Supplement of Atmos. Chem. Phys., 14, 10299–10314, 2014
http://www.atmos-chem-phys.net/14/10299/2014/
doi:10.5194/acp-14-10299-2014-supplement

Atmospheric Chemistry and Physics Open Access

Supplement of

A molecular-level approach for characterizing water-insoluble components of ambient organic aerosol particulates using ultrahigh-resolution mass spectrometry

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Supplementary Table 1. Percent area contributions from the major proton regions in the ^{1}H NMR spectra for the PSOM aerosol extracts.

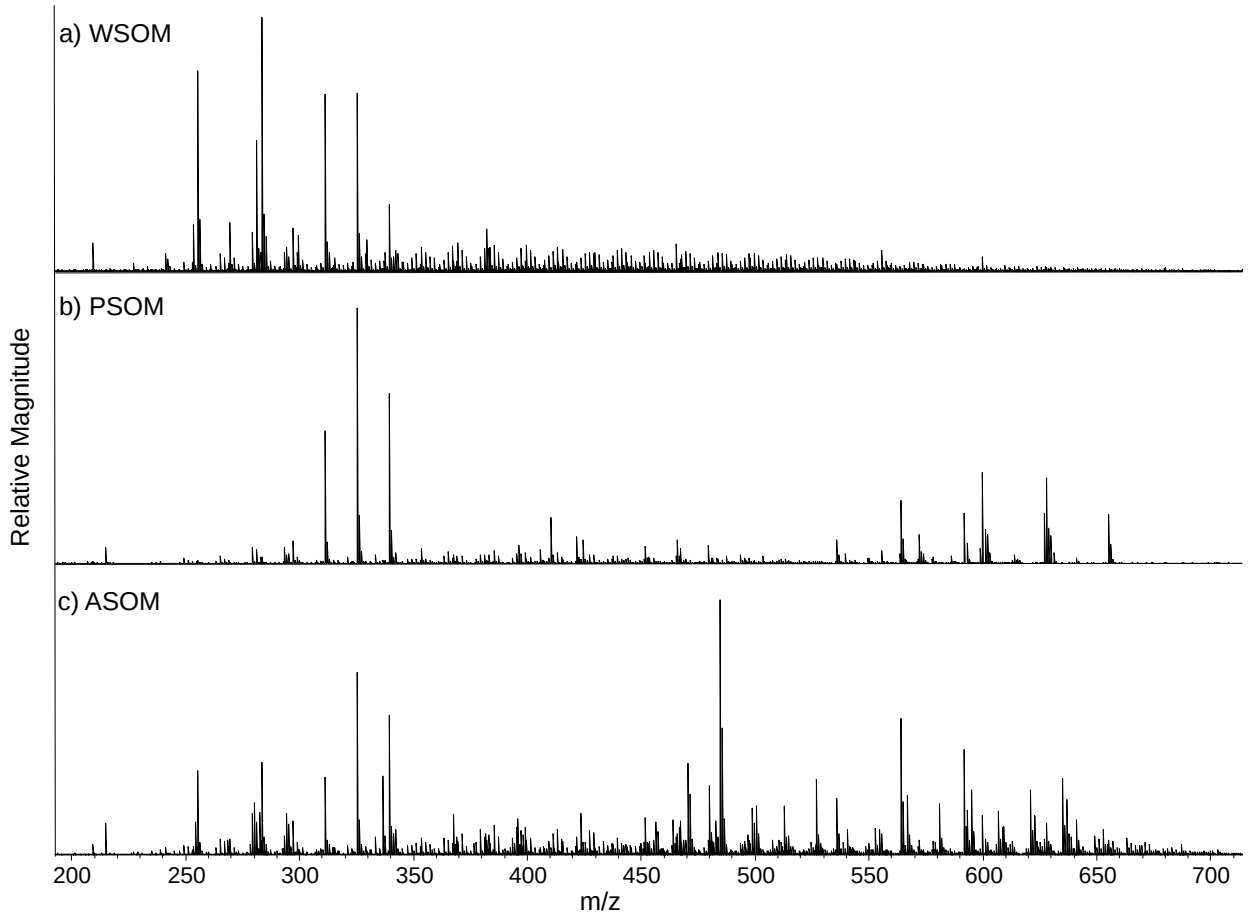
		% ^{1}H NMR spectral area		
Functional Group Region	**Chemical Shift (ppm)**	**16-17 August 2011**	**24-25 June 2013**	**25-26 June 2013**
H-C-O	0.7 – 1.95	2.5	2.5	6.4
H-C-C=	1.95 – 3.2	18.3	21.0	25.5
H-C	3.2 – 4.4	78.8	76.0	67.0
Calculated H/C		*1.98*	*1.98*	*1.94*

