

Supplementary Figure 2

A

Global: Needleman-Wunsch Protein alignment [Matrix: "BLOSUM55" Gap penalty: 10 Gap extension penalty: 1]
 BoGH13A_{FL}-GH13 only 1-448
 SusG-GH13 only 1-511
 %Identity 20.8% %Similar 37.2% %Gaps 29.7% Identical 116 Similar 208 Gap Count 27 Gap Length 160 Score 400 Length 557

BoGH13A_{FL}-GH13 only 316 V I Y E L L R D E T S S G N L A G A M E K L P Y L K E L G I D A I E L M P V Q E F A G N D S W . G Y N T G L Y F A L D A S Y G T Q N E Y K A F I D A C 390
 SusG-GH13 only 62 I S Y C L L L Y S R A D S O G D G Y G O L N G V T O K E D Y L N L G V K A L W L S R I H P C M S Y H G V D V T D Y T K V N P O L G T E S D F R L V T E A 139

BoGH13A_{FL}-GH13 only 391 H O N G I A V I F D V Y N H T N N D N P F A R M Y W D T F N N R P S T K N P W L N A V T P H Q K Y V 441
 SusG-GH13 only 140 H N R G I K I Y L D Y M N H T G T A H W F T E A S S S E S P Y R N Y . S F S E D P K T D I A A G K I A M I T O E G A A G Y N A A E F Q V S D E T G Q I T 339
 CBM58

BoGH13A_{FL}-GH13 only 442 F S P D D F N H T S E Q T A F V K R N L K Y L L D T Y H I D G F R F P T K G F T Q K O T T G D D L A A T D F A R 500
 SusG-GH13 only 340 Y F H S H E C T D W F A D L N Y G P V D Q A G E S P A Y Q A I A D A A K G W I A R G V D G L R L D A V K H I Y H S E T S E E N R 403

BoGH13A_{FL}-GH13 only 501 V S V L K E Y E A V K V Y K E D A M V T M H F C A N E E T T L A T E G I H F W R N M N H S Y C S A M G W K D N S D F S G L 564
 SusG-GH13 only 404 . R F L K M F Y E D M N A Y Y K Q G H T D D F Y M I G E V L S E Y D K V A P Y Y K L P A L F E F S E W Y R L E W G I N N S T G C Y F A K D I L S Y O O K 480

BoGH13A_{FL}-GH13 only 565 Y D T T R P N O F V G M E S H E E R C A Y K Q I E Y E N G A L K T N S E R L K O L S S N A A F F T V P S P K M L W O F G E M Y D I S I D E N G 640
 SusG-GH13 only 481 Y A N Y R S D Y I E A T K L S N H E D R T S S K L G K S A D K C K L A A A V L L T S A G H P Y I Y G E E L G L Y G T K D N G D 545

BoGH13A_{FL}-GH13 only 641 R T G K K R V L W E Y Q T E R K S L V D I Y T K L I T L R T H S D L F N A S S O F T W K V S Y N D W D N G R T L 697
 SusG-GH13 only 546 E Y V R S R M L W G D S Y T T N Y T D K T D A T V S K N V K T V A D Q G A D T H S L N I Y F S L T R L R N T Y P A L A E G N M T K H S V Y N E S Q E K D Y K 624

BoGH13A_{FL}-GH13 only 698 T L K A V N G K Q L H V Y A N E T N A S I D Y T I P E G T W Y L Y L E N G N P V E G E K K I S V P A H E F R L Y T N F A E 758
 SusG-GH13 only 625 P I A A W Y M T K D N E K L L V I H N E G G T A M O L P L T D K I E K V L F V N G E T Q O N T D S D S Y T L K E G G V A S V V F K L G N 692

B

Global: Needleman-Wunsch Protein alignment [Matrix: "BLOSUM40" Gap penalty: 10 Gap extension penalty: 1]
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 SusG-FL 1-692
 %Identity 21.1% %Similar 37.1% %Gaps 35.4% Identical 186 Similar 327 Gap Count 66 Gap Length 312 Score 577 Length 881

BoGH13A_{FL}-FL 1 M K D F K Y I W L L L L I L N S R . G A C S D D O L M P G E R P S S G T D P A P E E Q V L H D G F N F D P A I P K A D E P L T I T F K A R . E G S N F Y G Y 78
 SusG-FL 1 M N K H L H F L S L W L S M L M A R M T A C S D D K N I T D P A P E P E F R V E G 42

BoGH13A_{FL}-FL 79 A D D L Y L H S G T G A N W T G A R . T W G D N Q N K Y R L K K T K D N V S I T I S S I R H F Y S V A P S T P L O T I N L I V R D A E S Q O T Y D Y A 155
 SusG-FL 43 O W T A L T A S R D T W D E T K R A D I S Y Q L L E Y S F A D S D G D G Y G D L N G V T Q K L D Y L 92

BoGH13A_{FL}-FL 156 T L V E D S Q N G F I W E E P Q K A P L P I S G E E K E G I H I S A T S I M L V L Y D K . D S Q G G H K D C V F V T G N F N W K L D S R Y M M 277
 SusG-FL 93 N Q L G V K A L W L S R I H P C M S Y H G Y D V T D Y T K V N P O L G T E S D F R L V T E A H N R G I K I Y L D Y V M 152

BoGH13A_{FL}-FL 278 K Y D E T N H C W I I T E L T A G E T O F Q Y F Y S A S D G G Y T L C D P Y C E A L E K G V D T N F P T A Q A P Y S V V 293
 SusG-FL 153 N H T Q T A H P W F T E A S S S E S P Y R N Y . Y S F E E D P K T D I A A G K . I A M I T O E G A A G Y N A A E W F Q V S D E T A A V K G L L K 223

BoGH13A_{FL}-FL 294 E T N R P Q Y G W S A G E F E M K N K E R V I Y E L L R D E T S S G N L A G A M E K L P Y L K E I D A I E L M P V Q E F A 358
 SusG-FL 224 F T L D W S N A P S R I L V V S T G T K A E D N P D T G T D N A K Y L Y G E D I C K K E Y D K G N N I Y E L T V D E 283

BoGH13A_{FL}-FL 359 G N D S W G Y N T G L Y F A L D A S Y G T Q N E Y K A F I D A C H Q N G I A V I F D V Y N H T N N D N P F A R M Y W D T F N N R P S T K N P W L 431
 SusG-FL 284 . E S T W G L I R T S N A S F W P S G T K Y G A S S S E K L A L N K E F K L E N A G N P . A N I M F S Q O I T Y F H S H F C T D W F 350

BoGH13A_{FL}-FL 432 N A V T P H Q K Y V F S P D D F N H T S E Q T A F V K R N L K Y L L D T Y H I D G F R F P T K G F T Q K O T T G D D L A A T D F A R V S L K E Y E A 510
 SusG-FL 351 A D L N Y G R V D Q A G E S R . A Y G A I A D A A K G W I A R G V D G L R L D A V K H I Y H S E T S E E N R F L K M F Y E D 412

BoGH13A_{FL}-FL 511 V K A V K E D A M V T M H F C A N E E T T L A T E G I H F W R N M N H S Y C S A M G W K D N S D F S G L Y D T T R P N Q F 573
 SusG-FL 413 M N Y Y Y K Q G H T D D F Y M I G E V L S E Y D K V A P Y Y K L P A L F E F S E W Y R L E W G I N N S T G C Y F A K D I L S Y O O K M A N Y R S D Y I E 490

