

In addition, how these sustainable technologies can be pivotal in reducing poverty, hunger and income disparity. If correct measures are implemented at the outset, the future, which you will be part of, will be greener, a better place to live economically and socially.

With these thoughts, I am confident that you can play a key role in shaping Sri Lanka for the next millennia. Having being exposed to many challenges at the Institute

and the commitment you have shown to complete your research, is a clear indication that you are ready to face any challenge, locally or internationally. Now it's time for you to take the bull by the horns.

I wish all the presenters good luck in your future endeavors and remember to make your alma mater and your country proud.

### Kandiah Memorial Awards - 2022

Three Kandiah Memorial Awards are made annually to commemorate Professor A Kandiah, the first President of the Chemical Society of Ceylon. Professor Kandiah served in the University of Ceylon from 1933 and was the Professor of Chemistry at the University of Ceylon from 1934 until his death in 1951.

The Kandiah Memorial Awards for Basic Chemistry and Applied Chemistry are awarded for the best research contribution in Chemistry carried out by a postgraduate student registered at a Higher Education Institute and for work carried out in Sri Lanka with the exception of special analysis (less than 20% of findings) that cannot be done in the country.

- The Kandiah Award for Basic Chemistry is made for research predominantly in Basic Chemistry (Organic, Inorganic, Physical & Analytical).
- The Kandiah Award for Applied Chemistry is made annually for research in related areas such as polymer, food, biochemistry, biotechnology etc. where interdisciplinary research is involved, provided that chemistry has a central role & comprises at least 50% of the content.
- The Kandiah Memorial Graduateship Award is awarded to the best piece of research in the chemical sciences carried out by a Graduate Chemist of the Institute of Chemistry Ceylon registered with a Higher Educational Institute for a postgraduate degree.

### Kandiah Memorial Award for Applied Chemistry - 2022



**Ms. Yasuri Amarasekara** is expecting to start her Ph.D. degree at Macquarie University, Australia. Her research interests span the field of Peptide Chemistry, Cancer Cell Biology, Computational Chemistry, and

Nanomedicine. She has obtained her B.Sc. Special degree in Immunology and Integrative Molecular Biology from the Faculty of Science, University of Colombo. She received her postgraduate degree (Master's in Philosophy) from the Sri Lanka Institute of Nano Technology.

In terms of her experiences, she has worked as a Lecturer attached to the Department of Biomedical Sciences under the Faculty of Science at the NSBM Green University. She has also worked as a Research Assistant at the Centre for Scientific Computing and Advanced Drug Discovery at the University of Sri Jayewardenepura, Sri Lanka, where she focused on Computer-Aided Drug Discovery projects.

## Improving the Stability of XLAsp-P2 Through Nano conjugation

Ms. B.M. Yasuri D.E. Amarasekara

*Sri Lanka Institute of Nano Technology*

Antimicrobial (AMP) and Anti-cancer peptides (ACPs) recently have received significant attention as promising chemotherapeutic agents that avoid the drawbacks of current drugs. Many studies have verified that some synthetic and natural peptides possess a rapid and broad spectrum of anticancer activity towards tumor cells rather than normal cells such as human red blood cells. Moreover, these peptides were also verified to have the ability to overcome the multidrug-resistance mechanism and synergistic effects in combination treatment.

The current study mainly focuses on a peptide known as XLAspP2-RA, a peptide analog (EDLDED) designed based on a novel AMP, XLAsp-P2 (EDLDE). The natural peptide was initially isolated from the skin tissues of *Xenopus laevis* and has been reported to exhibit moderate antibacterial activity.<sup>1</sup> The analog sequence was designed based on the retro analog concept and possesses a rapid anticancer activity, with the IC<sub>50</sub> value of 5.36 µg/ml for RD cells. RD was derived directly from biopsy specimens of a pelvic Rhabdomyosarcoma (RMS), a malignant skeletal muscle cancer of pediatric patients.

Emerging evidence has shown that RMS's malignant growth involves a multistep process of signaling protein dysregulation that includes prolonged activation of serine/threonine kinases (Akt). Our *in silico* studies have indicated that peptides exhibited cancer-selective toxicity, mainly because that cancer cells are involved with the hyperactivation of Akt-1 protein. The present study used docking and (un) critical simulation analyses to identify XLAspP2-RA interacting residues of human Akt-1 protein. The results proved that peptide is an allosteric inhibitor of Akt-1 and exerts its inhibitory mechanism by binding to the allosteric site of Akt-1 and engaging the functionally important residues in various interactions. The exact binding mode of the peptide-based on the computational approach is presented, and various interacting residues within the allosteric site of this protein were identified and characterized. The quality of docking was assured by the negative dock score, which was -8.44 kcal/mol, and the identified various molecular

interactions between the protein and the ligand. In the docking and (un)binding simulation analyses, the Asn53, Gln59, Trp-80, and Lys268 were identified as the key residues among various important identified residues. The docked peptide-protein conformation is expected to serve as a suitable model for understanding the amino-acid environment mediating molecular interactions and thus, providing details for the inhibitory mechanism of the peptide. In the future, this study will help design novel peptidomimetics for human Akt isoforms, and it will help experimental biologists in testing and designing better inhibitors.

