Probing the Effect of Glucose on the Activity and Stability of a β-glucosidase: An All Atom Molecular Dynamic Simulation Investigation

Sukanya Konar[1], Sushant K. Sinha[2], Supratim Datta[2,3,4,*] and Pradip Kr. Ghorai[1,*]

[1]Indian Institute of Science Education and Research Kolkata, Department of Chemical Sciences, Mohanpur 741246, India
[2]Protein Engineering Laboratory, Department of Biological Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur, India and [3]Centre for Advanced Functional Materials, Indian Institute of Science Education and Research Kolkata, Mohanpur, India and [4]Centre for Climate Change and Environmental Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur, India

[*]To whom correspondence may be addressed: pradip@iiserkol.ac.in or supratim@iiserkol.ac.in

Table S1: The glycone, aglycone and gate-keeper residues of the B8CYA8

Glycone binding site	Aglycone binding site	Gatekeeper residues
Q20	V169	W168
H121	N222	F172
W122	P225	E173
N165	Y296	F177
N294	S297	N179
W401	W327	H180
N406		L223
E408		T224
W409		L242
K415		I246
F417		Y295
		M299
		V314
		K316
		E324
		M325
		P326
		A410
		Y411

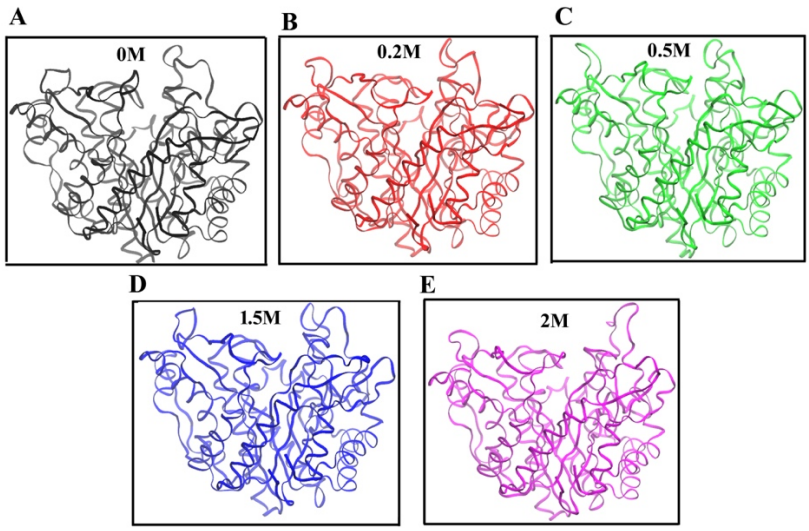

Figure S1: (A - E) are the last B8CYA8 structures for different glucose concentration at 335 K

