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

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**File S2: Peptide Sequence and Precursor Data**

Peptide Description:

|  |  |  |
| --- | --- | --- |
| **Sequence** | **Charge (z)** | **Observed *m*/*z*** |
| SRDPIYSNK | 2 | 540.27 |
| SQQLQNLR | 2 | 493.77 |
| LQESVIVEISKK | 3 | 458.26 |
| FQTLFK | 2 | 392.21 |

Ratio of 13C0 to 13C1; Precursor ion isotopic distribution was extracted for these four peptides, quantified and the ratio calculated:

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Method** | **m/z** | **Prediction** | **Replicate 1** | **Replicate 2** | **Replicate 3** | **Average** | **Standard Deviation** |
| HCD | 458.26 | 1.36 | 1.35 | 1.39 | 1.37 | 1.37 | 0.02 |
| CID | 458.26 | 1.36 | 1.34 | 1.36 | 1.37 | 1.36 | 0.02 |
| HCD | 392.21 | 2.17 | 2.17 | 2.31 | 2.14 | 2.21 | 0.09 |
| CID | 392.21 | 2.17 | 2.19 | 2.10 | 2.23 | 2.17 | 0.06 |
| HCD | 493.77 | 1.99 | 2.18 | 2.14 | 2.07 | 2.13 | 0.06 |
| CID | 493.77 | 1.99 | 1.98 | 2.02 | 2.02 | 2.01 | 0.02 |
| HCD | 540.27 | 1.77 | 1.82 | 1.73 | 1.63 | 1.73 | 0.10 |
| CID | 540.27 | 1.77 | 1.81 | 1.78 | 1.77 | 1.79 | 0.02 |

As indicated the predicted and average values from the replicates agree to within the precision of the measurements for these peptides, therefore no significant bias in the MS1 peptides were observed within this set.