Author Comments in Response to Referee Comments 2

RC2: 'Comment on egusphere-2026-116', Anonymous Referee #2, 26 Mar 2026

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The manuscript by Yee et al. presents an impressive effort to prepare a freely available library of GC/EI-MS mass spectra of semi-volatile organic aerosol compounds, UCB-GLOBES. The background and methodology is clearly presented, and the manuscript is in general very well written.

The usability of UCB-GLOBES is illustrated by examples of source reclassification of compounds observed in ambient studies, as well as prediction of selected key properties, and comparison between aerosols from laboratory studies and ambient studies. The UCB-GLOBES database will serve as a reference for researchers in the field.

We thank Referee # 2 for their encouraging comments and feedback on our manuscript. We have addressed all comments in line following those of Referee 2 with author responses in italics and blue. All references to line numbers are associated with those in the submitted manuscript for discussion.

Specific comments:

The range of in particular temperature, but also relative humidity, in laboratory studies is quite narrow compared to ambient environmental conditions. I suggest to add a short discussion about this limitation and the potential implications.

Thank you for this comment. We agree and have addressed this in three places in the manuscript:

Line 446: "For example, mismatches in simulated relative humidity and OA loadings could be a major source of disconnect (Porter et al., 2021) as well as the relative distribution of RO_2 fate (Kenagy et al., 2024). There are also limited laboratory simulations performed with mixed precursors (Takeuchi et al., 2022) rather than a single precursor, which could allow for cross-system reactions and new SOA products not currently represented in UCB-GLOBES that may better emulate atmospheric chemistry. While UCB-GLOBES MS represent oxidation of several major biogenic precursors and biomass burning intermediates, we recognize that the laboratory simulations are by no means exhaustive of all ambient SOA precursors and OA types."

Line 507: "While the majority of UCB-GLOBES data derives from laboratory simulations, we keep in mind that such simulations do not perfectly replicate environmental conditions (e.g., temperature, relative humidity) typical of many regions in the real atmosphere, and additional physicochemical properties (e.g., aerosol phase state, seed chemistry, volume to surface area ratio, etc.) cannot be perfectly controlled/simulated as complexly as in the real atmosphere. Thus, care and general knowledge of atmospheric chemistry must be taken in interpreting the applicability of mass spectral matches to real-world conditions."

We have also provided specific recommendations at the end of the Conclusions in address of Referee Comment #3, Line 516: "…we would benefit from technical advancements to conduct and catalogue organic species in atmospheric laboratory simulations that are closer to atmospheric conditions with higher relative humidities (> 75 % RH), lower organic aerosol mass loadings, and lower concentrations of precursors and oxidants. We also recommend new datasets simulating oxidation of a mixture of VOC precursors and their oxidation intermediates, as cross-VOC system reactions as would happen in the atmosphere are not sufficiently represented in UCB-GLOBES yet. Inherent to these recommendations are challenges to technical feasibility, ensuring experiments are at sufficient concentrations for detection, and trade-offs of adding too many variables to the experimental matrix. However, achievements toward these recommendations could provide some of the keys to elucidating the true mechanisms and chemical complexity in ambient observations."

Thermal desorption of aerosol samples is widely used but may fragment some compounds. Can the authors comment on potential implications regarding the database and its future applicability?

We appreciate this perspective and how it relates to interpretation and applicability of the UCB-GLOBES database. Thermal desorption of aerosol samples is conducted in our TD-GCxGC analysis from 50-320°C at a rate of 25°C/min (i.e. ~11 mins desorption time), with the goal of slowly volatilizing non-labile analytes into the GCxGC. Through testing of authentic standards, we are aware that certain compound types are not amenable to this analysis (whether through thermal treatment and/or not being amenable to our GC method). For example, organosulfates and organonitrates are not resolved in our analyses. However, there can certainly be larger compounds (e.g., oligomers) that may thermally fragment and be seen in their monomer form. In these cases, while the monomer form is the actual analyte observed in our TD-GCxGC analysis and rather than the nascent aerosol compound, it can still serve as a useful indicator of a particular source and/or mechanism. That is, the same nascent thermally labile aerosol compound present in multiple UCB-GLOBES datasets would be expected to appear as the same fragmented analyte in all

chromatograms being catalogued in UCB-GLOBES. That being said, we have previously resolved intact isoprene hemiacetal dimer with MS shown in Fig. S1D (Surratt et al., 2010) *as well as phenolic dimers of phenol, guaiacol, and syringol, suggesting that all or some fraction of dimer compounds survive the analysis.*

Minor comments:

Line 116: An ending parenthesis is missing at the end of the sentence.

*Thank you. This has been revised by deleting the opening parenthesis and using a comma instead, "…*Kováts chromatographic retention index, a proxy for elution time of compounds relative to a standard series such as n-alkanes that can be compared across instruments (Kováts, 1958)."

Page 17 (Line 330-) I suggest to divide the paragraph into 2-3 shorter paragraphs to improve readability.

Thank you, we have divided this into another paragraph beginning with, "Using UCB-GLOBES…"

References Cited

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