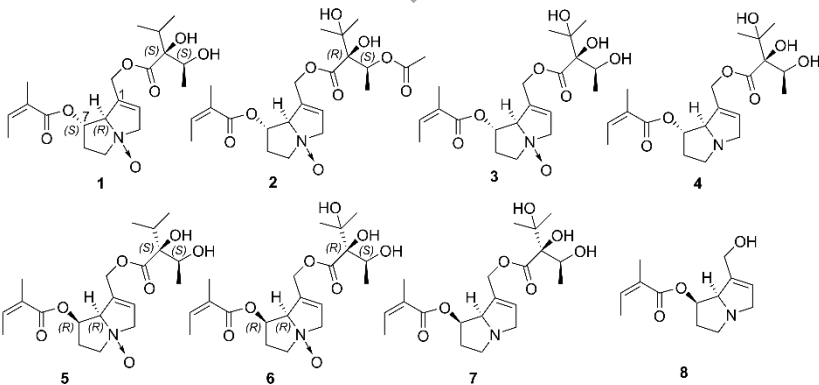


The enzyme acetylcholinesterase (AChE) acts in mammals and insects. Its inhibitors are considered to treat human disease (e.g., Alzheimer's disease) and to develop insecticides, with the recognized role of AChE as a target of environmentally safe insecticides of natural origin.



*Solenanthus lanatus* and *Echium confusum* plants



heliotridine-type pyrrolizidine alkaloids (PAs) isolated and *in vitro* tested as AChE inhibitors

Benamar et al. *Nat. Prod. Res.* 2016



Docking calculations

AutoDockVina (and PLANTS) calculations of the AChE complexes of PAs:  
**1** is the best inhibitor

*Torpedo californica* AChE (PDB: 6G1V):  
 E = -9.010 kcal/mol



*Drosophila melanogaster* AChE (PDB:6XYU)  
 E = -8.686 kcal/mol

ADME/Toxicity Prediction

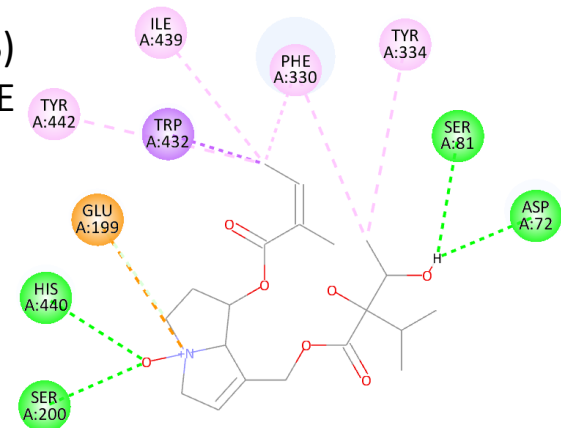
by using the tool AdmetSAR



No cancerogenic activity, but toxicity on humans



No environmental toxicity



**Interactions**

Attractive Charge	Pi-Cation
Conventional Hydrogen Bond	Pi-Sigma
Carbon Hydrogen Bond	Pi-Alkyl

