



Thompson, S. L., Yatavelli, R. L. N., Stark, H., Kimmel, J. R., Krechmer, J. E., Day, D. A., ... Jimenez, J. L. (2017). Field intercomparison of the gas/particle partitioning of oxygenated organics during the Southern Oxidant and Aerosol Study (SOAS) in 2013. *Aerosol Science and Technology*, 51(1), 30-56. <https://doi.org/10.1080/02786826.2016.1254719>

Peer reviewed version

Link to published version (if available):
[10.1080/02786826.2016.1254719](https://doi.org/10.1080/02786826.2016.1254719)

[Link to publication record in Explore Bristol Research](#)
PDF-document

This is the author accepted manuscript (AAM). The final published version (version of record) is available online via Taylor & Francis at <http://www.tandfonline.com/doi/full/10.1080/02786826.2016.1254719>. Please refer to any applicable terms of use of the publisher.

University of Bristol - Explore Bristol Research

General rights

This document is made available in accordance with publisher policies. Please cite only the published version using the reference above. Full terms of use are available:
<http://www.bristol.ac.uk/pure/about/ebr-terms>

Supplementary Information for**Field intercomparison of the gas/particle partitioning of oxygenated organics during the Southern Oxidant and Aerosol Study (SOAS)**

Samantha L. Thompson¹, Reddy L. N. Yatawelli^{1,§}, Harald Stark^{1,2}, Joel R. Kimmel^{2,7}, Jordan Krechmer¹, Douglas A. Day¹, Gabriel Isaacman⁴, Allen H. Goldstein^{4,5}, Anwar Khan⁶, Rupert Holzinger⁶, Felipe D. Lopez-Hilfiker³, Claudia Mohr^{3,§}, Joel A. Thornton³, John T. Jayne², Douglas R. Worsnop², Jose L. Jimenez^{1*}

¹Dept. of Chemistry and Biochemistry, and Cooperative Institute for Research in the Environmental Sciences (CIRES), University of Colorado, Boulder ² Aerodyne Research Inc. ³ Department of Atmospheric Sciences, University of Washington, Seattle ⁴ Department of Environmental Sciences, Policy and Management, University of California, Berkeley ⁵ Department of Civil and Environmental Engineering, University of California, Berkeley ⁶ Institute for Marine and Atmospheric Research Utrecht ⁷ Tofwerk AG, Thun, Switzerland

[§]now at Division of Atmospheric Sciences, Desert Research Institute, Reno, NV, 89512 USA

[§] now at Karlsruhe Institute of Technology (KIT)

*correspondence to J.L. Jimenez, jose.jimenez@colorado.edu

Table S1. Summary of Instruments. Table summarizing each instrument, what technique is used to separate gas/particle phase and ionize and detect analyte, and what class of compounds it detects. (see text for more detailed information on each of these).

Instrument	Techniques	Detects
Acetate-CIMS	FIGAERO Chemical Ionization ToF-MS	Acids
Iodide CIMS	FIGAERO Chemical Ionization ToF-MS	Acids Hydroxyl Oxidized Compounds
SV-TAG	Filter CTD collection GC EI Quadrupole MS	Hydrocarbons $\sim 13 < C < \sim 30$, Wide variety of oxygenates (esp. acids, carbonyls, alcohols), mostly limited to $O < 5$ compounds
TD-PTR-MS	Impactor CTD collection Chemical Ionization ToF-MS	Most hydrocarbons $C < 15$ Volatile and semivolatile oxygenated species

Table S2. Compounds compared between the A-CIMS, I-CIMS, and SV-TAG. Molecular formulas were identified in the two CIMS instruments, and compounds were identified in the SV-TAG. See main text for detailed interpretation. C* values are for 298 K.

Molecular Formula	Likely Compound	C* Value	ΔH_{vap} (KJ mol⁻¹)	Source
C ₅ H ₈ O ₅	Hydroxy glutaric acid	0.21	101	(Bilde and Pandis, 2001) (Salo et al., 2010)
C ₉ H ₁₄ O ₄	Pinic acid	10	109	(Bilde and Pandis, 2001)
C ₁₀ H ₁₆ O ₃	Pinonic acid	1000	98	(Müller et al., 2012)

Table S3. Possible compounds compared between the A-CIMS and the PTRMS, identified by their molecular formula. The possible compound listed is one of many possible isomers with the same molecular formula.

Molecular Formula	Possible Compound	C* (μg m⁻³) at 298 K	ΔH_{vap} (KJ mol⁻¹)	Source
C ₁₀ H ₂₀ O ₂	Decanoic acid	2.85x10 ³	101.8	(Nanolal et al., 2008)
C ₉ H ₁₈ O ₂	Nonanoic acid	9.1x10 ³	85.7	(Nanolal et al., 2008)
C ₈ H ₁₆ O ₂	Valproic acid	2.66x10 ⁴	82.8	(Nanolal et al., 2008)

