Atmos. Chem. Phys. Discuss.,
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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Evaluating the mutagenic potential of aerosol organic compounds using informatics based screening" *by* Stefano Decesari et al.

Anonymous Referee #2

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The authors present a proof of concept study for the evaluation of the mutagenic potential of species in secondary organic aerosol. By screening 104 different compounds for mutagenicity potential using in silico toxicological predictions, the authors were able to suggest groups of compounds as well as specific molecules which should undergo toxicological screening in the future. This methodology could lead to a more focused approach when investigating the health impacts of different types of SOA by relating SOA composition to potential health impacts. This is an interesting manuscript which is generally well written and should be published after some revisions.

Comments: - Have the compounds which were tested previously been measured in

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Discussion paper

atmospheric SOA, and if they have at what concentrations and which types of SOA (e.g. anthropogenic, biogenic, etc)? If they haven't been specifically measured can the authors give a rough estimation of the concentrations that could be expected in different types of SOA? Is there a trend of more of the toxic compounds being likely to be present in a specific type of SOA?

- Are the concentrations which would be expected in the respiratory tract upon inhalation of atmospheric SOA similar to the concentrations used during the Ames test and assumed in the models? When both positive and negative Ames tests results are reported due to testing conditions (Page 7, Line 2) are there any trends that have been observed for the range of results (e.g. a dependence on concentration, or a different experimental condition) and could some of the experimental results be discarded due to those conditions being unlikely to occur in the respiratory tract/ human body after inhalation?

- Are there any limitations to the two models used (the ACD/Impurity Profiling model and the Vega/CAESER model), for example, can they reliably predict the toxicity of any compound? What are the differences between them which leads to one giving a positive result whilst the other gives a negative result in some cases (as shown in Table 2)?

Minor comments:

- Introduction line 24: Did the author mean nearly three million deaths per year (rather than billion)? This should also include a reference.

- There are a lot of abbreviations throughout the text which should be written out in full for clarity (e.g. PaDEL, nHBDon, nHBAcc, KNIME).

- Section 2 should be renamed from 'Introduction' to 'Methods'.

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