Electronic supplementary information

Discrimination of Leucine and Isoleucine in Peptide Sequencing with the Orbitrap Fusion Mass Spectrometer

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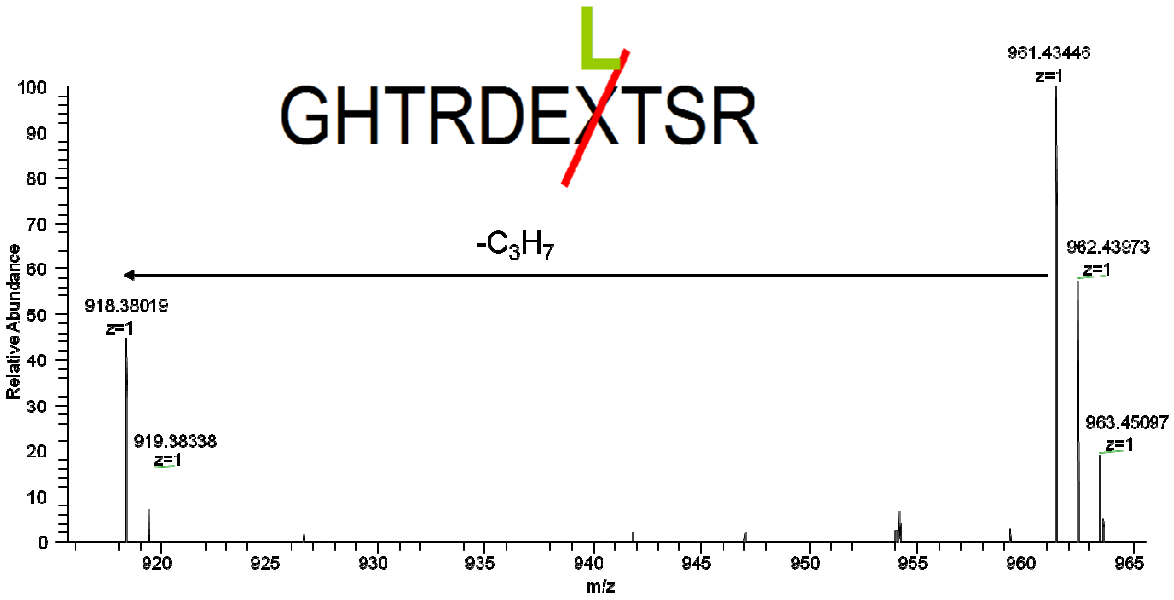

TOC

Table S1. Natural peptides used in the experiments

Name	Sequence*	Monoisoto-pic mass	Sequence comment
Ranatuerin 2R	AVNIPFKVKFRCKAAFC	1939.0325	Confirmed
Brevinin 1Ra	VIPFVASVAAEMMQHVYCAASRRC	2636.2485	Confirmed
Brevinin 1E	FLPLLAGLAANFLPKIFCKITRKC	2674.5220	Confirmed
Brevinin 2Ec	GILLDKLKNFAKTAGKGVLQSLLNT ASCKLSGQC	3516.9161	Confirmed
Ranatuerin 2Ra	KL/IL/IL/INPKFRCKAAFC	1748.9583	Non confirmed
Esculentin 2R	GL/IL/ISL/IVKGVAKL/IAGKTFAKEG GKFGL/IEFL/IACKVTNQC	3823.0893	Non confirmed

*Disulfide loop due to two cysteins is underlined

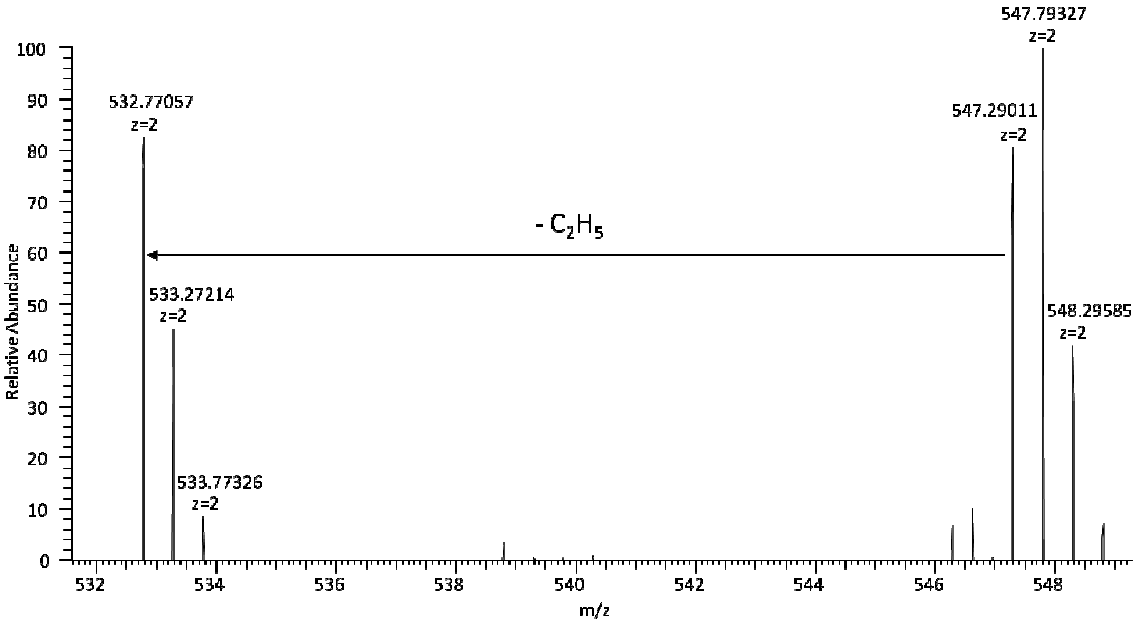

Fig.S1. EThcD spectrum of doubly charged z_9 ion of brevinin 1E.

