

Tofware 3 for TOF-ACSM

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Presented by

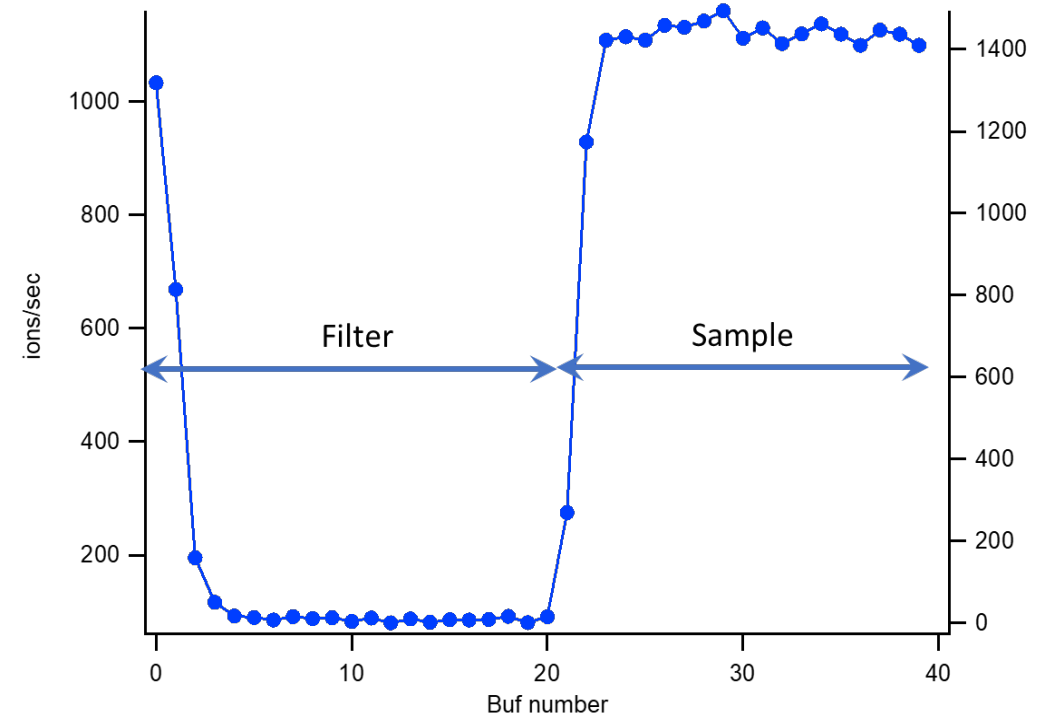
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Tofware 3

- Please upgrade!
 - Aerodyne is not supporting Tofware 2.5.13.
 - Tofware 2 has known bugs.
- Download Tofware 3.2.40208 from the Knowledge Base (support.aerodyne.com). Send an email to cacc-support@aerodyne.com if you need access.
 - Search for KA-01180
- Runs under Igor 7 or Igor 8 (but not Igor 6).
 - Windows or Macintosh operating system, except Catalina!
- Igor Licenses: We deliver the TOF-ACSM with a 1-seat license to run Acquility on the instrument computer and a 3-seat for data analysis by up to 3 people. If you need more licenses, go to www.wavemetrics.com.
- Tofware is proprietary and encrypted.
 - Tofwarelicense*.ibw in C:\Users\Documents\Wavemetrics\Igor Pro X User Files

What is New in Tofware 3? 2 Parts!

