

## Appendix A. Supplementary data

### Crystal structure of a homotrimeric verrucomicrobial exo- $\beta$ -1,4-mannosidase active in the hindgut of the wood-feeding termite *Reticulitermes flavipes*

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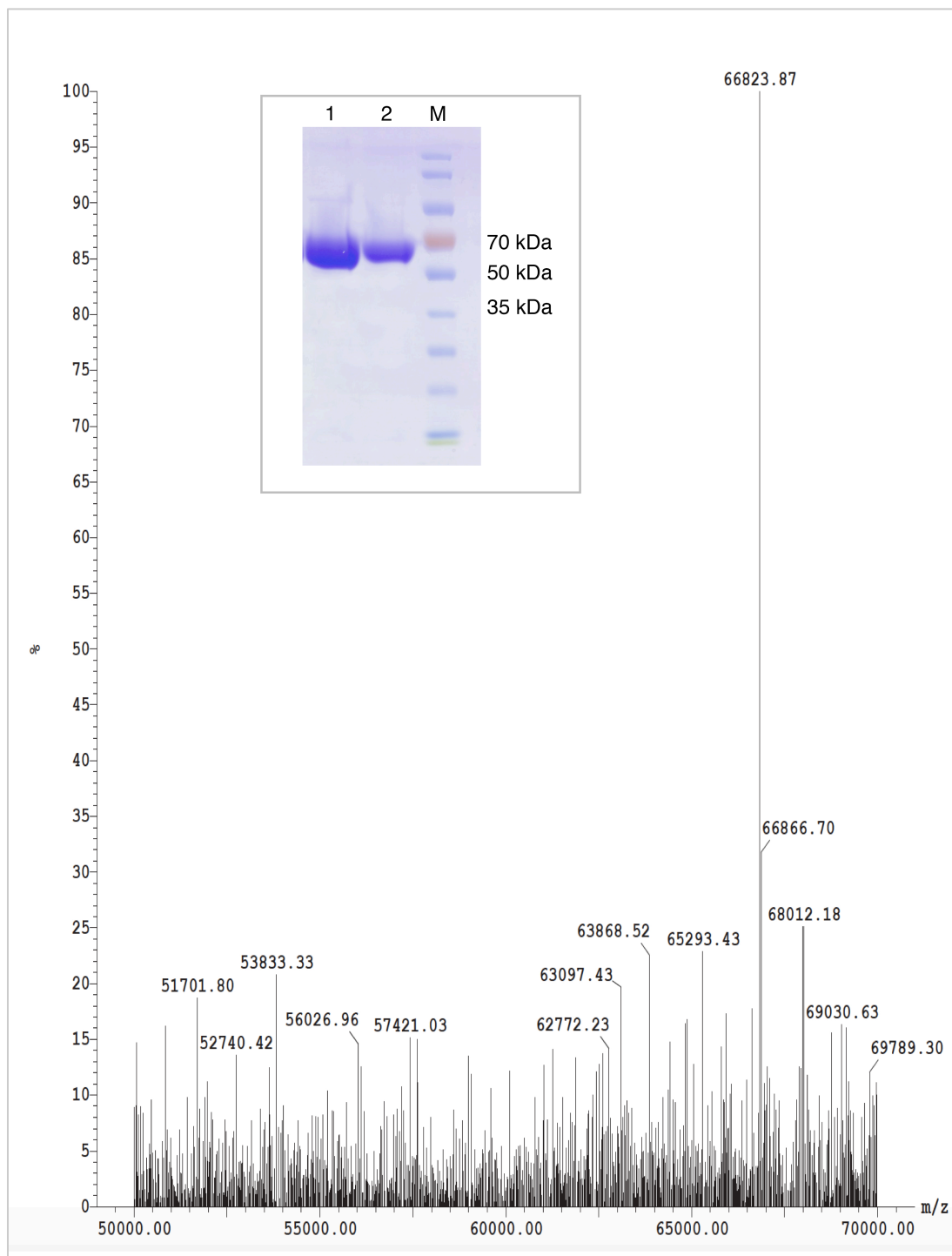
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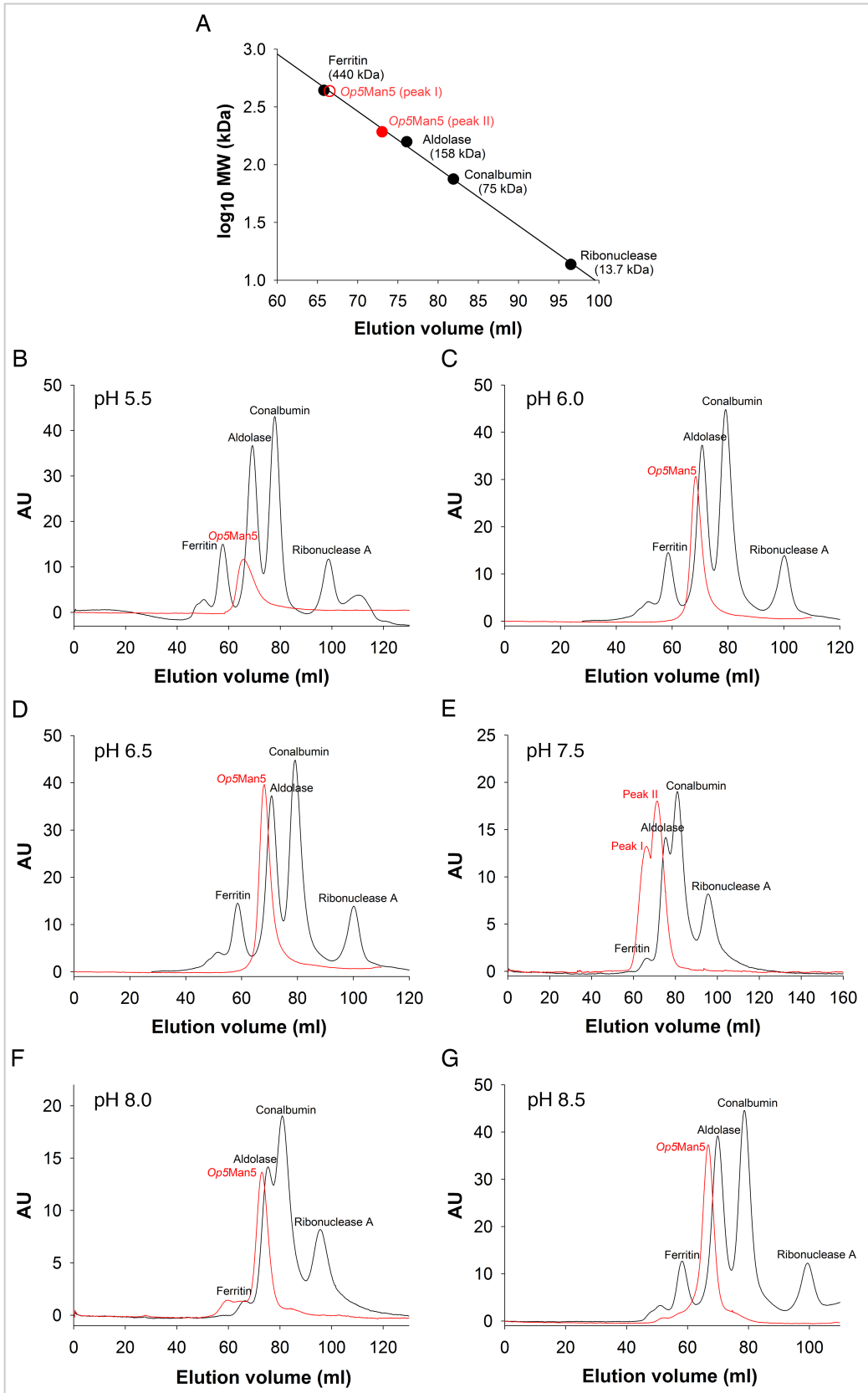
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**Figure S1**



