PROCEDURE

to plot Mass Spectroscopy and Thermogravimetry data from Netzsch Dispsav and Proteus in Origin software

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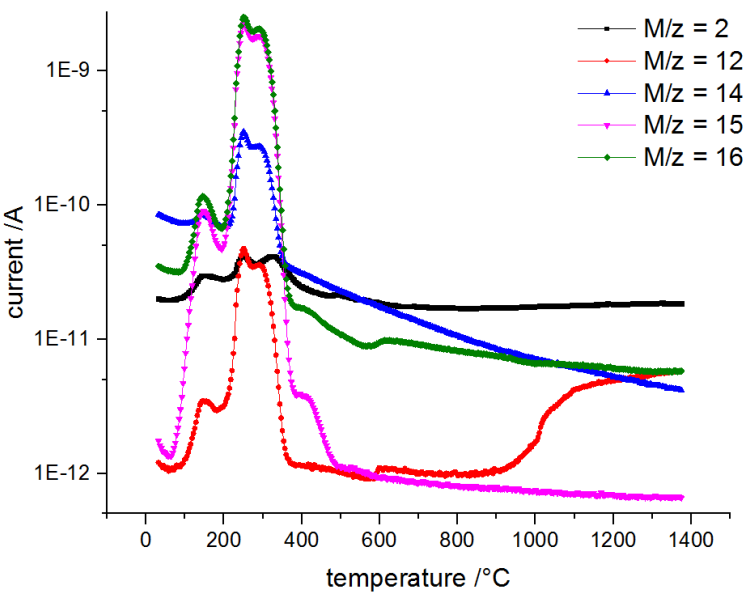
This is a guide to process and plot the mass spectroscopy (MS) and thermo-gravimetry (TG) data recorded from the Netzsch pieces of equipment in Origin 2016 software.[1] This also includes some scripts to automate the process.

The script source files and setup can be found at :

`https://github.com/sylvain-kern/tgmsplot-script`

along with this very procedure in `.pdf` or `.md` formats for user convenience.

[1] Origin 2016 - `https://www.originlab.com/index.aspx?go=PRODUCTS/Origin`

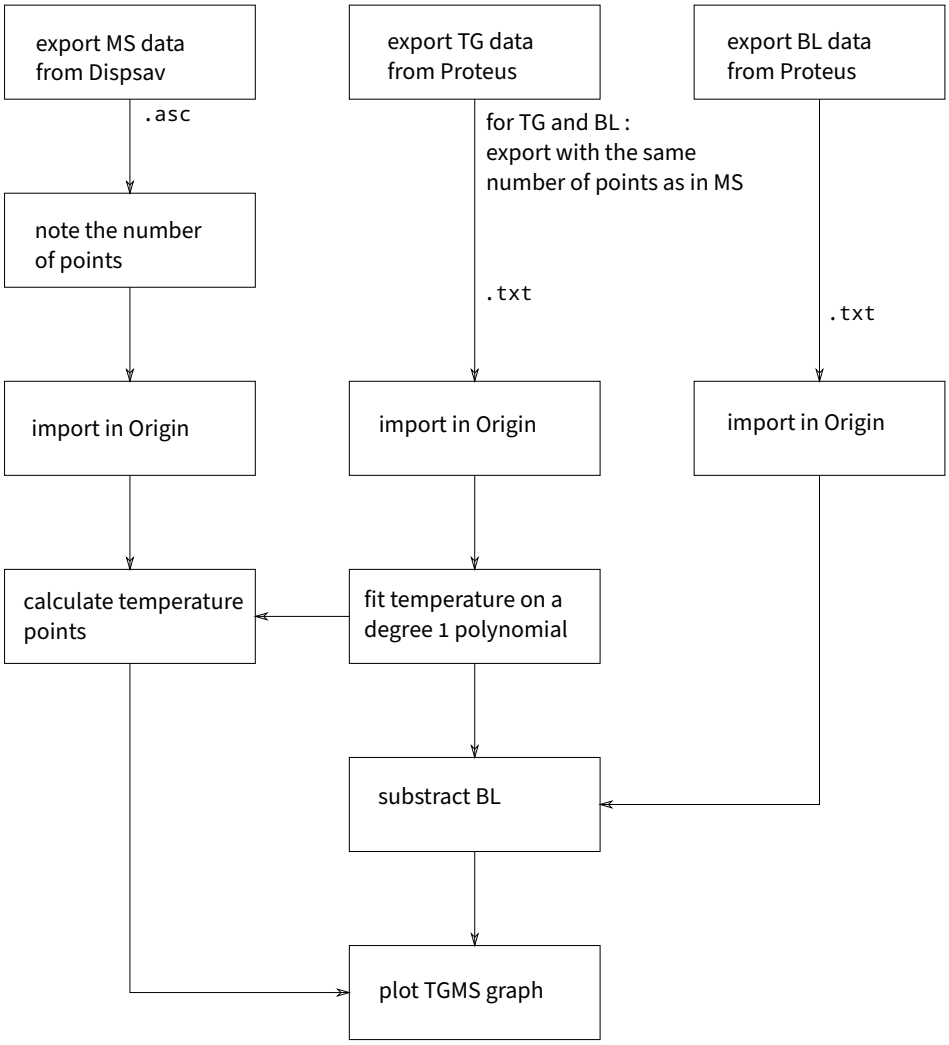


Contents

1 *Manual procedure*

Here is a way to get TGMS plots from data collected in the different Netzsch pieces of software, using Origin.

This is a visual overview of the procedure explained below.



However, this procedure can be quite repetitive, so a script that executes it automatically is presented in section 2.

