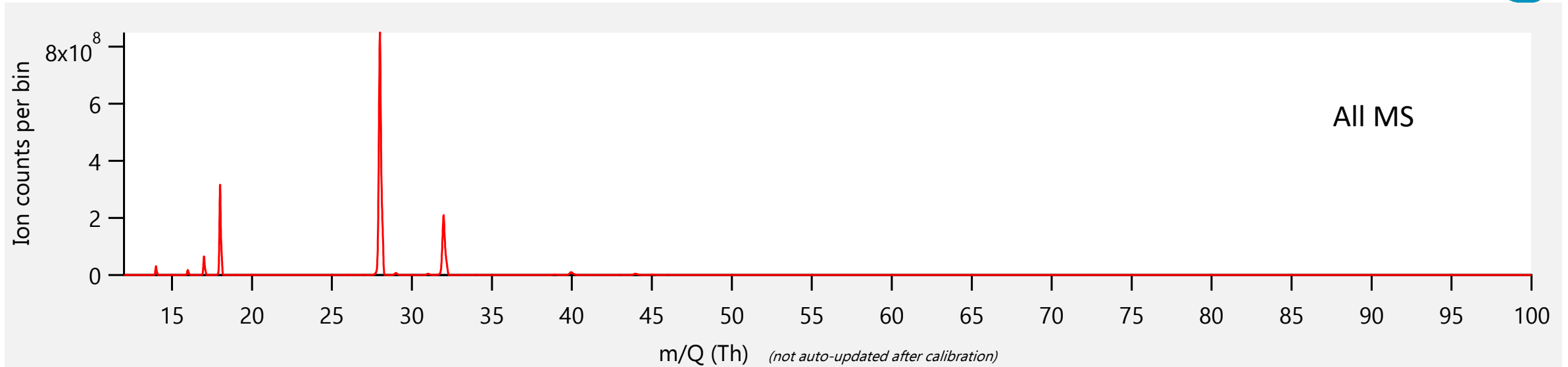
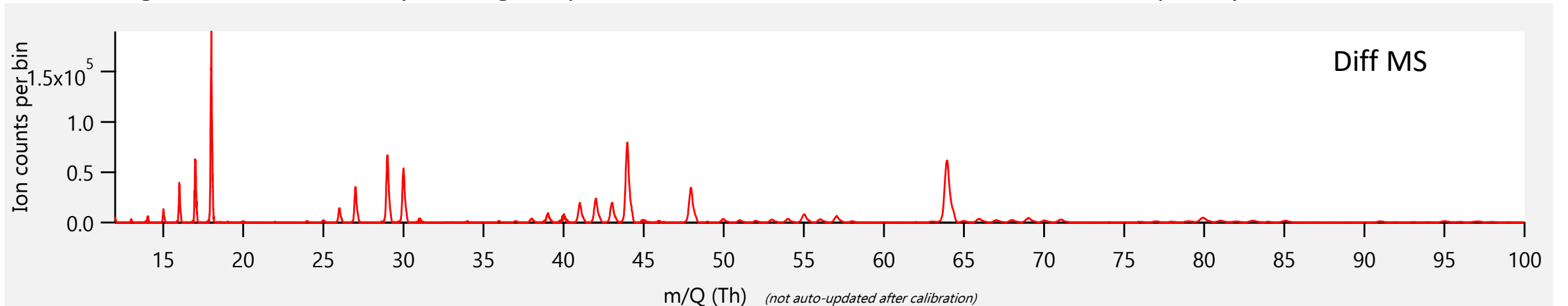


ACSM Settings/Frag
Frag Table, Species Table
Frag pattern diagnostics
Frag based analysis
Fragment time series

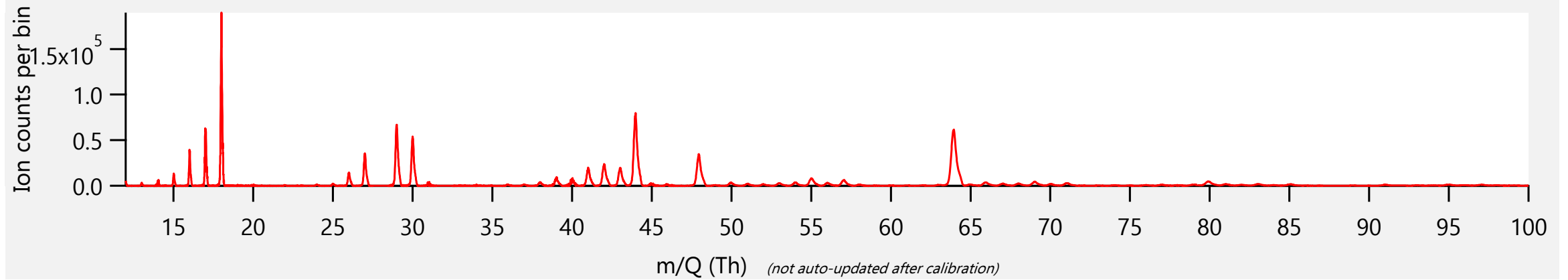
Dominant peaks in MS are gas-phase H₂O, N₂ and O₂



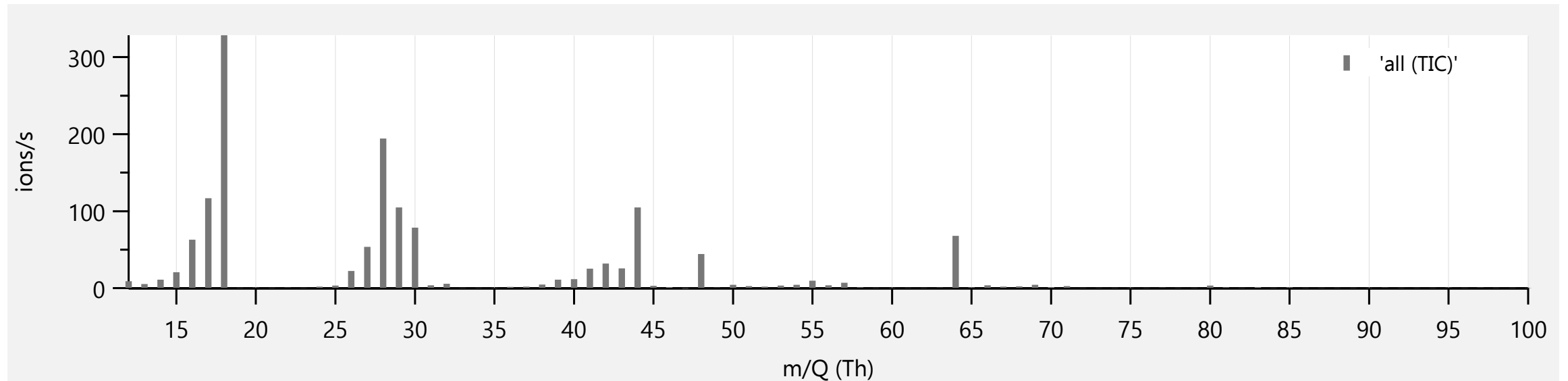
Subtracting filter MS from sample MS gives particle MS. Unlike AMS, air is subtracted completely.



Raw MS



Integrate each peak → Stick MS



Use Frag Table to assign signal at each m/Q to a particular species. Note that this is simpler than the AMS frag table because we do not have to remove gas-phase contributions via frag table. However, we still set Org[28]=Org[44] because Diff signal at 44 is very noisy due to high background of gas-phase CO₂.



