

## Peer Review

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

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In this manuscript, the author explores the feasibility of implementing projection-type mass spectrometry imaging (MSI) using commercially available time-of-flight mass spectrometry (TOF-MS) equipment with minimal modifications. The author performed detailed ion trajectory simulations using SIMION software to assess the effectiveness of post-extraction differential acceleration (PEDA) in improving mass resolution while preserving ion image quality.

Key findings include:

1. Determination of imaging conditions for ion image formation using realistic ion source potentials and detector configurations.
2. Demonstration of PEDA's potential to enhance time-of-flight focusing, with optimization of PEDA parameters (voltage and timing) for narrow mass ranges.
3. Analysis of how PEDA impacts ion image quality, showing minimal degradation in imaging performance under optimized conditions.
4. Insights into the effect of realistic voltage waveforms on PEDA performance, suggesting broader mass range applicability compared to idealized waveforms.

The study highlights the potential of PEDA to enable projection-type MSI using modified TOF-MS systems, offering a promising avenue for advancing spatial resolution in MSI without compromising mass resolution. This work could greatly influence the development of projection-type MSI, a field still in its early stages. Therefore, I recommend this manuscript for publication. However, I suggest the authors consider the following improvements:

1. The manuscript is dense and technical, making it challenging for non-specialists to follow. Key concepts, such as the relationship between PEDA parameters and ion imaging, could be explained more clearly for broader accessibility.
2. Figures and graphs are numerous but could be better integrated into the text for clarity. Providing captions with greater explanatory detail would enhance their utility.
3. I recommend adding a dedicated paragraph that clearly introduces the PEDA methodology as proposed and developed by the Osaka group. This should be followed by another paragraph highlighting the new contributions and

advancements made in this work beyond the Osaka group's findings. This structure would help general readers gain a better understanding of the PEDa method while immediately emphasizing the novelty and significance of this paper.

4. I recommend adding a conclusion section to summarize the key findings of this paper. Additionally, this section could include a discussion on the potential applications of the simulation results in real-world instrument implementation, highlighting both the advantages and the challenges associated with integrating the proposed methodology into practical systems. This would provide a clearer perspective on the impact and feasibility of the study's outcomes.

Overall, this manuscript offers a well-executed computational study with implications for advancing MSI technology. Addressing the presentation and clarity issues would make it more accessible to a wider audience, and experimental validation would significantly strengthen its conclusions.

## **Declarations**

**Potential competing interests:** No potential competing interests to declare.