

Supplement of Atmos. Chem. Phys., 20, 7875–7893, 2020
<https://doi.org/10.5194/acp-20-7875-2020-supplement>
© Author(s) 2020. This work is distributed under
the Creative Commons Attribution 4.0 License.



Atmospheric
Chemistry
and Physics
Open Access
EGU

Supplement of

A 1-year characterization of organic aerosol composition and sources using an extractive electrospray ionization time-of-flight mass spectrometer (EESI-TOF)

Lu Qi et al.

Correspondence to: Jay G. Slowik (jay.slowik@psi.ch) and André S. H. Prévôt (andre.prevot@psi.ch)

The copyright of individual parts of the supplement might differ from the CC BY 4.0 License.

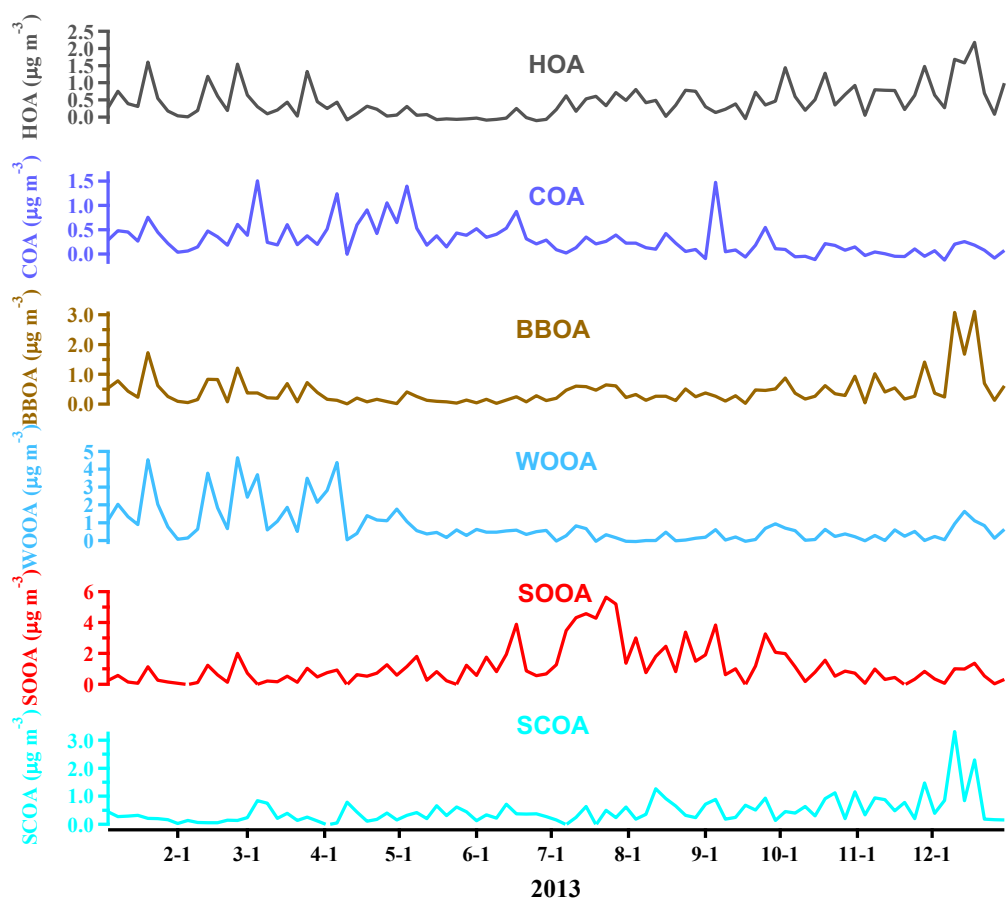


Fig. S1. Time series of AMS source apportionment factors.

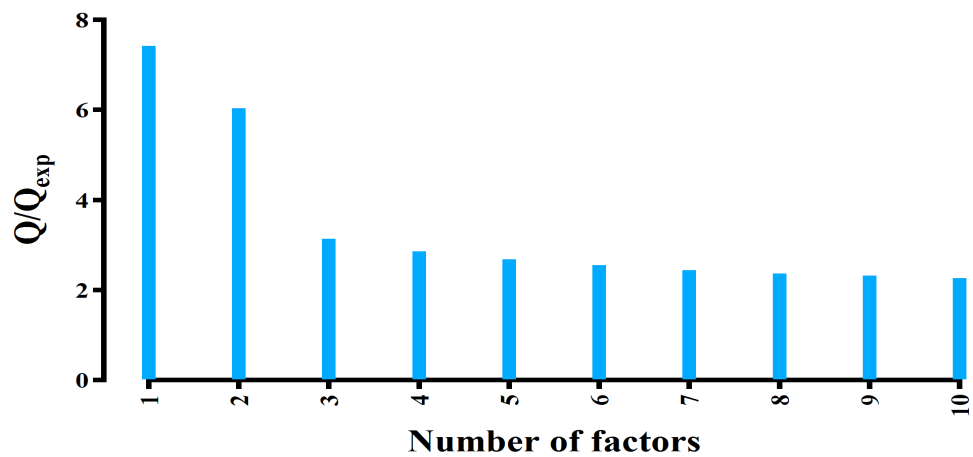
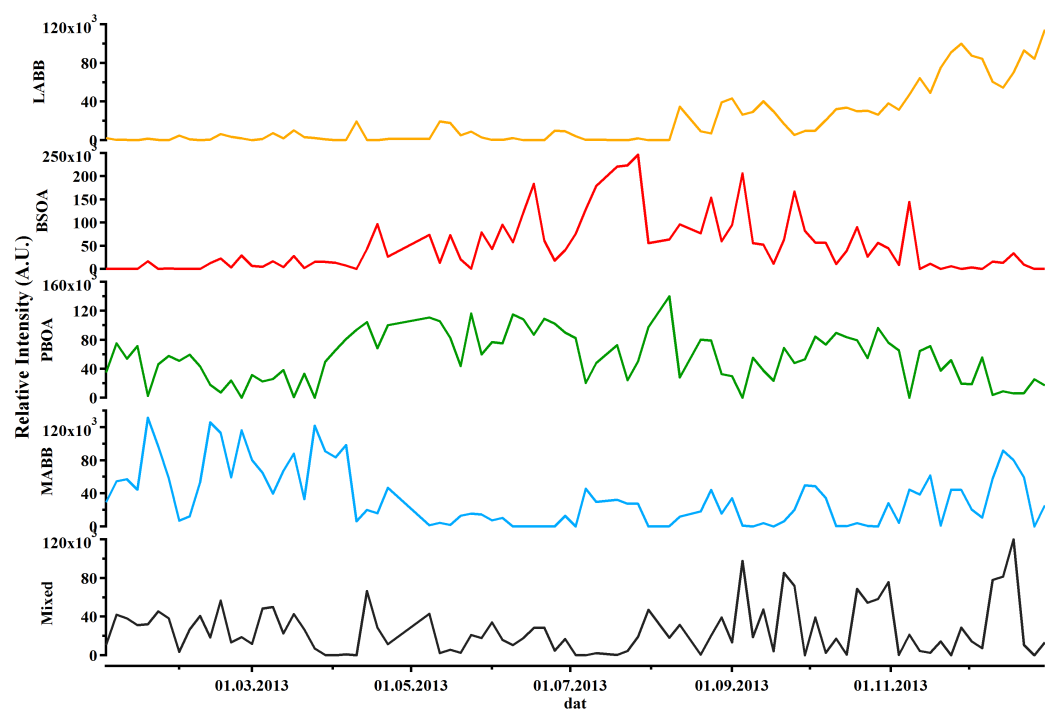
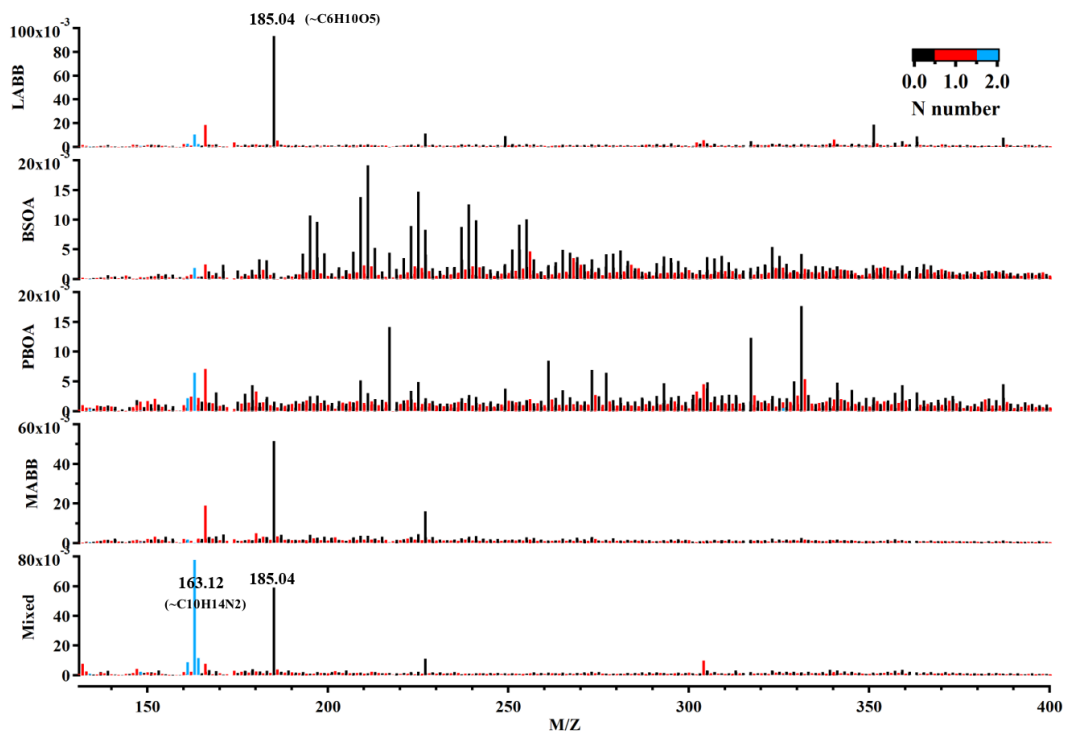


