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SUPPORTING INFORMATION

Mass spectral signatures of complex post-translational modifications in proteins: a proof-of-principle based on X-ray irradiated vancomycin

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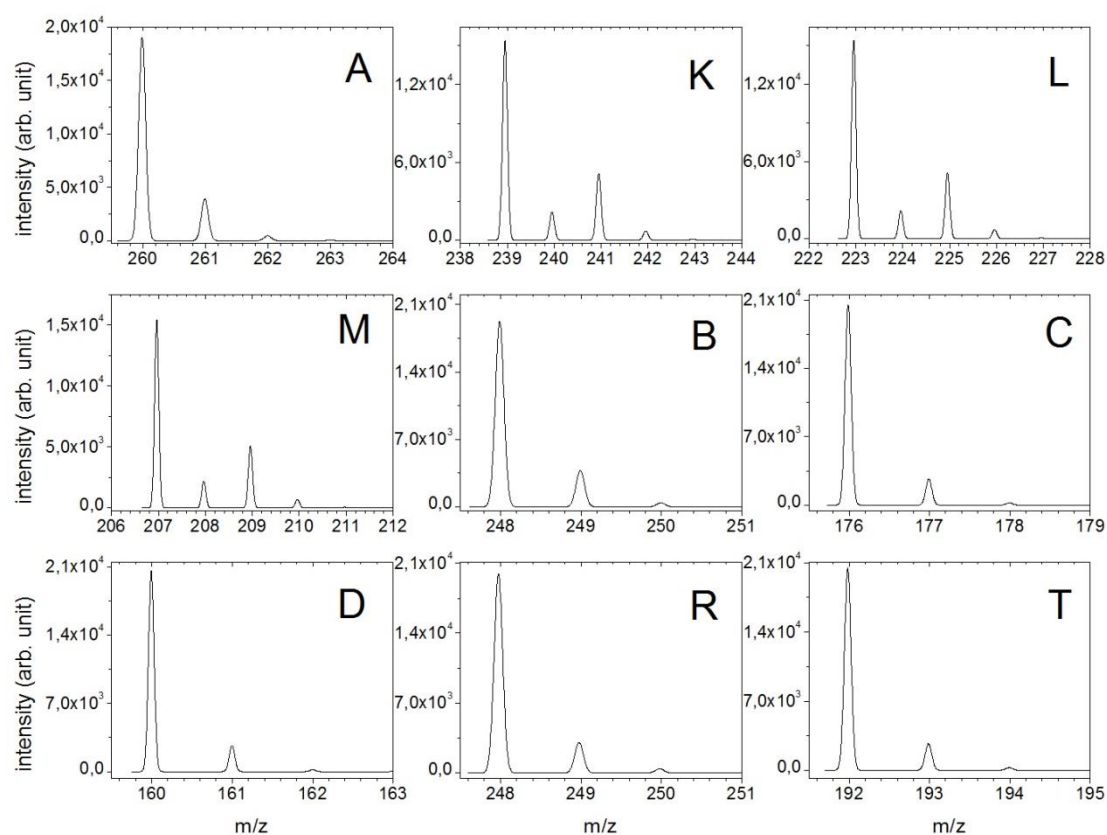


Figure S1. Simulated mass spectra of singly-charged internal fragments of vancomycin shown in Scheme 1, showing isotopic patterns. Gaussian functions with a mass resolving power of 2000 have been used. The fragments are indicated by the same letters as in Scheme 1.

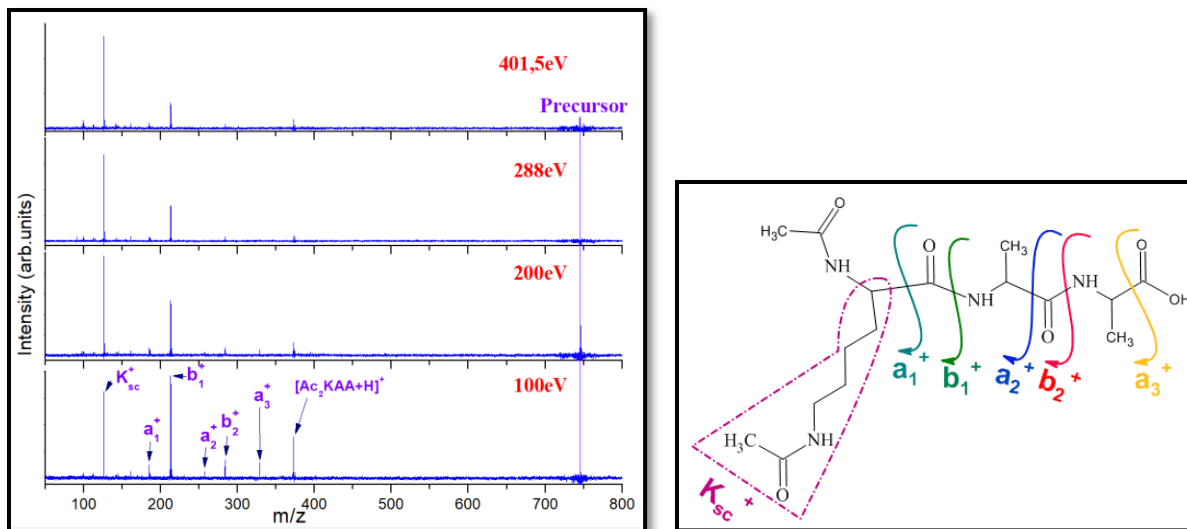


Figure S2. Left: mass spectra of $[R_2+H]^+$ after absorption of one photon of energy between 100 and 401.5 eV. The position of the precursor ion (m/z 745) is represented by purple dashes. The usual nomenclature for peptide backbone fragmentation is used for the main fragments observed after photoabsorption, illustrated on the scheme (right). Arrows indicate on which side of the cleaved bond the charge is located.