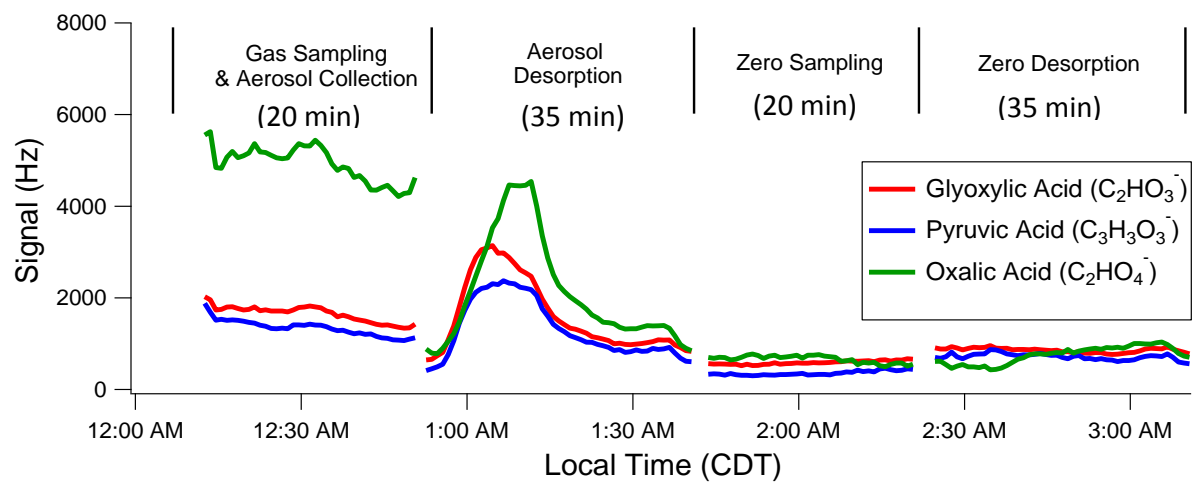


Figure S1. Example data of the FIGAERO sampling and heating cycles of the A-CIMS. Also shown is a zero sampling and zero desorption showing low background signals (see text for details on FIGAERO operation).

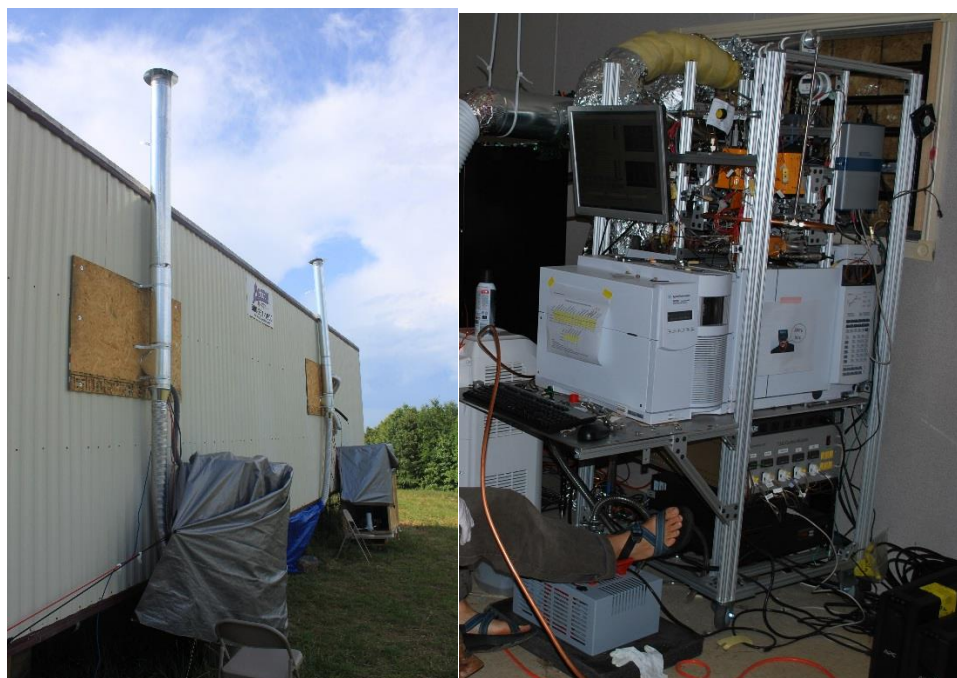
(A)



(B)



(C)



(D)



Figure S2. A picture of (A) the A-CIMS inlet setup, outside the trailer (left) and inside the trailer (right). (B) The I-CIMS setup outside the trailer (left) and inside (right). (C) The SV-TAG (left, foreground) and PTRMS setup (right, background) and SV-TAG setup inside the trailer (right). (D) The complete PTRMS setup outside.

