

Supplementary Table 1. Quality control outcomes and putative compound identifications for all PTR-TOF-MS detected ions. Color coding indicates filtering outcomes: green = compounds retained for final analysis after quality control and successful database matching (n=48); purple = masses without confident match in GLOVOCS database (± 0.015 Da window); dark gray = manually excluded ions comprising: compounds identified only in PTRwid Unified Mass List calculations, reagent/calibration ions and H_3O^+ water clusters, inorganic gases and halogen-associated peaks, isotopes of major compounds (acetone, acetic acid, dimethyl sulfide); light gray = compounds failing automated quality criteria during preprocessing (detection threshold < 0.025 ppbv, SNR < 0.1 , or IQR ratio < 0.02 ; see Methods). Putative chemical identities were assigned using GLOVOCS database matching with hierarchical classifications (class, superclass, subclass) provided where available.

Identified $m/z+1$ ¹	Instrument ions ²	Unwanted mass ³	Unwanted isotopes ⁴	Filtered out ⁵	No match found	Matched mass ⁶	Matched chemical formula ⁷	Remarks
19.024	X							Water
19.574		X						
19.583		X						
19.603		X						
20.010		X						
21.020	X							Primary ion isotope with O[18]
22.669		X						
22.731		X						
22.745		X						
22.771		X						
26.013		X						
28.008		X						

29.014	X							
29.996	X							
30.993		X						
31.999	X							
32.529		X						
32.590		X						
33.990		X						
36.015		X						
37.025	X							Water cluster
37.932		X						
38.027	X							Water cluster
39.026	X							Water cluster
39.961		X						
40.971		X						
41.034						41.039	C ₃ H ₄	
42.022						42.034	C ₂ H ₃ N	
43.013								Acetic acid fragment
44.002	X							
44.994	X							
45.030						45.033	C ₂ H ₄ O	
45.988	X							
47.012						47.013	CH ₂ O ₂	
48.001	X							
49.005						49.011	CH ₄ S	
49.993	X							
51.008		X						
51.932		X						

51.996		X						
52.932				X				
53.003		X						
53.930				X				
55.034	X							Water cluster
55.927		X						
56.045						56.049	C ₃ H ₅ N	
56.928				X				
57.058						57.045	C ₂ H ₄ N ₂	
57.929		X						
58.042						58.041	C ₃ H ₅ O	
59.049						59.049	C ₃ H ₆ O	
59.950					X			
60.049			X					Isotope of 59.049 (Acetone)
61.031						61.028	C ₂ H ₄ O ₂	
61.924				X				
62.033			X					Isotope of 61.031 (Acetic acid)
63.027						63.026	C ₂ H ₆ S	
63.982		X						
65.028			X					Isotope of 63.027 (DMS)
66.025				X				
66.981				X				
67.060				X				
67.962				X				
68.056				X				
69.073						69.070	C ₅ H ₈	
70.069				X				

70.964				X				
71.059						71.060	$C_3H_6N_2$	
71.951				X				
72.055				X				
72.955					X			
73.061						73.065	C_4H_8O	
73.961				X				
74.041						74.035	CH_3N_3O	
75.049						75.044	$C_3H_6O_2$	
75.961					X			
76.044				X				
77.036						77.039	C_6H_4	
77.959				X				
78.051						78.046	C_6H_5	
79.058						79.054	C_6H_6	
79.959					X			
80.057						80.049	C_5H_5N	
81.071								Monoterpenes fragment
82.071				X				
82.988				X				
83.085						83.086	C_6H_{10}	
83.954				X				
84.072						84.081	C_5H_9N	
84.972		X						
85.056						85.065	C_5H_8O	
85.969				X				
86.052				X				

