

Biocomplexity Faculty Search
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Dear Madame or Sir,

it is my pleasure to write a letter to strongly support the application of Dr. Danilo Roccatano for a biocomplexity faculty position at the Indiana University.

I am Professor of Computational Biology at the International University Bremen (IUB). The research focus of my group is to study structure formation of biomolecules and association of biomolecules using computer simulation methods. Dr. Danilo Roccatano has joined my group at IUB in July 2003 as a postdoctoral fellow.

Dr. Roccatano is a mature, independent, and original scientist. He has worked in the field of computational biology and biomolecular simulation since his PhD work and during postdoctoral stays in Prof. Alan Mark's Lab in Groningen, in Prof. DiNola's group in Rome and in L'Aquila and at IUB in my group. These postdoctoral stays allowed him to develop a high level of expertise in several areas of computational biology including molecular dynamics simulations of proteins, simulation of the folding of peptides, analysis of global protein motions and study of receptor-ligand interactions. In my group he works on protein dynamics and the dynamics of protein-nucleic acid complexes. He has already made very important contributions to the field, for example the study of the effect of cosolvents on the stability and dynamics of proteins and peptides (in part published in PNAS, 2001) and the folding mechanism of beta-hairpin peptides using long-time molecular dynamics simulations (published in Prot. Sci. 1999 and Proteins, 2002). These contributions have already made him a well know scientist in the biomolecular simulation field. During his entire scientific career he has been very productive and has an excellent publication record of ~25 papers in the area of computational biology and simulation in high-level Journals. He has demonstrated a high publication activity throughout all stages of his career with no signs of slowing down of his research activities. Dr. Roccatano's research focus, molecular simulations, is of increasing importance to better understand also many aspects of complex biological systems such as

interactions of several biomolecules forming an interaction network. The rapidly increasing availability of cluster computers, the refinement of force fields and several new methodologies will undoubtedly broaden the applicability of molecular simulation methods to larger systems of many interacting partners and much longer time scales.

Dr. Roccatano is very organized, very intelligent, a nice person and a loyal collaborator. He works well with a wide range of people, including theoretical and experimental scientists and students. He is very committed to his scientific work, is self-motivated, comes up with many excellent project ideas, and is very hard working. Dr. Roccatano has experience in guiding the research of PhD students and to build up collaborations with other experimental and computational scientist. For example, since his start in my lab he has already built up mostly by himself collaborations with two experimental groups at IUB. In collaboration with the group of Prof. Schwaneberg (Biochemical Engineering) he investigates the effect of organic cosolvents on the structure and dynamics of enzymes. Together with the group of Prof. Nau (Organic Chemistry) he compares molecular simulation results on peptide end-to-end contact formation with experimental fluorescence quenching data. This work is of fundamental importance for improving force field simulations on biomolecules. Both collaborations with experimental groups at IUB have already led to publications (Roccatano et al. JPC 108, 18734, 2004; Wong et al., A.E.Micro.Biol. in press) and several follow-up manuscripts are under preparation.

In summary, I consider Danilo Roccatano as an outstanding scientist with a broad and comprehensive knowledge and understanding of many aspects of computational biology and biomolecular simulation. He has very clear ideas on his future academic career and research. I thoroughly enjoy him as a member of my research group and I would clearly miss him and his expertise in my group. However, I know that he is strongly determined, eager and well prepared to start his own independent research group. I recommend Dr. Roccatano to you most highly as an excellent candidate for a biocomplexity faculty position at the Indiana University.

Sincerely yours,



Martin Zacharias