ECMC-P 2025 Conference

The 1st International Electronic Conference on Medicinal Chemistry and Pharmaceutics

01–30 November 2025 | Online

MDPI

PROBING THE INHIBITORY EFFCTS OF BARTERIA NIGRITANA SYNTHESIZED ZINC OXIDE NANOPARTICLES AGAINST ALPHA GLUCOSIDASE IMPLICATED IN DIABETES UPSURGE

•Ifeoma Felicia Chukwuma[1.2*], Victor Owukwube Apeh[3], and Joshua Chidubem Egbo[1].

•[1]Department of Biochemistry, Faculty of Biological Sciences, University of Nigeria, Enugu State, 410001, Nigeria:

•[2]Department of Genetics and Biotechnology, Faculty of Biological Sciences, University of Nigeria, Enugu State, 410001, Nigeria.

•[3]Federal University of Allied Health Sciences, Department of Applied Sciences, Enugu State, 01473, Nigeria; victorapeh@yahoo.com (V.O.A).

•*Correspondence: chukwuma.ifeoma@unn.edu.ng; odoifeoma1@gmail.com; (IFC).* Tel.: +234-7064614452.

INTRODUCTION & AIM

Diabetes mellitus (DM) is a metabolic endocrine disorder affecting carbohydrates, proteins, and lipid metabolism. The derangement in carbohydrate metabolism could impair insulin secretion, insulin action, or both.

Although all forms of DM have hyperglycemia (fasting blood glucose ⩾ 126 mg/dL) in common, the cause and clinical manifestations vary widely.

Although anti-DM drugs are effective as an anti-DM agent, prolonged usage could result in detrimental side effects. Hence the need for discovery of safe and effective agent.

The aim of this study is to investigate the inhibitory effects of *Barteria nigritiana* synthesized zinc oxide nanoparticle against alpha glucosidase implicated in diabetes upsurge'.

METHOD

The zinc nanoparticles was synthesized and characterized using GC- FID analysis. The 20compounds identified were docked against alpha- glucosidase using the XP glide docking tools of Schrodinger suite v12.4 and acarbose, was used as the standard drug.

Validation of the in silico experiment was done using *in vitro* analysis.

RESULTS & DISCUSSION

Table 1: The docking scores of top scoring compounds with *α*-glycosidase

S/N	COMPUNDS	DOCKING SCORE (Kcal/mol)	INTERACTING AMINO ACID
1	Resveratrol	-7.763	Tyr65, Asp62, Asp20, Hie332
2	2-hydroxy phenol	-7.025	Phe166, Arg400, Thr203,Asp303, Gln271
3	3,4-dihydroxy toluene	-7.018	Gly228,Phe166
4	Acarbose	–7.194	LYS467, GLU439,

