



BIOLOGICAL
CRYSTALLOGRAPHY

Volume 71 (2015)

Supporting information for article:

The first crystal structure of a glycoside hydrolase family 17 β -1,3-glucanosyltransferase displays a unique catalytic cleft

Zhen Qin, Qiaojuan Yan, Jian Lei, Shaoqing Yang, Zhengqiang Jiang and Shiwang Wu

Table S1 Primers used in this study.

Primers	Primer sequence (5'→3')	Bases (bp)
<i>RmBgt17A</i> -up ^a	ATTCGCGGAT <u>CCC</u> CAGACGTTCTATGGCATCAACTAT	36
<i>RmBgt17A</i> -down	ATTCCG <u>CTCGAG</u> TTAACAACCAGCCTCGATGGTAATA	37
E189A-up ^b	CTGTCAA AATTTC C GACAGGCTGG	26
E189A-down	G CGGAAATTTGACAGGCTTACCTAGGGAT	30
E158A-up	CATTCCTTACTGGG C AGGAGTTACC	26
E158A-down	G CCCAGTAAGGGAATGCGTTCATCA	25
Y102A-up	TTCTGAAGTGCTC GC TCGTGGCGAC	25
Y102A-down	GC GAGCACTTCAGAACCGACAATGAG	26
W157A-up	CGCATTCCCTTAC GC GGAAGGAGTT	25
W157A-down	GC GTAAGGGAATGCGTTCATCATTA	27
W157F-up	CGCATTCCCTTACT TC GAAGGAGTTAC	27
W157F-down	GA AGTAAGGGAATGCGTTCATCATTA	28

^a Restriction enzyme sites incorporated into the primers are underlined.

^b Mutations are indicated in box.