ACSM settings

Calibr.
Switching
Diags
Frag

Show species table
Show frag table

Frag pattern diagnostics

Make plot
NH4 meas vs pred

Frag based analysis

Make plot
Org f44 vs f43

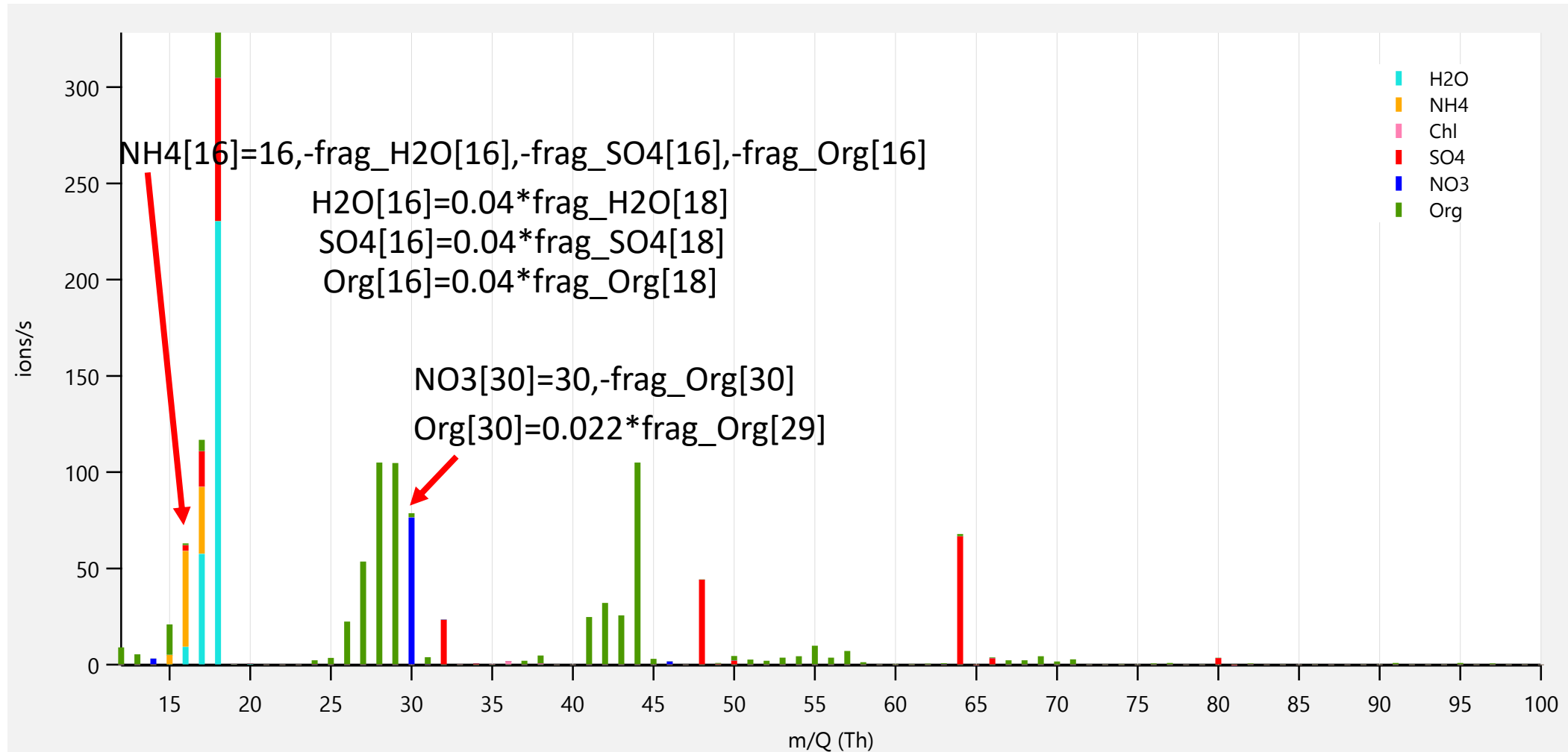
Fragment Time Series

Plot
m/Q 44
Org
☒ Fractional?

R0		1						
m/Q	Org	NO3	SO4	Chl	NH4	H2O	K	m/Q
12	12							12
13	13							13
14		0.04*frag_NO3[30],0.04*frag_NO3[46]						14
15	15,-frag_NH4[15]				0.1*frag_NH4[16]			15
16	0.04*frag_Org[18]		0.04*frag_SO4[18]		16,-frag_H2O[16],-frag_SO4[16],-frag_Org[16]	0.04*frag_H2O[18]		16
17	0.25*frag_Org[18]		0.25*frag_SO4[18]		17,-frag_H2O[17],-frag_SO4[17],-frag_Org[17]	0.25*frag_H2O[18]		17
18	0.225*frag_Org[44]		0.67*frag_SO4[64],0.67*frag_SO4[48],-			18,-frag_SO4[18],-frag_Org[18]		18
19	0.000691*frag_Org[18]		0.000691*frag_SO4[18],0.002*frag_SO			0.000691*frag_H2O[18],0.002*frag_H2O[17]		19
20	0.002*frag_Org[18]		0.002*frag_SO4[18]			0.002*frag_H2O[18]		20
21								21
22								22
23								23
24	24,-frag_SO4[24]		0.005*frag_SO4[48]					24
25	25							25
26	26							26
27	27							27
28	frag_Org[44]							28
29	29							29
30	0.022*frag_Org[29]	30,-frag_Org[30]						30
31	31,-frag_NO3[31]	0.00405*frag_NO3[30]						31
32		0.002*frag_NO3[30]	0.21*frag_SO4[48],0.21*frag_SO4[64],-					32
33			0.0079*frag_SO4[32]					33
34			0.022*frag_SO4[32]					34
35				35				35
36				36				36
37	37,-frag_Ch[37]			0.323*frag_Ch[35]				37
38	38,-frag_Ch[38],-frag			0.323*frag_Ch[36]				38
39							39	39
40								40
41	41,-frag_K[41]						0.0722*frag_K[39]	41
42	42							42
43	43							43
44	44							44