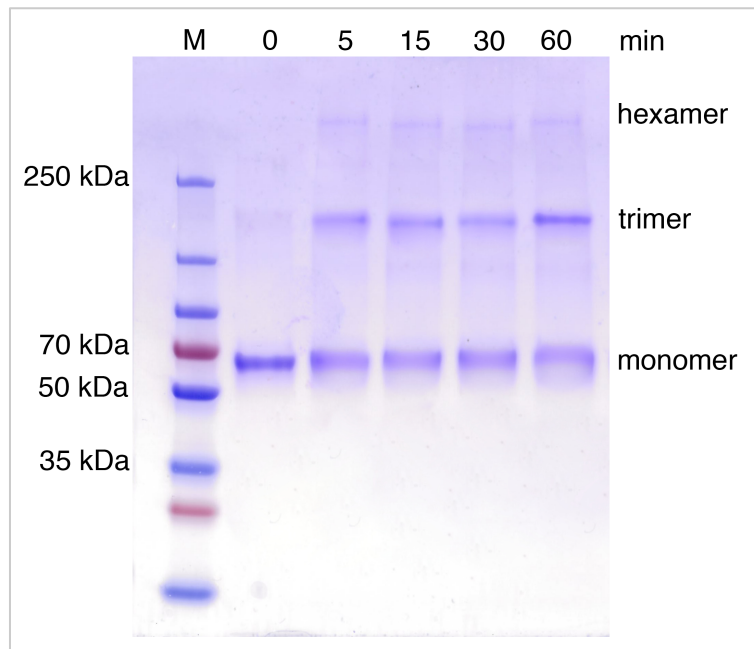
**Figure S1. Molecular mass of *Op5Man5*.** Liquid chromatography-tandem mass spectrometry (LC-MS/MS) of recombinant *Op5Man5* gives a molecular mass of 66,824 g/mol. The inset panel shows an SDS-PAGE gel of purified *Op5Man5* with different amounts of protein loaded in the two lanes. M, molecular weight reference proteins.

Figure S2



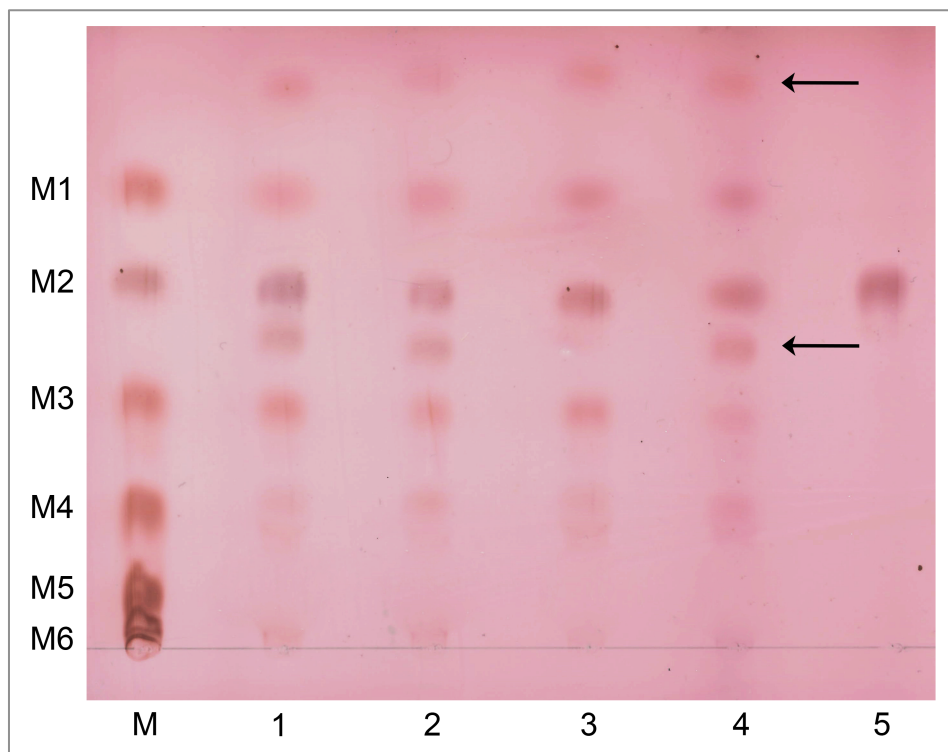
**Figure S2. SEC analysis of *Op5Man5*.** (A) Standard curve at pH 7.5 ( $R^2 = 0.9954$ ) based on the reference proteins (black filled circles), and the extrapolated molecular weights of the *Op5Man5* hexamer (peak I; ~434 kDa; red open circle) and trimer (peak II; ~214 kDa; red filled circle). SEC profiles of *Op5Man5* at different pH values (red curve) overlaid with the profiles of the reference proteins: (B) pH 5.5; (C) pH 6.0; (D) pH 6.5; (E) pH 7.5; (F) pH 8.0; and (G) pH 8.5. The SEC profile in (E) shows two distinct species: peak I (hexamer) and peak II (trimer).

