

O. Procedure for Processing of NMR data

1. Choice of data processing software
2. Installation of the software
3. Obtaining NMR measurement data
4. 1D processing
5. Data output
6. Arrangement of PDF data → Paste data to word processing software

1. Choice of Data Processing Software

If you process the NMR data with your own PC or laboratory owned PC or Mac PC, other than PC in NMR room, you should prepare the software by yourself. There are several data processing softwares, but we (administrators analytical devices & NMR in department of science) recommend you to use [ALICE2 Ver.6] (ALICE2) or [Delta Ver.5] (Delta) offered by JEOL. Both have the features as written below, so you had better choose the one, considering your work environment.

(1) ALICE2

This is available with MS-Windows. Furthermore, with a charge, the users of NMR room can use network-licensed [NetALICE2] (Network ALICE2 Client Version 6.1).

NetALICE2 with 10 licenses (10 users can use the software simultaneously.) is installed in the server PC on [Department of Chemistry and Polymer] network. The users can access it and use ALICE2 with any PC, which is connected to the network, with the easy initial setup.

Compliant Operating System: MS-Windows 95 / 98 / Me / NT4.0 / 2000 / XP

→ Windows VISTA / 7^{*}, MAC OS, Linux are unsupported.

Failure will occur in processing, but the software is available in XP mode.

→ You cannot use the software of network-licensed version without [Network for Department of Chemistry and Polymer] access environment.

(2) Delta

Multiplatform support (MS-Windows / Mac OSX / Linux) is available with free trial version of multi-language interface (Japanese, English, etc.), after the easy user and license registration. This is “NMR data processing only” version software for the NMR measurement with JEOL NMR.

Compliant OS: MS-Windows XP / Vista / 7, Mac OSX 10.3~, Linux

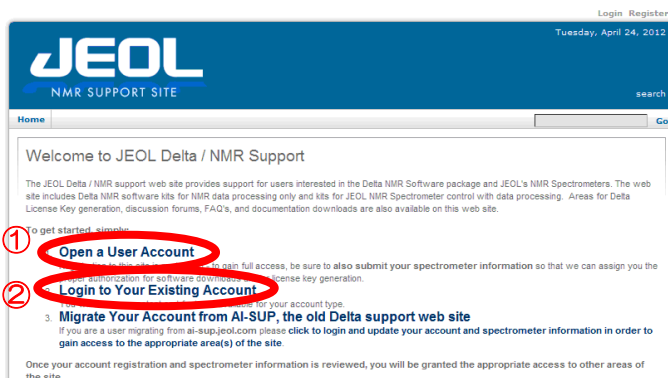
→ Sometimes, the installer does not work normally with MS-Windows XP Home Edition / Vista.

2. Installation and Setup of Delta

The newest revision of version 5 (5.02 in October, 2012) is available on JEOL NMR support website (<http://nmrsupport.jeol.com/Default.aspx>) after user registration, download and setup of the software.

① User Registration

On web browser, show <http://nmrsupport.jeol.com/Default.aspx>, and click [Open a User Account], then on [JEOL Delta/NMR Support Site Account Registration] page, complete user registration.

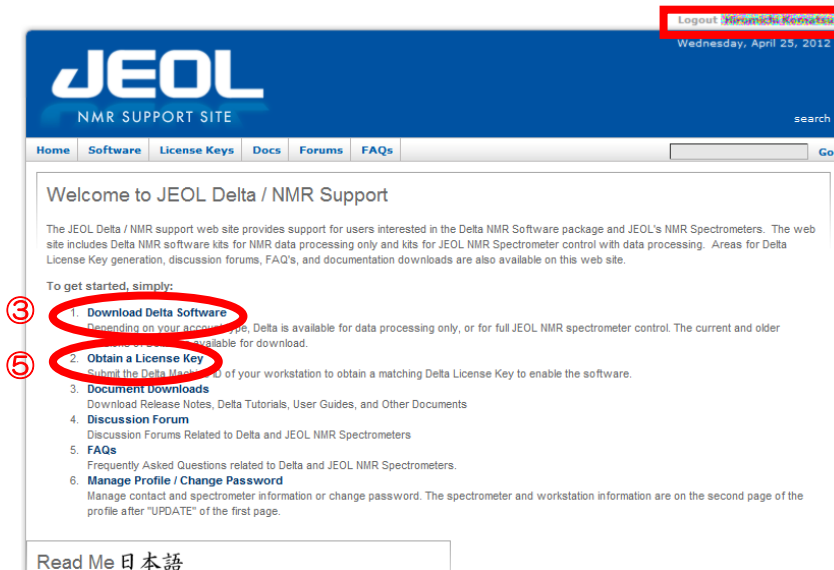


② Login

After user registration, show website ① (User Registration) again, click [Login to Your Existing Account], and on [User Log In] page, finish Login.

③ Download

Click [Download Delta Software], and on [Delta Software Download] page, download the latest revision.




④ Installation

Install the software by following the direction of installer.

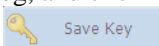
⑤ License Registration (→ aside from user registration)

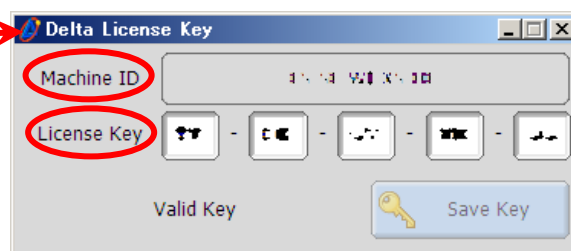
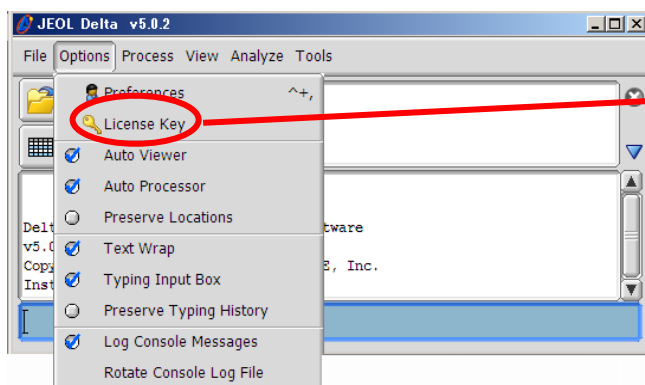
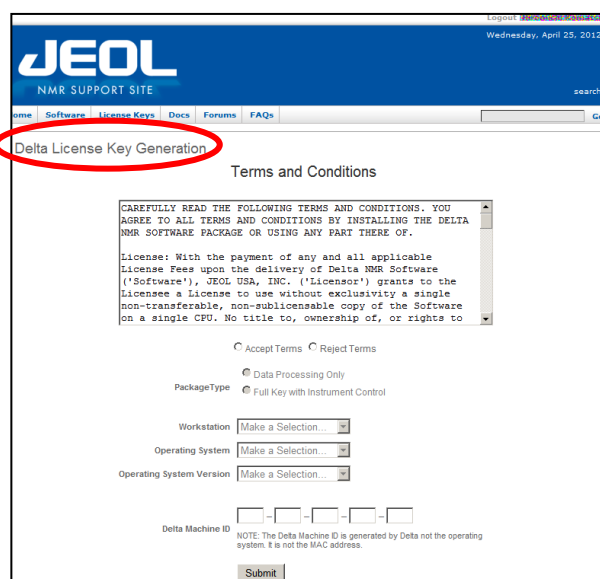
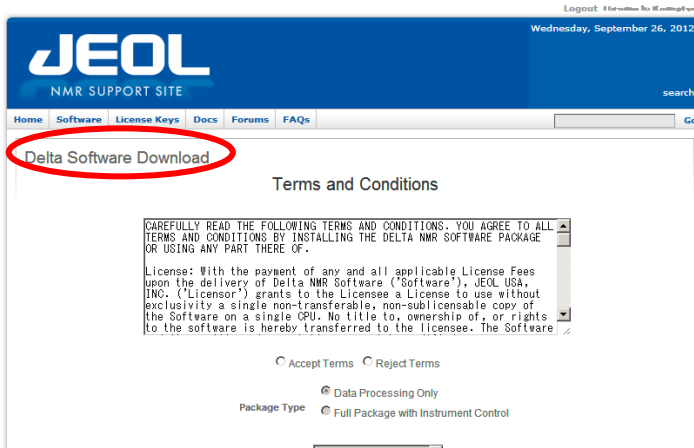
After setup, on the website same as ③, click [Obtain a License Key], and on [Delta License Key Generation] page, publish the license key (10 digits alphanumeric character) by license registration.

※ Fill [Delta Machine ID] column with [Machine ID] (10 digits character written in [Delta License Key] dialog BOX, which starts by the click of Delta icon  on each OS desktop, and from [Delta Console] menu bar, choice of [Options]→[License Key])

※ Without the key, usage time is limited to 15 minutes. This registration by the input of the key is required only once.



⑥ Setup of License Key

Input given 10 digits license key on ⑤ [Delta License Key] dialog, and click **Save Key** button .

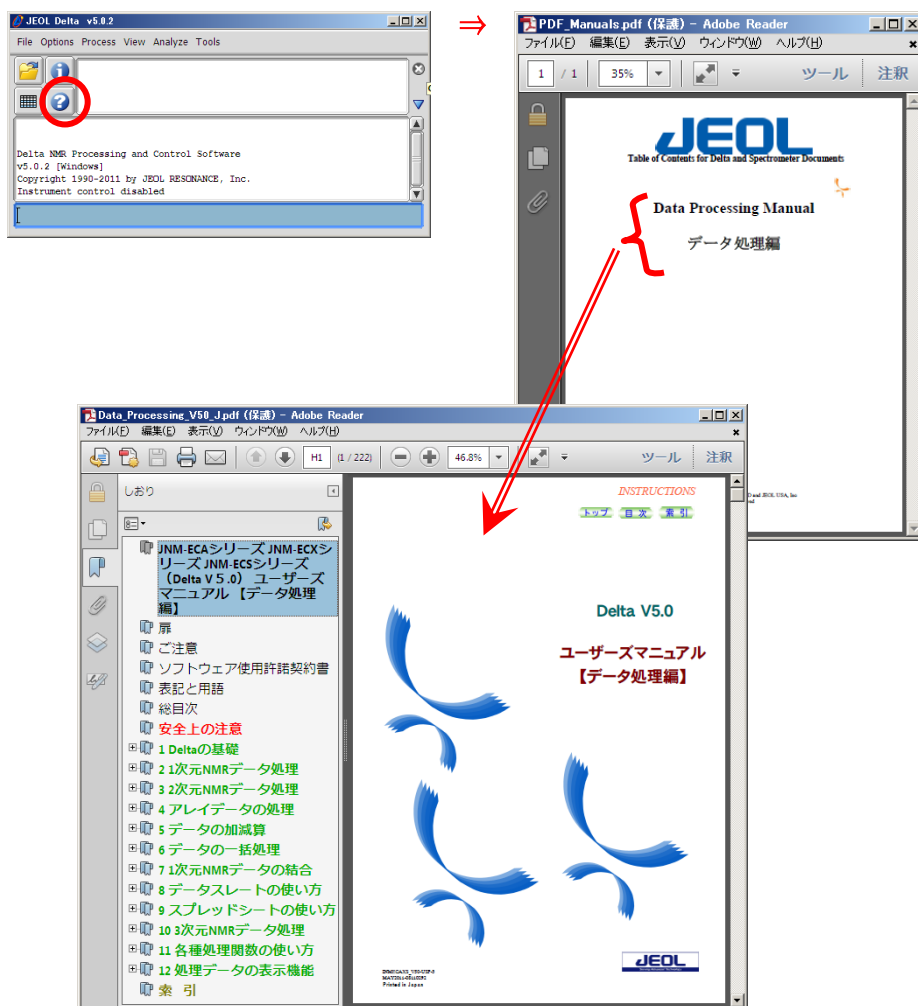


3. Manual

You can download manual made by JEOL by following next procedure.

