



Supplement of

Source characterization of volatile organic compounds measured by protontransfer-reaction time-of-flight mass spectrometers in Delhi, India

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Concentration weighted trajectory (CWT) analysis

Backward-trajectory analysis was performed using Hybrid Single-Particle Lagrangian Integrated Trajectory (HYSPLIT) model. The meteorological fields were obtained from the National Centers for Environmental Prediction (NCEP) Global Data Assimilation System (GDAS). (Stein et al., 2015) We performed hourly resolution back-trajectories for 6 hours, 12 hours, 24 hours and 48 hours. Owing to the short distance between the two sites (20 km) and short lifetime of VOCs, the 6-hour and 12-hour back-trajectories were found to be a good representation of the air mass transport between the two sites. The concentration weighted trajectory (CWT) analysis is widely used to reveal the potential source regions and spatial distribution of pollutants (Zheng et al., 2019). In this paper, the CWT analysis is based on the back-trajectories with an arriving height at 100 m above sea level for 6 hrs. Here, we utilized an Igor based tool, Zefir (Petit et al., 2017), to explore the CWT plots with a cell resolution of $0.2^{\circ} \times 0.2^{\circ}$.

Reference

- Petit, J. E., Favez, O., Albinet, A., and Canonaco, F.: A user-friendly tool for comprehensive evaluation of the geographical origins of atmospheric pollution: Wind and trajectory analyses, Environmental Modelling & Software, 88, 183-187, https://doi.org/10.1016/j.envsoft.2016.11.022, 2017.
- Stein, A. F., Draxler, R. R., Rolph, G. D., Stunder, B. J. B., Cohen, M. D., and Ngan, F.: NOAA's HYSPLIT Atmospheric Transport and Dispersion Modeling System, Bulletin of the American Meteorological Society, 96, 2059-2077, 10.1175/bams-d-14-00110.1, 2015.
- Zheng, H., Kong, S., Wu, F., Cheng, Y., Niu, Z., Zheng, S., Yang, G., Yao, L., Yan, Q., Wu, J., Zheng, M., Chen, N., Xu, K., Yan, Y., Liu, D., Zhao, D., Zhao, T., Bai, Y., Li, S., and Qi, S.: Intra-regional transport of black carbon between the south edge of the North China Plain and central China during winter haze episodes, Atmos. Chem. Phys., 19, 4499-4516, 10.5194/acp-19-4499-2019, 2019.



Fig. S1 Box-whisker plots of temperature during the cold and warm periods at the two sites. The comparisons of temperature change during different periods, and at each site are based on the periods when VOC measurements exist.



Fig. S2 Diurnal plots of averaged mixing ratio of NO_x, CO and each VOC family at each site.



Fig. S3 Q/Q_{exp} plots vs number of factors of (a) IITD and (b) MRIU.



Fig. S4 PMF results at IITD with the input of 154 ions (excluding $C_6H_6H^+$, $C_7H_8H^+$, $C_8H_{10}H^+$, and $C_9H_{12}H^+$), showing (a) factor profiles (b) factor time series. The selected secondary factors are labeled in the blue box.



Fig. S5 PMF results at IITD with the a-value=0.3, showing on the left the factor time series, and on the right the factor profiles. The shaded area spans the lower and higher constraints and the comparison between the gray area and the factor profile indicates in which direction the solution was pulled during the ME-2 run.



Fig. S6 (a) Factor profiles of raw PMF result at MRIU. (b) Factor profiles of PMF result at MRIU by constraining the two secondary factors as applied at IITD. (c) Factor time series of the two PMF results at MRIU, with the blue lines showing the unconstrained PMF results (corresponds to a), and the black lines showing the constrained results (b).



Fig.S7 Diurnal plot of the ratio of Traffic2 to Traffic1 at IITD. The shaded area represents the interquartile range.



Fig. S8 Concentration weighted trajectory (CWT) plots of PMF factors with the back-trajectory calculated for 6 hours at both sites. The green plots represent the IITD factors and the gold plots are the MRIU factors. In each plot, the white square represents the IITD site and the white circle represents the MRIU site.



Fig. S9 Comparison of the factor spectra of IITD SecVOC2 and MRIU SecVOC1.



Fig. S10 Diurnal patterns of factor concentrations and contributions (a) at IITD, (b) raw result at MRIU, and (c) constrained result at MRIU.



Fig. S11. Volume contributions of CH3OH, C2H4O, C3H6O, C2H4O2 and the six PMF factors at the two sites. The left pie represents the IITD site and the right pie the MRIU site.



Fig. S12 Diurnal patterns of isoprene and monoterpenes at the two sites. The squares represent the mean values and the circles the median values.



Fig. S13 CWT plots of maleic anhydride and PAN with the 6-hour back-trajectories at both sites. The green plots represent the IITD factors and the gold plots the MRIU factors. In each plot, the white square represents the IITD site and the white circle represents the MRIU site.

			. 111.044	$C6H6O2H^+$	0.086
Ion exact	T C 1	Averaged	111.080	$C7H10OH^+$	0.081
m/z (Th)	Ion formula	(ppby)	111.117	$C8H14H^{+}$	0.17
54 034	C3H3NH ⁺	0.17	112.112	C7H13NH ⁺	0.022
67 054	C5H6H ⁺	0.23	113.060	$C6H8O2H^+$	0.077
68 049	C4H5NH ⁺	0.25	113.096	$C7H12OH^+$	0.061
69.033	$C4H4OH^+$	0.26	113.132	$C8H16H^+$	0.019
69.035	C5H8H ⁺	0.20	115.075	$C6H10O2H^+$	0.12
70.065	$C4H7NH^+$	0.80	117.055	$C5H8O3H^+$	0.038
70.005	$C4H6OH^+$	0.32	117.070	$C9H8H^+$	0.028
73.028	C3H4O2H ⁺	0.32	117.091	$C6H12O2H^+$	0.035
73.020	C4H8OH ⁺	1.3	118.065	$C8H7NH^+$	0.028
75.005	C3H6O2H ⁺	0.92	119.049	$C8H6OH^+$	0.043
77.023	C2H4O2H ⁺	0.92	119.086	$C9H10H^+$	0.18
70.054	С6464+	2.8	121.065	$C8H8OH^+$	0.16
79.034 80.040	C5H5NH ⁺	2.8	121.101	C9H12H ⁺	1.3
81.022	C5H4OH+	0.13	123.044	$C7H6O2H^+$	0.073
01.033 01.070		0.10	123.080	$C8H10OH^+$	0.031
01.070 02.065		0.55	123.117	$C9H14H^+$	0.048
82.003		0.004	125.060	C7H8O2H ⁺	0.042
83.049	CSHOUH ⁺	0.26	125.096	C8H12OH ⁺	0.029
83.080	Conton Conton	0.60	125.132	C9H16H ⁺	0.064
84.081	C3H9NH ⁺	0.068	127.039	C6H6O3H ⁺	0.022
85.028	C4H4O2H ⁺	0.094	127.035	C7H10O2H ⁺	0.022
85.065	C5H8OH	0.24	127.112	C8H14OH ⁺	0.027
85.101	C6H12H ⁺	0.34	127.148	C9H18H ⁺	0.015
87.044	C4H6O2H ⁺	0.46	129.070	$C10H8H^+$	0.17
87.080	C3HI0OH ⁺	0.24	129.127	C8H16OH ⁺	0.033
89.060	C4H8O2H ⁺	0.70	131.070	C6H10O3H ⁺	0.012
91.039	C3H6O3H	0.064	131.086	C10H10H ⁺	0.021
91.054	C/H6H ⁺	0.38	131 143	C8H18OH ⁺	0.009
93.070	C/H8H	5.2	133.028	C8H4O2H ⁺	0.005
95.049	C6H6OH	0.17	133.065	C9H8OH ⁺	0.030
95.086	C/HI0H	0.17	133 101	C10H12H ⁺	0.088
96.081	C6H9NH	0.021	135.044	C8H6O2H ⁺	0.000
97.028	C5H4O2H	0.14	135.080	C9H10OH+	0.084
97.065	C6H8OH	0.15	135.000	$C10H14H^+$	0.001
97.101	C/HI2H	0.30	137.060	C8H8O2H ⁺	0.035
99.008	C4H2O3H ⁺	0.16	137.006	C9H12OH+	0.033
99.044	C5H6O2H ⁺	0.18	137.132	C10H16H ⁺	0.022
99.080	C6H10OH ⁺	0.15	139.075	C8H10O2H ⁺	0.14
101.060	C5H8O2H ⁺	0.15	139.073	C9H14OH+	0.010
101.096	C6H12OH ⁺	0.16	139.112	C10H18H ⁺	0.020
103.039	C4H6O3H ⁺	0.055	139.140	C6H5NO3H ⁺	0.025
103.075	C5H10O2H ⁺	0.049	140.034		0.05/
104.049	$C7H5NH^{+}$	0.16	141.12/		0.017
105.033	$C7H4OH^{+}$	0.091	141.104		0.012
105.070	$C8H8H^+$	0.38	145.080		0.040
107.049	$C7H6OH^+$	0.22	145.065		0.008
107.086	$C8H10H^+$	3.1	145.101	CHHI2H'	0.012

