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Measurement report: Extreme heat and wildfire emissions enhance volatile organic compounds in a temperate forest

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S1. Operation of PTR-ToF-MS 6000X2, Conversion of Raw Signals, and Definition of Mixing Ratio

In PTR-ToF-MS, hydronium ions are utilized to charge the VOCs through a non-dissociative proton transfer in the reaction chamber of the instrument. This technique can identify a wide range of compounds (e.g., carboxylic acids, carbonyls, and aromatic hydrocarbons) if the target compound has a proton affinity higher than water (691 kJ/mol). The protonation occurs as follows:

$$H_3O^+ + VOC \rightarrow H_2O + VOC{-}H^+ \ (S1)$$

The conversion of raw signals (counts per second) to mixing ratio (ppb) of an uncalibrated gas VOC can be performed using the following equation:

$$[VOC, ppb] = \frac{1}{k\Delta t} \times \frac{I(VOC^+)}{T(VOC^+)} \times \frac{I(H_3O^+)}{T(H_3O^+)} \ (S2)$$

Where RH^+ is the protonated gas compound, k is the proton-transfer-reaction rate coefficient, Δt is the reaction time, $I(VOC^+)$ and $I(H_3O^+)$ are the measured ion count rates for the RH^+ and the hydronium ion (H_3O^+), respectively. T (VOC^+) and $T(H_3O^+)$ are the transmission efficiencies for RH^+ and H_3O^+ ions (Worton et al., 2023; Taipale et al., 2008). All the values are readily available except for transmission efficiency value, which can be determined by generating a mass dependent transmission curve from compounds with known concentrations and reaction rate. The transmission is an instrument-specific parameter that depends on the transmission efficiencies of the lens system/ion guide, the mass filter (TOF), and the ion detector. Transmission Tool provided by the instrument developer (IONICON) was used to generate the transmission efficiencies of gas standards. The PTR-ToF-MS was operated with 2.6 mbar and 80°C drift tube pressure and temperature, with an E/N value of ~119 Townsend. The mass range was set up to 500 m/z. The single spectrum time was set to calculate the fluxes of the VOC, the results of which will be reported in subsequent works. One of the limitations of the PTR-ToF-MS technique is that it cannot distinguish isomers (e.g., α-pinene, β-pinene, and limonene) because of their identical exact mass (Blake et al., 2009).

.The term *mixing ratio* used in this manuscript is defined as the ratio of the moles of target analyte to the moles of all of atmospheric gases (i.e., N_2 and O_2). This can be expressed as the following equation:

$$R_i = \frac{n_i}{n_\Sigma - n_i} \approx \frac{n_i}{n_\Sigma} \ (S3)$$

Where R_i is the mixing ratio, n_i is the moles of gas analyte, and n_Σ is the total moles of atmospheric gases. The amount of organic gases in the atmosphere is significantly lower than the total gases.

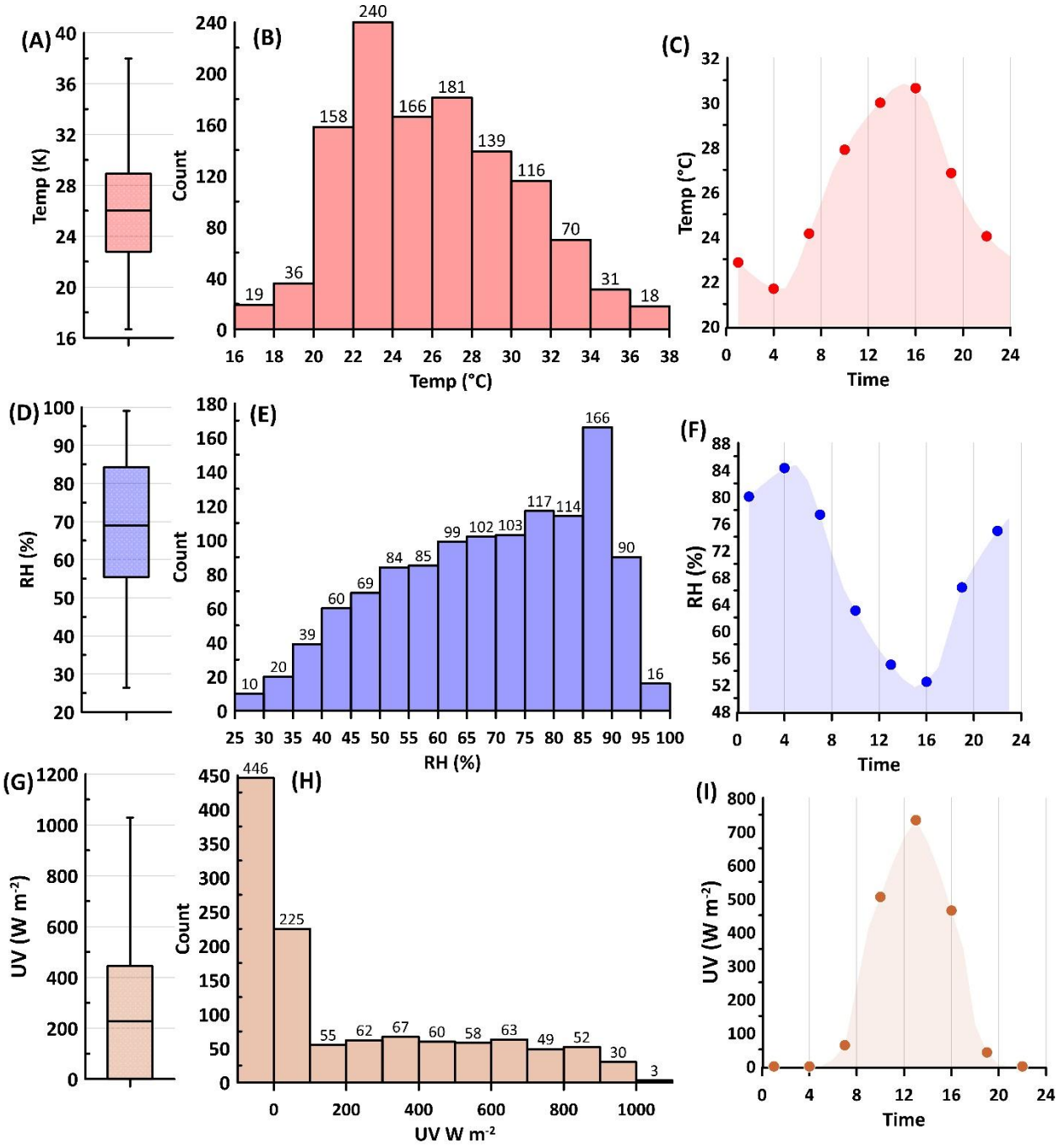


Figure S1. Box-Whisker plot, histogram, and diurnal profile of (A-C) temperature, (D-F) relative humidity, and (G-I) global solar radiation. Temperature and relative humidity were collected from a nearby airport monitoring site (KCOU) while global radiation was measured in Ashland, MO, 5.22 kilometers from the MOFLUX site.

