Supplementary Material

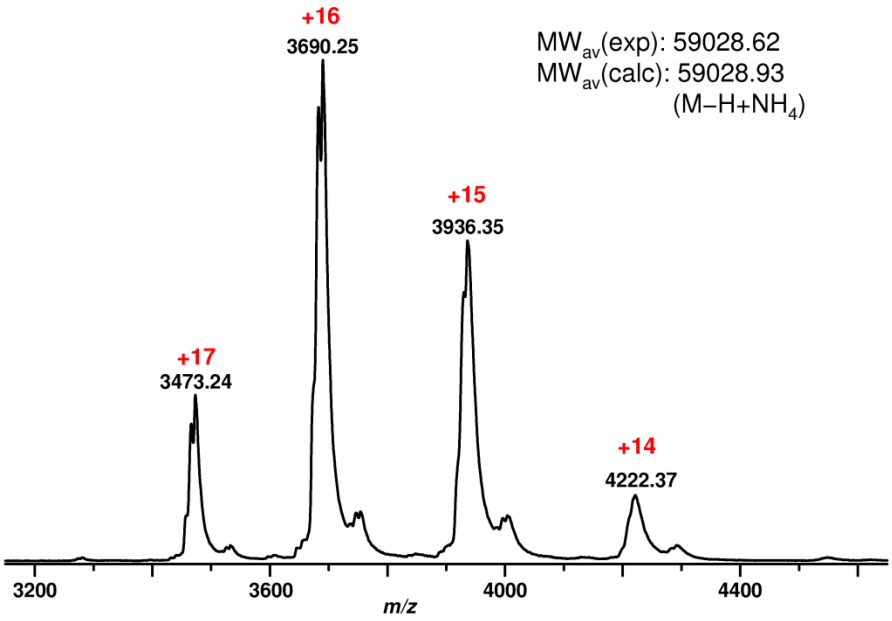


Fig. S1

Supplementary Figure 1. Mass scale expansion of nanoESI Q-Tof mass spectrum obtained from a SGSL solution in 10 mM NH_4OAc, pH 7.3.

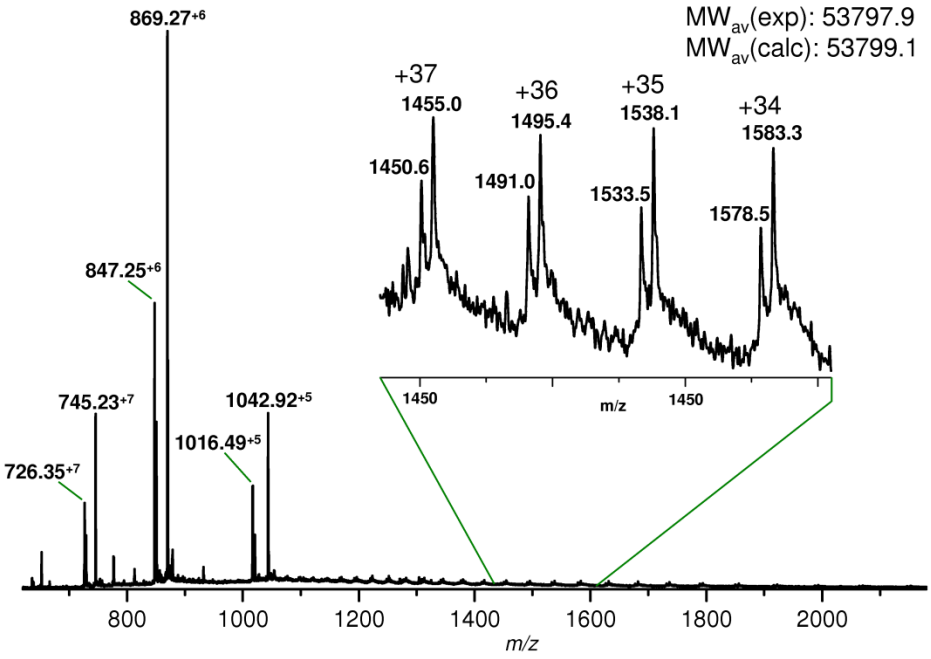


Fig. S2

Supplementary Figure 2. NanoESI Q-Tof mass spectrum of the intact purified SGSL dissolved in 50% ACN/2% formic acid.