 $C7H8OH^+$

 $C8H12H^{+}$

0.065

0.078

109.065

109.101

Table S1 List of ions and averaged mixing ratios included in the PMF analysis at IITD.

147.117 $C11H14H^+$ 0.049 148.112 $C10H13NH^+$ 0.015 149.060 $C9H802H^+$ 0.020 149.096 $C10H12OH^+$ 0.038 149.132 $C11H16H^+$ 0.11 150.128 $C10H15NH^+$ 0.012 151.039 $C8H603H^+$ 0.012 151.075 $C9H1002H^+$ 0.017 151.112 $C10H140H^+$ 0.014 151.148 $C11H18H^+$ 0.035 153.091 $C9H1202H^+$ 0.014 153.127 $C10H160H^+$ 0.046 153.164 $C11H20H^+$ 0.017 154.050 $C7H7N03H^+$ 0.034 155.070 $C8H1003H^+$ 0.011 155.086 $C12H10H^+$ 0.012 155.143 $C10H180H^+$ 0.016 155.179 $C11H22H^+$ 0.012 159.080 $C11H100H^+$ 0.006 159.117 $C12H14H^+$ 0.008 161.060 $C10H802H^+$ 0.011 163.039 $C9H603H^+$ 0.013 163.075 $C10H1002H^+$ 0.010 163.112 $C11H120H^+$ 0.010 163.133 $C8H1803H^+$ 0.011 163.148 $C12H18H^+$ 0.035 165.055 $C9H803H^+$ 0.005 165.164 $C12H20H^+$ 0.006 167.107 $C10H1402H^+$ 0.006 167.107 $C10H1402H^+$ 0.006 167.143 $C11H180H^+$ 0.008 167.143 $C11H180H^+$ 0.008	147.080	$C10H10OH^+$	0.034
148.112 C10H13NH ⁺ 0.015 149.060 C9H802H ⁺ 0.020 149.096 C10H12OH ⁺ 0.038 149.132 C11H16H ⁺ 0.11 150.128 C10H15NH ⁺ 0.012 151.039 C8H603H ⁺ 0.012 151.075 C9H1002H ⁺ 0.017 151.112 C10H140H ⁺ 0.014 153.055 C8H803H ⁺ 0.035 153.091 C9H1202H ⁺ 0.014 153.127 C10H160H ⁺ 0.046 153.164 C11H20H ⁺ 0.017 154.050 C7H7N03H ⁺ 0.034 155.070 C8H1003H ⁺ 0.016 155.179 C11H22H ⁺ 0.012 159.080 C11H100H ⁺ 0.006 159.17 C12H14H ⁺ 0.008 161.060 C10H802H ⁺ 0.012 163.039 C9H603H ⁺ 0.010 163.12 C11H100H ⁺ 0.010 163.13 C8H1803H ⁺ 0.011 163.148 C12H18H ⁺ 0.035 165.055 C9H803H ⁺ <t< td=""><td>147.117</td><td>$C11H14H^{+}$</td><td>0.049</td></t<>	147.117	$C11H14H^{+}$	0.049
149.060C9H802H $^+$ 0.020149.096C10H12OH $^+$ 0.038149.132C11H16H $^+$ 0.11150.128C10H15NH $^+$ 0.019151.039C8H603H $^+$ 0.012151.075C9H1002H $^+$ 0.017151.112C10H140H $^+$ 0.014151.148C11H18H $^+$ 0.031153.055C8H803H $^+$ 0.035153.091C9H1202H $^+$ 0.014153.127C10H160H $^+$ 0.046153.164C11H20H $^+$ 0.017154.050C7H7N03H $^+$ 0.034155.070C8H1003H $^+$ 0.016155.179C11H22H $^+$ 0.012159.080C11H100H $^+$ 0.006159.117C12H14H $^+$ 0.008161.060C10H802H $^+$ 0.011163.039C9H603H $^+$ 0.013163.075C10H1002H $^+$ 0.010163.132C11H140H $^+$ 0.010163.133C8H1803H $^+$ 0.011163.148C12H18H $^+$ 0.035165.055C9H803H $^+$ 0.005165.091C10H1202H $^+$ 0.014165.164C12H20H $^+$ 0.024167.070C9H1003H $^+$ 0.008167.179C12H22H $^+$ 0.011168.066C8H9N03H $^+$ 0.008167.179C12H22H $^+$ 0.011168.066C8H9N03H $^+$ 0.008167.179C12H22H $^+$ 0.011168.066C8H9N03H $^+$ 0.006169.195C12H10H $^+$ 0.006177.	148.112	C10H13NH ⁺	0.015
149.096 $C10H12OH^+$ 0.038 149.132 $C11H16H^+$ 0.11 150.128 $C10H15NH^+$ 0.019 151.039 $C8H6O3H^+$ 0.012 151.075 $C9H10O2H^+$ 0.017 151.112 $C10H14OH^+$ 0.014 151.148 $C11H18H^+$ 0.031 153.055 $C8H8O3H^+$ 0.035 153.091 $C9H12O2H^+$ 0.014 153.127 $C10H16OH^+$ 0.046 153.164 $C11H20H^+$ 0.017 154.050 $C7H7NO3H^+$ 0.034 155.070 $C8H10O3H^+$ 0.011 155.086 $C12H10H^+$ 0.012 155.143 $C10H18OH^+$ 0.016 155.179 $C11H22H^+$ 0.012 159.080 $C11H10OH^+$ 0.006 159.117 $C12H14H^+$ 0.008 161.060 $C10H8O2H^+$ 0.013 163.075 $C10H10O2H^+$ 0.010 163.132 $C11H10OH^+$ 0.010 163.133 $C8H18O3H^+$ 0.011 163.148 $C12H18H^+$ 0.035 165.055 $C9H8O3H^+$ 0.014 165.164 $C12H20H^+$ 0.006 167.179 $C12H22H^+$ 0.011 168.066 $C8H9NO3H^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C8H9NO3H^+$ 0.008 167.179 $C12H20H^+$ 0.006 169.195 $C12H20H^+$ 0.006 169.195 $C12H1NH^+$ 0.006 <	149.060	$C9H8O2H^+$	0.020
149.132C11H16H $^+$ 0.11150.128C10H15NH $^+$ 0.019151.039C8H603H $^+$ 0.012151.075C9H1002H $^+$ 0.017151.112C10H140H $^+$ 0.014151.148C11H18H $^+$ 0.031153.055C8H803H $^+$ 0.035153.091C9H1202H $^+$ 0.014153.127C10H160H $^+$ 0.046153.164C11H20H $^+$ 0.017154.050C7H7N03H $^+$ 0.034155.070C8H1003H $^+$ 0.016155.143C10H180H $^+$ 0.016155.179C11H22H $^+$ 0.012159.080C11H100H $^+$ 0.006159.117C12H14H $^+$ 0.008161.060C10H802H $^+$ 0.011163.039C9H603H $^+$ 0.013163.075C10H1002H $^+$ 0.010163.112C11H140H $^+$ 0.010163.133C8H1803H $^+$ 0.011163.148C12H18H $^+$ 0.035165.055C9H803H $^+$ 0.005165.091C10H1202H $^+$ 0.004167.070C9H1003H $^+$ 0.006167.107C10H1402H $^+$ 0.005167.143C11H180H $^+$ 0.008167.179C12H22H $^+$ 0.011168.066C8H9N03H $^+$ 0.018169.086C9H1203H $^+$ 0.005169.122C10H1602H $^+$ 0.008169.159C11H20H $^+$ 0.006177.127C12H16H $^+$ 0.006177.127C12H16H $^+$ 0.006	149.096	$C10H12OH^+$	0.038
150.128 $C10H15NH^+$ 0.019 151.039 $C8H6O3H^+$ 0.012 151.075 $C9H10O2H^+$ 0.017 151.112 $C10H14OH^+$ 0.014 151.148 $C11H18H^+$ 0.031 153.055 $C8H8O3H^+$ 0.035 153.091 $C9H12O2H^+$ 0.014 153.127 $C10H16OH^+$ 0.046 153.164 $C11H2OH^+$ 0.017 154.050 $C7H7NO3H^+$ 0.034 155.070 $C8H10O3H^+$ 0.011 155.086 $C12H10H^+$ 0.012 155.143 $C10H18OH^+$ 0.016 155.179 $C11H22H^+$ 0.012 159.080 $C11H10OH^+$ 0.006 159.117 $C12H14H^+$ 0.008 161.060 $C10H8O2H^+$ 0.011 163.039 $C9H6O3H^+$ 0.011 163.075 $C10H10O2H^+$ 0.010 163.112 $C11H14OH^+$ 0.010 163.133 $C8H18O3H^+$ 0.011 163.148 $C12H18H^+$ 0.035 165.055 $C9H8O3H^+$ 0.008 165.164 $C12H20H^+$ 0.004 167.107 $C10H14O2H^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C8H9NO3H^+$ 0.018 169.086 $C9H12O3H^+$ 0.005 167.143 $C11H18OH^+$ 0.006 177.127 $C12H24H^+$ 0.010 170.096 $C12H11NH^+$ 0.006 177.127 $C12H16OH^+$ 0.006	149.132	$C11H16H^+$	0.11
151.039 $C8H6O3H^+$ 0.012 151.075 $C9H10O2H^+$ 0.017 151.112 $C10H14OH^+$ 0.014 151.148 $C11H18H^+$ 0.031 153.055 $C8H8O3H^+$ 0.035 153.091 $C9H12O2H^+$ 0.014 153.127 $C10H16OH^+$ 0.046 153.164 $C11H2OH^+$ 0.017 154.050 $C7H7NO3H^+$ 0.034 155.070 $C8H10O3H^+$ 0.011 155.086 $C12H10H^+$ 0.013 155.143 $C10H18OH^+$ 0.016 155.179 $C11H22H^+$ 0.012 159.080 $C11H10OH^+$ 0.006 159.117 $C12H14H^+$ 0.008 161.060 $C10H8O2H^+$ 0.011 163.039 $C9H6O3H^+$ 0.013 163.075 $C10H10O2H^+$ 0.010 163.112 $C11H12OH^+$ 0.010 163.133 $C8H18O3H^+$ 0.011 163.148 $C12H18H^+$ 0.035 165.055 $C9H8O3H^+$ 0.014 165.164 $C12H2OH^+$ 0.006 167.107 $C10H14O2H^+$ 0.006 167.179 $C12H22H^+$ 0.011 168.066 $C8H9NO3H^+$ 0.018 167.179 $C12H22H^+$ 0.011 168.066 $C9H12O3H^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C9H12O3H^+$ 0.005 167.143 $C11H18OH^+$ 0.006 177.127 $C12H24H^+$ 0.005 <t< td=""><td>150.128</td><td>C10H15NH⁺</td><td>0.019</td></t<>	150.128	C10H15NH ⁺	0.019
