1   Supplemental Material for:

3 Stability assessment of organic sulfur and organosulfate compounds in filter samples for

4   quantification by Fourier Transform-Infrared Spectroscopy

5   Marife B. Anunciado[1], Miranda De Boskey[2], Laura Haines[2], Katarina Lindskog[2], Tracy

6   Dombek[2], Satoshi Takahama[3], Ann M. Dillner[1]

8   [1]Air Quality Research Center, University of California Davis, Davis, California, United States

9   [2]Research Triangle Institute, Research Triangle Park, North Carolina, United States

10   [3]Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland

11

Table S1. Reference wavenumbers and % transmissions from SBDS database [1] compared to wavenumbers obtained from laboratory standards for organosulfur and organosulfate compounds of interest. Percent transmissions increase with peak intensity.

Organosulfur or organosulfate compound	Wavenumber, reference	T % transmission	Wavenumber, laboratory standards
Methanesulfonic acid	1415	62	1414
	1342	4	1338
	1173	4	*
	1049	39	1061, 1050
	987	6	987
	895	7	900
	768	18	766
	536	6	535
	504	12	*
Hydroxymethanesulfonate, sodium salt	1432	60	1414
	1343	64	No peak
	1229, 1204, 1150		PTFE
	1086	31	1092
	1042	10	1041
	1033	10	No peak/shoulder of 1042
	933	79	934
	761		*
	732		*
	707		*
	605		*
	538		*
	522		*
Methyl sulfate, sodium salt	1458	16	1458
	1376	26	*

---

[1] Reference spectra of each compound was taken from https://sdbs.db.aist.go.jp/sdbs/cgi-bin/direct_frame_top.cgi.

1366	30	*
1209	12	*
1177	16	*
1154	25	*
		1135 (new peak)
1115	44	1115
1076	31	1073
999	16	1020, 1000
795	33	795
783	25	784
722	74	*
615	30	*
596	18	591
568	32	*

