MASS SPECTROMETRY CHARACTERIZATION OF OLIGOESTER FUNCTIONALIZED CYCLODEXTRINS

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Cyclodextrins (CD) ability to form inclusion complexes and hence to alter the physical-chemical properties of guest molecules has been exploited in order to increase the water mixing properties of hydrophobic drugs. To optimize the physical inclusion of specific guests, the polarity of native CD molecules should be adjusted. Generally this is achieved by attaching small alkyl or hydroxyalkyl substituents through ether linkages. Mass spectrometry is known to be a precise and fast method to achieve cyclodextrin derivatives characterization. The presentation deals with the use of ESI mass spectrometry to characterize CD derivatives obtained through ring opening oligomerization of β-butyrolactone[1], D,L-lactide (CDLA)[2], and other cyclic esters[3]. In MS/MS, depending on the chosen parent ion, the cyclodextrin-ester derivatives can be selectively cleaved at the level of the hemiacetal junction or at the level of the ester bonds. This distinct behavior in CID fragmentation conditions allows a direct access at the modified cyclodextrin substitution pattern.

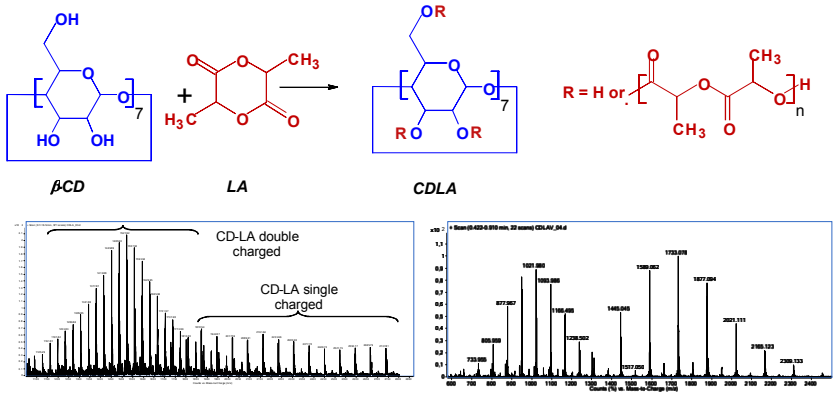

Figure 1. CDLA obtained through ROP of LA catalyzed by sparteine in DMSO or in DMF only

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