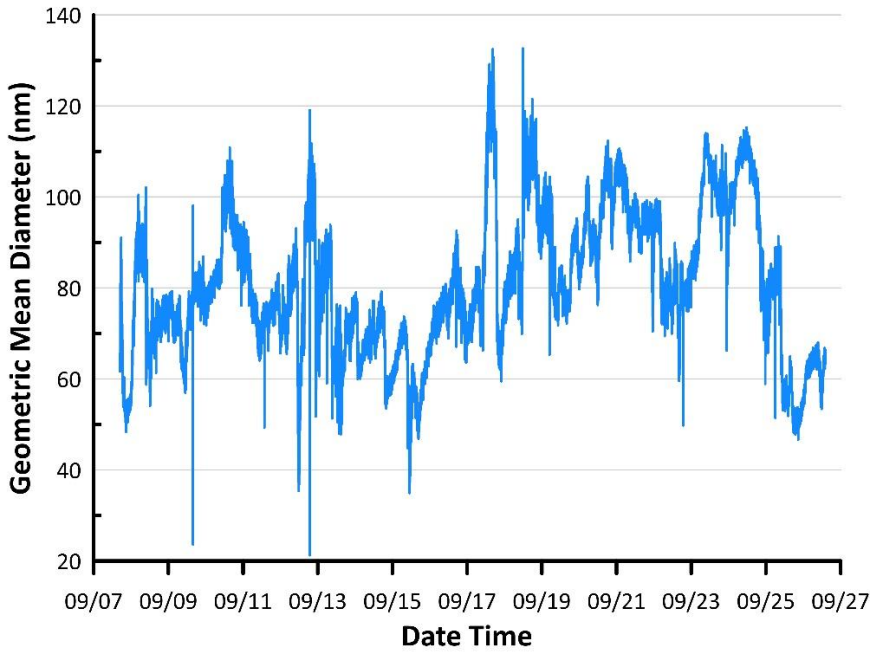


Figure S2. Geometric Mean Diameter (GMD) of the particles observed at MOFLUX. The real-time nanoparticle size measurements were implemented using a NanoScan Scanning Mobility Particle Sizer (SMPS, TSI) spectrometer with size distribution from 10 to 420 nm in one minute time interval. The time series of GMD shows that most of the particles have a diameter greater than 50 nm most of the time, with no apparent particle growth from smaller particles (~10 nm). Note that the particle measurements were performed after the VOC monitoring duration indicated in the main text.

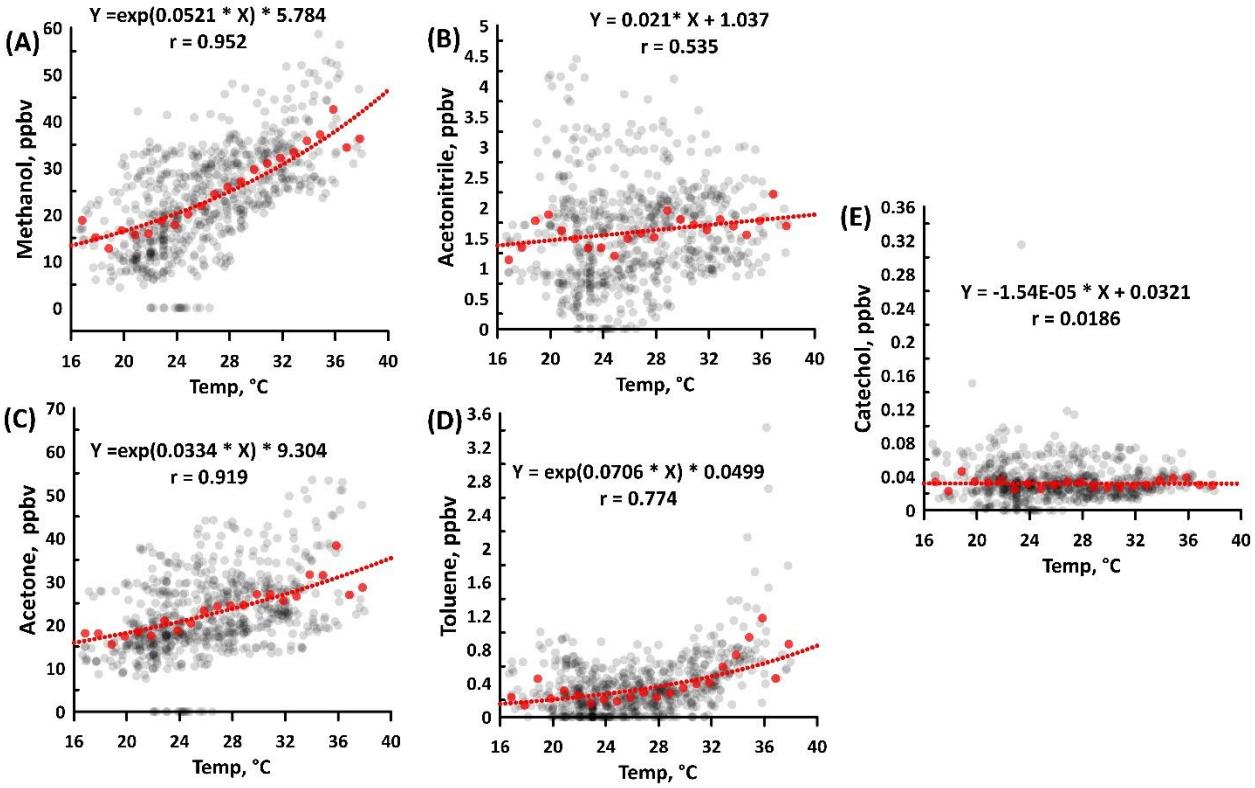


Figure S3. The correlation analysis of temperature and mixing ratios of other VOCs not included in Figure 3. Black symbols are hourly data while the red lines indicate the best-fit line of the binned mixing ratio of VOCs according to 1.0 °C of temperature

