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Crystal structure of DlyL, a mannose-specific lectin from *Dioclea lasiophylla* Mart. Ex Benth seeds that display cytotoxic effects against C6 glioma cells

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**Crystal structure of DlyL, a mannose-specific lectin from *Dioclea lasiophylla* Mart.
Ex Benth seeds that display cytotoxic effects against C6 glioma cells**

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Abstract

Lectins are a class of carbohydrate-binding proteins or glycoproteins with diverse specificities and functions. The determination and characterization of the three-dimensional structures of these proteins are keys to understanding their biological effects. Recent studies have explored the anticancer potential of *Diocleinae* lectins (from *Leguminosae* family), evaluating their antiproliferative effect and their ability to induce glioma cell death via apoptosis and autophagy. In this work, the three-dimensional structure of *Dioclea lasiophylla* seed lectin (DlyL) complexed with Xman (5-bromo-6-chloro-3-indolyl- α -D-mannopyranoside) was determined by X-ray crystallography. Moreover, interactions with relevant *N*-glycans were evaluated by molecular docking. DlyL presented the *jellyroll* motif, and both metal binding site (MBS) and carbohydrate-recognition domain (CRD) were determined and characterized. Molecular docking simulations indicated that DlyL interacts favorably with *N*-glycans, especially those of the complex and hybrid types, unlike previously studied *Diocleinae* lectins. DlyL also showed antitumor potential against rat C6 glioma cells impairing cell migration, inducing autophagy and cell death via activation of caspase 3. These results indicate that small structural differences among *Diocleinae* lectins can, in turn, result in differential modulation of autophagy and cell apoptosis processes.

Keywords: DlyL; crystal structure; glioma.

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