Supplementary Material for

Furoyl peroxynitrate (fur-PAN), a product of VOC-NO_x photochemistry from biomass burning emissions: Photochemical synthesis, calibration, chemical characterization, and first atmospheric observations.

James M. Roberts, et al.,

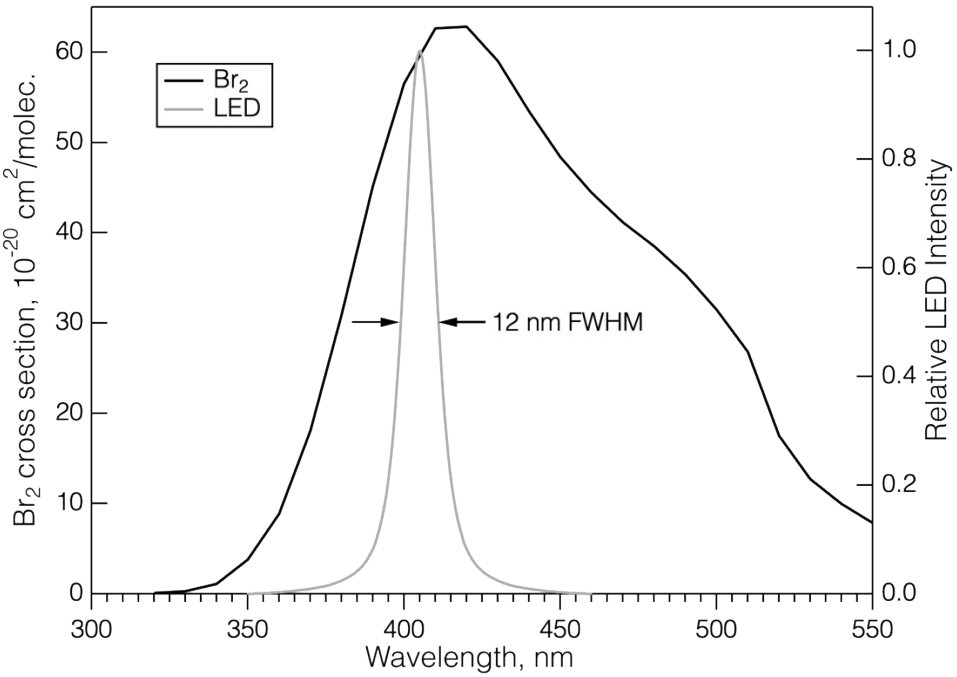

Figure S1. The absorption spectrum of Br_2 (black)[1] and the emission spectrum of the LED used in the photosource (grey).

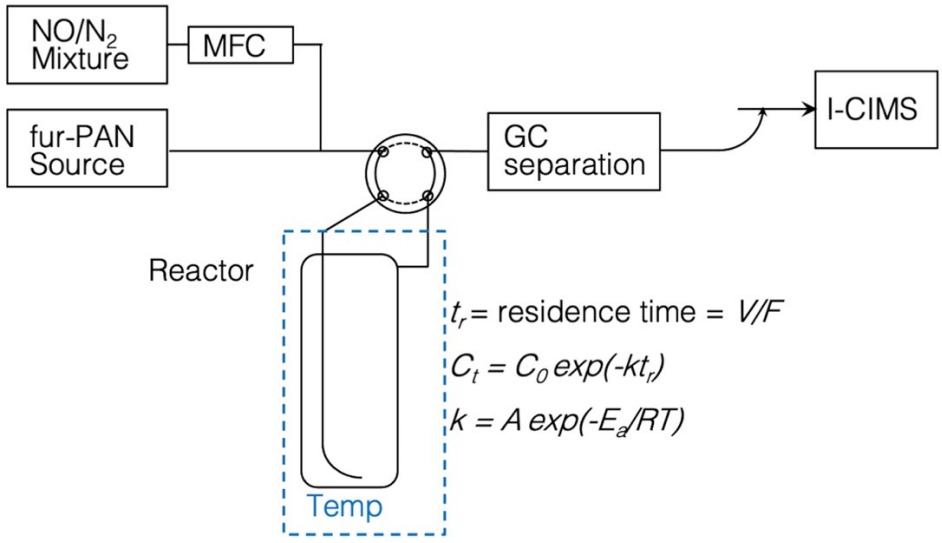

Figure S2. Schematic diagram of the reactor system for the measurement of the thermal decomposition of fur-PAN.

