**Analysis of isotopic labeling in peptide fragments by tandem mass spectrometry**

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**File S4: FTMS and ITMS Comparison**



FTMS data summarized as average labeling for three peptides fragmented at multiple CID energies measured in MS2. Statistics represent two samples each with evaluation at three scans nearest the apex of the eluted peptide peak.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Parent Mass & Products**  | **0** | **15** | **20** | **25** | **35** |
| **609.78** | 7.14±0.03 | 8.33±0.13 | 11.43±0.82 | --- | --- |
| **y8** | --- | 3.68±0.29 | 5.60±0.19 | --- | 6.77±0.09 |
| **b3** |  | 3.72±0.99 | 5.66±0.67 | --- | 6.12±0.25 |
|  |  |  |  |  |  |
| **514.3** | 7.07±0.03 | 8.54±0.19 | 11.88±0.14 | 14.53±0.08 | --- |
| **y5** | --- | 3.40±0.16 | 5.22±0.09 | 6.21±0.06 | 6.95±0.07 |
| **b5** | --- | 3.74±0.34 | 5.44±0.19 | 6.13±0.14 | 6.45±0.06 |
| **y3** | --- | 3.76±0.33 | 5.35±0.16 | 6.11±0.11 | 6.60±0.11 |
| **b7** | --- | 4.44±0.48 | 5.81±0.15 | 6.19±0.25 | 6.12±0.17 |
|  |  |  |  |  |  |
| **586.33** | 7.09±0.01 | 8.01±0.17 | 10.24±1.54 | 13.31±0.04 | --- |
| **y6** | --- | 2.89±0.20 | 5.08±0.09 | 6.07±0.12 | 6.57±0.32 |
| **b5** | --- | 3.03±0.28 | 5.36±0.20 | 6.00±0.37 | 5.94±0.06 |
| **y8** | --- | 2.78±0.19 | 5.04±0.13 | 6.10±0.10 | 6.69±0.10 |
| **b3** | --- | 2.16±1.12 | 4.89±0.49 | 5.57±0.58 | 6.31±0.36 |

ITMS data summarized as average labeling for three peptides fragmented at multiple CID energies measured in MS2. Statistics represent two samples each with evaluation at three scans nearest the apex of the eluted peptide peak.

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| --- | --- | --- | --- | --- | --- |
| **Parent Mass & Products** | **0** | **15** | **20** | **25** | **35** |
| **609.78** | 7.14±0.03 | 8.33±0.13 | 11.43±0.82 | --- | --- |
| **y8** | --- | 4.20±0.26 | 6.97±0.24 | --- | 7.19±0.19 |
| **b3** | --- | 4.81±0.74 | 7.80±0.91 | --- | 6.96±1.65 |
|  |  |  |  |  |  |
| **514.3** | 7.07±0.03 | 8.54±0.19 | 11.88±0.14 | 14.53±0.08 | --- |
| **y5** | --- | 4.20±0.24 | 6.89±0.15 | 7.15±0.06 | 7.16±0.06 |
| **b5** | --- | 4.35±0.38 | 7.29±0.21 | 7.44±0.26 | 7.53±0.34 |
| **y3** | --- | 4.68±0.45 | 7.07±0.22 | 6.97±0.25 | 7.27±0.29 |
| **b7** | --- | 4.79±0.41 | 7.22±0.20 | 7.58±0.38 | 7.23±0.67 |
|  |  |  |  |  |  |
| **586.33** | 7.09±0.01 | 8.01±0.17 | 10.24±1.54 | 13.31±0.04 | --- |
| **y6** | --- | 4.28±0.40 | 6.73±0.30 | 7.34±0.18 | 7.13±0.29 |
| **b5** | --- | 3.84±0.59 | 7.50±0.49 | 7.10±0.60 | 7.16±0.95 |
| **y8** | --- | 3.95±0.37 | 6.38±0.27 | 7.09±0.30 | 7.35±0.22 |
| **b3** | --- | 2.90±1.49 | 7.22±0.99 | 7.12±0.76 | 8.03±1.04 |