**Supporting Information**

# Extreme Heat and Wildfire Emissions Enhance Volatile Organic Compounds: Insights on Future Climate

Salvador, C.M.[1], Wood, J.[2], Cochran, E.[2], Seubert, H.[2], Kamplain, B.[2], Overby, S.[2], Birdwell, K.[1], Gu, L.[1], Mayes, M.A.[1]

[1]*Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, USA*
[2]*School of Natural Resources, University of Missouri, Columbia, MO, USA*

*Correspondence to:* Christian Mark Salvador (salvadorcg@ornl.gov) and Melanie Mayes (mayesma@ornl.gov)

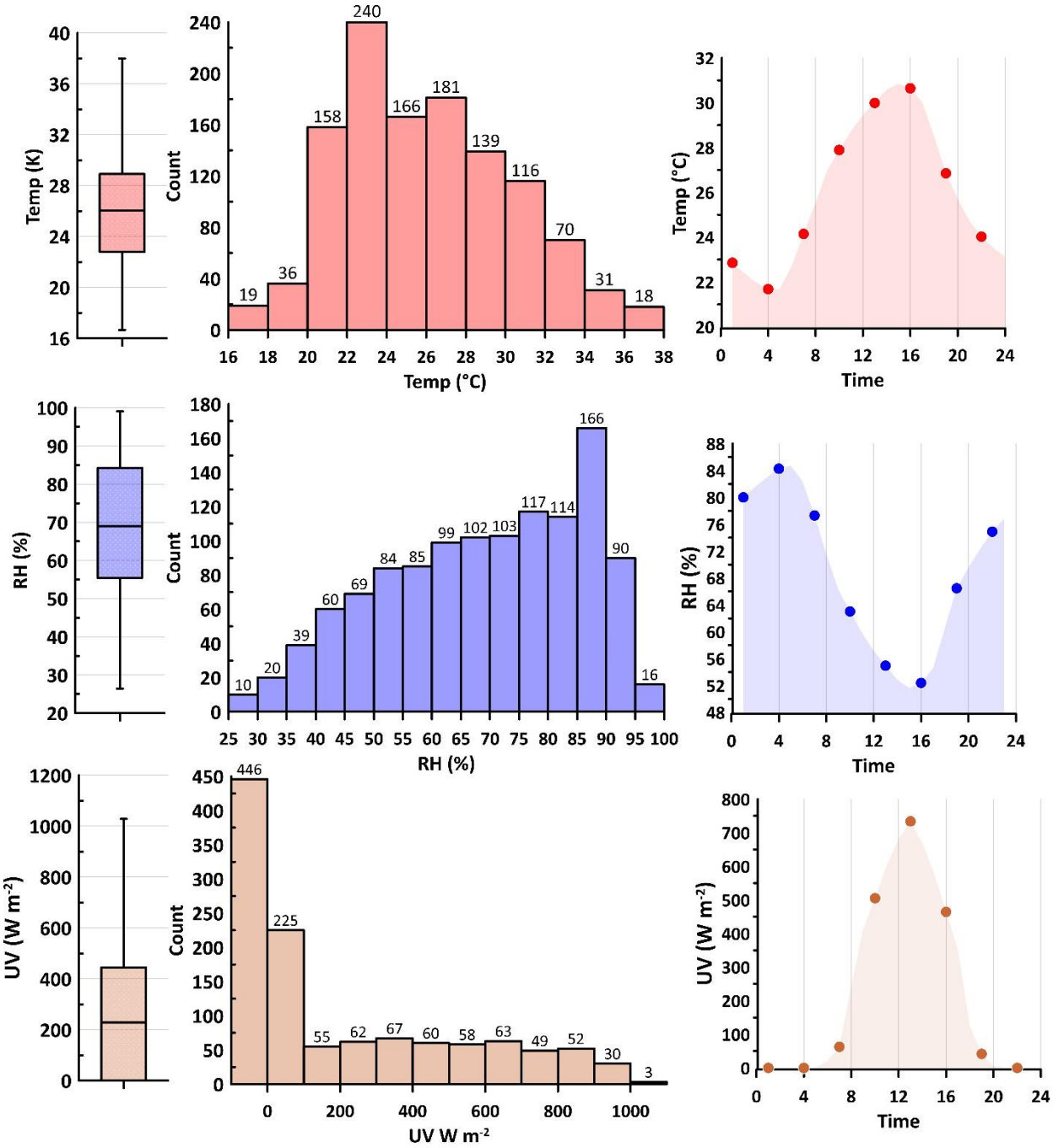


**Figure S1**. Box-Whisker plot, histogram, and diurnal profile of (top) temperature, (mid) relative humidity, and (bottom) global solar radiation. Temperature and relative humidity were collected from a nearby airport monitoring site (KCOU) while global radiation was measured in a were measured in weather site in Ashland, MO, 5.22 kilometers from the MOFLUX site.

