

# **w-type ions formed by Electron Transfer Dissociation of Cys-containing peptides investigated by infrared ion spectroscopy**

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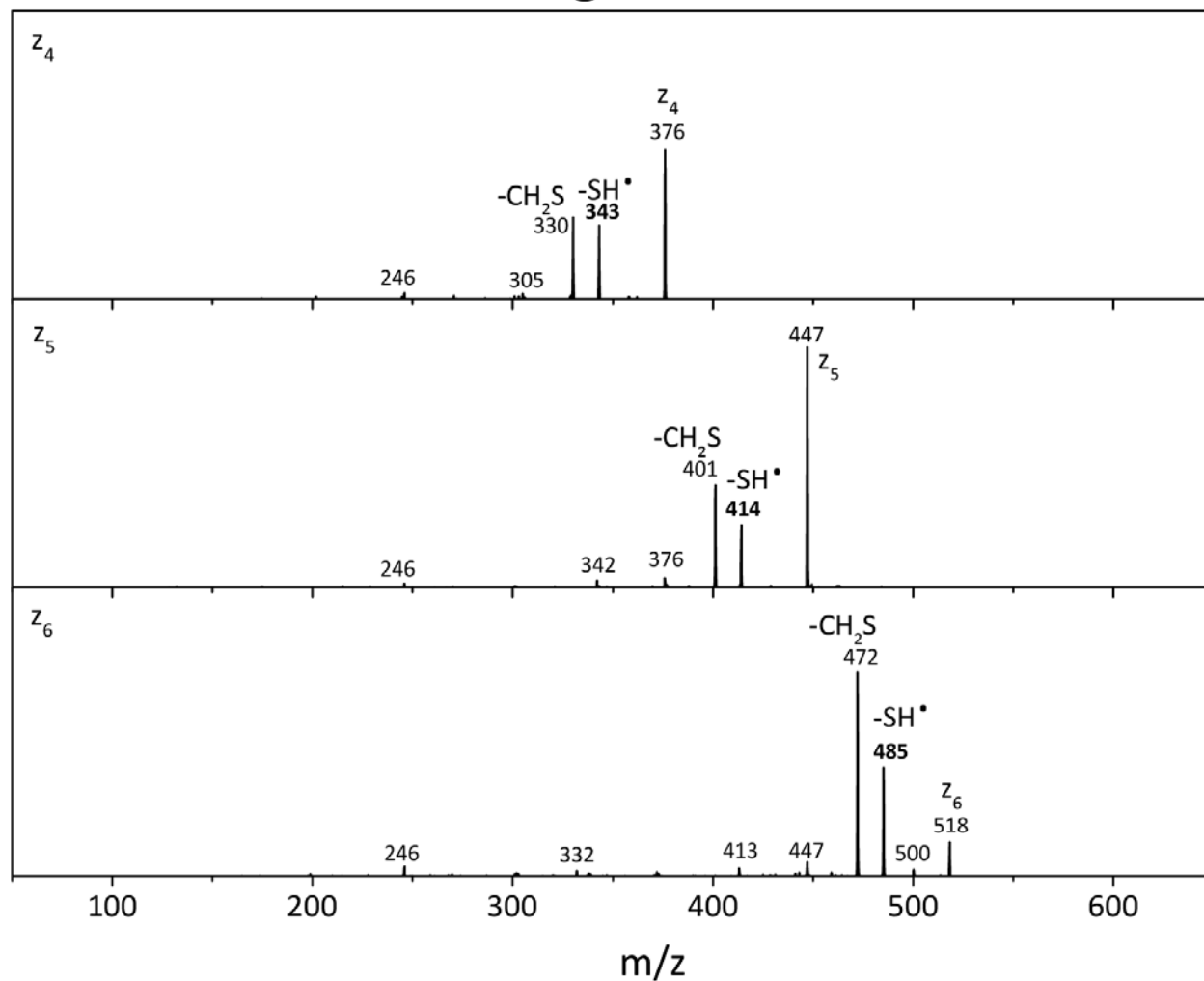
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## **Supporting Information**

