Towards new drugs for

Alzheimer's disease (AD)

via QSAR and molecular docking

FACTS AND FIGURES

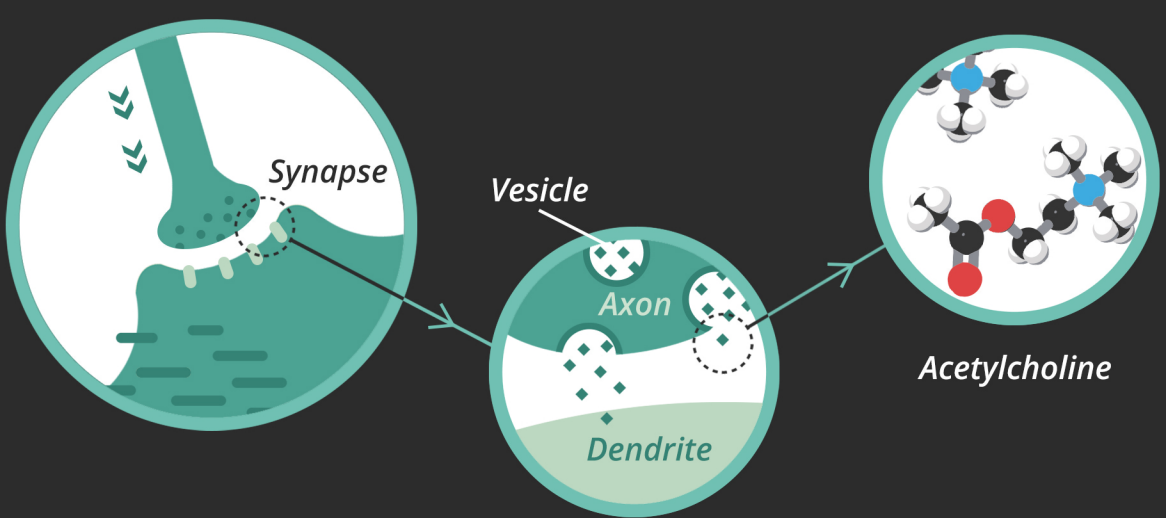
Among the top 10 most **burdensome** conditions in the **elderly.**

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.



AChE 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.

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Probing the origins of human acetylcholinesterase inhibition via QSAR modeling and molecular docking.
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