151.075 $C9H1002H^+$ 0.017 151.112 $C10H140H^+$ 0.014 151.148 $C11H18H^+$ 0.031 153.055 $C8H803H^+$ 0.035 153.091 $C9H1202H^+$ 0.014 153.127 $C10H160H^+$ 0.046 153.164 $C11H20H^+$ 0.017 154.050 $C7H7N03H^+$ 0.034 155.070 $C8H1003H^+$ 0.011 155.086 $C12H10H^+$ 0.013 155.143 $C10H180H^+$ 0.016 155.179 $C11H22H^+$ 0.012 159.080 $C11H100H^+$ 0.006 159.117 $C12H14H^+$ 0.008 161.060 $C10H802H^+$ 0.011 163.039 $C9H603H^+$ 0.013 163.075 $C10H1002H^+$ 0.010 163.112 $C11H120H^+$ 0.010 163.133 $C8H1803H^+$ 0.011 163.148 $C12H18H^+$ 0.035 165.055 $C9H803H^+$ 0.014 165.127 $C11H120H^+$ 0.006 167.107 $C10H1402H^+$ 0.006 167.107 $C10H1402H^+$ 0.006 167.179 $C12H22H^+$ 0.011 168.066 $C8H9N03H^+$ 0.018 169.086 $C9H1203H^+$ 0.008 167.179 $C12H22H^+$ 0.005 167.143 $C11H120H^+$ 0.006 177.127 $C12H24H^+$ 0.005 169.122 $C10H1602H^+$ 0.008 169.195 $C12H24H^+$ 0.005 <td>151.039</td> <td>$C8H6O3H^+$</td> <td>0.012</td>	151.039	$C8H6O3H^+$	0.012
151.112 $C10H14OH^+$ 0.014 151.148 $C11H18H^+$ 0.031 153.055 $C8H803H^+$ 0.035 153.091 $C9H12O2H^+$ 0.014 153.127 $C10H16OH^+$ 0.046 153.164 $C11H2OH^+$ 0.017 154.050 $C7H7NO3H^+$ 0.034 155.070 $C8H10O3H^+$ 0.011 155.086 $C12H10H^+$ 0.016 155.143 $C10H18OH^+$ 0.016 155.179 $C11H22H^+$ 0.012 159.080 $C11H10OH^+$ 0.006 159.117 $C12H14H^+$ 0.008 161.060 $C10H8O2H^+$ 0.012 161.096 $C11H12OH^+$ 0.010 163.039 $C9H6O3H^+$ 0.013 163.075 $C10H10O2H^+$ 0.010 163.112 $C11H14OH^+$ 0.010 163.133 $C8H18O3H^+$ 0.011 163.148 $C12H18H^+$ 0.035 165.055 $C9H8O3H^+$ 0.014 165.127 $C11H16OH^+$ 0.008 165.164 $C12H20H^+$ 0.005 167.107 $C10H14O2H^+$ 0.008 167.107 $C10H14O2H^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C9H12O3H^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C9H12O3H^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C9H12O3H^+$ 0.008 169.195 $C12H24H^+$ 0.006	151.075	C9H10O2H ⁺	0.017
151.148 $C11H18H^+$ 0.031 153.055 $C8H803H^+$ 0.035 153.091 $C9H12O2H^+$ 0.014 153.127 $C10H16OH^+$ 0.046 153.164 $C11H2OH^+$ 0.017 154.050 $C7H7NO3H^+$ 0.034 155.070 $C8H10O3H^+$ 0.011 155.086 $C12H10H^+$ 0.016 155.143 $C10H18OH^+$ 0.016 155.179 $C11H22H^+$ 0.012 159.080 $C11H10OH^+$ 0.006 159.117 $C12H14H^+$ 0.008 161.060 $C10H8O2H^+$ 0.012 161.096 $C11H12OH^+$ 0.010 163.039 $C9H6O3H^+$ 0.013 163.075 $C10H10O2H^+$ 0.010 163.112 $C11H14OH^+$ 0.010 163.133 $C8H18O3H^+$ 0.011 163.148 $C12H18H^+$ 0.035 165.055 $C9H8O3H^+$ 0.014 165.127 $C11H16OH^+$ 0.008 165.164 $C12H20H^+$ 0.004 167.107 $C10H14O2H^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C9H12O3H^+$ 0.008 167.179 $C12H22H^+$ 0.018 169.186 $C9H12O3H^+$ 0.008 167.196 $C11H12OH^+$ 0.008 167.197 $C12H22H^+$ 0.011 168.066 $C9H12O3H^+$ 0.005 167.143 $C11H18OH^+$ 0.008 167.196 $C12H20H^+$ 0.006 <	151.112	$C10H14OH^+$	0.014
153.055 $C8H803H^+$ 0.035 153.091 $C9H12O2H^+$ 0.014 153.127 $C10H16OH^+$ 0.046 153.164 $C11H20H^+$ 0.017 154.050 $C7H7N03H^+$ 0.034 155.070 $C8H1003H^+$ 0.011 155.086 $C12H10H^+$ 0.013 155.143 $C10H180H^+$ 0.016 155.179 $C11H22H^+$ 0.012 159.080 $C11H100H^+$ 0.006 159.117 $C12H14H^+$ 0.008 161.060 $C10H802H^+$ 0.012 163.039 $C9H6O3H^+$ 0.013 163.075 $C10H1002H^+$ 0.010 163.112 $C11H140H^+$ 0.010 163.133 $C8H1803H^+$ 0.011 163.148 $C12H18H^+$ 0.035 165.055 $C9H8O3H^+$ 0.014 165.164 $C12H20H^+$ 0.004 167.070 $C9H1003H^+$ 0.006 167.107 $C10H1402H^+$ 0.005 167.143 $C11H180H^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C8H9NO3H^+$ 0.018 169.086 $C9H12O3H^+$ 0.008 169.195 $C12H24H^+$ 0.006 177.127 $C12H10H^+$ 0.008 169.195 $C12H20H^+$ 0.006 177.164 $C13H20H^+$ 0.006 179.143 $C12H180H^+$ 0.006 179.179 $C13H22H^+$ 0.017 181.159 $C12H20OH^+$ 0.006 </td <td>151.148</td> <td>$C11H18H^+$</td> <td>0.031</td>	151.148	$C11H18H^+$	0.031
153.091 $C9H12O2H^+$ 0.014 153.127 $C10H16OH^+$ 0.046 153.164 $C11H2OH^+$ 0.017 154.050 $C7H7NO3H^+$ 0.034 155.070 $C8H10O3H^+$ 0.011 155.086 $C12H10H^+$ 0.013 155.143 $C10H18OH^+$ 0.016 155.179 $C11H22H^+$ 0.012 159.080 $C11H10OH^+$ 0.006 159.117 $C12H14H^+$ 0.008 161.060 $C10H8O2H^+$ 0.012 161.096 $C11H12OH^+$ 0.010 163.039 $C9H6O3H^+$ 0.013 163.075 $C10H10O2H^+$ 0.010 163.112 $C11H14OH^+$ 0.010 163.133 $C8H18O3H^+$ 0.011 163.148 $C12H18H^+$ 0.035 165.055 $C9H8O3H^+$ 0.005 165.091 $C10H12O2H^+$ 0.004 167.070 $C9H10O3H^+$ 0.006 167.107 $C10H14O2H^+$ 0.005 167.143 $C11H18OH^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C8H9NO3H^+$ 0.018 169.166 $C9H12O3H^+$ 0.008 169.159 $C11H2OOH^+$ 0.008 169.159 $C12H20H^+$ 0.006 177.148 $C12H11NH^+$ 0.006 177.127 $C12H16OH^+$ 0.008 177.164 $C13H20H^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.179 $C13H22H^+$ 0.017 </td <td>153.055</td> <td>$C8H8O3H^+$</td> <td>0.035</td>	153.055	$C8H8O3H^+$	0.035
153.127 $C10H16OH^+$ 0.046 153.164 $C11H20H^+$ 0.017 154.050 $C7H7NO3H^+$ 0.034 155.070 $C8H10O3H^+$ 0.011 155.086 $C12H10H^+$ 0.013 155.143 $C10H18OH^+$ 0.016 155.179 $C11H22H^+$ 0.012 159.080 $C11H10OH^+$ 0.006 159.117 $C12H14H^+$ 0.008 161.060 $C10H8O2H^+$ 0.013 163.039 $C9H6O3H^+$ 0.013 163.075 $C10H10O2H^+$ 0.010 163.112 $C11H12OH^+$ 0.010 163.133 $C8H18O3H^+$ 0.011 163.148 $C12H18H^+$ 0.035 165.055 $C9H8O3H^+$ 0.014 165.164 $C12H20H^+$ 0.004 167.107 $C10H12O2H^+$ 0.006 167.107 $C10H14O2H^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C8H9NO3H^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C8H9NO3H^+$ 0.008 167.122 $C10H16O2H^+$ 0.008 169.195 $C12H24H^+$ 0.010 170.096 $C12H11NH^+$ 0.006 177.127 $C12H16OH^+$ 0.008 177.164 $C13H20H^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.179 $C13H22H^+$ 0.017 181.159 $C12H20OH^+$ 0.006	153.091	C9H12O2H ⁺	0.014