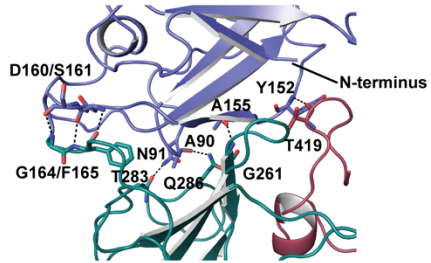
BoGH13A_{FL}-FL 574 V G Y M E S H E E R C A Y K Q I E Y E N G A L K T N S E R L K O L S S N A A F F T V P S . P K M L W O F G E M Y D I S I D E N G R T G K K R V L W 649
 SusG-FL 491 A T K L S N H E D R T S S K L G K S A D K C K L A A A V L L T S A G H P Y I Y G E E L G L Y G T K D N G D E Y V R S P M L W G D 556

BoGH13A_{FL}-FL 650 E Y Q T E R K S L V D I Y T K L I T L R Y T H S D L F N A S S O F T W K V S Y N D W D N 693
 SusG-FL 557 S Y T T N Y T D K T D A T V S K N V K T V A D Q G A D T H S L N I Y F S L T R L R N T Y P A L E G N M T K H S . V Y N E S Q E K D Y K . P I A A W Y M T K D N 635

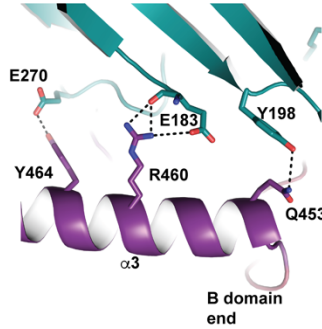
BoGH13A_{FL}-FL 694 G R T E T L K A V N G K O L H V Y A N E T N A S I D Y T I P E G T W Y L Y L E N G N P V E G E K K I S V P A H E F R L Y T N F A E 758
 SusG-FL 636 E K L E V I H N E G G T A M O L P L T D K I E K V L F V N G E T Q O N T D S D S Y T L K E G G V A S V V F K L G N 692