15

16   Note: * denotes a peak that is excluded from spectral characterization due to PTFE interference.

17

18

19

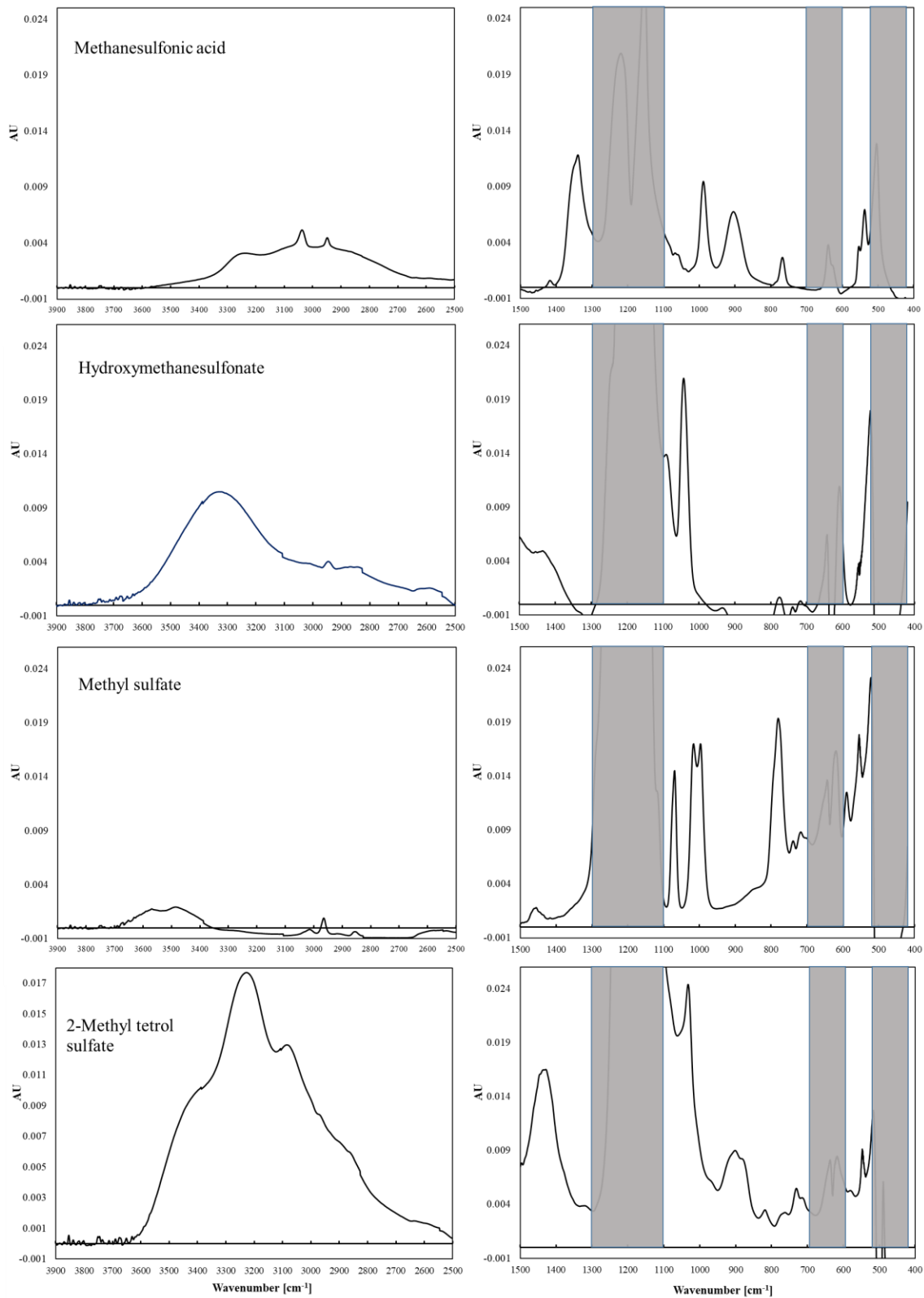



Figure S1. Baseline corrected spectra of selected compounds on PTFE filters.

22   Table S2. Vendor information for primary and secondary sources

Name of Solution or Salt	Primary Source	Secondary Source
1000 µg/mL Sulfate	SPEX CertiPrep (Metuchen, NJ)	NSI Lab Solutions (Raleigh, NC)
MSA	Sigma Aldrich, ≥ 99 % purity (St Louis, MO)	Acros Organics 99% purity (Fisher Scientific,Waltham, MA)
HMS	Alfa Aesar ,sodium salt, 95% purity (Ward Hill, MA)	TCI, sodium salt, >97.0% purity (Fisher Scientific, Waltham, MA)
MS	TCI, sodium salt, > 98.0 % purity (Fisher Scientific, Waltham, MA)	MP Biomedicals, potassium salt, 99.7% purity (Santa Ana, CA)

