***Session 5: Drug Design By Molecular Modeling***

# Frontier Research for HIV-1 Reverse Transcriptase Inhibitor Discovery

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***Abstract***

Three research platforms have been established for innovative research on Anti-AIDS drug discovery. Computational Drug Discovery platform includes structural modification of Natural products and organic syntheses, QSAR, quantum chemical calculations, virtual screening, *de novo* design, combinatorial library design, protein-ligand interaction simulations, large-scale Molecular Dynamics simulations, drug-likeness analysis and ADME/T prediction. In addition, Biological-physicochemical experimental platform has been set up to verify and realize the computational design based on several biophysical technologies, such as biological activity assay, including enzyme assay and cell-based assay, X-ray crystallographic and NMR spectroscopic studies on enzymes, enzyme kinetics study, and isothermal titration calorimetry (ITC), which can be used to determine ligand-receptor interaction and protein-protein/DNA interaction. Another goal is to set up a Development of methodology and nanopolymer platform to develop fluorescence resonance energy transfer materials for biological assay which might lead to high throughput screening technology development. It is hoped that the obtained results will provide drug candidates for drug development, and the platform as to how cooperative and interdisciplinary work can be carried out to further advance this crucial area of research.

***Keywords***: anti-HIV, Reverse Transcriptase, computer-aided drug design, biological testing.