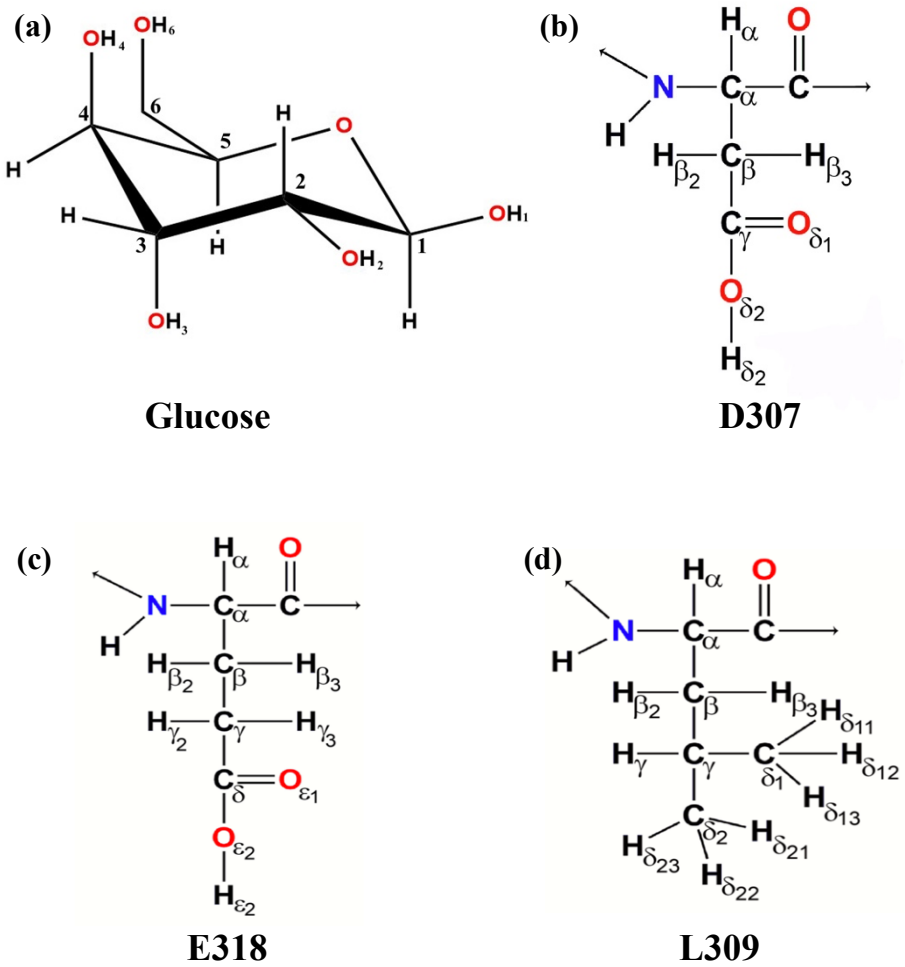

Figure S2: Atom notation for (a) Glucose, (b) D307, (c) E318 and (d) L309 amino acids

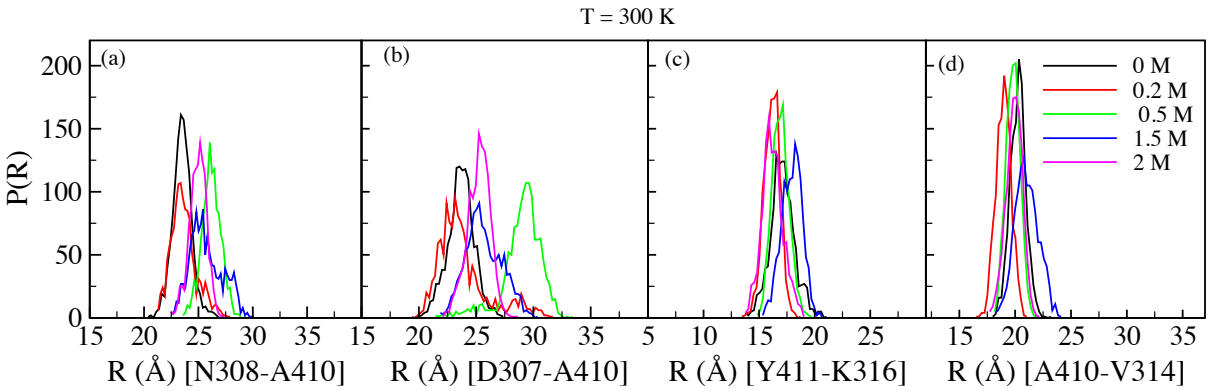

Figure S3: (a), (b), (c) and (d) show distance distribution [P(R)] for chosen pair of amino acids at 300 K

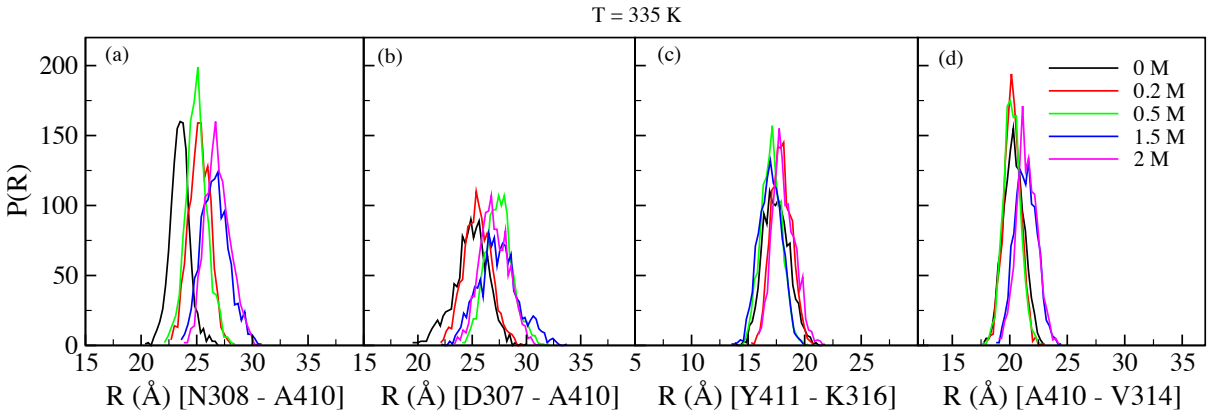

Figure S4: (a), (b), (c) and (d) show distance distribution [P(R)] for chosen pair of amino acids at 335 K

