

# I° Conference on Crystallography, Structural Chemistry and Biosystems



**Monday, 4 October 2021 - Wednesday, 6 October 2021**

## **Programme**

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# Monday 04 October 2021

## Registration (4 Oct 2021, 14:00-15:00)

## Opening (4 Oct 2021, 15:00-15:30)

time	title	presenter
15:00	Opening Remarks	Dr GIANNINI, Cinzia (CNR - Istituto di Cristallografia) Prof. ARMELAO, Lidia (CNR - Dipartimento di Scienze Chimiche e Tecnologie dei Materiali)
15:05	Nuove opportunità di finanziamento della ricerca	Prof. NICOLAIS, Luigi (Università di Napoli)

## Session: 1 (4 Oct 2021, 15:30-16:30)

-Conveners: Saviano, Michele (CNR - Istituto di Cristallografia)

time	title	presenter
15:30	Supra and Sub Molecular Investigation of Pathologic Tissues by X-Ray Scanning Microscopy	Dr GIANNINI, Cinzia (CNR - Istituto di Cristallografia)
15:45	Structure-based prediction of hERG-related cardiotoxicity: a benchmark study	Dr MANGIATORDI, Giuseppe Felice (CNR - Istituto di Cristallografia)
16:00	Structural Insights into the Intracellular Region of the Human Magnesium Transport Mediator CNNM4	Dr SILIQI, Dritan (CNR - Istituto di Cristallografia)
16:15	Synthesis of Porphyrin-Peptide conjugates and interaction with A $\beta$ 42: potential use of the systems as theranostic agents in Alzheimer's disease	Dr TOSTO, Rita (CNR - Istituto di Cristallografia)

## Coffe break (16:30-17:00)

## Session: 2 (4 Oct 2021, 17:00-18:15)

-Conveners: Capitelli, Francesco (CNR - Istituto di Cristallografia)

time	title	presenter
17:00	PNAs: a versatile synthetic tool in miRNAs targeting	Dr MOCCIA, Maria (CNR - Istituto di Cristallografia)
17:15	Visible light activeTiO <sub>2</sub> /Au nanorods for photocatalytic environmental remediation	Dr PETRONELLA, Francesca (CNR - Istituto di Cristallografia)
17:30	A survey of different approaches using ESI Mass Spectrometry for the characterization of metal binding sites in amyloid peptide fragments.	Dr DI NATALE, Giuseppe (CNR - Istituto di Cristallografia)
17:45	The Interdepartmental S&T Foresight Project	Dr BARTOLUCCI, Cecilia (CNR - Istituto di Cristallografia)
18:00	A year in Antarctica	Mr CATRICALÀ, Massimiliano (CNR - Istituto di Cristallografia)

## ePoster session: X-ray approaches (4 Oct 2021, 18:15-19:00)

**-Conveners: Bellia, Francesco (CNR - Istituto di Cristallografia)**

time	title	presenter
18:15	X-ray multilevel investigation of collagen in tissue engineering and pathology	Dr TERZI, Alberta (CNR - Istituto di Cristallografia)
18:20	Wide Angle and Small Angle X-ray Scattering for the structural characterization of fibers	Dr SIBILLANO, Teresa (CNR - Istituto di Cristallografia)
18:25	Molecular Replacement, new procedures and applications	Dr CASCARANO, Giovanni Luca (CNR - Istituto di Cristallografia)
18:30	Structural characterization of halide perovskites by X-ray measurements and advanced analysis	Dr CALIANDRO, Rocco (CNR - Istituto di Cristallografia)
18:35	The Structure of the Pro-domain of Mouse proNGF in Contact with the NGF Domain	Dr LAMBA, Dorian (CNR - Istituto di Cristallografia)
18:40	SUNBIM: a package for X-ray imaging of nano- and biomaterials using SAXS, WAXS, GISAXS and GIWAXS techniques	Dr SIBILLANO, Teresa (CNR - Istituto di Cristallografia)
18:45	Crystallographic investigation on whole anti-CD20 mAb	Dr CARROZZINI, Benedetta (CNR - Istituto di Cristallografia)
18:50	Single-crystal synchrotron X-ray diffraction study of new anthracene derivative compounds	Dr ALTAMURA, Davide (CNR - Istituto di Cristallografia)