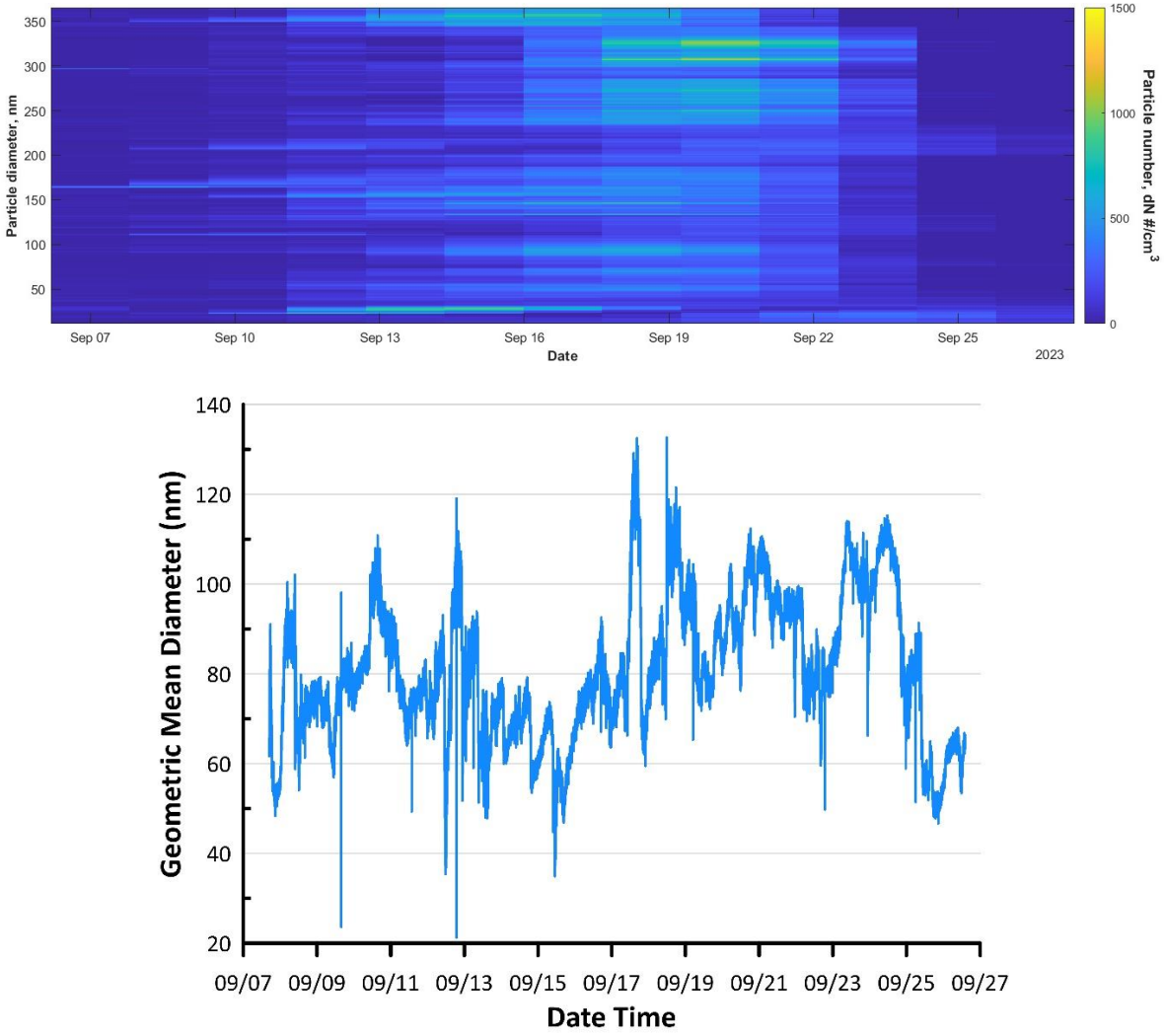


**Figure S2.** (Top) Particle size distribution and (bottom) geometric mean diameter (GMD) of the particles observed at MOFLUX. Note that the aerosol measurements were performed after the VOC collection data provided in the main text. The real-time nanoparticle size measurements were implemented using 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.

