Supplementary Materials: Primary Sequence and 3D Structure Prediction of the Plant Toxin Stenodactylin

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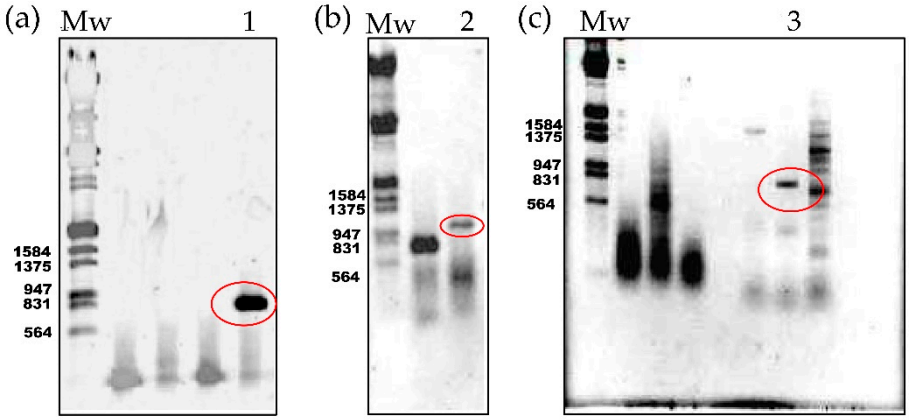

Figure S1. Amplification of stenodactylin A-chain (**a**, lane 1), A-chain and a part of B-chain (**b**, lane 2), B-chain (**c**, lane 3). MW: λ Hind III/EcoRI double digest DNA marker. The red circles indicate the amplificate.

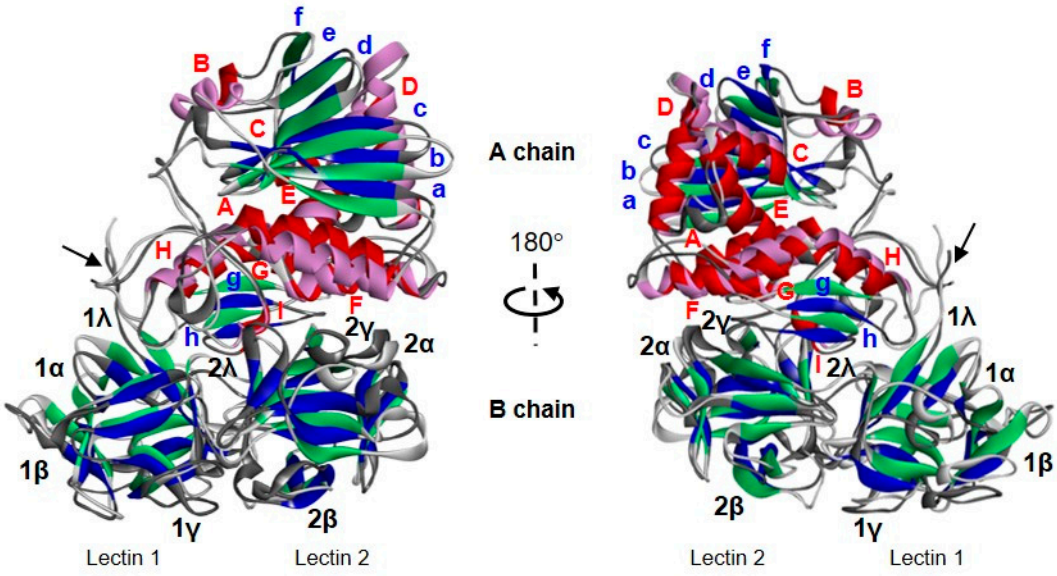

Figure S2. Superimposition of stenodactylin and ricin structure (Protein Data Bank accession number 2AAI). The three-dimensional structural modelling was carried out on the I-TASSER server and the figure was generated with Discovery Studio 2016. The α helices (red and purple in stenodactylin and ricin, respectively), the β chains (blue and green in stenodactylin and ricin, respectively), and the coils (dark and light grey in stenodactylin and ricin, respectively) are represented. The helices are labelled A to I and the strands of the β sheets are labelled a to h in the A chain. The structural domains and subdomains in the B chain are also indicated. Arrows indicates the position of the disulfide bond linking A and B chains.

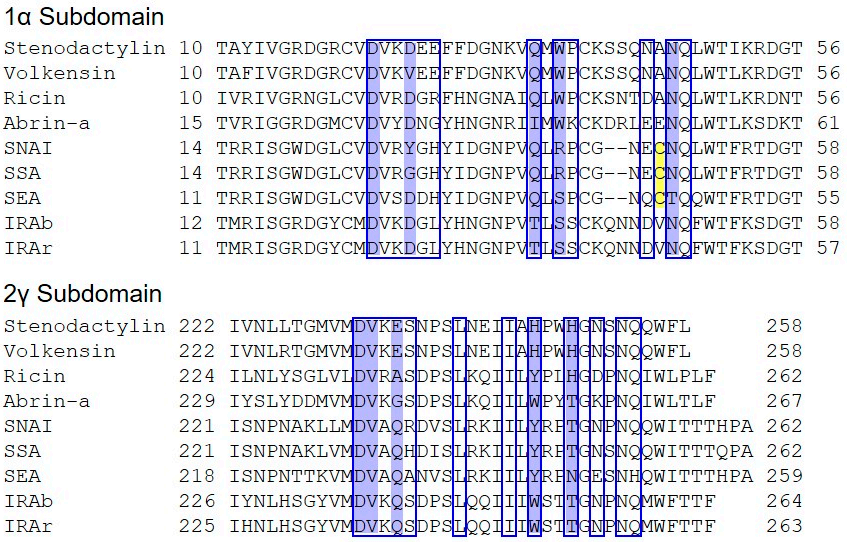

Figure S3. Alignment between the sugar-binding subdomains of stenodactylin, volkensin (acc.no CAD61022) ricin (acc.no P02879), abrin-a (acc.no P11140), SNAI (acc.no AAC49158), SSA, SEA (acc.no CAQ42478), IRAb (acc.no Q8W2E7) and IRAr (acc.no AAL55093). The putative amino acids that are present in the sugar-binding sites (boxed in blue) and those involved in sugar binding (high-lighted in blue) are represented, and they were assigned by comparison with the structure of ricin (acc.no 2AAI, 3RTI and 3RTJ). The cysteines involved in disulfide bridges between B-chains of tetrameric RIPs are high-lighted in yellow. The dash indicates a gap introduced into the sequences to maximize alignments.