

metabolomics Quality Assurance and quality Control Consortium (mQACC)
Priority-Setting Meeting
November 2020

Executive Summary

The metabolomics Quality Assurance and quality Control Consortium (mQACC) held a priority-setting meeting in November 2020 to assess the progress of the consortium since its establishment in 2017 following the *Think Tank on Quality Assurance and Quality Control for Untargeted Metabolomic Studies*, and establish further priorities for the consortium for the next three years. The report from the 2017 Think Tank was published by Beger, et al. (Towards quality assurance and quality control in untargeted metabolomics studies, *Metabolomics* 2019 Jan 3;15(1):4. doi: 10.1007/s11306-018-1460-7).

The November 2020 meeting was held as three virtual sessions, each with a specific objective, and the agenda may be found under Appendix A. The objective of Session 1 was to assess the current state of the consortium. The objective of Session 2 was to review and prioritize the objectives and recommended action points that were established at the *Think Tank on Quality Assurance and Quality Control for Untargeted Metabolomic Studies*. And, the objective of Session 3 was to identify new priorities for mQACC to accomplish over the next three years. The details of these three sessions are summarized in the meeting report. The key points from the meeting are below.

The objectives/action items from the 2017 Think Tank that were prioritized to be kept active were:

- Engage scientific journals to report that documented QC practices, including analysis of QC samples, should be part of the acceptance criteria for publication
- Obtain buy-in from scientific journals, companies, software developers, database developers, and funders
- Define acceptance criteria [e.g., scoring system (or explain why criteria were not met)]

Additional priorities that should be progressed over the next three years are:

- Define/recommend/disseminate QA/QC best practices/standards/protocols for both MS and NMR, including implementation
- Provide clear recommendations for authors, reviewers, editors as acceptance criteria
- Obtain buy-in from/engage scientific journals to report documented QC practices, including analysis of QC samples

Immediate action items to be completed by the February 2021 mQACC monthly meeting:

- The Best Practices Working Group Chairs, Jonathan Mosley and Ioanna Ntai, will work with Leo Cheng and Matt Lewis to develop a strategy to move forward the priority to define/recommend/disseminate QA/QC best practices/standards/protocols for both MS and NMR, including implementation.

- The newly established working group will develop a strategy to move forward the priorities to: 1) provide clear recommendations for authors, reviewers, editors as acceptance criteria; and 2) obtain buy-in from/engage scientific journals to report documented QC practices, including analysis of QC samples.

Session 1 Summary

The objective of the first session was to assess the current state of the consortium.

Prior to attending Session 1, attendees were tasked with completing the following:

- Read “Towards quality assurance and quality control in untargeted metabolomics studies,” *Metabolomics* 2019 Jan 3;15(1):4. doi: 10.1007/s11306-018-1460-7.
- Watch pre-recorded presentations: overview of mQACC and current status of each of the working groups
- Complete an online survey composed of two questions:
 1. What are the most important accomplishments achieved by mQACC in the last 3 years?
 2. What are most important areas where mQACC can improve in the next 3 years?

Key points raised in response to the compiled survey data:

- The consortium will need to prioritize the key objectives for the next three years as there are many competing interests.
- It was pointed out that supporting early career scientists is an objective of many consortia and societies; however, this is not one of the primary objectives of mQACC. Should this be discussed further for consideration?
- In order to improve awareness of mQACC, there needs to be increased outreach to the scientific community. For example, mQACC should engage with other associations and societies. Additionally, the mQACC Twitter account should be used for promotion and information dissemination.
- mQACC needs to interact with journals to define what QA/QC metrics should be reported. These metrics could be in the form of a short list of bullet points to a set of reporting standards. The question arose as to whether mQACC should publish an editorial in *Analytical Chemistry* to bring attention to this need.
- mQACC currently has no funding to support its activities. It was suggested that instrument vendors may be willing to sponsor various mQACC activities.
- Due to the large number of interests and priorities within mQACC, it was suggested that there is a need for more working groups, including volunteers to lead these groups, in order to assure the work within the consortium gets completed.

Session 1 Compiled Survey Answers

The data below were compiled from the full survey data to identify all of the unique answers for live polling during Session 1. Raw survey data can be found in Appendix B.

Question: What are the most important accomplishments achieved by mQACC in the last 3 years?