**Figure S3**



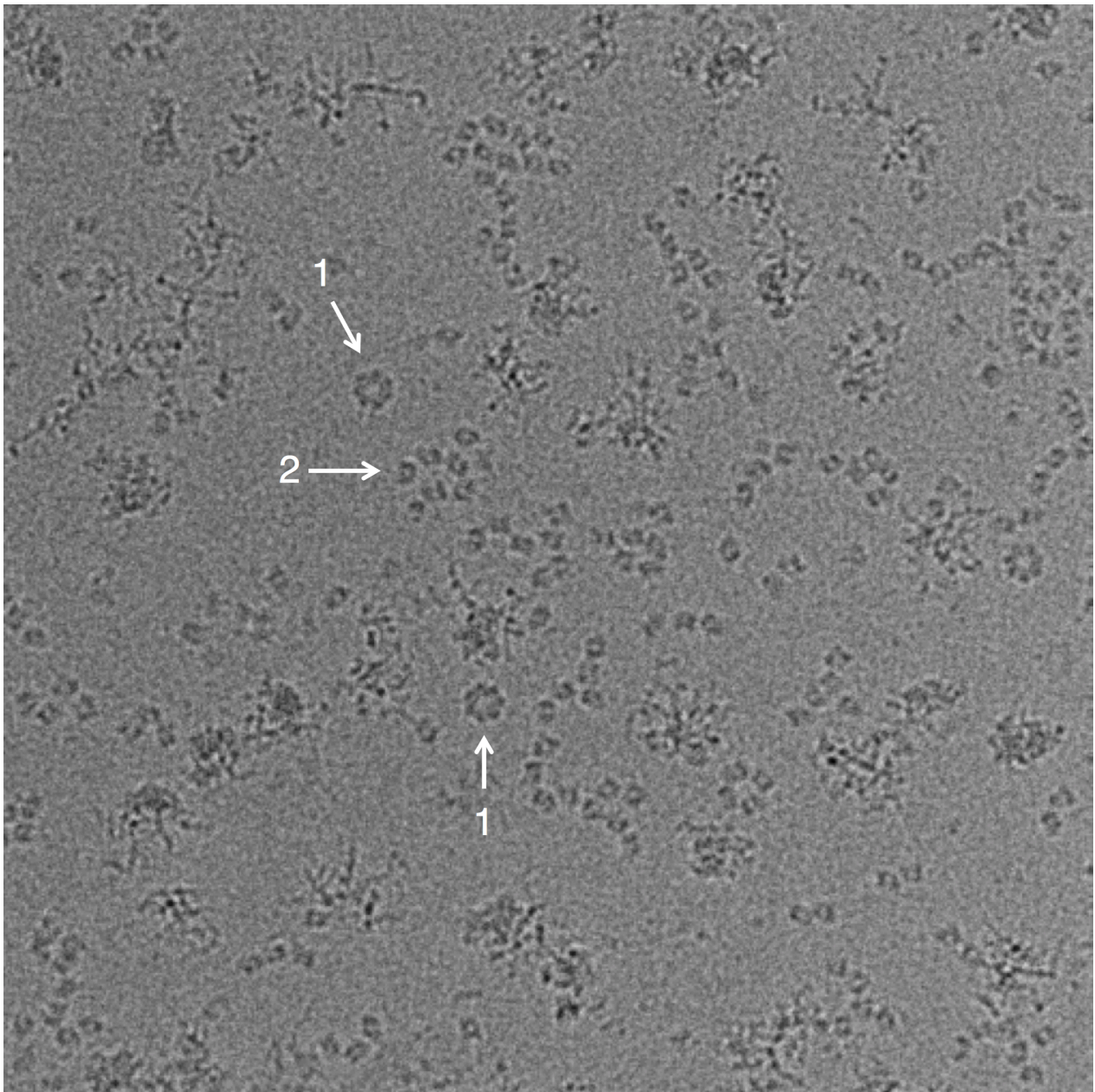
**Figure S3. Chemical cross-linking of *Op5Man5*.** Results of the crosslinking reaction as a function of time as represented by a Coomassie-stained SDS-PAGE. At  $t = 0$ , only the monomer band is present.

**Figure S4**



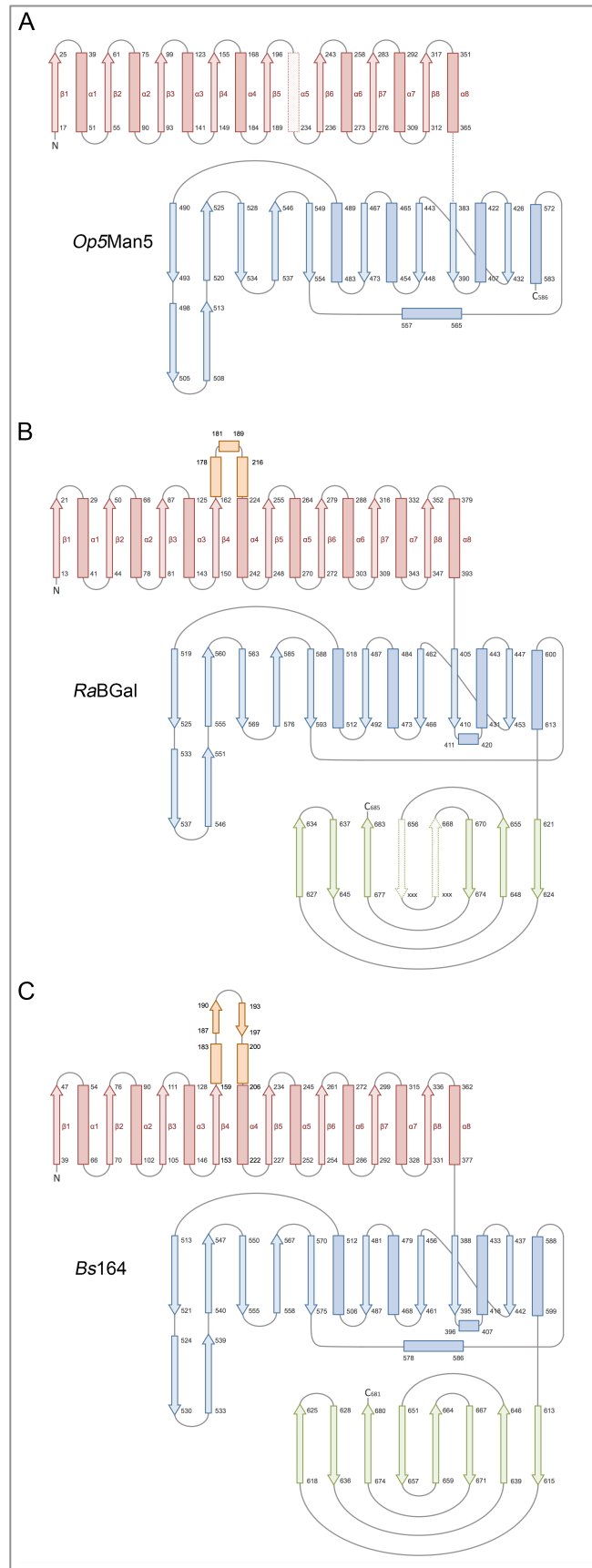
**Figure S4. Transglycosylation products.** TLC analysis of products from incubating M2 with methanol (lane 1), ethanol (lane 2), 1-propanol (lane 3), and hexanol (lane 4). Reference mannooligosaccharides: M1-M6 (lane M), and M2 (lane 5). Alkyl  $\beta$ -mannosides are indicated by arrows.

**Figure S5**



**Figure S5. Oligomeric species.** Electron micrograph showing two distinct species of *Op5GH5*, a hexameric or heptameric assembly (1) and the trimeric species (2).

