



*Supplement of*

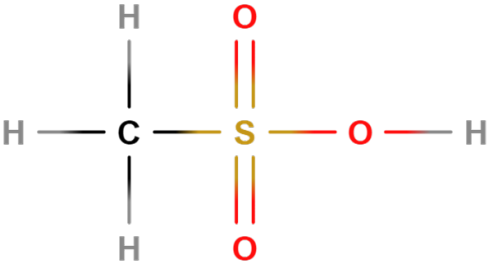
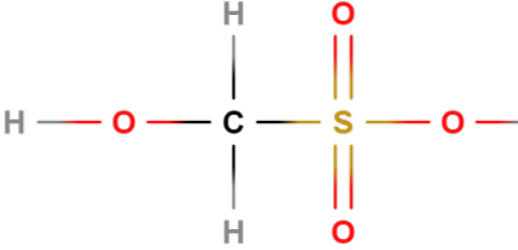
## **Stability assessment of organic sulfur and organosulfate compounds in filter samples for quantification by Fourier-transform infrared spectroscopy**

**Marife B. Anunciado et al.**

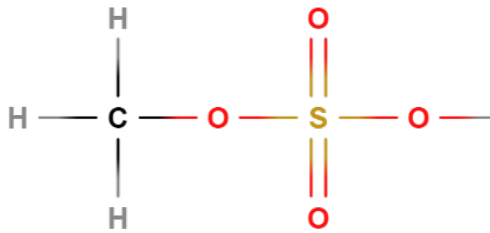
*Correspondence to:* Ann M. Dillner ([amdillner@ucdavis.edu](mailto:amdillner@ucdavis.edu))

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- 1 Table S1. Reference wavenumbers and % transmissions from SBDS database <sup>1</sup> compared to
- 2 wavenumbers obtained from laboratory standards for organosulfur and organosulfate compounds
- 3 of interest. Percent transmissions increase with peak intensity.

Organosulfur or organosulfate compound	Wavenumber, reference	T % transmission	Wavenumber, laboratory standards
Methanesulfonic acid (CH <sub>3</sub> SO <sub>3</sub> H) 	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 (HOCH <sub>2</sub> SO <sub>3</sub> H (Na)) 	1432	60
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 (CH <sub>3</sub> SO <sub>4</sub> H (Na))		1458	16
	1376	26	*

<sup>1</sup> Reference spectra of each compound was taken from [https://sdfs.db.aist.go.jp/sdfs/cgi-bin/direct\\_frame\\_top.cgi](https://sdfs.db.aist.go.jp/sdfs/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	*