23

24

25

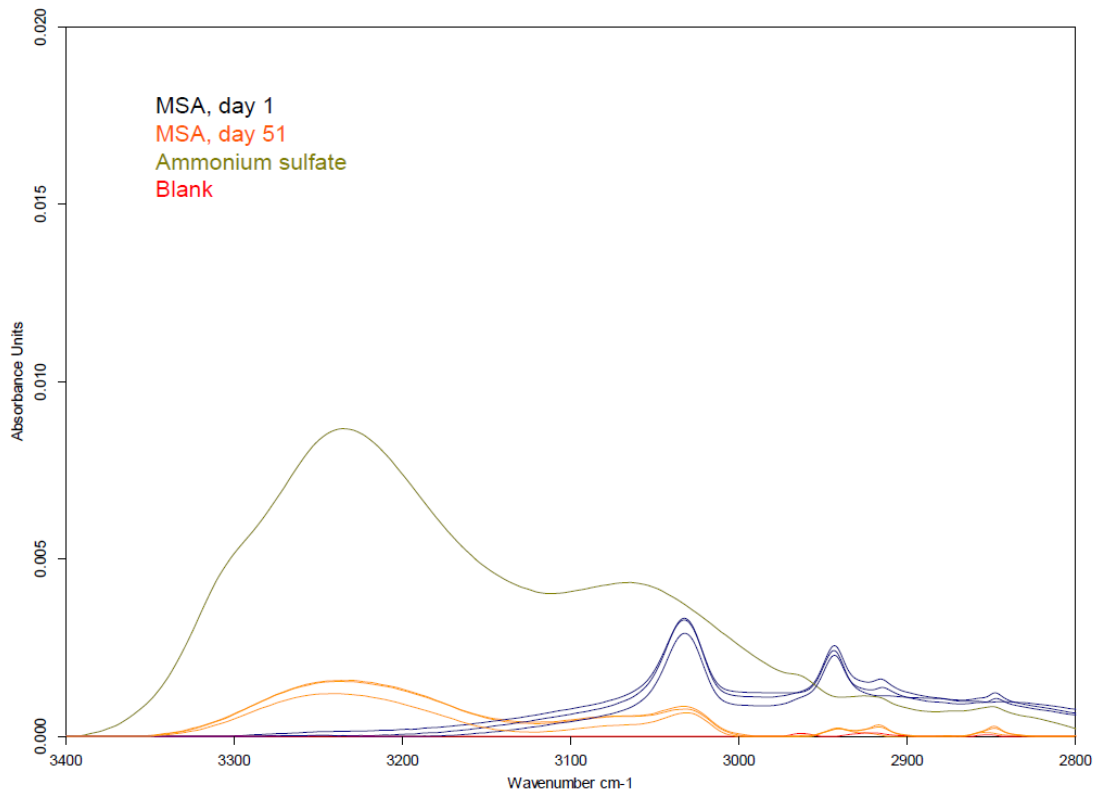
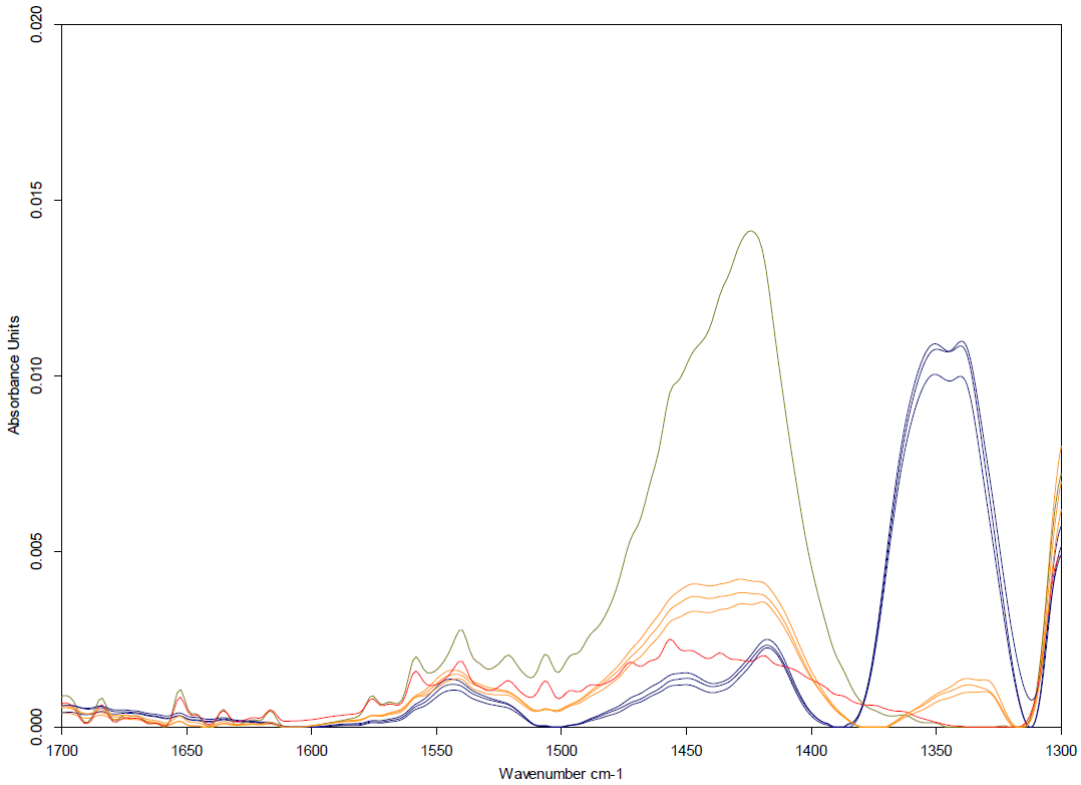



Figure S2. FT-IR spectra (split into two regions of four methanesulfonic acid (MSA) filters on day 1 in blue and day 51 in orange relative to ammonium sulfate (olive green) and blank (red).