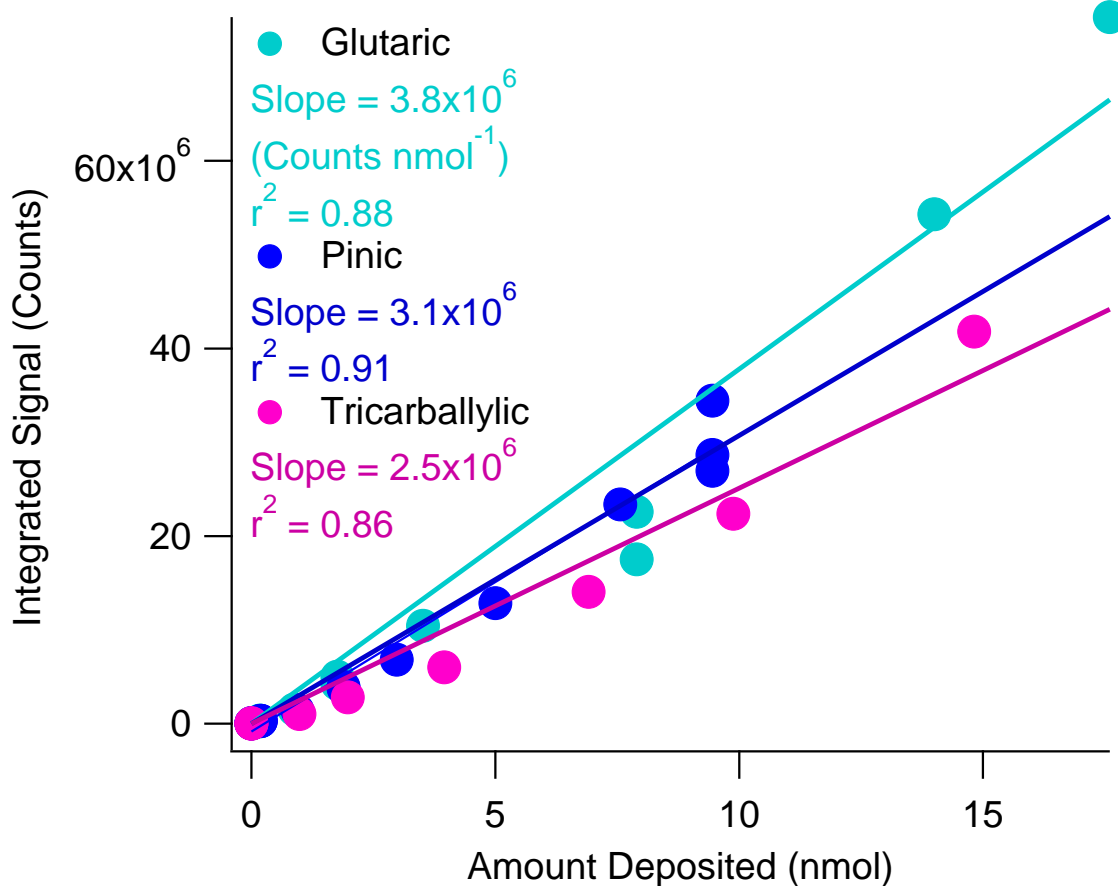


Figure S3. Example Calibration of FIGAERO A-CIMS. Thermal desorption profiles are integrated to measure total signal and plotted vs. amount of acid deposited on filter. Linear, repeatable calibrations are obtained.

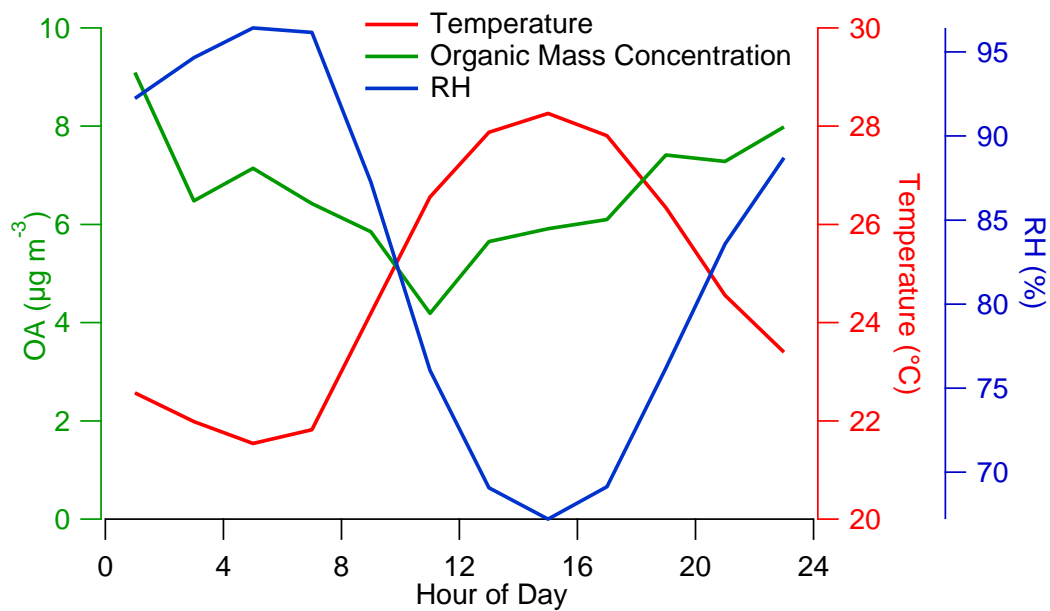


Figure S4. Average diurnal cycles over the 9-day period of organic aerosol concentration, temperature and relative humidity.