Compiled Answers:

Dissemination, Engagement and Awareness Training with the Metabolomics Community

- mQACC publications – Think Tank report and experimental processes publication
- Posters and presentations to disseminate information
- Presentation of workshops, including surveying, and posters to promote mQACC to the international metabolomics community; visibility; community engagement
- Building an international community interested in QA/QC; bridge the network between metabolomics researchers
- Developing engagement opportunities for early career researchers
- Creating awareness about the need and requirement for quality systems in the field of metabolomics and among MS community; promoting the concept of data quality for metabolomics; engagement/networking with metabolomics community

Operations

- Formation of productive task groups; the 4 working groups are making progress; deliver joint, relevant output
- Formation of a steering committee and larger scientific advisory board
- Coordinating multiple sub-projects and ensuring good communication; consistency with follow-up on specific topics
- Expansion of mQACC membership and enlisting interested investigators to join; engaging more consortium members for broad representative over current practices/viewpoints; linking fellow researchers

Community-Based Developments

- Engage scientific journals on the importance of QA/QC to metabolomics
- Cooperative development of best practices, reference materials, etc.
- Consensus on definitions
- Standard reference materials initiative; discussion/promotion of potential reference materials for untargeted metabolomics

Question: What are most important areas where mQACC can improve in the next 3 years?

Compiled Answers:

Dissemination, Engagement and Awareness Training with the Metabolomics Community

- More output and dissemination directed toward educating the community on best practices, including publications
- Organize QA/QC educational workshops and/or develop educational materials for proper experimental design
- Document and subsequently publish the complete experimental and data processing QA/QC procedure for metabolomics

- Disseminate mQACC goals in all geographical regions
- Development and dissemination of tools and materials to allow researchers to improve their QA/QC procedures; establish the website as a guiding tool in QA/QC
- Development of case studies for publication that exemplify good practice providing guidelines and recommendations for QA/QC/ illustrate why QA/QC practices are important and how they can impact data quality and interpretation
- Publish more articles on recommendations/current state of the field

Operations

- Focus on small number of do-able projects led by people who move them forward
- Integrate further/liase stronger with international and national metabolomics societies/networks (Metabolomics Society, MANA & other regional Societies, Eurachem) or networks in neighboring fields (NORMAN or other)
- It is unclear how new members to the group can become an active component of mQACC; improve engagement of members, so more participate regularly; attract more active scientists from diverse disciplines/institutions
- More working groups to cover other technologies (e.g., NMR)
- Each meeting should have at least one scientific discussion topic
- Recruit labs that are doing large studies, but not yet in mQACC; reach out to more laboratories
- Start a forum open to public; create a forum so people can ask questions and members can answer
- Better utilize website for knowledge transfer
- Regular meetings scheduled well in advance
- Identify how the consortium will develop long-term once best practices have been determined
- Identify funding opportunities to cover mQACC activities
- Establishing itself as the go-to for QA/QC in untargeted metabolomics; demonstrating leadership in the community through publications and events; as leaders, state what needs to be done for metabolite QA/QC
- Assure that there is no duplication of efforts across the working groups; working groups should be refreshed periodically; some working groups need better organization; introducing working group interactive session every 3 months
- Improve engagement of current and new members, so more participate regularly; constraining and constructively channeling participation and effort
- Identify how the consortium can contribute to encouraging good QA/QC practice
- As members increase, hard to understand individual roles in metabolomics QA/QC

Community-based Developments

- Coordination with publishers; get vendor/journal buy-in for standards and practices; encourage scientific journals to provide requirements for QA/QC practices; checklist to share with journals
- Provide recommendations on minimum data that is expected to be reported in publications; provide minimum acceptance criteria for publications
- Interlabs showcasing state of the field: challenges and best practices; focus on experimental work: DOE, PT, ring trials; create an interlab study like ABRF Workflow Interest Network (WIN) study
- Develop well characterized reference materials for QA/QC; develop market ready reference materials and standard mixes for routine use; define/develop test material for multiple purposes
- Develop best QA/QC practices and reporting for metabolomic biomarkers including pre-analytical, analytical, and data processing; set and publish minimum reporting standards for QA/QC; develop reporting standards reporting template for community
- Promotion of more drastic measures for the enforcement of QA/QC
- Get data from community so we know what they are doing
- Push forward issues on harmonization of applied methodologies in metabolomics
- Liaise with policy makers
- Develop human homeostasis database
- Develop disease-related databases
- Develop a set of best practices and a 'minimal viable product' for QC/QA in metabolomics
- Recommend spike-in standards and standardized sample preparation and storage
- Develop clear protocols for QA/QC for different instrument/technique type
- Provide open source QC software

Session 2 Summary

The objective of the second session was to review and prioritize the objectives and recommended action points that were established at the *Think Tank on Quality Assurance and Quality Control for Untargeted Metabolomic Studies*.

Prior to attending Session 2, attendees were tasked with completing a survey indicating whether each objective and action point identified at the 2017 Think Tank was completed, should be kept active, was not started, or should be dissolved. These objectives and actions points were outlined in Beger, et al. (doi: 10.1007/s11306-018-1460-7). The results of this survey are below.

