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Supporting information for article:

**Structure of a C1/C4-oxidizing AA9 lytic polysaccharide
monooxygenase from the thermophilic fungus *Malbranchea
cinnamomea***

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Table S1 Comparison of McAA9F to other structurally determined AA9 enzymes. The list of AA9 enzymes, structurally aligned to McAA9F using the Dali server, is ordered according to the shown root mean square deviation (RMSD) value and the structure-based sequence identity. The three-residue motif facilitating the formation of the succinimide in McAA9F is shown along with the corresponding motifs in other AA9 LPMOs.

Organism	Enzyme	PDB accession	RMSD (Å)	Identity (%)	Motif
<i>Malbranchea cinnamonea</i>	McAA9F	7ntl	/	/	ADG
<i>Thermoascus aurantiacus</i>	TaAA9A	2yet	1.1	54	IDG
<i>Aspergillus fumigatus</i>	AfAA9B	6h1z	1.2	55	ADG
<i>Trichoderma reesei</i>	HjAA9A	5o2w	1.2	52	ING
<i>Trichoderma reesei</i>	HjAA9B	2vtc	1.4	46	ING
<i>Neurospora crassa</i>	NcAA9M	4eis	1.5	40	IGG
<i>Heterobasidion irregulare</i>	HiAA9B	5nns	1.6	40	LAG
<i>Collariella virescens</i>	CvAA9A	5nlt	1.6	35	VNG
<i>Neurospora crassa</i>	NcAA9A	5foh	1.6	33	ADG
<i>Neurospora crassa</i>	NcAA9C	4d7u	1.7	35	VNG
<i>Thermothielavioides terrestris</i>	TtAA9E	3eii	1.8	35	NDG
<i>Neurospora crassa</i>	NcAA9D	4eir	1.8	33	VNG
<i>Neurospora crassa</i>	NcAA9F	4qi8	1.8	32	ANS
<i>Lentinus similis</i>	LsAA9B	6rs6	1.8	29	VNG
<i>Lentinus similis</i>	LsAA9A	5acf	1.9	33	VNG
<i>Thermothelomyces thermophilus</i>	MtPMO3	5ufv	2.1	34	IAG
<i>Phanerochaete chrysosporium</i>	PcAA9D	4b5q	2.2	31	PSG

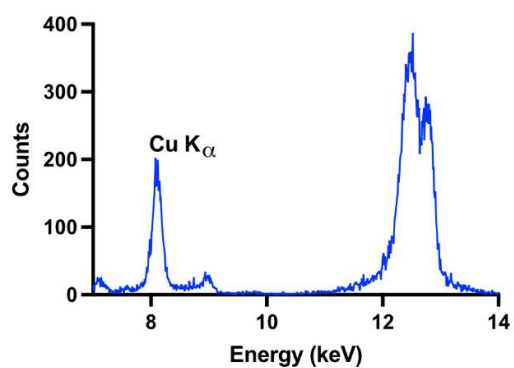


Figure S1 Energy scan of the *McAA9F* crystal. A peak corresponding to the copper K_{α} absorption edge was observed.

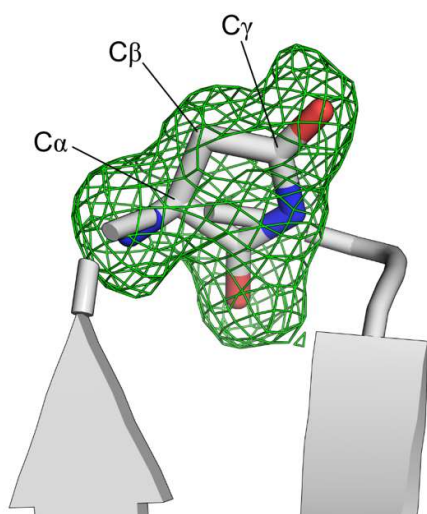


Figure S2 Succinimide observed in place of Asp10 in *McAA9F*. Electron density calculated in the form of a polder map (Liebschner *et al.*, 2017) where the succinimide was omitted is displayed around the succinimide and contoured at 3σ .

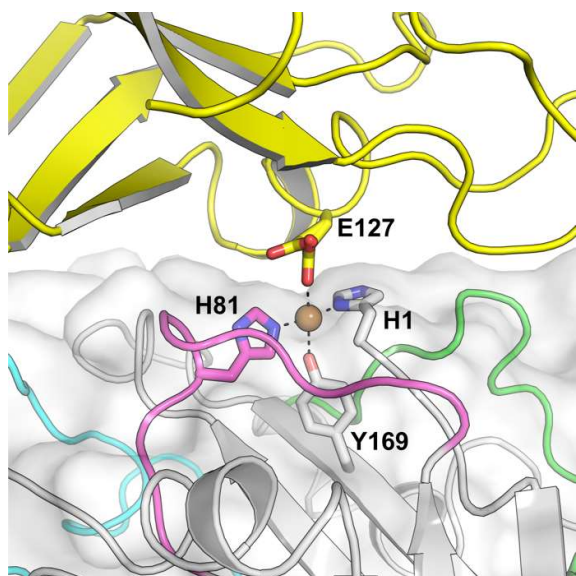


Figure S3 Crystal packing at the substrate binding face in *McAA9F*. Crystal contacts between a symmetry related molecule (yellow) and the substrate binding face of *McAA9F* (coloured as in Figure 3 with the loops L2, L3, and LC coloured green, magenta, and cyan).

Figure S4 Structure-based sequence alignment of AA9 LPMOs. The sequences of AA9 enzymes biochemically characterized but lacking a structure were aligned with Promals3D to the structure-based alignment of AA9 LPMOs with known structures obtained from Dali. Entries with a structure are noted with a pdb accession. The sequence numbering refers to McAA9F. Fully conserved residues are shown in white on a red background, blue frames indicate residues with similar physicochemical properties. The typical loop regions of LPMO, named L2, L3, LS, L8 and LC, are marked with blue, cyan, green, yellow and orange respectively. The conserved copper-binding residues are indicated by a red arrow below the alignment. Sequences are listed with the name assigned to the corresponding protein, and the PDB accession code is also written for structurally determined AA9 LPMOs. The sequences shown are from *M. Cinnamomea* (Mc), *Podospora anserina* (Pa), *T. reesei* (Hj), *Neurospora crassa* (Nc), *Heterobasidion irregulare* (Hi), *L. similis* (Ls), *Phanerochaete chrysosporium* (Pc), *T. aurantiacus* (Ta), *Myceliophthora thermophila* (Mt), *Gloeophyllum trabeum* (Gt), *Pestalotiopsis sp. NCi6* (Ps), *A. fumigatus* (Af), *Heterobasidion irregulare* (Hi), *Thielavia terrestris* (Tt), *Aspergillus nidulans* (An), and *C. virescens* (Cv).

Reference

Liebschner, D., Afonine, P. V., Moriarty, N. W., Poon, B. K., Sobolev, O. V., Terwilliger, T. C., Adams, P. D. (2017). *Acta Cryst D* **73**, 148-157.