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Discussions

Interactive comment on "Distinguishing molecular characteristics of aerosol water soluble organic matter from the 2011 trans-North Atlantic US GEOTRACES cruise" *by* A. S. Wozniak et al.

Anonymous Referee #3

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The chemical composition of WSOM is essential for tracking their sources and transformations in the atmosphere as well as assessing their environmental outcomes. In this manuscript, the authors employed a state-of-art ultra high resolution mass spectrometer for molecular level characterization of WSOM samples collected during the research cruise from North America to North Africa. Both the samples and data are valuable and rare, as considering the fact that recently there are only few studies on the detailed chemical composition of WSOM on marine aerosols. The authors also successfully applied the statistic method (PCA) on classifying and distinguishing the sources of WSOM based on the identified molecular formulas. The results and inter-

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pretations are reasonable. I recommend the publication of this manuscript after the authors addressing the following questions:

1. Page 10, line 1: the authors used naturally occurring fatty acids as the internal standards for calibrating the mass accuracy, which can dramatically increase the number of unambiguously identified formulas within WSOM samples. However, in the paper they cited (S and H, 2008), there is no detailed information about how to perform this calibration. Moreover, the studies of S and H are mainly focused on aquatic NOM samples, which might possess different chemical natures with the aerosol samples. I would encourage the authors providing more detailed information about this internal calibration in the supplementary material. For example, what kind of fatty acids were chosen as the internal calibrator? What are the criteria regulating their naturally occurring? How to re-correct the mass errors of other compounds by using the mass errors of the internal standards? I believe that the detailed description on this re-calibration method is very helpful in improving UHRMS data processing in atmospheric chemistry society and will make this paper highly cited in future. 2. Page 10, line 11: O/C $\leq$ 1.2 as one of the constraints of formula assignments. This may works well in aquatic NOM. However, in recent years, atmospheric scientists focusing on chamber studies of secondary organic aerosols do find some organic compounds with O/C greater than 1.2. Will the authors' dataset be changed if this constraint is extended to a larger value (e.g. O/C $\leq$ 3.0)?

Interactive comment on Atmos. Chem. Phys. Discuss., 14, 6427, 2014.