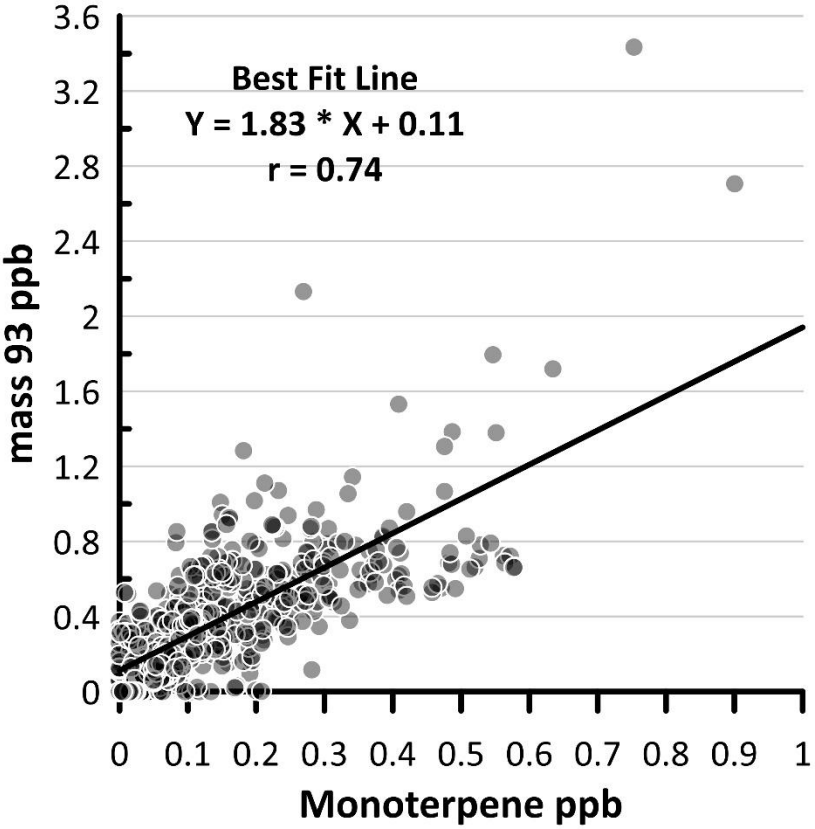
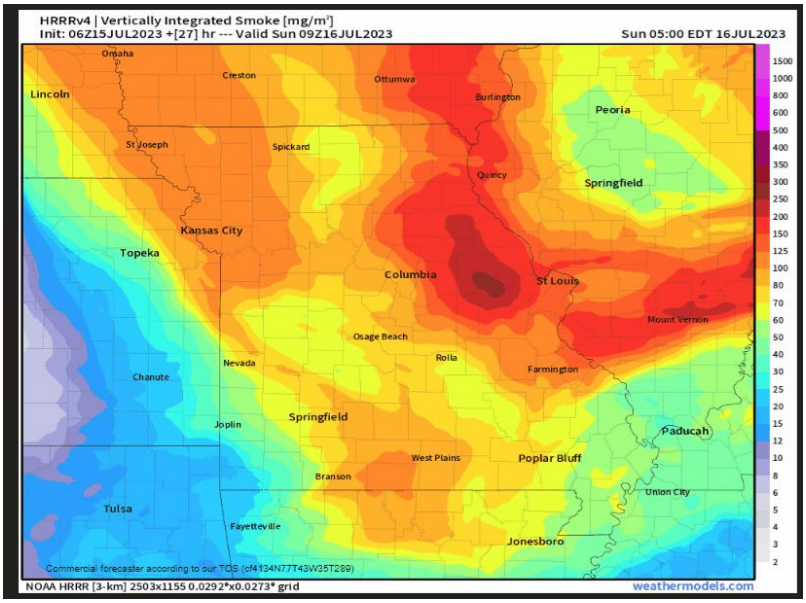


Figure S4. Correlation plot of mass 93 and monoterpene at mass 137.

(A)



(B)

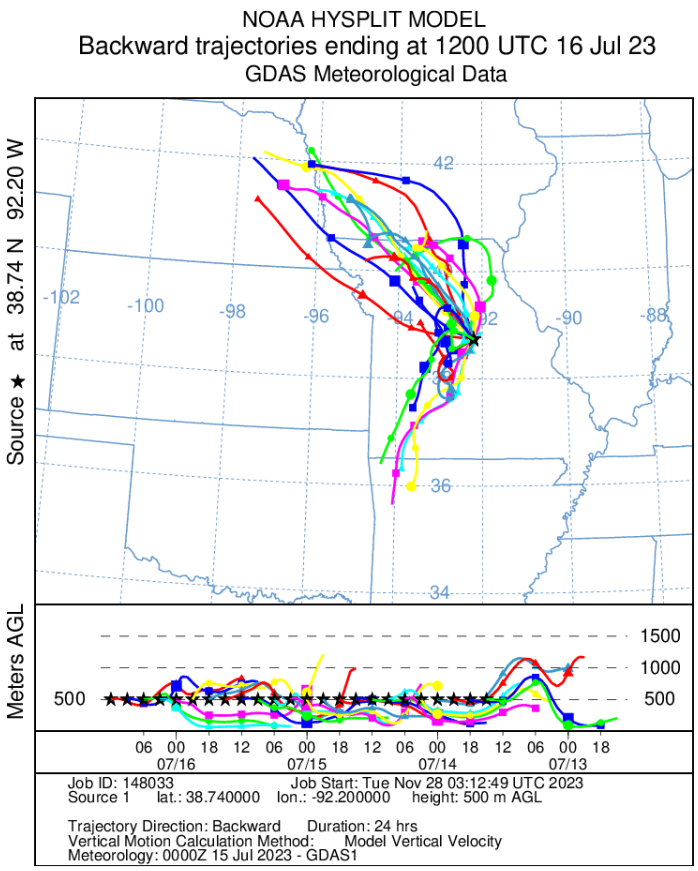


Figure S5. (A) Atmospheric dispersion of smoke observed during July 16, 2023. The smoke snapshot coincided with the day with highest smoke concentration observed during the MOFLUX VOC measurement. (B) Backward air parcel trajectory analysis of plumes arriving on the 16th of July (Stein et al., 2015).