## Tuesday 05 October 2021

### Session: 1 (5 Oct 2021, 09:00-10:30)

-Conveners: Siliqi, Dritan (CNR - Istituto di Cristallografia)

time	title	presenter
09:00	Advanced X-ray Characterization of Hierarchical Systems: from Biotissues to Electronic Devices	Dr ALTAMURA, Davide (CNR - Istituto di Cristallografia)
09:15	Structural Basis for Inhibition of Copper Trafficking by Platinum Anticancer Drugs	Dr CALIANDRO, Rocco (CNR - Istituto di Cristallografia)
09:30	Design and fabrication of biosensors for environmental and food safety monitoring.	Dr REA, Giuseppina (CNR - IC)
09:45	Multiple scale characterisation of ultrasmall nanocrystals by X-ray Total Scattering	Dr GUAGLIARDI, Antonella (CNR - Istituto di Cristallografia)
10:00	The XRD1 Synchrotron hard X-ray light source beamline as a tool for chemistry and science and technology of materials.	Dr BARBA, Luisa (CNR - Istituto di Cristallografia)
10:15	Functional disorder in complex materials	Dr CAMPI, Gaetano (CNR - Istituto di Cristallografia)

### Coffe break (10:30-11:00)

### Session: 2 (5 Oct 2021, 11:00-12:40)

-Conveners: Milardi, Danilo (CNR - Istituto di Cristallografia)

time	title	presenter
11:00	Disclosing the Major Structural Determinants Essential for Proneurotrophins Biological Functions	Dr COVACEUSZACH, Sonia (CNR - Istituto di Cristallografia)
11:15	Solving polycrystalline structures: from data collection to the development of innovative crystallographic methods	Dr RIZZI, Rosanna (CNR - Istituto di Cristallografia)
11:30	The role of stereochemistry in the inhibition of A $\beta$ Amyloid growth and toxicity by silybins.	Dr SCIACCA, Michele F.M. (CNR - Istituto di Cristallografia)
11:45	Structural investigation of calcium phosphates	Dr CAPITELLI, Francesco (CNR - Istituto di Cristallografia)
12:00	Natural polysaccharides from microalgae for the protection of cultural heritage	Dr ANTONACCI, Amina (CNR - Istituto di Cristallografia)
12:15	GHK-Hyaluronic acid conjugates affect the wound closure in the presence of copper ions	Dr NALETOVA, Irina (CNR - Istituto di Cristallografia)

### Lunch (12:40-14:00)

### ePoster session: Life Science (5 Oct 2021, 14:00-15:00)

-Conveners: Bellia, Francesco (CNR - Istituto di Cristallografia)

time	title	presenter
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14:00	VEGF bioactive fragments and their copper (II) complexes in angiogenesis	Dr ZIMBONE, Stefania (CNR - Istituto di Cristallografia) Prof. RIZZARELLI, Enrico (CNR - Istituto di Cristallografia)
14:05	Closing or opening proteasome doors by porphyrins.	Dr SANTORO, Anna Maria (CNR - Istituto di Cristallografia)
14:10	Hyaluronan-carnosine conjugates inhibit Amyloid- $\beta$ aggregation and toxicity	Dr BELLIA, Francesco (CNR - Istituto di Cristallografia)
14:15	Intrinsically disordered proteins (IDP) and metal ions: the case of amylin (HiAPP)	Dr MAGRÌ, Antonio (CNR - Istituto di Cristallografia) Dr RIZZARELLI, Enrico (CNR - Istituto di Cristallografia)
14:20	Antioxidant properties of Hyaluronate–Carnosine bioconjugates and their copper(II) complexes	Dr BOCCHIERI, Eleonora (CNR - Istituto di Cristallografia)
14:25	Structural determinants of quorum sensing specificity vs promiscuity	Dr COVACEUSZACH, Sonia (CNR - Istituto di Cristallografia)
14:30	A painful dance between Insulin degrading enzyme and two substrates: Insulin and OFQ/N	Dr AHMED, Iklas Mohamed Mohamud (CNR - Istituto di Cristallografia)
14:35	A re-investigation of copper coordination mode in the N-terminal 1-14 fragment of human Ctr1 protein.	Dr ATTANASIO, Francesco (CNR - Istituto di Cristallografia)
14:40	Cyclic synthetic peptide mimicking NGF enhances PC12 differentiation and BDNF/VEGF expression	Dr NALETOVA, Irina (CNR - Istituto di Cristallografia)

**Session: 3 (5 Oct 2021, 15:00-16:15)****-Conveners: Caliandro, Rocco (CNR - Istituto di Cristallografia)**

time	title	presenter
15:00	Rescuing proteostasis by small molecules	Dr MILARDI, Danilo (CNR - Istituto di Cristallografia)
15:15	Cross talk between Amyloid $\beta$ peptides and Ubiquitin: new perspective in Alzheimer's disease	Dr LANZA, Valeria (CNR - Istituto di Cristallografia)
15:30	Software for the Characterization of Polycrystalline Compounds	Dr CORRIERO, Nicola (CNR - Istituto di Cristallografia)
15:45	Competitive effectors of alpha-synuclein	Dr BELLIA, Francesco (CNR - IC)
16:00	Antimicrobial peptides (AMPs): Analysis, synthetic design and biological analysis.	Dr CAPORALE, Andrea (CNR - Istituto di Cristallografia)