On [Delta Console] window which starts by the click of Delta icon  on each OS desktop, click 

button, then select the language by the click of link on the cover of PDF file.

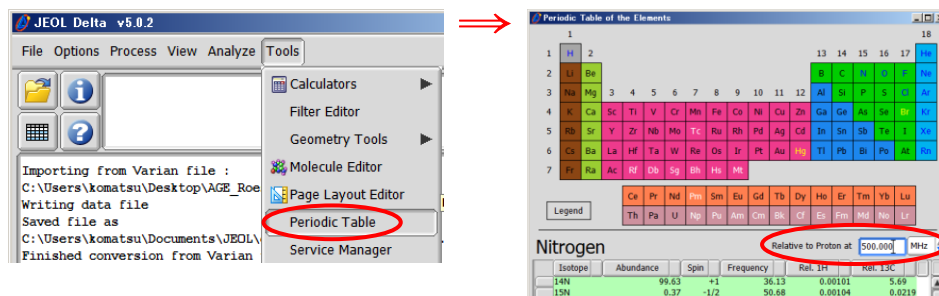


4. Each Window



(1) [Delta Console] window

On each OS desktop, click Delta icon  , [Delta Console] starts (Right figure).

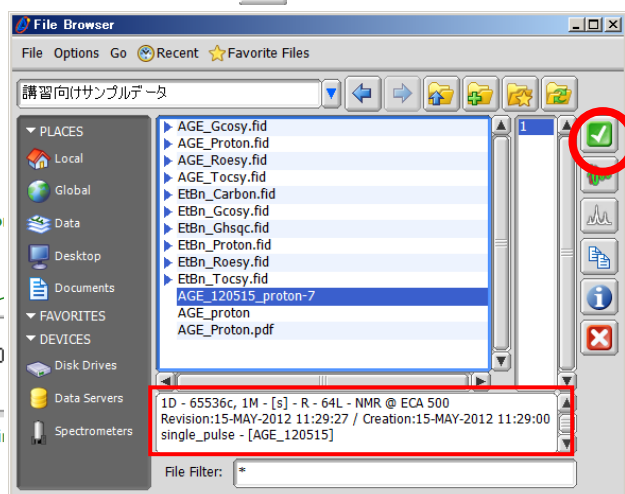
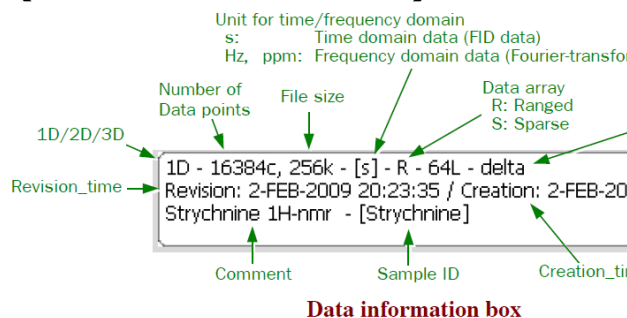
【Periodic table】 On menu bar, click [Tools]→[Periodic Table], input ^1H nuclear fundamental frequency on input BOX, then you can check the observation frequency of each nuclide.



(2) [File Browser] window


To open data file, on [Delta Console] window, click [File Browser] button  , or on menu bar, click [File]→[File Browser]. On [File Browser] window, choose the file, and click  (Right figure).

【Contents of Data information box】



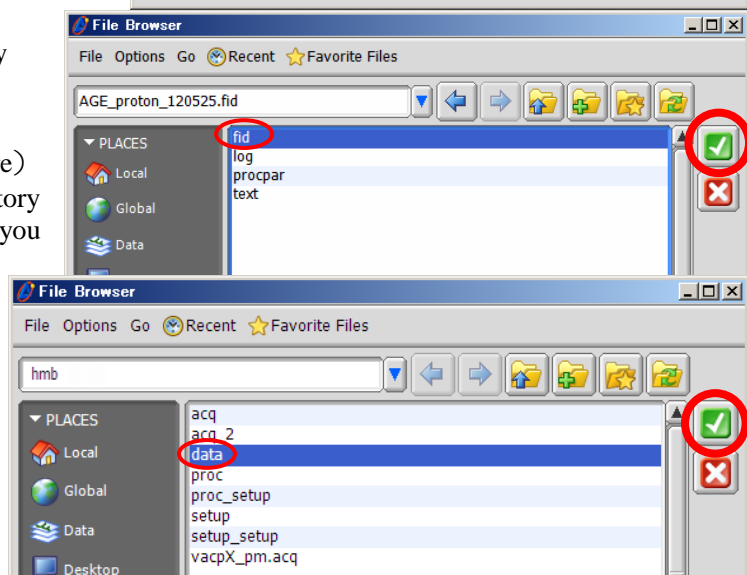
【Multi data format】

You can import NMR data measured by NMR made by other companies with the same procedure.


※ **Varian format** data (VnmrJ : Right figure) is not 1 file, and stored under 1 directory (data file, parameter file, etc.). When you open the file, choose “fid” file, and click .

Chemagnetics format data (Spinsight : Right figure) is the same as Varian one, and choose “data” file under the directory.

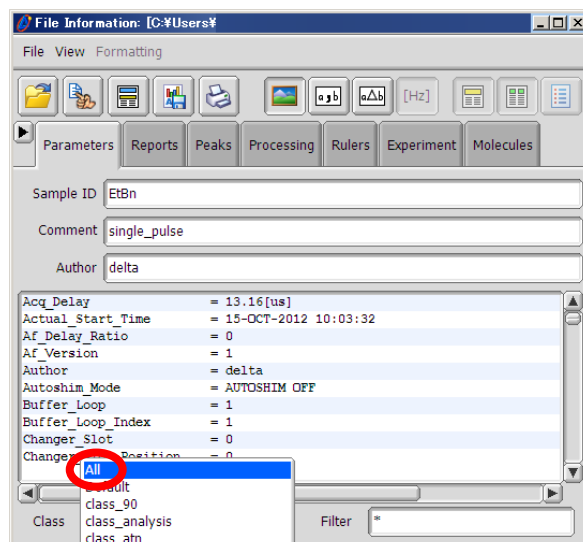
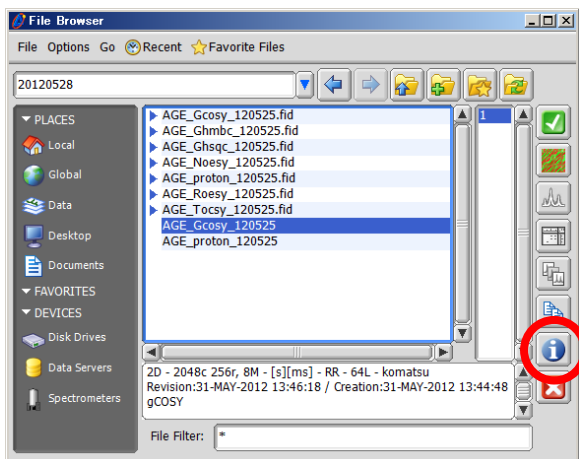
【JCAMP format】





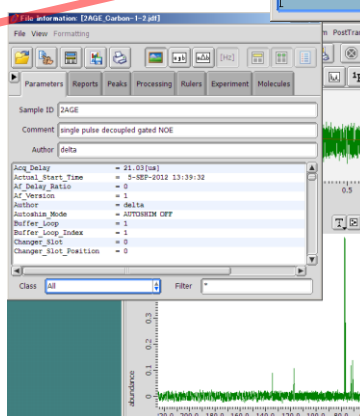
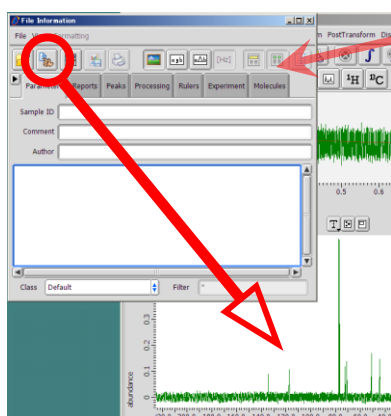
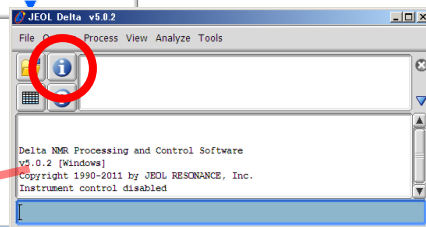
This data format is suggested to use each NMR data measured by NMR made by other companies, commonly. There are several filename extensions (.dx & .imp, etc.), but import is possible.

【File Information】 In the case of NMR data measured by JEOL NMR, choose the file, and click [information] button , [File information] window, which show the information of data, starts (Bottom figure).

※ You can check measurement parameter, when you choose [All] in [Class] pull-down in the lower part of the window.



※ As the method to obtain [File Information], on [Delta Console] window, click [Information] button , then after the click of [Select a file] button , with finger sign pointer, click data geometry. You can obtain [File Information] data shown in the geometry (This method is available for the NMR data measured by NMR made by other companies.).



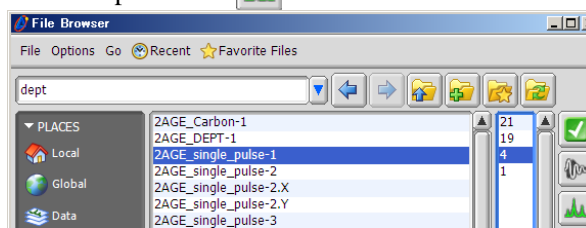
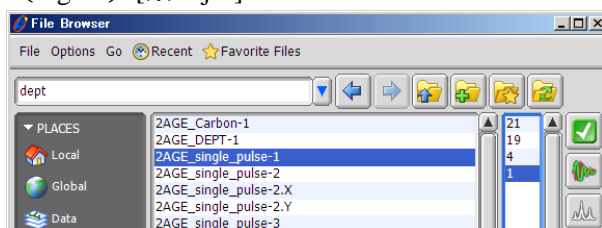
【Version of File】 In Delta, like [“Filename”-1-1.jdf] and [“Filename”-4-1.jdf],

[※-1.jdf] is FID data (measurement raw data). The number after [※-2], shows automatically saved Spectra Data performed processing on FID. (Spec of Delta software)

(Figure) [※-1.jdf] is FID data.

