SEPTEMBER 23-27 2024
19BMOS
BRAZILIAN MEETING ON ORGANIC SYNTHESIS
BENTO GONÇALVES, RS - BRAZIL

Synthesis and Neuroprotective Potential of Carvacrol-Derived Selenides-1,2,3-Triazoles for Alzheimer's Disease

Luana da S. Gomes,[1*] Érica de O. Costa,[1] Majory C. G. M. Schüler,[2] Aldo S. de Oliveira[2] and Vanessa Nascimento[1]

1) SupraSelen Laboratory, Department of Chemistry, Universidade Federal Fluminense, UFF, 24020-140.
2) Department of Chemistry, Federal University of Santa Catarina, UFSC, 89036-256.
e-mail: luanagomes@id.uff.br

Keywords: *Acetylcholinesterase, organochalcogen, natural product.*

ABSTRACT

Natural products inspire synthetic chemists, and modifying these compounds can lead to promising new structures. In this context, theoretical tools optimize and guide the synthesis of these compounds [1-2]. Thus, our research focused on carvacrol, known for its neuroprotective properties, and organochalcogen derivatives that also exhibit a range of biological activities [3]. In this work, we designed structural modifications in carvacrol to potentiate its neuroprotective effects, particularly for Alzheimer's disease. First, azides (**2a-i**) were synthesized from chlorides (**1a-i**) by reacting sodium azide (NaN_3) with acetonitrile (CH_3CN) and 18-crown-6 as a catalyst, produced an 87-92% yield. Finally, we obtained nine new carvacrol-derived selenides-1,2,3-triazoles (**4a-i**) via click chemistry with yields ranging from 44% to 63%. Figure 1 shows the synthetic routes and docking molecular of compound **4e**, revealing interactions with residues Trp286 and Tyr341, suggesting potential as a therapeutic for Alzheimer's.

.

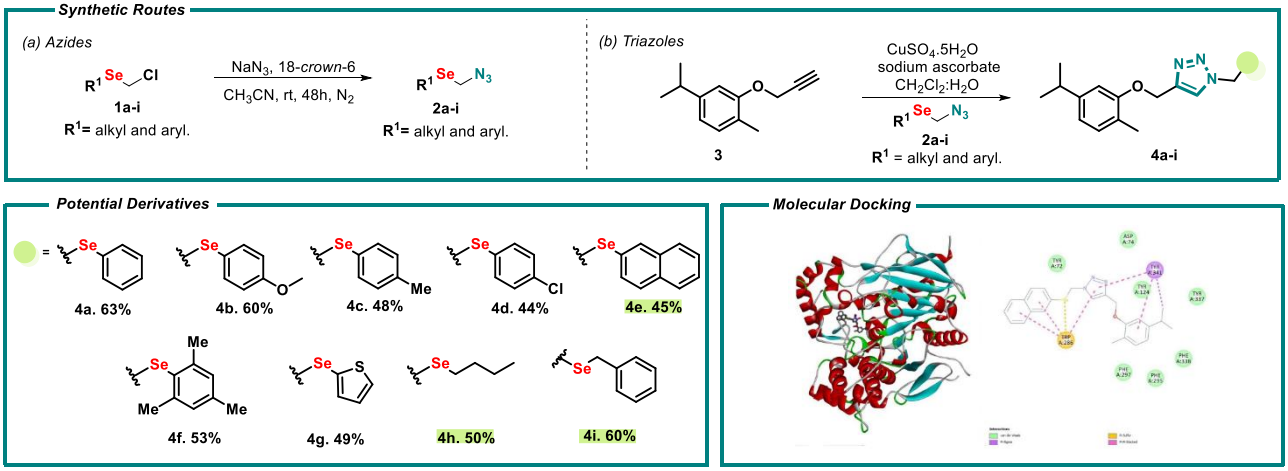

Figure 1. Synthetic routes for obtaining carvacrol derivatives and docking molecular of compound **4e**.

ACKNOWLEDGEMENTS

PPGQ-UFF, CAPES, FAPERJ and CNPq.

REFERENCES

[1] Zamaniam, M. Y. et al. *CNS & Neurological Disorders - Drug Target* **2024**, 20, 943.
[2] Ismail, Z. et al. *Nature Reviews Neurology* **2023**, 18, 131.
[3] Refaay, D. A. et al. *Medicinal Chemistry Research* **2022**, 31, 894.