29

30

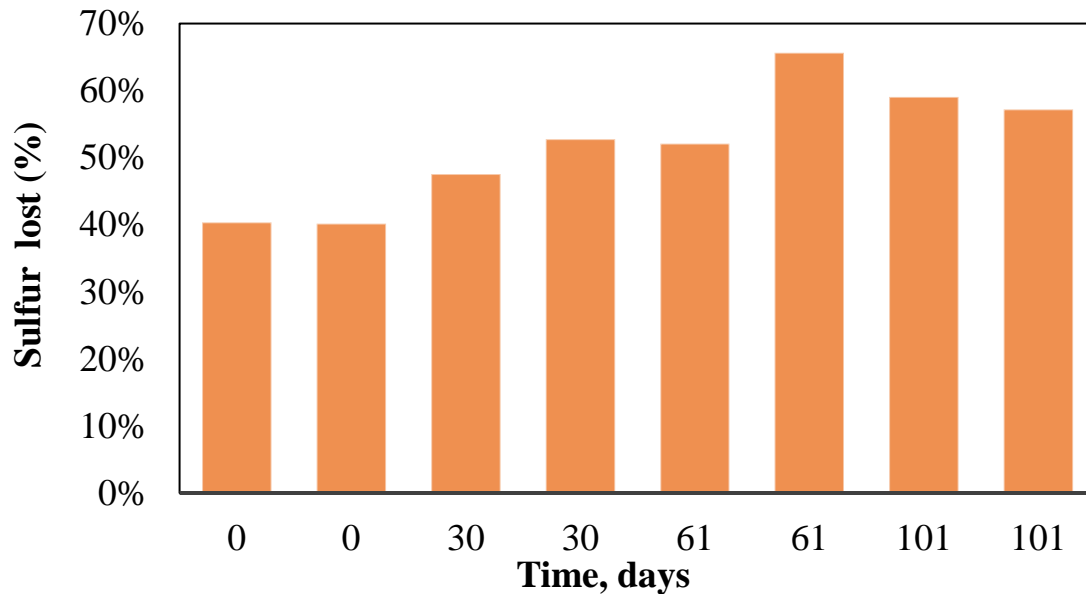



Figure S3. Percentage recovery of sulfur lost from PTFE filters over time as measured by
IC. At each time point, 2 filters were extracted and analyzed.

33

34

35

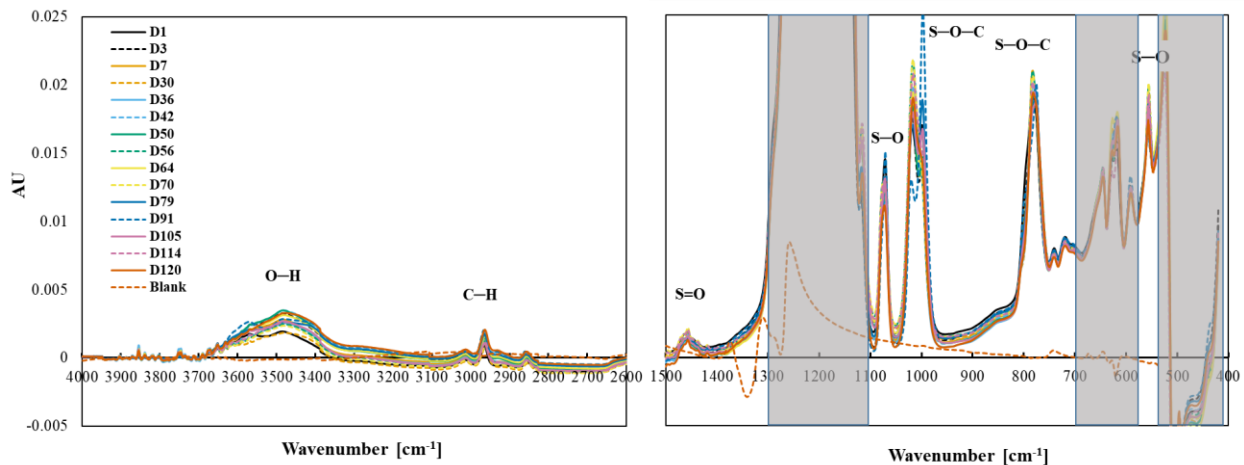



Figure S4. Same as Figure 7 except it include anomalous spectra collected on day 91.

