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Supplement of

Evidence for pyrazine-based chromophores in cloud water mimics containing methylglyoxal and ammonium sulfate

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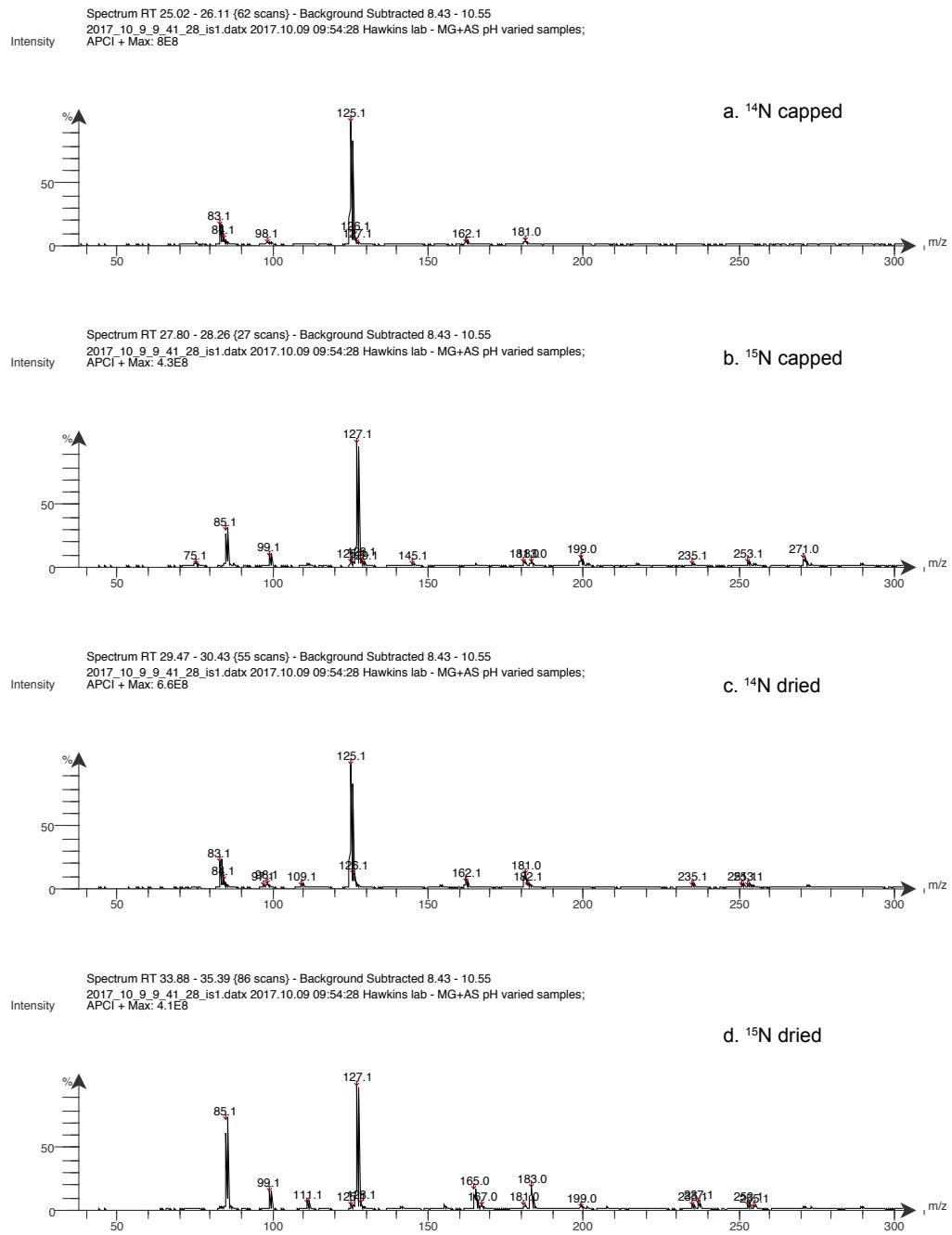


Figure S1. Methylglyoxal (1.0 M) and ammonium sulfate (1.0 M) reactions, adjusted to pH 5 analyzed by APCI after one week using low temperature and low fragmentation conditions.

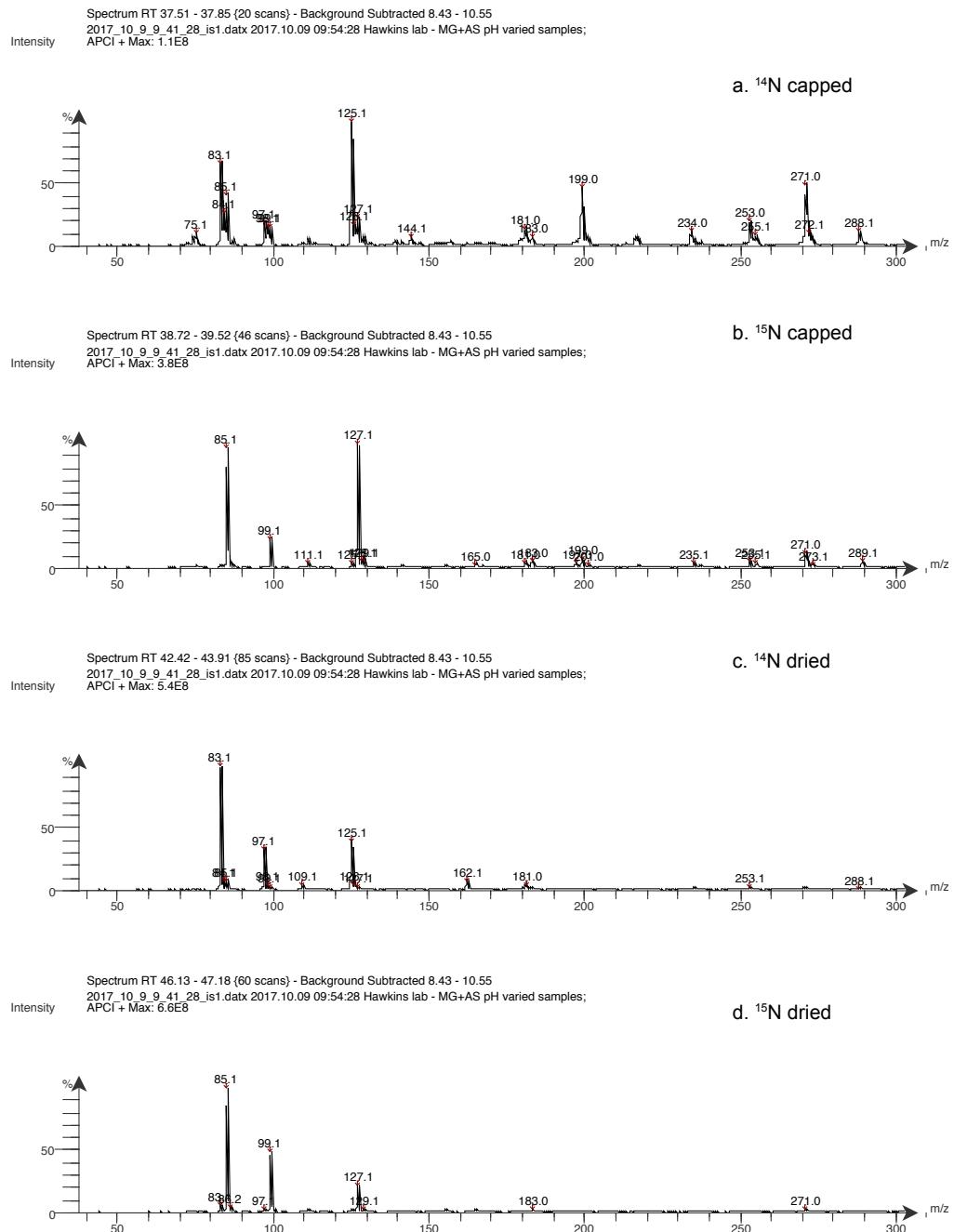


Figure S2. Methylglyoxal (1.0 M) and ammonium sulfate (1.0 M) reactions, adjusted to pH 7 analyzed by APCI after one week using low temperature and low fragmentation conditions.

