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Molecular characterization of atmospheric particulate organosulfates in three megacities at the middle and lower reaches of the Yangtze River

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Table S1. Comparison of air quality and meteorological conditions (arithmetic mean ± standard deviation) between the SH sampling days and the seasonal average.

Time	Air quality [a]						Meteorological conditions [b]		
	$PM_{2.5}$	PM_{10}	O_3	SO_2	NO_2	CO	Wind speed	Temperature	Relative humidity
	μg m^{-3}	μg m^{-3}	μg m^{-3}	μg m^{-3}	μg m^{-3}	mg m^{-3}	m s^{-1}	℃	%
28 - 29 Jul, 2013	52.5	75.0	184.5	19.0	38.5	0.69	1.7±0.8	34.8±2.2	49.4±8.3
1 Jun - 31 Aug, 2013	43.4±24.5	59.9±26.1	136.0±58.0	14.6±5.2	34.0±11.7	0.67±0.16	2.5±1.2	28.7±5.1	70.1±16.0
17 - 18 Jan, 2013	77.0	90.5	68.0	32.5	57.5	1.01	2.9±1.8	0.9±1.1	58.3±3.2
26 Dec, 2012 –28 Feb, 2013	78.4±48.1	84.4±46.6	72.0±23.1	27.5±15.0	54.7±21.5	0.99±0.40	2.3±1.1	5.8±3.9	71±16.5

[a] Arithmetic mean of 24h average concentrations

[b] Arithmetic mean of hourly average concentrations

Extraction efficiency and repeatability of the extraction protocol

5 µL of a 200 µM solution of methyl sulfate, octyl sulfate, dodecyl sulfate and camphor sulfonic acid were deposited on a quartz filter that was then extracted and analyzed as described in the main text. Three replicates were performed. The average chromatographic peak area obtained for each compound was compared to the average value obtained for three injections of a 1 µM standard solution (1 µM being the theoretical final concentration of the extract) to assess the extraction efficiencies. The repeatabilities were determined as the standard deviation obtained from the injection of the three replicates. Limits of detection (LODs) were estimated from calibration curves (0 to 2 µM) as $3.3*(\sigma_{slope}/a)$ with a the slope of the calibration curve and σ_{slope} standard deviation on the slope. They are reported in Table S2.

Table S2. Extraction efficiencies and repeatabilities of the extraction protocol and estimated limits of detection.

	Standard solution		Filter extract		Ext. Eff.	Estimated LOD (ng)
	Average area	Std. Dev.	Average area	Std. Dev.		
Methyl sulfate	4.6 108	1.6%	3.3 108	5.6%	71.4%	0.019
Octyl sulfate	3.2 1011	2.4%	3.0 1011	2.3%	95.0%	0.012
Dodecyl sulfate	5.9 1011	2.3%	5.7 1011	3.1%	97.7%	0.24*
Camphor sulfonic acid	1.3 1011	0.9%	1.2 1011	1.7%	94.0%	0.032

* High LOD due to the presence of dodecyl sulfate in the blank analysis.

Table S3. List of tentatively assigned OSs. Below are OSs and nitrooxy-OSs with an arbitrary intensity larger than 0.5% of the most abundant one in the same sample. Data for the NJSD sample is not included because a large amount of sample injection led to corruption of peaks and hence inaccurate retention times and worse peak resolution.

Neutral mass	Formula	Number of isomers	Retention times (min)	Sample ID	Potential precursor	Ref.
166.0301	$C_5H_{10}O_4S_1$	8	1.45	NJSN, SHWN	Isoprene	Szmigielski, 2015
			4.68; 4.85; 5.59; 5.82; 6.11; 7.58	NJSN, SHWD, SHWN		
			7.44	SHWD, SHWN		
168.0458	$C_5H_{12}O_4S_1$	3	6.18; 6.41; 6.78	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
177.9937	$C_5H_6O_5S_1$	3	2.95; 3.37	WHS, SHWN		
			1.31	SHWN		
180.0458	$C_6H_{12}O_4S_1$	3	6.48; 6.66	NJSN, WHW, SHWD, SHWN		
			8.31	WHW, SHWD, SHWN		
182.0251	$C_5H_{10}O_5S_1$	11	1.15	WHW, WHS, NJSN, SHSN	Isoprene	Riva et al., 2015a
			1.33; 3.35; 3.63; 4.85; 5.26	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			2.94	WHS, NJSH		
			5.40	WHW, WHS, NJSN, SHWN, SHSD, SHSN		
			5.48; 5.98	WHS		
			5.89	WHW, WHS		
182.0615	$C_6H_{14}O_4S_1$	6	6.86; 7.05; 7.23; 7.44; 7.56; 7.65	WHW, NJSN, SHWD, SHWN, SHSD, SHSN		
184.0407	$C_5H_{12}O_5S_1$	3	3.62; 4.57; 4.97	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
188.0145[p]	$C_7H_8O_4S_1$	4	5.40; 6.61	NJSN, SHWN	2-methyl-naphthalene	Riva et al., 2015b
			6.60	SHWN		
			4.80	NJSN		
189.9939	$C_6H_6O_5S_1$	3	1.25; 4.26; 5.84	WHW		

192.0095	$C_6H_8O_5S_1$	4	1.38	WHW		
			4.65; 4.93; 5.14	WHS, WHW		
193.9886	$C_5H_6O_6S_1$	5	1.15	WHW, WHS, SHWD, SHWN		
			1.33; 3.38; 4.34; 4.76	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
194.0250	$C_6H_{10}O_5S_1$	4	4.92; 5.31; 5.86	NJSN, SHWD, SHWN		
			6.09	SHWD,SHWN		
194.0614	$C_7H_{14}O_4S_1$	7	5.17	SHWD		
			5.28; 6.09; 6.93; 8.98	SHWD, SHWN		
			7.94; 8.21	SHWN		
196.0043	$C_5H_8O_6S_1$	5	1.34; 3.68; 4.69; 5.40	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			6.18	WHS, NJSN, SHWN, SHSN		
196.0407	$C_6H_{12}O_5S_1$	6	2.82	WHW, WHS, NJSN, SHWD, SHWN, SHSN		
			1.34; 5.18; 5.44 6.05	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			7.05	WHW, WHS, SHWN, SHSN		
196.0771	$C_7H_{16}O_4S_1$	3	8.00; 7.79; 8.42	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
198.0200	$C_5H_{10}O_6S_1$	7	1.34; 4.10; 4.74; 5.13; 5.30; 6.10	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN	Isoprene	Riva et al., 2015a
			5.84	NJSN, SHWD, SHWN, SHSD, SHSN		
198.0564	$C_6H_{14}O_5S_1$	4	5.89; 5.19; 6.06	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			6.19	WHW, WHS, SHWD, SHWN, SHSD, SHSN		
200.0146[p]	$C_8H_8O_4S_1$	5	5.40; 5.51; 5.89; 6.98; 7.95	SHWN	2-methyl-naphthalene	Riva et al., 2015b

200.0357	$C_5H_{12}O_6S_1$	1	1.36	WHW, WHS, NJSN, SHWN, SHSD, SHSN	Isoprene	Riva et al., 2015a
201.9938 [p]	$C_7H_6O_5S_1$	1	4.56	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN	2-methyl-naphthalene	Riva et al., 2015b
204.0096	$C_7H_8O_5S_1$	3	5.28; 6.94; 7.31	WHW		
206.0251	$C_7H_{10}O_5S_1$	5	4.81	WHS		
			5.19; 5.70; 5.85; 6.11	WHS, NJSN		
208.0043	$C_6H_8O_6S_1$	6	1.97	WHW, WHS, SHWD		
			1.34; 2.21; 4.53; 5.78	WHW, WHS, NJSN, SHWD, SHWN, SHSD		
			6.22	WHW, NJSN, WHS		
208.0771	$C_8H_{16}O_4S_1$	5	7.18	WHW, NJSN, SHWD		
			6.93	WHW, SHWD, SHWN		
			7.73; 8.34	WHW, NJSN, SHWD, SHWN		
			10.33	WHW		
209.9836	$C_5H_6O_7S_1$	2	0.98; 1.33	WHW, WHS, NJSN, SHWD, SHWN, SHSN		
210.0200	$C_6H_{10}O_6S_1$	8	1.36; 3.92; 4.65; 4.99; 5.27; 5.53	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			5.70	WHS, SHSN		
			6.19	WHS, NJSN, SHWN, SHSD,SHSN		
210.0563	$C_7H_{14}O_5S_1$	7	5.39	WHW, WHS, NJSN, SHWD, SHWN, SHSN		
			5.92; 6.13; 6.35; 6.77	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			8.13; 8.52	WHW, WHS, SHSD, SHSN, SHWD		
210.0928	$C_8H_{18}O_4S_1$	3	8.48; 8.76; 9.09	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
211.9993	$C_5H_8O_7S_1$	1	1.36	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN	Isoprene	Surratt et al., 2008
212.0356	$C_6H_{12}O_6S_1$	8	1.36; 5.24; 5.72; 6.06; 6.34	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		

			6.78	WHW, NJSN, SHWD, SHWN, SHSD, SHSN		
			7.01; 7.15	WHS, SHWD, SHWN		
212.0721	$C_7H_{16}O_5S_1$	5	5.59; 5.80; 6.48; 6.95; 7.10	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
213.9939	$C_8H_6O_5S_1$	1	5.86	WHW, SHWD, SHWN, SHSD		
214.0150	$C_5H_{10}O_7S_1$	1	1.34	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN	Isoprene	Surratt et al., 2008
216.0095[p]	$C_8H_8O_5S_1$	3	5.39; 5.76; 6.56	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN	2-methyl-naphthalene	Riva et al., 2015b
216.0306	$C_5H_{12}O_7S_1$	2	1.15; 1.29	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN	Isoprene	Surratt et al., 2008
217.9888	$C_7H_6O_6S_1$	5	1.34; 5.05; 5.24; 5.65; 6.99	WHW		
218.0251	$C_8H_{10}O_5S_1$	6	5.19; 5.73; 5.98	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			6.30; 7.86	WHW, WHS, SHWN		
			8.16	WHW, WHS		
221.9470	$C_5H_2O_8S_1$	1	0.92	WHS		
222.0200	$C_7H_{10}O_6S_1$	5	1.36; 1.62; 1.95; 2.42; 4.76	WHW, WHS		
222.0928	$C_9H_{18}O_4S_1$	6	12.36	WHW, WHS, SHWD		
			7.66; 8.72; 10.46; 12.87	WHW, WHS, SHWD, SHWN		
			12.44	WHW, WHS		
223.9993	$C_6H_8O_7S_1$	2	1.14; 1.34	WHW, WHS, NJSN, SHWD, SHWN		
224.0357	$C_7H_{12}O_6S_1$	5	1.37	WHW, NJSN, SHWD, SHSN	α-pinene	Surratt et al., 2008
			2.65	WHW, WHS, NJSN, SHSN		
			3.19	WHW, WHS, NJSN, SHWD, SHSN		
			5.17; 5.93	WHW, WHS, NJSN,		

