



17th-20th September 2023 / Chieti, University "G. d'Annunzio" of Chieti-Pescara

Scientific Program / Sunday, 17th September

| | |
|-------|--|
| 14.30 | REGISTRATION Auditorium Rectorate (University "G. d'Annunzio" of Chieti-Pescara) |
| 17.00 | OPENING CEREMONY Liborio Stuppia, Rector of the University "G. d'Annunzio" of Chieti-Pescara Amelia Cataldi, Head of the Department of Pharmacy of the University "G. d'Annunzio" of Chieti-Pescara Luigi Brunetti, President of the Faculty of Pharmacy of the University "G. d'Annunzio" of Chieti-Pescara Maria Laura Bolognesi, President of the Medicinal Chemistry Division - Italian Chemical Society Adriano Mollica, Chair of the Local Organizing Committee |
| 17.30 | Chair: Maria Laura Bolognesi, President of the Medicinal Chemistry Division - Italian Chemical Society MEDICINAL CHEMISTRY DIVISION - ITALIAN CHEMICAL SOCIETY AWARDS Chiara Borsari, University of Milan, Italy Antonella Ciancetta, University of Ferrara, Italy BEST DOCTORAL THESIS AWARDS FC: Francesca Annunziata, University of Milan, Italy DEVELOPMENT OF SUSTAINABLE AND EFFICIENT TAILOR-MADE PROCESSES FOR PHARMA AND FOOD APPLICATIONS FC: Giulia Bononi, University of Pisa, Italy DEVELOPMENT OF THERAPEUTIC AND DIAGNOSTIC AGENTS TARGETING TUMOR LIPID AND SUGAR METABOLISM |
| 18.00 | PRATESI MEDAL, MEDICINAL CHEMISTRY DIVISION - ITALIAN CHEMICAL SOCIETY Dario Neri, Philogen S.p.A., Italy & ETH Zürich, Switzerland THE DREAM OF PAUL EHRLICH |
| 18.45 | PL1: Kelly Chibale, University of Cape Town, South Africa MEDICINAL CHEMISTRY APPROACHES TO REPOSITIONING ANTICANCER HUMAN KINASE INHIBITORS FOR MALARIA |
| 20.00 | WELCOME BUFFET |

