Qeios

Peer Review

Review of: "A Computer Simulation Study on Ion Optics Aiming at the Realization of Projection-Type Mass Spectrometry Imaging"

Li Ding[1]

1. Ningbo University, China

Dear Editor,

This paper presents simulation work for projection type MALDI MSI where the mass resolution may be improved by a post-extraction differential acceleration method. The manuscript describes the simulation work in great detail, and the results brought out from the work seem trustworthy. However, the results show that the PEDA operation only offers good mass resolution for a very narrow mass range (deltaM/M ~1/3 judged from figure 12) for each T_delay parameter used. If this narrow range is still practically acceptable, I think the author should explain why such an uneven mass resolution can still meet the requirements of certain applications, and any technique in imaging data acquisition or processing that may be used so that the influence of a generally poor resolution for those unfocused mass ranges can be avoided.

The paper is also lacking a conclusion on what spatial resolution, together with what mass resolution, can be obtained by the simulation using practical parameters.

Other questions regarding the manuscript:

1) Page 3, line 10. “As a result, the spatial distributions of ions immediately after their generation are retained as ion images, and the first acceleration region works properly as an electrostatic lens.”

Do you mean that the ions’ distribution at their generation is retained as an object of the electrostatic lens? Even though it is the case, the large initial kinetic energy difference of ions can still cause a large chromatic aberration of this electrostatic lens, and this should not be ignored.

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2) Page 3, last line. You mentioned that the mass range may be extended using a method developed by Guo. If so, why did this simulation not take that advantage?

3) Figure 4: it would be clearer to include a diagram of the overall workbench containing regions of both potential arrays and the space (field free?) between them.

4) Page 8, line 6 from the bottom, "$10^3 ms^{-1}$"; Page 10, line 1; Page 19, line 1 "inR∆TOF"; there might be print errors in the PDF file?

5) Page 19, line 2, "Figure 12 shows the variation inR∆TOF for the narrow mass ranges in the vicinities of 100, 400, 900, and 1600 Da when the tdelay values optimized for these masses
were applied to each mass region." Are the varying R∆TOFs for masses in one small mass range obtained using one t-delay which is optimized for the middle mass in the range, rather than each using its t-delay optimized for its respective masses in the range?

6) Figure 13: Why does one point for the initial location of 200 um exhibit much poorer z focusing, and this point seems to be at the mass (1600?) for which the t-delay is just optimized? Is this from some random calculation errors, or based on certain coincidence?

7) Page 23, I don't feel it is necessary to employ so many plots in figure 15 to prove the point of computation quality. A few sentences of explanation instead of figure 15 should be enough.

Declarations

Potential competing interests: No potential competing interests to declare.