# Supplement

# Gouda cheese with modified content of β-casein as a source of peptides with ACE- and DPP-IV-inhibiting bioactivity: a study based on *in silico* and *in vitro* protocol

**Anna Iwaniak, Damir Mogut, Piotr Minkiewicz, Justyna Żulewska and Małgorzata Darewicz**

**Table S1.** Peptides with ACE- and DPP-IV-inhibitory activity encrypted in casein sequences. Data obtained using the BIOPEP-UWM database [13,61] (accessed January-March 2020).

| Sequence | \alpha_{S1}/A A[1] | \alpha_{S1}/A D[2] | \alpha_{S1}/B A | \alpha_{S1}/B D | \alpha_{S1}/C A | \alpha_{S1}/C D | \alpha_{S1}/D A | \alpha_{S1}/D D | \alpha_{S2}/A A | \alpha_{S2}/A D | β/A1 A | β/A1 D | β/A2 A | β/A2 D | β/A3 A | β/A3 D | β/B A | β/B D | β/C A | β/C D | β/E A | β/E D | β/F A | β/F D | κ/A A | κ/A D |
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| **AA[3]** | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 | 1 |
| AE | - | 2 | - | 2 | - | 2 | - | 2 | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| **AF** | - | - | - | - | - | - | - | - | - | - | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | - | - |
| AI | - | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 | - |
| AL | - | - | - | - | - | - | - | 1 | - | 3 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 2 |
| **AP** | 1 | 1 | 2 | 2 | 2 | 2 | 2 | 2 | - | - | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | - | - |
| AR | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 | - |
| AS | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 |
| AT | - | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 |
| AV | - | - | - | - | - | - | - | 1 | - | 2 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 3 |
| **AW** | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| **AY** | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| DA | 2 | - | 2 | - | 2 | - | 2 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| DQ | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
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| EH | - | - | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| **EI** | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 2 | 2 |
| **EK** | 2 | 2 | 2 | 2 | 1 | 1 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 1 | 1 | 3 | 3 | 2 | 2 | 2 | 2 | 1 | 1 |
| EP | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - | - | - | - | - | - | - | - | 2 | - | - | - | - | - | - | 1 |
| ES | - | 2 | - | 2 | - | 2 | - | 2 | - | 3 | - | 3 | - | 3 | - | 3 | - | 2 | - | 3 | - | 3 | - | 3 | - | 2 |
| ET | - | - | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| **EV** | - | - | 1 | 1 | 1 | 1 | 2 | 2 | 4 | 4 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| **EY** | - | - | - | - | - | - | - | - | 1 | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| FA | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - |
| FG | 1 | - | 1 | - | 1 | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| FL | - | - | - | - | - | - | - | - | - | 1 | - | 2 | - | 2 | - | 2 | - | 2 | - | 2 | - | 2 | - | 2 | - | 3 |
| **FP** | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | - | - |
| FQ | - | - | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - |
| **FR** | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| FY | 2 | - | 2 | - | 2 | - | 2 | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| **GA** | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 | 1 |
| **GE** | - | - | - | - | - | - | - | - | - | - | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| **GI** | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| GK | 1 | - | 1 | - | 2 | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| **GL** | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 | 1 |
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| GS | 2 | - | 2 | - | 2 | - | 2 | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| GT | 1 | - | 1 | - | 1 | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| **GV** | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | - | - | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | - | - |
| **GY** | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| HA | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| HI | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| HK | - | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - |
| **HL** | - | - | - | - | - | - | - | - | - | - | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| **HP** | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | - | - | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 2 | 2 |
| HS | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
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| IF | - | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| IG | 3 | - | 3 | - | 3 | - | 3 | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| IH | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - | 2 | - | 1 | - | 2 | - | 1 | - | 2 | - | 1 | - | 2 | - | - |
| II | - | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - |
| IL | - | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 2 |
| IN | - | - | - | - | - | - | - | - | - | 2 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 3 |
| **IP** | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 2 | 2 | 1 | 1 | 2 | 2 | 1 | 1 | 2 | 2 | 1 | 1 | 3 | 3 |
| IQ | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 |
| **IR** | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 | 1 |
| **KA** | - | - | - | - | - | - | - | - | 2 | 2 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | - | - |
| **KE** | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 3 | 3 | 2 | 2 | - | - |
| **KF** | - | - | - | - | - | - | - | - | 3 | 3 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | - | - |
| KH | - | 3 | - | 3 | - | 3 | - | 3 | - | 1 | - | 1 | - | 1 | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | - |
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| KK | - | 1 | - | 1 | - | 1 | - | 1 | - | 3 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 |
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| **KR** | - | - | - | - | - | - | - | - | 1 | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| KS | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 2 |
| KT | - | 1 | - | 1 | - | 1 | - | 1 | - | 4 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 |
| KV | - | 2 | - | 2 | - | 2 | - | 2 | - | 1 | - | 2 | - | 2 | - | 2 | - | 2 | - | 2 | - | 2 | - | 2 | - | - |
| **KY** | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | - | - | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| **LA** | 1 | 1 | 1 | 1 | 1 | 1 | 2 | 2 | 2 | 2 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 | 1 |
| LF | 1 | - | 1 | - | 1 | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| LG | 2 | - | 2 | - | 2 | - | 2 | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - |
| LH | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - |
| LI | - | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 |
| LL | - | 1 | - | 2 | - | 2 | - | 3 | - | 1 | - | 3 | - | 3 | - | 3 | - | 2 | - | 3 | - | 3 | - | 4 | - | - |
| **LN** | - | - | 1 | 1 | 1 | 1 | 1 | 1 | 4 | 4 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
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| LY | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - |
| MA | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | 2 |
| **ME** | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| **MF** | - | - | - | - | - | - | - | - | - | - | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | - | - |
| **MG** | - | - | - | - | - | - | - | - | - | - | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | - | - |
| MH | - | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - |
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| NT | - | - | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 3 |
| NV | - | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - |
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| PA | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 3 |
| PF | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - | 6 | - | 6 | - | 6 | - | 6 | - | 6 | - | 6 | - | 6 | - | 1 |
| **PG** | - | - | - | - | - | - | - | - | - | - | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | - | - |
| **PH** | - | - | - | - | - | - | - | - | - | - | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 2 | 2 |
| PI | - | 2 | - | 2 | - | 2 | - | 2 | - | 2 | - | 3 | - | 3 | - | 3 | - | 3 | - | 3 | - | 3 | - | 3 | - | 2 |
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| **PL** | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | - | - | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | - | - |
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| **PP** | - | - | - | - | - | - | - | - | - | - | 5 | 5 | 5 | 5 | 5 | 5 | 4 | 4 | 5 | 5 | 5 | 5 | 4 | 4 | 2 | 2 |
| **PQ** | 3 | 3 | 3 | 3 | 3 | 3 | 2 | 2 | 2 | 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | - | - |
| PS | - | 3 | - | 3 | - | 3 | - | 3 | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 |
| **PT** | - | - | - | - | - | - | - | - | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 4 | 4 |
| PV | - | - | - | - | - | - | - | - | - | - | - | 5 | - | 5 | - | 5 | - | 5 | - | 5 | - | 5 | - | 5 | - | 1 |
| PW | - | - | - | - | - | - | - | - | - | 2 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| PY | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 2 |
| QA | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 |
| QD | - | - | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 |
| QE | - | 1 | - | 2 | - | 2 | - | 2 | - | 2 | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | 2 |
| QF | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 |
| **QG** | 2 | 2 | 2 | 2 | 2 | 2 | 1 | 1 | 1 | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
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| **VP** | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 1 | 1 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 1 | 1 |
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| VRSP | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 | - |
| VRYL | - | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| VVPP | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - |
| WIQP | - | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| YAKP | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 | - |
| YPYY | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 |
| AMKPW | - | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| AVPYP | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - |
| AYFYP | 1 | - | 1 | - | 1 | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| FFVAP | - | - | 1 | - | 1 | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| FPIIV | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - |
| HLPLP | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - |
| IPIQY | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 |
| KDERF | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 | - |
| LPLPL | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - |

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **LPYPY** | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 | 1 |
| NLHLP | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - | - |
| PGPIP | - | - | - | - | - | - | - | - | - | 1 | - | - | - | - | - | 1 | - | - | - | - | - | 1 | - | - | - | - |
| RHPHP | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 | - |
| RYLGY | 1 | - | 1 | - | 1 | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| RYQKF | - | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| SLVYP | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - | - |
| SRYPS | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 | - |
| TKVIP | - | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| YAKPA | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 | - |
| ARHPHP | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 | - |
| AYFYPE | 1 | - | 1 | - | 1 | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| DKIHPF | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - | - |
| EKDERF | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 | - |
| EMPFPK | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - | - |
| FALPQY | - | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| KVLPVP | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - | - |
| LAYFYP | 1 | - | 1 | - | 1 | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| LHLPLP | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - | - |
| LKKISQ | - | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| PYVRYL | - | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| QSLVYP | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - | - |
| TTMPLW | 1 | - | 1 | - | 1 | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| VPITPT | - | - | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| VTSTAV | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 | - |
| VYPFPG | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - | - |
| YFYPEL | 1 | - | 1 | - | 1 | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| YIPIQY | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 | - |
| YKVPQL | 1 | - | 1 | - | 1 | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| YQEPVL | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - | - |
| YQQPVL | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | - | - | 1 | - | 1 | - | 1 | - | - | - | - |
| YYQQKP | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 | - |
| AVPYPQR | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - | - |

| Sequence | | | | | | | | | | | | | | | | | | | | | | | | | |
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| AYFYPEL | 1 | - | 1 | - | 1 | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| FPEVFGK | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| FPGPIPN | - | - | - | - | - | - | - | - | - | - | - | 1 | - | - | - | - | 1 | - | - | - | - | 1 | - | - | - |
| FPQYLQY | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| FSDKIAK | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 | - |
| GPFPIIV | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - |
| KVLPVPQ | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - |
| LHLPLPL | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - |
| LLYQQPV | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | - | 1 | - | 1 | - | 1 | - | - | - | - |
| LPQNIPP | - | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - |
| LTLTDVE | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - |
| NLHLPLP | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - |
| TESQSLT | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | - | 1 | - | 1 | - | 1 | - | - | - | - |
| TQSLVYP | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - |
| YPFPGPI | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - |
| AYFYPELF | 1 | - | 1 | - | 1 | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| DAYPSGAW | 1 | - | 1 | - | 1 | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| ENLHLPLP | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - |
| FALPQYLK | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| MKPWIQPK | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| NMAINPSK | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| QTQSLVYP | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - |
| RGPFPIIV | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - |
| SKVLPVPE | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | - | 1 | - | 1 | - | 1 | - | - | - | - |
| VYPFPGPI | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - |
| YPFPGPIP | - | - | - | - | - | - | - | - | - | - | - | 1 | - | - | - | 1 | - | - | - | 1 | - | - | - | - | - |
| YPVQPFTE | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | - | 1 | - | 1 | - | 1 | - | - | - | - |
| ALNEINQFY | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| AQTQSLVYP | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - |
| IPPLTQTPV | - | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - |
| LNVPGEIVE | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - |
| QSWMHQPHQ | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - |
| RPKHPIKHQ | 1 | - | 1 | - | 1 | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |

| Sequence | | | | | | | | | | | | | | | | | | | | | | | | | | |
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| VRGPFPIIV | - | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - |
| YPFPGPIPN | - | - | - | - | - | - | - | - | - | - | 1 | - | - | - | 1 | - | - | - | 1 | - | - | - | - | - | - | - |
| YPQRDMPIQ | - | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - |
| YYAKPAAVR | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 | - |
| FAQTQSLVYP | - | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - |
| GPVRGPFPII | - | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - |
| NIPPLTQTPV | - | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - |
| YIPIQYVLSR | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1 | - |
| YQQPVLGPVR | - | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | - | - | 1 | - | 1 | - | 1 | - | - | - |
| ALNEINQFYQK | - | - | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| TPVVVPPFLQP | - | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - |
| FFVAPFPEVFGK | - | - | - | - | - | - | 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| HPFAQTQSLVYP | - | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - |
| IHPFAQTQSLVYP | - | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - |
| KIHPFAQTQSLVYP | - | - | - | - | - | - | - | - | - | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | - | - |
| LVYPFPGPIPNSLPQ NIPP | - | - | - | - | - | - | - | - | - | - | 1 | - | - | - | 1 | - | - | - | 1 | - | - | - | - | - | - | - |
| Total number of peptides | 93 | 114 | 100 | 122 | 101 | 121 | 107 | 132 | 88 | 154 | 120 | 166 | 125 | 168 | 120 | 165 | 129 | 169 | 121 | 167 | 126 | 170 | 118 | 166 | 80 | 147 |

[1]A – ACE inhibitor, [2]D - DPP-IV inhibitory, [3]**bold** – sequence with dual (i.e., ACE- and DPP-IV-inhibitory) activity
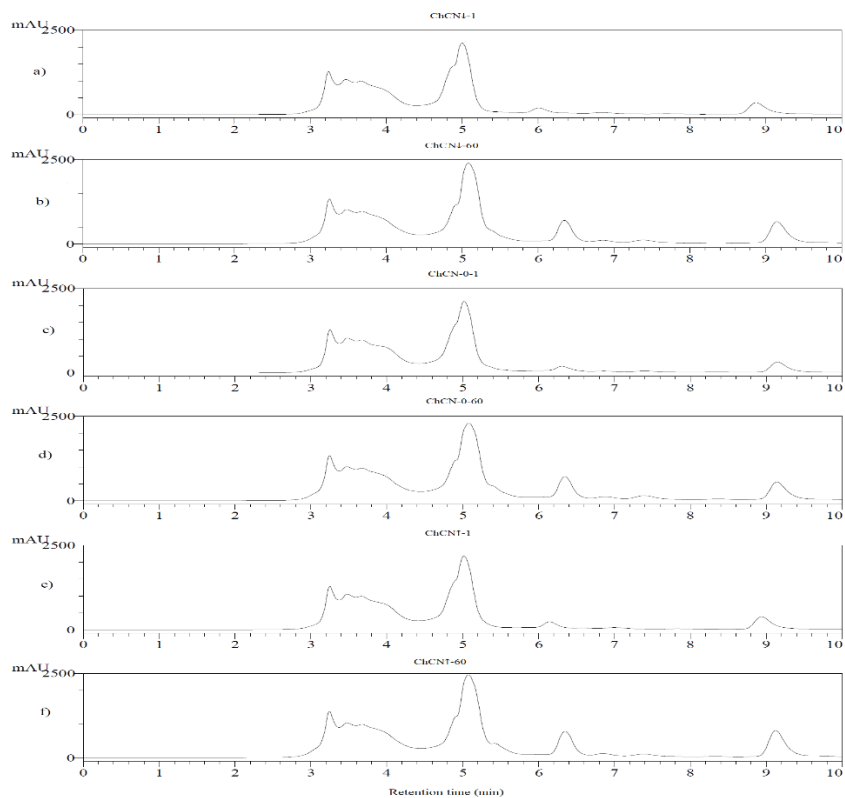
**Figure S1.** RP-HPLC chromatograms of water-soluble extracts derived from Gouda cheese with modified β-casein content before and after ripening (1st and 60th day, respectively), within the time interval 1-10 min. Abbreviations: ChCN↓-1 (a), ChCN↓-60 (b), ChCN-0-1 (c), ChCN-0-60 (d), ChCN↑-1 (e), ChCN↑-60 (f) – water-soluble extracts derived from Gouda cheese (Ch) with: reduced (↓), normative (0), and increased (↑) contents of
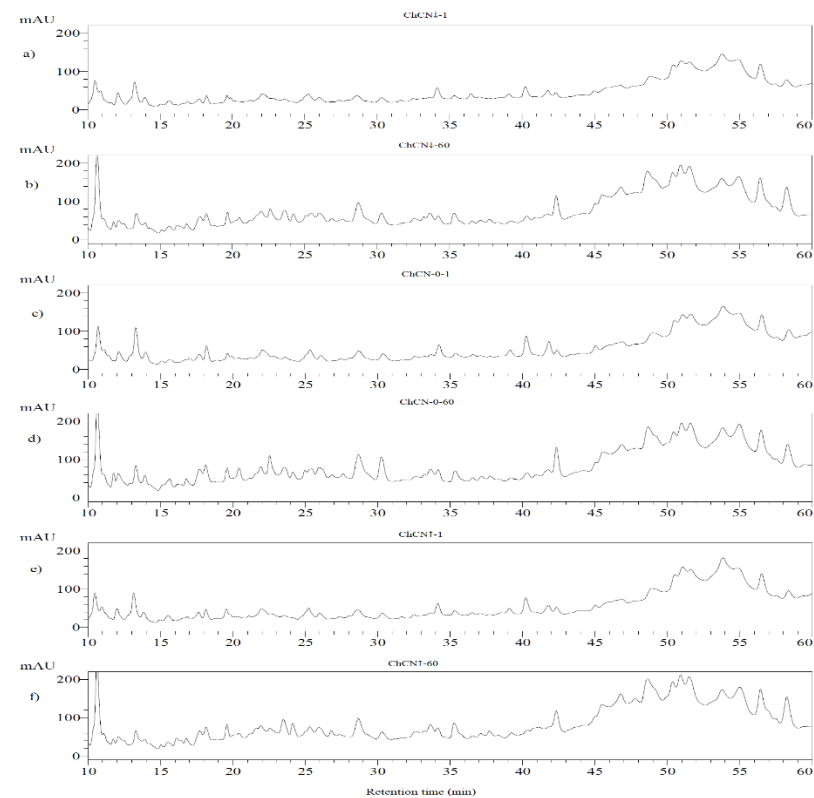


**Figure S2.** RP-HPLC chromatograms of water-soluble extracts derived from Gouda cheese with modified β-casein content before and after ripening (1st and 60th day, respectively), within the time interval 10-60 min. Abbreviations: ChCN↓-1 (a), ChCN↓-60 (b), ChCN-0-1 (c), ChCN-0-60 (d), ChCN↑-1 (e), ChCN↑-60 (f) – water-soluble extracts derived from Gouda cheese (Ch) with: reduced (↓), normative (0), and increased (↑) contents of

β-casein (CN) after 1 (suffix 1) and 60 (suffix 60) days of ripening, respectively (see Methods).

**Table S2.** RP-HPLC-MS/MS identification of peptides with ACE and/or DPP-IV-inhibitory activity in different Gouda cheese variants.

| Sequence | $t_R$[1] (min) | $m/z$[2] | ChCN ↓-1[3] | ChCN ↓-60 | ChCN 0- 1 | ChCN -0-60 | ChCN ↑-1 | ChCN ↑-60 | Casein[4] |
|---|---|---|---|---|---|---|---|---|---|
| AA[dual5] | 5.062 | 161.1 | - | + | - | + | - | + κ | $\kappa^A$ |
| **PP[dual]** | 32.179 | 213.1 | + | + | + | + | + | + | $\beta^{all}$, $\kappa^A$ |
| **VV[DPP-IVi6]** | 15.946 | 217.2 | + | + | + | + | + | + | $\alpha_{S2}^A$, $\beta^{all}$, $\kappa A$ |
| FG[ACEi7] | 18.761 | 223.1 | - | + | - | + | - | + | $\alpha_{S1}^{all}$ |
| **HA[DPP-IVi]** | 22.635 | 227.1 | + | + | + | + | + | + | $\alpha_{S1}^{all}$ |
| HV[DPP-IVi] | 6.113 | 255.1 | - | + | - | + | - | + | $\alpha_{S2}^A$ |
| **NK[ACEi]** | 20.370 | 261.2 | + | + | + | + | + | + | $\beta^{all}$ |
| TF[dual] | 14.969 | 267.1 | - | + | - | + | - | + | $\alpha_{S2}^A$ |
| **ME[dual]** | 27.981 | 279.1 | + | + | + | + | + | + | $\alpha_{S1}^{all}$, $\alpha_{S2}^A$ |
| EH[DPP-IVi] | 15.555 | 285.1 | - | + | - | + | - | + | $\alpha_{S2}^A$ |
| MH[DPP-IVi] | 18.512 | 287.1 | - | + | - | + | - | + | $\beta^{all}$ |
| **AIP[ACEi]** | 20.485 | 300.2 | + | + | + | + | + | + | $\kappa^A$ |
| IAK[ACEi] | 36.431 | 331.2 | - | + | - | + | - | + | $\kappa^A$ |
| **PPK[ACEi]** | 36.242 | 341.2 | + | + | + | + | + | + | $\kappa^A$ |
| **LNP[ACEi]** | 36.356 | 343.2 | + | + | + | + | + | + | $\alpha_{S2}^A$ |
| FAL[ACEi] | 21.381 | 350.2 | - | + | - | + | - | + | $\alpha_{S2}^A$ |
| FGK[ACEi] | 21.360 | 351.2 | + | - | + | - | + | - | $\alpha_{S1}^{all}$ |
| LNF[ACEi] | 29.027 | 393.2 | + | - | + | - | + | - | $\alpha_{S2}^A$ |
| AIPP[ACEi] | 16.044 | 397.2 | + | - | + | - | - | + | $\kappa^A$ |
| **PQR[ACEi]** | 25.706 | 400.2 | + | + | + | + | + | + | $\beta^{all}$ |
| FVAP[ACEi] | 25.270 | 433.2 | + | + | + | + | + | + | $\alpha_{S1}^{B,C,D}$ |

| Peptide | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| LPLP[ACEi] | 29.105 | 439.3 | - | + | - | + | - | + | $\beta$B |
| **GTQY[ACEi]** | 23.777 | 468.2 | + | + | + | + | + | + | $\alpha_{S1}$all |
| PFPE[ACEi] | 22.262 | 489.2 | - | + | - | + | - | + | $\alpha_{S1}$D |
| RYLG[ACEi] | 18.715 | 508.3 | - | + | - | + | - | - | $\alpha_{S1}$all |
| LQSW[ACEi] | 34.158 | 533.3 | + | - | + | - | + | + | $\beta$all |
| **WIQP[DPP-IVi]** | 22.460 | 543.3 | + | + | + | + | + | + | $\alpha_{S2}$A |
| **AVPYP[ACEi]** | 18.869 | 546.3 | + | + | + | + | + | + | $\beta$all |
| LPLPL[DPP-IVi] | 36.251 | 552.4 | + | - | + | - | + | - | $\beta$B |
| TKVIP[ACEi] | 22.863 | 557.4 | + | - | + | - | + | - | $\alpha_{S2}$A |
| **LFRQ[ACEi]** | 21.897 | 563.3 | + | + | + | + | + | + | $\alpha_{S1}$all |
| HLPLP[ACEi] | 26.979 | 576.3 | + | - | + | - | + | - | $\beta$B |
| FFVAP[ACEi] | 21.947 | 580.3 | + | - | + | - | + | - | $\alpha_{S1}$B,C,D |
| FPIIV[ACEi] | 20.820 | 588.4 | - | + | - | + | - | + | $\beta$all |
| **NLHLP[ACEi]** | 23.601 | 593.3 | + | + | + | + | + | + | $\beta$all |
| VPITPT[DPP-IVi] | 24.328 | 627.4 | + | + | + | + | + | + | $\alpha_{S2}$A |
| **AMKPW[ACEi]** | 27.366 | 632.3 | + | + | + | + | + | + | $\alpha_{S2}$A |
| **IPIQY[DPP-IVi]** | 29.073 | 633.3 | + | + | + | + | + | + | $\kappa$A |
| AYFYP[ACEi] | 24.033 | 660.3 | - | + | - | + | - | + | $\alpha_{S1}$all |
| **RYLGY[ACEi]** | 28.930 | 671.3 | + | + | + | + | + | + | $\alpha_{S1}$all |
| KDERF[ACEi] | 28.575 | 694.4 | - | - | + | - | + | - | $\kappa$A |
| ARHPHP[ACEi] | 52.565 | 714.4 | + | - | + | - | + | - | $\kappa$A |
| LKKISQ[ACEi] | 29.401 | 716.5 | - | - | + | - | + | - | $\alpha_{S2}$A |
| GPFPIIV[ACEi] | 31.149 | 742.4 | - | + | - | + | - | + | $\beta$all |
| DKIHPF[ACEi] | 22.606 | 756.4 | - | + | - | + | - | + | $\beta$all |
| LAYFYP[ACEi] | 31.494 | 773.4 | - | + | - | + | - | + | $\alpha_{S1}$all |
| LPQNIPP[DPP-IVi] | 25.077 | 778.4 | - | + | - | + | - | + | $\beta$all |
| **AYFYPE[ACEi]** | 17.108 | 789.3 | + | + | + | + | + | + | $\alpha_{S1}$all |

| Peptide | $t_R$ | m/z | ChCN↓-1 | ChCN↓-60 | ChCN-0-1 | ChCN-0-60 | ChCN↑-1 | ChCN↑-60 | Source |
|---|---|---|---|---|---|---|---|---|---|
| **LHLPLPL**[ACEi] | 18.087 | 802.5 | + | + | + | + | + | + | $\beta^B$ |
| NLHLPLP[ACEi] | 19.443 | 803.5 | + | - | + | - | + | - | $\beta^B$ |
| **FSDKIAK**[ACEi] | 21.871 | 808.5 | + | + | + | + | + | + | $\kappa^A$ |
| **AVPYPQR**[ACEi] | 24.422 | 830.4 | + | + | + | + | + | + | $\beta^{all}$ |
| **LLYQQPV**[ACEi] | 26.657 | 860.5 | + | + | + | + | + | + | $\beta^{A1, A2, A3, C, E, F}$ |
| DAYPSGAW[ACEi] | 29.459 | 866.3 | - | + | - | + | - | + | $\alpha_{S1}{}^{all}$ |
| **SKVLPVPE**[ACEi] | 25.869 | 868.5 | + | + | + | + | + | + | $\beta^{A1, A2, A3, C, E, F}$ |
| AYFYPEL[ACEi] | 18.075 | 902.4 | - | + | - | + | - | + | $\alpha_{S1}{}^{all}$ |
| **ENLHLPLP**[ACEi] | 20.145 | 932.5 | + | + | + | + | + | + | $\beta^B$ |
| FPQYLQY[ACEi] | 22.559 | 958.5 | + | - | + | - | + | - | $\alpha_{S2}{}^{A}$ |
| IPPLTQTPV[DPP-IVi] | 20.587 | 965.6 | + | - | + | - | + | - | $\beta^{all}$ |
| LNVPGEIVE[ACEi] | 20.910 | 969.5 | + | - | + | - | + | - | $\beta^{all}$ |
| AYFYPELF[ACEi] | 29.571 | 1049.5 | + | - | + | - | + | - | $\alpha_{S1}{}^{all}$ |
| RPKHPIKHQ[ACEi] | 16.101 | 1140.7 | - | + | - | + | - | + | $\alpha_{S1}{}^{all}$ |
| YPQRDMPIQ[ACEi] | 32.747 | 1147.5 | - | + | - | + | - | + | $\beta^{all}$ |