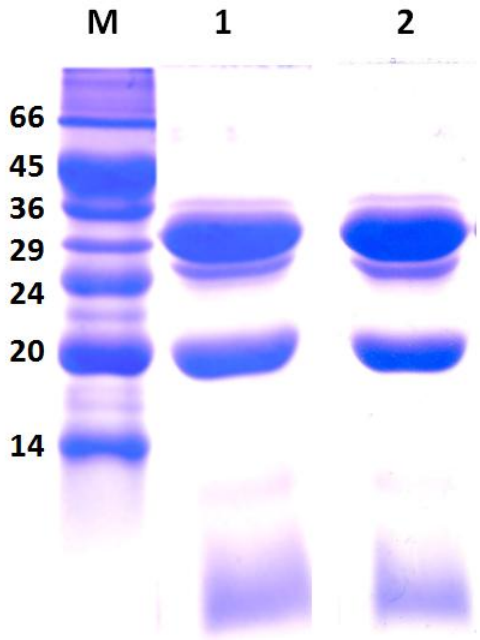


Figure S3

Supplementary Figure 3. SDS-PAGE of SGSL purified with and without protease inhibitor. Lane M: molecular weight markers; lane 1, SGSL purified in presence of cocktail; Lane 2: SGSL purified in the absence of cocktail. The standards used are: bovine serum albumin (Mr 66,000), ovalbumin (45,000), glyceraldehyde-3-phosphate dehydrogenase (36,000), carbonic anhydrase (29,000), trypsinogen (24,000), Trypsin inhibitor (20,000) and α-lactalbumin (14,200).

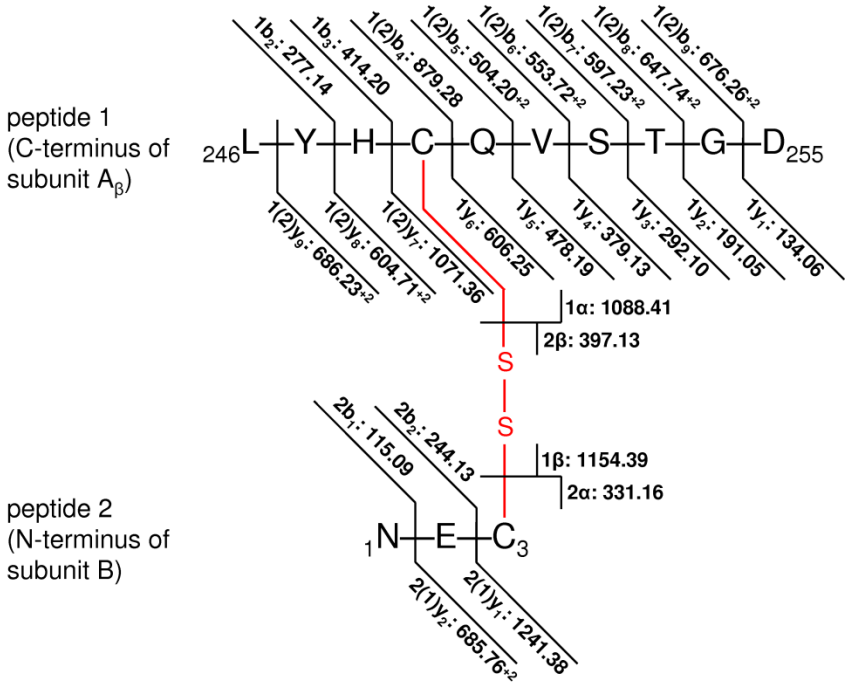


FIG S4

Supplementary Figure 4. Fragmentation scheme deduced from the low-energy-CID spectrum of the doubly charged precursor ions at *m/z* 742.77 derived from a digest of SGSL by thermolysin enabling the determination of the disulphide link between the peptides A_{β} $aa_{246-255}$ and B aa_{1-3} thus indicating the S-S bridge joining A_{β} and B (A_{β}:C_{249}-B:C_3; Fig. 1). Besides full sets of b and y type ions of both peptides, the typical asymmetric cleavage of the disulphide bridge is observed (Mormann *et al.*, 2008) Similarly, the disulphide bonds C_{19}-C_{38}, C_{60}-C_{77}, C_{149}-C_{164}, and C_{190}-C_{209} of the B chain were deduced from CID experiments on the doubly charged precursor ions at *m/z* 1547.79 (digest by thermolysin, aa_{12-25}-S-S-aa_{26-41}), the doubly charged precursor ions at *m/z* 672.34 (digest by thermolysin, aa_{57-60}-S-S-aa_{72-79}), the triply charged precursor ions at *m/z* 1166.16 (digest by thermolysin, $aa_{145-174}$ intra peptide S-S), and the triply charged precursor ions at *m/z* 1283.19 (tryptic digest, $aa_{183-202}$-S-S-$aa_{203-216}$), respectively.

