**Supplementary material I for**

# Collision-Induced Dissociation of Sodiated Glucose, Galactose, Mannose, and the Identification of Anomeric Configuration

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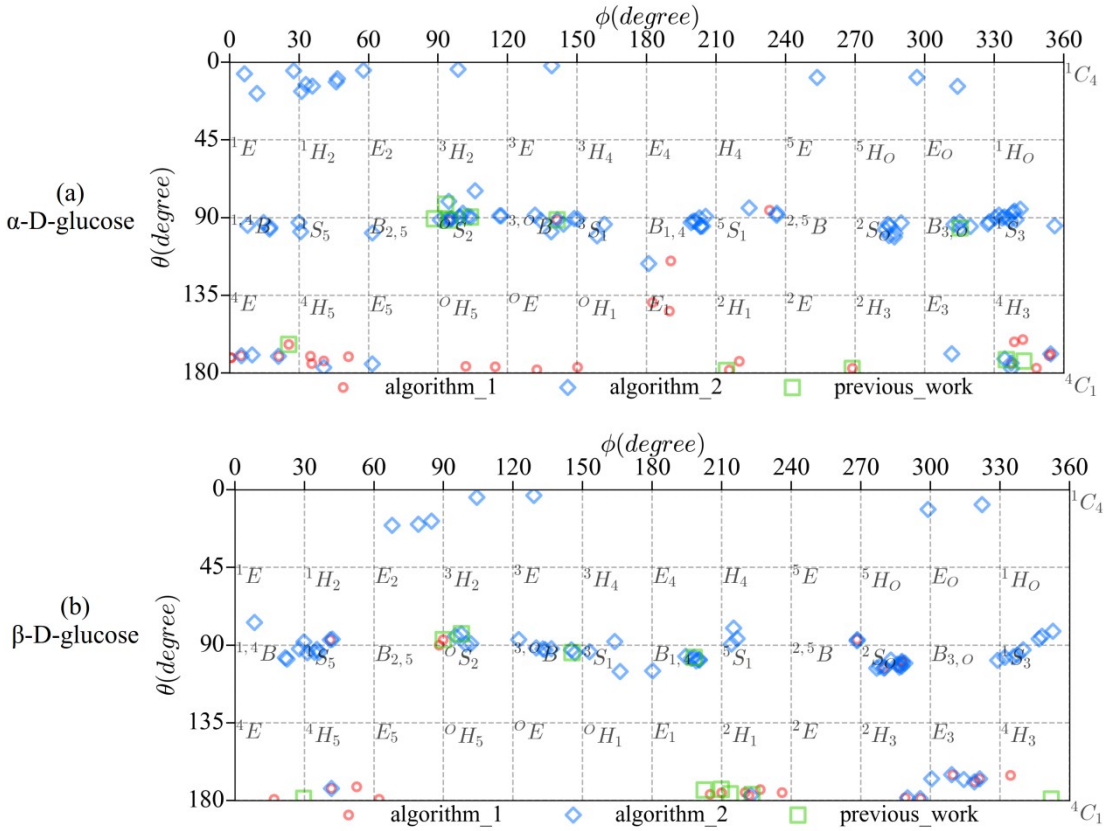


**Figure S1.** The sodiated conformers of (a) α-D-glucose and (b) β-D-glucose generated by algorithm 1 (red circle), algorithm 2 (blue diamond), and from the previous work[1] (green square) are plotted in the Mercator projections of the Cremer-Pople puckering sphere. The conformers from the previous work can be mostly covered by algorithm 1 and 2.

