Supporting Information

Stereostructural Elucidation of Glucose Phosphorylation by Raman Optical Activity

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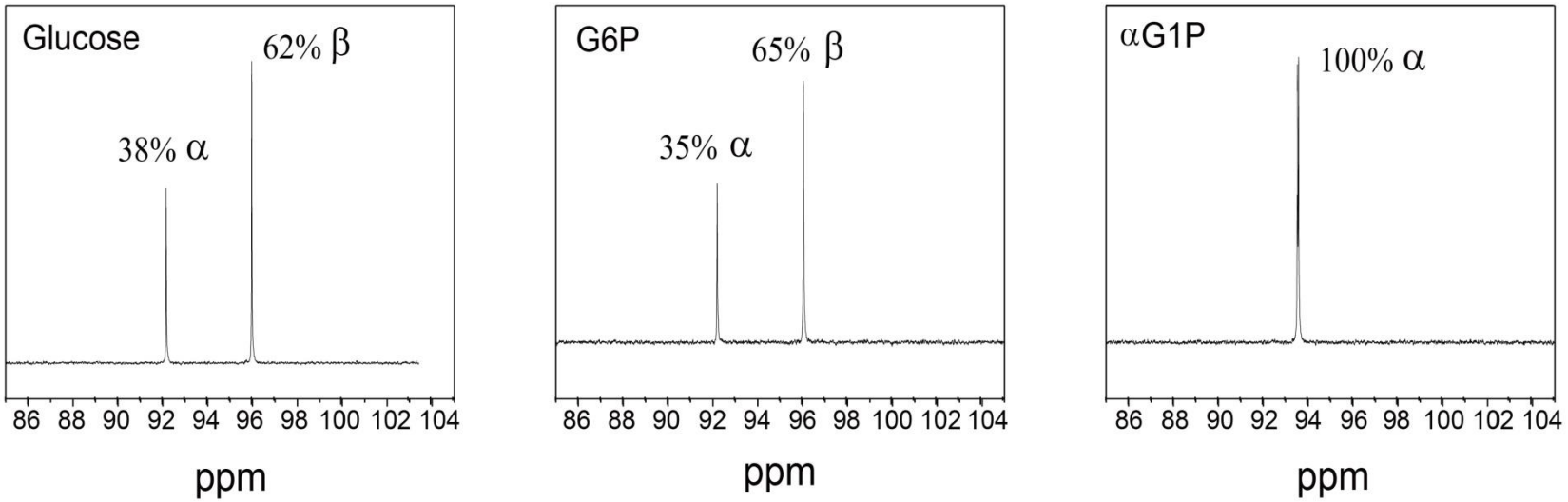

Figure S1. ^{13}C NMR results of glucose, G6P and αG1P. The integration value is shown on the top of each NMR signal.

