel Angel González Cardenete</b> , Universitat Politècnica de Valencia-CSIC, Spain

16:35 – 16:50	<b>OC3:</b> Development of functionalized amidrazones as an original nitrogen heterocycle for use in DEL Chemistry <b>Margaux Boutin</b> , Nantes Université, France
16:50 – 17:05	<b>OC4:</b> Phenolic cinnamic acid derivatives as selective COX-2 inhibitors: design, synthesis and biological activity studies <b>João Sousa Janela</b> , University of Coimbra, Portugal
17:05 – 17:20	<b>OC5:</b> Launching into the objective space: multi-objective optimization in REINVENT <b>Laura Landolfi</b> , University of Naples Federico II, Italy
17:20 – 17:35	<b>OC6:</b> NORUS: an AI-powered framework for assessing scientific originality and similarity <b>Marina Bilotta</b> , University "Magna Græcia" of Catanzaro, Italy
17:35 – 18:05	<b>FP1-FP10:</b> Flash Poster communications
18:05 – 19:30	<b>Welcome Reception</b> (included in conference registration cost) <i>Venue: Amphi Virginie Ferré, School of Pharmacy NU</i>

<b>Thursday 12<sup>th</sup> June 2025</b> <i>Venue: Amphi Virginie Ferré, School of Pharmacy NU</i>	
8:30 – 16:00	Registration open
<b>Session 3 COST Action OneHealth<i>drugs</i> - Session chairs</b> <b>Prof. Maria Paola Costi</b> , University of Modena and Reggio Emilia, Italy <b>Prof. Stefano Alcaro</b> , University of Catanzaro, Italy	
09:00 – 09:35	<b>KN3:</b> Leveraging medicinal chemistry for the United Nations Sustainable Development Goals <b>Prof. Maria Laura Bolognesi</b> , University of Bologna, Italy
09:35 – 09:45	<b>Gold sponsor presentation - CEM</b>
09:45 – 10:20	<b>KN4:</b> Purine nucleoside analogues as promising agents against protozoan pathogens in humans and livestock <b>Prof. Serge Van Calenbergh</b> , Ghent University, Belgium
10:20 – 11:20	<b>Coffee Break, Sponsor Exhibitions and Poster Session 1</b>
11:20 – 11:35	<b>OC7:</b> Development and characterization of Mucroporin-M1 analogues: improved stability, structural analysis and virucidal activity <b>Claudia Storti</b> , Universities of Pavia & Padova, Italy
11:35 – 11:50	<b>OC8:</b> Identification and further optimization of 4,5-dihydropyrazole scaffold as potential West Nile NS3 helicase inhibitors <b>Giulia Atzeni</b> , University of Cagliari, Italy

11:50 – 12:05	<b>OC9:</b> Structure-activity relationships and ADMETox profiling of novel isonipecotamide-based O-glycosides as highly potent DOACs for thromboembolic disorders <b>Caterina Deruvo</b> , University of Bari "Aldo Moro", Italy
12:05 – 12:35	<b>FP11-FP20:</b> Flash Poster communications
12:35 – 13:45	Lunch, Sponsor Exhibitions and Poster Viewing
<b>Session 4 - Session chairs</b> <b>Prof. Susan E. Matthews</b> , University of Sheffield, UK <b>Assoc. Prof. Shailesh Mistry</b> , University of Nottingham, UK	
13:45 – 14:20	<b>KN5:</b> Pleiotropic prodrugs: a polypharmacological approach to the treatment of neurodegenerative diseases <b>Prof. Christophe Rochais</b> , Université de Caen Normandie, France
14:20 – 14:55	<b>KN6:</b> Casein Kinase 1: where we are and where we are going <b>Dr. Stephanie Federico</b> , University of Trieste, Italy
14:55 – 16:00	Coffee Break, Sponsor Exhibitions and <b>Poster Session 2</b>
16:00 – 16:15	<b>OC10:</b> Design of melanostatin-based derivatives for application in Parkinson's disease <b>Beatriz Lopes Pires de Lima</b> , University of Porto, Portugal
16:15 – 16:30	<b>OC11:</b> Discovery of potent acyl-CoA synthetase long chain family member 4 (ACSL4) inhibitors with anti-ferroptotic properties <b>Emeline Charnelle</b> , University of Lille, France
17:00 – 19:00	<b>Optional Activity (prebooking only)</b> THE PERMANENT JOURNEY-HISTORIC HEART, Guided Tour of Nantes
19:00 – 20:00	GP <sub>2</sub> A committee meeting ( <i>committee only</i> ) Venue: Room 51 School of Pharmacy NU Meeting of Paul Ehrlich coordinators ( <i>coordinators only</i> ) Venue: Room 52 School of Pharmacy NU
20:30	<b>Conference Dinner (prebooking only)</b> Restaurant FELIX, 1 rue Lefèvre-Utile – 44000 Nantes

**Friday 13<sup>th</sup> June 2025**

**Venue: Amphi Virginie Ferré, School of Pharmacy NU**

**Session 5 - Session chair**

**Assoc. Prof. Niamh O'Boyle, TCD University of Dublin, Ireland**

9:00 – 9:35	<b>KN7:</b> Glycoconjugates as anti-virulence agents to combat fungal infection <b>Dr. Trinidad Velasco-Torrijos</b> , Maynooth University, Co. Kildare, Ireland
9:35 – 9:50	<b>OC12:</b> Targeting CtBP1 in Acute Myeloid Leukemia: optimization of HIPP derivatives and PROTAC development <b>Chaimae El Hadri</b> , Ghent University, Belgium
9:50 – 10:05	<b>OC13:</b> Development of orellanine conjugates for the treatment of cancer <b>Mark J. Lyons</b> , Trinity College Dublin, Ireland
10:05 – 10:25	<b>FP21-FP26:</b> Flash Poster communications
10:25 – 11:20	<b>Coffee Break, Sponsor Exhibitions and Poster Session 3</b>

