

The Workshop “Data Independent Acquisition Interest Group” of the ASMS Annual Conference 2016 in San Antonio took place in the Henry Gonzalez Convention Center Room 304 on the 7<sup>th</sup> of June 2016 from 17:45 till 19:00 moderated by Jarrett Egertson (University of Washington) and Ludovic Gillet (ETH Zürich). The workshop was very well attended, with almost the complete room of >200 seats occupied.

The aim of this workshop was to present the audience a brief description of the tools currently in use to analyze DIA data, and to propose a unified nomenclature to classify those tools. The focus was on tools to identify or detect peptides from DIA data.

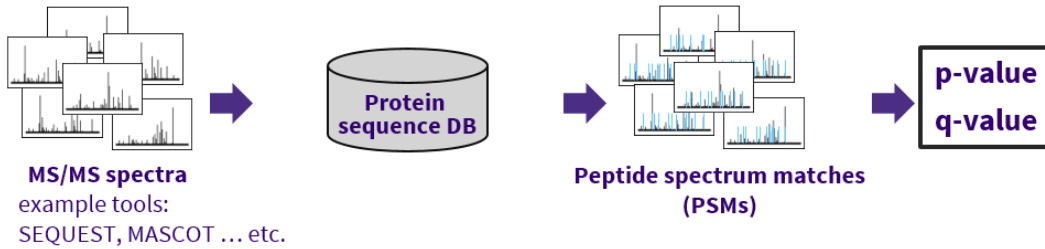
The invited scientists were: Alexey Nesvizhskii (University of Michigan) for DIAUmpire, Nuno Bandeira (University of San Diego) for MSPLIT-DIA, Scott Geromanos (Waters, Milford) for HD-MSE, Lukas Reiter (Biognosys, Schlieren, Switzerland) for Spectronaut, Sonia Ting (University of Washington) for PECAN, Pedro Navarro (University Mainz, Germany) for LFQBench, and Sam Payne (Pacific Northwest National Laboratory).

To have such a broad panel of guests was a great opportunity for the public to meet face-to-face the people behind the various software and to ask questions regarding the specificity of the tools for the DIA data analysis. From the interaction with the audience, one conclusion was that there is not too much concern within the community about the spectrum-centric vs. peptide-centric differentiation. In the minds of most, the greater concern was about whether to use analysis strategies that leverage a spectral library vs. strategies that do not and how many peptides can be analyzed regardless of approach.

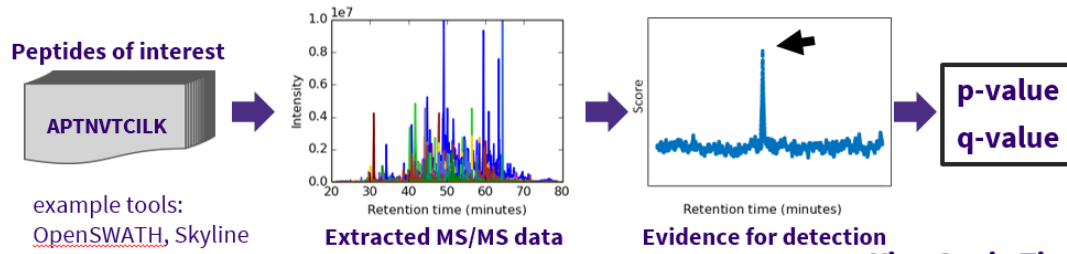
For analyses that use a spectral library, people expressed concern about longevity and general applicability of libraries. I.e. If one puts in a lot of effort to generate a huge spectral library, will it become invalid with a change in instrument platform? Some people that did cross-platform analysis spoke up and claimed that different instrument platforms didn't seem to significantly impact how well libraries worked. An important distinction within the strategies leveraging a spectral library was whether or not they used retention time information in conjunction with fragmentation spectra.

In summary, this workshop was a great platform to bring together software developers to represent the diversity of DIA querying strategies. The strong attendance indicates growing interest in DIA approaches. To capture this interest, a workshop about advances in DIA methodologies should be maintained in future ASMS annual conferences.

## Spectrum-centric analysis What peptides best explain the data?



## Peptide-centric analysis Which peptides are detected in our data?



Ying Sonia Ting, MCP 2015

	Spectrum-centric analysis	Peptide-centric analysis
Query unit	MS/MS spectrum	Peptide
Assumption	Each spectrum is generated from at least one peptide	Each peptide elutes once (for a short period of time) during liquid chromatography
Goal	Identify peptide(s) from each spectrum	Find evidence of detection for each peptide
Scoring	Candidate peptides from the sequence database compete with each other for the best scoring PSM	Candidate spectra from the acquired data compete with each other for the best scoring evidence of detection
Example tools	SEQUEST, Comet, MASCOT, X!Tandem, OMSSA, Probid, MS-GF+, MaxQuant	FT-ARM, OpenSWATH, Skyline, SALSA

(Gillet LC, *et. al.* Annu Rev Anal Chem, 2016)