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Physics-based approaches for protein identification[1] OLEG OBOLENSKY, YI-KUO YU, National Center for Biotechnology Information, NIH — In biomedical research it is often necessary to identify proteins present in a sample. Tandem mass spectrometry (MS/MS) techniques are routinely used for this purpose. The protein in question is digested into smaller pieces (peptides) and then these pieces are protonated and further fragmented in mass spectrometers. The obtained mass spectra are analyzed and the peptides (and eventually the original protein) are identified. Currently, mass spectrometry-based peptide identification methods rely solely on statistical analysis of the mass spectra, while information about physics of the peptide fragmentation processes is vastly underutilized. We demonstrate how the physical approaches can be applied to the problem of peptide identification and how they can complement the statistical analysis. In particular, we show that observability of more than 90 per cent of signal peaks in mass spectra of short singly charged peptides can be easily predicted by knowing the dissociation energies in the corresponding fragmentation channels.

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