

Supplementary material

Identification of water-soluble organic carbon in nonurban aerosols using ultrahigh-resolution FT-ICR mass spectrometry: organic anions

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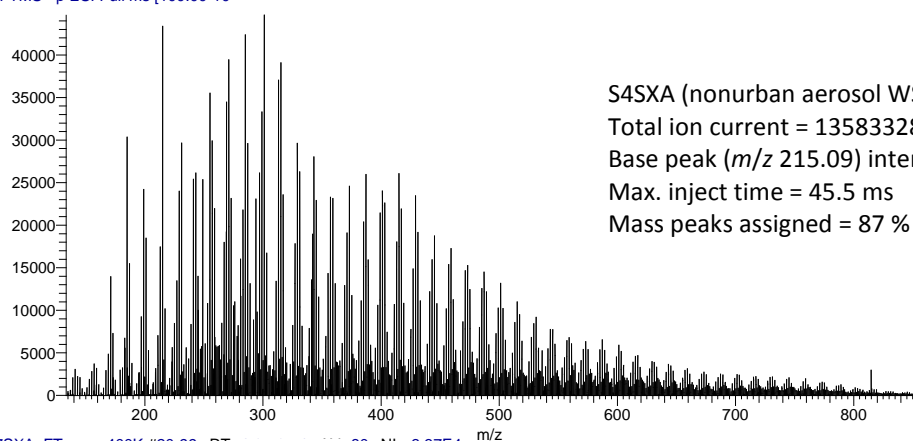
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A complete list of the assigned molecular formulas is provided via in Table S1, available as a separate Microsoft Excel 2007 workbook ('EN11167_TS1.xls'). A description of the provided data is as follows: column 'A' lists the averaged S4SXA negative ion mass-to-charge ratio (m/z) measured and internally recalibrated as described in the methods section; column 'B' lists the calculated neutral masses (Da) assuming the loss of 1 H for each identified m/z ; column 'C' lists the averaged S4SXA relative abundance (%; note relative abundances are relative to the base peak = 100 %) for each identified m/z ; column 'D' lists the averaged S4SXA absolute error (ppm) associated with each formula assignment; column 'E' indicates if the molecular formula and measured m/z were used in the internal recalibration procedure; column 'F' indicates if the molecular formula and measured m/z were detected in blank analyses and provides the blank relative abundance (%; base peak = m/z 564.2828); column 'G' lists the calculated double bond equivalents values for each identified m/z ; column 'H' lists the group assignments (based on the elemental composition); column 'I' lists the subgroup assignments; column 'J' provides the assigned molecular formula for each m/z ; column 'K' lists the number of carbon atoms in the assigned formula; column 'L' lists the number of hydrogen atoms in the assigned formula; column 'M' lists the number of nitrogen atoms in the assigned formula; column 'N' lists the number of oxygen atoms in the assigned formula; column 'O' lists the number of sulfur atoms in the assigned formula; column 'P' lists the S4SXA measured negative ion m/z measured and internally recalibrated as described in the methods section; column 'O' lists the S4SXA relative abundance (%) for each identified m/z ; column 'R' lists the S4SXA absolute error (ppm) associated with each formula assignment; column 'S' lists the S4SXAR1 (R1 indicates replicate measurement 1) measured negative ion m/z measured and internally recalibrated as described in the methods section; column 'T' lists the S4SXAR1 relative abundance (%) for each identified m/z ; column 'U' lists the S4SXAR1 absolute error (ppm) associated with each formula assignment; column 'V' lists the

