

## ***Interactive comment on “Seawater Analysis by Ambient Mass Spectrometry-Based Seaomics and Implications on Secondary Organic Aerosol Formation” by Nicolás Zabalegui et al.***

### **Anonymous Referee #2**

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This manuscript entitled “Seawater Analysis by Ambient Mass Spectrometry-Based Seaomics and Implications on Secondary Organic Aerosol Formation” by Zabalegui et al. presented a seawater “metabolomics” or “seaomics” analysis method by TM-DART-QTOF-MS. As the paper described, this method required very little sample preparation, and they were able to identify features unique to sea surface microlayer and underlying seawater. Additionally, after the untargeted chemical screening, they performed lab-to-the-field tests to look at the secondary organic aerosol potency. I appreciate they used such an experiment to add value to the untargeted chemical analysis. Based on their SOA experiment, they were able to associate certain chemical characteristics in samples with SOA formation potential. The paper presents an exciting future direction

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for organic characterization for a better understanding of how organic matter can impact atmospheric processes. The paper is well written, albeit some details were lacking.

Additionally, I am concerned about:

(1) The organic matter concentrations for the TM-DART-QTOF-MS. Marine metabolomics used solid-phase extraction not only for desalting the samples but also for further concentrating the samples. Open ocean seawater required concentrating a large volume (e.g. > 1000 x concentration factor) to perform metabolomics study. With only a concentrating factor of 6.67, they may only see a very limited class of organic compounds. If the samples were collected in high productivity waters, then 6.67 might have been fine. But, without knowing the organic carbon concentration, it is hard to assess the performance of such a method. The authors should include organic carbon concentrations if available. (2) While APCI-like ionization may be less prone to salt issues, electrospray ionization covers a large range of polar compounds representing important cell metabolites. Some of such metabolites may play important roles in SOA chemistry. I would appreciate they can further comment on this so that other scientists can make informed decisions on analytical strategies for future studies. (3) While I understand 11 features were the result of aggressive feature reduction after QA/QC, this is a rather small number for “omics”. Please see the specific comments below. I recommend publication of this manuscript in ACP after major revision and after the major concerns are addressed. Further specific comments are listed below.

Specific Comments: Line 40:  $N = 22$  is rather low. The authors discussed this in the Conclusion section, which I appreciate, but probably it should be discussed earlier.

Line 42 and lines 126 to 127: 11 species are also on the low end for untargeted. See the comments below.

Lines 78 to 80: Some of these are derived from biota, consider re-structure the sentence.

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Lines 176 to 177: Some of the particles need to be filtered. Centrifugation is usually not sufficient to remove all particulate matter. Please address this.

Line 178: "Extracted" may not be the correct word here. Based on the text, I assumed they meant removed. Extracted would make the reader think they have performed certain extraction protocols. Please rephrase.

Line 206 to 207: The repeat thawing and freezing process may affect the organic matter composition. What is the rationale for the thawing and re-freezing?

Lines 225 to 228: More details on sample extractions should be provided.

Line 345 and Figure 1: Based on the text, it reads like they extracted seawater. But in Figure 1, it looked like they extracted some kinds of solid (white cluster in the centrifuge tube). So, it is unclear to readers how they extract the samples.

Lines 226 and 345 to 363: Is a concentration factor of 6.67 enough? It might if the water samples were collected from high productivity water. Please include organic carbon concentration to justify this, if available.

Lines 365 to 405: The authors performed a large feature reduction, which is necessary to QA/QC untargeted data. However, from hundreds of total features down to 11 seems to be a bit aggressive. It would be nice to see how the PCA model changes at each step of feature reduction. In many untargeted environmental "omics" hundreds of features are typical even after substantial feature reduction. Therefore, it would be good to see a more detailed narrative and interpretations based on various levels of feature reduction.

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