New method identifies up to twice as many proteins and peptides in mass spectrometry data

November 10 2015, by Ioana Patringenaru

An international team of researchers developed a method that identifies up to twice as many proteins and peptides in mass spectrometry data than conventional approaches. The method can be applied to a range of fields, including clinical settings and fundamental biology research for cancer and other diseases. The key to the new method's improved performance is its ability to compare data to so-called spectral libraries—essentially a pattern-matching exercise—rather than individual spectra or a database of sequences.

The team describes their results in the Nov. 9 issue of *Nature Methods*. "You can integrate our method with existing pipelines to increase performance by up to three- to four-fold," said Nuno Bandeira, a professor at the Jacobs School of Engineering and the Skaggs School of Pharmacy at UC San Diego, the study's senior author.

The advance is particularly important because many research teams are now switching to an approach known as data-independent acquisition, which captures a wealth of raw data instead of running data analysis on a few elements at random, (selected from a distribution based on peptide intensities). The amount of data collected has created a bottleneck for existing computational tools. "We needed a new data analysis method," said Bandeira.

Bandeira's research group focuses on building spectral network

algorithms, which analyze pairs of overlapping peptides spectra produced during mass spectrometry experiments. The spectra are produced when an enzyme digests proteins, breaking them down into subcomponents, including peptides. The algorithms detect patterns that the pairs have in common and then look for these patterns in other spectra. This considerably speeds up the process of identifying peptides and by extension, proteins.

Traditional methods compare spectra either against databases or against spectra that have already been identified.

In the Nature Methods study, researchers showed that they were able to identify twice as many peptides in human samples when compared to traditional methods. They also observed 40 percent more protein-on-protein interactions. "The results are more stable and easier to reproduce" when compared to traditional methods, Bandeira said.

Next steps include speeding up the process, which takes roughly twice as long as traditional methods. The method also will have to be fine-tuned for the next generation of mass spectrometers.

"We also want to start seeing how we can capitalize on this to analyze a full cohort of data," Bandeira said.

Provided by University of California - San Diego

data (2015, November 10) retrieved 27 April 2024 from https://phys.org/news/2015-11-method-proteins-peptides-mass-spectrometry.html