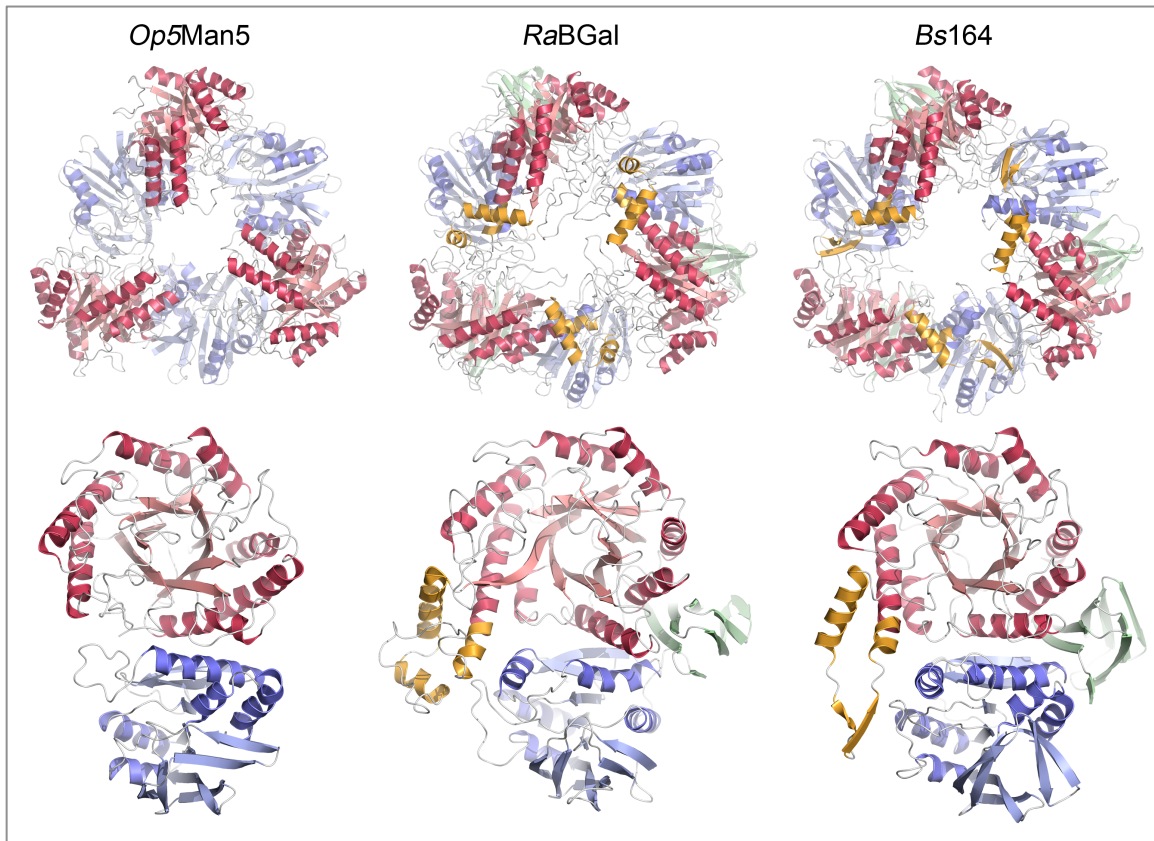
Figure S6





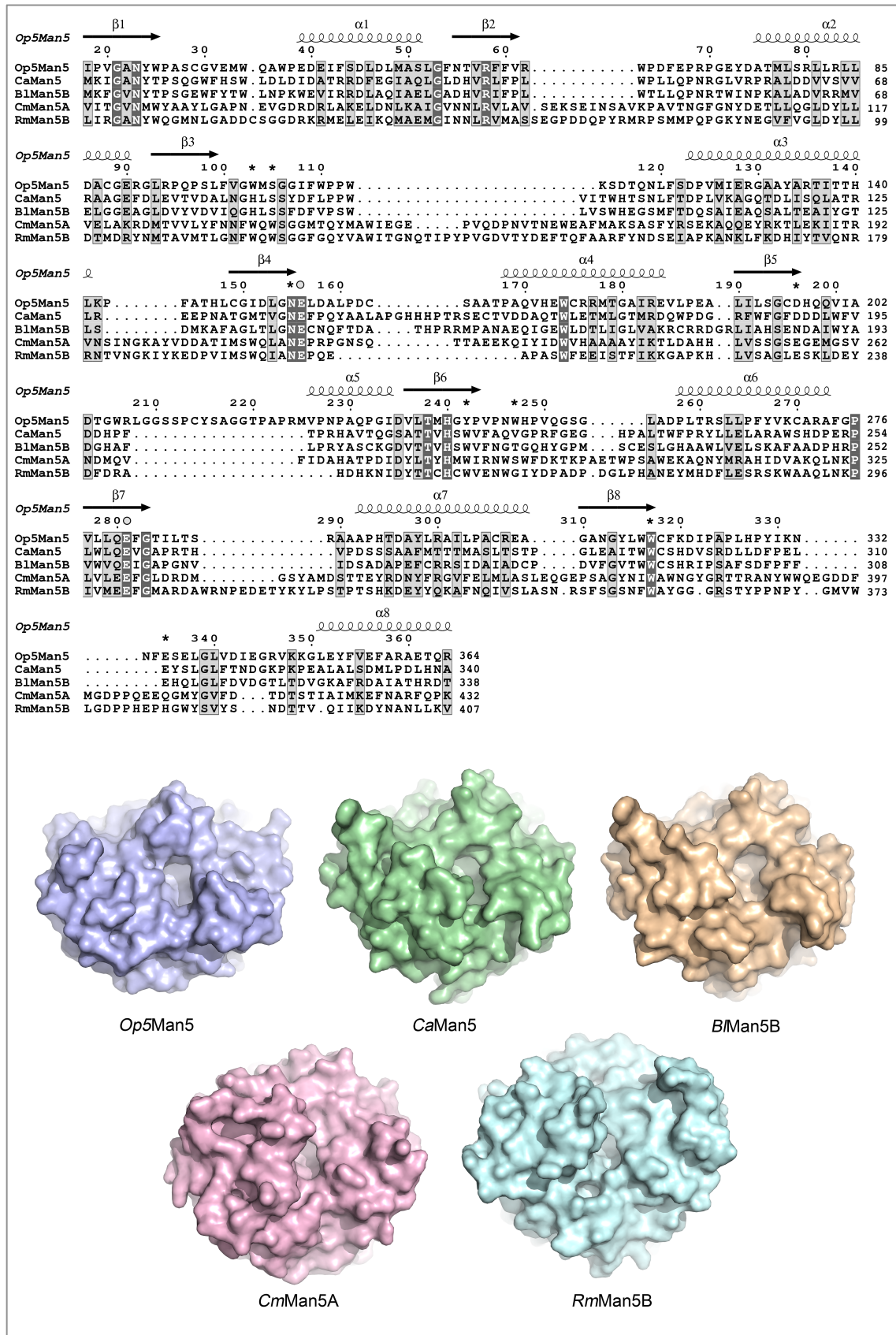
**Figure S6. Topological similarity of *Op5Man5*, *RaBGal* and *Bs164*.** The N-terminal folds as a TIM barrel (domain A; red), and continues into a Rossmann-like mixed-sheet domain (domain B; blue). Except for a helical extension (orange) in the A-domain of *RaBGal* and *Bs164*, and an additional peripheral  $\alpha$ -helix in the B domain of *Op5Man5*, the topology of the A and B domains are identical in the three enzymes. The C-terminal domain (domain C; green) in *RaBGal* and *Bs164* features a Greek-key fold that is not present in *Op5Man5*. Two  $\beta$ -strands in the Greek-key domain of *RaBGal* are partly disordered, which is indicated as dashed arrows. The unmodeled region in *Op5Man5* comprising residues 210-221 is shown as a dashed, unfilled rectangle indicating a possible  $\alpha$ -helix that is either very flexible or partly unfolded. A second unmodeled region is the linker peptide between domains A and B in *Op5Man5* (residues 366-382). Note that the deposited *Bs164* models have a sequence offset of +10 residues relative the sequence deposited in UniProt (entry I9SUA3), and the numbering used in the topology diagram is that of the models.