Scientific Program / Monday, 18th September

| | |
|--|--|
| Aula Magna (Department of Pharmacy) Chair: Adriano Mollica | |
| 9.00 | PL2: Steven Ballet, Vrije Universiteit Brussel, Belgium DEVELOPMENT OF GENERIC G PROTEIN PEPTIDOMIMETICS ABLE TO STABILIZE ACTIVE STATE G_s PROTEIN-COUPLED RECEPTORS FOR APPLICATION IN DRUG DISCOVERY |
| Aula Magna (Department of Pharmacy) Chairs: Adriano Mollica, Francesco Epifano | |
| Aula 3 (Department of Pharmacy) Chairs: Patrizia Diana, Salvatore Genovese | |
| 10.00 | KN1: Paolo Rovero, University of Florence, Italy THE CONTRIBUTION OF PEPTIDE RESEARCH TO THE FIGHT AGAINST SARS-COV-2: FROM VACCINES TO ANTIVIRALS |
| KN2: Alessia Bertamino, University of Salerno, Italy DESIGN AND DEVELOPMENT OF NEW SOLUBLE EPOXIDE HYDROLASE INHIBITORS AS PHARMACOLOGICAL TOOLS IN INFLAMMATORY DISEASE | |
| 10.30 | OC1: Marina Sala, University of Salerno, Italy GREENING THE SOLID-PHASE PEPTIDE SYNTHESIS: FURTHER CHALLENGES TO IMPROVE SUSTAINABILITY IN THE DEVELOPMENT OF THERAPEUTIC PEPTIDES |
| OC2: Valeria Pittalà, University of Catania, Italy RECENT ADVANCES IN THE DISCOVERY OF HEME OXYGENASE-1 INHIBITORS WITH ANTICANCER ACTIVITY | |
| 10.50 | FC1: Michela Buonocore, University of Salerno, Italy EXPLOITING THE FEATURES OF SHORT PEPTIDES TO RECOGNIZE SPECIFIC CELL SURFACE MARKERS |
| FC2: Manuela Giovanna Basilicata, University of Salerno, Italy IN VITRO CHEMICAL AND METABOLIC STABILITY AND IN VIVO PHARMACOKINETIC STUDIES OF A CONFORMATIONALLY RESTRICTED RETIGABINE ANALOGUES AS NOVEL NEURONAL KV7 CHANNEL ACTIVATORS | |
| 11.00 COFFEE BREAK | |
| 11.20 | OC3: Federica Moraca, University of Naples "Federico II", Italy DISCOVERING ALZHEIMER'S A β-AMYLOID FIBRILLOGENESIS INHIBITOR PEPTIDES THROUGH A COMBINED 3D-GRID PHARMACOPHORE AND METADYNAMICS STRATEGY |
| OC6: Alessandra Anna Altomare, University of Milan, Italy THINNED APPLE POLYPHENOLS ALLEVIATE INFLAMMATION IN A MOUSE MODEL OF DNBS-INDUCED COLITIS: LABEL-FREE QUANTITATIVE PROTEOMICS STUDIES | |
| 11.40 | OC4: Emanuela Salvati, University of Salerno, Italy FLEXIBLE SPATIAL-MASS SPECTROMETRY STRATEGY APPLIED TO TRAUMATIC BRAIN INJURY AND ITS ASSOCIATION WITH ALZHEIMER'S DISEASE |
