

SUPPORTING INFORMATION

Gas-Phase Detection of Fluorotelomer Alcohols and Other Oxygenated PFAS by Chemical Ionization Mass Spectrometry

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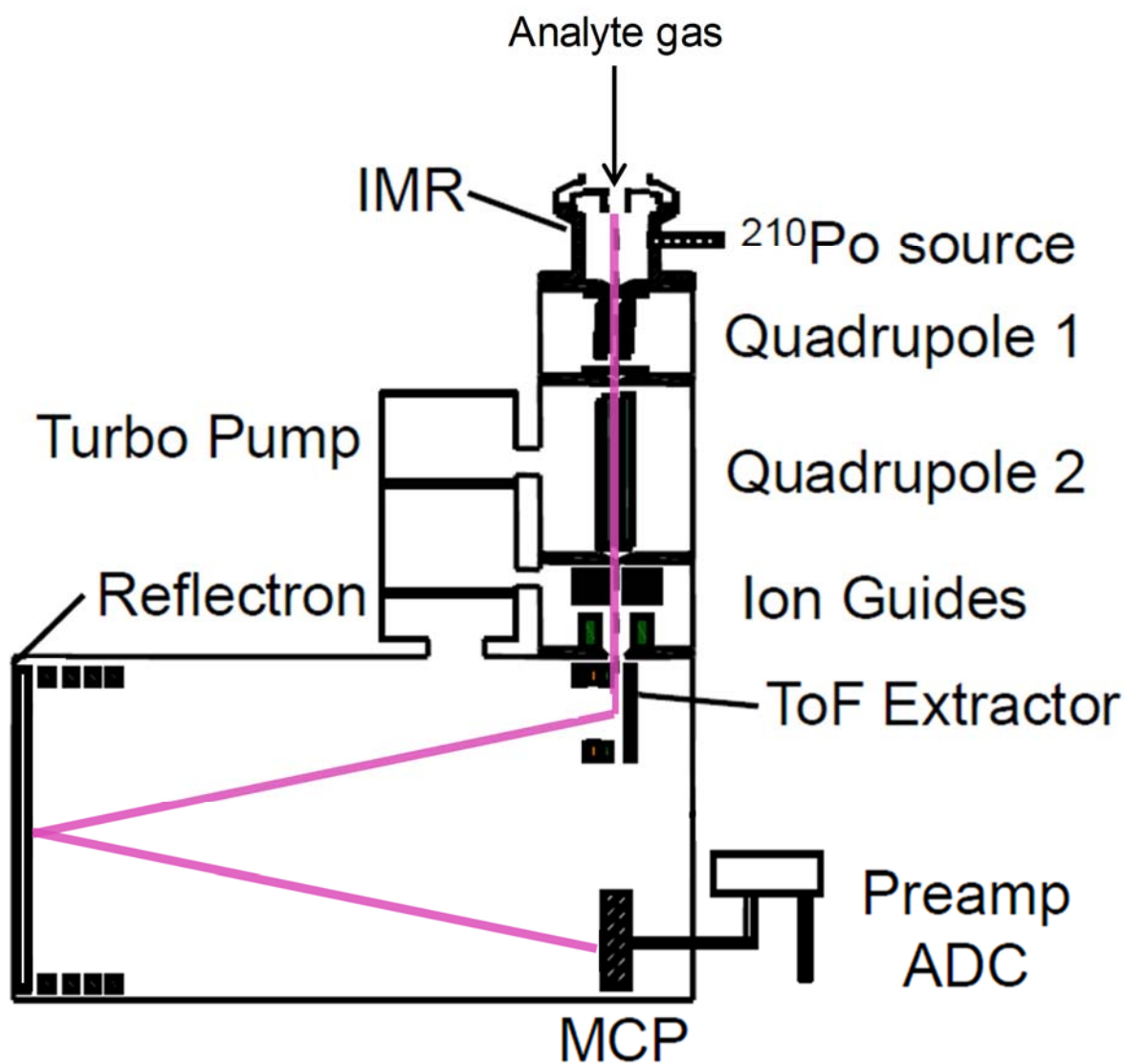


Figure S1. Schematic of the CIMS showing main elements of each vacuum region. The pink line illustrates the ion flight path through the instrument. IMR: ion-molecule reaction chamber; MCP: micro-channel plate detector; ADC: analog-to-digital converter.