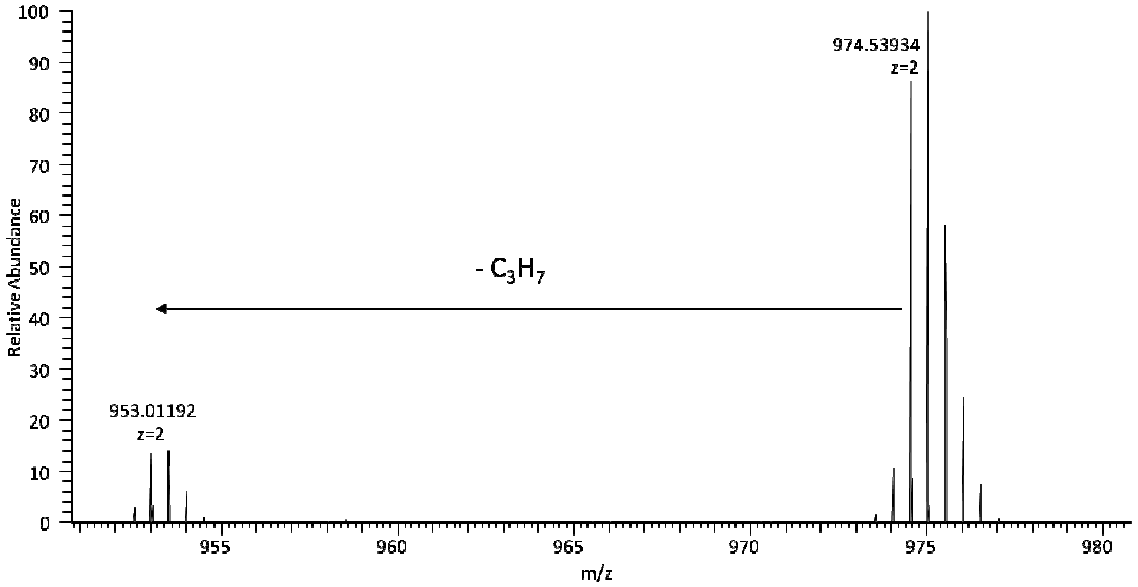

Fig.S2. EThcD spectrum of doubly charged z_{17} ion of brevinin 1E.

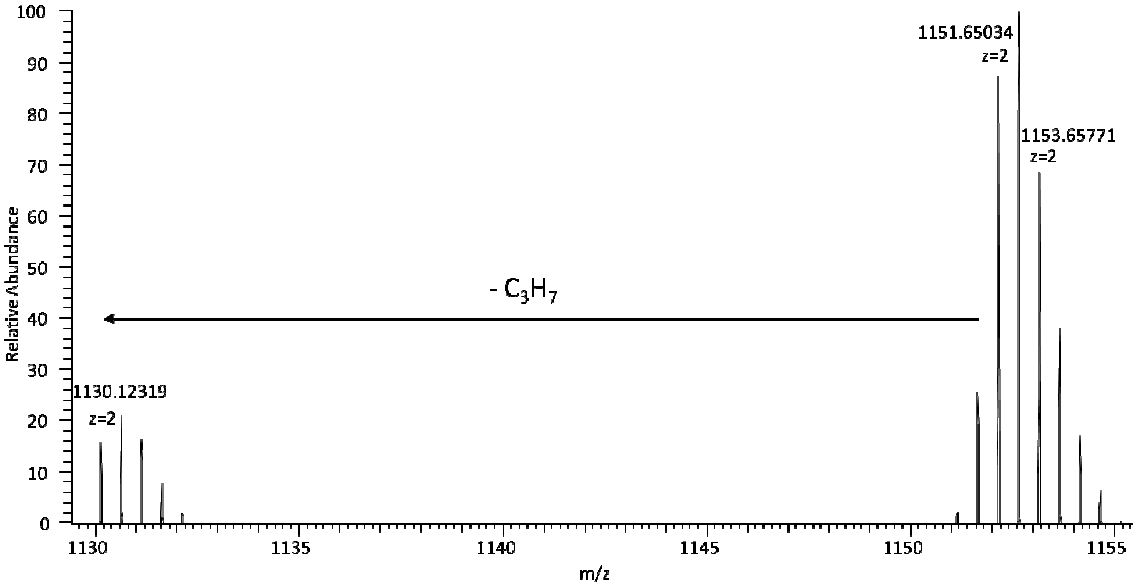

Fig.S3. EThcD spectrum of doubly charged z_{21} ion of brevinin 1E.

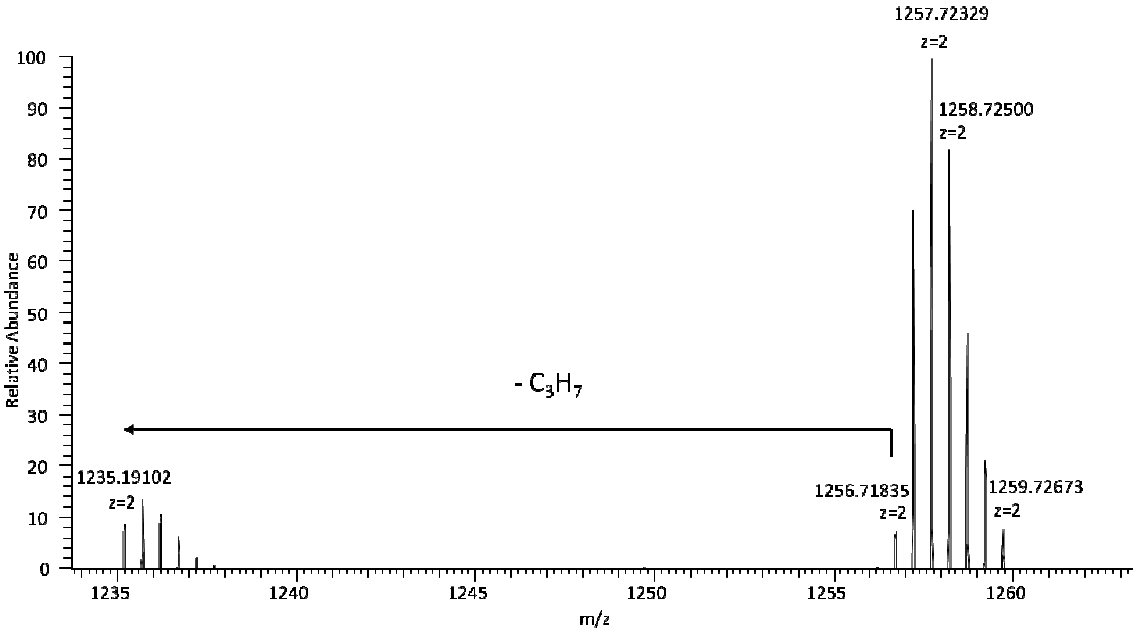

Fig.S4. EThcD spectrum of doubly charged z_{23} ion of brevinin 1E.