| OC7: Marco Paolino, University of Siena, Italy DONEPEZIL-LIKE DUAL TARGET AChE AND MAO-B INHIBITORS WITH PHOTOMODULABLE INHIBITORY ACTIVITY | |
| 12.00 | OC5: Claudia Mugnaini, University of Siena, Italy A DUAL-TARGET APPROACH FOR THE TREATMENT OF ALZHEIMER'S DISEASE |
| OC8: Filippo Basagni, University of Bologna, Italy FYN/GSK-3β DOUBLE KINASE INHIBITORS TO INVESTIGATE NEUROINFLAMMATORY PROCESSES IN NEURODEGENERATIVE DISEASES | |
| 12.30 LUNCH 14.00 POSTER SESSION & COMMERCIAL EXHIBITION | |
| Aula Magna (Department of Pharmacy) Chair: Stefano Alcaro | |
| 15.10 | PL3: Zoe Cournia, Biomedical Research Foundation, Academy of Athens, Greece EXPLOITING ALLOSTERY FOR COMPUTER-AIDED DRUG DESIGN TO TARGET ONCOGENES |
| Aula Magna (Department of Pharmacy) Chairs: Stefano Alcaro, Violetta Cecchetti | |
| Aula 3 (Department of Pharmacy) Chairs: Gianluca Sbardella, Stefano Moro | |
| 16.00 | KN3: Alessandro Accetta, Chiesi Farmaceutici, Italy MEDICINAL CHEMISTRY OF INHALED DRUGS: EXAMPLES FROM VALIDATION TO PRECLINICAL CANDIDATES |
| KN4: Giovanni Bottegoni, University of Urbino, Italy IN SILICO POLYPHARMACOLOGY STUDIES FOR CNS CONDITIONS | |
| 16.30 | OC9: Bruno Cerra, University of Perugia, Italy INTEGRATED FLOW PLATFORM TO STREAMLINE THE SYNTHESIS OF BIOLOGICALLY-ACTIVE STEROIDS |
| OC11: Valentina Straniero, University of Milan, Italy PK7: A SYNAPTIC TARGETING COMPOUND TO OVERCOME PARKINSON'S DISEASE | |
| 16.50 | OC10: Vincenzo Maria D'Amore, University of Naples "Federico II", Italy A DYNAMICAL AND ATOMISTIC RESOLUTION VIEW OF THE G PROTEIN COUPLED RECEPTOR A2A ACTIVATION MECHANISM |
| OC12: Federico Ricci, University of Messina, Italy LEARNING ON HUMAN TYROSINASE: FROM HOMOLOGY MODELLING TO NEW INHIBITORS SELECTION | |
| 17.10 | FC3: Elisa Patacchini, "Sapienza" University of Rome, Italy STRUCTURE-BASED DRUG DESIGN OF NEW SIGMA1 AGONISTS FOR HUNTINGTON'S DISEASE TREATMENT |
| FC4: Alessandro Andreani, IIT, Genova, Italy TARGETING THE CONSERVED, ACTIVE SITE OF SPLICING MACHINES WITH SPECIFIC AND SELECTIVE SMALL MOLECULE MODULATORS | |
| 17.30 COCKTAIL AND JAZZ CONCERT at Teatro Marrucino, Chieti | |

