Electronic Supplementary Material (ESI) for RSC Advances.

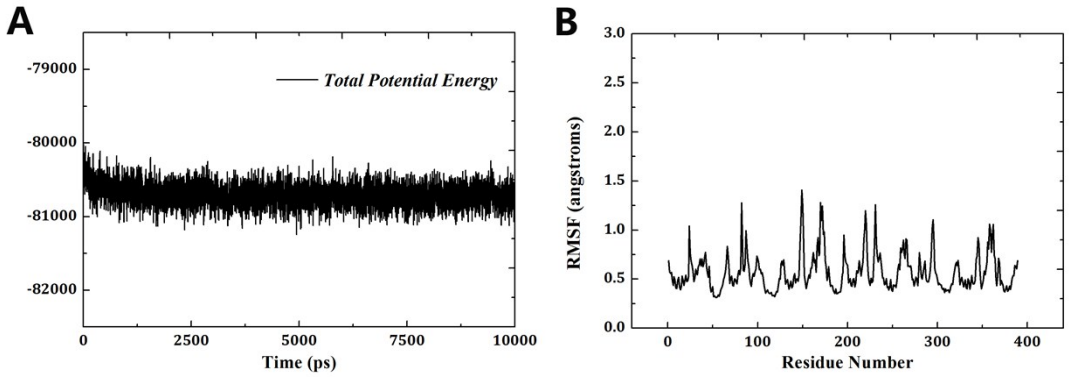

Figure S1. MD simulation results of *Ra*CE and some important residues for MAN binding. A. The total potential energy curve of the complex (kcal/mol). B. The per-residue RMSF values of the protein *Ra*CE backbone atoms with respect to the crystal structure.

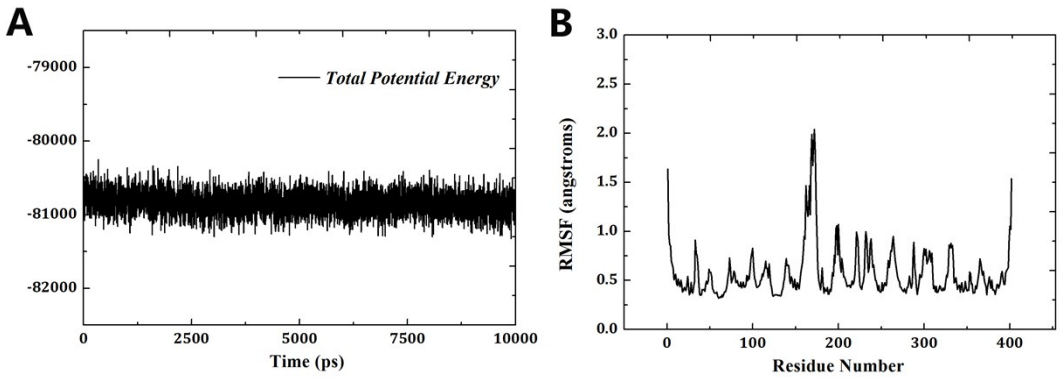

Figure S2. MD simulation results of pAGE and some important residues for ManNAc binding. A. The total potential energy curve of the complex (kcal/mol). B. The per-residue RMSF values of the protein pAGE backbone atoms with respect to the crystal structure.

Table S1. The key distances (with deviation) between MAN and the residues of *Ra*CE of TS1, intermediates and TS2

	Distance(Å)		
	TS1	I	TS2
O7-HE2(H184)	2.42±0.03	2.33±0.02	5.05±0.03
O24-HE2(H184)	2.43±0.03	2.04±0.03	2.91±0.03
HO7-OD1(N180)	1.80±0.02	2.42±0.03	5.41±0.03
O7-HH(Y110)	1.90±0.03	1.73±0.02	3.49±0.02
O24-HE2(H374)	2.21±0.02	1.73±0.02	3.21±0.02
O11-2HH1(R52)	2.70±0.02	3.03±0.03	3.70±0.01
O10-2HH2(R52)	2.22±0.03	2.51±0.03	2.90±0.03
O24-2HH2(R52)	4.41±0.02	3.92±0.03	2.11±0.03
O7-2HH1(R52)	5.71±0.03	5.39±0.03	1.90±0.02

Table S2. The key distances (with deviation) between ManNAc and the residues of pAGE of TS1, intermediates and TS2

	Distance(Å)		
	TS1	I	TS2
HN7-NE2(H248)	2.92±0.01	3.10±0.03	4.41±0.02
O8-NE2(H248)	3.31±0.02	3.13±0.01	4.31±0.02
O10-2HH1(R60)	2.20±0.03	3.39±0.02	3.89±0.03
O-2HH1(R60)	1.81±0.03	1.89±0.03	3.01±0.03
O24-HE2(H382)	1.82±0.02	2.14±0.03	3.18±0.02
N7-2HH1(R60)	4.29±0.03	4.01±0.03	2.20±0.02