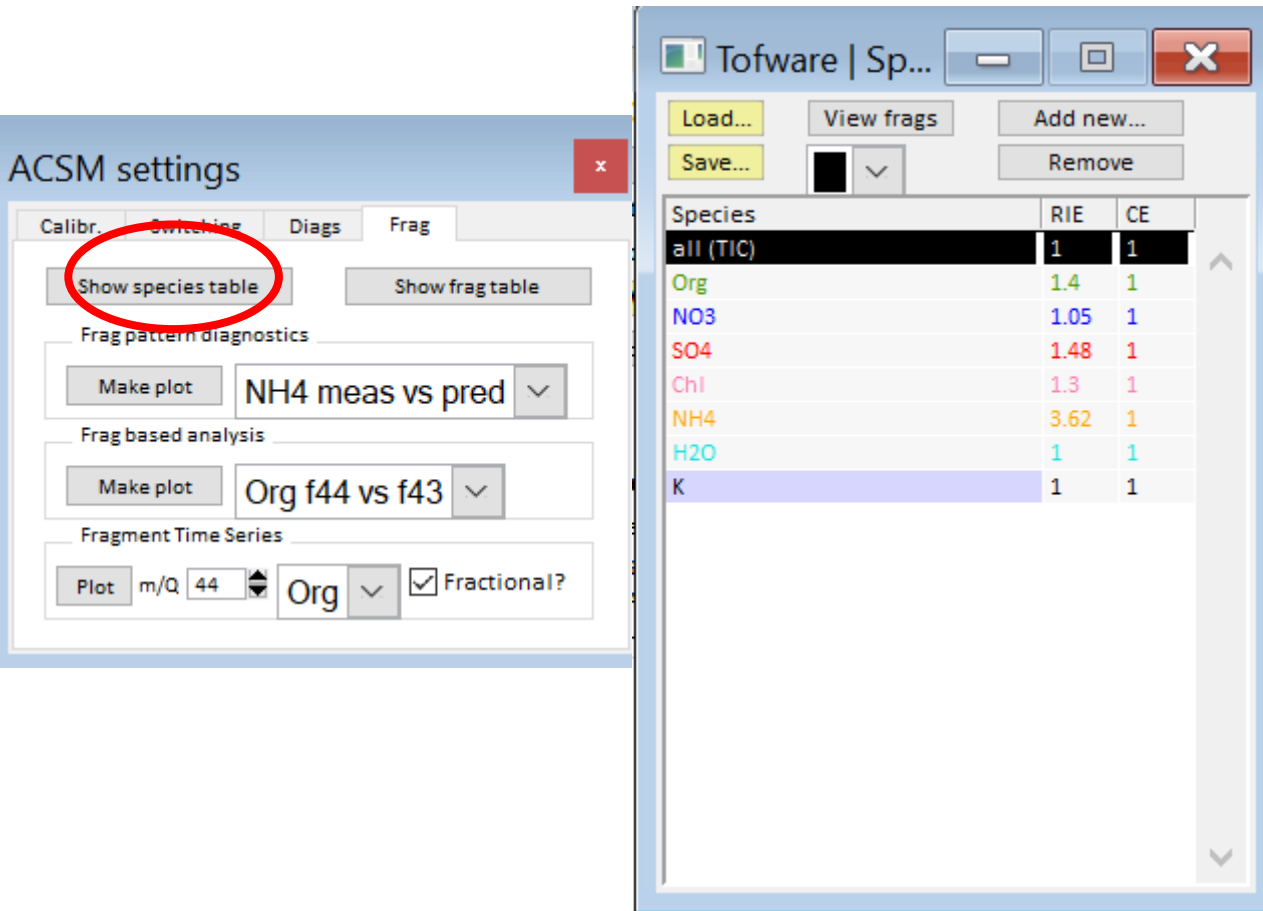
Applying the Frag Table: For example, diff signal at m/Q 16 gets distributed among NH₄, H₂O, SO₄ and Org, and diff signal at m/Q 30 gets distributed among NO₃ and Org.

Frag table is based on many AMS ambient data sets. Might not apply to laboratory experiments!



Applying the Species Table

Sorted ions into different species. Now need to convert to mass loading using the RIE's for each species → Species (or batch) Table

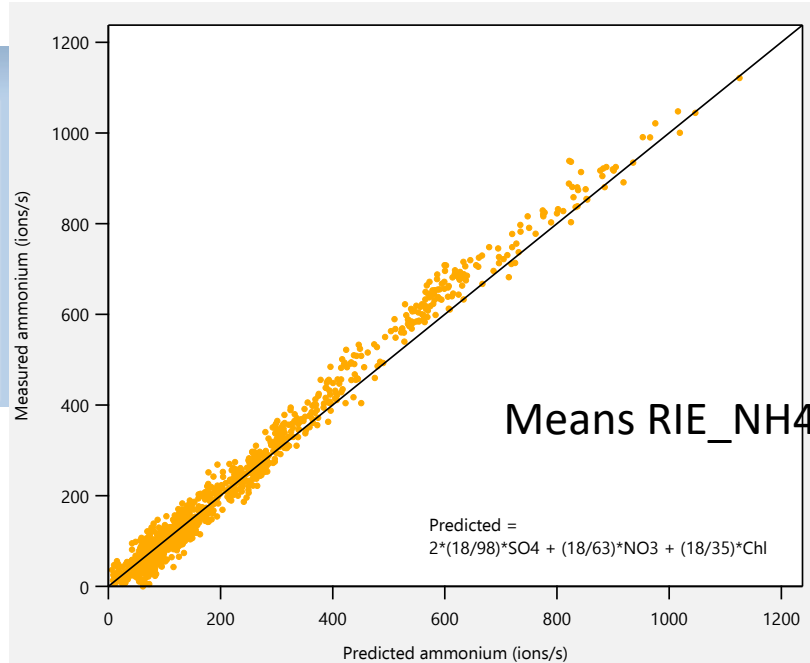
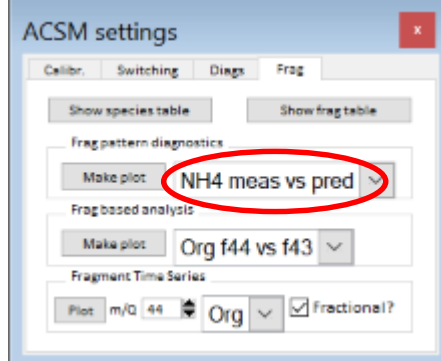


The image shows two windows from the Tofware software. The 'ACSM settings' window on the left has tabs for 'Calibr.', 'Switching', 'Diags', and 'Frag'. The 'Frag' tab is selected, and the 'Show species table' button is circled in red. Below this are sections for 'Frag pattern diagnostics', 'Frag based analysis', and 'Fragment Time Series'. The 'Tofware | Sp...' window on the right displays a table of species with their respective RIE and CE values.

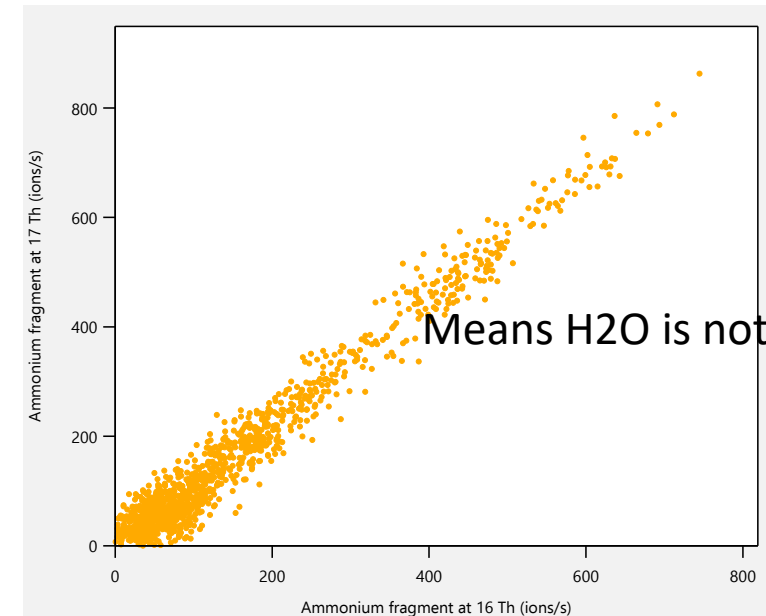
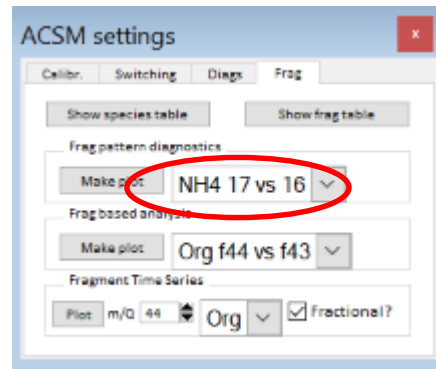
Species	RIE	CE
all (TIC)	1	1
Org	1.4	1
NO3	1.05	1
SO4	1.48	1
Chl	1.3	1
NH4	3.62	1
H2O	1	1
K	1	1

- RIE for each species
 - New in Acquility 2.3.1/Tofware 2.5.13: RIE_NH4 and RIE_SO4 are imported from datafiles.
 - RIE_Org, RIE_ChI are defaults.
- CE should be the same for all species!
 - ~0.5 for ambient with standard vaporizer
 - ~1 for ambient with capture vaporizer
 - Composition dependent collection efficiency (CDCE) for ambient (Middlebrook et al., 2012) for standard vaporizer
 - Laboratory experiments – measure for your experiment!
- You can Save the species and frag table for loading into another experiment.
- When you close tofware, whatever is in this table will be saved as the default for the next time you start tofware.

