

Discovery and Characterization of Cancer Mutations on DNA Transaction Enzymes

Tuesday, 26 September 2023 13:30 (30 minutes)

We have developed a comprehensive approach to find and characterize the impact of cancer mutants on target proteins, and have applied it to DNA modification enzymes. This approach is an extension of conventional genome wide-association studies (GWAS). Our approach employs a new method for discovery and statistical validation of single nucleotide polymorphisms (SNPs) on specific genes called HyDn-SNP-S, followed by atomistic simulations via molecular dynamics (MD) and/or quantum mechanics/molecular mechanics (QM/MM) techniques. We will present the details of our mutant discovery and characterization approach, as well as examples of characterization of cancer mutations on DNA modification enzymes. Our simulations provide insights at the atomic level about how these mutations affect protein structure and/or function. Furthermore, experimental results validating our predictions will be presented.

Primary author: CISNEROS, G. Andres (University of Texas at Dallas)

Presenter: CISNEROS, G. Andres (University of Texas at Dallas)

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