153.164 $C11H20H^+$ 0.017 154.050 $C7H7NO3H^+$ 0.034 155.070 $C8H10O3H^+$ 0.011 155.086 $C12H10H^+$ 0.013 155.143 $C10H18OH^+$ 0.016 155.179 $C11H22H^+$ 0.012 159.080 $C11H10OH^+$ 0.006 159.117 $C12H14H^+$ 0.008 161.060 $C10H8O2H^+$ 0.012 161.096 $C11H12OH^+$ 0.010 163.039 $C9H6O3H^+$ 0.013 163.075 $C10H10O2H^+$ 0.010 163.112 $C11H14OH^+$ 0.010 163.133 $C8H18O3H^+$ 0.011 163.148 $C12H18H^+$ 0.035 165.055 $C9H8O3H^+$ 0.005 165.091 $C10H12O2H^+$ 0.014 165.164 $C12H20H^+$ 0.008 167.107 $C10H14O2H^+$ 0.008 167.107 $C10H14O2H^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C8H9NO3H^+$ 0.018 169.086 $C9H12O3H^+$ 0.005 169.122 $C10H16O2H^+$ 0.008 169.195 $C12H24H^+$ 0.010 170.096 $C12H11NH^+$ 0.006 177.127 $C12H16OH^+$ 0.008 177.164 $C13H20H^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.179 $C13H22H^+$ 0.017 181.159 $C12H20OH^+$ 0.006	153.127	C10H16OH ⁺	0.046
154.050 $C7H7NO3H^+$ 0.034 155.070 $C8H10O3H^+$ 0.011 155.086 $C12H10H^+$ 0.013 155.143 $C10H18OH^+$ 0.016 155.179 $C11H22H^+$ 0.012 159.080 $C11H10OH^+$ 0.006 159.117 $C12H14H^+$ 0.008 161.060 $C10H8O2H^+$ 0.012 161.096 $C11H12OH^+$ 0.010 163.039 $C9H6O3H^+$ 0.013 163.075 $C10H10O2H^+$ 0.010 163.112 $C11H14OH^+$ 0.010 163.133 $C8H18O3H^+$ 0.011 163.148 $C12H18H^+$ 0.035 165.055 $C9H8O3H^+$ 0.005 165.055 $C9H8O3H^+$ 0.008 165.164 $C12H20H^+$ 0.014 167.107 $C10H12O2H^+$ 0.008 167.107 $C10H14O2H^+$ 0.008 167.107 $C10H14O2H^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C8H9NO3H^+$ 0.008 167.179 $C12H22H^+$ 0.001 169.086 $C9H12O3H^+$ 0.008 169.159 $C11H2OOH^+$ 0.008 169.159 $C12H24H^+$ 0.010 170.096 $C12H11NH^+$ 0.006 177.164 $C13H20H^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.179 $C13H22H^+$ 0.017 181.159 $C12H20OH^+$ 0.006 <td>153.164</td> <td>$C11H20H^+$</td> <td>0.017</td>	153.164	$C11H20H^+$	0.017
155.070 $C8H1003H^+$ 0.011 155.086 $C12H10H^+$ 0.013 155.143 $C10H180H^+$ 0.016 155.179 $C11H22H^+$ 0.012 159.080 $C11H100H^+$ 0.006 159.117 $C12H14H^+$ 0.008 161.060 $C10H802H^+$ 0.012 161.096 $C11H120H^+$ 0.010 163.039 $C9H603H^+$ 0.013 163.075 $C10H1002H^+$ 0.010 163.112 $C11H140H^+$ 0.010 163.133 $C8H1803H^+$ 0.011 163.148 $C12H18H^+$ 0.035 165.055 $C9H803H^+$ 0.005 165.091 $C10H1202H^+$ 0.014 165.164 $C12H20H^+$ 0.006 167.107 $C10H1402H^+$ 0.008 167.107 $C10H1402H^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C8H9N03H^+$ 0.018 169.086 $C9H12O3H^+$ 0.005 169.122 $C10H1602H^+$ 0.008 169.159 $C11H200H^+$ 0.008 169.195 $C12H24H^+$ 0.010 170.096 $C12H11NH^+$ 0.006 177.164 $C13H20H^+$ 0.006 179.143 $C12H180H^+$ 0.006 179.143 $C12H180H^+$ 0.006 179.179 $C13H22H^+$ 0.017 181.159 $C12H200H^+$ 0.006	154.050	C7H7NO3H ⁺	0.034
155.086 $C12H10H^+$ 0.013 155.143 $C10H180H^+$ 0.016 155.179 $C11H22H^+$ 0.012 159.080 $C11H100H^+$ 0.006 159.117 $C12H14H^+$ 0.008 161.060 $C10H802H^+$ 0.012 161.096 $C11H120H^+$ 0.010 163.039 $C9H603H^+$ 0.013 163.075 $C10H1002H^+$ 0.010 163.112 $C11H140H^+$ 0.010 163.133 $C8H1803H^+$ 0.011 163.148 $C12H18H^+$ 0.035 165.055 $C9H803H^+$ 0.005 165.091 $C10H1202H^+$ 0.014 165.127 $C11H160H^+$ 0.008 165.164 $C12H20H^+$ 0.024 167.070 $C9H1003H^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C8H9N03H^+$ 0.018 167.179 $C12H22H^+$ 0.018 169.086 $C9H12O3H^+$ 0.008 169.195 $C11H200H^+$ 0.008 169.195 $C12H24H^+$ 0.010 170.096 $C12H11NH^+$ 0.006 177.164 $C13H20H^+$ 0.006 177.164 $C12H180H^+$ 0.006 179.143 $C12H180H^+$ 0.006 179.179 $C13H22H^+$ 0.017 181.159 $C12H20OH^+$ 0.006	155.070	$C8H10O3H^+$	0.011
155.143 $C10H18OH^+$ 0.016 155.179 $C11H22H^+$ 0.012 159.080 $C11H10OH^+$ 0.006 159.117 $C12H14H^+$ 0.008 161.060 $C10H8O2H^+$ 0.012 161.096 $C11H12OH^+$ 0.010 163.039 $C9H6O3H^+$ 0.013 163.075 $C10H10O2H^+$ 0.010 163.112 $C11H14OH^+$ 0.010 163.133 $C8H18O3H^+$ 0.011 163.148 $C12H18H^+$ 0.035 165.055 $C9H8O3H^+$ 0.005 165.091 $C10H12O2H^+$ 0.014 165.127 $C11H16OH^+$ 0.008 165.164 $C12H20H^+$ 0.004 167.070 $C9H10O3H^+$ 0.008 167.177 $C10H14O2H^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C8H9NO3H^+$ 0.018 169.086 $C9H12O3H^+$ 0.008 169.195 $C12H22H^+$ 0.010 170.096 $C12H11NH^+$ 0.006 177.127 $C12H20H^+$ 0.005 177.127 $C12H16OH^+$ 0.008 177.164 $C13H20H^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.179 $C13H22H^+$ 0.017 181.159 $C12H20OH^+$ 0.006	155.086	$C12H10H^+$	0.013
155.179 $C11H22H^+$ 0.012 159.080 $C11H10OH^+$ 0.006 159.117 $C12H14H^+$ 0.008 161.060 $C10H802H^+$ 0.012 161.096 $C11H12OH^+$ 0.010 163.039 $C9H6O3H^+$ 0.013 163.075 $C10H1002H^+$ 0.010 163.112 $C11H14OH^+$ 0.010 163.133 $C8H1803H^+$ 0.011 163.148 $C12H18H^+$ 0.035 165.055 $C9H8O3H^+$ 0.005 165.091 $C10H12O2H^+$ 0.014 165.127 $C11H16OH^+$ 0.008 165.164 $C12H20H^+$ 0.024 167.070 $C9H10O3H^+$ 0.006 167.177 $C10H14O2H^+$ 0.005 167.143 $C11H18OH^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C8H9NO3H^+$ 0.018 169.195 $C12H12M^+$ 0.005 169.122 $C10H16O2H^+$ 0.009 169.195 $C12H24H^+$ 0.010 170.096 $C12H11NH^+$ 0.006 177.127 $C12H16OH^+$ 0.008 177.164 $C13H20H^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.179 $C13H22H^+$ 0.017 181.159 $C12H20OH^+$ 0.006	155.143	$C10H18OH^+$	0.016
159.080 $C11H10OH^+$ 0.006 159.117 $C12H14H^+$ 0.008 161.060 $C10H802H^+$ 0.012 161.096 $C11H12OH^+$ 0.010 163.039 $C9H6O3H^+$ 0.013 163.075 $C10H1002H^+$ 0.010 163.112 $C11H14OH^+$ 0.010 163.133 $C8H18O3H^+$ 0.011 163.148 $C12H18H^+$ 0.035 165.055 $C9H8O3H^+$ 0.005 165.091 $C10H12O2H^+$ 0.014 165.127 $C11H16OH^+$ 0.008 165.164 $C12H20H^+$ 0.004 167.107 $C10H14O2H^+$ 0.005 167.107 $C10H14O2H^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C8H9NO3H^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C9H12O3H^+$ 0.008 169.122 $C10H16O2H^+$ 0.008 169.122 $C10H16O2H^+$ 0.008 169.195 $C12H24H^+$ 0.016 177.091 $C11H12O2H^+$ 0.006 177.148 $C13H18H^+$ 0.006 177.127 $C12H16OH^+$ 0.008 177.164 $C13H20H^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.179 $C13H22H^+$ 0.017 181.159 $C12H20OH^+$ 0.006	155.179	C11H22H ⁺	0.012
159.117 $C12H14H^+$ 0.008 161.060 $C10H802H^+$ 0.012 161.096 $C11H12OH^+$ 0.010 163.039 $C9H603H^+$ 0.013 163.075 $C10H1002H^+$ 0.010 163.112 $C11H14OH^+$ 0.010 163.133 $C8H1803H^+$ 0.011 163.148 $C12H18H^+$ 0.035 165.055 $C9H803H^+$ 0.005 165.091 $C10H1202H^+$ 0.014 165.127 $C11H16OH^+$ 0.008 165.164 $C12H20H^+$ 0.024 167.070 $C9H1003H^+$ 0.006 167.107 $C10H1402H^+$ 0.005 167.143 $C11H18OH^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C8H9NO3H^+$ 0.008 169.122 $C10H1602H^+$ 0.009 169.159 $C11H20OH^+$ 0.008 169.195 $C12H24H^+$ 0.010 170.096 $C12H11NH^+$ 0.006 177.127 $C12H16OH^+$ 0.008 177.164 $C13H20H^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.179 $C13H22H^+$ 0.017 181.159 $C12H20OH^+$ 0.006	159.080	$C11H10OH^+$	0.006