1.1 *Exports*

1.1.1 *Export MS data from Dispsav*

1. Open Aëolos Dispsav.
2. Go to the `Process` tab, go to `Cycles...` and open the desired `.mdc` .
3. Then go to `File > Convert to ASCII...` .
4. Save the `.asc` file into a chosen folder.
5. Open this `.asc` file with a notepad and note the number of points and the maximum time, which appear in the header lines or in the last line of the two firsts columns.

1.1.2 *Export TG data form Netzsch Proteus*

1. Open Proteus Analysis.
2. Go to `File > Open...` and open the `.ngb-ss1` file of your choice.
3. Then go to `Extras > Export Data...`. Choose the range and number of points[2]. The number of points must be exactly the same as in the `.asc` file exported from Dispsav. Check that the maximum time matches too.

[2] Since the TG and MS experiments have been made at the same time with the same temperature increase, the temperature measurements and the step should match for the MS and TG.

1.1.3 *Export baseline data*

The baseline data is in the same form than the TG data, so the steps are exacly similar than those on the paragraph above. Again, export it with exactly the same number of points and maximum time as in the MS.

1.2 *Imports in Origin*

The data treatments will be executed on Origin software. To continue, open Origin.

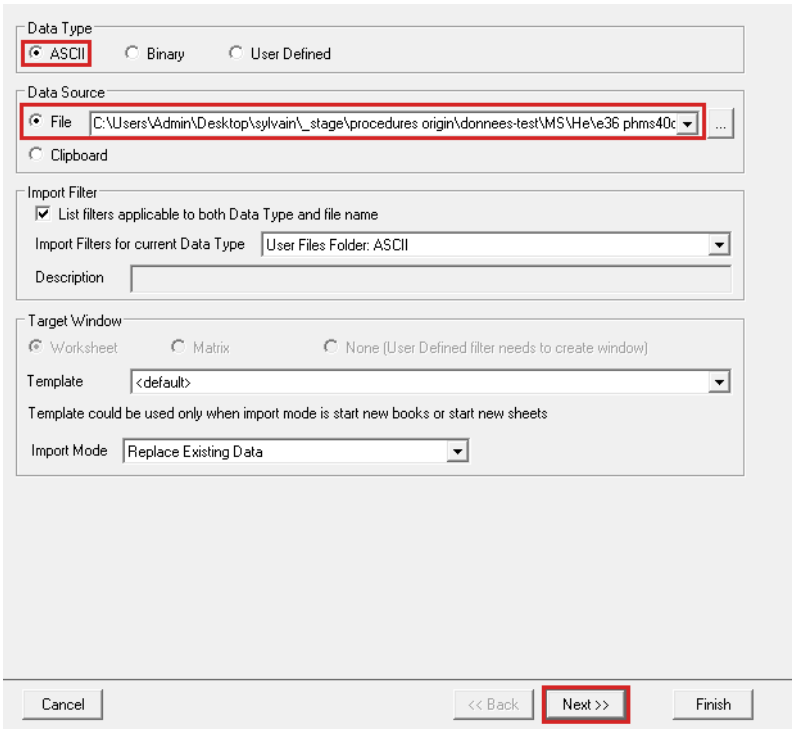
This procedure has been made using Origin 2016 version 93E. The software may differ a bit if you use more recent versions of the software. For more help, see Origin's user guide: `www.originlab.com/doc/User-Guide`

1.2.1 *Import MS data in ASCII format*

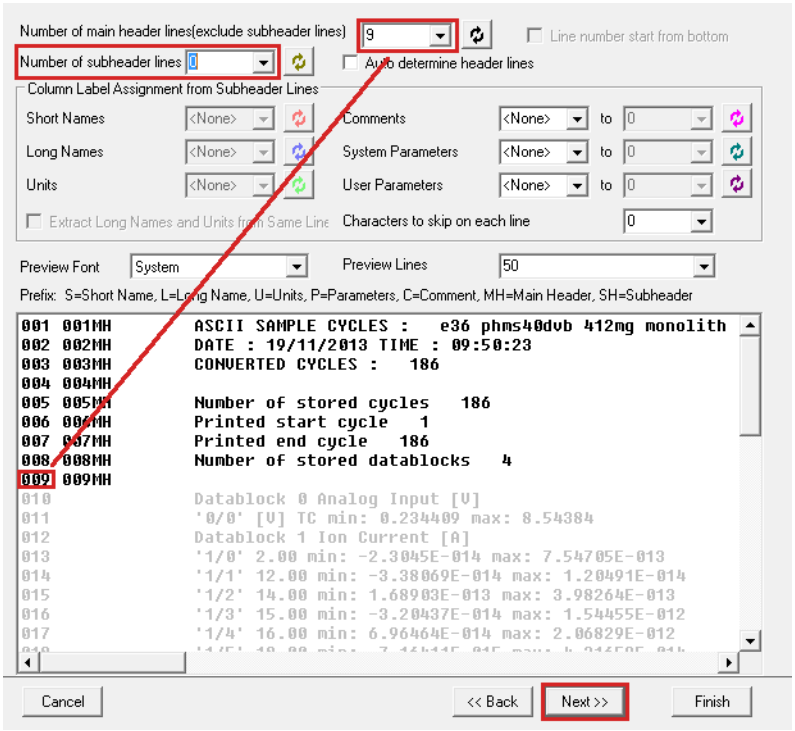
Here are the steps to import the first MS data worksheet, *i.e* the relative intensity extrema for each M/z.

1. On Origin, go to `File > Import > Import Wizard` or press `Ctrl+3`.
2. On the `Import Wizard - Source` window, select the MS data file you saved. Make sur the data type ASCII is selected, and click `Next`.

If the `Import` line does not appear on the `File` menu, make sure an Origin project is open by clicking `File > New > Project`.