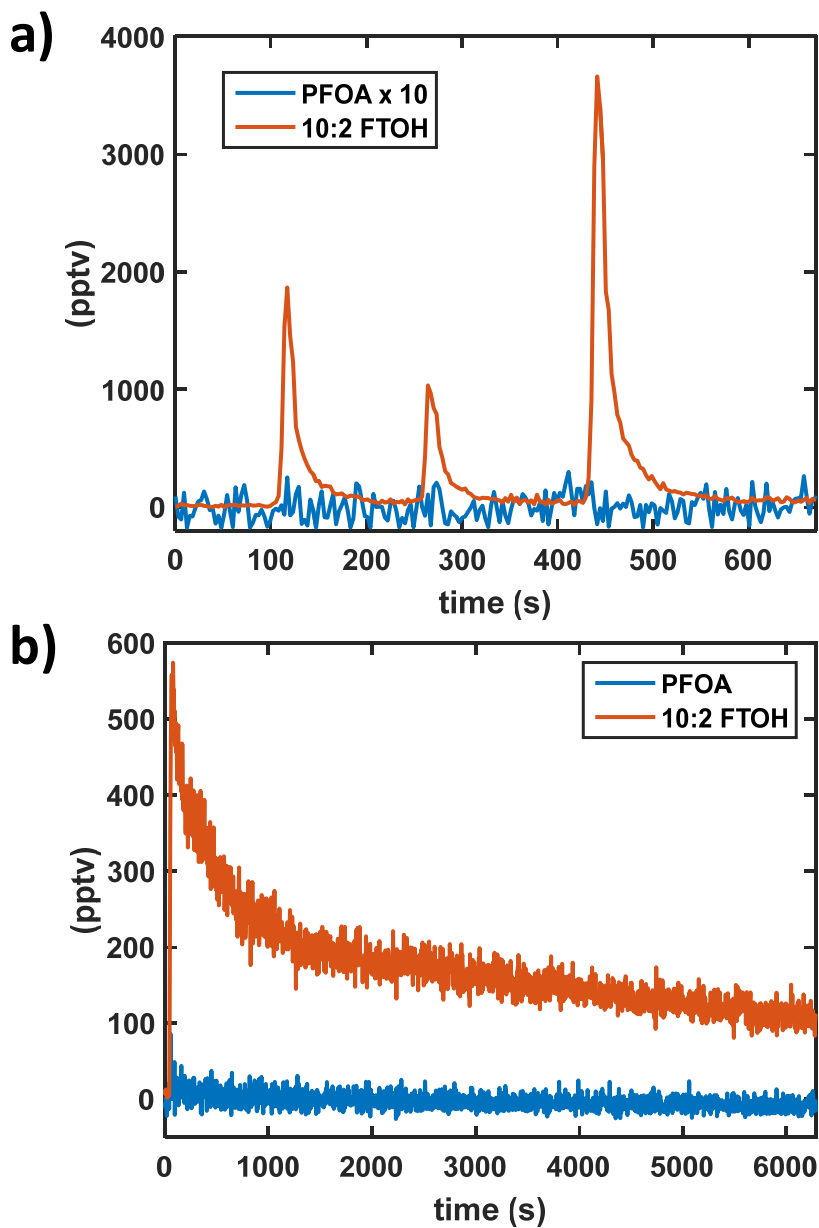


Figure S2. Time series of perfluorooctanoic acid (PFOA) and 10:2 fluorotelomer alcohol (FTOH) mixing ratios during (a) the 10:2 FTOH calibration and (b) sampling of the Zonyl FSA fluoro-product. The initial spike in 10:2 FTOH marks the beginning of (a) calibration injection or (b) product sampling. The average PFOA mixing ratio during each period was $-0.13 \pm 10.48(1\sigma)$ pptv and $-2.34 \pm 10.20(1\sigma)$ pptv, respectively. These are below the estimated PFOA detection limit of 5.9 pptv, indicating that significant PFOA was not produced from the calibration or sampling setups.