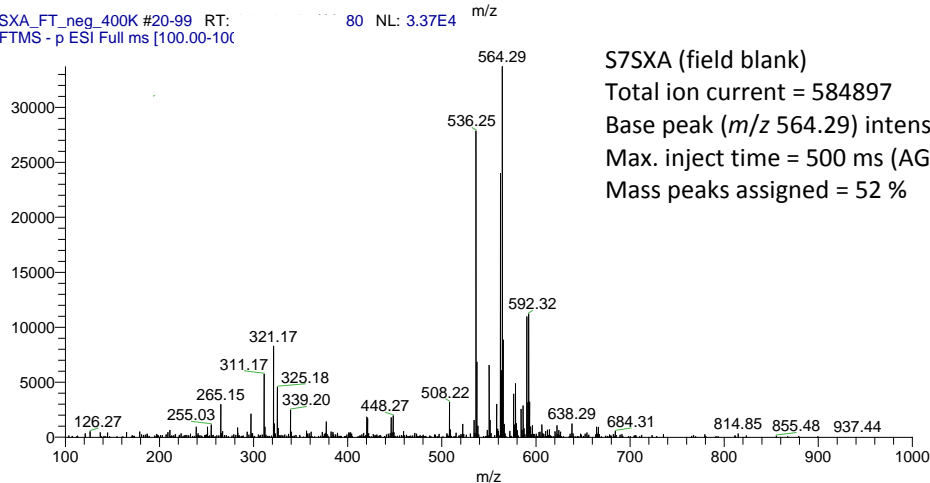
S4SXAR2 (R2 indicates replicate measurement 2) measured negative ion m/z measured and internally recalibrated as described in the methods section; column 'W' lists the S4SXAR2 relative abundance (%) for each identified m/z ; column 'X' lists the S4SXAR2 absolute error (ppm) associated with each formula assignment; column 'Y' lists the S4SXAR3 (R3 indicates replicate measurement 3) measured negative ion m/z measured and internally recalibrated as described in the methods section; column 'Z' lists the S4SXAR3 relative abundance (%) for each identified m/z ; column 'AA' lists the S4SXAR3 absolute error (ppm) associated with each formula assignment; column 'AB' lists the S4SXAR4 (R4 indicates replicate measurement 4) measured negative ion m/z measured and internally recalibrated as described in the methods section; column 'AC' lists the S4SXAR4 relative abundance (%) for each identified m/z ; column 'AD' lists the S4SXAR4 absolute error (ppm) associated with each formula assignment; column 'AE' indicates if the identified formula was matched to the α -pinene/O₃ SOA molecular formulas presented in Putman et al.^[1]; column 'AF' indicates if the identified formula was matched to the limonene/O₃ SOA molecular formulas presented in Kundu et al.^[2]; column 'AG' indicates if the identified formula was matched to the caryophyllene/O₃ SOA molecular formulas identified by L. R. Mazzoleni, S. Kundu, R. Fisseha, A. L. Putman, T. A. Rahn (unpubl. data); column 'AH' indicates if the identified formula was matched to the α -pinene/O₃ SOA molecular formulas identified by Mazzoleni et al.(unpubl. data) column 'AI' indicates if the identified formula was matched to the β -pinene/O₃ SOA molecular formulas identified by Mazzoleni et al. (unpubl. data), and column 'AJ' indicates all other matches including those from Chan et al.,^[3] Laskin et al.,^[4] Nozière et al.^[5] and Surratt et al.^[6]

S4SXA_FT_neg_400K_rep #33-204
T: FTMS - p ESI Full ms [100.00-10



S4SXA (nonurban aerosol WSOC sample)
Total ion current = 13583328
Base peak (m/z 215.09) intensity = 47709
Max. inject time = 45.5 ms
Mass peaks assigned = 87 %

S7SXA_FT_neg_400K #20-99 RT:
T: FTMS - p ESI Full ms [100.00-100



S7SXA (field blank)
Total ion current = 584897
Base peak (m/z 564.29) intensity = 35794
Max. inject time = 500 ms (AGC timed out)
Mass peaks assigned = 52 %

Fig. S1. The average mass spectra for the sample (S4SXA) and the field blank without any post-processing. See also Fig. 1 in the main paper.

