

For a peptide with molecular weight M , the positively charged ion will be $[M+H]^+$, while the negatively charged ion will be $[M-H]^-$. So the mass of the peptide acquired in positive mode is 2 Da more than that acquired in negative mode.

The MS/MS of m/z 651.35 in positive mode, corresponding to m/z 649.39 in the negative mode precursor ion scan, provides the sequence information of the phosphopeptide of interest. In this case, the data confirms that S12 is phosphorylated, as illustrated below.