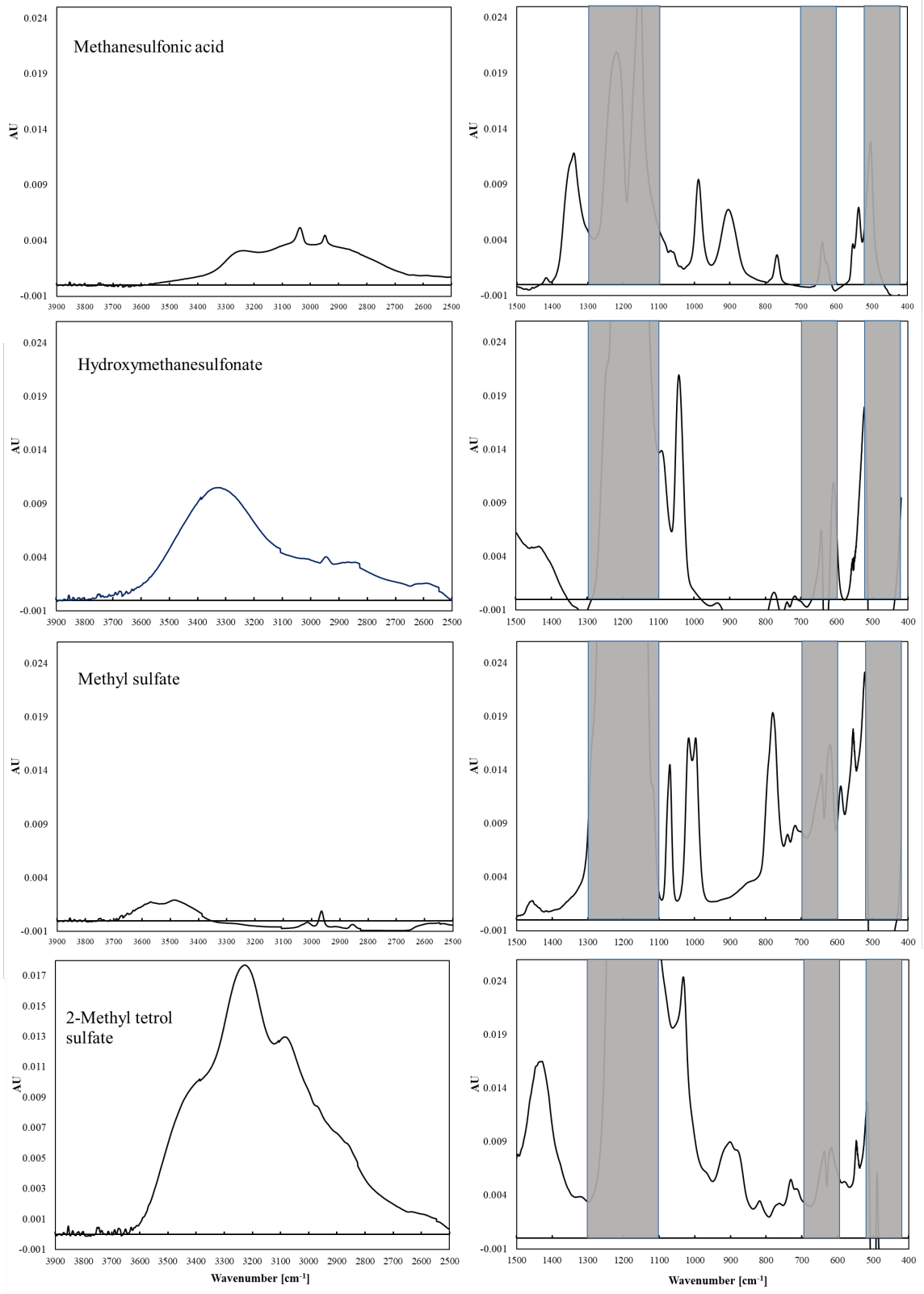
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5 Note: \* denotes a peak that is excluded from spectral characterization due to PTFE interference.

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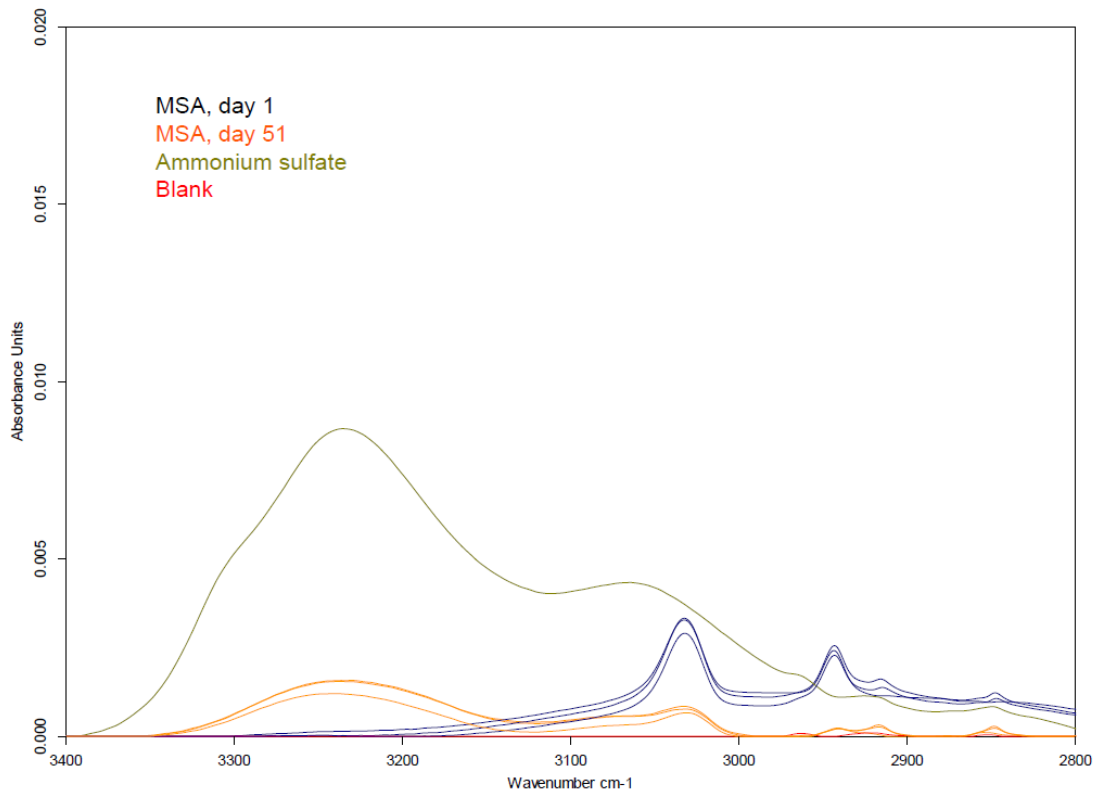
Figure S1. Baseline corrected spectra of selected compounds on PTFE filters.