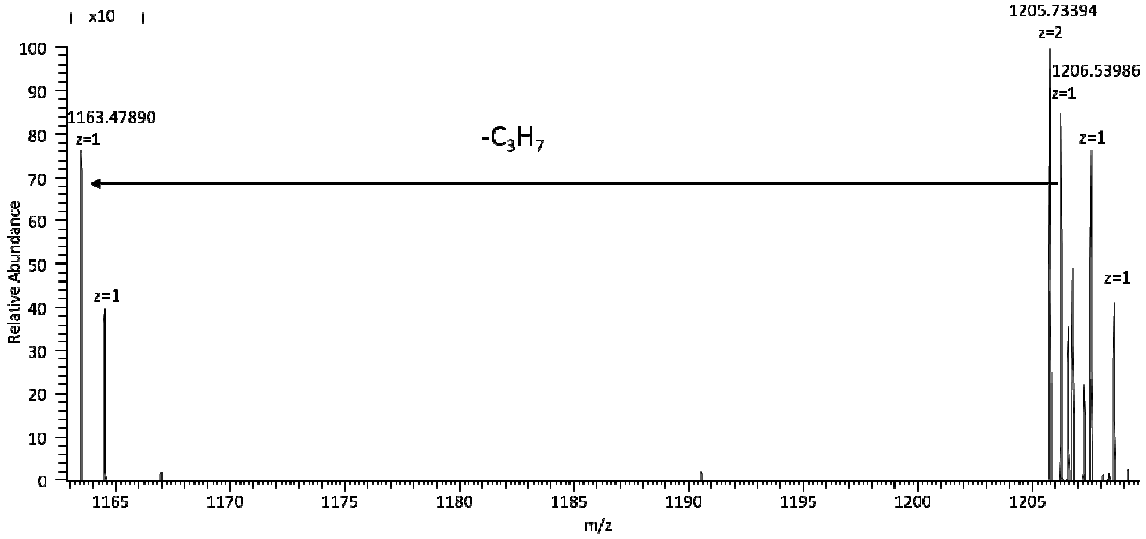

Fig.S5. EThcD spectrum of singly charged z_{12} ion of brevinin 2Ec. Pay attention that the precursor ion with monoisotopic mass 1206.53986 is not the base peak in the selected cluster of isobaric ions

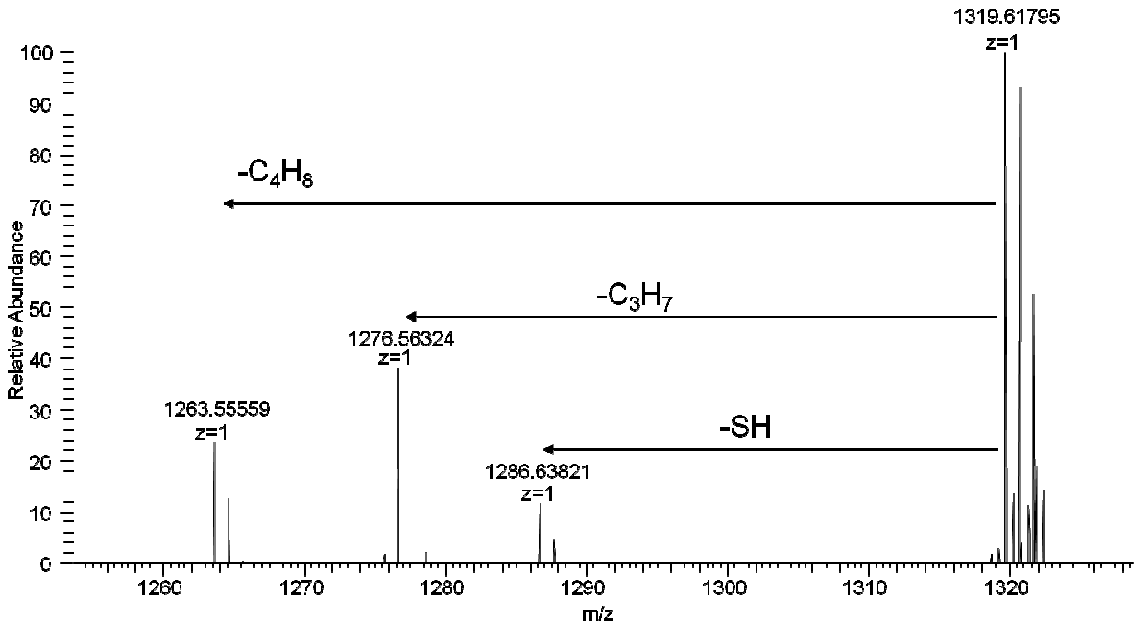

Fig.S6. EThcD spectrum of singly charged z_{13} ion of brevinin 2Ec.

