EXPERIMENTAL AND COMPUTATIONAL ASSESSMENT OF *Discorea bulbifera* DERIVED BIOCHAR AND HYDROCHAR FOR IBUPROFEN RELEASE

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AUGUST, 2024

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A DISSERTATION SUBMITTED TO THE SCHOOL OF POST GRADUATE STUDIES IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE AWARD OF THE DEGREE OF MASTER OF SCIENCE (M.Sc) IN BIOCHEMISTRY IN THE DEPARTMENT OF BIOCHEMISTRY, COLLEGE OF SCIENCE AND TECHNOLOGY, COVENANT UNIVERSITY, OTA, OGUN STATE, NIGERIA

AUGUST, 2024

ACCEPTANCE

This is to attest that this dissertation is accepted in partial fulfillment of the requirements for the award of a Master of Science (M.Sc.) in Biochemistry in the Department of Biochemistry, college of Science and Technology, Covenant University, Ota, Nigeria.

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

Prof. Akan B. Williams
(Dean, School of Postgraduate Studies) **Signature and Date**

DECLARATION

I, NNAJI, PRECIOUS CHINYERE (22PCP02386) hereby declare that this research work was carried out by me under the supervision of Prof. Olubanke O. Ogunlana (Supervisor) of the Department of Biochemistry, College of Science and Technology, Covenant University, Ota, Ogun State. I attest the dissertation has not been presented either wholly or partially for the award of any degree elsewhere. All sources of data and scholarly information used in this dissertation were duly acknowledged.

NNAJI, PRECIOUS CHINYERE

Signature and Date

CERTIFICATION

We certify the dissertation titled "**EXPERIMENTAL AND COMPUTATIONAL ASSESSMENT OF *Discorea bulbifera* DERIVED BIOCHAR AND HYDROCHAR FOR IBUPROFEN RELEASE"** is an original work carried out by **NNAJI PRECIOUS CHINYERE (22PCP02386)** in the Department of Biochemistry, College of Science and Technology, Covenant University, Ota, Ogun State, Nigeria under the supervision of Prof. Olubanke O. Ogunlana. We have examined and found this work acceptable as part of the requirement for the award of Master of Science (M.Sc.) degree in Biochemistry.

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Prof. Solomon O. Rotimi
(Head of Department) **Signature and Date**

Prof. Joseph O. Adebayo
(External Examiner) **Signature and Date**

Prof. Akan B. Williams
(Dean, School of Postgraduate Studies) **Signature and Date**

DEDICATION

This dissertation is dedicated to God Almighty, who granted me grace among the living, intellectual and physical strength to complete this work. I also dedicate this work to my beautiful daughter Nnaji Goodtidings Nwaihe and my Darling Husband Dr. Nnaji, Nnaemeka Joshua who single handedly sponsored me to school and also gave me maximum encouragements.

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TABLE OF CONTENTS

CHAPTER FOUR: RESULTS AND DISCUSSION

CHAPTER SIX: CONCLUSION AND RECOMMENDATION

LIST OF FIGURES

LIST OF TABLES

LIST OF ABBREVIATIONS

IBU	Ibuprofen
BC	Biochar
HC	Hydrochar
DFT	Density functional theoretical
R2	Coefficients of correlation
A_{IBU}	Concentration of untrapped ibuprofen.
T_{IBU}	Initial concentration of ibuprofen
C_0	Initial Ibuprofen concentrations
C_e	Final Ibuprofen concentration
HRBC	Human red blood cell
ELUMO	Lowest unoccupied molecular orbital energy
EHOMO	Highest occupied molecular orbital energy
1HD2	Human Peroxiredoxin 5 protein
SEM	Scanning electron microscope
EDX	Energy dispersive X-ray analysis
pH_{zpc}	Zero-point charge pH
EA	Elemental analysis
TPD	Temperature programmed desorption
XPS	X-ray photoelectron spectroscopy
FTIR	Fourier transformed infrared
PAHs	Polycyclic aromatic hydrocarbons
MO	Determinant of moisture ash
VM	Volatile matter
FC	Fixed carbon
CS	Carboxymethyl chitosan
TLR	Toll-like receptor
CLRs	C-type lecithin receptors
PRRs	Pattern-recognizing receptors
COX	Cyclooxygenase
NSAIDs	Nonsteroidal anti-inflammatory medicine

ABSTRACT

The efficacy of ibuprofen in inflammation management depends on efficient delivery to the targeted site. Utilising a delivery agent would involve ibuprofen adsorption and release for improved delivery. This work studies the utilisation of *Discorea bulbifera* derived biochar and hydrochar for ibuprofen release. The biochar was prepared in a muffle furnace at 300 ^{o}C for 90 min and the hydrochar was prepared in a hydrothermal autoclave at 200 ^{o}C for an hr. Characterisation of the chars was performed using several techniques such as Brunauer-Emmett-Teller (BET) analysis, Fourier transform infrared spectroscopy (FTIR), powder X-ray diffraction (XRD), electron dispersive X-ray (EDX), and scanning electron microscopy (SEM). The following biochemical assays were carried out; Protein albumin denaturation assay, hypotonic solution induced hemolysis stabilizing assay, Heat induced hemolysis stabilizing assay. Ibuprofen equilibrium adsorption was performed at 180 min adsorption time, using concentrations (5–200 mg L^{-1}). The equilibrium of adsorption was evaluated using the Freundlich, Temkin, and Langmuir isotherm models. Non−linear Freundlich adsorption isotherm gave the best descriptions of ibuprofen adsorptions onto the studied chars. Freundlich adsorption capacities of biochar and hydrochar are 21.977 and 19.921 mg. g^{-1}, respectively. Egg albumin denaturation inhibition anti−inflammatory results show that biochar (≈ 85 %) performed better than hydrochar (≈ 70 %). Similar trend was observed at lower concentrations of the chars for heat induced hemolysis inhibition studies and as concentration increased, the trend changed such that hydrochar (≈ 38 %) performed better than biochar (≈ 17 %). Ibuprofen equilibrium adsorption performed using initial ibuprofen concentrations (5–200 mg L^{-1}) was established in 2 hours, for biochar and hydrochar, and the highest ibuprofen removals occurred at pH 4. Density functional theoretical calculations gave results which are in excellent agreements with adsorption studies. Both biochar and hydrochar showed good performance as long−term adsorbents for the removal of ibuprofen and results from *in vitro* and computational studies indicate they have great promise for ibuprofen delivery.

KEYWORDS: Ibuprofen, Hydrochar, Biochar, Density Functional Theoretical