Scientific Program / Tuesday, 19th September

| | |
|--|---|
| Aula Magna (Department of Pharmacy) Chair: Gianluca Sbardella | |
| 9.00 | PL4: Thomas Lundbäck, AstraZeneca, Gothenburg, Sweden APPLICATION OF THE CELLULAR THERMAL SHIFT ASSAY IN DRUG DISCOVERY |
| Aula Magna (Department of Pharmacy) Chairs: Gianluca Sbardella, Marco De Vivo | |
| Aula 3 (Department of Pharmacy) Chairs: Giancarlo Aldini, Cristina Maccallini | |
| 10.00 | KN5: Simona Collina, University of Pavia, Italy SMALL MOLECULES INTERFERING WITH HUR-RNA COMPLEXES: A PROMISING STRATEGY TO DISCOVER ANTICANCER AGENTS |
| KN6: Enrica Calleri, University of Pavia, Italy APPLICATIONS OF PROTEIN-BASED ANALYTICAL METHODS IN DRUG DISCOVERY | |
| 10.30 | OC13: Marta Serafini, University of Oxford, United Kingdom THE DEVELOPMENT OF HYPOXIA-ACTIVATED PROTACS (HAP-TACS) TO SELECTIVELY DEGRADE BRD4 IN HYPOXIC CANCER CELLS |
| OC14: Lorenza Marinaccio, University "G. d'Annunzio" of Chieti-Pescara, Italy LYCOPENE EXTRACTION WITH α-PINENE, NATURAL VOLATILE DEEP EUTECTIC SOLVENT MENTHOL-THYMOL AND EXTRA VIRGIN OLIVE OIL | |
| 10.50 | FC5: Camilla Pecoraro, University of Palermo, Italy DISCOVERY OF PYRAZOLE-PYRIMIDINES AS NOVEL CDK7 INHIBITORS: SYNTHESIS AND PRELIMINARY BIOLOGICAL EVALUATION |
| FC6: Chiara Lambona, "Sapienza" University of Rome, Italy TARGETING ROS PRODUCTION THROUGH INHIBITION OF NADPH OXIDASE | |
| 11.00 COFFEE BREAK | |
| Aula Magna (Department of Pharmacy) Chairs: Ivana Cacciatore, Cosimo D. Altomare | |
| Aula 3 (Department of Pharmacy) Chairs: Giancarlo Aldini, Letizia Giampietro | |

