

## Mass-based classification (MBC) of peptides: Highly accurate precursor ion mass values can be used to directly recognize peptide phosphorylation

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Accurate mass values as obtainable by Fourier transform ion cyclotron resonance mass spectrometry (FTICR-MS) were employed in a theoretical study to differentiate between nonmodified and phosphorylated peptides. It was found that for peptide masses up to 1,000 u more than 98% of all theoretical monophosphorylated peptides (all possible combinations of proteinogenic amino acids having one phosphorylation on S, T, or Y) can be distinguished from nonphosphorylated peptides directly by their mass, if mass values are determined with an accuracy of better than  $\pm 0.1$  ppm. At a peptide mass of 1,500 u still 70% of all possible monophosphorylated peptides are distinguishable from nonmodified peptides by their accurate mass alone. In contrast to established techniques of data-dependent multidimensional mass spectrometry, only the mass of the precursor ion is necessary to decide upon subsequent fragment ion analysis of a peptide for sequence analysis in an LC-MS/MS investigation of a complex sample, when using a precalculated mass distribution table of theoretical peptides. A mass distribution table of nonphosphorylated and monophosphorylated peptides with a bin width of 0.1 mu was made available via the open web site [www.peptidecomposer.com](http://www.peptidecomposer.com).

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