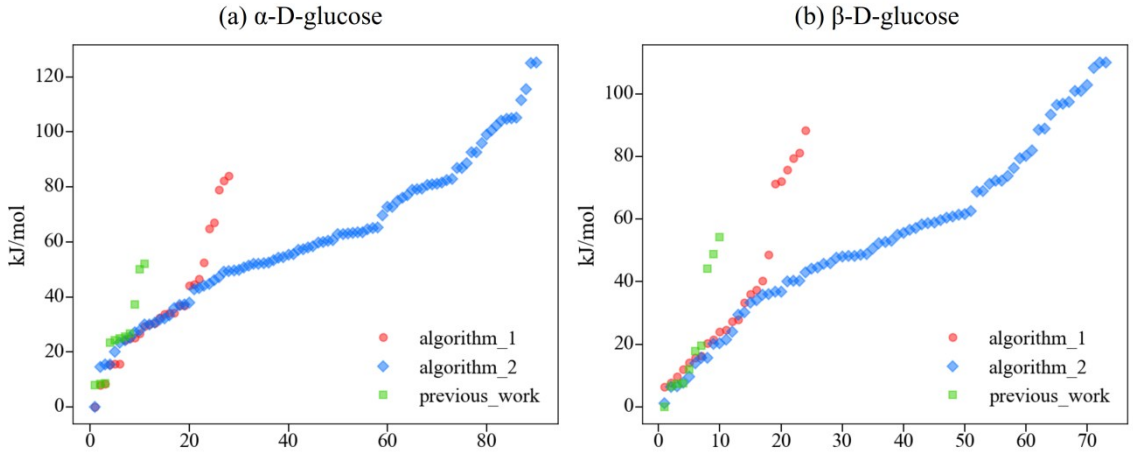


**Figure S2.** Relative energies of the sodiated conformers generated by algorithm 1 (red circle), algorithm 2 (blue diamond), and from the previous work[1] (green square). The abscissa is numbering of the conformers.