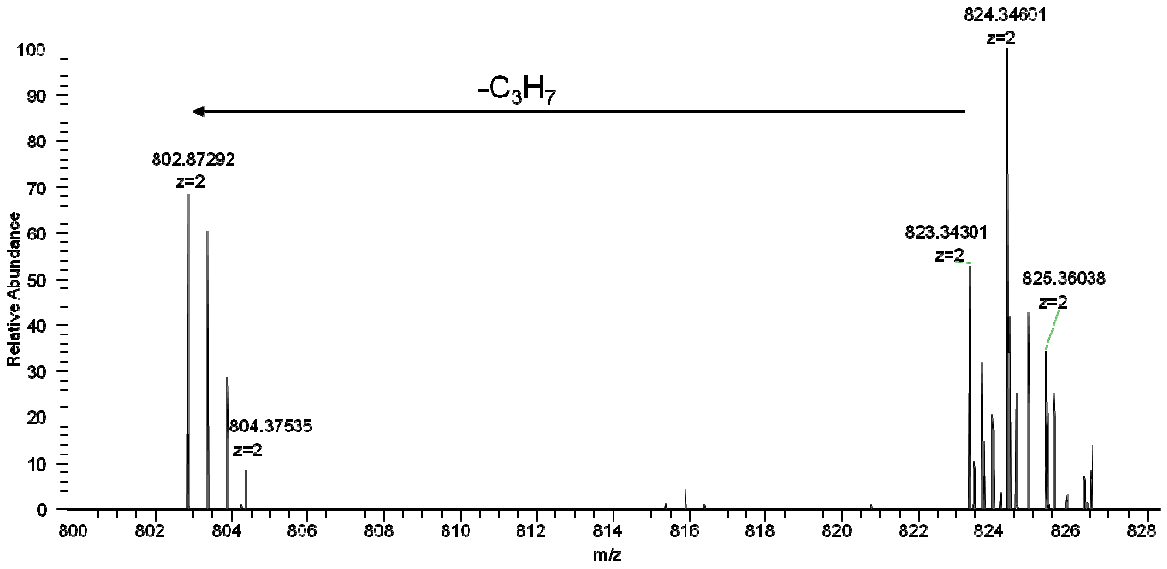

Fig.S7. EThcD spectrum of doubly charged z_{16} ion of brevinin 2Ec. The interferences with isobaric precursor peaks (ca Fig.S8) are not important for the L/I determination.

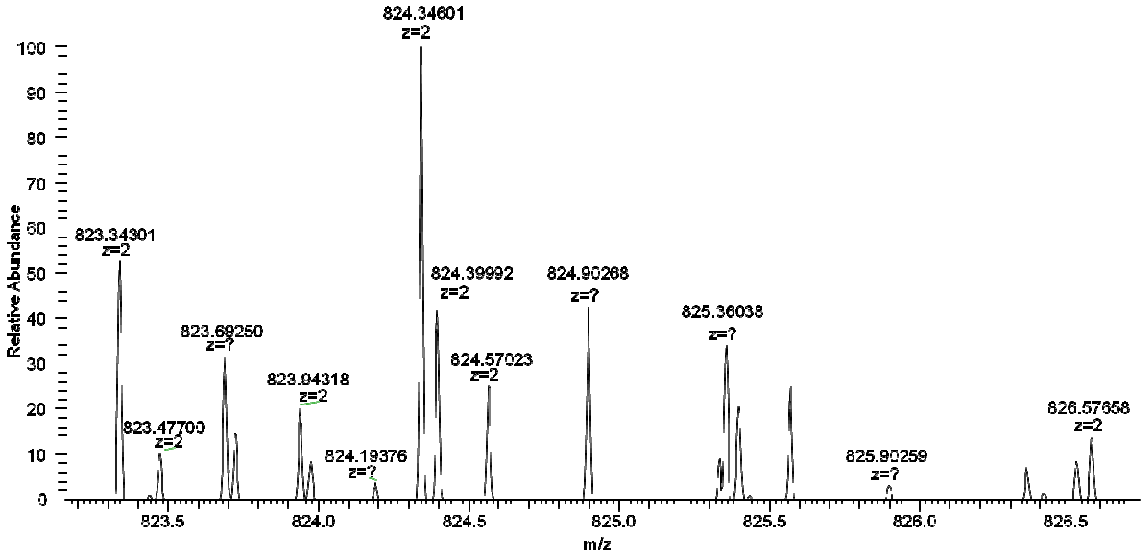

Fig.S8. Cluster of the precursor ions used for the fragmentation of z_{16} ion of brevinin 2Ec. Monoisotopic z_{16} ion has m/z value 824.39992, being a minor constituent among other selected ions.

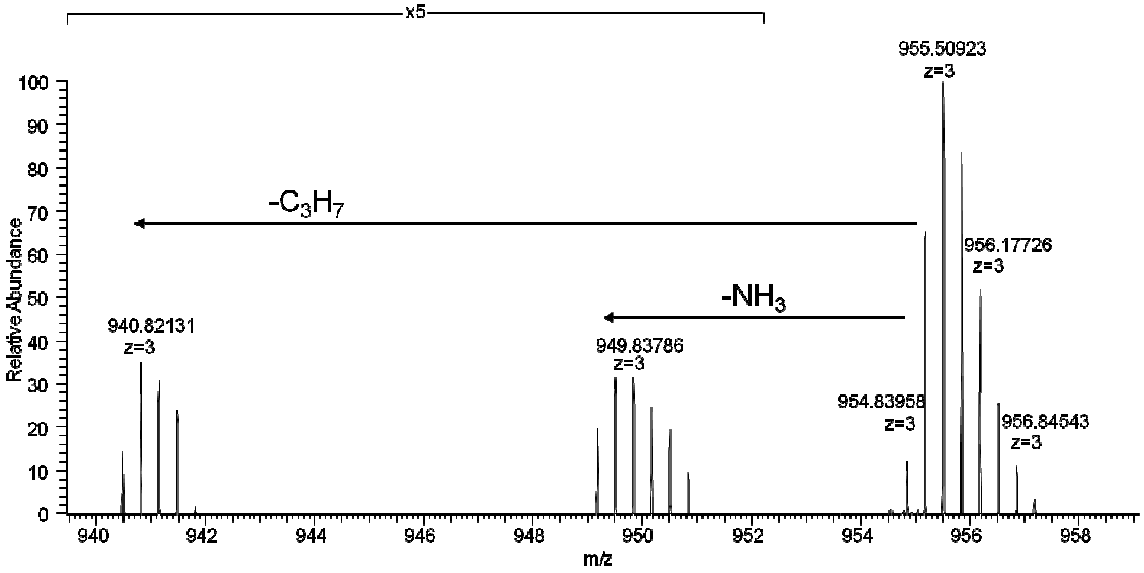

Fig.S9. EThcD spectrum of triply charged z_{28} ion of brevinin 2Ec.