**Session 6 - Session chair**

**Prof. Diego Muñoz-Torrero, University of Barcelona, Spain**

11:20 – 11:35	<b>OC14:</b> Unlocking new allosteric chemotypes for AKT1 modulation in cancer <b>Marta Casciari</b> , University of Perugia, Italy
11:35 – 11:50	<b>OC15:</b> Design, synthesis and screening of novel prenylated chalcones as potential anti-cancer agents <b>Mouna Hind Laiche</b> , Royal College of Surgeons in Ireland, Dublin
11:50 – 12:05	<b>OC16:</b> Discovery of highly potent BET inhibitors based on a tractable tricyclic scaffold <b>Jaffer M. Zaidi</b> , University of Nottingham, UK
12:05 – 12:20	<b>OC17:</b> Another way of predicting PROTAC permeability <i>in silico</i> <b>Laura Márquez Cantudo</b> , Universidad CEU San Pablo, Madrid, Spain
12:20 – 13:15	<b>Lunch, Sponsor Exhibitions and Poster Viewing</b>

**Session 7 - Session chairs**

**Assoc. Prof. Florence McCarthy, Prof. Fernanda Borges, Prof. Maria Paola Costi,  
Prof. Pascal Marchand**

	<b>PE MedChem Euro-PhD Label communications PEA1-PEA8</b>
13:15 – 13:30	<b>PEA1:</b> Design and synthesis of SARS-COV-2 helicase inhibitors <b>Dr. Erica Sanna</b> , University of Cagliari, Italy
13:30 – 13:45	<b>PEA2:</b> New prospects on the benzo[ <i>b</i> ]thiophene-3-ol scaffold: design, synthesis, and biological evaluation of novel monoamine oxidase inhibitors & photocatalytic functionalization of dehydroalanine-derived peptides <b>Dr. Francesca Arrighi</b> , Sapienza University of Rome, Italy
13:45 – 14:00	<b>PEA3:</b> MAATrica: a measure for assessing consistency and methods in medicinal and nutraceutical chemistry papers <b>Dr. Giulia Panzarella</b> , University "Magna Græcia" of Catanzaro, Italy
14:00 – 14:15	<b>PEA4:</b> Targeting proteins involved in neurodegenerative diseases and cancer: from traditional structure-based approaches to Artificial Intelligence models <b>Dr. Lisa Lombardo</b> , University of Messina, Italy
14:15 – 14:30	<b>PEA5:</b> Unraveling the mechanism of action of the innovative antileishmanial agent H80 through fluorescence imaging and multi-omics profiling <b>Dr. Lorenzo Tagliazucchi</b> , University of Parma, Italy
14:30 – 14:45	<b>PEA6:</b> Exploring triazole and thiazole systems for antiviral applications <b>Dr. Roberta Bivacqua</b> , University of Palermo, Italy
14:45 – 15:00	<b>PEA7:</b> Development and characterization of novel 2-arylbenzofuran derivatives as potent and selective human monoamine oxidase B inhibitors: new tools to tackle neurodegenerative diseases <b>Dr. Michele Coluccia</b> , Sapienza University of Rome, Italy
15:00 – 15:15	<b>PEA8:</b> Identification of small heterocycles to tackle emerging infectious threats <b>Dr. Giada Cernicchi</b> , University of Perugia, Italy
15:15 – 15:50	<b>KN8:</b> Expediting drug discovery for undruggable targets using AI <b>Prof. Michele Vendruscolo</b> , University of Cambridge, UK
15:50 – 16:15	<b>Prize Announcements</b> (Early career presentations, flash poster and poster presentations) <b>Other Announcements &amp; Conference Close</b>

## LIST OF FLASH POSTER COMMUNICATIONS

Number	Last name	First name	Affiliation	Country
FP01	Lemaitre	Thomas	Université de Caen Normandie	France
FP02	Sarnari	Chiara	University of Perugia	Italy
FP03	Buttitta	Giorgio	Sapienza University of Rome	Italy
FP04	Faloci	Federico	University of Padova	Italy
FP05	Scaviner	Mathieu	Nantes Université	France
FP06	Primavera	Erika	University of Perugia	Italy
FP07	Magniez	Antoine	Université de Caen Normandie	France
FP08	Coderch Boué	Claire	Universidad CEU San Pablo, Madrid	Spain
FP09	Lafon	Juliette	University of Lille	France
FP10	Leblond	Auriane	Université d'Angers	France
FP11	Aliyeva	Gunel	Baku State University	Azerbaijan
FP12	Almeida	Hugo	University of Porto	Portugal
FP13	Ganter	Benedikt	University of Hamburg	Germany
FP14	Rijono	Desiree	University of Hamburg	Germany
FP15	Hébert	Olivier	Université de Caen Normandie	France
FP16	Demuru	Laura	University of Cagliari	Italy
FP17	Onali	Alessia	University of Cagliari	Italy
FP18	Gréverie	Marie	Université de Picardie Jules Verne, Amiens	France
FP19	Cornu	Marie	Université de Caen Normandie	France
FP20	Van Hauwermeiren	Anouk	Ghent University	Belgium
FP21	Lo Mascolo	Fabiana	University of Palermo	Italy
FP22	Marra	Maria	Università della Calabria	Italy
FP23	Chieffallo	Martina	University of Calabria	Italy
FP24	Scarcelli	Eva	University of Calabria	Italy
FP25	Dal Ponte	Nicolò	University of Padova	Italy