Fragmentation Diagnostics: These were developed as checks for the AMS fragmentation table. For example, org44 vs org43 going through the origin confirms that air contributions were being subtracted correctly. Subtracting air is not relevant for the ACSM, but frag table diagnostics are still useful.

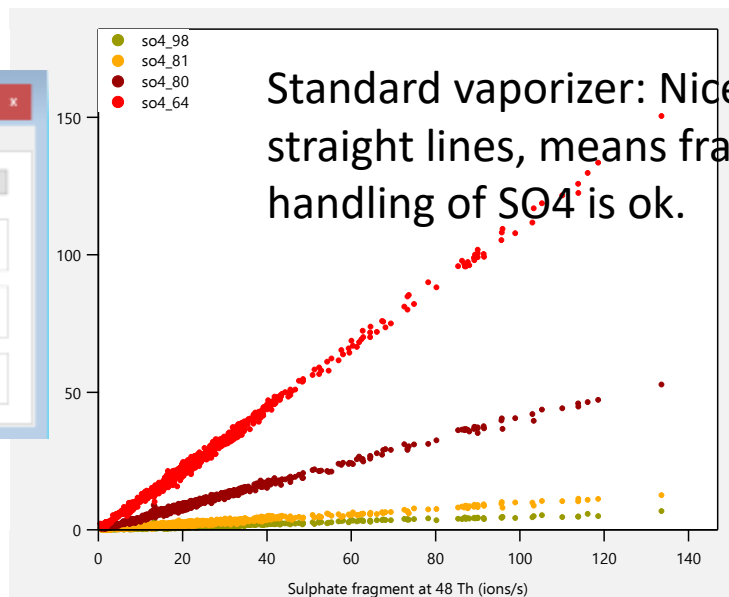
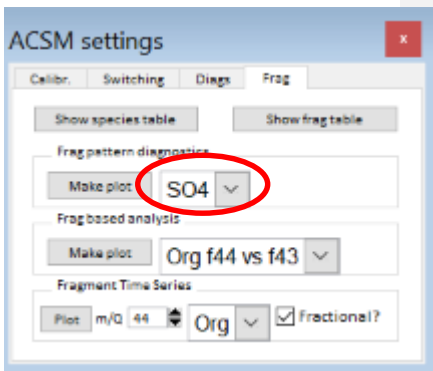


Means RIE_NH4, RIE_SO4 ok.

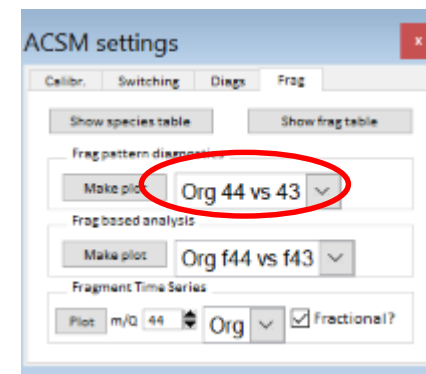
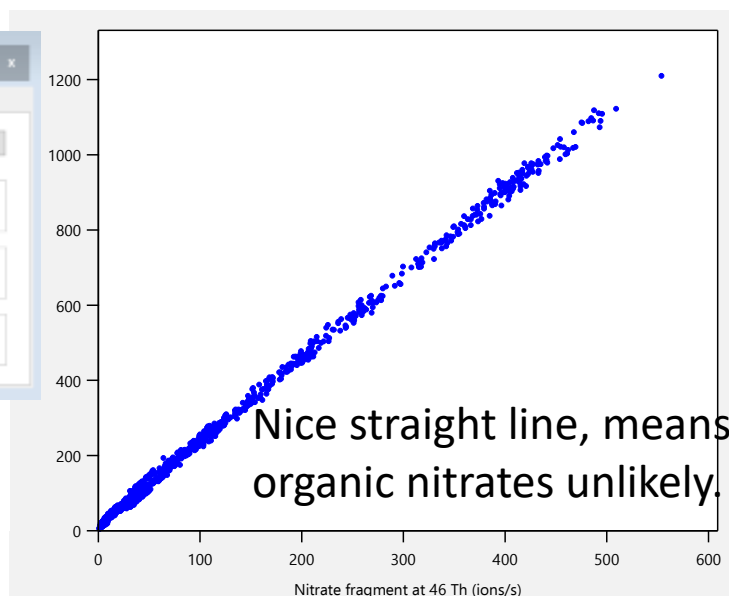
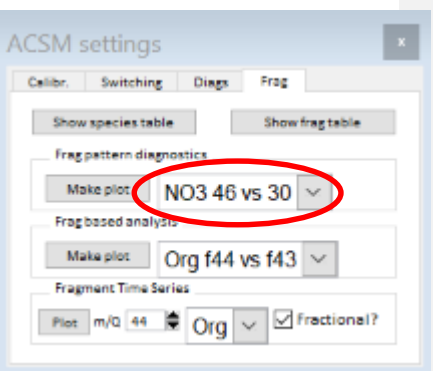
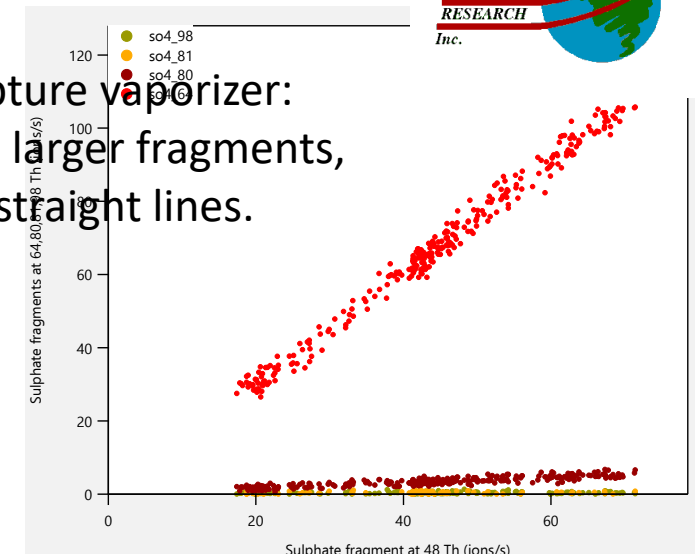


Means H2O is not interfering with NH4.

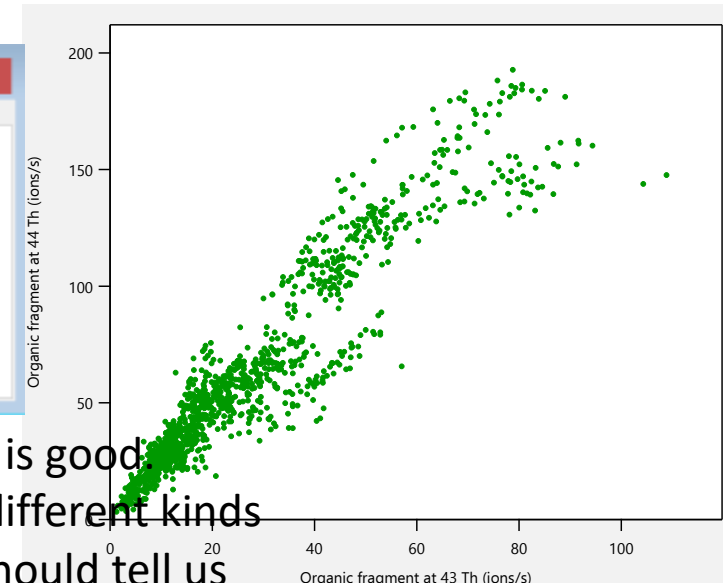
Frag pattern diagnostics (cont.)