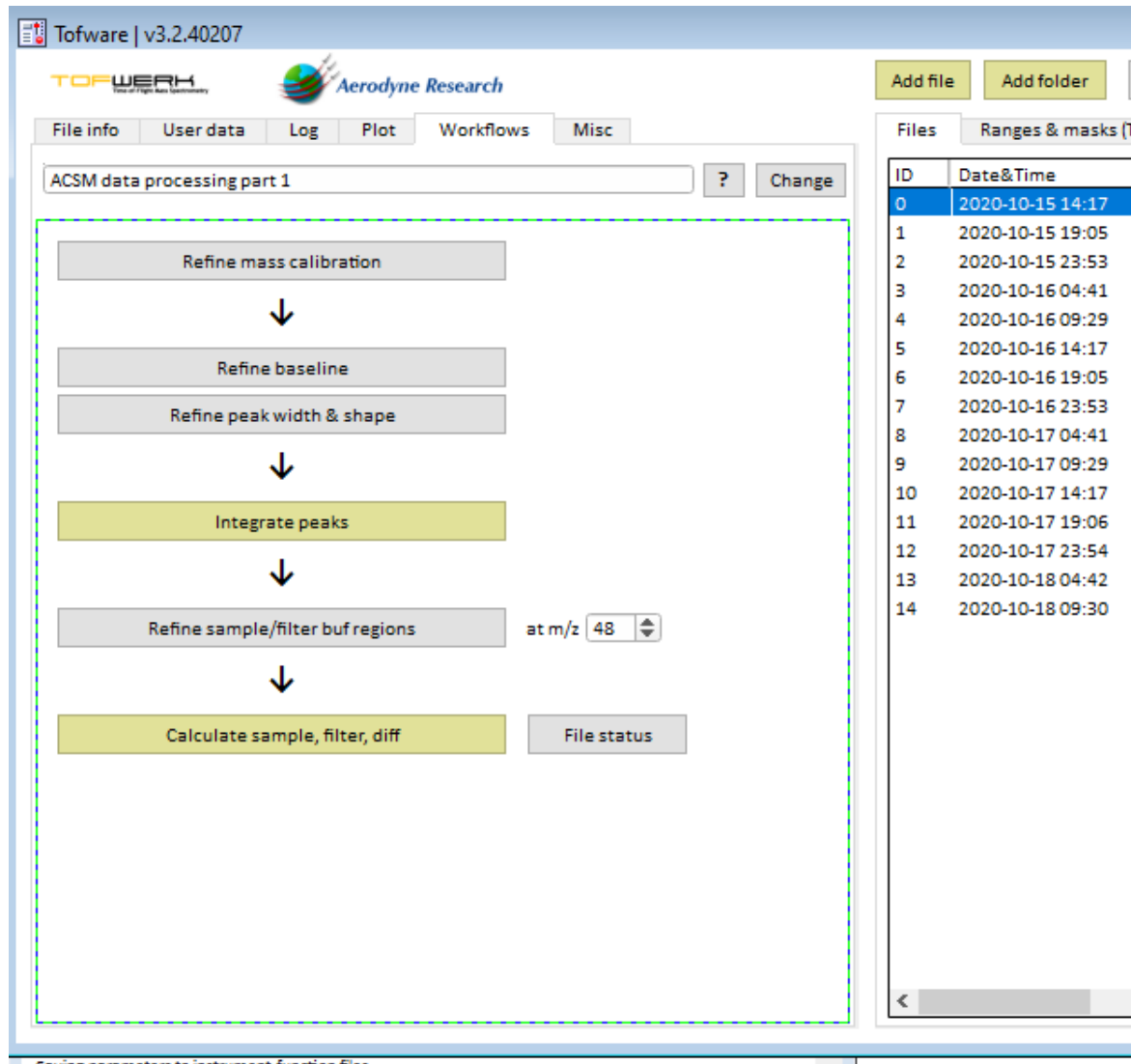
- Big change in indexing between Tofware 2 and Tofware 3 → 2 part analysis
- Part 1 indexes and analyzes 1 sec mass spec data
 - Acquility 2.3.9 – 20 s filter/20 s sample
 - Integrate MS peaks to unit mass resolution (UMR)
 - Calculate diff data



Part 2

- Part 2 indexes and analyzes on sampling time base (40 s, 10 minutes, etc.)
 - Check IE, RIEs and CE (including CDCE), apply AB correction
 - Calculate mass loading in $\mu\text{g}/\text{m}^3$
 - Plot mass spectra
 - Calculate MS and err matrices for PMF
- Concept of Workflows
 - Set of steps for data analysis

Workflow 1



- Yellow buttons are required actions, grey buttons are optional
- Saves _dif files for loading into Workflow 2.

Workflow 2

Tofware | v3.2.40207

TOPWERK Aerodyne Research

File info User data Log Plot Workflows Misc

ACSM data processing part 2 ? Change

☐ Capture Vaporizer?