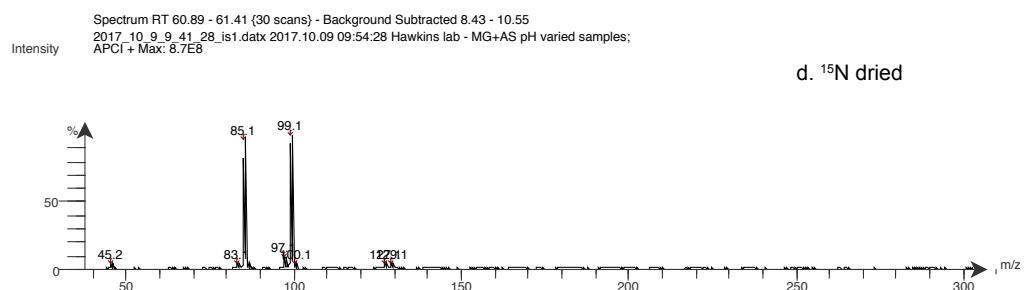
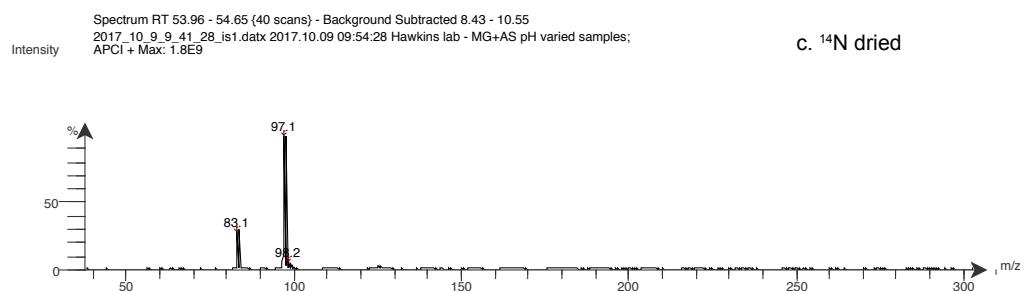
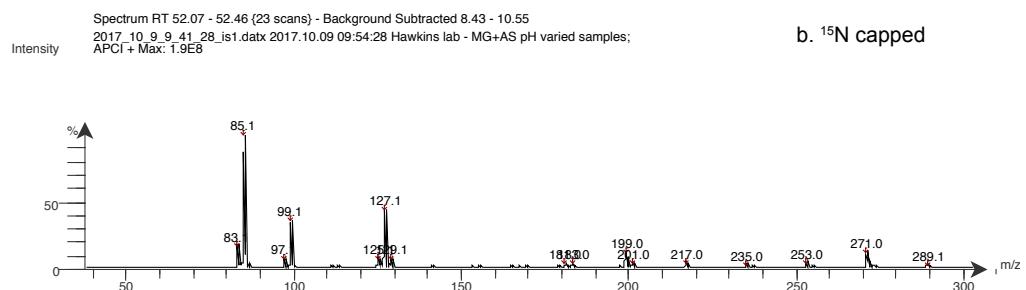
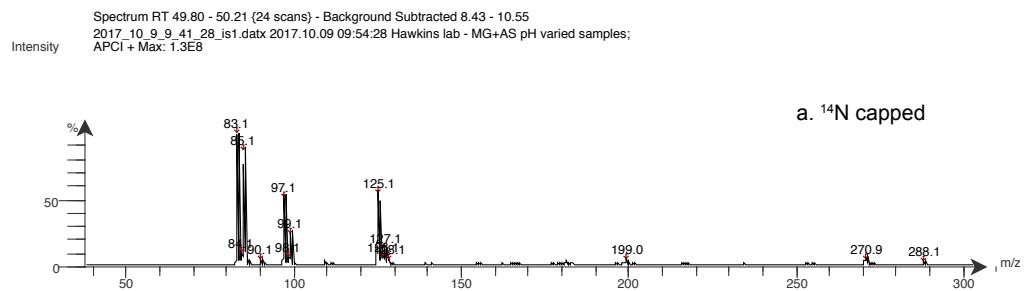


Figure S3. Methylglyoxal (1.0 M) and ammonium sulfate (1.0 M) reactions, adjusted to pH 9 analyzed by APCI after one week using low temperature and low fragmentation conditions.

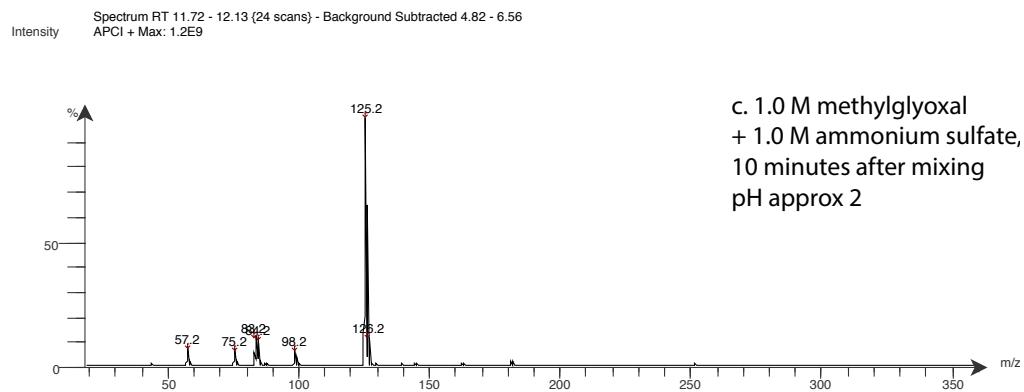
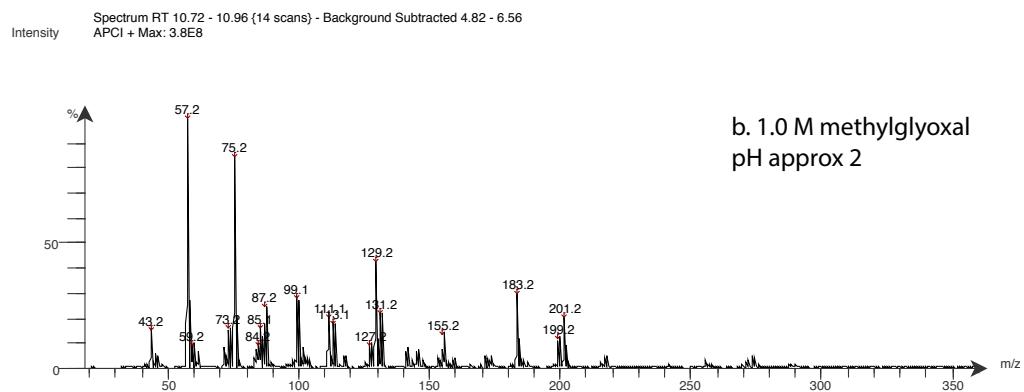
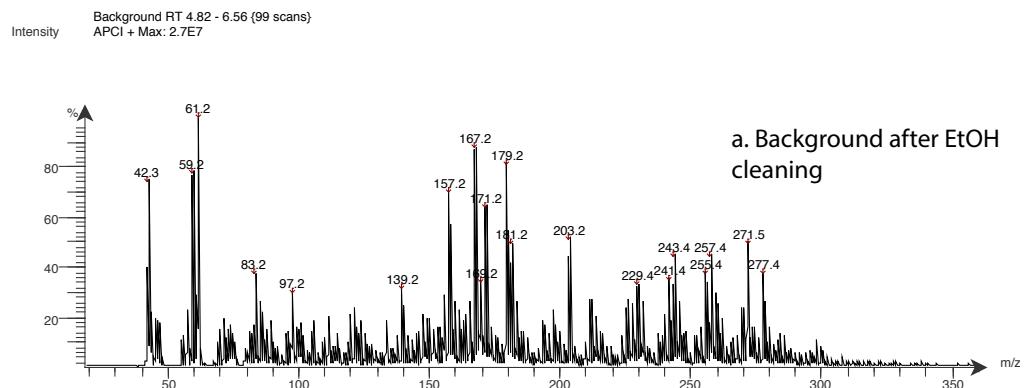