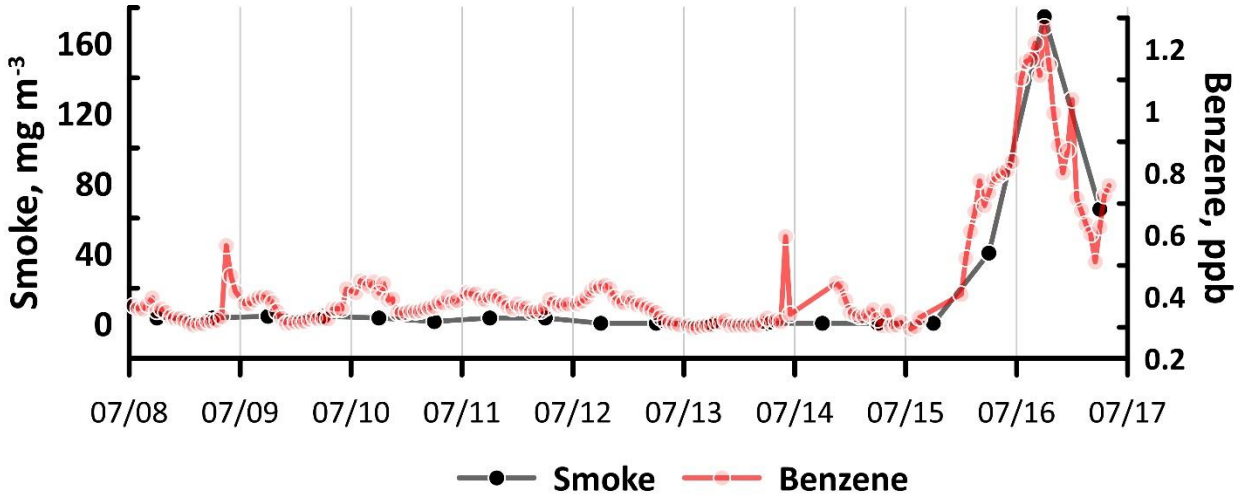


Figure S6: The time series profile of benzene and smoke between July 8 to 17.

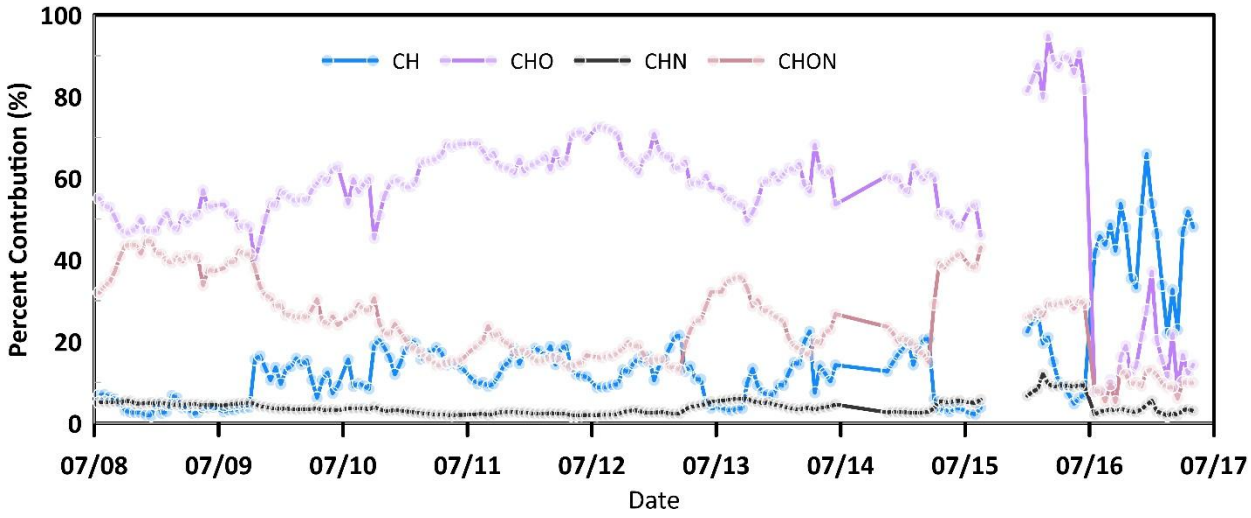


Figure S7: Time series profile of percent contribution of each VOC class to total concentration during the intensive observation period with enhanced temperature and combustion plume transport at MOFLUX. $C_xH_yO_wS_v$ compounds were not included due to low mixing ratio compared to other categories.

Table S1. List of all identified ions with the corresponding suggested molecular formula measured from MOFLUX site. N/A – No possible suggested molecular formula; ***mDa*** – Absolute difference of experimental (Exp) m/z and monoisotopic (Theor) mass in terms of milliDalton; ***DU*** – Degree of Unsaturation; ***O:C*** – oxygen to carbon ratio; ***H:C*** – hydrogen to oxygen ratio; ***Csat*** – effective saturation mass mixing ratio (μg m^{-3}); ***Ave Conc*** – concentration of the VOC between July 8 to 17.

Exp. Mass [M+H]	Molecular Formula	Theor. Mass [M]	mDa	DU	O:C	H:C	Csat	Ave Conc. (ppb)
40.023	C_2HN	39.011	4.59	3	0.00	0.50	5.43	0.059
41.035	C_3H_4	40.031	-4	2	0.00	1.33	10.45	5.753
42.006	C_2HO	41.003	-3.92	2.5	0.50	0.50	9.53	0.009
42.031	C_2H_3N	41.027	-2.61	2	0.00	1.50	5.43	0.892
42.044	C_3H_5	41.039	-2.2	1.5	0.00	1.67	10.45	0.037
43.014	C_2H_2O	42.011	-4.02	2	0.50	1.00	9.53	12.872
43.031	CH_2N_2	42.022	2.4	2	0.00	2.00	6.88	0.019
43.050	C_3H_6	42.047	-4.09	1	0.00	2.00	10.45	1.073
44.019	CHNO	43.006	6.24	2	1.00	1.00	9.30	0.253
44.064	C_3H_7	43.055	2.24	0.5	0.00	2.33	10.45	0.040
44.977	CS	43.972	-1.95	2	0.00	0.00	11.40	0.137
44.997	CO_2	43.990	-0.25	2	2.00	0.00	9.80	0.071
45.025	CH_2NO	44.014	4.11	1.5	1.00	2.00	9.30	2.400
45.031	C_2H_4O	44.026	-2.2	1	0.50	2.00	9.53	4.864
45.988	CHS	44.980	1.28	1.5	0.00	1.00	11.40	0.961
46.023	CH_3NO	45.022	-5.74	1	1.00	3.00	9.30	0.159
46.032	CH_3NO	45.022	2.97	1	1.00	3.00	9.30	0.668
46.062	C_2H_7N	45.058	-3.37	0	0.00	3.50	5.43	0.009
47.007	CH_2O_2	46.006	-5.66	1	2.00	2.00	9.80	0.839
47.017	CH_2O_2	46.006	4.64	1	2.00	2.00	9.80	0.124
47.040	CH_4NO	46.029	3.81	0.5	1.00	4.00	9.30	0.504
47.047	C_2H_6O	46.042	-2.19	0	0.50	3.00	9.53	1.030
47.991	HNS	46.983	0.81	1	0.00	0.00	9.98	0.006
48.007	HNO_2	47.001	-1.29	1	0.00	0.00	9.58	0.029
48.049	CH_5NO	47.037	4.32	0	1.00	5.00	9.30	0.043
49.008	CH_4S	48.003	-2.32	0	0.00	4.00	11.40	0.016
49.999	HO_3	48.993	-1.02	0.5	0.00	0.00	11.28	0.012
51.043	N/A				0.00	0.00		0.132
53.038	C_4H_4	52.031	-0.56	3	0.00	1.00	9.98	0.069
54.034	C_3H_3N	53.027	0.3	3	0.00	1.00		0.024
55.017	C_3H_2O	54.011	-1.09	3	0.33	0.67	8.90	0.061
55.039	C_3H_4N	54.034	-2.84	2.5	0.00	1.33		1.133
55.054	C_4H_6	54.047	-0.17	2	0.00	1.50	9.98	0.722
56.021	C_3H_3O	55.018	-4.84	2.5	0.33	1.00	8.90	0.007
56.059	C_4H_7	55.055	-3.27	1.5	0.00	1.75	9.98	0.015