Airbeam correction, diagnos. and Hz unit conversion

↓

Species & frag diagnostics panel

↓

Composition dependent collection efficiency (CDCE)

↓

Standard analysis plots

↓

Export 2D matrix for PMF/ME-2/SoFi

Results and general plotting options

ACSM data and plotting options

☒ Use ug/m3 units (else ions/s)

☒ Use the airbeam correction (if generated)

☐ Use the CDCE (if generated)

☒ New plot ☐ Append to top plot

Data set

☒ Difference ☐ Sample ☐ Filter

ACSM species and fragments time series plots

Species: Org,NO3,SO4,NH4,ChI,

☐ Calculate, plot errors

> Specialty time series

ACSM average mass spectra plots

Species: Org,NO3,SO4,NH4,ChI,H2O,

The RIE is not applied to species in mass spectral plots.

AB, CDCE file correction status

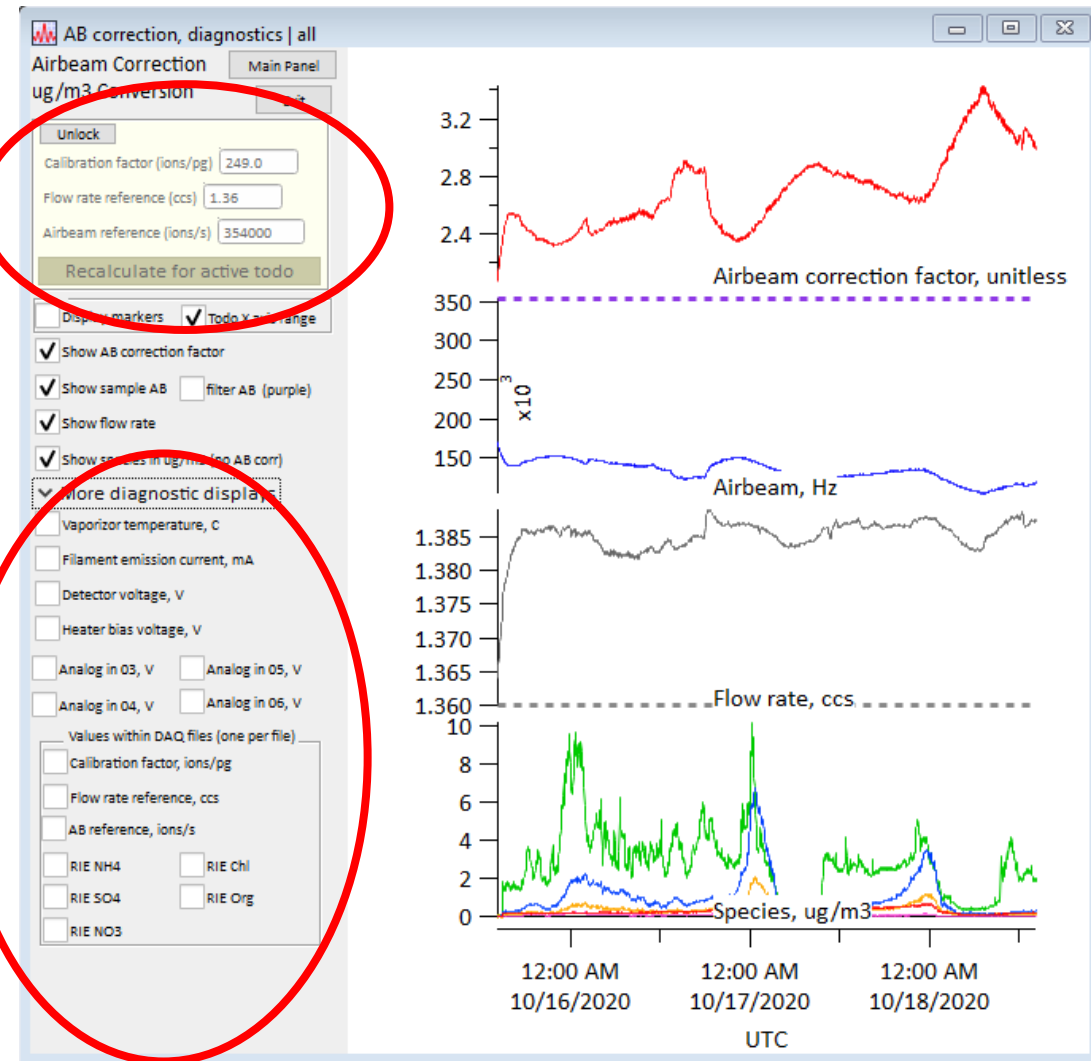
Files Ranges & masks (T

ID	Date&Time
0	2020-10-15 14:17
1	2020-10-15 19:05
2	2020-10-15 23:53
3	2020-10-16 04:41
4	2020-10-16 09:29
5	2020-10-16 14:17
6	2020-10-16 19:05
7	2020-10-16 23:53
8	2020-10-17 04:41
9	2020-10-17 09:29
10	2020-10-17 14:17
11	2020-10-17 19:06
12	2020-10-17 23:54
13	2020-10-18 04:42
14	2020-10-18 09:30

- Yellow buttons are required actions, grey buttons are optional
- Left: Analysis Panels
- Right: Plot time series and mass spectra
- Some analysis options not available for capture vaporizer

Workflow 2: AB Correction Panel

- Loads calibration data from first datafile. Can change if needed.
- Quick access to instrument diagnostics.



Workflow 2: Species and Frag Panel

m/Q	Org	NO3	SO4	Chl	NH4	H2O	K	m/Q
10								10
11								11
12	12							12
13	13							13
14	0.04*frag_NO3[30].0							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].-fra	0.04*frag_H2O[18]		16
17	0.25*frag_Org[18]		0.25*frag_SO4[18]		17.-frag_H2O[17].-fra	0.25*frag_H2O[18]		17
18	0.225*frag_Org[44]		0.67*frag_SO4[64].0			18.-frag_SO4[18].-fra		18
19	0.000691*frag_Org[1]		0.000691*frag_SO4[0.000691*frag_H2O[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[3						31
32		0.002*frag_NO3[30]	0.21*frag_SO4[48].0					32
33			0.0079*frag_SO4[32]					33
34			0.022*frag_SO4[32]					34
35								35