161.060 $C10H8O2H^+$ 0.012 161.096 $C11H12OH^+$ 0.010 163.039 $C9H6O3H^+$ 0.013 163.075 $C10H10O2H^+$ 0.010 163.112 $C11H14OH^+$ 0.010 163.133 $C8H18O3H^+$ 0.011 163.148 $C12H18H^+$ 0.035 165.055 $C9H8O3H^+$ 0.005 165.055 $C9H8O3H^+$ 0.008 165.164 $C12H20H^+$ 0.014 165.164 $C12H20H^+$ 0.006 167.107 $C10H12O2H^+$ 0.006 167.107 $C10H14O2H^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C8H9NO3H^+$ 0.018 169.086 $C9H12O3H^+$ 0.009 169.159 $C11H2OOH^+$ 0.008 169.159 $C12H24H^+$ 0.010 170.096 $C12H11NH^+$ 0.006 177.127 $C12H16OH^+$ 0.008 177.164 $C13H20H^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.179 $C13H22H^+$ 0.017 181.159 $C12H20OH^+$ 0.006	159.117	$C12H14H^{+}$	0.008
161.096 $C11H12OH^+$ 0.010 163.039 $C9H6O3H^+$ 0.013 163.075 $C10H10O2H^+$ 0.010 163.112 $C11H14OH^+$ 0.010 163.133 $C8H18O3H^+$ 0.011 163.148 $C12H18H^+$ 0.035 165.055 $C9H8O3H^+$ 0.005 165.091 $C10H12O2H^+$ 0.014 165.127 $C11H16OH^+$ 0.008 165.164 $C12H20H^+$ 0.004 167.070 $C9H10O3H^+$ 0.006 167.107 $C10H14O2H^+$ 0.005 167.143 $C11H18OH^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C8H9NO3H^+$ 0.018 169.086 $C9H12O3H^+$ 0.009 169.122 $C10H16O2H^+$ 0.009 169.159 $C11H20OH^+$ 0.006 175.148 $C13H18H^+$ 0.016 177.091 $C11H12O2H^+$ 0.005 177.127 $C12H24H^+$ 0.006 177.164 $C13H20H^+$ 0.006 179.086 $C14H10H^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.179 $C13H22H^+$ 0.017 181.159 $C12H20OH^+$ 0.006	161.060	C10H8O2H ⁺	0.012
163.039 $C9H6O3H^+$ 0.013 163.075 $C10H10O2H^+$ 0.010 163.112 $C11H14OH^+$ 0.010 163.133 $C8H18O3H^+$ 0.011 163.148 $C12H18H^+$ 0.035 165.055 $C9H8O3H^+$ 0.005 165.091 $C10H12O2H^+$ 0.014 165.127 $C11H16OH^+$ 0.008 165.164 $C12H20H^+$ 0.024 167.070 $C9H10O3H^+$ 0.006 167.107 $C10H14O2H^+$ 0.005 167.143 $C11H18OH^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C8H9NO3H^+$ 0.018 169.086 $C9H12O3H^+$ 0.005 169.122 $C10H16O2H^+$ 0.009 169.159 $C11H20OH^+$ 0.008 169.195 $C12H24H^+$ 0.010 170.096 $C12H11NH^+$ 0.006 177.127 $C12H16OH^+$ 0.008 177.127 $C12H16OH^+$ 0.008 177.143 $C12H18OH^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.179 $C13H22H^+$ 0.017 181.159 $C12H20OH^+$ 0.006	161.096	C11H12OH ⁺	0.010
163.075 $C10H10O2H^+$ 0.010 163.112 $C11H14OH^+$ 0.010 163.133 $C8H18O3H^+$ 0.011 163.148 $C12H18H^+$ 0.035 165.055 $C9H8O3H^+$ 0.005 165.091 $C10H12O2H^+$ 0.014 165.127 $C11H16OH^+$ 0.008 165.164 $C12H20H^+$ 0.024 167.070 $C9H10O3H^+$ 0.006 167.107 $C10H14O2H^+$ 0.005 167.143 $C11H18OH^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C8H9NO3H^+$ 0.005 169.122 $C10H16O2H^+$ 0.009 169.159 $C12H24H^+$ 0.010 170.096 $C12H11NH^+$ 0.006 177.127 $C12H16OH^+$ 0.008 177.127 $C12H16OH^+$ 0.008 177.127 $C12H18OH^+$ 0.006 179.086 $C14H10H^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.179 $C13H22H^+$ 0.017 181.159 $C12H20OH^+$ 0.006	163.039	$C9H6O3H^+$	0.013
163.112 $C11H14OH^+$ 0.010 163.133 $C8H18O3H^+$ 0.011 163.148 $C12H18H^+$ 0.035 165.055 $C9H8O3H^+$ 0.005 165.091 $C10H12O2H^+$ 0.014 165.127 $C11H16OH^+$ 0.008 165.164 $C12H20H^+$ 0.024 167.070 $C9H10O3H^+$ 0.006 167.107 $C10H14O2H^+$ 0.005 167.143 $C11H18OH^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C8H9NO3H^+$ 0.018 169.086 $C9H12O3H^+$ 0.009 169.122 $C10H16O2H^+$ 0.009 169.159 $C11H20OH^+$ 0.008 169.195 $C12H24H^+$ 0.010 170.096 $C12H11NH^+$ 0.006 177.127 $C12H16OH^+$ 0.008 177.127 $C12H16OH^+$ 0.008 177.164 $C13H20H^+$ 0.006 179.086 $C14H10H^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.179 $C13H22H^+$ 0.017 181.159 $C12H20OH^+$ 0.006	163.075	$C10H10O2H^+$	0.010
163.133 $C8H18O3H^+$ 0.011 163.148 $C12H18H^+$ 0.035 165.055 $C9H8O3H^+$ 0.005 165.091 $C10H12O2H^+$ 0.014 165.127 $C11H16OH^+$ 0.008 165.164 $C12H20H^+$ 0.024 167.070 $C9H10O3H^+$ 0.006 167.107 $C10H14O2H^+$ 0.005 167.143 $C11H18OH^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C8H9NO3H^+$ 0.018 169.086 $C9H12O3H^+$ 0.005 169.122 $C10H16O2H^+$ 0.009 169.159 $C11H20OH^+$ 0.008 169.195 $C12H24H^+$ 0.010 170.096 $C12H11NH^+$ 0.006 177.127 $C12H16OH^+$ 0.008 177.164 $C13H20H^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.179 $C13H22H^+$ 0.017 181.159 $C12H20OH^+$ 0.006	163.112	C11H14OH ⁺	0.010
163.148 $C12H18H^+$ 0.035 165.055 $C9H8O3H^+$ 0.005 165.091 $C10H12O2H^+$ 0.014 165.127 $C11H16OH^+$ 0.008 165.164 $C12H20H^+$ 0.024 167.070 $C9H10O3H^+$ 0.006 167.107 $C10H14O2H^+$ 0.005 167.143 $C11H18OH^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C8H9NO3H^+$ 0.005 169.122 $C10H16O2H^+$ 0.009 169.159 $C12H24H^+$ 0.010 170.096 $C12H11NH^+$ 0.006 177.127 $C12H16OH^+$ 0.008 177.164 $C13H20H^+$ 0.006 179.086 $C14H10H^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.179 $C13H22H^+$ 0.017 181.159 $C12H20OH^+$ 0.006	163.133	$C8H18O3H^+$	0.011
165.055 $C9H8O3H^+$ 0.005 165.091 $C10H12O2H^+$ 0.014 165.127 $C11H16OH^+$ 0.008 165.164 $C12H20H^+$ 0.024 167.070 $C9H10O3H^+$ 0.006 167.107 $C10H14O2H^+$ 0.005 167.143 $C11H18OH^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C8H9NO3H^+$ 0.018 169.086 $C9H12O3H^+$ 0.009 169.122 $C10H16O2H^+$ 0.009 169.159 $C11H20OH^+$ 0.008 169.195 $C12H24H^+$ 0.010 170.096 $C12H11NH^+$ 0.006 177.127 $C12H16OH^+$ 0.008 177.164 $C13H20H^+$ 0.006 179.086 $C14H10H^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.179 $C13H22H^+$ 0.017 181.159 $C12H20OH^+$ 0.006	163.148	$C12H18H^{+}$	0.035
165.091 $C10H12O2H^+$ 0.014 165.127 $C11H16OH^+$ 0.008 165.164 $C12H20H^+$ 0.024 167.070 $C9H10O3H^+$ 0.006 167.107 $C10H14O2H^+$ 0.005 167.143 $C11H18OH^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C8H9NO3H^+$ 0.018 169.086 $C9H12O3H^+$ 0.009 169.122 $C10H16O2H^+$ 0.009 169.159 $C11H20OH^+$ 0.008 169.195 $C12H24H^+$ 0.010 170.096 $C12H11NH^+$ 0.006 177.127 $C12H16OH^+$ 0.008 177.127 $C12H16OH^+$ 0.008 177.164 $C13H20H^+$ 0.006 179.086 $C14H10H^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.179 $C13H22H^+$ 0.017 181.159 $C12H20OH^+$ 0.006	165.055	$C9H8O3H^+$	0.005