The primary objectives and actions items that were prioritized to remain active by over 50% of the attendees were:

- Engage scientific journals to report that documented QC practices, including analysis of QC samples, should be part of the acceptance criteria for publication

- Obtain buy-in from scientific journals, companies, software developers, database developers, and funders
Define acceptance criteria [e.g., scoring system (or explain why criteria were not met)]

Survey Results

Question 1: For each of the priorities identified at the 2017 mQACC Think Tank, please indicate whether you feel that priority has been completed, should be kept actively going, has not started, or should be dissolved as a priority.

Answers:

#	Question	Completed		Keep active		Not started		Dissolve		Total
1	Publish a workshop report to communicate the meeting proceedings to the metabolomics community and allow new members to join the consortium.	78.05%	32	14.63%	6	2.44%	1	4.88%	2	41
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	21.43%	9	71.43%	30	7.14%	3	0.00%	0	42

	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.	2.38%	1	54.76%	23	42.86%	18	0.00%	0	42
4	Document and subsequently publish the complete experimental procedure for metabolomics, including the QC practices.	11.90%	5	54.76%	23	28.57%	12	4.76%	2	42
5	Establish a community forum to discuss the development of reference standards, and interlaboratory comparison exercises.	2.38%	1	78.57%	33	16.67%	7	2.38%	1	42
6	Engage the community to identify key reference materials that need to be developed.	2.38%	1	85.71%	36	11.90%	5	0.00%	0	42
7	Form a steering committee and larger scientific advisory board.	38.10%	16	28.57%	12	30.95%	13	2.38%	1	42
8	Identify funding opportunities to hold meetings and continue the group discussion and planning.	0.00%	0	53.66%	22	41.46%	17	4.88%	2	41

9	Organize workshop(s) on QA/QC at the Metabolomics Society meeting to promote community engagement in these efforts.	21.43%	9	76.19%	32	2.38%	1	0.00%	0	42
---	---	--------	---	--------	----	-------	---	-------	---	----

For each of the recommended action items identified at the 2017 Think Tank for the question indicated below, please indicate whether you feel that priority has been completed, should be kept actively going, has not started, or should be dissolved as an action item.

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

Answers:

#	Question	Completed		Keep active		Not started		Dissolve		Total
1	Document complete experimental processes and reporting from study design to data analysis	7.50%	3	70.00%	28	20.00%	8	2.50%	1	40
2	Focus is not just analytical but study protocols	2.38%	1	54.76%	23	35.71%	15	7.14%	3	42
3	Training and education, different for researchers and users new to the scientific discipline versus experienced researchers in the discipline	0.00%	0	61.90%	26	33.33%	14	4.76%	2	42
4	Define the best practices and those that should be avoided in sample collection, processing and storage	2.38%	1	73.81%	31	23.81%	10	0.00%	0	42

Question 3: What are the current gaps that should be addressed to establish widespread best practices for QC protocols in untargeted metabolomics?

Answers:

#	Question	Completed		Keep active		Not started		Dissolve		Total
1	Obtain buy in from scientific journals, companies, software developers, database developers, and funders	2.44%	1	39.02%	16	46.34%	19	12.20%	5	41
2	Define best QC practices	9.52%	4	88.10%	37	2.38%	1	0.00%	0	42
3	Need agreement and to encourage/enforce QC practices	0.00%	0	78.57%	33	16.67%	7	4.76%	2	42
4	Educate community about QC procedures	2.38%	1	83.33%	35	11.90%	5	2.38%	1	42

Question 4: What is needed to establish QC acceptance criteria reporting across the wider community?

Answers:

#	Question	Completed		Keep active		Not started		Dissolve		Total
1	Establish minimum acceptance criteria, including creating a broad-based scoring system [For example, one QC scoring scheme could include: (i.e. 0 = none, 1 = pooled, 2 = pooled and SRM)]	0.00%	0	35.71%	15	54.76%	23	9.52%	4	42
2	Create reporting standards/SOPs for the entire analytical process	2.38%	1	69.05%	29	26.19%	11	2.38%	1	42

Question 5: What should be the minimum QA and QC reporting standards for publications and databases?

Answers:

#	Question	Completed		Keep active		Not started		Click to write Scale Point 4		Total
1	Define acceptance criteria [e.g. scoring system (or explain why criteria were not met)]	0.00%	0	57.14%	24	38.10%	16	4.76%	2	42
2	QC metadata should be reported (e.g. sample order, QC sample reference material used) and define elements under each category with adequate details for reproducibility	0.00%	0	69.05%	29	30.95%	13	0.00%	0	42

Question 6: What are the key characteristics of high-availability test material sample types for metabolomics?