[1]$t_R$ – retention time (min), [2]all precursor ions of identified peptide are $(M+H)^+$; [3]ChCN↓-1, ChCN↓-60, ChCN-0-1, ChCN-0-60, ChCN↑-1, ChCN↑-60 – water-soluble extracts derived from Gouda cheese with: reduced (↓), normative (0), and increased (↑) content of β-casein after 1st (suffix 1) and 60th (suffix 60) day of ripening, respectively, [4]letters assigned to the casein sources refer to their specific genetic variant, whereas term "all" means the presence of a peptide in all genetic variants of specific casein that had been *in silico* analyzed, [5]dual - ACE and DPP-IV inhibitor; [6]DPP-IVi - DPP-IV inhibitor; [7]ACEi - ACE inhibitor; **bold** - peptides identified in all cheese variants.
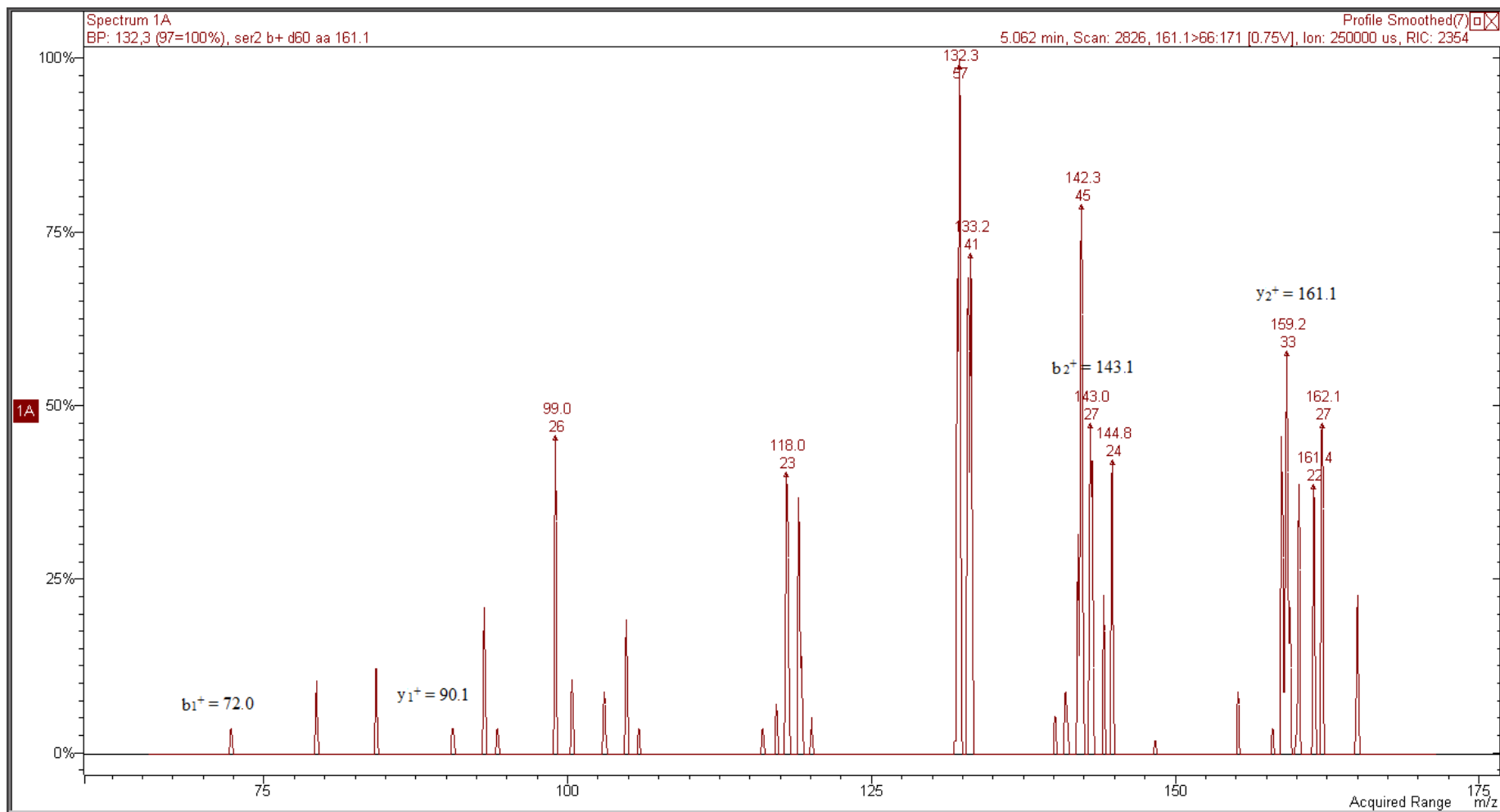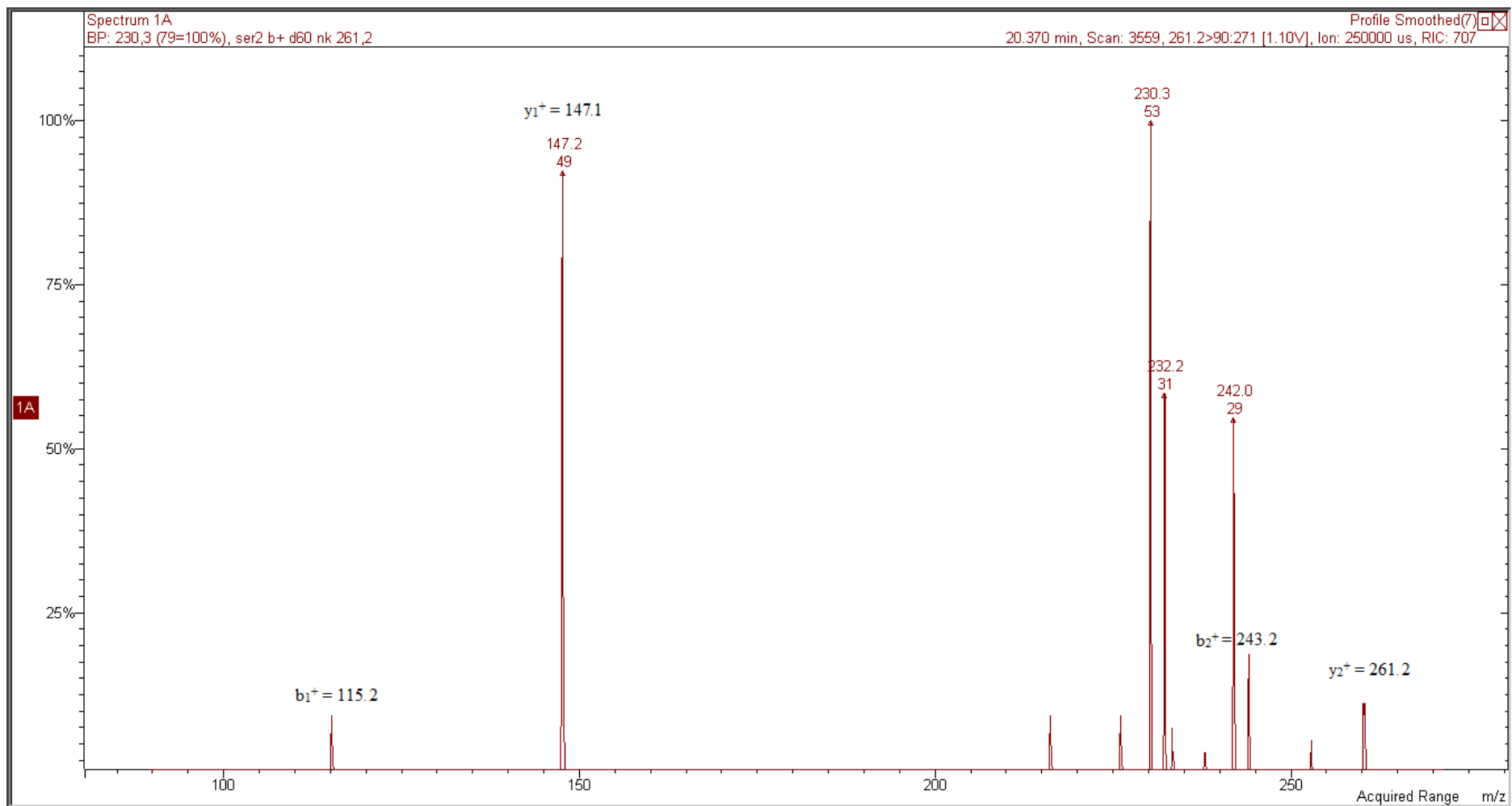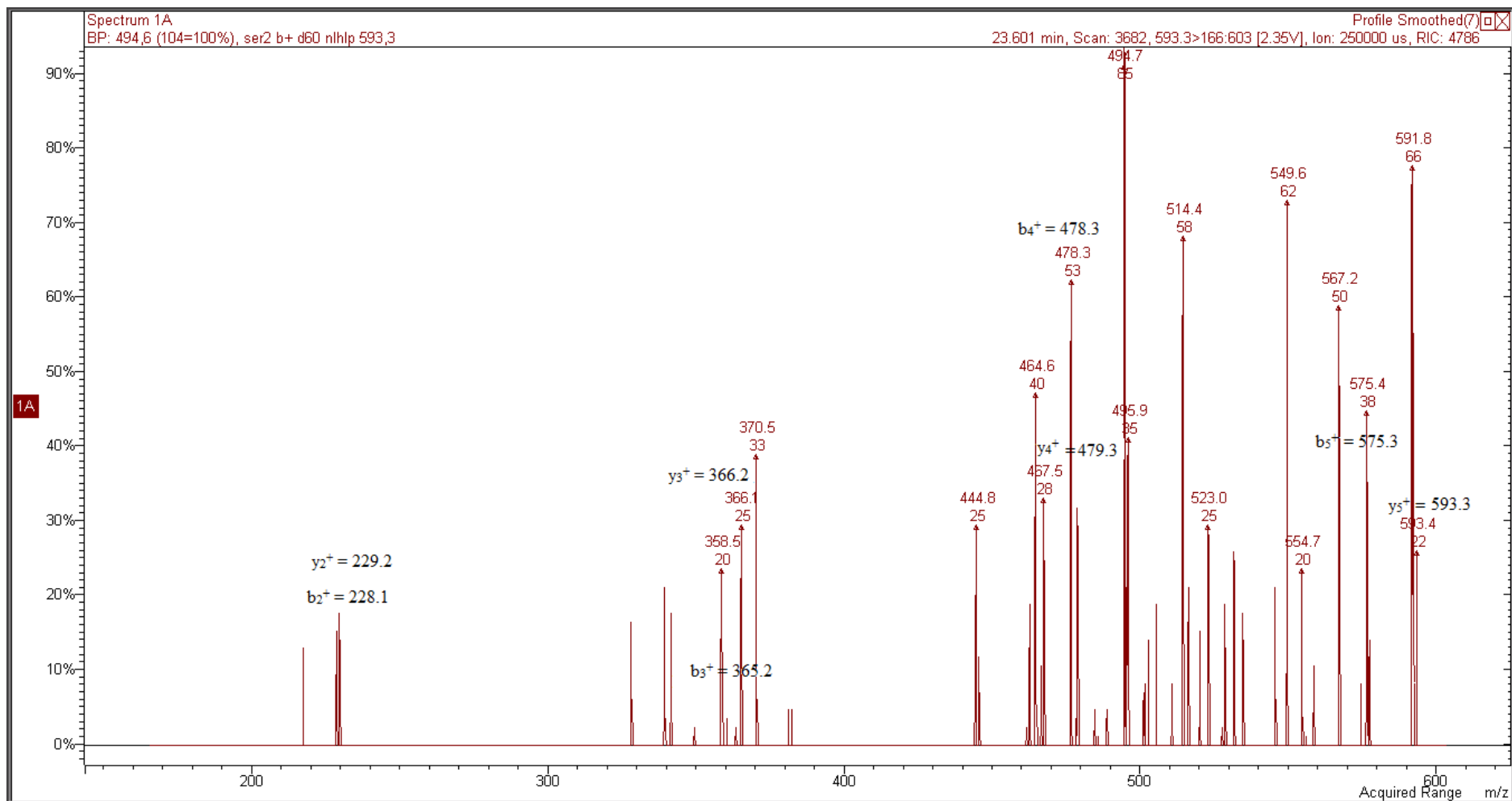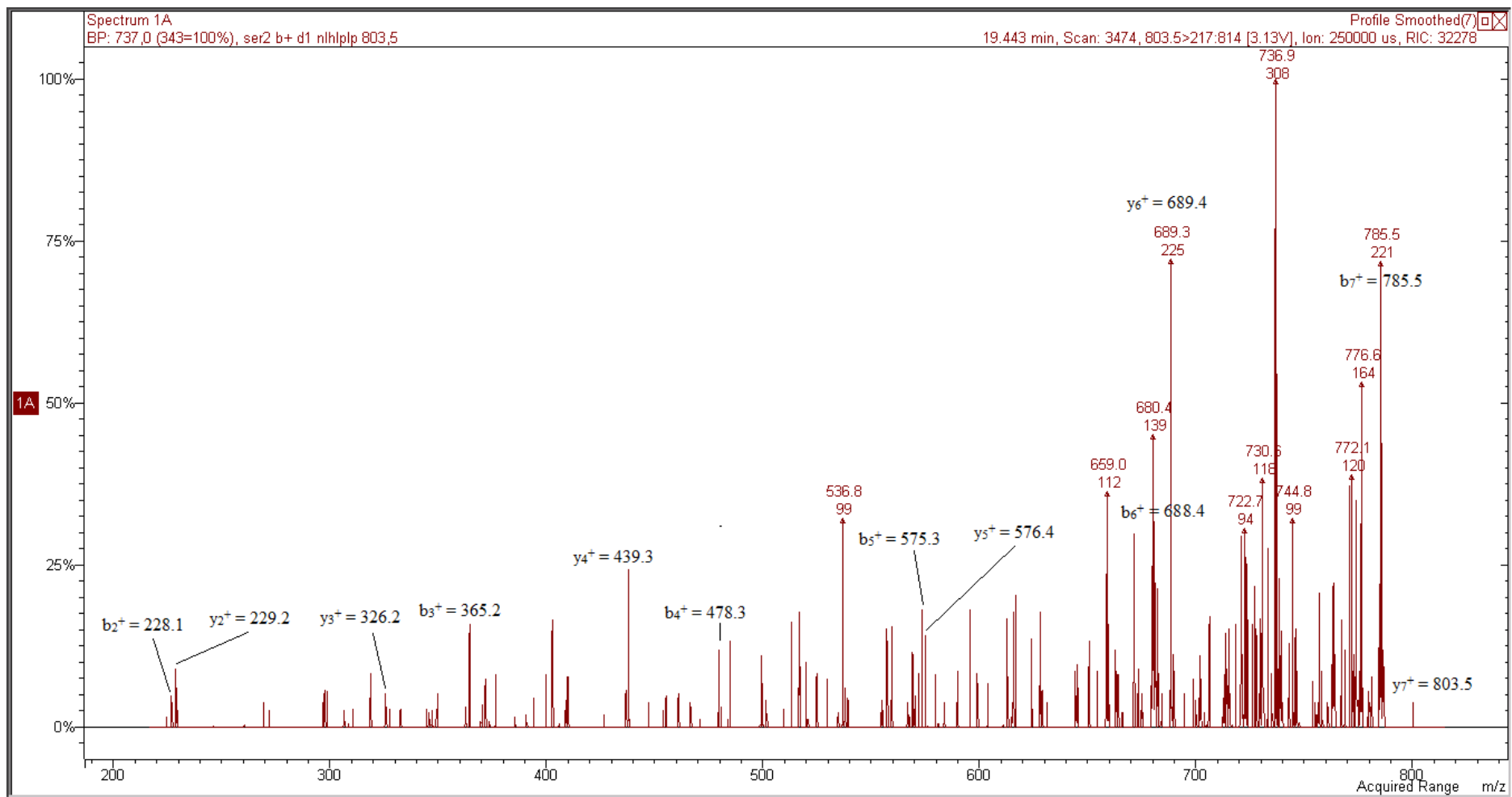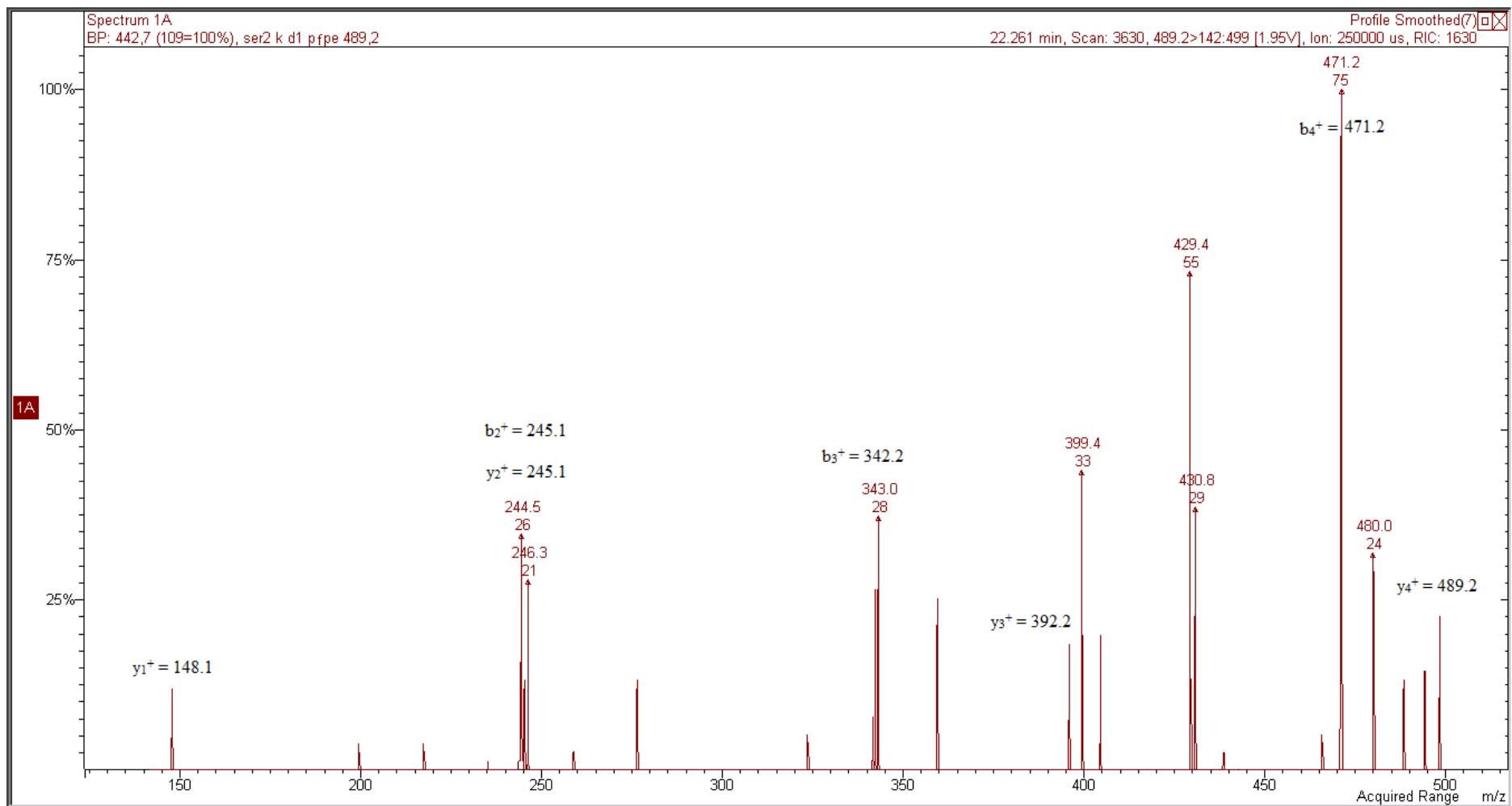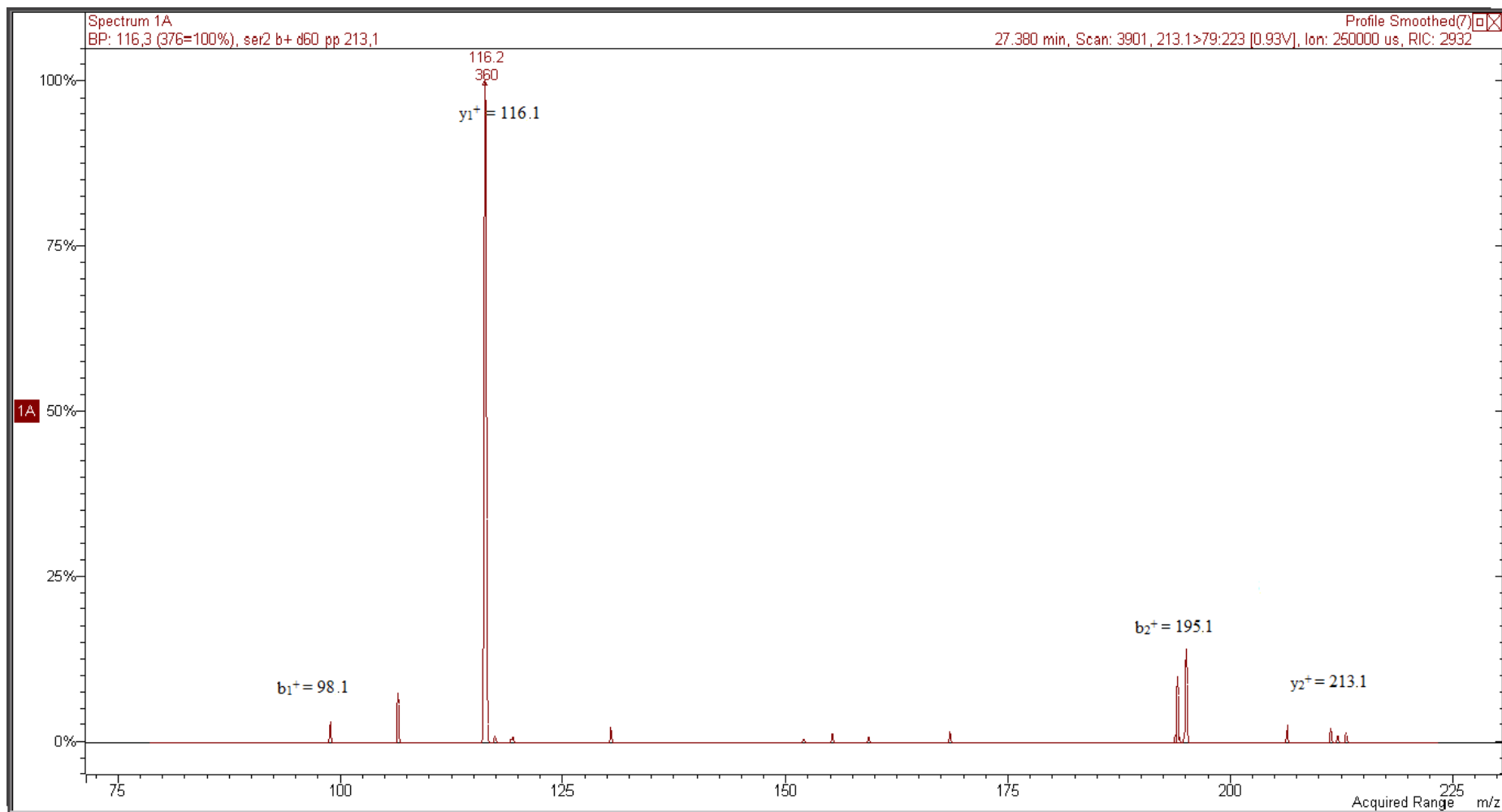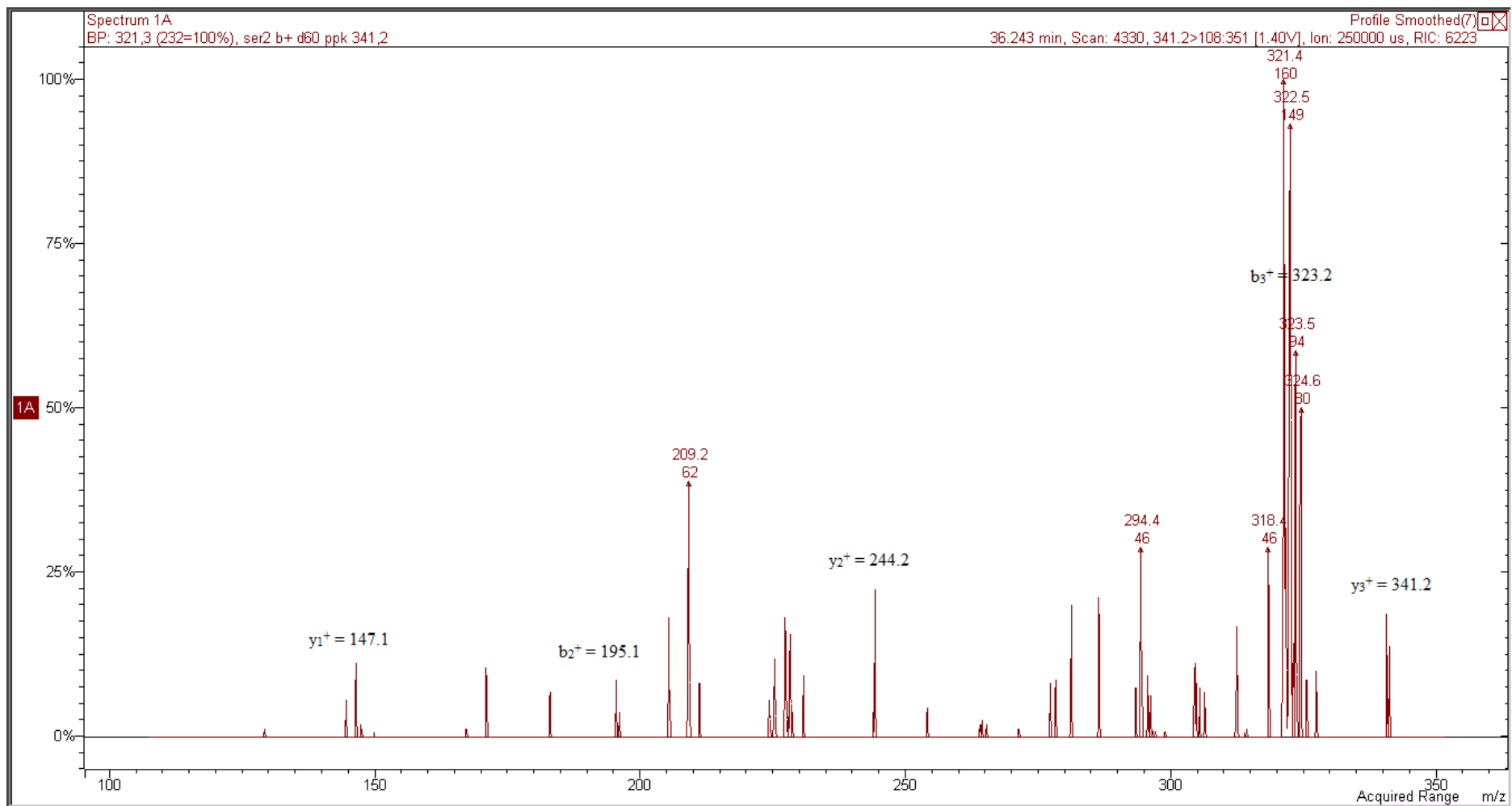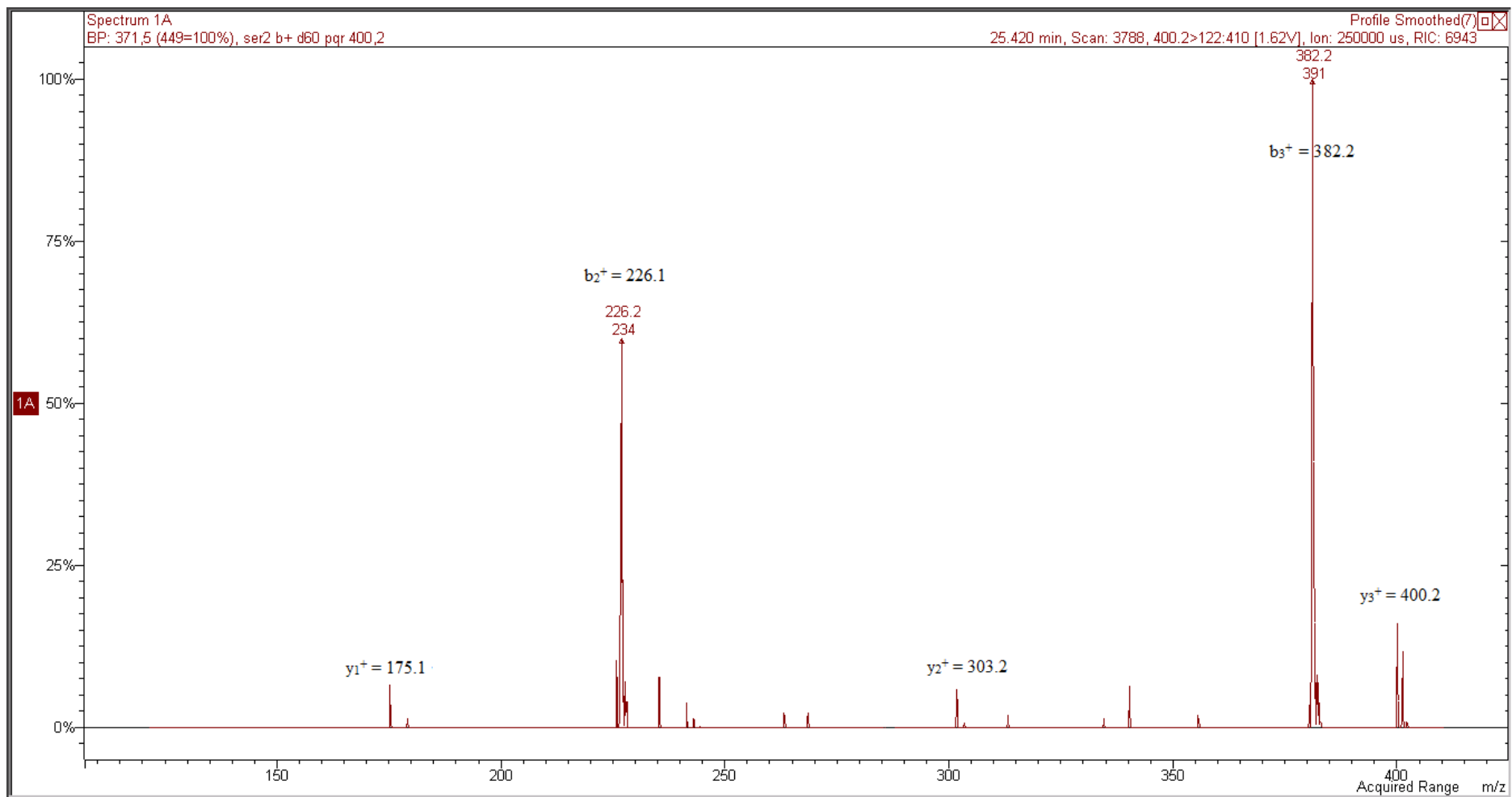