165.127 $C11H16OH^+$ 0.008 165.164 $C12H20H^+$ 0.024 167.070 $C9H10O3H^+$ 0.006 167.107 $C10H14O2H^+$ 0.005 167.143 $C11H18OH^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C8H9NO3H^+$ 0.018 169.086 $C9H12O3H^+$ 0.005 169.122 $C10H16O2H^+$ 0.009 169.159 $C12H24H^+$ 0.010 170.096 $C12H11NH^+$ 0.006 177.127 $C12H16OH^+$ 0.008 177.127 $C12H16OH^+$ 0.008 177.164 $C13H20H^+$ 0.006 179.086 $C14H10H^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.179 $C13H22H^+$ 0.017 181.159 $C12H20OH^+$ 0.006	165.091	$C10H12O2H^+$	0.014
165.164 $C12H20H^+$ 0.024 167.070 $C9H10O3H^+$ 0.006 167.107 $C10H14O2H^+$ 0.005 167.143 $C11H18OH^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C8H9NO3H^+$ 0.018 169.086 $C9H12O3H^+$ 0.009 169.122 $C10H16O2H^+$ 0.009 169.159 $C11H20OH^+$ 0.008 169.195 $C12H24H^+$ 0.010 170.096 $C12H11NH^+$ 0.006 177.127 $C12H16OH^+$ 0.008 177.127 $C12H16OH^+$ 0.008 177.164 $C13H20H^+$ 0.006 179.086 $C14H10H^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.179 $C13H22H^+$ 0.017 181.159 $C12H20OH^+$ 0.006	165.127	$C11H16OH^+$	0.008
167.070 $C9H10O3H^+$ 0.006 167.107 $C10H14O2H^+$ 0.005 167.143 $C11H18OH^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C8H9NO3H^+$ 0.018 169.086 $C9H12O3H^+$ 0.005 169.122 $C10H16O2H^+$ 0.009 169.159 $C11H20OH^+$ 0.008 169.195 $C12H24H^+$ 0.010 170.096 $C12H11NH^+$ 0.006 175.148 $C13H18H^+$ 0.016 177.127 $C12H16OH^+$ 0.008 177.164 $C13H20H^+$ 0.006 179.086 $C14H10H^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.179 $C13H22H^+$ 0.017 181.159 $C12H20OH^+$ 0.006	165.164	$C12H20H^+$	0.024
167.107 $C10H14O2H^+$ 0.005 167.143 $C11H18OH^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C8H9NO3H^+$ 0.018 169.086 $C9H12O3H^+$ 0.005 169.122 $C10H16O2H^+$ 0.009 169.159 $C11H2OOH^+$ 0.008 169.195 $C12H24H^+$ 0.010 170.096 $C12H11NH^+$ 0.006 175.148 $C13H18H^+$ 0.016 177.127 $C12H16OH^+$ 0.008 177.127 $C12H16OH^+$ 0.008 177.164 $C13H20H^+$ 0.006 179.086 $C14H10H^+$ 0.006 179.179 $C13H22H^+$ 0.017 181.159 $C12H20OH^+$ 0.006	167.070	C9H10O3H ⁺	0.006
167.143 $C11H18OH^+$ 0.008 167.179 $C12H22H^+$ 0.011 168.066 $C8H9NO3H^+$ 0.018 169.086 $C9H12O3H^+$ 0.005 169.122 $C10H16O2H^+$ 0.009 169.159 $C11H20OH^+$ 0.008 169.195 $C12H24H^+$ 0.010 170.096 $C12H11NH^+$ 0.006 177.148 $C13H18H^+$ 0.016 177.127 $C12H16OH^+$ 0.008 177.164 $C13H20H^+$ 0.006 179.086 $C14H10H^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.179 $C13H22H^+$ 0.017 181.159 $C12H20OH^+$ 0.006	167.107	$C10H14O2H^+$	0.005
167.179 $C12H22H^+$ 0.011 168.066 $C8H9NO3H^+$ 0.018 169.086 $C9H12O3H^+$ 0.005 169.122 $C10H16O2H^+$ 0.009 169.159 $C11H20OH^+$ 0.008 169.195 $C12H24H^+$ 0.010 170.096 $C12H11NH^+$ 0.006 175.148 $C13H18H^+$ 0.016 177.091 $C11H12O2H^+$ 0.005 177.127 $C12H16OH^+$ 0.008 177.164 $C13H20H^+$ 0.006 179.086 $C14H10H^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.179 $C13H22H^+$ 0.017 181.159 $C12H20OH^+$ 0.006	167.143	$C11H18OH^+$	0.008
168.066 $C8H9NO3H^+$ 0.018 169.086 $C9H12O3H^+$ 0.005 169.122 $C10H16O2H^+$ 0.009 169.159 $C11H20OH^+$ 0.008 169.195 $C12H24H^+$ 0.010 170.096 $C12H11NH^+$ 0.006 175.148 $C13H18H^+$ 0.016 177.091 $C11H12O2H^+$ 0.005 177.127 $C12H16OH^+$ 0.008 177.164 $C13H20H^+$ 0.020 179.086 $C14H10H^+$ 0.006 179.143 $C12H18OH^+$ 0.017 181.159 $C12H20OH^+$ 0.006	167.179	$C12H22H^{+}$	0.011
169.086 $C9H12O3H^+$ 0.005 169.122 $C10H16O2H^+$ 0.009 169.159 $C11H20OH^+$ 0.008 169.195 $C12H24H^+$ 0.010 170.096 $C12H11NH^+$ 0.006 175.148 $C13H18H^+$ 0.016 177.091 $C11H12O2H^+$ 0.005 177.127 $C12H16OH^+$ 0.008 177.164 $C13H20H^+$ 0.020 179.086 $C14H10H^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.179 $C13H22H^+$ 0.017 181.159 $C12H20OH^+$ 0.006	168.066	C8H9NO3H ⁺	0.018
169.122 $C10H16O2H^+$ 0.009 169.159 $C11H20OH^+$ 0.008 169.195 $C12H24H^+$ 0.010 170.096 $C12H11NH^+$ 0.006 175.148 $C13H18H^+$ 0.016 177.091 $C11H12O2H^+$ 0.005 177.127 $C12H16OH^+$ 0.008 177.164 $C13H20H^+$ 0.006 179.086 $C14H10H^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.179 $C13H22H^+$ 0.017 181.159 $C12H20OH^+$ 0.006	169.086	C9H12O3H ⁺	0.005
169.159 $C11H20OH^+$ 0.008 169.195 $C12H24H^+$ 0.010 170.096 $C12H11NH^+$ 0.006 175.148 $C13H18H^+$ 0.016 177.091 $C11H12O2H^+$ 0.005 177.127 $C12H16OH^+$ 0.008 177.164 $C13H20H^+$ 0.020 179.086 $C14H10H^+$ 0.006 179.143 $C12H18OH^+$ 0.006 179.179 $C13H22H^+$ 0.017 181.159 $C12H20OH^+$ 0.006	169.122	$C10H16O2H^+$	0.009
169.195 C12H24H ⁺ 0.010 170.096 C12H11NH ⁺ 0.006 175.148 C13H18H ⁺ 0.016 177.091 C11H12O2H ⁺ 0.005 177.127 C12H16OH ⁺ 0.008 177.164 C13H20H ⁺ 0.006 179.086 C14H10H ⁺ 0.006 179.143 C12H18OH ⁺ 0.006 179.179 C13H22H ⁺ 0.017 181.159 C12H20OH ⁺ 0.006	169.159	$C11H20OH^+$	0.008
170.096 C12H11NH ⁺ 0.006 175.148 C13H18H ⁺ 0.016 177.091 C11H12O2H ⁺ 0.005 177.127 C12H16OH ⁺ 0.008 177.164 C13H20H ⁺ 0.020 179.086 C14H10H ⁺ 0.006 179.143 C12H18OH ⁺ 0.006 179.179 C13H22H ⁺ 0.017 181.159 C12H20OH ⁺ 0.006	169.195	$C12H24H^{+}$	0.010
175.148 C13H18H ⁺ 0.016 177.091 C11H12O2H ⁺ 0.005 177.127 C12H16OH ⁺ 0.008 177.164 C13H20H ⁺ 0.020 179.086 C14H10H ⁺ 0.006 179.143 C12H18OH ⁺ 0.006 179.179 C13H22H ⁺ 0.017 181.159 C12H20OH ⁺ 0.006	170.096	C12H11NH ⁺	0.006
177.091 C11H12O2H ⁺ 0.005 177.127 C12H16OH ⁺ 0.008 177.164 C13H20H ⁺ 0.020 179.086 C14H10H ⁺ 0.006 179.143 C12H18OH ⁺ 0.006 179.179 C13H22H ⁺ 0.017 181.159 C12H20OH ⁺ 0.006	175.148	$C13H18H^{+}$	0.016
177.127 C12H16OH ⁺ 0.008 177.164 C13H20H ⁺ 0.020 179.086 C14H10H ⁺ 0.006 179.143 C12H18OH ⁺ 0.006 179.179 C13H22H ⁺ 0.017 181.159 C12H20OH ⁺ 0.006	177.091	$C11H12O2H^+$	0.005
177.164C13H20H+0.020179.086C14H10H+0.006179.143C12H18OH+0.006179.179C13H22H+0.017181.159C12H20OH+0.006	177.127	C12H16OH ⁺	0.008
179.086C14H10H+0.006179.143C12H18OH+0.006179.179C13H22H+0.017181.159C12H20OH+0.006	177.164	$C13H20H^+$	0.020
179.143C12H18OH+0.006179.179C13H22H+0.017181.159C12H20OH+0.006	179.086	$C14H10H^{+}$	0.006
179.179C13H22H+0.017181.159C12H200H+0.006	179.143	$C12H18OH^{+}$	0.006
181.159 C12H20OH ⁺ 0.006	179.179	$C13H22H^{+}$	0.017
	181.159	$C12H20OH^+$	0.006

