COMPUTATIONAL MODELLING OF THE NUCLEOCAPSID PROTEIN FOR THE PREDICTION AND DELIVERY OF COVID- 19 DRUG TARGETS

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(18PCH01811)

DECEMBER 2020

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A DISSERTATION SUBMITTED TO THE SCHOOL OF POSTGRADUATE STUDIES IN PARTIAL FULFILMENT OF THE REQUIREMENTS FOR THE AWARD OF MASTER OF SCIENCE (M.Sc.) DEGREE IN MANAGEMENT INFORMATION SYSTEM IN THE DEPARTMENT OF COMPUTER AND INFORMATION SCIENCES, COLLEGE OF SCIENCE AND TECHNOLOGY, COVENANT UNIVERSITY.

DECEMBER 2020

ACCEPTANCE

This is to attest that this dissertation was accepted in partial fulfillment of the requirements for the award of Master of Science (M.Sc.) degree in Management Information System in the Department of Computer and Information Science, College of Science and Technology, Covenant University, Ota, Ogun State, Nigeria.

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(Secretary, School of Postgraduate Studies) **Signature and Date**

Prof. Akan B. Williams
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DECLARATION

I, **BISHUNG JANET UGUMMAYE** with matriculation number **18PCH01811**, hereby declare that this dissertation entitled **COMPUTATIONAL MODELLING OF THE NUCLEOCAPSID PROTEIN FOR THE PREDICTION AND DELIVERY OF COVID- 19 DRUG TARGETS** was carried out by me under the supervision of Prof. Victor C. Osamor. This project is an original study in the Department of Computer and Information Sciences, College of Science and Technology, Covenant University, Ota, Nigeria. All scholarly information used in this study is fully acknowledged.

BISHUNG, JANET UGUMMAYE _____

Signature and Date

CERTIFICATION

This is to certify that the dissertation titled **"COMPUTATIONAL MODELLING OF THE NUCLEOCAPSID PROTEIN FOR THE PREDICTION AND DELIVERY OF COVID-19 DRUG TARGETS"** was carried out by **BISHUNG JANET UGUMMAYE** with matriculation number 18PCH01811 under the supervision of Prof. Victor C. Osamor in the Department of Computer and Information Science, College of Science and Technology, Covenant University, Ota, Ogun State.

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(Dean, School of Postgraduate Studies) **Signature and Date**

DEDICATION

This dissertation is dedicated to God for his grace and to me for the strength to pull through.

ACKNOWLEDGEMENTS

All praise to God, the creator of the universe, the source of all good inspirations and insights and all wise God for his unlimited grace, mercies, insights, directions, and wisdom all through my academic pursuit in Covenant University. It's His doing and he deserves all the glory.

I would like to appreciate my awesome parents Mr. and Mrs. Matthias Bishung and my siblings for their support physically, spiritually, and financially from the beginning of this academic pursuit to the completion.

Immense appreciation to the Chancellor of Covenant University, Dr David Oyedepo for his vision, which birthed a world class academic institution where sound academic excellence can be obtained, and sound academic research can be made. I also want to appreciate the entire management of Covenant University for seeing that the vision has been fulfilled towards accomplishing great excellence through the master's academic programme.

My sincere gratitude goes to my dissertation supervisor, Prof Victor C. Osamor, for his diligent and great guidance towards the completion of the dissertation. Despite his busy schedule, he made time to guide, instruct and made sure the work was done timely and with excellence. I also appreciate the Head of Department of Computer and Information Sciences (CIS), Dr. Olufunke O. Oladipupo, the PG Coordinator, the former Head of Department, Prof. Ambrose A. Azeta, and the entire faculty members for their remarks during the numerous presentations during the cause of this project work.

Finally, I would like to appreciate my lovely friends Okezie Fiona, Awal Abdulganiyu, Atainyang Idara, Koyejo Ooreofe, Ejiobih Chukwuebuka, Ani Osinachi Sylvester, Edosomwan Boma, Okezie Chidinma, who assisted me in one capacity or the other to make this work a reality, and my colleagues for making this journey a remarkable one despite the challenges we faced throughout the programme.

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ABSTRACT

The Severe acute respiratory syndrome coronavirus 2, which is the causative agent of the Coronavirus Disease 2019 (COVID-19) pandemic is more than a threat to public health. This is due to an inadequate understanding of the molecular keys that constitute its viral protein chemistry. Since its outbreak in December 2019, there have been a series of research, trials, tests carried out and genomic analysis was done to ascertain infection, hinder transmission, and evolve clinical intervention. With several deaths and no hope for a cure anytime soon, more in-depth knowledge of the virus is urgently needed. This project aims to investigate the structural, molecular makeup, and epidemiology of Coronavirus and further make use of computational models to derive a three-dimensional structure of the Nucleocapsid protein of the virus in other to find drug targets that can help inhibit the replication of the virus and make it visible for the human immune system fight off the virus. During this work, the structural, molecular makeup, and epidemiology of Coronavirus were analyzed alongside a detailed understanding of the selected nucleocapsid protein. Homology modeling and model validation was performed to confirm the authenticity of the structure predicted. The result showed a likelihood of the N-protein being a suitable protein to be used in its test phase because of its stability and the various drug targets found during the work. With the knowledge harnessed, we will be a step closer to finding a therapeutic drug that will inhibit the spread of this deadly virus.

Keywords: Drug targets, COVID-19, Nucleocapsid Protein, protein, clinical trials. Artificial intelligence