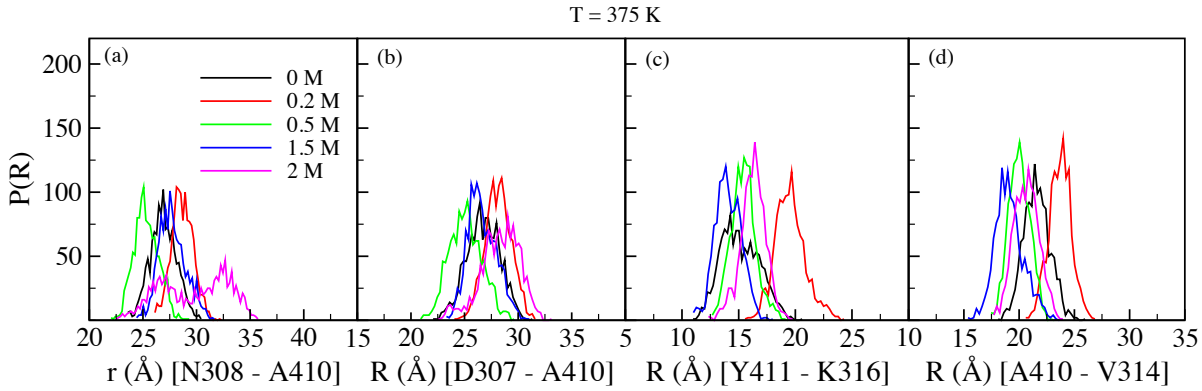

Figure S5: (a), (b), (c) and (d) show distance distribution [P(R)] for chosen pair of amino acids at 375 K