Supplementary Table 2. Percent OC extraction for PSOM extracts using ^{1}H NMR and WSOM using TOC analysis.

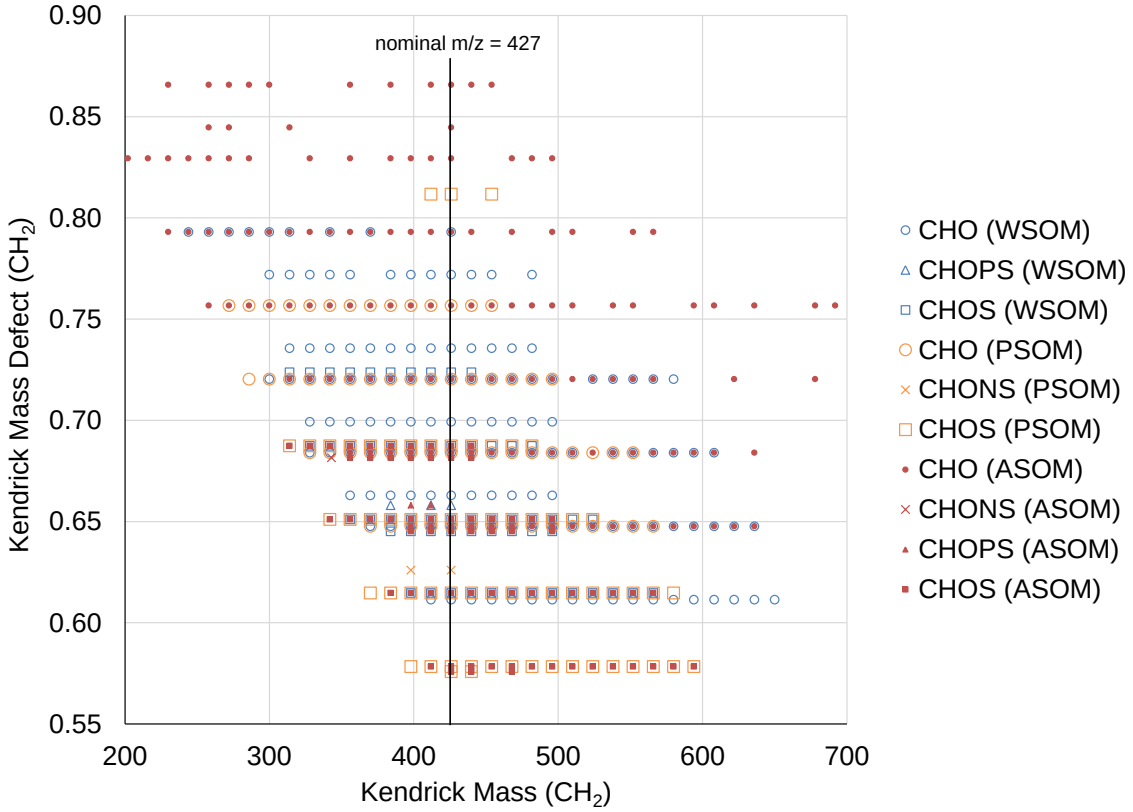
Aerosol Sample	Initial OC mass (mg)	Spectral Area (intensity units)	**Calc DOC (mg)	%PSOC	%WSOC (by TOC)
16-17 August 2011	*0.045	2.4×10^{10}	0.041	90.3	37.0 ± 2.2
24-25 June 2013	0.039	1.1×10^{10}	0.021	53.8	54.3 ± 3.8
25-26 June 2013	0.049	9.1×10^{9}	0.018	36.5	60.3 ± 3.6
Glucose	0.114	2.5×10^{9}	-	-	-