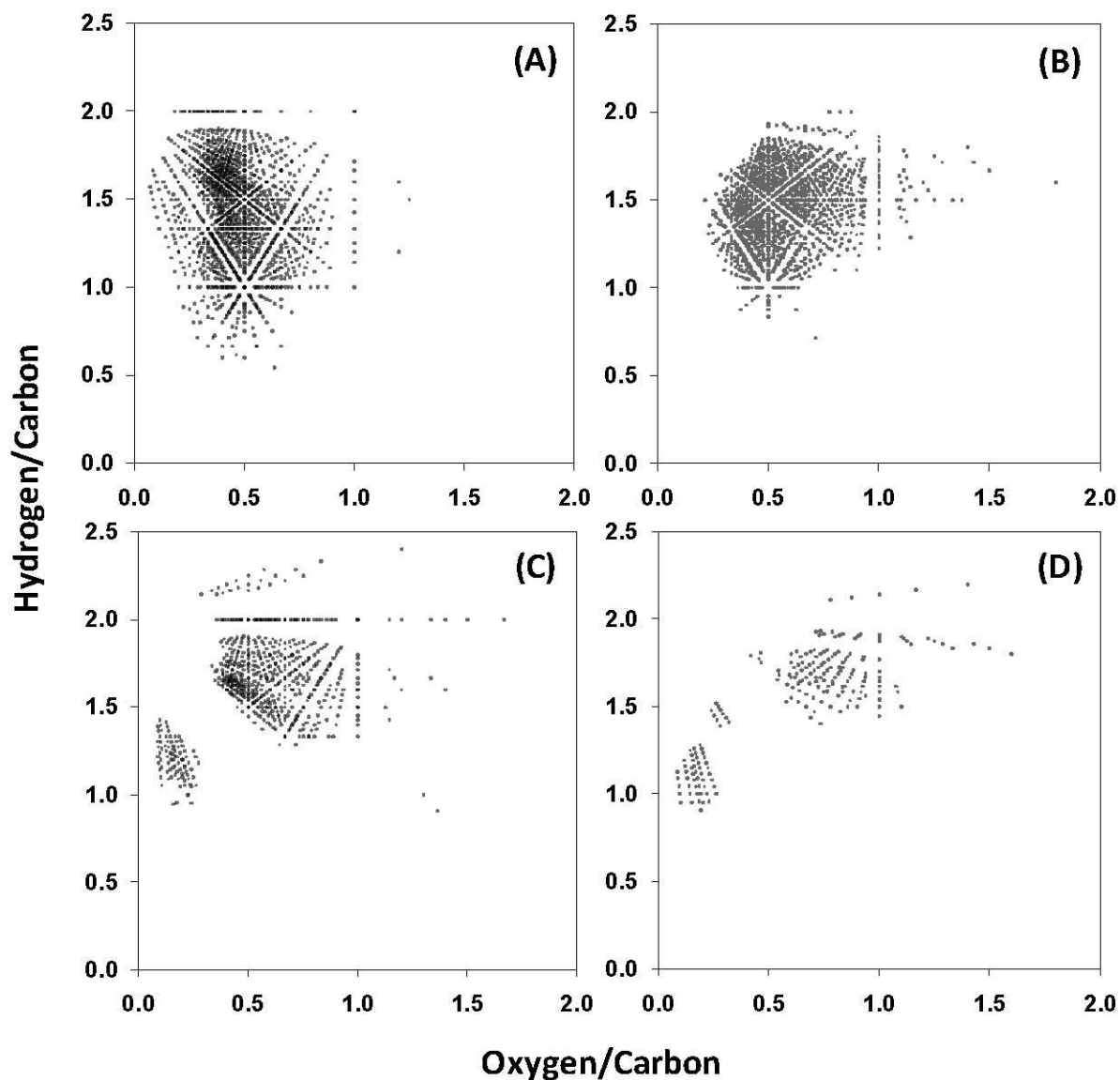


Fig. S2. Elemental ratio plots: (A) 1506 compounds containing only C, H and O atoms; (B) 1385 compounds containing only C, H, N and O atoms; (C) 641 compounds containing only C, H, O and S atoms and (D) 205 compounds containing C, H, N, O and S atoms. See also Fig. 2 in the main paper for the isoabundance elemental ratio plots.