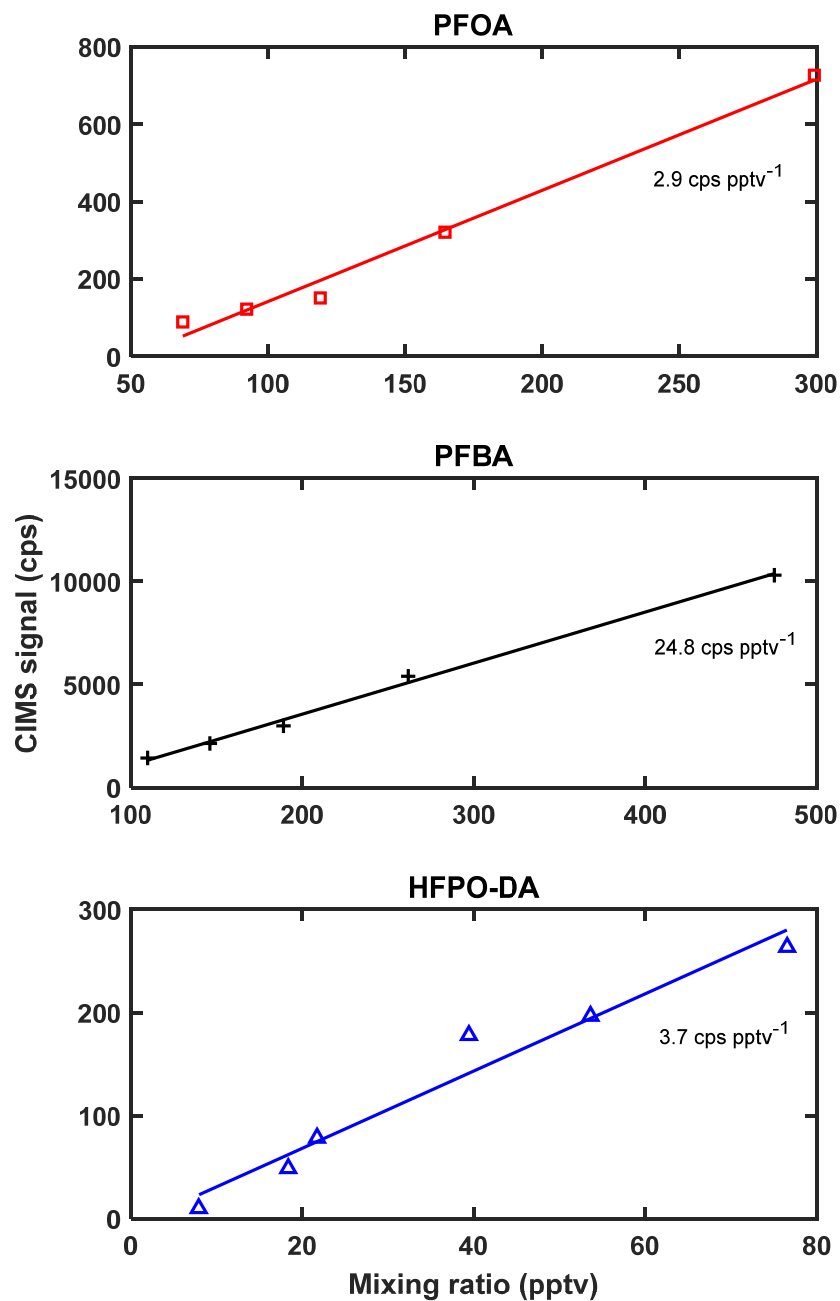


Figure S3. CIMS calibration curves for perfluorooctanoic acid (PFOA); perfluorobutanoic acid (PFBA); and hexafluoropropylene oxide dimer acid (HFPO-DA) with the corresponding calibration factors.

