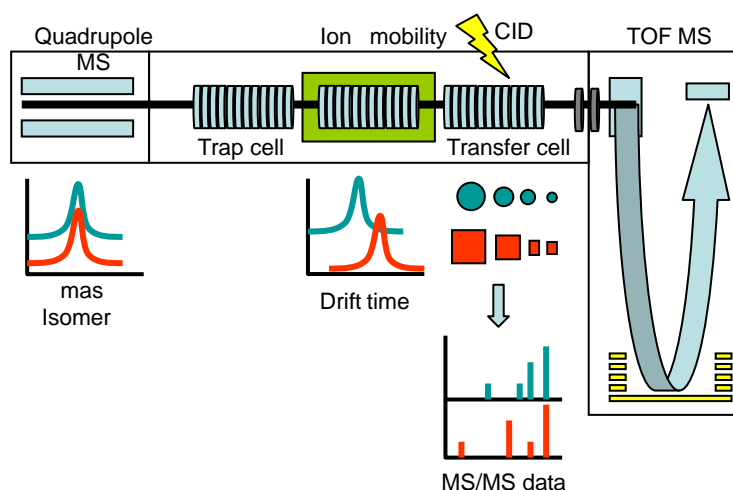


Isomeric Oligosaccharides Analyses Using Negative-ion Electrospray Ionization Ion Mobility Spectrometry Combined with Collision-induced Dissociation MS/MS

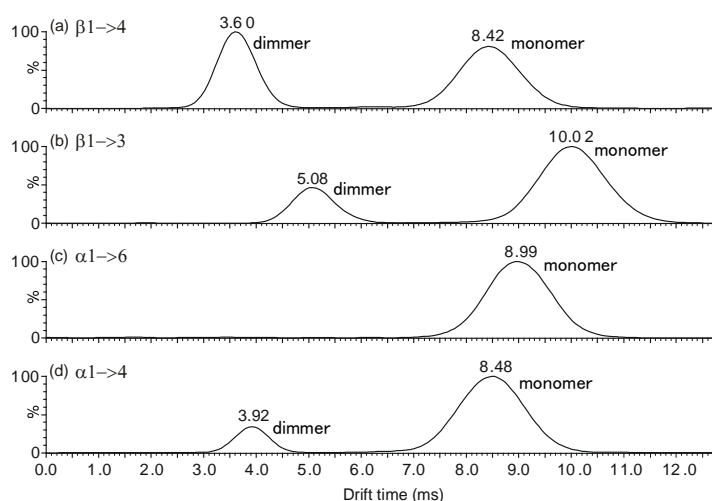
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Molecular interactions and/or self-assembling of biomolecules are one of the most interesting topics in biosciences. When a biomolecule shows their activity in cell, it is a big question that the molecule works as mono-mer or dimer, or multimers. Due to solve the issues it is required to analyze how the biomolecules are in the cell, they are monomer, or dimer, or multi-mers. We analyzed multi-mer formation of the biomolecules with ion mobility-mass spectrometry (IM-MS). IM-MS can analyze the multimer formation of isomeric sugar chains with the different glycosyl bonds such as α 1-4, α 1-6, β 1-3, and β 1-4 linkages. Addition to that, negative-ion electrospray ionization (ESI) quadrupole IM time-of-flight mass spectrometry allowed the combination of IM separation and collision-induced dissociation (CID) MS/MS product ion analysis. Multimer formations of hexa-saccharide linkage isomers differ from each other, and their molecular shapes were analyzed by ion mobility spectrometry (IMS). The product ion spectra of the oligosaccharide isomers were measured by negative-ion CID-MS/MS for each IM separated peak. The spectrum for each isomer was distinct, and their corresponding linkage structures were identified by MS/MS analysis.



Scheme of the instrument of ion mobility time-of-flight mass spectrometry (Q-IM(TOF)MS). We can decompose the precursor ions at the both former and later cells of the IM cell. The precursor ions were selected at quadrupole MS, and then we can detect the product ions' ion mobility MS at the "Trap cell". When we analyze the structural information of the IM peak, we can decompose the ions after separating them by IM drift time at the "Transfer cell".



Ion mobility spectra of the deprotonated molecules at m/z 989 of cellohexaose (a), laminarihexaose (b), isomaltohexaose (c), maltohexaose (d).

IM spectra of β 1-4 linked hexose (a), β 1-3 linked hexose (b), α 1-6 linked hexose (c), α 1-4 linked hexose. The early detected peaks were doubly charged dimmers, the lately detected peaks were singly charged monomers. We can distinguish all of them with the complex multimer formation analysis. Cellohexaose can more easily form the dimer than maltohexaose because the straight structure of the chains. Isomaltohexaose can not form the dimer because of the high flexibility at their glycosyl bonds.