Contribution ID: **160** Type: **Oral**

Electrostatic Influence on the Excited-State Twisting of Thioflavin T Binding to Bimolecular G-Quadruplex DNA: A Computational Study

Thioflavin T (ThT), a cationic fluorescent dye, and the bimolecular G-quadruplex (biGQ) DNA (two guanine-rich single-stranded DNAs, 5'-TGAGGGAGGGGT-3') have been used to develop an optical sensor for potassium ion (K^+) detection based on the fluorescence characteristic of ThT in different environments. Fluorescence intensity of free ThT in non-viscous media is extremely low due to the twisting of the central C-C single bond of the dye on the excited state. In the absence of K^+, ThT fluorescence is weak because of a low ThT/single-stranded DNA binding stability. However, the biGQ structure is formed in the presence of K^+ leading to the fluorescence enhancement of ThT. The enhancement by the twisting hindrance is found when ThT is embedded into a confined space of biGQ. The detail of the ThT/biGQ system at a molecular level is not completely understood, despite the fact that the ThT/biGQ-based optical sensor is effective for K^+ detection. In this study, molecular simulations are performed using a hybrid quantum mechanical/molecular mechanical (QM/MM) approach to investigate the excited-state twisting of ThT. Our QM/MM simulations show that electrostatic interactions with the negatively charged phosphate groups in the backbone of biGQ play a significant role in the excited-state intramolecular charge transfer process that relates to the twisting of ThT. Importantly, a better understanding achieved from this study would be very beneficial for designing more effective ThT/GQ-based optical sensors.

Authors: THONGYOD, Wutthinan (Faculty of Science, Prince of Songkla University); Dr PUNWONG, Chutintorn (Faculty of Science, Prince of Songkla University)

Co-authors: Dr BURANACHAI, Chittanon (Faculty of Science, Prince of Songkla University); Dr PENGPAN, Teparksorn (Faculty of Science, Prince of Songkla University)

Presenter: THONGYOD, Wutthinan (Faculty of Science, Prince of Songkla University)

Track Classification: Biological Physics, Biosensors and Chemical Sensors