The 12th KPSI Seminar
Place: ITBL G201 room, KPSI, QST
Time& Date: 13:15-, (WED) 2-NOV-2016

Title of Presentation:

Molecular Dynamics Simulations, as a Tool to Understand Human Telomeric DNA G-quadruplexes

Outline of Presentation:

I. An introduction to Molecular Dynamics (MD) simulations, from conventional to enhanced sampling techniques (methodology in details to understand part II);
II. MD simulations on human telomeric DNA G-quadruplexes, for the understanding of their stabilities, folding pathways and ligand-binding behaviours;
III. Future work in QST;

Abstract:

Molecular Dynamics (MD) simulation has been widely used to study biomolecules on their structures, interactions and conformational fluctuations.

In conventional MD simulations, the evolution of atomistic motions is governed by the unbiased energy functions at an integration time-scale of femtosecond. As a result, with current computing resources and the reachable time-scales (nano- or micro-second), conventional MD simulations can only sample local conformational changes around free energy minima. To observe large conformational fluctuations associated with transitions between free energy minima, such as the folding/unfolding of biomolecules, enhanced sampling techniques are required.

In our studies, we employed both conventional and enhanced sampling techniques to understand DNA G-quadruplexes adopted by human telomeric sequence. G-quadruplex is a non-canonical yet crucial secondary structure of nucleic acids, which has proven its importance in cell aging, anti-cancer therapies, gene expression and genome stability. In our work, we examined the stabilities, folding pathways and ligand-binding behaviours of human telomeric DNA G-quadruplexes, which aims to assist experimentalists to not only stabilize the structures but also intervene their formation in genome.

At the end, I will introduce my future work to be carried out here in QST.