Fig. S2. Q/Q_{exp} for the solutions consisting of 1 to 10 factors.

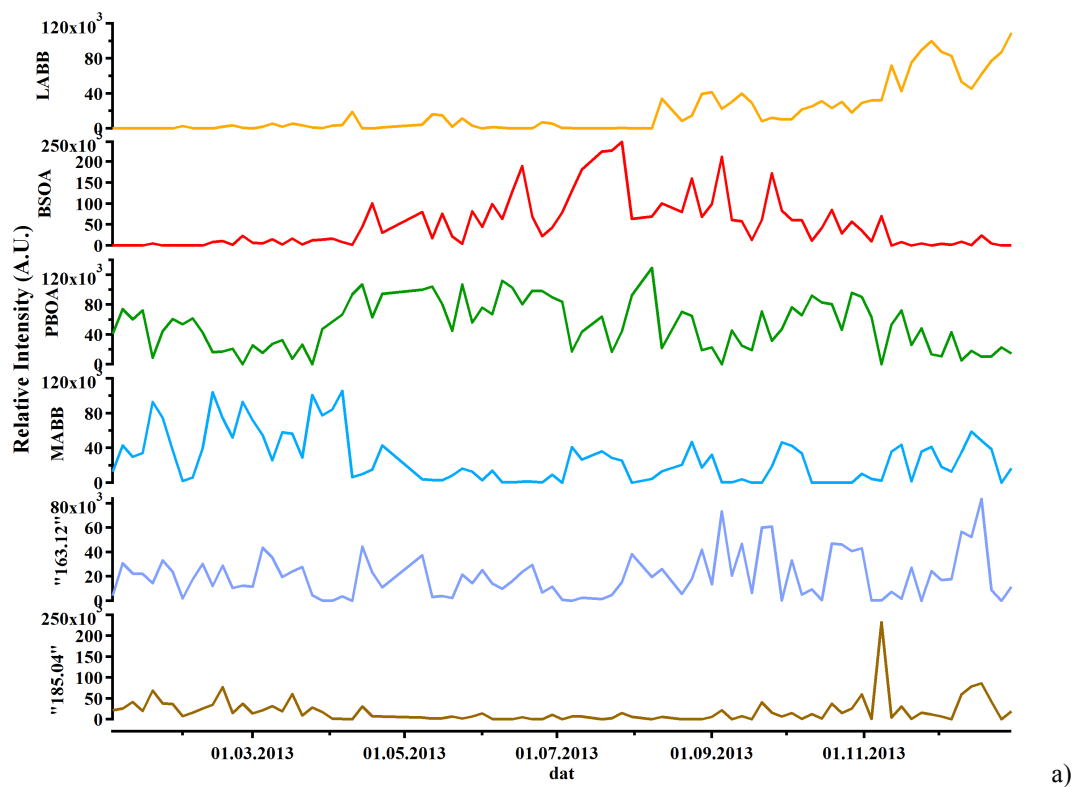


a)