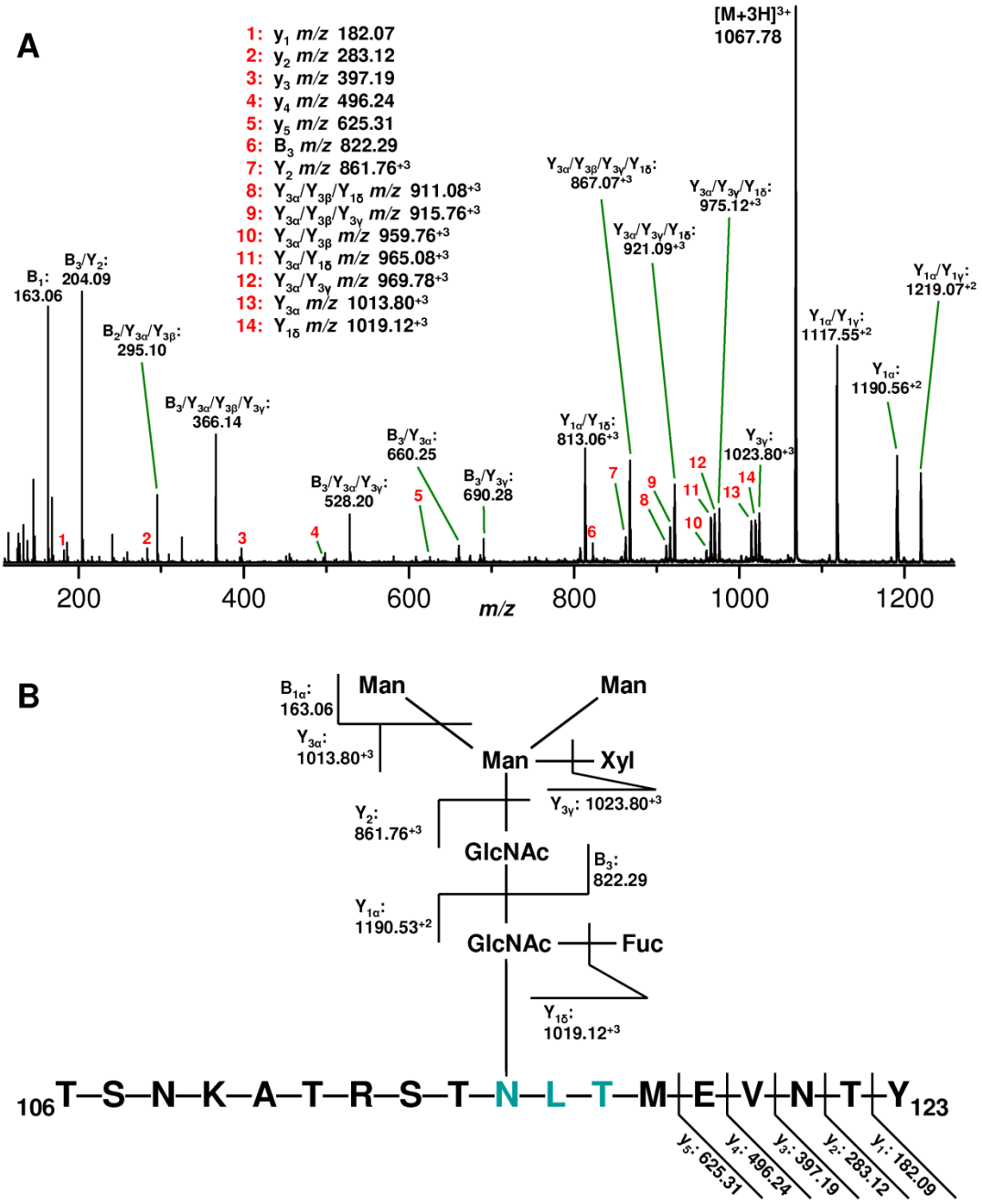


FIG S5

Supplementary Figure 5. **(a)** NanoESI Q-Tof fragment ion spectrum obtained from a CID experiment on the triply charged precursor *N*-glycopeptide ions with *m/z* 1067.78 derived from a chymotryptic digest of SGSL. **(b)** Corresponding fragmentation scheme.