3. On the `Import Wizard - Header Lines` window, specify the number of header lines –*i.e.* the number of lines which will be ignored by Origin. Leave the `Number of subheader lines` at `0`, and `Long Names` at `0` too.

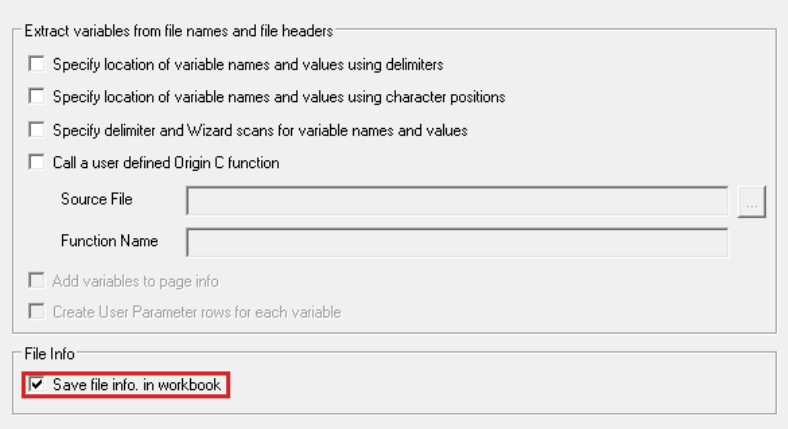


The data preview should look like this: header lines in black and data lines

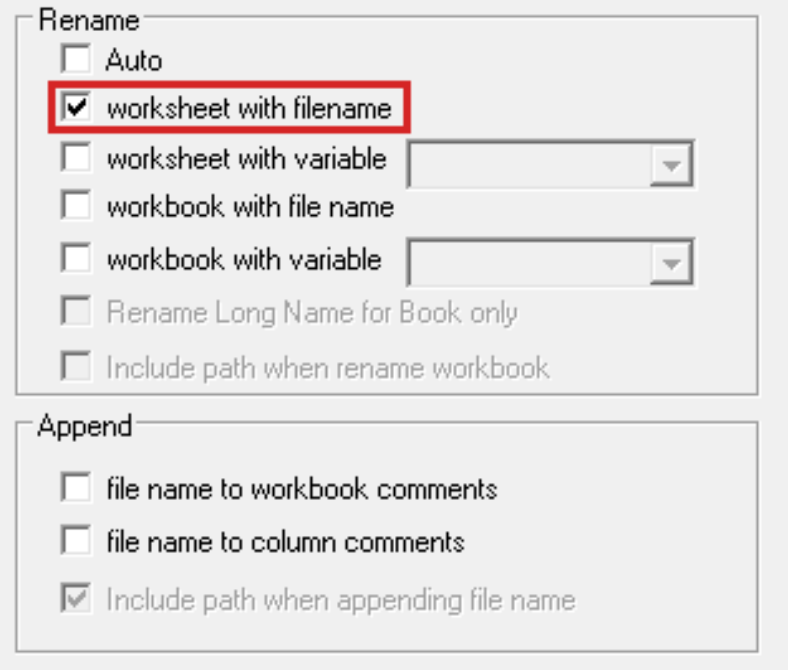
in gray.

Then, click `Next`.

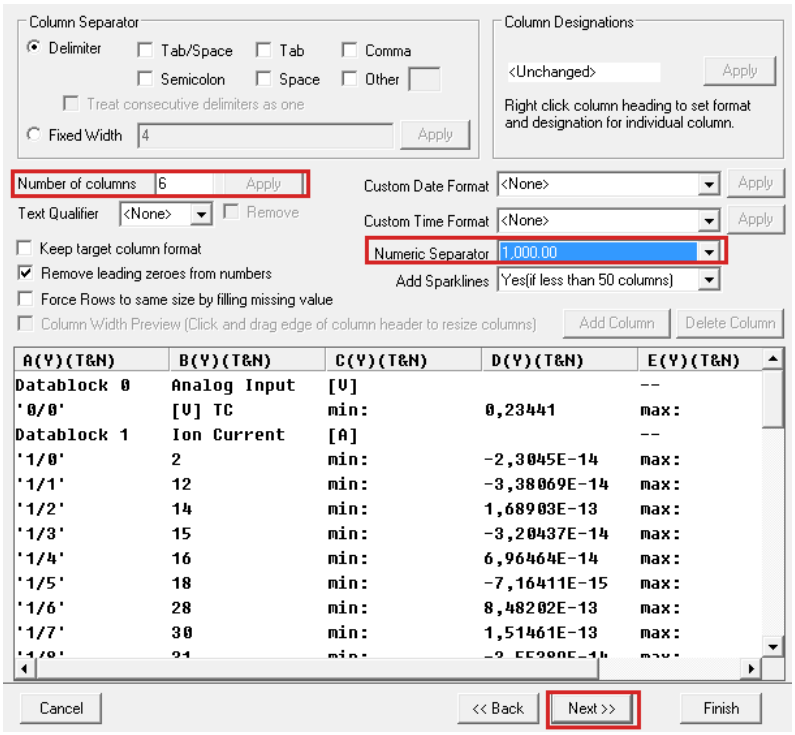
4. On `Variable Extraction` window, verify that the `Save file into a workbook` box is ticked. Leave the other boxes blank and click `Next`.



