Towards new drugs for Alzheimer’s disease (AD) via QSAR and molecular docking

FACTS AND FIGURES

- Among the top 10 most burdensome conditions in the elderly.
- 50 million cases worldwide and forecasted to triple in 30 years.
- Over 800 billion USD in costs globally.

MECHANISMS

Acetylcholine (ACh) deficiency is responsible for AD per the cholinergic hypothesis.

ACH E INHIBITION

Acetylcholinesterase (AChE) breaks down ACh. Inhibiting AChE could be a valuable pathway for treating Alzheimer’s.

We performed a QSAR study of 2,570 compounds and molecular docking study of a diversity set of 30 compounds with AChE inhibitory activity

CONCLUSION

QSAR and molecular docking revealed that aromatic, heteroaromatic and heterocyclic rings were preferable moieties for interacting with the hydrophobic pocket of AChE.