Supporting Informations

Analysis of glycosyl bond cleavage and there related isotope effects in collision-induced dissociation quadrupole/time-of-flight mass Spectrometry of isomeric trehaloses

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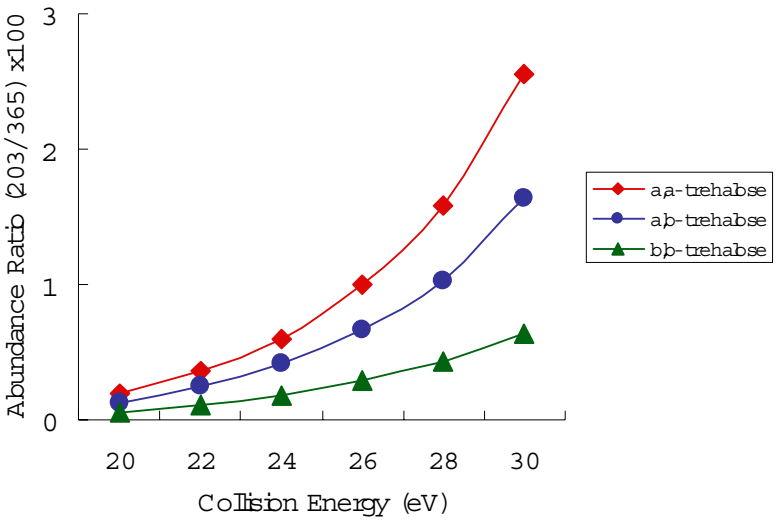
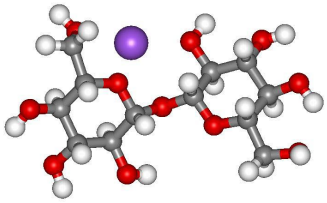


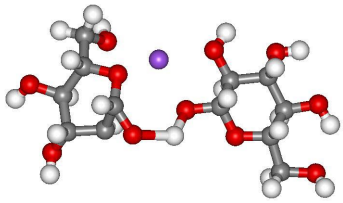
SI-1. Abundance ratio of ion m/z 203/365.

Red diamond plots -♦- are the data of α,α-trehalose, blue circle plots -●- are that of α,β-trehalose, and green square plots -▲- are that of β,β-trehalose.

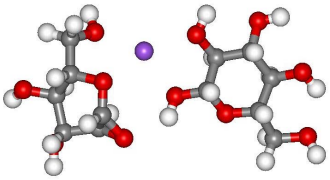
(a)



(b)

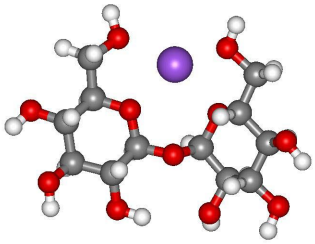


(c)

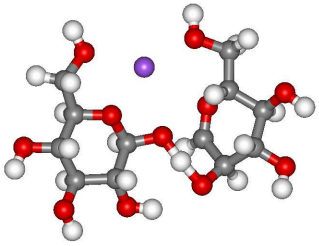


SI-2. Optimized structures of [β,β-trehalose + Na]$^{+}$ (a), the transition state (b) and the intermediate (c) product of reaction path (B) in Figure 6-b.

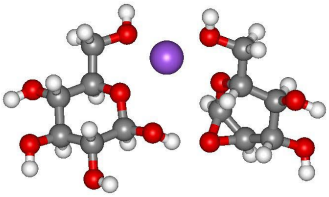
(a)



(b)



(c)



SI-3. Optimized structures of [α,β-trehalose + $Na]^+$ (a), the transition state (b) and the intermediate (c) product of reaction path (B) in Figure 6-c.