**Figure S3.** MS/MS spectrum of AA peptide.
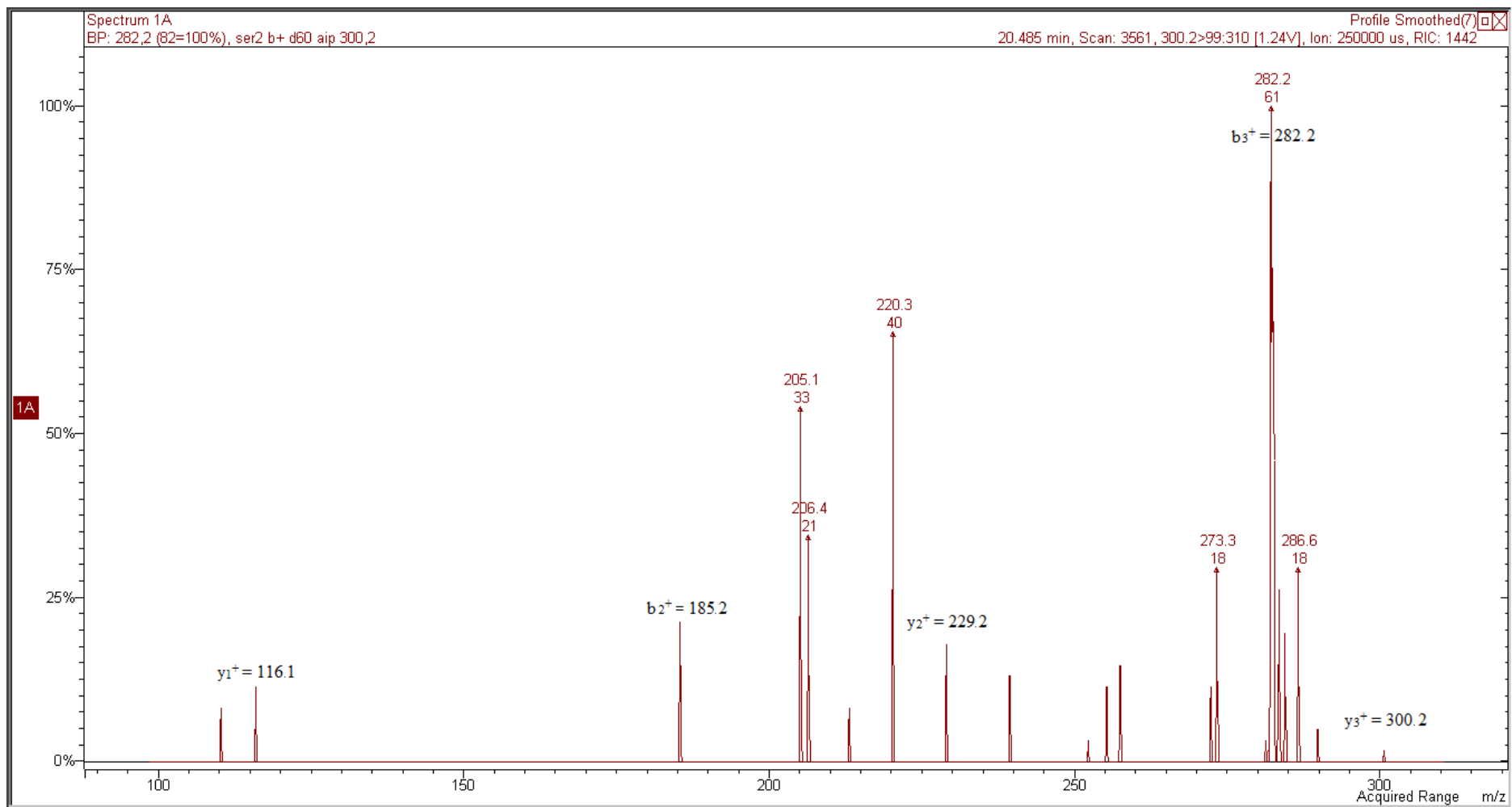
**Figure S4.** MS/MS spectrum of AIP peptide.
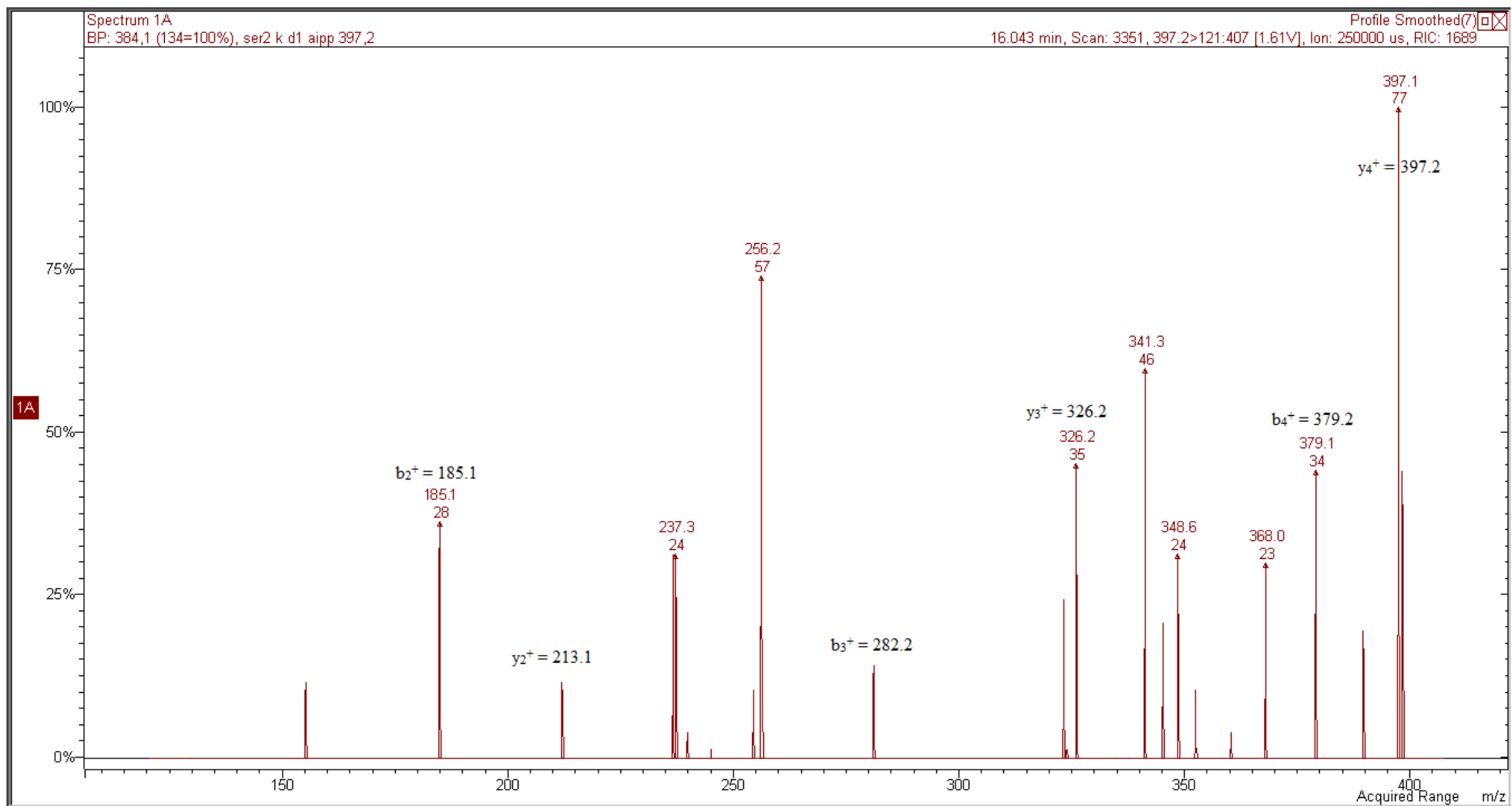
**Figure S5.** MS/MS spectrum of AIPP peptide.
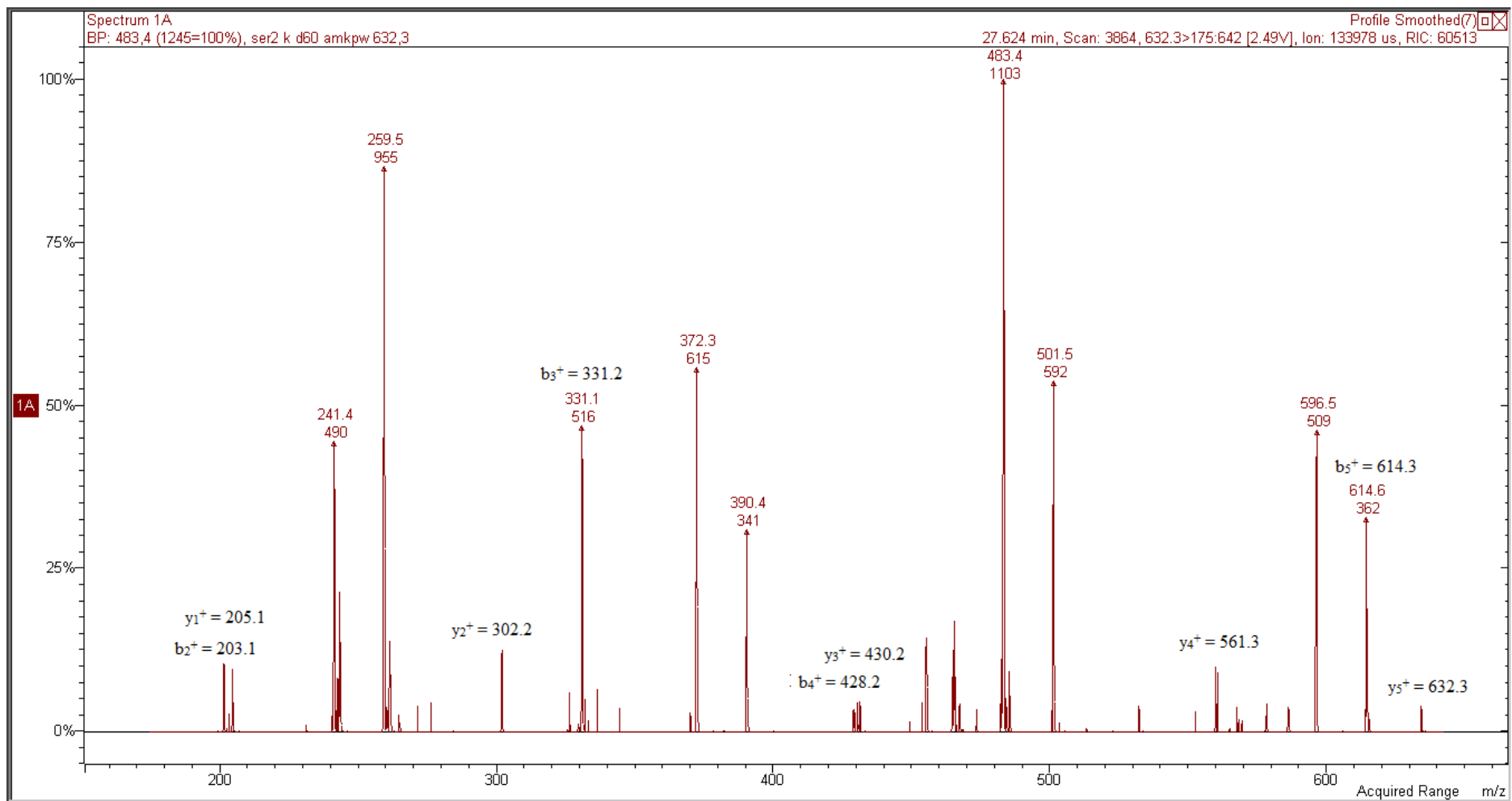
**Figure S6.** MS/MS spectrum of AMPKW peptide.
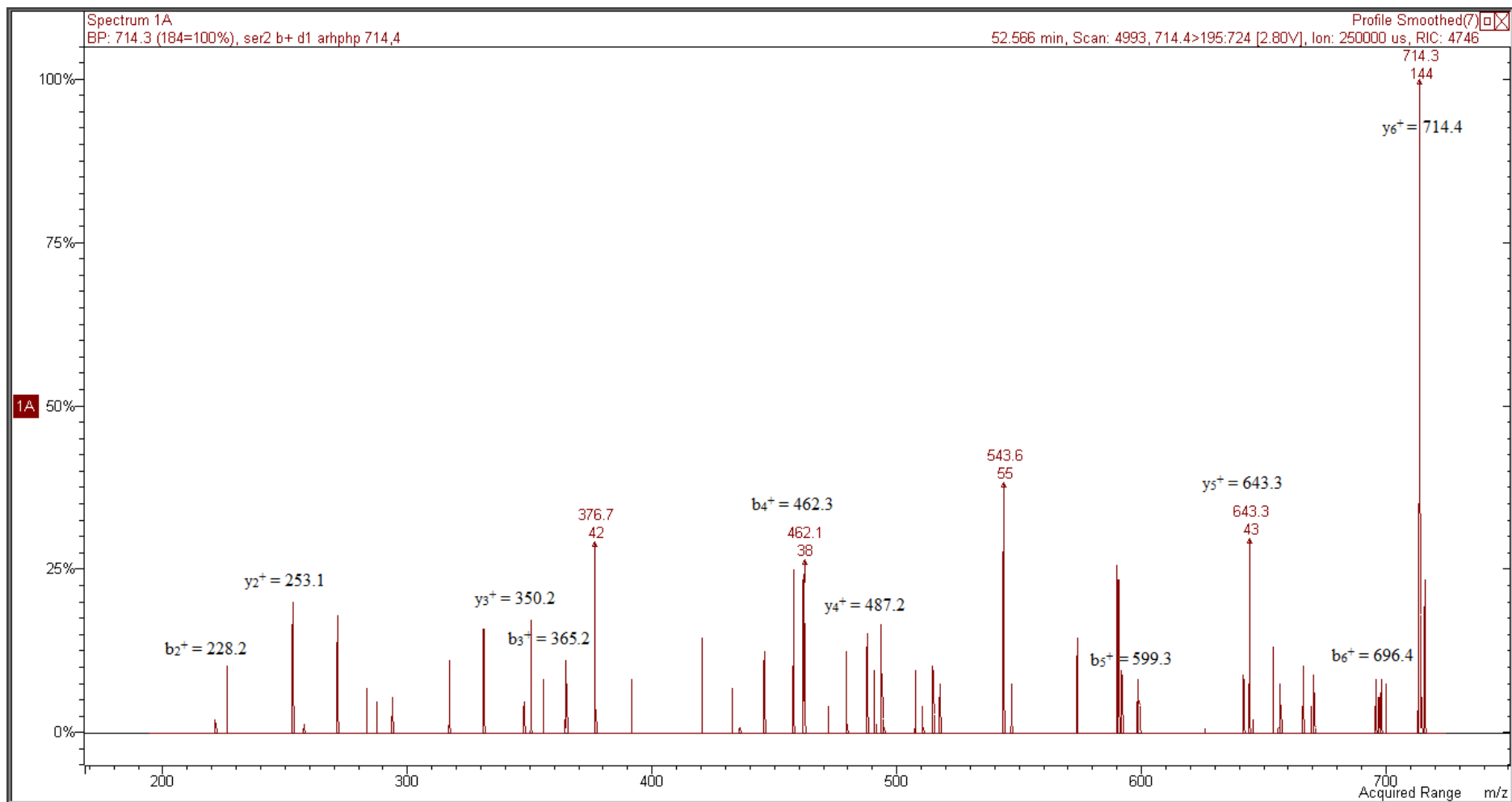
**Figure S7.** MS/MS spectrum of ARHPHP peptide.
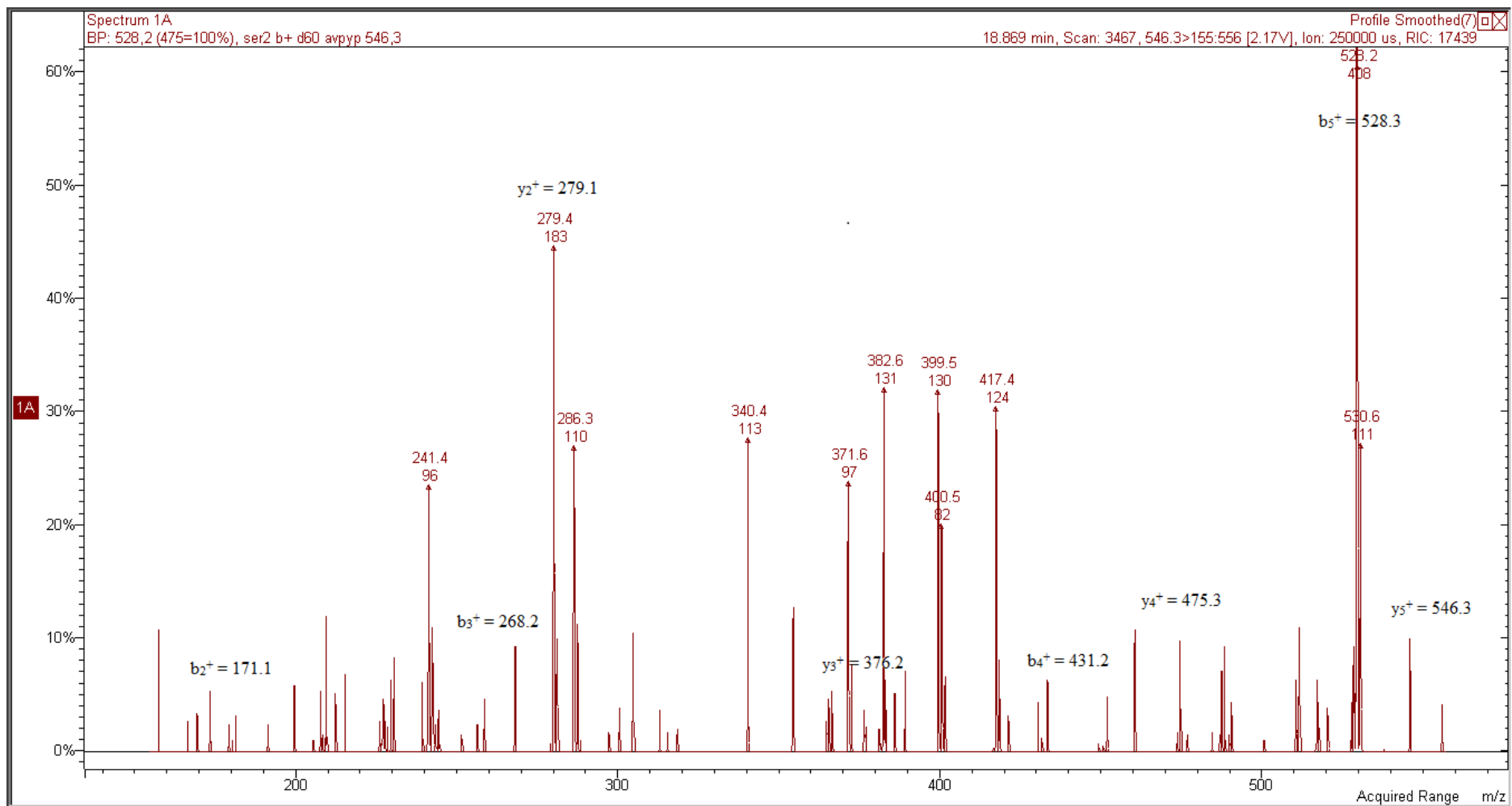
**Figure S8.** MS/MS spectrum of AVPYP peptide.
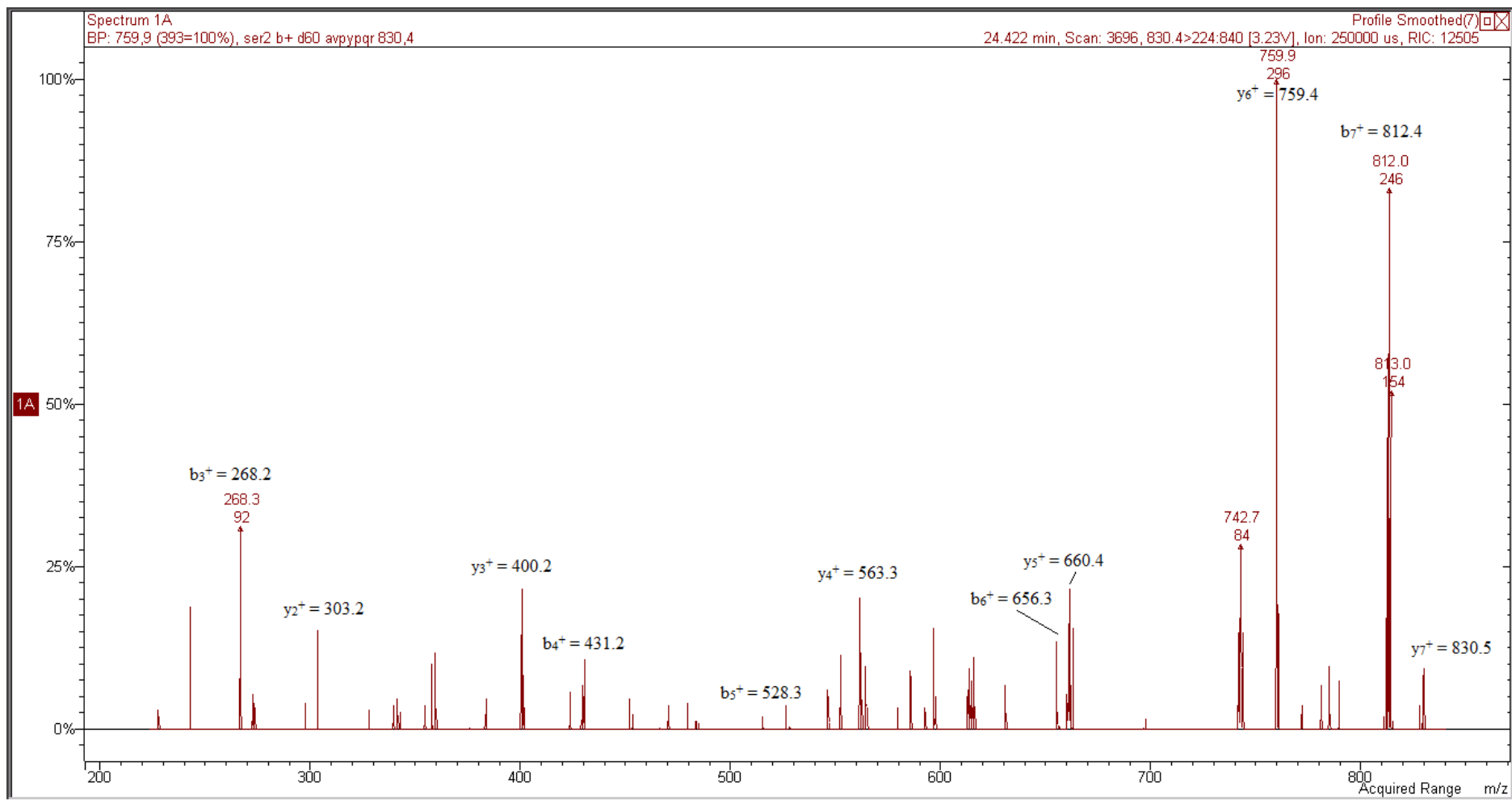
**Figure S9.** MS/MS spectrum of AVPYPQR peptide.
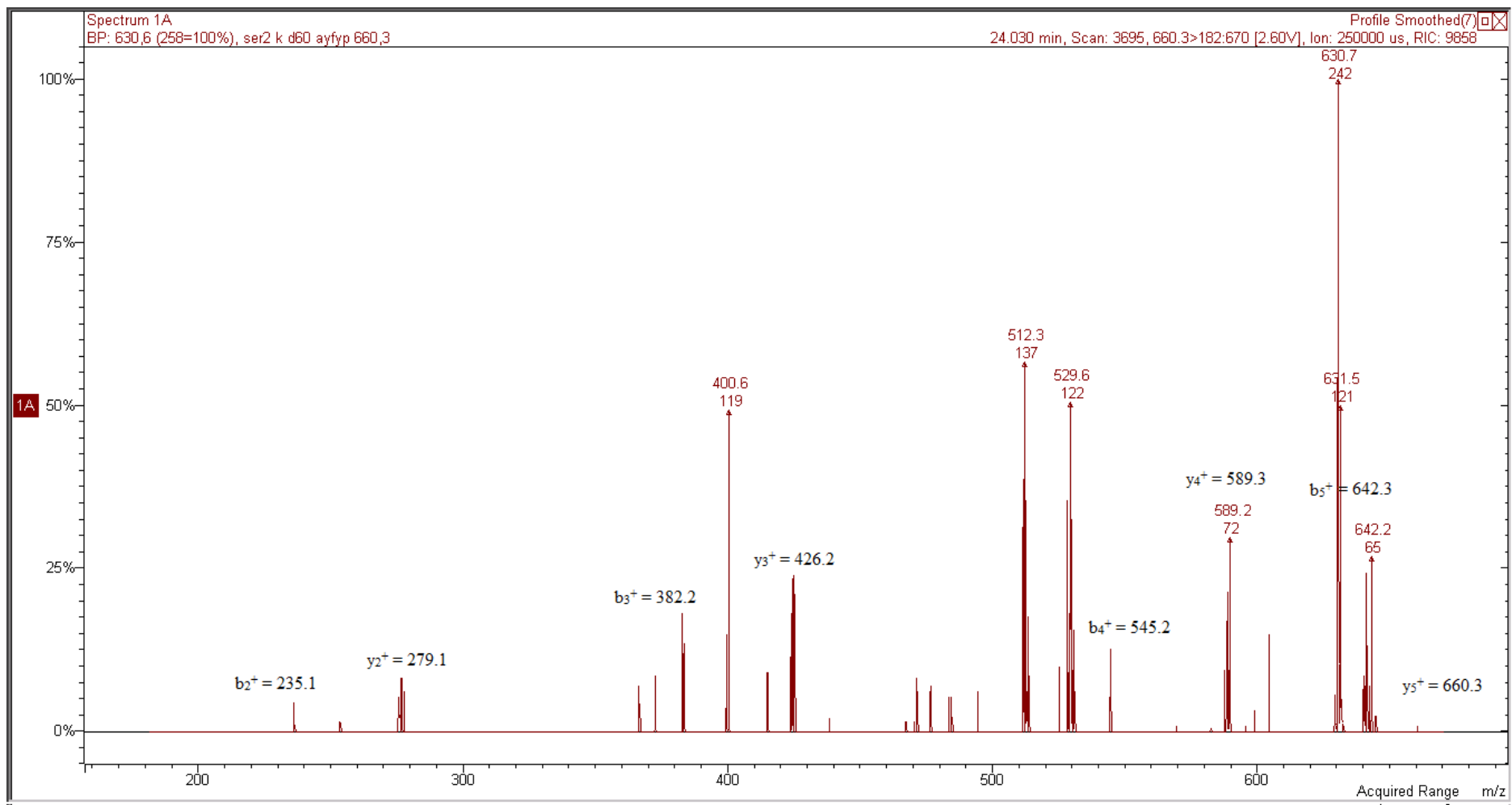
**Figure S10.** MS/MS spectrum of AYFYP peptide.
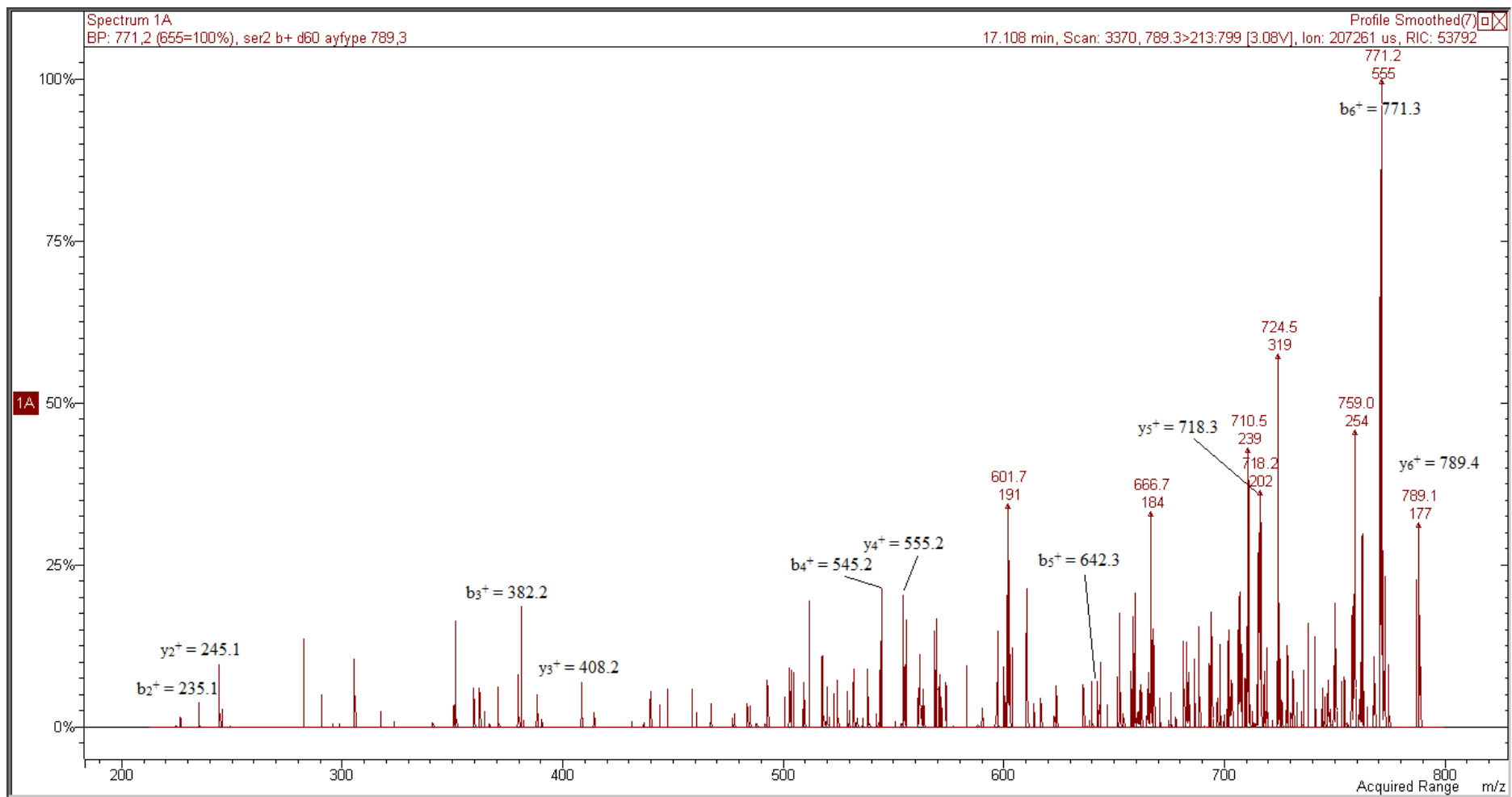
**Figure S11.** MS/MS spectrum of AYFYPE peptide.
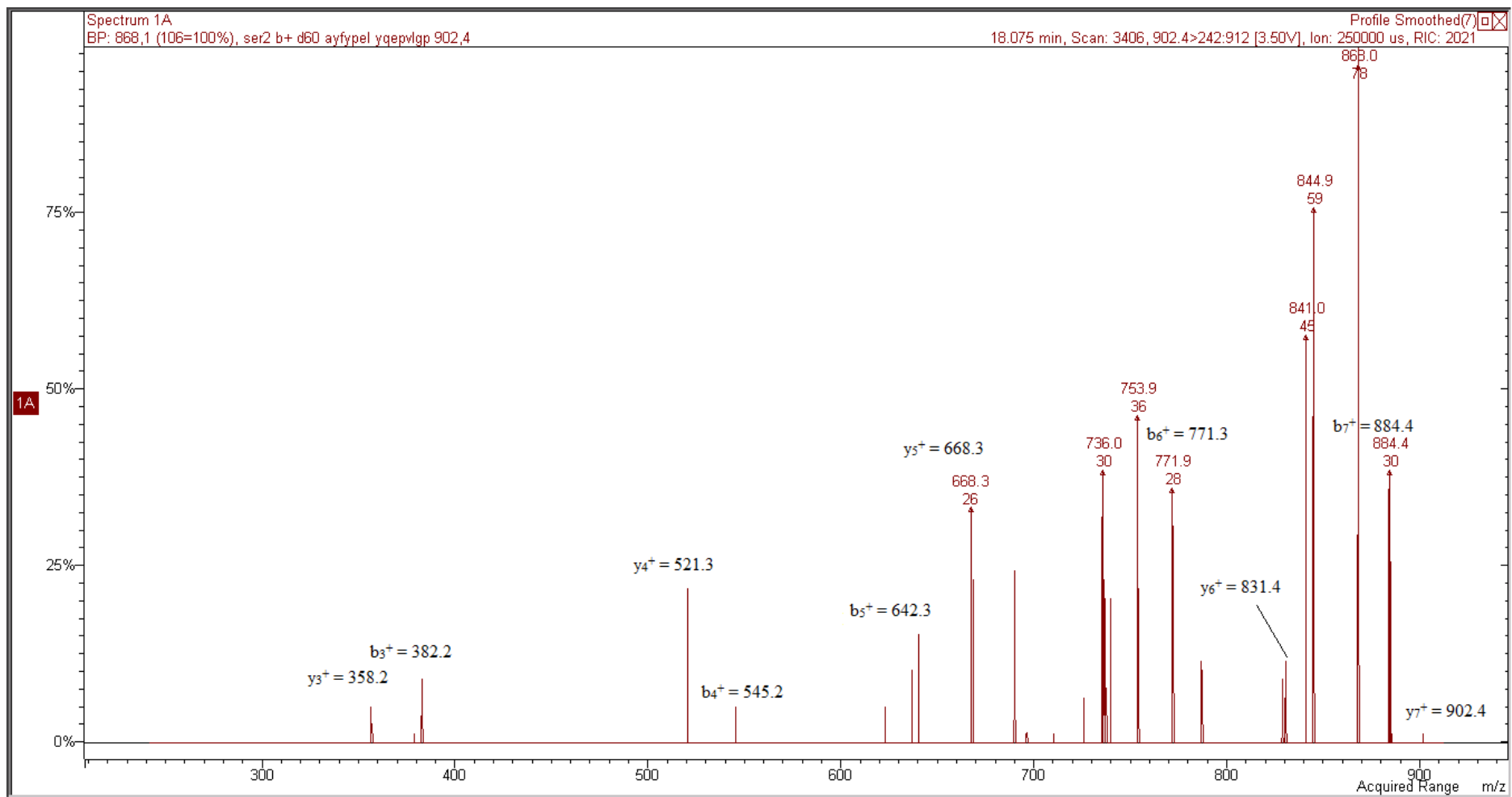
**Figure S12.** MS/MS spectrum of AYFYPEL peptide.
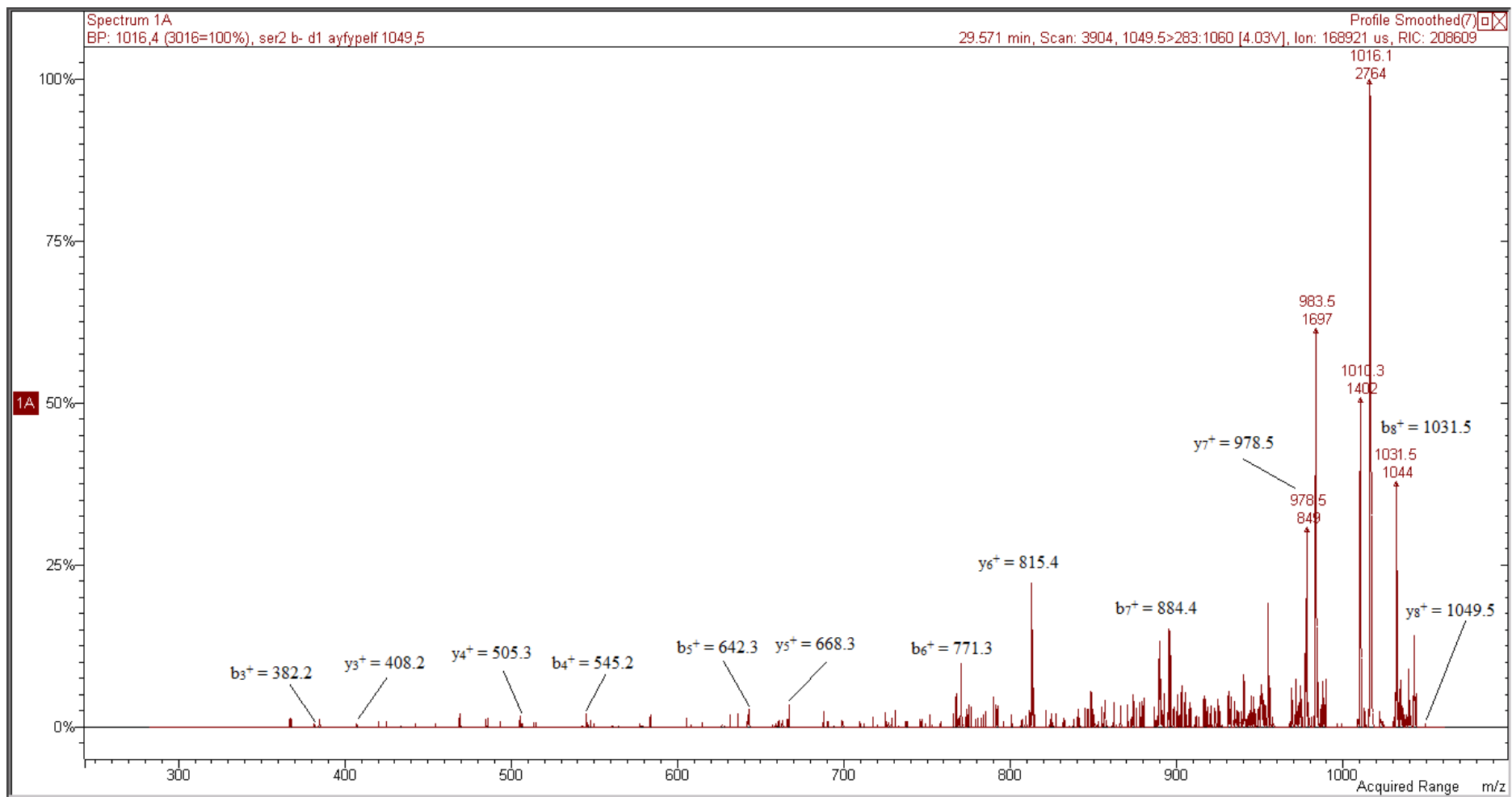
**Figure S13.** MS/MS spectrum of AYFYPELF peptide.
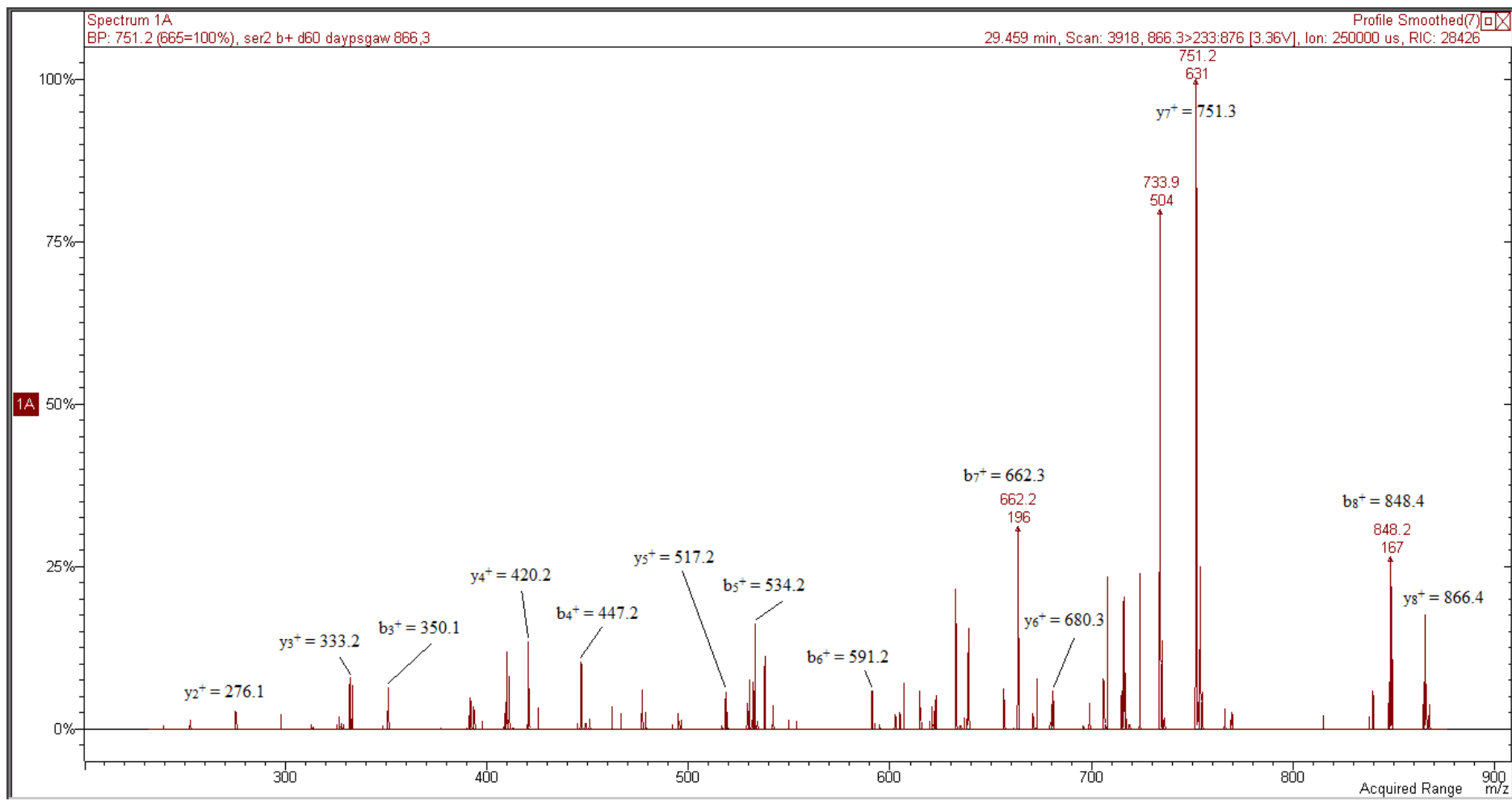
**Figure S14.** MS/MS spectrum of DAYPSGAW peptide.
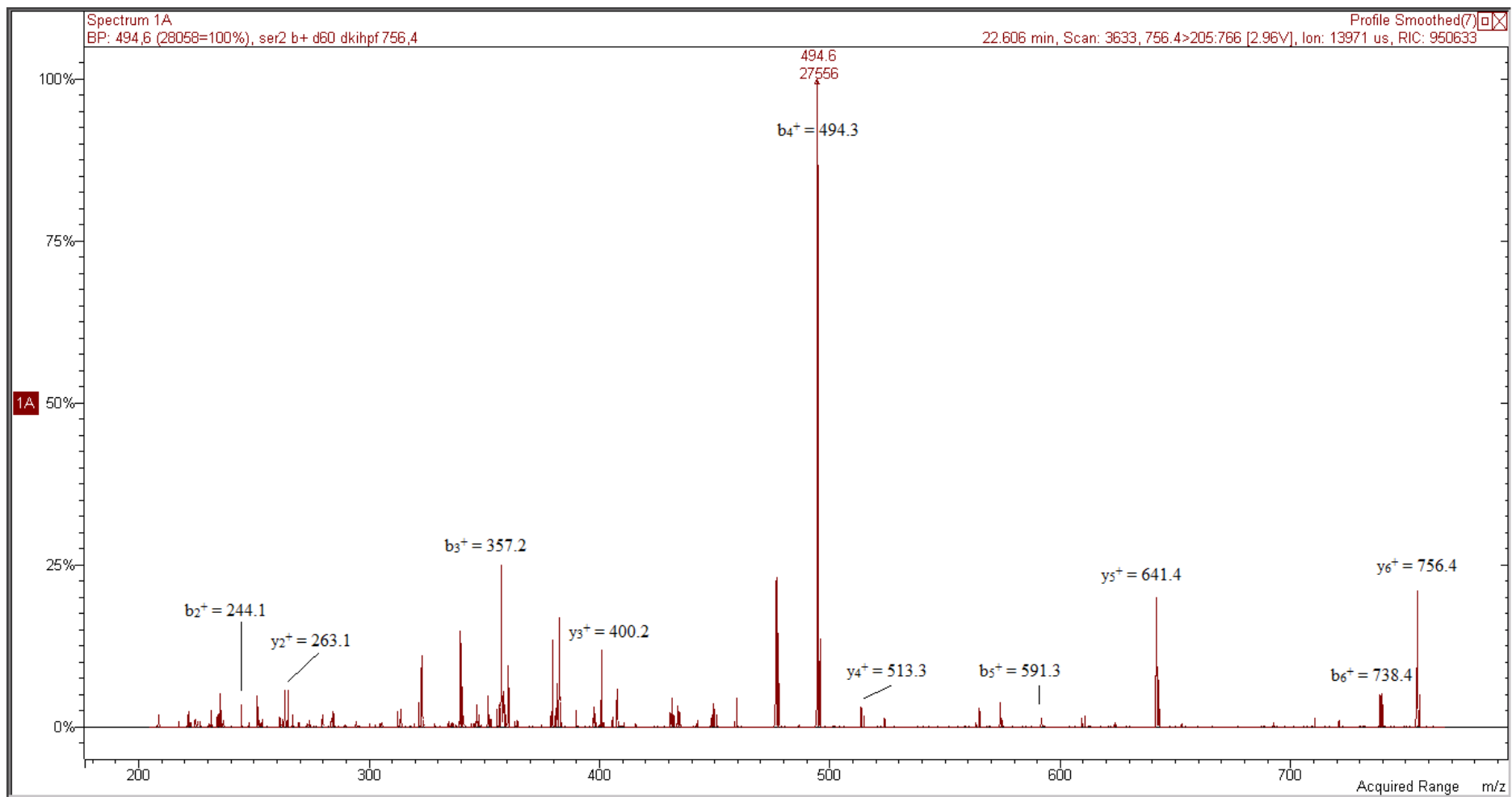