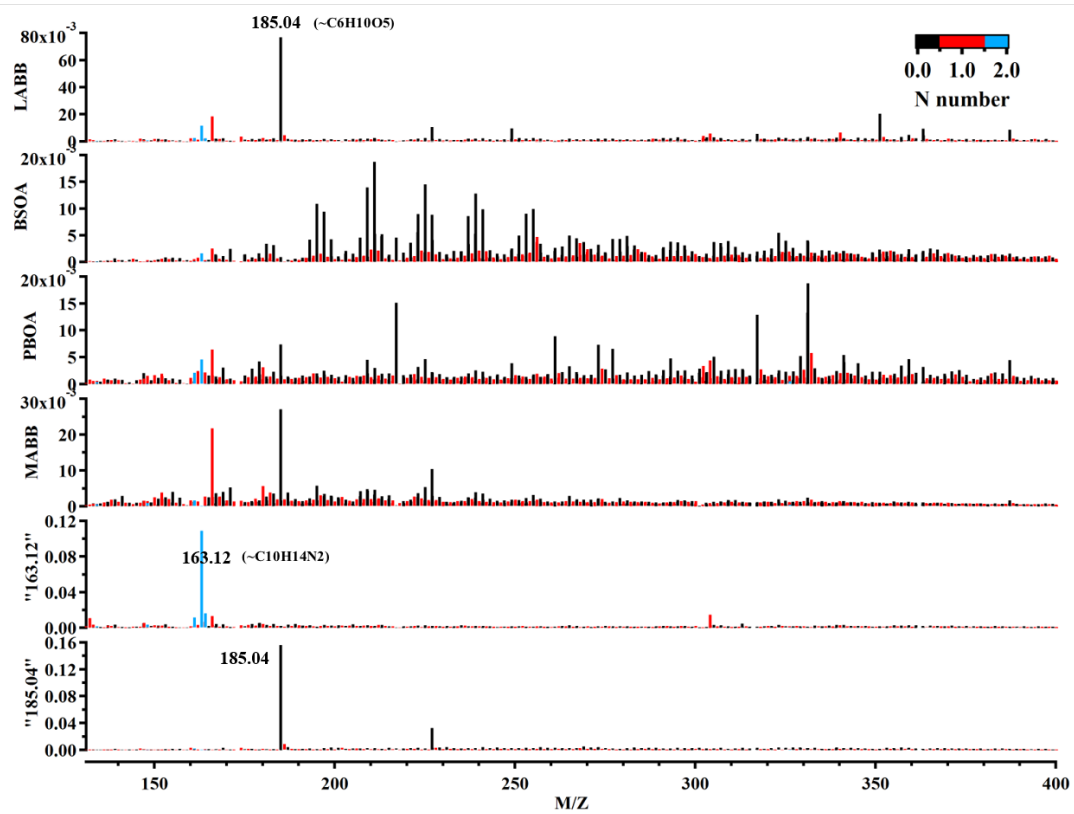


b)

Fig. S3. Time series (a) and profiles (b) of the EESI-TOF 5-factor PMF solution.

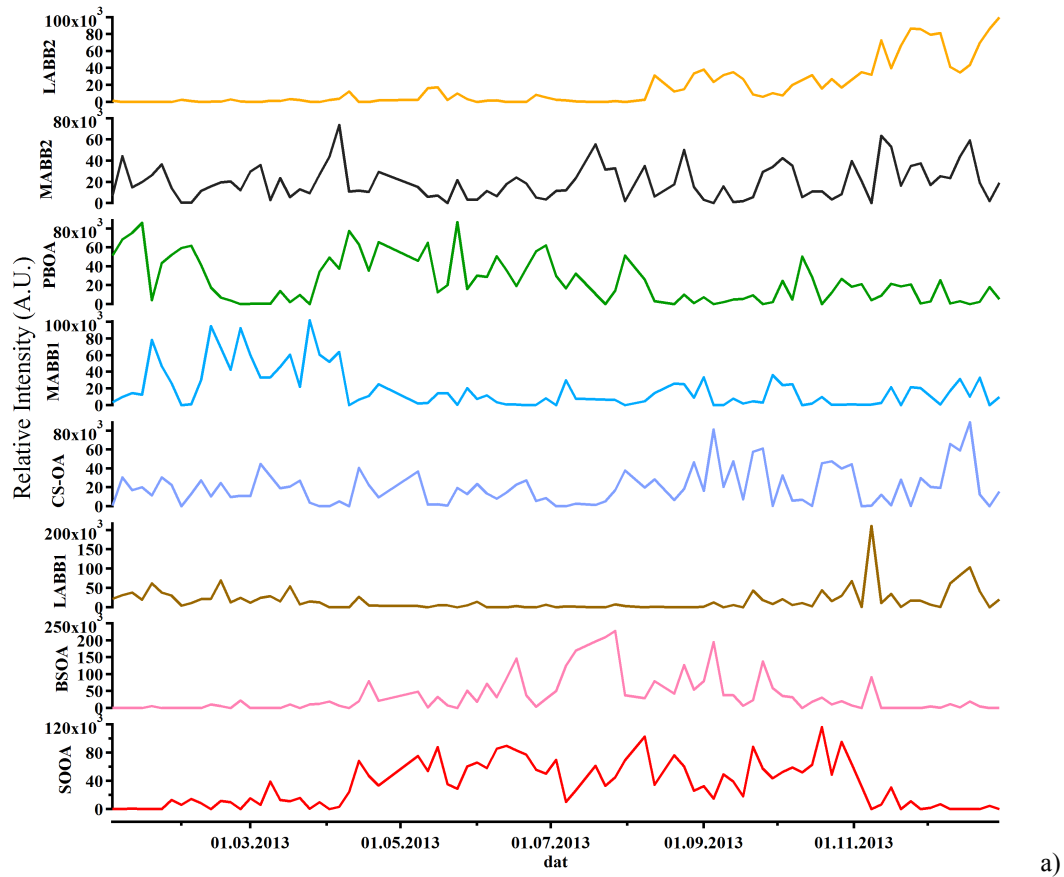


a)

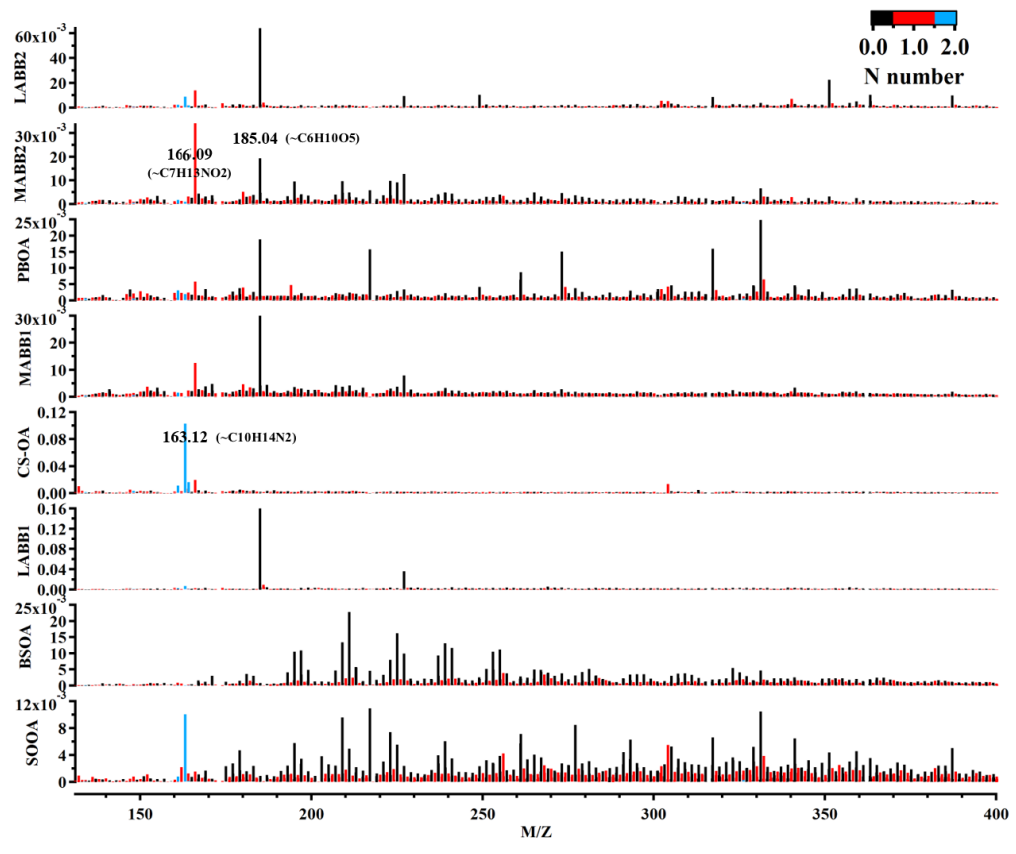


b)

Fig. S4. Time series (a) and profiles (b) of the EESI-TOF 6-factor PMF solution.



a)



b)

Fig. S5. Time series (a) and profiles (b) of EESI-TOF eight-factors solution.