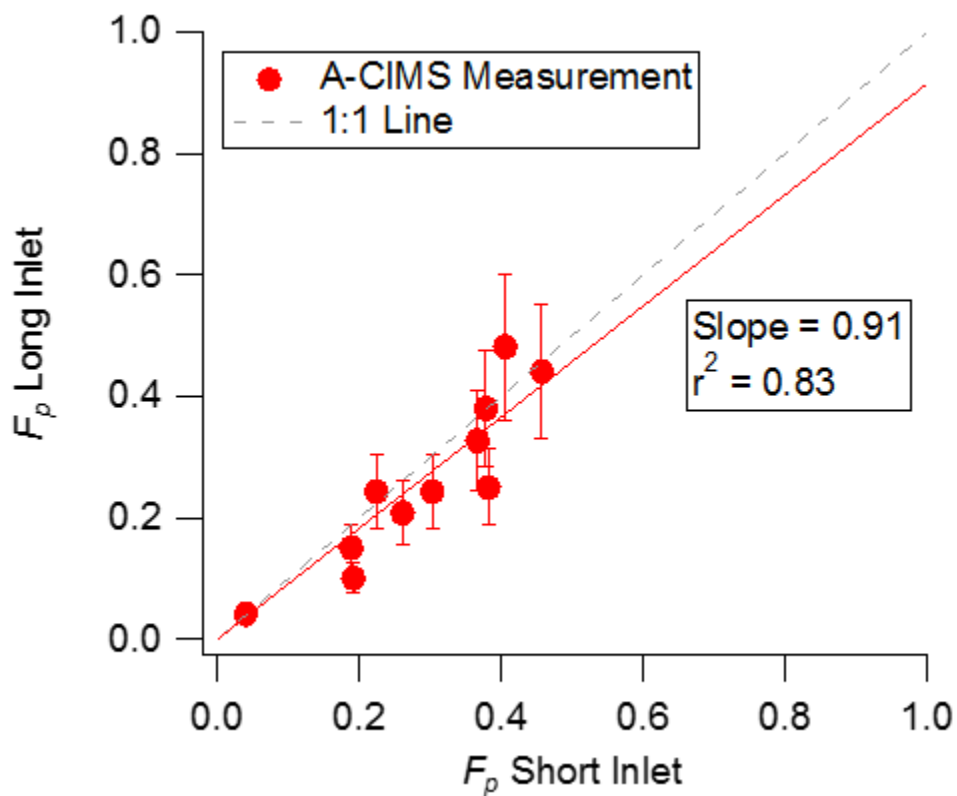


Figure S5. Comparison of average F_p from the A-CIMS for all acids compared in this study, for the long inlet configuration (6 m long) vs the short inlet configuration (0.5 m long). Average temperature and relative humidity during the two periods were not significantly different (Long Inlet: 25.2 \pm 3.3 $^{\circ}$ C, 81 \pm 16% and Short Inlet: 24.9 \pm 2.7 $^{\circ}$ C, 92 \pm 10%). Most of the points fall within error of the 1:1 line. A small effect of larger gas-phase losses in the longer inlet cannot be ruled out. However this difference is far smaller than the differences between the different instruments.

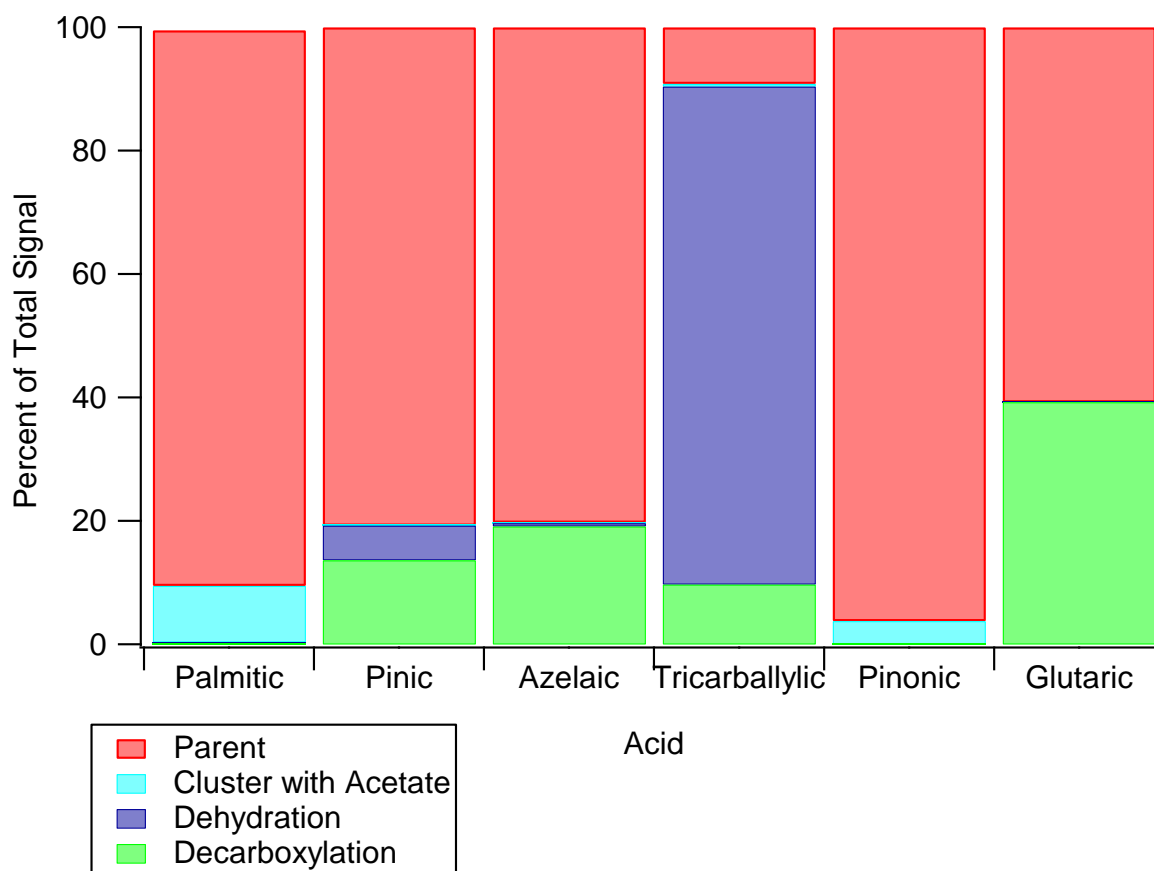


Figure S6. Percent of the total signal observed during calibration experiments with pure acids, for the parent molecule, thermal decomposition products, and the cluster with the acetate reagent ion. Experiments were carried out with the acetate CIMS by calibrating each compound individually and measuring the signal for the decomposition products. For monoacids, the decarboxylation and dehydration products are not measurable.