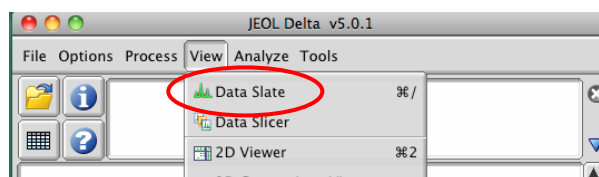





Others are spectra data .

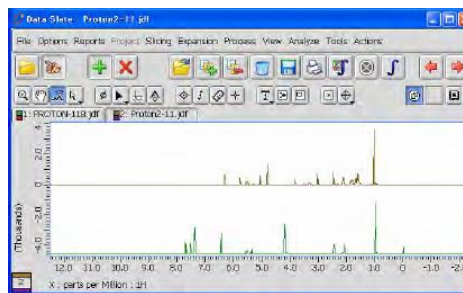
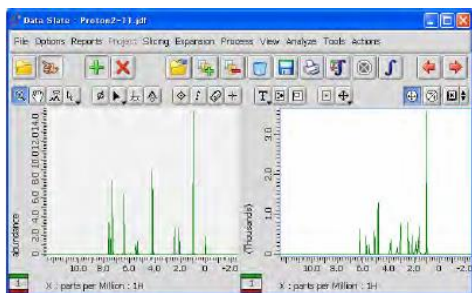



(3) [Data Slate] window

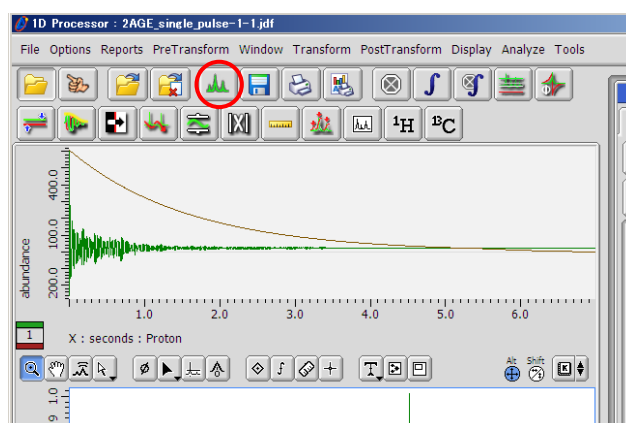
This is the viewer of processed spectra data, and usable regardless of the dimension of data. It can show several spectra. (Example : bottom-left figure (Horizontally) and bottom-right figure (Overlay))



On menu bar of [Delta Console], click [View]→[Data Slate], [Data Slate] starts. On the menu bar, click [File]→[Open ▶]→[Open], or [Open Data File] button  (※ It is not [Open Data From Disk] button ), and on [Open file] window, choose the file and click .



※ Another method to show on [Data Slate] window, is, on the already opened [1D Processor] window or [nD Processor] window, click [Put into Data Slate] button .





I Processing of 1D Measurement Data

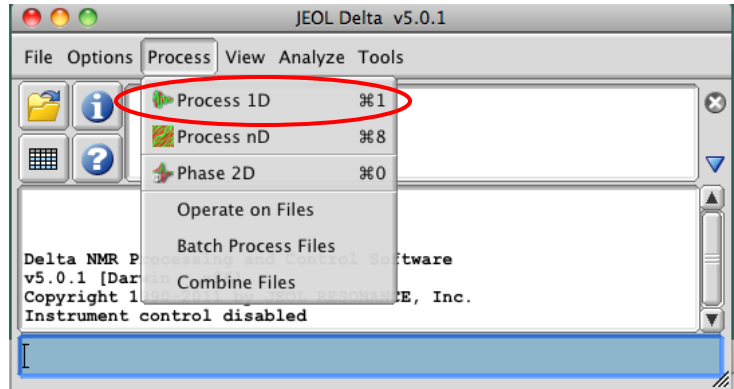
1. [1D Processor] window

For data processing

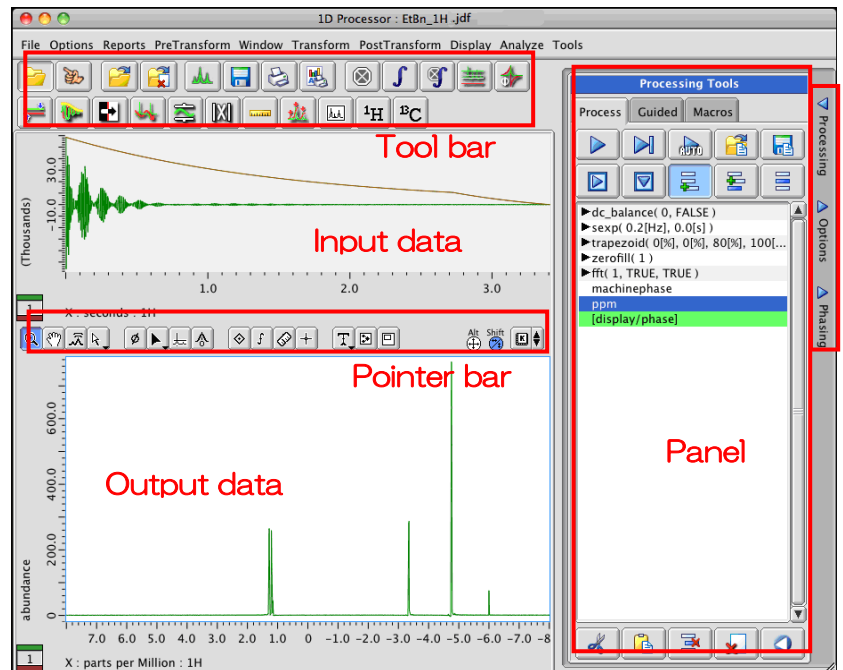
- ※ When you perform 1D measurement with JEOL NMR, (If Deliver data automatically is checked ,) this window automatically starts after measurement.

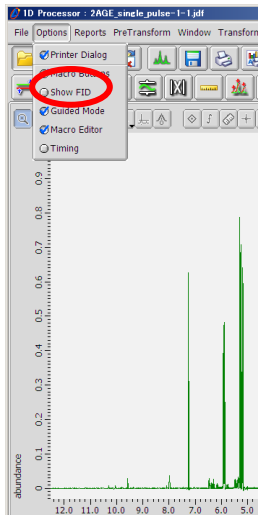
On the menu bar of [Delta Console] window, choose [Process]→[Process 1D], then [1D Processor] window starts.

On the tool bar, click [Open Data] button , and on [Open Data] window, choose the file, and click .



[Name of each part]

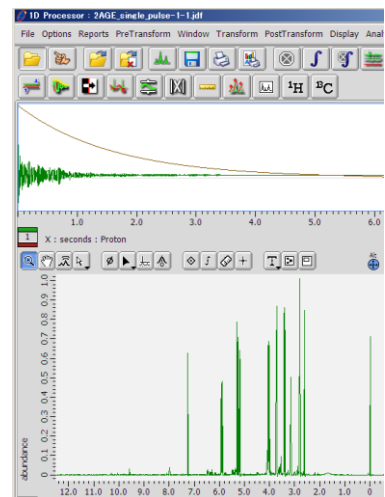
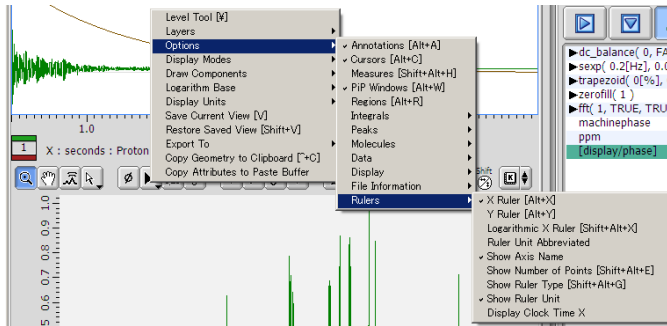




※ If Input data is not shown, you can see by checking of [Show FID] check BOX in the menu bar, [Option].

※ The vertical axis scale of [abundance] can be deleted. In the context menu shown by long press of right-button of mouse, click [Options]→[Ruler]→uncheck ✓ of [Y Ruler]

(Bottom figure). (on the right example, the vertical axis of Input data (FID) is unshown.)



2. Process List — Processing Tools

On [1D Processor] window, Input data is shown in the upper part, while corresponding processed output data is shown in the lower part.

(Example) Without [fft] (Fast Fourier Transform) in the list, processed FID itself is shown on the Output data part, so spectrum is not shown.

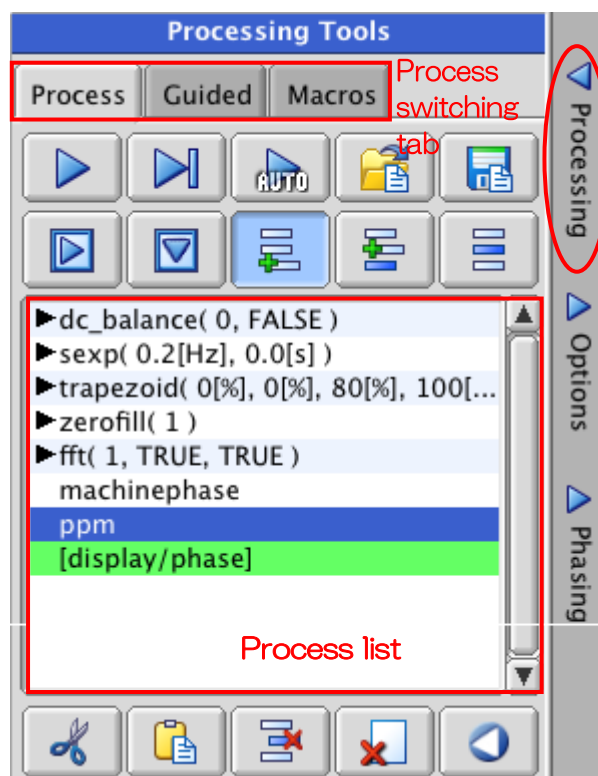
On the process list, contents and conditions of data processing are described.

You can input the conditions of processing by the click of [▶] of each process and unfolding (It changed to [▼].) .

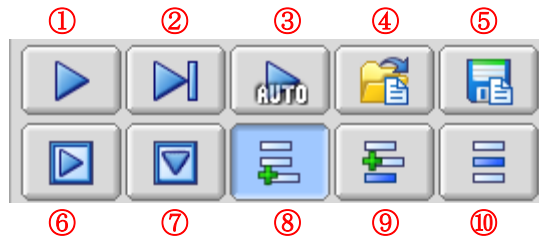
In the representative measurement sequence, fundamental process list is set (^1H ^{13}C buttons, etc.) . After measurement, this process is automatically performed. You can change, delete, and add these processes.

※ Sometimes, fundamental process list cannot be prepared for the data measured by NMR made by other companies. In that case, you should deal with it from the first by yourself, or arrange the fundamental process list.

[Native Scale] Without the setting of the reference, in Delta program, Axis is shown with the calculated values based on observed frequency of rock signals of each solvent. (Only with the data measured by JEOL NMR. With the one by NMR made by other companies, calculation is not performed, and center of observation is scaled to be 0 ppm.)