Figure S4. Methylglyoxal (1.0 M) and ammonium sulfate (1.0 M) reactions, at pH 2 analyzed by APCI after 10 min using low temperature and low fragmentation conditions. Methylglyoxal at pH 2 is shown in (b) as a control.

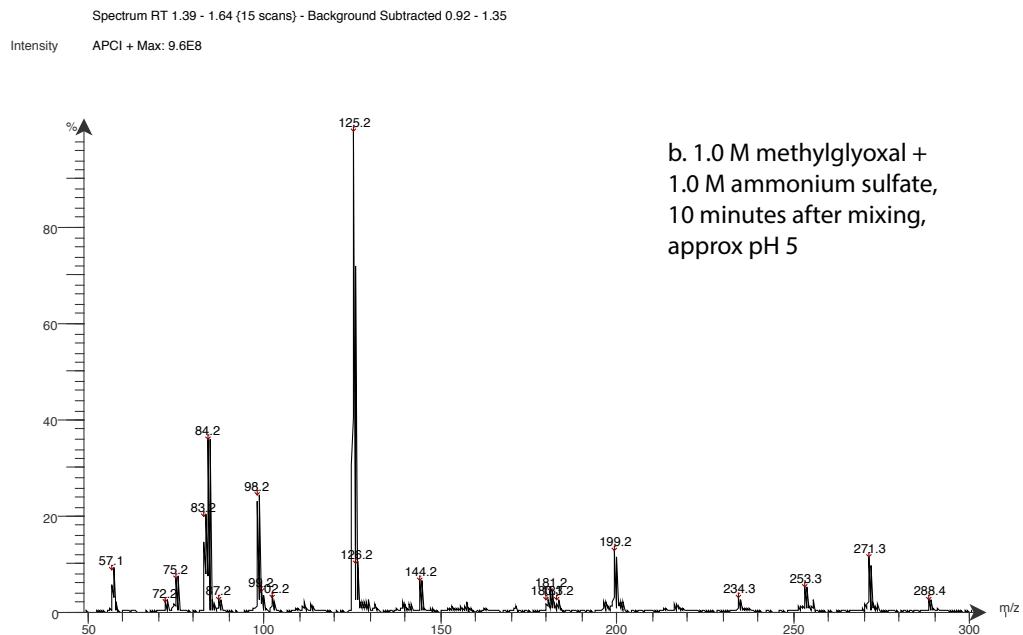
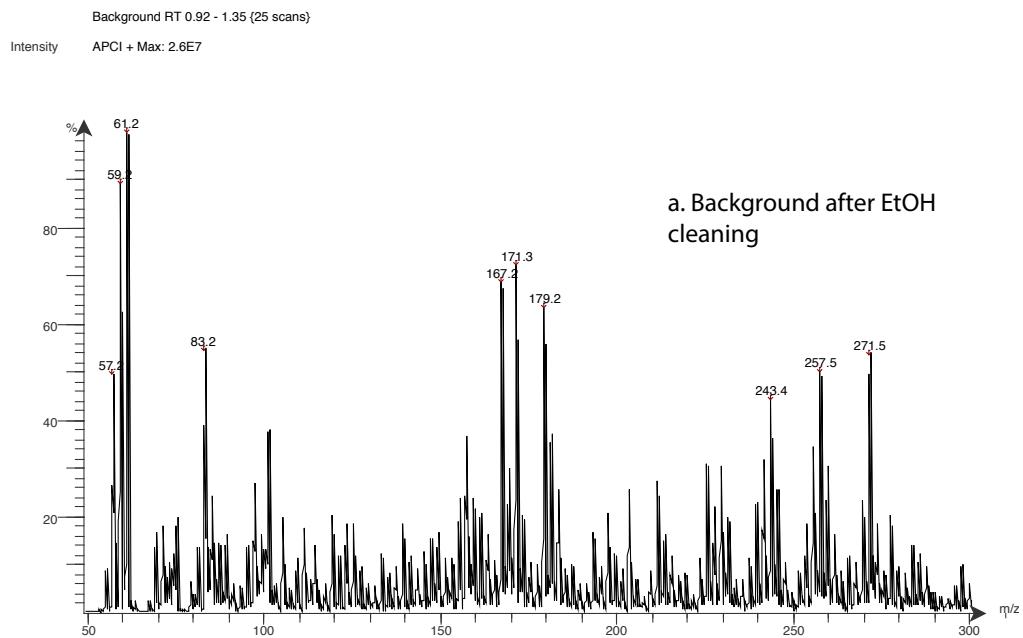


Figure S5. Methylglyoxal (1.0 M) and ammonium sulfate (1.0 M) reactions, adjusted to pH 5 analyzed by APCI after 10 min using low temperature and low fragmentation conditions.