				SHWD, SHWN, SHSD, SHSN		
224.0720	$C_8H_{16}O_5S_1$	7	5.72; 5.95; 6.44; 7.60	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			9.21	WHW, WHS, SHWD, SHWN, SHSN		
			9.74	WHW, WHS, SHWN, SHSN		
			10.35	WHS		
224.1085	$C_9H_{20}O_4S_1$	4	9.00; 9.16; 9.37; 9.81	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
225.9785	$C_5H_6O_8S_1$	2	0.97	WHW, SHWD, SHWN		
			1.25	SHWN		
226.0150	$C_6H_{10}O_7S_1$	7	1.36; 2.72; 3.25; 4.57; 4.98	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN	3-Z-Hexenal	Shalamzari et al., 2014
			6.41; 7.02	NJSN, SHWD, SHWN, SHSD, SHSN		
226.0514	$C_7H_{14}O_6S_1$	5	5.84; 6.10; 6.56; 7.19	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			8.01	WHS, SHWD, SHWN		
226.0878	$C_8H_{18}O_5S_1$	4	6.73; 7.47; 7.73; 7.86	WHW, WHS, NJSN, SHWD, SHWN, SHSD		
227.0102	$C_5H_9O_7N_1S_1$	1	1.15	WHW, WHS		
227.9943	$C_5H_8O_8S_1$	1	1.34	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN	α-pinene	Surratt et al., 2008
228.0096 [p]	$C_9H_8O_5S_1$	4	5.80; 6.31; 6.69	WHW, SHWD, SHWN	2-methyl-naphthalene	Riva et al., 2015b
			8.86	SHWD		
228.0306	$C_6H_{12}O_7S_1$	5	1.36; 1.97; 2.38; 2.87; 4.76	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN	Isoprene	Riva et al., 2015a
228.0667	$C_7H_{16}O_6S_1$	4	5.57	WHS		
			4.97; 5.42; 5.76	WHS, SHWN		
229.0260	$C_5H_{11}O_7N_1S_1$	2	6.82; 7.22	WHW, NJSN, SHWD, SHWN, SHSD, SHSN		
229.9886 [p]	$C_8H_6O_6S_1$	4	3.49; 3.79	WHW, WHS	2-methyl-naphthalene	Riva et al., 2015b
			5.68	WHW, SHWD, SHWN		

			6.57	WHW, WHS, NJSN, SHWD, SHWN, SHSD		
230.0098	$C_5H_{10}O_8S_1$	1	1.11	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
230.0251[p]	$C_9H_{10}O_5S_1$	3	5.94; 6.17; 6.40	WHW, WHS, NJSN, SHWD, SHWN	2-methyl-naphthalene	Riva et al., 2015b
232.0044	$C_8H_8O_6S_1$	7	6.84	WHW, WHS		
			5.74; 6.10; 6.31; 7.29	WHW, WHS, SHWD, SHWN		
			5.30; 7.86	WHW, WHS, SHWN		
232.0407	$C_9H_{12}O_5S_1$	4	6.30	WHS, NJSN, SHWD	2-methyl-naphthalene	Riva et al., 2015b
			6.41; 6.61; 6.82	WHS, NJSN, SHWD, SHWN		
232.0772	$C_{10}H_{16}O_4S_1$	1	6.86	WHW		
234.9789	$C_6H_5O_7N_1S_1$	5	1.36	WHW, WHS, SHWD		
			5.61; 6.74; 7.11; 7.27	WHW, WHS, SHWD, SHWN		
236.0357	$C_8H_{12}O_6S_1$	2	4.98; 5.67	WHW, WHS, NJSN, SHWN		
236.0721	$C_9H_{16}O_5S_1$	5	5.73	WHW, WHS, SHWD, SHSD, SHSN		
			6.44; 7.35; 7.58; 7.91	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
238.0149	$C_7H_{10}O_7S_1$	4	1.36; 3.87; 4.81	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			5.55	WHW, WHS, SHWN, SHSD, SHSN		
238.0514	$C_8H_{14}O_6S_1$	2	5.24; 5.65	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN	α-pinene	Surratt et al., 2008
238.0877	$C_9H_{18}O_5S_1$	4	6.52; 7.23; 9.12	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			10.18	WHW, WHS		
238.1242	$C_{10}H_{22}O_4S_1$	4	9.57; 9.88; 10.10; 10.61	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
239.9942	$C_6H_8O_8S_1$	3	1.15; 5.10; 5.20	WHS		
240.0307	$C_7H_{12}O_7S_1$	3	4.84; 5.27	WHW, WHS, NJSN,	Limonene	Surratt et

				SHWD, SHWN, SHSD, SHSN	al., 2008
			6.64	WHS	
240.0671	$C_8H_{16}O_6S_1$	11	4.92; 5.47; 6.35; 6.52; 6.84; 7.29; 7.91; 8.17	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN	
			8.27	WHS, SHWN, SHSD, SHSN	
			8.81	WHS	
			9.72	WHW, WHS, SHWD	
240.1034	$C_9H_{20}O_5S_1$	6	6.68; 7.39; 8.01; 8.41; 8.54	WHS, SHWD, SHWN	
			7.92	WHS, SHWN	
241.0259	$C_6H_{11}O_7N_1S_1$	2	7.22; 7.32	NJSN, SHWD, SHWN, SHSN	
242.0099	$C_6H_{10}O_8S_1$	5	1.28	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN	
			4.84; 5.43	WHW, WHS, NJSN, SHWN, SHSD, SHSN	
			5.73	SHSD, SHSN	
			5.85	WHW, WHS, NJSN, SHWD, SHSD, SHSN	
242.0251	$C_{10}H_{10}O_5S_1$	3	6.64	SHWN	
			5.90; 6.89	WHS, SHWN	
242.0463	$C_7H_{14}O_7S_1$	4	1.36; 4.97; 5.84	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN	
			6.05	WHS, SHSN	
242.0826	$C_8H_{18}O_6S_1$	6	5.05; 5.53; 6.22; 6.47; 6.69; 7.10	WHS, SHWN, WHW	
243.0052	$C_5H_9O_8N_1S_1$	6	1.12	WHW, WHS, NJSN, SHWN, SHSN	
			5.40	WHW, WHS, NJSN, SHWN, SHSD, SHSN	
			5.63; 6.18; 6.80	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN	
			6.03	NJSN, SHSN	
243.0416	$C_6H_{13}O_7N_1S_1$	2	7.50	NJSN, SHWN, SHSN	

			8.07	SHWN, SHSN		
243.9890	$C_5H_8O_9S_1$	1	1.05	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
244.0044	$C_9H_8O_6S_1$	4	5.14; 5.55; 6.86; 7.10	WHW, WHS, SHWD, SHWN		
244.0254	$C_6H_{12}O_8S_1$	2	1.34	WHW, WHS, NJSN, SHSD, SHWN, SHSN		
			1.80	WHS, SHSN		
244.0407	$C_{10}H_{12}O_5S_1$	6	6.59; 6.89; 6.97; 7.03; 7.20	WHS, NJSN, SHWN		
			6.06	SHWN		
245.0207	$C_5H_{11}O_8N_1S_1$	2	5.74; 5.95	NJSN	Isoprene	Surratt et al., 2008
246.0200	$C_9H_{10}O_6S_1$	5	5.52; 6.27; 6.39; 6.69; 6.88	WHS, SHWN		
246.0565	$C_{10}H_{14}O_5S_1$	3	6.28; 7.23; 8.95	WHW		
248.0357	$C_9H_{12}O_6S_1$	4	5.17; 5.34; 5.70	WHW, SHWN		
			8.21	WHW		
248.0721	$C_{10}H_{16}O_5S_1$	4	5.88	WHW, WHS	α-pinene	Surratt et al., 2008
			6.30; 6.91; 7.49	WHW, WHS, NJSN, SHWN, SHSD		
248.9945	$C_7H_7O_7N_1S_1$	7	4.95; 6.59; 6.93; 7.05; 7.75; 8.38	WHW, WHS		
			5.59	WHW		
250.0514	$C_9H_{14}O_6S_1$	2	5.22; 6.17	WHW, WHS, NJSN, SHSD, SHSN	Limonene; Terpinolene	Surratt et al., 2008
250.0877	$C_{10}H_{18}O_5S_1$	5	6.34; 6.70; 7.03; 7.23	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN	α-pinene; β-pinene; Terpinolene	Surratt et al., 2008
			5.27	WHW		
250.1243	$C_{11}H_{22}O_4S_1$	1	8.93	SHWD, SHWN		
251.9940	$C_7H_8O_8S_1$	5	5.01; 5.49	WHS		
			1.36; 2.39; 4.88	WHS, SHSD		
252.0306	$C_8H_{12}O_7S_1$	5	1.34; 1.85; 4.80; 5.53; 6.24	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN	Isoprene	Schindelka et al., 2013

252.0670	$C_9H_{16}O_6S_1$	7	5.98; 6.24; 7.61; 7.96; 8.08	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN	Limonene; β-caryo-phyllene	Chan et al., 2011
			4.90	WHW, WHS, NJSN, SHWD, SHWN, SHSN		
			10.26	WHW, WHS		
252.1035	$C_{10}H_{20}O_5S_1$	3	7.86	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			8.93	WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			10.75	WHS, SHSD		
252.1399	$C_{11}H_{24}O_4S_1$	3	10.57; 10.91; 11.39	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
254.0099	$C_7H_{10}O_8S_1$	5	1.36; 2.63; 4.97; 5.55	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			6.02	WHS		
254.0463	$C_8H_{14}O_7S_1$	5	1.34	WHW, WHS, NJSN, SHWD, SHSD, SHSN	Isoprene; α-terpinene	Schindelka et al., 2013; Surratt et al., 2008
			5.13; 5.35; 5.55; 6.15	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
254.0827	$C_9H_{18}O_6S_1$	8	5.52; 6.89; 7.16; 7.50; 7.96; 8.56	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			8.99; 9.59	WHW, WHS, SHWN		
254.1190	$C_{10}H_{22}O_5S_1$	3	8.69; 8.80; 9.07	WHS		
255.0414	$C_7H_{13}O_7N_1S_1$	4	1.34	WHW, WHS, SHWD, SHSN		
			7.47; 7.71; 7.92	WHW, WHS, NJSN, SHWD, SHWN, SHSN		
256.0256	$C_7H_{12}O_8S_1$	3	1.36; 4.85	WHW, WHS, NJSN, SHWN, SHSD, SHSN		
			5.95	WHS		
256.0618	$C_8H_{16}O_7S_1$	7	3.29	WHW, WHS, SHSD, SHSN		
			3.85	WHW, WHS, NJSN, SHSD, SHSN		
			5.53; 5.80; 6.34	WHW, WHS, NJSN, SHWD, SHWN, SHSD,		

				SHSN		
			6.55	WHS, SHSD, SHSN		
			6.81	WHW, WHS, SHWN, SHSD, SHSN		
256.9845	$C_5H_7O_9N_1S_1$	1	6.49	NJSN		
257.0208	$C_6H_{11}O_8N_1S_1$	5	1.15	WHS, SHWN, SHSN		
			6.15; 6.43; 7.05; 7.23	WHS, NJSN, SHWN, SHSN		
257.0572	$C_7H_{15}O_7N_1S_1$	3	8.17; 8.35	SHWD, SHWN, SHSN		
			8.56	SHWN, SHSN		
258.0048	$C_6H_{10}O_9S_1$	1	1.34	WHW, WHS, NJSN, SHWN, SHSD, SHSN		
258.0201	$C_{10}H_{10}O_6S_1$	5	4.94; 5.95; 6.70; 6.85	WHW, WHS, SHWD, SHWN, SHSD	naphthalene	Riva et al., 2015b
			5.45	WHW, SHWD, SHWN, SHSD		
258.0412	$C_7H_{14}O_8S_1$	1	1.34	WHS, NJSN, SHSD, SHSN		
259.0000	$C_5H_9O_9N_1S_1$	3	4.43; 5.14	WHS, NJSN, SHSD		
			5.81	NJSN, SHSD		
259.0364	$C_6H_{13}O_8N_1S_1$	3	5.84; 6.05; 6.55	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
259.9993	$C_9H_8O_7S_1$	3	5.56; 5.94; 6.18	WHW, WHS, NJSN, SHWD, SHWN, SHSD		
260.0203	$C_6H_{12}O_9S_1$	2	1.02; 1.16	WHS		
260.0357	$C_{10}H_{12}O_6S_1$	2	6.86; 7.28	WHS, SHSN		
261.0157	$C_5H_{11}O_9N_1S_1$	4	2.46; 2.94; 3.53; 4.43	WHS, NJSN, SHWN, SHSD, SHSN	Isoprene	Surratt et al., 2008
262.0149	$C_9H_{10}O_7S_1$	2	5.03; 5.39	WHS		
262.0513	$C_{10}H_{14}O_6S_1$	5	6.03; 6.22; 6.47; 6.84	WHW, SHSD		
			9.00	WHW		
263.0102	$C_8H_9O_7N_1S_1$	4	7.37	WHW, WHS, NJSN, SHWN		
			7.99	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			7.65; 8.60	WHW		
264.0306	$C_9H_{12}O_7S_1$	3	5.07; 6.07; 6.28	WHS, NJSN, SHSD, SHSN		
264.0670	$C_{10}H_{16}O_6S_1$	2	5.49; 6.60	WHW, WHS, NJSN, SHSD	β-pinene	Surratt et al., 2008