Supplementary Figure 3

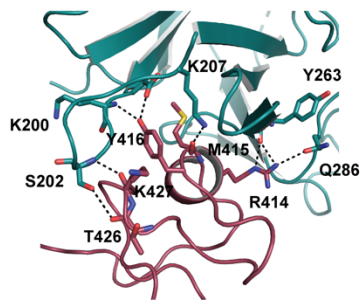
A CBM98, CBM48 and B domain



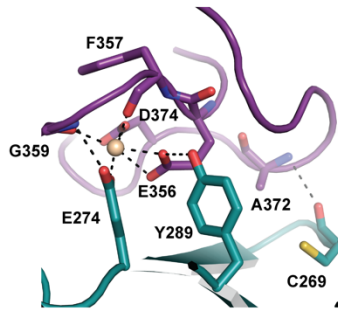
B CBM48 and $\alpha 3$



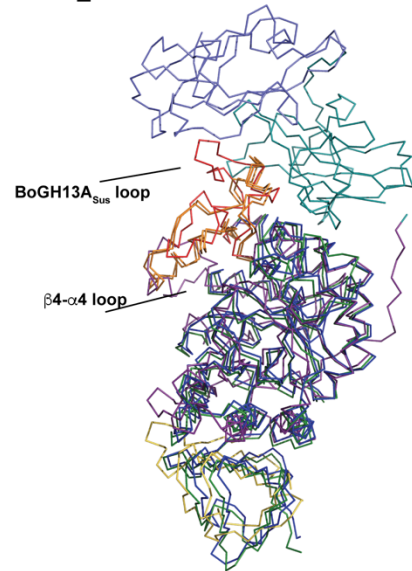
C CBM48 and B domain



D Ca^{2+} Binding

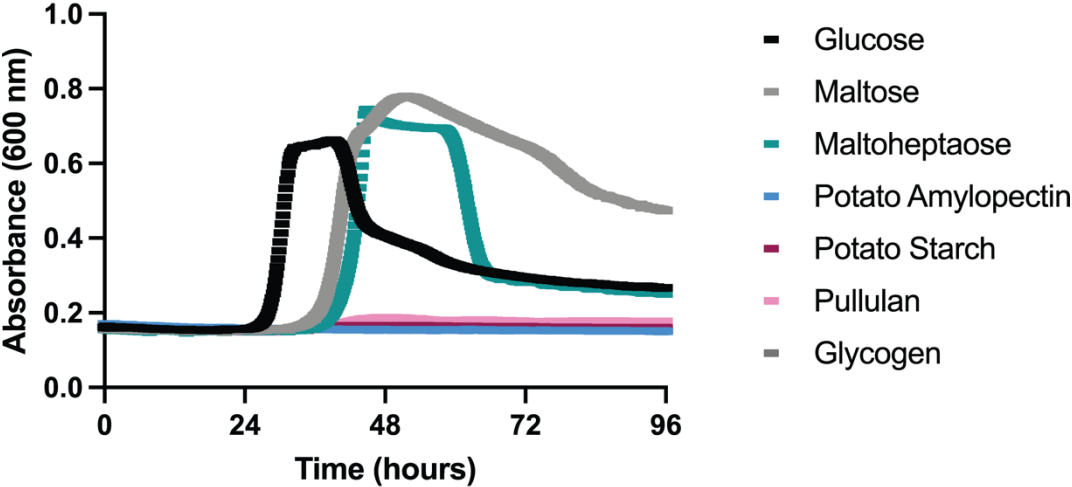


E

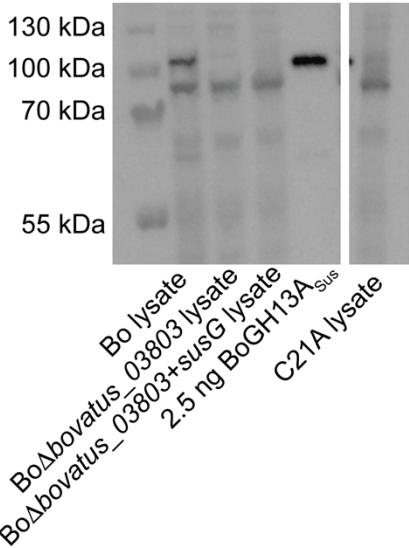


Supplementary Figure 4

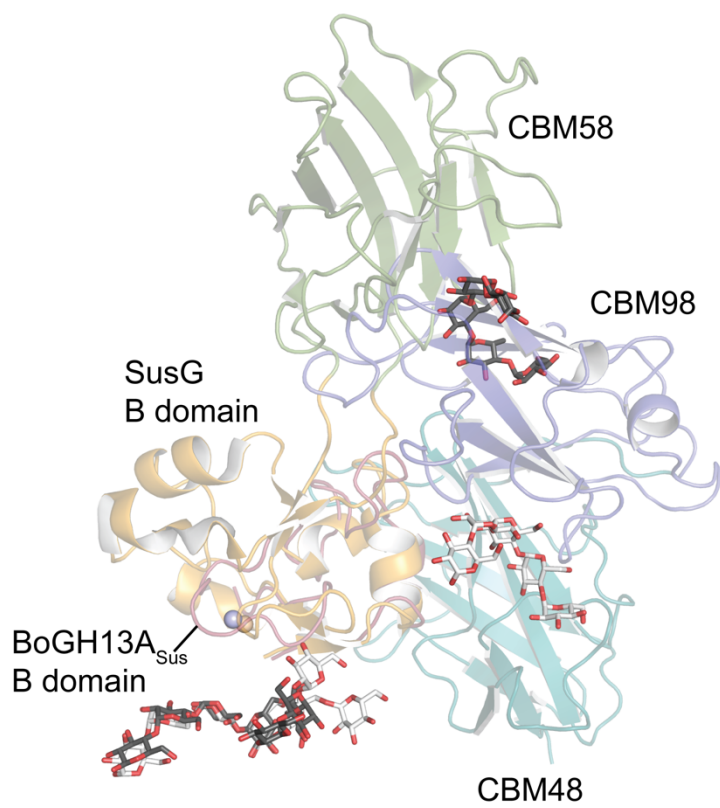
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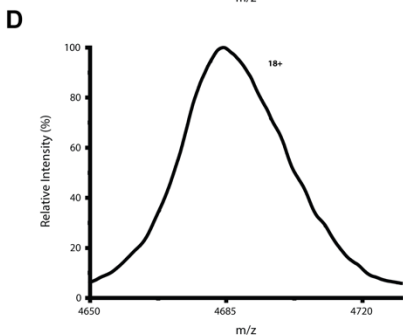
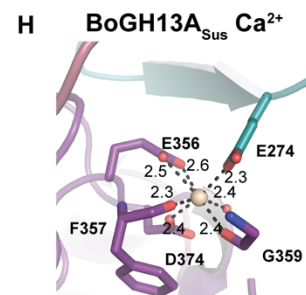
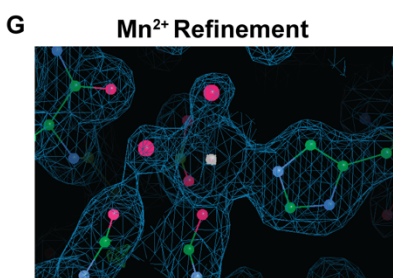
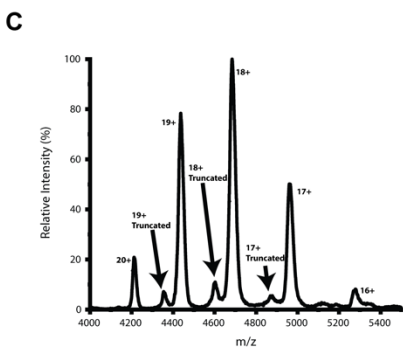
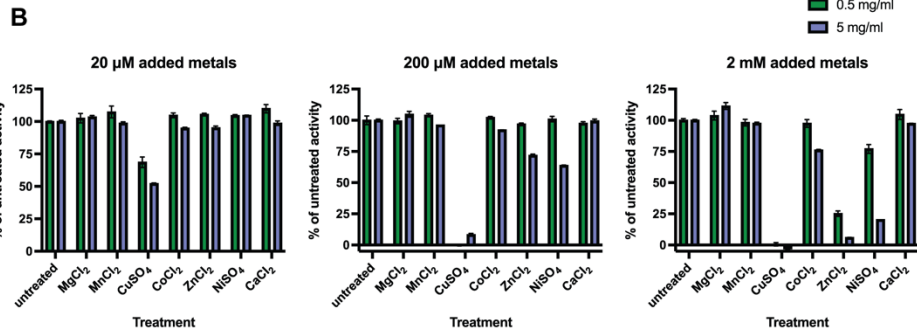
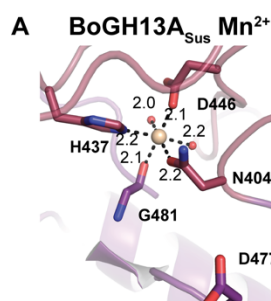
B



Supplementary Figure 5



Supplementary Figure 6



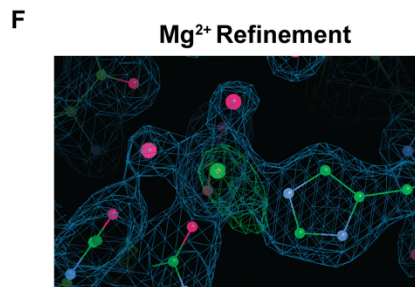
I

ID	Res.	Metal	Occupancy	B factor (e ²) ¹	Ligands	Valence ²	nVECSUM ³	Geometry ^{4,5}	gRMSD ⁶ (°) ¹	Vacancy ⁷	Bidentate	Alt. metal
F-1	CA	Ca	1	25.9 (25.8)	O ₇	2	0.11	Octahedral	9.2°	0	1	
F-2	CA	Ca	1	25.6 (25.4)	O ₇	2	0.17	Octahedral	10.4°	0	1	
F-3	CA	Ca	1	26.8 (25)	O ₇	1.8	0.068	Octahedral	9°	0	1	
F-4	CA	Ca	1	27.4 (23.8)	O ₇	1.9	0.12	Octahedral	10.6°	0	1	
F-5	MN	Mn	1	31.2 (31)	O ₇ N ₁	2.4	0.091	Octahedral	5.1°	0	0	
F-6	MN	Mn	1	33.2 (33.4)	O ₇ N ₁	2	0.067	Octahedral	6.5°	0	0	
F-7	MN	Mn	1	35 (35.2)	O ₇ N ₁	2.1	0.078	Octahedral	4.3°	0	0	
F-8	MN	Mn	1	33.2 (25.8)	O ₇ N ₁	2.2	0.046	Octahedral	6.2°	0	0	

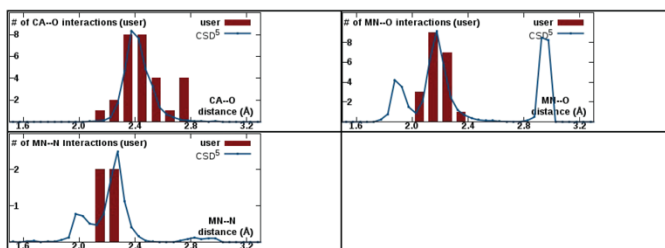
Legend: Not applicable | Outlier | Borderline | Acceptable

