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Supporting Information
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Richard A. Scheltema, Anas Kamleh, David Wildridge, Charles Ebikeme,
David G. Watson, Michael P. Barrett, Ritsert C. Jansen and Rainer Breitling

Increasing the mass accuracy of high-resolution
LC-MS data using background ions – a case study
on the LTQ-Orbitrap
Supporting Information Figure 1

**Figure 1** | Detected background ion. The graph shows all peaks (mass-over-charge value against scan number) assigning to a single background ion from an Orbitrap LTQ measurement. A window size of 2 ppm and a threshold of 18% were used for the collection of the peaks. The discrete distance between groups of mass-values can be attributed to the discrete Fourier Transform that is used for deconvoluting the signal into mass values.
Supporting Information Figure 2

Figure 2 | Use of weighted mean for mass estimation. For the mass estimation a weighted mean is calculated, which exploits the fact that the accuracy of the mass measurement decreases for less intense peaks. The top graph shows a typical mass chromatogram from the Orbitrap LTQ data, which has a retention time of 141 (most intense peak). The bottom graph shows the associated mass values. It can clearly be seen that the highly intense peaks have a mass close to the mean and show little variation. The less intense peaks in the tail of the elution profile scatter far more around the mean.
**Supporting Information Table 1**

<table>
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<th>Name</th>
<th>Mass</th>
<th>Formula</th>
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**polyethylene glycol**

(M+H)+; M='C(2n)H(4n+2)O(n+1)'

**polypropylene glycol**

(M+H)+; M='H[OCH(CH3)CH2]nOH'
## Supporting Information Table 2

Table 2 | Commonly occurring background ions for negative-mode electrospray ionization.

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<tr>
<th>Name</th>
<th>Mass</th>
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