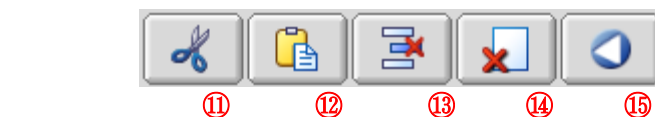
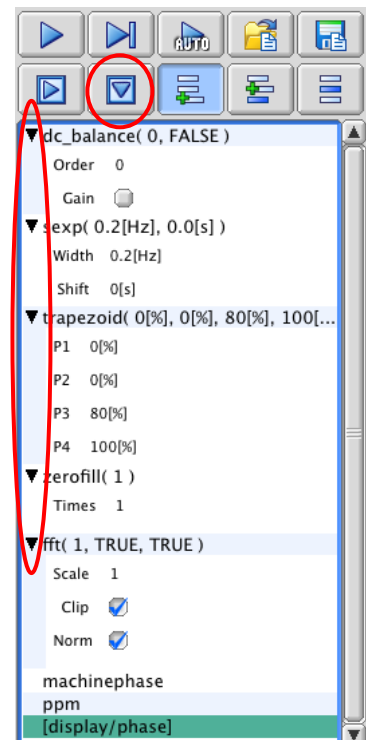


【Explanation for Buttons】 Refer to the explanation on each button shown by right click.



- ① Process : Implementation of process, Click when you modify the process.
 ※ Click this button when you find the process lines except the lowest line of [display/phase] are green. It means there exist unprocessed.
- ② Sequential Process : The process was applied one by one, different from ①.
- ③ Auto Process : Toggle Button, When you add or delete or arrange the process , it was automatically applied. ※ CPU was occupied, and PC processing will be slowed.
- ④ Load : Call-out of Process List
 ※ To read process from another process window on PC/Mac desktop, paste and overwrite the process by drag & drop (with handprint pointer) between windows.
 ※ With right button of mouse
- ⑤ Save : Saving Process List
 【Multi-nucleus measurement】 Use it when you save reference of external standard (If you did not use internal standard in the measurement.).

- ⑥ Cancel of Unfolding : Hiding all process
- ⑦ Unfolding All : (Right figure)
 ※ You can check and modify process conditions in full detail.
- ⑧ Addition : Process is added to the ending line.
- ⑨ Insert : Process is added to the one line before the selected line.
- ⑩ Exchange : The selected process is exchanged for the added process.



- ⑪ Cut : Cutting the selected process
- ⑫ Paste : Pasting cut/buffer
- ⑬ Delete : Deleting the selected process
- ⑭ Clear : Deleting all process
- ⑮ Restore : Restoring standard process list


3. Processing

```

▶dc_balance( 0, FALSE )
▶sexf( 0.2[Hz], 0.0[s] )
▶trapezoid( 0[%], 0[%], 80[%], 100[...
▶zerofill( 1 )
▶fft( 1, TRUE, TRUE )
  machinephase
  ppm
  [display/phase]

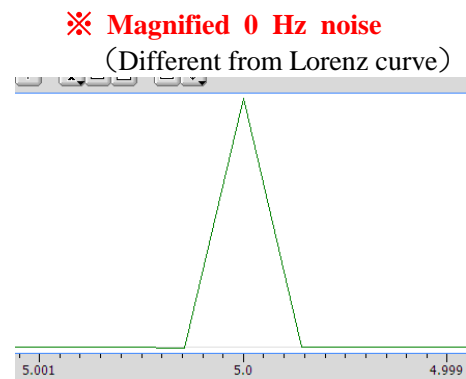
```

3 - 1 . Processing before FT (PreTransform)—Input data

(1) DC Balance  : Removal of DC offset

When direct current element is biased on [Data Slate] window signal, FID center deviates from zero. In the spectra obtained after FT, False sharp signal peak (0 Hz noise) on the observation center frequency appears. This processing is performed to solve the problem.

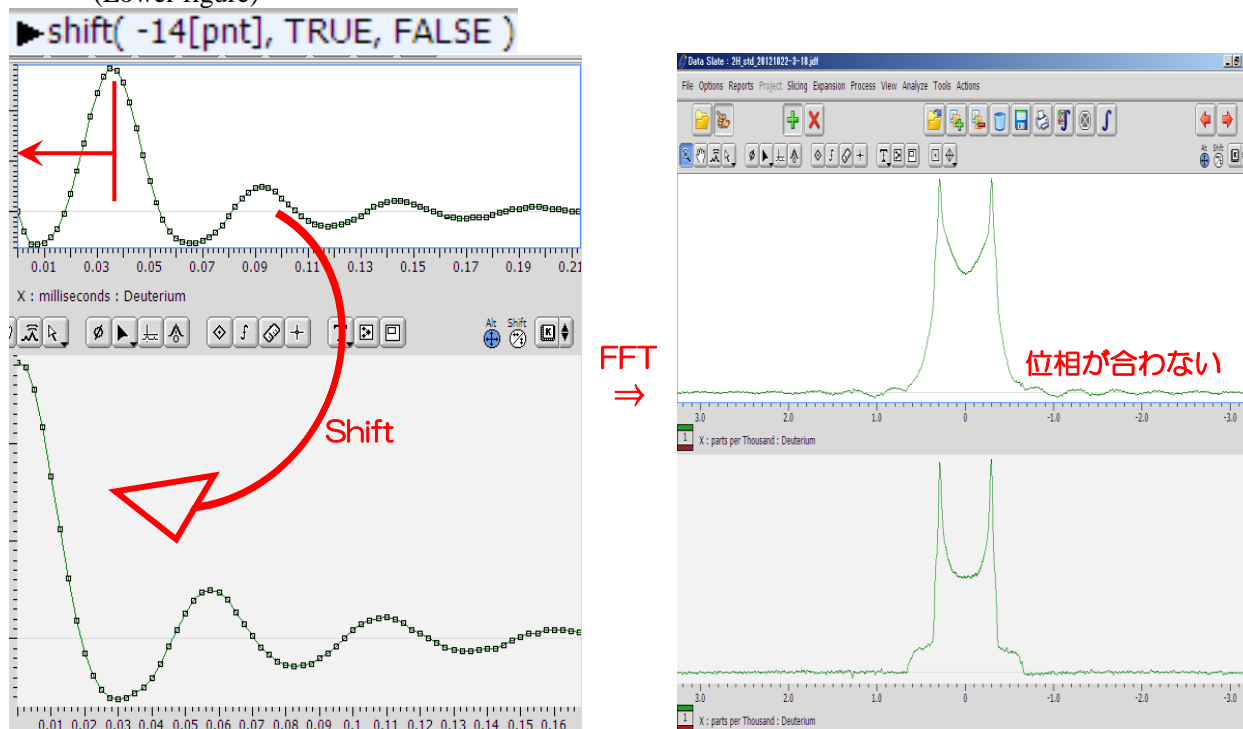
(Ex.) FID before DC offset processing & spectra (Upper figure), and processed (Lower)



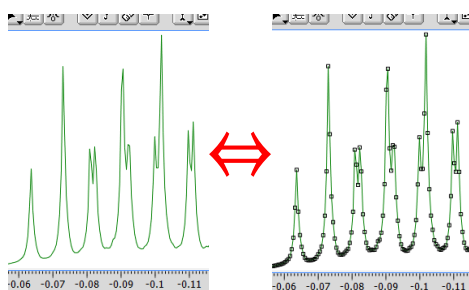
(2) Shift : FID Shift

Use FID shift in data processing of solid echo measurement. You can set point number to shift FID. Normally use this for removing points before obtaining FID by inputting minus value.

(Ex.) ^2H signal echo FID (Quadrupole Echo) & spectra(Upper figure), and The ones after removing 14 points (Lower figure)



[Dotted View] **Alt** key \oplus **n** switches Line view of FID/FT spectra \Leftrightarrow Dotted view.




(3) Window Function

To improve seeming S/N and dispersion of spectra, FID multiplies by window function, and dispersion FT is performed.

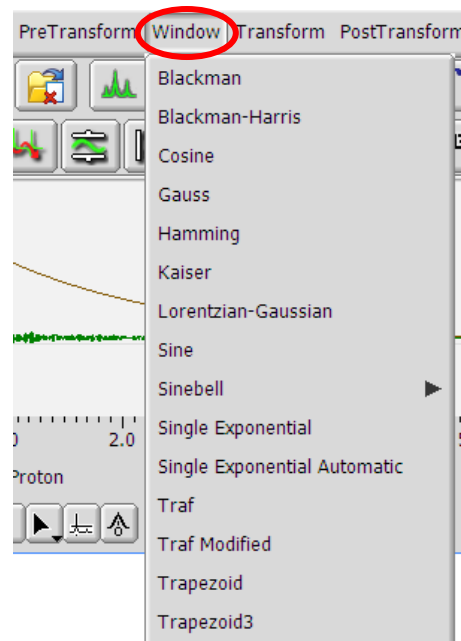
※ It is difficult to improve both S/N & resolution.

Select required window function on menu bar [Window].

※ When you click the toolbar [Window] button , the process registered in the button is performed.

① Improvement of S/N

(i) Exponential Function $f(t) = \exp(-\pi b t)$



Parameter b : Broadening factor BF[Hz]

= 0~Large

⇒The larger BF is, the faster it decays.(= 0 means that FID does not multiply by window function.)

[Single Exponential] : $sexp(\text{Width}=\text{BF value[Hz]}, \text{shift value[s]})$

▶ $sexp(0.2[\text{Hz}], 0.0[\text{s}])$

※ FID signal intensity decays exponentially with time, however noise element does not decay. Therefore noise contribution is high in the last of FID relatively.

Especially it is important in lowly sensitive ^{13}C spectra.

※ If BF is too large, signal element with noise element decays, and peak line width of spectra (Half maximum full-width) is too broaden. (Integration value is the same, so peak height is decreased.)
Reversely, it seems S/N decreases.

Index: FID multiplies by the same value as digital resolution ($\times 1$ or $\times 1/2$ to 2)

(Ex.) Digital resolution is 0.2 Hz, then BF should be ca. 0.2 Hz.

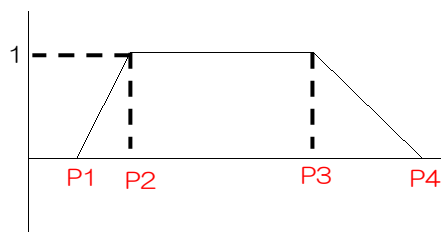
[Digital resolution]=[Observation range]/[Data point number]

(Ex.) [Single Exponential] processing result for 0.2 Hz of digital resolution

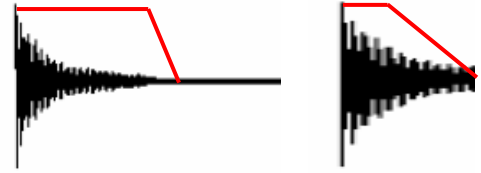


(ii) Trapezoid Function $trapezoid(P1[\%], P2[\%], P3[\%], P4[\%])$

▶ $trapezoid(0[\%], 0[\%], 80[\%], 100[\%])$



※ In the case you continue to acquire data even after FID decays thoroughly, data contains lots of noise. Cut the latter part of the data (Left figure). When you stop acquiring the data before FID decays thoroughly (due to its long decay time), tail of peak waves after FT (truncation). Reduce it by yourself.