E

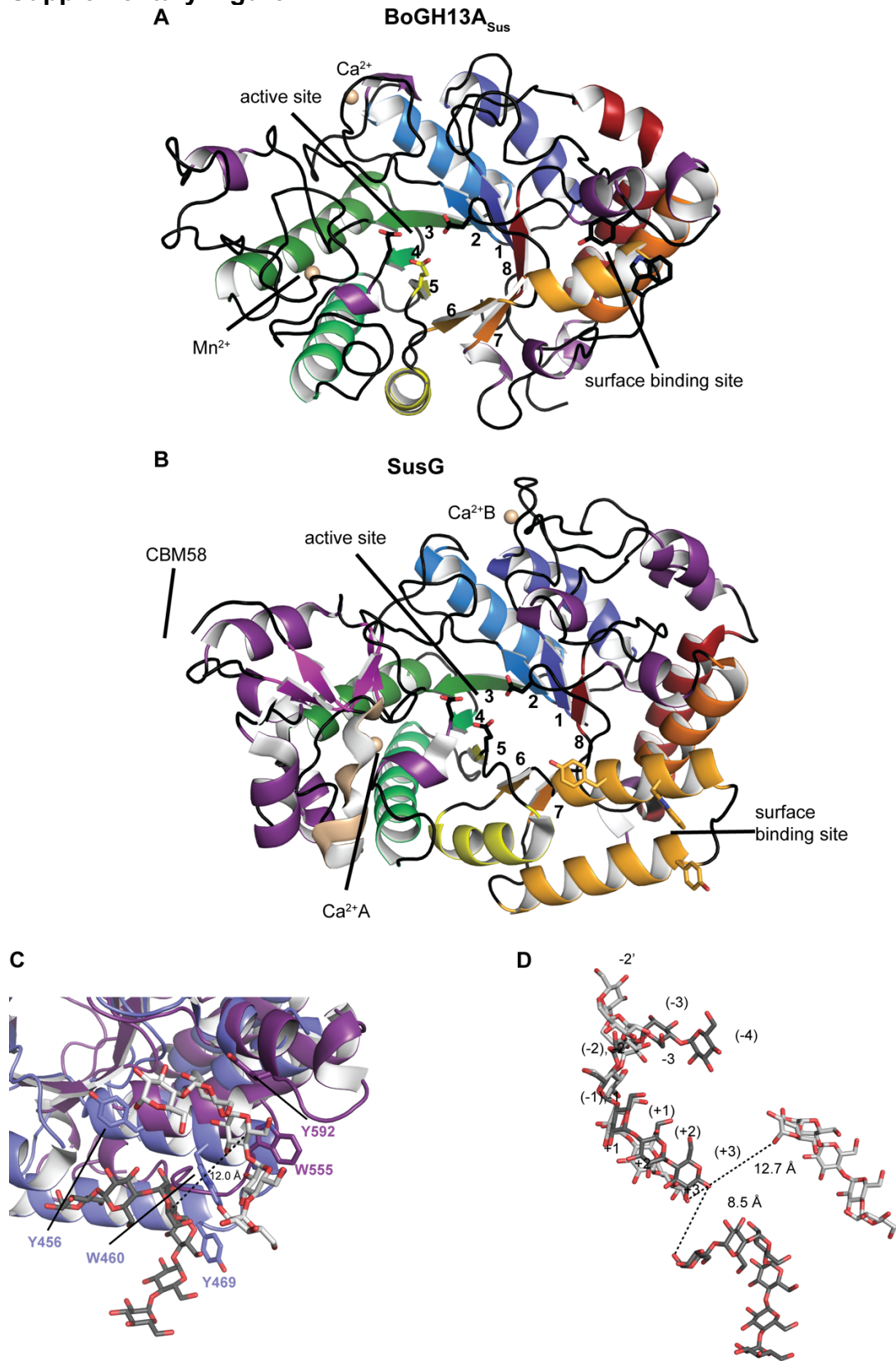
Observed Mass	84123 +/- 4 Da
Expected Mass based on peptide sequence	83975 Da
Observed-Expected (Δ)	148 Da +/- 4 Da
Mass of Calcium ion	40 Da
Mass of 3 Waters	54 Da
Δ-Calcium-3 Waters	54 Da +/- 4 Da
Mass of Manganese Ion	55 Da



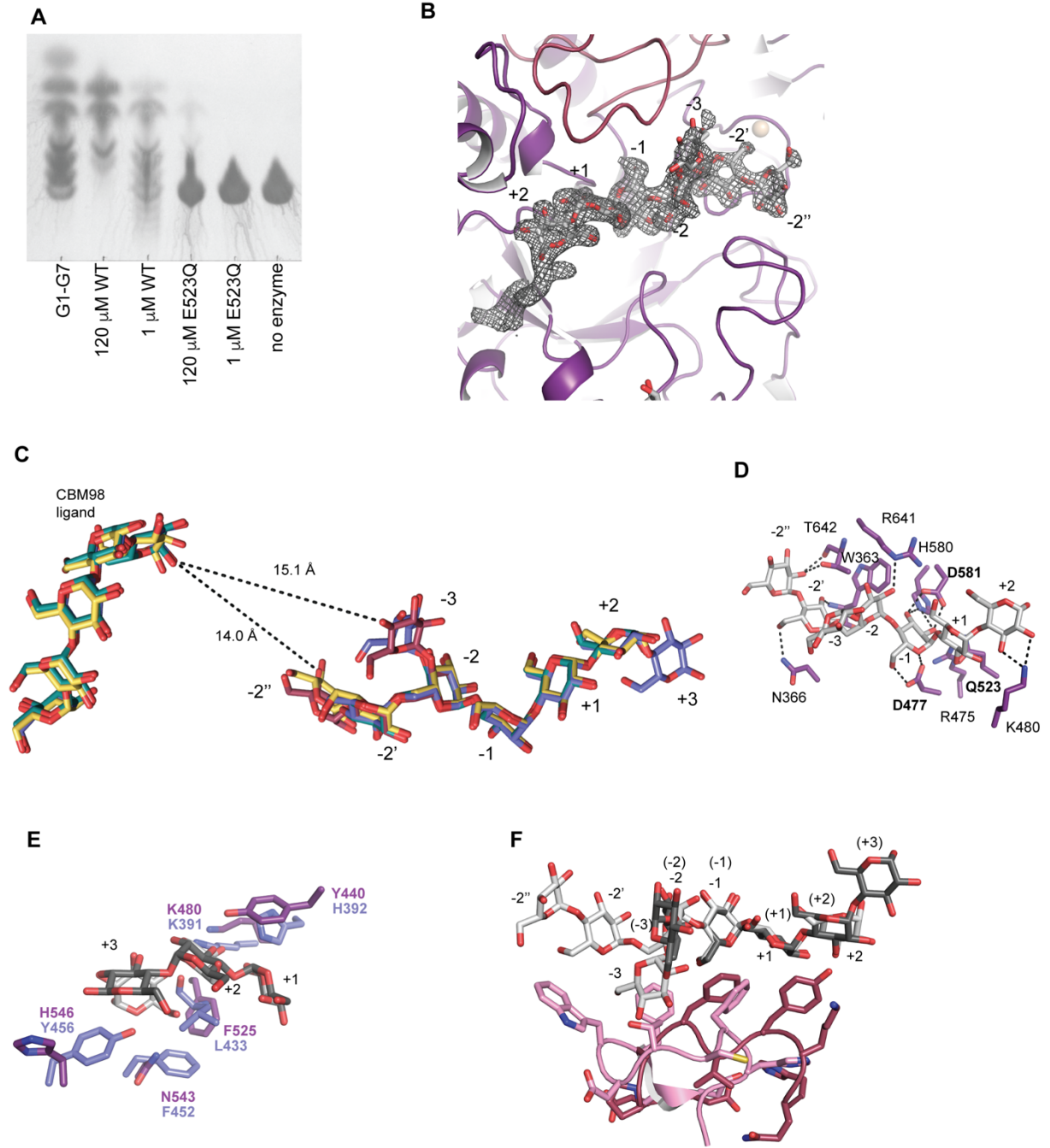
Metal-ligand distance distributions for XYZOUT-job42.pdb in comparison with CSD



