Clement AGONI

Technology Centre:	Food for Health Ireland (FHI)
Academic Mentor	Professor Dennis Shields
Company Partner:	NURITAS
Company Mentor:	Dr. Hansel Gómez Martínez

Dr. Clement Agoni has completed his Ph.D. (2021) in Pharmaceutical Chemistry at the University of KwaZulu Natal (South Africa), MMedSc (2018) in Pharmaceutical Chemistry at the University of KwaZulu Natal (South Africa), and a BSc (2014) in Medical Laboratory Technology at University of Cape Coast (Ghana). Before moving to Ireland, Clement worked as a postdoctoral research fellow at the Department of Pharmaceutical Sciences, Faculty of Science, Tshwane University of Technology

Professor Denis Shields

Professor Denis Shields is a full professor of clinical bioinformatics in the School of Medicine, University College Dublin. His research group analyses peptides, focussing on potentially therapeutic bioactives and on deepening understanding of the role of proteolysis in disease and health. Current applications include the design of peptides targeting SARS-CoV-2, profiling peptide distributions in Inflammatory Bowel Disease, and profiling the pattern of proteolysis and peptide generation in bean sprouts. The group's peptide analysis software is provided to academics worldwide (bioware.ucd.ie). He has led successive PhD programmes in computational biology (2007-2026; funded by Irish Research Council, Wellcome Trust, and Science Foundation Ireland; and co-funded with the Joint Research Centre of the European Union). He has worked in industry as Biometrics Manager at ICON Clinical Research where he prepared clinical trial results for regulatory approval, and Managing Director at Surgen Ltd, a campus company, providing biobanking and genetics analysis services in clinical trials.

Dr. Hansel Gómez Martínez

Dr. Hansel Gómez Martínez is a Principal Data Scientist and Bioinformatician at NURITAS. He forms part of the team in NURITAS working on implementing AI and molecular modelling methodologies to help us find bioactive peptides binding to specific targets. He has directly been involved in the training of Machine Learning predictors for peptide bioactivity and the implementation of methods for protein-protein docking, molecular dynamics simulations, and free energy calculations to estimate the binding affinity of peptides to protein receptors. Dr. Gómez has extensively employed Molecular modelling techniques for the last ten years using different levels of theory, from coarse-grained applications to molecular mechanics and quantum mechanics. He also has extensive teaching experience in different areas, including Biochemistry, General Chemistry, Physical Chemistry, Enzymology, and Data Science and Machine Learning methods at three different academic institutions: the University of Havana, the Autonomous University of Barcelona, and the University of Barcelona. During his period as an academic, Dr. Gómez was awarded several times by the Spanish Ministry of Science and was funded to briefly join the Max Planck Institute for Coal Research and moved to Brazil for a few months to work at the Chemistry Institute, Federal University of Rio de Janeiro. Dr. Gómez also has much experience using several HPC facilities around Europe. He is currently the administrator of all the scientific computational resources at NURITAS, which also includes the AWS cloud.

Food for Health Ireland (FHI)

Food for Health Ireland (FHI) brings together leaders in industry and research to improve global health through innovation in food. From start-ups to established multinationals, the centre has spent more than a decade working with the food industry to deliver commercial impact through pioneering research solutions. FHI's extensive research infrastructure, combined with world-class technical expertise, makes it a leader in the development of novel food ingredients with proven health benefits. With the global functional food market forecast to be worth more than €450bn by 2028, FHI aims to position Ireland as a global leader in this space by providing strategic R&D support to Irish companies and multinationals.

NURITAS

Is a biotechnology company that uses AI to mine therapeutic peptides from natural food sources that can be used in therapeutic and preventative fields. They combine computational biology with nutritional science at the molecular level to develop preventative and curative peptide-based treatments for disease with industry-leading speed and accuracy. The company's unique, disruptive computational approach to discovery uses artificial intelligence, deep learning, and genomics to rapidly and efficiently predict and then provide access to discover new patentable bioactive peptides in multiple therapeutic areas. NURITAS will fully support Clement's project in different ways by granting him access to all their computational resources, including the Oracle and Amazon Cloud, so that he can work on the project without any limitations from the computational power perspective. NURITAS is also ideally situated to provide an optimal working environment since all the team members working in different areas of expertise will support Clement if necessary. Clement will also have access to formation programs, including industry programs that will improve his skills while providing him experience on how to deploy his research in a production environment of a biotechnology company. All the resulting data resulting from this project will also be used to train new machine learning models to speed up the discovery process in future projects in NURITAS and, hence, will positively impact the company's business model.

Host Institution

University College Dublin (UCD) and the Conway Institute of Biomolecular and Biomedical Research have strong academic reputations, industry linkages, and a bioinformatics centre of excellence. UCD also co-locates extensive science research facilities on a single campus, and among its five core research pillars are three that are core to this proposal: Agri-Food, ICT, and Health. As a European research leader in the integration of computational and experimental/clinical research, UCD is also supported by Systems Biology Ireland and the UCD Centre for Bioinformatics, led by my academic mentor Shields and including Desmond Higgins (one of the top ten scientists in the world for his multiple sequence alignment CLUSTAL software) and Kenneth Wolfe (FRS; twice awarded ERC advanced grants). Also, UCD hosts a high-performance computer (sonic cluster) and researchers additionally have access to the Irish Centre for High End Computing. UCD also plays host to Food for Health Ireland, which provides a multidisciplinary and inter-sectoral organisation bringing together industry and academia. It's core staff support commercialisation, dissemination, training, coordination, and industry relationships

Clement's project

"Structural modelling of peptide target interactions for peptides of natural origins"

The centrality of peptides in crucial physiological processes such as protein-protein Interactions, signal regulation, and transduction presents peptides as promising potential leads for, or alternatives to, drugs. Naturally sourced bioactive peptides have strong safety profiles and easier regulatory approval processes, as they can be derived by natural processes (food grade protease digestion) from a well characterised food component (protein). The central research question is whether structural modelling can accelerate the development of peptides from natural sources for therapeutic purposes while also improving our understanding of their mechanisms of action. This is challenging because peptides adopt more flexible structures than small molecules. This study aims to assemble a pipeline identifying naturally occurring peptides to test their binding to therapeutic targets using molecular modelling techniques and then combine findings with machine learning to prioritize peptides with promising therapeutic activity. Thus, the study seeks to accelerate existing methods for discovering bioactive peptides from natural protein as it will incorporate computational techniques that are relatively faster than experimental methods. For bioactive peptide mixtures, the identification of lead bioactives by this method can accelerate the description and refinement of bioactive components.