

Hydrogen-deuterium exchange of α -carbon protons and fragmentation pathways in N-methylated glycine and alanine-containing peptides derivatized by quaternary ammonium salts.

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Recently, we developed a selective and efficient method of hydrogen-deuterium exchange (HDX) at the α -carbon (α -C) of sarcosine residue (N-methylglycine) in model peptides [Bąchor et al. *J. Mass Spectrom.* 2014, 49, 43]. Here, we report the influence of quaternary ammonium (QA) group on HDX at the α -C of sarcosine and N-methylalanine in peptides. The obtained results suggest a significant acceleration of the HDX in sarcosine residue caused by the presence of QA. The effect depends on the distance between the sarcosine residue and QA moiety. The deuterons, introduced at α -C, are resistant to the back-exchange in acidic aqueous solution. The collision induced dissociation of the deuterium-labeled analogs of QA-tagged oligosarcosine peptides without mobile hydrogen revealed the mobilization of the hydrogens localized at α -C of sarcosine residue.

Słowa kluczowe

HDX of peptides, quaternary ammonium salts, ESI-MS/MS, sarcosine, charge-remote fragmentation

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