Answers:

#	Question	Completed		Keep active		Not started		Dissolve		Total
1	Develop test materials for inter-laboratory comparisons	0.00%	0	92.68%	38	7.32%	3	0.00%	0	41
2	Quantitative/semi-quantitative comparisons	0.00%	0	61.90%	26	38.10%	16	0.00%	0	42
3	Inexpensive materials	0.00%	0	47.62%	20	47.62%	20	4.76%	2	42
4	Same sample for all technologies—must cover wide range of characteristics	0.00%	0	53.66%	22	36.59%	15	9.76%	4	41
5	Develop key data quality metrics for each	0.00%	0	50.00%	21	50.00%	21	0.00%	0	42

platform and test material									
----------------------------	--	--	--	--	--	--	--	--	--

Question 7: What best use practices should be established for test material samples by the community?

Answers:

#	Question	Completed		Keep active		Not started		Dissolve		Total
1	Define best practices	2.50%	1	80.00%	32	17.50%	7	0.00%	0	40
2	Need consensus, including when you run the test material and timing of use, to allow for data harmonization	0.00%	0	60.00%	24	37.50%	15	2.50%	1	40
3	Context dependent (i.e., highly dependent on matrix)	0.00%	0	50.00%	20	45.00%	18	5.00%	2	40
4	Determine if test materials should be accompanied by SOPs	2.44%	1	41.46%	17	53.66%	22	2.44%	1	41
5	Test materials should be used in conjunction with other QC samples	4.88%	2	73.17%	30	19.51%	8	2.44%	1	41
6	Use for lab qualification, instrument qualification, training	2.44%	1	56.10%	23	39.02%	16	2.44%	1	41

The results of this survey were reviewed during the session and attendees were then asked to prioritize those objectives and action items that were indicated to be kept active. Additionally, attendees were asked whether those objectives and action items that were considered not started should be initiated. This was done via live polling during the session, and the results of the polling are below.

Live Polling Results

Question 1: What is the most important priority from the 2017 Think Tank to keep active?

Poll Option	Count	Total	Results
		Votes	
Publish a white paper which could include QA/QC procedures; use of QC samples as best practices; QA/QC being a developing principle; and a description of the QC procedures performed in experienced labs	10	37	27%
Engage scientific journals to report that documented QC practices, including analysis of QC samples, should be part of the acceptance criteria for publication	21	37	57%
Document and subsequently publish the complete experimental procedure for metabolomics, including the QC practices	3	37	8%
Establish a community forum to discuss the development of reference standards and interlaboratory comparison exercises	2	37	5%
Engage the community to identify key reference materials that need to be developed	1	37	3%
Identify funding opportunities to hold meetings and continue the group discussion and planning	0	37	0%
Organize workshop(s) on QA/QC at the Metabolomics Society meeting to promote community engagement in these efforts	0	37	0%

Question 2: What is the most important gap that should be addressed to establish widespread best practices for QA in untargeted metabolomics?

Poll Option	Count	Total Votes	Results
Document complete experimental processes and reporting from study design to data analysis	12	37	32%
Focus is not just analytical but study protocols	3	37	8%
Training and education, different for researchers and users new to the scientific discipline versus experienced researchers in the discipline	9	37	24%
Define the best practices and those that should be avoided in sample collection, processing and storage	13	37	35%
Obtain buy in from scientific journals, companies, software developers, database developers, and funders	22	38	58%
Define best QC practices	8	38	21%
Need agreement and to encourage/enforce QC practices	2	38	5%
Educate community about QC procedures	6	38	16%

Question 3: What is the most important strategy to implement minimum QA and QC reporting standards for publications and databases?

Poll Option	Count	Total Votes	Results
Define acceptance criteria [e.g. scoring system (or explain why criteria were not met)]	20	39	51%
QC metadata should be reported (e.g. sample order, QC sample reference material used) and define elements under each category with adequate details for reproducibility	19	39	49%

Question 4: What is the most important characteristic of high-availability test materials for metabolomics?

Poll Option	Count	Total Votes	Results
Develop test materials for inter-laboratory comparisons	14	39	36%
Quantitative/semi-quantitative comparisons	3	39	8%
Inexpensive materials	4	39	10%
Same sample for all technologies—must cover wide range of characteristics	3	39	8%
Develop key data quality metrics for each platform and test material	15	39	38%

Question 5: What is the most important next step for the community to establish test material samples?