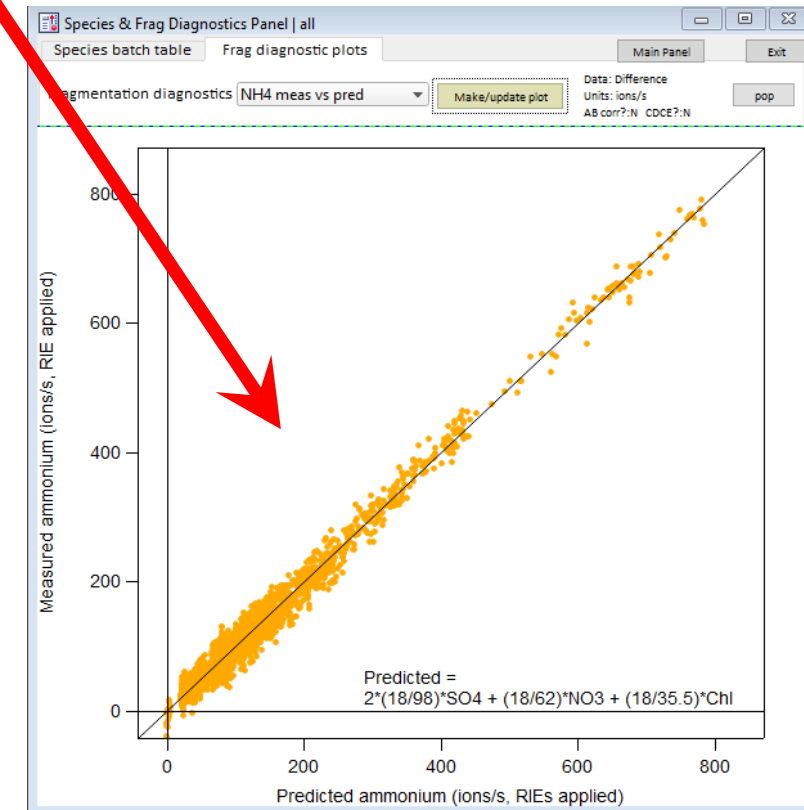
Species & Frag Diagnostics Panel | all

Species batch table **Frag diagnostic plots**

Load from H5 file View frags Add new species