**Figure S15.** MS/MS spectrum of DKIHPF peptide.
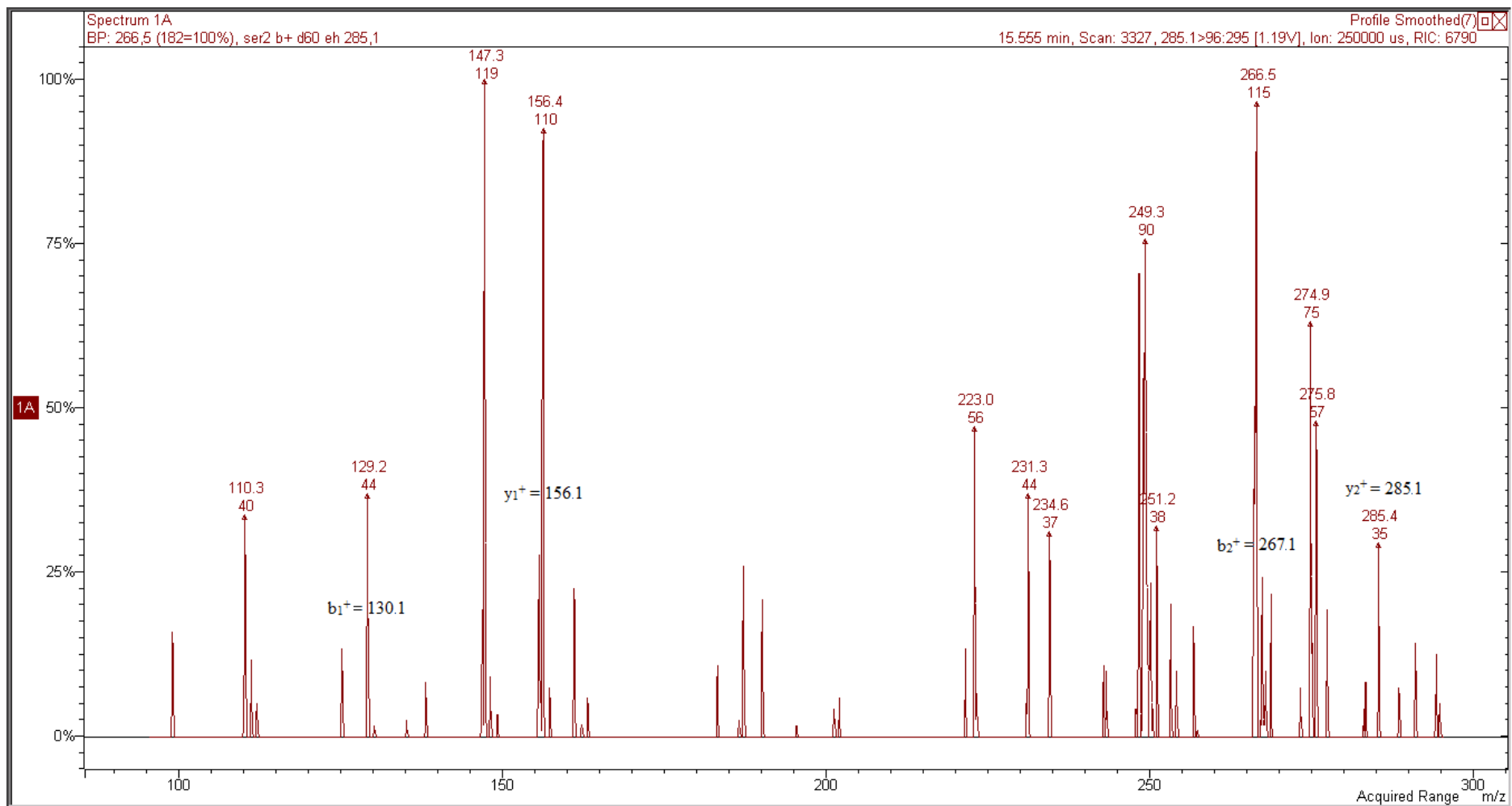
**Figure S16.** MS/MS spectrum of EH peptide.
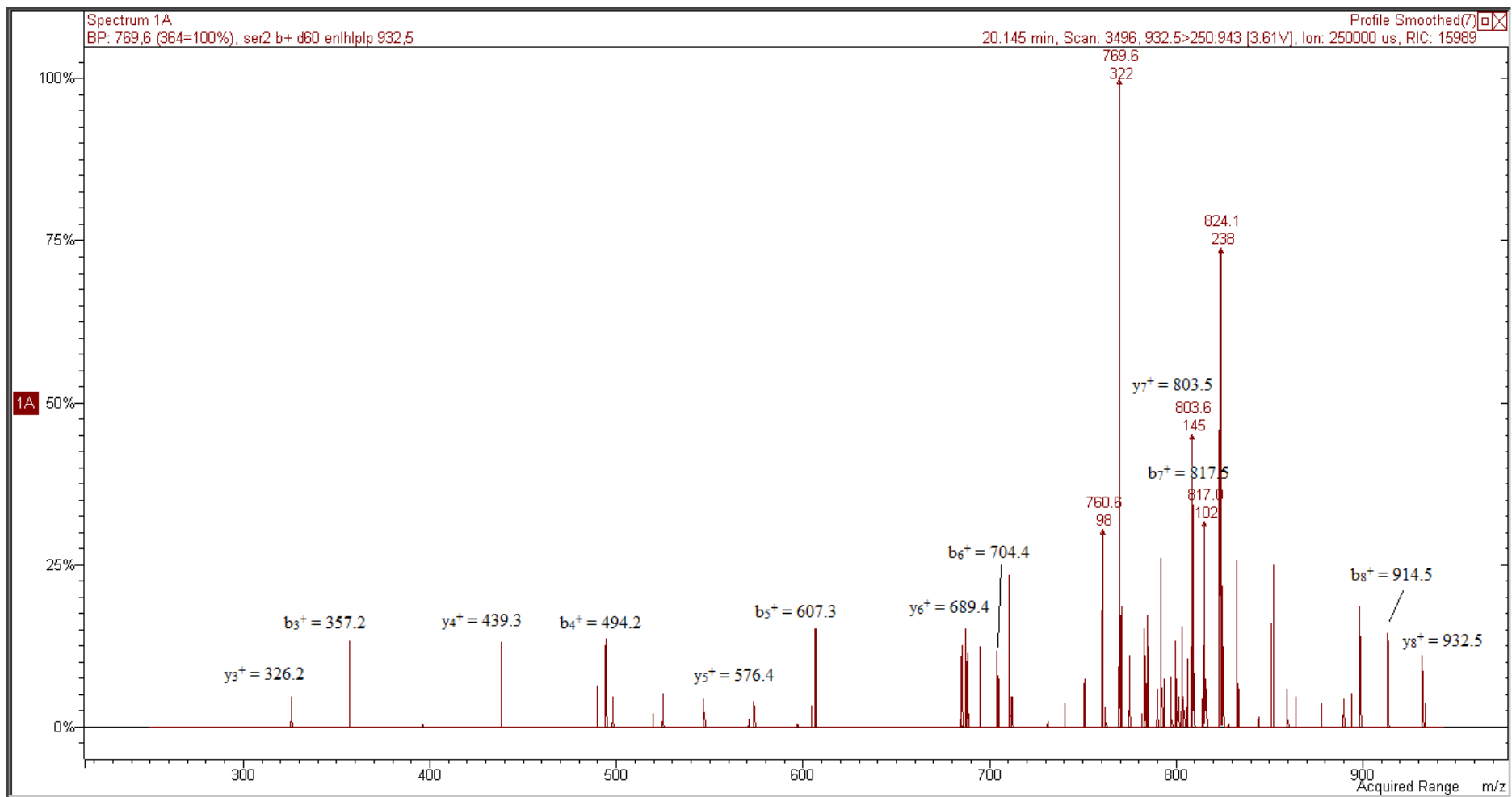
**Figure S17.** MS/MS spectrum of ENLHLPLP peptide.
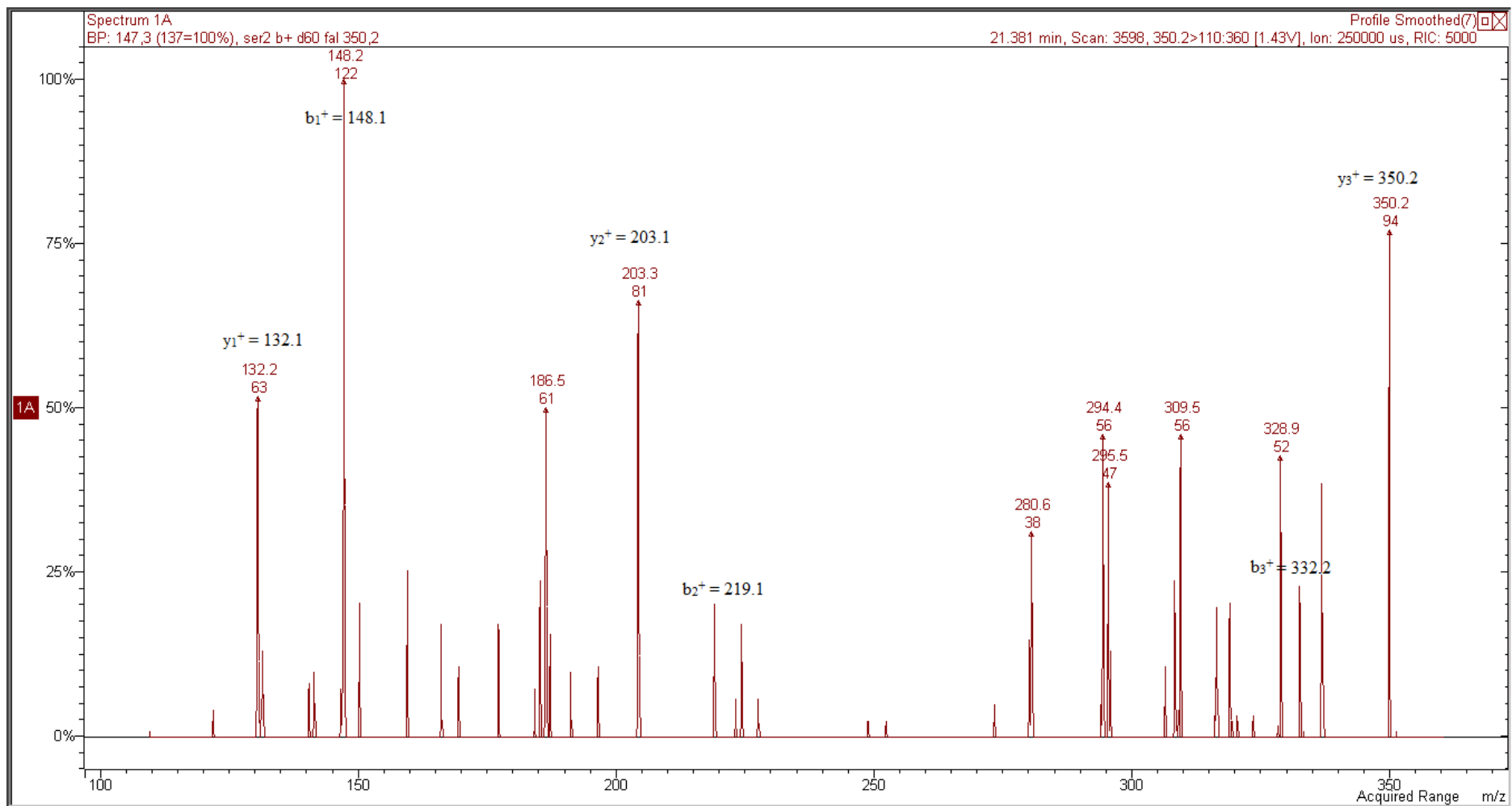
**Figure S18.** MS/MS spectrum of FAL peptide.
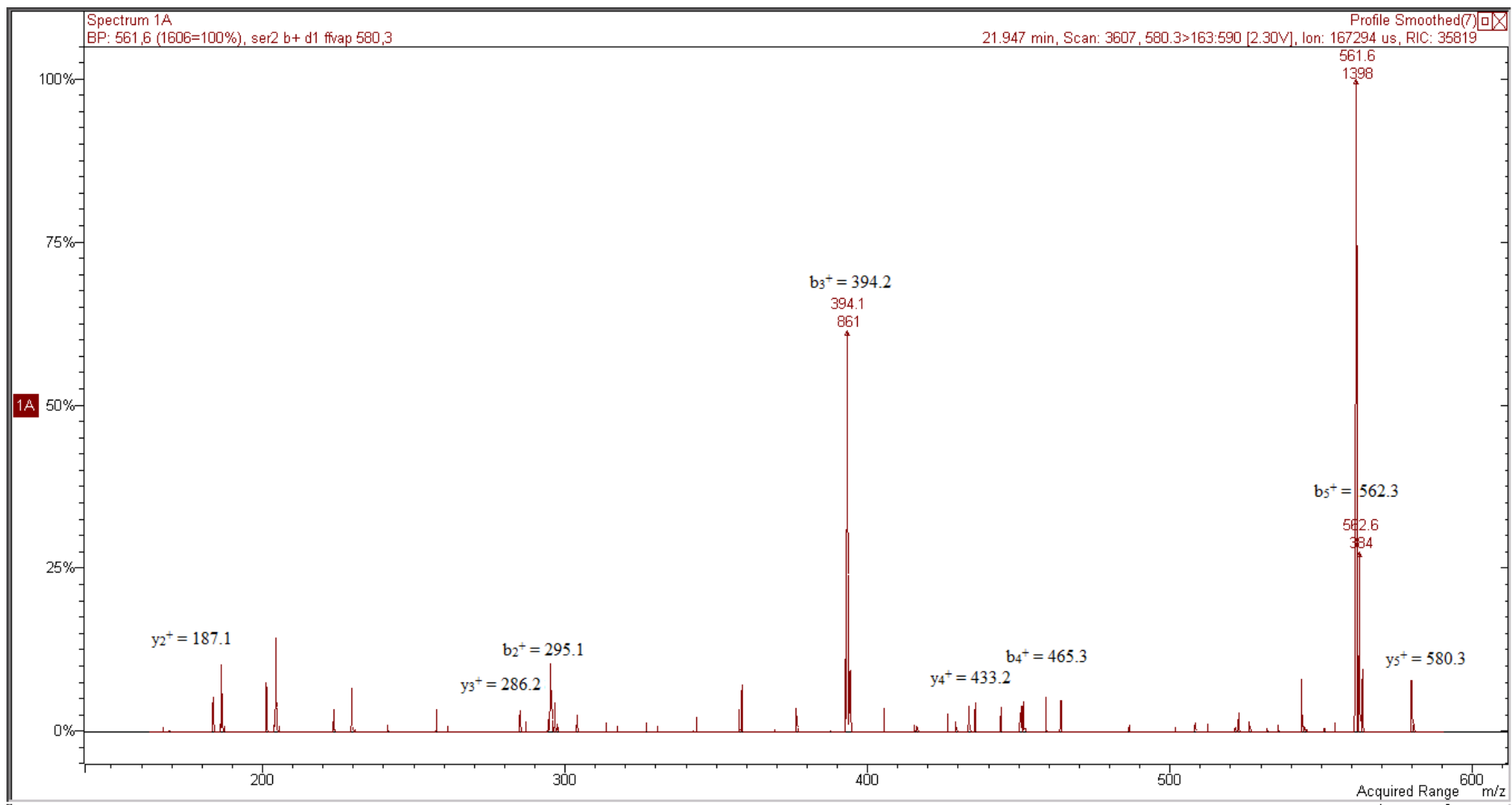
**Figure S19.** MS/MS spectrum of FFVAP peptide.
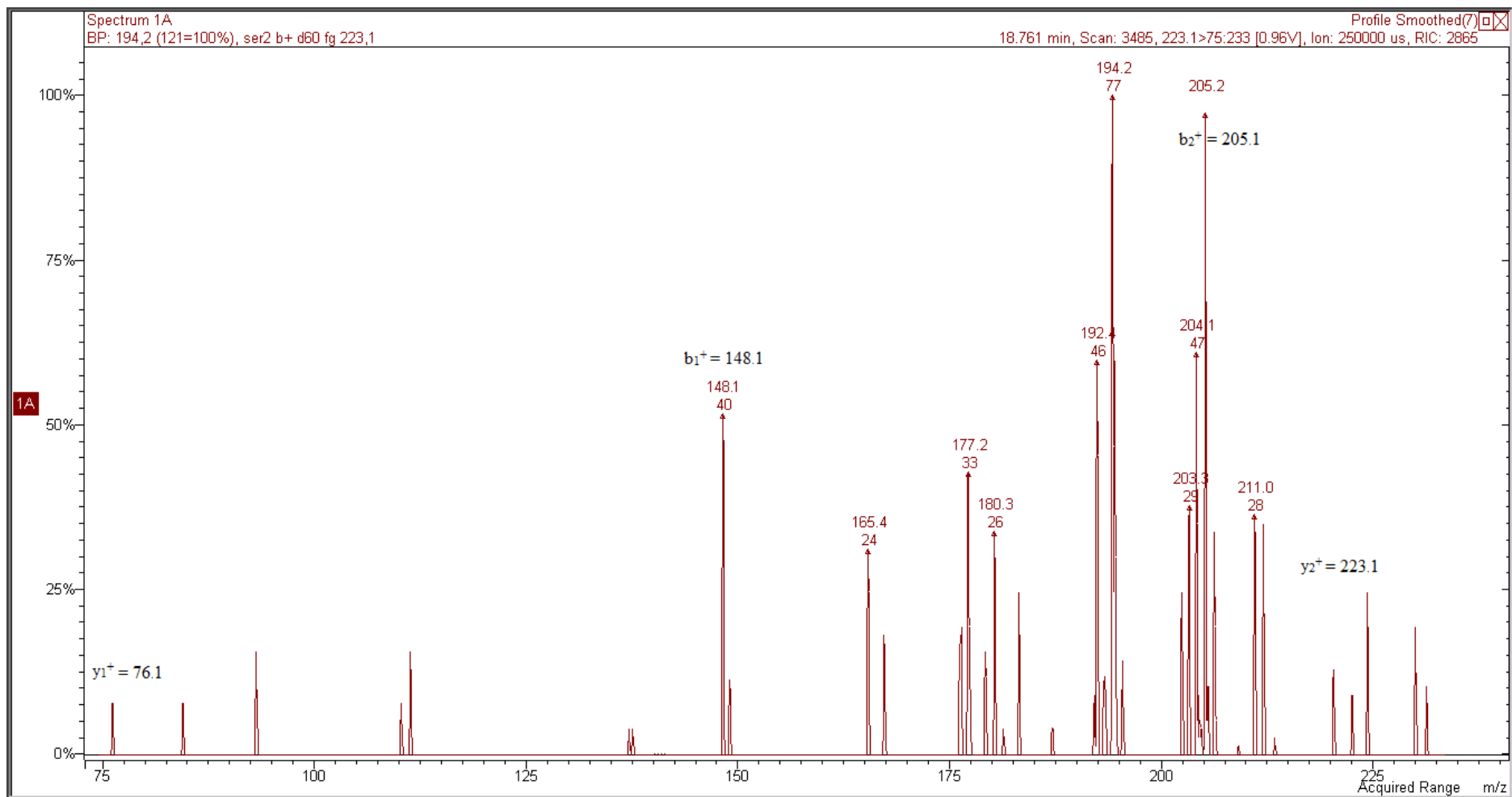
**Figure S20.** MS/MS spectrum of FG peptide.
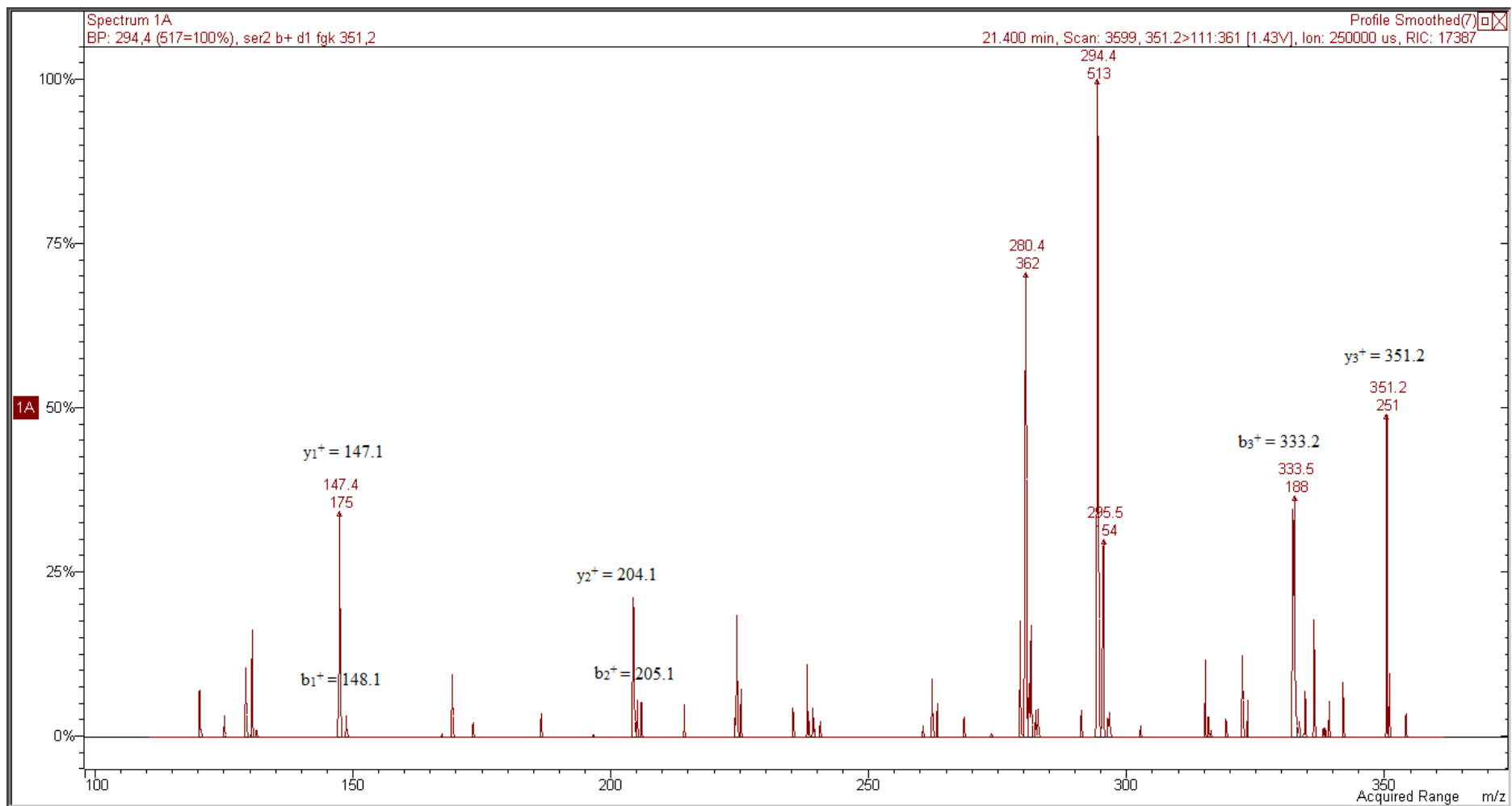
**Figure S21.** MS/MS spectrum of FGK peptide.
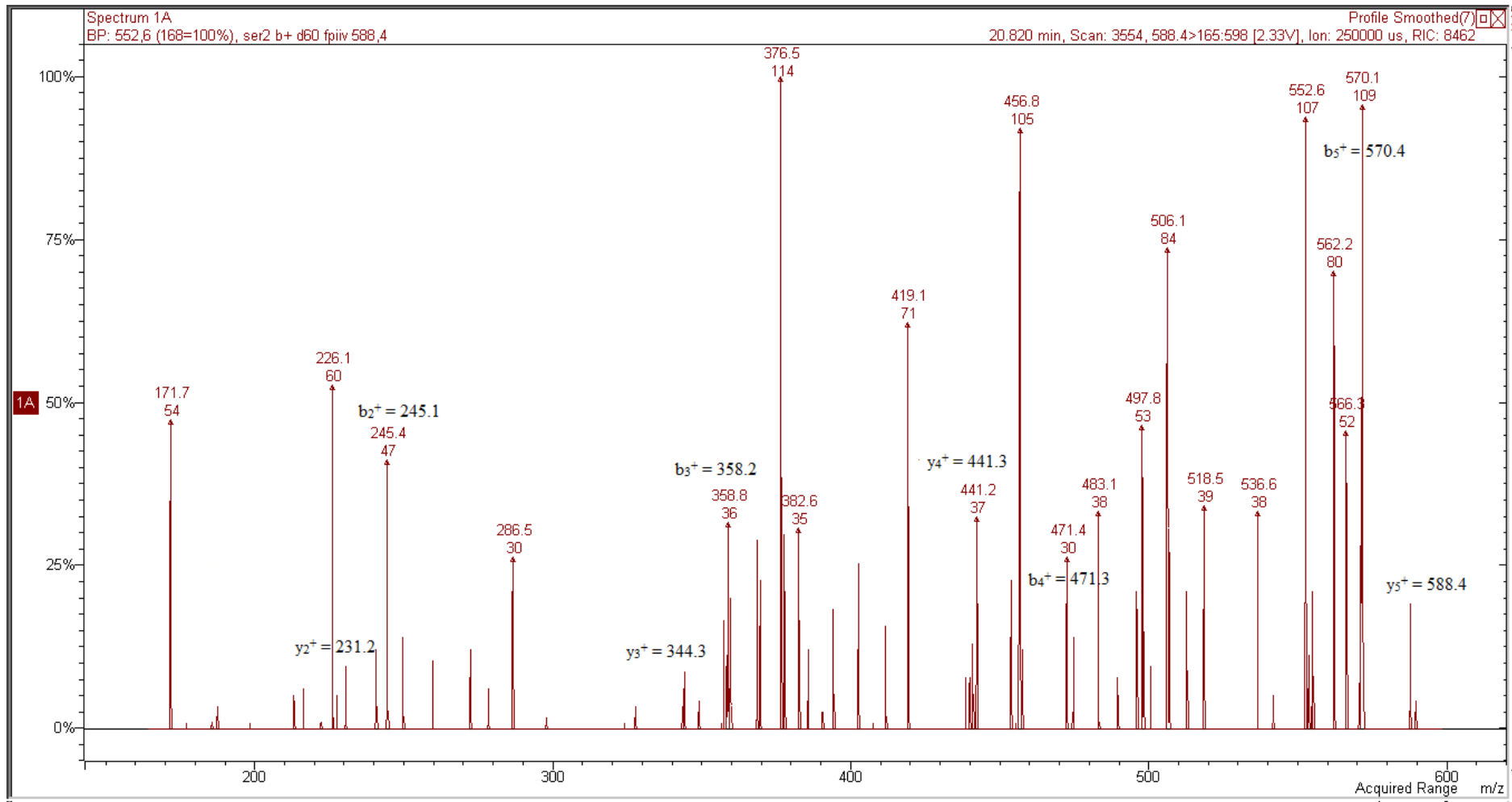
**Figure S22.** MS/MS spectrum of FPIIV peptide.
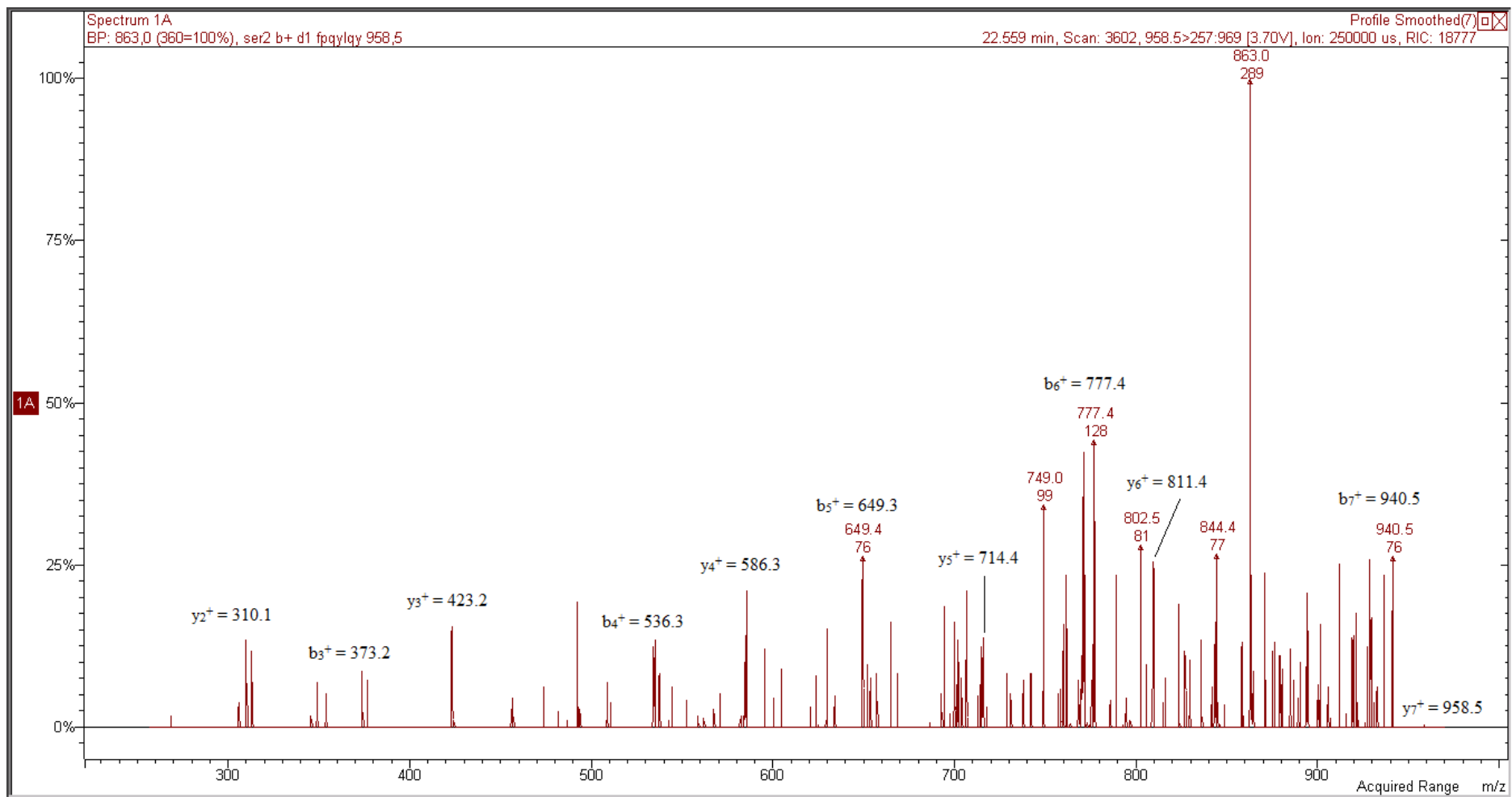
**Figure S23.** MS/MS spectrum of FPQYLQY peptide.
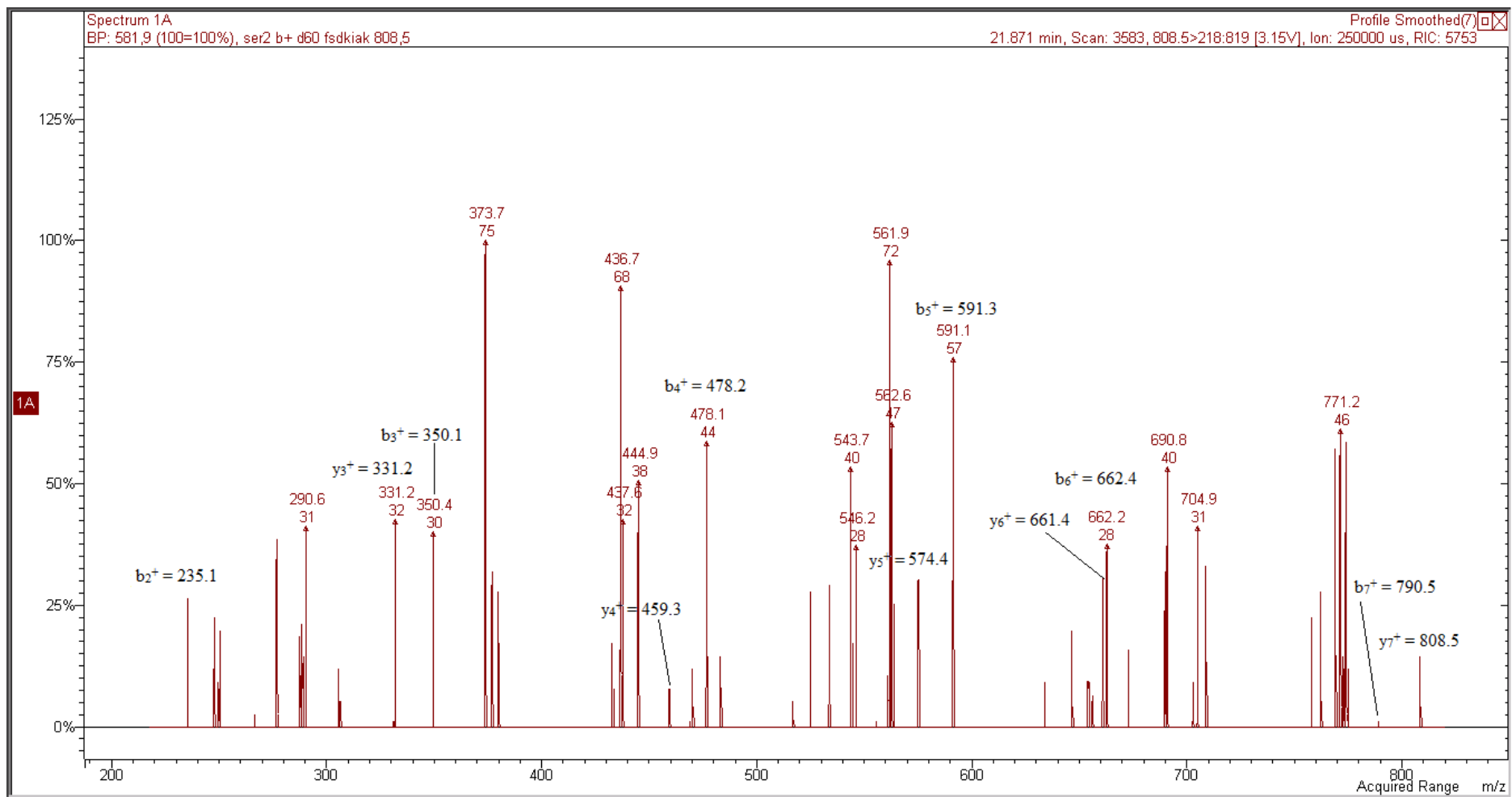
**Figure S24.** MS/MS spectrum of FSDKIAK peptide.
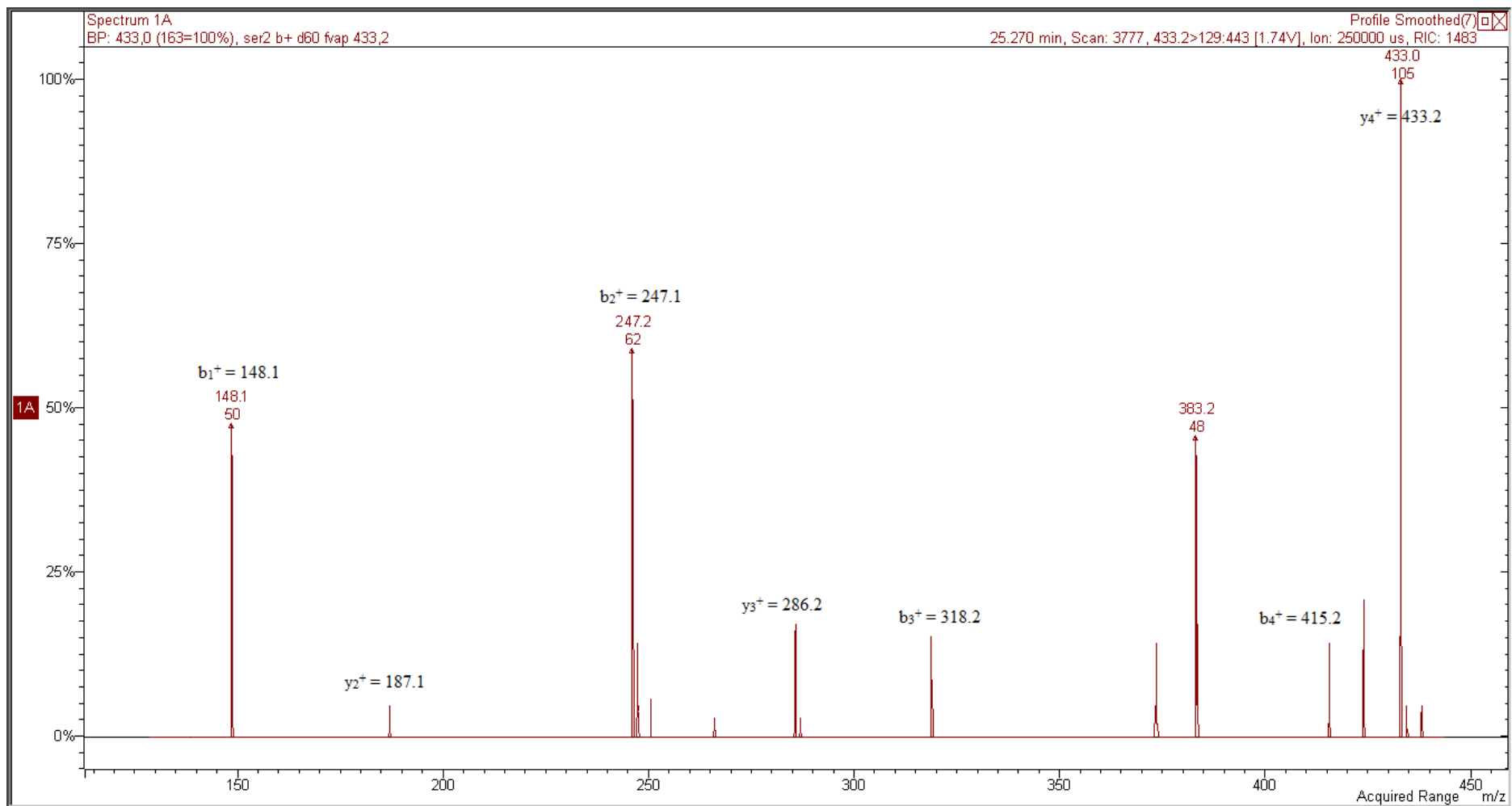
**Figure S25.** MS/MS spectrum of FVAP peptide.
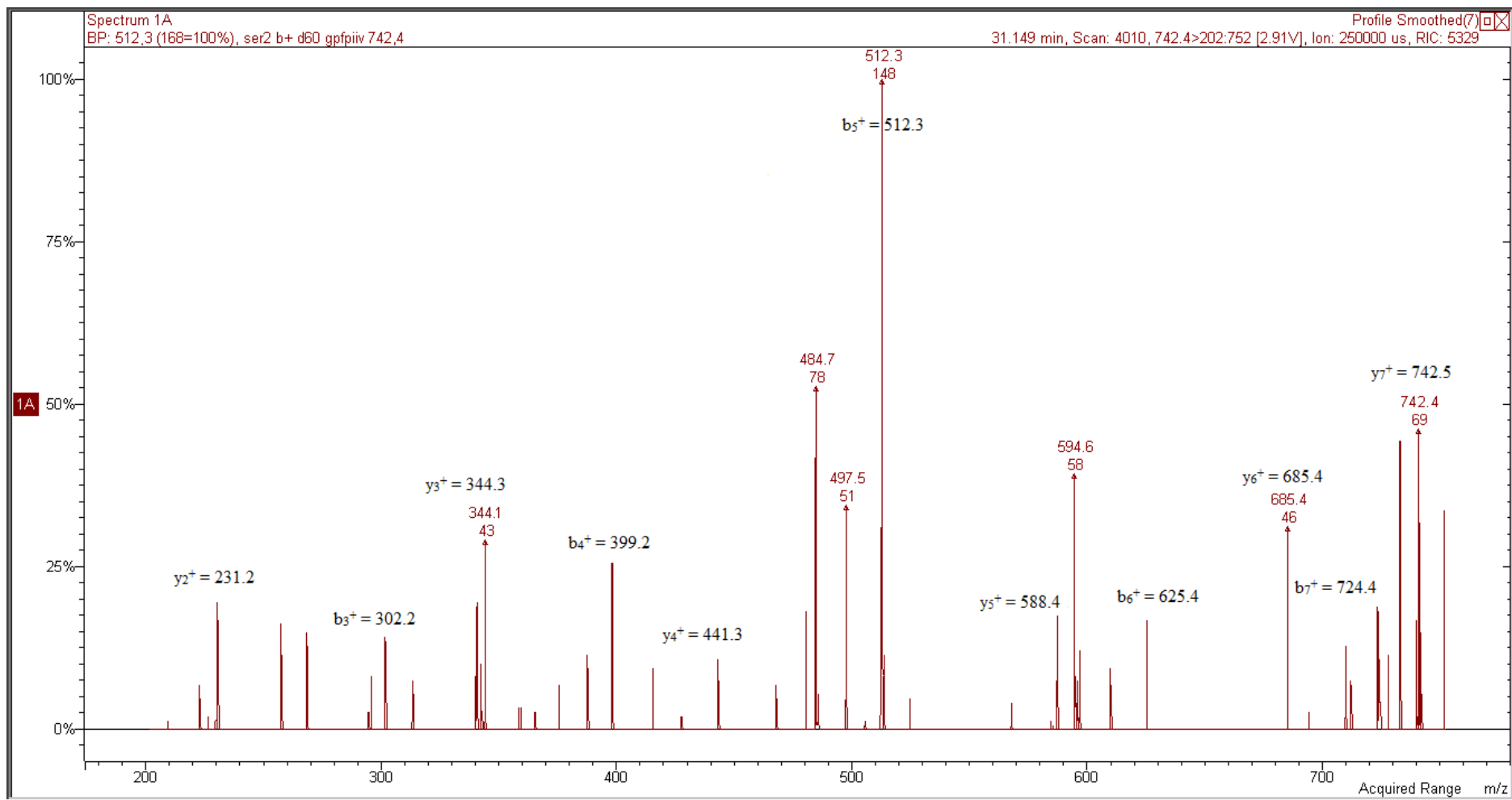
