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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Technical Note: Development of chemoinformatic tools to enumerate functional groups in molecules for organic aerosol characterization" *by* G. Ruggeri and S. Takahama

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We thank both reviewers for their extremely useful comments. Based on a general consensus that the focus of the Technical Note should be on the novelty of the tool itself and less on the example applications, we have made a few general changes:

- Methods (Section 2.1) describing the SMARTS pattern development is expounded

- Example Applications (Section 3.2) is made much more concise
- Conclusion (Section 4) is modified to summarize the chemoinformatic tools, more than interpretation from the specific applications presented

We address specific comments to the reviewer below:

1. **Comment** P. 33642: Usually one uses the term low-NOx reaction to mean that organic peroxy radicals have reacted with HO2 or other RO2 radicals, or perhaps by autooxidation. If an organic nitrate contributes 26% of the gas-phase mass of products then this does not seem to qualify. The authors should make clear what they mean by low-NOx

   Response We have omitted the definition of low NO_x in the manuscript and just specified that the α-pinene simulation was carried in the presence of NO_x (initial ratio α-pinene/NO_x is 1.25). In line 25, page 33638 we modified the sentence as follows:

   "Furthermore, the gas phase composition generated by α-pinene photooxidation in the presence of NO_x (α-pinene/NO_x ratio of 1.25), with propene as a radical initiator, was simulated using the Kinetic Pre-Processor (KPP, Damian et al., 2002; Sandu and Sander, 2006; Henderson, 2016) incorporating mechanistic information taken from MCMv3.2."

2. **Comment** My understanding is that the present classification method does not separate positional isomers. Is this correct?

   Response Yes this is the case for most of the chemoinformatic patterns described in this manuscript. Only in the case of conjugated aldehyde ketone and ester with an alkene or a benzene ring the relative position of these two functional

ACPD
15, C12880–C12884, 2016

groups is specifically described by the SMARTS pattern (Substructures 40-48). We have therefore added a statement in section 2.1:

"Positional arguments can be included by querying specific structural information from the internal representations of molecular graphs according to implementations in various software packages, or formulating SMARTS patterns which require specificity in the arrangement of neighboring atoms (Barley et al., 2011; Topping et al., 2016). In this work, positional information of FGs are used only for conjugated aldehyde, ketone, and ester with an alkene or benzene ring (Table 1, substructures 40-48)."

3. **Comment** P. 33643: In the Conclusions it would be useful to summarize the value of this approach and clarify its advantages over getting this information other ways.

   Response We have restructured the conclusion in order to give more importance to the chemoinformatic patterns developed than to the example application. In this way we hope to better convey the importance of the validation of the chemoinformatic patterns described in the manuscript. The Conclusion (Section 4) has been modified as follows:

   "We introduced the application of chemoinformatic tools that allow us to perform substructure matching in molecules to enumerate FGs present in compounds relevant for organic aerosol chemistry. We developed 50+ substructure patterns and validated them over a list of 125 compounds that were selected in order to account for all the functional groups (FGs) represented. We demonstrate how these tools can facilitate intercomparisons between GC-MS and FTIR measurements, and mapping of compounds onto the VBS space described by pure component vapor pressure and oxidation state.

   "We further introduce a novel approach for defining a set of patterns which accounts for each atom in a chemical system once and only once (except for poly-

ACPD

15, C12880–C12884, 2016

functional carbon atoms associated with multiple FGs); this condition is confirmed by an atomic-level validation scheme applied to chemically explicit α-pinene and 1,3,5-TMB degradation mechanisms. This validation scheme provides an intermediate resolution between molecular speciation and atomic composition, and permits apportionment of conventionally aggregated quantities such as O:C, H:C, and N:C to contributions from individual FGs. We illustrate its application to the photochemical degradation of α-pinene from speciated simulations using MCMv3.2."

References

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Please also note the supplement to this comment:
http://www.atmos-chem-phys-discuss.net/15/C12880/2016/acpd-15-C12880-2016-

ACPD

15, C12880–C12884, 2016

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ACPD

15, C12880–C12884, 2016