

Supplementary material for the article:

Alkaloid Profiling, Anti-Enzymatic and Antiproliferative Activity of The Endemic Chilean Amaryllidaceae *Phycella cyrtanthoides*

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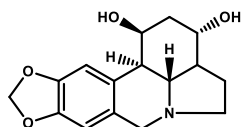
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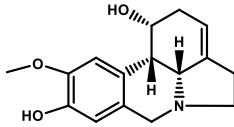
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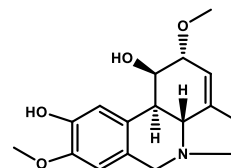
3-hydroxydihydrocaranine (13)
(Bulbs)



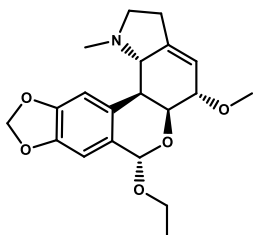
Kirkine (25)
(Bulbs)



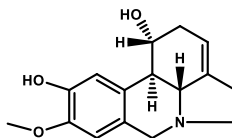
10-O-dimethylgalanthine (31)
(Bulbs)



2-alpha-methoxy-6-O-ethyloduline (22)
(Leaves)



10-norpluviine (24)
(Leaves)



3-O-acetylnarcissidine (30)
(Leaves)

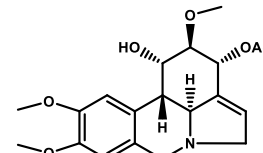


Figure S1. Alkaloids subjected to docking assays in the corresponding catalytic sites of *Torpedo californica* acetylcholinesterase (TcAChE) and human butyrylcholinesterase (hBuChE).

Material and Methods

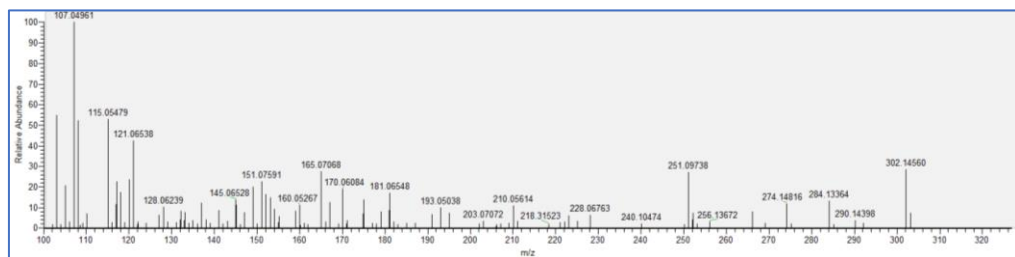
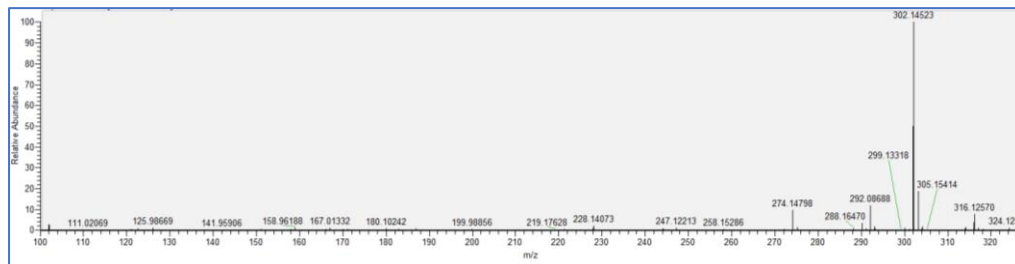
- Docking experiments

Docking experiments were performed using Autodock 4.2 [1] and polar hydrogen atoms of both enzymes were added treating them as rigid bodies. Grid maps were calculated using the autogrid option and were centred on the putative catalytic site of each enzyme considering their known catalytic residues: Ser200 for acetylcholinesterase (TcAChE) [2,3] and Ser198 for butyrylcholinesterase (hBuChE) [4,5] respectively. The volumes chosen for the grid maps were made up of $60 \times 60 \times 60$ points, with a grid-point spacing of 0.375 \AA . Docked compound complexes were built using the Lamarckian Genetic Algorithm [6] which involved 100 runs. The lowest docked-energy binding cluster positions were chosen to be analyzed according to the potential intermolecular interactions between inhibitors and the enzymes. The different complexes were visualised in a Visual Molecular Dynamics program (VMD) and Pymol [7].