**Figure S26.** MS/MS spectrum of GPFPIIV peptide.
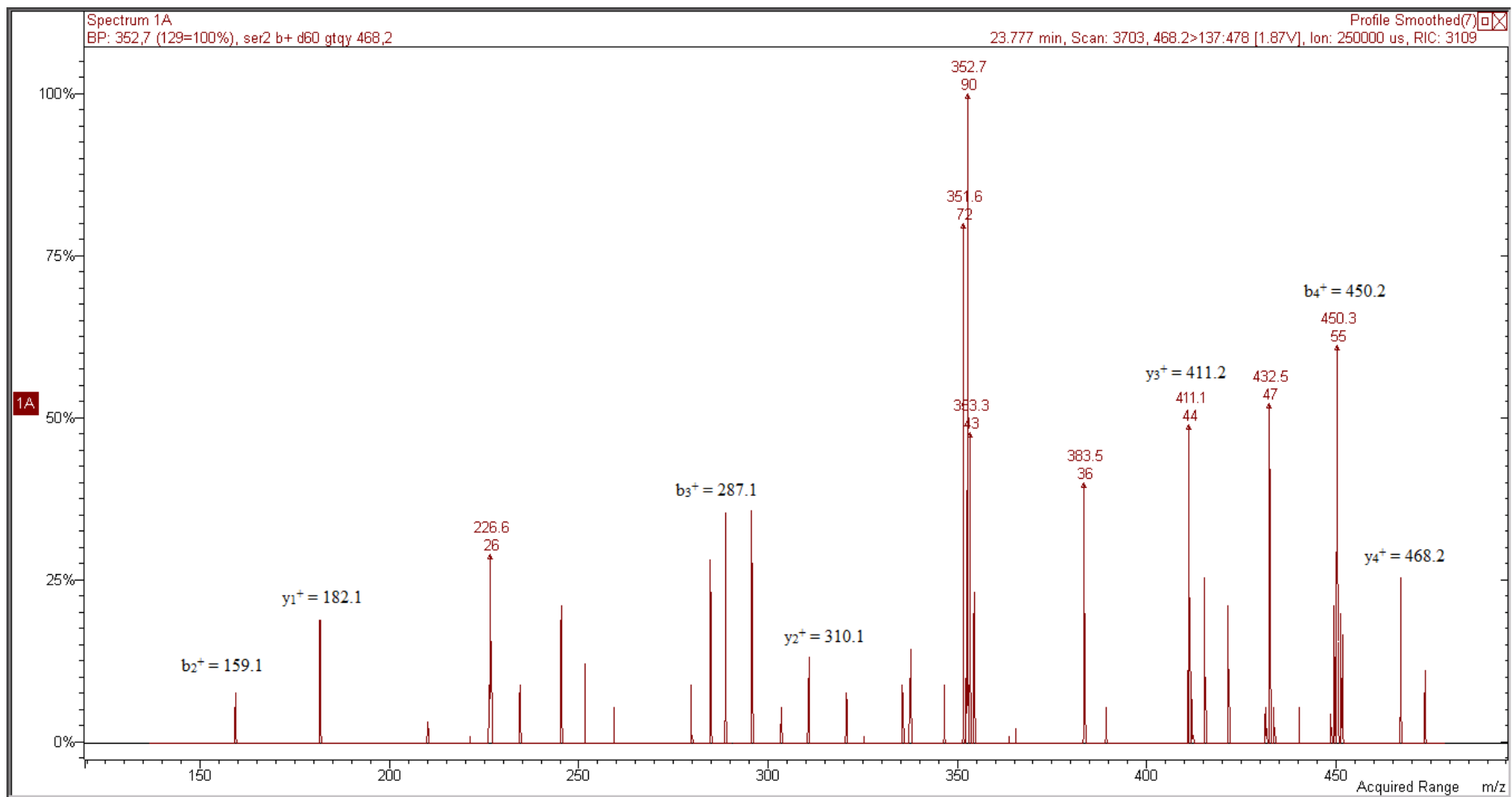
**Figure S27.** MS/MS spectrum of GTQY peptide.
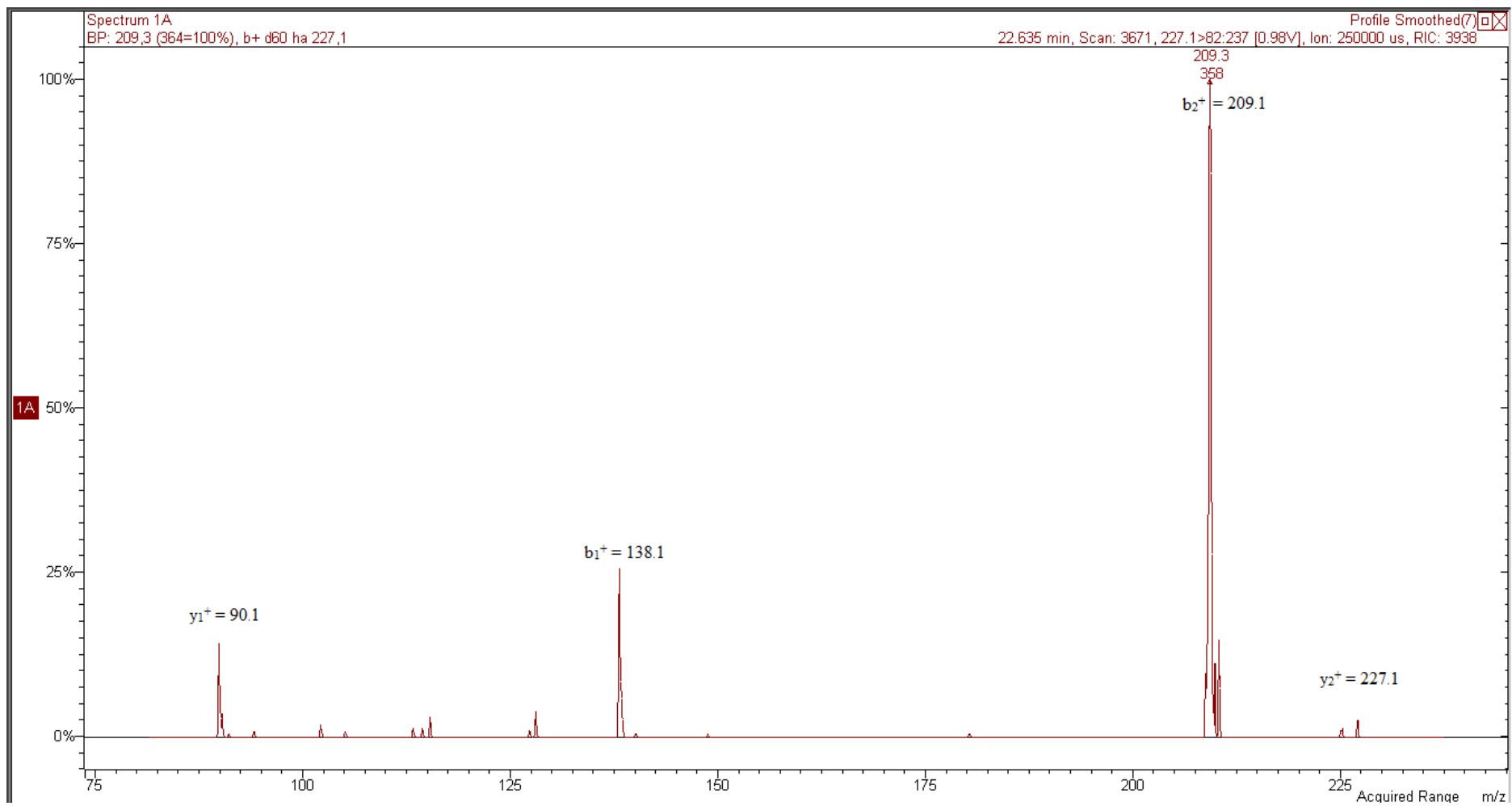
**Figure S28.** MS/MS spectrum of HA peptide.
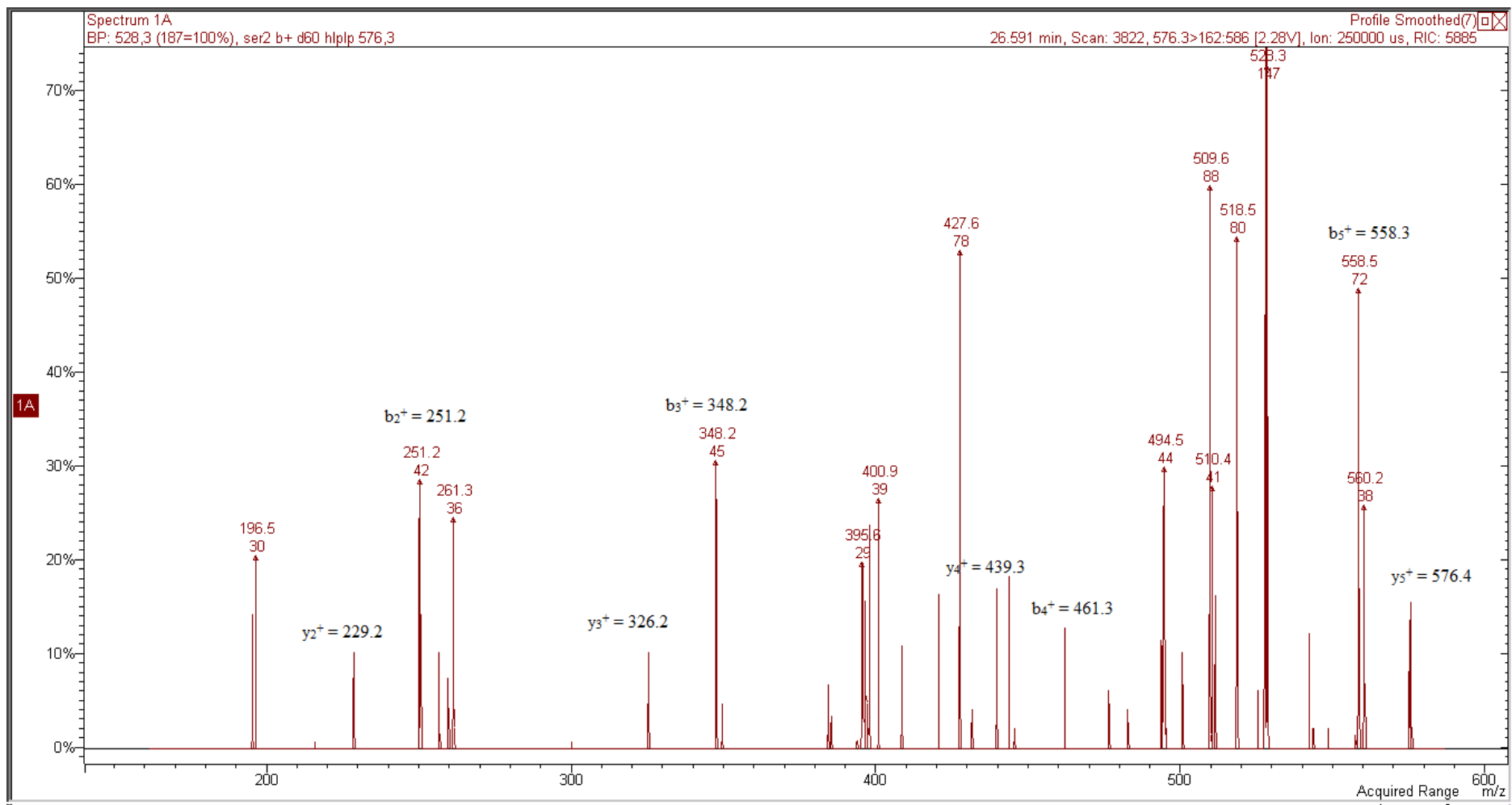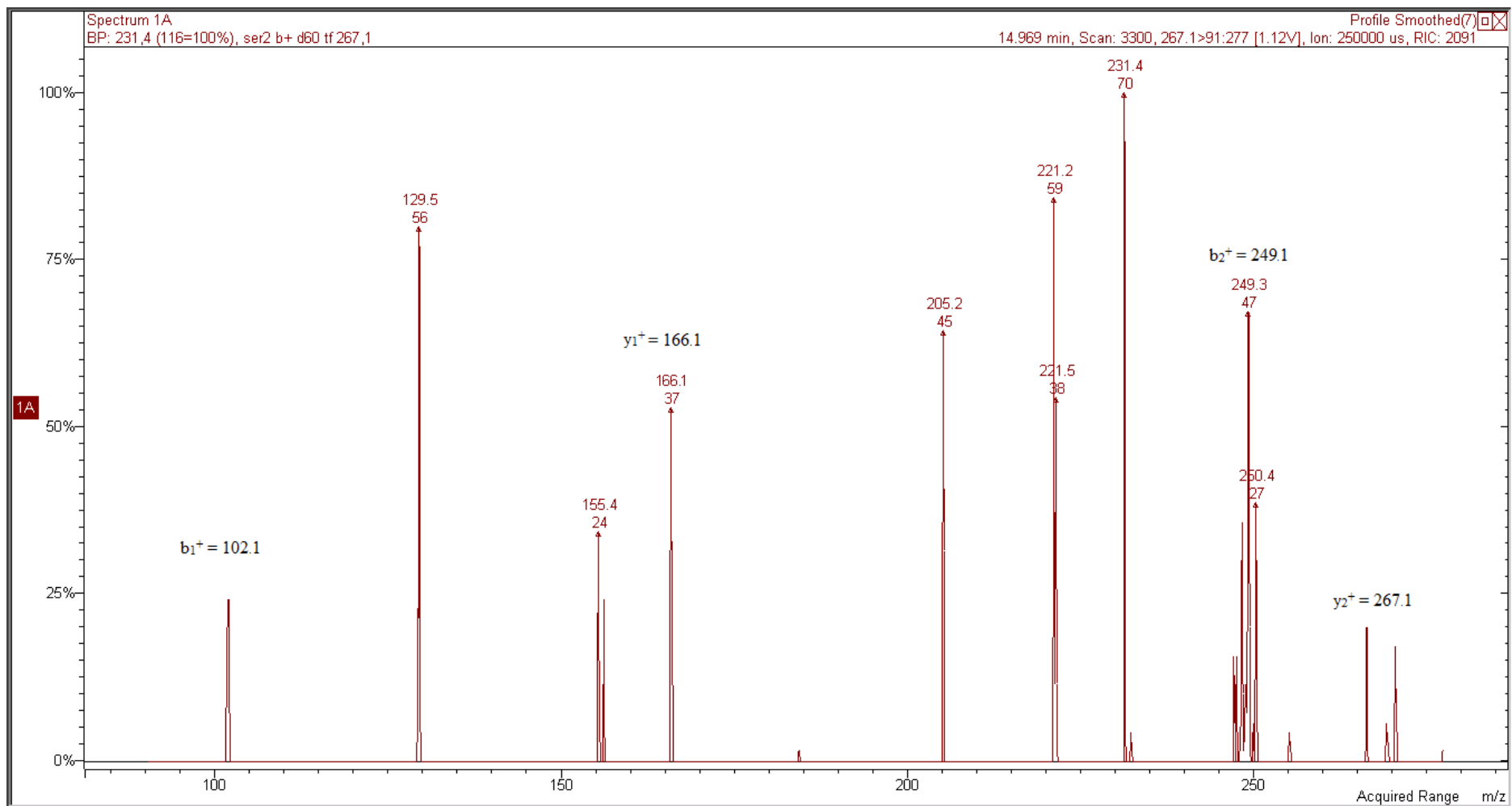
**Figure S29.** MS/MS spectrum of HLPLP peptide.
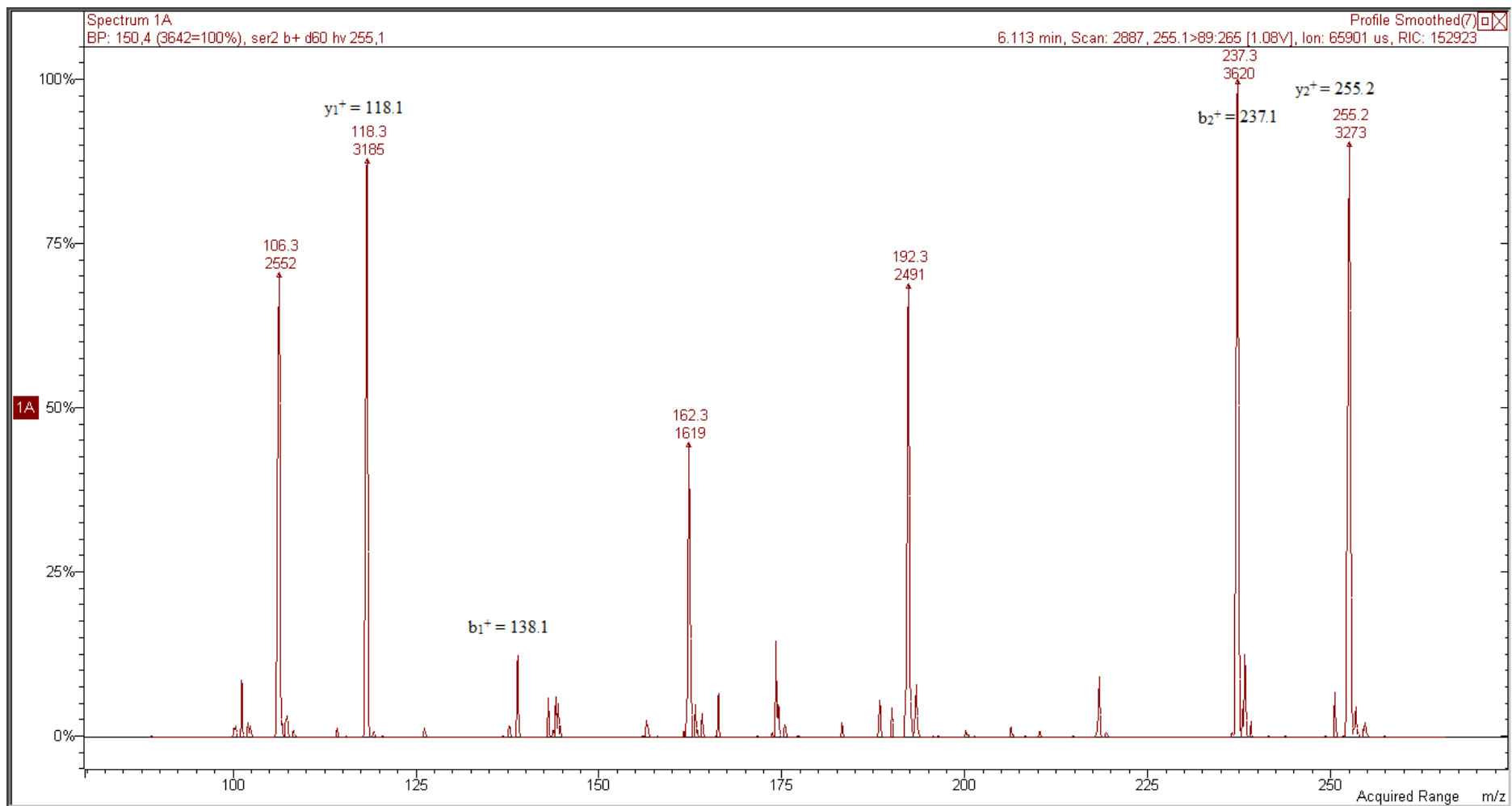
**Figure S30.** MS/MS spectrum of HV peptide.
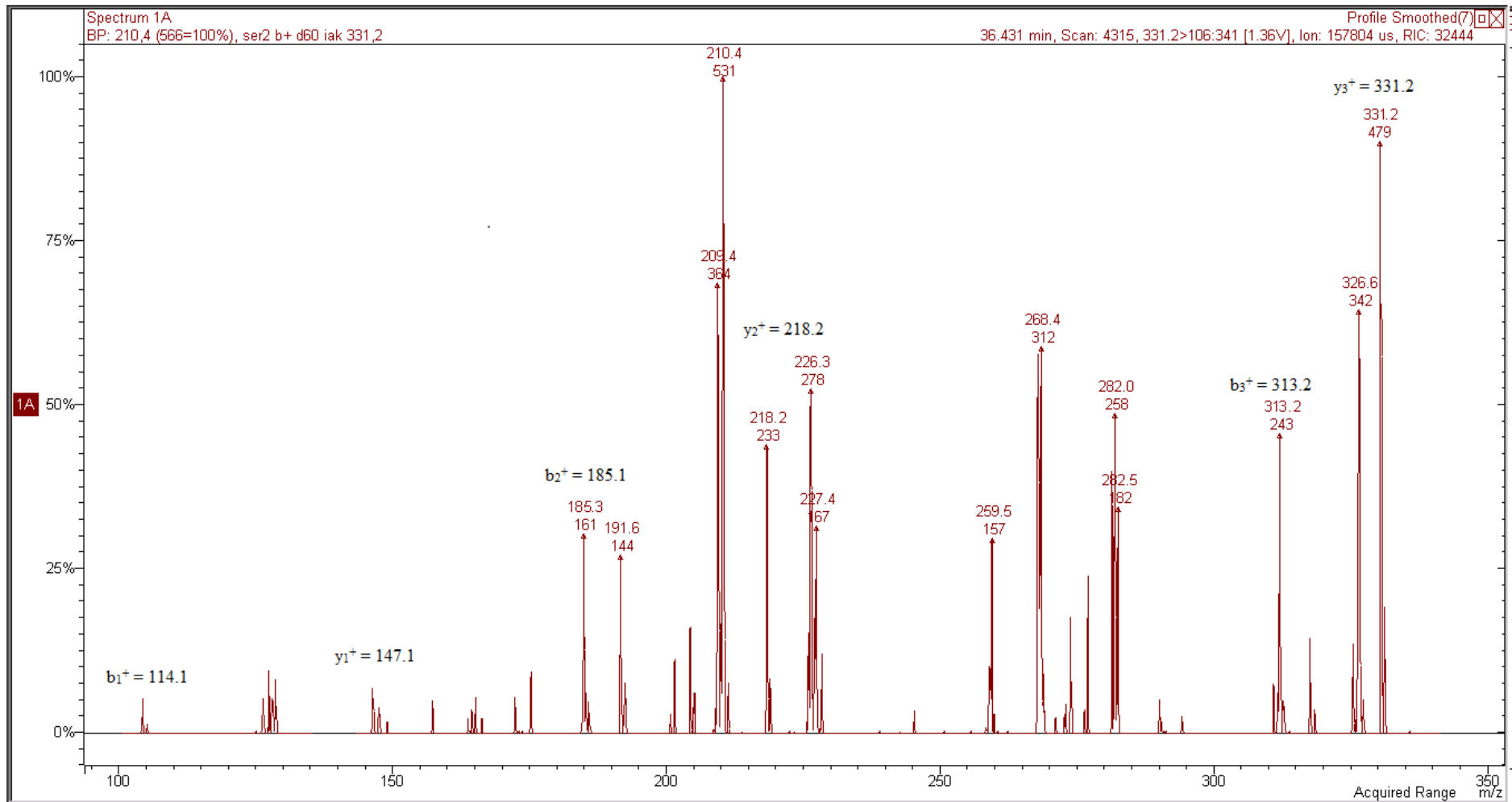
**Figure S31.** MS/MS spectrum of IAK peptide.
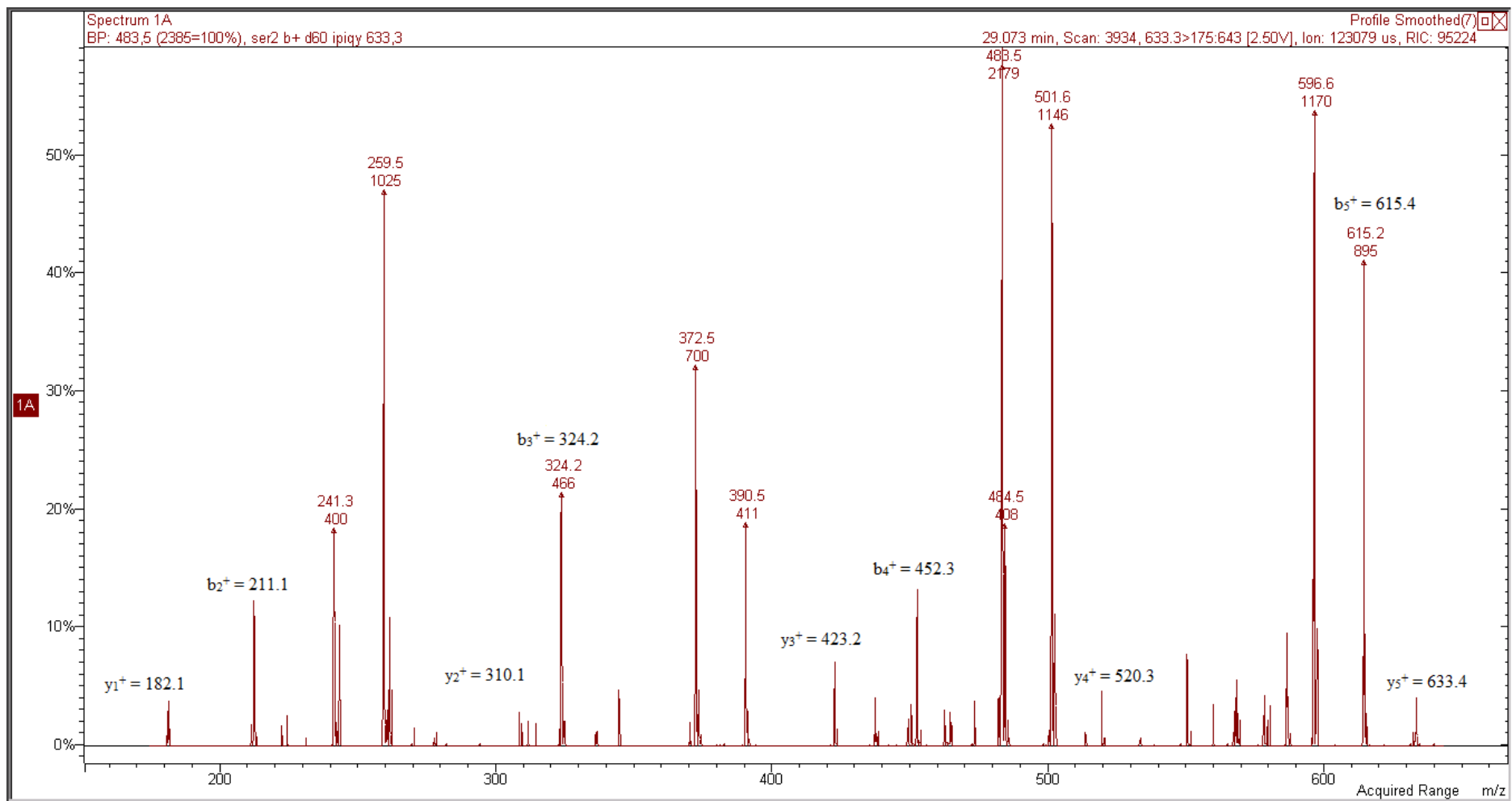
**Figure S32.** MS/MS spectrum of IPIQY peptide.
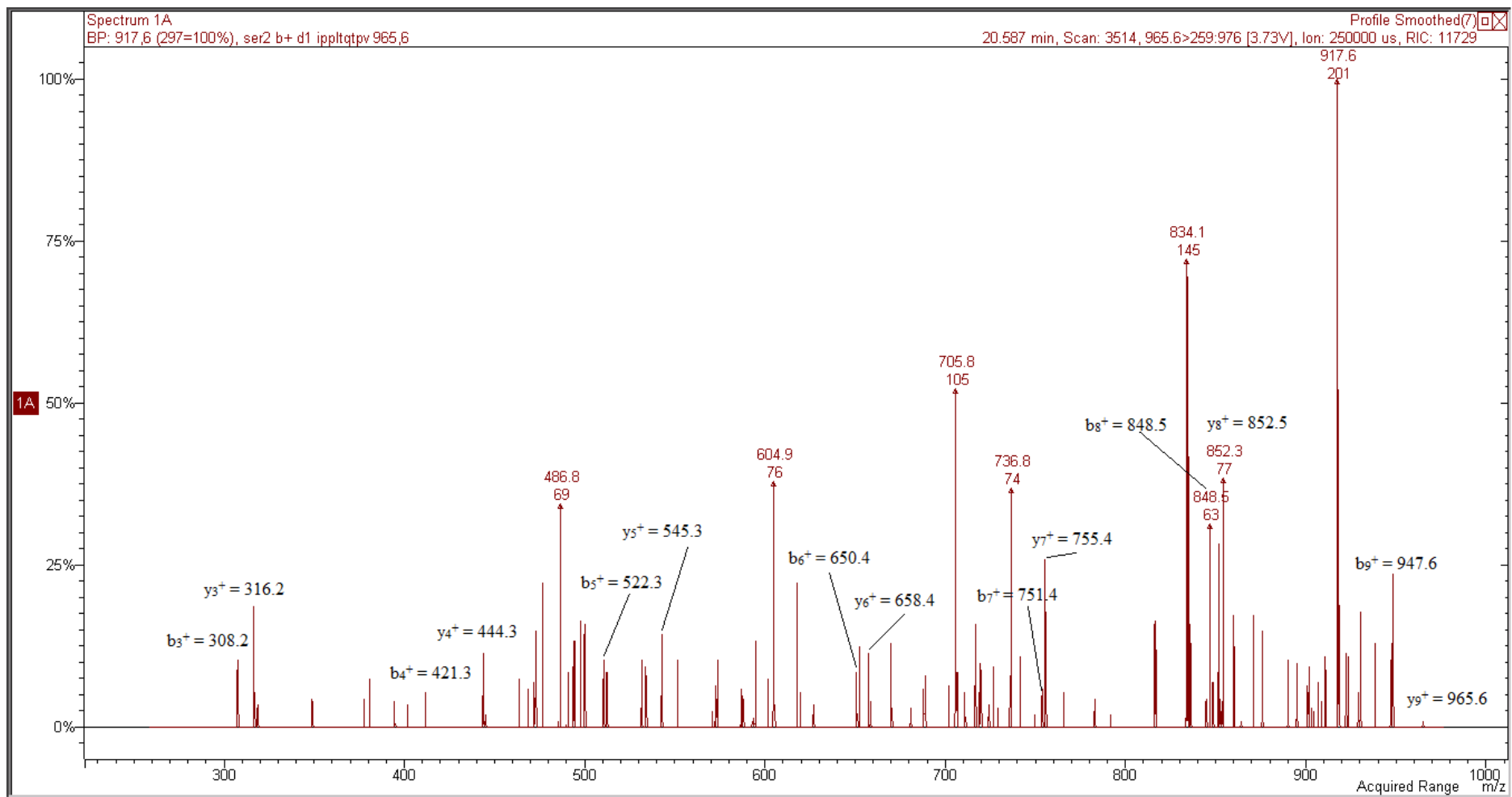
**Figure S33.** MS/MS spectrum of IPPLTQTPV peptide.
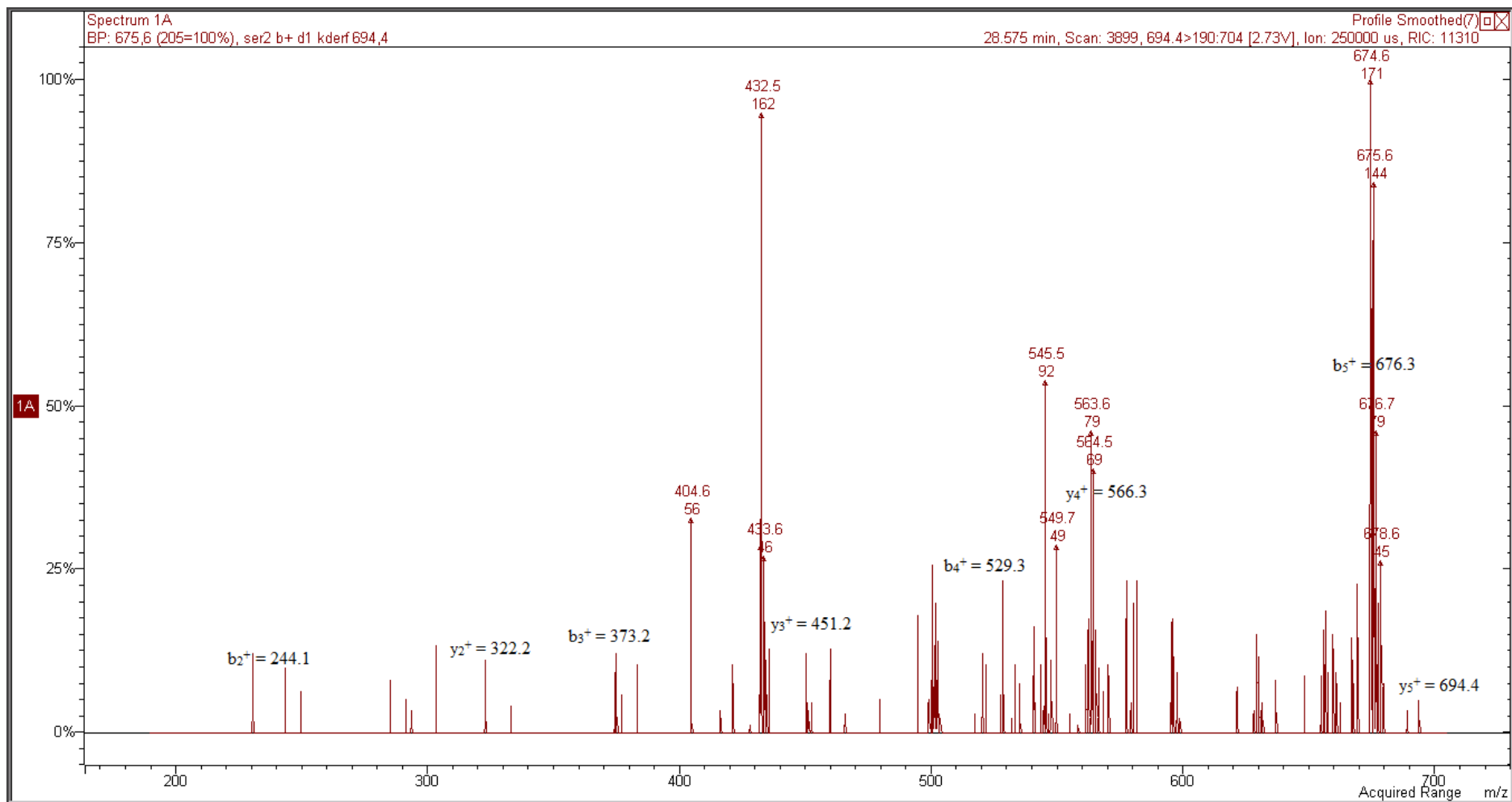
**Figure S34.** MS/MS spectrum of KDERF peptide.
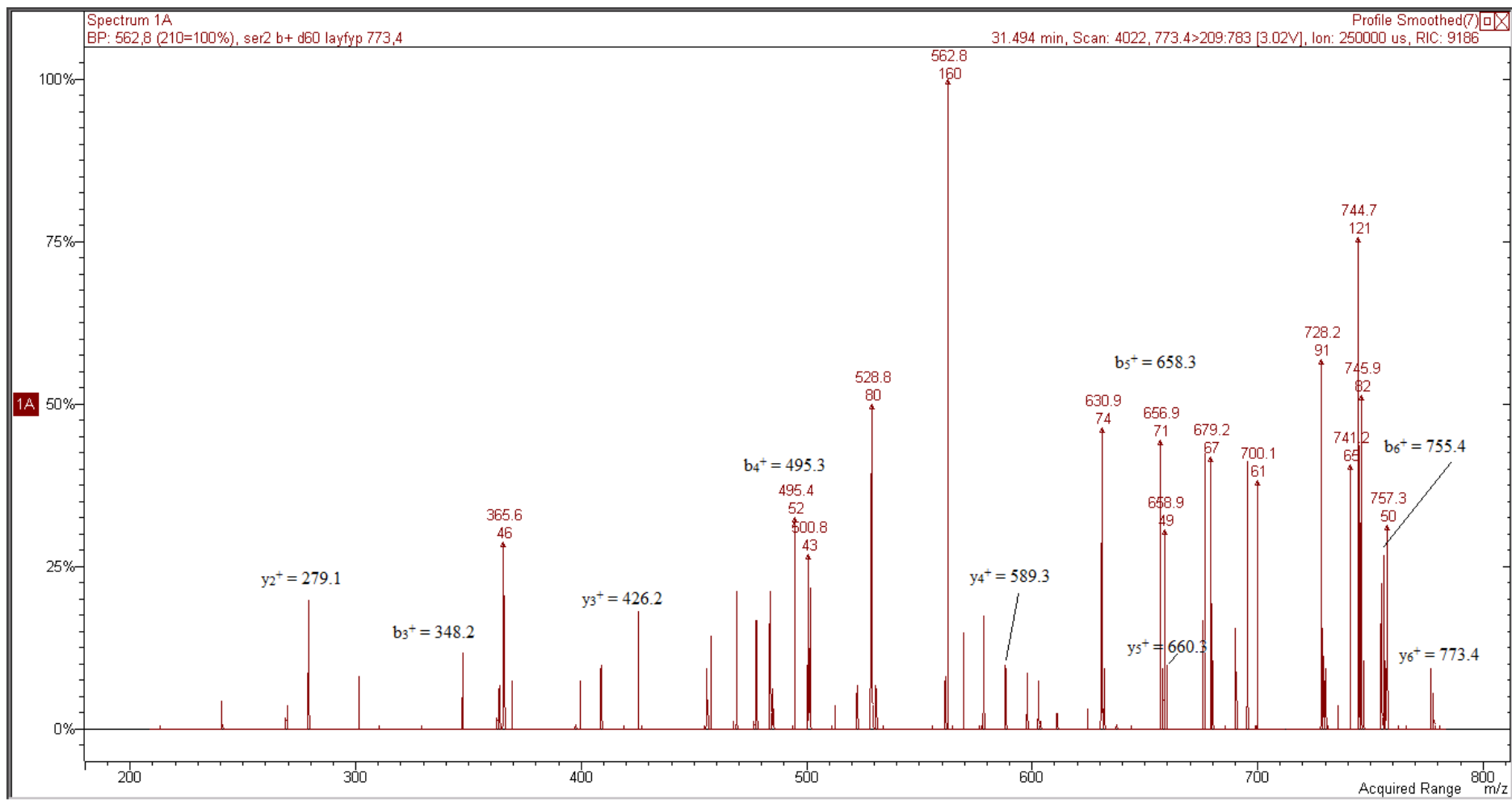
**Figure S35.** MS/MS spectrum of LAYFYP peptide.
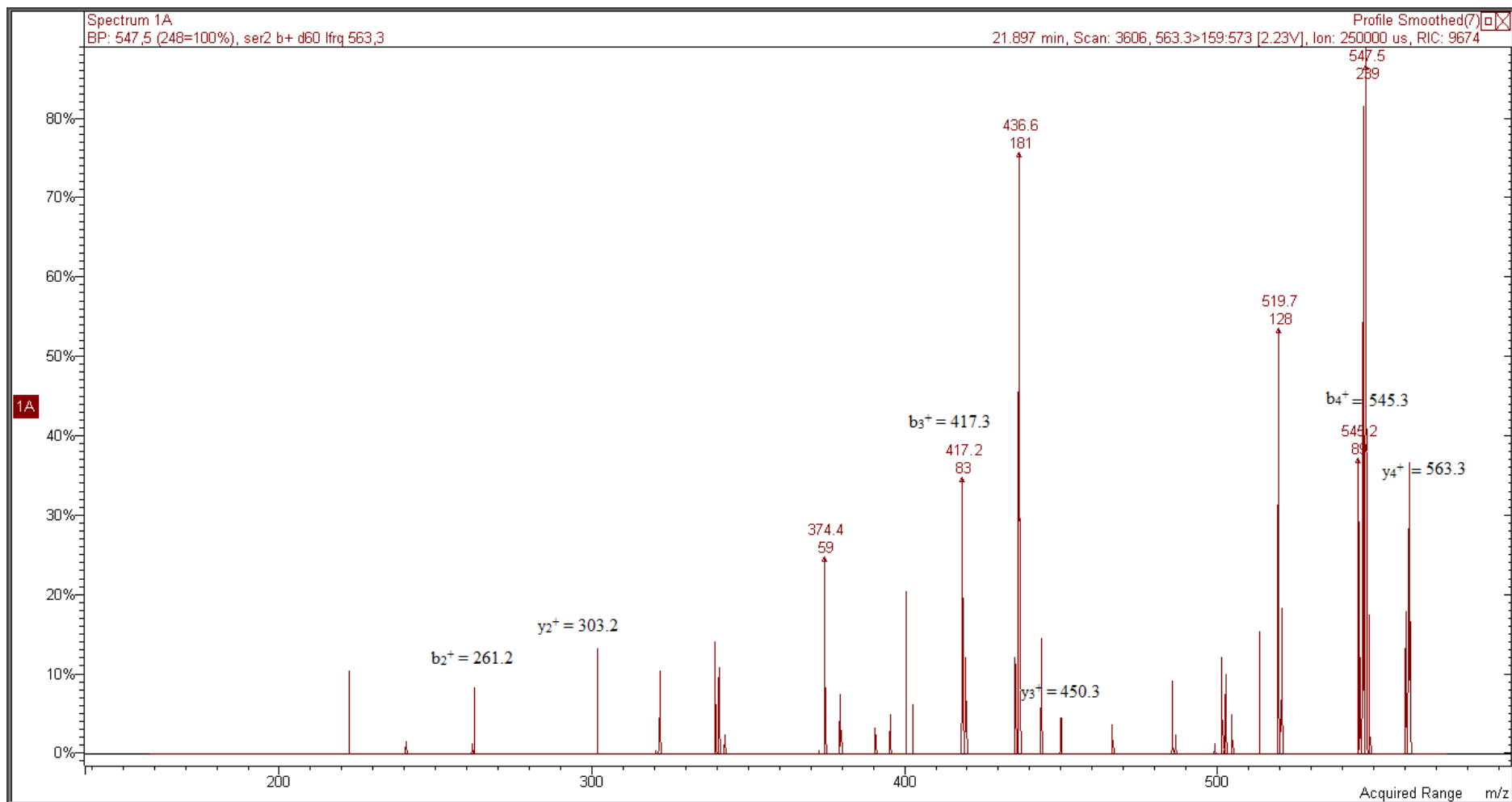
**Figure S36.** MS/MS spectrum of LFRQ peptide.
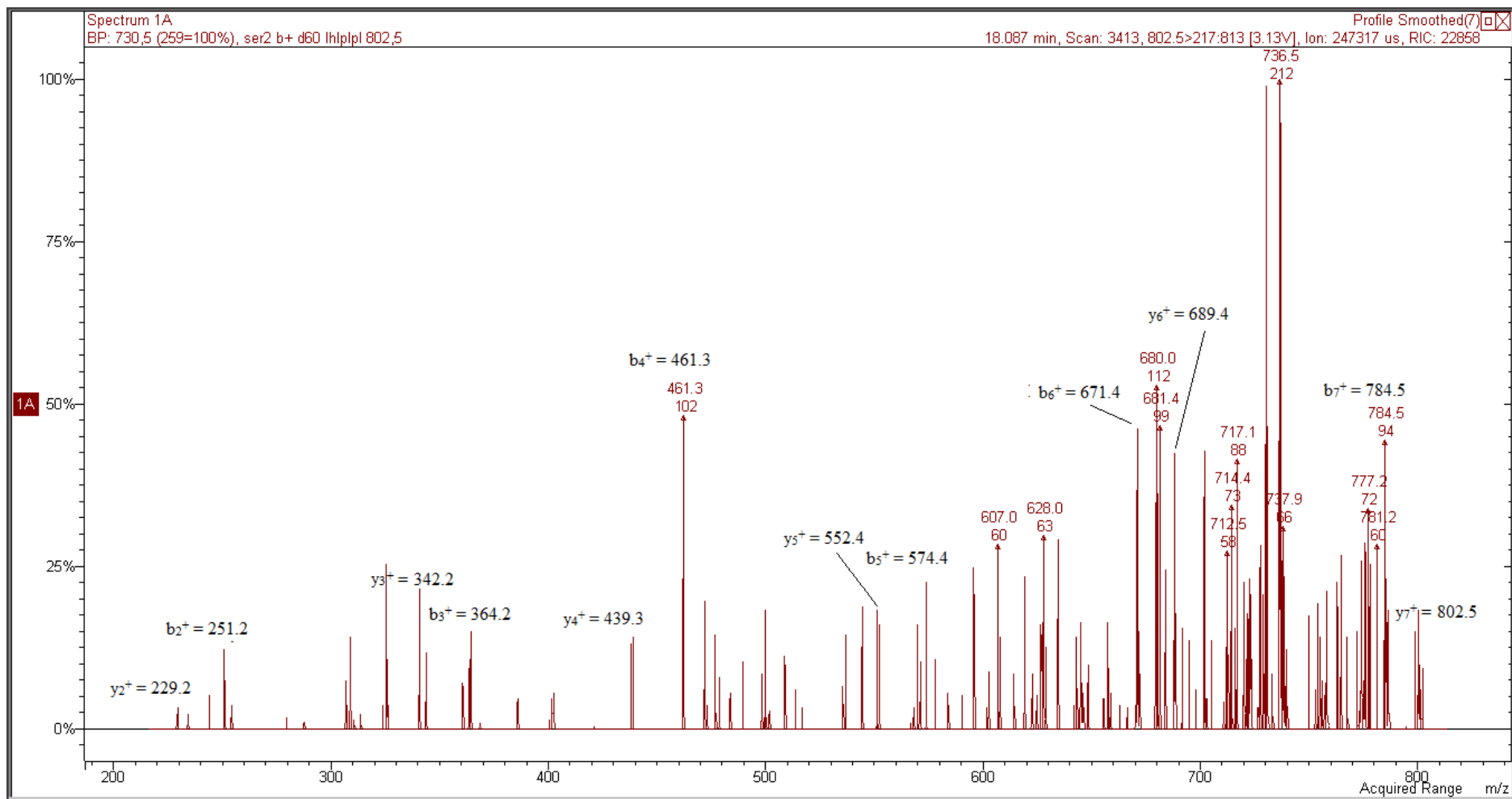
