Supporting Information

Identification of [6-Hydroxy-2-(hydroxymethyl)-5-oxo-5,6-dihydro-2*H*-pyran-3-yl]-cysteine (HHPC) as a Cysteine-specific Modification Formed from 3,4-Dideoxyglucosone-3-ene (3,4-DGE)

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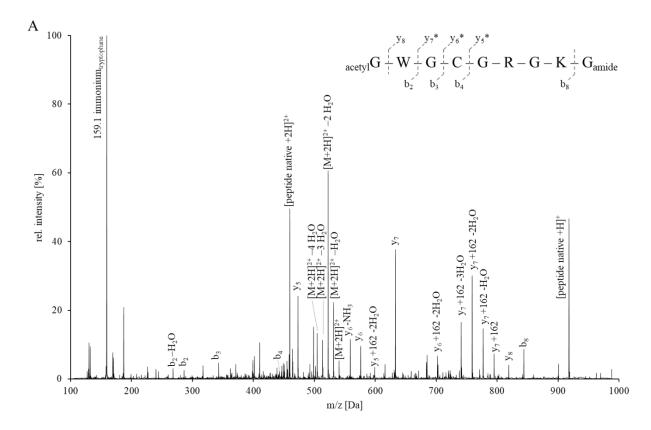
Figure S-1, pp S2–S4

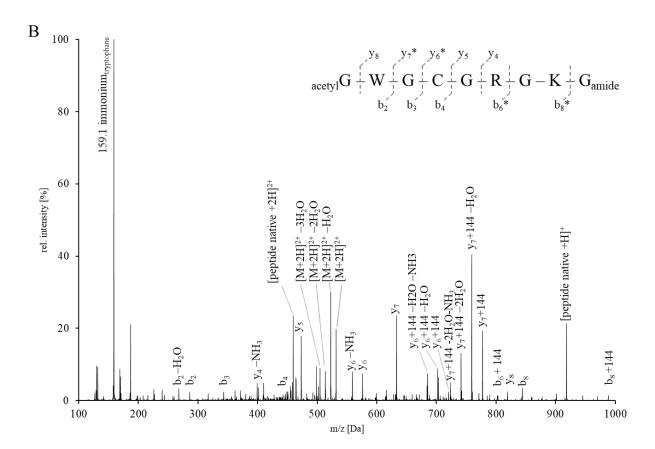
Enhanced product ion spectra of the modified nonapeptide Ac-GWGCGRGKG-NH₂ after incubation with 3,4-dideoxyglucosone-3-ene, which resulted in a mass shift of (A) \pm 162 Da, (B) \pm 144 Da, (C) \pm 142 Da, and (D) \pm 126 Da. All detected peptide fragments are marked in the peptide sequence and modified peptide fragments are highlighted with an asterisk. Binding sites of modification products were determined according to the detected modified and unmodified peptide fragments of b- and y-series.

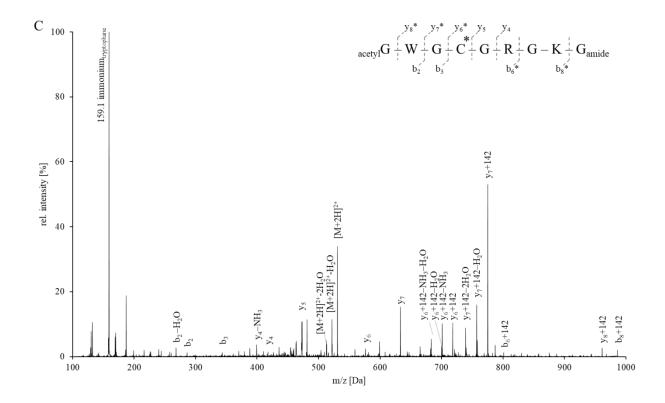
Scheme S-1, p. S5

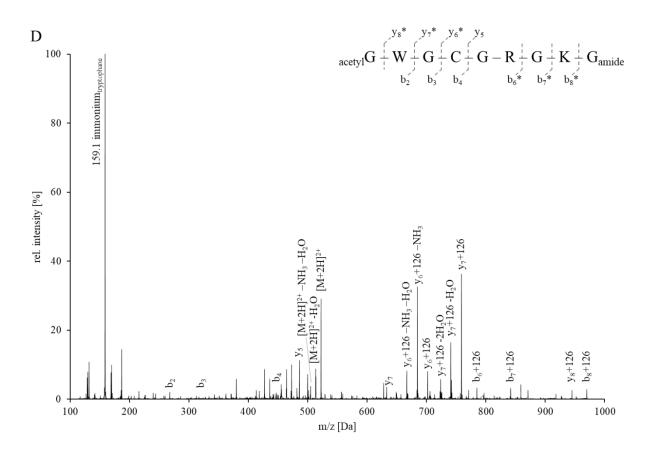
The glycating agent 3,4-dideoxyglucosone-3-ene (3,4-DGE) and its hydration products 3-deoxyglucosone (3-DG) and 3-deoxyglactosone (3-DGal).

Figure S-1









Scheme S-1