

CADD PROGRAM, DE BARON RESORT, LANGKAWI 6 - 8 DECEMBER 2017)

Day 1	Seminar, Wednesday, 6 th December 2017	
09.00	Opening: Introductory Remark: Prof. Habibah A Wahab Welcome Remark (Officiation): Prof. Dato' Muhamad Jantan, Deputy Vice Chancellor (R&I), USM	
09.30	Keynote	Chair: Prof. Kenneth Merz Jr Title: Exploration of Molecular Recognition processes
10.10	Invited 1	Prof Dr. Asif Khan
10.30	COFFEE BREAK	
10.45	Invited 2	Prof. Mohd Basyaruddin Abdul Rahman
11.05	Invited 3	Prof. Muchtaridi Title: Modification of Chalcone Compound Isolated from <i>Eugenia aquae</i> Leaves as Novel Therapeutic Compounds Targeted Breast Cancer
11.25	Invited 4	Dr. Maywan Hariono Title: Synthesis of Novel Flavone Hydrazone: <i>In-Vitro</i> Evaluation of α -Glucosidase Inhibition, QSAR Analysis and Docking Studies
12.45	Invited 5	Assoc. Prof Dr. Vannajan Sanghiran Lee Title: Structure and Dynamics in Protein Design
13.05	LUNCH	
14.00	Invited 6	Prof. Kam Zhang Title: Scaffold-based Discovery of An Oncogenic BRAF Mutant Selective Inhibitor for Treating Metastatic Melanoma
14.20	Invited 7	Prof. Fumio Hirata Title: Structural Fluctuation of Protein and "Anfinsen's Dogma"
14.40	Invited 8	Prof. Stephen Doughty
15.00	Invited 9	Dr. Nurul Hashimah
15.20	Invited 10	Dr. Shirley Siu Title: Biomolecular Force Fields for Alkanethiol Self-Assembled Monolayers (SAMs): Comparison and Tuning
15.40	TEA BREAK	
16.00	Invited 11	Prof. Dr Norio Yoshida Title: pKa Prediction in Biological Systems Based on the Statistical Mechanics Theory of Liquids Combined with the Electronic Structure Theory
16.20	Invited 12	Dr. Choong Yee Siew Title: Structural insights of 16.3 kDa heat shock protein from <i>Mycobacterium tuberculosis</i>
16.40	Invited 13	Prof. Richard Bryce Title: Computational tools for drug design: modelling biomolecular conformation using molecular dynamics simulations
17.00	Keynote	Prof. Alan Mark Title: Validating of protein: ligand complexes: Reconciling theory and experiment
17.40	END OF SEMINAR	
20.30	DINNER & CULTURAL SHOW	

CADD WORKSHOP PROGRAM, DE BARON RESORT LANGKAWI, LANGKAWI

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	DAY 1 (6.12.17)	DAY 2 (7.12.17)		DAY 3 (8.12.17)			(9.12.17)	
0900	Seminar – See Seminar Program	Introduction to the course (Choong Yee Siew)		Solvation (Fumio Hirata)			ISLAND HOPPING	
0910		Force Field (Ken Merz)						
1000		Protein Structure & Modeling (Alan Mark)		Free Energy (Norio Yoshido)				
1045		Tea Break						
		HANDS- ON SESSIONS			HANDS-ON SESSION			
1100		BEGINNERS Unix (Choong Yee Siew)	INTERMEDIATE Using VMD in Molecular Modelling (Choi Sy Bing)	CADD 3 (Lecture) Cheminformatics - Similarity searching (Siti Zuraidah)	MD 3 Free Energy Calculation (MM/PBSA & 3DRISM) (Choong Yee Siew/Hassan Hadi)	BIOINFO 3 Sequence Alignment Homology Modelling (Modeller/SwissModel) (Choi Sy Bing & Yap Beow Keat)		
1150				CADD 4 Pharmacophore Modelling (Maywan)				
1300	LUNCH							
	Seminar	PARALLEL LECTURES			PARALLEL LECTURES			
1400		CADD 2 Docking (Ezatul Ezleen)	MD 2 Statistical Mechanics for Biomolecular system (Vannajan)	BIONFO 2 Sequence Alignment & Homology Modeling (Asif Khan)	CADD 5 (3D-QSAR) (Maywan)	MD 5 Principle Component Analysis in MD (Stephen Doughty)	BIONFO 5 Treading and fold recognition (Asif Khan)	
1450		CADD 2 (Lecture & hand-on) Molecular Docking (Siti Azma, Ezatul)	MD 3 & BIOINFO 3 Principles of MD (Shirley Siu)		CADD 6 (Hand-on) Pharmacophore Modelling (Maywan)	MD 6 Replica Exchange MD (Richard Bryce)	BIONINFO 6 <i>Ab initio</i> -using MD on protein folding (Choong Yee Siew)	
1540	Tea Break							
	Seminar	HANDS- ON SESSIONS			HANDS- ON SESSIONS			
1600		CADD 2 (Lecture & hand-on) Molecular Docking (Siti Azma, Ezatul)	MD2 & BIOINFO 2 Setting-up, Equilibration & Production (Hassan Hadi)		CADD 6 (Hand-on) Pharmacophore Modelling (Maywan)	MD 4 Advanced Sampling – Replica Exchange (Yusuf)	BIOINFO 4 Function Prediction using molecular docking (Choi Sy Bing)	
1700								
1710								
1800	DINNER							
2000	STUDENTS' PRESENTATION				-			
2100	END OF DAY							