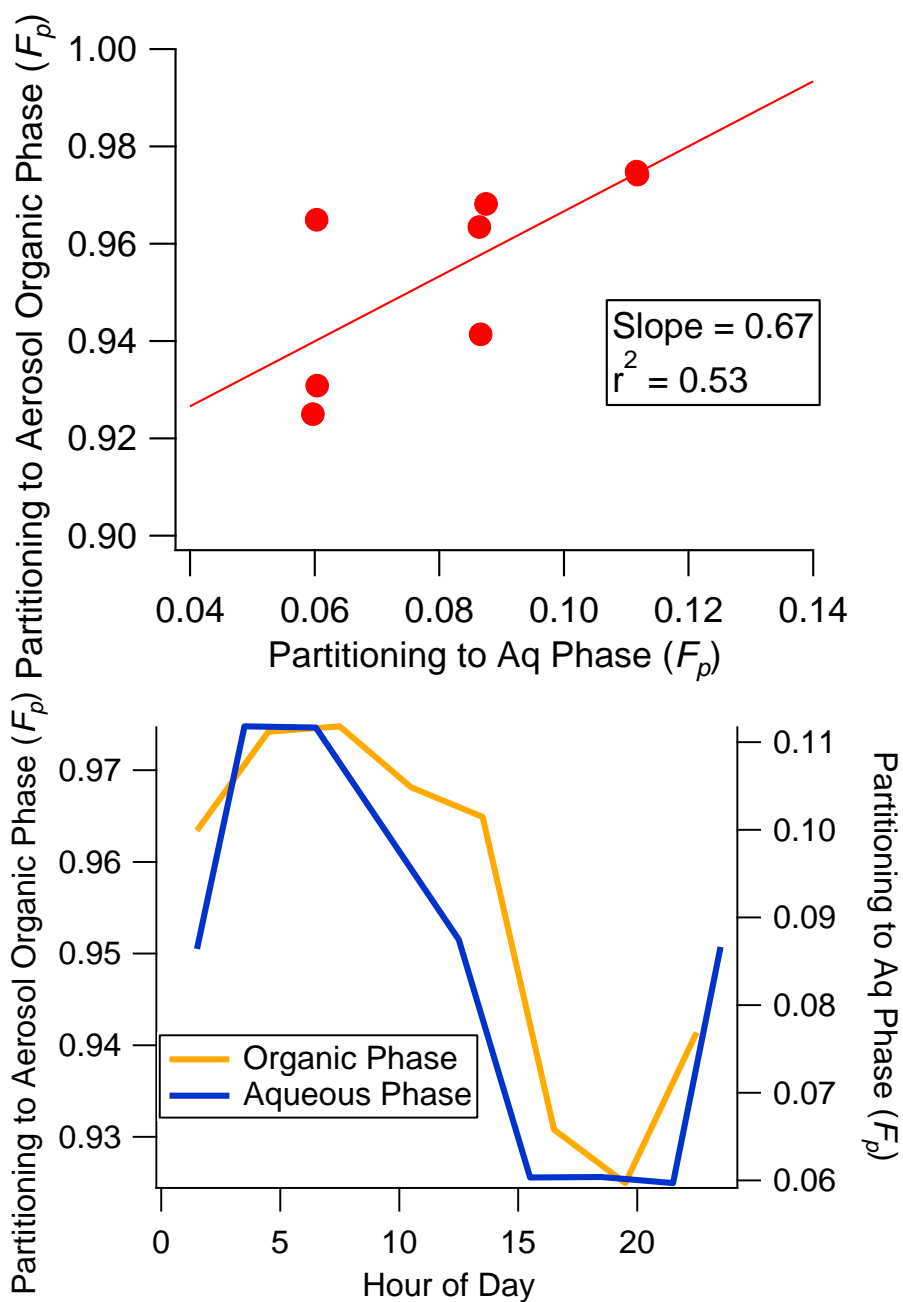
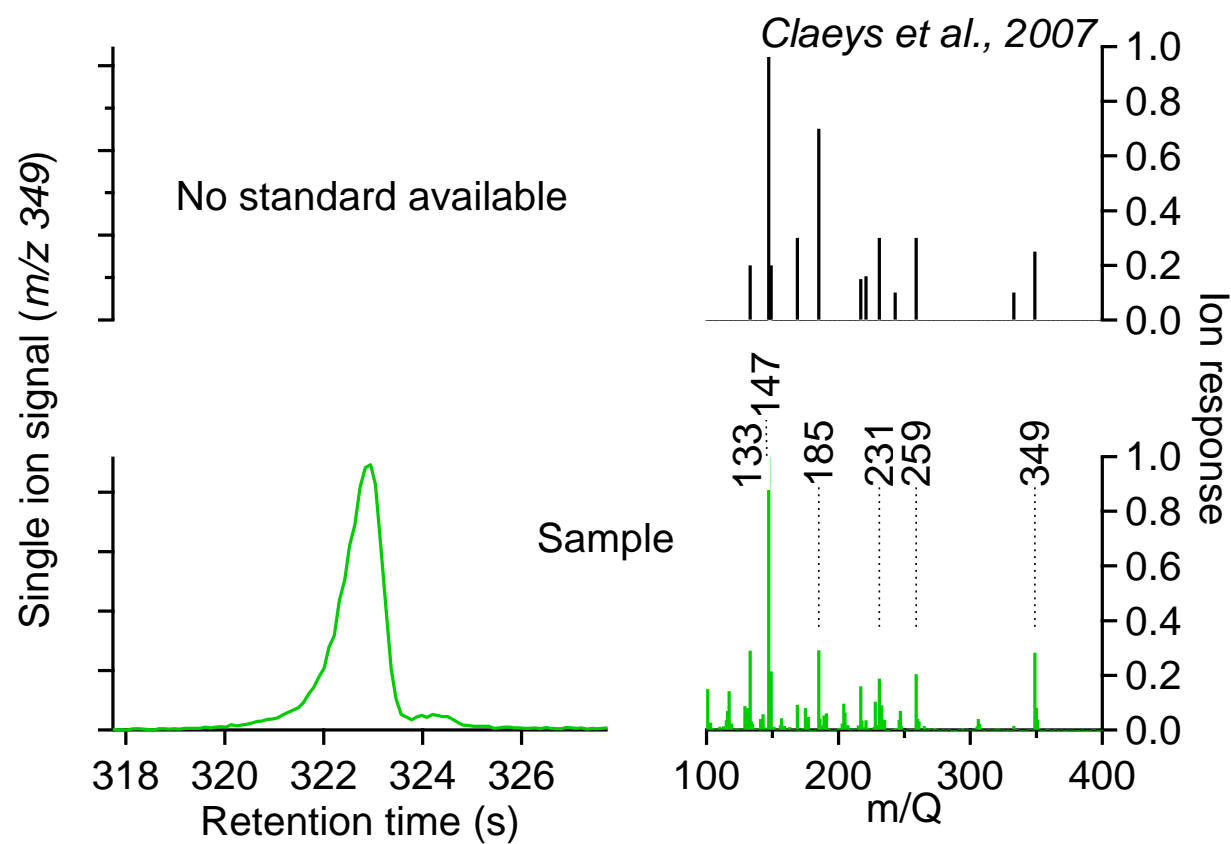
