Seminars in Biotechnology BTEC 592 & BTEC 692

"Molecular Modelling Techniques in Modern Drug Design"

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13:30
GTU Congress Center, Red Hall

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Dr. Ilke Ugur Marion is the co-founder and managing partner of Meddenovo Drug Design and Consultancy Company. Meddenovo is the first computational drug design company in Turkey and is established by the prestigious TÜBİTAK Techno techno-initiative capital support program.

Dr. Ilke Ugur Marion obtained her Ph.D. in a joint program between Bogazici University and Université de Lorraine (Nancy, France), focusing on the biochemical understanding of posttranslational modifications in enzymes. She worked on a wide range of molecular modeling projects, including enzyme design, transition metal chemistry, and polymerization, with an intense collaboration with pioneer experimental chemists and biologists.

She was a visiting scientist at the University of California, Los Angeles (UCLA), and the Free University of Brussels (VUB). She worked as a postdoctoral associate at the Technical University of Munich (TUM), first in Chemistry and then in the Life Sciences Department. She was involved in several projects focusing on drug and enzyme design in collaboration with the Roche Company.

Since 2017, she has worked with Ashwin-Ushas Corporation (USA) as a computational chemist in a remote fashion. Together, they investigate oxygen activation reaction catalyzed by hemoproteins. She is also enrolled in METU Chemistry Department as a postdoctoral scientist, where she develops computational methods for drug design.

Abstract

Computational chemistry methods are an indispensable part of modern rational drug design. There are diverse methods, software, and approaches used successfully in this field. Although approaches differ, computational chemists explore three key elements in drug design: 1. drug interactions with the target, 2. drug interactions with its environment, 3. drug characterization in isolation. As a result of researching these factors, critical data such as target validation, drug candidate selection, use of the drug in different indications, determination of the pharmacokinetic and dynamic properties of the drug, redesign of the pharmaceutical form of the drug, and toxicity are obtained. It is known that safely transferring these data to the following stages of drug design reduces drug design costs by 30%.

In order to increase efficiency in drug modeling, the drug and target protein must be examined in detail using more than one computational chemistry method. Our talk aims to introduce these different computational chemistry approaches while talking about the success stories of drugs whose design started in the computer environment and reached the patient.