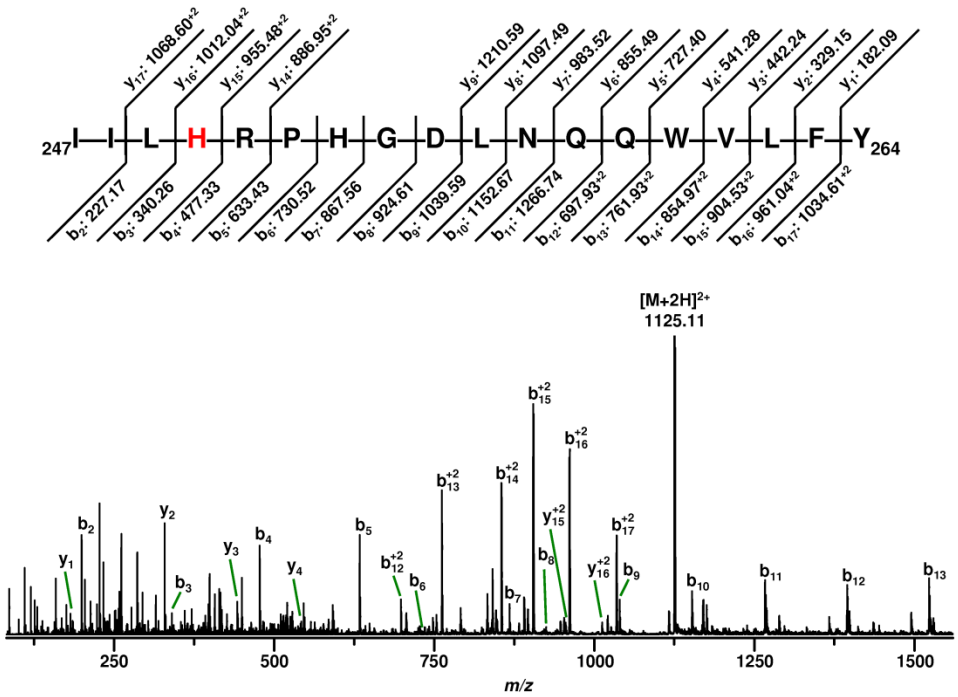


FIG S6

Supplementary Figure 6. CID spectrum of the doubly charged precursor ions at *m/z* 1125.11 derived from tryptic digest of SGSL. The insert shows the corresponding fragmentation scheme and His_{250} is highlighted in red.