264.1034	$C_{11}H_{20}O_5S_1$	2	7.32; 7.83	WHW		
266.0099	$C_8H_{10}O_8S_1$	6	2.16	WHS		
			1.36; 5.14; 5.45; 5.60; 6.11	WHS, SHWN		
266.0252	$C_{12}H_{10}O_5S_1$	1	7.43	WHW, WHS, NJSN, SHWD, SHWN		
266.0462	$C_9H_{14}O_7S_1$	4	2.68; 5.51; 6.18; 6.56	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
266.0826	$C_{10}H_{18}O_6S_1$	5	6.24; 6.77; 6.93	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN	α-pinene; α-terpinene; Terpinolene	Surratt et al., 2008
			8.80	WHS, SHSD, SHSN		
			9.37	WHS		
266.1190	$C_{11}H_{22}O_5S_1$	4	7.73	WHW, WHS, SHWD, SHWN, SHSD, SHSN		
			8.51; 8.90	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			12.27	WHS		
266.1554	$C_{12}H_{26}O_4S_1$	3	12.24; 12.54	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			16.75	SHWD, SHSN		
268.0253	$C_8H_{12}O_8S_1$	5	1.37; 4.93; 5.57	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			6.31	WHW, WHS, NJSN, SHWN, SHSD, SHSN		
			6.55	WHW, WHS, NJSN, SHWD, SHWN, SHSN		
268.0620	$C_9H_{16}O_7S_1$	5	5.74; 6.30; 7.02	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN	Isoprene; Limonene	Riva et al., 2015a
			7.47	WHW, WHS, NJSN, SHWD, SHSD, SHSN		
			7.74	WHS, NJSN, SHSN		
268.0983	$C_{10}H_{20}O_6S_1$	10	7.40; 7.62; 7.77; 8.12; 8.57; 9.21	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			8.30	WHS, SHWN, SHSD, SHSN		

			8.80	WHS, SHSD, SHSN
			9.70; 10.36	WHW, WHS, SHWN
268.1347	$C_{11}H_{24}O_5S_1$	3	9.20; 9.39; 9.77	WHS
269.0572	$C_8H_{15}O_7N_1S_1$	2	8.22; 8.61	WHW, WHS, NJSN, SHWD, SHWN, SHSN
270.0048	$C_7H_{10}O_9S_1$	2	1.36; 2.98	WHS, NJSN, SHWN, SHSD, SHSN
270.0411	$C_8H_{14}O_8S_1$	8	1.36; 4.85; 5.22; 5.39; 5.63; 7.28	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN
			1.79	WHW, WHS, SHWN, SHSD, SHSN
			6.39	WHS, SHWD, SHSD
270.0776	$C_9H_{18}O_7S_1$	9	4.93; 5.03; 5.49; 5.97; 6.10; 6.40; 6.91	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN
			7.33	WHW, WHS, SHSN
			7.60	WHW, WHS, NJSN, SHSN
271.0364	$C_7H_{13}O_8N_1S_1$	7	4.81	WHW, NJSN, SHWN, SHSN
			5.09	WHW, NJSN, SHSN
			5.28; 5.77	WHW, NJSN, SHWN, SHSN
			6.45	WHW, NJSN, SHWN
			6.56; 6.74	WHW, NJSN, SHWN, SHSD, SHSN
271.0729	$C_8H_{17}O_7N_1S_1$	4	8.46	WHW, WHS, SHWD, SHWN, SHSN
			8.60; 8.82; 9.19	WHW, WHS, SHWD, SHWN, SHSD, SHSN
272.0205	$C_7H_{12}O_9S_1$	3	2.50	WHW, WHS, SHSD
			1.36; 5.07	WHW, WHS, NJSN, SHWN, SHSD, SHSN
272.0357	$C_{11}H_{12}O_6S_1$	3	5.45; 5.99; 6.22	WHW, SHWN
273.0158	$C_6H_{11}O_9N_1S_1$	5	5.11; 5.89; 6.11; 6.59; 6.78	WHS, NJSN, SHWN, SHSD, SHSN
273.0522	$C_7H_{15}O_8N_1S_1$	3	6.13; 6.35; 6.86	NJSN, SHWN, SHSN

274.0150	$C_{10}H_{10}O_7S_1$	4	4.92; 5.42; 5.67; 6.64	WHW, WHS, SHWD, SHWN	naphthalene	Riva et al., 2015b
274.0303	$C_{14}H_{10}O_4S_1$	1	9.26	WHW, WHS, SHWD, SHWN		
274.0362	$C_7H_{14}O_9S_1$	1	1.36	SHSD, SHSN		
274.9951	$C_5H_9O_{10}N_1S_1$	2	2.72; 3.68	NJSN, SHSD		
275.0104	$C_9H_9O_7N_1S_1$	2	8.04; 8.31	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
276.0307	$C_{10}H_{12}O_7S_1$	7	5.10; 5.44; 5.70; 5.81; 6.02; 6.15; 6.39	WHS	naphthalene	Riva et al., 2015b
277.0259	$C_9H_{11}O_7N_1S_1$	4	6.05	NJSN, SHWN, SHSN		
			8.14	WHW		
			8.42; 8.61	WHW, WHS, NJSN, SHWN, SHSN		
278.0463	$C_{10}H_{14}O_7S_1$	3	5.18; 5.39; 5.78	WHW, WHS, NJSN, SHWN, SHSD, SHSN		
280.0255	$C_9H_{12}O_8S_1$	2	5.09; 6.18	SHSD, SHSN		
280.0619	$C_{10}H_{16}O_7S_1$	4	5.44; 6.01; 6.35; 7.47	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN	α-pinene; β-pinene; Limonene; α-terpinene; γ-terpinene	Surratt et al., 2008
280.0982	$C_{11}H_{20}O_6S_1$	7	6.69; 7.11; 7.56; 7.96	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			8.86	WHW, WHS, SHWN, SHSD, SHSN		
			9.09	WHW, WHS, SHWD, SHWN, SHSN		
			9.53	WHW WHS		
280.1347	$C_{12}H_{24}O_5S_1$	6	7.98;10.10	WHW, WHS, SHWD, SHWN, SHSD, SHSN		
			9.13; 9.63	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			10.66	WHS, SHSD		
			11.26	WHS		
280.1709	$C_{13}H_{28}O_4S_1$	4	12.36	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		

			13.08	WHW, WHS, NJSN, SHWD, SHWN, SHSN		
			13.69	WHS, NJSN, SHWD, SHWN		
			14.28	WHW, WHS, SHWD		
281.0207	$C_8H_{11}O_8N_1S_1$	3	1.37; 6.81; 7.11	WHS		
282.0412	$C_9H_{14}O_8S_1$	4	1.37	WHW, WHS, NJSN, SHWD, SHSD, SHSN		
			5.31; 6.52	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			7.12	WHW, WHS, SHWD, SHWN, SHSD, SHSN		
282.0776	$C_{10}H_{18}O_7S_1$	6	6.24; 6.52; 6.80; 7.06	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN	α-pinene; β-pinene; Limonene; α-terpinene; Terpinolene	Surratt et al., 2008
			7.79	WHW, WHS, SHWD, SHWN, SHSD, SHSN		
			8.18	WHW, WHS		
282.1139	$C_{11}H_{22}O_6S_1$	11	6.45; 6.57; 7.86; 8.09; 8.35; 8.72; 9.00; 9.19	WHW, WHS, SHWD, SHWN, SHSD		
			9.87	WHW, WHS, SHWD, SHWN		
			10.46; 11.18	WHW, WHS		
282.1503	$C_{12}H_{26}O_5S_1$	4	8.52; 9.81; 10.14; 10.51	WHS		
283.0000	$C_7H_9O_9N_1S_1$	4	6.76	WHS		
			7.12	WHS, SHWN		
			7.48; 7.61	WHS, SHWD, SHWN		
283.0729	$C_9H_{17}O_7N_1S_1$	1	8.72	SHWD, SHWN		
284.0203	$C_8H_{12}O_9S_1$	9	1.36; 3.82; 4.68; 4.99; 5.39; 6.10	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			3.70	WHW, WHS, NJSN, SHSD, SHSN		
			3.91	WHW, WHS, SHSD, SHSN		
			5.94	WHW, WHS, NJSN		
284.0566	$C_9H_{16}O_8S_1$	6	5.31; 5.57; 5.88; 6.24	WHW, WHS, NJSN, SHWD, SHWN, SHSD,	α-terpinene	Surratt et al., 2008

				SHSN		
			6.59	WHS, SHSD		
			6.64	WHW, WHS, SHWN, SHSD, SHSN		
284.0932	$C_{10}H_{20}O_7S_1$	10	5.13; 5.99; 6.22; 6.64; 7.09; 7.41	WHW, WHS, NJSN, SHWN, SHSD, SHSN	β-pinene; Terpinolene	Surratt et al., 2008
			5.27	WHW, WHS, SHWN, SHSD, SHSN		
			8.16; 8.25	WHS, SHSD		
			8.00	WHS		
284.9946	$C_{10}H_7O_7N_1S_1$	3	5.51; 5.73; 9.34	WHW, SHWN		
285.0156	$C_7H_{11}O_9N_1S_1$	2	6.35	NJSN, SHSD, SHSN		
			7.06	NJSN, SHSN		
285.0522	$C_8H_{15}O_8N_1S_1$	2	6.99; 7.28	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
285.9997	$C_7H_{10}O_{10}S_1$	2	1.16;1.34	WHS, NJSN, SHSD, SHSN		
286.0360	$C_8H_{14}O_9S_1$	3	1.37; 3.12; 5.51	WHS, NJSN, SHSD, SHSN		
286.1242	$C_{14}H_{22}O_4S_1$	1	11.35	NJSN		
287.0313	$C_7H_{13}O_9N_1S_1$	7	5.59	WHW, WHS, NJSN, SHWN, SHSN		
			5.70; 6.07; 6.35; 6.52; 6.98	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			7.33	WHS, SHWN, SHSD, SHSN		
287.0677	$C_8H_{17}O_8N_1S_1$	5	8.30	WHS, SHWN, SHSN		
			6.99; 7.48; 8.13; 8.64	WHW, WHS, NJSN, SHWD, SHWN, SHSN		
288.0153	$C_7H_{12}O_{10}S_1$	2	1.16; 1.36	WHS, SHSD, SHSN		
288.0307	$C_{11}H_{12}O_7S_1$	2	7.23; 7.45	WHS	2-methyl-naphthalene	Riva et al., 2015b
288.0459	$C_{15}H_{12}O_4S_1$	1	9.79	WHW, SHWN		
288.1399	$C_{14}H_{24}O_4S_1$	1	8.31	NJSN		
289.0259	$C_{10}H_{11}O_7N_1S_1$	5	5.94	WHW, SHWD, SHWN		
			6.36	WHW, SHWD		
			8.38; 8.60; 8.85	WHW, WHS, NJSN, SHWD, SHWN		
291.0417	$C_{10}H_{13}O_7N_1S_1$	4	6.53; 8.85;	WHW		

