

## Unusual Covalent Bond Breaking Reactions in the Non-Covalent Complexes of $\beta$ -Cyclodextrins and Nucleobases/Nucleosides

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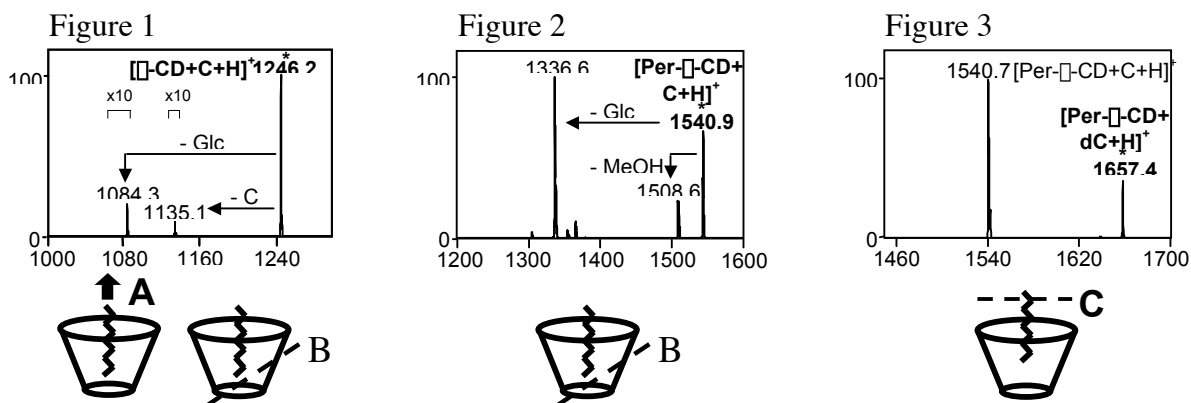
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### Introduction:

Cyclodextrins<sup>1</sup> are cyclic oligosaccharides consisting of 6, 7 or 8 glucopyranose (Glc) units, usually referred to as  $\alpha$ ,  $\beta$ , or  $\gamma$ -cyclodextrins respectively. In solution, their large inner cavity makes them ideal hosts to form inclusion complexes with more hydrophobic compounds.<sup>2</sup> Recent gas phase studies have shown that inclusion complexes of protonated amino acids and cyclodextrins (formed via electrospray ionization (ESI)) can be examined by ion-molecule reactions or collision-induced dissociation (CID).<sup>3,4,5</sup>

### Results:

Collision-induced dissociation (CID)<sup>5,6</sup> has been used to probe the fragmentation behaviour of  $\beta$ -cyclodextrin-nucleobase/nucleoside complexes. Examples of such experiments are shown for the  $\beta$ -cyclodextrin-cytosine [ $\beta$ -CD+C+H]<sup>+</sup> (Figure 1), permethylated  $\beta$ -cyclodextrin-cytosine [Per- $\beta$ -CD+C+H]<sup>+</sup> (Figure 2) and permethylated  $\beta$ -cyclodextrin-deoxycytidine [Per- $\beta$ -CD+dC+H]<sup>+</sup> (Figure 3) complexes respectively. Under these conditions, the inclusion complexes either: (A) dissociate as shown in Figure 1; (B) result in cleavage of the host oligosaccharide as shown in Figures 1 and 2; (C) result in cleavage of the guest molecule as shown in Figure 3. This study has shown that the preferred dissociation pathway of these complexes depends on the structures of both the cyclodextrin and guest molecule. In order to better understand the competition between these reaction channels, various other complexes have been generated and examined. These results will be discussed in greater detail.



### References:

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