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Comparison Of Different Pooled Quality Control Samples To Improve Data Quality During An Interbatch Experiment In Untargeted UHPLC-HRMS Analysis On Two Different MS Platforms

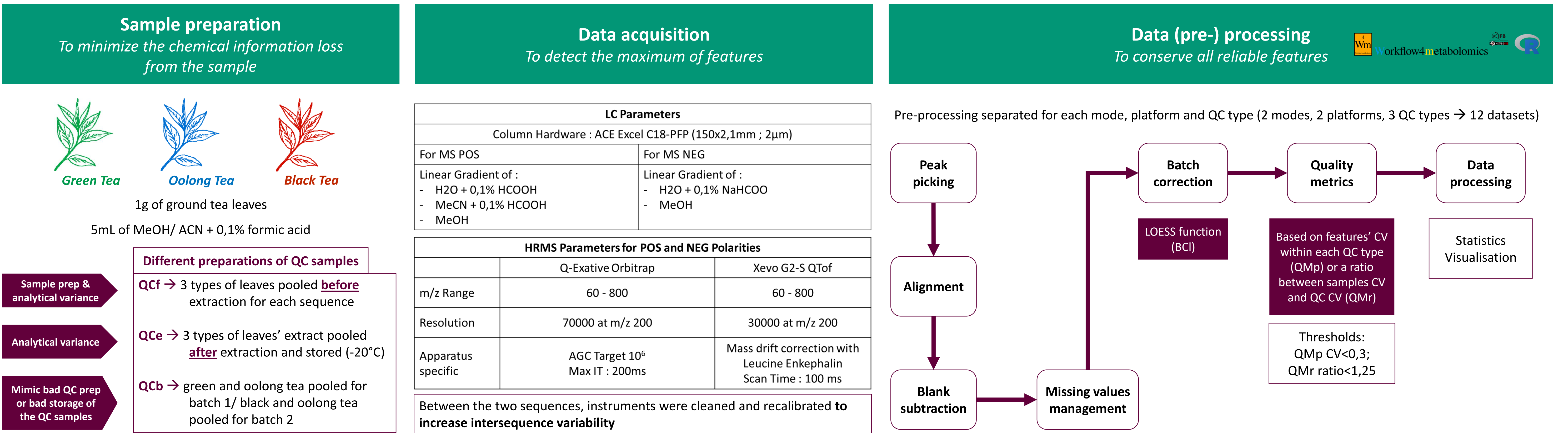
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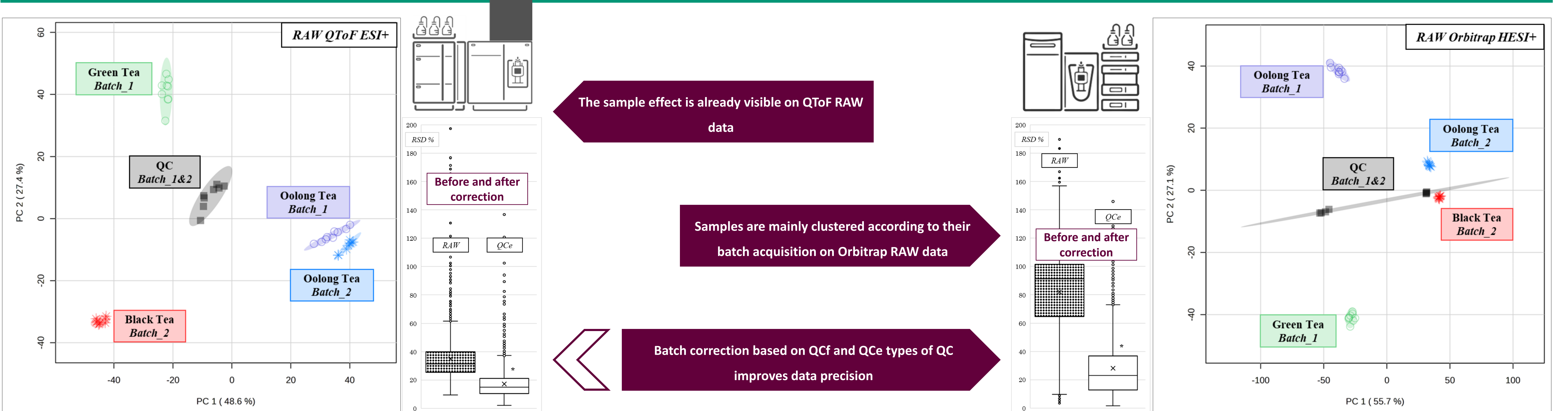
Correcting inter/ intra batch effect is still an important step during data pre-processing because it can introduce a lot of variability and mask the studied effect in the dataset. For that, measures to improve data quality must be taken in order to obtain precise and repeatable data. These measures commonly rely on quality control (QC) samples used in metabolomics approaches for three main reasons: (i) the initial conditioning of the column; (ii) the correction of analytical drift especially between batches; and (iii) the evaluation of measurement precision. During the pre-processing, data are then corrected and filtered based on the QC samples to improve data quality of the dataset¹.

However, depending on QC composition and pre-processing method applied, a significant part of the data can be lost² in the process which is an issue especially in untargeted metabolomics that is dedicated to extract and detect the maximum of features within a sample. This loss especially concern low intense features in the samples that are not always detected in the QC samples.