This reactor is a hybrid between a plug-flow reactor and a continuous stirred-tank reactor (CSTR). In both kinds of reactors, the residence time is defined as the Volume/Flow Rate and mixing relies partly on diffusion. The time scale for diffusive mixing is $r^2/3.6D$ [2], which for our reactors is on the order of 5–20 seconds. This would be the maximum uncertainty in the residence times in the reactor. The shorter mixing times correspond to the 250cc reactor operated at the highest temperatures (50°C), which also correspond to the shortest residence times. The longer mixing times correspond to the 1000cc reactor operated at the lowest temperature (24°C) Consequently, the mixing times are much shorter than the residence times, 100–1620 seconds, so there would be at most a 5% uncertainty in the reaction times. Also, unlike linear flow tubes in which there can be induction times due to flow mixing and establishment of laminar flow, the analyte and carrier gas are already well mixed when they enter the reactor, so no such time offset pertains.

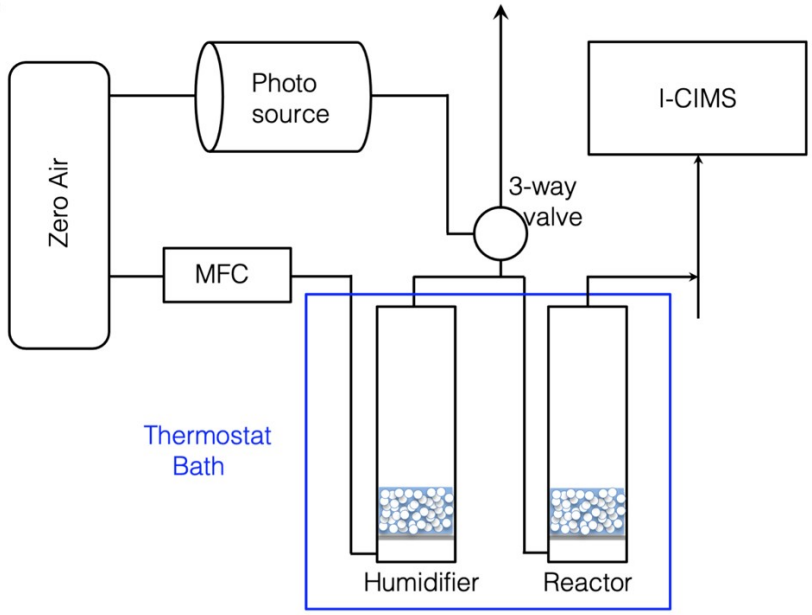

Figure S3. Schematic diagram of the bubble flow reactor system for the measurement of the Henry's Law solubility of fur-PAN.

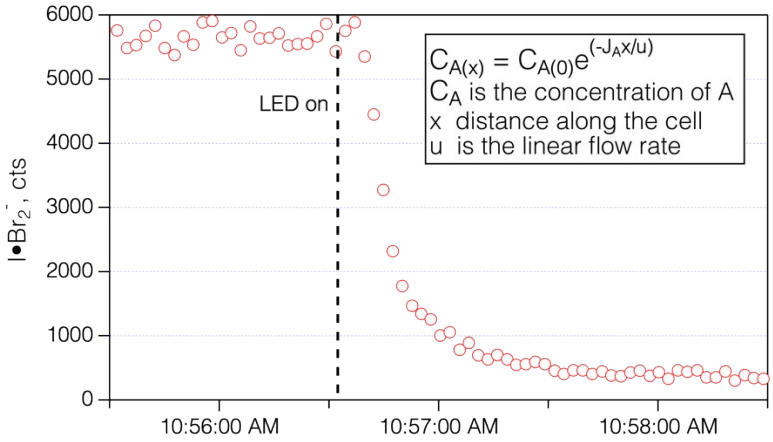

Figure S4. Photolysis profile of the Br_2 signal in the quadrupole I-CIMS.