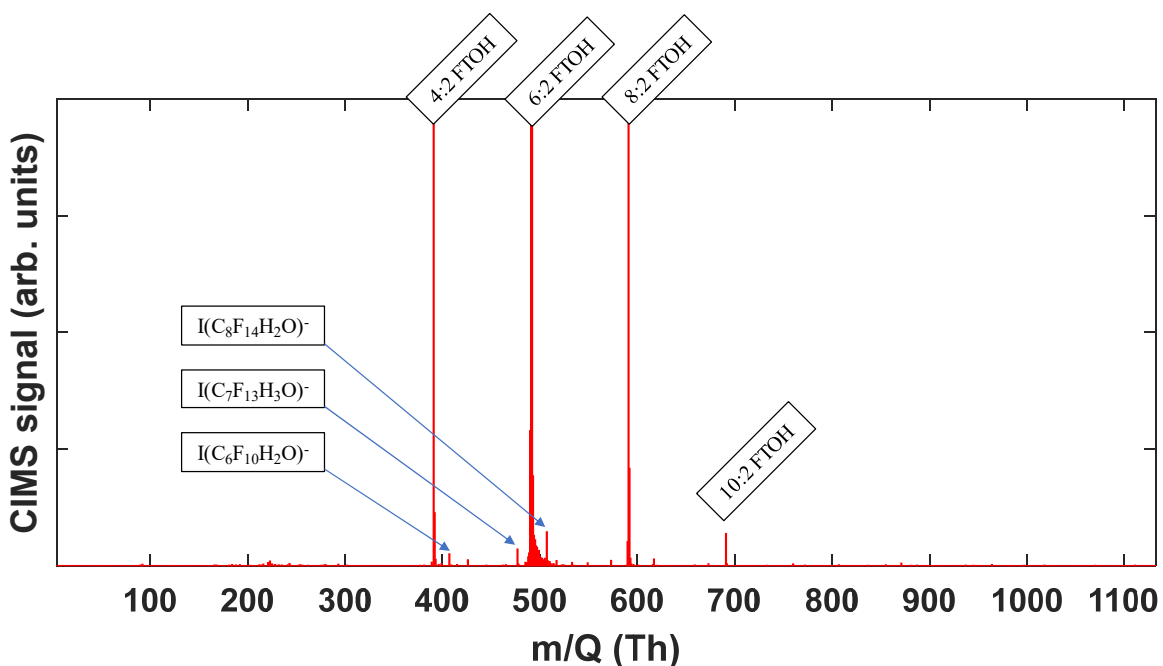


Figure S4. Unit mass resolution difference mass spectrum illustrating the enhancement of PFAS signals while sampling Masurf FS-115 relative to background sampling. The difference mass spectrum is produced by subtracting the background mass spectrum from the product sampling mass spectrum, which illustrates the enhanced peaks during product sampling. Known and probable molecular composition assignments for some of the observed peaks are provided.

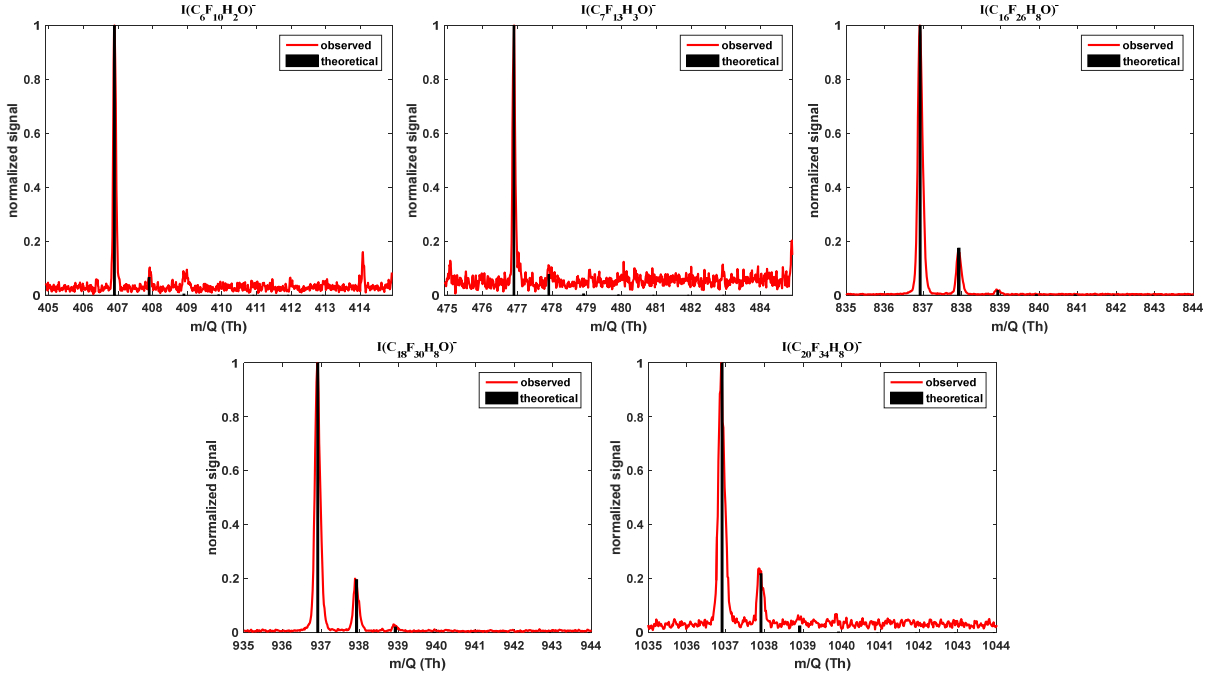


Figure S5. Isotopic distribution for molecular composition assignments from Masurf FS-115 mass spectra.