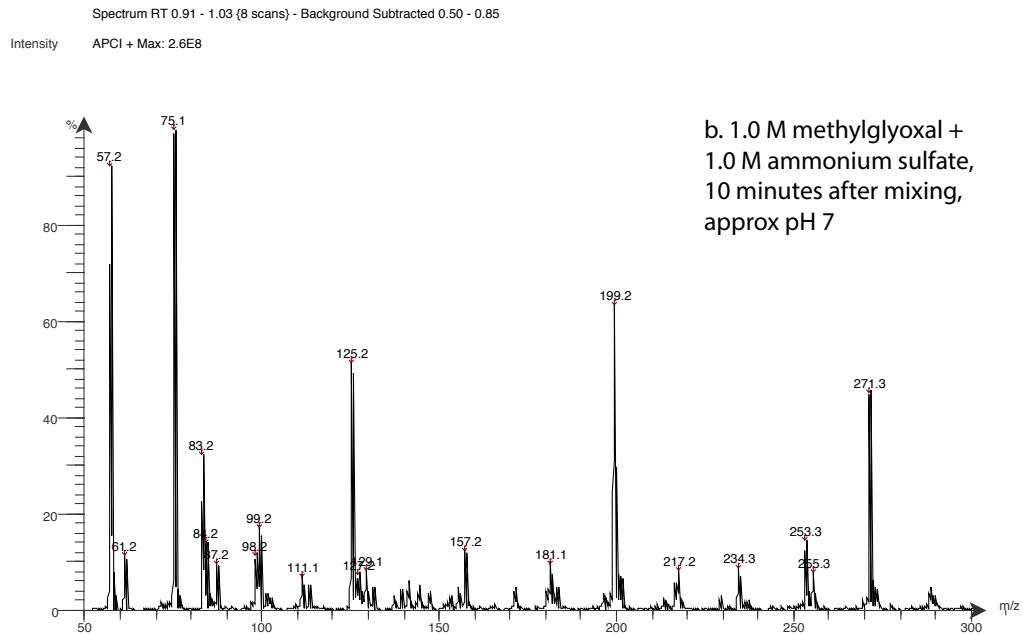
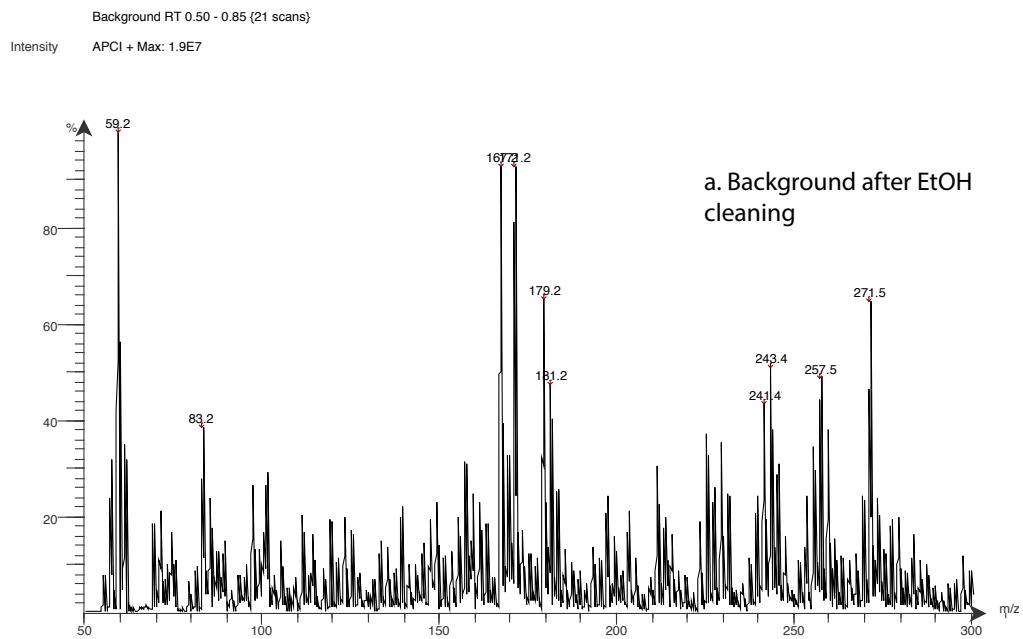


Figure S6. Methylglyoxal (1.0 M) and ammonium sulfate (1.0 M) reactions, adjusted to pH 7 analyzed by APCI after 10 min using low temperature and low fragmentation conditions.

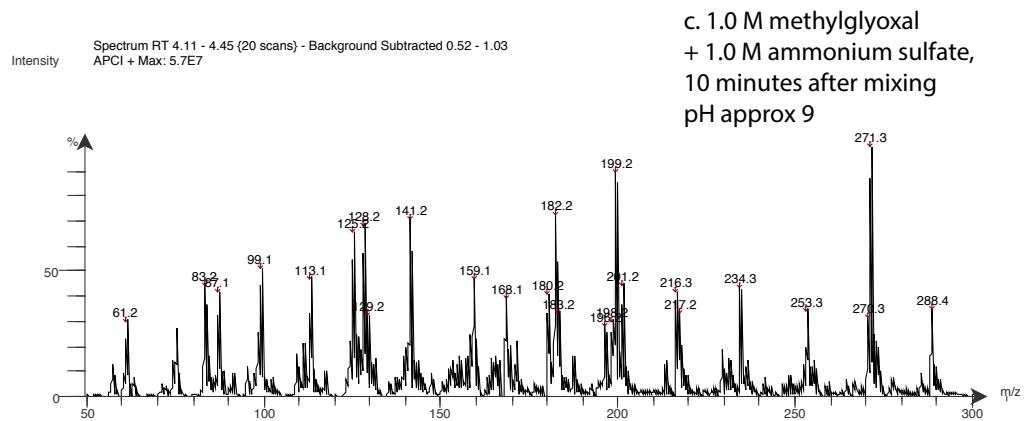
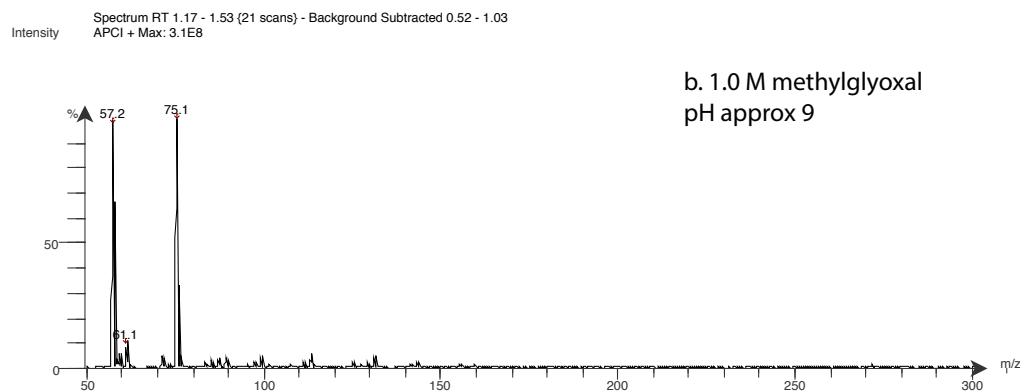
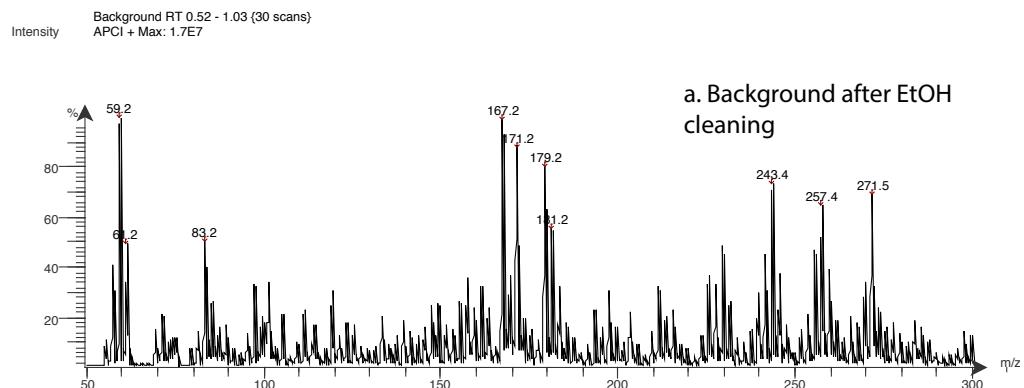


Figure S7. Methylglyoxal (1.0 M) and ammonium sulfate (1.0 M) reactions, adjusted to pH 9 analyzed by APCI after 10 min using low temperature and low fragmentation conditions. Methylglyoxal adjusted to pH 9 is shown in (b) as a control.