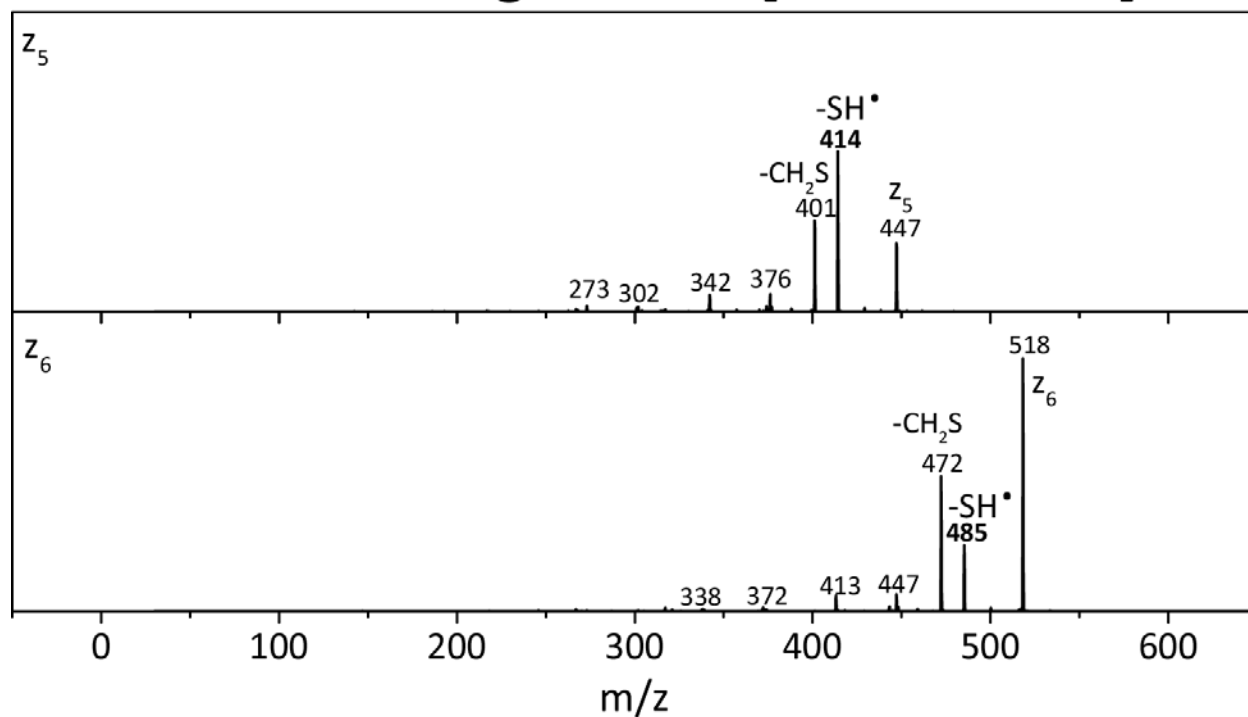
**Additional figures:** CID mass spectra of z<sup>\*</sup>-type ETD fragment ions containing a Cys residue which is not at the cleavage site. The z<sup>\*</sup>-type fragments with Cys at the cleavage site are discussed in the main text. Computed spectra for additional conformers of the vinyl-group N-terminal structures of the z<sub>3</sub> – 33 and z<sub>4</sub> – 33 ions presented in Figure 2 of the main text.

