

2016 SATU Joint Research Scheme Program Host Application Form

Date: 2016/4 /26 (year /month/day)

1. Host University

University Malaya

2. Host Unit

Department of Chemistry, Faculty of Science

3. Joint Research Project Title

Cell Membrane Targeting Peptide: Computational Custom-Tailored Peptide Design and Synthesis

4. Principal Investigator

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SATU Presidents' Forum

of Southeast and South Asia and Taiwan Universities
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6. Project Details

Project Description	<p>As an advanced approach to identify suitable targeting molecules is required for various diagnostic and therapeutic interventions, we propose a procedure to devise peptides with customizable features to improve affinity by using an iterative computer-assisted optimization strategy. An algorithm according to the structural parameters and the interaction energy criterion will be utilized to breed peptides <i>in-silico</i> and the "optimized" peptides will be determined and tested in an appropriate <i>in-vitro</i> assay. As a proof of concept, two models from our previous work: (i) a diverse sets of lead peptides with improved affinity against protein membrane target model for dengue virus envelope (DENV2) (Baharuddin, et.al, 2014) and (ii) antimicrobial peptides toward bacteria membrane lipid model, will be investigated.</p> <p>The strategy consisting:</p> <ol style="list-style-type: none"> 1. Determine the binding site and the sequence of residues on the surface of the target protein on which the peptide will be docked. 2. Search for common substrate and calculate the pair-wised decomposition interaction energy. 3. Design, improve, and evaluate the binding interactions/affinity with structural modification and point mutations using automated mutation and in-house docking protocol. 4. Explore peptide-membrane interactions with coarse-grained molecular dynamics simulation. 5. Experimental in vitro activity testing and cell based assay for membrane protein.
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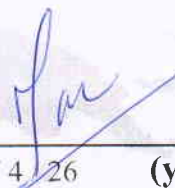
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7. Acknowledgement (Signed by the President or SATU representative to show recognition)

Name
title

PROFESSOR DR. NOORSAADAH ABD. RAHMAN
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(signature)

Date: 2016 / 4 / 26 (yyyy/mm/dd)

Please email satu@email.ncku.edu.tw before 2016.4. 29(Fri.) for application with the subject line: < 2016 SATU JRS host application –School Name>. Thank you.