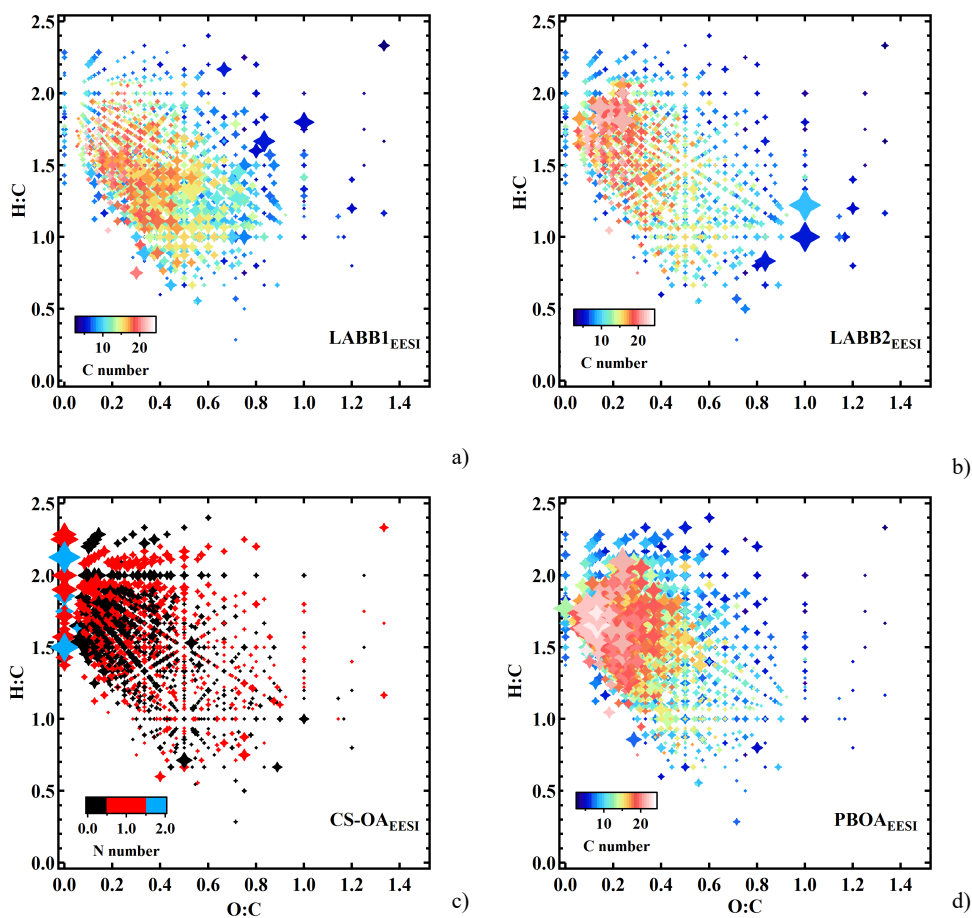


Fig. S6. Van Krevelen plots (atomic H:C vs. O:C ratio) of the LABB1_{EESI}, LABB2_{EESI}, CS-OA_{EESI} and PBOA_{EESI} factor mass spectra. Points are sized by the fraction of each ion apportioned to LABB1_{EESI}, LABB2_{EESI}, CS-OA_{EESI} and PBOA_{EESI}, colored by number of carbon atoms and nitrogen number, respectively.

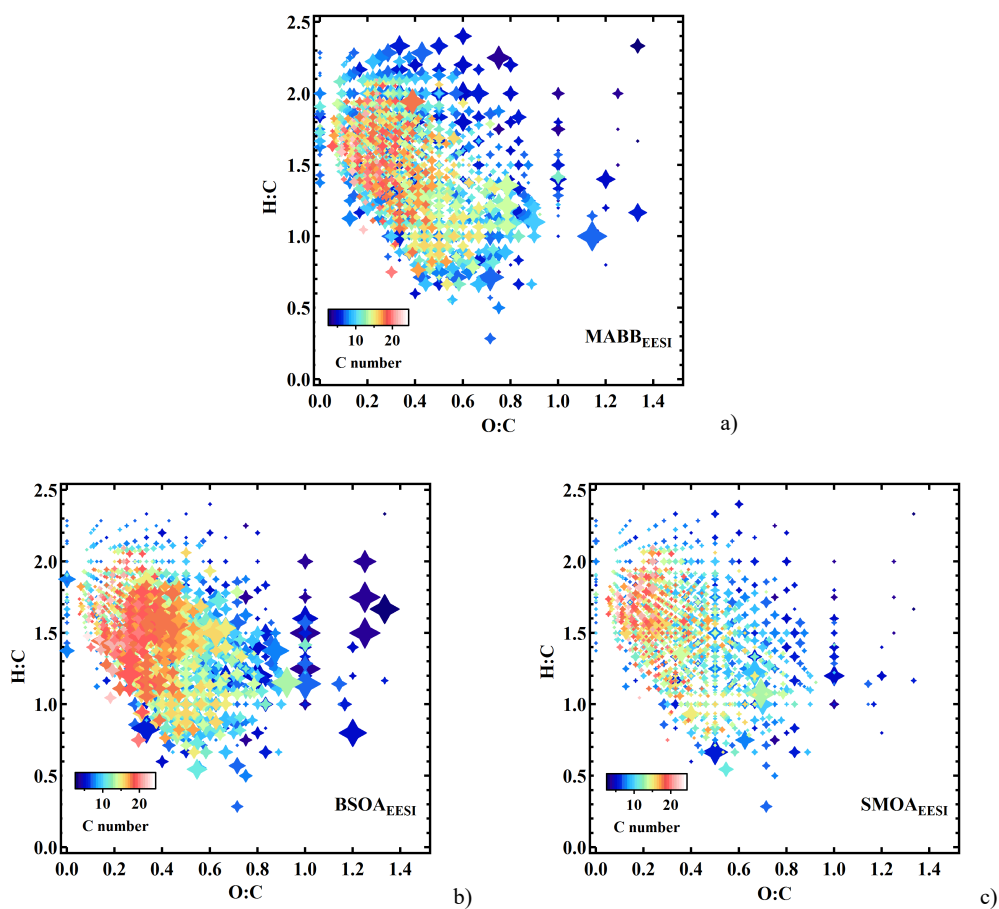


Fig. S7. Van Krevelen plot (atomic H:C vs. O:C ratio) of the MABB_{EESI}, SMOA_{EESI} and BSOA_{EESI} factor mass spectra. Points are sized by the fraction of each ion apportioned to each factor and colored by number of carbon atoms and nitrogen number.