## CID on ETD fragments of AAAACAK

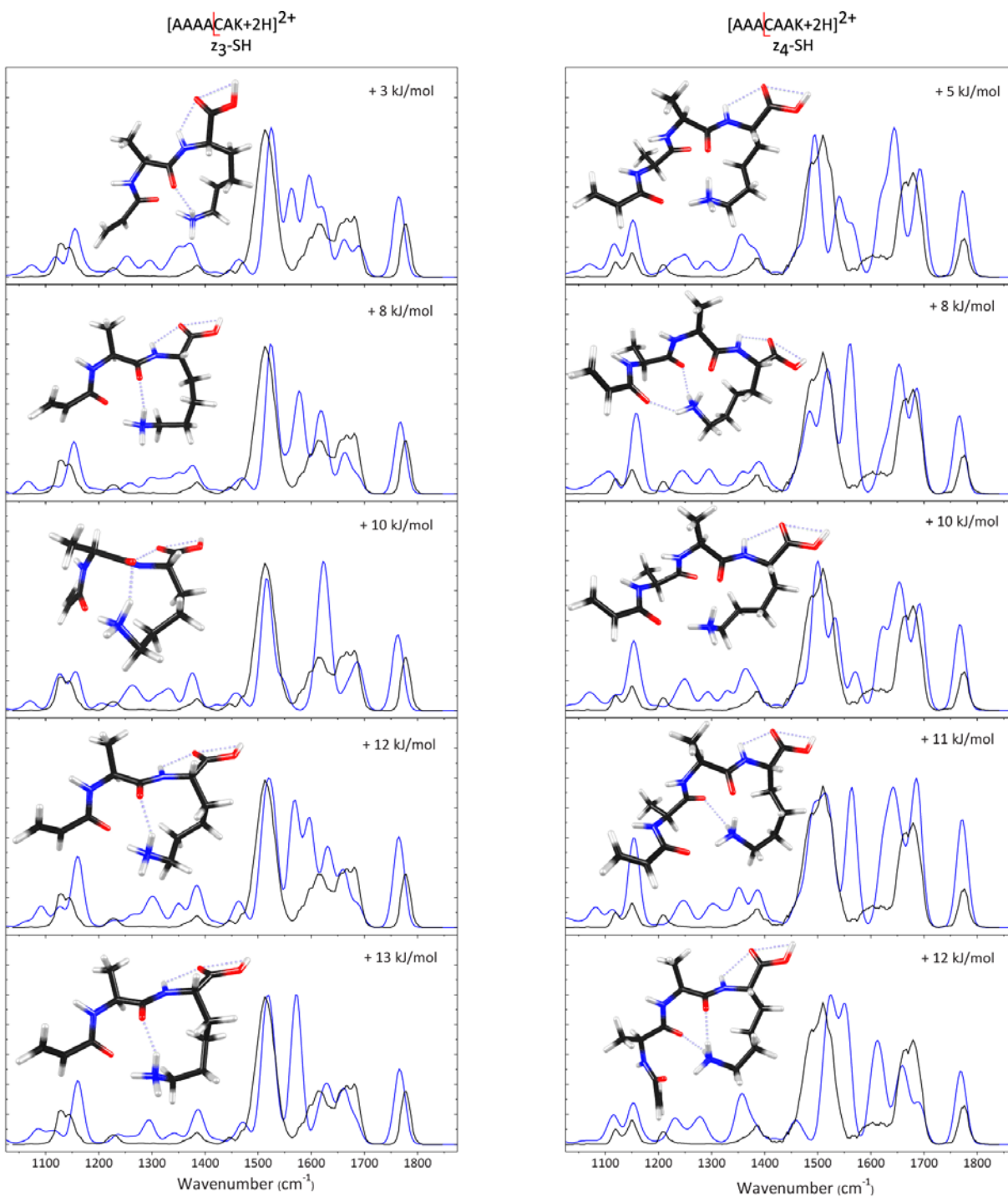


**Figure S1.** Mass spectra of CID applied on  $z^\bullet$ -ions obtained from ETD of  $[AAAACAK+2H]^{2+}$ . The mass peaks corresponding to loss of the radical thiol group are indicated.

## CID on ETD fragments of [AAACAAK+2H]<sup>2+</sup>



**Figure S2.** Mass spectra upon CID fragmentation of  $z^*$ -ions obtained by ETD on [AAACAAK+2H]<sup>2+</sup>. The mass peaks corresponding to loss of the radical thiol group are indicated.



**Figure S3.** Additional conformers and their computed IR spectra of the  $z_3 - 33$  and  $z_4 - 33$  ions under discussion.