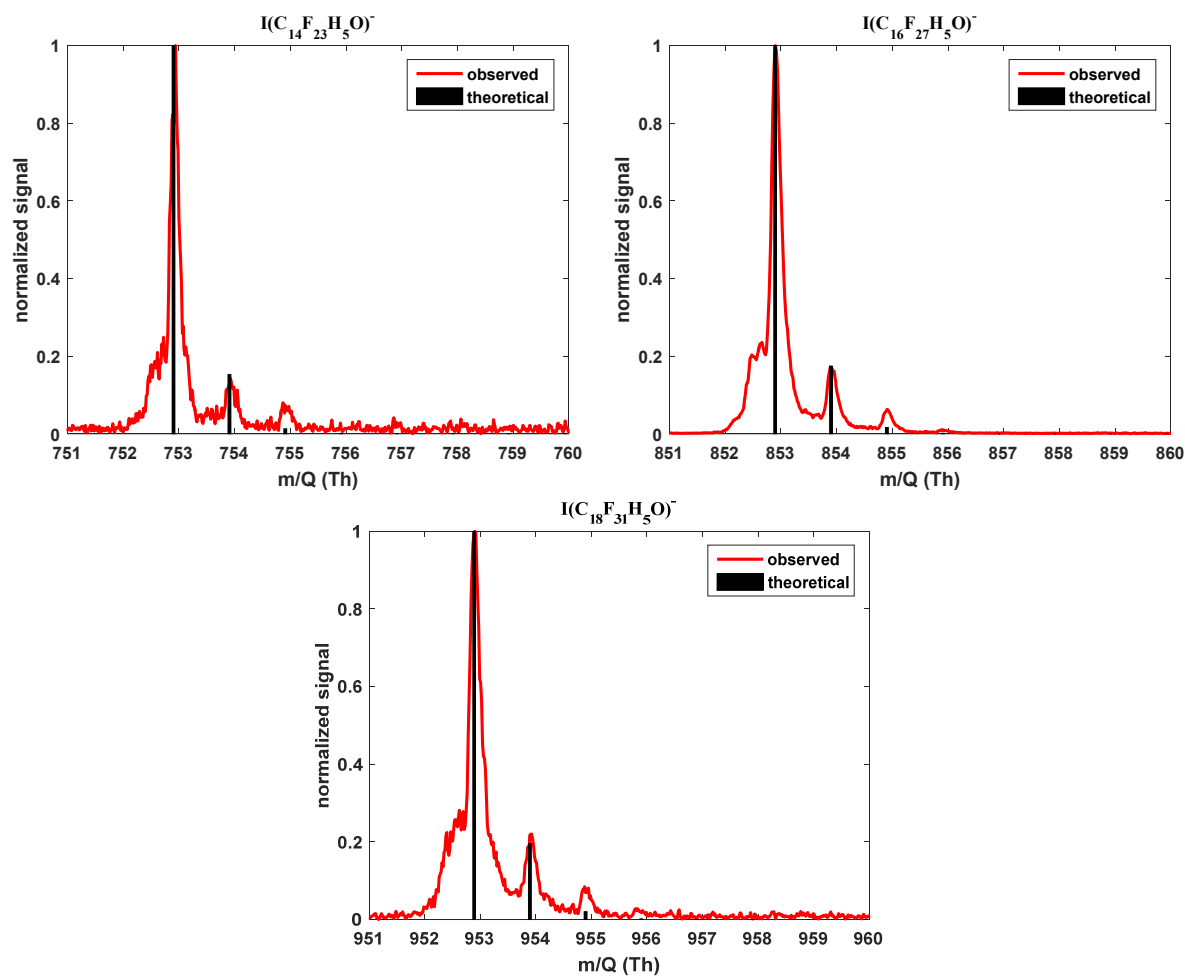


Figure S6. Isotopic distribution for molecular composition assignments from Zonyl FSA mass spectra.