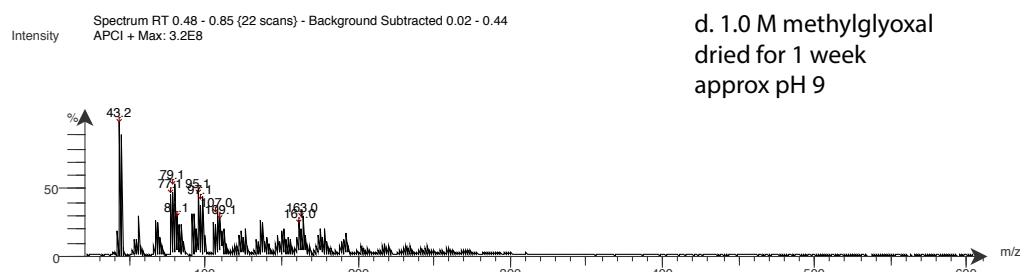
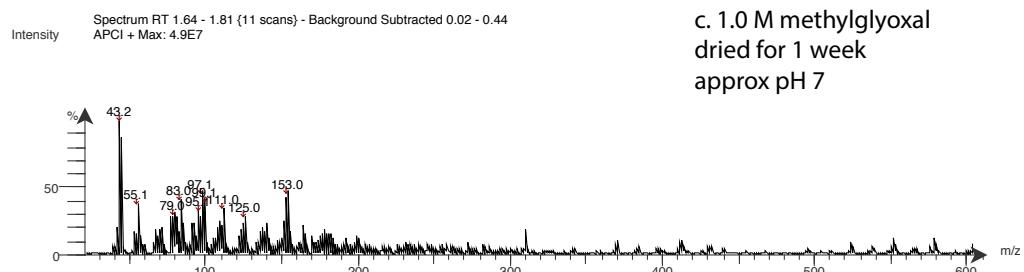
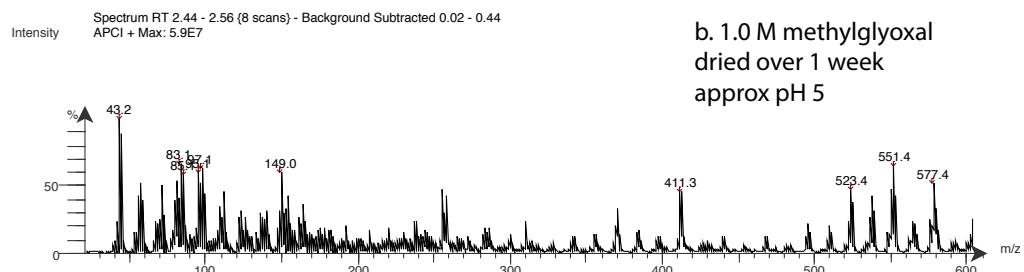
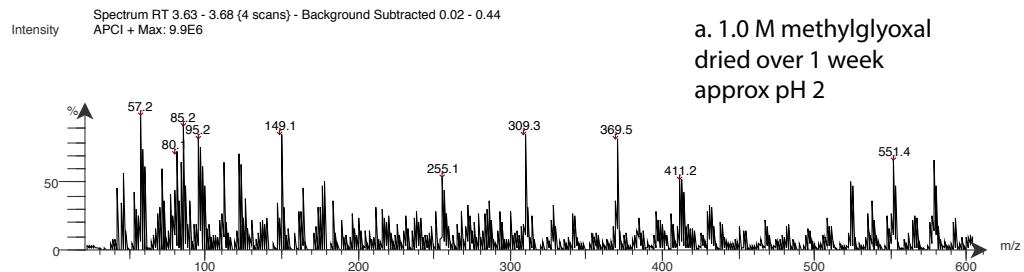


Figure S8. Methylglyoxal (1.0 M) prepared at a) pH 2, b) pH 5, c) pH 7, and d) pH 9 and allowed to dry uncovered for one week in the hood. The products observed in the reactions with AS do not appear in these samples.

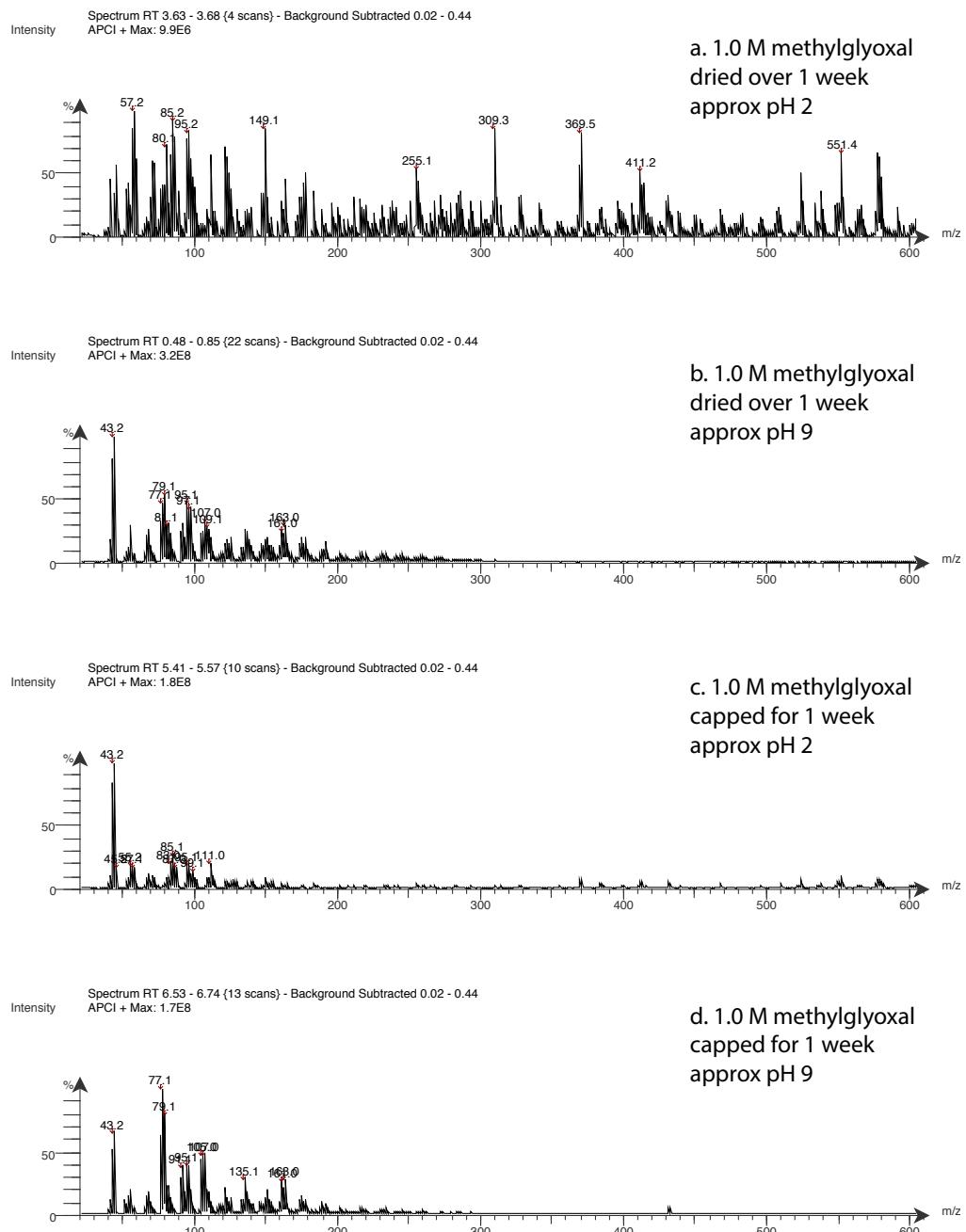


Figure S9. Methylglyoxal (1.0 M) prepared at a) pH 2 and b) pH 9 and allowed to dry uncovered for one week in the hood (reproduced from Fig S8). In (c) and (d), duplicate capped samples are shown. The products observed in the reactions with AS do not appear in these samples.