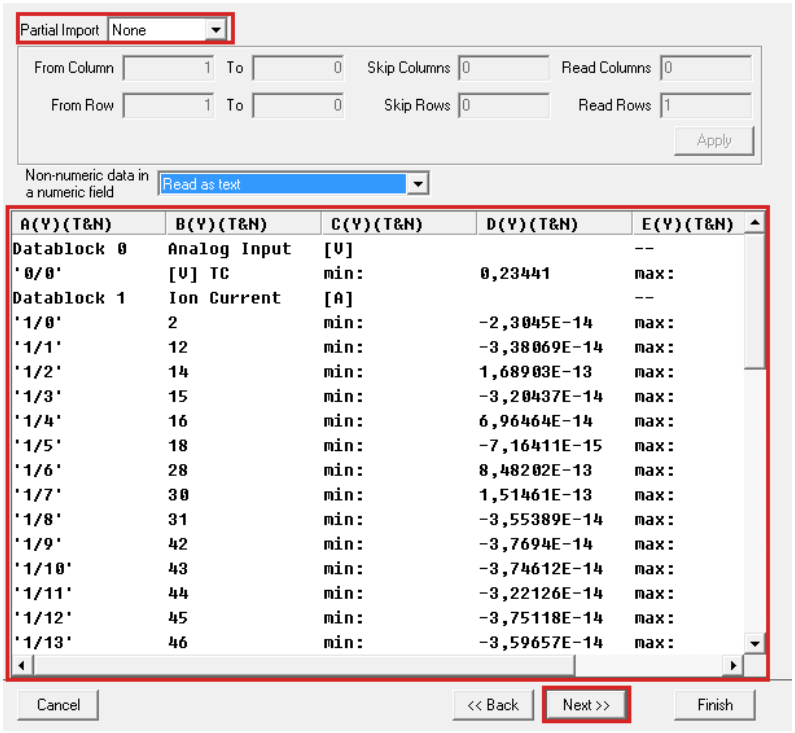
5. On `File name options`, tick the `Worksheet with filename` box and leave the others alone. Then go `Next`.



6. On `Data Columns`, select the number of columns there are in the imported file, – here 6, click `Apply` and make sure that the data is properly formatted in the preview window. Select the `1,000.00` numeric separator and go to the `Next` page.



7. On `Data Selection`, just leave `Partial import` to `None` click `Next` – the data should be correctly displayed in the window below, just like in the last step. Then go `Next`.



8. On `Save Filters`, leave everything as it is, unless you want to save this

import filter for a next time. Click `Finish`.

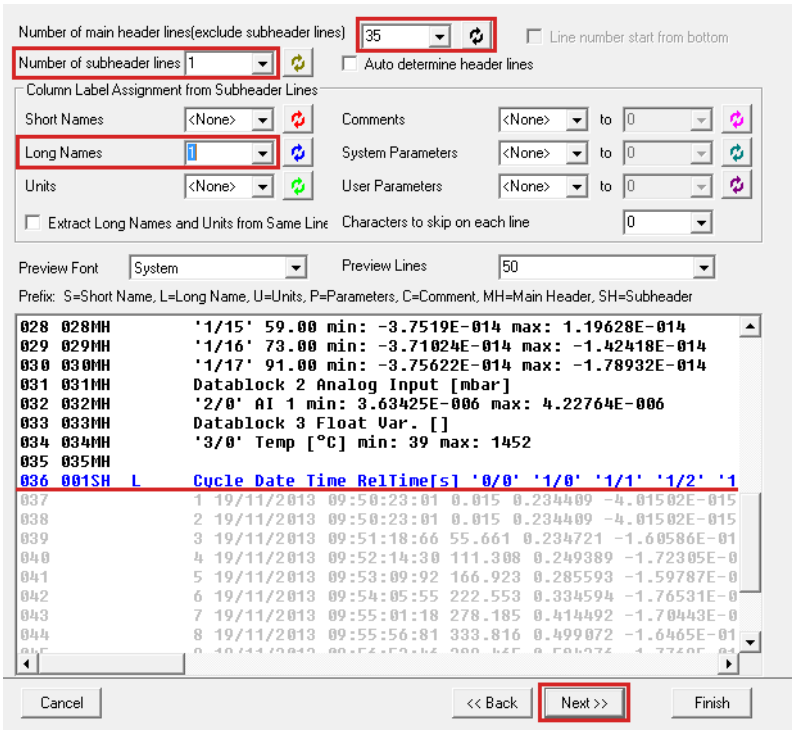
Now your worksheet should look like this:[3]

	A(X)	B(Y)	C(Y)	D(Y)	E(Y)	F(Y)
Long Name						
Units						
Comments						
F(x)=						
Sparklines						
1	Datablock 0	Analog Input	[V]		--	
2	'0/0'	[V] TC	min:	0,23441	max:	8,54384
3	Datablock 1	Ion Current	[A]		--	
4	'1/0'	2	min:	-2,3045E-14	max:	7,54705E-13
5	'1/1'	12	min:	-3,38069E-14	max:	1,20491E-14
6	'1/2'	14	min:	1,68903E-13	max:	3,98264E-13
7	'1/3'	15	min:	-3,20437E-14	max:	1,54455E-12
8	'1/4'	16	min:	6,96464E-14	max:	2,06829E-12
9	'1/5'	18	min:	-7,16411E-15	max:	4,31659E-14
10	'1/6'	28	min:	8,48202E-13	max:	2,08033E-12
11	'1/7'	30	min:	1,51461E-13	max:	4,36167E-13
12	'1/8'	31	min:	-3,55389E-14	max:	8,21005E-15
13	'1/9'	42	min:	-3,7694E-14	max:	-7,51887E-15
14	'1/10'	43	min:	-3,74612E-14	max:	3,30935E-14
15	'1/11'	44	min:	-3,22126E-14	max:	1,21587E-13
16	'1/12'	45	min:	-3,75118E-14	max:	8,46162E-14
17	'1/13'	46	min:	-3,59657E-14	max:	-1,62815E-14
18	'1/14'	58	min:	-3,71239E-14	max:	-4,52501E-15
19	'1/15'	59	min:	-3,7519E-14	max:	1,19628E-14
20	'1/16'	73	min:	-3,71024E-14	max:	-1,42418E-14
21	'1/17'	91	min:	-3,75622E-14	max:	-1,78932E-14
22	Datablock 2	Analog Input	[mbar]		--	
23	'2/0'	AI 1	min:	3,63425E-6	max:	4,22764E-6
24	Datablock 3	Float Var.	[]		--	
25	'3/0'	Temp [°C]	min:	39	max:	1452
26	--		--		--	
27	Cycle	Date	Time	RelTime[s]	'0/0'	'1/0'
28	1	19/11/2013	09:50:23:01	0,015	0,23441	-4,01502E-15
29	2	19/11/2013	09:50:23:01	0,015	0,23441	-4,01502E-15
30	3	19/11/2013	09:51:18:66	55,661	0,23472	-1,60586E-14
31	4	19/11/2013	09:52:14:30	111,308	0,24939	-1,72305E-14
32	5	19/11/2013	09:53:09:92	166,923	0,28559	-1,59787E-14