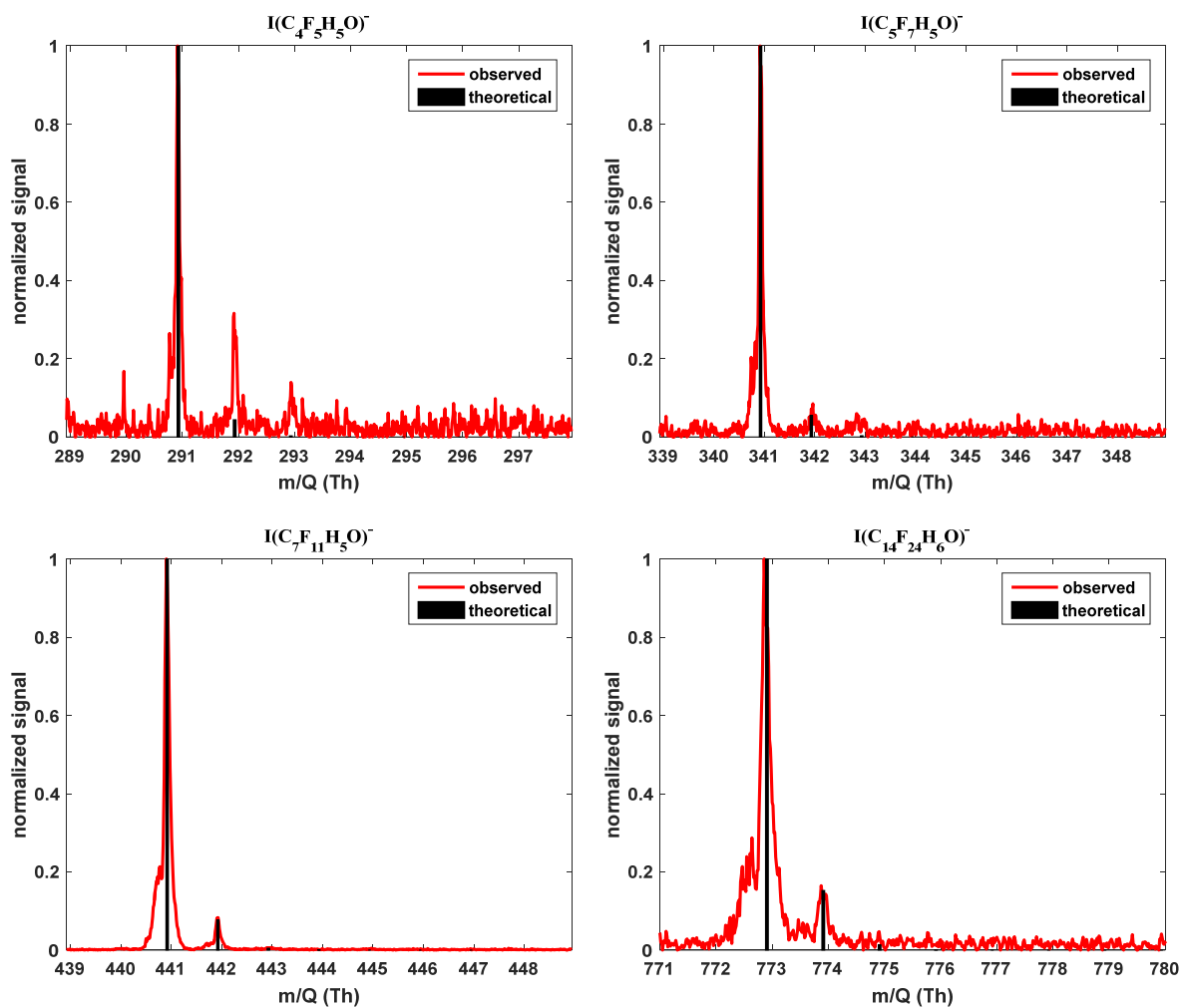


Figure S7. Isotopic distribution for molecular composition assignments from Capstone FS-35 mass spectra.