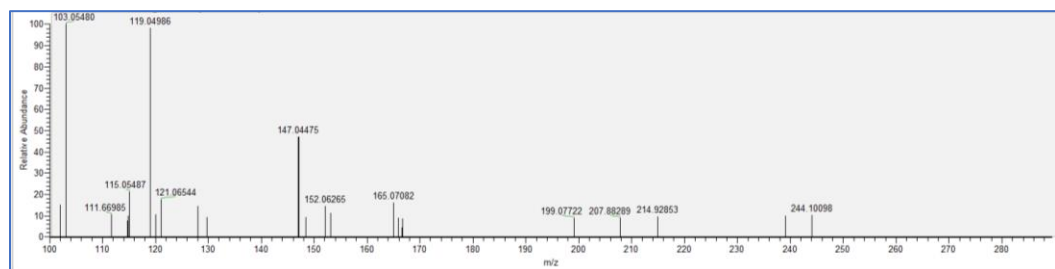
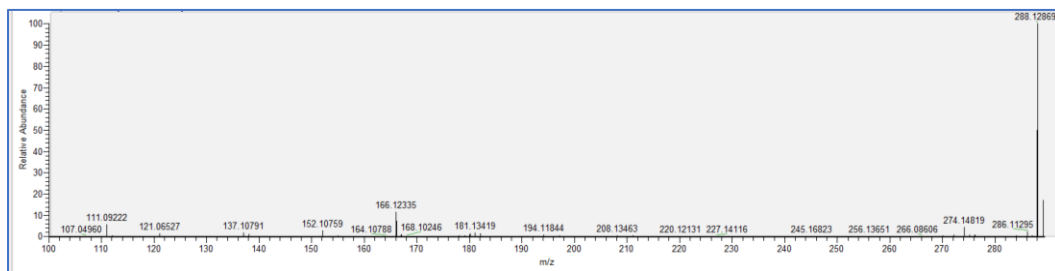
Results

- Alkaloid profile of *Phycella cyrtanthoides* extracts

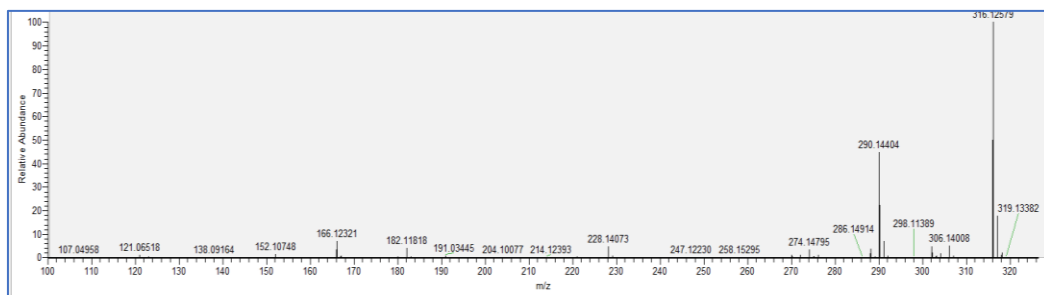
The MS/MS spectrum of peak 3, identified as Powelline



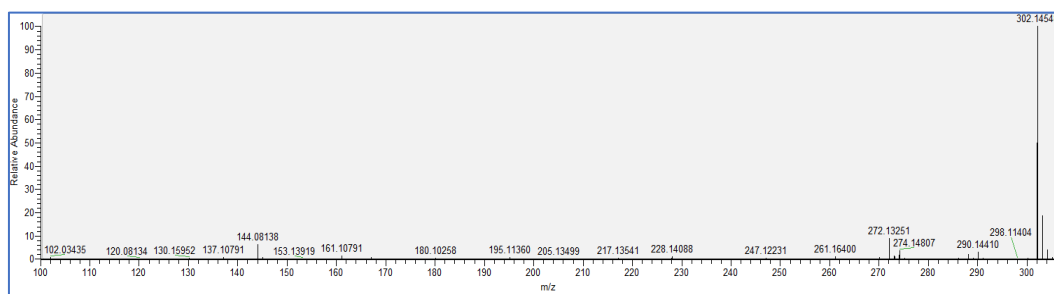
The MS/MS spectrum of peak 4, identified as Lycorine



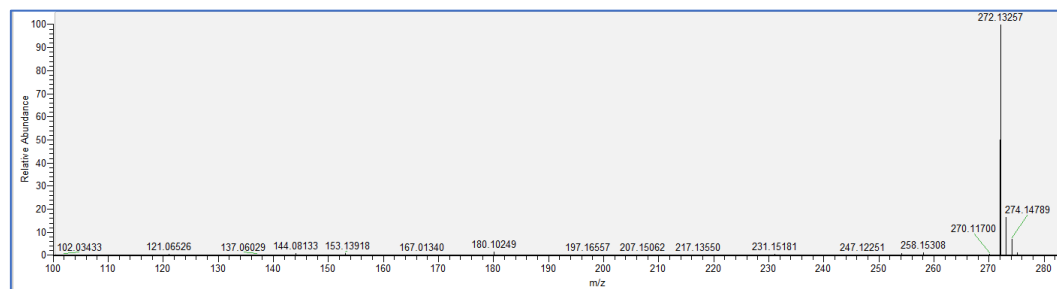
The MS/MS spectrum of peak 6, identified as Hippeastrine



The MS/MS spectrum of peak 20, identified as Haemanthamine



The MS/MS spectrum of peak 23, identified as Vittatine



- Antiproliferative effects

Plant organs/cells	A549	HBL-100	HeLa	SW1573	T-47D	WiDr
bulbs	<2,5	<2,5	<2,5	<2,5	<2,5	<2,5
leaves	<2,5	<2,5	<2,5	<2,5	<2,5	<2,5
cisplatin	4.9 ± 0.2	1.9 ± 0.2	1.8 ± 0.5	2.7 ± 0.4	17 ± 3.3	23 ± 4.3

All values were expressed as means ± SEM (n = 3). Cisplatin was used as reference compound

Table S1. Antiproliferative activity (GI₅₀, in µg/mL) of *P. cyrtanthoides*, against human solid tumor cell lines.

References

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