In addition to the cytotoxicity and undergoing inhibitory mechanism of XLAspP2-RA, we proved that it could increase the efficacy of the peptide against RD cells when it is encapsulated with drug carriers such as fHNT. The induced effect is shown to permit the use of relatively low concentrations of peptides and drugs to achieve significant anticancer effects *in vitro*. This dose reduction minimizes drug side effects on normal cells and enables an effective apoptosis-mediated anticancer effect. Our present study has implications in that XLAspP2-RA peptide may become a promising anticancer therapeutic agent with high anticancer selectivity and a strong induced effect in combination therapy. Our studies mainly illustrate the mechanism of XLAspP2-RA peptide-induced cell death and may be helpful in the design of chemotherapeutics against RMS cell lines.

Furthermore, in the model study, we investigate the potential of GO as an efficient system for sustaining the antibacterial activity of CEF. Upon successful encapsulation of CEF into GO, the anticipated sustained release of CEF was achieved. Moreover, the GO-PEG-CEF composite showed an enhanced antibacterial activity compared to positive control on gram-positive bacteria. GO-PEG-CEF could be an effective nano-based antibiotic system with synergistic antibacterial mechanisms to treat infections caused by gram-positive bacteria.

In the future, the bioavailability of the peptide after release from fHNT-XLAspP2-RA composites can be

confirmed by *in vitro* studies using kinetic assays. The research can be taken further to the next level within *in vivo* studies on different animal models. Additionally, the tubular ends and surface of drug-loaded fHNT can be modified with pH-sensitive polymers, followed by the preparation of oral tablets for gastrointestinal drug delivery. Such aminosilane functionalized nanomaterials have been used in some previous studies, and they displayed no toxicity upon oral consumption.<sup>2,3</sup> These milestones by aminosilane modified nanomaterials indicate the promising usage of the peptide-loaded fHNT.

#### Contribution

This study, therefore, focused on peptide-nano hybrids, exposing new pathways in therapeutic applications. Ms. B.M. Yasuri D.E. Amarasekara carried out this project in her M. Phil degree. She has completed the work at the Sri Lanka Institute of Nano Technology

under the supervision of Dr. Laksiri Weerasinghe. In this project, she managed the methodologies and validated the methods. Further, she did all the formal analysis by herself, and she was able to publish the work in two international journals.

#### References

1. Zhang Y, Liu S, Li S, Cheng Y, Nie L, Wang G, et al. Novel short antimicrobial peptide isolated from *Xenopus laevis* skin. *J Pept Sci.* 2017; 23(5):403–9.
2. Yang Y, Chen Y, Leng F, Huang L, Wang Z, Tian W. Recent advances on surface modification of halloysite nanotubes for multifunctional applications. *Appl Sci.* 2017; 7(12).
3. Grimes WR, Luo Y, McFarland AW, Mills DK. Bi-functionalized clay nanotubes for anti-cancer therapy. *Appl Sci.* 2018; 8(2):1–12.

### Professor M. U. S. Sultanbawa Award for Research in Chemistry

Awarded for the best research paper presented at the Annual Sessions of the Institute of Chemistry Ceylon, for the unique, distinguished and significant contribution made to the cause of Science, Chemistry, Education and Research in Sri Lanka.

#### Professor M. U. S. Sultanbawa Award for Research in Chemistry - 2022



**Ms. Imesha Lakmini Hettige** graduated from the University of Sri Jayewardenepura with B.Sc. Honours Degree (First Class Honours) in Chemistry in 2019, becoming the batch-top, and also obtained the Graduateship in Chemistry (First Class Honours) from the College of Chemical Sciences, Institute of Chemistry Ceylon in 2018, ranking third in the batch. During her undergraduate studies, she received several awards such as the Prof. Tuley de Silva Gold Medal for obtaining highest overall marks at the B.Sc. Chemistry Special Degree, Prof. W S Fernando Gold Medal for Physical and Inorganic Chemistry and Prof.

A. M. Abeysekera Gold Medal for Organic Chemistry at the University of Sri Jayewardenepura, as well as the Graduate Chemist Silver Jubilee Commemoration Award, Mr and Mrs Gamini Gunasekara and Family Prize, Rasanthika Nayomi Jayathissa Memorial Prize, W.R.O. Fernando Memorial Prize and Professor G.C.N. Jayasuriya Memorial Scholarship and others at the Institute of Chemistry Ceylon. She conducted her research on “Synthesis and characterization of platinum complexes with ethylenediamine and diethylenetriamine sulphonamide ligands towards biological applications” which was selected for the Professor M U S Sultanbawa Award for Research in Chemistry – 2021, under the supervision of Professor Theshini Perera at the University of Sri Jayewardenepura. She just recently started working on her PhD research project for which she was awarded the Postgraduate Research Scholarship from the ARC Industrial Transformation Training Centre for Fragment-Based Design (CFBD) at the Monash Institute of Pharmaceutical Sciences, Faculty of Pharmacy and Pharmaceutical Sciences, Monash University, Australia.