Abstract

Development of Bioactive Molecules for the Treatment of Alzheimer's Disease †

Amisha Punmiya *, Ruchita Gharat and Arati Prabhu

Department of Quality Assurance, SVKM's Dr. Bhanuben Nanavati College of Pharmacy, Vile Parle, Mumbai 400056, India

*   Correspondence: amishapunmiya@gmail.com
†   Presented at the 8th International Electronic Conference on Medicinal Chemistry, 1–30 November 2022; Available online: https://ecmc2022.sciforum.net/.

Abstract: A series of novel thiophene pyrazolines were designed as potential bioactive molecules against Alzheimer's disease. The probable binding modes of these molecules in AChE were evaluated using in silico techniques, and promising molecules were then synthesized and characterized. Their biological activities were profiled to confirm their potential as multifunctional molecules for the treatment of Alzheimer's disease by addressing multiple pathological mechanisms. While the anti-oxidant activities of the synthesized molecules needed further optimization, the series showed excellent potential in mitigating the multiple causative factors via Aβ aggregation inhibition, AChE inhibition, metal chelation, and inhibition of advanced glycation products.

Keywords: Alzheimer's disease; multifunctional; antioxidant; amyloid aggregation; docking; cholinesterase; neurodegenerative

Supplementary Materials: The following are available online at https://www.mdpi.com/article/10.3390/ECMC2022-13470/s1.

Author Contributions: Conceptualization, A.P. (Arati Prabhu); methodology, A.P. (Amisha Punmiya) and R.G.; investigation, A.P. (Amisha Punmiya) and R.G.; formal analysis, A.P. (Amisha Punmiya), R.G. and A.P. (Arati Prabhu); resources, A.P. (Arati Prabhu); data curation, A.P. (Arati Prabhu); writing—original draft preparation, A.P. (Amisha Punmiya), R.G.; writing—review and editing, A.P. (Arati Prabhu); supervision, A.P. (Arati Prabhu); project administration, A.P. (Arati Prabhu). All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: The data presented in this study are available on request from the corresponding author.

Conflicts of Interest: The authors declare no conflict of interest.