

## ***Interactive comment on “Identification of particulate organosulfates in three megacities at the middle and lower reaches of the Yangtze River” by X. K. Wang et al.***

**Anonymous Referee #4**

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General comments:

I feel that the manuscript is not suitable for publication in its current form for a number of reasons. My first concern is lack of chromatograms and mass spectra in the manuscript or supporting information. I understand that showing a large number of extracted ion chromatograms is not practical. However, the authors need to show at least chromatograms from major peaks in the main manuscript or supporting information. The authors can discuss about the differences in organosulfates at different locations directly using chromatograms. That is far more effective than descriptive texts. Second, the authors discuss about seasonal and diurnal variations from extremely small

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sets of data. While the authors can discuss about the differences in these sampling days, they should not be discussed as seasonal or diurnal patterns. Third, I find the manuscript extremely difficult to follow. It is extremely densely written. The authors should seek a language editing service to make sure that the manuscript can be read smoothly.

Technical comments:

Page 21419 line 13 onwards: The authors should also address Kahnt et al (2015) here.

Kahnt, A., Behrouzi, S., Vermeylen, R., Shalamzari, M. S., Vercauteren, J., Roekens, E., Claeys, M., and Maenhaut, W.: One-year study of nitro-organic compounds and their relation to wood burning in PM<sub>10</sub> aerosol from a rural site in Belgium, *Atmos. Environ.*, 81, 561–568, Doi 10.1016/J.Atmosenv.2013.09.041, 2013.

Page 21420 line 10: Do the authors mean ‘OS’ measurements instead of identification? I am not aware of a study dealing with OS identification from Shanghai aerosols.

Page 21421 line 4: Do the authors mean 24 h samples? Daily samples mean a sampling was performed every day. I can only find two 24 h samples in the Table 1.

Page 21422 line 11: ‘Th’ and ‘m/z’ are used simultaneously. Both are a unit of mass-to-charge ratio, and it is redundant here. I recommend using ‘m/z’ as recommended by IUPAC.

Page 21423 line 1 and throughout the manuscript: A term ‘identification’ should be reserved for a compound that is positively identified from the comparison to an authentic standard compound. ‘Pseudo-molecular ion’ should be ‘quasi-molecular ion’.

Page 21423 line 16: The authors claim the detection of about 200 organosulfates from the UHPLC/(–)ESI-MS analysis but I am a little skeptical if these compounds eluted from the column as peaks. The authors must show more extracted ion chromatograms in the main manuscript and supporting information. In supporting information, the authors show only four extracted ion chromatograms for an m/z value range between m/z

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351.1849 and  $m/z$  351.1853 without showing their mass spectra. From the description of the data processing, the authors did not seem to consider an isotope distribution of a detected compound, and relied solely on the ratio of H/C, O/C, N/C, S/C, and DBE. The authors should show corresponding mass spectra to assure readers that the compounds shown here are indeed organosulfates.

Pages 21422-21423: In connection to the previous concern, how did the authors calibrate  $m/z$  values? Have the authors used a lock mass function or were they calibrated externally? This should be clearly stated in the manuscript.

Figure S1 in supporting information: Figure S1 should show the intensity of the peak.

Page 21425 line 10: How do the authors know that they are all nitrooxy-organosulfates? They are other structures that can contain nitrogen such as heterocyclic compounds, nitrophenolic compounds, etc.

Figure 2. The authors should caution the readers that these are a number of isomers separated by the authors' method. For example, the  $C_{10}H_{17}O_7N_1S_1$  compounds show only three isomers for a certain method but it can be separated into six isomers when the method is further optimized.

Page 21426 line 27-29 and throughout manuscript: Is it a nitrate group or nitrooxy group? How do the authors know without MSn experiments?

Page 21427: The authors cannot discuss seasonal differences from such a limited number of samples.

Page 21429 onwards about KD and VK diagrams: I find this section very difficult to read and get information out of it. I recommend the authors summarizing most important information here instead of describing every single detail about the diagrams.

Page 21432: These isoprene originating organosulfates tend to elute very early in the chromatogram, and their MS intensities can be potentially influenced by co-eluting compounds in this region (ion suppression). How have the authors corrected for this?

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If not, how do the authors know that they are not affected by the ion suppression?

Page 21433 onwards: Seasonal and diurnal variations cannot be discussed when the number of sampling day is so limited even they are similar to average seasonal conditions.

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Interactive comment on Atmos. Chem. Phys. Discuss., 15, 21415, 2015.