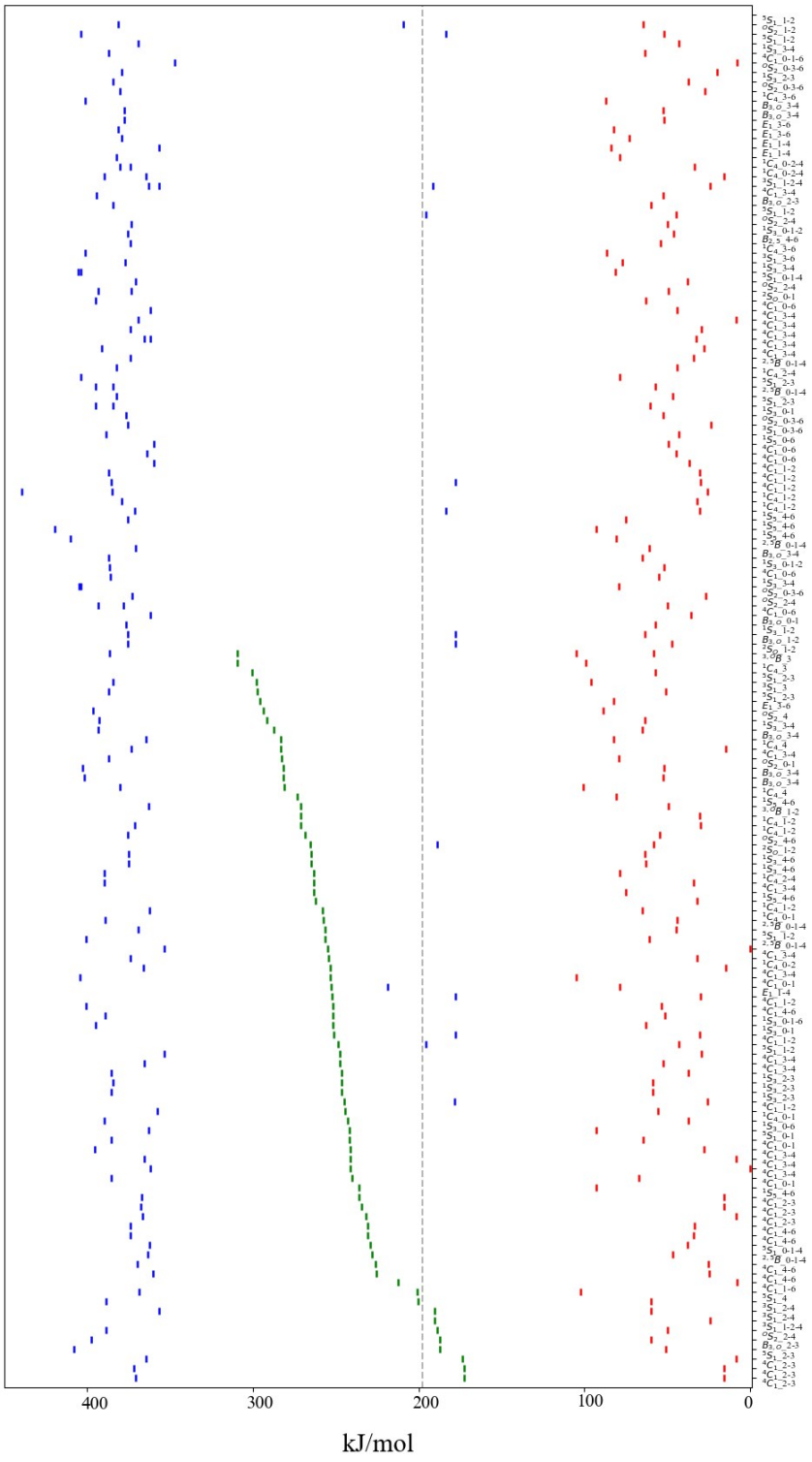


**Figure S3.** Full energy diagram of sodiated α-D-glucose with sodiated energy (dashed line) of 197.5 kJ/mol, the equilibrium energies (red), and the corresponding TS energies of dehydration (green) and ring-opening (blue) reactions.