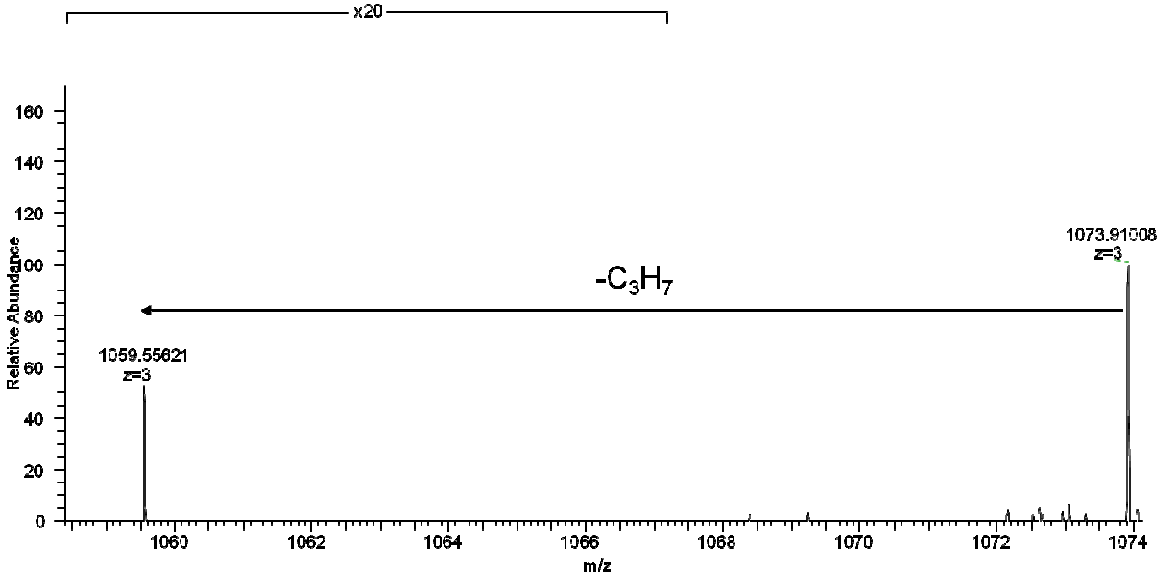

Fig.S10. EThcD spectrum of triply charged z_{31} ion of brevinin 2Ec. Only monoisotopic peak is selected as precursor

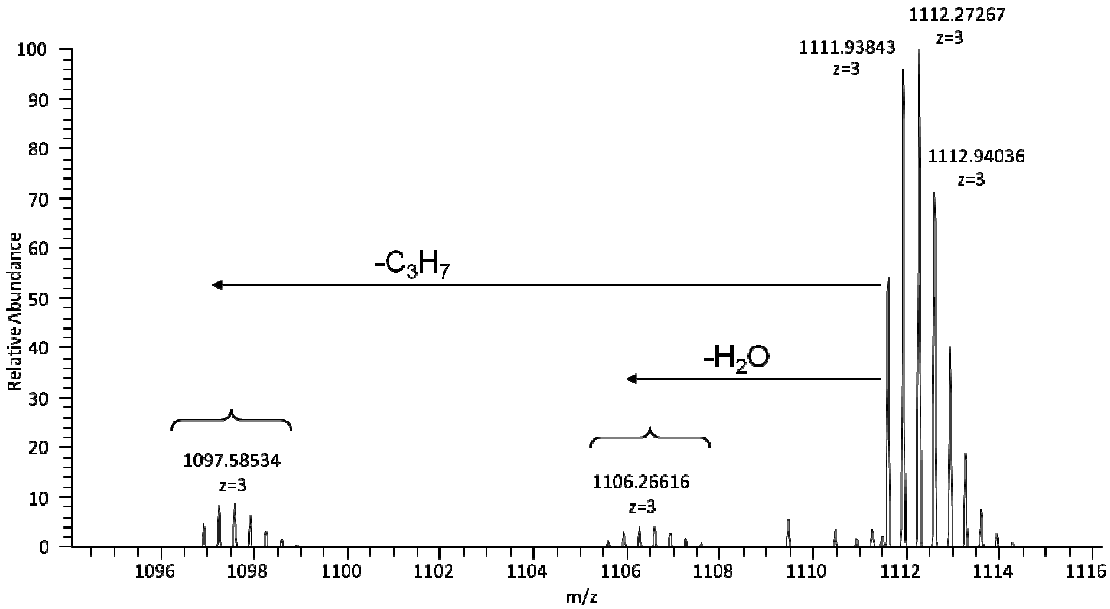

Fig.S11. EThcD spectrum of triply charged z_{32} ion of brevinin 2Ec.