**Figure S7**



**Figure S7. Structural comparison of *Op5Man5*, *RaBGal* and *Bs164*.** Overview of the trimer and monomer structure of *Op5Man5* (this work), *RaBGal* (PDB code 5E9A) and *Bs164* (PDB code 6T75). The same colors are used as in Fig. S5.

Figure S8



**Figure S8. Comparison of the catalytic TIM-barrel domains of GH5  $\alpha$ -1,4-mannosidases.** (A) Structure-based sequence alignment of the catalytic TIM-barrel domains of *Op5Man5*, *CaMan5* (PDB 6GVB<sup>31</sup>), *B/Man5B* (PDB 6MPA<sup>47</sup>), *CmMan5A* (PDB 1UUQ<sup>20</sup>) and *RmMan5B* (PDB 4LYP<sup>17</sup>). Surface representations of the TIM-barrel domains are shown to highlight the differences in shape of the entrance to the binding pockets.



Figure S10

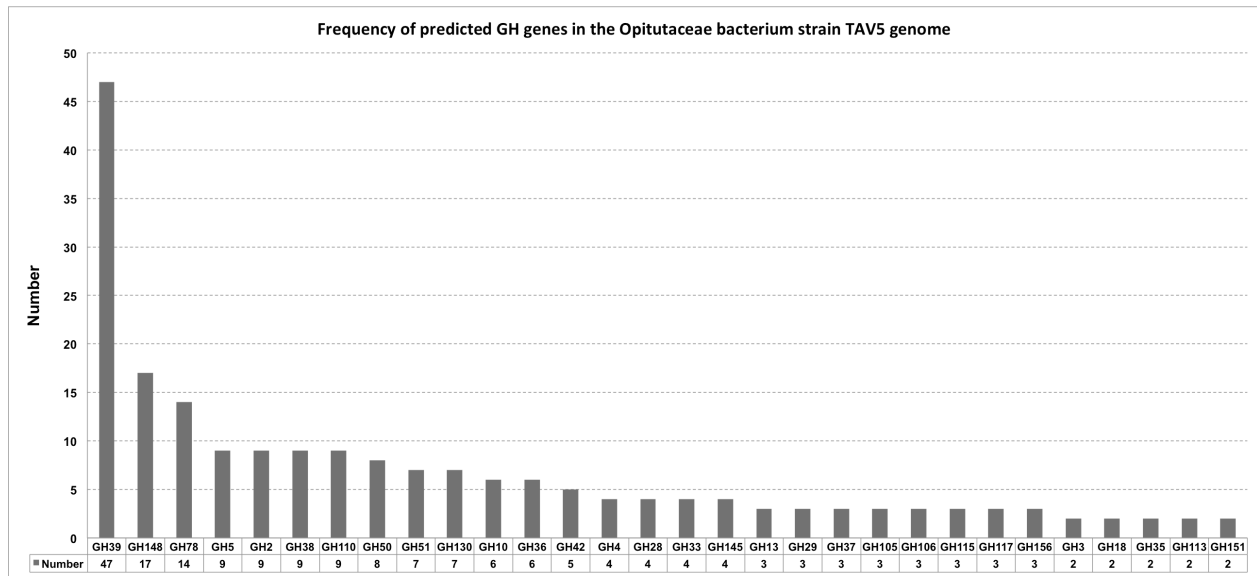
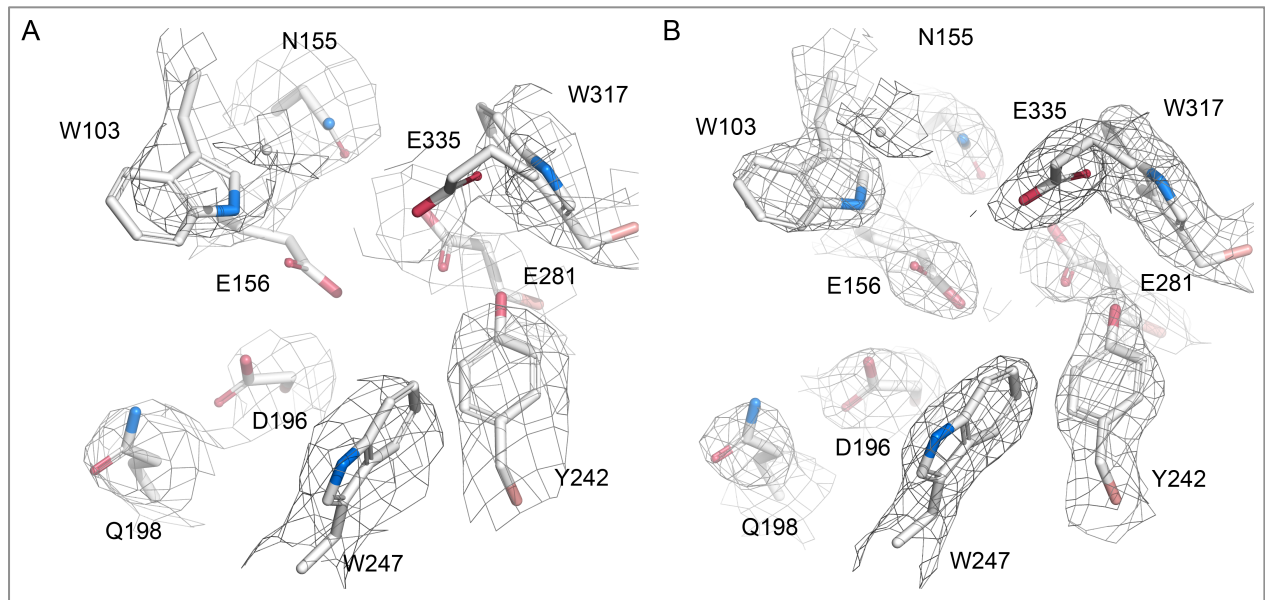


Figure S10. GH genes in the *Opitutaceae* bacterium strain TAV5 genome. The distribution of GH genes in the genome of *Opitutaceae* bacterium strain TAV5 according to GH family.

**Figure S11**



**Figure S11. Quality of the cryo-EM and final X-ray map.** Comparison of the map quality in the region of the active site. The 3.7 Å cryo-EM map (A) is of good overall quality, especially for aromatic residues, but lacks detectable signal for some side chains (E156, D196, E335), for which the 2.2 Å  $2F_o - F_c$  electron-density map (B) provided additional information.