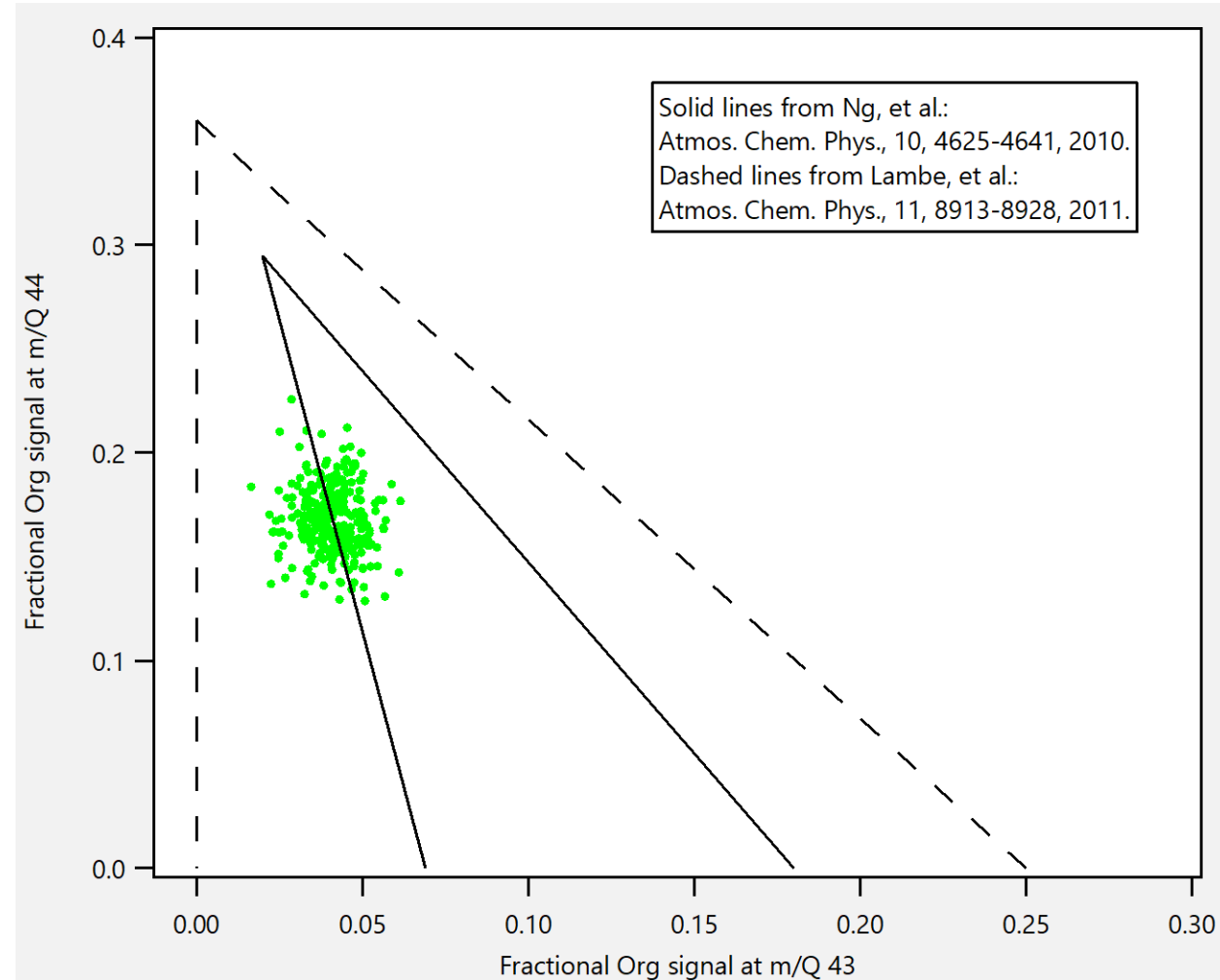
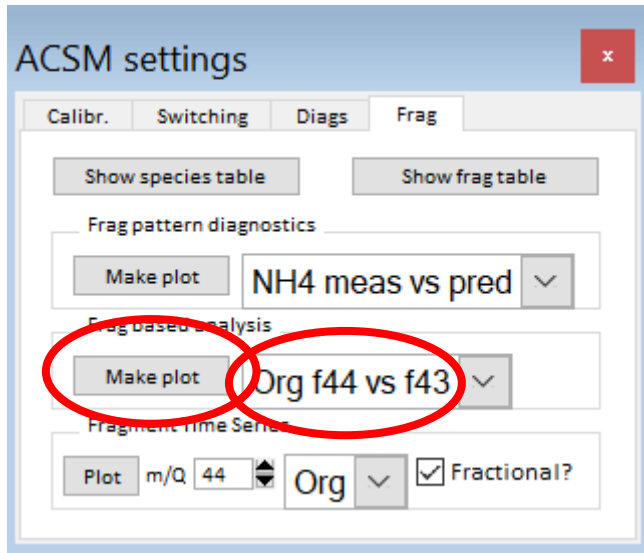
SO4 with Capture vaporizer:
Less signal at larger fragments,
but still nice straight lines.