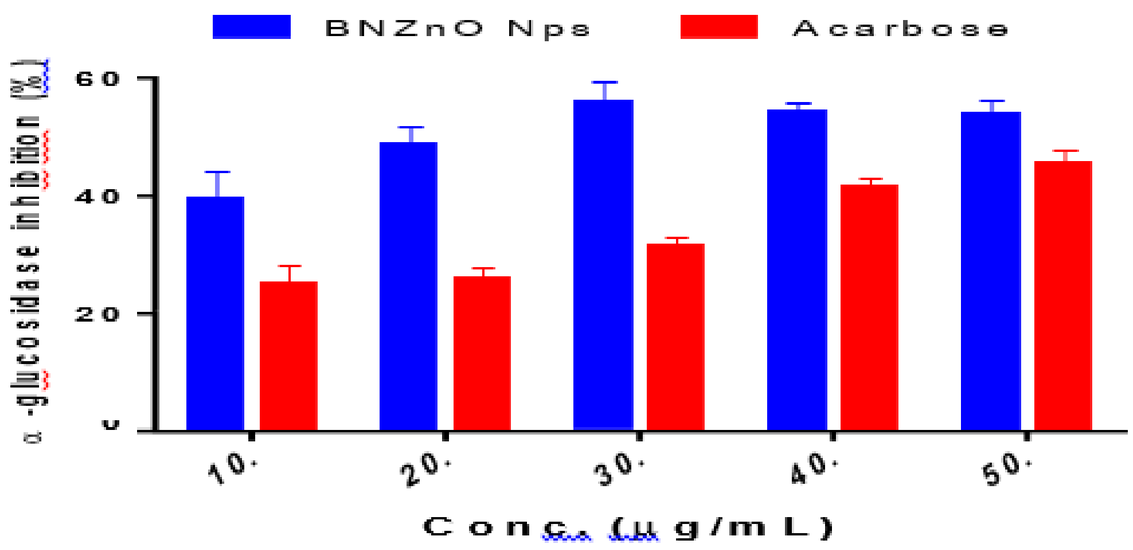

Figure 2. Effects of BNZnNPs on α-glucosidase enzyme

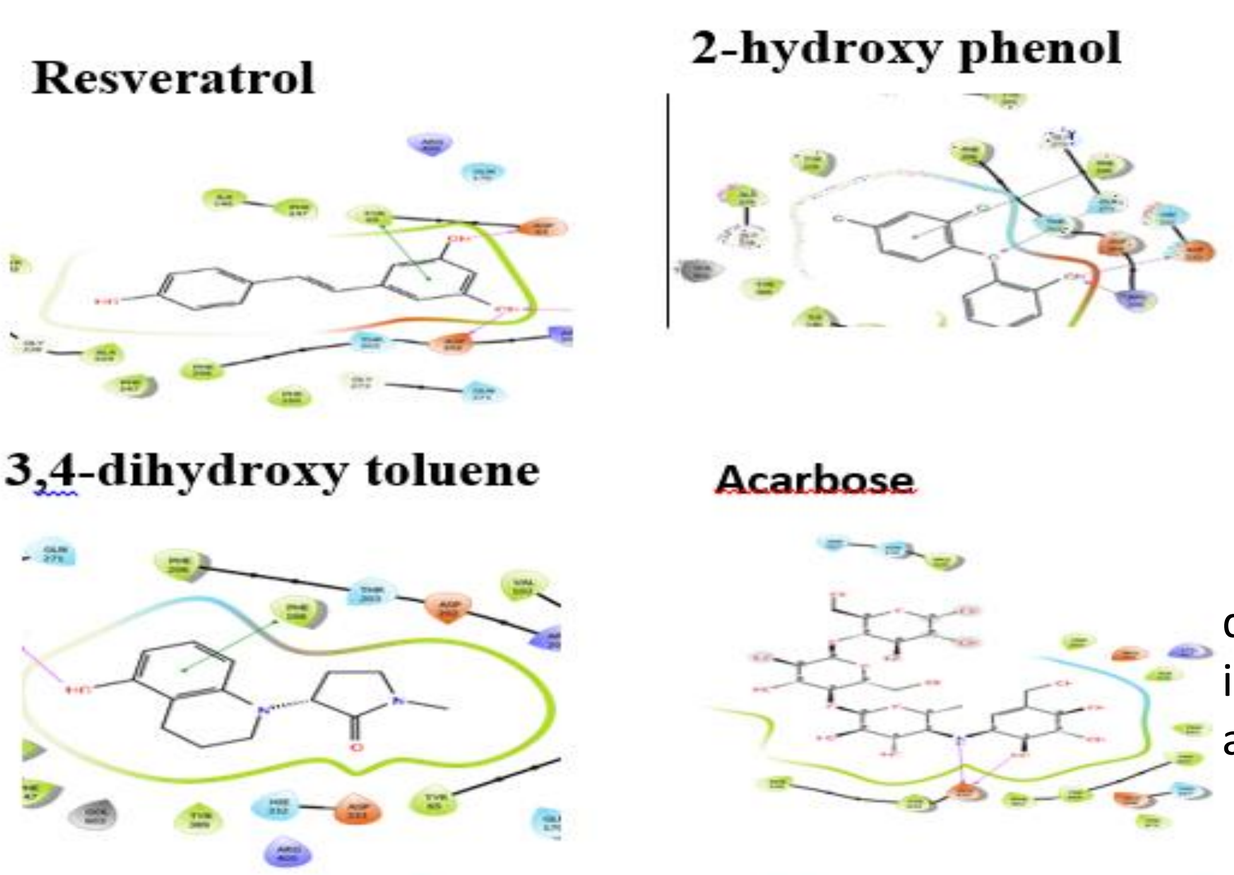

Figure 1: 2D Molecular interactions of the top compounds with alpha glucosidase.

CONCLUSION

The findings from this study show that BNZnNPs compounds interacted favorably with amino acids within and around the binding sites of α-glucosidase.

Furthermore, validation of the BNZnNPs's efficacy as an anti-DM therapy using α -glucosidase inhibition *in vitro* also authenticated its anti-diabetic potential.

Hence, this study validates the use of *B.nigritana* as an anti-diabetic agent in folk medicine practice and brings the plant into the spotlight in searching for novel and safe anti-diabetic agents for drug development.

FUTURE WORK / REFERENCES

Future research is needed to confirm the anti-daibetic activity of the nanoparticles using animal models before proceeding to clinical trials to determine the efficacy in humans.