

Accepted Manuscript

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PII: S0141-8130(17)32782-4
DOI: <http://dx.doi.org/10.1016/j.ijbiomac.2017.08.174>
Reference: BIOMAC 8167

To appear in: *International Journal of Biological Macromolecules*

Received date: 28-7-2017
Revised date: 29-8-2017
Accepted date: 30-8-2017

Please cite this article as: Benildo Sousa Cavada, David Alencar Araripe, Ivanice Bezerra Silva, Vanir Reis Pinto-Junior, Vinicius Jose Silva Osterne, Antonio Hadson Bastos Neco, Eva Pollyanna Peixe Laranjeira, Claudia Figueiredo Lossio, Jorge Luiz Almeida Correia, Alana Freitas Pires, Ana Maria Sampaio Assreuy, Kyria Santiago Nascimento, Structural studies and nociceptive activity of a native lectin from *Platypodium elegans* seeds (nPELa), *International Journal of Biological Macromolecules* <http://dx.doi.org/10.1016/j.ijbiomac.2017.08.174>

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Structural studies and nociceptive activity of a native lectin from *Platypodium elegans* seeds (nPELa)

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Highlights

- We present the three-dimensional structure of *Platypodium elegans* Hook seed lectin (PELa).
- Molecular docking and dynamics analysis of PELa structure was performed.
- We evaluated the nociceptive effect of PELa in rats.

Abstract

A native lectin (nPELa), purified from seeds of the species *Platypodium elegans*, Dalbergieae tribe, was crystallized and structurally characterized by X-ray diffraction crystallography and bioinformatics tools. The obtained crystals diffracted to 1.6 Å resolution, and nPELa structure was solved through molecular substitution. In addition, nPELa has a metal binding site and a conserved carbohydrate recognition domain (CRD) similar to other Dalbergieae tribe lectins, such as PAL (*Pterocarpus angolensis*) and CTL (*Centrolobium tomentosum*). Molecular docking analysis indicated high affinity of this lectin for different mannosides, mainly trimannosides, formed by α -1,3 or α -1,6 glycosidic bond, as evidenced by the obtained scores. In addition, molecular dynamics simulations were performed to demonstrate the structural behavior of nPELa in aqueous solution. In solution, nPELa was highly stable, and structural modifications presented at its carbohydrate recognition site allowed interaction between the lectin and the different ligands. Different modifications were observed during simulations for each one of the glycans, which included different hydrogen bonds and hydrophobic

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