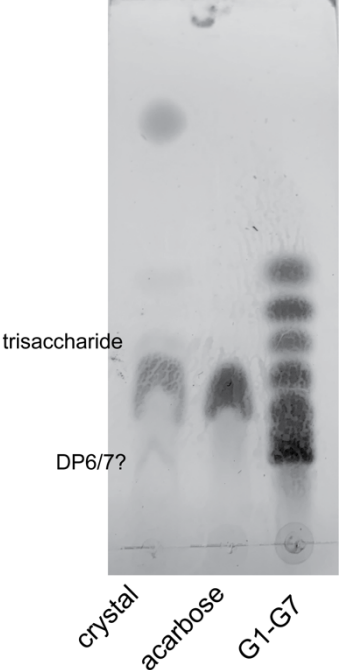
Supplementary Figure 7



Supplementary Figure 8



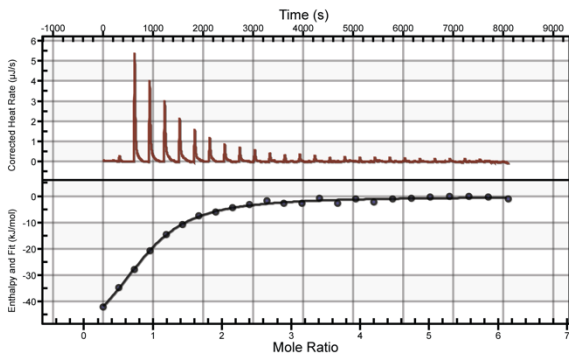
Supplementary Figure 9



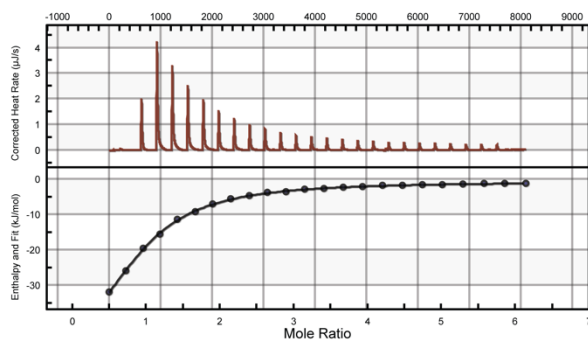
Supplementary Figure 10

CBM98

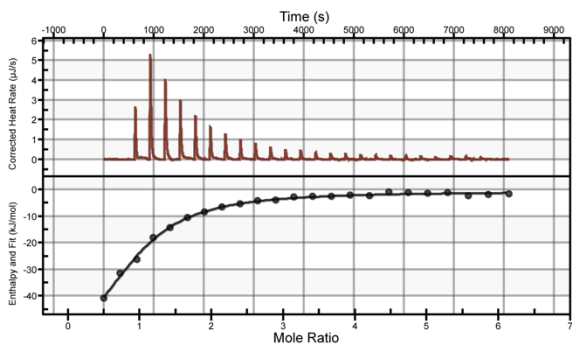
2 mM maltoheptaose



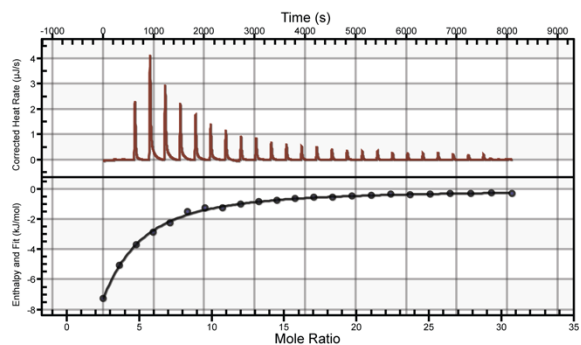
2 mM α -cyclodextrin



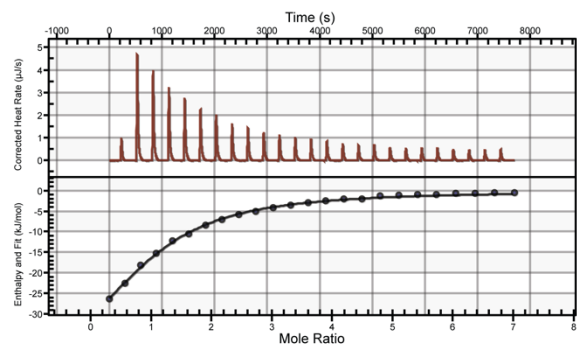
2 mM β -cyclodextrin



10 mM maltotriose



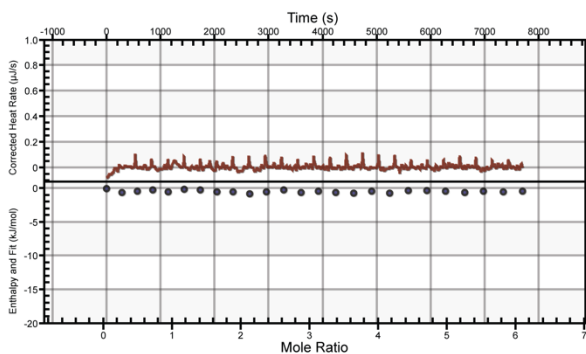
5 mg/ml potato amylopectin



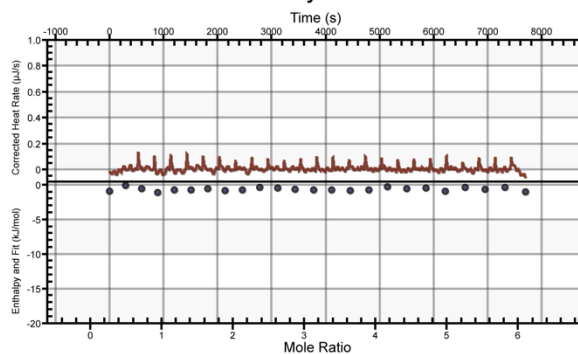
Supplementary Figure 11

CBM98-W92,98A

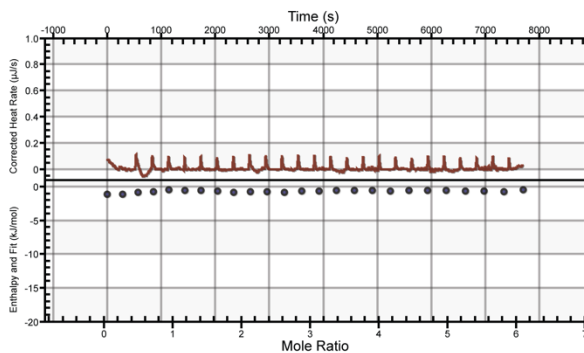
2 mM maltoheptaose



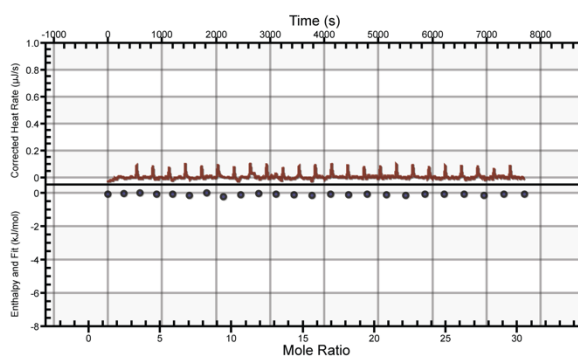
