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Supplementary Data

Improving Detection Thresholds and Robust Event Filtering in Single-Particle and Single-Cell ICP-MS Analysis

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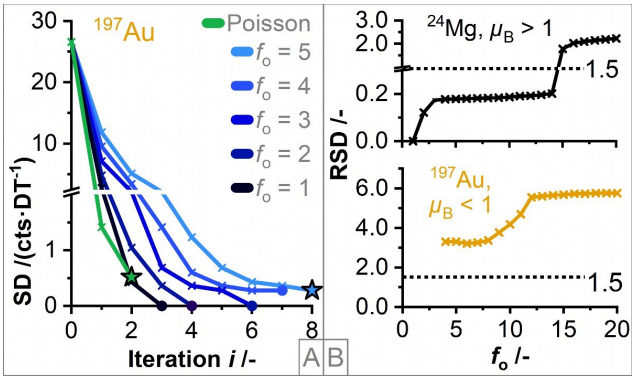

Fig. S 1. Panel A. For a data set of 50 nm AuNP (^{197}Au, DT = 1 ms), the outlier test requires a value of at least f_o = 4 to obtain a SD greater than zero. Star symbols (★) mark the final stopping point of the algorithm. Panel B shows the relative SD (RSD) depending on f_o. For the AuNP (^{197}Au, DT = 1 ms), μ_B is smaller than one which causes all observed RSD to be larger than 1.5. Data from a sample of *C. reinhardtii* (^{24}Mg, DT = 1 ms) are shown as a reference that agrees with the expectation to observe RSD > 1.5 after the transition to masking effects. For the AuNP data, no points f_o < 4 are shown because the RSD cannot be computed for μ_B = 0.

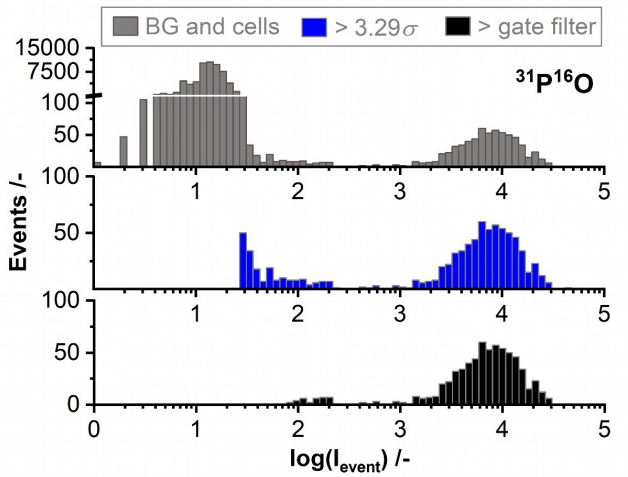

Fig. S 2. Data from a sample of *C. reinhardtii* ($^{31}P \rightarrow {}^{31}P^{16}O$, DT = 1 ms) is processed according to the modular workflow. At the top, a mixed histogram of split-corrected cell signals and uncorrected BG is shown (gray). In the middle, only the split-corrected cell events above the "$3.29\sigma_B$" criterion (Y_D) are shown (blue). At the bottom, the cell signals (black) are filtered with the secondary gate filter ($2 \cdot Y_D$), reducing the remaining false-positive BG contribution.

Table S 1. The key parameters of the improved "$f_o \cdot \sigma_B$" outlier test are shown for three samples that were chosen for the respective BG levels to exemplify the algorithm. SD and μ_B refer to the remaining BG signal after the test with the given value of f_o. The value of f_o was determined via the incrementing algorithm to guarantee SD > 0. The region with the transition to masking effects was determined with a step size of $\Delta f_o = 0.01$ and is indicated by f_{mask}. The data supplement Fig. 2, Fig. 3, and Fig. S 1.

Sample, *m*/*z*	μ_B [cts·DT^{-1}]	SD [cts·DT^{-1}]	f_o	f_{mask} transition, $\Delta f_o = 0.01$
AuNP (50 nm), ^{197}Au	0.1	0.3	5	11.19 → 11.20
S. cerevisiae, $^{31}P \rightarrow {}^{31}P^{16}O$	7.4	3.6	3	6.53 → 6.54
C. reinhardtii, ^{24}Mg	235.8	40.8	3	14.53 → 14.54