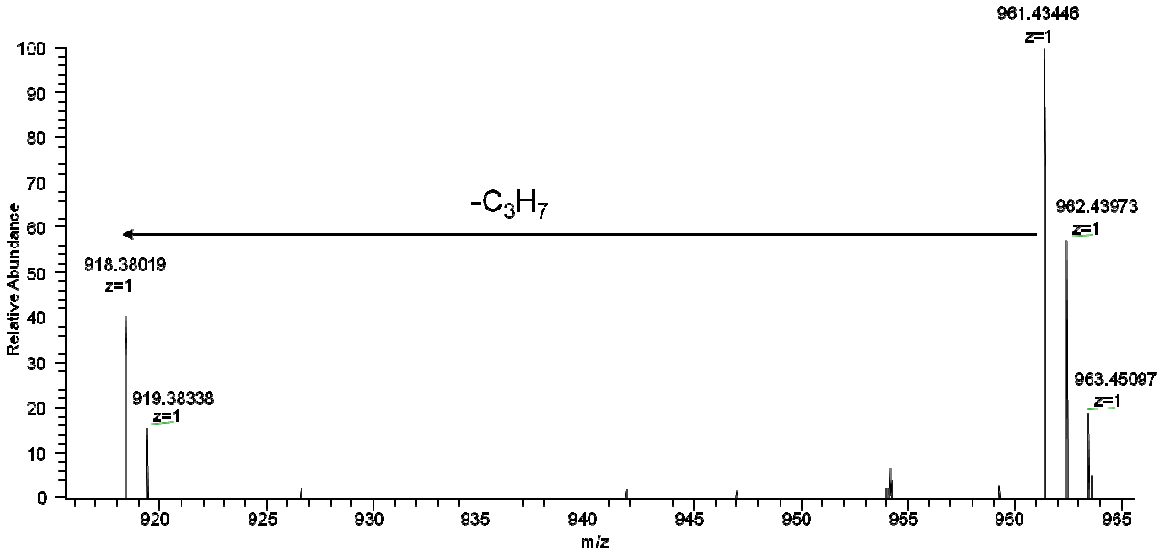

Fig.S12. EThcD spectrum of singly charged z_9 ion of esculentin 2R.

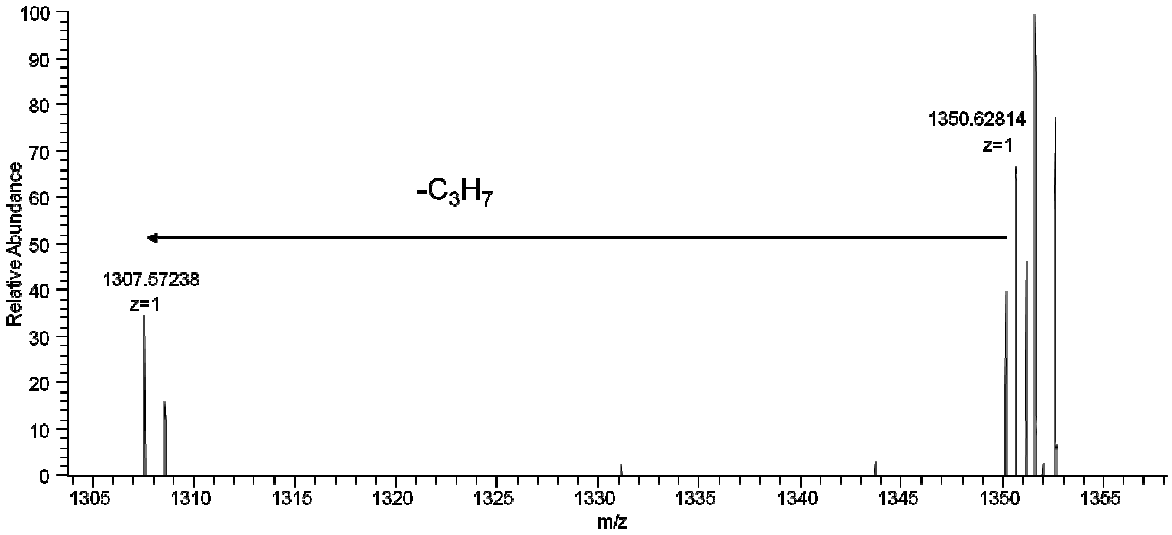

Fig.S13. EThcD spectrum of singly charged z_{12} ion of esculentin 2R. The interferences with isobaric precursor peaks are not important for the L/I determination

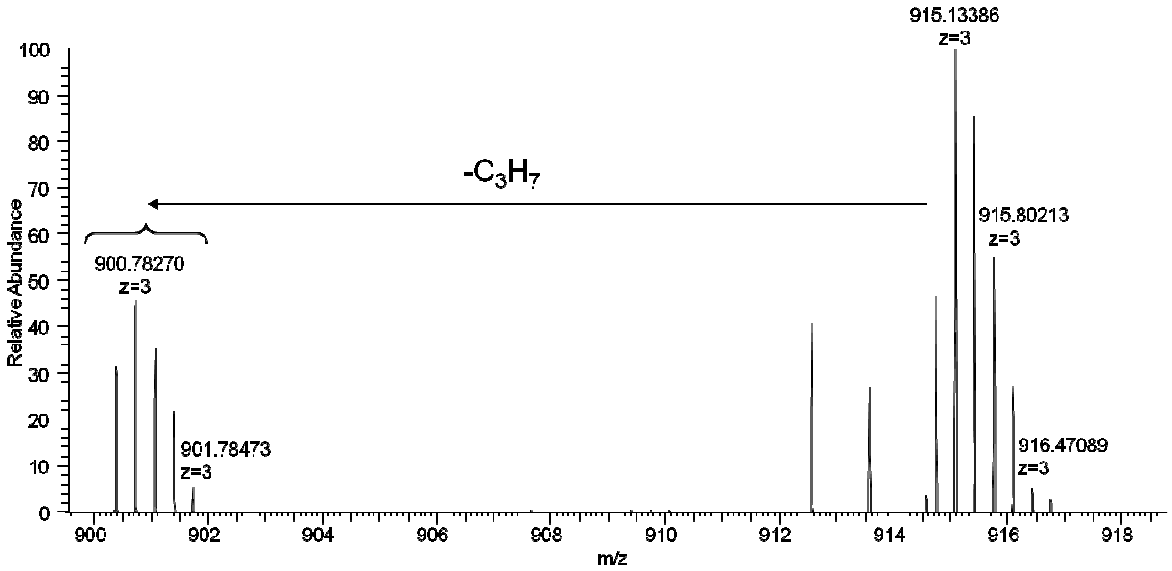

Fig.S14. EThcD spectrum of triply charged z_{26} ion of esculentin 2R.