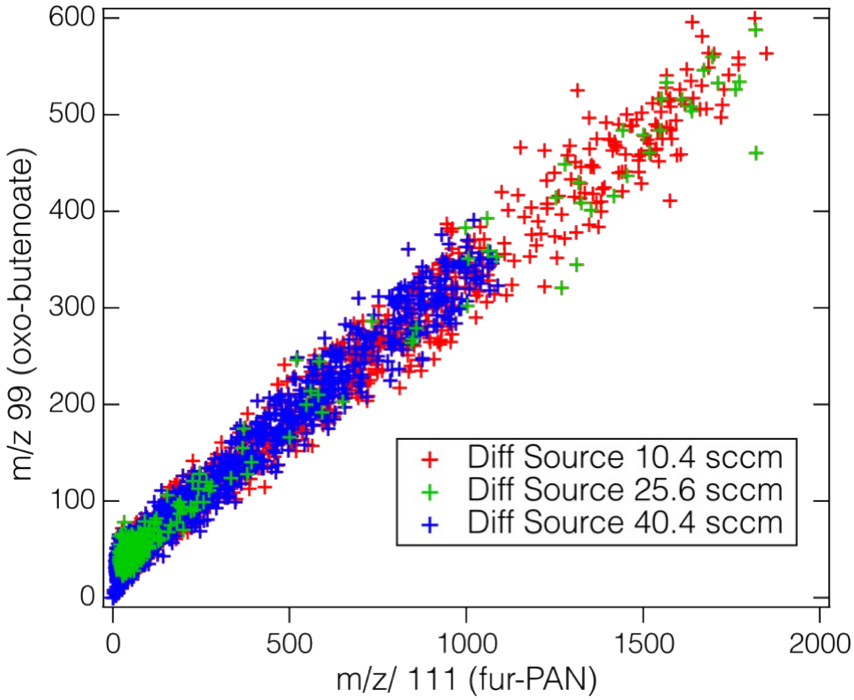

Figure S5. The I^-CIMS response at m/z 99 (oxo-butenoate) vs. the response at m/z 111 (furoate) under a variety of photosource conditions.

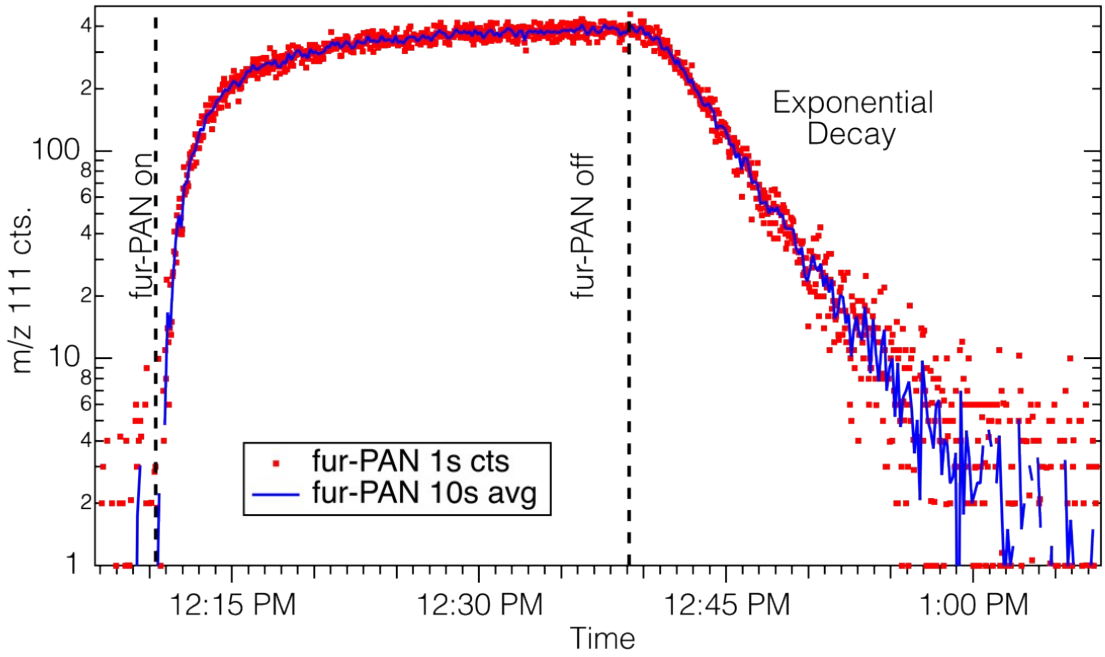

Figure S6. Example equilibration and exponential decay profile from a fur-PAN solubility measurement in which 25mL of DI water was equilibrated with a flow of 725 ambient cc/min containing fur-PAN.