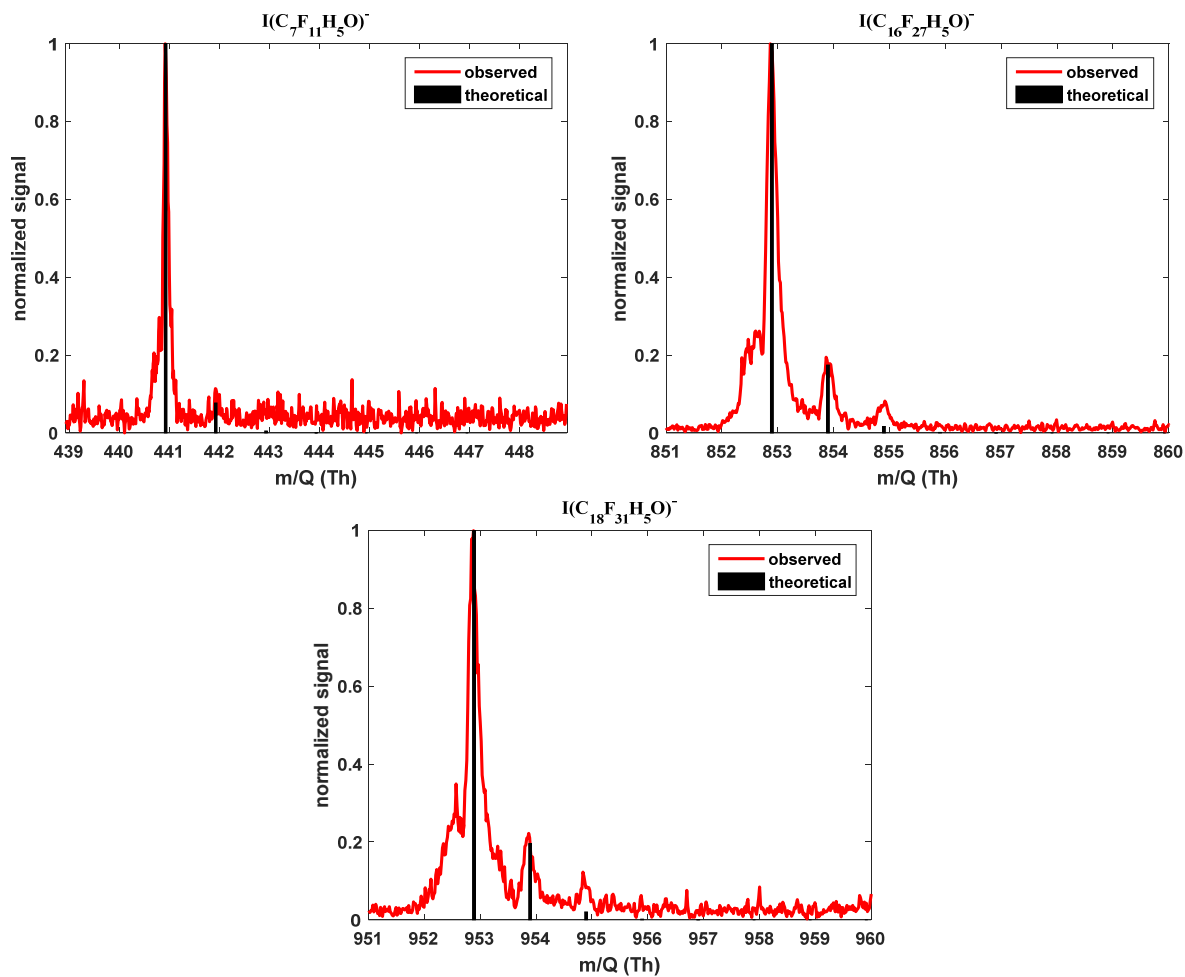


Figure S8. Isotopic distribution for molecular composition assignments from Arctic 3 AFFF mass spectra.

Table S1. CIMS Specifications

Manufacturer:	TOFWERK AG	www.tofwerk.com/products/api-tof/
	Aerodyne Research Inc.	www.aerodyne.com/products/chemical-ionization-time-flight-mass-spectrometer-tof-cims
ToF analyzer type:	HTOF	
Purchase date:	Autumn 2011	
Mass resolving power*:	3000 - 7000 (M/ Δ M, FWHM)	
Mass range:	1 - 20000 Th	
Mass accuracy (manufacturer):	4 ppm	
Mass accuracy (this study)**:	8.7 \pm 4.8 (1 σ) ppm	
ToF Power Supply version:	TPS1	
Analysis software (version):	Toftools (2.5.13)	www.tofwerk.com/software/toftware/

*M = peak center location; Δ M = Full Width at Half Maximum of peak

**calculated from Table 2 mass errors