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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 #1

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Unfortunately I failed to find any recommendations on not considering phosphorous for molecular formulae assignment in Wozniak et al paper. The authors did consider this element and eliminated all molecular formulas containing phosphorous from the final list of formulae as they found them insignificant in their environment (and those environments considered by Wozniak et al references). As emphasised in my previous comment, this may not be the case for Yangtze river environment.

Moreover, neither Fuller et al nor Wozniak et al (referenced paper in this section) provide any recommendation for not considering isotopic patterns. For molecular formulae assignment procedure, I strongly recommend considering isotopic pattern/ratio section

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of the highly cited work by Kind and Fiehn (2007) and references therein, which strongly emphasise the importance of this step for accurate molecular formulae assignment.

Reference:

Kind T, Fiehn O. Seven Golden Rules for heuristic filtering of molecular formulas obtained by accurate mass spectrometry. BMC Bioinformatics. (2007) Mar 27, 8:105.

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

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