**Table S1. Reported activity on pNP-βMan for a selection of retaining glycoside hydrolases with exo-β-1,4-mannosidase activity (EC 3.2.1.25).**

Enzyme name	Gene name	Organism name	UniProt accession	CAZy subfamily	<sup>a</sup> Molecular weight (g mol <sup>-1</sup> )	PDB accession	Oligomeric state	<sup>b</sup> K <sub>m</sub> (mM)	<sup>c</sup> k <sub>cat</sub> (s <sup>-1</sup> )	<sup>d</sup> k <sub>cat</sub> /K <sub>m</sub> (s <sup>-1</sup> mM <sup>-1</sup> )	Specific activity U mg <sup>-1</sup>	Transglycosylation activity	Reference	Digital object identifier	
<b>GH5 (Bacteria)</b>															
Op5Man5	OPIT5_10225	<i>Opiritaceae</i> bacterium strain TAV5, Verrucomicrobia	W0J1H8	–	66,062	This work	homotrimer / hexamer	1.0	238.9	238.9	–	Yes	This work		
TthMan5	Theth_0949	<i>Pseudothermotoga (Thermotoga) thermarum</i> strain DSM 5069, Thermotogae	F7YX66	19	70,687	n.a.	oligomer	4.4	1924	441	–	n.a.	Shi <i>et al.</i> 2013	10.1186/1472-6750-13-83	
CaMan5_18	PAZ_c15370	<i>Cutibacterium acnes (Propionibacterium acnes)</i> , Actinobacteria	A0A2B717A6	18	45,701	6GVB	homodimer	10.4	7.8	0.75	–	n.a.	Reichenbach <i>et al.</i> 2018	10.1371/journal.pone.0204703	
BtMan5B	BLD_0195 (BL1333)	<i>Bifidobacterium longum</i> strain DJO10A, Actinobacteria	B3DQP5	18	47,441	6MPA	homodimer	<sup>d</sup> n.a.	<sup>d</sup> n.a.	<sup>d</sup> n.a.	–	n.a.	Cordeiro <i>et al.</i> 2019	10.1016/j.jmb.2018.12.017	
CmMan5A	man5A	<i>Cellvibrio mixtus</i> strain NCIMB 8633, Proteobacteria	Q6QT42	7	51,623	1UUU	monomer	1.6	0.033	0.021	–	Yes	Dias <i>et al.</i> 2004	10.1074/jbc.M401647200	
<b>GH5 (Eukaryota, Fungi)</b>															
RmMan5B	man5B	<i>Rhizomucor miehei</i> strain CAU432, zygomycete fungus	A0A075C6T6	7	51,321	4LYP, 4LYQ	monomer	n.a.	n.a.	n.a.	1.93	Yes	Zhou <i>et al.</i> 2014	10.1107/S1399004714019762	
LrMan5B	LRAMOS04528	<i>Lichtheimia ramosa</i> , zygomycete fungus	A0A077WZ93	–	50,996	n.a.	n.a.	1.38	19.7	14.3	–	n.a.	Xie <i>et al.</i> 2019	10.1016/j.jbio.2019.04.007	
AcMan5	acman5	<i>Lichtheimia (Absidia) corymbifera</i> strain D1, zygomycete fungus	A0A141PG32	–	49,797	n.a.	n.a.	n.a.	n.a.	n.a.	2.65	Yes	Li <i>et al.</i> 2015	10.1016/j.molcatb.2015.09.018	
<b>GH2 (Bacteria)</b>															
BtMan2A	BT_0458	<i>Bacteroides thetaiotaomicron</i> strain VPI-548, Bacteroidetes	Q8AAK6	–	99,506	2JE8	homodimer	0.19	128	667	–	No	Tailford <i>et al.</i> 2007	10.1074/jbc.M610964200	
TmMan2	TM_1624	<i>Thermotoga maritima</i> strain MSB8, Thermotogae	Q9X1V9	–	92,373	n.a.	monomer	0.49	8.4	17.2	–	Yes	Zhang <i>et al.</i> 2009	10.1016/j.molcatb.2009.04.005	
TnMan2	man2	<i>Thermotoga neapolitana</i> strain DSM 5068, Thermotogae	Q93M25	–	92,197	n.a.	homodimer	3.1	67.8	24.2	–	n.a.	Duffaud <i>et al.</i> 1997	10.1128/AEM.63.1.169-177.1997	
ManB	manB	<i>Thermobifida (Thermomonospora) fusca</i> strain TM5, Actinobacteria	Q8KLI9	–	94,228	n.a.	n.a.	0.18	9.34	51.9	–	Yes	Beki <i>et al.</i> 2003	10.1128/aem.69.4.1944-1952.2003	
CjMan2A	man2	<i>Cellulomonas fimi</i> strain ATCC 484, Actinobacteria	Q9XCV4	–	93,696	n.a.	monomer	0.3	<sup>d</sup> 167	<sup>d</sup> 500	–	n.a.	Stoll <i>et al.</i> 1999	10.1128/AEM.65.6.2598-2605.1999	
Man2S27	bma	<i>Streptomyces sp. S27</i> , Actinobacteria	D2DFB5	–	92,580	n.a.	n.a.	0.23	305	1320	–	Yes	Shi <i>et al.</i> 2011	10.1016/j.enzymictec.2011.06.003	
NixH	XCC2891	<i>Xanthomonas campestris pv. campestris</i> strain ATCC 3391, Proteobacteria	Q8P6S4	–	100,196	n.a.	n.a.	7.4	1552	209.8	–	n.a.	Dupoiron <i>et al.</i> 2015	10.1074/jbc.M114.624593	
DtMan	DICTH_1692	<i>Dictyoglomus thermophilum</i> strain DSM 3960, Firmicutes	B5YAN4	–	96,130	5N6U	homodimer	0.47	298	617	–	n.a.	Guillot <i>et al.</i> 2017	10.1016/j.biochi.2017.03.020	
–	–	<i>Paenibacillus polymyxa (Bacillus polymyxa)</i> strain A-8, Firmicutes	U5N3E2	–	96,836	n.a.	n.a.	n.a.	n.a.	n.a.	38	n.a.	Bai <i>et al.</i> 2014	10.1371/journal.pone.0111622	
–	–	<i>Paenibacillus polymyxa (Bacillus)</i> strain A-8, Firmicutes, recombinant	U5N3E2	–	96,836	n.a.	n.a.	n.a.	n.a.	n.a.	0.7	n.a.	Bai <i>et al.</i> 2014	10.1371/journal.pone.0111622	
<b>GH2 (Eukaryota)</b>															
MndA	mndA	<i>Aspergillus niger</i> strain ATCC 46890, ascomycete fungus	Q9UUZ3	–	104,390	n.a.	homodimer	0.30	67.5	225	–	Yes	Ademark <i>et al.</i> 1999	10.1016/s0168-1656(99)00172-8	
MndA	mndA	<i>Aspergillus niger</i> strain ATCC 46890, ascomycete fungus	Q9UUZ3	–	104,390	n.a.	homodimer	0.46	67.5	217	–	Yes	Reddy <i>et al.</i> 2013	10.1016/j.febslet.2013.08.029	
MndB	mndB	<i>Aspergillus (Emericella) nidulans</i> strain ATCC 38163, ascomycete fungus	Q5B7W2	–	96,367	n.a.	n.a.	0.22	1.32	6.0	–	n.a.	Reddy <i>et al.</i> 2013	10.1016/j.febslet.2013.08.029	
bMann9	man9	<i>Thermothelomyces thermophilus</i> strain C1, ascomycete fungus	I2C092	–	97,352	n.a.	n.a.	0.41	15	37	–	n.a.	Dotsenko <i>et al.</i> 2012	10.1134/S0006297912110090	
TtMan2A	–	<i>Hypocrea jecorina (Trichoderma reesi)</i> strain Z12, ascomycete fungus	n.a.	–	n.a.	n.a.	homodimer, putative	0.12	<sup>d</sup> 5.2	<sup>d</sup> 43	–	n.a.	Kulminkaya <i>et al.</i> 1999	10.1016/S0141-0229(99)00056-3	
TtMan2A	–	<i>Hypocrea lixii (Trichoderma harzianum)</i> strain IOC-3844, ascomycete fungus	A0A075B5H6	–	105,388	4CVU	monomer	n.a.	n.a.	n.a.	3.2	Yes	Nascimento <i>et al.</i> 2014	10.1111/febs.12894	
ManbA	Manba	<i>Mus musculus</i> (lysosomal)	Q8K214	–	100,831	6DDU	monomer	1.42	72.2	51	–	n.a.	Gytz <i>et al.</i> 2019	10.1111/febs.14731	
–	manba	<i>Capra hircus</i> (lysosomal), goat kidney	Q95327	–	101,386	n.a.	n.a.	9	n.a.	n.a.	1.08	n.a.	Frei <i>et al.</i> 1982	10.1042/bj2490871	
–	manba	<i>Homo sapiens</i> (lysosomal), human serum	n.a.	–	(90,000)	n.a.	n.a.	2.7	n.a.	n.a.	n.a.	n.a.	Bernard <i>et al.</i> 1986	10.1016/0020-711x(86)90255-7	
–	manba	<i>Homo sapiens</i> (lysosomal), human urine	n.a.	–	(100,000)	n.a.	n.a.	2.4	n.a.	n.a.	n.a.	n.a.	Bernard <i>et al.</i> 1986	10.1016/0020-711x(86)90255-7	
–	manba	<i>Homo sapiens</i> (lysosomal), human placenta	O00462	–	(75,000)	n.a.	n.a.	2.2	n.a.	n.a.	n.a.	n.a.	Noeske & Mersmann 1983	10.1515/bchm2.1983.364.2.1645	
–	manba	<i>Homo sapiens</i> (lysosomal), human placenta	O00462	–	100,895	n.a.	n.a.	2.5	n.a.	n.a.	12.7	n.a.	Samra & Athar 2008	Acta Biochim. Pol. 55, 479-490, 2008	
AkMnsd	AkMnsd	<i>Aplysia kurodai</i> (gut), Kuroda's sea hare	H1AFK3	–	105,059	n.a.	n.d.	0.10	6.2	62	–	n.a.	Zahura <i>et al.</i> 2012	10.1016/j.cbpb.2012.02.003	