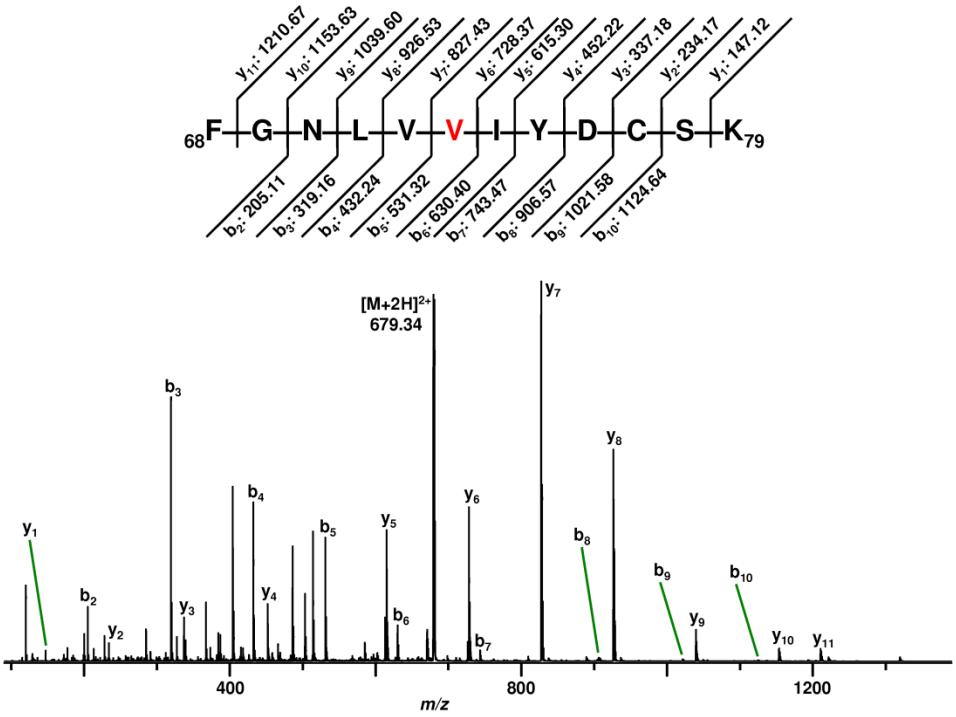
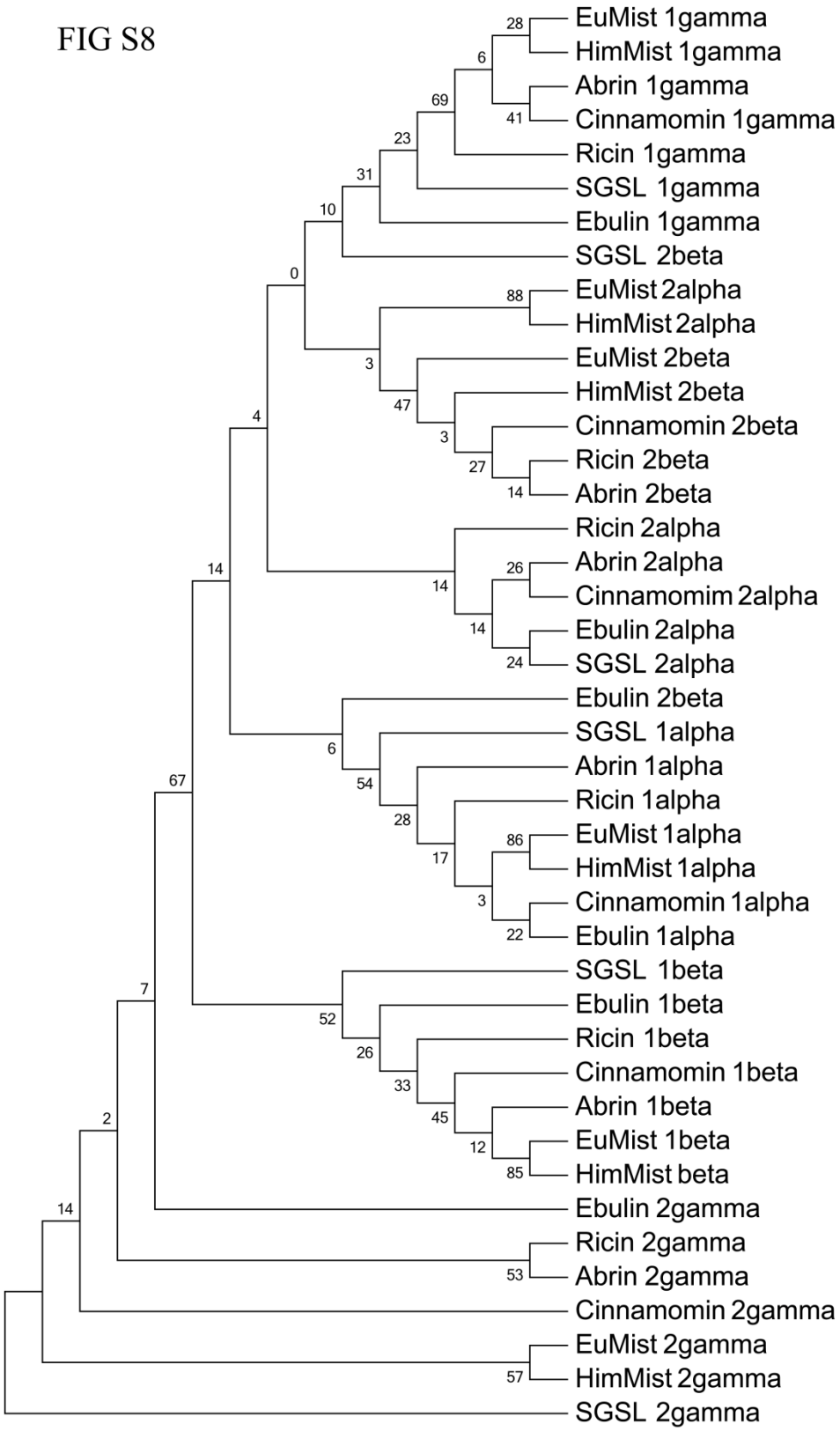


FIG S7

Supplementary Figure 7. CID spectrum of the doubly charged precursor ions at *m/z* 679.34 derived from tryptic digest of SGSL and subsequent reduction. The insert shows the corresponding fragmentation scheme.Val_{73} is highlighted in red.

FIG S8



Supplementary Figure 8. Phylogenetic tree generated from the alignment of three leaves of each β-trefoil lectin domain of type II RIPs of known structure. Each branch of the tree reflects the polypeptide sequence of the corresponding sub-domains of the lectin chain.