Think Tank on

uality Assurance &

uality Control for Untargeted

Think Tank 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.

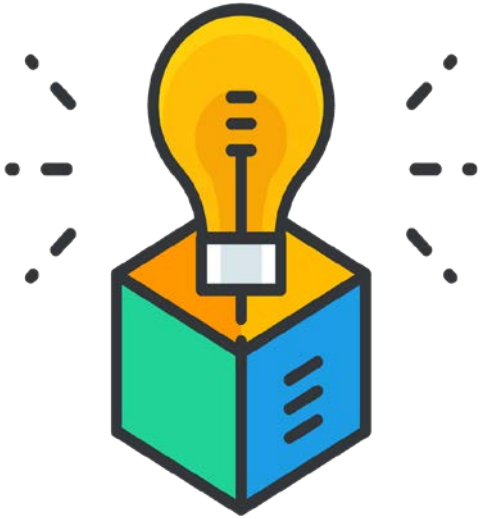

Image courtesy of Venngage

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

Think Tank Agenda

Image courtesy of Venngage

Session 1:

Meeting Introduction

Speaker: Warwick Dunn, University of Birmingham

Quality control: an unbiased data cleaning protocol controlled by relative information content

Speaker: David Broadhurst, Edith Cowan University

Think Tank Agenda

Session 2: Taming the unknown: pragmatic approaches to quality control in untargeted metabolic phenotyping

Speaker: Ian Wilson, Imperial College London

World Café:

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

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Session 3: Reporting standards for QA/QC in untargeted metabolomics

Speaker: Richard Beger, Food and Drug Administration

World Café:

- What is needed to establish QC acceptance criteria reporting across the wider community?
- What should be the minimum QA and QC reporting standards for publications and databases?

Think Tank Agenda

Session 4: Test materials for untargeted metabolomics

Speaker: Dan Bearden, National Institute of Standards and Technology

World Café:

- What are the key characteristics of high-availability test material sample types for metabolomics?
- What best use practices should be established for test material samples by the community?

Think Tank
Priorities & Action Plan

Agreed upon a set of priorities for immediate action as follows:

- Workshop on QA/QC at the Metabolomics 2018 – Lead: Dan Bearden
- Think Tank workshop report – Leads: Rick Beger and Rick Dunn
- Manuscript documenting the complete experimental procedure for untargeted metabolomics, including the QC practices – Leads: Annie Evans and Claire O'Donovan
- Identify 2-3 reference materials that need to quickly move forward – Lead: Katrice Lippa

Once the immediate priorities are addressed, the group will then systematically review and begin to address other priorities identified.

Post-Think Tank
Continued Collaboration

Quality Assurance & Quality Control

Consortium (mQACC)

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

mQACC Mission

To engage the metabolomics community to communicate and promote the development, dissemination and harmonization of best QA/QC practices in untargeted metabolomics.

mQACC Objectives

- To identify, catalog, harmonize and disseminate QA/QC best practices for untargeted metabolomics.
- To establish mechanisms to enable the metabolomics community to adopt QA/QC best practices.
- To promote and support systematic training in QA/QC best practices for the metabolomics community.
- To encourage the prioritization and development of reference materials applicable to metabolomics research.

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