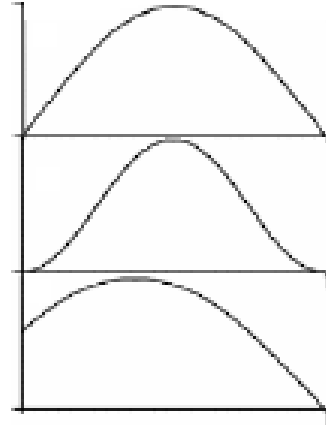
※ This is important in the process of zerofill (later discussion).

② Improvement of spectrum separation

(iii) sine-bell function

In the right figure, beginning at the top,

- sine-bell
- sine-bell (order 2)
- shifted sine-bell



In Delta,

- [Sinebell] : Design [Shift] & [Size] values
- [Sinebell(order 2)] : Same
- [Sinebell(order 4)] : Same
- [Sinebell Shift] : Design $[\pi/n]$ value & apply N

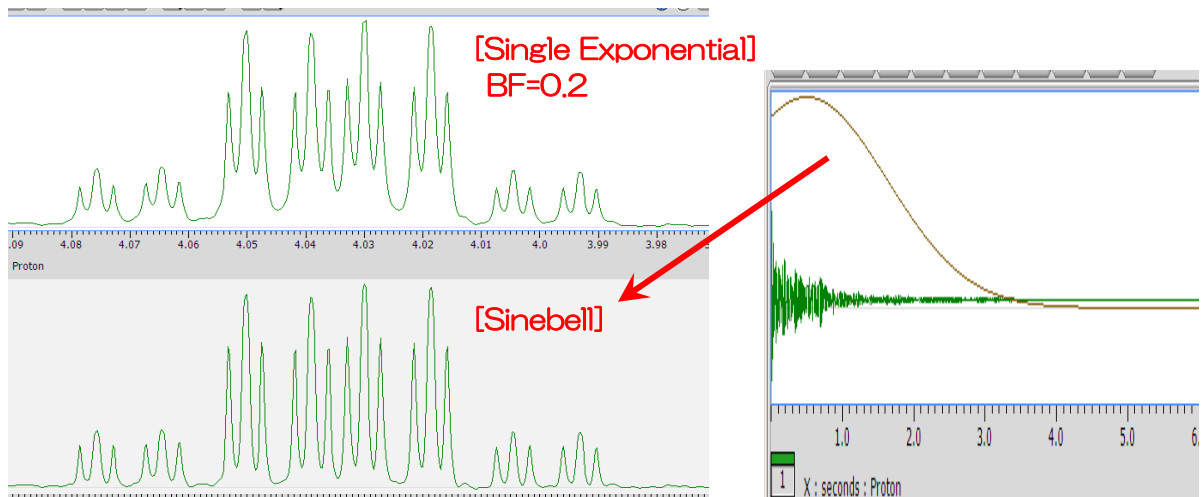
Sinebell

shifted

※ You suppress fast decay (broad element) in primary part of FID, and emphasize sharp element in middle part.

※ You reduce the intensity of FID in primary part, so peak intensity decreases & quantity is lost.

(Ex) Processing result of [Single Exponential] to ca. 0.2 Hz of digital resolution data (upper figure) & Processing result of [Sinebell] (lower figure)



(4) Zerofill

Use it in the case you want to increase apparent digital resolution.

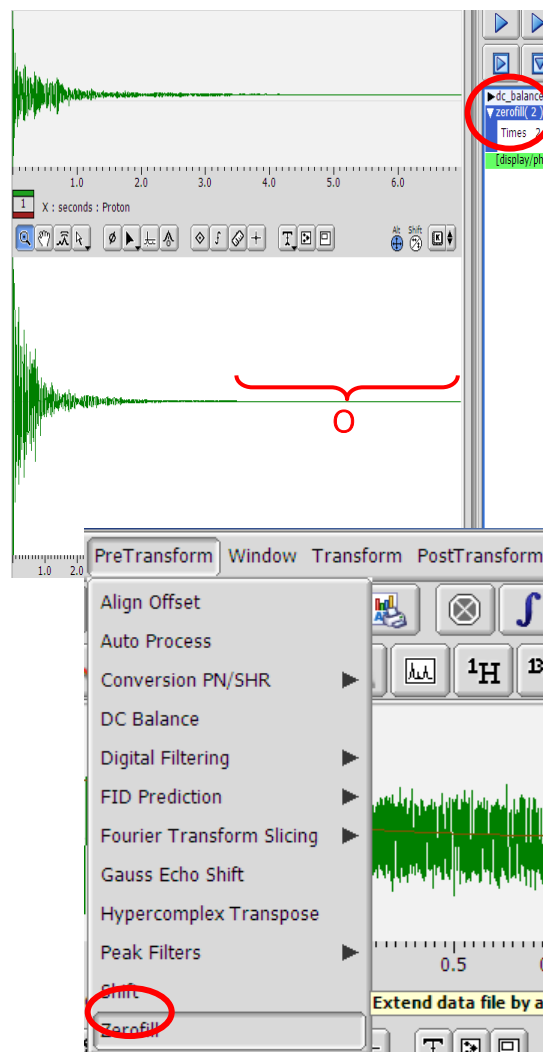
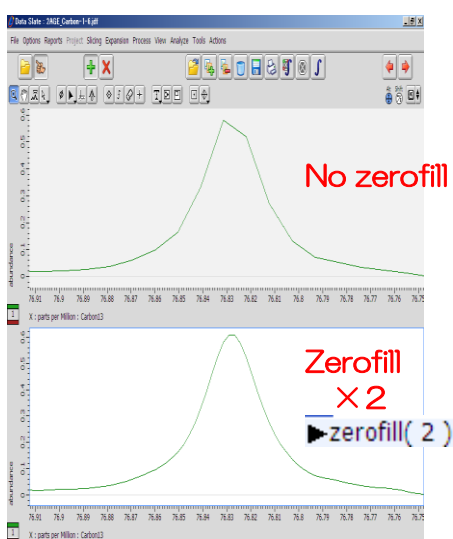
In Delta, select [PreTransform] in menu bar → [Zerofill], then design scale factor of number of data, and execute it.

※ After zerofill, number of data point should be 2^n ($\times 1$, $\times 2$, $\times 4$, $\times 8$,...) related to FFT algorithm.

※ In the case 「1」 is input, zerofill is not executed.

▶ zerofill(1)

When you add zero data point to tail of FID & multiply the data point by 2, these points are the ones between the original point and the point, after FT (bottom scheme).

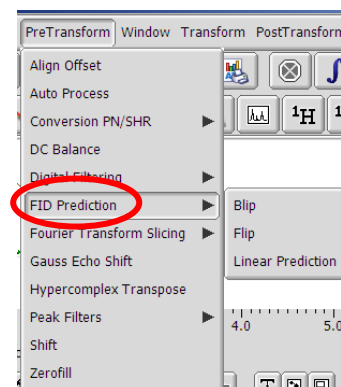


※ It is better that the end of FID is zero by performing window function to avoid truncation (preceding discussion) . ⇒ Combine [Single Exponential] with [Trapezoid]

※ Quantity of calculation increases with the square of data points, so time for FFT processing increases exponentially.

【Scale factor】 When you increase the number of zero point infinitely in 1D data, spectrum becomes smooth, but resolution does not become more than double. (more than quadruple zerofill is just interpolation by trigonometric.) You can theoretically interpolate unused imaginary part of N points of data from original 2N points of FID data. Therefore, in 1D data, double zerofill is special compared to more than double zerofill. In homonuclear 2D data, zerofill should be performed to make the number of F1 data points equal digital resolution of F2 axis (directly observing axis).


【FID Prediction】 Sometimes, prediction of frequency is used, instead of sequential zero value,





3-2. Processing after FT (PostTransform) — Output Data Part

(1) Hot key





In Output data part, [Key Shortcuts] is assigned to each mode selected by pointer bar. You can check by click of  button in each mode.


※ In pointer bar, you can check the explanation of the button by right-click on each button.


Check   to assign each mode to **Alt** key & **Shift** key of keyboard.

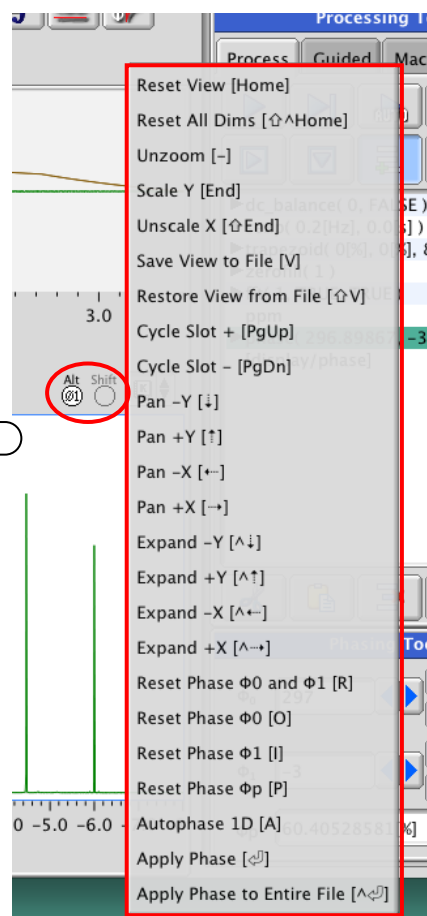
In each mode,

Space key + Assignment of range
 ⇒ Magnification of spectrum range 

Home key ※ On Mac keyboard, **Fn** + 
 ⇒ Back to display

 key ⇒ Back to the previous status

End key ※ On Mac keyboard, **Fn** + 
 ⇒ Auto-scaling of Y axis
 (with max intensity peak height)





Apple Keyboard



【Magnification】 To save magnified spectrum, select [Save Current View] in context menu displayed with long click of right button of mouse, on spectrum. Then, the data is saved with new version number. After that, saving data as the other name by [File]→[Save As...], does not reflect magnification. If you want to apply the magnification to data saved as the other name, open the data and magnify it again, then execute [Save Current View]. If you want to reflect magnified information of a data to the other data, drag & drop among the data with Zoom pointer.

(2) Phase correction

- ◎ [Machine Phase]  : Sequence measurements except for [Single Pulse] are not supported, because phase is seeked from the calculation based on measurement condition, which is independent of peak of spectrum. ※ Array measurement is not supported with even [Single Pulse].
- ◎ [AutoPhase]  : Phase is seeked from peak of spectrum, so long range of pulse sequence is supported. For high resolution, adjustment is required in many cases.

※ When you set a number of [phase] processing in process list, processed with $[\Phi_0]+[\Phi_1]$ value.

※ In the case you use [AutoPhase], delete [Machine Phase] (or, replace) .

