Schedule for the Croucher Advanced Study Institute

'Structure-based screening and design of ligands for protein targets'

December 14 (Monday)

10:00 am - 4:00 pm Registration and setting up of posters

Venue: 1/Fl., Teaching Complex at Western Campus (TCW), The Chinese University of

Hong Kong (CUHK)

2:00 pm Workshop conducted by Brian Shoichet, John Irwin, Mike Keiser

Venue: 103, Pi Ch'iu Building, CUHK

Coordinators: S.Au, Jacky Ngo, Terrence Lau and Kenneth Leung

December 15 (Tuesday)

Venues:

Lectures: LT3 (U/G), TCW, CUHK Registration and Coffee/Tea: 1/Fl., TCW

8:30 am Registration

9:00 – 9:30 am Opening ceremony

9:30 -10:30 am "Structural Biology, Informatics and Fragment-Based

Approaches to Lead Discovery"

T. Blundell, Department of Biochemistry, University of Cambridge,

Cambridge

Chair: K.B. Wong

10:30 – 11:15 am Coffee break

 $11:15-12:30~\mathrm{pm}$ "New Ligands for Old Targets and New Targets for Old

Druas"

Brian Shoichet, University of California, San Francisco, California

Chair: K.H. Sze

2:00 – ~ 6:00 pm Workshop conducted by Brian Shoichet, John Irwin, Mike Keiser

<u>Venue</u>: 103, Pi Ch'iu Building

December 16 (Wednesday)

Venues:

Lectures: LT3 (U/G), TCW, CUHK Registration and Coffee/Tea: 1/Fl., TCW

9:15 -10:15 am "Drug Design Driven by Computational Biophysics and

Chemistry"

Prof. Weiliang Zhu, Shanghai Institute of Materia Medica, Shanghai

Chair: G. Zhu

10:15 -11:00 am Coffee and poster session 1

11:00 - 11:45 am "Automated Docking Screens: A Feasibility Study"

John Irwin, University of California, San Francisco, California

11:45 am-12:30 pm "Predicting Drug Off-Targets"

Mike Keiser, University of California, San Francisco, California

Chair: M. Waye

2:00 - ~ 6:00 pm Workshop conducted by Brian Shoichet, John Irwin, Mike Keiser

<u>Venue</u>: 103, Pi Ch'iu Building

December 17 (Thursday)

Venues:

Lectures: LT3 (U/G), TCW, CUHK

Registration and Coffee: 1/Fl., TCW

9:15 -10:15am "Challenges and Opportunities for Computational

Docking in Structure based Drug Design"

Arthur Olson, The Scripps Research Institute, California

Chair: R. Wong

10:15 – 11:00am Coffee and poster session 2

 $11:00 \ am \ -12 \ noon$ "The Structure-based Screening and Verification of

Novel Cdc25 Phosphatase Inhibitors"

Seong Eon Ryu, Hanyang University, Seoul

 $12\ \mathrm{noon}$ - $12:45\ \mathrm{pm}$ "Application of High Throughput Crystallography in Drug

Discovery: Fragment-based Screening"

Cheng Yang, Rigaku Americas Corporation, Texas

Chair: K.W. Tsui

2:00 - ~6:00 pm Workshop conducted by Brian Shoichet, John Irwin, Mike Keiser

<u>Venue</u>: 103, Pi Ch'iu Building

December 18 (Friday)

Venues:

Lectures: LT3 (U/G), TCW, CUHK

Registration and Coffee: 1/Fl., TCW

9:15 – 10:15 am "Past, Present and Future of Structure-Based Design"

Irwin Kuntz, University of California, San Francisco, California

Chair: P.C. Shaw

Compounds"

Stefano Forli, The Scripps Research Institute, California

11:00 – 11:30 am Coffee

11:45 am – ~ 6:00 pm Workshop conducted by Arthur Olson and Stefano Forli

Venue: 103, Pi Ch'iu Building

Coordinators: S.Au, Jacky Ngo, Terrence Lau and Kenneth Leung

December 19 (Saturday)

Venue: 102, Pi Ch'iu Building

Coffee: same venue

9:30 – late afternoon Workshop conducted by Arthur Olson and Stefano Forli

Venue: <u>102</u>, Pi Ch'iu Bldg