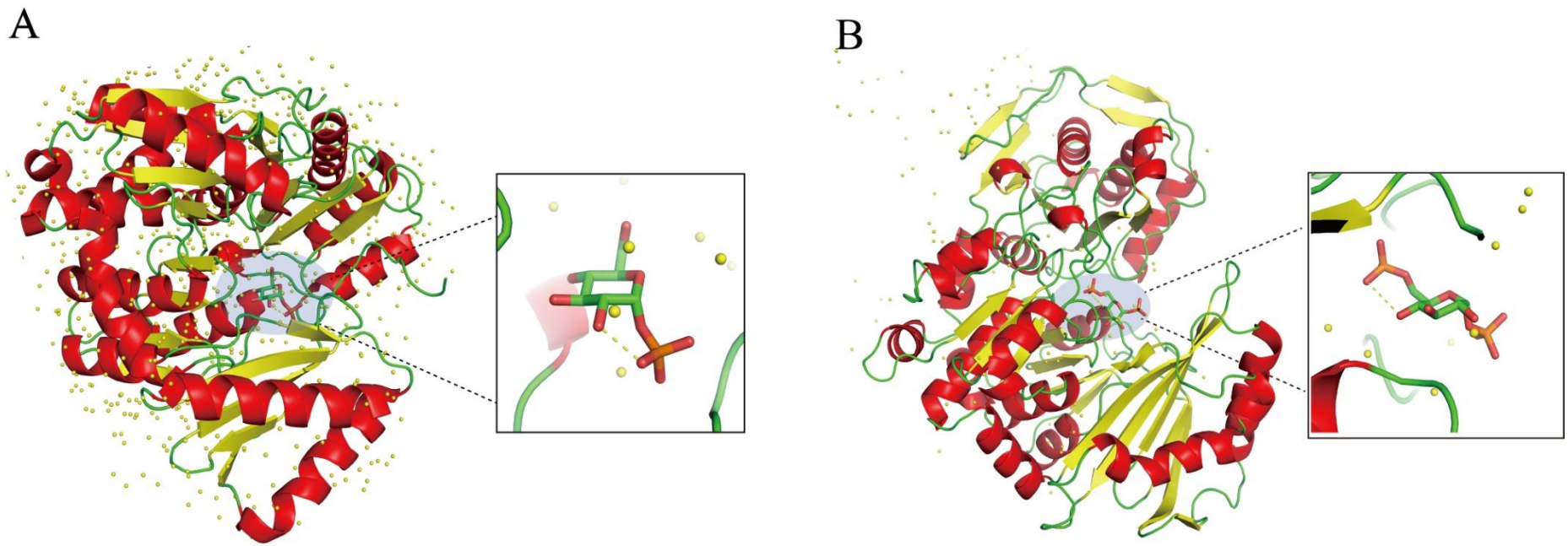

Figure S2. Crystal structures and close-up views of A) αG1P (PDB ID 5BMP) and B) an intermediate, αG16P (PDB ID 1C47) in their complexes with α-phosphoglucomutase. The intramolecular hydrogen bonds between the phosphate groups and their adjacent –OH groups are shown in dashed yellow lines. The yellow dots are presented for the oxygen atoms of water.

Table S1. Raman and ROA band assignments of glucose, G6P and αG1P. Take calculation works on glucose[1], G6P solids[2], D-gluconic acid[3], galactose[4], beta-D-xylose[5], methyl-beta-D-glucose[6] and our simulation results as reference.

	Glucose		G6P		αG1P		Assignments
Region	Raman	ROA	Raman	ROA	Raman	ROA	
low wavenumber region				(-) 375		(-) 360	C-C,C-O stretching; Ring deformation; PO_3 twisting and rocking
				(+) 406		(+) 388	C-C,C-O stretching; Ring deformation; O-H twisting, O6-H twisting
	444	(-) 436	422	(-) 428	435	(-) 432	Ring deformation; Ring breathing; O-H twisting; CH_2 rocking; PO_3 symmetric stretching
	515	(-) 512	450	(-) 505			Ring breathing; OH twisting; PO_3 asymmetric stretching;
		(+) 554	505	(+) 540	538	(+) 528	Ring breathing; OH twisting;
anomeric region	847	(-) 844,**α**	853	(-) 860, **α**	843	(-) 840, **α**	C-O-C stretching;CH_2 bending; C6-O6-H bending; C5-H wagging
	900	(-) 897, **β**	913	(-) 912, **β**	870		C-O-C stretching;CH_2 bending; C6-O6-H bending; C5-H wagging
						(+) 920	C-C,C-O stretching; PO_3 stretching
fingerprint region			980	(+) 980	968	(+) 968	PO_3 symmetric stretching
		(-) 993		(-) 1005		(-) 995	C-C,C-O stretching; C5-C6 stretching C-O-H bending; CH_2 rocking; PO_3 symmetric stretching
	1018	(-) 1028		(-) 1036		(-) 1022	C-C, C-O stretching; C1-C2-C3 deformation;

							C3-C4, C2-O2, C1-O1 stretching
							C-O-H bending; C-H wagging
	1064	(+) 1049	1066		1048	(+) 1053	O1- C5-O5-C5-C6-O6 stretching;
							C1-O1-H, C6-O6-H bending; CH_2 rocking;
		(-) 1066			1061	(-) 1070	C-C stretching; C-O stretching
	1125	(-) 1108		(-) 1110	1108	(-) 1102	Ring deformations
						(-) 1125	PO_3 stretching
		(+) 1152	1130	(+) 1153	1133	(+) 1146	Ring deformations
		(-) 1228		(-) 1234		(-) 1224	C-H wagging; C-O-H bending; CH_2 twisting
H_2 and COH	1265	(+)1266, **β**	1279	(+) 1267, **β**	1269	(-) 1264	C-H wagging; C-O-H bending; CH_2 twisting
deformations	1332	(-) 1315	1335	(-) 1315	1337	(-) 1337	Ring H torsion; C-O-H bending
region	1368	(+) 1365	1372	(+) 1367	1366	(+) 1363	Ring H torsion; C-O-H bending
	1462	(+) 1465	1462	(-) 1455	1462		CH_2 scissoring; CH_2 twisting
							Weak OH wagging

α or **β** refers to an anomer which has an axial or equatorial hydroxyl group at C1.

References

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