File : D:\MassHunter\GCMS\1\data\LNH\171012_pH2b.D
 Operator :
 Acquired : 12 Oct 2017 15:10 using AcqMethod pyrazineSearch.M
 Instrument : 5975 GCMS
 Sample Name: pH2
 Misc Info :
 Vial Number: 2

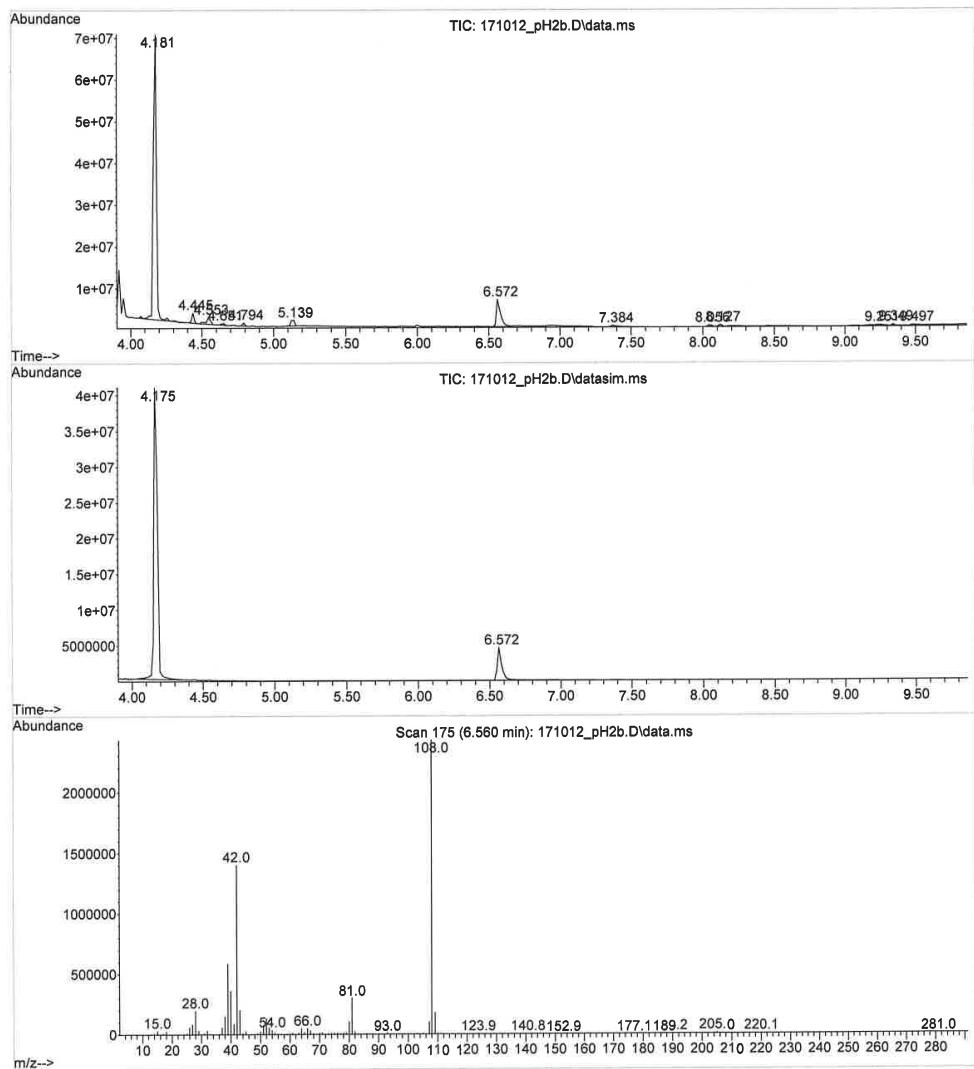


Figure S10. Top: Total ion chromatogram for the ethyl acetate extract of a dried pH 2 sample. Middle: sum of all ions selected for SIM showing a peak at 4.175 min corresponding to the pyrazine internal standard and a second peak at 6.572 min corresponding to 2,5-dimethylpyrazine. Bottom: Electron impact spectrum acquired at retention time 6.560 (during 2,5-DMP elution) with prominent fragments at m/z 108, 42, and 81.

Library Searched : D:\MassHunter\Library\NIST14.L
Quality : 91
ID : Pyrazine, 2,5-dimethyl-

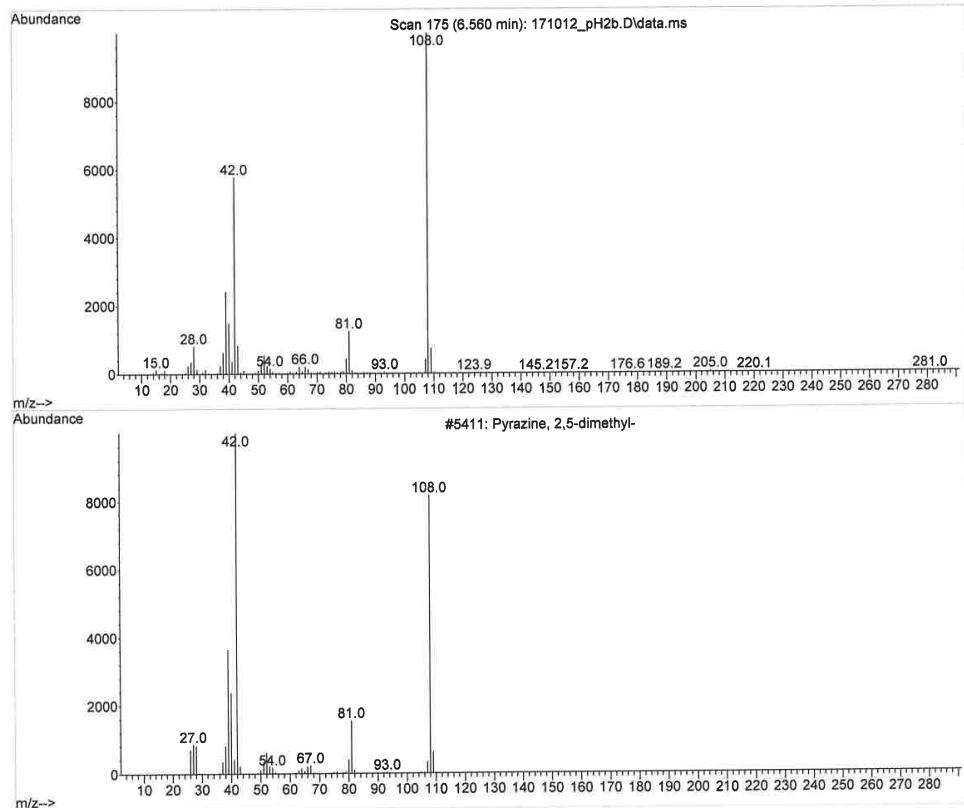


Figure S11. Top: spectrum obtained during elution of (proposed) 2,5-DMP peak from column. Bottom: NIST reference spectrum for electron impact ionization of 2,5-DMP.

