

Bioinformatics Institute (BII)								
No.	Department	A*STAR Supervisor's Name	Designation	Email	Project Title	Project Description	Degree Awarded By Upon Graduation	Website Link (if any)
1	Translational Research Division	Dr Prakash Arumugam	Principal Investigator and Adjunct at Singapore Institute for Food and Biotechnology Innovation(SIFBI)	prakasha@bii.a-star.edu.sg	Chemical Genomics Group 1. Genome scale CRISPR screens to unravel Mode-of-action of bioactive compounds  Chemical Genomics Group 2. Synthetic Biology approach to produce natural sunscreens in yeast.	1. Use of CRISPR/Cas9 as a tool to manipulate genomes has provided the opportunity to perform genetic screens in mammalian cells and probe interesting questions in biology. The objective of the project is to use the Genome-wide CRISPR Knockout assay) in mammalian cells to identify factors that modulate resistance to therapeutic drugs and nutraceuticals. This will help in discovery of new therapeutic targets /nutraceuticals and mechanisms of drug resistance.  2. Ultraviolet rays from the sun can have serious damaging effects on our health such as cancer, premature ageing and inflammation. Current solutions to this problem in the form of sunscreens such as TiO2 and avobenzone are unhealthy and not eco-friendly. The objective of this project is to produce natural sunscreen compounds known as mycosporines in microbial systems in large amounts to attract industrial interest.	NTU	
2	Biomolecular Function Discovery Division	Dr Birgit Eisenhaber	Senior Principal Investigator	birgite@bii.a-star.edu.sg	Gene Function Prediction / Annotator Group Discovery of biomolecular mechanisms with sequence analysis and data mapped onto genomes, analysis of omics clinical data, prediction of gene function from sequence.	For decades to come, sequencing of DNA, RNA and other biological macromolecules (in context with other omics technologies) will be the main source about living systems. The discovery of biomolecular mechanisms that link genomes with phenotypes is the most important challenge in life science, the basis for rational applications in medicine, industry, etc. At the same time, ~10000 human genes have scarce or no functional annotation (PUBMED-ID: 30265449). The student's project consists of two stages: (i) In a personalized tutorial, the student is familiarized with modern methods in sequence-based function discovery. Exercises include examples with already functionally characterized genes and the goal is to extract the function just from the sequences and associated omics data that can be verified from known data. (ii) The actual research project will be dedicated to a set of omics data (the actual topic will change over time as this is a hot area of research) and the attempt to discover the underlying mechanisms and gene functions there. This effort will require using existing web-based tools, some office-level IT skills and, desirably but not obligatorily, some scripting skills (PERL, PYTHON or similar). The ability to digest biological literature is critical. For students that have more advanced IT skills, we can consider the development of a computerized tool for a selected class of data-derived function predictions. In this case, the life science background is not that important.	NTU / NUS	