37

38

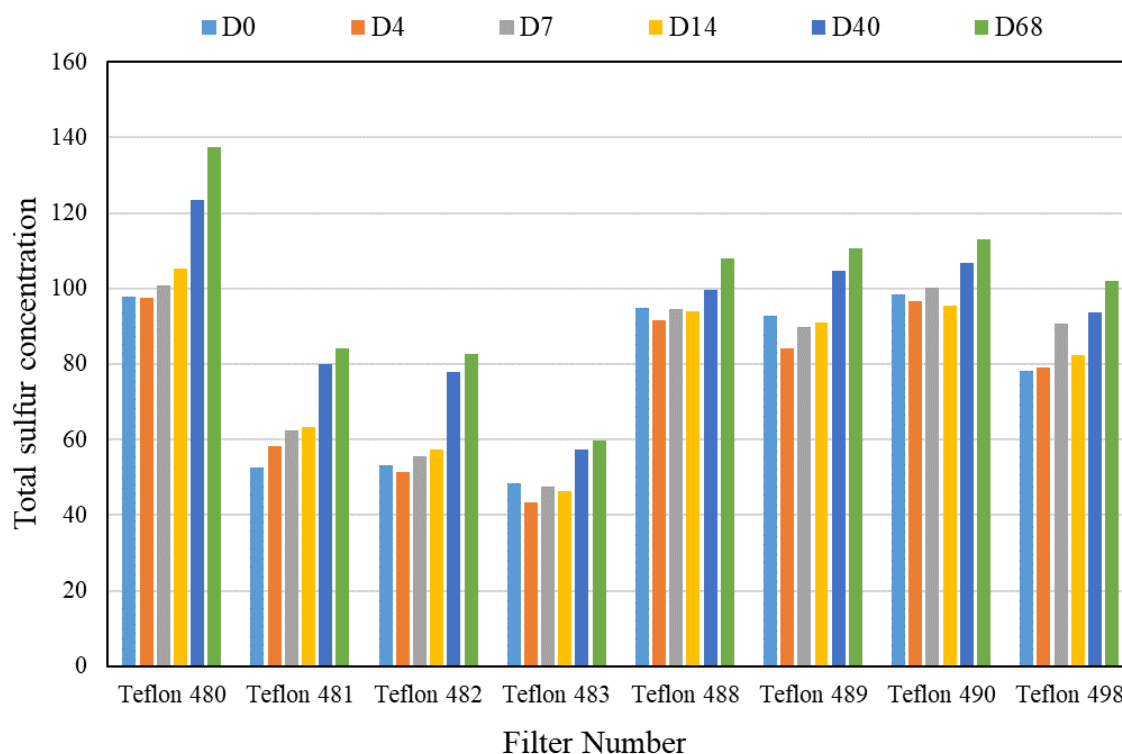
Eight PTFE filters were extracted on day 0 and recoveries of MTS averaged 78 ± 22% for ICP-

OES. Recoveries of QC samples were 97 ± 6%, suggesting inconsistent and incomplete

41   extraction. However, the extracts with the filters remaining in the extraction liquid were

42   analyzed over time and the extraction efficiency increases over time and averages $100 \pm 24\%$ on

43   day 68 (Figure S5). This suggest that improved extraction procedures could increase extraction

44   efficiency. Further work may be need to improve the consistency of the extraction.

45

46   Figure S5. Total sulfur concentrations via ICP-OES for eight 2-MTS filter samples analyzed six

47   times over a two month period. D0 stands for day 0, D4 is the fourth day, etc.