2 mM α -cyclodextrin



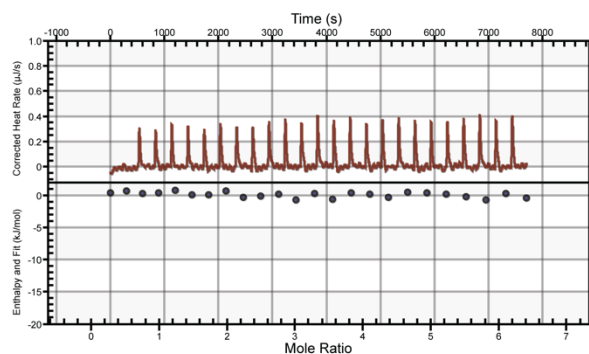
2 mM β -cyclodextrin



10 mM maltotriose



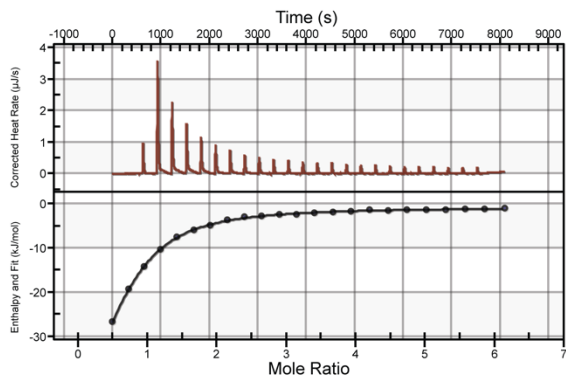
5 mg/ml potato amylopectin



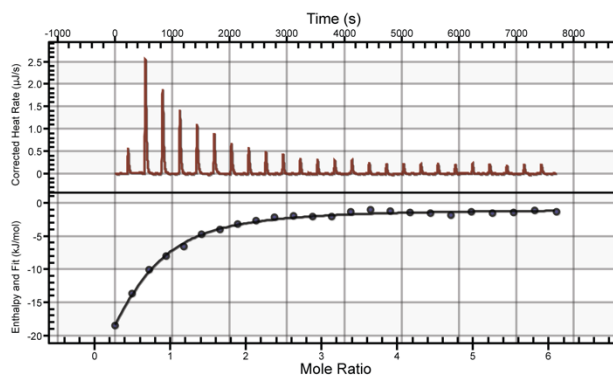
Supplementary Figure 12

CBM98-CBM48

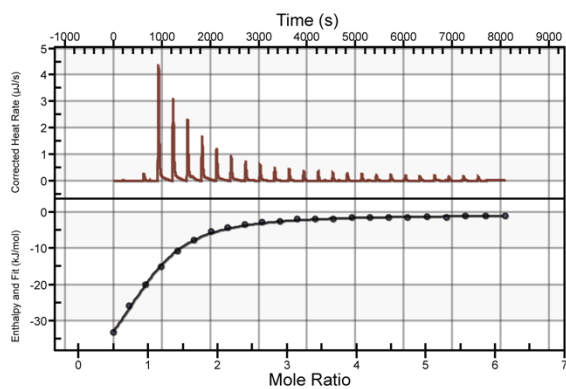
2 mM maltoheptaose



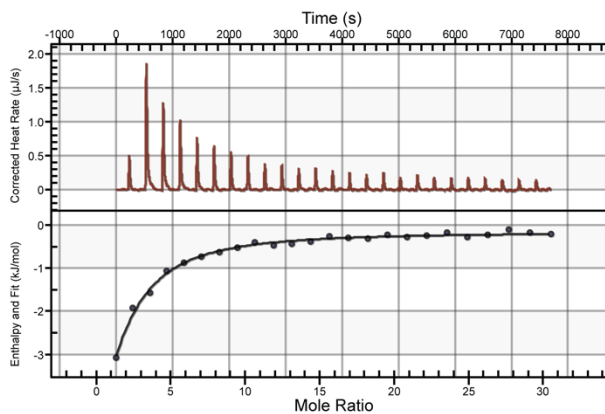
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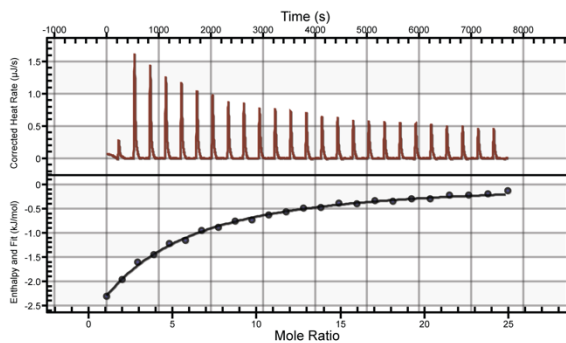
2 mM β -cyclodextrin



10 mM maltotriose



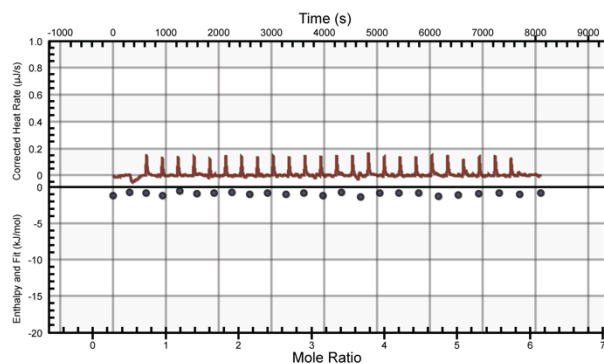
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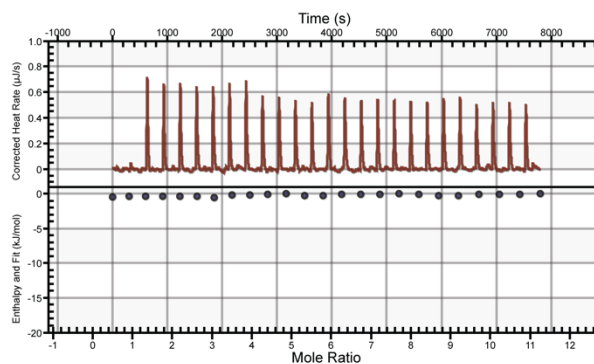
Supplementary Figure 13