In this study, we chose to analyse different types of tea and we compared three ways of preparing pooled QC samples analysed in both positive and negative mode on two MS platforms (QToF and Orbitrap). We applied common pre-processing steps adapted to our dataset and evaluated the performances of the different QC types in terms of precision and ability to conserve low intense features.



Results



	Data loss (QToF)			
	ESI+		ESI-	
	QMr	QMp	QMr	QMp
QCf	3%	43%	0%	19%
QCe	0%	8%	0%	21%
QCb	9%	90%	4%	98%

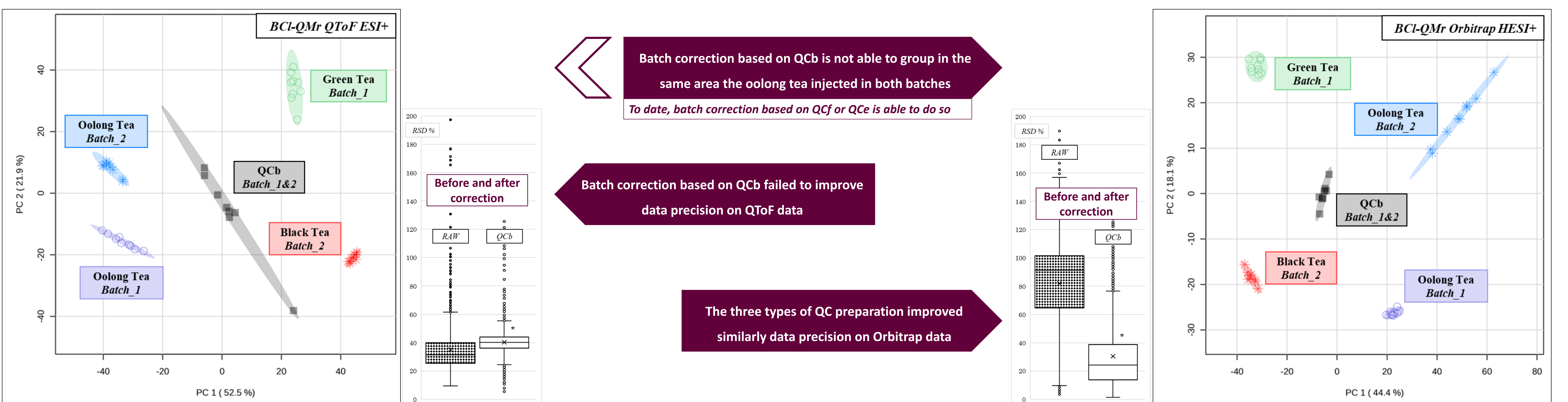
	Count of 10 lowest int. features (QToF)			
	ESI+		ESI-	
	QMr	QMp	QMr	QMp
QCf	10	1	10	2
QCe	9	6	10	1
QCb	9	0	10	0

Ratio quality metrics filtering approach is less prone to data loss and allows low intense features' conservation

The three types of QC preparation give similar results on Orbitrap data

	Count of 10 lowest int. features (Orbitrap)			
	HESI+		HESI-	
	QMr	QMp	QMr	QMp
QCf	10	3	10	5
QCe	10	4	10	2
QCb	10	5	10	2

	Data loss (Orbitrap)			
	HESI+		HESI-	
	QMr	QMp	QMr	QMp
QCf	2%	36%	2%	41%
QCe	1%	36%	1%	44%
QCb	2%	39%	2%	39%



Conclusion

QC samples to correct batch effect and improve data quality are more and more used but not enough described in published articles impacting the reproducibility of the studies³. We show in this work that the type of QC preparation and the choice of data filtration affect differently the data matrices in terms of precision and conservation of low intense features. On the one hand, it appears that QCe and QCf are good basis for batch correction, quality improvement of the dataset and low intense data conservation that are reliable in our study. On the other hand, our results give evidence that QC preparation and storage must be controlled, otherwise (QCb type here) it may decrease data precision, cause a severe loss of data, and not be able to group the same samples injected in different batches.

References

- Maertens A., Holle J., Mollenhauer B., Wegner A., Kirwan J., Hiller K. 2023. « Instrumental Drift in Untargeted Metabolomics: Optimizing Data Quality with Intraudy QC Samples ». *Metabolites* 13 (5): 665. <https://doi.org/10.3390/metab13050665>
- Dunn WB., Broadhurst D., Begley P., Zelena E., Francis-McIntyre S., Anderson N., Brown M., et al. 2011. « Procedures for Large-Scale Metabolic Profiling of Serum and Plasma Using Gas Chromatography and Liquid Chromatography Coupled to Mass Spectrometry ». *Nature Protocols* 6 (7): 1060-83. <https://doi.org/10.1038/nprot.2011.335>
- Broeckling, CD., Beger RD., Cheng LL., Cumeras R., Cuthbertson DJ., Dasari S., Davis WD., et al. 2023. « Current Practices in LC-MS Untargeted Metabolomics: A Scoping Review on the Use of Pooled Quality Control Samples ». *Analytical Chemistry* 95 (51): 18645-54. <https://doi.org/10.1021/acs.analchem.3c02924>