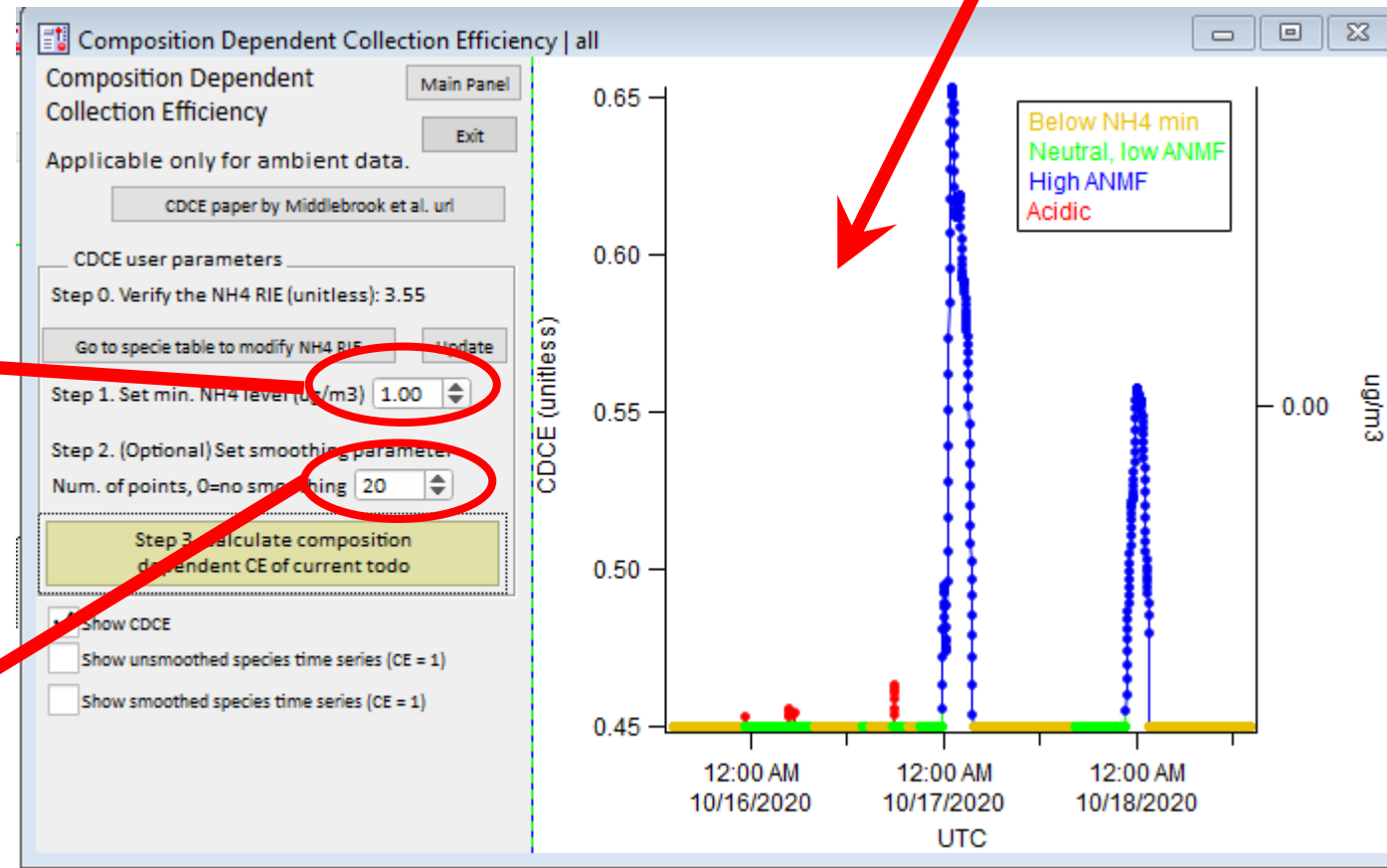
Save to H5 file Remove species

Species	RIE	CE
all (TIC)	1	1
Org	1.4	1
NO3	1.05	1
SO4	0.94	1
Chl	1.3	1
NH4	3.55	1
H2O	1	1
K	1	1