◎ Manual phase correction

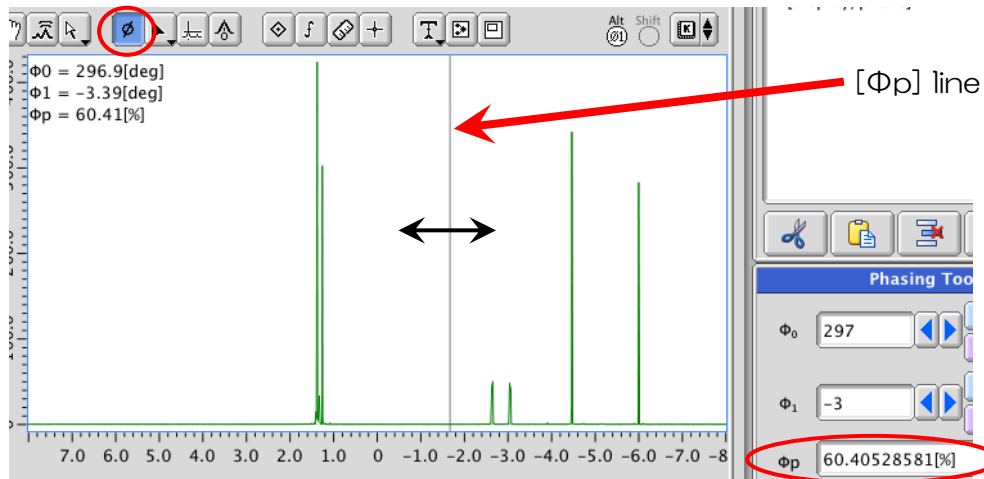
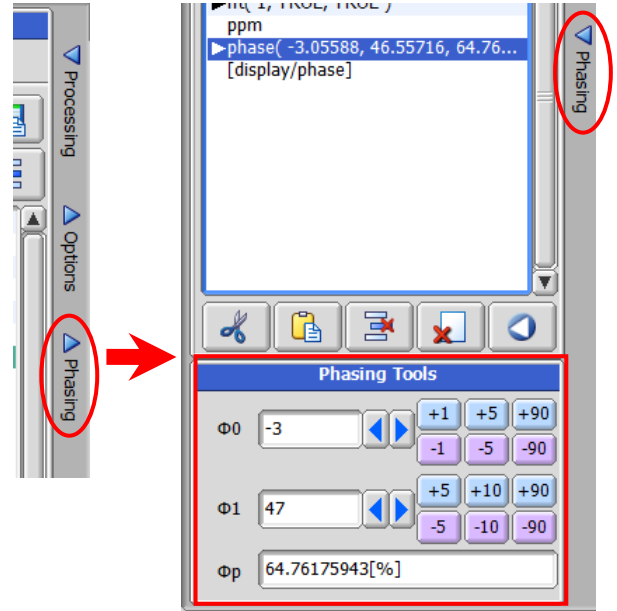
Click [►Phasing] in Panel switching button, spread [Phasing Tools] panel.

Select [Phase] mode  of pointer bar, click [AutoPhase] button .

※ Line appears on $[\Phi_p]$ (Pivot Point of Phase Correction) (Bottom scheme: On [%]age within the range of the observation, value is shown.) (⇒ Automatically it is set on the max intensity if peak. If it is not set, move the line with pointer by drag & drop.)

Near Pivot Point, adjust $[\Phi_0]$, and correct 0-dimensional phase.

Next, adjust $[\Phi_1]$ on the point as far as possible from Pivot Point and correct 1D phase.





[[Φ_0], [Φ_1]] [Φ_0] corrects the difference between primary phase of magnetization and phase of standard signal transmit into receiver. The phase should be corrected on the whole spectrum uniformly.


[Φ_1] corrects the phase originated from delay time. The phase should be corrected, dependent on frequency.

(3) Baseline Correction


① Auto-baseline correction



[PostTransform] in menu bar → [Baseline Correction▶] → [Base Correct] (or, [Base Correct]  on tool bar) Apply [base_correct] into process list, Click process button  & execute

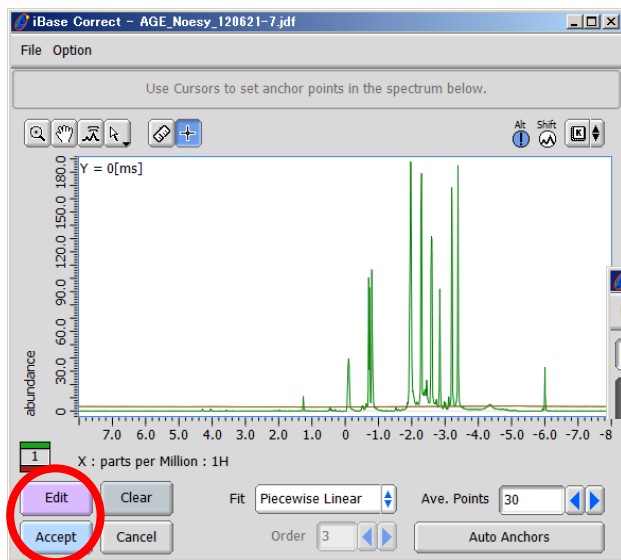
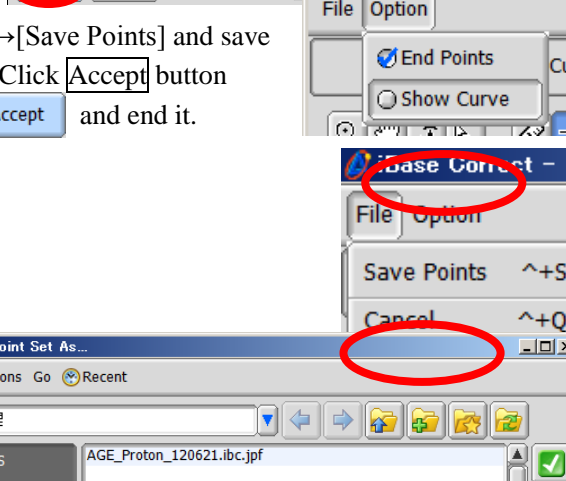
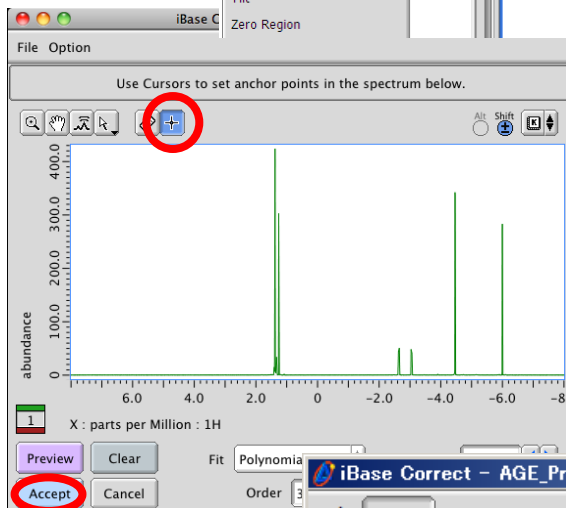
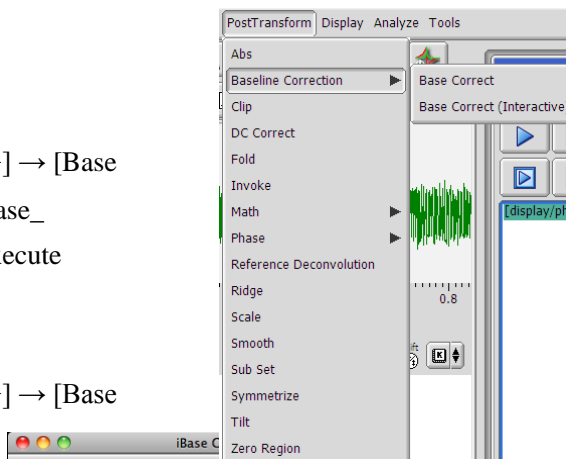
② Manual baseline correction

[PostTransform] in menu bar → [Baseline Correction▶] → [Base Correct (Interactive)] & apply [ibase_correct] into process list, and click process button  & execute.


On [iBase Correct] window (Right figure), select the suitable [Fit] (interpolation of base point) ([Piecewise Linear] is recommended.) . Set parameter [Ave Pnts] (= number of points for calculation of the intensity of base point by averaging) ※ you can use default setting.

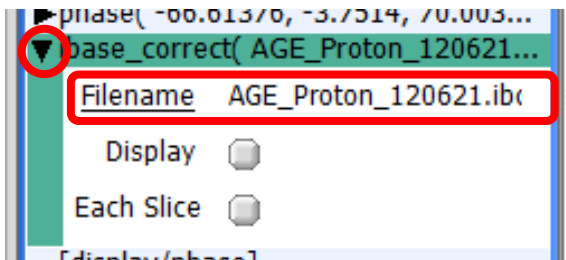
Select the pointer bar, [Create cursor] button  mode, and click several parts without signal (=baseline) (max 32 points) ※ Check [Option]→[Show Curve] (Right figure) .


Click [Preview] button  & check the spectrum. The spectrum does not look good, click [Edit] button  and try again. If it is good, select [File]→[Save Points] and save it. Click [Accept] button




and end it. Click [Accept] button

Finally, spread  [ibase_correct] in process list, click [Filename], and open the saved file & register it.

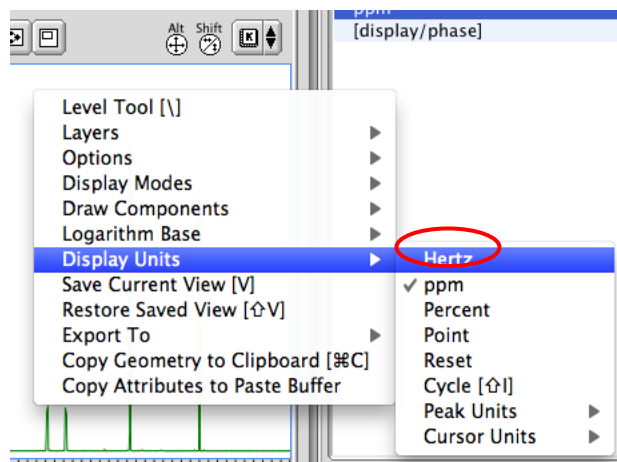


※ If you skip this operation, every time when you execute process list , on [iBase Correct] window, you repeat the operations.

(4) Unit of axis : PPM \leftrightarrow HZ


After FFT, Hz is displayed. Apply ppm display  into process list & execute it. (This process is applied in normal auto processing.)



※ It is the fastest way that in Output data part, on popup menu by right click, select [Display Units]→[Hertz] (in this case, contents of process list is ignored temporarily.)