			8.98; 9.20			
292.1711	$C_{14}H_{28}O_4S_1$	1	12.54	WHW		
294.0412	$C_{10}H_{14}O_8S_1$	4	5.24; 5.99; 6.13; 7.24	NJSN, SHSD		
294.0777	$C_{11}H_{18}O_7S_1$	2	5.82; 6.36	WHS, NJSN, SHWN, SHSD		
294.1141	$C_{12}H_{22}O_6S_1$	9	6.91; 7.11; 7.35; 7.62; 7.78; 8.16; 8.61	WHW, WHS, SHWD, SHWN, SHSD, SHSN		
			9.03	WHS, SHSD		
			9.77	WHW, WHS, SHWD, SHSN		
294.1503	$C_{13}H_{26}O_5S_1$	7	8.42	WHW, WHS, SHWD		
			9.56; 9.82	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			10.39	WHW, WHS, NJSN, SHWN, SHSD, SHSN		
			10.88	WHW, WHS, NJSN, SHWN, SHSD		
			11.19, 12.45	WHS		
294.1868	$C_{14}H_{30}O_4S_1$	4	9.43	WHW, NJSN, SHWD, SHWN, SHSD, SHSN		
			13.60	WHW, NJSN, SHWD, SHSD, SHSN		
			13.83	SHSN		
			16.52	WHW, SHWD, SHWN, SHSD, SHSN		
295.0729	$C_{10}H_{17}O_7N_1S_1$	4	8.37; 8.82; 8.95	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN	α-pinene; β-pinene; α-terpinene; Terpinolene	Surratt et al., 2008
			9.17	SHWD, SHWN		
296.0567	$C_{10}H_{16}O_8S_1$	4	5.38; 6.70	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			6.59	WHS, NJSN, SHWN, SHSD, SHSN		
			7.78	WHW, WHS, SHWD, SHWN, SHSD, SHSN		
296.0931	$C_{11}H_{20}O_7S_1$	7	5.93; 6.59; 7.15	WHS, NJSN, SHSD, SHSN, SHWN		
			7.78	WHS, SHSD, SHSN,		

				SHWN		
			8.01	WHS		
			8.14	WHS, SHSN, SHWN		
			8.48	WHS, SHSN		
296.1295	$C_{12}H_{24}O_6S_1$	8	7.73; 8.33; 8.57; 8.93; 9.31	WHW, WHS, SHWD, SHWN, SHSD, SHSN		
			9.81	WHW, WHS, SHWN, SHSD, SHSN		
			10.60	WHW, WHS		
			11.27	WHW, WHS, SHWN		
296.1660	$C_{13}H_{28}O_5S_1$	5	9.56; 9.85; 10.62; 10.89; 11.35	WHS		
297.0520	$C_9H_{15}O_8N_1S_1$	2	6.94; 7.43	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN	Limonene	Surratt et al., 2008
297.0884	$C_{10}H_{19}O_7N_1S_1$	2	9.56; 9.70	WHW, SHWN		
298.0301	$C_{16}H_{10}O_4S_1$	1	9.77	WHW, SHWN		
298.0360	$C_9H_{14}O_9S_1$	5	1.34; 5.06; 5.24	WHW, WHS, NJSN, SHWN, SHSD, SHSN		
			6.65	WHW, WHS, SHWN		
			6.73	WHW, WHS		
298.0724	$C_{10}H_{18}O_8S_1$	8	5.53; 5.97; 6.11; 6.40; 7.22	WHW, WHS, NJSN, SHWN, SHSD, SHSN	α-pinene; α-terpinene	Surratt et al., 2008
			6.77	WHW, WHS, SHWN, SHSD, SHSN		
			6.93; 7.39	WHW, WHS, SHSD, SHSN		
298.1087	$C_{11}H_{22}O_7S_1$	10	5.88; 6.19; 6.51; 6.61; 7.16; 7.44; 7.60; 7.73; 8.87; 8.98	WHS		
298.1241	$C_{15}H_{22}O_4S_1$	1	9.72	WHW		
299.0677	$C_9H_{17}O_8N_1S_1$	3	7.57; 8.12	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			8.58	WHS, NJSN, SHSN		
300.0152	$C_8H_{12}O_{10}S_1$	6	1.19; 1.36; 1.61; 5.09	WHS, NJSN, SHSD, SHSN		
			1.80, 1.93	WHS, SHSN		

300.0516	$C_9H_{16}O_9S_1$	1	4.85	WHS, NJSN		
300.1399	$C_{15}H_{24}O_4S_1$	3	8.98; 10.96; 11.83	WHW		
300.9894	$C_{10}H_7O_8N_1S_1$	1	5.84	WHW		
301.0106	$C_7H_{11}O_{10}N_1S_1$	4	5.57; 5.77; 6.01; 6.40	SHSD, SHSN		
301.0468	$C_8H_{15}O_9N_1S_1$	6	5.93; 6.23; 6.86; 7.14; 7.67; 7.87	WHW, WHS, NJSN, SHWN, SHSD, SHSN		
301.0833	$C_9H_{19}O_8N_1S_1$	2	7.23; 7.96	WHS, NJSN, SHWN		
302.0097	$C_{11}H_{10}O_8S_1$	4	6.41; 6.59; 7.33; 7.40	SHWN		
302.0309	$C_8H_{14}O_{10}S_1$	2	1.16; 1.34	WHS, SHSD	Isoprene	Surratt et al., 2008
302.1190	$C_{14}H_{22}O_5S_1$	1	12.08	WHW		
306.0007	$C_5H_{10}O_{11}N_2S_1$	7	6.22; 6.44; 6.63; 6.80; 6.98; 7.61; 7.45	WHS, NJSN, SHWD, SHWN, SHSD, SHSN	Isoprene	Surratt et al., 2008
308.0048	$C_6H_{12}O_{12}S_1$	3	6.61; 6.80; 6.99	NJSN		
308.0933	$C_{12}H_{20}O_7S_1$	2	6.99; 7.49	WHS, SHSD, SHWN		
308.1296	$C_{13}H_{24}O_6S_1$	4	8.31; 8.54; 9.22	WHS, SHSD		
308.1296	$C_{13}H_{24}O_6S_1$	4	10.44	WHS		
308.1659	$C_{14}H_{28}O_5S_1$	6	9.24; 10.53	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
308.1659	$C_{14}H_{28}O_5S_1$	6	10.88	WHW, WHS, NJSN, SHWN, SHSD, SHSN		
308.1659	$C_{14}H_{28}O_5S_1$	6	11.22	WHW, WHS, NJSN, SHSD, SHSN		
308.1659	$C_{14}H_{28}O_5S_1$	6	11.85	WHW, WHS, NJSN, SHWD, SHSD, SHSN		
308.1659	$C_{14}H_{28}O_5S_1$	6	12.11	WHW, WHS, NJSN, SHWN, SHSD, SHSN		
308.2021	$C_{15}H_{32}O_4S_1$	3	10.96; 12.18	WHS, WHW		
308.2021	$C_{15}H_{32}O_4S_1$	3	16.74	WHS		
309.0521	$C_{10}H_{15}O_8N_1S_1$	2	8.00; 8.37	NJSN		
310.0361	$C_{10}H_{14}O_9S_1$	4	4.76; 5.45; 5.86; 6.22	WHS, NJSN, SHSD		
310.0726	$C_{11}H_{18}O_8S_1$	5	5.17; 5.92; 6.64; 7.12	WHS, NJSN, SHWN, SHSD, SHSN		

			7.24	WHS, SHSD, SHSN		
310.1088	$C_{12}H_{22}O_7S_1$	11	6.31; 6.48; 6.97; 7.44; 7.75; 7.95; 8.16	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			8.33	WHS, SHWD, SHSD, SHSN		
			8.69	WHW, WHS, NJSN, SHWD, SHSD, SHSN		
			8.86	WHW, WHS, SHSD		
			9.17	WHS,, SHSD, SHSN		
310.1450	$C_{13}H_{26}O_6S_1$	12	6.99; 7.64; 8.72; 9.06; 9.22; 9.52; 9.95	WHS, SHWN		
			10.16; 10.49; 11.39; 12.22; 13.49	WHS		
310.1815	$C_{14}H_{30}O_5S_1$	7	9.72	WHW, WHS, NJSN, SHWD, SHWN, SHSD		
			10.17	WHW, WHS, NJSN, SHWD, SHWN, SHSD		
			11.27	WHW, WHS, SHWD, SHWN, SHSD		
			11.47	WHW, WHS, SHWN		
			12.40	WHW, WHS, NJSN, SHWN, SHSN		
			14.63	WHW, WHS, SHWD, SHWN		
			15.14	NJSN, SHSD, SHSN, SHWN		
311.0102	$C_{12}H_9O_7N_1S_1$	1	9.28	NJSN, SHWD, SHWN		
311.0677	$C_{10}H_{17}O_8N_1S_1$	7	6.60	WHW, WHS, NJSN	α-pinene; β-pinene; α-terpinene; γ-terpinene	Surratt et al., 2008
			6.73	WHW, WHS, NJSN, SHWN, SHSN		
			7.05; 7.69; 7.84	WHW, WHS, NJSN, SHWN, SHSD, SHSN		
			8.73	WHW, WHS, NJSN, SHWN, SHSN		
			8.96	WHW, WHS, NJSN, SHWN		
312.0518	$C_{10}H_{16}O_9S_1$	3	6.44	WHW, WHS, NJSN, SHSD, SHSN		

			5.45; 6.55	WHW, WHS, NJSN, SHWN, SHSD, SHSN		
312.0882	$C_{11}H_{20}O_8S_1$	8	5.18; 6.40; 6.59; 6.89; 7.29	WHS, SHWN, SHSD		
			7.54; 7.69; 7.91	WHS		
312.1245	$C_{12}H_{24}O_7S_1$	4	6.66; 7.65; 8.17; 8.85	WHS		
313.0470	$C_9H_{15}O_9N_1S_1$	6	6.07; 6.36; 6.82; 7.05; 7.29; 7.53	WHW, WHS, NJSN, SHWN, SHSD, SHSN	Limonene	Surratt et al., 2008
313.0834	$C_{10}H_{19}O_8N_1S_1$	7	6.70; 6.85	WHW, WHS, NJSN, SHWN, SHSN		
			7.06; 7.45; 7.67; 8.37; 8.72	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
314.0310	$C_9H_{14}O_{10}S_1$	2	1.36; 5.28	WHS, NJSN, SHSD, SHSN		
314.0675	$C_{10}H_{18}O_9S_1$	5	5.17; 5.51; 5.88; 6.07	WHS, NJSN, SHSD, SHSN		
			6.66	SHSD		
315.0627	$C_9H_{17}O_9N_1S_1$	9	6.41; 6.68; 7.03; 7.43	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			8.00	WHW, WHS, SHWD, SHWN, SHSD, SHSN		
			8.25, 8.60	WHW, WHS, NJSN, SHWN, SHSD, SHSN		
			8.41	WHS, SHWN, SHSD, SHSN		
			8.81	WHW, WHS, NJSN, SHSD, SHSN		
315.0992	$C_{10}H_{21}O_8N_1S_1$	1	8.14	SHWN		
318.0412	$C_{12}H_{14}O_8S_1$	2	6.99; 7.26	SHSD		
320.1298	$C_{14}H_{24}O_6S_1$	5	7.41; 7.91; 8.17 8.29; 8.76;	WHS	β-caryo-phyllene	Chan et al., 2011
321.0157	$C_{10}H_{11}O_9N_1S_1$	1	6.06	SHWN	naphthalene	Riva et al., 2015b
321.0521	$C_{11}H_{15}O_8N_1S_1$	1	6.60	WHW		
322.1090	$C_{13}H_{22}O_7S_1$	5	6.65; 6.97; 7.71; 7.98	WHS, SHSD		