To import the second MS piece of data, see the following steps.

1. Create a new worksheet by right-clicking a worksheet tab on the bottom, " `Add` ".
2. Open `File > Import > Import Wizard` or press `Ctrl+3`.
3. On the `Import Wizard - Source` window, select the MS data file you saved. Make sur the data type ASCII is selected, and click `Next`.
4. On the `Import Wizard - Header Lines` window, specify the number of header lines –*i.e.* the number of lines which will be ignored by Origin. This time, put the `Number of subheader lines` at 1, and `Long Names` at 1 too.

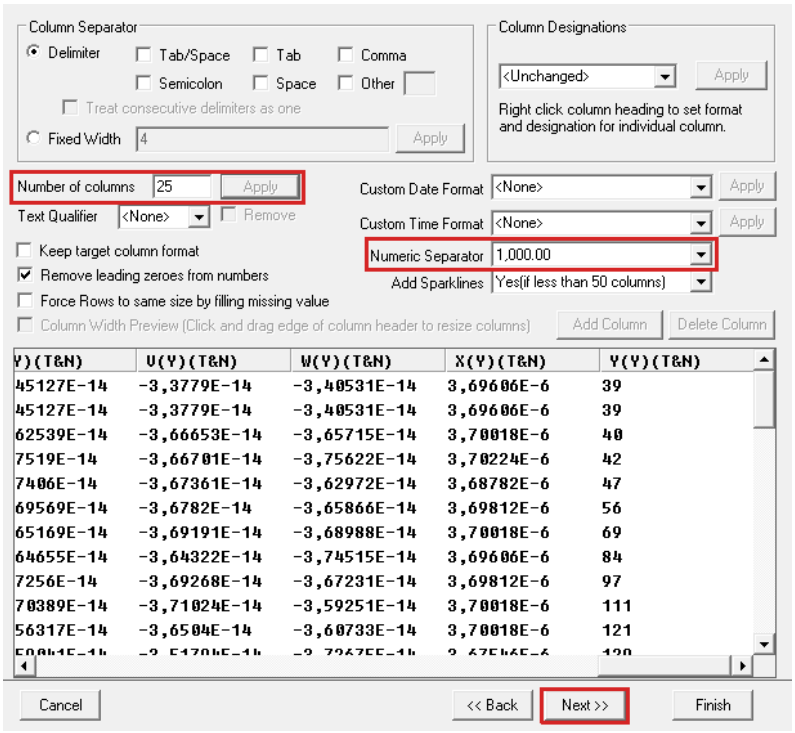
[3] It is possible that Origin creates another empty worksheet with the same name as the one you created, and I don't know why. You can just delete it by right-clicking on it `> Delete`.



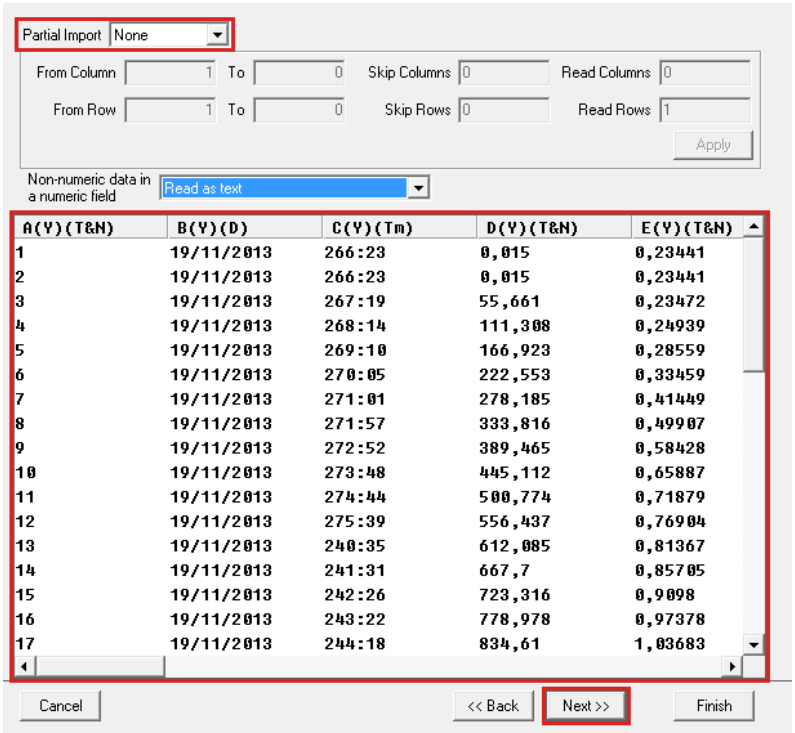
The data preview should look like this, with the subheader lines highlighted in blue.