**Break (16:15-17:00)****Session: 4 (5 Oct 2021, 17:00-18:40)****-Conveners: Covaceuszach, Sonia (CNR - Istituto di Cristallografia)**

time	title	presenter
17:00	Free radicals induced DNA damage: Chemical, Analytical, Biological, and Diagnostic Aspects	Dr MASI, Annalisa (CNR - Istituto di Cristallografia)
17:15	Carnosine and trehalose-carnosine tune the activity and expression of endogenous protection factors and their crosstalk with metal homeostasis	Dr ATTANASIO, Francesco (CNR - Istituto di Cristallografia)
17:30	Insights into the PPAR $\gamma$ phosphorylation and its inhibition mechanism	Dr MONTANARI, Roberta (CNR - Istituto di Cristallografia)
17:45	Peptide therapeutics: $\beta$ -sheet breaker conjugates for neuroprotection and amyloid detection.	Dr PAPPALARDO, Giuseppe (CNR - IC)
18:00	Reverse engineering and 3D additive manufacturing from research to the clinical assistance	Dr CLEMENTE, Fabrizio (CNR - Istituto di Cristallografia)
18:15	Privacy @CNR: panoramica generale su argomento, organizzazione e adempimenti	Dr CHIARELLA, Caterina (CNR - Istituto di Cristallografia)

**ePoster session: Software and Tools (5 Oct 2021, 18:40-19:00)**

**-Conveners: Bellia, Francesco (CNR - Istituto di Cristallografia)**

time	title	presenter
18:40	Ceftazidime and other cephalosporins inhibit bacterial NAD biosynthesis by targeting NadD enzymes. Implication for the treatment of chronic infections.	Dr PESARESI, Alessandro (CNR - Istituto di Cristallografia)
18:45	Geant4, a Monte-Carlo simulation tool for nuclear medicine and molecular radiotherapy	Dr MAZZONE, Annamaria (CNR - Istituto di Cristallografia)
18:50	ICT methods and tools for health	Dr CLEMENTE, Fabrizio (CNR - Istituto di Cristallografia)

## Wednesday 06 October 2021

### **Session: 1 (6 Oct 2021, 09:00-10:20)**

**-Conveners: Montanari, Roberta (CNR - Istituto di Cristallografia)**

time	title	presenter
09:00	Toward Personalized Medicine: RGD-Peptide as Scaffold for the Comprehension of Structural Determinants for Integrin Specific Recognition	Dr SAVIANO, Michele (CNR - Istituto di Cristallografia)
09:15	Protein Crystallization in Hydrated Deep Eutectic Solvents	Dr BELVISO, Benny Danilo (CNR - Istituto di Cristallografia)
09:30	Surface Plasmon Resonance, a powerful tool for ligand binding investigation	Dr CAPELLI, Davide (CNR - Istituto di Cristallografia)
09:45	ICT solution for Scientific Communication and Learning	Dr RIGHINI, Guido (CNR - Istituto di Cristallografia)
10:00	The synthetic heptapeptide Semax, a fragment of the ACTH hormone, sustains differentiated neuroblastoma, by improving the cellular bioenergetic: investigations toward New Therapeutic Solutions	Dr TOMASELLO, Marianna Flora (CNR - Istituto di Cristallografia)

### **Coffe break (10:20-11:00)**

### **Session: 2 (6 Oct 2021, 11:00-13:00)**

**-Conveners: Giannini, Cinzia (CNR - Istituto di Cristallografia)**

time	title	presenter
11:00	In vitro and in vivo approaches to the study of Alzheimer's disease	Dr GIUFFRIDA, Maria Laura (CNR - Istituto di Cristallografia)
11:15	New insight into the physiological activities of Amyloid Beta monomers	Dr ZIMBONE, Stefania (CNR - Istituto di Cristallografia)
11:30	CNR Hard X-ray diffraction activities at Elettra 2.0	Dr CASSETTA, Alberto (CNR - Istituto di Cristallografia)
11:45	Algae-Based Biosensors	Dr SCOGNAMIGLIO, Viviana (CNR - Istituto di Cristallografia)
12:00	Cockayne syndrome: a DNA repair defective syndrome with neurodegenerative features	Dr PASCUCCI, Barbara (CNR - Istituto di Cristallografia)
12:15	3D electron and X-ray powder diffraction multi-technique approach for structural investigation of new challenging lead chalcogenide nanocrystals	Dr MOLITERNI, Anna (CNR - Istituto di Cristallografia)
12:30	Kinetic analysis for the new enzymology	Dr PESARESI, Alessandro (CNR - Istituto di Cristallografia)
12:45	IC-CNR activities in Cultural Heritage	Dr TARQUINI, Ombretta (CNR - Istituto di Cristallografia)

### **Concluding remarks (6 Oct 2021, 13:00-13:15)**