

## Meet Our Editorial Board Member

### Prof. Walter Filgueira de Azevedo Jr.

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Prof. De Azevedo was born in Rio de Janeiro/RJ Brazil in 1963, and since his early age, he got fascinated by science. This passion for science did not become productive for few years, since he had to work to support his family; therefore he had to postpone beginning his education in university.

Finally, in 1986, he started the physics course at the University of São Paulo. He was a little bit old to start a university course, but with determination not to give up his dreams, he moved on. During his undergraduate course, he had the opportunity to start working with X-ray diffraction crystallography and small-angle X-ray scattering. Learning crystallography and its importance to explore the molecular world was very important for his education. It was crystal clear that the investigation of the molecular world would be his research focus in the next decades. In 1990, he graduated in physics (BSc in Physics) at the University of São Paulo (USP). In 1992, he completed his Master's degree in applied physics also at USP, working under the supervision of Prof. Yvonne P. Mascarenhas. Prof. Mascarenhas is the founder of crystallography in Brazil and greatly helped in his career as a scientist. She is an example of dedication to science and education. His dissertation was about X-ray diffraction crystallography applied to the study of organometallics compounds [1].

During his PhD, he worked under the supervision of Prof. Sung-Hou Kim (University of California, Berkeley. Department of Chemistry, USA), on a split PhD program with a fellowship from Brazilian Research Council (CNPq)(1993-1996). During these three years, he had the opportunity to learn protein crystallography and structural bioinformatics and their application to the drug design. The enthusiastic and inspiring academic environment at the University of California (Berkeley) was a turning point in his scientific career. Prof. Kim played a role in providing this opportunity. His PhD thesis was about the crystallographic structure of human Cyclin-Dependent Kinase 2 (CDK2) in complex with inhibitors [2]. In his thesis, he described the structure of CDK2 and the details of intermolecular interactions between CDK2, roscovitine [2] and flavopiridol [3]. Roscovitine and flavopiridol are competitive CDK2 inhibitors [4]. In 1996, he returned to Brazil. In April 1997, after completing his PhD, he moved to São José do Rio Preto (SP, Brazil) (UNESP) and worked there from 1997 to 2005. In 1997, he started the Laboratory of Biomolecular Systems- UNESP - São Paulo State University. Since 2005, he has been in Porto Alegre/RS (Brazil). His current position is of a professor and a researcher at the Pontifical Catholic University of Rio Grande do Sul (PUCRS).

As a professor, he aims to use scientific training to teach science to a new generation of Brazilian students. Many of his former PhD students are now active scientists working in Brazil and abroad. For instance, Prof. Fernanda Canduri who works at the University of Sao Paulo (Sao Paulo, Brazil) and Dr. José Henrique Pereira who works at Lawrence Berkeley National Laboratory (California, USA).

His research interests are focused on the application of protein-ligand docking simulations to the discovery and development of drugs. Moreover, he is also interested in the development of machine learning algorithms and their application to molecular docking simulations, protein-ligand interactions, and drug repurposing.

In the last two years, he worked on the development of bioinformatics tools to study protein-ligand interactions and their application to drug design and discovery. He developed the program SAnDReS (www.sandres.net) [5], which makes use of supervised machine learning techniques to generate computational models for the prediction of ligand-binding affinity. This program is also able to evaluate the performance of docking programs such as Molegro Virtual Docker [6]. The focus is the use of such computational methodologies to bring deeper insights into the problem of protein-ligand interactions, which may facilitate the discovery and development of new drugs [6, 7]. He aspires to use this computational tool to face major challenges in the development of drugs for neglected diseases [8] that affect the developing countries such as tuberculosis and malaria.

He has published over 160 scientific papers about protein structures and computer simulation methods applied to the study of biological systems (H-index: 38). These publications have over 5000 citations. He is a section editor for Current Medicinal Chemistry (Drug Design and Discovery) and a regional editor for Current Drug Targets. He is also a member of the editorial board of the following journals: Current Bioinformatics, PeerJ, Jacobs Journal of Computer Science, and Journal of Biochemistry.

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