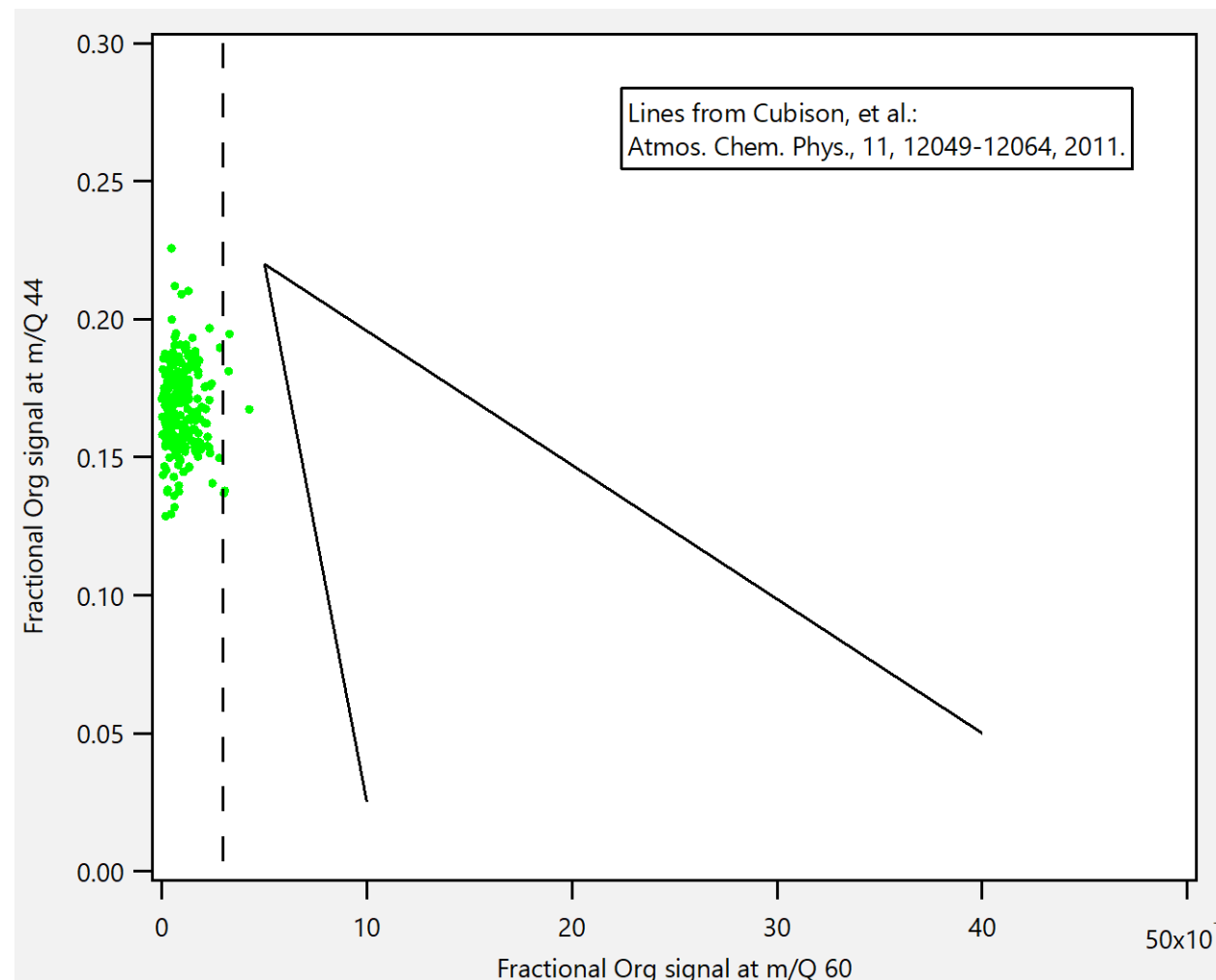
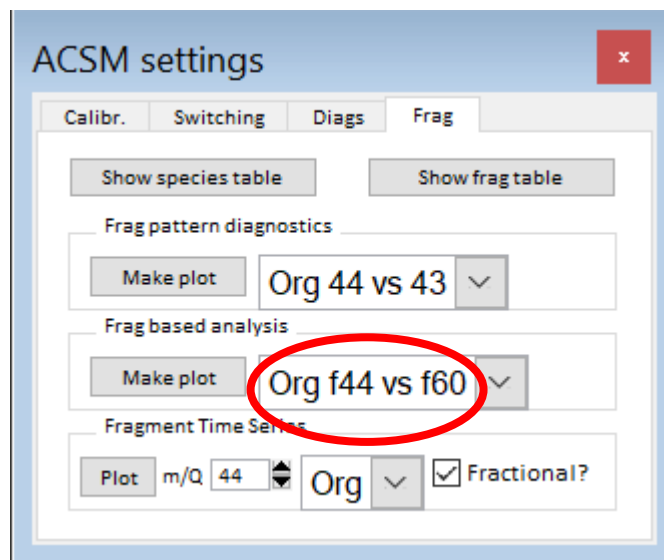
Going through origin is good.
Scatter means have different kinds
of organics → PMF should tell us
something.



Frag based analysis



f44 (i.e., signal at m/Q 44 over total organics) is indicative of oxygenated organics and f43 is indicative of hydrocarbon-like organics. Typically, ambient falls inside solid triangle, but this is capture vaporizer which causes more thermal decomposition and therefore more 44 than standard vaporizer.



f60 is indicative of levoglucosan from biomass burning. If you had biomass burning contribution, then points should fall inside the solid lines.