			8.22	WHS
322.1453	$C_{14}H_{26}O_6S_1$	4	7.95; 9.37; 9.88; 11.31	WHS
322.1817	$C_{15}H_{30}O_5S_1$	3	11.32	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN
			11.76	WHS, SHWN, SHSD, SHSN
			12.37	WHS
322.2179	$C_{16}H_{34}O_4S_1$	4	12.15; 16.71	WHW, WHS, NJSN, SHWD, SHWN, SHSD
			14.91	WHW, WHS, SHWD
			16.40	WHW, WHS
324.0883	$C_{12}H_{20}O_8S_1$	4	6.26; 7.10; 7.36; 7.47	WHS, SHSD
324.1245	$C_{13}H_{24}O_7S_1$	6	9.07; 9.83	WHS
			7.43; 7.98; 8.31	WHS, SHWN, SHSD
			8.52	WHS, SHSD
324.1608	$C_{14}H_{28}O_6S_1$	10	9.20; 9.59; 10.62; 11.11	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN
			9.83; 11.24	WHW, WHS, NJSN, SHWN, SHSD, SHSN
			10.14	WHW, WHS, SHWN, SHSD, SHSN
			10.89; 12.37	WHW, WHS
			13.68	WHS
324.1971	$C_{15}H_{32}O_5S_1$	5	9.86; 10.89; 11.35; 12.76; 14.51	WHS
325.0470	$C_{10}H_{15}O_9N_1S_1$	3	6.56; 6.95; 7.43	NJSN, SHSN
326.0133	$C_{10}H_{14}O_8S_2$	1	7.58	WHW
326.0675	$C_{11}H_{18}O_9S_1$	2	5.70	WHS, NJSN, SHSD, SHSN
			6.64	WHS, SHSD, SHSN
326.1040	$C_{12}H_{22}O_8S_1$	4	6.84; 7.06; 7.36; 8.42	WHS
326.1403	$C_{13}H_{26}O_7S_1$	7	7.24; 7.75; 7.66; 8.12; 8.38; 8.70; 8.85	WHS

			5.19	WHS, SHSD, SHSN		
327.0626	$C_{10}H_{17}O_9N_1S_1$	7	6.27; 6.63; 7.49; 7.74; 8.50	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN	β-pinene; Limonene; Terpinolene	Surratt et al., 2008
			8.73	WHS, NJSN, SHSD, SHSN		
327.0992	$C_{11}H_{21}O_8N_1S_1$	4	8.56; 8.78; 9.28	SHWN, SHSD, SHSN		
			9.60	SHSN		
327.1356	$C_{12}H_{25}O_7N_1S_1$	1	11.02	SHWN		
328.0467	$C_{10}H_{16}O_{10}S_1$	3	4.71; 5.02; 5.82	WHS, NJSN, SHSD, SHSN		
328.1345	$C_{16}H_{24}O_5S_1$	1	14.48	SHWD		
329.0419	$C_9H_{15}O_{10}N_1S_1$	6	6.19; 6.43; 6.53; 6.80; 7.06; 7.50	WHS, NJSN, SHSD, SHSN		
329.0783	$C_{10}H_{19}O_9N_1S_1$	9	5.70; 5.85; 6.01; 6.41; 7.01; 7.29; 7.49; 8.11	WHW, WHS, NJSN, SHSN, SHWN	Limonene	Surratt et al., 2008
			8.89	WHW, WHS, SHSN		
331.0213	$C_8H_{13}O_{11}N_1S_1$	3	5.45	WHS, NJSN, SHWN, SHSD, SHSN		
			5.90; 6.19	WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
332.1298	$C_{15}H_{24}O_6S_1$	6	7.87; 8.16; 8.44; 9.08	WHW, WHS, NJSN		
			9.60	WHW,WHS		
			10.19	WHW		
336.0882	$C_{13}H_{20}O_8S_1$	5	6.05; 6.27; 6.44; 6.86; 6.94	WHS, NJSN, SHSD		
336.1611	$C_{15}H_{28}O_6S_1$	5	8.22; 9.29; 10.01; 10.58; 12.22	WHS		
336.1974	$C_{16}H_{32}O_5S_1$	2	12.15	WHS, SHWD, SHWN, SHSD, SHSN		
			12.68	WHS, SHWN, SHSD, SHSN		
337.0836	$C_{12}H_{19}O_8N_1S_1$	1	7.87	NJSN		
338.1040	$C_{13}H_{22}O_8S_1$	2	6.20; 6.40	WHS		
338.1404	$C_{14}H_{26}O_7S_1$	9	7.03; 7.20; 7.86; 8.52;	WHS, SHWN, SHSD, SHSN		

			8.90			
			9.13	WHS, SHSN		
			9.41; 9.72; 10.57	WHS		
338.1764	$C_{15}H_{30}O_6S_1$	9	8.22	WHS, SHSD		
			9.25; 14.12	WHS		
			9.70; 10.01; 10.84; 11.39	WHW, WHS, SHWN, SHSD		
			10.48	WHW, WHS		
			12.15	WHW,WHS, SHWN		
338.2130	$C_{16}H_{34}O_5S_1$	7	9.28	WHW, WHS, SHWD, SHSD		
			10.84	WHS, SHWN		
			11.01	WHS, SHWD, SHWN, SHSD		
			11.13	WHW, WHS, SHWD, SHWN		
			11.62; 12.48; 12.78	WHW, WHS, NJSN, SHWD, SHWN, SHSD		
340.1195	$C_{13}H_{24}O_8S_1$	9	7.66; 8.22; 8.41; 8.51	WHS		
			7.27; 7.50; 7.81; 8.73; 8.93	WHS, SHWN		
340.1559	$C_{14}H_{28}O_7S_1$	8	7.66; 8.24; 8.56; 8.94; 9.17; 9.30; 9.60; 9.97	WHS		
341.0421	$C_{10}H_{15}O_{10}N_1S_1$	3	6.78; 6.95; 7.29	WHW, WHS, NJSN, SHSD, SHSN		
341.0784	$C_{11}H_{19}O_9N_1S_1$	4	7.57; 7.66; 7.95; 9.08	WHS, NJSN		
341.1511	$C_{13}H_{27}O_7N_1S_1$	1	11.79	SHWN		
342.0624	$C_{11}H_{18}O_{10}S_1$	3	5.45; 5.73; 5.99	WHS, NJSN, SHSD, SHSN		
342.0989	$C_{12}H_{22}O_9S_1$	2	6.60; 7.11	WHS		
343.0576	$C_{10}H_{17}O_{10}N_1S_1$	7	6.44; 6.68; 7.57	WHW, WHS, NJSN, SHWN, SHSD, SHSN	α-pinene; β-pinene; α-terpinene	Surratt et al., 2008
			7.70; 7.77	WHW, WHS, NJSN, SHSD, SHSN		
			8.11	WHS, NJSN, SHSD, SHSN		
			8.21	SHSD, SHSN		

343.1304	$C_{12}H_{25}O_8N_1S_1$	3	8.85; 8.96; 9.22	SHWN		
345.0369	$C_9H_{15}O_{11}N_1S_1$	3	6.05; 6.57; 6.93	WHS, NJSN, SHSN		
345.0733	$C_{10}H_{19}O_{10}N_1S_1$	7	5.39; 5.59; 5.76; 7.07; 7.23; 7.32	WHW, WHS, NJSN, SHWN, SHSN		
			6.93	WHW, WHS, NJSN, SHSN		
346.0760	$C_{11}H_{22}O_8S_2$	1	7.31	SHWD		
348.1246	$C_{15}H_{24}O_7S_1$	10	6.80; 6.89; 6.97; 7.07; 7.33; 7.73; 7.86; 8.03; 8.31; 8.51	WHS, NJSN	β-caryo-phyllene	Chan et al., 2011
350.1038	$C_{14}H_{22}O_8S_1$	5	6.44; 6.66; 6.93; 7.16; 7.33	WHS, SHSD	β-caryo-phyllene	Chan et al., 2011
350.1404	$C_{15}H_{26}O_7S_1$	6	7.39; 7.54; 7.74; 8.34; 8.43	WHS, NJSN, SHWN, SHSD	β-caryo-phyllene	Chan et al., 2011
			8.53	WHS		
350.1766	$C_{16}H_{30}O_6S_1$	7	9.35; 9.90; 10.14; 10.42; 10.71; 11.37; 12.10	WHS, WHW		
350.2130	$C_{17}H_{34}O_5S_1$	7	11.27; 11.49; 11.70; 12.09; 12.42; 13.12; 13.98	WHS		
		4	12.09; 12.42; 13.12; 13.98	SHSD		
352.0829	$C_{13}H_{20}O_9S_1$	4	5.92; 6.23; 6.35; 6.48	SHSD		
352.1198	$C_{14}H_{24}O_8S_1$	2	6.89; 7.74	WHS, SHSD	β-caryo-phyllene	Chan et al., 2011
352.1557	$C_{15}H_{28}O_7S_1$	5	7.29; 8.30; 9.08	WHS, SHSD		
			9.47; 11.37	WHS		
352.1922	$C_{16}H_{32}O_6S_1$	10	10.25; 10.38; 10.67; 11.27	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			10.50; 10.89	WHW, WHS, SHWD,		

				SHWN, SHSD, SHSN		
			11.63; 12.32	WHW, WHS, NJSN, SHWN		
			13.55	WHS		
			16.75	WHW		
352.2287	$C_{17}H_{36}O_5S_1$	2	11.82; 12.45	WHS		
354.0988	$C_{13}H_{22}O_9S_1$	4	5.99; 6.09; 6.28; 7.09	WHS, SHSD		
354.1353	$C_{14}H_{26}O_8S_1$	9	7.48; 7.67; 7.94; 8.43; 8.54; 8.67; 8.81; 9.09; 9.99	WHS		
354.1718	$C_{15}H_{30}O_7S_1$	5	8.08; 9.04; 9.37; 9.51; 9.77	WHS		
354.2079	$C_{16}H_{34}O_6S_1$	3	15.58	SHWD		
			16.34	WHW, SHWD		
			16.68	NJSN, SHWN, SHSD, SHSN		
355.0942	$C_{12}H_{21}O_9N_1S_1$	3	8.21; 8.46; 8.77	WHW, WHS, NJSN, SHWN, SHSN		
356.1659	$C_{18}H_{28}O_5S_1$	2	7.69	SHWD, SHWN		
			15.77	NJSN, SHWD, SHWN, SHSD ,SHSN		
357.0735	$C_{11}H_{19}O_{10}N_1S_1$	4	6.78; 6.98; 7.22; 7.36	WHS, NJSN		
361.0684	$C_{10}H_{19}O_{11}N_1S_1$	2	6.47; 7.29	SHSD		
363.1356	$C_{15}H_{25}O_7N_1S_1$	6	10.53	WHW, WHS, NJSN, SHWN	β-caryo-phyllene	Chan et al., 2011
			10.88	WHW, WHS, NJSN, SHWD, SHWN, SHSN		
			11.18	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			11.32	SHSD, SHSN		
			11.50	WHW, WHS, SHSD, SHSN		
			11.93	WHW, WHS, NJSN, SHWN		
363.9484	$C_9H_4O_{12}N_2S_1$	1	0.84	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		