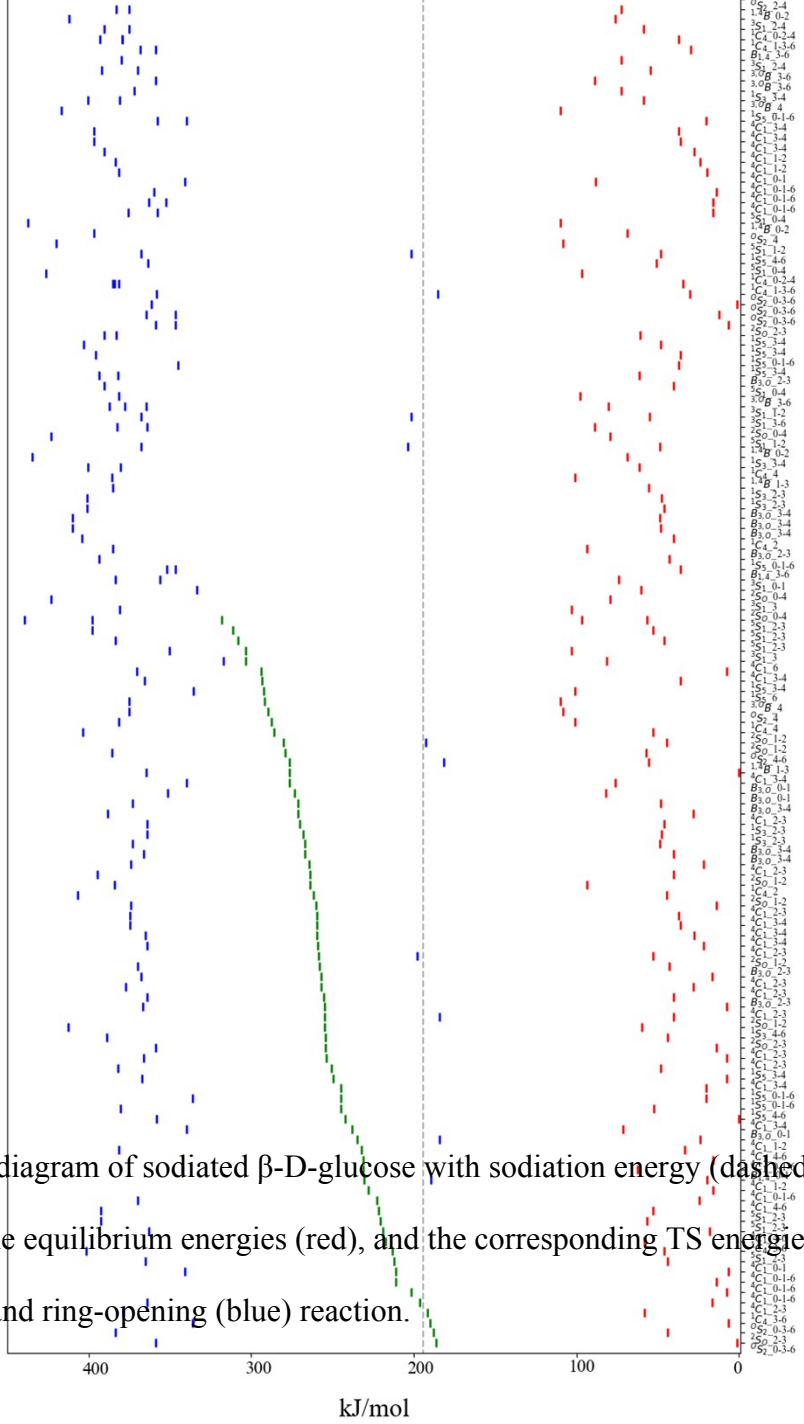


**Figure S4.** Full energy diagram of sodiated β-D-glucose with sodiation energy (dashed line) of 194.2 kJ/mol, the equilibrium energies (red), and the corresponding TS energies of dehydration (green) and ring-opening (blue) reaction.

