CompBioMed
A Centre of Excellence in Computational Biomedicine

e-Seminar Series

e-Seminar #27
DNA Point Mutations in the Absence and Presence of Electric Fields

19 October 2022 2pm CEST / 1pm BST (1h duration)

Register for free here: https://attendee.gotowebinar.com/register/7233407048686103820

DNA mutations can occur spontaneously or can be induced by external factors such as electric fields, intercalators, radiations, etc. One of the point mutation mechanisms, known as the Löwdin's mechanism, is the double proton transfer process between DNA base pairs. A Quantum Mechanics/Molecular Mechanics (QM/MM) multiscale study was completed on a realistic model of DNA to evaluate the kinetics and thermodynamics of this mutation in the absence and presence of electric fields. The results show that it is unlikely for the AT base pair to undergo double proton transfer even in the presence of the electric field, while the GC base pairs have higher probabilities of undergoing point mutations, especially in the presence of electric fields in the order of 109 Vm-1. This model explains the experimentally observed mutation bias of the conversion of the GC to AT base pairs.

This is the 27th in a series of online e-Seminars organised by CompBioMed.

Watch the full series at www.compbiomed.eu/training!

Dr. Alya A. Arabi is Associate Professor in the Department of Biochemistry, College of Medicine and Health Sciences at UAEU (2020-). She is Honorary Lecturer in the Department of Chemistry at University College London, UK (2017-).

In 2012, Dr. Arabi received her PhD in Chemistry from Dalhousie University, Canada. In 2008, she was awarded a Bachelor of Sciences Honors degree with highest aggregate from Mount Saint Vincent University joint with Dalhousie University, Canada. Dr. Arabi received numerous prestigious awards including the Killam Predoctoral Scholarship, NSERC Alexander Graham Bell Graduate Scholarship-Doctoral, and the 2nd Khalifa Fund Techo-preneur Award in the UAE.

Dr. Arabi accepted Adjunct Faculty positions at Mount Saint Vincent University, Canada, and Abu Dhabi University, UAE (2012-2013). She then joined the College of Natural and Health Sciences at Zayed University, UAE, as an Assistant Professor (2014-2018), and as an Associate Professor (2018-2020).

Her research interests lie in the investigation of biochemical systems using computational tools. She studies the effect of external factors such as electric fields and intercalators on mutations in DNA, and bioisosterism in drug design.

Moderated by Tim Weaving, **UCL**

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 823712.

Organised in collaboration with: Avicenna Alliance Association for Predictive Medicine, VPH Institute Building the Virtual Physiological Human