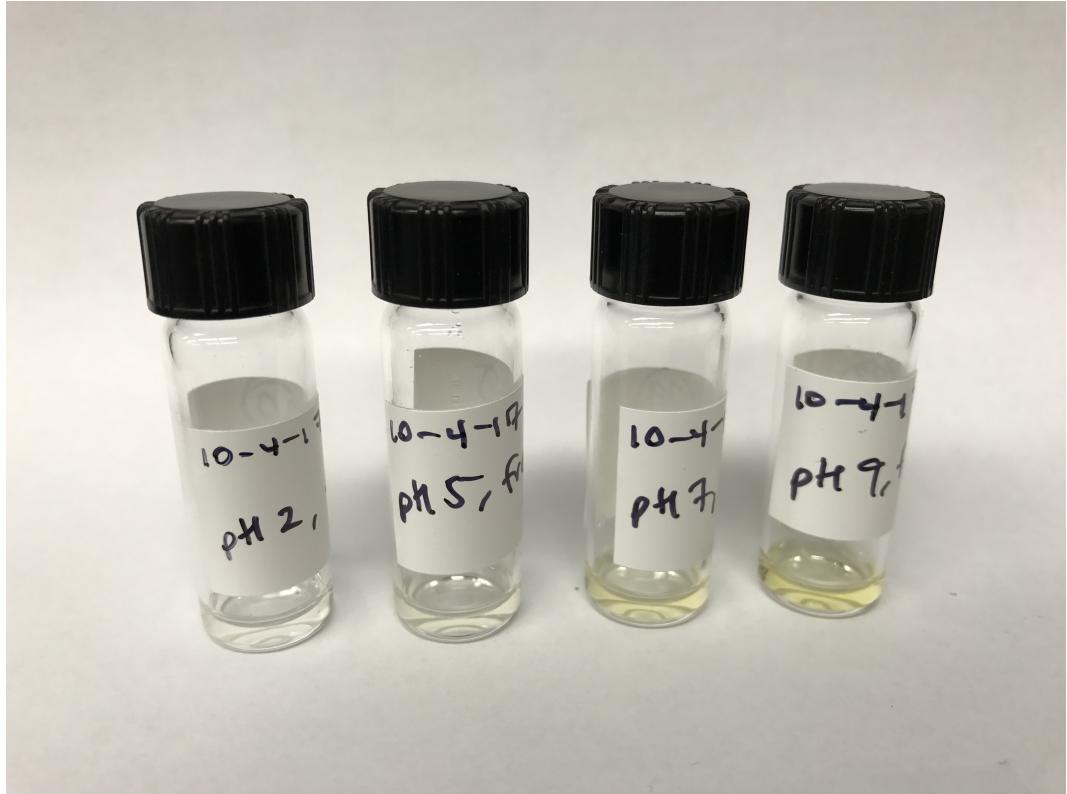


Figure S12. Image taken after 24 hours of reaction time between methylglyoxal and AS in capped samples. A pH dependence on absorbance is immediately visible.

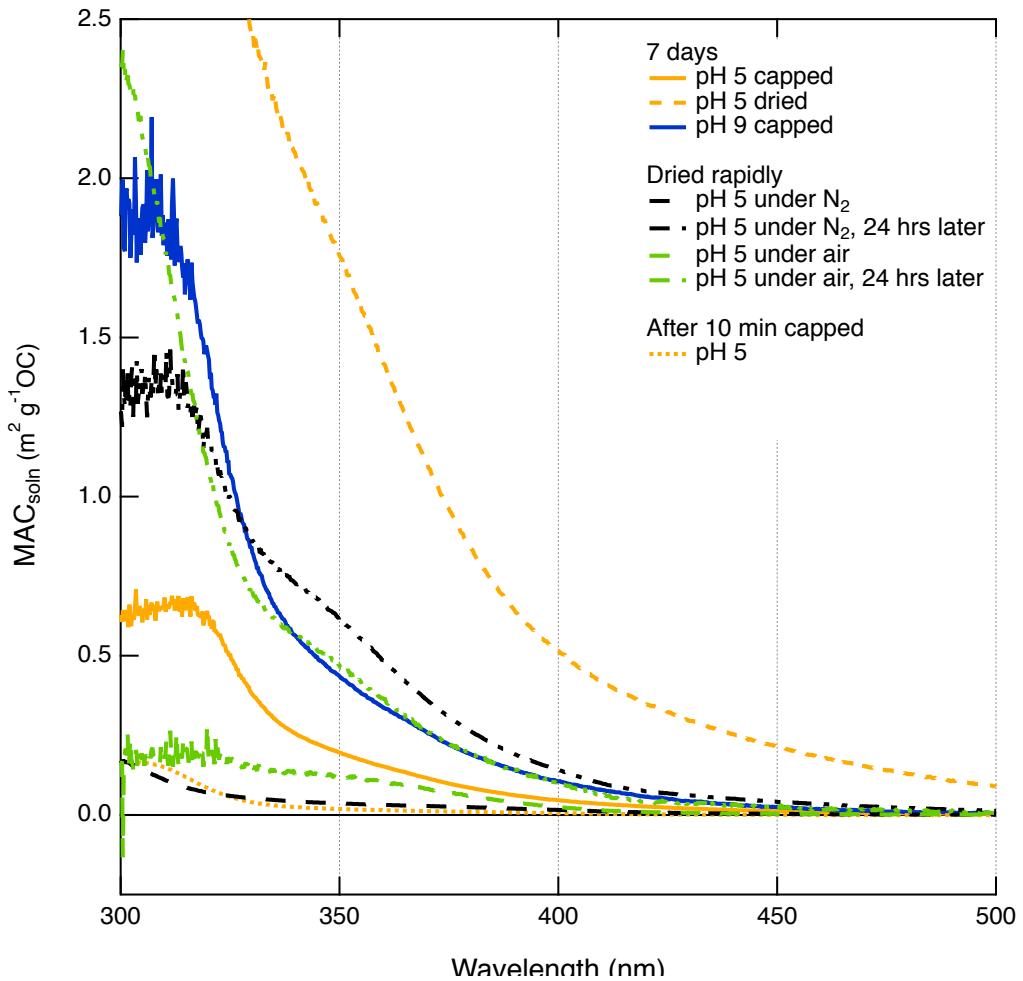


Figure S13. UV-visible absorbance spectra for methylglyoxal (1.0 M) and ammonium sulfate (1.0 M) at pH 5 under a variety of drying conditions.