Exp. Mass [M+H]	Molecular Formula	Theor. Mass [M]	mDa	DU	O:C	H:C	Csat	Ave Conc. (ppb)
57.032	C_3H_4O	56.026	-1.19	2	0.33	1.33	8.90	1.102
57.070	C_4H_8	56.063	0.17	1	0.00	2.00	9.98	0.773
58.068	C_3H_7N	57.058	3.15	1	0.00	2.33		0.025
59.049	C_3H_6O	58.042	0.03	1	0.33	2.00	8.90	
59.967	N/A				0.00	0.00		0.064
59.994	CHNS	58.983	3.26	2	0.00	1.00	8.60	0.009
60.023	$C_2H_3O_2$	59.013	2.9	1.5	1.00	1.50	8.73	0.013
60.049	C_2H_5NO	59.037	4.59	1	0.50	2.50		0.743
61.029	$C_2H_4O_2$	60.021	0.25	1	1.00	2.00	8.73	3.293
61.053	C_2H_6NO	60.045	1.07	0.5	0.50	3.00		0.053
61.980	CHOS	60.975	-2.4	1.5	1.00	1.00	10.30	0.007
62.028	CH_3NO_2	61.016	4.61	1	2.00	3.00		0.111
62.060	C_2H_7NO	61.053	0.13	0	0.50	3.50		0.028
63.026	C_2H_6S	62.019	-0.65	0	0.00	3.00	10.93	0.094
63.044	$C_2H_6O_2$	62.037	-0.5	0	1.00	3.00	8.73	0.057
65.024	CH_4O_3	64.016	0.65	0	3.00	4.00	9.45	0.011
65.039	C_5H_4	64.031	0.91	4	0.00	0.80	9.50	0.008
65.059	N/A				0.00	0.00		0.030
67.054	C_5H_6	66.047	-0.24	3	0.00	1.20	9.50	0.417
68.057	C_5H_7	67.055	-4.93	2.5	0.00	1.40	9.50	0.090
68.998	C_3O_2	67.990	0.94	4	0.67	0.00	7.89	0.033
69.032	C_4H_4O	68.026	-1.32	3	0.25	1.00	8.34	0.218
69.070	C_5H_8	68.063	0.01	2	0.00	1.60	9.50	
70.068	C_4H_7N	69.058	2.59	2	0.00	1.75	15.28	0.025
71.012	$C_3H_2O_2$	70.006	-0.62	3	0.67	0.67	7.89	0.128
71.050	C_4H_6O	70.042	0.46	2	0.25	1.50	8.34	7.228
71.068	C_4H_8N	70.066	-5.25	1.5	0.00	2.00	15.28	0.019
71.086	C_5H_{10}	70.078	-0.01	1	0.00	2.00	9.50	0.058
72.045	C_3H_5NO	71.037	0.68	2	0.33	1.67	8.35	0.755
72.087	C_4H_9N	71.074	5.8	1	0.00	2.25	15.28	0.011
72.998	C_2H_2NS	71.991	-0.21	2.5	0.00	1.00	5.43	0.015
73.028	$C_3H_4O_2$	72.021	-0.04	2	0.67	1.33	7.89	0.386
73.046	$C_2H_4N_2O$	72.032	6.21	2	0.50	2.00	5.73	0.013
73.065	C_4H_8O	72.058	-0.02	1	0.25	2.00	8.34	
74.007	C_2H_3NS	72.999	1.14	2	0.00	1.50	5.43	0.056
74.029	$C_2H_3NO_2$	73.016	5.84	2	1.00	1.50	5.03	0.039
74.060	C_3H_7NO	73.053	0.31	1	0.33	2.33	8.35	2.073
74.994	C_2H_2OS	73.983	3.93	2	0.50	1.00	9.53	0.027
75.044	$C_3H_6O_2$	74.037	0.42	1	0.67	2.00	7.89	2.256
75.065	C_3H_8NO	74.061	-2.93	0.5	0.33	2.67	8.35	0.082
75.944	N/A				0.00	0.00		0.008