| | | |
|-------|--|--|
| 11.20 | OC15: Marco Lolli , University of Torino, Italy POTENT HUMAN DIHYDROOROTATE DEHYDROGENASE INHIBITORS BASED ON THE 2-HYDROXYPIRAZOLE [1,5-A]PYRIDINE SCAFFOLD AGAINST ACUTE MYELOGENOUS LEUKEMIA: BE PREPARED TO THE CLINIC | OC18: Serena Montanari , University of Bologna, Italy MICROALGAE: BIOACTIVES EXTRACTION AND CHARACTERIZATION FOR NUTRACEUTICAL USAGE |
| 11.40 | OC16: Luca Pinzi , University of Modena, Italy DESIGN, SYNTHESIS AND IN VITRO EVALUATION OF HSP90/HDAC6 DUAL INHIBITORS BASED ON A 2-AMINO-PYRROLOPYRIMIDINE SCAFFOLD FOR THE TARGETING OF AGGRESSIVE PROSTATE CANCER | OC19: Erika Baldini , University of Ferrara, Italy CHEMICAL CHARACTERIZATION AND VALORIZATION OF <i>Helichrysum italicum</i> AND MEDICINAL MUSHROOMS FOR NUTRACEUTICAL APPLICATIONS |
| 12.00 | OC17: Anna di Porzio , University of Naples "Federico II", Italy DEVELOPMENT OF A NOVEL MULTI-TARGET ANTICANCER APPROACH BASED ON G-QUADRUPLEX STABILIZATION AND INHIBITION OF HUMAN CARBONIC ANHYDRASES | OC20: Greta Petrella , University of Rome "Tor Vergata", Italy A PERSONALIZED URINARY METABOLIC PROFILE FOR BLADDER CANCER PATIENTS: AN APPLICATION OF THE SYNHMET METHOD |
| 12.30 | LUNCH | |
| 14.00 | POSTER SESSION & COMMERCIAL EXHIBITION | |
| | Aula Magna (Department of Pharmacy) Chairs: Isabella Romeo, Chiara Borsari | Aula 3 (Department of Pharmacy) Chairs: Azzurra Stefanucci, Antonella Ciancetta |
| 15.30 | KN7: Chiara Borsari , University of Milan, Italy (Premio DCF) MEDCHEM STRATEGIES TO SELECTIVELY TARGET THE PI3K-mTOR PATHWAY FOR ONCOLOGY APPLICATIONS | KN8: Antonella Ciancetta , University of Ferrara, Italy (Premio DCF) MIDAS: A COMBINED ENHANCED SAMPLING MOLECULAR DYNAMICS AND FRAGMENT-BASED APPROACH TO LOCATE ALLOSTERIC BINDING SITES IN G PROTEIN-COUPLED RECEPTORS |
| 16.00 | FC7: Michela Puxeddu , "Sapienza" University of Rome, Italy NOVEL PYRROLE TUBULIN ASSEMBLY INHIBITOR AS ANTICANCER AGENT INDUCING FERROPTOSIS | FC13: Anna Marta Pasiaka , University of Bologna, Italy APPLICATION OF CLICK CHEMISTRY IN THE DEVELOPMENT OF NOVEL ANTILEISHMANIAL PROTEOLYSIS TARGETING CHIMERAS |
| 16.10 | FC8: Jessica Sebastiani , "Sapienza" University of Rome, Italy RS6077 AS NEW INDUCER OF CELL DEATH IN A LYMPHOMA TUMOR IN VIVO | FC14: Matteo Lusardi , University of Genova, Italy STRUCTURAL FUNCTIONALIZATION OF TRI-SUBSTITUTED PYRAZOLE DERIVATIVES AND PRELIMINARY EVALUATION OF THEIR ANTIMALARIAL ACTIVITY |
| 16.20 | FC9: Rosa Sparaco , University of Naples "Federico II", Italy MOLECULAR HYBRIDS BETWEEN ANTIGLAUCOMA DRUGS AND H₂S DONORS: SYNTHESIS AND IN VITRO H₂S RELEASING PROPERTIES | FC15: Francesco Melfi , University "G. d'Annunzio" of Chieti-Pescara NATURE-INSPIRED ANTIBACTERIAL AGENTS: SYNTHESIS AND BIOLOGICAL ACTIVITY OF EUGENOL DERIVATIVES AGAINST <i>H. pylori</i> STRAINS |
| 16.30 | FC10: Francesco Samarelli , University of Bari, Italy NOVEL AZEPINO[4,3-b]INDOLE DERIVATIVES AS LIGANDS OF THE CANNABINOID-ACTIVATED ORPHAN RECEPTORS GPR18 AND GPR55 WITH POTENTIAL AGAINST NEURODEGENERATIVE DISEASES | FC16: Letizia Crocetti , University of Florence, Italy EBSELEN ANALOGUES AS HUMAN NEUTROPHIL ELASTASE (HNE) INHIBITORS AND ANTIOXIDANT AGENTS |
| 16.40 | FC11: Alessia Alberico , University of Naples "Federico II", Italy GREEN AND AFFORDABLE KETOAMIDES SYNTHESIS AS VERY POTENT BROAD-SPECTRUM COV_s MAIN PROTEASE INHIBITORS: X-RAY STRUCTURE AND BIOLOGICAL PROFILE | FC17: Aleksei Smirnov , University of Camerino, Italy DUAL ANTA-INHIBITORS TARGETING PROTEIN KINASE CK1Δ AND A₂A ADENOSINE RECEPTOR USEFUL IN NEURODEGENERATIVE DISORDERS |
| 16.50 | FC12: Giovanni Graziano , University of Bari, Italy N-ADAMANTYL-ANTHRANIL AMIDE DERIVATIVES: NEW SELECTIVE LIGANDS FOR THE CANNABINOID RECEPTOR SUBTYPE 2 (CB₂R) | FC18: Emanuele Fabbrizi , "Sapienza" University of Rome, Italy FIRST-IN CLASS SPECIFIC INHIBITORS OF THE MITOCHONDRIAL DEACYLASE SIRTUIN 4 |
| 17.00 | COFFEE BREAK | |
| | Aula Magna (Department of Pharmacy) | |
| 17.30 | ASSEMBLEA DELLA DIVISIONE DI CHIMICA FARMACEUTICA - SOCIETÀ CHIMICA ITALIANA (DCF-SCI GENERAL MEETING) | |
| 20.30 | SOCIAL DINNER at "Tenuta Di Sipio" Winery | |