ACSM settings

Calibr. Switching Diags **Frag**

Show species table Show frag table

Frag pattern diagnostics

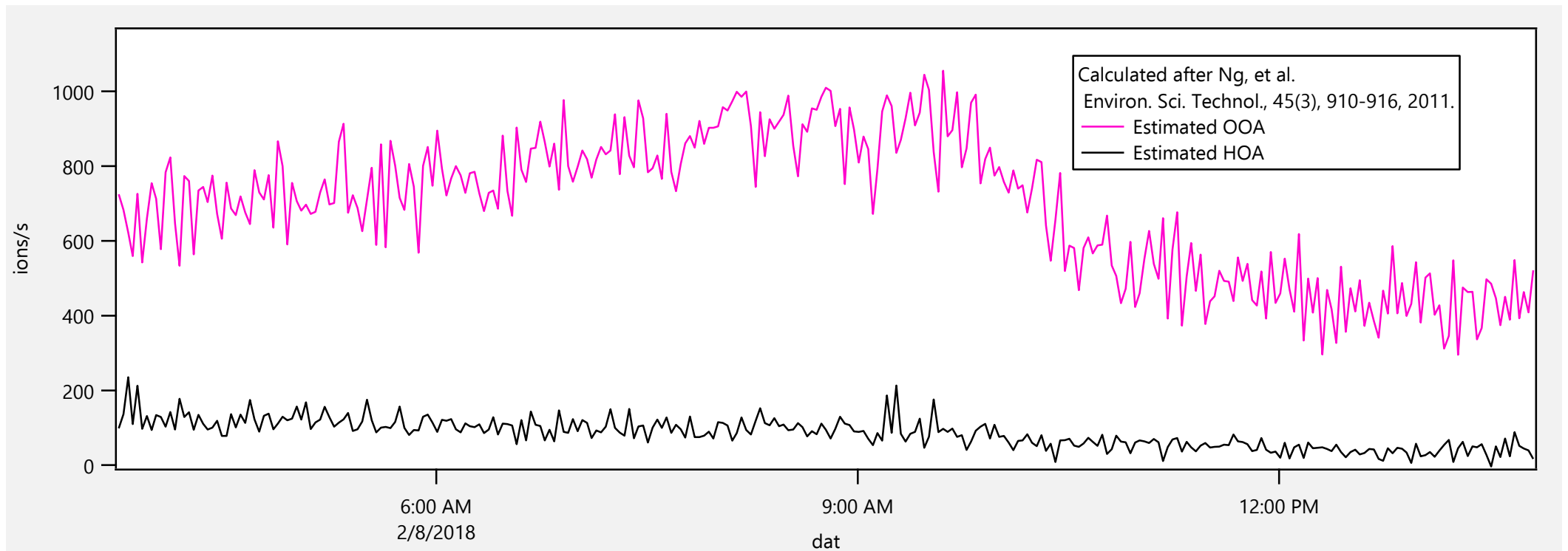
Make plot Org 44 vs 43

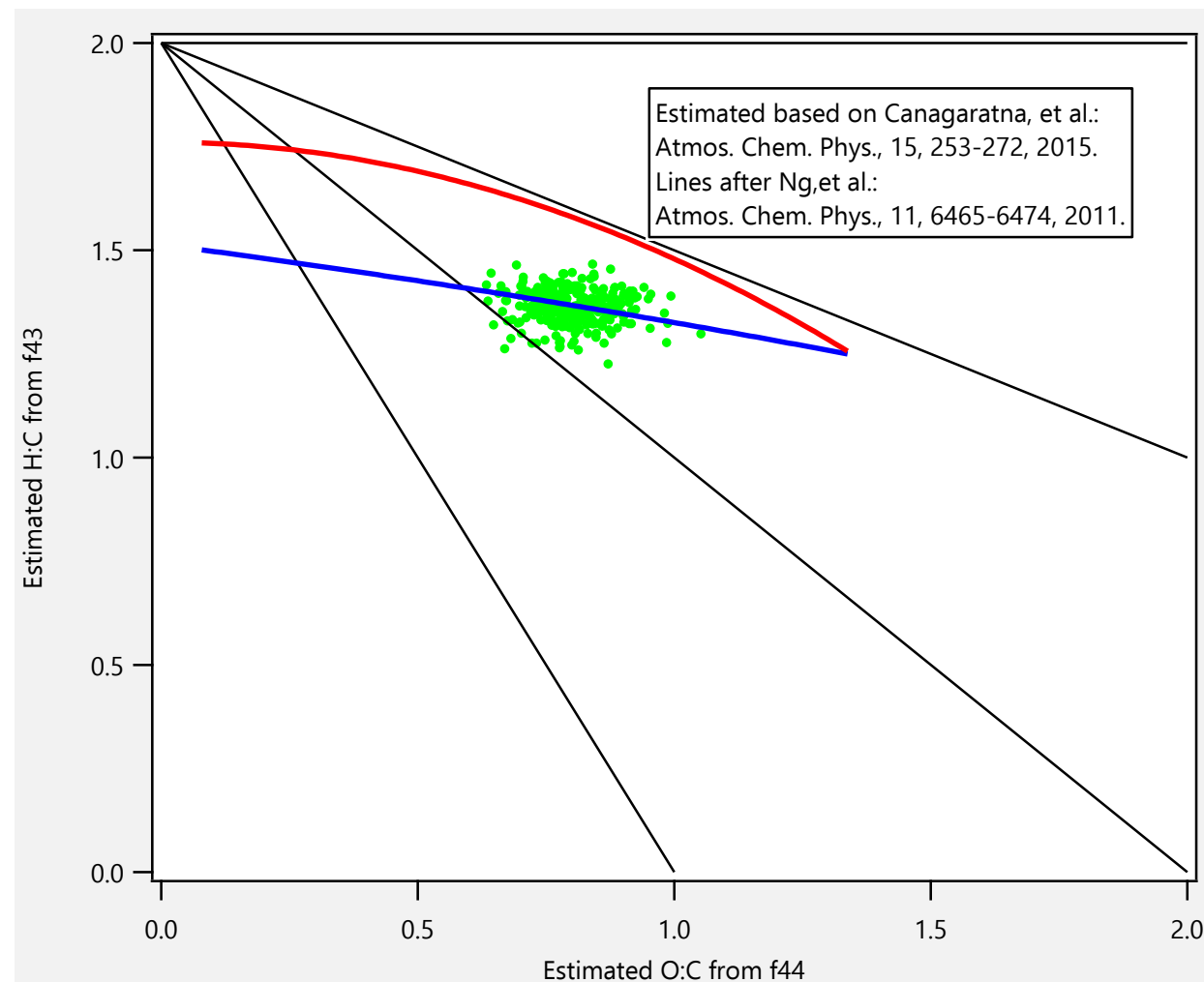
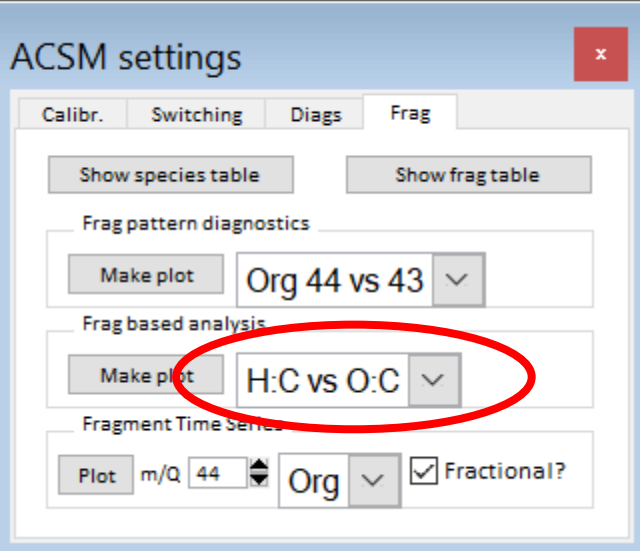
Frag based analysis

Make plot **Poor Person's PMF**

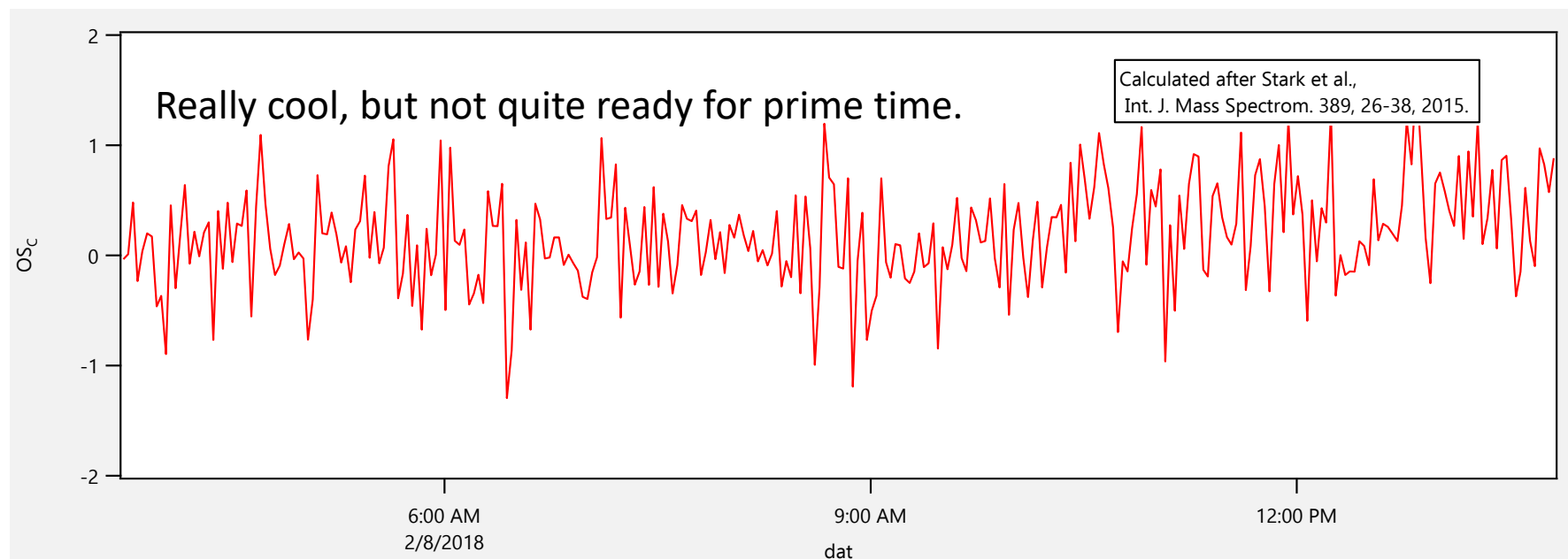
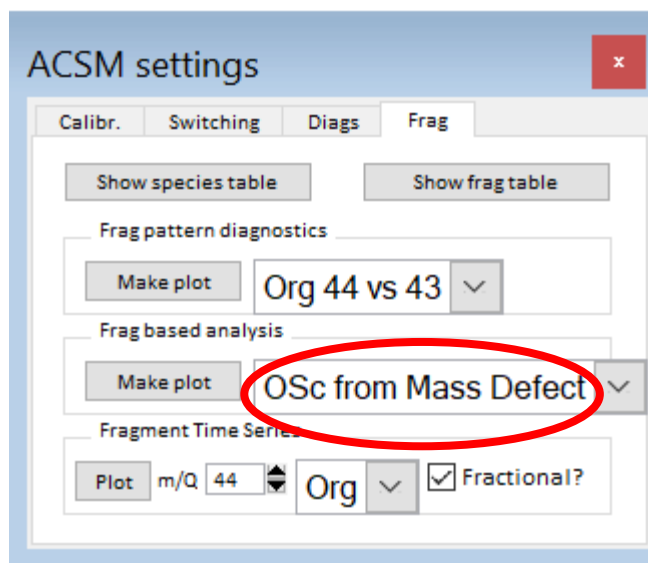
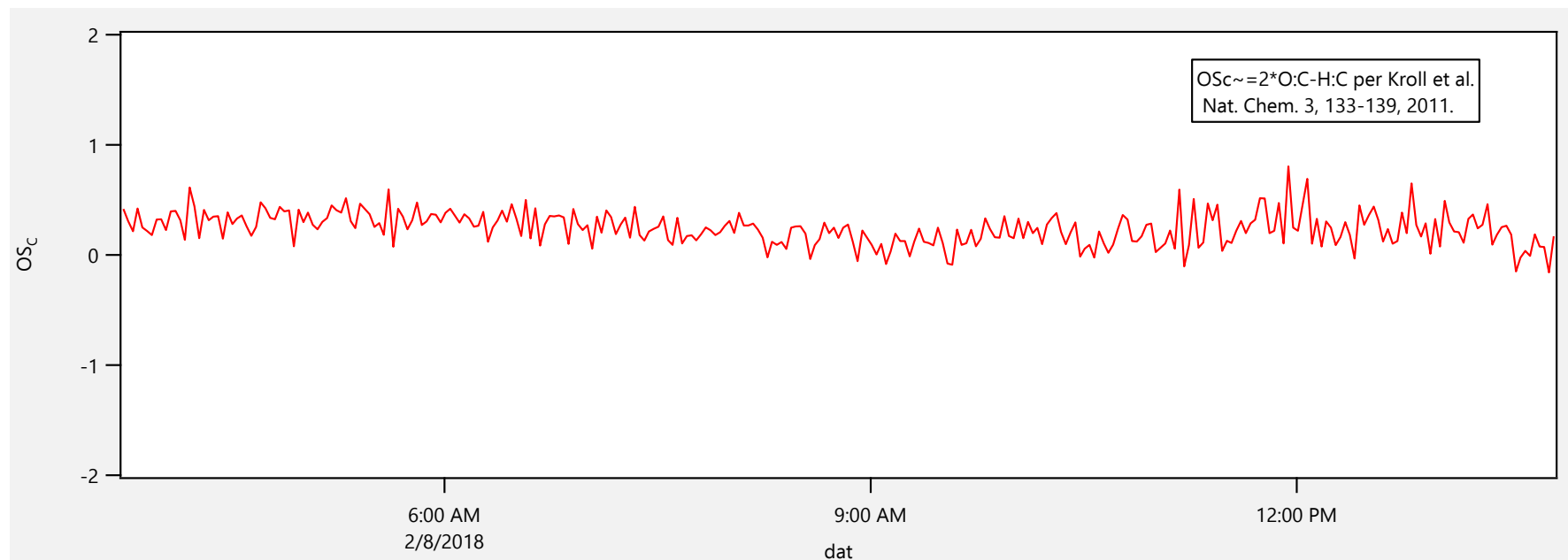
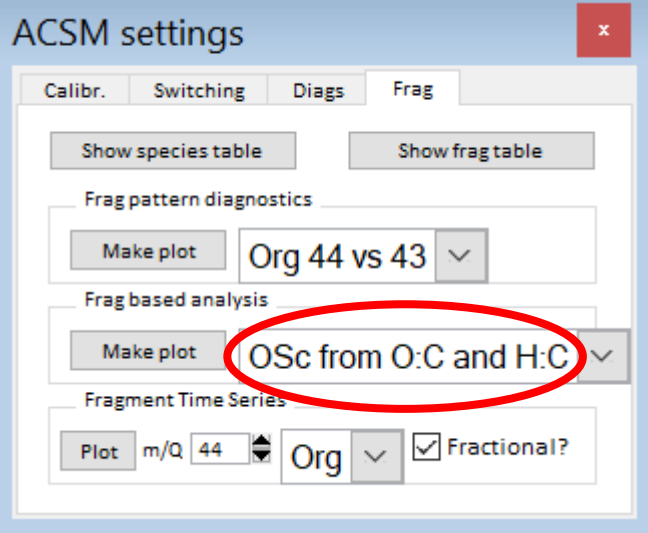
Fragment Time Series