Poll Option	Count	Total Votes	Results
Define best practices	7	38	18%
Need consensus, including when you run the test material and timing of use, to allow for data harmonization	17	38	45%
Context dependent (i.e., highly dependent on matrix)	3	38	8%
Test materials should be used in conjunction with other QC samples	3	38	8%
Use for lab qualification, instrument qualification, training	8	38	21%

Question 6: Should creating reporting standards/SOPs for the entire analytical process be a priority to start in the next 3 years?

Poll Option	Count	Total Votes	Results
Yes	34	37	92%
No	3	37	8%

Question 7: Determining if test materials should be accompanied by SOPs is important to start in the next 3 years?

Poll Option	Count	Total Votes	Results
Yes	28	37	76%
No	9	37	24%

Session 3 Summary

The objective of the third session was to identify new priorities for mQACC to accomplish over the next three years.

Prior to the session, attendees were tasked with completing a survey to identify new objectives for the consortium to move forward over the next three years.

The top priorities were identified as:

- Define/recommend/disseminate QA/QC best practices/standards/protocols for both MS and NMR, including implementation
- Provide clear recommendations for authors, reviewers, editors of acceptance criteria
- Obtain buy-in from/engage scientific journals to report documented QC practices, including analysis of QC samples

Key points raised in response to the identified priorities:

- Define/recommend/disseminate QA/QC best practices/standards/protocols for both MS and NMR, including implementation falls under the existing Best Practices Working Group (BPWG); therefore, this priority will be led by this working Group.
- Currently, the BPWG focuses on mass spectrometry; therefore, an NMR component will need to be added to the working group. Leo Cheng and Matt Lewis have agreed to lead the NMR component as a subgroup of the BPWG.
- The following priorities were determined to be similar in nature, so it was decided that they could be addressed together:
 - provide clear recommendations for authors, reviewers, editors as acceptance criteria; and
 - obtain buy-in from/engage scientific journals to report documented QC practices, including analysis of QC samples
- To address these combined priorities, a new working group will be formed and led by Rick Dunn and Clare O'Donovan. Additional members of the working group will be Rick Beger, Julia Kuligowski, Georgios Theodoridis, Ian Wilson.

Compiled Answers from Survey

These data were compiled from the full survey data to identify all of the unique answers for live polling during Session 3. Raw survey data can be found in Appendix C.

Question: Choose the most important priority that mQACC should focus on over the next 3 years.

Answers:

- High impact publications
- Obtain buy-in from/engage scientific journals to report documented QC practices, including analysis of QC samples
- Provide clear recommendations for authors, reviewers, editors as acceptance criteria
- Obtain buy in from vendors, software developers and database developers
- Secure funding for our activities
- Promote/raise awareness about the need for QA/QC among research community
- Educate/train the research community on QA/QC for untargeted metabolomics
- Engage with other organizations/groups for further development of mQACC objectives
- Agree on the minimum QA and QC reporting standards for publications and databases
- Define/recommend/disseminate QA/QC best practices/standards/protocols for both MS and NMR
- Getting members into working groups
- More focused working groups, e.g., sample collection QMS, data analysis QMS, NMR, journal engagement
- Study design and metabolite annotation/identification
- Harmonization using standard reference materials
- Remembering that we are only a recommendation body and propose recommendations accordingly
- Collection and storage quality control

The results of this survey were reviewed during the session and attendees were then asked to prioritize these points via live polling. The results of the polling are below.

Question: Choose the 3 most important priorities that mQACC should focus on over the next 3 years.

Live Polling Results

Poll Option	Count	Total Votes	Results
High impact publications	3	37	8%
Obtain buy in from/engage scientific journals to report documented QC practices, including analysis of QC samples	11	37	30%
Provide clear recommendations for authors, reviewers, editors as acceptance criteria	21	37	57%
Obtain buy in from vendors, software developers and database developers	7	37	19%
Secure funding for our activities	0	37	0%
Promote/raise awareness about the need for QA/QC among research community	5	37	14%

Educate/train the research community on QA/QC for untargeted metabolomics	11	37	30%
Engage with other organizations/groups for further development of mQACC objectives	3	37	8%
Agree on the minimum QA and QC reporting standards for publications and databases	9	37	24%
Define/recommend/disseminate QA/QC best practices/standards/protocols for both MS and NMR, including implementation	23	37	62%
Getting members into working groups	2	37	5%
More focused working groups, e.g. sample collection QMS, data analysis QMS, NMR, journal engagement	4	37	11%
Study design and metabolite annotation/identification	2	37	5%
Harmonization using standard reference materials	7	37	19%
Remembering that we are only a recommendation body and propose recommendations accordingly	1	37	3%
Collection and storage quality control	1	37	3%

Appendix A: Meeting Agenda

mQACC virtual meeting 2020

The 2020 mQACC virtual meeting has two main objectives:

1. To review the progress and reflect on the progress observed in the last three years
2. To define the objectives and action points for the next three years

The agenda for each session is detailed below.

