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ANOTHER JOURNAL ON PROTEINS AND PEPTIDES RESEARCH

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We are pleased to announce the launch of World Research Journal of Peptide and Protein-a new peer reviewed journal published by Bioinfo publication.

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In World Research Journal of Peptide and Protein, as in other open access journals, the costs are covered by the author in the form of a publication processing fee.

Our new journal does not try to be the same as those journals already dedicated to this field. The journal considers research in protein structure and function, comparative structural analysis, molecular dynamics, peptide research. The journal welcomes cutting edge research in modern techniques of sequencing, proteomics, and development and use of new resources, technologies and techniques, as well as how findings can be applied to biological research and in an industrial context. Works in X-ray crystallography, nuclear magnetic resonance (NMR), electron paramagnetic resonance (EPR), circular dichroism (CD), magnetic circular dichroism (MCD), and (resonance) Raman (RR) spectroscopy, atomic force (AFM) and electron microscopy (EM) are welcome. The journal also features applications of computational, statistical and mathematical methods of significance to the protein and peptide sciences. It publishes reviews, regular research papers and short communications. There is no restriction on the length of papers.

In this first issue, experimental (CD, fluorescence and NMR) and computation techniques have been applied to the study of peptides and proteins. Two contributions are original articles and two contributions are reviews. All the papers have been subjected to a critical reviewing process.

In the first paper, Wah and D. Laurentz have structurally characterized two peptides corresponding to two motifs from the C-terminal domain of the *T. brucei* transcription factor IIB (TFIIB) [1]. TFIIB plays crucial roles in RNA transition initiation. It binds DNA, RNA polymerase II, the TATA box binding protein and organizes other transcription initiation factors [2-3]. These two motifs have no counterpart in the human protein and in a recent crystallographic study their structures couldn't be determined because of lack of electronic density [1]. The two peptides are found intrinsically disordered by CD, fluorescence and NMR experiments. On the bases of these results, the authors proposed that these regions could play an important role in mediating interactions with other transcription factors, compensating the low positive charge density of *T. brucei* TFIIB.

In the second paper, Marabotti and Milanesi review the bioinformatics tools available in finding inhibitors of protein-protein interactions. The discovery of drugs targeting protein-protein interactions is an active field and the computational approach can be a valid support for the scientists. The authors have covered a large amount of literature in this review. Particularly, tools for the analysis of protein-protein interfaces and for the identification of pockets on the protein surface and methods for identifying the presence of clefts in unbound protein interfaces, like molecular dynamics simulations and docking have been described. Fragment-

based drug discovery approach has also been extensively explained. The information enclosed in the paper will be rather useful for the field.

Marcelo Marti' and co-workers also present a review of computational methods. They summarize selected techniques for the calculation of the binding free energy between a drug-like compound and its macromolecular target. This is a key concept for understanding molecular recognition processes, with direct implications in the design of molecular devices and the interpretation of biochemical processes and drug discovery. The paper first reviews the so-called End Point-based techniques [4], which include the widely used molecular mechanics-Poisson Boltzmann Surface Area (MM/PBSA) and molecular Mechanics-Generalized born surface area (MM-GB SA) strategies, that combine a molecular mechanics force field with a continuum solvation model to determine the direct protein-ligand interaction energy in the complex and the solvent associated free energy change respectively [5-6]; then, it discusses methods based on the explicit description of solvent (water) molecules, with particular emphasis to several applications of the inhomogeneous fluid solvation theory method [7-8].

The final part of the manuscript discusses free energy methods designed for elucidating the association/dissociation processes, including steered molecular dynamics [9], multiple-step trajectory combination [10], and brute-force sampling methods [see for example 11]. The manuscript ends with practical considerations for the choice of techniques, which can be very interesting for non-expert researchers in the field.

Finally, the last paper, by Vendruscolo group, reports a new tool for protein structure analysis, which includes structure comparison, generation of annotated structural alignments, and annotated superposition of structures. This method produces an accurate analysis of structural conservation in a family of proteins. The annotated alignment and superposed structures are used to characterize the local and global structural information content, to refine the sequence alignment and to produce fragments and 3D probability density functions for comparative modeling. The tool, called ARABESQUE, could be at the basis for a new hybrid modeling programs that combine information derived from the probability density functions with experimental data such as NMR chemical shifts [12], residual dipolar couplings [13] and low-resolution electron density maps [14].

We would like to thank all the authors for their cooperation in helping us to bring together this first issue, and we thank the referees for their efforts. It is a pride and an honor to be able to work with all of you.

It is our hope that the scientific community working in the field of protein and peptide research will find this new journal useful. We are looking forward to receiving some of your very best manuscripts for publication in this journal!

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