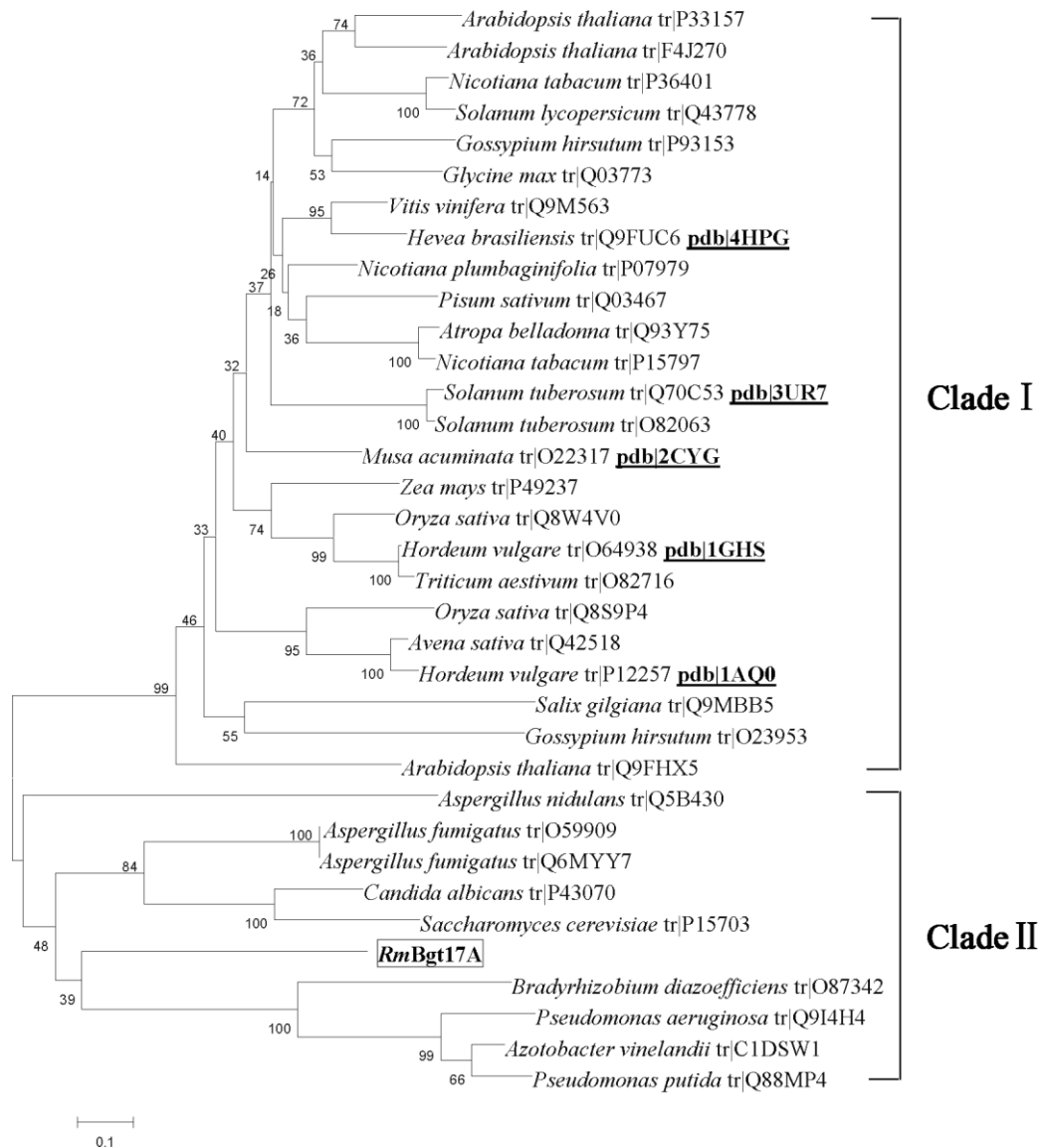


Figure S1 Phylogenetic tree of the GH family 17 members. Neighbor-joining tree showing phylogenetic relationships between *RmBgt17A* and other Uniprot and PDB entries. The sequence alignment was created with MUSCLE. Bootstrap values are expressed as percentages of 1,000 replications. The scale bar indicates branch length. The phylogenetic tree was constructed using the neighbor-joining method with program MEGA4.

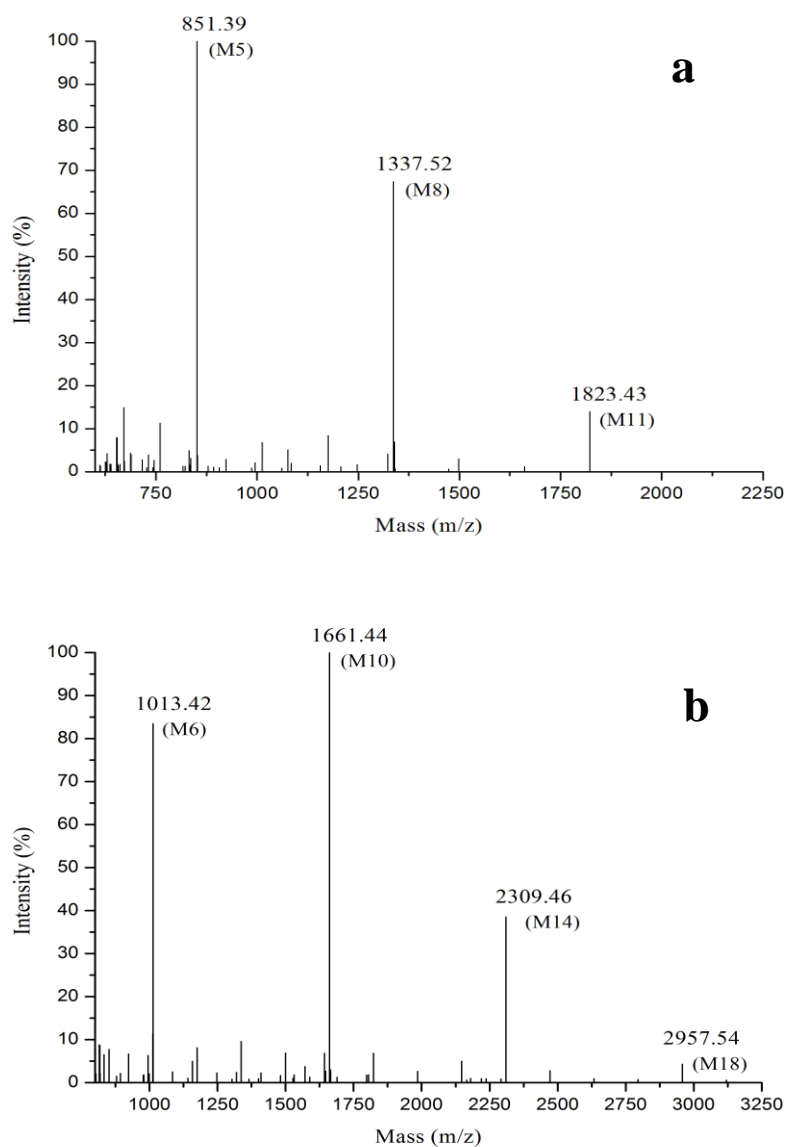


Figure S2 MALDI-TOF MS analysis of the transglycosylation products by *RmBgt17A*. The peaks in the spectra correspond to the monoisotopic masses of sodium adducts $[M+Na]^+$ of the laminarioligosaccharides. (a) Transglycosylation products deriving from laminaripentaose, which contain octasaccharide and undecasaccharide. (b) Transglycosylation products deriving from laminarihexaose, which contain decasaccharide, tetradecasaccharide and octadecasaccharide.

