BRC Science Highlight
February 2019

Peak Annotation and Verification Engine for Untargeted LC-MS Metabolomics

Background/objective

Metabolomics continues to play an increasing role in numerous research areas including bioenergy. While liquid chromatography mass spectrometry (LC-MS) has emerged as a commonly used platform for generating metabolomics data, these datasets contain thousands of peaks that represent both analytical artifacts and actual metabolites. Researchers developed the Peak Annotation and Verification Engine (PAVE), which offers substantial improvement over previously developed tools for metabolite peak annotation.

Approach

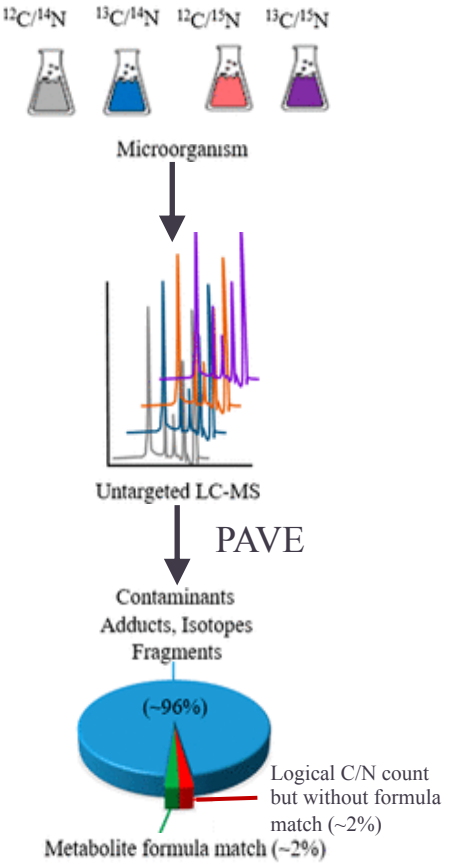
- Extracts from *S. cerevisiae* and *E. coli* grown on unlabeled, ^{13}C labeled, ^{15}N labeled, and both $^{13}C/^{15}N$ labeled media were analyzed via untargeted LC-MS.
- PAVE was used to process LC-MS data, eliminating artifacts and annotating remaining metabolite peaks.
- PAVE results were compared with other recently published methods.

Results

- PAVE reduced ~45,000 total LC-MS peaks to ~1,500 and ~600 putative metabolites credentialed with C and N counts for *S. cerevisiae* and *E. coli*, respectively, and correctly identified most well-known core metabolites.

Significance

- PAVE incorporates improved analytical and algorithmic performance, exceeding that of the previous state-of-the-art and presenting a significant step toward comprehensive annotation of metabolites detected via LC-MS.
- PAVE opens the possibility for metabolome annotation of less-studied microbes that might have unique properties amenable to industrial bioproduct and biofuel production.



PAVE processes LC-MS data from isotope-labeled microbes, eliminates the majority of peaks as instrumental artifacts, and matches approximately half of the remaining peaks with known metabolites.

Wang et al. 2018. "Peak Annotation and Verification Engine for Untargeted LC-MS Metabolomics." ***Analytical Chemistry.*** *91:1838-1846*. DOI: 10.1021/acs.analchem.8b03132

CABBI CENTER FOR ADVANCED BIOENERGY AND BIOPRODUCTS INNOVATION
U.S. DEPARTMENT OF ENERGY