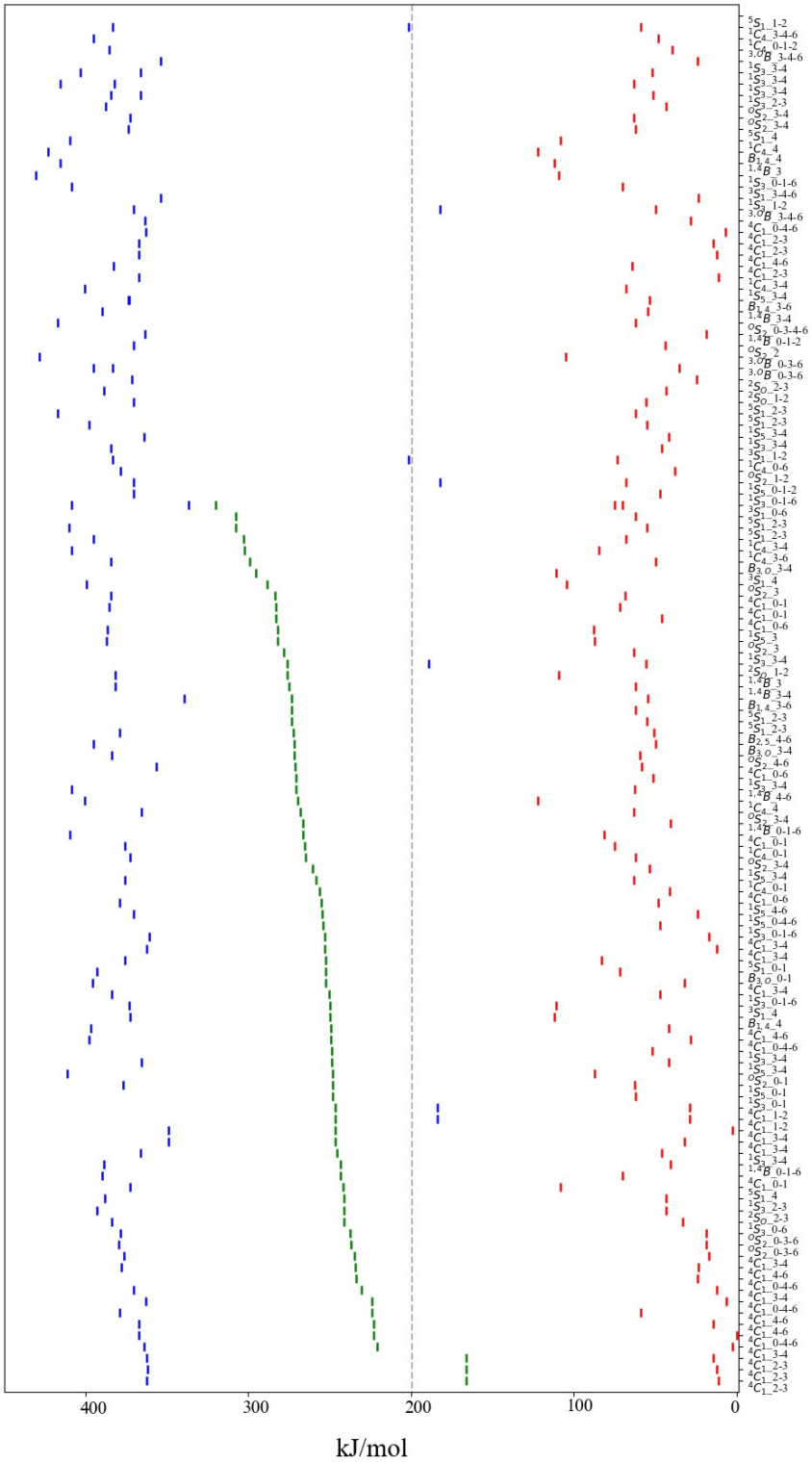


**Figure S5.** Full energy diagram of sodiated α-D-galactose with sodiated energy (dashed line) of 199.4 kJ/mol, the equilibrium energies (red), and the corresponding TS energies of dehydration (green) and ring-opening (blue) reactions.

