Exploration of the interactions between maltase-glucoamylase and its potential peptide inhibitors by Molecular Dynamics Simulation

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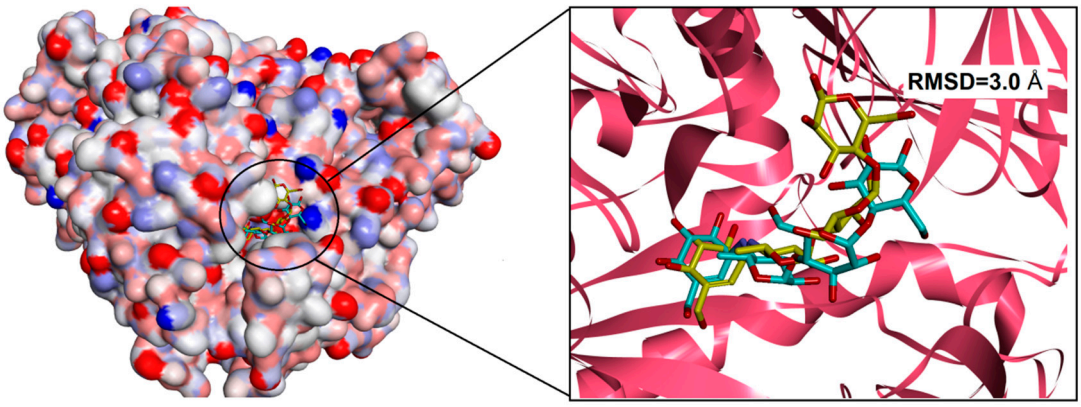

Figure S1 The comparison between the re-docked acarbose (blue) and the reference for the crystal structure (yellow).

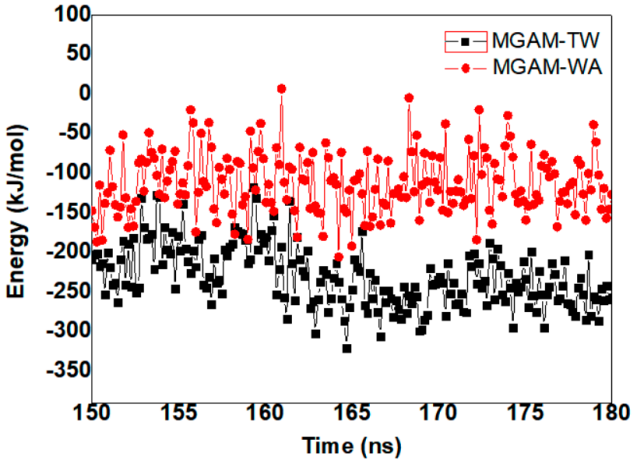

Figure S2. The binding energy distribution of MGAM-TW and MGAM-WA.

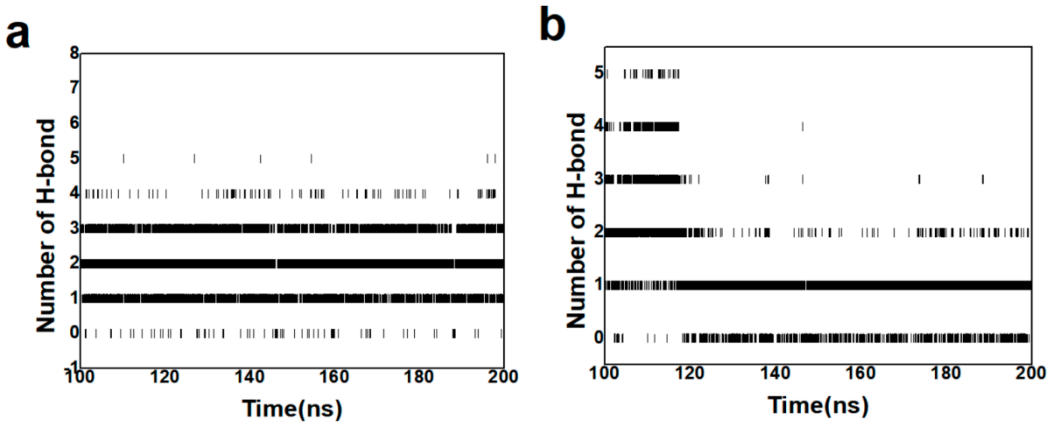

Figure S3 The number of H-bonds evolution along time (a) MGAM-TW (b) MGAM-WA.