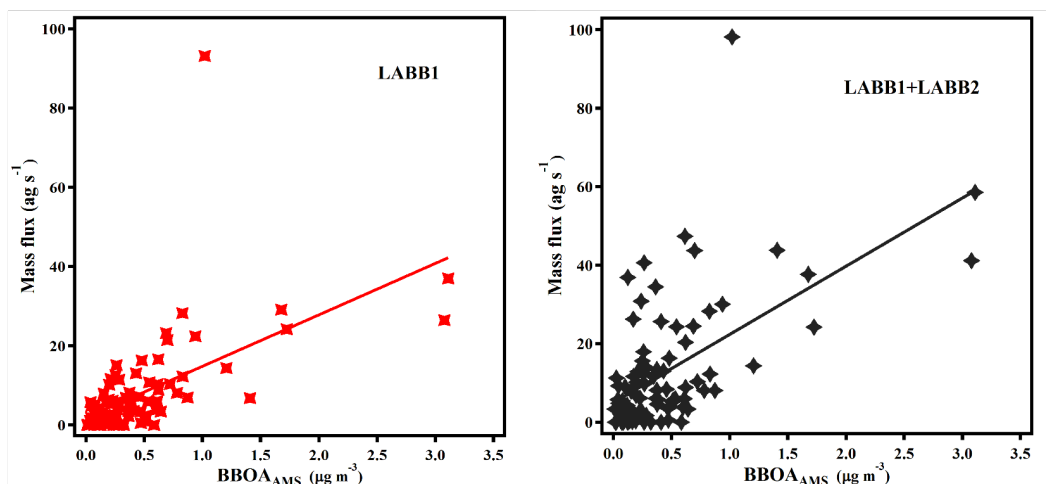


Fig. S8. Scatter plot of the LABB1_{EESI} factor and LABB1_{EESI}+LABB2_{EESI} factor as a function of the

BBOA_{AMS} factor.

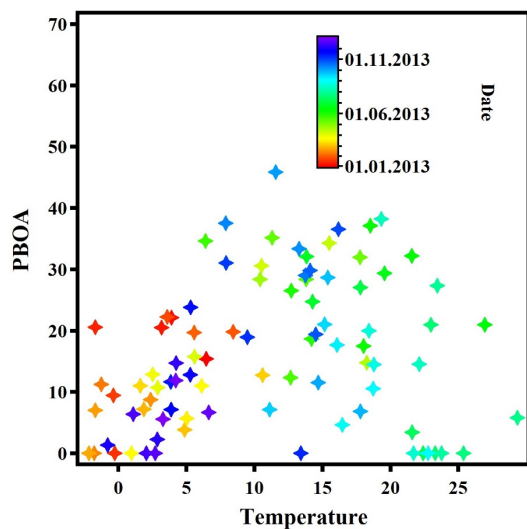


Fig. S9. The scatter plot of the temperature as a function of the PBOA factor of the EESI-TOF PMF.

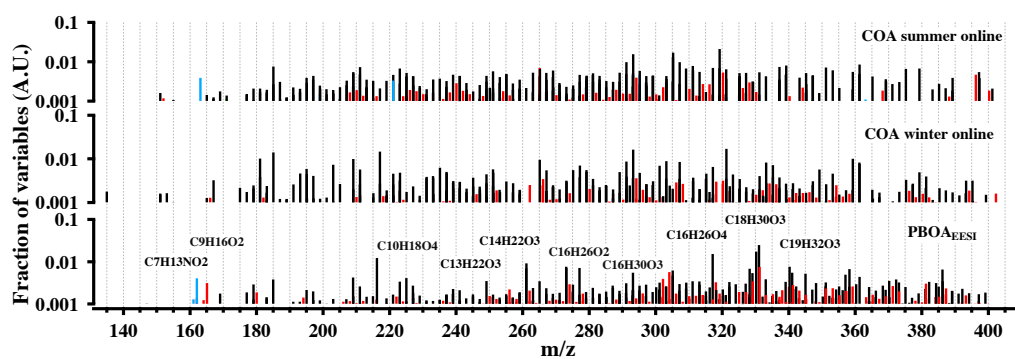
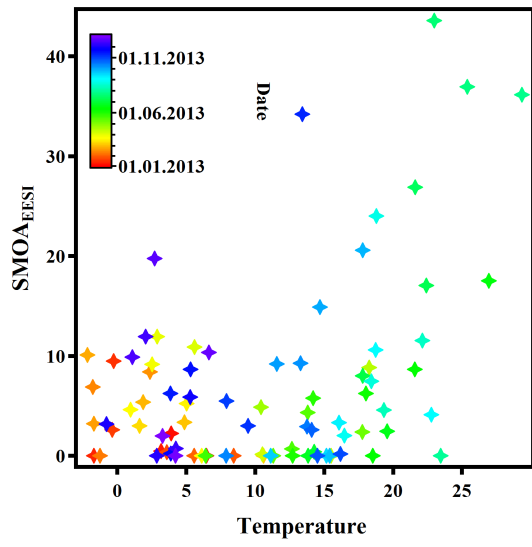
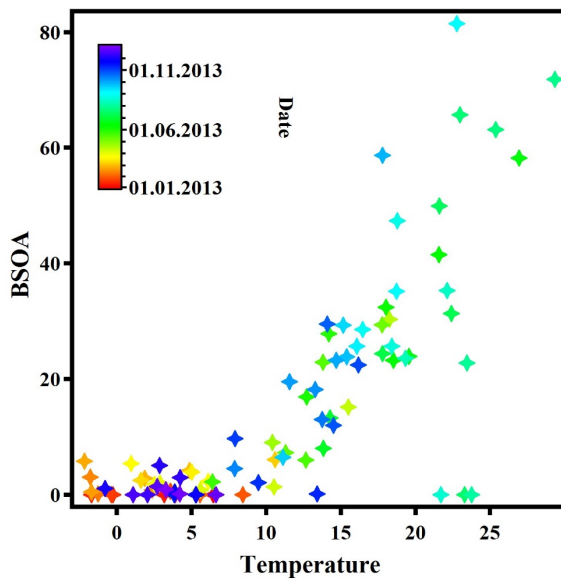


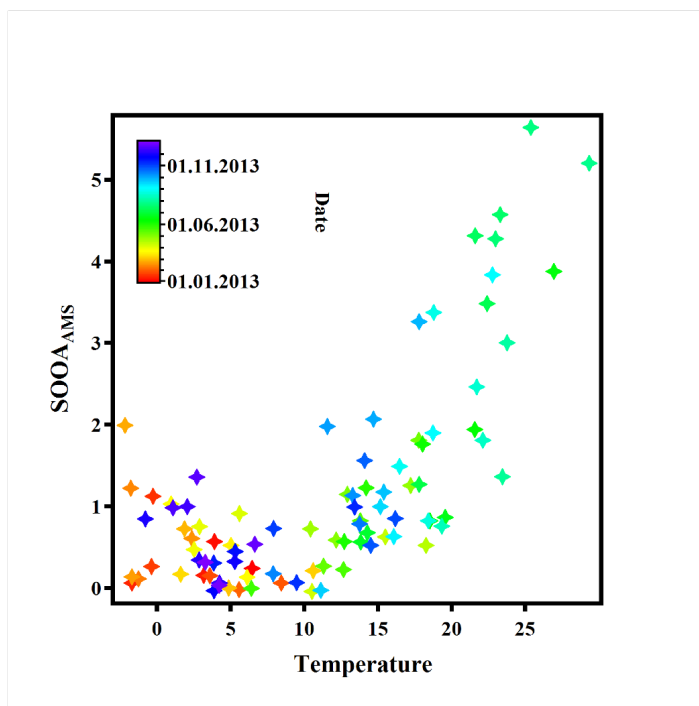
Fig. S10. The mass spectrum comparison between the PBOA factor and reference COA EESI factor (Qi et al., 2019, Stefenelli et al., 2019).



a)



b)



c)

Fig. S11. The scatter plot of the temperature as a function of the SMOA_{EESI} factor (a), BSOA_{EESI} factor (b) and SOOA_{AMS} factor of the EESI-TOF PMF.