Session 1

Date: Monday November 9th (90 minutes maximum)

Objective: To define what mQACC was constructed to do and define what has been done

0-5 minutes: Technical introduction on how to use Webex and other interactive software

5-15 minutes: Quick recap on the five pre-session presentations and describe objective of this session

15-40 minutes: Discussion session – What are the most important accomplishments in the last 3 years?

40-80 minutes: Discussion session – How can mQACC *improve* in the next 3 years?

80-90 minutes: Summarize session one, Introduction to session 2

Session 2

Date: Thursday November 12th (90 minutes)

Objective: To revisit the 9 objectives/23 recommended action points developed from the 2017 Think Tank meeting

0-5 minutes: Introduction to the session

10-20 minutes: Presentation of results of pre-session 2 homework

20-65 minutes: Discussion session on the 23 objectives and recommended action points.

60-80 minutes: Slido online voting

80-90 minutes: Summarize session two, Introduction to session 3, Introduction to pre-session 3 homework

Session 3

Date: Wednesday November 18th (120 minutes)

Objective: To define any new objectives/action points and to rank priorities/action points based on importance and action lead person

0-5 minutes: Introduction to the session

10-20 minutes: Presentation of results of pre-session 3 homework

20-50 minutes: Discussion session

50-60 minutes: Bio-break/Coffee break

60-70 minutes: Slido poll – prioritizing new and current objectives

70-110 minutes: Report of Slido poll and defining lead personnel

110-120 minutes: Close virtual meeting

Appendix B: mQACC Meeting Session 1 Full Survey Results

Survey Question 1: What are the most important accomplishments achieved by mQACC in the last 3 years? Please list a maximum of 3.

Answers:

1. Introductory manuscripts. 2. Workshops. 3. Building community.

1. Representation and promotion of the consortia at international meetings 2. Formation of productive task groups 3. Dissemination of objectives: pubs (Beger et al, and Evans et al), BP workshops

1) white paper on QA/QC. 2) standard reference materials initiative

1. Provide a forum for discussion of QC/QA procedures in metabolomics! 2. Provide a repository for presentations and information on QC/QA 3. Survey metabolomics groups for their practices.

1. Developing a community of researchers interested in QAQC 2. Coordinating multiple subprojects and ensuring good communication 3. Best practices publication

Coordination of activities and manuscripts relevant in the field.

1) Current Practices publication; 2) Think Tank Report; 3) workshops

1. gained community awareness through conference presentations/workshops 2. article publication on QA/QC practices in untargeted metabolomics 3. expansion of mQACC membership panel

1. Survey on QC practices 2. consensus on definitions 3. visibility at conferences promoting better practices in untargeted metabolomics

publications and posters at presentations. disseminating information.

1) publish a workshop from the meeting 2) engage scientific journals on the importance of QA/QC to metabolomics 3) organize QA/QC workshops at the metabolomics society meeting
not sure. Far too little content discussed in meetings.

1. Set the best QC practice 2. Set the minimum and best reporting standards

QC paper in metabolomics

1. Experimental processes publication 2. Best Practices Working Group community engagement efforts 3. Promotion of mQACC to inform the community and enlist interested investigators to join

1) publications (Think Tank Report and the Experimental Processes manuscript) 2) workshops at multiple conferences

I joined too recently to judge

1. getting international community to work together to address issues of QA/QC in metabolomics 2. workshops to raise visibility about current practices and mQACC itself 3. publications

1. Bring together people from diverse disciplines/institutions 2. Deliver joined, relevant output

1. Creating awareness about the need and requirement for quality systems in the field of metabolomics and among MS community 2. Developing engagement opportunities for early career researchers

1) community engagement for consortia awareness (conferences, posters) 2) polling questions to members of the community in workshops 3) publication on best practices survey

1: building a thriving community; 2: seminal publications; 3: publicizing the consortium

1) Publication by Beget et al. to disseminate mQACC creation and goals. 2) Participation of mQACC in different conferences that contributed to membership increase. 3) Publication by Evans et al.

1. mQACC workshops 2. engaging more people within the consortium for getting a more representative overview of the current practices/viewpoints 3. discussion/development of new reference materials

1. Establish a community forum to discuss the development for QA/QC procedures. 2. Promote mQACC to community to generate awareness 3. Form a steering committee and larger scientific advisory board.