Then, click `Next`.

5. On `Variable Extraction` window, verify that the `Save file into a workbook` box is ticked. Leave the other boxes blank and click `Next`.
6. On `File name options`, tick the `Worksheet with filename` box and leave the others alone. Then go `Next`.
7. On `Data Columns`, select the number of columns there are in the imported file, – here 25, click `Apply` and make sure that the data is properly formatted in the preview window. Select the `1,000.00` numeric separator and go to the `Next` page.



8. On `Data Selection`, just leave `Partial import` to `None` and click `Next` – the data should be correctly displayed in the window below, just like in the last step. Then go `Next`.



9. On `Save Filters`, leave everything as it is, unless you want to save this

import filter for a next time. Click `Finish`.

Now you have two worksheets, one with M/z data, the other with the actual MS curves.

To make future worksheet reference easier, I renamed the worksheets with the respective names "`mz sheet`", "`ms data`". To do the same, right-click a worksheet tab on the bottom, "`Name and Comments...`" and fill the "`Short Name`" field.

	A(X)	B(Y)	C(Y)	D(Y)	E(Y)	F(Y)
Long Name						
Units						
Comments						
F(x)=						
Sparklines						
1	Datablock 0	Analog Input	[V]		--	
2	'0/0'	[V] TC	min:	0,23441	max:	8,54384
3	Datablock 1	Ion Current	[A]		--	
4	'1/0'	2	min:	-2,3045E-14	max:	7,54705E-13
5	'1/1'	12	min:	-3,38069E-14	max:	1,20491E-14
6	'1/2'	14	min:	1,68903E-13	max:	3,98264E-13
7	'1/3'	15	min:	-3,20437E-14	max:	1,54455E-12
8	'1/4'	16	min:	6,96464E-14	max:	2,06829E-12
9	'1/5'	18	min:	-7,16411E-15	max:	4,31659E-14
10	'1/6'	28	min:	8,48202E-13	max:	2,08033E-12
11	'1/7'	30	min:	1,51461E-13	max:	4,36167E-13
12	'1/8'	31	min:	-3,55389E-14	max:	8,21005E-15
13	'1/9'	42	min:	-3,7694E-14	max:	-7,51887E-15
14	'1/10'	43	min:	-3,74612E-14	max:	3,30935E-14
15	'1/11'	44	min:	-3,22126E-14	max:	1,21587E-13
16	'1/12'	45	min:	-3,75118E-14	max:	8,46162E-14
17	'1/13'	46	min:	-3,59657E-14	max:	-1,62815E-14
18	'1/14'	58	min:	-3,71239E-14	max:	-4,52501E-15
19	'1/15'	59	min:	-3,7519E-14	max:	1,19628E-14
20	'1/16'	73	min:	-3,71024E-14	max:	-1,42418E-14
21	'1/17'	91	min:	-3,75622E-14	max:	-1,78932E-14
22	Datablock 2	Analog Input	[mbar]		--	
23	'2/0'	AI 1	min:	3,63425E-6	max:	4,22764E-6
24	Datablock 3	Float Var.	[]		--	
25	'3/0'	Temp [°C]	min:	39	max:	1452
26	--		--		--	
27	Cycle	Date	Time	RelTime[s]	'0/0'	'1/0'
28	1	19/11/2013	09:50:23:01	0,015	0,23441	-4,01502E-15
29	2	19/11/2013	09:50:23:01	0,015	0,23441	-4,01502E-15
30	3	19/11/2013	09:51:18:66	55,661	0,23472	-1,60586E-14
31	4	19/11/2013	09:52:14:30	111,308	0,24939	-1,72305E-14
32	5	19/11/2013	09:53:09:92	166,923	0,28559	-1,59787E-14

