

mQACC: A community-led effort to strengthen quality assurance (QA) and quality control (QC) practices in metabolomics research and reporting

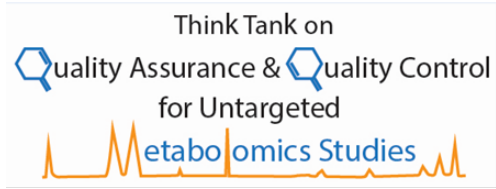
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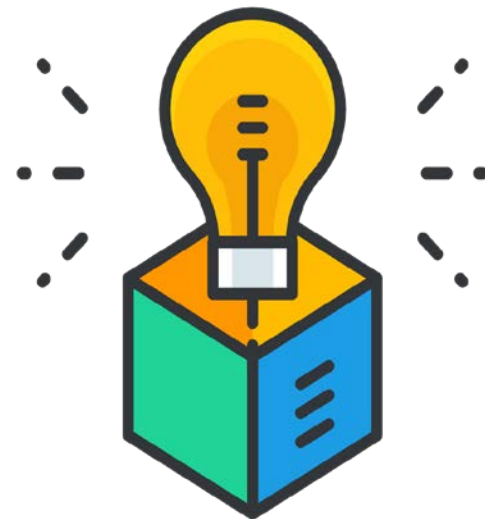




- Two-day 'Think Tank' was held on October 19-20, 2017 at the National Cancer Institute's Shady Grove Campus in Rockville, MD, USA.
- The four organizers were
 - Dr. Richard Beger (Food and Drug Administration, USA)
 - Dr. Dan Bearden (National Institute of Standards and Technology, USA)
 - Dr. Warwick Dunn (University of Birmingham, UK)
 - Dr. Krista Zanetti (National Cancer Institute, USA)
- 38 internationally recognized experts in metabolomics and QA/QC processes attended including NIH program staff:
 - from the US, Europe, and Australia
 - scientists and stakeholders from instrument manufacturers, commercial laboratories, and government and academic institutions

Meeting Objectives

- Identify the most useful metrics for assessing study and data quality for untargeted metabolomic studies.
- Identify and prioritize processes to ensure appropriate reporting of QA/QC data.
- Identify and prioritize the types of test materials that are needed in the field of metabolomics for QA/QC in untargeted studies.

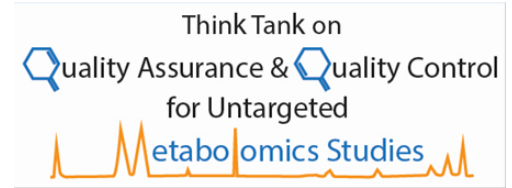


How did we intend to meet these objectives?

- Think Tank = Working Meeting
- Bring stakeholders together to identify key points that are actionable
 - High-level discussion
 - Implementation will be part of the next steps
- Prioritize ideas
- Develop a plan of action for continued collaboration to address key priorities



How the Think Tank was operated



- Each session had
 - presentations from leading experts to initiate discussions,
 - facilitated breakout sessions to discuss six different questions.
 - each attendee had the opportunity to provide input for each of the questions posed.
- The information gathered was collated and reported to the larger group.
- The information was then prioritized through an open voting process (see next slide)

Six World Café questions were discussed

- Question 1: What are the current gaps that should be addressed to establish widespread best practices for QA in untargeted metabolomics?
- Question 2: What are the current gaps that should be addressed to establish widespread best practices for QC protocols in untargeted metabolomics?
- Question 3: What is needed to establish QC acceptance criteria reporting across the wider community?
- Question 4: What should be the minimum QA and QC reporting standards for publications and databases?
- Question 5: What are the key characteristics of high-availability test material sample types for metabolomics?
- Question 6: What best use practices should be established for test material samples by the community?

Paper to be submitted

Taming the unknown: pragmatic approaches to quality control in untargeted metabolic phenotyping

Question 2: What are the current gaps that should be addressed to establish widespread best practices for QC protocols in untargeted metabolomics?

Top priorities:

- Obtain buy in from scientific journals, companies, software developers, database developers, and funders
- Define best QC practices
 - Need agreement and to encourage/enforce
- Educate community re: QC procedures

Reporting standards for QA/QC in untargeted metabolomics

Question 4: What should be the minimum QA and QC reporting standards for publications and databases?