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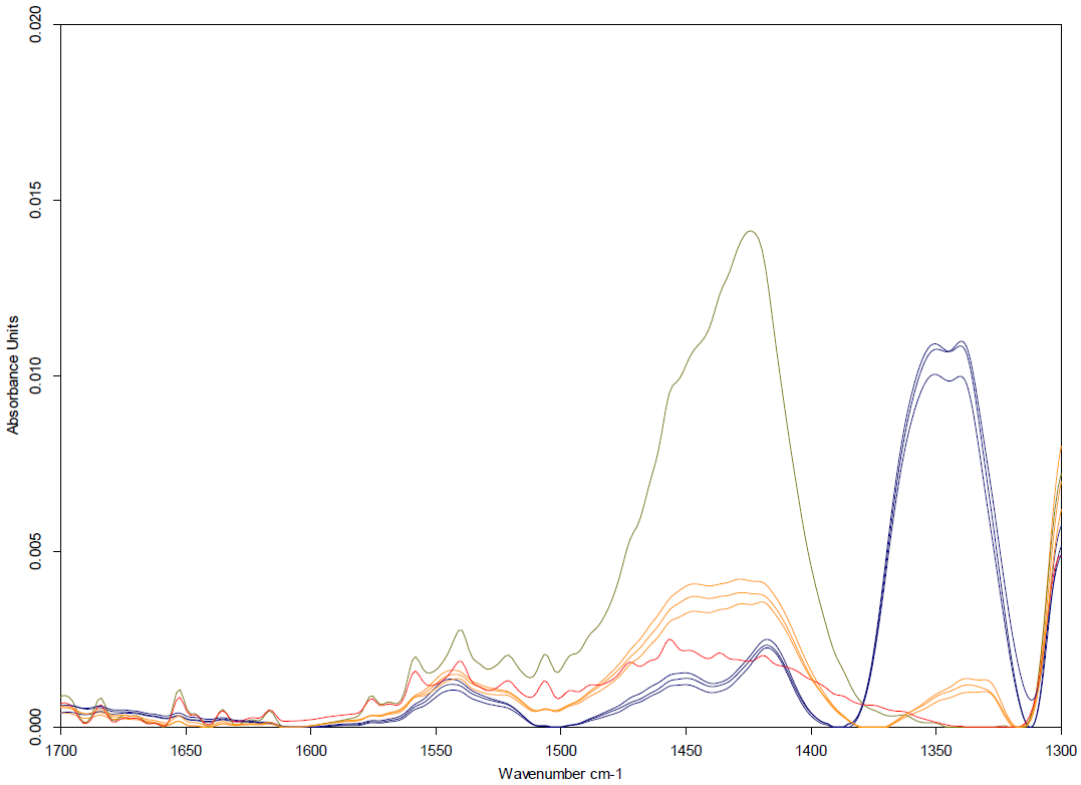
Table S2. Vendor information for primary and secondary sources