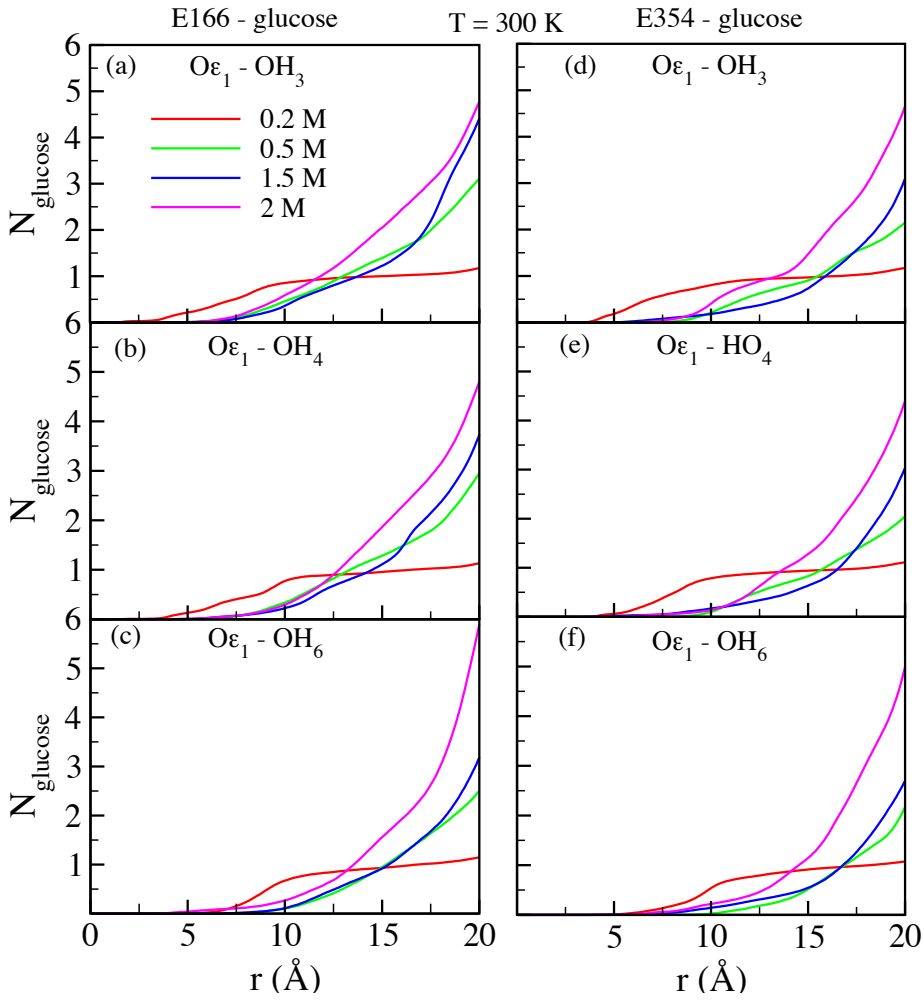

Figure S6: (a), (b) and (c) represent numbers of glucose ($N_{glucose}$) as a function of the distance (r_d) between different hydroxyl groups of glucose (OH_3, OH_4, OH_6) and the $O\varepsilon_1$ of E166 at 300 K. (d-f) represents represent numbers of glucose ($N_{glucose}$) as a function r_d between the same hydroxyl groups as above and the $O\varepsilon_1$ of E354 at 300 K.

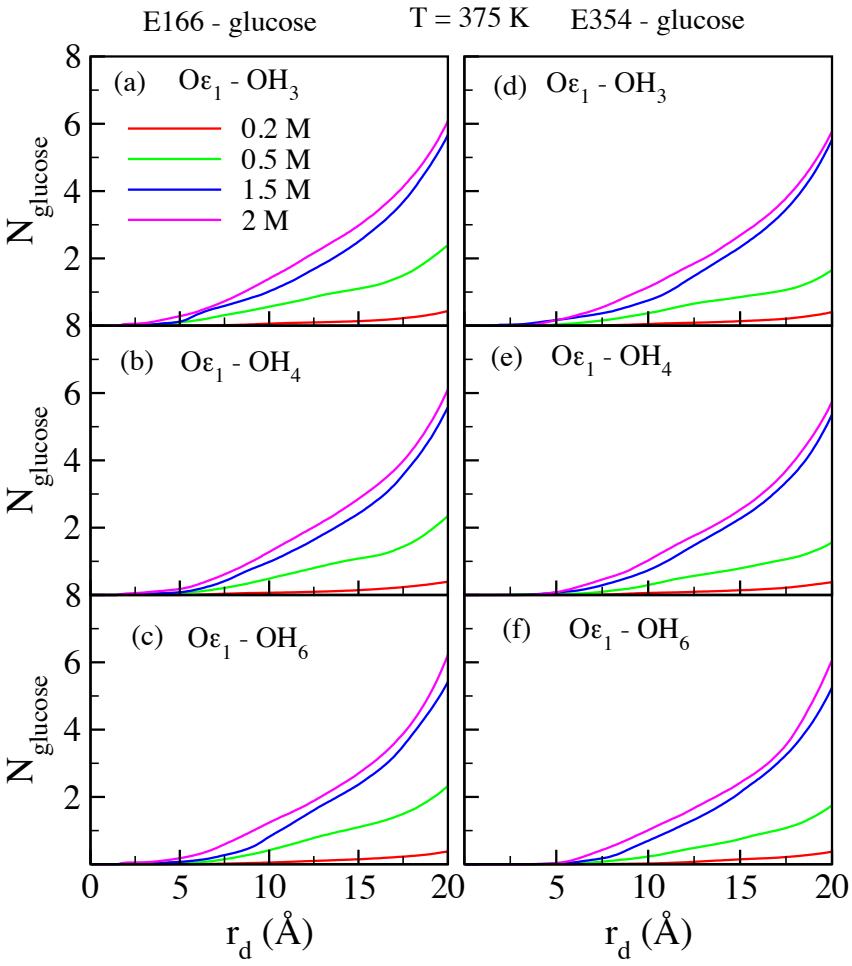

Figure S7: (a), (b) and (c) represent numbers of glucose ($N_{glucose}$) as a function of the distance (r_d) between different hydroxyl groups of glucose (OH_3, OH_4, OH_6) and the $O\varepsilon_1$ of E166 at 375 K. (d-f) represents represent numbers of glucose ($N_{glucose}$) as a function r_d between the same hydroxyl groups as above and the $O\varepsilon_1$ of E354 at 375 K.