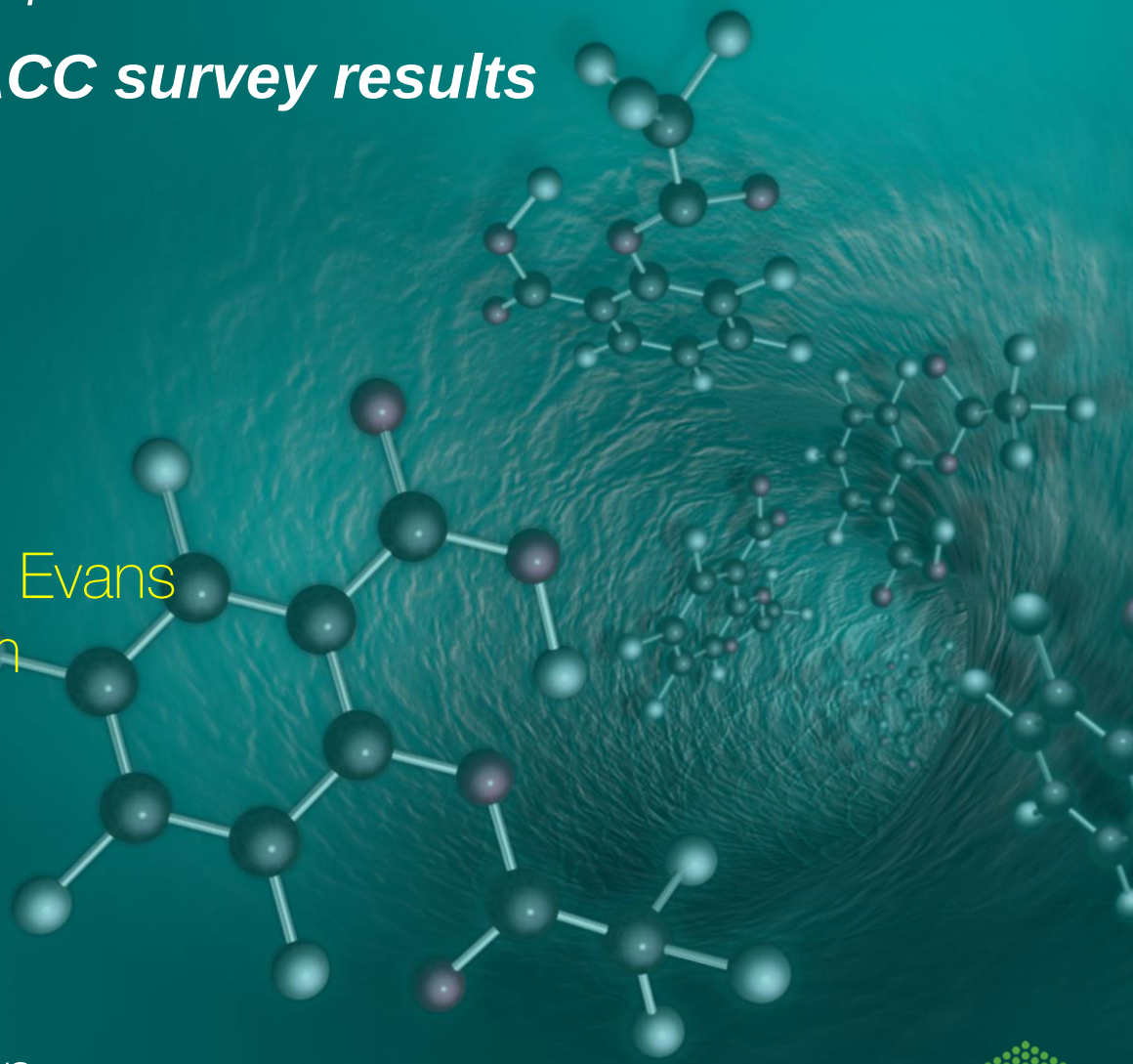
Discussion of QA/QC practices

-presentation of mQACC survey results



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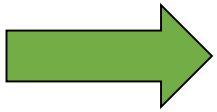
EMBL-EBI

So what actually happens in practice?