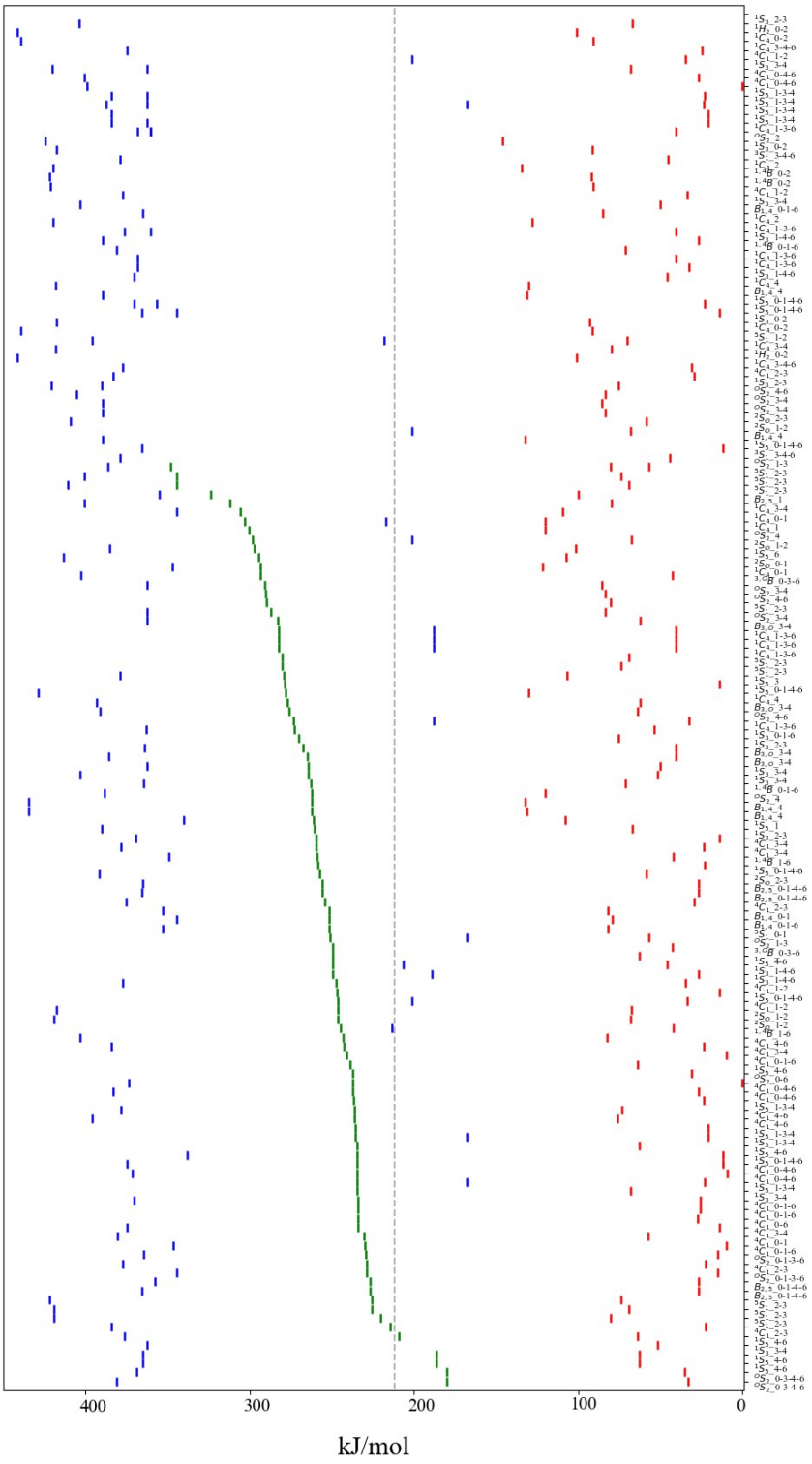


**Figure S6.** Full energy diagram of sodiated β-D-galactose with sodiated energy (dashed line) of 212 kJ/mol, the equilibrium energies (red), and the corresponding TS energies of dehydration (green) and ring-opening (blue) reactions.