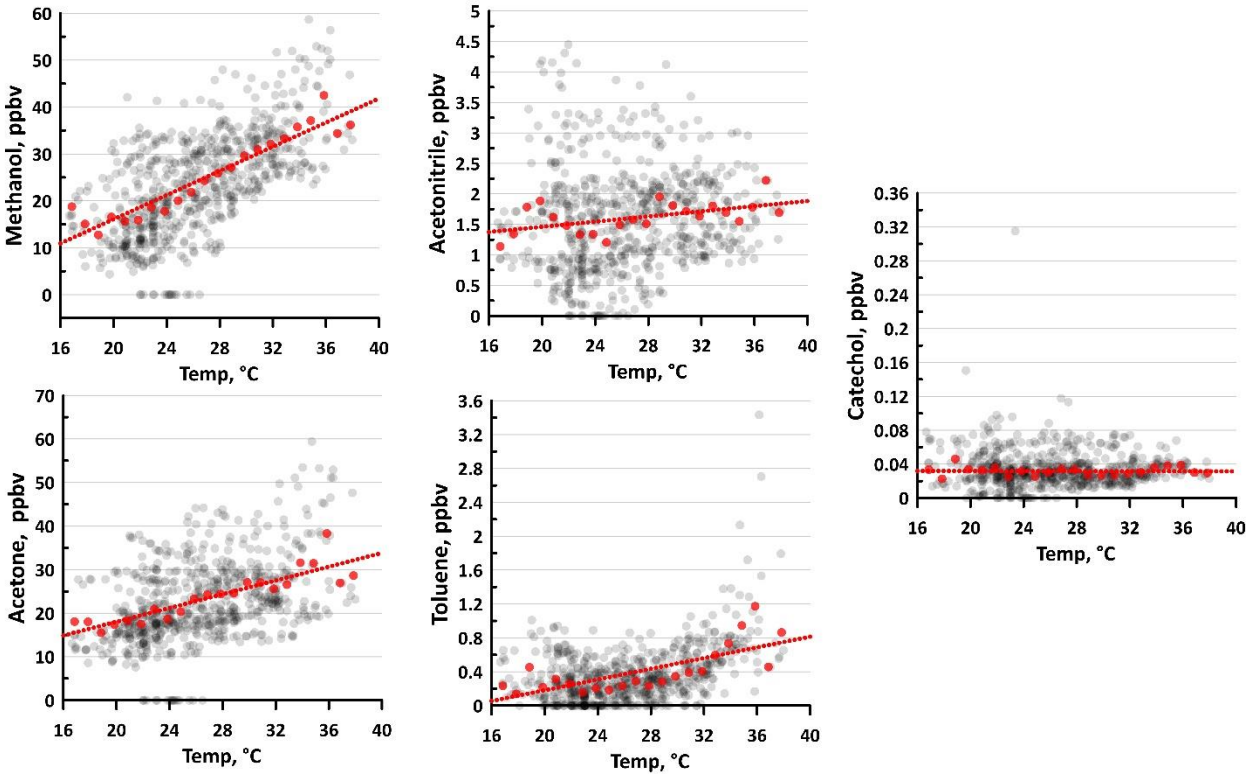


**Figure S3.** The correlation analysis of temperature and mixing ratios of other VOCs not included in Figure 3. Black symbols are hourly data while the red lines indicate the best-fit line of the binned mixing ratio of VOCs according to 1.0 °C of temperature