**Figure S37.** MS/MS spectrum of LHLPLP peptide.
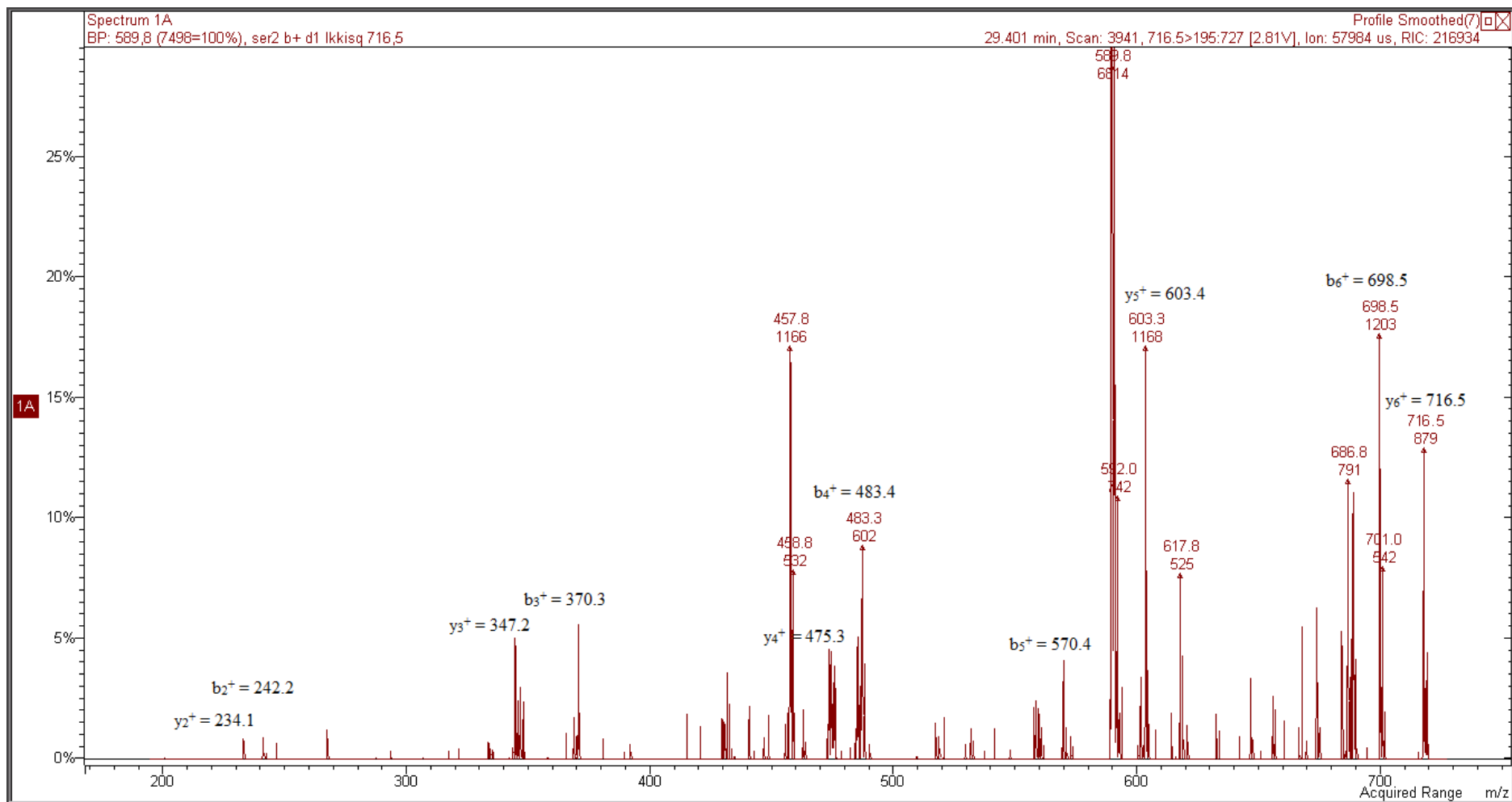
**Figure S35.** MS/MS spectrum of LKKISQ peptide.
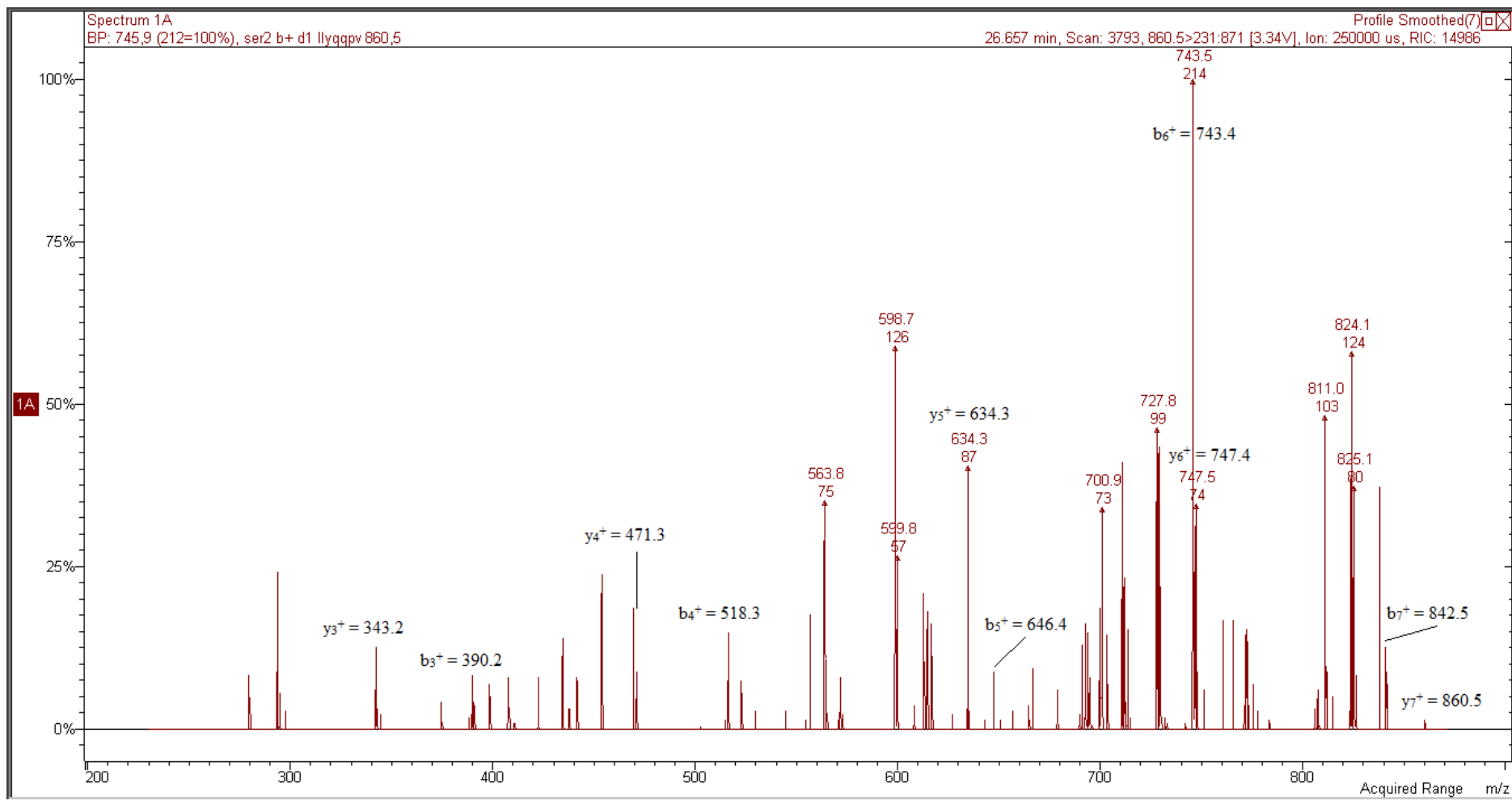
**Figure S39.** MS/MS spectrum of LLYQQPV peptide.
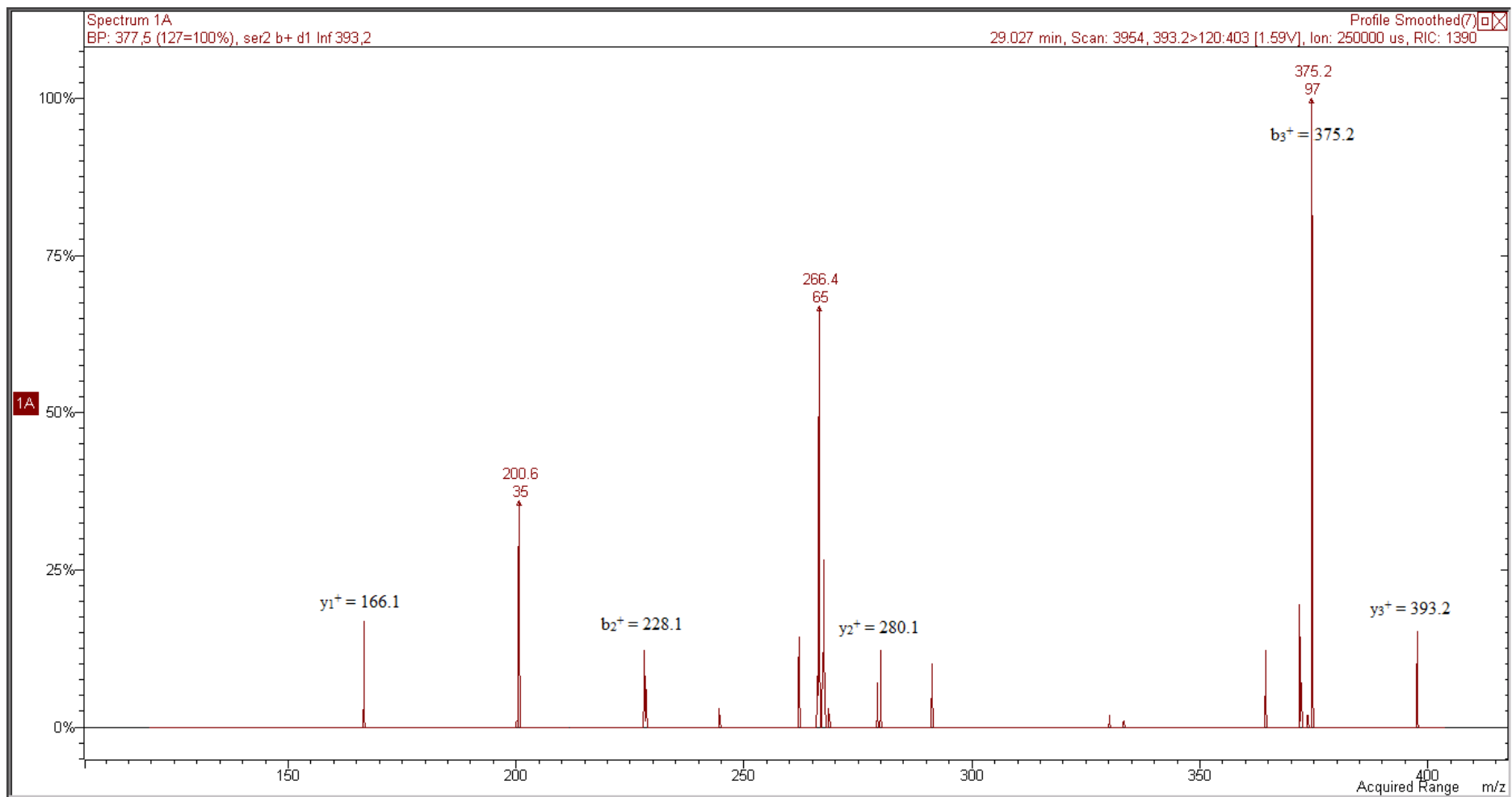
**Figure S40.** MS/MS spectrum of LNF peptide.
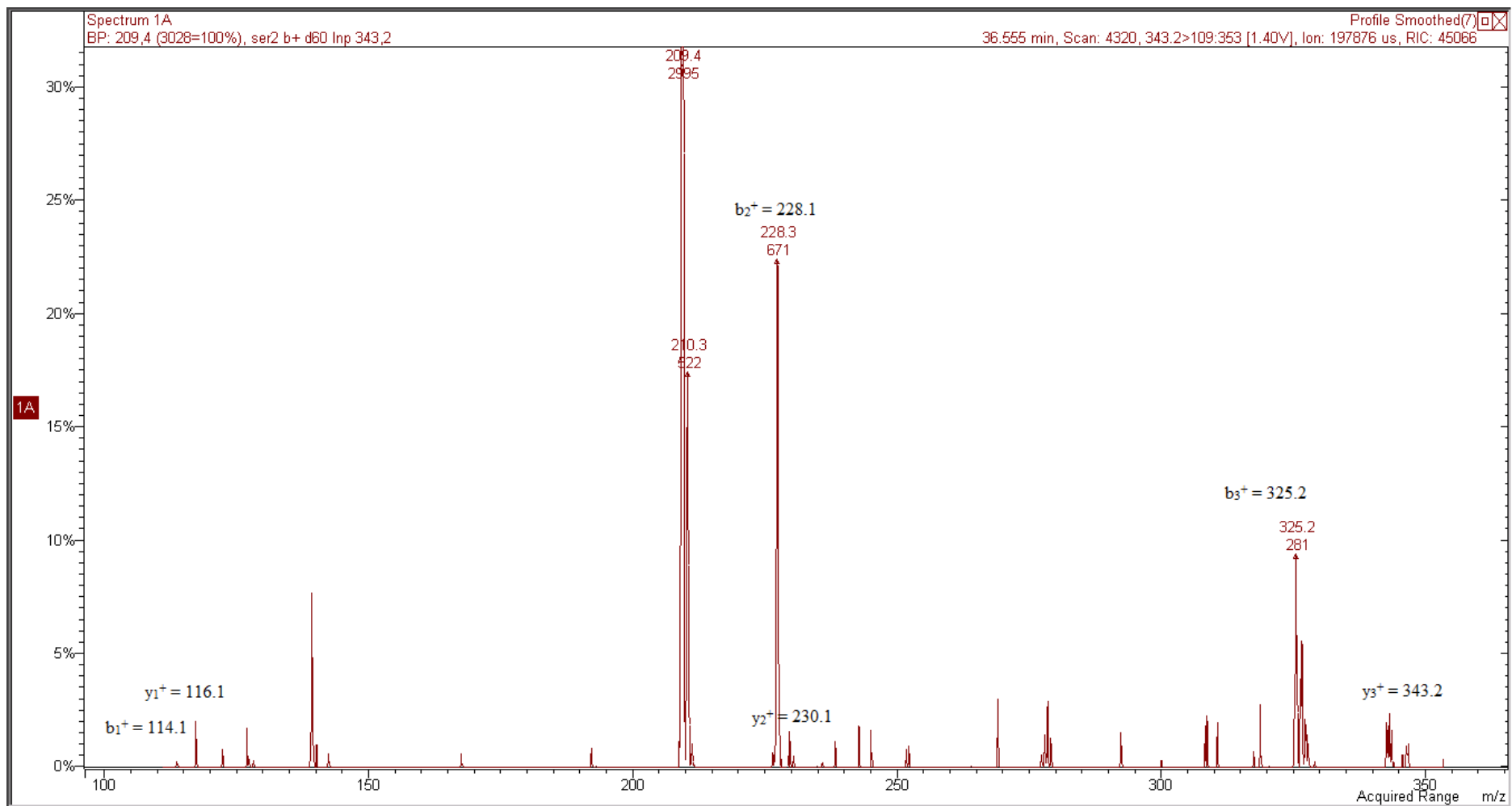
**Figure S41.** MS/MS spectrum of LNP peptide.
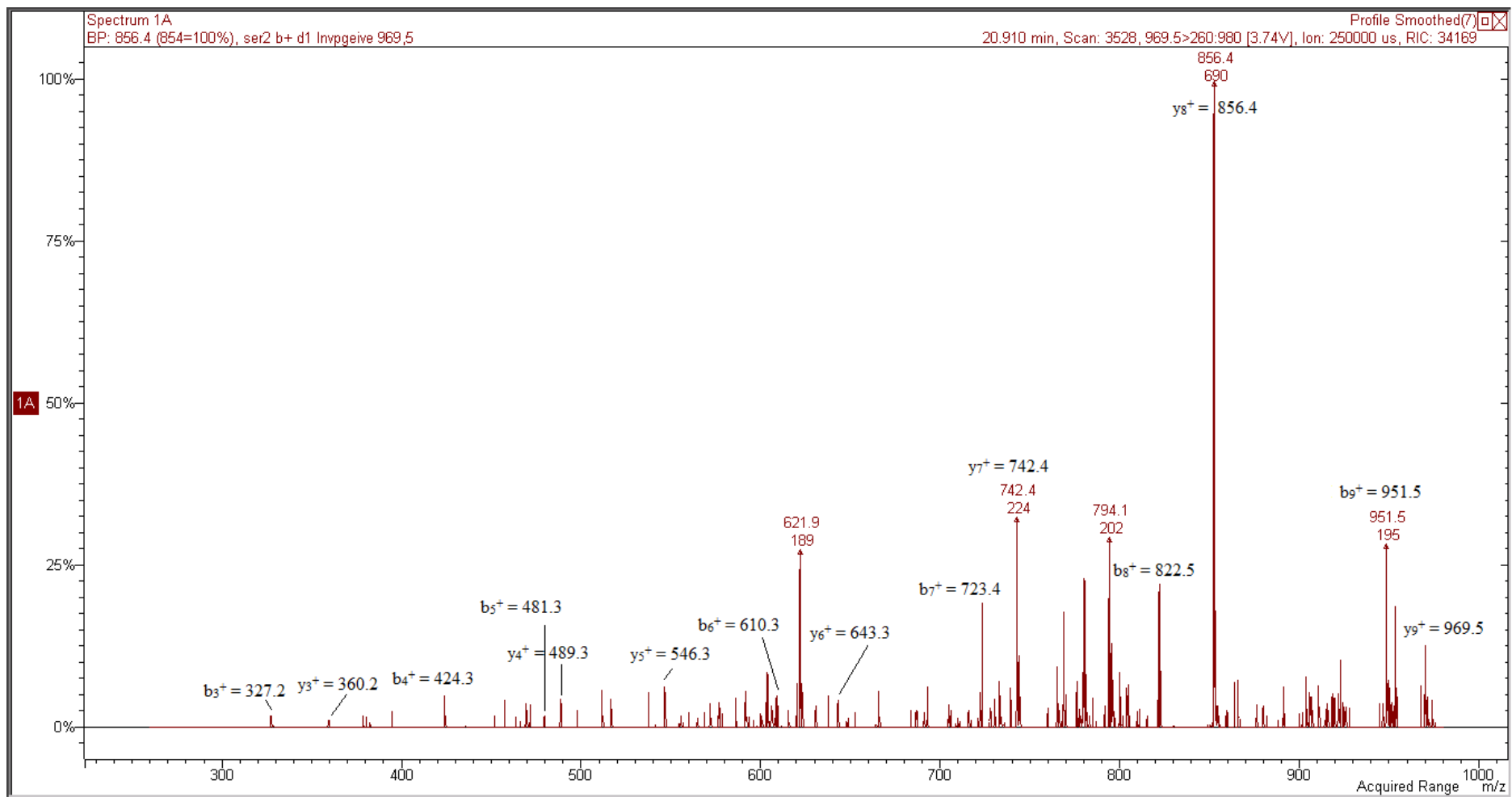
**Figure S42.** MS/MS spectrum of LNVPGEIVE peptide.
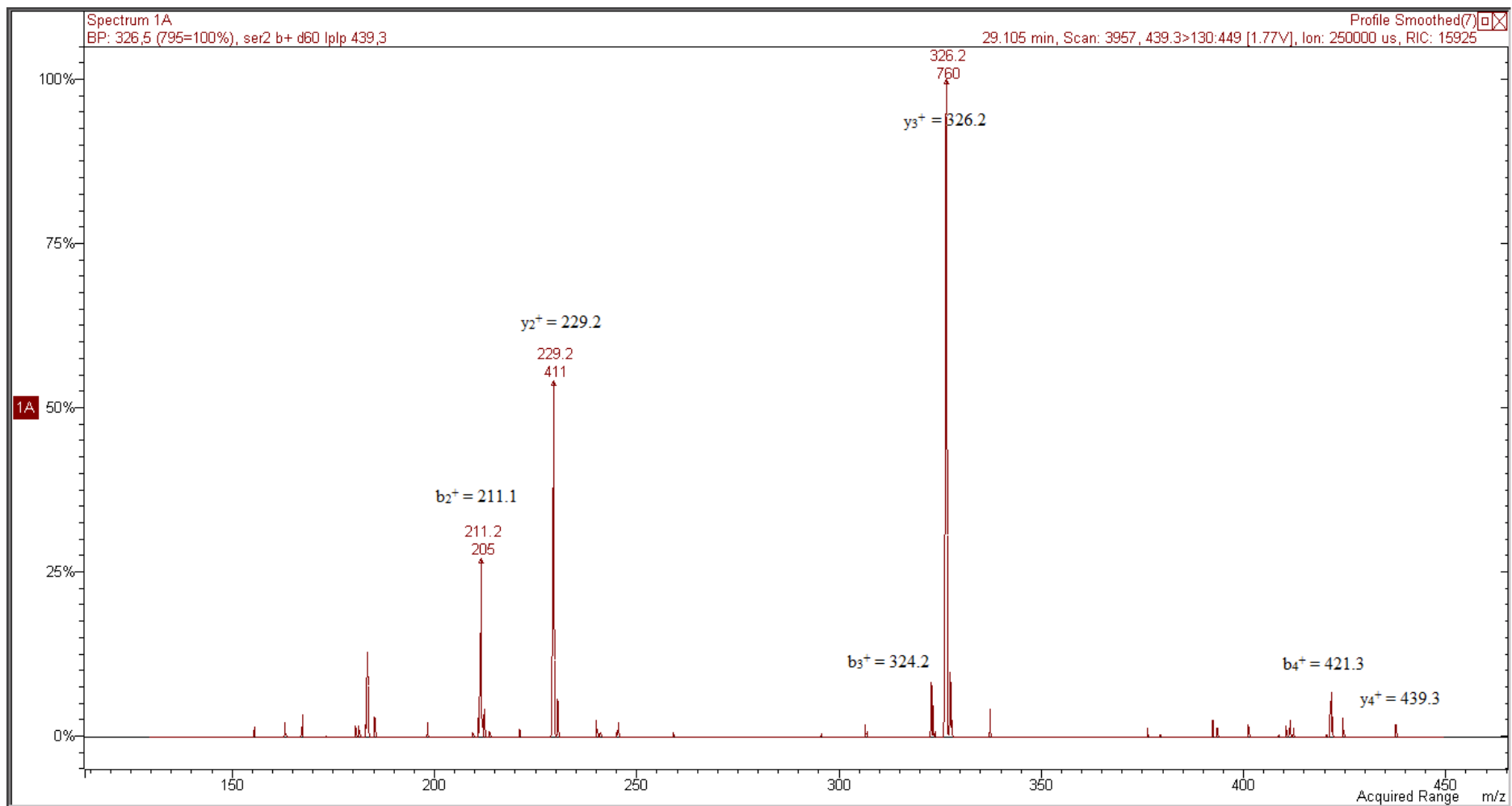
**Figure S43.** MS/MS spectrum of LPLP peptide.
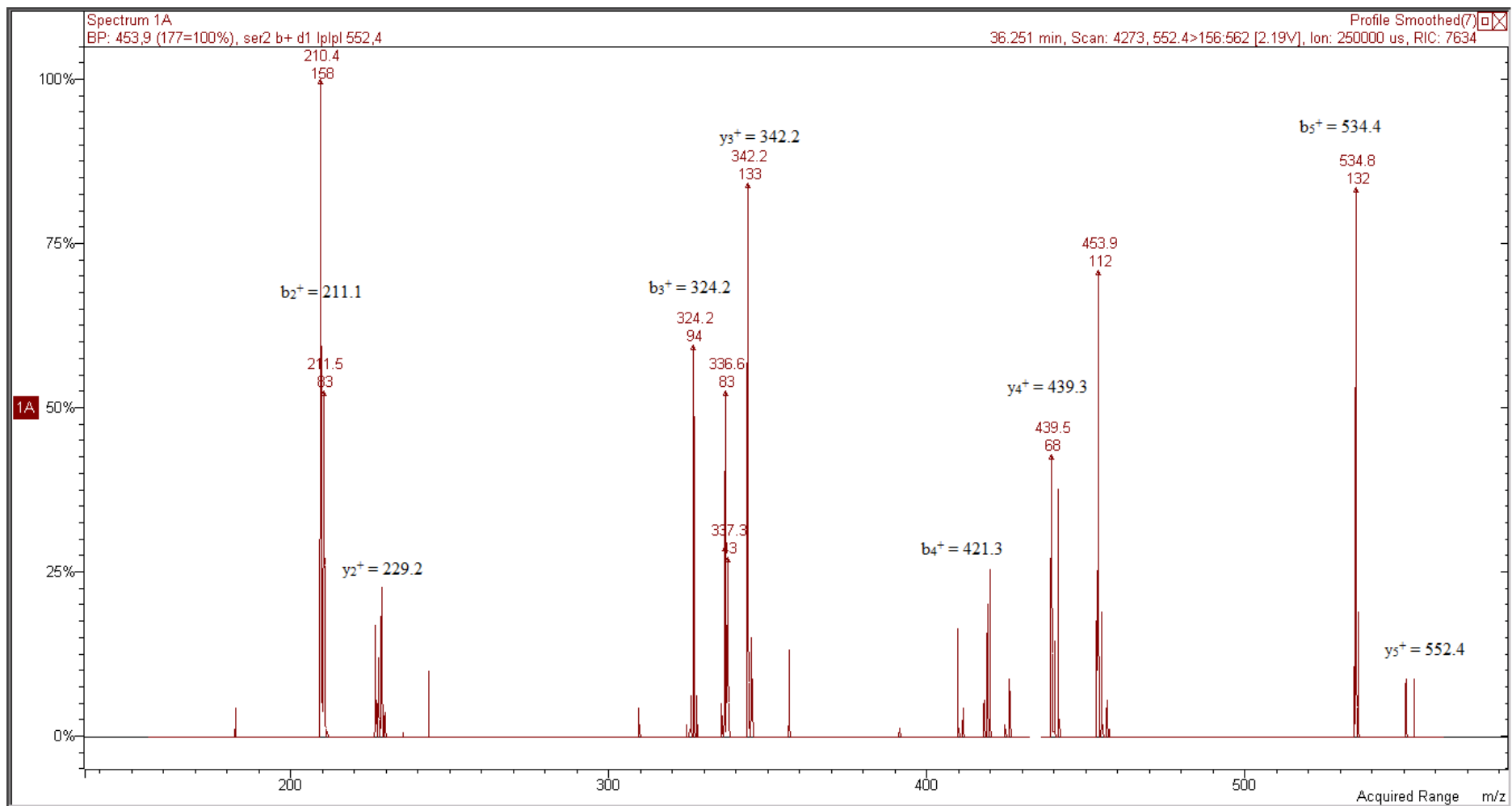
**Figure S44.** MS/MS spectrum of LPLPL peptide.
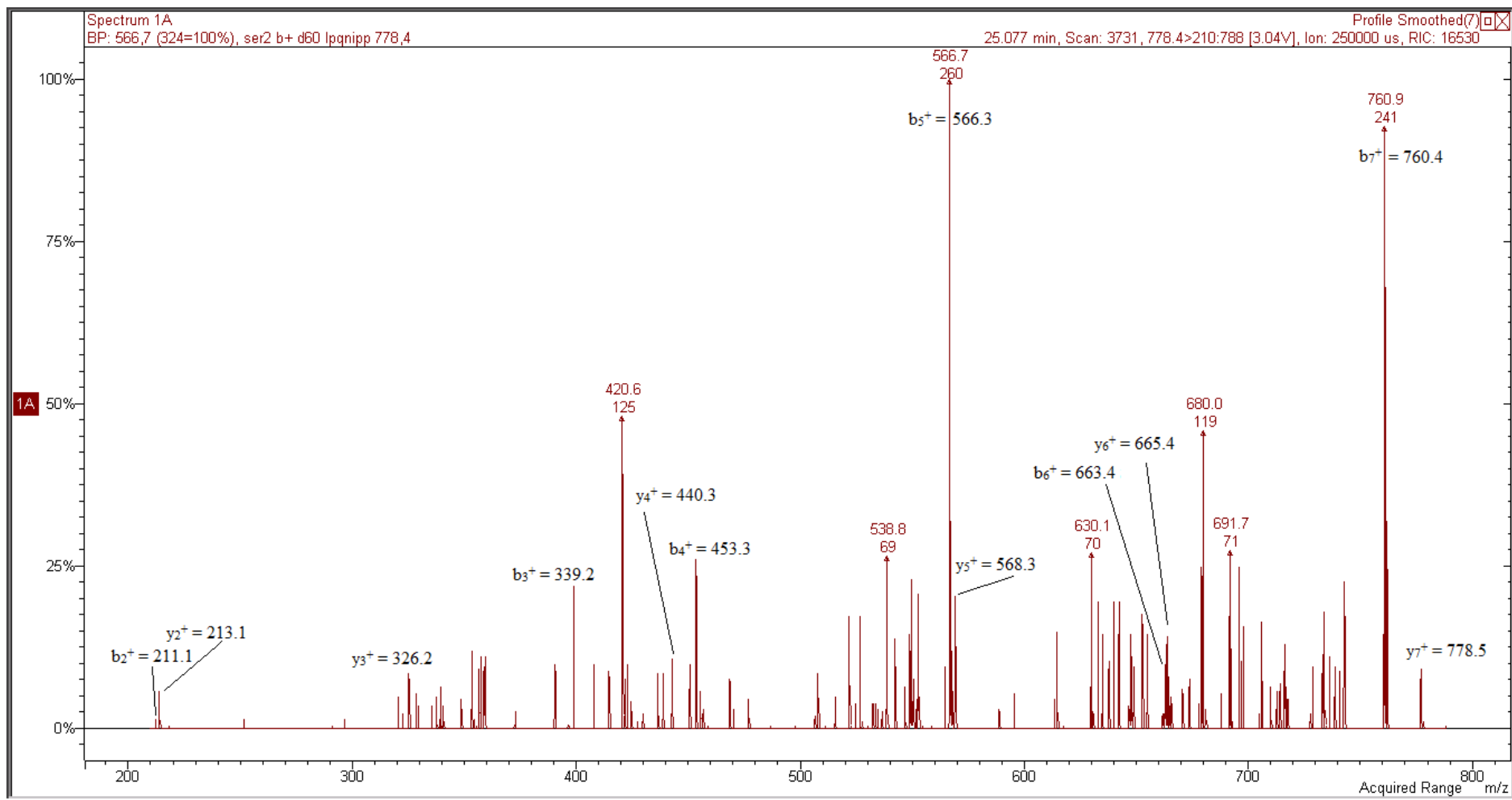
**Figure S45.** MS/MS spectrum of LPQNIPP peptide.
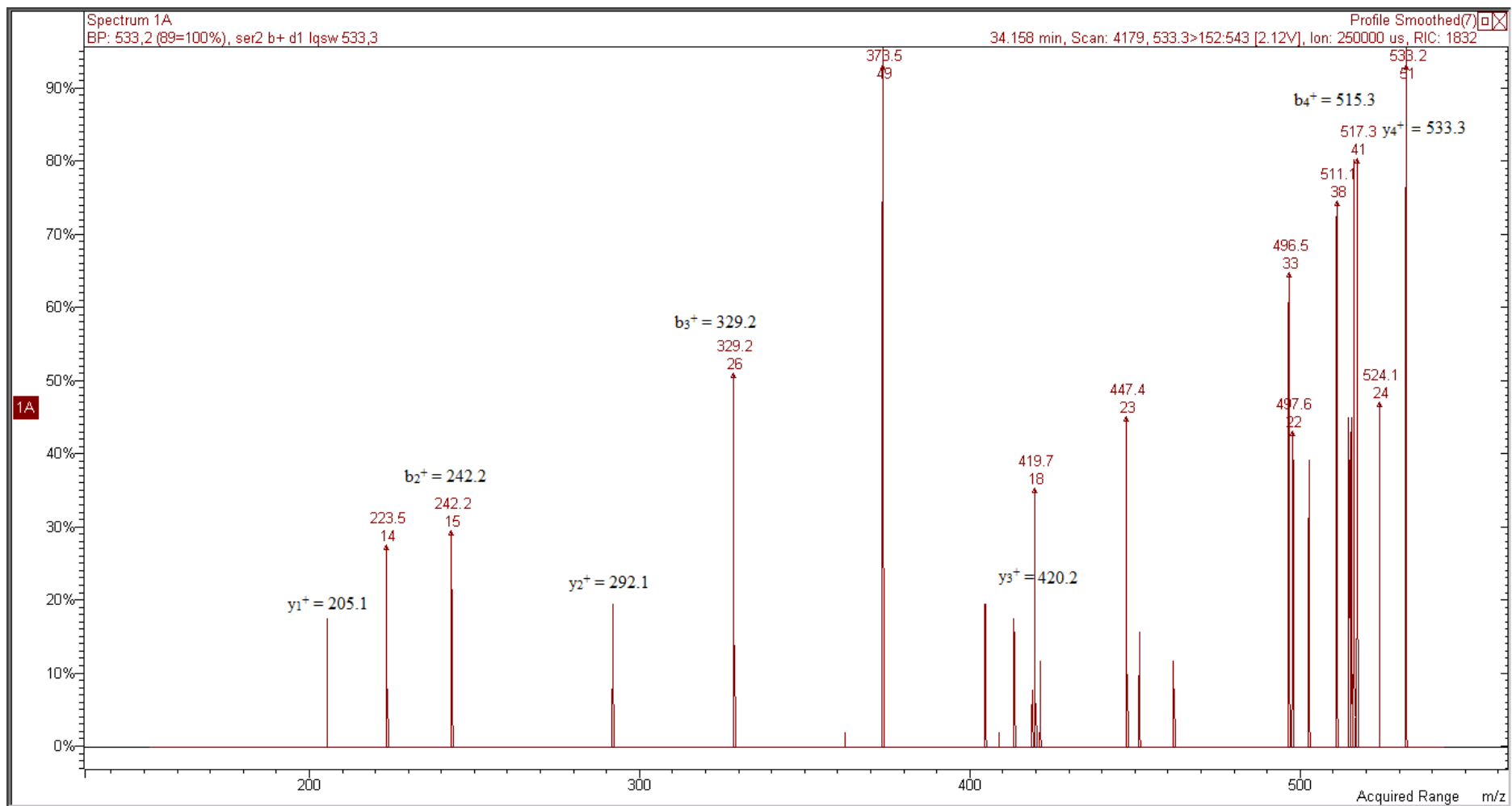
**Figure S46.** MS/MS spectrum of LQSW peptide.
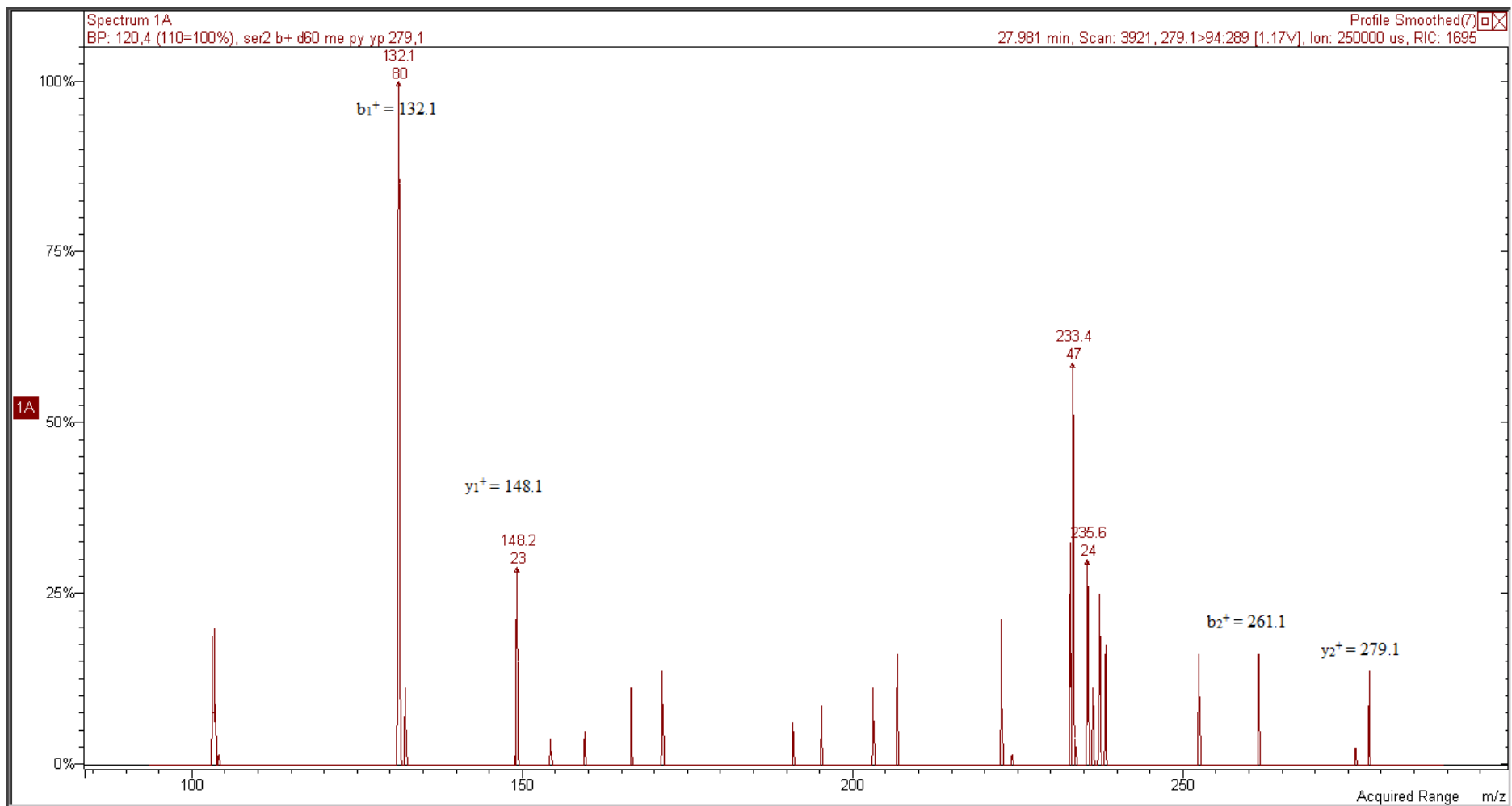
**Figure S47.** MS/MS spectrum of ME peptide.
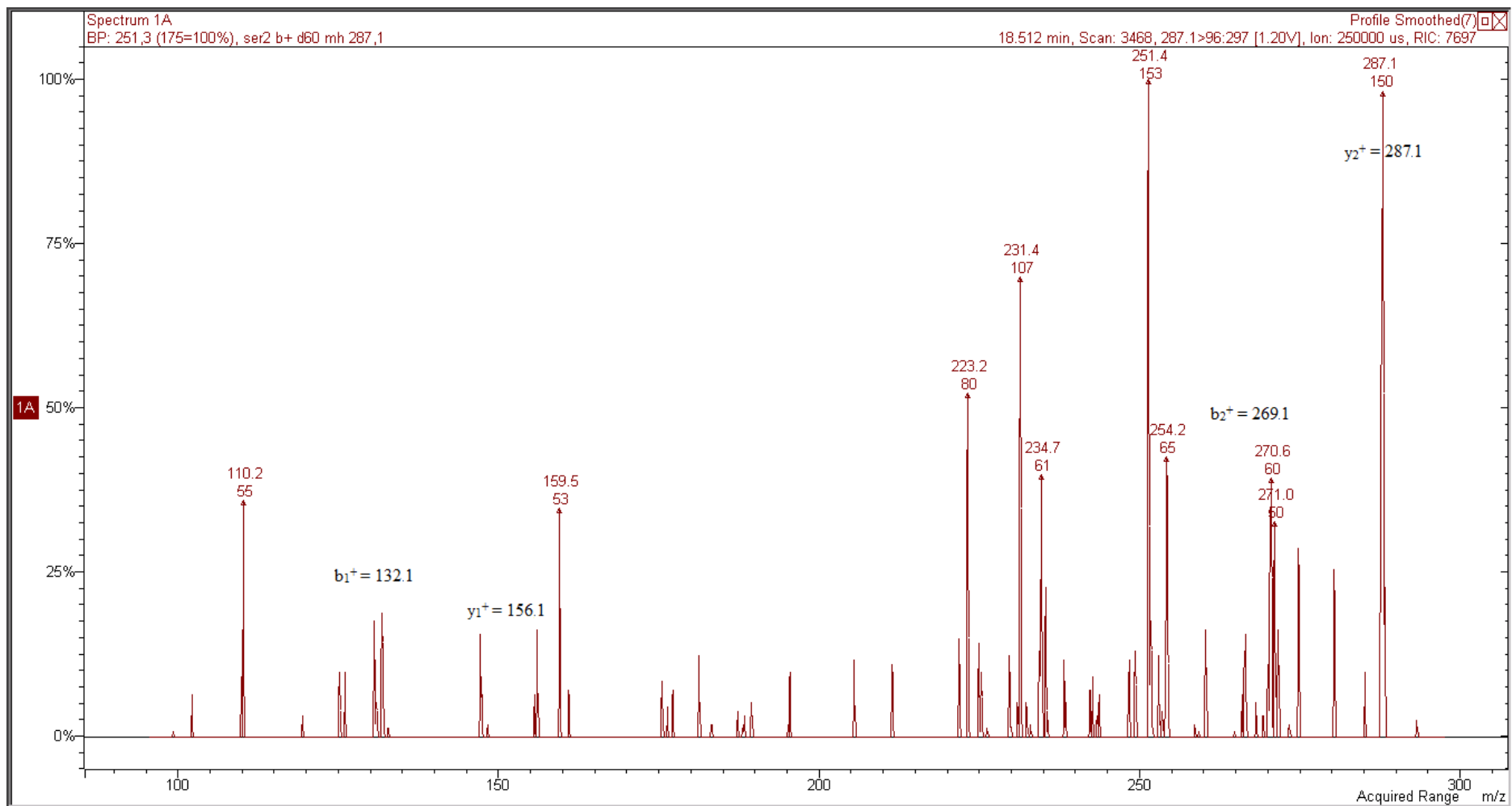
**Figure S48.** MS/MS spectrum of MH peptide.

