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Topic of Research : **Exploring Biomarkers of Alzheimer Disease Through Computational Approaches Exploiting Curcumin and its Analogous as Therapeutics.**

Finding of the study

The present research provides a comprehensive computational framework for identifying reliable biomarkers and exploring novel therapeutic candidates for Alzheimer's disease by integrating transcriptomics, artificial intelligence, network pharmacology, and structure-based drug discovery. Analysis of multiple gene expression datasets revealed extensive molecular alterations associated with disease progression, demonstrating that Alzheimer's disease is regulated by complex biological mechanisms rather than a single pathological pathway. Functional enrichment analysis further indicated that dysregulated genes are closely linked with neuroinflammation, immune responses, synaptic dysfunction, and disturbances in cellular homeostasis, all of which contribute to neuronal degeneration.

To improve the reliability of biomarker discovery, three independent machine learning algorithms were employed, and only the genes consistently selected by all models were considered. This integrative strategy identified MED13L, CLIP3, GFAP, CXCR4, POLR3C, NFKBIA and LINC00643 as the most promising biomarkers. Their excellent diagnostic performance suggests that these genes may support the early detection of Alzheimer's disease and provide valuable targets for future experimental validation.

The study also demonstrated that curcumin exerts its therapeutic potential through a multi-target mechanism instead of acting on a single protein. Network pharmacology identified APP, MAPK1, PPARG, RARA, and STAT3 as central regulatory proteins involved in amyloid metabolism, inflammatory signalling, neuronal survival, and disease progression. Subsequent virtual screening, ADMET profiling, molecular docking, and 100 ns molecular dynamics simulations identified several curcumins and its analogous compounds with favourable pharmacokinetic properties, strong binding affinity, and stable interactions with these therapeutic targets. These findings indicate that the selected compounds possess significant potential for further drug development.

Overall, this study not only proposes novel molecular biomarkers for Alzheimer's disease diagnosis but also provides computational evidence supporting curcumin analogues as promising multi-target therapeutic candidates. The findings contribute to a deeper understanding of Alzheimer's disease biology and establish a strong scientific foundation for future in vitro, in vivo, and clinical investigations aimed at translating these computational discoveries into practical therapeutic applications.