Exp. Mass [M+H]	Molecular Formula	Theor. Mass [M]	mDa	DU	O:C	H:C	Csat	Ave Conc. (ppb)
76.044	$C_2H_5NO_2$	75.032	4.66	1	1.00	2.50	5.03	0.094
76.069	C_3H_9NO	75.068	-6.54	0	0.33	3.00	8.35	0.006
77.023	$C_2H_4O_3$	76.016	-0.04	1	1.50	2.00	8.17	0.045
77.043	C_3H_8S	76.035	1.22	0	0.00	2.67	10.45	0.011
77.058	$C_3H_8O_2$	76.052	-1.52	0	0.67	2.67	7.89	0.023
79.033	CH_6N_2S	78.025	0.22	0	0.00	6.00	6.88	0.009
79.054	C_6H_6	78.047	-0.18	4	0.00	1.00	9.03	0.102
80.055	C_5H_5N	79.042	5.02	4	0.00	1.00	12.10	0.030
80.995	C_4O_2	79.990	-1.64	5	0.50	0.00	7.18	0.057
81.035	C_5H_4O	80.026	1.67	4	0.20	0.80	7.80	0.043
81.070	C_6H_8	80.063	0.13	3	0.00	1.33	9.03	0.348
82.036	C_5H_5O	81.034	-5.4	3.5	0.20	1.00	7.80	0.005
82.074	C_6H_9	81.070	-4.08	2.5	0.00	1.50	9.03	0.017
82.987	C_3NS	81.975	4.63	4.5	0.00	0.00		0.025
83.050	C_5H_6O	82.042	0.6	3	0.20	1.20	7.80	0.451
83.086	C_6H_{10}	82.078	0.15	2	0.00	1.67	9.03	0.183
84.049	C_4H_5NO	83.037	4.84	3	0.25	1.25	7.88	0.042
84.087	C_5H_9N	83.074	6.42	2	0.00	1.80	12.10	0.013
84.965	N/A				0.00	0.00		0.025
85.029	$C_4H_4O_2$	84.021	0.23	3	0.50	1.00	7.18	0.164
85.064	C_5H_8O	84.058	-0.46	2	0.20	1.60	7.80	0.254
85.101	C_6H_{12}	84.094	0.08	1	0.00	2.00	9.03	0.013
86.025	$C_3H_3NO_2$	85.016	1.31	3	0.67	1.00	5.45	0.020
87.007	$C_3H_2O_3$	86.000	-0.68	3	1.00	0.67	7.15	0.025
87.046	$C_4H_6O_2$	86.037	1.52	2	0.50	1.50	7.18	0.697
87.077	$C_5H_{10}O$	86.073	-2.95	1	0.20	2.00	7.80	0.023
88.017	C_3H_5NS	87.014	-4.22	2	0.00	1.67		0.036
88.032	C_4H_7S	87.027	-2.58	1.5	0.00	1.75	9.98	0.446
88.064	$C_3H_7N_2O$	87.056	0.99	1.5	0.33	2.33	3.75	1.435
88.078	C_4H_9NO	87.068	2.31	1	0.25	2.25	7.88	0.013
89.022	$C_3H_4O_3$	88.016	-1.1	2	1.00	1.33	7.15	0.043
89.055	$C_4H_8O_2$	88.052	-5.07	1	0.50	2.00	7.18	0.275
90.021	$C_2H_3NO_3$	89.011	2.12	2	1.50	1.50	4.83	0.023
90.042	C_3H_7NS	89.030	4.43	1	0.00	2.33		0.243
90.058	$C_3H_7NO_2$	89.048	3.28	1	0.67	2.33	5.45	0.016
91.031	$C_2H_4NO_3$	90.019	4.3	1.5	1.50	2.00	4.83	0.026
91.054	C_7H_6	90.047	-0.52	5	0.00	0.86	8.55	0.031
92.031	$C_2H_5NO_3$	91.027	-2.94	1	1.50	2.50	4.83	0.010
92.059	C_7H_7	91.055	-3.11	4.5	0.00	1.00	8.55	0.009
93.006	$C_2H_4O_2S$	91.993	5.39	1	1.00	2.00	8.73	0.007
93.037	C_6H_4O	92.026	3.19	5	0.17	0.67	7.28	0.739

Exp. Mass [M+H]	Molecular Formula	Theor. Mass [M]	mDa	DU	O:C	H:C	Csat	Ave Conc. (ppb)
93.070	C_7H_8	92.063	-0.07	4	0.00	1.14	8.55	0.330
93.956	$CHOS_2$	92.947	1.88	1.5	1.00	1.00	10.30	0.140
94.041	CH_7N_3S	93.036	-2.13	0	0.00	7.00	5.03	0.598
94.070	C_6H_7N	93.058	4.48	4	0.00	1.17	10.73	0.059
95.013	$C_5H_2O_2$	94.006	-0.11	5	0.40	0.40	6.53	0.054
95.026	$C_4H_2N_2O$	94.017	1.8	5	0.25	0.50		0.067
95.049	C_6H_6O	94.042	-0.12	4	0.17	1.00	7.28	0.102
95.085	C_7H_{10}	94.078	-0.1	3	0.00	1.43	8.55	0.028
95.951	$HNOS_2$	94.950	-5.8	1	0.00	0.00	9.78	0.050
96.051	C_6H_7O	95.050	-5.55	3.5	0.17	1.17	7.28	0.007
96.959	O_4S	95.952	-0.16	1	0.00	0.00	11.08	0.031
97.028	$C_5H_4O_2$	96.021	0.08	4	0.40	0.80	6.53	0.075
97.065	C_6H_8O	96.058	0.04	3	0.17	1.33	7.28	0.055
97.101	C_7H_{12}	96.094	0.02	2	0.00	1.71	8.55	0.041
97.949	HO_2S_2	96.942	0.29	0.5	0.00	0.00	11.48	0.007
98.032	$C_5H_5O_2$	97.029	-4.67	3.5	0.40	1.00	6.53	0.017
98.063	C_5H_7NO	97.053	2.72	3	0.20	1.40	7.40	0.012
98.952	$H_2O_2S_2$	97.950	-4.48	0	0.00	0.00	11.48	0.027
98.980	H_2O_4S	97.967	5.55	0	0.00	0.00	11.08	0.014
99.007	$C_4H_2O_3$	98.000	-1	4	0.75	0.50	6.29	0.006
99.015	$C_3H_2N_2O_2$	98.012	-3.66	4	0.67	0.67	6.25	0.024
99.045	$C_5H_6O_2$	98.037	0.57	3	0.40	1.20	6.53	0.816
99.082	$C_6H_{10}O$	98.073	1.4	2	0.17	1.67	7.28	0.196
100.040	$C_4H_5NO_2$	99.032	1.1	3	0.50	1.25	5.28	0.168
100.077	C_5H_9NO	99.068	1.01	2	0.20	1.80	7.40	0.012
100.938	N/A				0.00	0.00		0.057
101.024	$C_4H_4O_3$	100.016	0.18	3	0.75	1.00	6.29	0.107
101.061	$C_5H_8O_2$	100.052	0.99	2	0.40	1.60	6.53	0.493
101.097	$C_6H_{12}O$	100.089	1.11	1	0.17	2.00	7.28	0.026
102.056	$C_4H_7NO_2$	101.048	0.75	2	0.50	1.75	5.28	0.081
102.092	$C_5H_{11}NO$	101.084	0.26	1	0.20	2.20	7.40	0.006
102.934	$C_3H_2S_2$	101.960	-32.67	3	0.00	0.67	10.45	0.024
103.040	$C_4H_6O_3$	102.032	0.73	2	0.75	1.50	6.29	0.058
103.061	$C_5H_{10}S$	102.050	3.1	1	0.00	2.00	9.50	0.006
103.086	$C_4H_{10}N_2O$	102.079	-0.79	1	0.25	2.50		0.045
104.048	C_7H_5N	103.042	-1.88	6	0.00	0.71	9.80	0.039
104.070	$C_4H_9NO_2$	103.063	-1.1	1	0.50	2.25	5.28	0.017
104.933	N/A				0.00	0.00		0.005
105.034	C_4H_8OS	104.030	-2.66	1	0.25	2.00	8.34	0.070
105.070	C_8H_8	104.063	-0.08	5	0.00	1.00	8.08	0.020
106.037	C_3H_7NOS	105.025	4.39	1	0.33	2.33	8.35	0.007