CBM98-CBM48-W92,98A

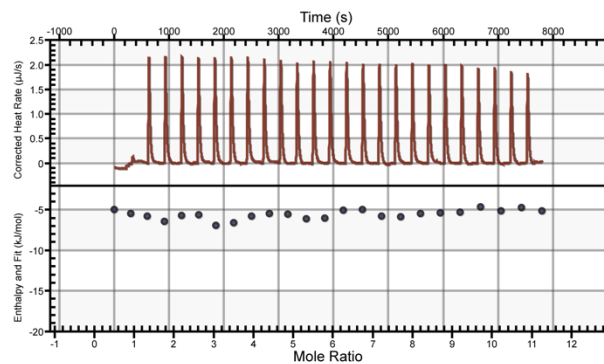
2 mM maltoheptaose



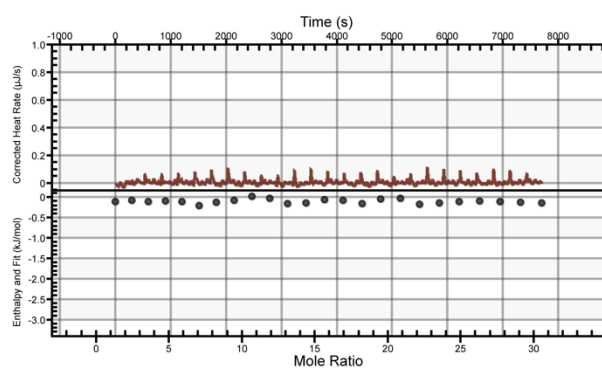
1 mM α -cyclodextrin



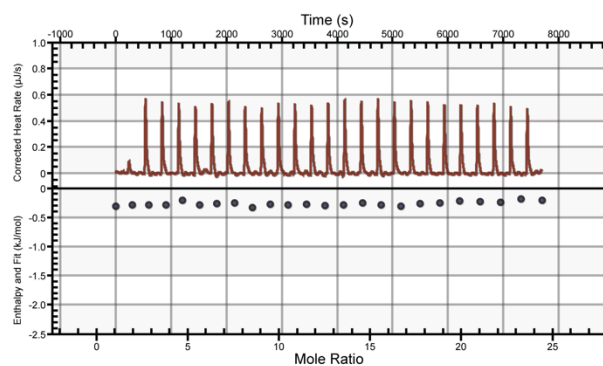
1 mM β -cyclodextrin



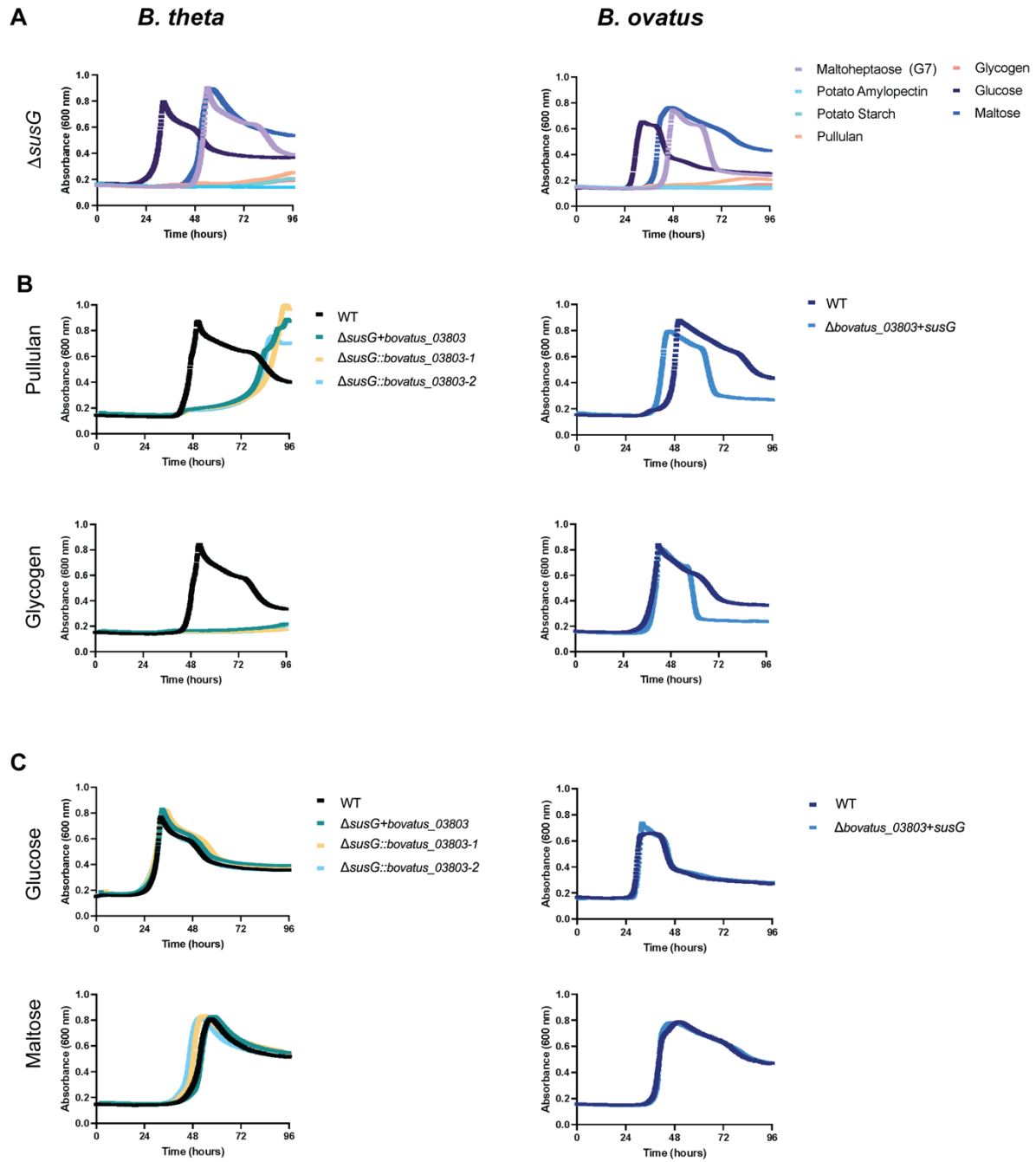
10 mM maltotriose



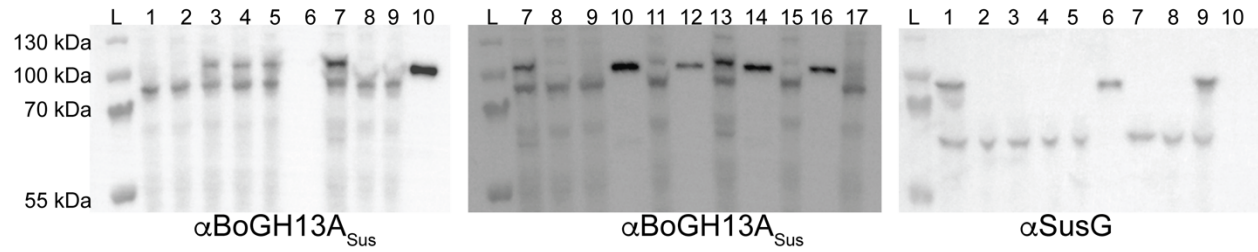
5 mg/ml potato amylopectin



Supplementary Figure 14

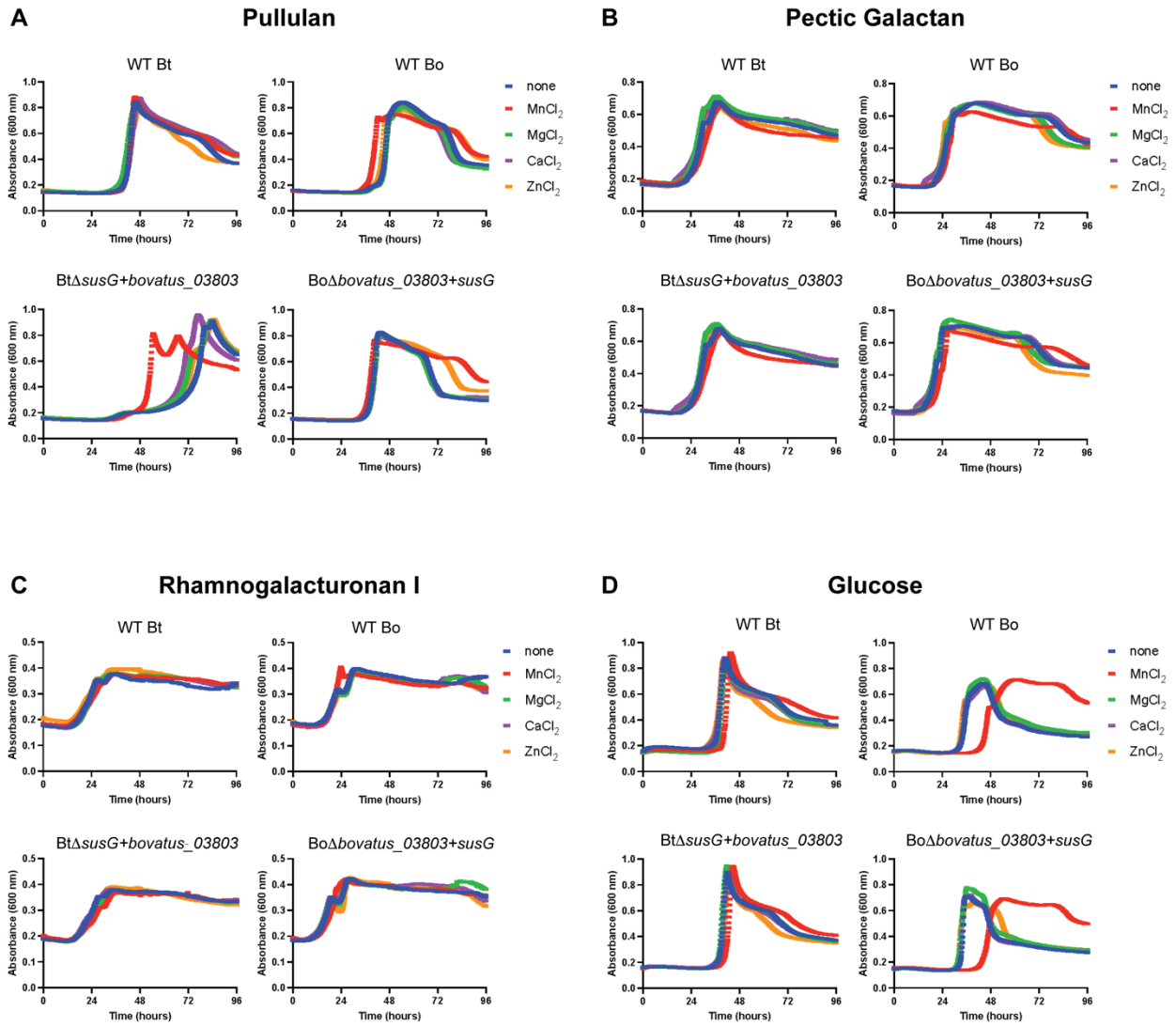


Supplementary Figure 15

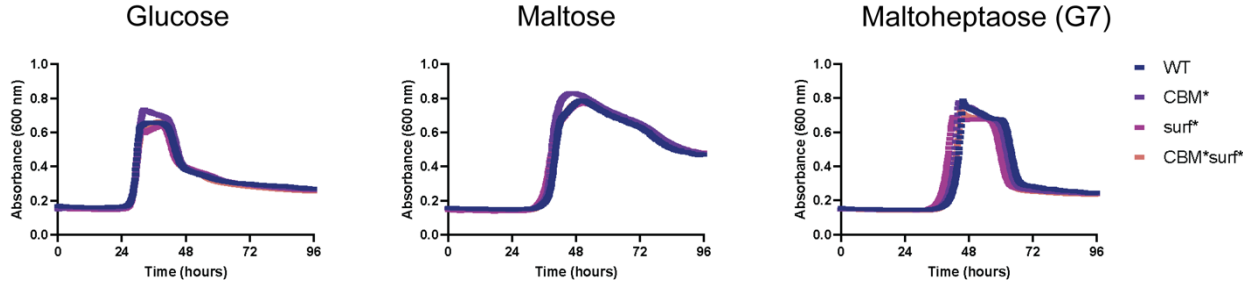


- | | | |
|---|---|-----------------------|
| L - ladder | 7 - Bo lysate | 13 - surf* lysate |
| 1 - Bt lysate | 8 - <i>Bo</i> Δ <i>bovatus_03803</i> lysate | 14 - 2.5 ng surf* |
