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Pharmacokinetics and inhibitory activities of UPLC-detected compounds of *Voacanga africana* roots on acetylcholinesterase and monoamine oxidase B: Potential drug candidates for neurological disorders

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INTRODUCTION & AIM

- Neurological disorders are the leading causes of disability and one of the leading causes of death in the world.
- Acetylcholinesterase (AChE) and monoamine oxidase B (MAO-B) are implicated in various neurological disorders, particularly Alzheimer's and Parkinson's diseases, which are the most prevalent neurodegenerative disorders.
- Inhibitors of these enzymes increase the levels of neurotransmitters in the brain, thereby altering deranged processes in neurological disorders.
- *Voacanga africana* is a widely used medicinal plant in Africa for the treatment of several diseases, including mental disorders (Bekoe et al., 2024).
- This study therefore investigated the pharmacokinetic properties and inhibitory potential of compounds detected in the roots of *V. africana,* on AChE and MAO-B, using *in silico* tools.

METHOD

Extract of *Voacanga africana* roots

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UPLC-ESI-MS/MS
(negative mode)

↓

19 known compounds

\+ **Rivastigmine** (standard) — Molecular docking — \+ **Rosiglitazone** (standard)

ACHE (PDB ID: 4EY7) | **MAO-B** (PDB ID: 4A7A)

↓

Drug likeness and pharmacokinetics prediction

- **Tools used:**

Molecular docking: AutoDock Vina (Trott and Olson, 2010)

Drug likeness: SwissADME

Pharmacokinetics: vNN-ADMET

RESULTS & DISCUSSION

Table 1: Binding affinities of top-scoring compounds against ACHE and MAO-B

Compounds	Molecular weight	ACHE (Kcal/mol)	MOA-B (Kcal/mol)
Tsangibeilin B, rel-	350.4	-12.4	-12.1
Pinocembrin 7-[4-(1-hydroxyethyl)phenyl] ether	376.4	-10.8	-11.2
Elisabatin B	292.4	-11.3	-10.2
Obochalcolactone	550.6	-9.6	-11.1
Hedyotol C	584.6	-9.8	-11.2
Standard		-8.0	-9.8

Table 2: Drug-likeness properties of top-scoring compounds

Compounds	nHBA	nHBD	CLogP	NOR	TPSA (Å²)
Tsangibeilin B, rel-	4	1	3.42	3	55.76
Pinocembrin 7-[4-(1-hydroxyethyl)phenyl] ether	5	2	3.69	4	75.99
Elisabatin B	2	1	4.58	1	37.30
Obochalcolactone	7	2	5.22	7	102.29
Hedyotol C	11	4	2.57	11	145.53

nHBA: Number of hydrogen bond acceptors; nHBD: Number of hydrogen bond donors; CLogP: Consensus LogP, NOR: Number of rotatable bonds; TPSA: Topological surface area

Table 3: Pharmacokinetic properties of top-scoring compounds

Compounds	HLM	CYP1A2 Inhibitor	CYP3A4 Inhibitor	CYP2D6 Inhibitor	CYP2C9 Inhibitor	CYP2C19 Inhibitor	BBB	P-gp Inhibitor/ Substrate
Tsangibeilin B, rel-	Yes	No	No	No	No	No	Yes	Yes/Yes
Pinocembrin 7-[4-(1-hydroxyethyl)phenyl] ether	Yes	Yes	No	No	No	Yes	No	No/Yes
Elisabatin B	Yes	No	No	No	No	No	No	No/No
Obochalcolactone	Yes	No	No	No	Yes	Yes	No	No/Yes
Hedyotol C	Yes	No	No	No	No	No	No	No/Yes

HLM: The human liver microsomal stability assay; CYP: Cytochrome P450; BBB: Blood-brain barrier

CONCLUSION

- The top-scored compounds, especially tsangibeilin B, rel- inhibited AChE and MAO-B activities with better binding affinities compared to their respective standards. They also showed favorable pharmacokinetic profiles.
- These compounds therefore have potential in various neurological disorders in which AChE and MAO-B activities are implicated.

FUTURE WORK / REFERENCES

Bekoe, E. O., Opare, J. A. A., Lartey, M., & Amoateng, P. (2024). Ethnomedicinal uses, biological activities, and toxicity of *Voacanga africana* Stapf Ex Scott-Elliot. *Advances in Traditional Medicine*, *24*(2), 431–448. https://doi.org/10.1007/S13596-023-00709-Y

Trott, O. & Olson, A. J. (2010). AutoDock vina: Improving the speed and accuracy of docking with a new scoring function, efficient optimization, and multithreading. *Journal of Computational Chemistry*, *31*(2), 455–461. https://doi.org/10.1002/JCC.21334