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	Biomolecular Sequence to Function Division	Dr Sebastian Maurer-Stroh	Executive Director	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 inlcuding AI to predict effects of mutations on protein structure and function relevant for human diseases	NUS	
2	Biomolecular Sequence to Function	Dr Roland Huber	Assistant Principal Investigator	rghuber@bii.a-star.edu.sg	Structure and Function of RNA Structural genomics of RNA. Regulation, structure-function relations, and design of RNA. Focus on viral pathogens, host-virus interactions, surveillance of viral pathogens, identification and annotation of functional elements and structure-based drug discovery on RNA targets.	Reassortment of genomic segments between different viruses coexisting in the same host are one driver of the emergence and potential cross-species transmission of new strains of Influenza viruses and hence are a key concern for potential pandemics. Moreover, the efficient production of Influenza vaccines relies on the integration of newly identified surface antigens into strains that are optimized for efficient viral production in suitable biotechnological processes. Structural studies of the viral ribonucleoproteins have largely focused on the protein assembly. We are constructing detailed structural models comprising of viral RNA, the viral nucleoproteins and the viral polymerases. EM studies of these assemblies have allow us to integrate near-atomic resolution models of the protein components with RNA structures modelled based on cross-linking and chemical probing data of the Influenza genome. We are aiming to create a comprehensive interaction site model that rationalizes the mutual recognition of segments and the spatial organization of these complexes at the time of viral packaging.	NTU / NUS	https://www.a-star.edu.sg/bii/research/bsfd/fsrna
3	Biomolecular Sequence to Function Division	Dr Kumar Selvarajoo	Senior Principal Investigator	kumar_selvarajoo@bii.a-star.edu.sg	A systems biology platform to integrate dynamic metabolomics and fluxomics data into a computational model	The student will curate metabolomics and fluxomics data, both inhouse and across databases, to develop a kinetic model. The model will be subsequently used to simulate metabolic pathways of engineering microbes (E.coli and Yeast)	NUS	

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)
4	Biomolecular Sequence to Function Division	Dr Kumar Selvarajoo	Senior Principal Investigator	kumar_selvarajoo@bii.a-star.edu.sg	Artificial Intelligence for Biological Pathway Discovery	The student will develop Machine Learning (ML) algorithms to train transcriptomics, proteomics and/or metabolomics data to finally develop a ML model that will accurately predict proteomics/metabolomics data from transcriptomics data, for example, to predict mutant microbe's metabolomics response based on transcriptomics data	NUS	
5	Biomolecular Sequence to Function Division	Dr Birgit Eisenhaber	Senior Principal Investigator	birgite@bii.a-star.edu.sg	Gene Function Prediction / Annotator GroupDiscovery 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	

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)
6	Biomolecular Sequence to Function Division	Dr Frank Eisenhaber	A*STAR Senior Fellow / Senior Principal Investigator	franke@bii.a-star.edu.sg	Gene Function Prediction / Annotator GroupDiscovery 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	
7	Biomolecular Structure to Mechanism Division	Dr Chandra Verma	Deputy Director (Research)	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.	1. Atomistic modelling and simulations of properties of proteins/peptides to understand characteristics such as aggregation, gellation, solubility, liquid-liquid phase transitions to develop machine learning methods for use in the food, cosmetic, pharma industry 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 3. Atomostic modelling and simulations of novel antimicrobials targeting membranes 4. Atomistic modelling and simulations of rigorous understanding of hydration properties of proteins and peptides with a view to applyimng machine learning methods for design of proteins, therapeutics 5. Atomistic modelling and simulations for developing rapid analytic methods to explore the role of SNPs in protein structue, dynamics, function and effects on therapeutics 6. Applications of Machine Learning/AI methods to accelerate MD simulations of biomolecules	NTU / NUS	

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)
8	Biomolecular Structure to Mechanism Division	Dr Peter J Bond	Senior Principal Investigator	peterjb@bii.a-star.edu.sg	Multiscale Simulation, Modelling & Design Group Computational design and development of novel antimicrobial peptides.	There is an ever growing crisis of bacterial multidrug resistance, which threatens to make existing antibiotic therapies redundant. As part of the Multiscale Simulation, Modelling & Design Group in BII, a computational modelling 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. This will be iteratively validated via wet lab experiments in the group of Prof. EE Pui Lai Rachel (NUS Pharmacy), towards the development of new molecules with optimized antimicrobial properties for use against drug-resistant bacterial pathogens.	NUS	https://www.a-star.edu.sg/bii/research/bsmd/msmd https://www.ee-research-group.com
9	Biomolecular Structure to Mechanism Division	Dr Peter J Bond	Senior Principal Investigator	peterjb@bii.a-star.edu.sg	Multiscale Simulation, Modelling & Design Group Computational design and experimental development of novel nucleotide sensors.	Dysfunction of nucleotide binding to proteins is the cause of several diseases (e.g. cancers and Parkinson's), and the ability to track the amounts of nucleotides in living cells would represent a revolution in improved diagnostic and treatment strategies. In this project, we will develop biologically inspired fluorescence-based sensors, based on existing proteins whose normal function in the cell is to sense ATP. As part of the Multiscale Simulation, Modelling & Design Group in BII, we will use computational approaches to model protein structure/dynamics and predict side-directed point mutations to tune nucleotide selectivity, and design novel protein-sensor chimeras. Alongside this, in the group of Prof. Thorsten Wohland (NUS DBS / Chemistry), molecular biology approaches will be used to engineer the designed mutants that may be fused to fluorescent constructs, towards the development of novel in vitro and in vivo biosensors with broad therapeutic and diagnostic potential.	NUS	https://www.a-star.edu.sg/bii/research/bsmd/msmd https://www.dbs.nus.edu.sg/staffs/thorsten-wohland/

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)
10	Biomolecular Structure to Mechanism Division	Dr Igor N Berezovsky	Senior Principal Investigator	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 mutaitons. Chromatin structural dynamics and epigenetic regulation. Evolution of protein function, protein thermostability molecular adaptation.	1. Depelopment of theoretical models of allostery and their implementation in computatinoal framewogks. Analysis of the allosteric regulation in protieins and engineerings of allosteric signalling in protein design efforts. 2. Using models of allostery developed in the group for teh analysis of different allosteric effectors aimed at fragment-based design of new drug candidates. 3. Developement and using models of chromatin organization and whole-genoome 3D reconstruction complememnted by teh analysis of the high-throughput epigenetic data with the goal to understand it in norm and pathology. 4. Bioinformatics, sequence/struture 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 desinged proteins.	NUS	https://www.a-star.edu.sg/bii/research/bmad/pebm
11	Biomolecular Structure to Mechanism Division	Dr Hao Fan	Senior Principal Investigator	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.	1. In silico prediction of cancer drug response to kinase mutants. 2. Directed computational evolution of industrial enzymes. 3. Structure-based functional mechanism study and chemical toxicity prediction for nuclear receptors and transporters. 4. AI-guided protein-ligand scoring function development. 5. Structure-based functional mechanism study and ligand discovery for GPCRs	NUS	https://web.bii.a-star.edu.sg/~fanh/
12	Cellular Image Informatics Division	Dr Lee Hwee Kuan	Deputy Director (Training and Talent)	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.	Adjunct position at NUS/NTU	
13	Cellular Image 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	

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)
14	Cellular Image 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	