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Silvio Sammartano, Editor
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Guido Crisponi, Editor
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Editors:

Silvio Sammartano ***(President of the Scientific Committee of ISMEC 2011)***
Dipartimento di Chimica Inorganica,
Chimica Analitica e Chimica Fisica
Università degli Studi di Messina
V.le F. Stagno d'Alcontres 31
98166 Messina, ITALY
ssammartano@unime.it

Guido Crisponi ***(President of ISMEC Group)***
Dipartimento di Scienze Chimiche
Università degli Studi di Cagliari
Cittadella Universitaria
09042 Monserrato – Cagliari, ITALY
crisponi@unica.it

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Contacts:
Organizing Committee ISMEC 2011
email: *ismec2011@mat520.unime.it*
Phone +39 090 6765761/58/49
Fax +39 090 392827
Congress website: *http://mat520.unime.it/ismec2011*
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The interaction of DNA with metal complexes: experimental and computational studies

Giampaolo BARONE, Angelo SPINELLO, Alessio TERENZI

Dipartimento di Chimica "Stanislao Cannizzaro", Università di Palermo, Viale delle Scienze, Edificio 17, 90128 Palermo, Italy,
gbarone@unipa.it

We have recently reported on the interaction of native calf thymus DNA with cationic first row transition metal complexes, in aqueous solutions at neutral pH, investigated by spectroscopic techniques such as circular dichroism, absorption and fluorescence in the UV-visible wavelength range [1,2]. Such techniques revealed the occurrence of essentially two kinds of molecule-DNA interaction, specifically intercalation [1] and groove binding [2]. The interaction type has been assigned by interpreting the experimental spectra on the basis of "finger print" criteria, by monitoring the shape, intensity and wavelength of the spectral bands recorded as a function of the molecule/DNA molar ratio.

Of course, such procedure cannot furnish atomic level details of the molecule-DNA interaction. For this reason we are recently making use of computational methods as supporting tool for the structural interpretation of the experimental spectra. For example, quantum chemical calculations have been employed to rationalise the electronic transitions of the absorption and emission spectra of a DNA-intercalating zinc(II) Schiff base complex [3]. Moreover, quantum chemical – molecular mechanical (QM/MM) hybrid methods have been applied to simulate the intercalative interaction of proflavine with DNA models [4].

Such computational approach has been at present extended by the use of molecular dynamics (MD) simulations of the metal complex-DNA systems, by explicitly including counterions and the water solvent. The MD simulations are preliminary to the application of the QM/MM calculations and are performed i) to obtain a DNA conformation relaxed at the experimental conditions and ii) to explore a wider conformational space of the DNA-molecule system. In the present communication the first examples of the application of this combined experimental/computational approach to study the interaction of DNA with first row transition metal complexes will be shown.

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