87.061				X				
87.952				X				
88.057				X				
88.970					X			
89.052						89.060	C ₄ H ₈ O ₂	
89.963					X			
90.961		X						
91.961					X			
92.061				X				
93.059						93.057	C ₆ H ₆ N	
93.960					X			
95.047						95.047	C ₆ H ₆ O	
95.955					X			
97.008						97.011	C ₅ H ₄ S	
97.957				X				
98.043				X				
99.045						99.044	C ₅ H ₆ O ₂	
99.994				X				
100.039						100.039	C ₄ H ₅ NO ₂	
100.950					X			
101.051						101.060	C ₅ H ₈ O ₂	
101.967				X				
102.048				X				
102.951		X						
103.062						103.058	C ₅ H ₁₀ S	
103.962					X			
104.049						104.049	C ₇ H ₅ N	

104.958				X				
105.062						105.055	$C_4H_8O_3$	
105.955					X			
106.966					X			
107.076						107.070	$C_4H_{10}O_3$	
107.970					X			
108.960		X						
109.960					X			
110.965					X			
111.087						111.092	$C_6H_{10}N_2$	
111.966				X				
112.063				X				
113.049						113.042	C_6H_8S	
114.038		X						
115.067						115.075	$C_6H_{10}O_2$	
116.060				X				
116.909					X			
117.077						117.073	$C_6H_{12}S$	
117.953				X				
118.911		X						
119.953					X			
120.932		X						
121.087						121.086	$C_5H_{12}O_3$	
121.959					X			
122.959				X				
123.082						123.092	$C_8H_{10}O$	
123.946	X							Impurities from Teflon rings

124.953		X						
125.094						125.094	C ₈ H ₁₂ O	
125.959		X						
126.968						126.970	C ₂ H ₆ S ₃	
127.951					X			
128.949				X				
129.095						129.091	C ₇ H ₁₂ O ₂	
129.947				X				
130.066				X				
130.985				X				
131.056				X				
131.914				X				
132.017				X				
133.065				X				
133.921				X				
135.008				X				
135.093				X				
135.953				X				
136.035				X				
136.959				X				
137.126						137.132	C ₁₀ H ₁₆	
137.962				X				
138.121				X				
139.031				X				
139.097						139.112	C ₉ H ₁₄ O	
139.978				X				
140.015				X				

140.089				X			
141.092					141.091	$C_8H_{12}O_2$	
141.953				X			
142.926				X			
143.124				X			
143.925				X			
144.917				X			
145.090				X			
146.996				X			
147.049				X			
148.030				X			
149.048				X			
150.053				X			
151.102				X			
152.110				X			
153.097					153.091	$C_9H_{12}O_2$	
154.089				X			
155.094				X			
156.073				X			
157.069					157.065	$C_{11}H_8O$	
158.037				X			
159.039				X			
159.091				X			
160.982				X			
161.069				X			
161.928				X			
162.961				X			

164.025				X				
165.004				X				
167.087				X				
169.089				X				
171.107				X				
173.039				X				
174.053				X				
175.035				X				
177.032				X				
178.953				X				
180.936				X				
182.020				X				
183.098				X				
185.012				X				
185.128				X				
187.049				X				
189.016				X				
189.969				X				
191.019				X				
192.032				X				
193.041				X				
195.015				X				
196.170				X				
198.194				X				
199.183				X				
202.978				X				
203.939	X							

204.942	X						
205.998				X			
207.033			X				
209.021			X				
212.998			X				
219.935			X				
220.933				X			
221.937			X				
223.056			X				
224.064			X				
225.030			X				
226.022			X				
227.018			X				
230.931			X				
233.909			X				
234.913			X				

¹Identified in PTRwid Unified Mass List calculations (see Methods).

²Including reagent ions and internal calibration gases as well as primary ion water clusters.

³Including inorganic gases, and peaks associated with halogens.

⁴Isotopes of abundant compounds (i.e., Acetone, Acetic acid, and DMS).

⁵Not excluded manually like the first four groups but filtered out in the preprocessing (see Methods).

⁶Matched masses in the GLOVOCs database.

⁷Chemical formula of the matched masses in the GLOVOCs database.