Società Chimica Italiana

SCI2021

XXVII CONGRESSO NAZIONALE DELLA
SOCIETÀ CHIMICA ITALIANA

LA CHIMICA GUIDA LO SVILUPPO SOSTENIBILE

14–23 SETTEMBRE 2021

Sessioni Plenarie – ABC – ANA

BOOK OF ABSTRACTS
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Benvenuti a SCI2021!

Il Congresso Nazionale della Società Chimica Italiana, giunto alla sua XXVII edizione, si svolgerà in modo virtuale da martedì 14 settembre a giovedì 23 settembre 2021. Come di consueto, sarà un punto di incontro e di confronto per tutto il mondo della chimica in Italia su argomenti di grande attualità.

Il congresso sarà aperto dalla ***plenary lecture*** **del Prof. Stanley Whittingham, premio Nobel per la Chimica 2019**, e prevede interventi di una serie di illustri oratori, fra cui **il premio Nobel per la Chimica 1981, Prof. Roald Hoffmann**. Il congresso si articolerà in sessioni plenarie di interesse generale e sessioni parallele, a cura delle Divisioni della Società Chimica Italiana. Nel pomeriggio di mercoledì 22 settembre sono previsti eventi satellite di interesse industriale, accessibili gratuitamente per gli iscritti al congresso.

Nelle attuali necessità di distanziamento sociale, il congresso si svolgerà tutto in modalità live telematica, con presentazioni, discussioni e tavole rotonde in diretta. Gli interventi verranno comunque registrati e resi disponibili ai partecipanti nelle due settimane successive alla chiusura del congresso, con possibilità di contatto e discussione con i presentatori.

Understanding the thermodynamics and coordination chemistry of metal-binding proteins: the common thread to elucidate metal acquisition processes at host/pathogen interface

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Several studies have shown that the disruption of metal homeostasis in bacterial and fungal cells can be a powerful tool to design new antimicrobial drugs with a high rate of selectivity and specificity. To prevent infections, in fact, the human organism reduces the bioavailability of essential micronutrients by means of an innate immune response termed "nutritional immunity"; on the contrary, pathogens rely on specialized metal-binding proteins and molecular systems which capture the metal ions from the competitive host environment forming stable complexes [1]. Understanding the properties, structure and action mechanisms of the involved metal chelators is the very first step to elucidate the dynamics behind the metal transfer mechanisms and to rationally design novel metal-based antibiotic therapeutics [2].

An outstanding example is given by the thermodynamic and spectroscopic characterization of the zinc and copper binding sites of the periplasmic protein ZinT, expressed by *Escherichia coli* and *Salmonella enterica* [3, 4]. The chosen unstructured fragments, which serve as models to simulate the coordination and transport of metal ions in ZinT protein, correspond to the 24–29 and 166–178 amino acid sequences and are protected at their amino- and carboxyl-termini: Ac-^{24}HGHHSH^{29}-Am and Ac-^{166}DHIIAPRKSSHFH^{178}-Am (*E. coli*), Ac-^{24}HGHHAH^{29}-Am and Ac-^{166}DHIIAPRKSAHFH^{178}-Am (*S. enterica*).

A deep investigation on the thermodynamics and coordination chemistry of the formed Zn(II) and Cu(II) complexes was performed through different experimental techniques. The protonation and complex-formation equilibria were studied by means of potentiometric acid-base titrations. ESI mass spectra of the solutions under examination allowed to confirm the stoichiometries of the formed species and, through UV-Vis, CD and EPR spectroscopies at variable pH values, the metal coordination spheres and the geometry of the complexes were explored. Finally, the obtained results allowed a comparison with other biologically relevant metal-binding systems, such as the antimicrobial peptide calcitermin (VAIALKAAHYHTHKE) which can, in principle, participate in human nutritional immunity, competing with ZinT for the metal ion acquisition.

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