	A(X)	B(Y)	C(Y)	D(Y)	E(Y)	F(Y)	G(Y)	H(Y)	I(Y)	J(Y)
Long Name	Cycle	Date	Time	RelTime[s]	'0/0'	'1/0'	'1/1'	'1/2'	'1/3'	'1/4'
Units										
Comments										
F(x)=										
Sparklines										
1	1	19/11/2013	266:23	0,015	0,23441	-4,01502E-15	-1,77078E-14	3,16359E-13	-2,22537E-14	1,24057E-13
2	2	19/11/2013	266:23	0,015	0,23441	-4,01502E-15	-1,77078E-14	3,16359E-13	-2,22537E-14	1,24057E-13
3	3	19/11/2013	267:19	55,661	0,23472	-1,60586E-14	-3,04259E-14	3,05827E-13	-2,81147E-14	1,15784E-13
4	4	19/11/2013	268:14	111,308	0,24939	-1,72305E-14	-3,24716E-14	3,07468E-13	-2,95645E-14	1,18719E-13
5	5	19/11/2013	269:10	166,923	0,28559	-1,59787E-14	-3,24532E-14	3,05755E-13	-3,18105E-14	1,10384E-13
6	6	19/11/2013	270:05	222,553	0,33459	-1,76531E-14	-3,38069E-14	3,03437E-13	-3,16278E-14	1,1715E-13
7	7	19/11/2013	271:01	278,185	0,41449	-1,70443E-14	-3,25024E-14	3,09316E-13	-3,20437E-14	1,17971E-13
8	8	19/11/2013	271:57	333,816	0,49907	-1,6465E-14	-3,24101E-14	3,00756E-13	-3,05478E-14	1,07659E-13
9	9	19/11/2013	272:52	389,465	0,58428	-1,7769E-14	-3,22245E-14	3,07359E-13	-3,09377E-14	1,19047E-13
10	10	19/11/2013	273:48	445,112	0,65887	-2,3045E-14	-3,21291E-14	3,04119E-13	-3,07255E-14	1,17341E-13
11	11	19/11/2013	274:44	500,774	0,71879	-1,34928E-14	-3,28612E-14	3,09499E-13	-2,84843E-14	1,12819E-13
12	12	19/11/2013	275:39	556,437	0,76904	-7,37815E-15	-3,20597E-14	3,12775E-13	-2,2633E-14	1,16392E-13
13	13	19/11/2013	240:35	612,085	0,81367	-3,33125E-15	-3,13307E-14	3,14447E-13	-1,68297E-14	1,13196E-13
14	14	19/11/2013	241:31	667,7	0,85705	-1,68108E-16	-3,06631E-14	3,17941E-13	-1,1553E-14	1,16477E-13
15	15	19/11/2013	242:26	723,316	0,9098	8,8639E-16	-2,99781E-14	3,21972E-13	-4,27881E-15	1,19216E-13
16	16	19/11/2013	243:22	778,978	0,97378	-6,005E-16	-2,90485E-14	3,24711E-13	3,20446E-15	1,16354E-13
17	17	19/11/2013	244:18	834,61	1,03683	2,12603E-15	-2,92614E-14	3,29083E-13	1,02303E-14	1,12432E-13
18	18	19/11/2013	245:13	890,287	1,10362	5,05878E-15	-2,8566E-14	3,29458E-13	1,05663E-14	1,15834E-13
19	19	19/11/2013	246:09	945,918	1,16728	5,69251E-15	-2,97839E-14	3,24581E-13	1,22779E-14	1,09476E-13
20	20	19/11/2013	247:04	1001,56	1,22346	8,66174E-15	-2,84457E-14	3,24231E-13	1,41242E-14	1,11472E-13
21	21	19/11/2013	248:00	1057,24	1,27309	8,16862E-15	-2,81908E-14	3,1733E-13	1,2665E-14	1,12228E-13
22	22	19/11/2013	248:56	1112,87	1,31803	1,02724E-14	-2,86008E-14	3,15808E-13	1,37961E-14	1,09708E-13
23	23	19/11/2013	249:51	1168,52	1,36766	1,41284E-14	-2,94103E-14	3,16762E-13	1,05988E-14	1,07114E-13
24	24	19/11/2013	250:47	1224,18	1,4229	1,61157E-14	-2,83991E-14	3,11669E-13	1,34446E-14	1,05271E-13
25	25	19/11/2013	251:43	1279,84	1,47783	1,53086E-14	-2,81487E-14	3,11362E-13	1,26339E-14	1,07345E-13
26	26	19/11/2013	252:38	1335,45	1,53869	2,26782E-14	-2,78393E-14	3,03697E-13	1,50824E-14	1,08367E-13
27	27	19/11/2013	253:34	1391,11	1,59799	3,22898E-14	-2,80246E-14	3,05174E-13	1,83356E-14	1,08553E-13
28	28	19/11/2013	254:30	1446,72	1,65292	4,22103E-14	-2,69212E-14	3,05427E-13	2,24047E-14	1,13193E-13
29	29	19/11/2013	255:25	1502,35	1,7041	5,00289E-14	-2,54983E-14	3,05693E-13	2,88262E-14	1,09825E-13
30	30	19/11/2013	256:21	1558,03	1,75404	6,05523E-14	-2,6125E-14	3,10922E-13	3,55058E-14	1,12767E-13
31	31	19/11/2013	257:17	1613,73	1,80741	6,33115E-14	-2,52149E-14	3,01834E-13	4,14654E-14	1,14063E-13
32	32	19/11/2013	258:12	1669,41	1,85859	6,77693E-14	-2,62309E-14	3,10436E-13	4,62842E-14	1,18852E-13
33	33	19/11/2013	259:08	1725,07	1,91696	7,06243E-14	-2,4359E-14	3,14671E-13	5,53112E-14	1,15505E-13
34	34	19/11/2013	260:04	1780,75	1,97251	6,93469E-14	-2,46477E-14	3,12584E-13	6,29995E-14	1,20038E-13
35	35	19/11/2013	260:59	1836,43	2,0315	6,73743E-14	-2,39839E-14	3,13653E-13	6,73589E-14	1,17664E-13
36	36	19/11/2013	261:55	1892,11	2,08237	5,98744E-14	-2,40557E-14	3,10882E-13	7,39515E-14	1,19244E-13
37	37	19/11/2013	262:51	1947,8	2,1373	5,92559E-14	-2,24065E-14	3,12893E-13	8,24638E-14	1,17948E-13
38	38	19/11/2013	263:46	2003,5	2,18693	5,55978E-14	-2,10131E-14	3,15581E-13	8,98063E-14	1,15048E-13
39	39	19/11/2013	264:42	2059,18	2,24217	5,37044E-14	-2,13031E-14	3,1496E-13	9,75074E-14	1,14343E-13
40	40	19/11/2013	265:38	2114,85	2,29679	5,41937E-14	-1,94182E-14	3,29961E-13	1,1428E-13	1,17647E-13

1.2.2 *Import TG data in `.txt` format*

This is a bit shorter than the MS import but it is the same idea.

1. Create a new worksheet and switch to it.
2. Reach `File > Import > Import Wizard` and browse the desired file.
3. Filter the file the same way as for the MS file (headers and column numbers)

1.2.3 *Import baseline data in `.txt` format*

The steps are the same than the TG import in paragraph 1.2.2 since the files are formatted in the same way.

1.3 *Preliminary treatments*

You can rearrange the columns of your worksheets the way you want, delete some of the useless information, put names, units, comments etc…

sThe following steps treat the data to prepare the TGMS plots.