364.1196	$C_{15}H_{24}O_8S_1$	5	6.76; 7.41; 7.56; 7.77; 7.86	NJSN	β-caryo-phyllene	Chan et al., 2011
364.1925	$C_{17}H_{32}O_6S_1$	3	9.72; 9.92; 11.49	WHS		
364.2286	$C_{18}H_{36}O_5S_1$	8	11.66; 12.01; 12.31; 13.01; 13.45; 13.64; 13.86; 14.76	WHS		
365.1150	$C_{14}H_{23}O_8N_1S_1$	3	8.78; 9.11; 9.29	WHS, NJSN		
366.1715	$C_{16}H_{30}O_7S_1$	12	7.61	WHS, SHSD		
			8.74; 9.22; 9.65	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			10.08	WHW, WHS, SHWD, SHWN, SHSD, SHSN		
			10.46	WHW, WHS, SHWN		
			10.79	WHW, WHS, SHWD, SHSN		
			11.15	WHW, WHS		
			11.44; 12.50	WHS, SHWD		
			12.36	WHS		
			12.89	NJSN, SHSD, SHSN		
366.2078	$C_{17}H_{34}O_6S_1$	8	10.86; 11.02; 11.39; 12.35	WHW, WHS, SHSD, SHWN		
			12.64; 13.43	WHW, WHS, SHSD		
			13.23; 13.92	WHW, WHS		
366.2440	$C_{18}H_{38}O_5S_1$	2	12.89; 16.74	WHS		
368.1144	$C_{14}H_{24}O_9S_1$	5	6.69; 6.88; 7.09; 7.16; 7.24	WHS, SHSD		
368.1509	$C_{15}H_{28}O_8S_1$	6	8.11; 8.34	WHW, WHS		
			9.13	WHS		
			10.00	WHW, WHS, SHWN		
			9.52; 10.18	WHW, WHS, SHWD, SHWN		
368.1873	$C_{16}H_{32}O_7S_1$	8	8.51; 8.93; 9.19; 9.55; 9.82; 10.10	WHW, WHS, NJSN		
			8.31; 10.42	WHW, WHS		
369.1098	$C_{13}H_{23}O_9N_1S_1$	2	8.48; 9.50	NJSN		
369.9841	$C_{10}H_{10}O_{13}S_1$	2	10.48; 10.70	SHSD, SHSN		

371.1618	$C_{14}H_{29}O_8N_1S_1$	2	10.27; 11.17	WHS		
374.1041	$C_{16}H_{22}O_8S_1$	2	9.35; 9.60	WHW, WHS, NJSN, SHWN, SHSD, SHSN		
376.1924	$C_{18}H_{32}O_6S_1$	3	9.30	WHW, NJSN		
			9.07; 11.45	WHW		
377.1149	$C_{15}H_{23}O_8N_1S_1$	4	9.03; 9.28; 9.55; 9.88	WHS, NJSN		
378.2081	$C_{18}H_{34}O_6S_1$	4	9.64; 10.95; 12.01; 12.45	WHW, WHS		
379.1305	$C_{15}H_{25}O_8N_1S_1$	8	8.60; 9.06	WHS, NJSN		
			8.77; 9.17; 9.33; 9.75; 10.22; 11.27	WHS, NJSN, SHSN		
380.1511	$C_{16}H_{28}O_8S_1$	3	7.12; 7.43; 9.19	WHS	β-caryo-phyllene	Chan et al., 2011
380.1652	$C_{20}H_{28}O_5S_1$	1	14.98	NJSN		
380.1871	$C_{17}H_{32}O_7S_1$	6	9.17; 10.27; 11.18; 11.98; 12.48; 12.63	WHS		
380.2233	$C_{18}H_{36}O_6S_1$	11	8.96; 16.68	WHS		
			9.22	WHW, WHS, NJSN, SHWN		
			9.61	WHS, NJSN		
			11.56; 11.78; 12.00; 12.27	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN		
			12.67	WHW, WHS, SHSD		
			13.29; 14.15	WHW, WHS		
381.1463	$C_{15}H_{27}O_8N_1S_1$	2	9.08; 9.97	NJSN		
381.9843	$C_{11}H_{10}O_{13}S_1$	2	7.84; 10.48	NJSN, SHSD, SHSN		
382.1302	$C_{15}H_{26}O_9S_1$	4	6.93; 7.26; 7.07; 7.50	WHS		
382.1666	$C_{16}H_{30}O_8S_1$	3	8.51; 10.07; 10.48	WHS		
382.2031	$C_{17}H_{34}O_7S_1$	4	8.59; 8.94; 10.09; 11.09	WHS		
382.2395	$C_{18}H_{38}O_6S_1$	1	13.24	SHWD		
384.1972	$C_{20}H_{32}O_5S_1$	1	14.12	NJSN, SHWD, SHWN, SHSD, SHSN		
385.1049	$C_{13}H_{23}O_{10}N_1S_1$	6	7.37; 7.53; 7.90; 8.25; 8.47; 8.80	WHS, NJSN, SHSN		
385.9429	$C_9H_6O_{15}S_1$	1	0.85	WHW, SHWD, SHSD,		

				SHSN
390.0991	$C_{16}H_{22}O_9S_1$	1	7.58	SHSD
391.0245	$C_{10}H_{17}O_{11}N_1S_2$	4	6.36	WHW, NJSN
			6.60; 6.91; 7.06	WHW, WHS, NJSN, SHWN, SHSN
393.1100	$C_{15}H_{23}O_9N_1S_1$	1	8.85	NJSN
394.2030	$C_{18}H_{34}O_7S_1$	10	8.83; 12.09; 12.41	WHS
			9.35; 9.66; 10.97; 11.31; 11.50; 11.79; 12.72	WHW, WHS
394.2393	$C_{19}H_{38}O_6S_1$	4	12.33; 12.74; 13.12; 13.41	WHS
395.1255	$C_{15}H_{25}O_9N_1S_1$	7	8.16; 8.63; 8.96; 9.11; 9.69; 9.83; 10.13	WHS, NJSN
396.1823	$C_{17}H_{32}O_8S_1$	5	8.93; 9.22; 10.49; 10.67; 10.89	WHS
396.2186	$C_{18}H_{36}O_7S_1$	5	7.45	WHS
			9.43; 10.47; 10.66	WHS, NJSN
			11.56	WHW, WHS
397.1410	$C_{15}H_{27}O_9N_1S_1$	2	7.92; 8.52	NJSN
398.1194	$C_{22}H_{22}O_5S_1$	1	5.68	SHSD
398.2345	$C_{18}H_{38}O_7S_1$	1	16.42	SHWD
402.1306	$C_{13}H_{26}O_{10}N_2S_1$	1	12.23	SHWD
408.2188	$C_{19}H_{36}O_7S_1$	4	10.18; 10.82; 11.58; 11.75	WHS
408.2548	$C_{20}H_{40}O_6S_1$	5	10.96; 13.50; 13.75; 13.97; 14.76	WHS
409.1048	$C_{15}H_{23}O_{10}N_1S_1$	2	8.77; 9.87	NJSN
410.1978	$C_{18}H_{34}O_8S_1$	6	7.91; 9.70; 10.23; 11.05	WHW, WHS
			10.58	WHS
			11.35	WHW, WHS, NJSN, SHWD, SHWN, SHSD, SHSN
410.2344	$C_{19}H_{38}O_7S_1$	3	9.47; 9.90; 11.37	WHS

411.1205	$C_{15}H_{25}O_{10}N_1S_1$	2	7.86; 8.47	WHS, NJSN
412.1222[a]	$C_{16}H_{28}O_8S_2$	2	4.76; 5.21	WHW, WHS
413.1362	$C_{15}H_{27}O_{10}N_1S_1$	2	7.81; 8.69	NJSN
413.1725	$C_{16}H_{31}O_9N_1S_1$	3	10.17; 10.91; 11.17	WHW, WHS
413.9742	$C_{11}H_{10}O_{15}S_1$	1	10.69	NJSN, SHWN, SHSD, SHSN
417.1464	$C_{18}H_{27}O_8N_1S_1$	1	10.39	WHW
418.1330[b]	$C_{15}H_{30}O_9S_2$	1	1.19	SHSD
422.2342	$C_{20}H_{38}O_7S_1$	3	9.28; 9.44	SHWN
			16.58	SHWD
422.2705	$C_{21}H_{42}O_6S_1$	3	11.08; 12.39; 16.71	WHS
424.2136	$C_{19}H_{36}O_8S_1$	6	9.64; 11.01; 11.35; 11.18; 11.88; 12.11	WHS
425.0998	$C_{15}H_{23}O_{11}N_1S_1$	2	7.86; 8.00	NJSN
425.9192	$C_{11}H_6O_{14}S_2$	1	0.83	WHW, NJSN, SHWD, SHWN, SHSD
425.9743	$C_{12}H_{10}O_{15}S_1$	1	7.84	NJSN, SHSD, SHSN
426.2293	$C_{19}H_{38}O_8S_1$	8	9.60; 9.92; 10.10; 10.34; 10.66; 11.04; 11.80; 12.87	WHS
427.1154	$C_{15}H_{25}O_{11}N_1S_1$	1	6.76	NJSN
436.2864	$C_{22}H_{44}O_6S_1$	4	11.40; 11.79; 12.41; 13.19	WHS
438.0108	$C_{14}H_{14}O_{14}S_1$	1	11.45	NJSN
438.1354	$C_{21}H_{26}O_8S_1$	1	9.64	NJSN
440.0843[c]	$C_{12}H_{24}O_{15}S_1$	1	1.18	SHWD, SHWN, SHSD
440.1724	$C_{18}H_{32}O_{10}S_1$	1	8.65	WHS, SHWD
441.2037	$C_{18}H_{35}O_9N_1S_1$	3	10.39	WHS, NJSN
			12.37; 12.78	WHW, WHS, NJSN, SHWN, SHSN
442.0512[d]	$C_{25}H_{14}O_6S_1$	1	8.29	NJSN
442.2607	$C_{20}H_{42}O_8S_1$	1	16.71	SHWD
443.1106	$C_{15}H_{25}O_{12}N_1S_1$	1	7.92	NJSN
452.0727	$C_{27}H_{16}O_5S_1$	1	11.14	WHW
453.9304	$C_{16}H_6O_{12}S_2$	1	0.86	SHWD, SHSD, SHSN
456.1098	$C_{20}H_{24}O_{10}S_1$	1	1.19	SHWD, SHSD
456.1460	$C_{21}H_{28}O_9S_1$	1	8.09	NJSN
457.1989	$C_{18}H_{35}O_{10}N_1S_1$	2	9.43; 9.88	WHS

484.0526	$C_{16}H_{20}O_{15}S_1$	1	10.75	SHWN, SHSD
494.2136[e]	$C_{29}H_{34}O_5S_1$	1	6.73	NJSN
495.9773	$C_{19}H_{12}O_{12}S_2$	1	11.15	NJSN
499.9235	$C_9H_8O_{22}S_1$	1	0.84	NJSN, SHWD, SHWN, SHSD
521.9178	$C_{10}H_6O_{21}N_2S_1$	1	0.86	SHWD, SHSD, SHSN
525.9679[f]	$C_{11}H_{14}O_{18}N_2S_2$	1	8.91	NJSN, SHSD
531.9747	$C_{13}H_{12}O_{19}N_2S_1$	2	9.55; 12.81	NJSN, SHSD
533.9332	$C_{15}H_6O_{18}N_2S_1$	1	16.22	WHW, NJSN, SHWN, SHSD, SHSN
539.9671	$C_{20}H_{12}O_{14}S_2$	1	8.37	NJSN, SHSD, SHSN
545.9742[g]	$C_{22}H_{10}O_{15}S_1$	1	11.91	NJSN
550.1753[h]	$C_{20}H_{38}O_{13}S_2$	1	1.34	SHSD
575.9650[i]	$C_{14}H_{12}O_{21}N_2S_1$	1	9.53	NJSN
581.9719[j]	$C_{29}H_{10}O_{10}S_2$	1	10.23	NJSN
589.9054	$C_{17}H_6O_{18}N_2S_2$	2	0.86	SHWD, SHSD, SHSN
			10.30	SHWD
589.9641[k]	$C_{23}H_{10}O_{17}S_1$	1	8.91	NJSN
631.9687[l]	$C_{11}H_{20}O_{26}S_2$	1	11.13	NJSN
645.9682[m]	$C_{21}H_{14}O_{18}N_2S_2$	1	13.65	SHWD
649.9218[n]	$C_{13}H_{14}O_{26}S_2$	3	14.21; 14.35; 14.81	NJSN
651.8755	$C_{10}H_8O_{27}N_2S_2$	1	0.85	SHWD, SHSD
696.8671	$C_{11}H_7O_{32}N_1S_1$	1	0.85	SHSD
699.9188	$C_{16}H_{12}O_{29}S_1$	1	16.72	SHSD
725.8798[o]	$C_{17}H_{10}O_{28}S_2$	3	0.86	SHWD, SHSD, SHSN
			16.63	SHSD
			16.75	NJSN, SHWD, SHWN, SHSD, SHSN

[a] Other formula within 2 ppm: $C_{15}H_{24}O_{13}$.