Name of Solution or Salt	Primary Source	Secondary Source
1000 $\mu\text{g/mL}$ Sulfate	SPEX CertiPrep (Metuchen, NJ)	NSI Lab Solutions (Raleigh, NC)
MSA	Sigma Aldrich, $\geq 99\%$ 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)

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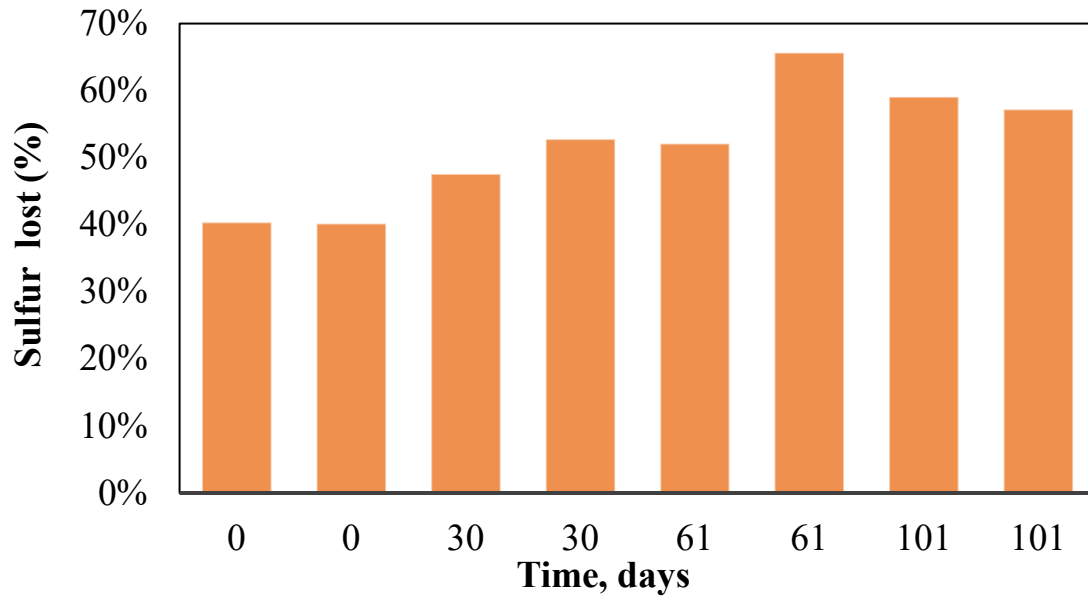
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15 Figure S2. FT-IR spectra (split into two regions of four methanesulfonic acid (MSA)  
 16 filters on day 1 in blue and day 51 in orange relative to ammonium sulfate (olive green)  
 17 and blank (red).