Top priorities:

- Define acceptance criteria [e.g. scoring system (or explain why criteria were not met)]
- QC metadata should be reported (e.g. sample order, QC sample reference material used) → define elements under each category with adequate details for reproducibility

Test materials for untargeted metabolomics

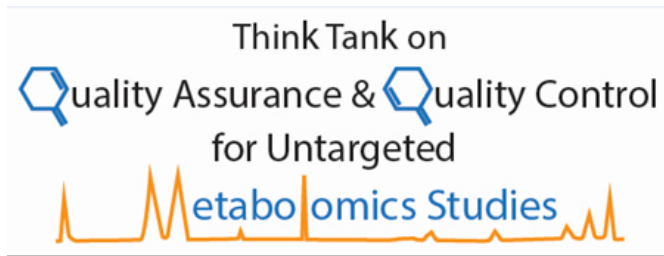
Question 5: What are the key characteristics of high-availability test material sample types for metabolomics?

Top priorities:

- Develop test materials for inter-laboratory comparisons
 - Quantitative/semi-quantitative comparisons
 - Inexpensive materials
- Same sample for all technologies – must cover wide range of characteristics
- Must determine the purpose for which test materials will be used

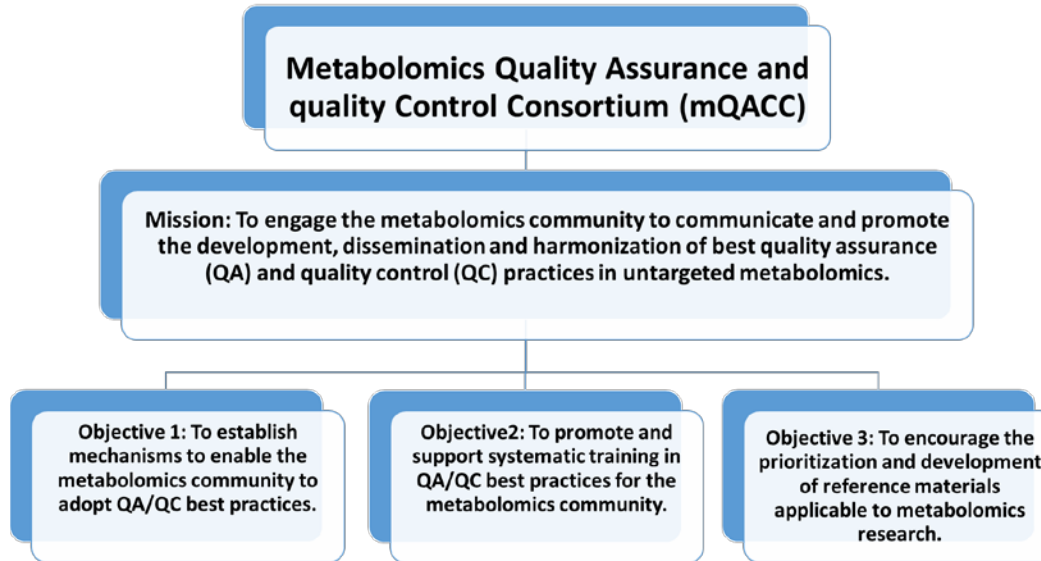
The consensus priorities agreed were:

- 1. Publish a workshop report** to communicate the meeting proceedings to the metabolomics community and allow new members to join the consortium.
- 2. Publish a white paper** which could include: (1) metabolomics practices with a focus on QA/QC procedures; (2) an emphasis on the use of QC samples as best practices and give examples of current use; (3) a discussion of metabolomics QA/QC being a developing principle, the need to develop standards, and the need for the wider community to be involved in the process; and (4) a description of the QC procedures performed in experienced labs to begin a community dialogue on the topic.
- 3. Engage scientific journals** to report that the community believes that good, documented QC practices, including analysis of QC samples, should be part of the acceptance criteria for publication.
- 4. Document and subsequently publish the complete experimental procedure for metabolomics, including the QC practices**
- 5. Establish a community forum** to discuss the development of reference standards, and interlaboratory comparison exercises.
- 6. Engage the community to identify key reference materials that need to be developed.**
- 7. Form a steering committee and larger scientific advisory board.**
- 8. Identify funding opportunities** to hold meetings and continue the group discussion and planning.
- 9. Organize workshop(s) on QA/QC at the Metabolomics Society** meeting to promote community engagement in these efforts.



- From the Think Tank has developed the Metabolomics Quality Assurance and Quality Control Consortium (mQACC)
- Provides a structure for the Think Tank participants to not only continue these efforts, but expand them to include the broader metabolomics community

<https://epi.grants.cancer.gov/Consortia/mQACC/>
- The group has continued to be active with monthly TCs and working groups are operating and progressing well
 - Reference and Test Material Working Group
 - Dissemination of Current QA/QC Practices Working Group



- Importantly, this is an inclusive and democratic group which we hope will continue to grow
- **Input from the community would be highly welcomed!**

<https://epi.grants.cancer.gov/Consortia/mQACC/>