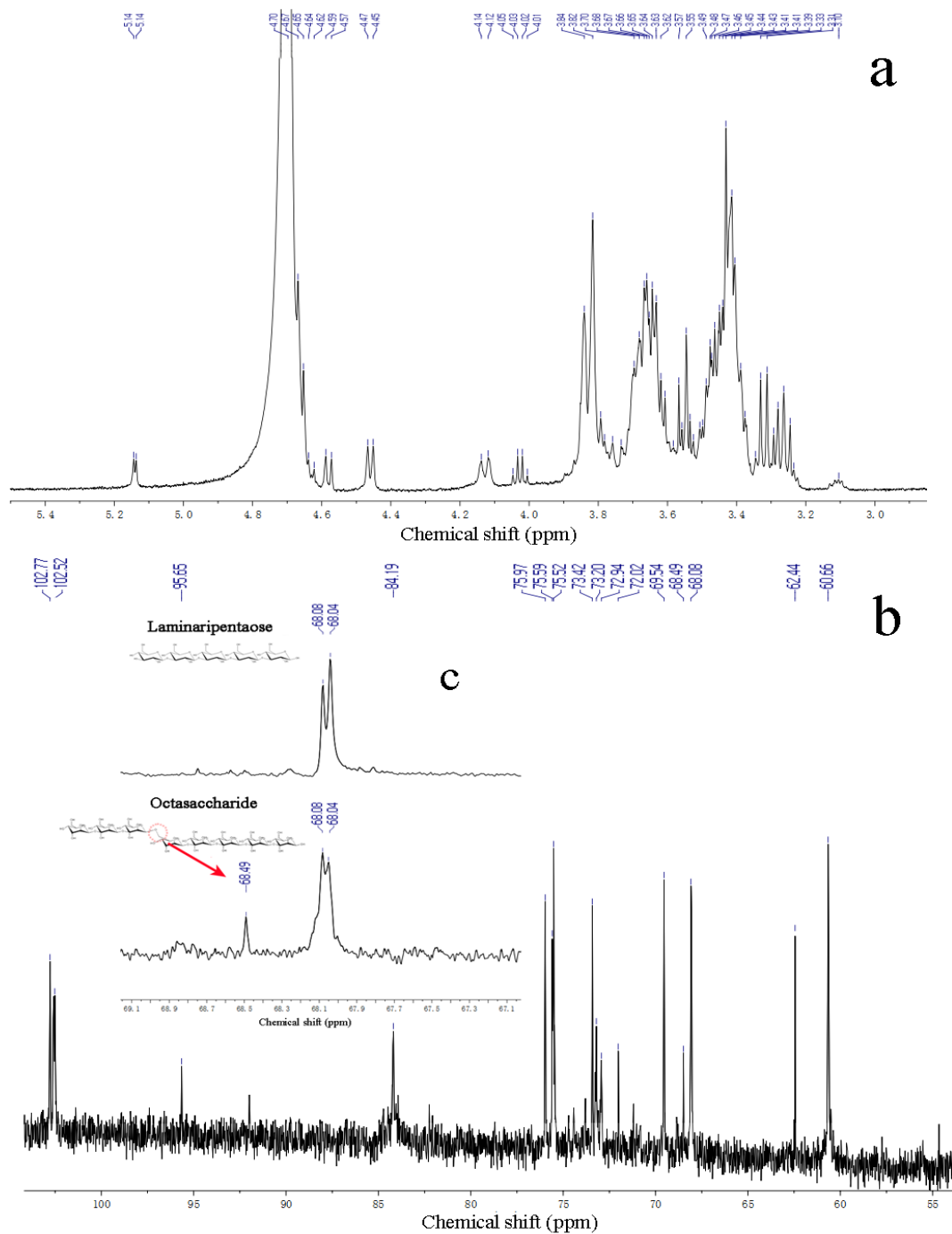


Figure S3 NMR data of the transglycosylation product (octasaccharide). (a) One-dimensional ^1H spectra of octasaccharide. (b) One-dimensional ^{13}C spectra of octasaccharide. (c) The enlarged picture of one-dimensional ^{13}C spectra of laminaripentaose and octasaccharide. A characteristic chemical shift at 68.49 ppm, indicating a β -1,6 linkage form in the transglycosylation product.