*There is a known error in the initial mass measurement of this aerosol, and was omitted from the results

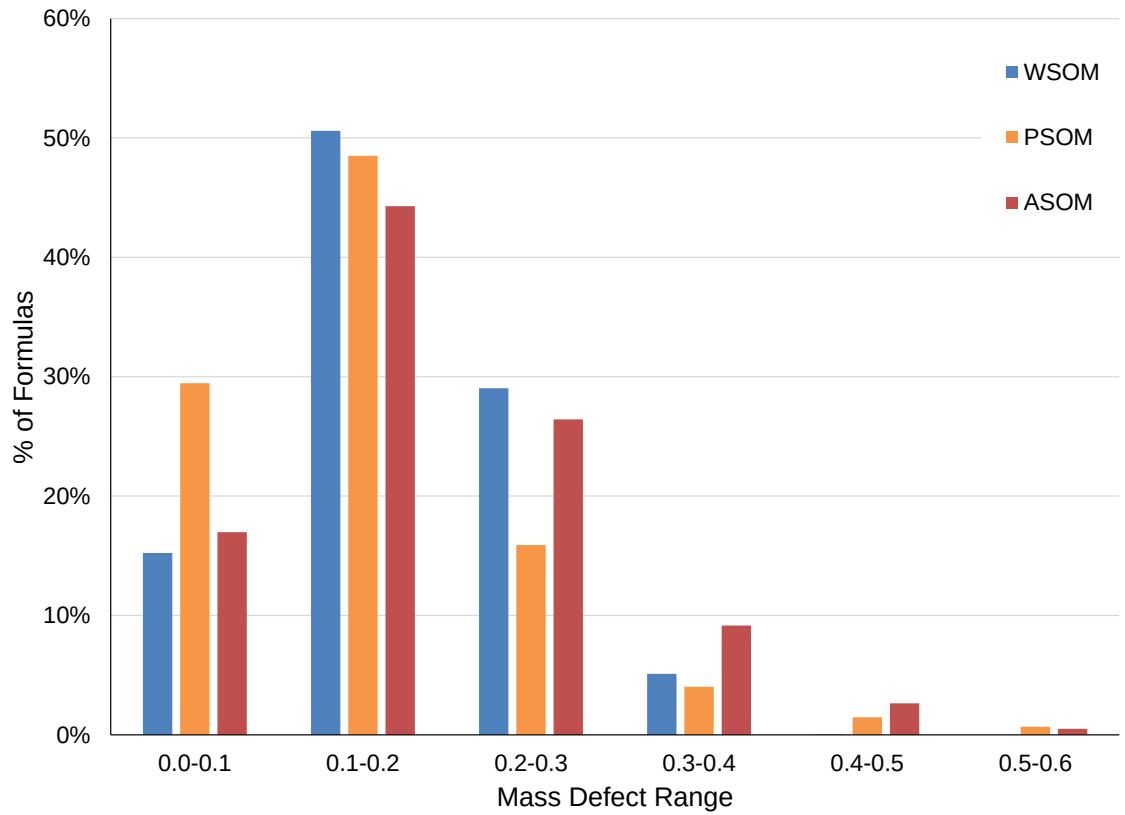
**Calculated by multiplying the spectral area by the glucose response factor (2.6×10^{11} intensity units/mg H), and then converting mg H to mg C using the H/C ratio calculated in Supplementary Table 1.