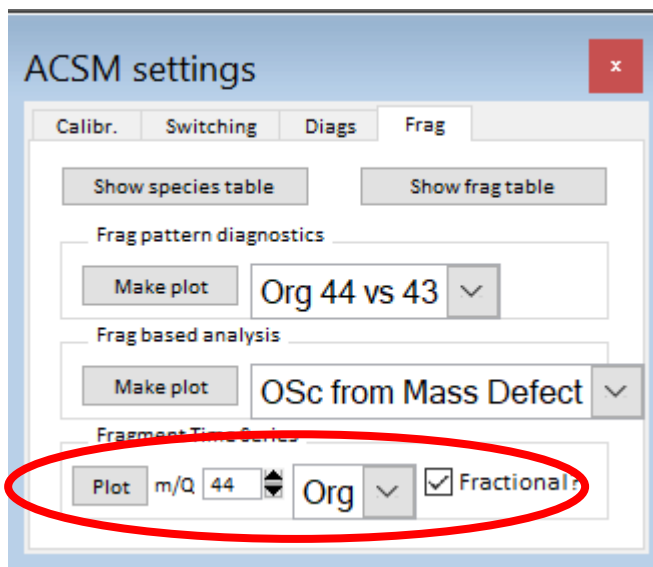
Plot m/Q 44 Org ☒ Fractional?



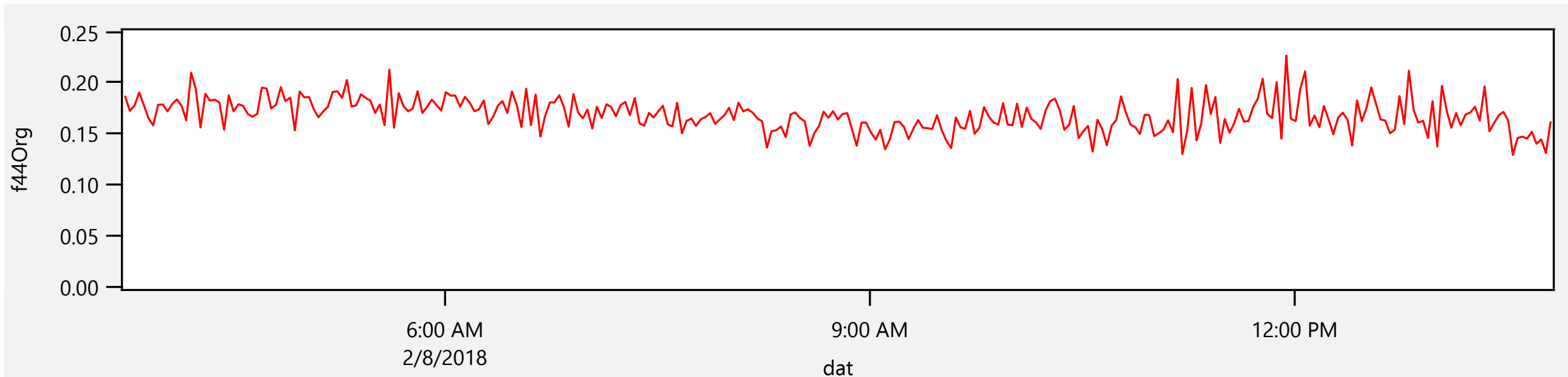


Ambient data should fall inside colored lines, but this is capture vaporizer. Also, this is using UMR parameterization from Canagaratna et al. 2015, which increases both O:C and H:C, while lines are from older parameterization.





This part of the panel allows you to plot an m/Q after it has been pushed through the frag table, either as a ratio to the species (this slide) or as a time series (next slide).



ACSM settings

Calibr. Switching Diags **Frag**

Show species table Show frag table

Frag pattern diagnostics

Make plot Org 44 vs 43

Frag based analysis

Make plot OSc from Mass Defect

Fragment Time Series

Plot m/Q 30 Org ☐ Fractional?