(5) Reference setting 

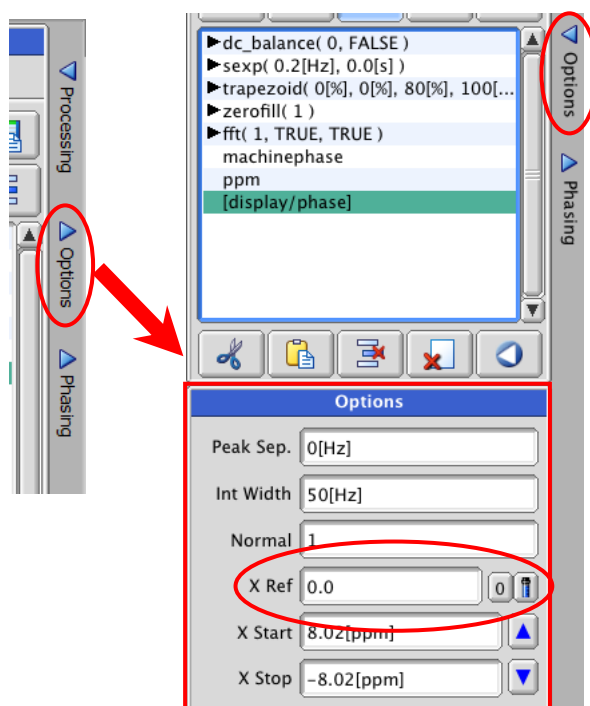
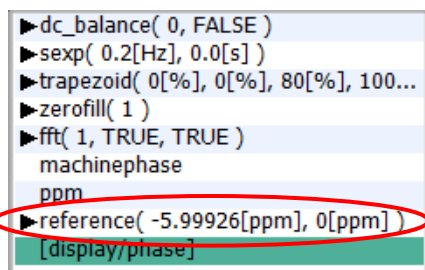
On pointer bar, select [Reference] mode .

Click panel switch button ▶[Options], spread [Options] panel, then input reference value ppm on [X Ref] column.

※ When you click  button, 0.0[ppm] (TMS reference value). When you click  button, reference value of the solvent signal is automatically input ((Ex) When the solvent is CDCl₃, it is input as

X Ref 7.24[ppm]   (CHCl₃) .)


Click the pointer on the top of reference peak, the applied into process list (Bottom figure) .




【Native scale】 When you do not set the reference, on Delta program, calculated value based on observed frequency of lock signal of each solvent is used.

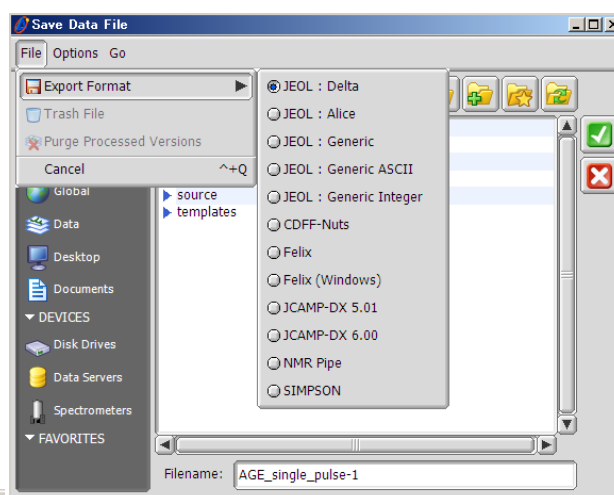
【Definition】 Reference of ¹H is defined as 0 ppm of chemical shift of the peak of TMS in infinitely-diluted CDCl₃ measured at 20°C.

4. Save of Spectrum Data / Export

On tool bar, click [Save] button . the spectrum is saved as the file name which is the same as measured raw data, but version is automatically updated. (On menu bar, you can save as other name.)

To export the data, select [File]→[Save as...], on the [Save Data File] window, select [File]→[Export Format ▶], and select the format & directory for the save. Input the file name & click  button.

When you select [ASCII], you can save the file as ASCII format (Bottom figure) .



X	Real	Imaginary	
12.50527892421294		-0.00072659382672	(
12.50499262709586		-0.00065328444215	(
12.50470632997878		-0.00027404904602	(
12.5044200328617		-0.00051193185336	(
12.50413373574462		-0.00091470314186	(
12.50384743862755		-0.00089003559101	(
12.50356114151047		-0.00064140504007	(


※ In Delta v5, The function which changes the width & type of spectrum, and font size of axis are not implemented. (As for font size, use "Page Layout Editor" (Later discussion)). By ASCII format, peak pick & intensity integration & separation of wave can be performed with KaleidaGraph or Origin, gnuplot (Freeware). Other graph soft.

In addition, the spectrum which is output by PDF is vector data. So, you can use Adobe Illustrator or Inkcape (Freeware) to change the line width.

(v4 offered the function above, from Preference.)

5. Final Data Processing (Peak pick, Intensity integration, Deconvolution)

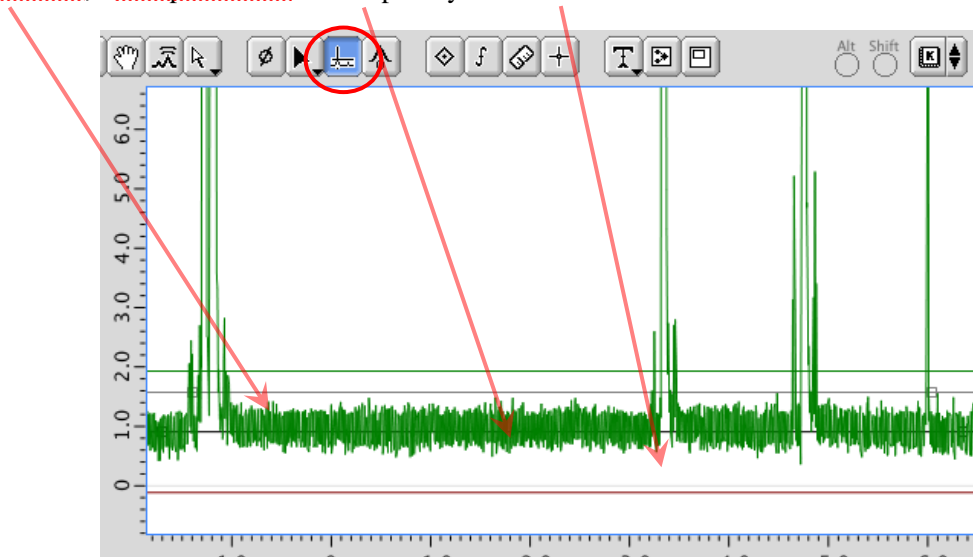
This processing is not reflected in process list.


In addition, if you accidentally click process execute button , all the result are deleted.

Without [1D Processor] window, but with [Data Slate] window, the same processing can be used (As described above, it can be processed with other graph soft.) .

(1) Peak pick

Click [Compute and Show Statics] button  on tool bar, then 3 markers like peak threshold level, noise threshold level, base plane level are temporarily shown.

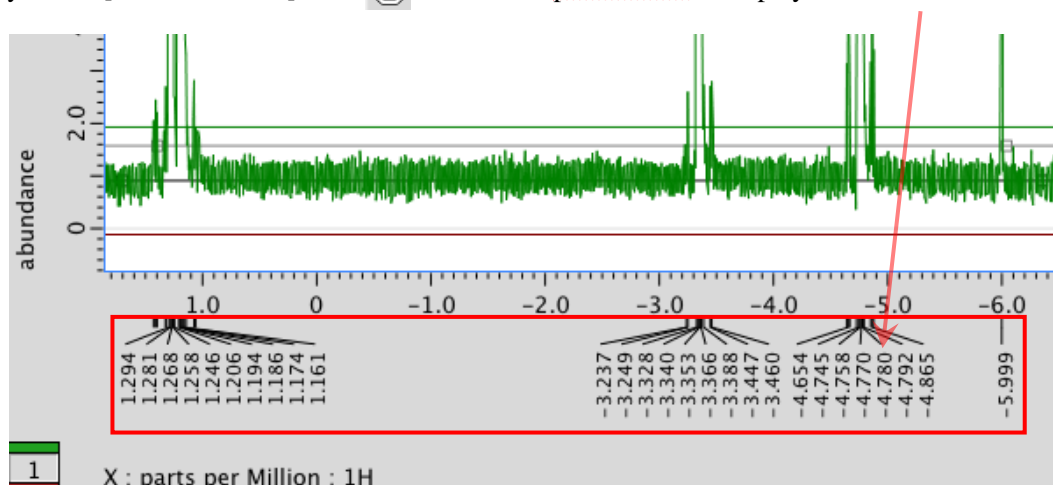


Next, with pointer bar select [Peak]mode , move pointer on peak threshold marker, then pointer changes into peak threshold icon. You can move it by drag & drop.


It is the same for noise threshold marker & base plane level marker.

※ In the case of peak threshold marker, you set the location by double-click of pointer.

Finally, Click [Auto Peak Pick] icon  in tool bar, peak marker is displayed.



① Selection of peak


With pointer bar select [Select] mode , click peak marker.
In the case of multiple selections, click them with keyboard **Shift** key.

※ You can highlight it with dragging mouse over it.

② Deletion of peak

Select the peak marker (①), type keyboard **Backspace** key. ※ With Mac, **Delete**

③ Addition of peak

With pointer bar select [Peak] mode , click the peak top where you want to add the pointer (Peak top is automatically picked.) .

※ The peak should be higher than peak threshold.


If you do the operation with **Shift** key, peak marker which shows the position is generated (Sometimes, in deconvolution, this method is used (later discussion) .

④ Display of J-value among peaks


Select 2 peaks, and click , and from pull-down menu, select [J coupling].

(2) Integration

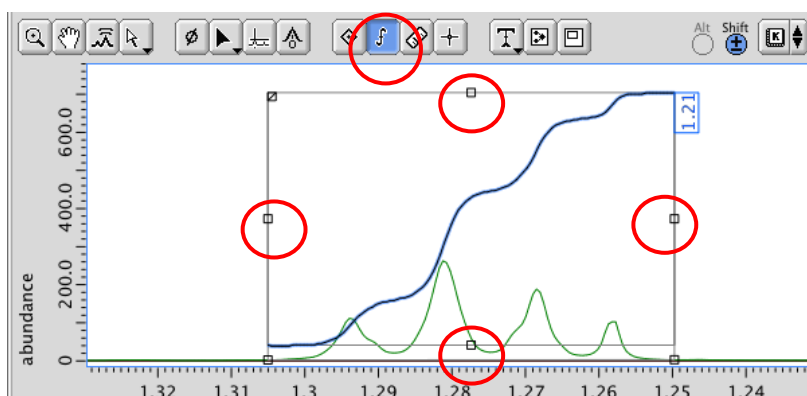
◎ Auto-integration

Click [Auto Integration] button  in tool bar.

◎ Manual integration

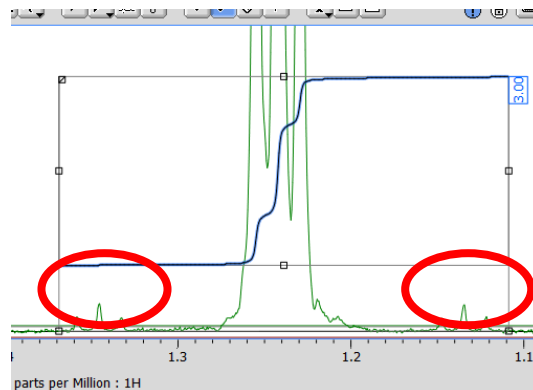
With pointer bar select [Integral] mode , drag & drop the pointer from left to right end of integration range.

To correct integration range & zoom-in or zoom-out of integration curve, select the integration, and drag & drop one of 4 grab boxes □.



Deletion or addition of integration is the same for Chapter (1).