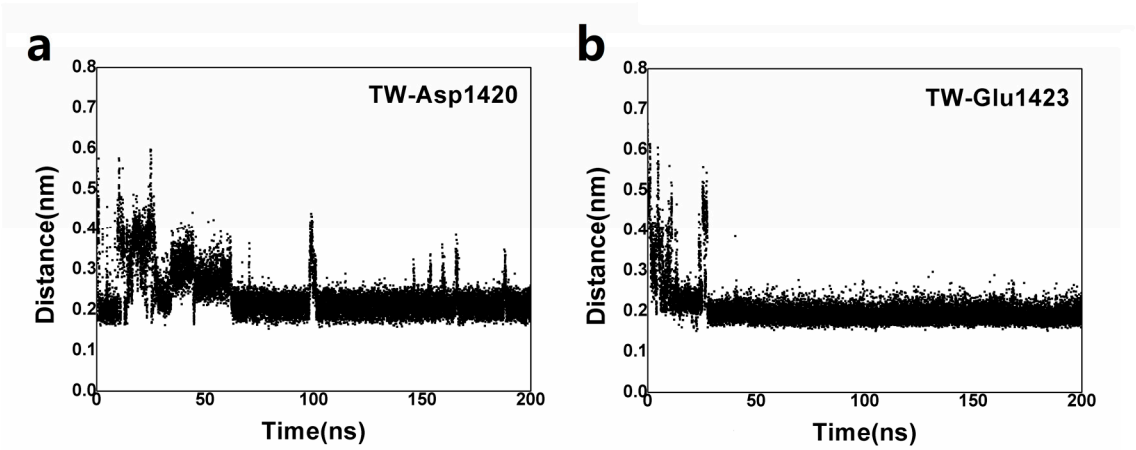

Figure S4. The distances between TW and Asp1420/Glu1423 in MGAM-TW complex.

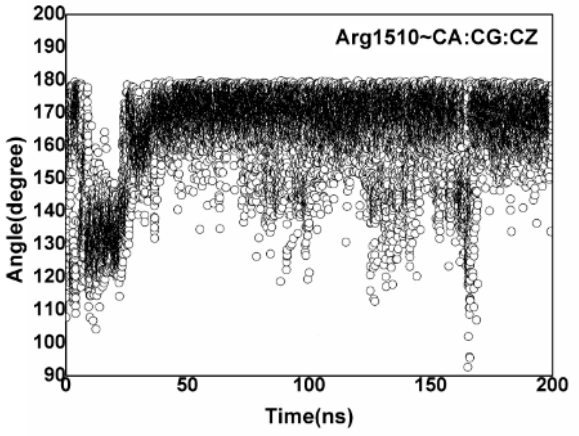

Figure S5 The angle deflection of Arg1510 side chain during the simulations in MGAM-TW complex.

Table S1. The cluster size of WA in cluster 7 to cluster 12.

Cluster	**7**	**8**	**9**	**10**	**11**	**12**
size	58	14	9	6	2	2

Table S2 The probability of H-bonds in the MGAM-TW complex.

Acceptor		**Donor**		**Presence (%)**
MGAM-Asp1420	C=O	MGAM-Thr1^{pep}	NH (amino group)	82.25%
MGAM-Glu1423	COO-	MGAM-Trp2^{pep}	NH (indole group)	95.21%

Table S3. Molecular systems.

Simulations	MGAM-TW complex	MGAM-WA complex
Force field	Gromos 54 A7 force field	Gromos 54 A7 force field
Time (ns)	200	200
Number of solvent	41895	41908
Number of ions	28 NA+	28 NA+