Supporting Information

Molecular Recognition of Methyl α-D-Mannopyranoside by Antifreeze (Glyco)Proteins

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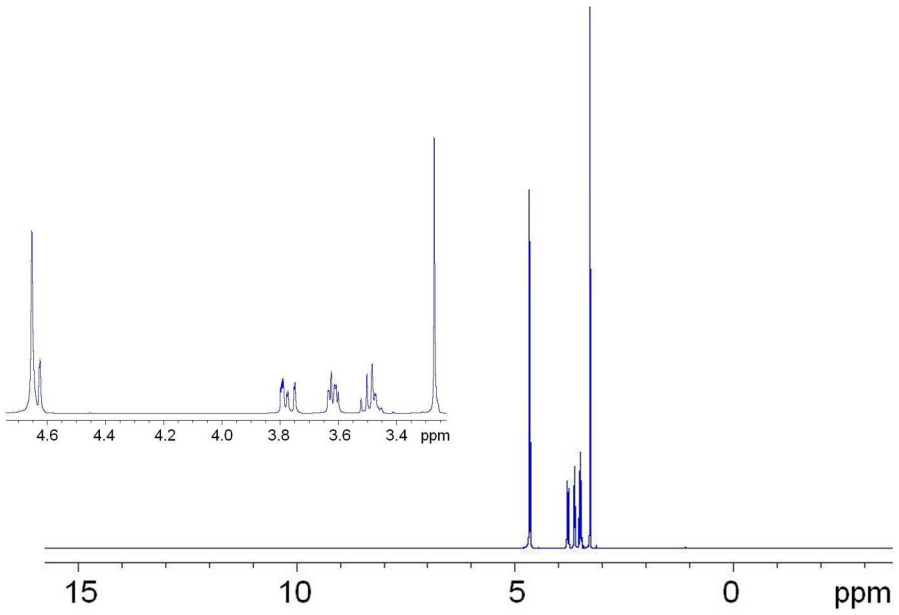

Figure S1. ^{1}H NMR spectrum of MDM in D_2O (500 MHz).

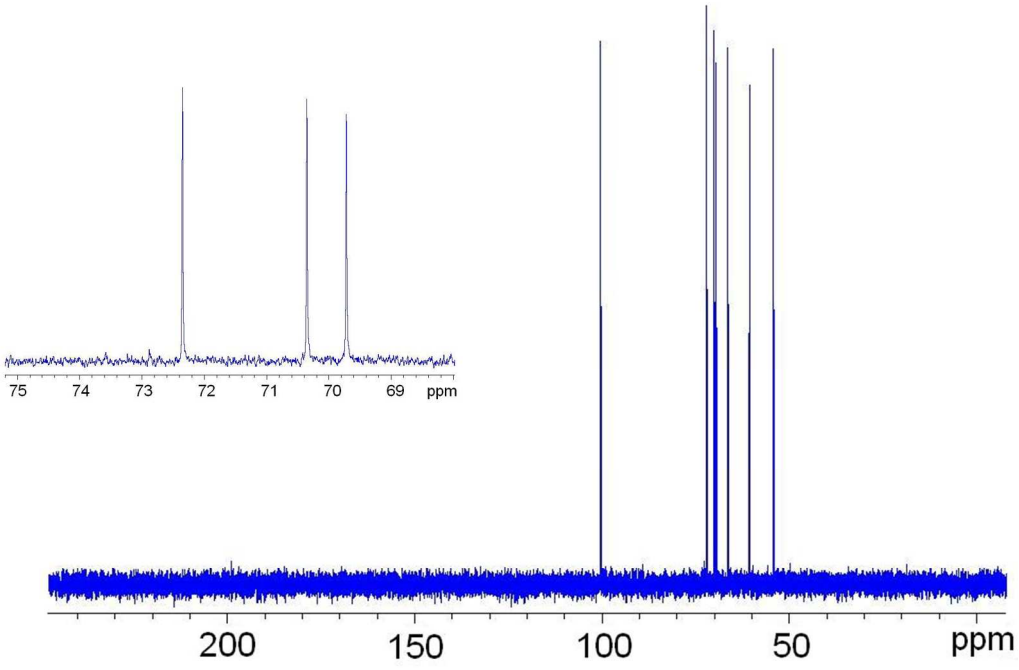

Figure S2. ^{13}C NMR spectrum of MDM in D_2O (125.8 MHz).