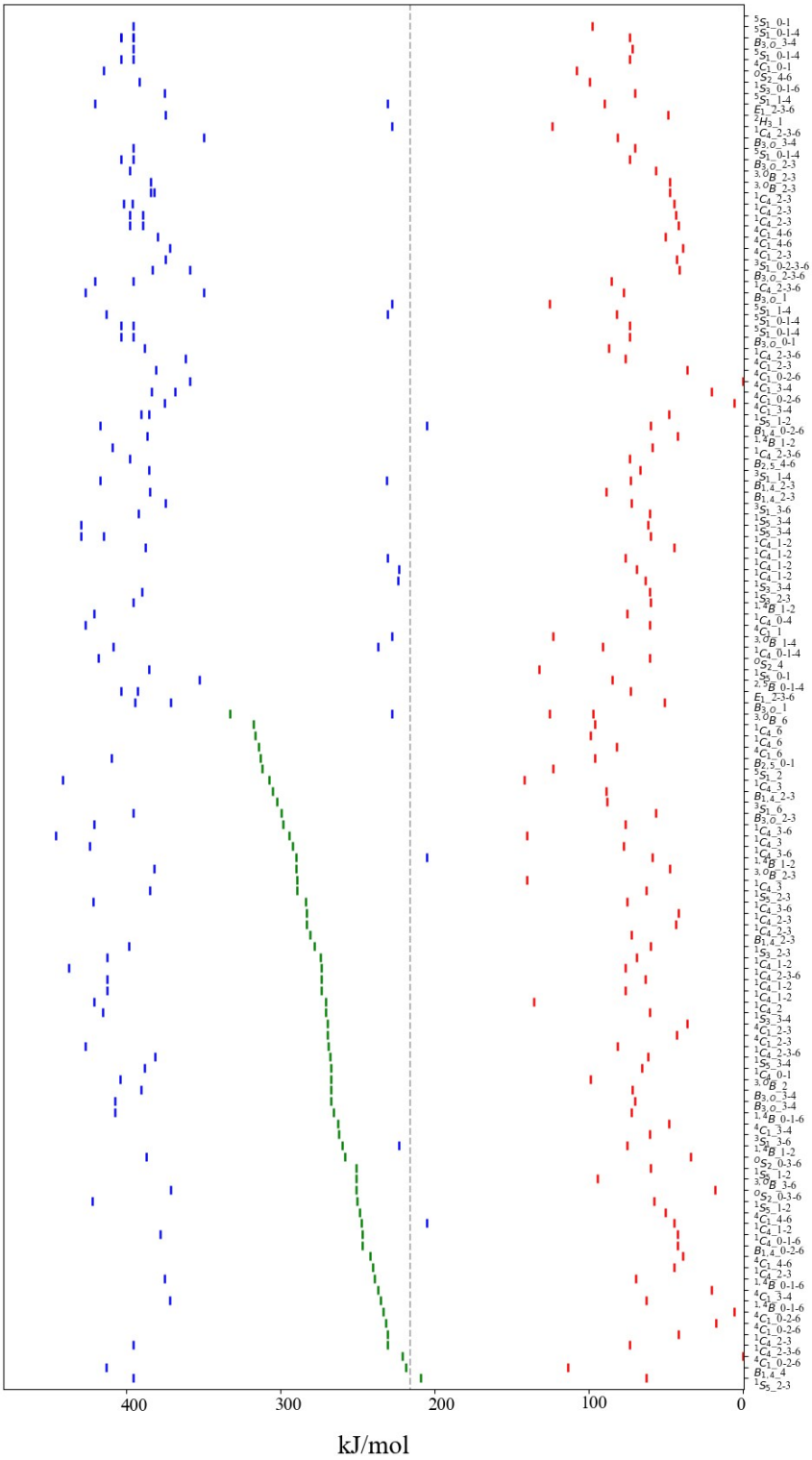


**Figure S7.** Full energy diagram of sodiated α-D-mannose with sodiated energy (dashed line) of 215.6 kJ/mol, the equilibrium energies (red), and the corresponding TS energies of dehydration (green) and ring-opening (blue) reactions.