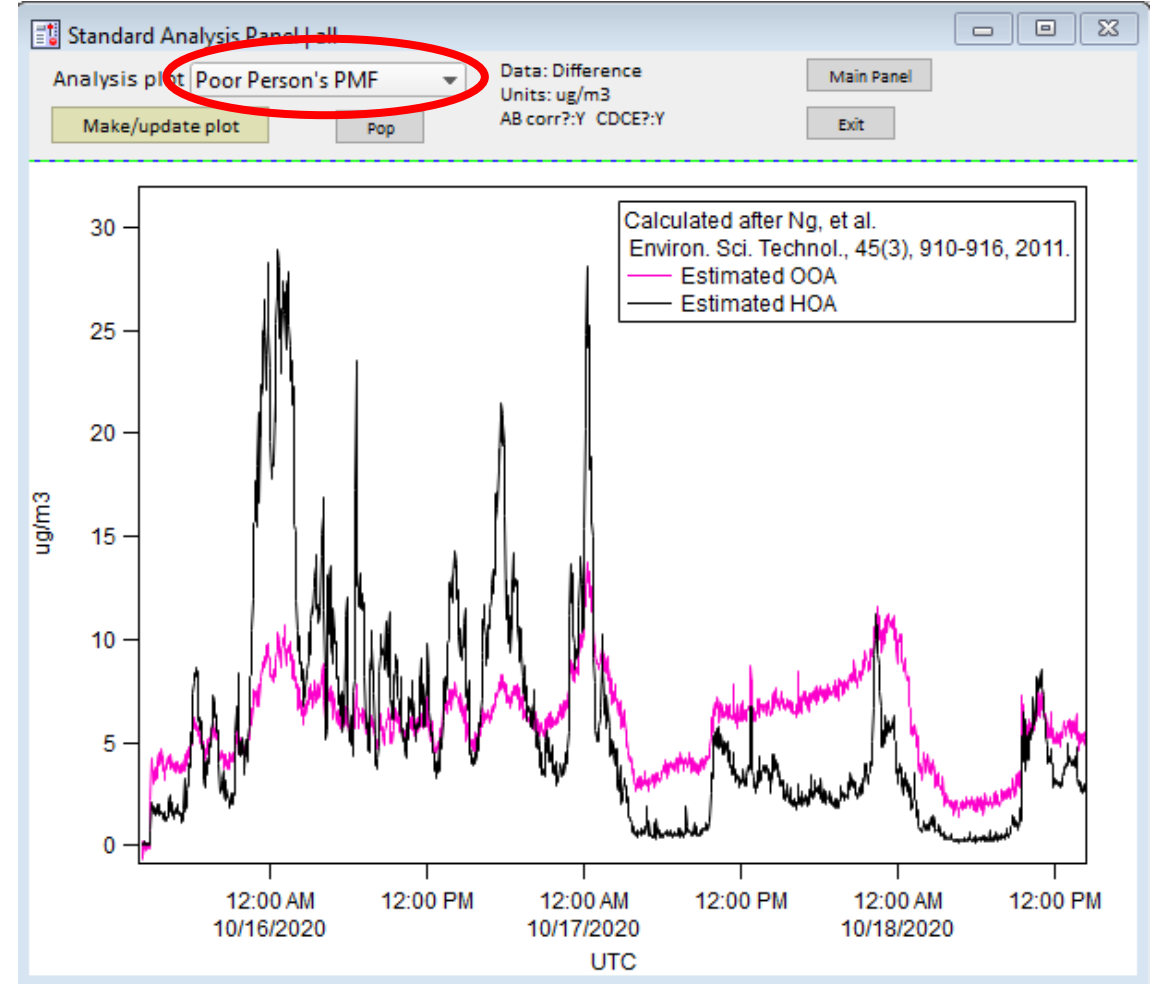
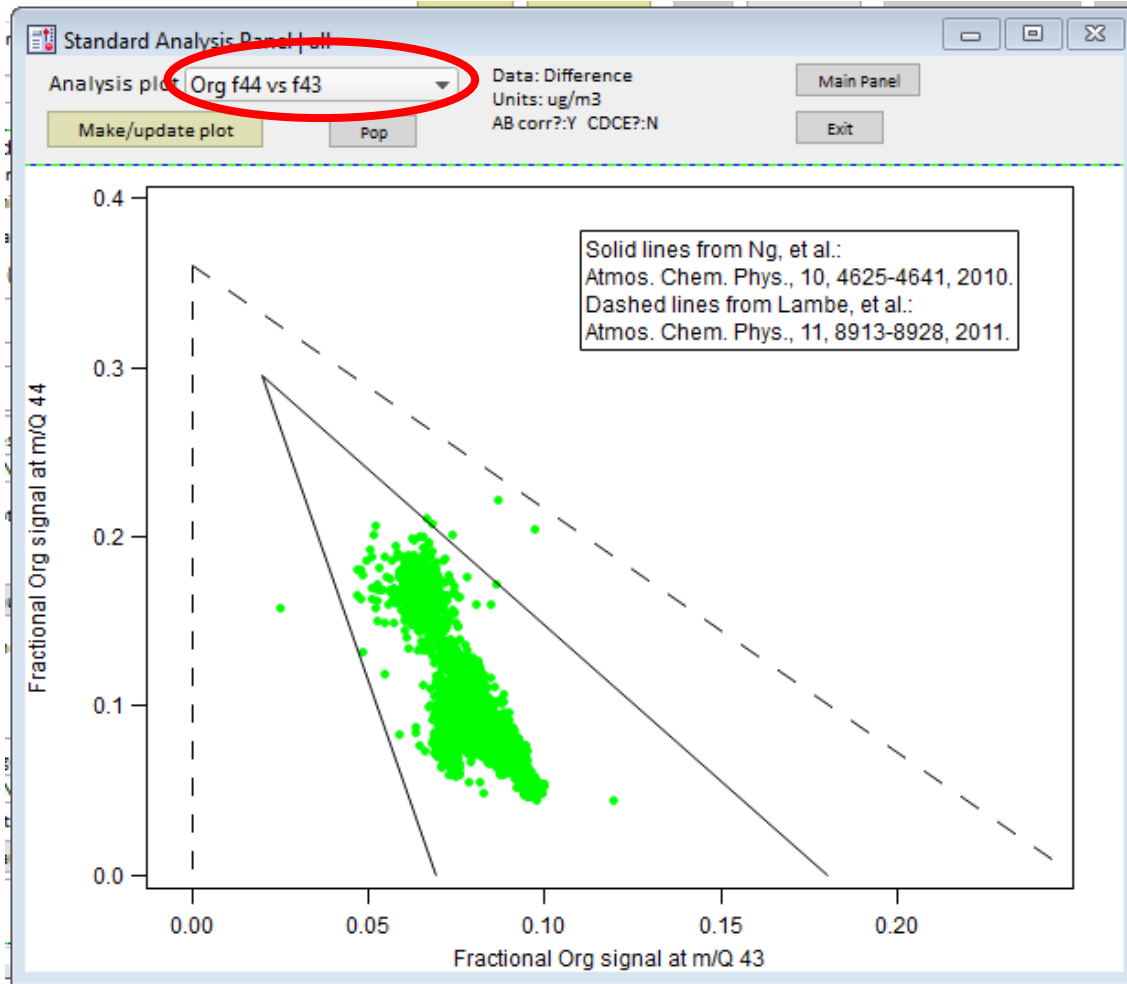


Workflow 2: CDCE Panel (Standard Vaporizer)

- Graph of which factor is controlling CDCE.



Workflow 2: Standard Analysis Plots



Workflow 2: PMF Export

- Improvements to error calculation.
- Using non-baseline subtracted signals for ion counting statistics.
- Electronic noise typically small, and set = 0 as default, but new panel to investigate.
- Please give us feedback!