1. Manuscript publications 2. Raise the public recognition through conference and workshop 3. Bridge the network between metabolomics researchers

1. Visibility 2. Consistency with follow ups on specific topics 3. Inclusions of many new members

1) QA/QC best practices manuscript Evans et al. 2) Surveys on topics at metabolomics meetings 3) 4 working groups making progress

1. Created the consortium so all labs can contribute and share 2. Workshops to promote mQACC and to raise the awareness 3. Published surveys & consensus on how the other labs are doing

1. the building of a community 2. the workshops 3. the publication of the paper

1. Linking fellow researchers 2. promotion of quality measures 3. promotion of reference material

1. engagement with metabolomics community 2. cooperative development of best practices, reference materials, etc. 3. widening our own community base that is driven by metabolomics QA/QC

1) promoting the concept of data quality for metabolomics. I think prior to this metabolomics was seen as a relative, exploratory low precision methodology. I think that is now changing.

1. manuscripts so people know we exist 2. network (advising other tangential groups/HHEAR, etc.) 3. received data from community so we know what they are doing

1. Interaction with the metabolomics community at conferences and through polls 2. Publication of experimental processes manuscript 3. Growth of mQACC 3.

1. Bring together scientists working long on the specific field 2. Push forward issues on harmonization of applied methodologies in metabolomics

1) recommendations for QA/QC in various presentations 2) surveys on best practices for QA/QC 3) discussion of potential reference materials for untargeted metabolomics

1. growing in membership 2. publishing content 3. gathering data from wider community at conferences

I have been added to the committee in Nov 2019. I joined to learn more on quality standards that people in this field are working on and got a handful information while being a part of the committee.

Highlighting the need for QA/QC in metabolomics Identifying what common practice is Identifying what best practice should be

Survey Question 2: What are most important areas where mQACC can improve in the next 3 years? Please list a maximum of 3.

Answers:

1. Move toward statements of need and minimal requirements. 2. Development of case studies that exemplify good practice. 3. Coordination with publishers in some context.

1. More outputs directed toward educating the community on BP 2. Interlabs showcasing state of the field: challenges and BP 3.

1) Continuing to exist 2) The Broadhurst paper 3) The Working partys

Help disseminate tools and materials to allow researchers to improve their QA/QC procedures

1. Get vendor/journal buy in for standards and practices 2. Have a set of best practices and a 'minimal viable product' for QC/QA in metabolomics

1. Focus on small number of do-able projects led by people who move them forward. 2. Integrate further with Metabolomics Society, MANA & other regional Societies 3. Publish further best practice

It is unclear how new members to the group can become an active component of the mQACC group and have full benefit.

1) Establishing itself as the go-to for QA/QC in untargeted metabolomics; 2) releasing a test material for untargeted metabolomics; 3) publishing a set of minimum reporting standards for QAQC.

- develop market ready reference materials and standard mixes for routine use
- continue education aspects at conferences
- encourage scientific journals to provide requirements for QA/QC practices

1. Standardize more processes. 2. Agree upon Terms and definitions 3. Hold in person conference and training seminar

1) develop clear protocols for QA/QC for different instrument / technique type 2) develop well characterized reference materials for QA/QC 3) organize QA/QC workshops at metabolomics society meeting

each meeting should have at least one scientific discussion topic. Not just WG.

Best QA, QC practice and reporting for metabolomic biomarkers including pre-analytical, analytical, and data processing.

recommend spike-in standards recommend standardized sample preparation and storage

1. Assure that there is no duplication of efforts across the working groups 2. Improve engagement of members, so more participate regularly 3. Some working groups need better organization

1) reference materials 2) reporting standards 3) educational material for proper experimental design

1). Data analysis and reporting standard. 2). Human homeostasis data base. 3). Disease related data bases.

1. additional papers with case studies to illustrate why QA/QC practices are important and how they can impact data quality and interpretation 2. checklist to share with journals

1. define/develop test material for multiple purposes

1. Training workshops 2. Tools development for QA systems

1) providing guidelines and recommendations for QA and QC 2) reference material development and experimental implementation 3) reporting - what and how

1: gaining momentum; 2: constraining and constructively channeling participation and effort; demonstrating leadership in the community through publications and events

1) Provide recommendations on minimum data that is expected to be reported in publications. 2) Disseminate best practices for QC samples. 3) Disseminate mQACC goals in all geographical regions.

1. provide clear recommendations on how to perform QC/QA in metabolomics 2. provide minimum acceptance criteria for publications 3. Provide training/education on QC/QA 2.