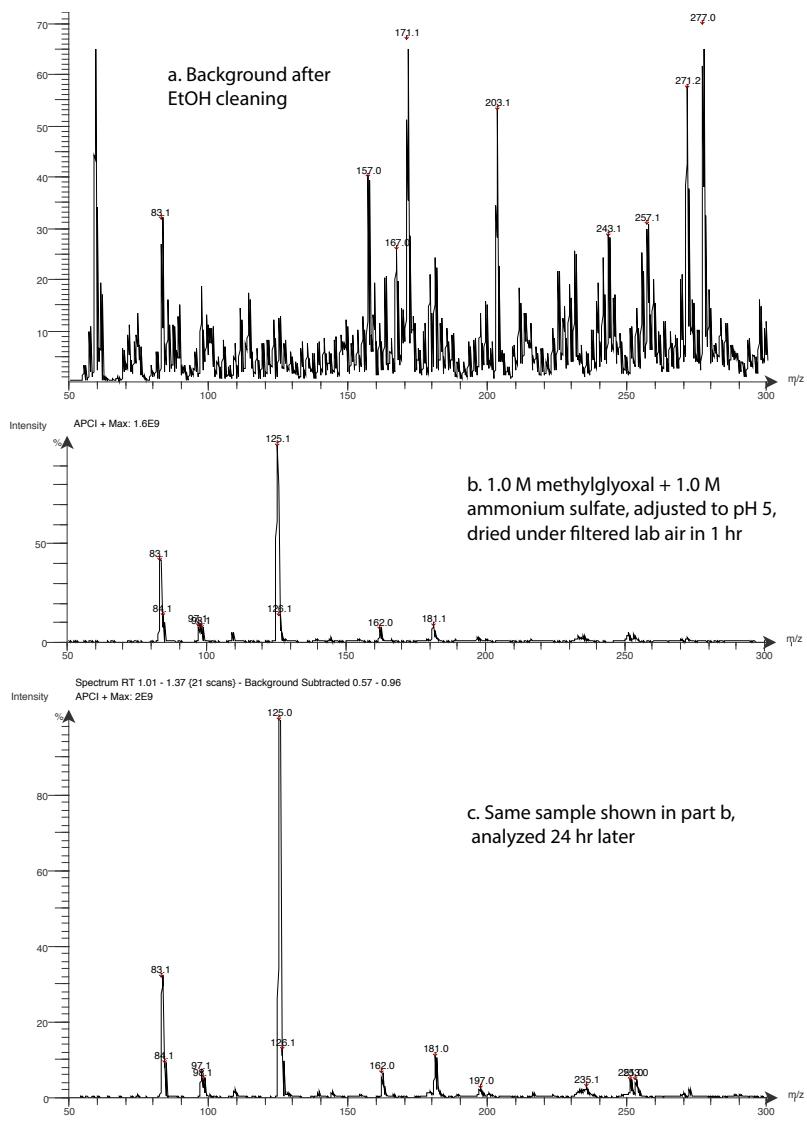


Figure S14. Methylglyoxal (1.0 M) and ammonium sulfate (1.0 M), adjusted to pH 5 and evaporated to dryness over the course of one hour using HEPA-filtered laboratory air. The sample was analyzed a) immediately by APCI and b) 24 hours later when additional chromophores were observed.

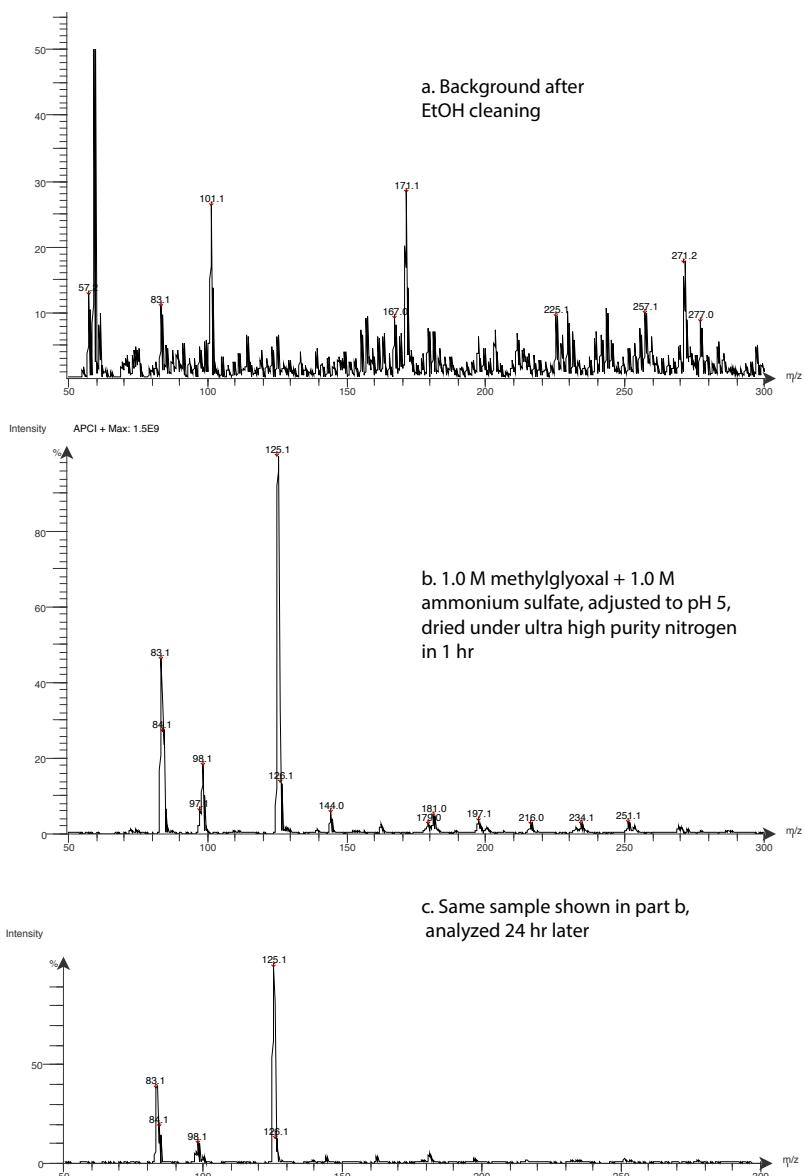
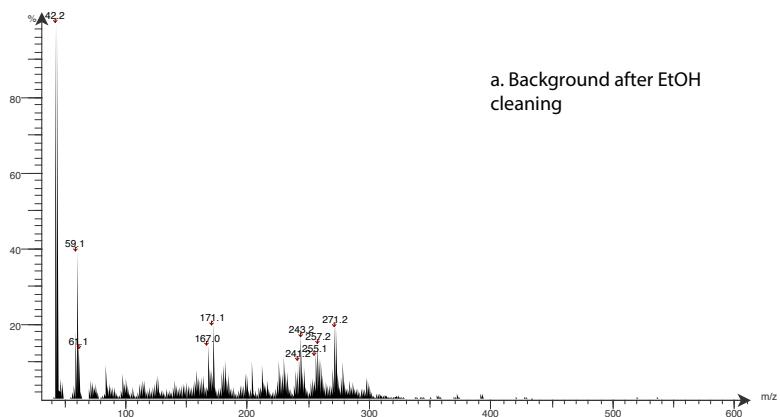


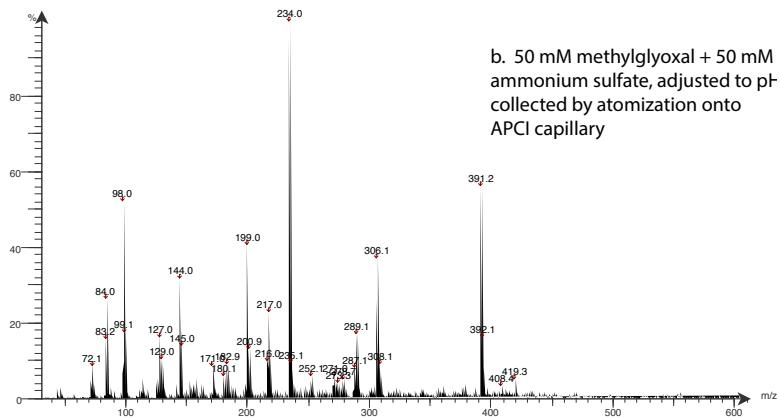
Figure S15. Methylglyoxal (1.0 M) and ammonium sulfate (1.0 M), adjusted to pH 5 and evaporated to dryness over the course of one hour using ultra high purity nitrogen. The sample was analyzed a) immediately by APCI and b) 24 hours later when additional chromophores were observed.

Background RT 0.18 - 0.55 (22 scans)
2018_6_5_16_38_30_ls1.datx 2018.06.05 16:39:06 Hawkins MG+AS control sample atomizer;
APCI + Max: 8.9E7



a. Background after EtOH
cleaning

Spectrum RT 0.59 - 0.68 (6 scans) - Background Subtracted 0.18 - 0.55
2018_6_5_16_38_30_ls1.datx 2018.06.05 16:39:06 Hawkins MG+AS control sample atomizer;
APCI + Max: 1.1E8



b. 50 mM methylglyoxal + 50 mM
ammonium sulfate, adjusted to pH
collected by atomization onto
APCI capillary

Figure S16. Methylglyoxal (50 mM) and ammonium sulfate (50 mM), adjusted to pH 5 atomized and dried using diffusion dryers and impacted directly onto the APCI capillary. The sample was analyzed immediately by APCI.