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3	Biomolecular Function Discovery Division	Dr Frank Eisenhaber	Executive Director & Division Head	franke@bii.a-star.edu.sg	Gene Function Prediction / Annotator Group	Discovery of biomolecular mechanisms with sequence analysis and data mapped onto genomes, analysis of omics clinical data, prediction of gene function from sequence.  For decades to come, sequencing of DNA, RNA and other biological macromolecules (in context with other omics technologies) will be the main source about living systems. The discovery of biomolecular mechanisms that link genomes with phenotypes is the most important challenge in life science, the basis for rational applications in medicine, industry, etc. At the same time, ~10000 human genes have scarce or no functional annotation (PUBMED-ID: 30265449). The student's project consists of two stages: (i) In a personalized tutorial, the student is familiarized with modern methods in sequence-based function discovery. Exercises include examples with already functionally characterized genes and the goal is to extract the function just from the sequences and associated omics data that can be verified from known data. (ii) The actual research project will be dedicated to a set of omics data (the actual topic will change over time as this is a hot area of research) and the attempt to discover the underlying mechanisms and gene functions there. This effort will require using existing web-based tools, some office-level IT skills and, desirably but not obligatorily, some scripting skills (PERL, PYTHON or similar). The ability to digest biological literature is critical. For students that have more advanced IT skills, we can consider the development of a computerized tool for a selected class of data-derived function predictions. In this case, the life science background is not that important.	NTU	
4	Biomolecular Function Discovery Division	Dr Sebastian Maurer-Stroh	Executive Director (Designate), Adjunct Asst Prof at DBS (NUS)	sebastianms@bii.a-star.edu.sg	Protein Sequence Analysis Group 1. Computational sequence and structure analysis to combat viral infectious diseases. 2. Computational sequence and structure analysis to study protein allergenicity in novel food 3. Computational sequence and structure analysis using AI for enzyme design 4. Computational sequence and structure analysis using AI for evaluating genetic variants in human diseases (early childhood)	1. Computational sequence and structure analysis to combat viral infectious diseases. => study virus evolution and interpret effects of mutations, contribute tools for better surveillance 2. Computational sequence and structure analysis to study protein allergenicity in novel food => use and develop tools to predict protein allergenicity in novel food from the sequence and structure 3. Computational sequence and structure analysis using AI for enzyme design => Learn and develop workflows using AI for optimizing enzyme structures for stability and increased output 4. Computational sequence and structure analysis using AI for evaluating genetic variants in human diseases (early childhood) => Apply and develop workflows of computational methods including AI to predict effects of mutations on protein structure and function relevant for human diseases	NUS	

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5	Biomolecular Modeling and Design Division	Dr Chandra Verma	Senior Principal Investigator & Head of Research Division, Adjunct Professor DBS (NUS), Adjunct Professor SBS (NTU), Adjunct Principal Research Scientist (SERI)	chandra@bii.a-star.edu.sg	Atomistic Simulations & Design in Biology Group Molecular modelling & simulations of biomolecular mechanisms; design of drugs, peptides, proteins, enzymes, antibodies in oncology; inflammation, antimicrobials. Machine learning/AI in drug design.	<ol style="list-style-type: none"> <li>1. Atomistic modelling and simulations of properties of proteins/peptides to understand characteristics such as aggregation, gelation, solubility, liquid-liquid phase transitions to develop machine learning methods for use in the food, cosmetic, pharma industry</li> <li>2. Atomistic modelling and simulations of proteins and interactions in the p53 pathway to develop novel therapeutics including stapled peptides, cyclic peptides, p53 reactivating molecules, minibodies</li> <li>3. Atomistic modelling and simulations of novel antimicrobials targeting membranes</li> <li>4. Atomistic modelling and simulations of rigorous understanding of hydration properties of proteins and peptides with a view to applying machine learning methods for design of proteins, therapeutics</li> <li>5. Atomistic modelling and simulations for developing rapid analytic methods to explore the role of SNPs in protein structure, dynamics, function and effects on therapeutics</li> <li>6. Applications of Machine Learning/AI methods to accelerate MD simulations of biomolecules</li> </ol>	NTU / NUS	
6	Biomolecular Modeling and Design Division	Dr Hao Fan	Principal Investigator; Adjunct Associate Prof at Synthetic Biology Translational Research Programme in NUS School of Medicine, and in Ctr for Computational Biology in DUKE-NUS Medical School	fanh@bii.a-star.edu.sg	Structure-based Ligand Discovery & Design Group Developing and applying computational methods including protein structure prediction, chemical/peptide/protein docking, MD simulation, and AI to study protein-ligand interactions, such as biomarker/drug design, chemical toxicity prediction, and enzyme design.	<ol style="list-style-type: none"> <li>1. In silico prediction of cancer drug response to kinase mutants.</li> <li>2. Directed computational evolution of cytochrome P450 enzymes.</li> <li>3. Molecular interactions between endocrine-disrupting chemicals and nuclear receptors.</li> <li>4. AI-guided protein-ligand scoring function development.</li> <li>5. Ligand discovery for GPCRs</li> </ol>	NUS	<a href="http://www.a-star.edu.sg/bii/research/bmad/slidd">www.a-star.edu.sg/bii/research/bmad/slidd</a>

