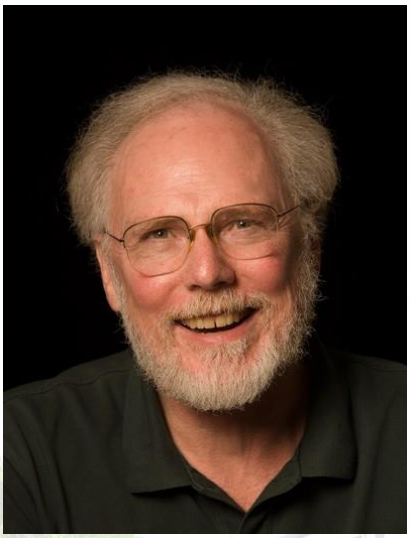
1st Symposium on Biophysics Postgraduate Research in Hong Kong

October 28, 2014, Science Center North Block G25, CUHK



Keynote Speaker:

Prof J. Andrew McCammon
Department of Chemistry & Biochemistry,
Department of Pharmacology,
Howard Hughes Medical Institute,
Center for Theoretical Biological Physics,
University of California at San Diego

COMPUTER-AIDED DRUG DESIGN

The selective character of the binding and reactivity of key biological molecules is essential for life. Properly understood, such selectivity can be exploited in the design of drugs, novel antibodies or enzymes, sensors, or a host of other materials or devices. This talk will provide a brief overview of how computer simulations can be used quantitatively to interpret the selectivity of molecular behavior. Particular emphasis will be placed on proper accounting of the flexibility of the receptor in the design of ligands. The potential of new generations of computing hardware and methodology to dramatically transform this area of work will be emphasized.

The symposium has been supported by the Postgraduate Students Conference/Seminar Grant of the Research Grants Council, Hong Kong.

Schedule:

10am – 12noon Student presentations (10-12 minute talk and 2-3 minute Q&A); Posters in the SC North lobby.

10:00am Chiang, YingChih (CUHK)
10:15am Ge, Zhenpeng (CUHK)
10:30am Chen, Chong (CUHK)
10:45am Zhai, He (CUHK)
11:00am Chan, Chun (CityU)
11:15am Jiang, Hanlun (HKUST)
11:30am Gu, Shuo (HKUST)

2:00pm – 4:20pm Platforms (30 minute talk and 5 minute Q&A)

2:00pm Prof. Chen, Guanhua (HKU)
Directional rotation of Escherichia coli's Flagellar Motor: mechanisms revealed by structural modeling

2:35pm Prof. Fan, Jun (CityU)
Multiscale molecular dynamics simulations of actin filament and BAR-PH proteins

3:10pm Prof. Tang, Leihan (HKBU)
Energy dissipation and transient response in an adaptive molecular circuit

3:45pm Prof. Wong, Kin-Yiu (HKBU)
Towards Biomolecular Calculations without Samplings: a "Wormhole" Path-Integral Theory for Quantum Free Energy

4:30pm – 5:30pm Keynote talk
Prof. J. Andrew McCammon (UCSD)
Computer-aided drug design

Venue: Science Center North Block G25, Chinese University of Hong Kong.

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