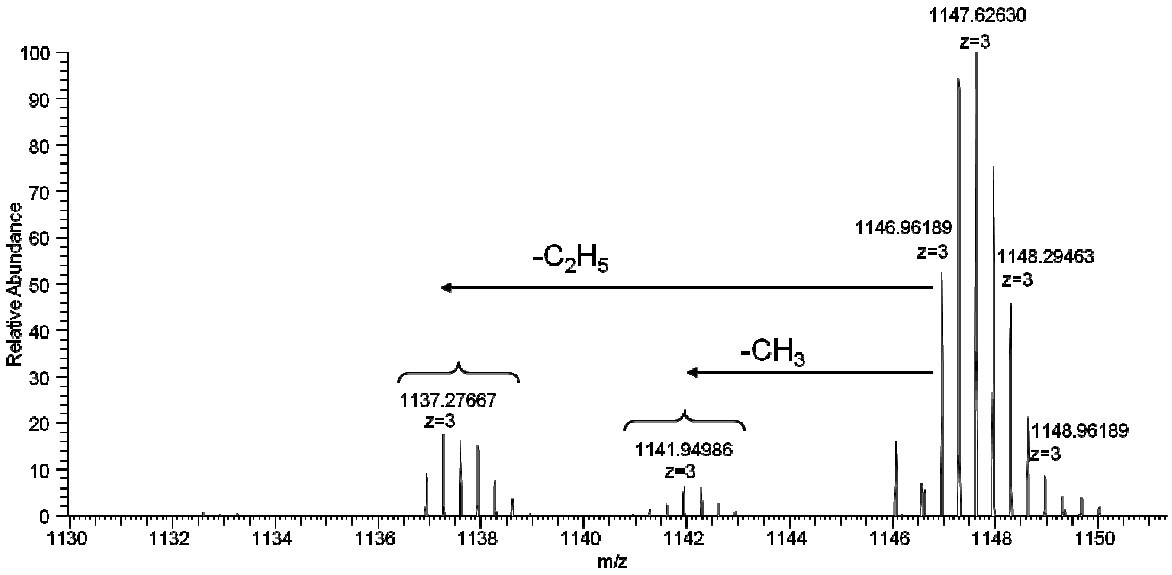

Fig.S15. EThcD spectrum of triply charged z_{33} ion of esculentin 2R.

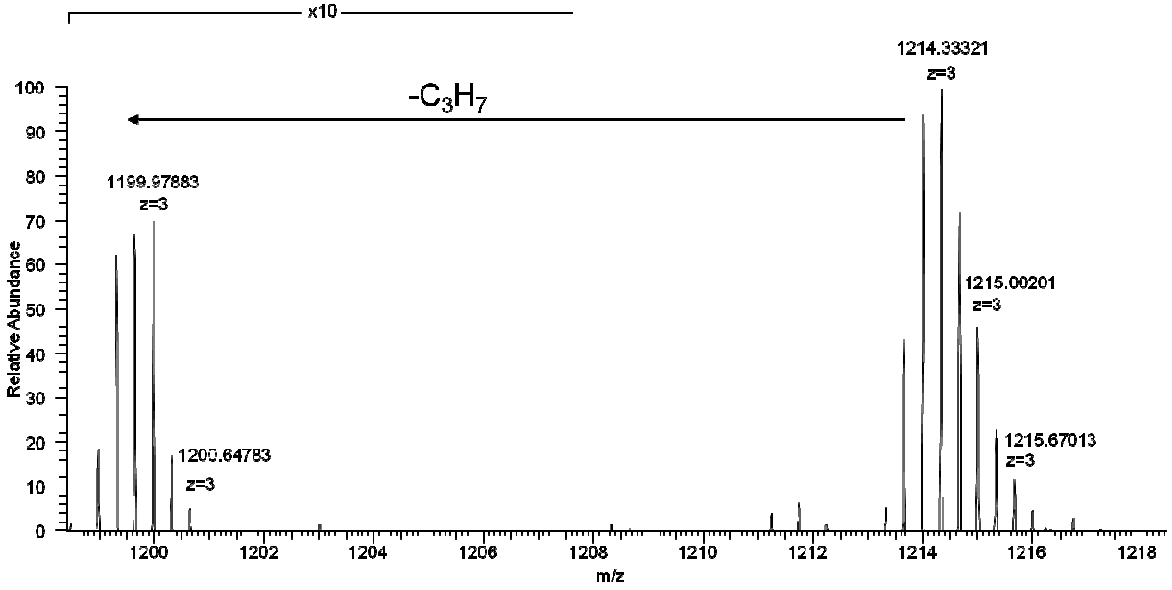

Fig.S16. EThcD spectrum of triply charged z_{35} ion of esculentin 2R.

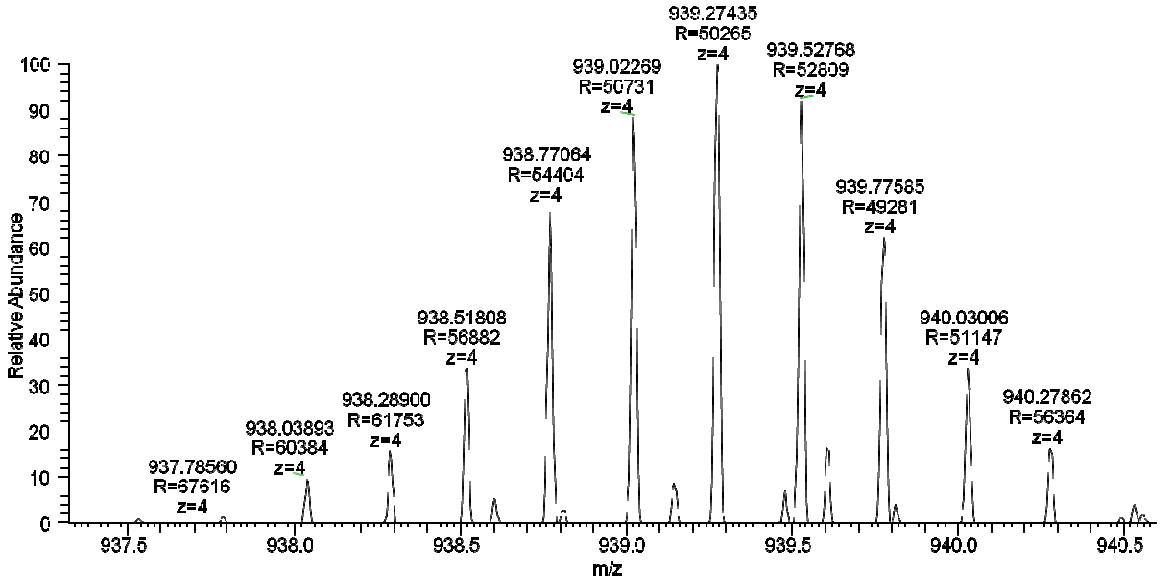

Figure S17. Isolation of z_{36}^{+4} ion formed in ETD spectrum of esculentin 2R.