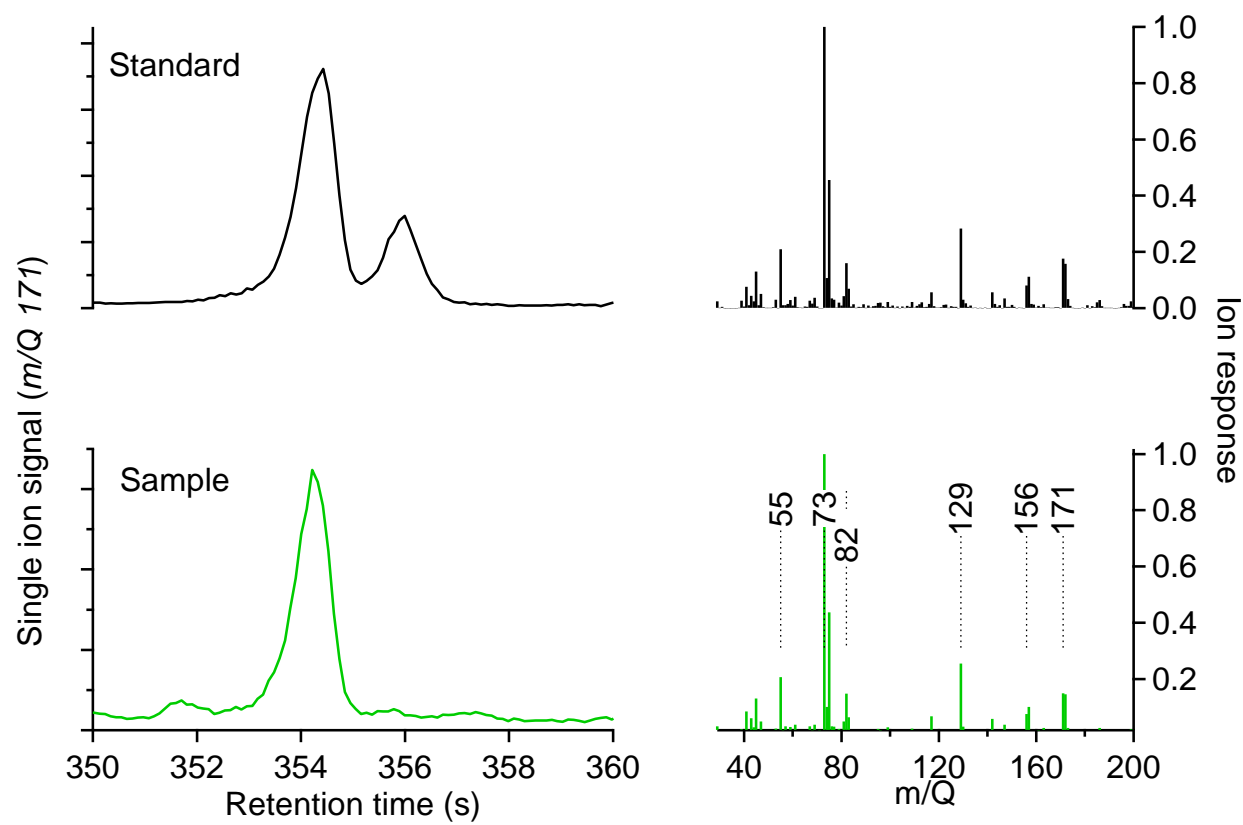


