

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 #1

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Zabalegui et al present an analysis of surface microlayer seawater samples collected from Cape Verde. Extracted SML samples were analyzed via DART-MS approaches to characterize organic species present. The intent of the work is to relate seawater organic composition (both in the SML and underlying water) to the production of VOC that can go on and form secondary organic aerosol. To this end, the investigators conducted a parallel experiment where secondary organic aerosol was measured following the OH oxidation of VOC formed from illuminated SML surfaces. The paper describes a new application of DART-MS to SML characterization and novel measurements of SML in the ocean. The paper is likely publishable in ACP, following the authors attention to the following general and specific comments.

C1

General Comments:

The direct link between SOA formation and seawater composition is not well established chemically. A few things might help in this discussion: 1) Describe in more detail what differentiates the SML samples that lead to SOA formation (e.g., where the collected at different times, do they have different organic/inorganic ratios, surface temperature, DMS). This begs the question why a more direct experiment wasn't done to link SML composition to SOA (like measuring the VOC). 2) Figures such as F5 and S8 are confusing. Objectively, these appear to be the same figure, but yield different conclusions regarding the relationship between PC scores and SOA formation. I think a bit more discussion is needed to guide the reader through this relationship. For example, it is not clear what to take from text such as line 374: “results suggest that SML samples that led to particle formation were 375 enriched on boron-containing organic compounds and other unidentified molecules (Table S5)” In Table S5 there appears to be a slight increase in average intensity for the peaks listed, but these are likely only a very, very small subset of all the organic compounds present.

Specific Comments:

Line 53: I would suggest removing “secondary” as these processes influence the marine aerosol of both primary and secondary nature.

Line 60: The work of Brüggemann did not prove that abiotic sources of VOCs are comparable to biological sources. This was a modeling study that scaled up laboratory experiments to the global scale.

Line 91: It would be helpful to include a short discussion here on the ionization process and the bias that it can introduce when attempting a holistic analysis. DART ionization proceeds in a very similar fashion to high pressure $\text{H}_3\text{O}^+(\text{H}_2\text{O})_n$ ion chemistry. As such, it is selective and dehydration reactions are common. It would be helpful to describe the advantages, but also the limitations when compared to ESI.

C2

Line 135: Were surface tension measurements made to more quantitatively make this comparison? Without this (or comparable information) the dilution conditions seem arbitrary? Could it also be done with IC measurements of [Cl-]?

Line 175: What was the rationale for using negative ion mode with DART? Was positive ion mode also looked at? I was under the impression that most DART analysis was done in positive mode? Again, it would be very helpful to include some discussion of the ionization process and its selectivity.

Interactive comment on Atmos. Chem. Phys. Discuss., <https://doi.org/10.5194/acp-2019-852>, 2019.