**Figure S48.** MS/MS spectrum of NK peptide.

**Figure S50.** MS/MS spectrum of NLHLP peptide.

**Figure S51.** MS/MS spectrum of NLHLPLP peptide.

**Figure S52.** MS/MS spectrum of PFPE peptide.
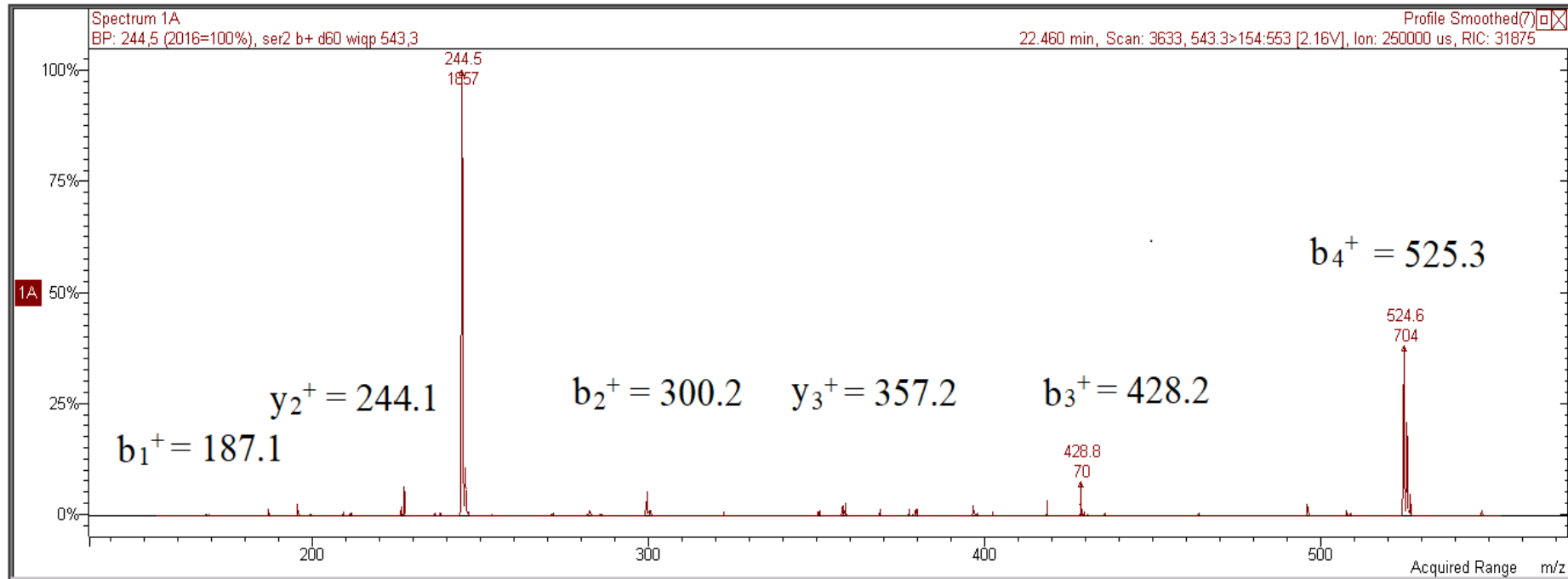
**Figure S53.** MS/MS spectrum of PP peptide.