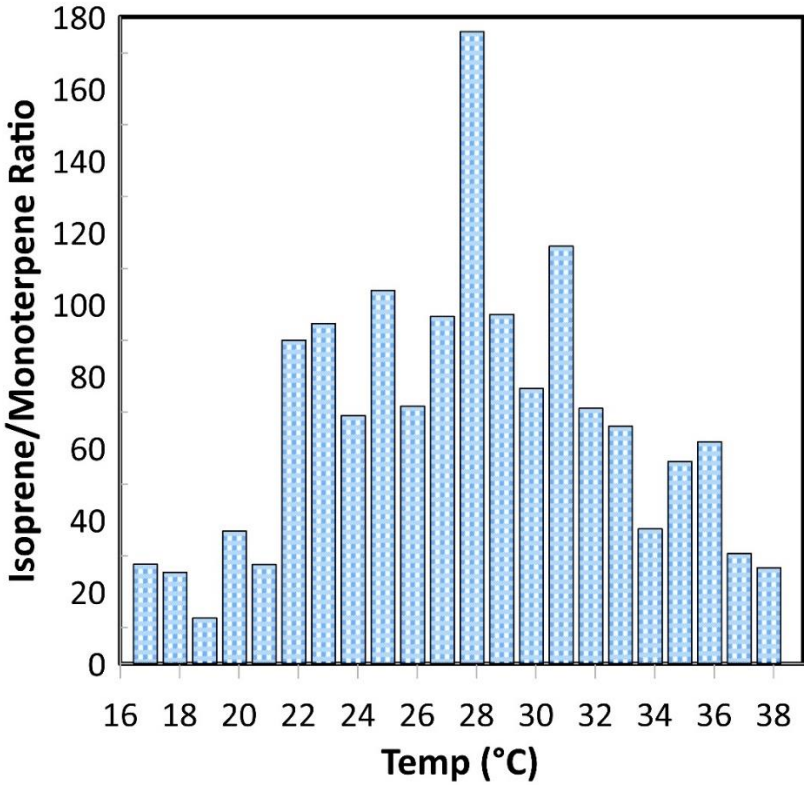


**Figure S4.** Ratio of monoterpene and isoprene mixing ratio binned to temperature. A bell-shaped profile was observed from the plot of temperature and ratio, with the maximum occurring at 28°C.

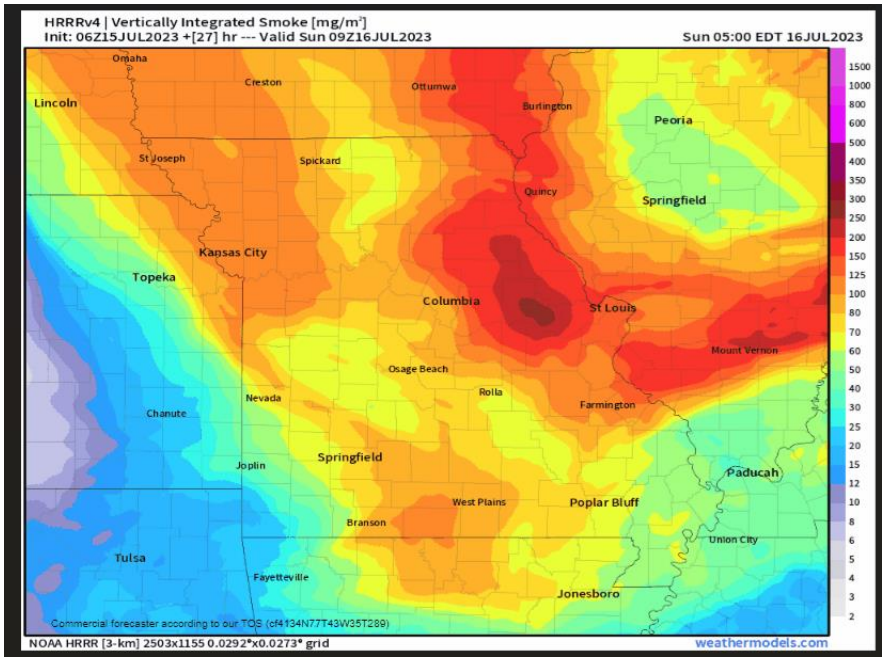


**Figure S5.** Atmospheric dispersion of the smoke observed during July 16, 2023. The smoke snapshot coincided with the day with highest smoke concentration observed during the MOFLUX VOC measurement.

**Text S1**. Calculation of Ozone Forming Potential

The impact of transported wildfire emissions on the formation of ozone was calculated using the incremental reactivity, based on the response of the ozone levels to the incremental increase of benzene, divided by the mixing ratio of benzene. The ozone formation potential (Carter, 1994, 2009) of toluene in MOFLUX during the long range transport of biomass burning from Canada was determined as the products of the toluene and the maximum incremental reactivity coefficient (MIR) given by the following equation:

$$OFP_{benzene} = [benzene] \times MIR$$

## Reference


Carter, W. P. L.: Development of Ozone Reactivity Scales for Volatile Organic Compounds, Air & Waste, 44, 881-899, 10.1080/1073161X.1994.10467290, 1994.

Carter, W. P. L.: Updated Maximum Incremental Reactivity Scale and Hydrocarbon Bin Reactivities for Regulatory Applications, California Air Resources Board Contract 07-339, 2009.

**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 |