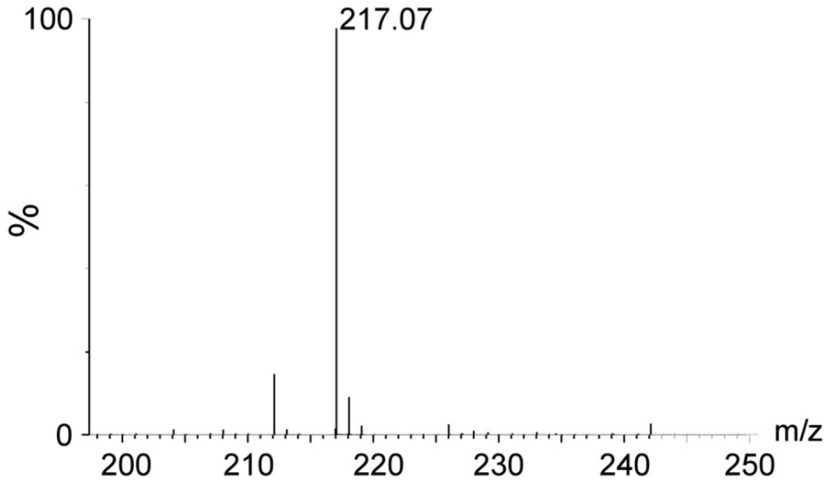

Figure S3. LC-MS spectrum of MDM. Calculated mass for $C_7H_{14}O_6Na$ is 217.07 and observed mass is 217.07.

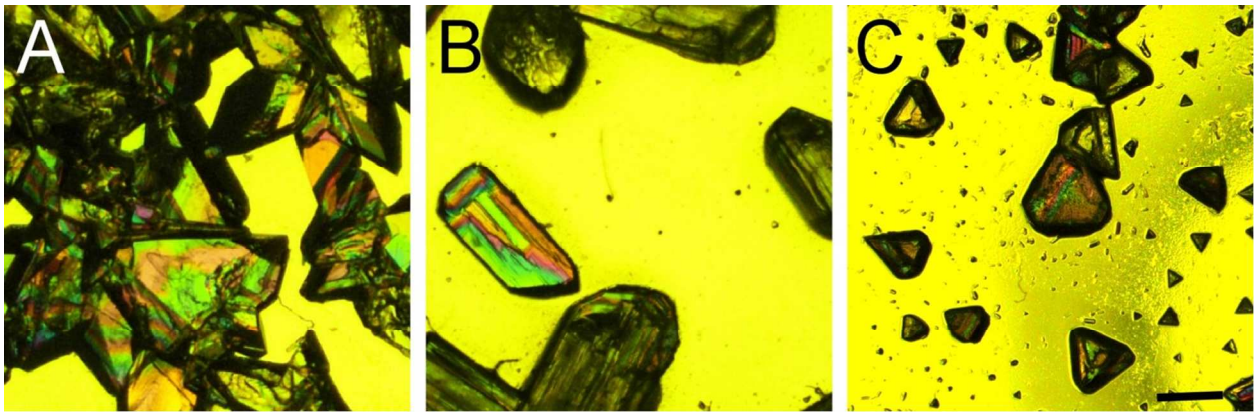

Figure S4. Optical micrographs of the MDM crystals obtained in the presence of the seed MDM crystals and (A) AFGP8, (B) AFGP1-5, and (C) DAFP1. The length of the scale bar, 1 mm, is the same in all the panels.

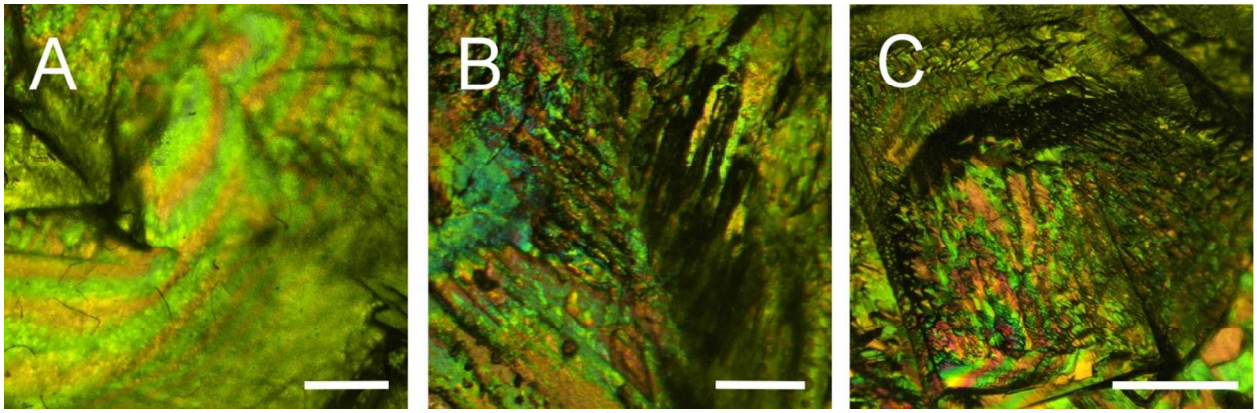

Figure S5. Optical micrographs of the MDM crystals obtained in the presence of the controls: (A) Gal1-β-3GalNAc, (B) denatured DAFP1, (C) LCA. The length of the scale bar is 1 mm.