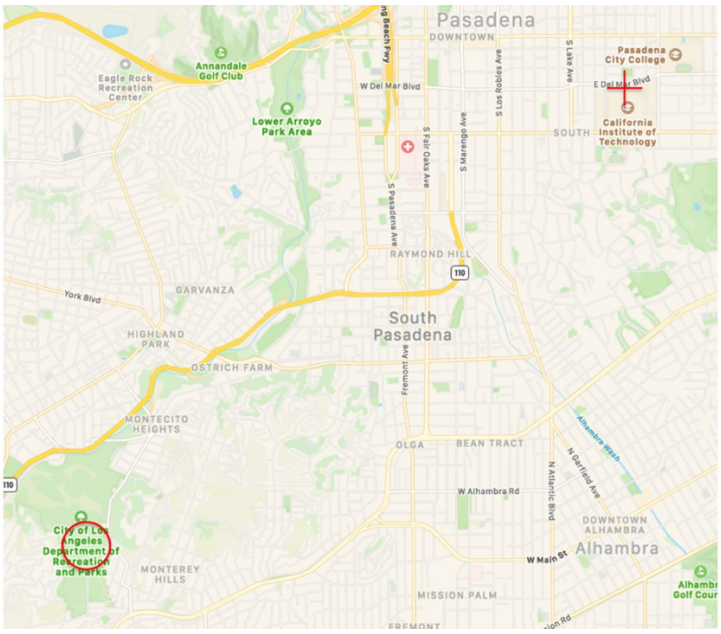

Figure S7. Map of the South Pasadena area showing the location of the Debs Park fire (red circle) and SUNVEx Pasadena measurement site (red cross). The distance between the two is approximately 8 km.

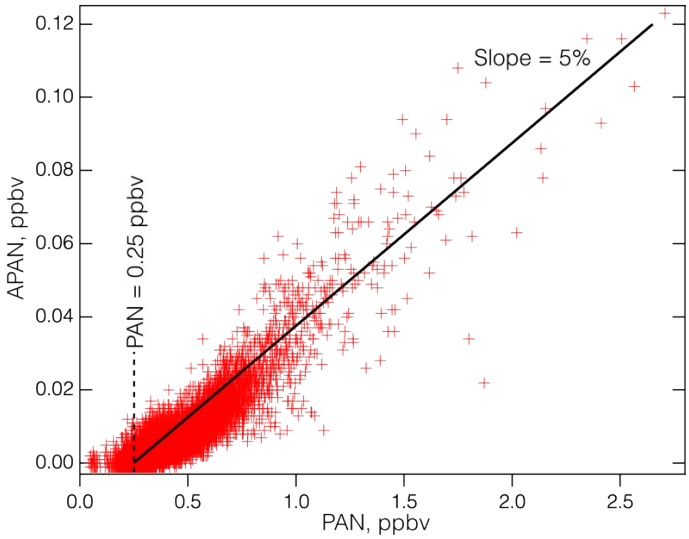

Figure S8. Measurements of APAN and PAN from the SENEX 2013 campaign during the July 2 (local time) flight of the NOAA WP-3 aircraft that sampled agricultural fires in the southeastern U.S. (see Decker et al., 2019). The black line is drawn for a ratio of APAN to PAN of 5%, with a background PAN mixing ratio of 0.25 ppbv.

References

1. H. Keller-Rudek, G. K. Moortgat, R. Sander and R. Sörensen, The MPI-Mainz UV/VIS spectral atlas of gaseous molecules of atmospheric interest, *Earth Syst. Sci. Data*, 2013, **5**, 365-373.
2. D. R. Hanson, J. B. Burkholder, C. J. Howard and A. R. Ravishankara, Measurement of OH and HO_2 radical uptake coefficients on water and sulfuric acid surfaces, *J. Phys. Chem.*, 1992, **96**, 4979-4985.