181.195	$C13H24H^{+}$	0.008
183.138	$C11H18O2H^+$	0.005
183.211	$C13H26H^{+}$	0.008
185.190	$C12H24OH^{+}$	0.005
189.091	$C12H12O2H^+$	0.008
193.159	$C13H20OH^+$	0.011
195.102	$C11H14O3H^{+}$	0.004
195.138	$C12H18O2H^+$	0.006
197.117	$C11H16O3H^+$	0.005
197.154	$C12H20O2H^+$	0.007
	181.195 183.138 183.211 185.190 189.091 193.159 195.102 195.138 197.117 197.154	181.195 C13H24H ⁺ 183.138 C11H18O2H ⁺ 183.211 C13H26H ⁺ 185.190 C12H24OH ⁺ 189.091 C12H12O2H ⁺ 193.159 C13H20OH ⁺ 195.102 C11H14O3H ⁺ 195.138 C12H18O2H ⁺ 197.117 C11H16O3H ⁺ 197.154 C12H20O2H ⁺

		Averaged
Ion exact	Ion formula	mixing ratio
m/z (1h)		(ppbv)
54.034	$C3H3NH^{+}$	0.15
67.054	$C5H6H^{+}$	0.13
69.034	$C4H4OH^{+}$	0.21
69.070	$C5H8H^{+}$	1.3
70.065	$C4H7NH^{+}$	0.059
71.049	$C4H6OH^+$	0.29
73.028	$C3H4O2H^{+}$	0.14
73.065	$C4H8OH^+$	1.3
75.044	$C3H6O2H^+$	0.90
77.023	$C2H4O3H^{+}$	0.050
79.054	$C6H6H^+$	1.8
80.050	$\rm C5H5NH^{+}$	0.069
81.034	$C5H4OH^{+}$	0.043
81.070	$\rm C6H8H^{+}$	0.25
82.065	$C5H7NH^+$	0.043
83.049	$C5H6OH^+$	0.16
83.086	$C6H10H^+$	1.3
85.028	$C4H4O2H^+$	0.13
85.065	$C5H8OH^+$	0.22
85.101	$C6H12H^+$	0.24
87.044	$C4H6O2H^+$	0.54
87.080	$C5H10OH^+$	0.24
89.060	$C4H8O2H^+$	0.43
91.039	$C3H6O3H^+$	0.033
93.070	$C7H8H^+$	2.6
95.049	C6H6OH ⁺	0.14
95.086	$C7H10H^+$	0.060
96.081	C6H9NH ⁺	0.026
97.028	$C5H4O2H^+$	0.12
97.065	$C6H8OH^+$	0.094
97.101	$C7H12H^{+}$	0.38
99.008	$C4H2O3H^{+}$	0.060
99.044	$C5H6O2H^+$	0.069
99.080	$C6H10OH^+$	0.16
101.060	$C5H8O2H^+$	0.25
101.096	C6H12OH ⁺	0.21
103.039	$C4H6O3H^+$	0.040
103.075	C5H10O2H ⁺	0.13
104.049	$C7H5NH^{+}$	0.10
105.070	$C8H8H^+$	0.17
107.049	$C7H6OH^+$	0.084
107.086	$C8H10H^+$	1.3
109.065	$C7H8OH^+$	0.033
109.101	$C8H12H^+$	0.12
111.044	$C6H6O2H^+$	0.065