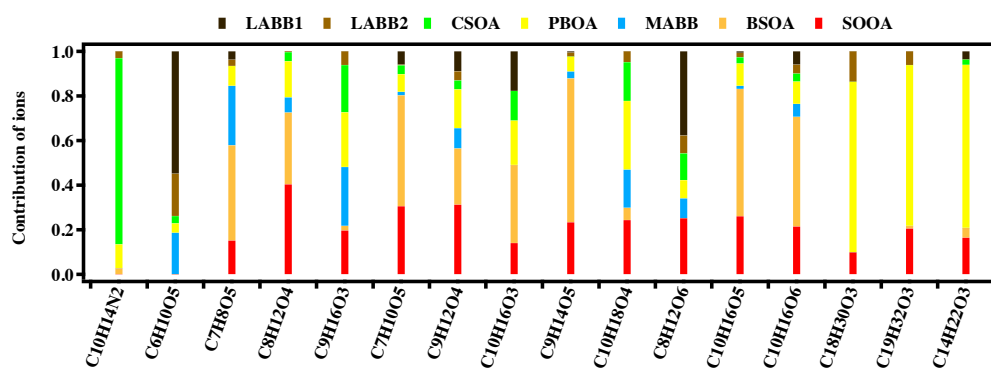


Fig. S12. Contribution of each ions to each factor from EESI-TOF PMF analysis.

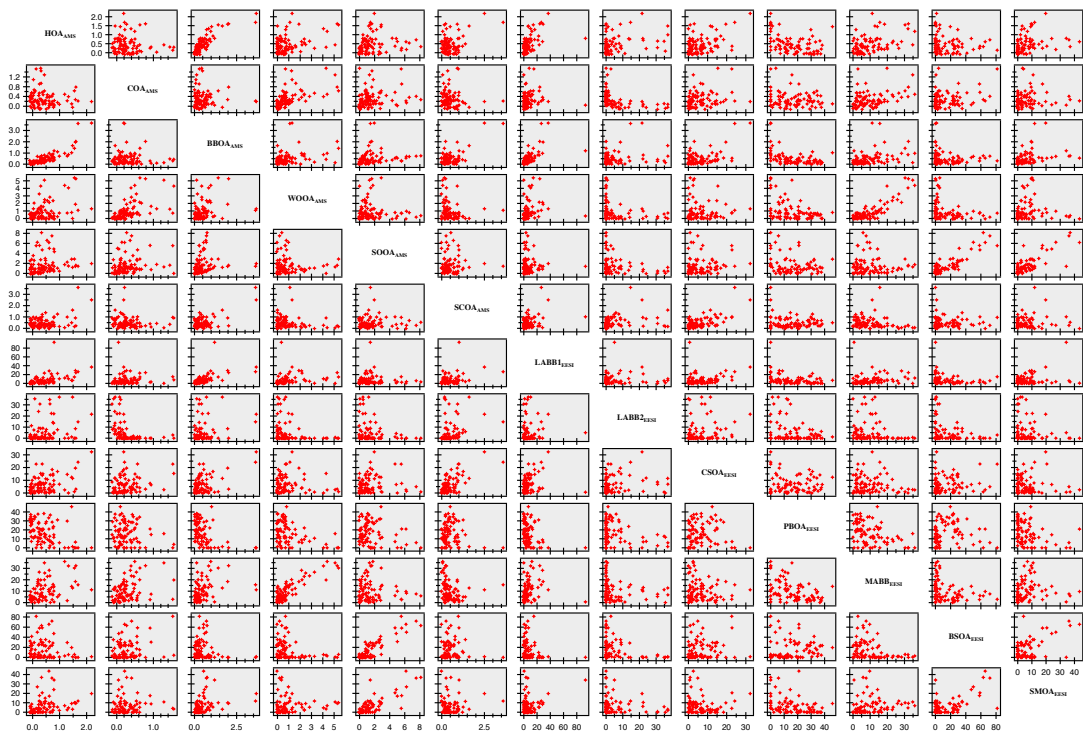


Fig. S13. Correlation between all the AMS and EESI factors.

Table S1. The list of the distinguished molecules of each factor.

Factor name	Formula	m/z			
LABB1	C5H8O4	132.042		C11H16O7	260.09
	C5H9NO5	163.048		C11H16O8	276.085
	C6H10O5	162.053		C12H14O3	206.094
	C7H11NO6	205.059		C12H14O4	222.089
	C8H12O6	204.063		C12H14O7	270.074
	C8H15NO5	205.095		C12H15NO4	237.1
	C8H7NO3	165.043		C12H15NO5	253.095
	C9H11NO3	181.074		C12H15NO6	269.09
	C9H13NO3	183.09		C12H16O4	224.105
	C9H8O3	164.047		C12H16O7	272.09
	C10H11NO4	209.069		C12H16O8	288.085
	C10H11NO5	225.064		C13H14O5	250.084
	C10H11NO6	241.059		C13H14O6	266.079
	C10H12O4	196.074		C13H16O4	236.105
	C10H12O6	228.063		C13H16O5	252.1
	C10H12O7	244.058		C13H16O6	268.095
	C10H13NO5	227.079		C13H17NO4	251.116
	C10H14O7	246.074		C14H14O5	262.084
	C11H12O4	208.074		C14H16O5	264.1
	C11H12O5	224.069		C14H17NO6	295.106
	C11H13NO4	223.085		C14H18O5	266.115
	C11H13NO5	239.079		C14H18O7	298.105
	C11H13NO6	255.074		C14H20O8	316.116
	C11H13NO7	271.069		C15H16O6	292.095
	C11H14O4	210.089		C15H16O8	324.085
	C11H14O6	242.079		C15H18O5	278.115
	C11H14O7	258.074		C15H18O6	294.11
	C11H14O8	274.069		C15H20O6	296.126
	C11H15NO4	225.1		C15H20O8	328.116
				C15H22O8	330.132
				C16H18O5	290.115

	C16H2005	292.131
	C16H2006	308.126
	C16H22010	374.121
	C16H2205	294.147
	C16H2206	310.142
	C16H2207	326.137
	C16H23NO5	309.158
	C16H2409	360.142
	C17H2005	304.131
	C17H2205	306.147
	C17H2206	322.142
	C17H2408	356.147
	C17H2409	372.142
	C18H2007	348.121
	C18H2206	334.142
	C18H2208	366.132
	C18H2405	320.162
	C18H2407	352.152
	C18H2408	368.147
	C19H1806	342.11
	C19H2206	346.142
	C19H2207	362.137
	C19H2606	350.173
	C20H2405	344.162
LABB2	C5H6O6	162.016
	C6H5NO5	171.017
	C6H6O6	174.016
	C6H6O7	190.011
	C7H4O5	168.006
	C8H4O6	196.001
	C13H22O3	226.157
	C13H24O3	228.173