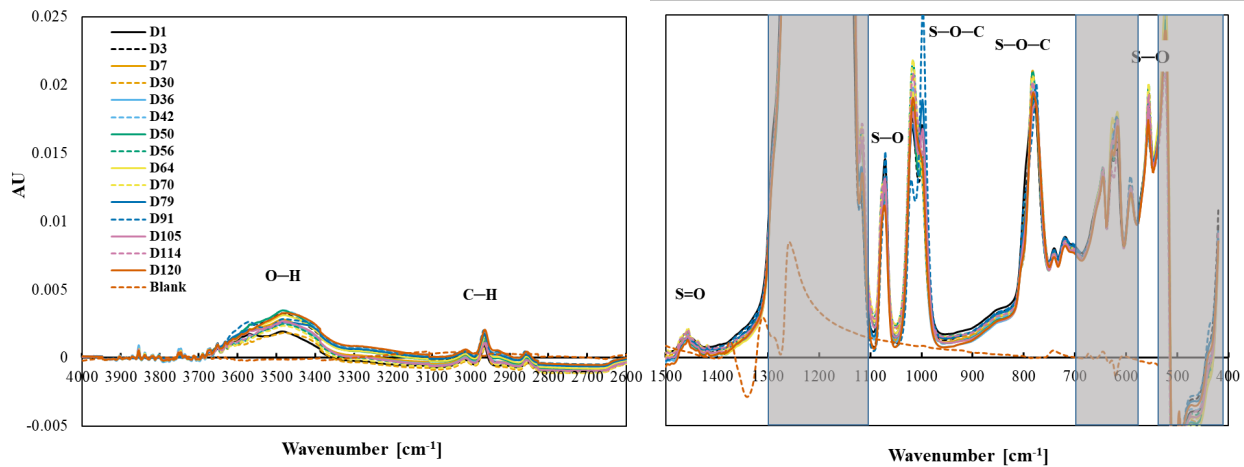
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20 Figure S3. Percentage recovery of sulfur lost from PTFE filters over time as measured by  
21 IC. At each time point, 2 filters were extracted and analyzed.  
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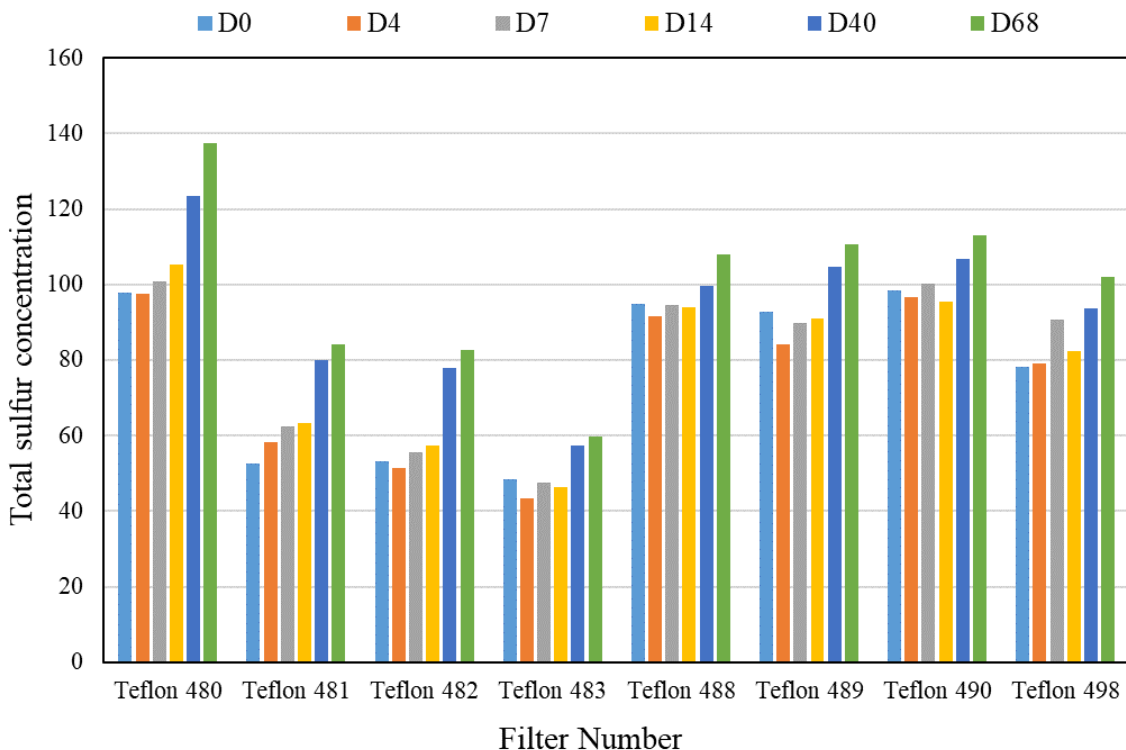
25 Figure S4. Same as Figure 7 except it include anomalous spectra collected on day 91.  
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28 Eight PTFE filters were extracted on day 0 and recoveries of MTS averaged  $78 \pm 22\%$  for ICP-

29 OES. Recoveries of QC samples were  $97 \pm 6\%$ , suggesting inconsistent and incomplete

30 extraction. However, the extracts with the filters remaining in the extraction liquid were  
31 analyzed over time and the extraction efficiency increases over time and averages  $100 \pm 24\%$  on  
32 day 68 (Figure S5). This suggest that improved extraction procedures could increase extraction  
33 efficiency. Further work may be need to improve the consistency of the extraction.



34  
35 Figure S5. Total sulfur concentrations via ICP-OES for eight 2-MTS filter samples analyzed six  
36 times over a two month period. D0 stands for day 0, D4 is the fourth day, etc.