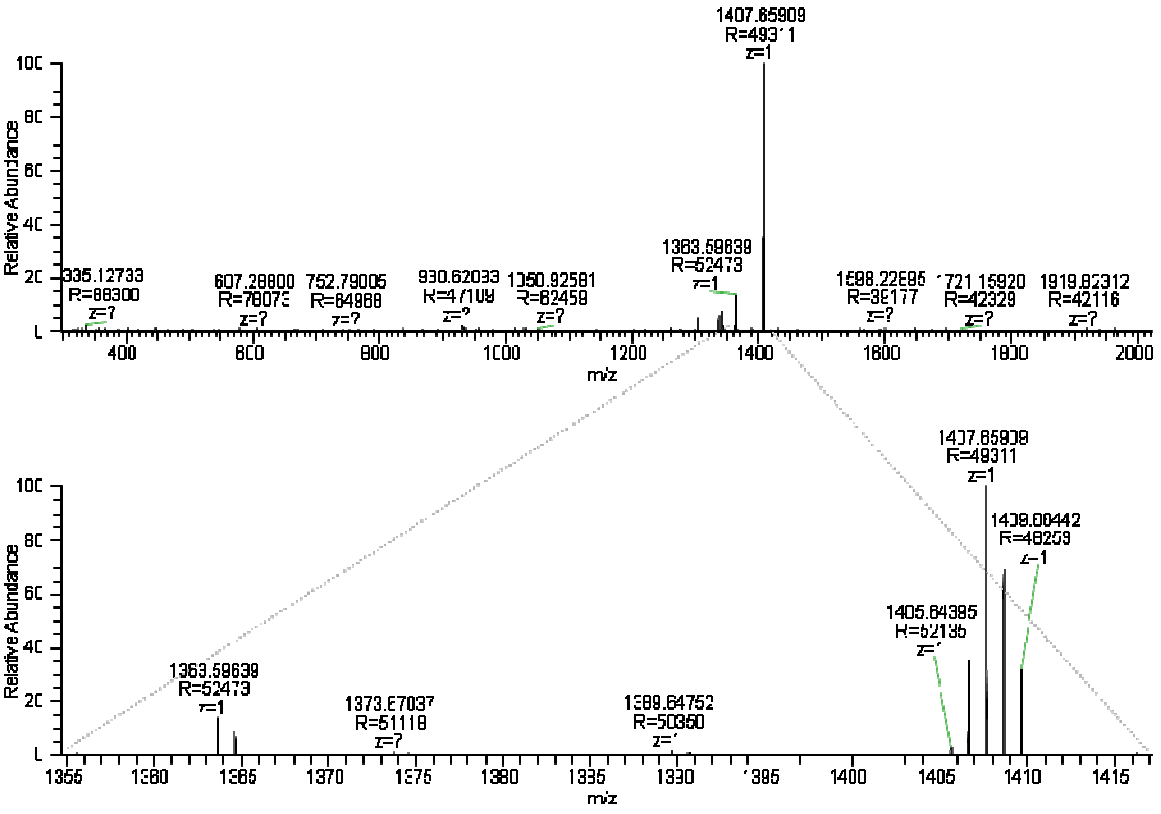

Fig.S18. EThcD spectrum of singly charged z_{14} ion of brevinin-2Ec.

Fig.S18 demonstrates an example of the radical site migration. In this case z_{14} ion has two Leu residues in the second and third positions to the radical center at N-terminus. The targeted low

abundant *w*-ion of m/z 1363.5964 is present in the spectrum recorded at 30 eV. At lower energies its intensity is negligible.

On the other hand there are no peaks of *w*-ions or any other secondary fragments (even with 50x zoom) in the spectrum of z_{18} ion (Fig.S19), in which Leu occupies the third position from N-terminus.

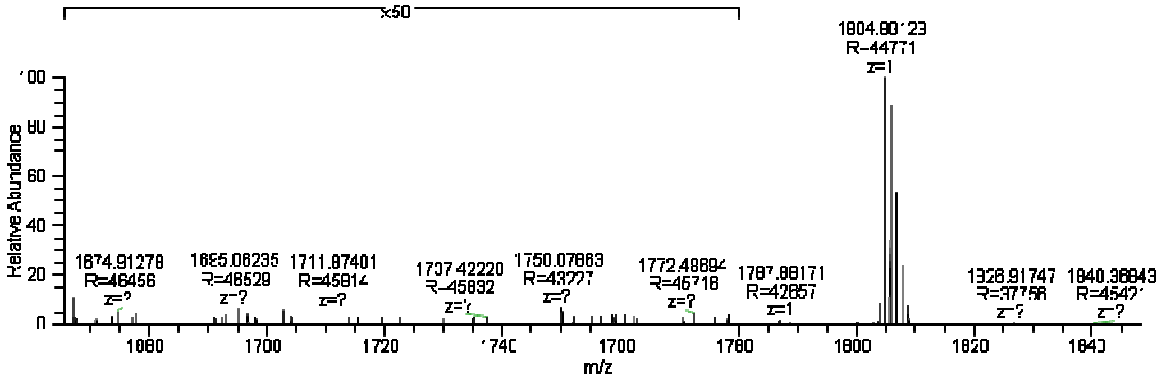

Fig.S19. EThcD spectrum of singly charged z_{18} ion of brevinin-2Ec.