|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Sample** | **Compound** | **Retention time (min)** | **Measured m/z** | **Ion formula [M-H]-** | **Calculated m/z [M-H]-** | **Error [ppm]** | **Error [mmu]** |
| Enzymatic reaction mix (S4 Fig.) | Dipeptide **1** | 4.9 | 202.1092 | C9H16NO4 | 202.1085 | 3.5 | 0.7 |
| Dipeptide **2** | 6.2 | 216.1241 | C10H18NO4 | 216.1241 | 0 | 0 |
| Tetrapeptide **3** | 5.4-5.6 | 401.2345 | C19H33N2O7 | 401.2293 | 12.9 | 5.2 |
| Octapeptide **4** | 6.1-6.2 | 785.4608 | C38H65N4O13 | 785.4554 | 6.9 | 5.4 |