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7	Biomolecular Modeling and Design Division	Dr Peter Bond	Senior Principal Investigator, Adjunct Asst Prof at DBS (NUS)	peterjb@bii.a-star.edu.sg	Multiscale Simulation, Modelling & Design Group Multiscale modelling and simulation of biomolecules, towards novel therapeutic development. Focus on modelling of viral and bacterial pathogens, and host immune receptors / antibodies.	As part of the Multiscale Simulation, Modelling & Design Group in BII, a computational modelling and simulation approach will be used to investigate the molecular mechanisms by which synthetic antimicrobial peptides interact with bacterial membranes to induce bacterial cell lysis and/or aggregation. This will be performed in order to understand how different sequences in a library of peptides influence such interactions, and to design new peptides, and will be iteratively validated via wet lab experiments collaboratively in the group of Prof. EE Pui Lai Rachel (NUS Pharmacy).	NUS	
8	Biomolecular Modeling and Design Division	Dr. Igor N. Berezovsky	Senior Principal Investigator, Adjunct Associate Professor DBS (NUS)	igorb@bii.a-star.edu.sg	Physics & Evolution of Biological Macromolecules Group Protein dynamics and allosteric regulation of protein function. Design of allosteric drugs and allosteric effects of mutations. Chromatin structural dynamics and epigenetic regulation. Evolution of protein function, protein thermostability molecular adaptation.	<ol style="list-style-type: none"> <li>1. Development of theoretical models of allostery and their implementation in computational frameworks. Analysis of the allosteric regulation in proteins and engineering of allosteric signalling in protein design efforts.</li> <li>2. Using models of allostery developed in the group for the analysis of different allosteric effectors aimed at fragment-based design of new drug candidates.</li> <li>3. Development and using models of chromatin organization and whole-genome 3D reconstruction complemented by the analysis of the high-throughput epigenetic data with the goal to understand it in norm and pathology.</li> <li>4. Bioinformatics, sequence/structure analysis of genomes and proteomes of extremophiles, and simulations towards understanding of molecular mechanisms of adaptation to extreme environments and ways of engineering them in newly designed proteins.</li> </ol>	NUS	
8	Imaging Informatics Division	Dr Chiam Keng Hwee	Senior Principal Investigator	chiamkh@bii.a-star.edu.sg	Biophysical Modelling Group Biophysical modeling of cellular and molecular processes involved in cell motility and cell interactions with the microenvironment	Development of computational models to describe the signaling pathways and biophysics of how cells sense environmental cues and respond by migrating in the direction of the cues	NTU / NUS	
10	Imaging Informatics Division	Dr Lee Hwee Kuan	Senior Principal Investigator, Adjunct Asst Prof at NUS	leehk@bii.a-star.edu.sg	Computer Vision & Pattern Discovery Group Artificial Intelligence for healthcare: theory and applications. Project involves close collaborations with hospitals.	Theory and applications of Artificial Intelligence on the healthcare domain. This includes clinical domains such as cancers (digital pathology and radiology), cardiology (ultrasound, CT, EGM, patient data), skin diseases (multiple imaging techniques) and others. On the theoretical part, we identify big AI problems specific to real world healthcare problems. These theoretical efforts will form the basis of our next generation AI capabilities in the laboratory.	NUS/NTU	

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11	Imaging Informatics Division	Dr Loo Lit Hsin	Senior Principal Investigator	loolh@bii.a-star.edu.sg	Complex Cellular Phenotype Analysis Group High-throughput phenotypic profiling for predicting the efficacy of cancer immunotherapy agents.	The objective is to identify phenotypic markers that are predictive of cellular responses to cancer immunotherapy and other anti-cancer agents.	NUS	
12	Translational Research (APD Lab)	Dr Su Tran-To Chinh	Research Scientist	chinhstranto@bii.a-star.edu.sg	Structure-based Antibody Drug Development Structural modeling integrated with machine learning for therapeutics design.	The project aims to integrate structural computational modeling and machine learning to assist in studying and design of biologics to speed up drug development via protein-protein interactions, e.g. antibody-antigen and viral target proteins.	NTU	