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Structural insight into industrially-relevant glucoamylases: flexible positions of starch-binding domains

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	25	30	40	
AnigerGA A T	D S W L S N	A T V A R T A I L N N I G A D	49
HresinaeGA D	I S S F I A S	R A I A L O G A I L N N I O P D	24
PoxalicumGA	R P D P K G G N	I T P F I H K	E G E R S L Q G I I D N L G G R	31
	50	60	70	80
AnigerGA	G A W V S C A D S G I V V A S P S T D N P D V F Y T W T R D S	80		
HresinaeGA	G S A V P G A G A G F V V A S P S K A N P D V F Y T W S R D S	55		
PoxalicumGA	K K T P G T A A G L F I A S P N T E N P N Y Y Y T W T R D S	62		
	90	100		
AnigerGA	G V L R A T L V L R N G D T S L S T I E N	104		
HresinaeGA	A C T L K M I I D E P I L G N T T F Q T I L E Q	79		
PoxalicumGA	A L T A K C L I D L F E D S R A K F P I D R K Y I E T G L R D	93		
	110	120	130	
AnigerGA	V I S A Q A I V Q G I S N P S G D . L S S G A G L G E P K E N	134		
HresinaeGA	V I H A Q A V L Q T V S N P S G T F L P D G V G L G E P K E M	110		
PoxalicumGA	V S S Q A I L L G S V S N P S G T . K D G S G L G E P K E	123		
	140	150	160	
AnigerGA	V E T A Y T G S H S R F Q R D G P A L R A T A M I G F G Q W	165		
HresinaeGA	V G T R F N G E F W G R P Q R D G P A L R A I A L M T Y S N W	141		
PoxalicumGA	I D L N P F S G A W G R P Q R D G P A L R A T A M I T Y A N Y	154		
	170	180	190	
AnigerGA	L D N G Y T S T A T D I V N F L V R N D L S Y V A Q Y W N Q	196		
HresinaeGA	L I K N G Q F A E A K T K I N P I I A N D L S Y V G Q Y W N Q	172		
PoxalicumGA	L I S H G Q K S D V S Q V M N F I I A N D L A Y V G Q Y W N	185		
	200	210	220	
AnigerGA	T E Y D L W E E V N G S S F P T T A V Q H R A L V E G S A F F	227		
HresinaeGA	S G F D L W E E T Y A S S F P T T I Q N Q H R A L V E G A Q L A	203		
PoxalicumGA	T G F D L W E E V D G S S F P T T A V Q H R A L V E G S Q L A	216		
	230	240	250	
AnigerGA	T A V G S S C S W C D S G A E I L C Y L Q S F W T G S F L	258		
HresinaeGA	H L E V T C I G C D L Q A E V L C F L Q S F W N G K Y V	233		
PoxalicumGA	K K L K S C D A C D S P Q I L C F L Q S F W N G K Y T	247		
	260	270	280	
AnigerGA	A F D . . S S R S G K A N T L L O S A H T F O P E A A C U	287		
HresinaeGA	S N I N V N N G S T G L G N S I L O A I S T F D I D A Y C D	264		
PoxalicumGA	S N I N T Q A S S R S G I L D S V E P S T H T F D P E A A C D	278		
	290	300	310	
AnigerGA	D S F F Q P C S P R A A N H K E V V D S F S S I Y T L N D	318		
HresinaeGA	S P L L Q P C H S Q S L A N F K V L T D T F A N L Y T T I N A	295		
PoxalicumGA	D A F F Q P C S A R A L A N H K K V Y V D S F R S I Y K I N A C	309		
	320	330	340	
AnigerGA	L S D S E A V A V G R Y P E D T W Y N G N P W F L C T L A A A	349		
HresinaeGA	I P E G Q G V A V G R Y A E D V Y M G G N P W Y L I T T A A A	326		
PoxalicumGA	L A E G S A A N V G R Y P E D V S Q G N P W Y L A T L G A S	340		
	350	360	370	380
AnigerGA	F Q L Y D A L Y C M D K Q G S E H T D V S L D F E N A L Y S	380		
HresinaeGA	F L Y D A V A Q M K A R H V L T V D E T S L A F P K D I Y P	357		
PoxalicumGA	F L Y D A L Y Q M D R L G K L E V S E T S L S F F K D F D A	371		
	390	400		
AnigerGA	D A A T G T Y S S . . S S S T Y S S I V D A V K T F A D G F V	409		
HresinaeGA	E V T V R E Y K S G N A N S P F A Q I M D A V T A Y A D S Y V	388		
PoxalicumGA	T Y K I G S Y S R . . N S K T Y K K L T Q S I K S Y A D G F I	400		
	410	420	430	440
AnigerGA	S I V E T H A A S N G S M S C Q Y D K S D G E Q L S A R D L T	440		
HresinaeGA	A I A E K Y I P S N G S L S E O F N R D T G T P I S A I D L T	419		
PoxalicumGA	Q L V Q Q Y T P S N G S L A E Q Y D R N T A A P L S A N D L T	431		
	450	460	470	
AnigerGA	N S Y A A L L T A N N R R N S V V F A S W G E T S A S S V V G	471		
HresinaeGA	N S Y A A F I T M S Q R H A G Q Y F S S N G S R N A L P P T	450		
PoxalicumGA	N S F A S F L T A T Q E R D A V V F P S W G A K S A N K V E T	462		
	480	490	500	
AnigerGA	T C A A T S A I G T V S S V T V T S W P S I V A T G G T T T T	502		
HresinaeGA	T C S A S S T P C I V T P	463		
PoxalicumGA	T C S A S P V V G T V K .	474		
	510	520	530	
AnigerGA	A T P T G S G S V T S T S K T T A T A S K T S T S T S S C	533		
HresinaeGA	A T A A G A P N V T S S C	476		
PoxalicumGA	. A P T A T F S S K T K	486		
	540	550	560	
AnigerGA	T . T P T A V A V C F D L T A T T X G E N I Y L V S I S Q	563		
HresinaeGA	Q V S I T F N I N A T T Y Y G E N L Y I G N S S D	502		
PoxalicumGA	V P A K D I V P I T P Y L I E N Y Y G E N V F M S N I T A	517		
	570	580	590	
AnigerGA	L C D H E T S D G I A S S D K Y S S D P L W Y V T V T L	593		
HresinaeGA	L C A W N I A D A Y P L S A S A Y T Q D R P L W S A I P L L	532		
PoxalicumGA	L C G N W D A K K G F P I T A N L Y T Q D Q N I W F A S V E F I	548		
	600	610	620	
AnigerGA	P A G E S F E V K F I R I S D D S V E W E S D P N R E Y T V	624		
HresinaeGA	N A G E V I S Y Q Y V R Q E S D C D Q P Y I Y E T V N R T L T V	563		
PoxalicumGA	P A S T P F E V K Y Y K V P N G D I T W E K G P N R V F V A	579		
	630	640		
AnigerGA	Q A C G T S T A T V T T R	640		
HresinaeGA	A . C G G A A V T T D A W M G P V G S S G N C	587		
PoxalicumGA	T G C P V Q P H S . N A V W Q F	595		