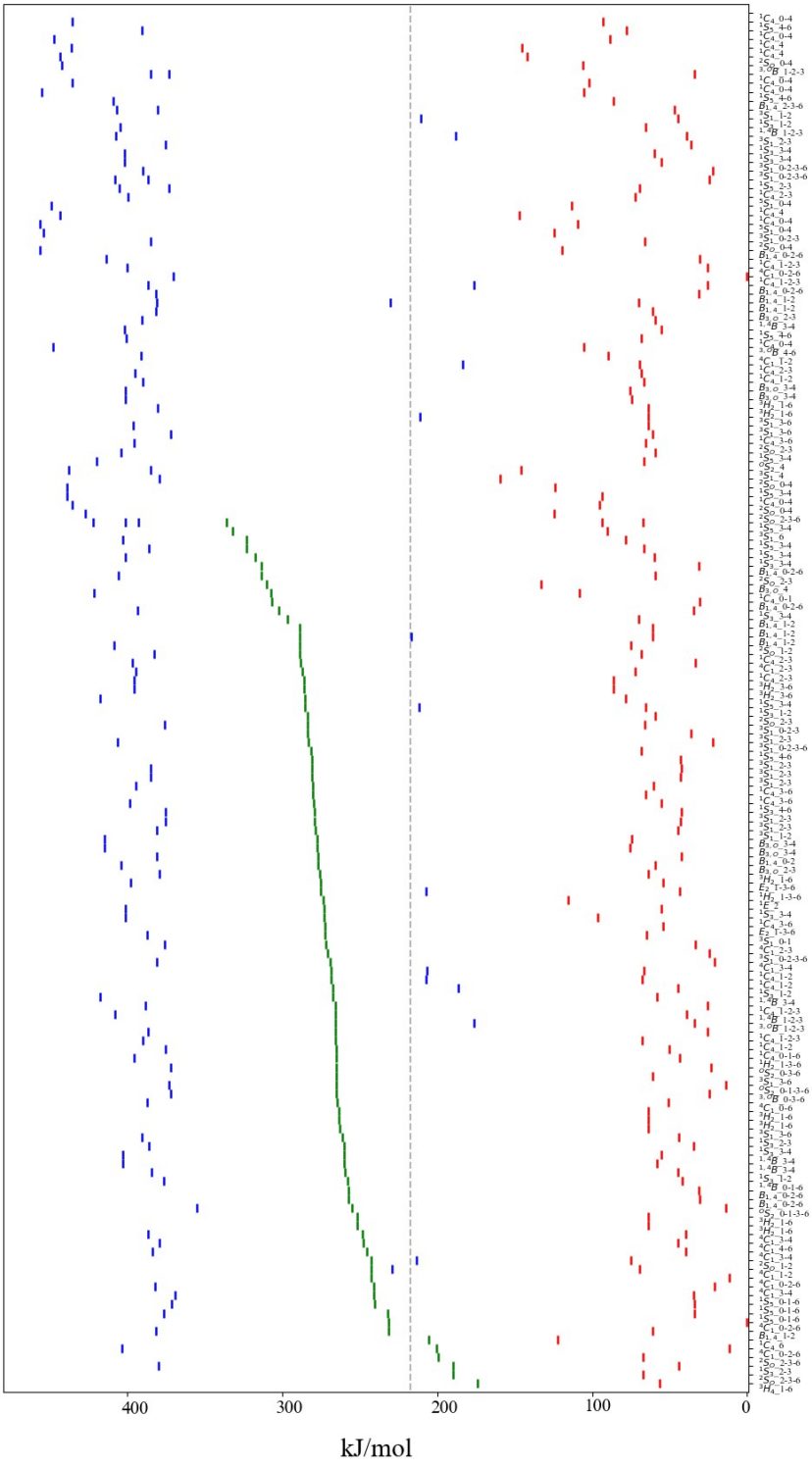


**Figure S8.** Full energy diagram of sodiated β-D-mannose with sodiated energy (dashed line) of 217.5 kJ/mol, the equilibrium energies (red), and the corresponding TS energies of dehydration (green) and ring-opening (blue) reactions.

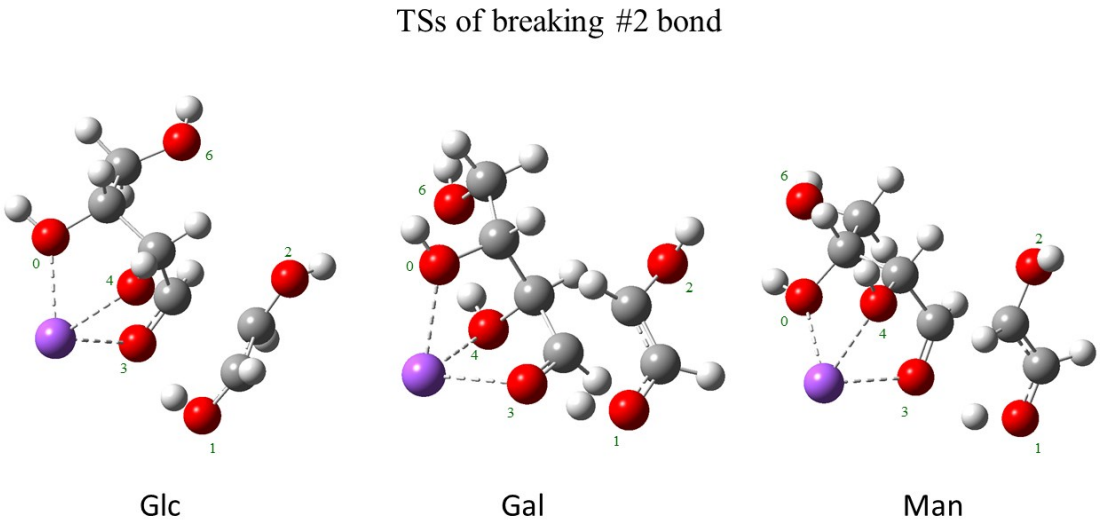


**Figure S9.** Transition state geometries of breaking #2 bond after ring opening.

**Coordinate files in Supplementary material II**

The xyz coordinate files of TS of dehydration and cross-ring dissociation and their corresponding stable conformers in Fig. 4. Those conformers with the same Cremer-Pople puckering index and the same absorption sites of sodium cation to oxygen atoms are grouped into the same file. The file names are labelled by the puckering index and the absorption sites found in the conformers of Fig. 4. In each xyz file, the odd frame represents the local minimum of TS, and the even frame indicates the TS with respect to the corresponding conformer. The coordinates are sorted by the TS energies in ascending order.

# Reference

1. J. L. Chen, H. S. Nguan, P. J. Hsu, S. T. Tsai, C. Y. Liew, J. L. Kuo, W. P. Hu, and C. K. Ni., *Phys. Chem. Chem. Phys.*, 2017, **19**, 15454.