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Androtoxin B is a neurosteroidal alkaloid from venom of the jellyfish *Cassiopea andromeda* and a potent acetylcholinesterase inhibitor

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Objectives: Marine venoms have been rarely studied for their acetylcholinesterase (AChE) inhibitory activities. The aim of this study was to isolate novel compounds with antiAChE activity from the venom of upside-down jellyfish *Cassiopea andromeda.*

Methods: The compounds of the fractionated venom on gel filtration chromatography were identified by analyzing gas chromatography–mass spectroscopy data. The structure of the isolated compound that showed the most potent antiAChE activity in a docking study was elucidated by different spectral data, including ^{1}H-NMR and ^{13}C-NMR.

Results: Three compounds, including a neurosteroidal alkaloid androtoxin B, were identified from two venom fractions. This neurosteroidal alkaloid showed strong acetylcholinesterase inhibitory activity (IC_{50}: 2.24±0.1 μM) compared with the reference standard, galantamine. The results obtained by a docking study demonstrated that androtoxin B had close contact with two of the three amino acid residues of the catalytic triad of acetylcholinesterase gorge and was accommodated within a peripheral hydrophobic pocket composed of numerous aromatic site chains.

Conclusion: The neurosteroidal alkaloid isolated from *Cassiopea andromeda* is a potent antiAChE agent with strong binding to both the catalytic and peripheral sites of acetylcholinesterase that correlated well with the experimental data. Further studies are required to determine whether androtoxin B could be a potential treatment for Alzheimer's disease.