Table S1. Cont.

Enzyme name	Gene name	Organism name	UniProt accession	CAZy subfamily	<sup>a</sup> Molecular weight (g mol <sup>-1</sup> )	PDB accession	Oligomeric state	<sup>b</sup> K <sub>m</sub> (mM)	<sup>c</sup> k <sub>cat</sub> (s <sup>-1</sup> )	<sup>d</sup> k <sub>cat</sub> /K <sub>m</sub> (s <sup>-1</sup> mM <sup>-1</sup> )	Specific activity U mg <sup>-1</sup>	Transglycosylation activity	Reference	Digital object identifier
<b>GH1 (Archaea)</b>														
BmnA	bmnA	<i>Pyrococcus furiosus</i> strain DSM 3638	Q51733	–	59,069	n.a.	tetramer	0.79	<i>31</i>	<i>39</i>	–	n.a.	Bauer et al. 1996	10.1074/jbc.271.39.23749
PFTG	PF0356	<i>Pyrococcus furiosus</i> strain DSM 3638	Q8U3U9	–	56,327	n.a.	tetramer	0.09	0.30	3.0	–	Yes	Park et al. 2011	10.1016/j.nbt.2011.05.002
BglB	PH0501	<i>Pyrococcus horikoshii</i> strain OT3	O58237	–	56,458	n.a.	tetramer	0.44	4.2	9.8	–	n.a.	Kaper et al. 2002	10.1021/bi011935a
TkβGly	–	<i>Thermococcus kodakarensis</i> strain KOD1	Q9YGB8	–	56,266	n.a.	homodimer	1.1	51	47	–	n.a.	Hwa et al. 2015	10.1016/j.enzymetec.2015.05.002
<b>GH1 (Eukaryota, Plantae)</b>														
HvBII	–	<i>Hordeum vulgare subsp. vulgare</i> , barley	B5A496	–	57,425	n.a.	n.a.	0.25	3.1	12.7	–	Yes	Kuntothom et al. 2010	10.1021/bi101112c
Os7BGlu26	OsI_27163	<i>Hordeum vulgare subsp. indica</i> , barley	A2YPH1	–	58,498	4JHO	monomer	0.48	0.35	0.71	–	n.a.	Tankrathok et al. 2013	10.1107/S0907444913020568
LeMsIde	–	<i>Solanum lycopersicum (Lycopersicon esculentum)</i> , tomato	Q8VWL8	–	59,288	n.a.	n.a.	0.55	<i>10</i>	<i>18</i>	–	n.a.	Mo & Bewley 2002	10.1007/s00425-001-0725-x
BGLU44	BGLU44	<i>Arabidopsis thaliana</i> , thale cress	Q9LV33	–	58,984	n.a.	n.a.	0.43	<i>6</i>	<i>14</i>	–	n.a.	Xu et al. 2004	10.1007/s11103-004-0790-1
<b>GH113 (Bacteria)</b>														
RtGH113	ROSINTL182_05483	<i>Roseburia intestinalis</i> strain L1-82	–	–	36,057	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	La Rosa et al. 2019	10.1038/s41467-019-08812-y
<b>GH164 (Bacteria)</b>														
Bs164	HMPREF1071_03408	<i>Bacteroides salyersiae</i> strain CL02T12C01	I9SUA3	–	76,732	6T50, 6T75	homotrimer	3.6	40	11	–	n.a.	Armstrong & Davies 2020	10.1074/jbc.RA119.011591
<b>Not classified in CAZy</b>														
–	–	<i>Bacillus mannanilyticus</i> strain DSM 16130 (AM-001), bacteria, firmicutes	n.a.	–	(94,000)	n.a.	n.a.	1.3	n.a.	n.a.	38.8	Yes	Akino et al. 1988	10.1080/00021369.1988.10868864
–	–	<i>Tremella fuciformis</i> , basidiomycete fungus	n.a.	–	(140,000)	n.a.	n.a.	2.1	n.a.	n.a.	0.21	n.a.	Sone & Misaki 1978	10.1093/oxfordjournals.jbcchem.a132003
–	–	<i>Laetiporus (Polyporus) sulphureus</i> , basidiomycete fungus	n.a.	–	(64,000)	n.a.	n.a.	1.6	n.a.	n.a.	4.2	n.a.	Wan et al. 1976	10.1016/s0021-9258(17)33308-2
–	–	<i>Athelia (Sclerotium) rolfsii</i> , basidiomycete fungus	–	–	(57,500)	n.a.	n.a.	n.a.	n.a.	n.a.	<i>41</i>	n.a.	Gübitz et al. 1996	10.1016/S0960-8524(96)00093-4
GM-1 (isoenzyme)	–	<i>Phlebia radiata</i> strain ATCC 64658, basidiomycete fungus	n.a.	–	(104,600)	n.a.	n.a.	0.3	<i>74</i>	<i>247</i>	–	n.a.	Prendecka et al. 2007	Pol. J. Microbiol. 56, 139-147, 2007
GM-2 (isoenzyme)	–	<i>Phlebia radiata</i> strain ATCC 64658, basidiomycete fungus	n.a.	–	(89,500)	n.a.	n.a.	1.8	<i>72</i>	<i>40</i>	–	n.a.	Prendecka et al. 2007	Pol. J. Microbiol. 56, 139-147, 2007
–	–	<i>Thermoascus aurantiacus</i> Miehe, ascomycete fungus	n.a.	–	(99,900)	n.a.	monomer	1.1	6.1	<i>5.5</i>	–	Yes	Gomes et al. 2007	10.1016/j.enzymetec.2006.08.011
–	–	<i>Helix pomatia</i> , Roman snail	n.a.	–	(94,000)	n.a.	n.a.	1.43	<i>159</i>	<i>111</i>	–	n.a.	McCleary 1983	10.1016/0008-6215(83)88314-1