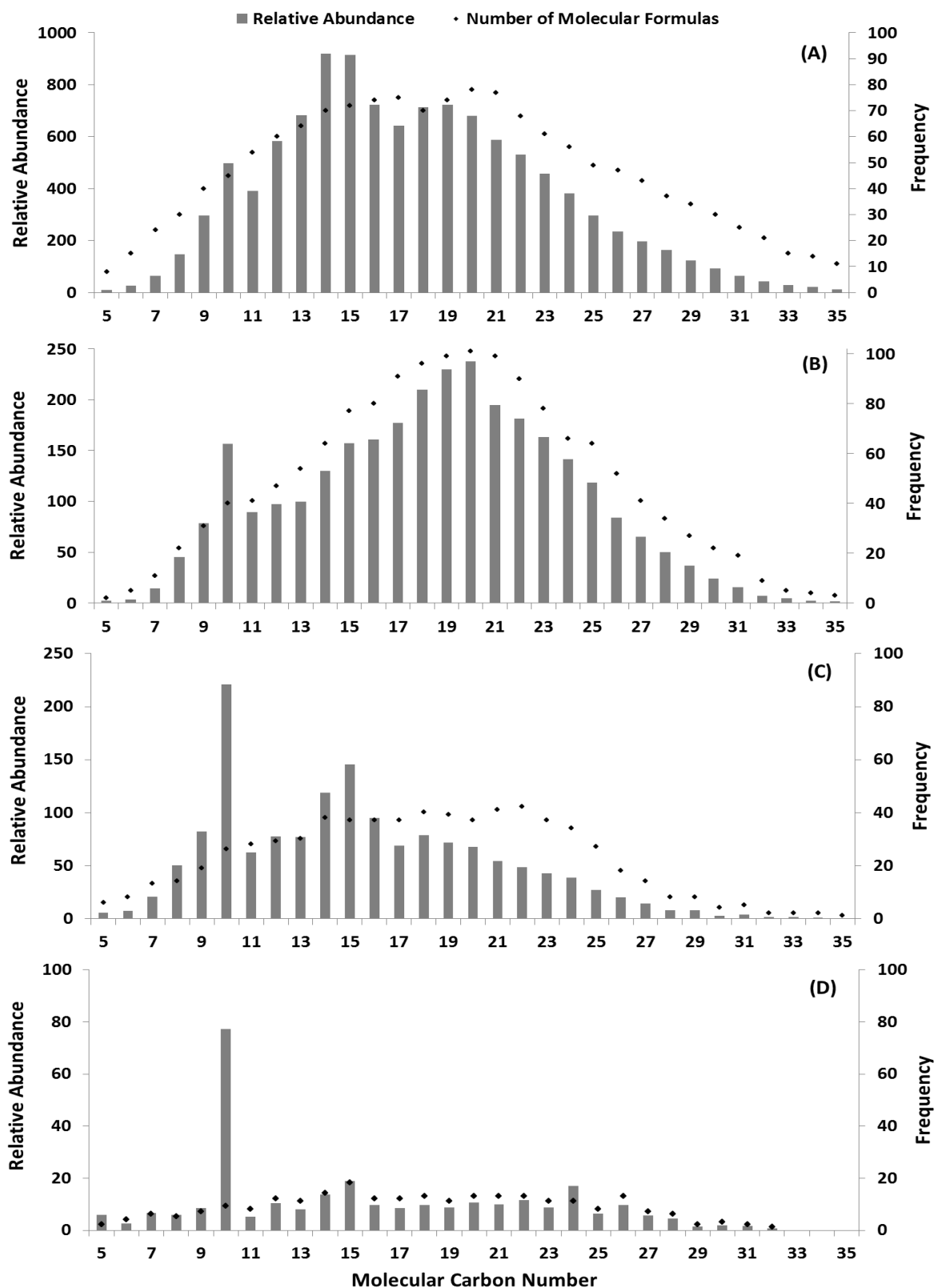


Fig. S3. Relative abundance for each elemental groups with respect to the number of carbon atoms identified in the molecular formulas: (A) 1506 compounds containing only C, H and O atoms; (B) 1385 compounds containing only C, H, N and O atoms; (C) 641 compounds containing only C, H, O and S atoms; and (D) 205 compounds containing C, H, N, O and S atoms.

References

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