

## Clinical Chemistry Interest Group Report for the 69th ASMS Conference in Philadelphia

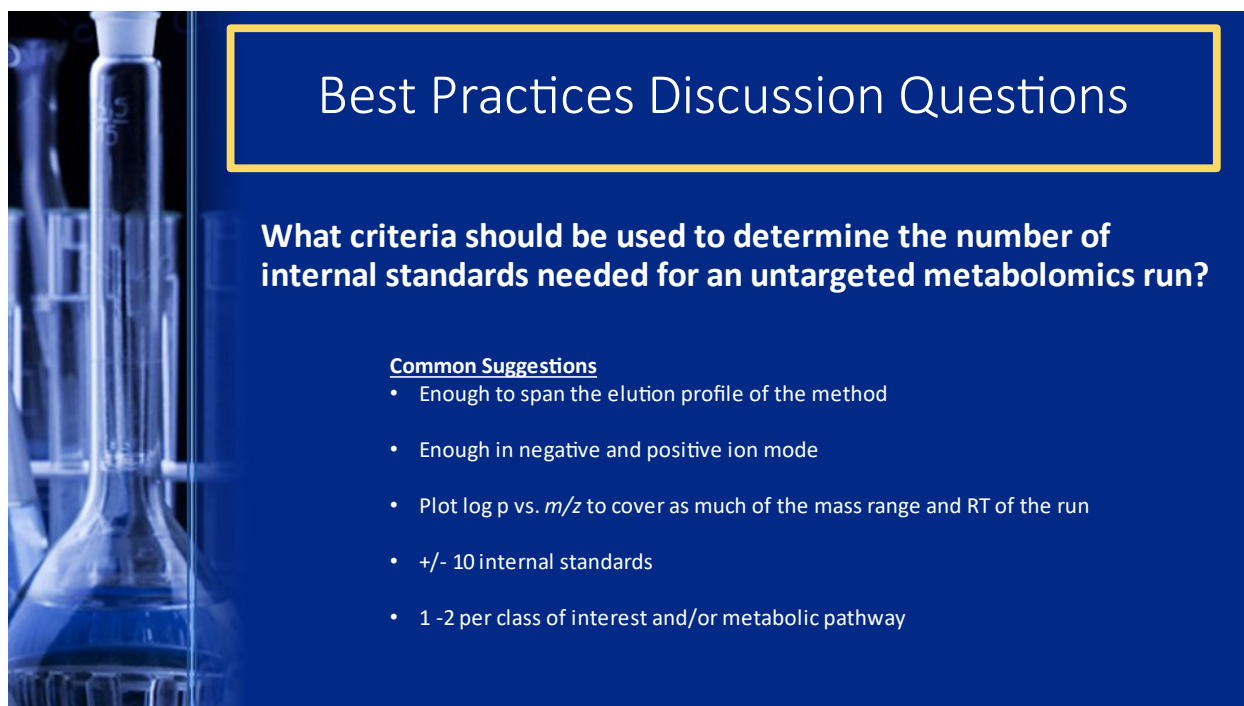
*Submitted 12-12-2021 by Dr. Donald Chace, Co-Chair of the ASMS Clinical Chemistry Interest Group*

### **Achieving Harmonized Clinical Laboratory Testing: Current Best Practices & Future Approaches**

**Candace Ulmer, Don Chace, Tim Garrett**

The above workshop was held during the Tuesday evening session and was done in person by Dr. Donald Chace and Dr. Timothy Garrett. The presentation was organized by Dr. Candice Z. Ulmer. There was still restricted travel because of Covid for many attendees. The presentation was also broadcast on Zoom. Thirty plus people attended the workshop.

Our focus and that of the attendees (based on their participation) was quality assurance in metabolomics studies specifically. Example slides are below.



**Best Practices Discussion Questions**

**What criteria should be used to determine the number of internal standards needed for an untargeted metabolomics run?**

Common Suggestions

- Enough to span the elution profile of the method
- Enough in negative and positive ion mode
- Plot  $\log p$  vs.  $m/z$  to cover as much of the mass range and RT of the run
- +/- 10 internal standards
- 1 -2 per class of interest and/or metabolic pathway



## Best Practices Discussion Questions

**Is a universal system suitability testing (SST) sample AND assay - specific SST sample needed in untargeted metabolomics?**

Use of SSS	Purpose	Frequency
Before Analysis	Confirm instrument performance	Before the start of a run (after several priming injections)
During a run	Confirm and monitor performance of instrument during the entire run	Depends on stability of instrument; if changes in parameters are common, consider more injections
After instrument maintenance, power outage, break in vacuum, tuning/calibration	Confirm instrument is within performance specifications and stable prior to sample analysis	Multiple injections, approx. 5-10

We also had extensive discussion with regard to instrument performance across a run which is applicable to both untargeted (discovery) and targeted (practice).



## Best Practices Discussion Questions

**What criteria should be used to assess instrument performance across a run?**

Common Suggestions

- Peak area/height
- QI/CI ratios
- Mass accuracy (select endogenous metabolites, IS, manufacturer mass calibrant(s))
- Peak shape/width
- Pump traces
- S/N

We had active participation in discussing the need for “rules” and QA/QC in metabolomics, so studies are better compared across laboratories. Clearly, this is where the interest of the attendees was focused and will likely serve as a potential focus of next years workshop topic.