Quantification in untargeted mass spectrometry-based metabolomics
Kloet, F.M. van der

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**Author:** Kloet, Frans van der  
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1. Binning algorithms should account for variable binsizes. (Chapter 4)

2. The most interesting data is often acquired under uncontrolled conditions. (Chapter 3)

3. High resolution mass spectrometry implies a better separation of mass peaks. Unfortunately, however, it does not simplify automatic processing of the data. (Chapter 5)

4. Visualisation of data often leads to unexpected results and new insights. (Chapter 5)

5. Results from using univariate analysis based on some modified version of the t-test tend to be fairly robust. However, the simplification ignores the fact that changes in a biological system are often multifactorial. (Zhen Zhang et al. *Cancer Proteomics*; 2283—2286, 2005.)

6. The nonlinear response generated by detector saturation cannot be compensated for by an stable isotope labeled internal standard. Therefore, matrix ion suppression/enhancement across different samples should be carefully evaluated (G. Liu et al. *Anal. Chem.* 82, 9671—9677 (2010).)

7. A mass spectrometer capable of 3 ppm mass accuracy but 2% isotopic pattern accuracy usually removes more than 95% of false candidates and outperforms even a (non-existing) mass spectrometer capable of 0.1 ppm mass accuracy but no isotopic pattern accuracy. (Tobias Kind et al. *BMC Bioinformatics* 2006, 7:234)

8. Metabolomics is downstream:—changes in the metabolome are amplified relative to changes in the transcriptome and proteome, and are arguably numerically more tractable (Kell, D. B. et al. *Nat. Rev. Microbiol.* 3, 557—65 (2005))

9. Absolute quantitation in untargeted metabolomics is a contradiction.

10. Nothing is a waste of time if you use the experience wisely. (Aguste Rodin)

11. The interpretation of its data is so complex that the true potential of metabolomics hardly ever is revealed.