Discussion

- within the mQACC Consortium
- at the mQACC workshop last year in Seattle



Created a survey to discover common and differing QA/QC practices

Credit: Annie Evans – Metabolon

Who participated?

Total: 23 laboratories

- 16 from Academia
- 4 from Governmental organizations
- 3 from Industry

Thanks so much to all who participated!

What did we ask?

Do you perform system suitability testing?

i.e. do you test that a method and associated instrumentation is fully functioning before analysis of experimental samples?

100%

a) If yes, do you check chromatographic performance? 64%
b) If yes, do you check MS performance? 90%
c) If yes, do you use a solution of standards and/or a biological sample for this purpose? 100%

What did we ask?

Blanks

a) Do you use a process/extraction blank? 100%

b) Do you use a system suitability blank? 70%

What did we ask?

Do you use internal standards?: 91%

If yes, how do you use these standards?

To assess RSDs	70%
To assess chromatographic performance	80%
For Chromatographic alignment	45%
To assess sensitivity	70%
To assess mass stability	80%
To assess mass accuracy	80%

What did we ask?

Do you use pooled QC/Intra-study QC samples: 96%

If yes, how do you use these?

To assess peak quality	76%
To filter for peak quality	60%
To assess process RSDs	71%
To condition column	76%

What did we ask?

Do you use long-term reference QC samples/ intra-laboratory QC samples? 52%

Do you use NIST SRM 1950 or generate/purchase your own?

23%/77%

What did we ask?

Do you use Standard Reference Materials/Inter-laboratory QC samples? 33%

If yes: which ones? SRM 1950 most common..all used NIST standards

Do you use technical replicates of experimental samples? 36%

If yes

a) Do you perform multiple replicates for all experimental samples or just a subset? ?|36%

b) If yes, is it a process replicate or a injection replicate? 33%/66%

What did we ask?

Run order

a) Do you balance samples based on the meta data? Eg equal number of males/females 81%

b) Do you randomize experimental sample injection order per batch? 91%

What did we ask?

Compound identification

a) Do you use publicly available databases (eg Metlin or Lipid Maps) for compound identification? 91%

b) Do you use authentic standards to confirm metabolite identification (MS1)? 100%

   a) If yes, do you do only for compounds of primary statistical interest? 65%

   b) If yes do you have an inhouse authentic standard library/database? 76%

   c) Do you report MSI confidence levels for all compounds reported/published? 68%

What did we ask?

Data acceptance criteria

a) Do you manually review peak integrations? 82%

b) Do you manually review peak alignment? 50%

c) Do you use statistical analysis to assess data quality? 85%

What did we ask?

Quality assurance

a) Is your lab run under any formal accreditation? 10%

b) Do you have an independent QA group? 29%

c) Do you have formalized document control processes? Eg SOPs 50%

d) Do you have a formalized document system? Eg tracking incidents or deviations 50%

What did we ask?

e) Do you have SOPs for all laboratory processes? 65%

f) Do you have lab atmospheric monitoring? 62%

g) Do you have refrigerator/freeze temp monitoring? 91%

h) Do you have an established preventative maintenance, calibration and tuning schedule for equipment? 100%

What did we ask?

i) Do you maintain log books or files for tracking purposes? 85%

j) Are your lab processes and quality systems audited on a routine basis by an independent group? 27%

k) Do you have a formal sample tracking system? 32%

l) Do you have formalized staff training and documentation of completed training? 55%

What did we ask?

m) Do you have a formal new instrument and equipment validation processes? 81%

n) Do you have a formalized process for QC review and approval involving multiple people? 50%

o) Do you have an established data storage and archival process for all data? 71%

p) Do you upload study raw spectral data into public repositories such as MetaboLights/Metabolomics Workbench? 55%

Conclusions and next steps

- QC seems to be progressing in agreement except with regards to reference standards
- still a lot of work to do in QA
- Lots more data to process
- Publication to come!
- Feedback most welcome!!!