

Internal Seminar

Potential Novel Dengue Virus NS2B-NS3 Protease Inhibitors from Natural Scaffolds: A Preliminary Study

Suman Sinha

Universiti Sains Malaysia, Penang

Dengue is transmitted by the bite of a mosquito infected with one of the five dengue virus serotypes. As far as anti-dengue drug discovery is concerned, among few established therapeutic targets, NS2B-NS3 protease is quite popular and well-studied because of its role in production of mature viruses as well as maintaining infectivity. The current work describes the computational and experimental initiatives in the molecular design and synthesis of novel NS2B-NS3pro inhibitors from specific natural scaffolds. In the preliminary stages of the investigation, based on literature reports, molecular docking analysis and subsequent enzymatic assay of two specific natural compounds against NS2B-NS3pro, it was proved that these compounds are active with IC_{50} of 108 μ M and 878 μ M. Further design based on molecular docking studies led to the synthesis of eighteen compounds. Finally, enzymatic inhibition studies led to the identification compound SS-2 and SS-5 which showed IC_{50} of 37.92 μ M and 0.0065 μ M respectively. Overall, the structure based design approach and subsequent experimental validation through the present work successfully proved the concept of rational drug design.

Friday, Mar 24th 2017

10:30 AM (Tea/Coffee at 10:15 AM)

Seminar Hall, TCIS