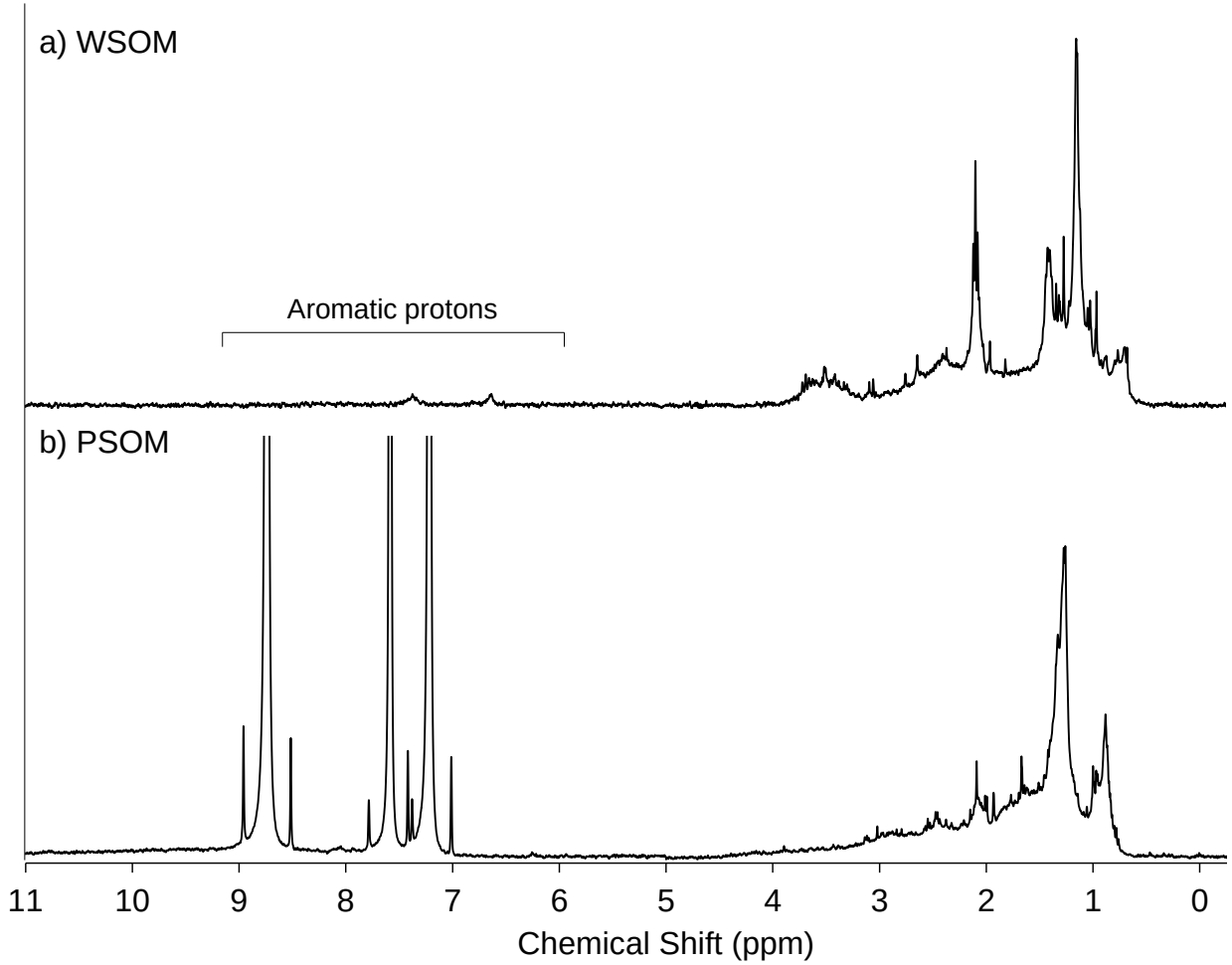
Supplemental Figure 1. A representative full FTICR mass spectrum for each a) WSOM, b) PSOM, and c) ASOM.



Supplemental Figure 2. Kendrick mass defect (CH_2) plot for formulas identified at m/z=427 in Figure 2 of the manuscript. The different colors represent the different solvents, and the different shapes represent different formula types. A vertical line identifies the formulas at m/z=427 in Figure 2 of the manuscript.



Supplemental Figure 3. The percentage of molecular formulas sorted by measured mass defect (the decimal value of the measured m/z) for each of the solvents.



Supplemental Figure 4. Full ^{1}H NMR spectra for a) WSOM and b) PSOM for the aerosol particulate sample collected 25-26 June 2013. The strong signal (off scale) in the PSOM spectra in the aromatic region is from protons that have been exchanged in the pyridine-D_5 solvent, which overwhelms any possible aromatic signal from the sample.