

International Symposium on Grids & Clouds 2018 (ISGC 2018) in conjunction with Frontiers in Computational Drug Discovery (FCDD)

Friday, 16 March 2018

Workshop on Frontiers in Computational Drug Discovery (09:00 - 11:10)

time	[id] title	presenter
09:00	[100] Registration & overview of the workshop	Dr LIN, Jung-Hsin

Workshop on Frontiers in Computational Drug Discovery (11:30 - 12:30)

time	[id] title	presenter
11:30	[102] Fundamentals in structure biology	Dr LIN, Jung-Hsin

Workshop on Frontiers in Computational Drug Discovery - Conference Room 2, BHSS (14:00 - 15:30)

time	[id] title	presenter
14:00	[101] Introduction to Protein Data Bank (PDB) and molecular graphics (PyMOL)	SUEN, Ching-Shu

Workshop on Frontiers in Computational Drug Discovery - Conference Room 2, BHSS (16:00 - 18:00)

time	[id] title	presenter
16:00	[103] Molecular graphics (UCSF Chimera) and analytics for biomolecule-drug interactions (LigPlot+, PDB2PQR, etc.)	Ms CHU, Pei-Ying

Saturday, 17 March 2018

Workshop on Frontiers in Computational Drug Discovery - Conference Room 2, BHSS (09:00 - 10:30)

time	[id] title	presenter
09:00	[104] Quantum chemical calculations of drug-like molecules	Dr LIN, Jung-Hsin

Workshop on Frontiers in Computational Drug Discovery - Conference Room 2, BHSS (11:00 - 12:30)

time	[id] title	presenter
11:00	[105] Hands-on tutorials of quantum chemical calculation with Gaussian and visualization of molecular orbitals and chemical spectra (GaussView)	Dr CHOU, Ching-Yu

Workshop on Frontiers in Computational Drug Discovery - Conference Room 2, BHSS (14:00 - 15:30)

time	[id] title	presenter
14:00	[106] Principle of molecular docking	Dr LIN, Jung-Hsin

Workshop on Frontiers in Computational Drug Discovery - Conference Room 2, BHSS (16:00 - 18:00)

time	[id] title	presenter
16:00	[107] Hands-on tutorials of AutoDock 4.0 and AutoDock vina	Ms CHU, Pei-Ying

Sunday, 18 March 2018**Workshop on Frontiers in Computational Drug Discovery - Conference Room 2, BHSS (09:00 - 10:30)**

time	[id] title	presenter
09:00	[108] Deep learning approaches in computation drug discovery	Dr LIN, Jung-Hsin
09:50	[168] Improving Scoring-Docking-Screening Powers of Protein-Ligand Scoring Functions using Random Forest	Prof. ZHANG, Yingkai

Workshop on Frontiers in Computational Drug Discovery - Conference Room 2, BHSS (11:00 - 12:30)

time	[id] title	presenter
11:00	[192] Hands-on Tutorial of Δ vina	Ms CHU, Pei-Ying Prof. ZHANG, Yingkai
11:30	[109] Hands-on Tutorial of DeepChem and Gnina	Ms CHU, Pei-Ying

Workshop on Frontiers in Computational Drug Discovery - Conference Room 2, BHSS (14:00 - 15:30)

time	[id] title	presenter
14:00	[110] Molecular dynamics simulations for drug-target complexes	Dr LIN, Jung-Hsin

Workshop on Frontiers in Computational Drug Discovery - Conference Room 2, BHSS (16:00 - 18:00)

time	[id] title	presenter
16:00	[111] Hands-on Tutorial of AMBER16 (xLEaP, sander, pmemd, cpptraj)	Dr CHOU, Ching-Yu

Monday, 19 March 2018

Workshop on Frontiers in Computational Drug Discovery - Conference Room 2, BHSS (09:00 - 10:30)

time	[id] title	presenter
09:00	[112] Quantum mechanical/molecular mechanical molecular dynamics simulations	Prof. ZHANG, Yingkai

Workshop on Frontiers in Computational Drug Discovery - Conference Room 2, BHSS (11:00 - 12:30)

time	[id] title	presenter
11:00	[113] Hands-on Tutorial of AMBER16 (sqm, sander, pmemd)	Dr CHOU, Ching-Yu

Workshop on Frontiers in Computational Drug Discovery - Conference Room 2, BHSS (14:00 - 15:30)

time	[id] title	presenter
14:00	[167] Potential of mean force and free energy calculations	Dr LIN, Jung-Hsin
14:50	[114] Gaussian accelerated molecular dynamics simulation (GaMD)	Prof. MIAO, Yinglong

Workshop on Frontiers in Computational Drug Discovery - Conference Room 2, BHSS (16:00 - 18:00)

time	[id] title	presenter
16:00	[115] Hand-on Tutorial of AMBER16 (sander, pmemd, WHAM, UI) and Gaussian accelerated molecular dynamics (GaMD)	Dr CHOU, Ching-Yu Prof. MIAO, Yinglong