	C15H28O4	272.199
	C16H25NO3	279.184
	C16H28O3	268.204
	C16H29NO5	315.205
	C17H28O3	280.204
	C17H29NO2	279.22
	C17H30O5	314.209
	C17H31NO	265.241
	C17H31NO2	281.236
	C17H31NO5	329.22
	C17H33NO2	283.251
	C17H35NO4	317.257
	C18H31NO5	341.22
	C18H32O3	296.235
	C18H32O5	328.225
	C18H33NO3	311.246
	C18H33NO4	327.241
	C18H34O3	298.251
	C18H34O5	330.241
	C19H32O5	340.225
	C19H33NO5	355.236
	C19H33NO6	371.231
	C19H34O4	326.246
	C19H36O3	312.267
	C19H36O4	328.262
	C20H29NO4	347.21
	C20H35NO3	337.262
	C20H38O5	358.272
	C21H38O3	338.282
	C21H38O5	370.272
	C21H40O3	340.298
	C21H40O4	356.293

	C21H42O5	374.303
	C22H37NO2	347.283
	C22H38O2	334.287
	C22H40O3	352.298
	C24H31NO2	365.236
CS-OA	C6H11N2	111.092
	C6H13NO	115.1
	C6H13NO3	147.09
	C6H9NO	111.068
	C7H10N	108.081
	C7H10O	110.073
	C7H11N	109.089
	C7H11NO	125.084
	C7H12N	110.097
	C7H12O	112.089
	C7H13N2	125.108
	C7H13NO	127.1
	C7H14O	114.105
	C7H14O3	146.094
	C7H15N	113.121
	C7H15NO	129.115
	C7H15NO2	145.11
	C7H15NO3	161.105
	C7H15NO4	177.1
	C7H16N	114.128
	C7H16O	116.12
	C8H10O	122.073
	C8H12O	124.089
	C8H13N	123.105
	C8H14N	124.113
	C8H14N2	138.116
	C8H14O	126.105

	C8H14O2	142.099
	C8H15NO	141.115
	C8H15NO2	157.11
	C8H16	112.125
	C8H16N	126.128
	C8H16O	128.12
	C8H16O2	144.115
	C8H16O3	160.11
	C8H17N2	141.139
	C8H17NO	143.131
	C8H17NO3	175.121
	C8H17NO4	191.116
	C8H18N	128.144
	C8H18O	130.136
	C8H18O3	162.126
	C9H15N	137.121
	C9H15NO	153.115
	C9H17NO	155.131
	C9H18O3	174.126
	C9H18O4	190.121
	C9H19NO	157.147
	C9H19NO3	189.137
	C9H20O	144.152
	C9H20O2	160.146
	C9H20O3	176.141
	C10H14O3	182.094
	C10H15N2	163.124
	C10H15NO	165.115
	C10H17NO	167.131
	C10H18O	154.136
	C10H19N	153.152
	C10H19NO	169.147

C10H19NO2	185.142
C10H20O	156.152
C10H21NO	171.162
C10H21NO3	203.152
C10H21NO4	219.147
C10H22O	158.167
C11H16O	164.12
C11H18O	166.136
C11H18O2	182.131
C11H18O3	198.126
C11H19N	165.152
C11H19NO	181.147
C11H20O	168.152
C11H20O3	200.141
C11H21N	167.168
C11H21NO	183.162
C11H21NO2	199.157
C11H22O	170.167
C11H23NO3	217.168
C11H23NO4	233.163
C12H18O	178.136
C12H19NO2	209.142
C12H20O2	196.146
C12H20O3	212.141
C12H21NO2	211.157
C12H22O	182.167
C12H23NO	197.178
C12H23NO2	213.173
C12H25NO	199.194
C12H25NO4	247.178
C13H20O	192.152
C13H20O2	208.146

C13H21NO	207.162
C13H21NO2	223.157
C13H22O2	210.162
C13H23NO	209.178
C13H23NO2	225.173
C13H24O	196.183
C13H25NO	211.194
C13H26O3	230.188
C13H26O4	246.183
C13H27NO3	245.199
C14H21NO2	235.157
C14H22O	206.167
C14H22O2	222.162
C14H23NO2	237.173
C14H24O3	240.173
C14H24O3	240.173
C14H25NO2	239.189
C14H27NO2	241.204
C14H29NO3	259.215
C15H22O2	234.162
C15H23NO4	281.163
C15H24O2	236.178
C15H26O3	254.188
C15H27NO	237.209
C15H27NO2	253.204
C15H27NO3	269.199
C15H27NO6	317.184
C15H28O3	256.204
C15H29NO2	255.22
C15H29NO3	271.215
C15H30O3	258.22
C16H27NO3	281.199

	C16H31NO3	285.231
	C17H28O2	264.209
	C17H30O3	282.22
	C18H32O4	312.23
PBOA	C9H16O2	156.115
	C9H17NO2	171.126
	C12H18O2	194.131
	C12H19NO	193.147
	C12H22O5	246.147
	C13H18O4	238.121
	C13H21NO3	239.152
	C13H21NO4	255.147
	C13H23N	193.183
	C14H21NO3	251.152
	C14H22O3	238.157
	C14H22O4	254.152
	C14H23NO3	253.168
	C14H24O6	288.157
	C14H26O5	274.178
	C14H29NO4	275.21
	C15H20O4	264.136
	C15H22O4	266.152
	C15H23NO2	249.173
	C15H23NO3	265.168
	C15H25NO	235.194
	C15H26O	222.198
	C15H26O4	270.183
	C16H22O3	262.157
	C16H24O3	264.173
	C16H26O4	282.183
	C16H27NO	249.209
	C16H30O3	270.22

	C16H30O3	270.22
	C17H22O4	290.152
	C17H25NO3	291.184
	C17H25NO4	307.178
	C17H27NO4	309.194
	C18H24O4	304.168
	C18H26O4	306.183
	C18H27NO5	337.189
	C18H28O4	308.199
	C18H29NO2	291.22
	C18H30O2	278.225
	C18H30O3	294.22
	C18H30O4	310.215
	C18H32O7	360.215
	C19H24O5	332.162
	C19H28O3	304.204
	C19H28O4	320.199
	C19H30O3	306.22
	C19H30O4	322.215
	C19H31NO2	305.236
	C19H32O3	308.235
	C19H33NO2	307.251
	C19H34O6	358.236
	C19H34O7	374.231
	C20H26O5	346.178
	C20H30O5	350.209
	C20H31NO4	349.225
	C20H33NO3	335.246
	C20H34O6	370.236
	C20H35NO2	321.267
	C21H30O5	362.209
	C21H34O2	318.256

	C21H34O4	350.246
	C21H44O5	376.319
	C22H34O3	346.251
	C22H36O2	332.272
	C22H37NO3	363.278
	C22H39NO2	349.298
	C23H38O3	362.282
MABB	C4H7NO4	133.038
	C4H9NO3	119.058
	C5H10O3	118.063
	C5H11NO3	133.074
	C5H11NO4	149.069
	C5H12O3	120.079
	C5H7NO6	177.027
	C5H9NO2	115.063
	C5H9NO3	131.058
	C5H9NO4	147.053
	C6H10O2	114.068
	C6H10O3	130.063
	C6H11NO2	129.079
	C6H11NO3	145.074
	C6H11NO4	161.069
	C6H11NO5	177.064
	C6H12O2	116.084
	C6H12O3	132.079
	C6H12O4	148.074
	C6H13NO2	131.095
	C6H14O2	118.099
	C6H14O3	134.094
	C6H5NO4	155.022
	C6H6O2	110.037
	C6H7NO8	221.017