**Figure S54.** MS/MS spectrum of PPK peptide.

**Figure S55.** MS/MS spectrum of PQR peptide.
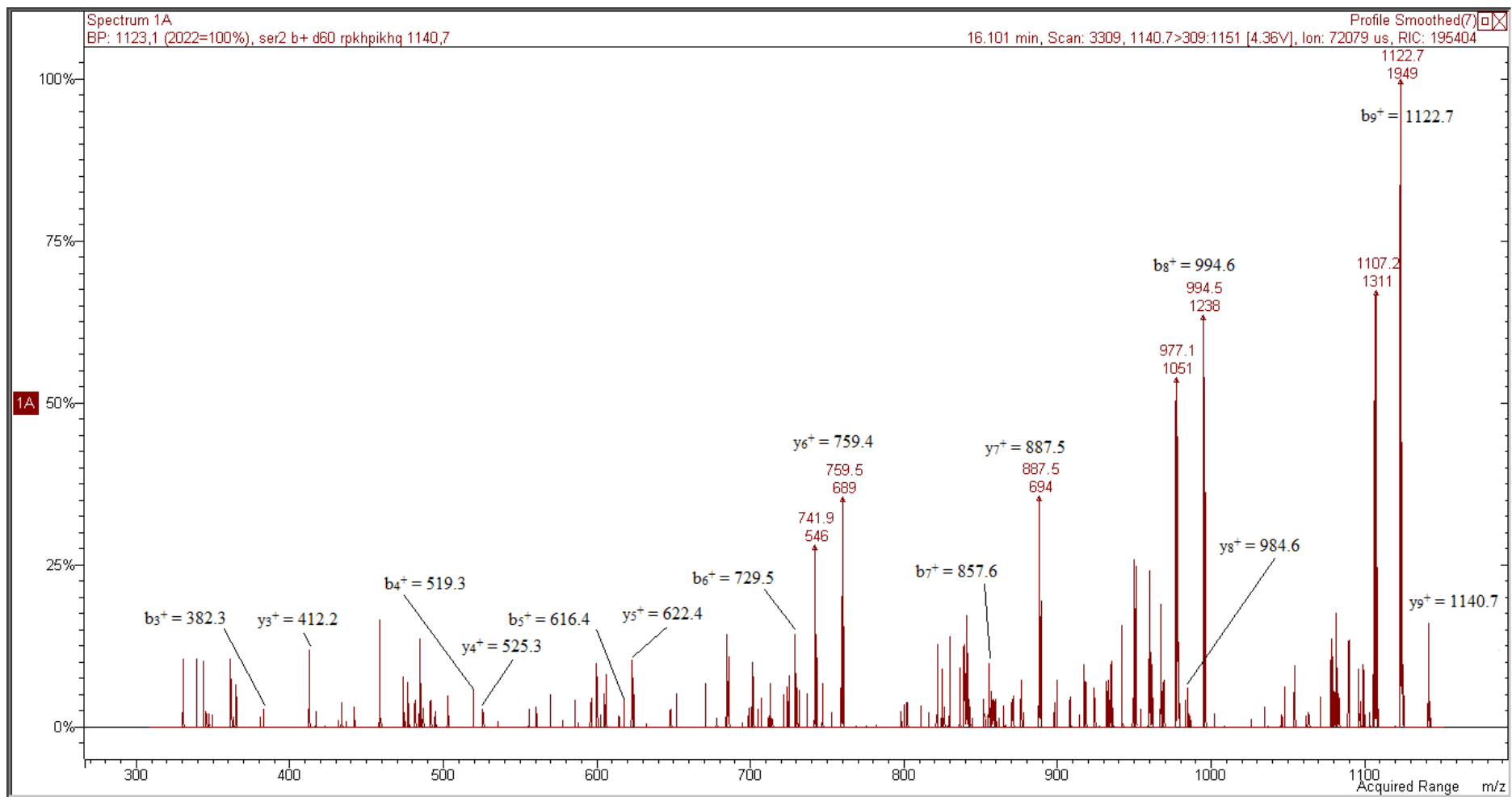
**Figure S56.** MS/MS spectrum of RPKHPIKHQ peptide.
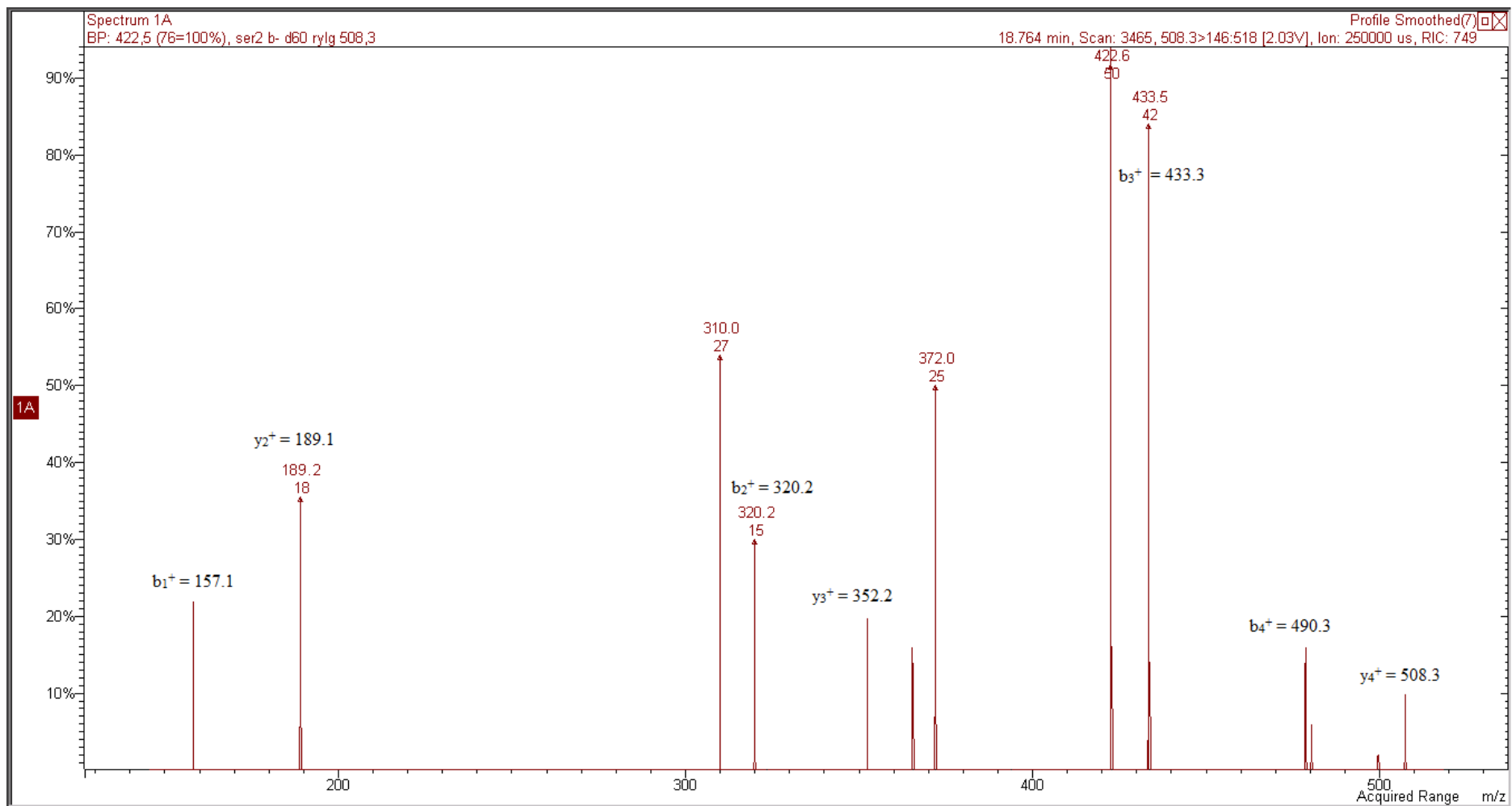
**Figure S57.** MS/MS spectrum of RYLG peptide.
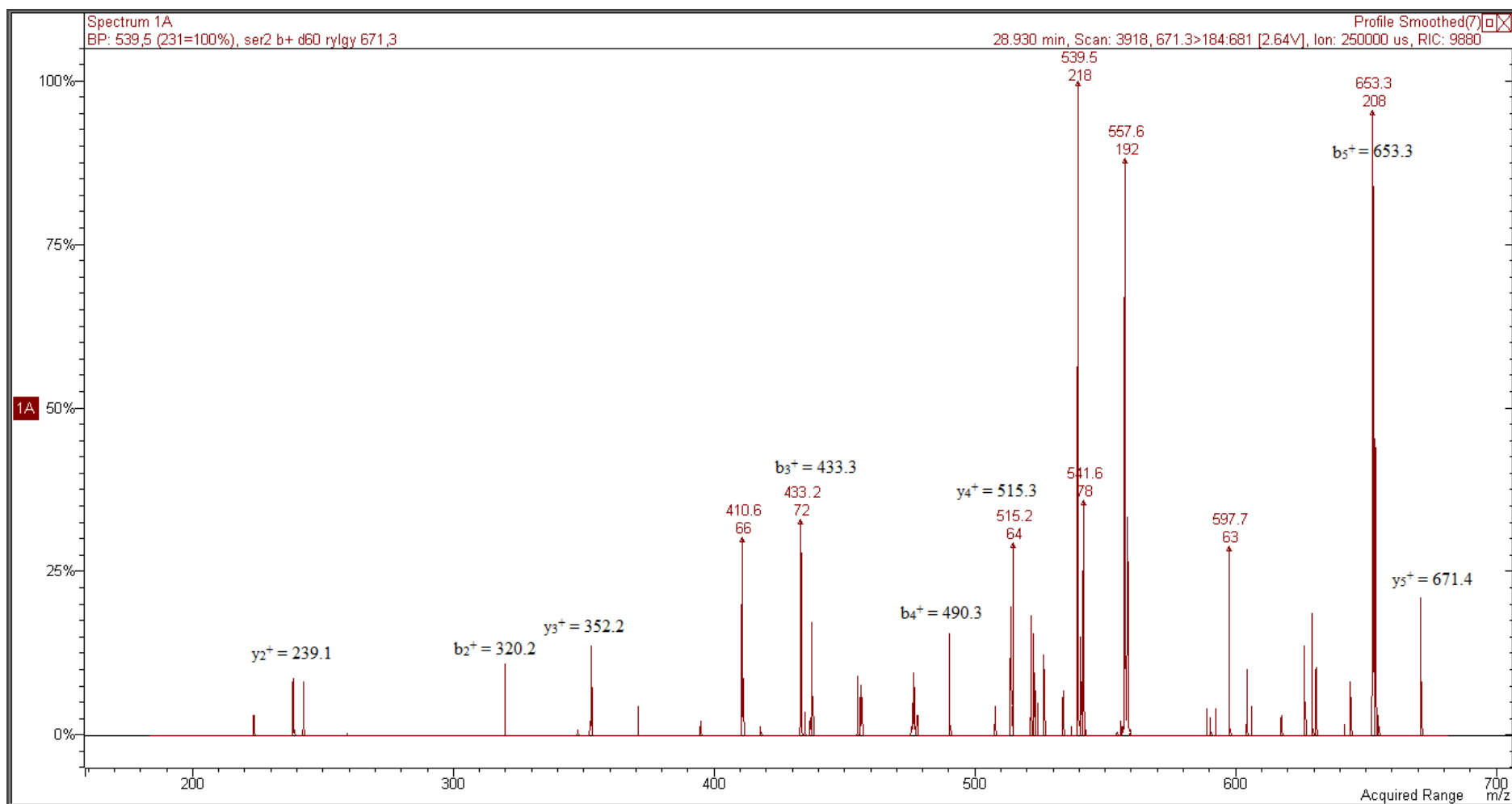
**Figure S58.** MS/MS spectrum of RYLGY peptide.
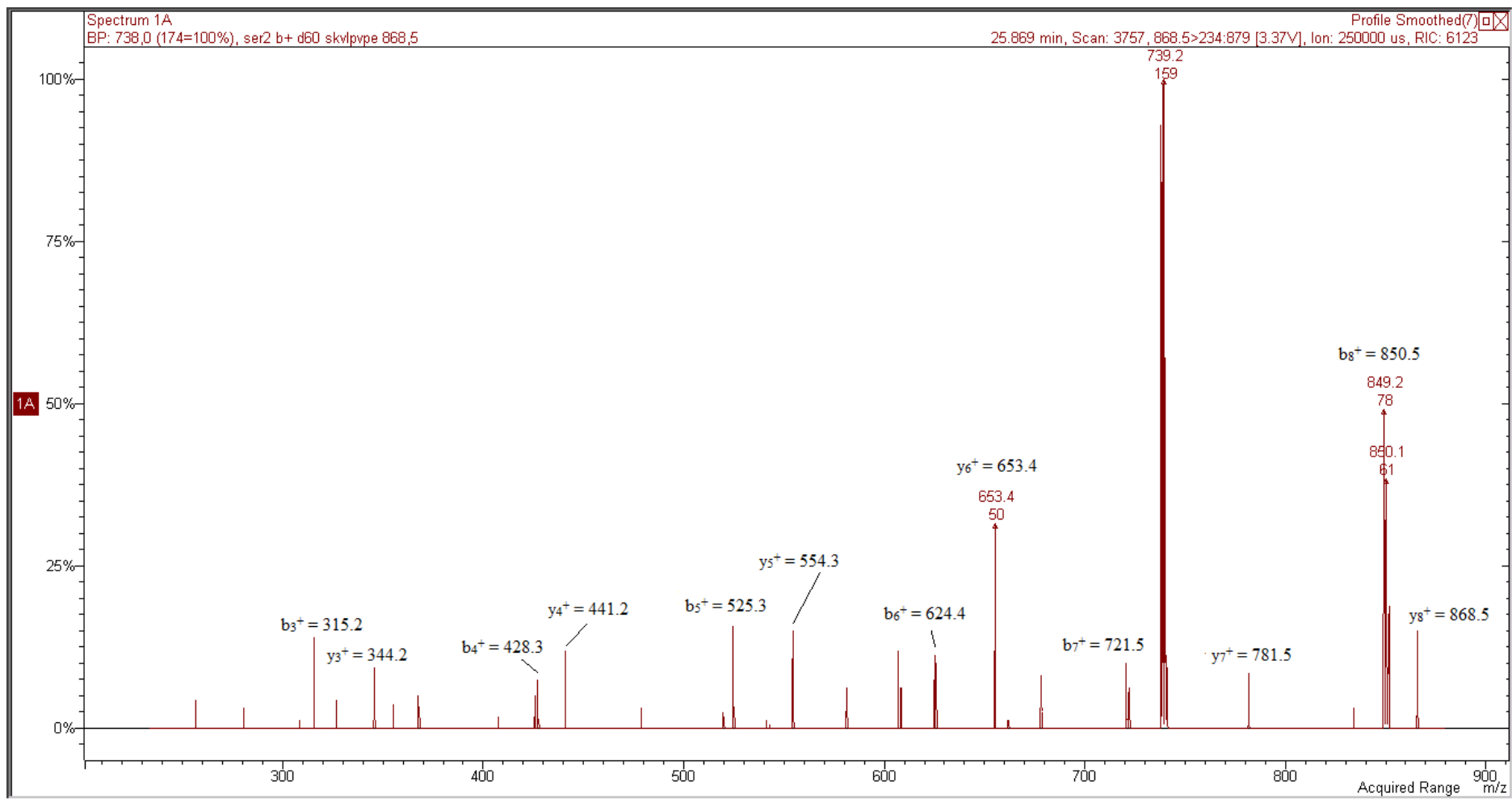
**Figure S59.** MS/MS spectrum of SKVLPVPE peptide.

**Figure S60.** MS/MS spectrum of TF peptide.
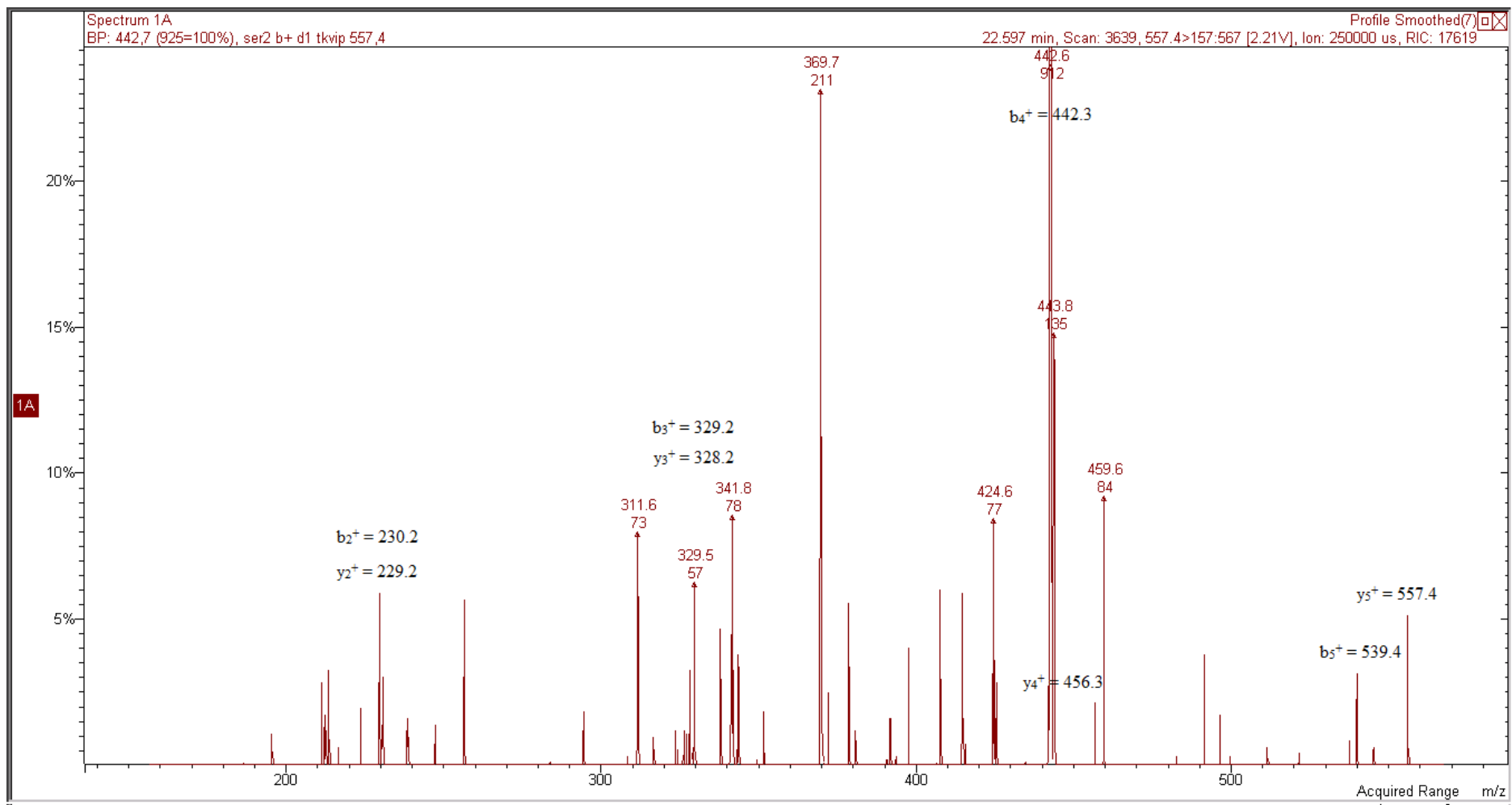
**Figure S61.** MS/MS spectrum of TKVIP peptide.
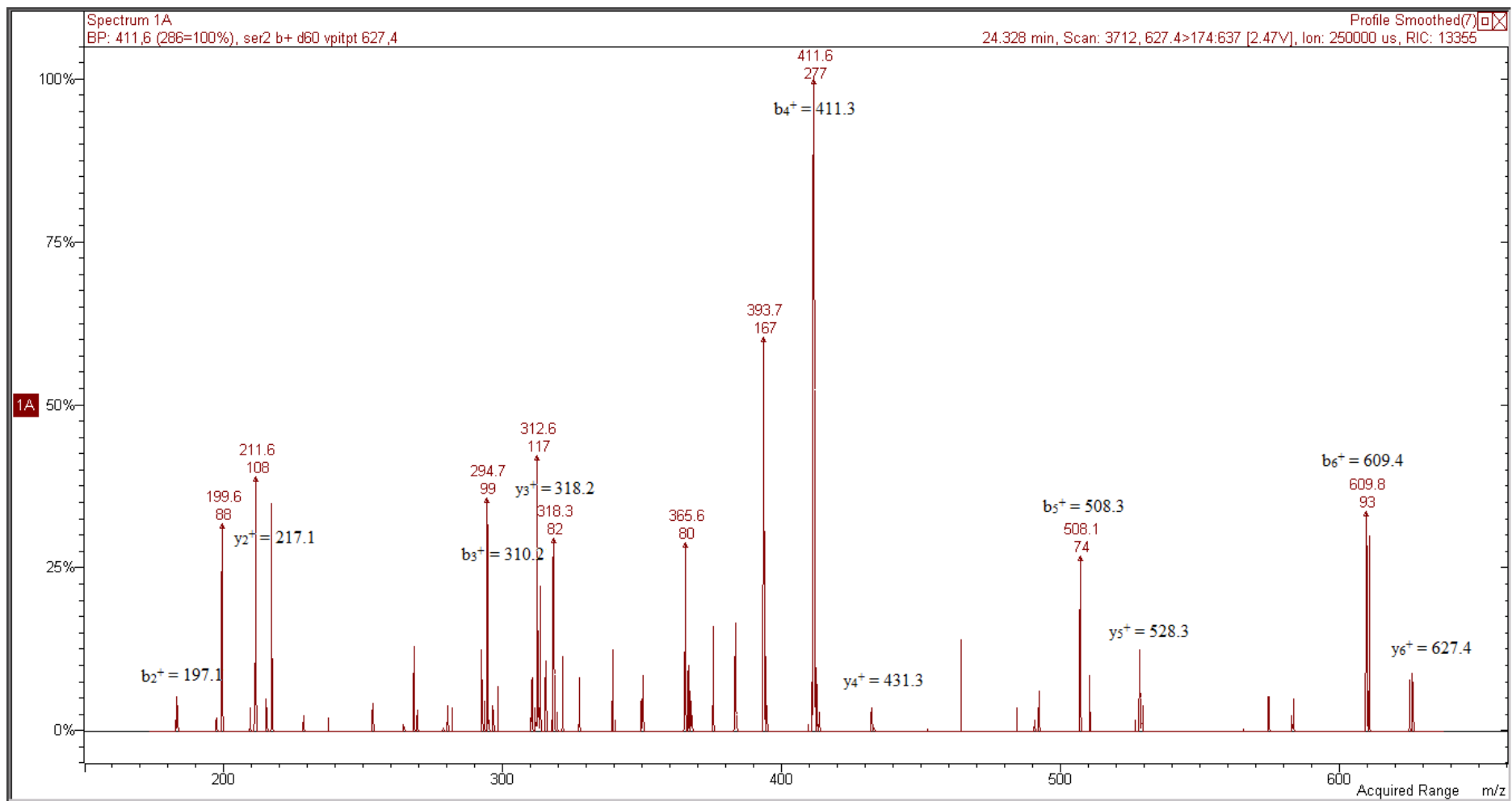
**Figure S62.** MS/MS spectrum of VPITPT peptide.
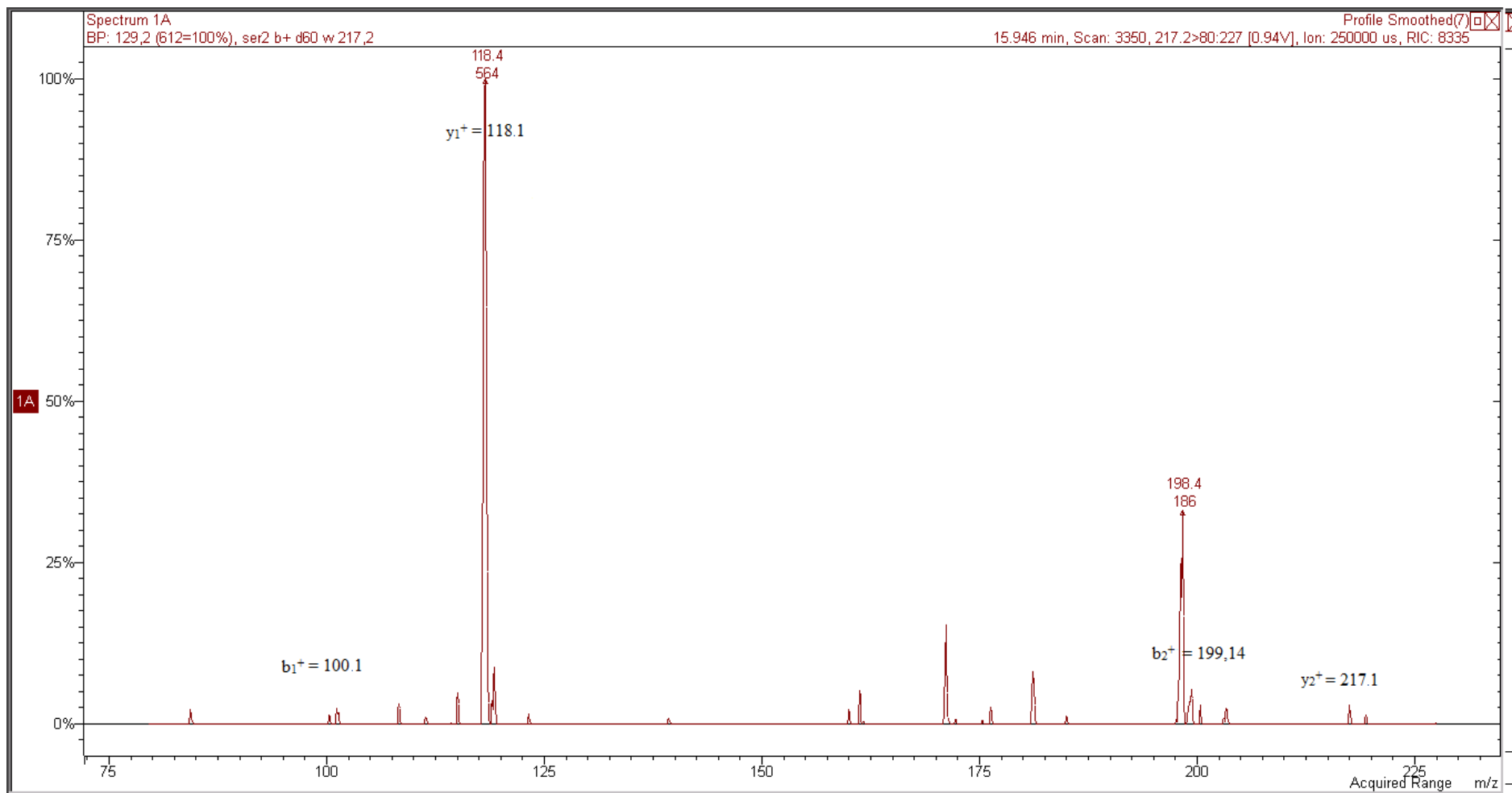
**Figure S63.** MS/MS spectrum of VV peptide.
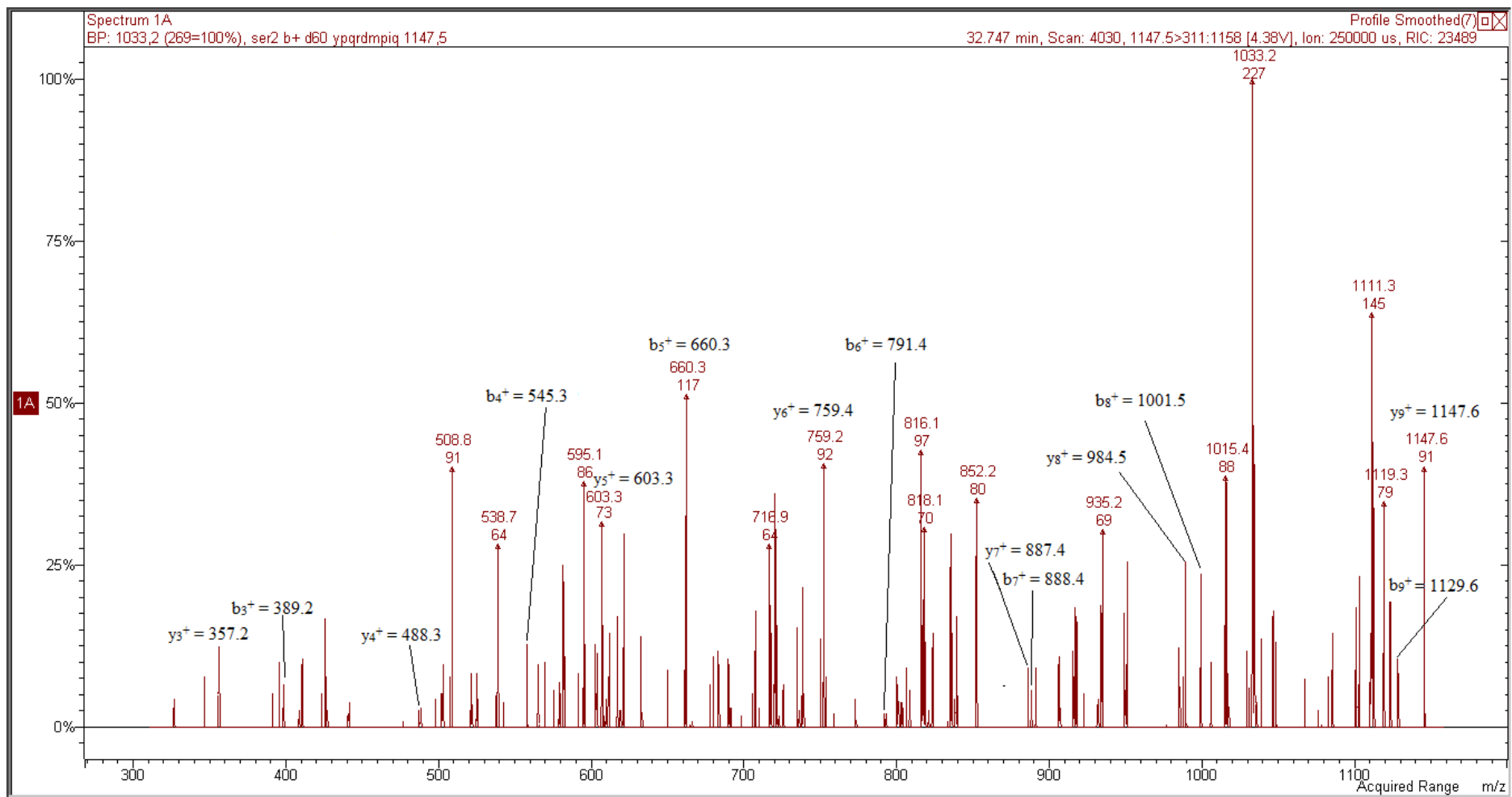
**Figure S64.** MS/MS spectrum of WIQP peptide.

**Figure S64.** MS/MS spectrum of YPQRDMPIQ peptide.