Exp. Mass [M+H]	Molecular Formula	Theor. Mass [M]	mDa	DU	O:C	H:C	Csat	Ave Conc. (ppb)
106.963	$C_2H_2OS_2$	105.955	1.12	2	0.50	1.00	9.53	0.035
107.050	C_7H_6O	106.042	0.66	5	0.14	0.86	6.78	0.025
107.085	C_8H_{10}	106.078	-0.53	4	0.00	1.25	8.08	0.083
107.970	$C_2H_3OS_2$	106.963	-0.11	1.5	0.50	1.50	9.53	0.023
108.044	C_6H_5NO	107.037	-0.39	5	0.17	0.83	6.93	0.006
108.082	C_7H_9N	107.074	0.72	4	0.00	1.29	9.80	0.044
108.959	CO_4S	107.952	-0.41	2	4.00	0.00	9.16	0.488
109.048	$C_3H_8O_4$	108.042	-1.54	0	1.33	2.67	6.56	0.067
109.067	C_7H_8O	108.058	2.01	4	0.14	1.14	6.78	0.033
109.101	C_8H_{12}	108.094	-0.08	3	0.00	1.50	8.08	0.018
109.958	HN_2OS_2	108.953	-2.51	1.5	0.00	0.00	7.88	0.010
110.044	$C_2H_7NO_4$	109.038	-1.18	0	2.00	3.50	4.63	0.006
110.960	$CH_2O_2S_2$	109.950	2.8	1	2.00	2.00	9.80	0.010
111.044	$C_6H_6O_2$	110.037	-0.06	4	0.33	1.00	5.93	0.026
111.054	$C_5H_6N_2O$	110.048	-1.69	4	0.20	1.20		0.018
111.081	$C_7H_{10}O$	110.073	0.26	3	0.14	1.43	6.78	0.027
111.117	C_8H_{14}	110.110	0.17	2	0.00	1.75	8.08	0.012
111.975	HNO_4S	110.963	4.89	1	0.00	0.00	9.18	0.006
112.046	$C_6H_7O_2$	111.045	-6.18	3.5	0.33	1.17	5.93	0.009
112.078	C_6H_9NO	111.068	1.91	3	0.17	1.50	6.93	0.007
112.951	O_5S	111.947	-2.92	1	0.00	0.00	10.88	0.008
113.024	$C_5H_4O_3$	112.016	0.88	4	0.60	0.80	5.53	0.386
113.064	$C_6H_8O_2$	112.052	4.59	3	0.33	1.33	5.93	0.085
113.096	$C_7H_{12}O$	112.089	-0.29	2	0.14	1.71	6.78	0.046
114.016	$C_4H_3NO_3$	113.011	-2.37	4	0.75	0.75	3.88	0.024
114.055	$C_5H_7NO_2$	113.048	-0.05	3	0.40	1.40	4.95	0.066
114.092	$C_6H_{11}NO$	113.084	0.26	2	0.17	1.83	6.93	0.077
115.008	$C_4H_2O_4$	113.995	5.42	4	1.00	0.50	5.58	0.017
115.040	$C_5H_6O_3$	114.032	1.03	3	0.60	1.20	5.53	0.081
115.077	$C_6H_{10}O_2$	114.068	1.64	2	0.33	1.67	5.93	0.097
115.109	$C_7H_{14}O$	114.105	-2.74	1	0.14	2.00	6.78	0.027
116.071	$C_5H_9NO_2$	115.063	0.3	2	0.40	1.80	4.95	3.128
116.907	N/A				0.00	0.00		0.176
117.016	$C_4H_4O_4$	116.011	-2.24	3	1.00	1.00	5.58	0.019
117.044	$C_4H_8N_2S$	116.041	-4.2	2	0.00	2.00		0.009
117.071	C_9H_8	116.063	0.62	6	0.00	0.89	7.60	0.152
117.102	$C_5H_{12}N_2O$	116.095	-0.34	1	0.20	2.40		0.489
118.048	$C_4H_7NO_3$	117.043	-1.47	2	0.75	1.75	3.88	0.014
118.074	C_9H_9	117.070	-3.6	5.5	0.00	1.00	7.60	0.015
118.105	$C_6H_{13}O_2$	117.092	5.67	0.5	0.33	2.17	5.93	0.027
118.904	N/A				0.00	0.00		0.160