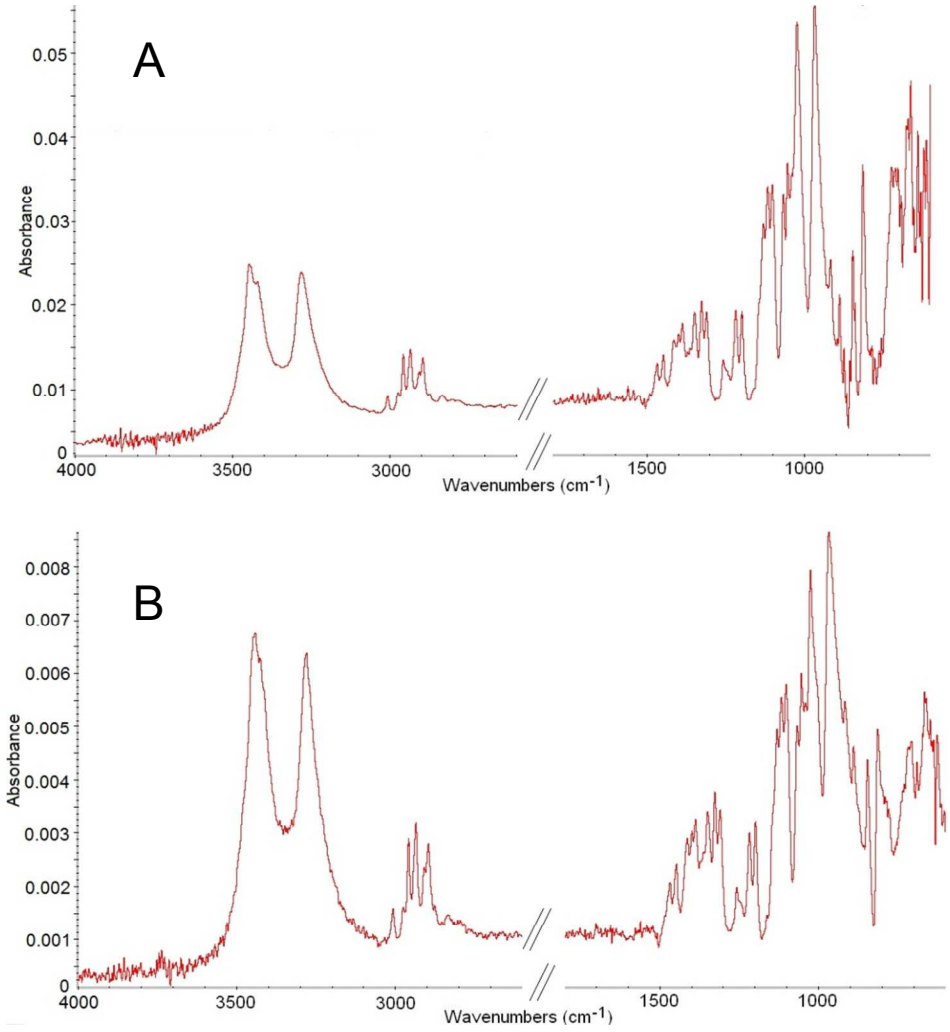

Figure S6. Representative ATR-FTIR spectra of the MDM crystals in the absence and presence of AF(G)Ps. The ATR-FTIR spectra of MDM crystals in the absence of AF(G)Ps (A) and in the presence of DAFP1 (B).

Table S1. Sample results of methyl α-D-mannopyranoside (MDM) crystal growth in the presence of additives.

Sample[a]	Polypeptide concentration (μM)	Induction time (day)[b]	Complete time (day)[b]	Twin defects (%)[c]
MDM	0	12	14	> 75%
MDM/denatured DAFP1	170.0	12	14	> 75%
MDM + LCA	275.4	12	14	> 75%
MDM + Gal1-β-3GalNAc	408.0	12	14	> 75%
MDM + DAFP1	14.0	12	17	< 5%
MDM + DAFP1	0.15	12	16	< 5%
MDM + AFGP1-5	1.89	12	15	< 15%
MDM + AFGP1-5	1.00	12	14.5	< 15%
MDM + AFGP8	170.0	12	14	< 40%
MDM + AFGP8	112.2	12	14	< 40%

[a] Each sample contained 510 mM MDM on day 1. Results of each MDM alone and in the presence of each of the three control compounds, the denatured DAFP1, *Lens culinaris* lectin (LCA), and 2-acetamido-2-deoxy-O-(β-D-galactopyranosyl)-D-galactose (Gal1-β-3GalNAc) are listed for comparison. [b] The day the first solid was observed. Complete means no more weight loss from the vial. Time errors are less than 8 hours. [c] The identity and quality of single crystals were examined using polarized microscope and single crystal x-ray diffraction. The estimated percentages of crystals with twin defects are listed.