| 2 - Bt Δ <i>susG</i> lysate | 9 - <i>Bo</i> Δ <i>bovatus_03803+susG</i> lysate | 15 - CBM*surf* lysate |
| 3 - Bt Δ <i>susG+bovatus_03803</i> lysate | 10 - 2.5 ng BoGH13A _{Sus} | 16 - 2.5 ng CBM*surf* |
| 4 - Bt Δ <i>susG::bovatus_03803-1</i> lysate | 11 - CBM* lysate | 17 - C21A lysate |
| 5 - Bt Δ <i>susG::bovatus_03803-2</i> lysate | 12 - 2.5 ng CBM* | |
| 6 - 2.5 ng SusG | | |

Supplementary Figure 16

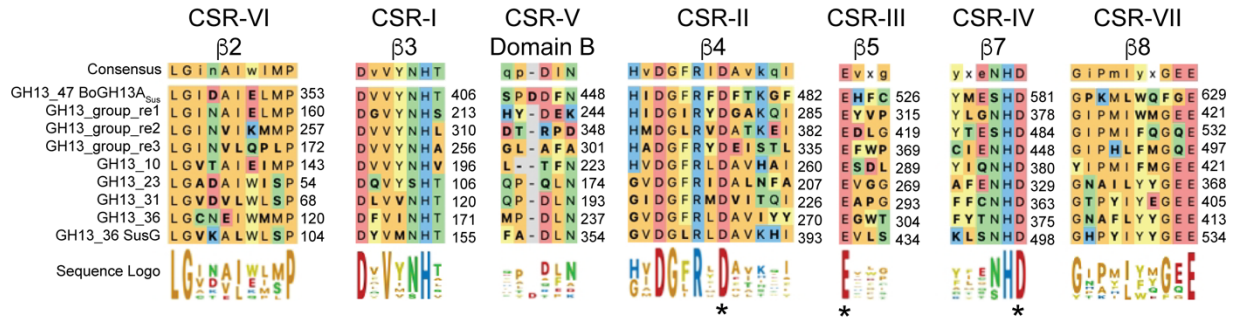


Supplementary Figure 17

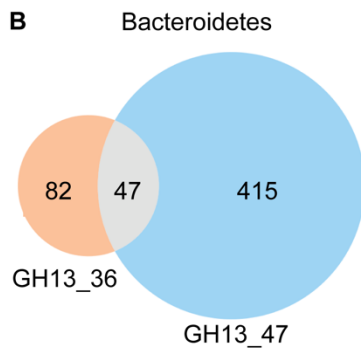


Supplementary Figure 18

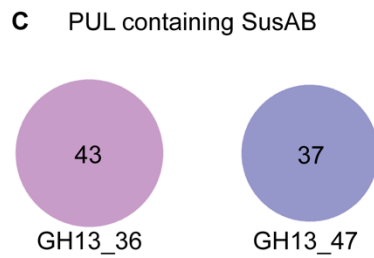
A



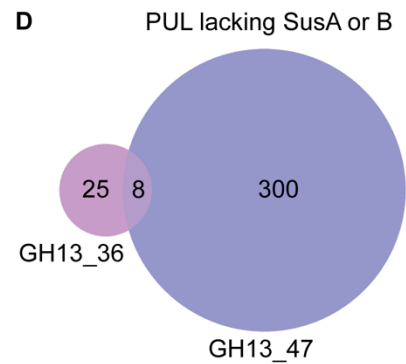
B



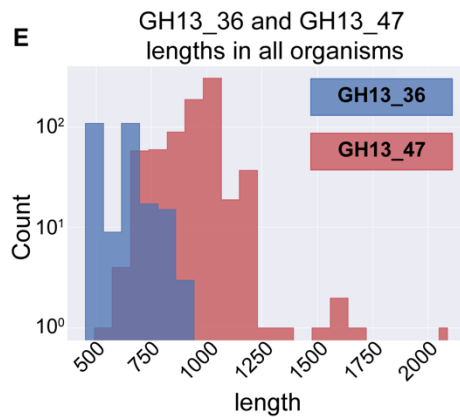
C



D



E



F