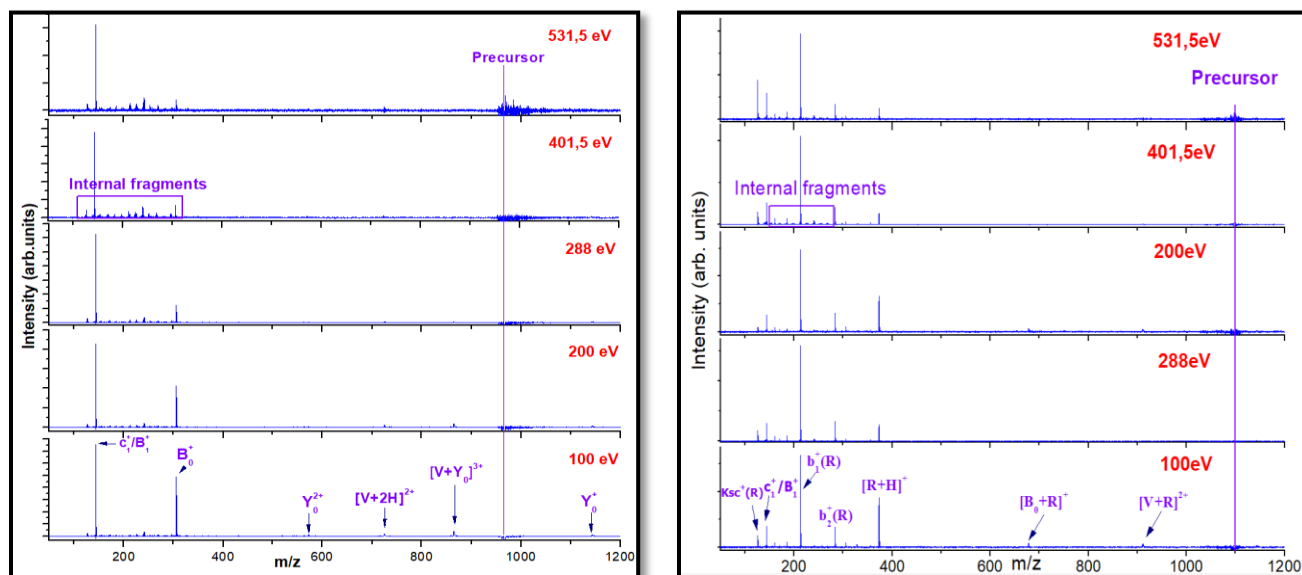


Figure S3. Mass spectra of $[V_2+3H]^{3+}$ (left) and $[V+R_2+2H]^{2+}$ (right) after absorption of one photon of energy between 100 and 531.5 eV. The position of the precursor ions (m/z 967.2 (left) and 1097.6 (right)) is represented by purple dashes. The usual nomenclature is used for the peptide backbone as well as for oligosaccharide fragmentation and hence for the main fragments observed after photoabsorption (cf. Fig. 1). Fragments of R are spotted by (R). Internal fragments of vancomycin formed by at least two bond cleavages are indicated.

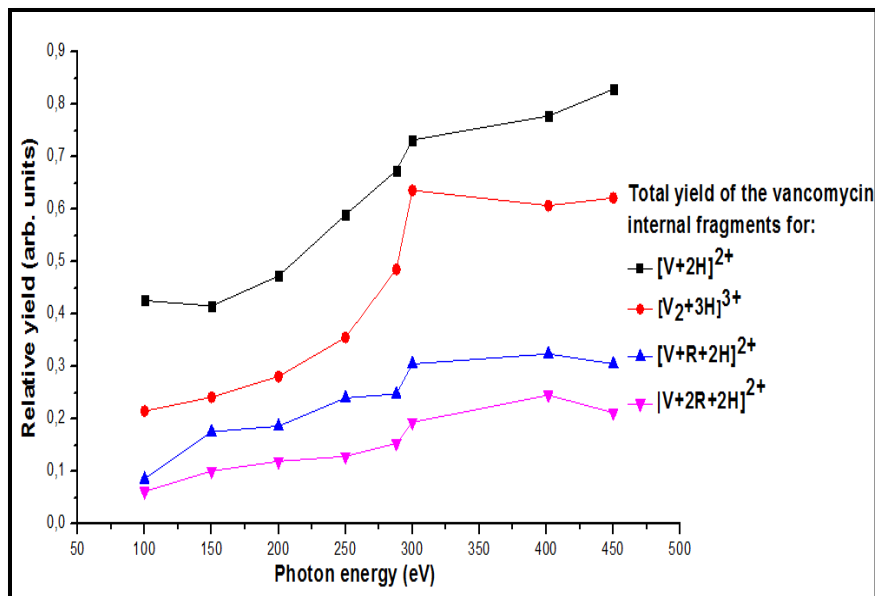


Figure S4. Total yield of the internal fragments of vancomycin formed by photoabsorption by different molecular systems: $[V+2H]^{2+}$, $[V_2+3H]^{3+}$, $[V+R+2H]^{2+}$ and $[V+2R+2H]^{2+}$ as a function of photon energy. All yields have been normalized by the detector efficiency and the total yield of photoinduced cations.