–	–	<i>Helix aspersa</i> Müller ( <i>Cornu aspersum</i> ), brown garden snail	n.a.	–	(77,800)	n.a.	monomer	0.77	<i>64</i>	<i>83</i>	–	n.a.	Charrier & Rouland 2001	10.1002/jez.1042
–	–	<i>Achatina fulica</i> , giant African snail	n.a.	–	n.a.	n.a.	n.a.	6.5	n.a.	n.a.	6.67	n.a.	Sugahara et al. 1972	10.1016/0005-2744(72)90344-0
–	–	<i>Turbo cornutus</i> , horned turban sea snail	n.a.	–	n.a.	n.a.	n.a.	7.1	n.a.	n.a.	3.8	n.a.	Muramatsu & Egami 1967	10.1093/oxfordjournals.jbcchem.a128726
–	–	<i>Aplysia fasciata</i> , mottled sea hare	n.a.	–	(130,000)	n.a.	homodimer	2.4	<i>192</i>	<i>80</i>	–	Yes	Andreotti et al. 2005	10.1016/j.jbiotec.2005.06.003
–	–	<i>Hordeum vulgare</i> , malted barley	n.a.	–	(88,000)	n.a.	n.a.	0.3	n.a.	n.a.	0.6	n.a.	Houston et al. 1974	10.1016/0005-2744(74)90052-7
–	–	<i>Lactuca sativa L. cv. Grand Rapids</i> , garden lettuce	n.a.	–	n.a.	n.a.	n.a.	0.3	n.a.	n.a.	n.a.	n.a.	Ouellette & Bewley 1986	10.1007/BF00392128
–	–	<i>Cyamopsis tetragonolobus</i> (guar seeds)	–	–	(59,000)	n.a.	n.a.	0.5	<i>15</i>	<i>30</i>	15.6	n.a.	McCleary 1982	Meth. Enzymol. 160, 589-595, 1982
–	–	<i>Gallus gallus</i> , hen oviduct	n.a.	–	(100,000)	n.a.	n.a.	2.9	n.a.	n.a.	n.a.	n.a.	Sukeno et al. 1972	10.1021/bi00758a026

<sup>a</sup>Theoretical molecular weight of a protein monomer derived from the amino-acid sequence. Numbers in soft brackets refer to the experimentally determined molecular weight by SDS-PAGE and is given when the sequence is not available.

<sup>b</sup>Italicized values were derived estimates calculated from the data reported in the original reference

<sup>c</sup>n.a., information not available

<sup>d</sup>Activity confirmed but substrate saturation not reached, which prevented deduction of the catalytic constants

<sup>e</sup>Substrate inhibition was observed and the values are estimates.

<sup>f</sup>The derived values assume that the  $k_{cat}$  value is  $2.95 \cdot 10^3 \mu\text{mol} \mu\text{g}^{-1} \text{min}^{-1}$ , and not  $2.95 \cdot 10^3 \mu\text{mol} \text{min} \mu\text{g}^{-1}$  as given in the original reference

**Table S2. Data collection, phasing and refinement statistics**

<b>Data collection<sup>a</sup></b>	
Synchrotron, beamline	Diamond Light Source, I03
Wavelength (Å)	0.826561
Space group / mol per a.s.u.	$P2_12_12_1$ / 3 (one homotrimer)
Cell dimensions: <i>a</i> , <i>b</i> , <i>c</i> (Å), $\alpha$ , $\beta$ , $\gamma$ (°)	102.14, 162.45, 168.18, 90, 90, 90
Resolution (Å), nominal	49.15–2.20 (2.30–2.20)
Unique reflections	141664 (17459)
$R_{\text{sym}}$	0.107 (1.865)
$I / \sigma I$	11.9 (1.3)
Completeness (%)	99.7 (99.4)
Redundancy	13.3 (12.6)
CC(1/2) <sup>b</sup>	99.9 (76.8)
Wilson <i>B</i> factor (Å <sup>2</sup> )	45.16
<b>Refinement</b>	
Resolution (Å)	48.87–2.20 (2.28–2.20)
Completeness	99.64 (99.39)
No. reflections work	141605 (13961)
No. reflections free	2012 (197)
$R_{\text{work}}$	0.203 (0.385)
$R_{\text{free}}$	0.227 (0.401)
N <sup>o</sup> . non-hydrogen atoms: all, protein, water	13299, 13134, 165
N <sup>o</sup> . protein residues, all chains	1662
Missing residues chain A, B, C	41, 38, 41
Mean <i>B</i> factors protein, water (Å <sup>2</sup> )	56.9, 52.0
R.m.s deviation bond lengths (Å), bond angles (°)	0.008, 0.89
Ramachandran, MolProbity: allowed, favored, outliers (%)	99.94, 97.14, 0.06
PDB ID	7BOB

<sup>a</sup> Statistics for outer-shell reflections are given in parentheses.

<sup>b</sup> Percentage of correlation between intensities from random half-datasets as given by XSCALE. Values given represent correlations significant at the 0.1% level.<sup>48</sup>