1.4 *Place the M/z labels on MS columns*

1. Switch to the "`mz sheet`" worksheet.
2. Create a new column by right-clicking on the empty gray space in the worksheet and selecting `Add new column`.
3. Right-click on the new column header and select `Set column values...`.
4. On the text area, type the following :

   ```
   "M/z = "+col(M/z)$
   ```

   Now the new column should have proper labels.
5. Delete the meaningless labels such as "`M/z = Ion current`", select the block of cells with the right label, right-click on it and select `Copy` (or press `Ctrl+C`).
6. Go to the "`ms data`" worksheet, select the leftmost columns with ms data (you can find it with the cycle number), right-click on it at the row "`Long Name`" and click `Paste transpose`.

The MS columns should now be properly labeled.

1.5 *Calculate the relative intensity on mz sheet*

1.5.1 *Polynomial regression of the temperature curve in TG data*

Since temperature *vs.* time is not given in the MS data, it is needed to whether fit a curve, whether interpolate the data, to get new temperature points corresponding to MS time points.

Assuming the temperature growth is more or less I chose to fit a degree one polynomial in this case.

The fit must only consider the points where the temperature grows – approximately – linearly, therefore it must omit all points from segment 2 and 3. The temperature increase shows some variations at the beginning, until a stabilized growth settles. Usually, this variation becomes marginal around $T = 200\,°C$.

1.5.2 *Baseline mass loss data interpolation and substraction*[4]

If the exports are correct, with the same number of points, just skip this step.

The time points for TG and baseline may not be the same. If it is the case, we will want to interpolate the baseline mass loss data in order to get the correct values to substract from TG ones, since the baseline data does not follow a predictable model.

[4] This is only needed if the TG and baseline data don't have the same measurement points. If they have been exported from Proteus with the same settings, please ignore this part.

1.6 *Plotting graphs*

1.6.1 *For TG*

1.6.2 *For MS*

1.6.3 *Plot TGMS graph*

2 *Origin scripting for automated plots*

To reduce the time spent on overly repetitive tasks, I produced a LabTalk – Origin's scripting language – file run by Origin to execute the procedure detailed above in section 1.

2.1 *Scripts installation*

2.1.1 *Automatic installation*

Go to the following address:

https://github.com/sylvain-kern/tgmsplot-script

and reach for the `setup.exe` file in the `setup` folder. Download it and run it[5]. The setup creates a `tgmsplot-script` folder in the Origin files directory a and puts the script files in it. When installing, verify the destination folder, by default it is

```
C:\Program Files\OriginLab\Origin2016
```

but it can change with your version of Origin, so check your software version and where the program files are stored.

[5] Do not worry if Windows freaks out and thinks it is a virus, I do not have an authentification certificate indeed, so I can not guarantee to Windows that my program is safe (do not worry, it actually is).

2.1.2 *Manual installation*

Download the folder that contains the source files on the project repository:

https://github.com/sylvain-kern/tgmsplot-script.

Place the `tgmsplot-script` in the following folder (check that this folder is the right for your software files):

```
C:\ProgramFiles\OriginLab\Origin2016\
```

If you have a different version of Origin, it may not be '`...$\backslash $Origin2016`' but whatever your version is.

2.1.3 *Button groups installation*[6]

For more information about this step, check https://www.originlab.com/doc/Origin-Help/UserDef-Custom-Toobar-Button.

[6] The button bitmap :

1. On Origin, go to `View > Toolbars` or press `Ctrl+T`. Go to the `Button groups` tab. Click `New`.
2. Choose a name for the button group.
3. Select "4" for the number of buttons.
4. For the bitmap, and browse for the file located at:

```
C:\ProgramFiles\OriginLab\Origin2016\tgmsplot-script\button-b
↪  itmap\bitmap.bmp
```

5. Then, right-click on the buttons that appear on the right pane, and assign them to the script files, respectively :
   - `import-ms.ogs`
   - `import-tg.ogs`
   - `plot-vs-time.ogs`
   - `plot-vs-temp.ogs`
6. Drag and drop the buttons in your favourite toolbar on Origin.

2.2 *Usage*

2.2.1 *Using buttons*

If the buttons are installed, just click on them to use the program.

2.2.2 *Using the `run.file` command*

Open the command window –this icon  on the right of the top toolbar. Then run the following command:

```
run.file("C:\ProgramFiles\Origin2016\tgmsplot-script\<file>")
```

A file browser window appears, select the file you want to load.

To import only the MS data, run the following in the command window:[7] you wand to load. Click `Ok` then do the same for the TG and baseline files.

```
run.file("C:\Program
↪  Files\Origin2016\tgmsplot-script\import-ms.ogs")
```

The same goes for TG and BL data:

[7] Note that the scipt will NOT work if the file name contains accents or fancy characters.

The MS curves are not to scale on the y axis, which is not ticked. The TGMS plot is only meant to give a qualitative overview and not precise quantitative information.

```
run.file("C:\Program
↪  Files\Origin2016\tgmsplot-script\import-tg.ogs")
```

```
run.file("C:\Program
↪  Files\Origin2016\tgmsplot-script\import-bl.ogs")
```

Then, execute the plot program:

```
run.file("C:\Program Files\Origin2016\tgmsplot-script\plot.ogs")
```

2.2.3 *Script and execution details*

The source folder contains the following files:

2.3 *Issues*

In progress …

3 *Merge several Origin projects : the `Append` function*

To compare several experiments imported in separated Origin projects, it is possible to merge the `.opj` files with the following procedure :

1. open a new Origin project ;
2. go on `File > Append` and select the first project you want to import ;
3. repeat the last step for the other project to append.

If the temperature increase and the number of points are the same, it is possible to copy/paste the desired data on one single worksheet and plot it directly.