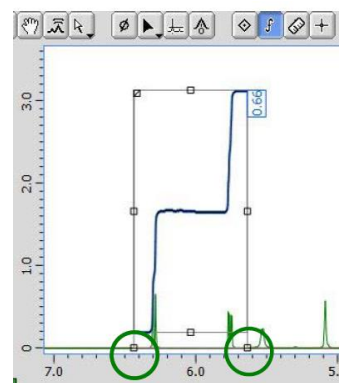
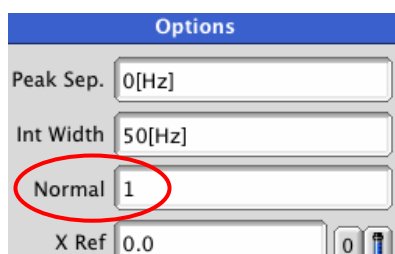
※Satellite peak in both side of main peak should be take in integration range(Right figure).



① Setting of integration reference

Click [▶Options] in panel switch button, and spread [Options] panel, input reference on [Normal] column.


Select reference integration, click , select [Normalize] in pull-down menu.

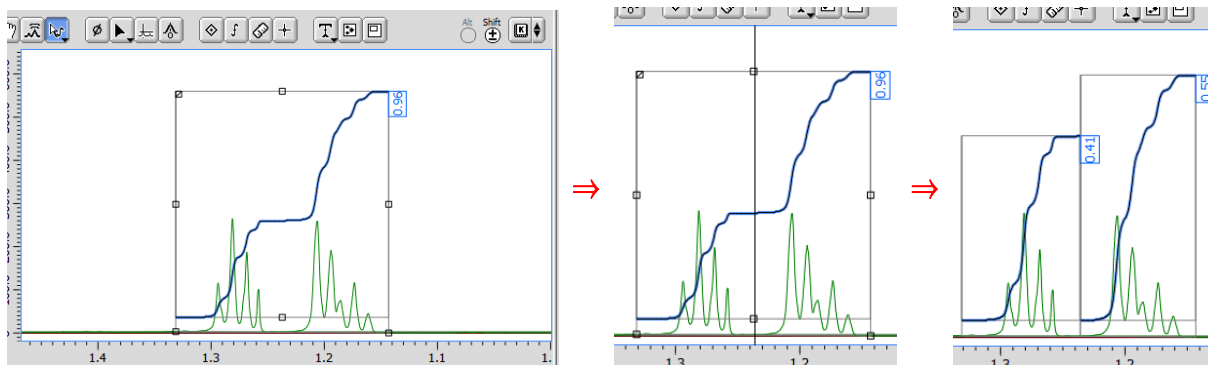


② Correction of integration baseline

Select integration curve, drag & drop lower grab box, with checking integration baseline.

③ Separation of integration curve

Select integration curve, and click left-upper grab box , then pointer turns into scissors, so you drug & drop it to the desired position.





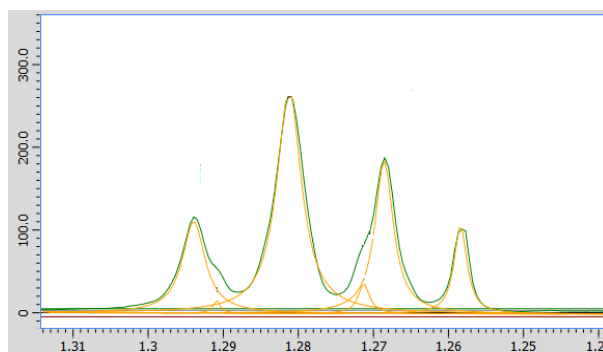
(3) DECONVOLUTION

Use it when signals are overlapping, and it is difficult to obtain each integration (integration ratio).

Pick peaks in the range (peak number & position), and magnify the range.


Select [Options] from popup menu by right-click on spectrum → [Peaks] → check [Deconvolve] ✓

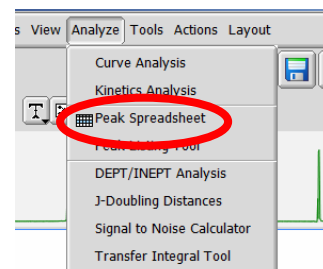
With pointer bar [Peak] mode , click , select wave shape of peak from pull-down menu ([Fit Lorentzian] or [Fit Gaussian] or [Fit Mixed]).



[Lorentzian] In the case of solvent, normally Lorentzian (or Mixed).

© Result of peak pick

On [2D Viewer] or [Data Slate] window, select [Analyze] in menu bar →  Peak Spreadsheet]. You can check [Spread Sheet] window.



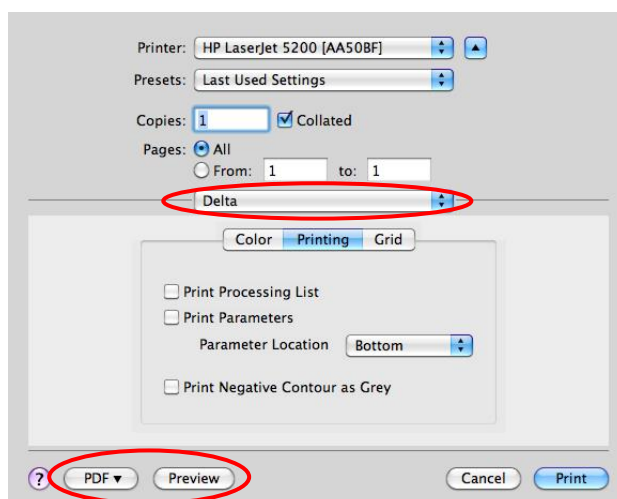
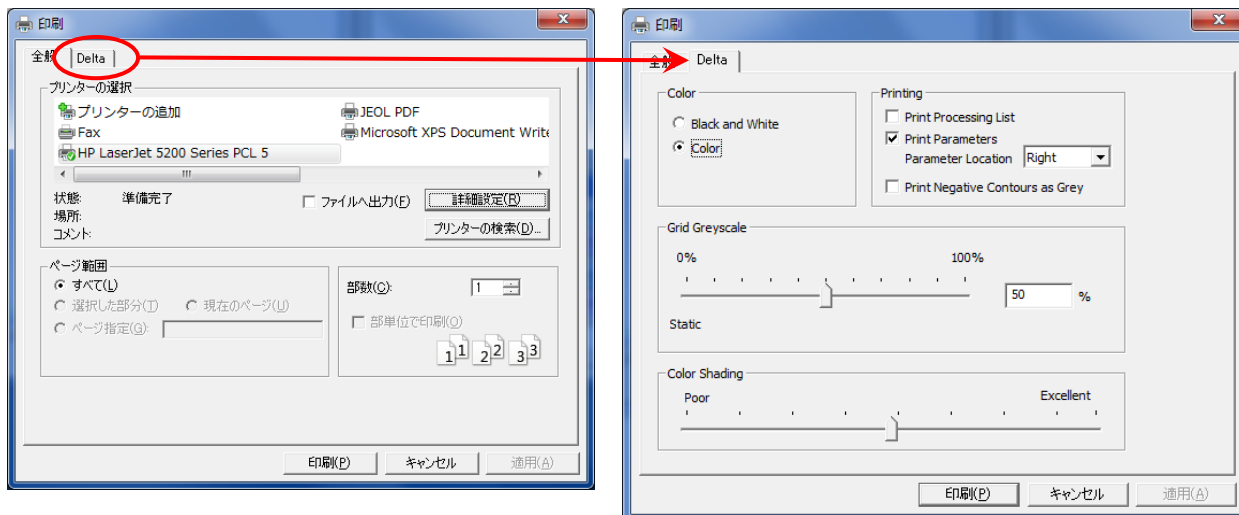
X	X Fold	Class	Normal	Integral	Intensity	Slope	Offset	G/L Mix
[ppm]						[abn/ppm]		
7.206	0	MD	3.000	3.647k	267.862	-11.264	0.365	0.000
7.193	0	MD	2.085	2.535k	187.116	-11.264	0.507	0.000
7.185	0	MD	0.537	652.867	61.132	-11.264	0.600	0.000
7.173	0	MD	1.105	1.343k	116.370	-11.264	0.737	0.000
7.160	0	MD	0.383	465.999	44.238	-11.264	0.876	0.000
1.239	0	MI	3.000	11.062k	0.000	-66.615m	79.959m	0.000

6. Printing

(1) Setting of printing

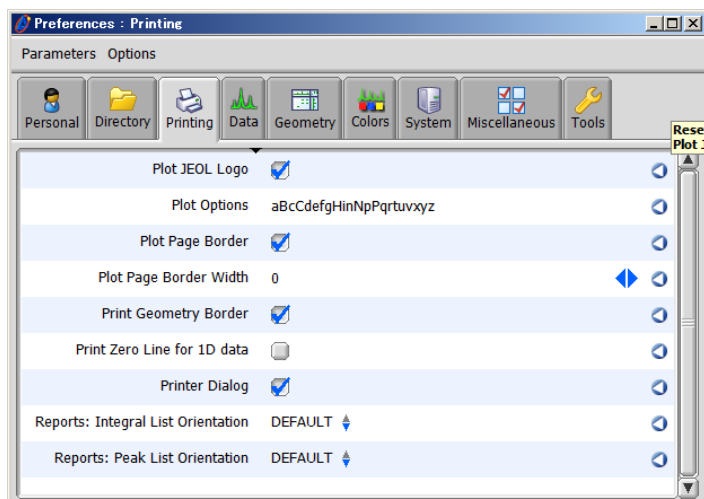
Click [Print Processed Data] button  in tool bar.

For detail setting, use [Delta] tab on [Print] window (Upper figure : Windows, Lower figure : Mac) .




【Fundamental setting】 On [Delta Console], select [Options]→[Preferences]. You can change the setting on [Printing] tab.

(Ex) If you do not print frame, uncheck [Plot Page Border] ✓ (For temporal use, select [Options] on context menu by right-click→[Display]→Uncheck [Plot Border] ✓) .

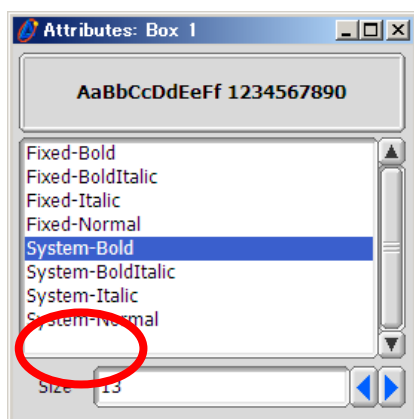


(2) Page Layout Editor

Select [Tools] in menu bar → [Page Layout Editor]. You can change font size.

On the window, select [Template] in menu bar. On <empty> box, you incorporate the data to print (Use Fingering .)

To change font size, select the box (Red frame), select [Box] in menu bar → [Attributes...]. In dialog box, use [Size] input box.



※ Default value is 13. This value is set on [Delta Console, which is opened by selecting [Options] → [Preferences], and then in [Tools tab] on the window (Lower figure) .

(3) PDF Output

In MS-Windows, when you install Delta, the PDF driver soft, 「JEOL PDF」 (in fact 「novaPDF」) is also installed. If you are not a MacOS X user, you can export PDF output.

※ Of course, Adobe Acrobat is enough.

※ When you use this PDF soft for the output by the soft other than Delta, Lower message is put on the lower part of the page.

「Create PDF files without this message by purchasing novaPDF printer (<http://www.novapdf.com>)」