Figure S7. Comparison of the diurnal profiles of the predicted partitioning for the organic vs. the aerosol water phases for hydroxy glutaric acid.

(A) hydroxy glutaric acid



(B) pinic acid



(C) pinonic acid

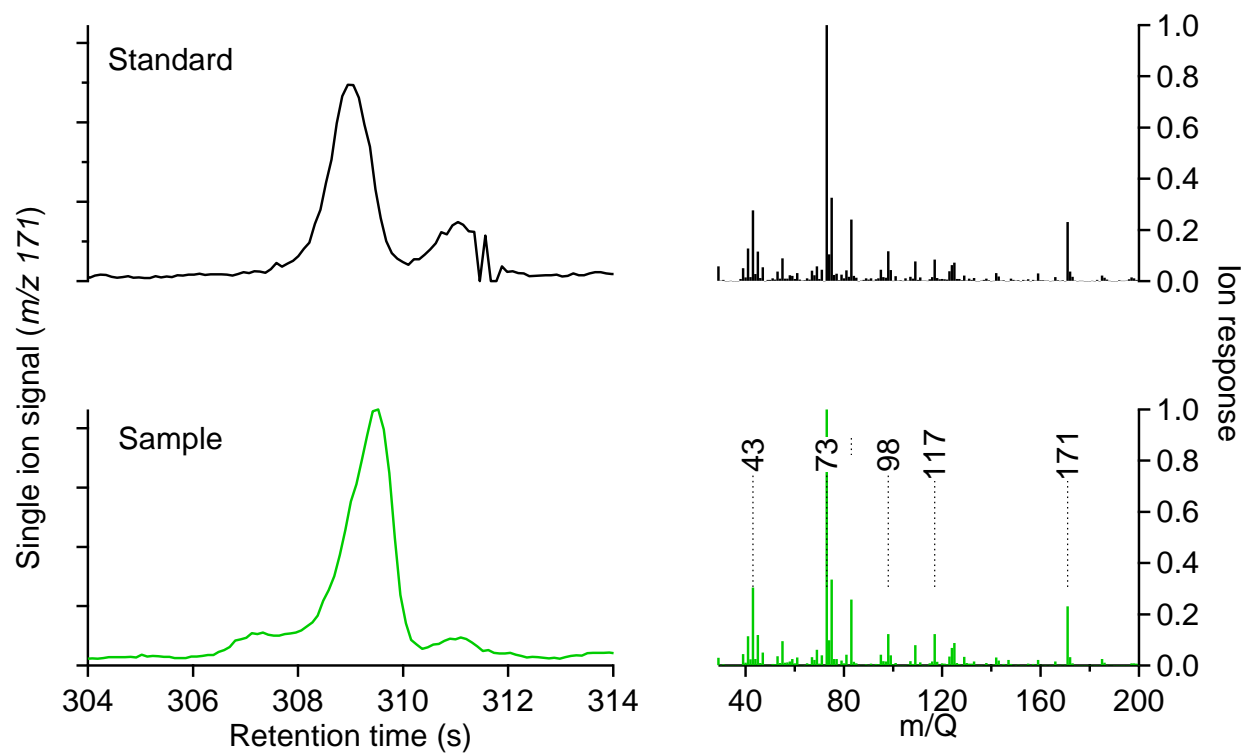


Figure S8. Gas chromatogram and mass spectra used for identification of the three compounds compared with the SV-TAG instrument. Standards shown in black when available and ambient sample shown in green.