[b] Other formula within 2 ppm: $C_{14}H_{26}O_{14}$.

[c] Other formula within 2 ppm: $C_{33}H_{12}O_2$.

[d] Other formula within 2 ppm: $C_{17}H_{18}O_8N_2S_2$.

[e] Other formula within 2 ppm: $C_{17}H_{38}O_{12}N_2S_1$.

[f] Other formula within 2 ppm: $C_{10}H_{10}O_{23}N_2$..

[g] Other formula within 2 ppm: $C_{14}H_{14}O_{17}N_2S_2$.

[h] Other formulas within 2 ppm: $C_{19}H_{34}O_{18}$.

[i] Other formula within 2 ppm: $C_{22}H_8O_{19}$.

[j] Other formula within 2 ppm: $C_{16}H_{10}O_{22}N_2$.

[k] Other formula within 2 ppm: $C_{15}H_{14}O_{19}N_2S_2$.

[l] Other formulas within 2 ppm: $C_{24}H_{12}O_{15}N_2S_2$; $C_{10}H_{16}O_{31}$.

[m] Other formulas within 2 ppm: $C_{29}H_{10}O_{16}S_1$; $C_{20}H_{10}O_{23}N_2$.

[n] Other formula within 2 ppm: $C_{12}H_{10}O_{31}$

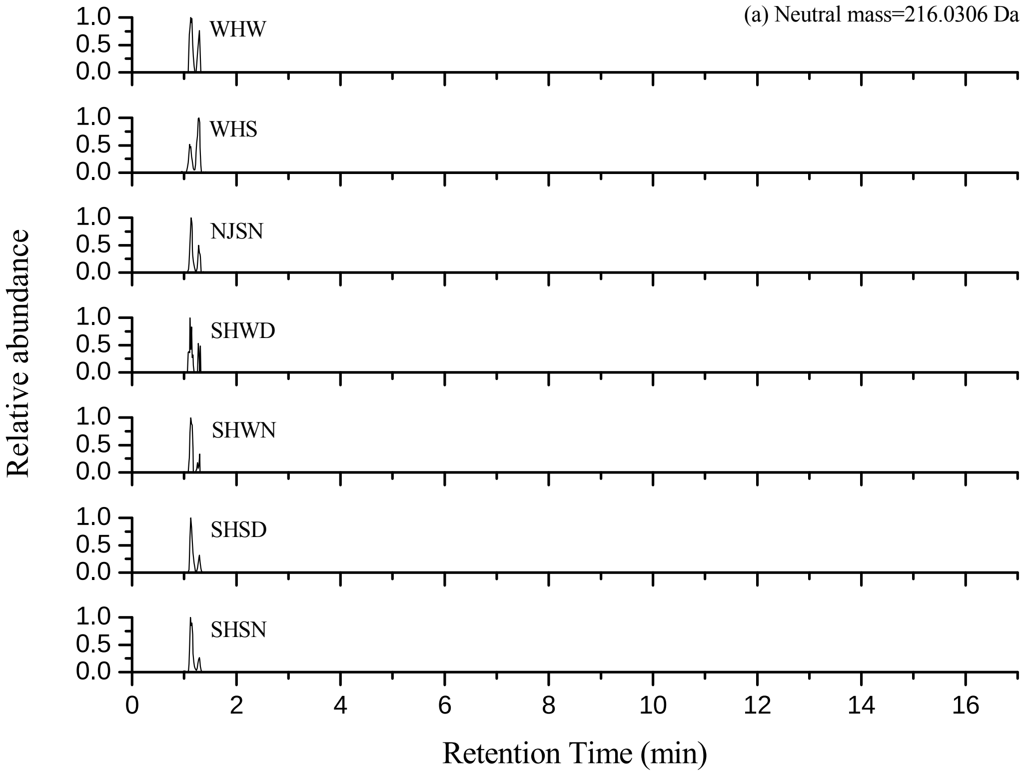
[o] Other formula within 2 ppm: $C_{16}H_{6}O_{33}$.

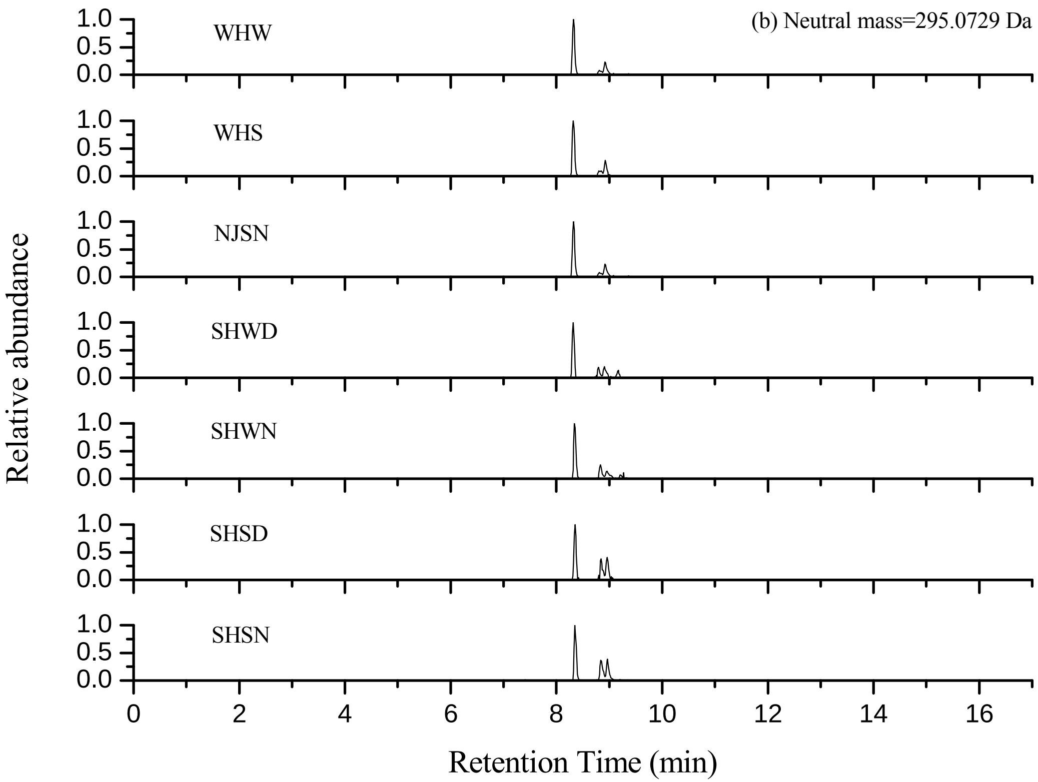
[p] Potentially being sulfonates.

Table S4. Isomer ratios for selected OSs in Figure 3.

ID	Formula	Trace	Number of isomers	Retention times (min)	Intensity ratios of isomers (%)	Potential precursor	Ref.
A	$C_5H_8O_7S_1$	WHS	1	1.36	100	Isoprene	Surratt et al., 2008
		NJSN	1	1.36	100		
		SHSD+SHSN	1	1.36	100		
B	$C_5H_{12}O_7S_1$	WHS	2	1.15; 1.29	37.4: 62.6	Isoprene	Surratt et al., 2008
		NJSN	2	1.15; 1.29	79.4: 20.6		
		SHSD+SHSN	2	1.15; 1.29	73.5: 26.5		
C	$C_6H_{10}O_7S_1$	WHS	5	1.36; 2.72; 3.25; 4.57; 4.98	6.8: 27.8: 52.0: 11.6: 1.8	3-Z-Hexenal	Shalamzari et al., 2014
		NJSN	7	1.36; 2.72; 3.25; 4.57; 4.98; 6.41; 7.02	10.1: 19.8: 41.7: 9.7: 2.1: 6.6: 10.0		
		SHSD+SHSN	7	1.36; 2.72; 3.25; 4.57; 4.98; 6.41; 7.02	10.7: 17.0: 45.7: 9.5: 4.1: 1.0: 2.0		
D	$C_7H_{12}O_7S_1$	WHS	3	4.84; 5.27; 6.64	27.0: 72.9: 0.1	Limonene	Surratt et al., 2008
		NJSN	2	4.84; 5.27	51.4: 48.6		
		SHSD+SHSN	2	4.84; 5.27	44.6: 55.4		
E	$C_9H_{18}O_6S_1$	WHS	8	5.52; 6.89; 7.16; 7.50; 7.96; 8.56; 8.99; 9.59	0.5: 24.6: 45.3: 14.6: 10.5: 3.9: 0.1: 0.5	Not known	
		NJSN	6	5.52; 6.89; 7.16; 7.50; 7.96; 8.56	2.7: 29.0: 46.6: 14.9: 5.9: 0.9		
		SHSD+SHSN	6	5.52; 6.89; 7.16; 7.50; 7.96; 8.56	0.8: 30.5: 46.4: 17.2: 4.4: 0.7		
F	$C_5H_{11}O_9N_1S_1$	WHS	4	2.46; 2.94; 3.53; 4.43	33.8: 13.9: 43.8: 8.5	Isoprene	Surratt et al., 2008
		NJSN	4	2.46; 2.94; 3.53; 4.43	24.7: 17.2: 51.4: 6.7		
		SHSD+SHSN	4	2.46; 2.94; 3.53; 4.43	22.2: 28.6: 42.8: 6.4		