111.080	$C7H10OH^+$	0.045
111.117	$C8H14H^{+}$	0.21
113.060	$C6H8O2H^+$	0.071
113.096	$C7H12OH^{+}$	0.067
115.075	C6H10O2H ⁺	0.13
117.055	$C5H8O3H^+$	0.024
117.091	$C6H12O2H^+$	0.25
118.065	$C8H7NH^{+}$	0.023
119.049	C8H6OH ⁺	0.023
119.086	$C9H10H^+$	0.061
121.101	$C9H12H^+$	0.61
123.044	$C7H6O2H^+$	0.039
123.080	$C8H10OH^+$	0.020
123.117	$C9H14H^+$	0.056
125.060	$C7H8O2H^+$	0.027
125.096	$C8H12OH^+$	0.038
125.132	C9H16H ⁺	0.095
127.039	$C6H6O3H^+$	0.022
127.075	$C7H10O2H^+$	0.030
127.112	$C8H14OH^{+}$	0.070
129.070	$C10H8H^+$	0.077
129.127	$C8H16OH^+$	0.043
131.070	$C6H10O3H^+$	0.012
133.065	C9H8OH ⁺	0.025
133.101	$C10H12H^+$	0.060
135.044	$C8H6O2H^+$	0.024
135.117	$C10H14H^{+}$	0.25
137.060	$C8H8O2H^+$	0.034
137.132	$C10H16H^+$	0.077
139.075	$C8H10O2H^+$	0.021
139.112	$C9H14OH^{+}$	0.029
139.148	$C10H18H^+$	0.038
140.034	$C6H5NO3H^+$	0.040
141.127	$C9H16OH^+$	0.028
143.086	$C11H10H^+$	0.062
147.117	$C11H14H^{+}$	0.056
149.132	$C11H16H^+$	0.13
153.164	$C11H20H^+$	0.023
154.050	$C7H7NO3H^{+}$	0.028
155.143	$C10H18OH^+$	0.018
168.066	C8H9NO3H ⁺	0.019
175.148	$C13H18H^{+}$	0.026
177.164	$C13H20H^+$	0.043
179.179	$C13H22H^{+}$	0.022
181.195	$C13H24H^{+}$	0.012

Table S2 List of ions and averaged mixing ratiosincluded in the PMF analysis at MRIU