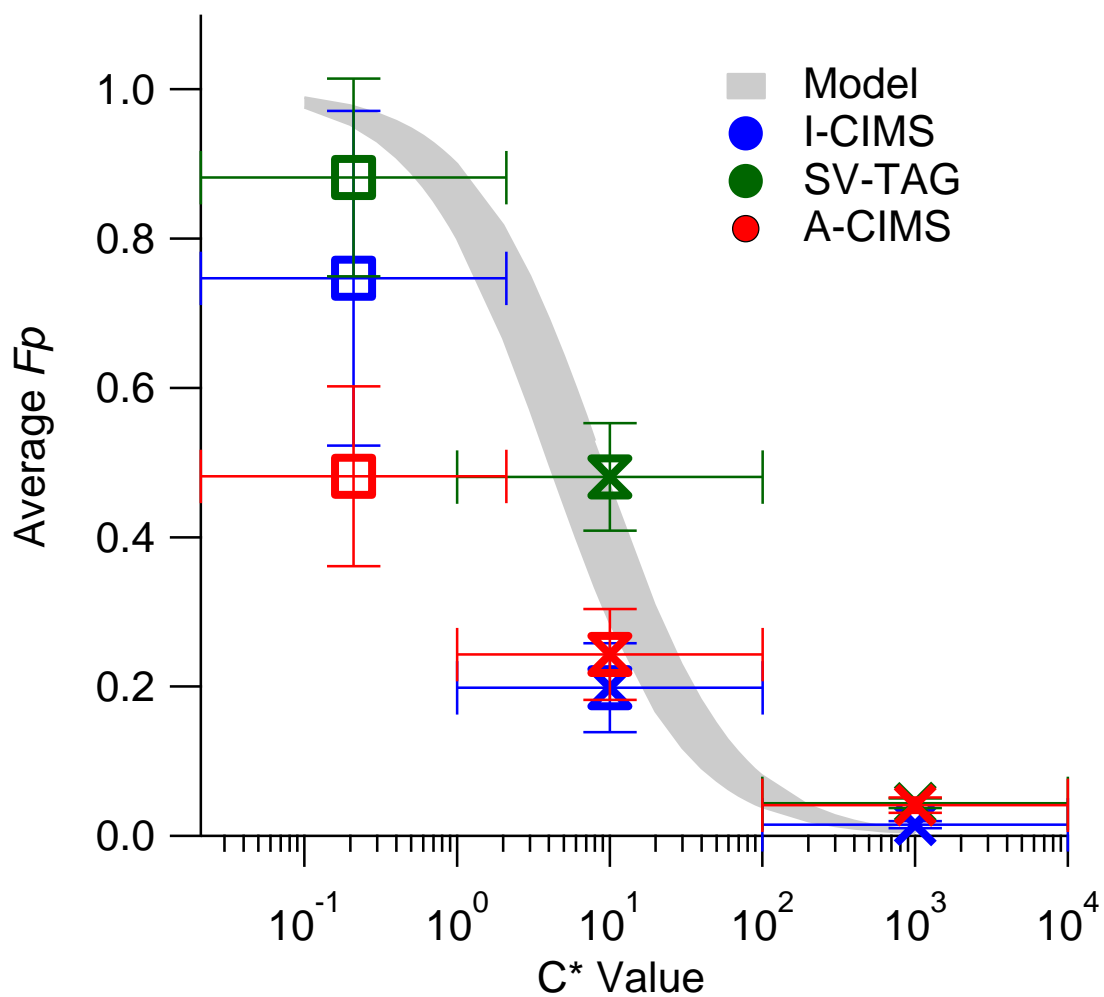


Figure S9. Average measured partitioning values vs their calculated C^* values. Grey band shows modelled F_p vs C^* values using the ambient conditions at the site (temperature and organic aerosol concentration).

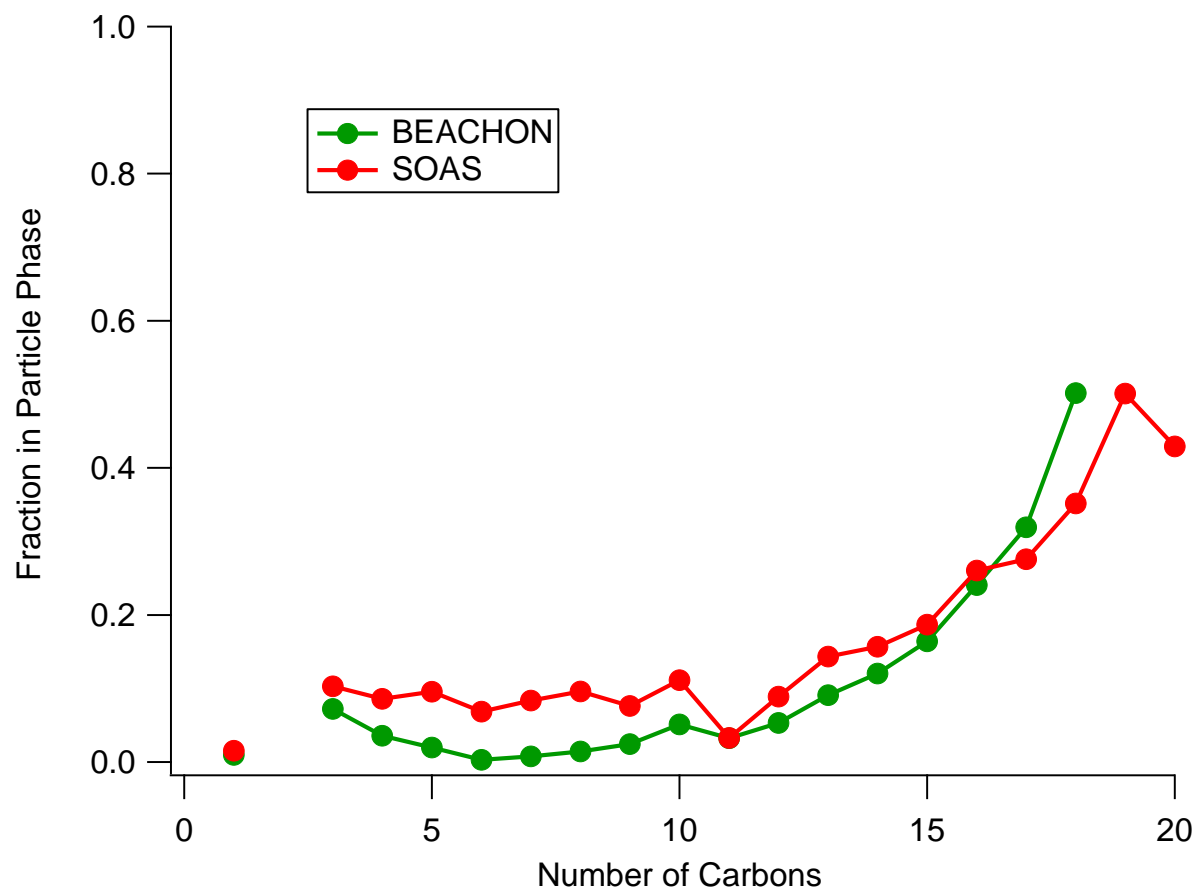


Figure S10. Fraction in the particle phase as a function of carbon number. This shows results from this campaign compared to a previous campaign with a similar instrumental setup.