Scientific Program / Wednesday, 20th September

| | | |
|-------|--|--|
| | Aula Magna (Department of Pharmacy) Chairs: Alessandra Ammazalorso, Mariangela Agamennone | Aula 3 (Department of Pharmacy) Chairs: Simone Carradori, Francesco Epifano |
| 9.00 | KN9: Enza Lacivita , University of Bari, Italy TARGETING FORMYL PEPTIDE RECEPTORS TO TACKLE INFLAMMATION IN NEUROLOGICAL DISORDERS AND CANCER | KN10: Alessia Petrocchi , IRBM, Italy THE DISCOVERY OF I-0436650, A POTENT AND SPECIFIC ALLOSTERIC SHP2 INHIBITOR FOR THE CANCER THERAPY |
| 9.30 | OC21: Samuele Maramai , University of Siena, Italy 1,4,5-TRISUBSTITUTED 1,2,3-TRIAZOLE DERIVATIVES AS HSP90 INHIBITORS: SYNTHESIS, EVALUATION, AND STRUCTURAL CHARACTERIZATION | OC26: Tommaso Felicetti , University of Perugia, Italy FROM 2,1-BENZOTHIAZINE 2,2-DIOXIDE DERIVATIVES TO SULFONYL ANTHRANILIC ACID ANALOGUES AS POTENT PAN SEROTYPE DENGUE INHIBITORS |
| 9.50 | OC22: Maria Giulia Nizi , University of Perugia, Italy PROGRESS ON POTENT AND SPECIFIC PARP INHIBITORS: A SAR STUDY AROUND THE [1,2,4]TRIAZOLO [3,4-b]BENZOTHIAZOLE SCAFFOLD | OC27: Francesca Galvani , University of Parma, Italy QM/MM MODELLING OF MGL CARBAMOYLATION BY PIPERAZINE AZOLE UREAS REVEALS THE ROLE OF LEAVING GROUP EXPULSION AND DISCRIMINATES INHIBITORS WITH HIGH AND LOW POTENCY |
| 10.10 | OC23: Lidia Ciccone , University of Pisa, Italy MOLECULAR INTERACTION OF PCSK9 WITH AN INHIBITORY NANOBODY, CAP1 AND HLA-C:FUNCTIONAL REGULATION OF LDLR LEVELS | OC28: Laura Braconi , University of Florence, Italy TETRAZOLE AND OXADIAZOLE DERIVATIVES OF TARIQUIDAR AS POTENT MDR REVERSERS |
| 10.30 | OC24: Antonella Messori , University of Rome "Sapienza", Italy INDOLYL DIKETO ACID DERIVATIVES AS INHIBITORS OF NSP13 OF SARS-COV-2 THAT BLOCK VIRAL REPLICATION | OC29: Carmen Cerchia , University of Naples "Federico II", Italy A NEW ANTIDIABETIC AGENT SHOWING PPAR α/γ DUAL AGONISM AND MITOCHONDRIAL PYRUVATE CARRIER INHIBITION |
| 10.50 | OC25: Erika Del Grosso , University of Eastern Piedmont, Italy VALIDATION OF A NEW LC-HRMS METHOD FOR THE QUANTIFICATION OF THE CHEMICAL CHAPERONE 4-PHENYLBUTYRIC ACID (4-PBA) IN CELL CULTURE MEDIA | OC30: Serena Vittorio , University of Milan, Italy ENSEMBLE OF STRUCTURE AND LIGAND-BASED CLASSIFICATION MODELS FOR HERG LIABILITY PROFILING |
| 11.10 | COFFEE BREAK | |
| | Aula Magna (Department of Pharmacy) Chairs: Cristina Campestre, Barbara De Filippis | Aula 3 (Department of Pharmacy) Chairs: Marialuigia Fantacuzzi, Serena Fiorito |
| 11.30 | OC31: Emanuele Amata , University of Catania, Italy SYNTHESIS, COMPUTATIONAL INSIGHTS AND EVALUATION OF NOVEL SIGMA RECEPTORS LIGANDS | OC33: Ana Caballero , Pharmacelera, Barcelona, Spain THE ROLE OF HYDROPHOBICITY IN DRUG DISCOVERY: FROM 3D-QSAR MODELS TO HUGE CHEMICAL LIBRARIES EXPLORATION |
| 11.50 | OC32: Barbara Vergani , Italfarmaco, Milan, Italy 2-DIFLUOROMETHYL-1,3,4-OXADIAZOLE – TOWARDS ABSOLUTE SELECTIVITY VS HDAC6 | OC34: Daniele Aiello , University of Modena and Reggio Emilia, Italy LEAD OPTIMIZATION OF HUMAN THYMIDYLATE SYNTHASE DIMER DISRUPTERS: FROM COMPUTATIONAL STUDIES TO EVALUATION OF THEIR BIOLOGICAL PROFILES |
| | Aula Magna (Department of Pharmacy) Chairs: Maria Laura Bolognesi, Adriano Mollica | |
| 12.10 | PL5: Ana Martinez , Centro de Investigaciones Biológicas-CSIC, Spain MODULATING TDP-43 PATHOLOGY WITH PROTEIN KINASE INHIBITORS: A NEW AVENUE FOR ALS THERAPY | |
| 13.00 | CLOSING REMARKS AND POSTER PRIZES | |
| 13.30 | LIGHT LUNCH | |

PATRONAGES



SPONSOR