	C6H8O2	112.052
	C6H9NO2	127.063
	C7H10O2	126.068
	C7H11NO2	141.079
	C7H12O2	128.084
	C7H13NO3	159.09
	C7H13NO4	175.085
	C7H13NO5	191.079
	C7H14O2	130.099
	C7H16O2	132.115
	C7H16O3	148.11
	C7H5NO3	151.027
	C7H5NO4	167.022
	C7H5NO5	183.017
	C7H6O4	154.027
	C7H7NO5	185.032
	C7H7NO8	233.017
	C7H8O6	188.032
	C7H9NO2	139.063
	C7H9NO3	155.058
	C8H10O2	138.068
	C8H13NO2	155.095
	C8H15NO3	173.105
	C8H15NO6	221.09
	C8H18O2	146.131
	C8H6O4	166.027
	C8H7NO6	213.027
	C8H8O4	168.042
	C8H9NO	135.068
	C8H9NO7	231.038
	C9H10O8	246.038
	C9H11NO7	245.054

C9H11NO8	261.048
C9H13NO2	167.095
C9H15NO2	169.11
C9H15NO3	185.105
C9H17NO5	219.111
C9H18O2	158.131
C9H19NO5	221.126
C9H6O6	210.016
C9H7NO4	193.038
C9H7NO5	209.032
C9H8O7	228.027
C9H9NO6	227.043
C10H10O9	274.032
C10H11NO3	193.074
C10H11NO8	273.048
C10H11NO9	289.043
C10H12O2	164.084
C10H12O9	276.048
C10H14O2	166.099
C10H15NO2	181.11
C10H17NO2	183.126
C10H17NO3	199.121
C10H17NO4	215.116
C10H19NO4	217.131
C10H19NO5	233.126
C10H20O3	188.141
C10H9NO6	239.043
C10H9NO7	255.038
C11H11NO7	269.054
C11H13NO3	207.09
C11H13NO8	287.064
C11H14O2	178.099

C11H16O2	180.115	
C11H17NO3	211.121	
C11H17NO4	227.116	
C11H19NO4	229.131	
C11H21NO5	247.142	
C11H9NO7	267.038	
C11H9NO8	283.033	
C12H11NO6	265.059	
C12H17NO5	255.111	
C12H19NO3	225.137	
C12H19NO4	241.131	
C12H19NO5	257.126	
C12H21NO4	243.147	
C12H21NO5	259.142	
C12H21NO6	275.137	
C13H13NO7	295.069	
C13H19NO3	237.137	
C14H11NO9	337.043	
C14H15NO10	357.07	
C14H17NO11	375.08	
C14H19NO10	361.101	
C14H19NO11	377.096	
C15H15NO10	369.07	
C15H21NO3	263.152	
BSOA	C3H5NO4	119.022
	C4H5NO4	131.022
	C4H6O4	118.027
	C4H6O5	134.022
	C4H7NO5	149.032
	C5H6O3	114.032
	C5H6O4	130.027
	C5H7NO4	145.038

C5H8O5	148.037
C6H5NO2	123.032
C6H7NO4	157.038
C7H10O6	190.048
C7H11NO5	189.064
C7H11NO7	221.054
C7H8O7	204.027
C8H11NO7	233.054
C8H12O5	188.069
C8H9NO4	183.053
C9H12O6	216.063
C9H13NO5	215.079
C9H13NO6	231.074
C9H13NO7	247.069
C9H14O5	202.084
C9H8O5	196.037
C9H8O6	212.032
C10H10O5	210.053
C10H10O6	226.048
C10H14O6	230.079
C10H15NO7	261.085
C10H16O5	216.1
C10H16O6	232.095
C11H17NO5	243.111
C11H17NO6	259.106
C11H17NO7	275.101
C11H18O5	230.115
C11H19NO7	277.116
C11H9NO5	235.048
C12H11NO5	249.064
C12H17NO7	287.101
C12H18O5	242.115

C12H18O6	258.11
C12H19NO6	273.121
C12H19NO7	289.116
C12H20O5	244.131
C13H13NO5	263.079
C13H15NO5	265.095
C13H19NO6	285.121
C13H20O5	256.131
C13H20O7	288.121
C13H22O6	274.142
C14H20O6	284.126
C14H22O5	270.147
C14H22O6	286.142
C14H23NO4	269.163
C14H24O5	272.162
C14H25NO5	287.173
C15H21NO7	327.132
C15H22O6	298.142
C15H22O7	314.137
C15H23NO10	377.132
C15H23NO5	297.158
C15H23NO6	313.153
C15H23NO7	329.148
C15H23NO9	361.137
C15H24O5	284.162
C15H24O7	316.152
C15H25NO5	299.173
C15H25NO6	315.168
C15H25NO7	331.163
C15H26O5	286.178
C15H28O5	288.194
C16H15NO5	301.095

	C16H17NO5	303.111
	C16H19NO5	305.126
	C16H24O10	376.137
	C16H24O5	296.162
	C16H24O6	312.157
	C16H24O7	328.152
	C16H26O5	298.178
	C17H24O7	340.152
	C17H25NO8	371.158
	C17H26O5	310.178
	C17H27NO5	325.189
	C17H27NO6	341.184
	C17H27NO7	357.179
	C17H29NO5	327.205
	C18H20O4	300.136
	C18H23NO3	301.168
	C18H26O3	290.188
	C18H26O5	322.178
	C18H27NO7	369.179
	C18H28O5	324.194
	C18H28O7	356.184
	C18H28O8	372.179
	C18H29NO6	355.2
	C18H29NO7	371.195
	C18H30O5	326.209
	C19H21NO5	343.142
	C19H23NO5	345.158
	C19H25NO5	347.173
	C19H28O6	352.189
	C19H28O7	368.184
	C21H26O4	342.183
SOOA	C5H7NO3	129.043

	C6H4O3	124.016
	C6H7NO2	125.048
	C6H8O4	144.042
	C7H10O4	158.058
	C7H10O5	174.053
	C7H11NO4	173.069
	C7H12O4	160.074
	C7H12O5	176.069
	C7H2O5	165.99
	C7H8O4	156.042
	C8H10O4	170.058
	C8H10O5	186.053
	C8H12O3	156.079
	C8H12O4	172.074
	C8H13NO4	187.085
	C8H13NO6	219.074
	C8H14O4	174.089
	C8H14O5	190.084
	C9H11NO5	213.064
	C9H12O4	184.074
	C9H12O5	200.069
	C9H14O3	170.094
	C9H14O4	186.089
	C9H14O6	218.079
	C9H15NO4	201.1
	C9H15NO6	233.09
	C9H16O4	188.105
	C9H16O5	204.1
	C10H14O4	198.089
	C10H14O5	214.084
	C10H16O4	200.105
	C10H17NO6	247.106

C10H18O5	218.115
C11H16O4	212.105
C11H16O5	228.1
C11H18O4	214.121
C12H16O3	208.11
C12H20O4	228.136
C13H18O3	222.126
C13H20O4	240.136

C14H18O3	234.126
C14H19NO5	281.126
C14H20O3	236.141
C15H20O3	248.141
C15H22O3	250.157
C16H24O2	248.178
C16H25NO4	295.178
C16H26O2	250.193