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Addition/Correction

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Correction to "Pregnancy-Induced Metabolic Phenotype Variations in Maternal Plasma"

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In the process of curating and describing the data and methods of this publication for submission as a Data Note in the journal *GigaScience*,[1,2] certain discrepancies between the actual methods and the reported methods came to light. In most cases, these are minor and do not affect the results as described in the original article.[3] Yet one discrepancy involving randomization of the samples in one analysis could be of more concern when interpreting those results.

The full details of each run of mass spectrometry can be visualized fully in the figure presented in the supplemental file to the Data Note.[1] The corrections to be noted concern distribution of quality control (QC) samples within the run and between batches of samples and randomization of samples in the positive ion mode, nontargeted, global metabolomics analysis.

QC Erratum 1

The methods state that QC samples were injected once every 10 samples. This was the case in the targeted lipidomics analysis, but in fact the nontargeted data had a higher frequency of QCs, roughly every sixth sample. This would actually be likely to improve the robustness of the drift correction algorithm applied later.

QC Erratum 2

The methods state that the QC was injected five times at the start and end of each run, but this was performed only on the negative-ion mode data (not reported in original article; provided in the Data Note). Furthermore, each of the reported methodologies was run as two batches, and the QCs were not injected between batches. The lack of QCs between batches may reduce the effectiveness of the drift and batch correction algorithm.

Randomization

Randomization of sample order is not mentioned in the methods, yet it is apparent from the Data Note that randomization was applied to only one of the two reported analyses (targeted lipidomics). The nontargeted, positive-ion mode data was not randomized, and so systematic error is likely to have entered the raw data. The data were run as two batches, and so metabolite drift would have to be consistent across both batches to greatly affect the subsequent analyses. Furthermore, a drift and batch correction algorithm was applied that should have reduced some of this systematic effect.

REFERENCES

(1) Luan, H.; Meng, N.; Liu, P.; Fu, J.; Chen, X.; Rao, W.; Jiang, H.; Xu, X.; Cai, Z.; Wang, J. Non-targeted metabolomics and lipidomics LC-MS data from maternal plasma of 180 healthy pregnant women. *GigaScience* **2015**, *4*, 16.

(2) Luan, H.; Meng, N.; Liu, P.; Fu, J.; Chen, X.; Rao, W.; Jiang, H.; Xu, X.; Cai, Z.; Wang, J. Non-targeted metabolomics and lipidomics LC-MS data from maternal plasma of 180 healthy pregnant women. *GigaScience Database* **2015**, http://dx.doi.org/10.5524/100108.

(3) Luan, H.; Meng, N.; Liu, P.; Feng, Q.; Lin, S.; Fu, J.; Davidson, R.; Chen, X.; Rao, W.; Chen, F.; Jiang, H.; Xu, X.; Cai, Z.; Wang, J. Pregnancy-induced metabolic phenotype variations in maternal plasma. *J. Proteome Res.* **2014**, *13* (3), 1527−1536.

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