

**PE 5 - Thermodynamic Study of Chitooligosaccharide Binding to Chitinase B of *Serratia marcescens***

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Chitooligosaccharides consisting of 1,4- $\beta$ -linked N-acetylglucosamine (GlcNAc) and glucosamine have a variety of interesting applications, such as elicitation of plant defence responses, fungicidal, insecticidal, and anti-malarial activity, and activity as signal molecule, e.g. in relation to bone growth. The origin of this behaviour stems from their ability to bind with chitinases and related proteins such as chitinase-like lectins. We have undertaken a detailed thermodynamic study of the binding of a chitinase natural substrate, (GlcNAc)<sub>6</sub>, and a potent chitinase inhibitor, allosamidin, to the family 18 chitinase B (ChiB) of *Serratia marcescens*, in order to elucidate the binding mechanism. The major driving force of chitooligosaccharide binding is an increase in the entropy change of the reaction ( $\Delta S_r$ ), while there are relative moderate and positive changes in the enthalpy of reaction ( $\Delta H_r$ ). A parameterization of the entropy term shows that the conformation entropy change ( $\Delta S_{conf}$ ) is large and positive for allosamidin binding, and the solvation entropy change ( $\Delta S_{solv}$ ) is large and positive for (GlcNAc)<sub>6</sub> binding.