G	$C_9H_{16}O_7S_1$	WHS	5	5.74; 6.30; 7.02; 7.47; 7.74	71.9: 15.4: 11.6: 0.9: 0.2	Limonene	Surratt et al., 2008
		NJSN	5	5.74; 6.30; 7.02; 7.47; 7.74	90.8: 7.4: 1.6: 0.4: 0.1		
		SHSD+SHSN	5	5.74; 6.30; 7.02; 7.47; 7.74	87.4: 8.4: 4.0: 0.1: 0.1		
H	$C_{10}H_{17}O_7N_1S_1$	WHS	3	8.37; 8.82; 8.95	69.1: 10.5: 20.4	α-pinene, β-pinene, α-terpinene and terpinolene	Surratt et al., 2008
		NJSN	3	8.37; 8.82; 8.95	51.4: 38.3: 10.3		
		SHSD+SHSN	3	8.37; 8.82; 8.95	47.8: 25.9: 26.3		
I	$C_5H_{10}O_{11}N_2S_1$	WHS	7	6.22; 6.44; 6.63; 6.80; 6.98; 7.61; 7.45	2.2: 12.9: 26.8: 23.7: 16.0: 10.0: 8.4	Isoprene	Surratt et al., 2008
		NJSN	7	6.22; 6.44; 6.63; 6.80; 6.98; 7.61; 7.45	1.8: 10.4: 25.7: 27.0: 15.1: 13.6: 6.4		
		SHSD+SHSN	7	6.22; 6.44; 6.63; 6.80; 6.98; 7.61; 7.45	1.6: 13.9: 20.0: 24.8: 21.1: 12.7: 5.9		
J	$C_{16}H_{32}O_6S_1$	WHS	9	10.25; 10.38; 10.50; 10.67; 10.89; 11.27; 11.63; 12.32; 13.55	33.3: 16.7: 7.1: 8.1: 6.4: 7.6: 8.6: 9.2: 3.0	Not known	
		NJSN	6	10.25; 10.38; 10.67; 11.27; 11.63; 12.32	42.4: 21.3: 7.8: 7.3: 10.9: 10.3		
		SHSD+SHSN	6	10.25; 10.38; 10.50; 10.67; 10.89; 11.27	43.8: 21.6: 11.0: 10.9: 6.6: 6.1		
K	$C_{15}H_{25}O_7N_1S_1$	WHS	5	10.53; 10.88; 11.18; 11.50; 11.93	0.8: 2.6: 17.4: 77.6: 1.6	β-caryophyllene	Chan et al., 2011
		NJSN	4	10.53; 10.88; 11.18; 11.93	0.2: 26.3: 69.8: 3.7		
		SHSD+SHSN	4	10.88; 11.18; 11.32; 11.50	0.3: 2.8: 96.8: 0.1		


(a) Neutral mass=216.0306 Da
WHW
WHS
NJSN
SHWD
SHWN
SHSD
SHSN
Relative abundance
1.0
0.5
0.0
0
2
4
6
8
10
12
14
16
Retention Time (min)



(b) Neutral mass=295.0729 Da
WHW
WHS
NJSN
SHWD
SHWN
SHSD
SHSN
Relative abundance
1.0
0.5
0.0
0
2
4
6
8
10
12
14
16
Retention Time (min)

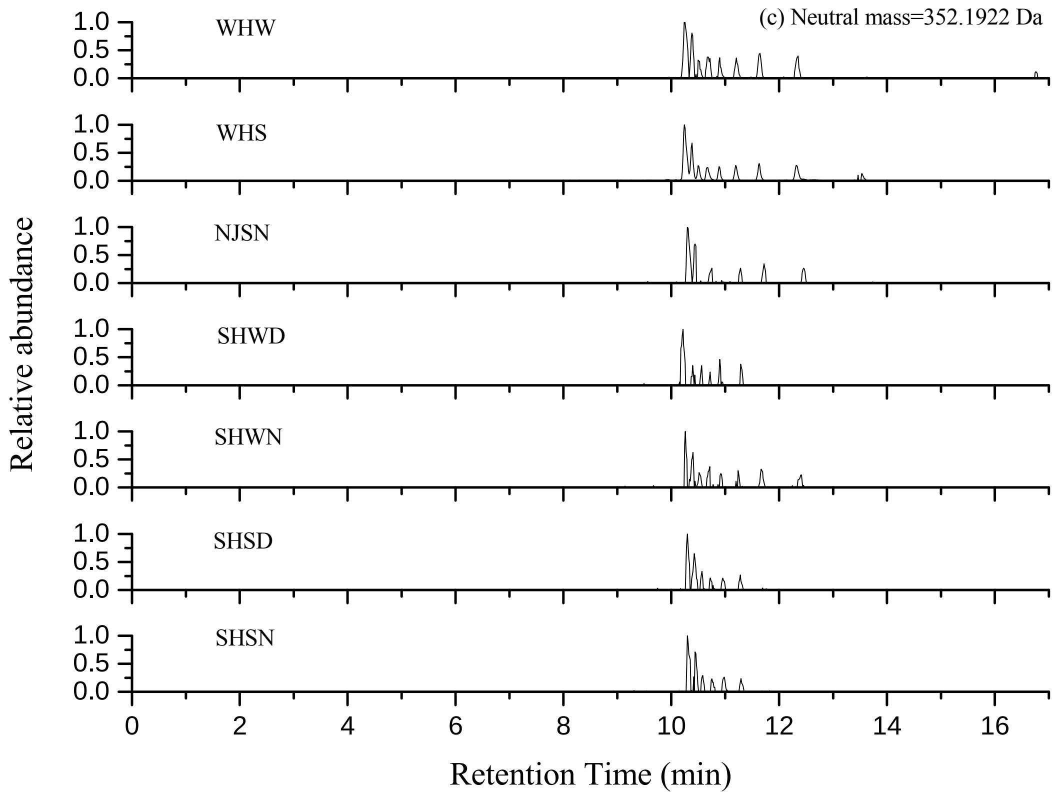


Figure S1. LC chromatograms of three deprotonated OSs (a) $C_5H_{12}O_7S_1$ (potentially from isoprene); (b) $C_{10}H_{17}O_7N_1S_1$ (potentially from various monoterpenes); (c) $C_{16}H_{32}O_6S_1$ (with an unknown precursor). Chromatograms for the NJSD sample are not included because a large amount of sample injection led to corruption of peaks and hence inaccurate retention times and worse peak resolution.

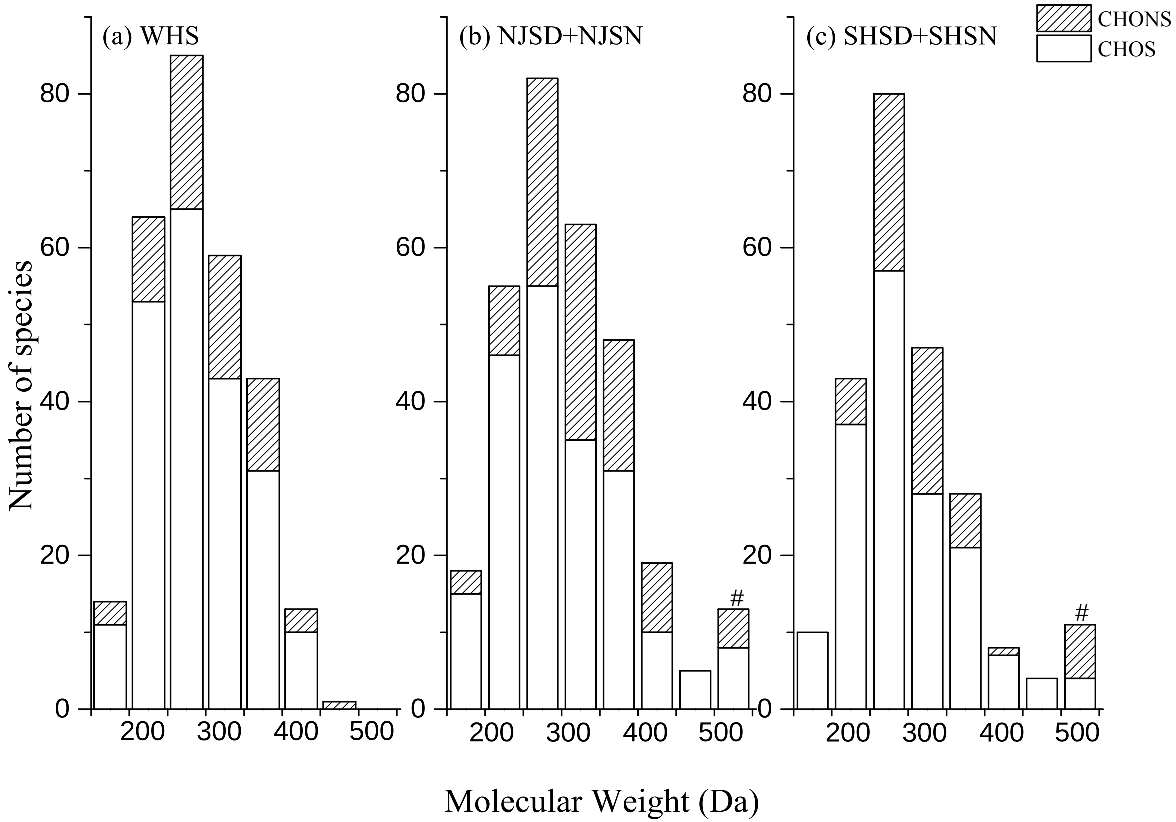


Figure S2. Number of CHOS and CHONS in the different mass ranges. The bins are 50 Da wide. The last bin with a # sign includes all species with a molecular weight larger than 500 Da.

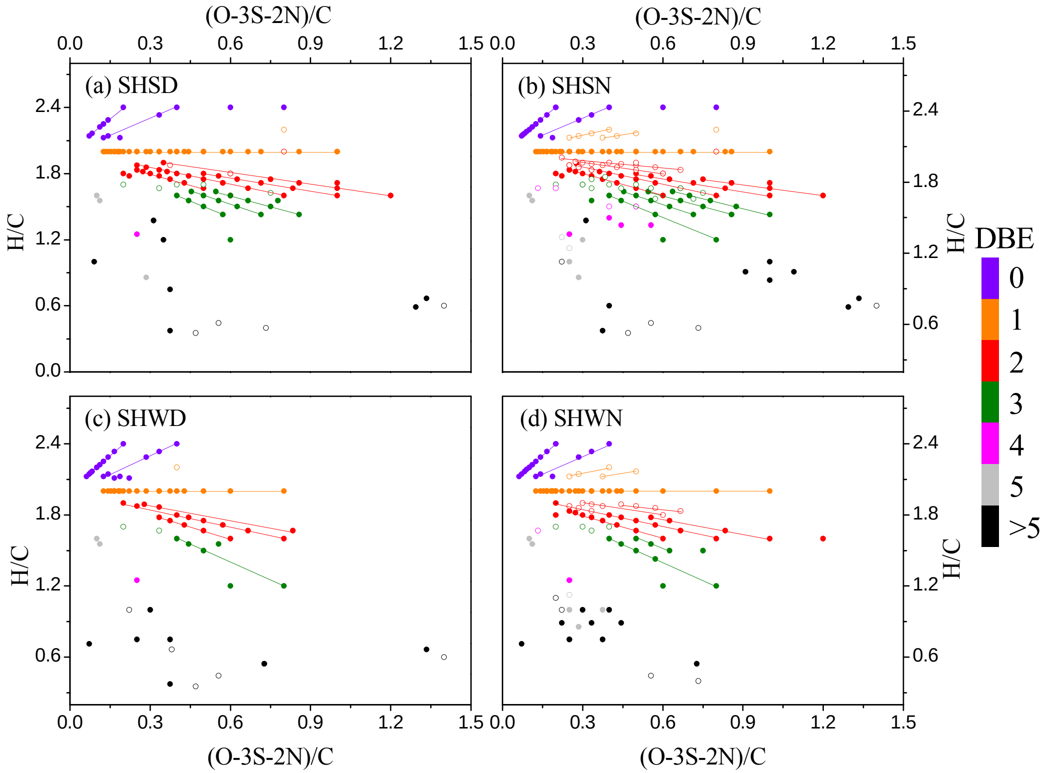


Figure S3. (a-d) Van Krevelen diagrams for CHOS and CHONS detected in Shanghai samples. The filled and open circles denote CHOS and CHONS, respectively. Note that only compounds with a relative abundance greater than or equal to 0.5% of that of $C_{10}H_{17}O_7N_1S_1$ in the SHSN sample are shown in this figure.

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