Figure S1 Sequence alignment of AnGA, HrGA and PoGA obtained using MUSCLE (Edgar, 2004) and visualized using ALINE (Bond & Schüttelkopf, 2009). Amino acids identical for all three proteins are outlined in red, for two – in yellow. The catalytic acid and base are marked with a star.

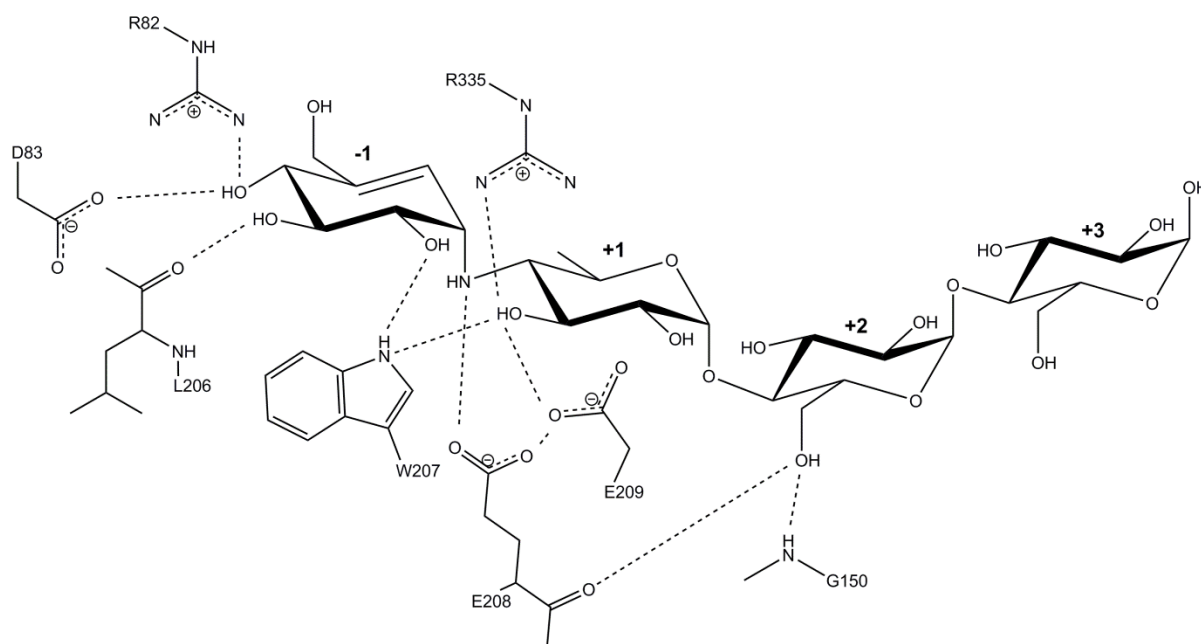


Figure S2 Schematic representation of the interaction of acarbose in the active site of HrGA. Hydrogen bonds are shown as dotted lines and the monomers of acarbose are numbered according their position in the subsites of the GA binding site Figure was prepared using ChemDraw (Perkin Elmer Informatics Inc.).