1. Document and subsequently publish the complete experimental and data processing QA / QC procedure for metabolomics 2. Make available reference standards 3. Identify funding opportunities

1. Create a inter lab study like ABRF Workflow Interest Network (WIN) study and send survey and samples to different labs and compare the results. 2. Start a forum and open to public

1. Establish the website as a guiding tool in QAQC 2. Develop and promote use of reference materials 3. Run educational workshops in QAQC procedures

1) Develop reporting standards reporting template for community 2) Provide open source QC software 3) continue QC/QA education

1. increase more scientific interactions and also between groups 2. recruit labs that are doing large studies but not yet in mQACC 3. create a forum so people can ask questions and members can answer

1. reaching out to more laboratories 2. providing guides 3. training

1. Focus on experimental work: DOE, PT, ring trials 2. Liaison with policy makers 3. Stronger liaison with professional bodies e.g. Eurachem or networks in neighboring fields (NORMAN or other)

1. as members increase, hard to know who who/individual roles in metabolomics QA/QC 2 is. task/working groups to refreshed periodically 3. better utilize website for knowledge transfer inter/externally

Keep up the good work. Metabolomics will fail if it does not become a better, more reproducible science. I think most metabolomics data produced is irreproducible.

1. specialized tasks/outputs from working groups 2. engagement of new members 3. assess how effective mQACC can be with so many members 4. as leaders, states what needs to be done for metabolite QAQC

1. Regular meetings and scheduled well in advance

1. promotion of more drastic measures for the enforcement of QA/QC 2. liaison with international and national metabolomics societies/networks 3. attract more active scientists of the field

1) identify most important reference material for untargeted metabolomics and work towards development 2) publish more articles on recommendations/current state of the field

1. More working groups to cover other technologies (e.g. NMR), 2. get funds to cover various activities

Introducing subcommittee interactive session in every 3 months.

Identify how the consortium will develop long term once best practice has been determined.

Identify how the consortium can contribute to encouraging good QA/QC practice

Appendix B: mQACC Meeting Session 3 Full Survey Results

Survey Question: Using the information from the first two Sessions, think about what you feel is the most important priority for mQACC to move forward over the next three years. This can include new and/or ongoing initiatives that you feel remain a key target for the consortium.

What is the one most important priority that mQACC should focus on over the next three years?

Answers:

I believe it is time to educate the grant funders and journal publishers.

High impact publications

Obtaining buy-in from scientific journals, companies, etc. and securing funds for our activities

Defining standards and protocols for QC for both MS and NMR

Educate, promote, and raise awareness among research community, cores, publisher, and funder.

Creating awareness about the need of quality system in Metabolomics

encourage journals to provide requirements for QA/QC; we need to define those & provide training

Engagement with other organizations/groups to further develop mQACC objectives e.g. funders/academia

Dissemination of best practices for QA/QC (through publications, examples, protocols, training)

Define guidelines for routine and robust QA/QC practices in untargeted metabolomics.

Focus = Quality: Quality data should be mQACC focus. It easy to implement QA/QC. No technical bias

Agree on the minimum QA and QC reporting standards for publications and databases.

Recommend the best practices for generating good quality of metabolomics data.

Describe best the QA/QC procedures for non-Targeted Metabolomics and to get the message out

Engage scientific journals to report that documented QC practices, including analysis of QC samples.

Defining best practices

Engaging scientific journals, let them know plans and get early input

Obtain buy in from scientific journals, companies, software developers, database developers, funding

Define QC best practices for the community AND journals, companies, etc.

Documenting best practices throughout the entire experimental process including study design

More focused working groups e.g. sample collection QMS, data analysis QMS, NMR, journal engagement

Obtain buy in from scientific journals, companies, software/database developers, and funders

I believe buy-in from scientific journals, companies and funding agencies

discussing best practices, harmonizing how to report QA/QC and engaging journals, founders, etc.

Harmonization using standard reference materials

Provide clear recommendation for authors, reviewers, editors as acceptance criteria

minimum standards how metabolics data is generated, analyzed and reported

getting people into working groups

Collection and storage quality control

define and publish best practices and get buy-in from journals, software developers, funding agency.

Remembering that we are only a recommendation body and propose recommendations accordingly.

Raising awareness of QA/QC, ideally at the instrument vendor end

Define best QC practices and then engage with journals, DBs, funders, agencies to facilitate QCs

study design and metabolite annotation/identification

Appendix C: Session recordings

Session One: <https://cbiit.webex.com/cbiit/ldr.php?RCID=71a89deb4532414a83f3a8323e418d05>

Session Two: <https://cbiit.webex.com/cbiit/ldr.php?RCID=ed2a96e39b9d4ddea78b900e381d425a>

Session Three: <https://cbiit.webex.com/cbiit/ldr.php?RCID=fb00c9a620324fb18fd7f08a8ba972ce>