Exp. Mass [M+H]	Molecular Formula	Theor. Mass [M]	mDa	DU	O:C	H:C	Csat	Ave Conc. (ppb)
119.035	$C_4H_6O_4$	118.027	1.21	2	1.00	1.50	5.58	0.024
119.054	C_8H_6O	118.042	4.66	6	0.13	0.75	6.28	0.013
119.086	C_9H_{10}	118.078	0.17	5	0.00	1.11	7.60	0.054
119.951	N/A				0.00	0.00		0.014
120.048	C_7H_5NO	119.037	3.51	6	0.14	0.71	6.45	0.011
120.089	$C_5H_{13}NS$	119.077	4.95	0	0.00	2.60	12.10	0.006
120.900	N/A				0.00	0.00		0.047
121.065	C_8H_8O	120.058	0.41	5	0.13	1.00	6.28	0.089
121.102	C_9H_{12}	120.094	0.52	4	0.00	1.33	7.60	0.015
121.952	N/A				0.00	0.00		0.012
121.982	N/A				0.00	0.00		0.009
122.031	$C_3H_7NO_2S$	121.020	3.47	1	0.67	2.33	5.45	0.012
122.068	$C_4H_{11}NOS$	121.056	4.09	0	0.25	2.75	7.88	0.008
123.045	$C_7H_6O_2$	122.037	0.44	5	0.29	0.86	5.35	0.017
123.117	C_9H_{14}	122.110	0.17	3	0.00	1.56	7.60	0.017
123.946	N/A				0.00	0.00		0.083
123.974	N/A				0.00	0.00		0.016
124.044	$C_6H_5NO_2$	123.032	4.5	5	0.33	0.83	4.57	0.007
124.960	N_2O_4S	123.958	-4.95	2	0.00	0.00	7.28	0.012
124.981	$CH_4N_2OS_2$	123.977	-2.68	1	1.00	4.00	6.95	0.013
125.060	$C_7H_8O_2$	124.052	0.19	4	0.29	1.14	5.35	0.024
125.096	$C_8H_{12}O$	124.089	0.01	3	0.13	1.50	6.28	0.024
125.960	N/A				0.00	0.00		0.353
126.056	$C_6H_7NO_2$	125.048	0.75	4	0.33	1.17	4.57	0.005
126.092	$C_7H_{11}NO$	125.084	0.76	3	0.14	1.57	6.45	0.013
126.968	CH_2O_5S	125.962	-1.47	1	5.00	2.00	8.90	0.161
127.035	$C_6H_6O_3$	126.032	-3.87	4	0.50	1.00	4.83	0.013
127.047	$C_5H_6N_2O_2$	126.043	-3.1	4	0.40	1.20	5.30	0.007
127.079	$C_7H_{10}O_2$	126.068	4.04	3	0.29	1.43	5.35	0.019
127.112	$C_8H_{14}O$	126.105	-0.04	2	0.13	1.75	6.28	0.020
127.942	N/A				0.00	0.00		0.013
127.966	N/A				0.00	0.00		0.013
128.071	$C_6H_9NO_2$	127.063	0.2	3	0.33	1.50	4.57	0.013
128.108	$C_7H_{13}NO$	127.100	0.91	2	0.14	1.86	6.45	0.017
129.039	C_6H_8OS	128.030	1.84	3	0.17	1.33	7.28	0.009
129.060	$C_6H_8O_3$	128.047	5.28	3	0.50	1.33	4.83	0.017
129.092	$C_7H_{12}O_2$	128.084	1.29	2	0.29	1.71	5.35	0.036
129.126	$C_8H_{16}O$	128.120	-1.09	1	0.13	2.00	6.28	0.015
130.054	$C_5H_7NO_3$	129.043	4.03	3	0.60	1.40	3.40	0.018
130.123	$C_7H_{15}NO$	129.115	0.56	1	0.14	2.14	6.45	0.009
131.036	$C_5H_6O_4$	130.027	2.31	3	0.80	1.20	4.70	0.025

Exp. Mass [M+H]	Molecular Formula	Theor. Mass [M]	mDa	DU	O:C	H:C	Csat	Ave Conc. (ppb)
133.080	$C_6H_{12}O_3$	132.079	-5.52	1	0.50	2.00	4.83	0.035
136.023	$C_3H_5NO_5$	135.017	-1.45	2	1.67	1.67	3.23	0.338
136.945	N/A				0.00	0.00		0.006
137.025	$C_7H_4O_3$	136.016	1.58	6	0.43	0.57	4.17	0.021
137.133	$C_{10}H_{16}$	136.125	0.12	3	0.00	1.60	7.13	0.137
138.020	$C_6H_3NO_3$	137.011	0.93	6	0.50	0.50	2.93	0.017
138.136	$C_{10}H_{17}$	137.133	-4	2.5	0.00	1.70	7.13	0.016
139.038	$C_7H_6O_3$	138.032	-1.37	5	0.43	0.86	4.17	0.013
139.075	$C_8H_{10}O_2$	138.068	-0.66	4	0.25	1.25	4.80	0.023
139.112	$C_9H_{14}O$	138.105	0.56	3	0.11	1.56	5.78	0.093
141.057	$C_7H_8O_3$	140.047	2.68	4	0.43	1.14	4.17	0.017
141.127	$C_9H_{16}O$	140.120	-0.89	2	0.11	1.78	5.78	0.034
143.072	$C_7H_{10}O_3$	142.063	1.83	3	0.43	1.43	4.17	0.009
143.105	$C_8H_{14}O_2$	142.099	-1.76	2	0.25	1.75	4.80	0.019
143.143	$C_9H_{18}O$	142.136	-0.34	1	0.11	2.00	5.78	0.023
145.053	$C_6H_8O_4$	144.042	3.46	3	0.67	1.33	3.91	0.012
145.133	$C_7H_{16}N_2O$	144.126	-0.14	1	0.14	2.29	10.85	0.439
146.136	N/A				0.00	0.00		0.034
151.106	$C_{10}H_{14}O$	150.105	-6.04	4	0.10	1.40	5.29	0.013
153.054	$C_8H_8O_3$	152.047	-0.42	5	0.38	1.00	3.55	0.022
153.091	$C_9H_{12}O_2$	152.084	-0.51	4	0.22	1.33	4.25	0.010
153.128	$C_{10}H_{16}O$	152.120	0.21	3	0.10	1.60	5.29	0.021
155.105	$C_9H_{14}O_2$	154.099	-1.76	3	0.22	1.56	4.25	0.012
155.144	$C_{10}H_{18}O$	154.136	0.86	2	0.10	1.80	5.29	0.010
156.102	$C_8H_{13}NO_2$	155.095	0.09	3	0.25	1.63	3.72	0.020
157.121	$C_9H_{16}O_2$	156.115	-1.51	2	0.22	1.78	4.25	0.005
159.114	$C_7H_{14}N_2O_2$	158.106	0.7	2	0.29	2.00	4.35	0.450
160.116	$C_{11}H_{13}N$	159.105	4.22	6	0.00	1.18	7.23	0.035
161.131	$C_{12}H_{16}$	160.125	-1.08	5	0.00	1.33	6.18	0.007
163.119	$C_{10}H_{14}N_2$	162.116	-3.87	5	0.00	1.40	12.33	0.009
179.066	$C_{10}H_{10}O_3$	178.063	-4.47	6	0.30	1.00	2.37	0.021
187.144	$C_{14}H_{18}$	186.141	-4.03	6	0.00	1.29	5.23	0.007
192.138	$C_{12}H_{17}NO$	191.131	0.11	5	0.08	1.42	4.08	0.031
230.175	$C_{12}H_{23}NO_3$	229.168	0.23	2	0.25	1.92	0.07	0.048