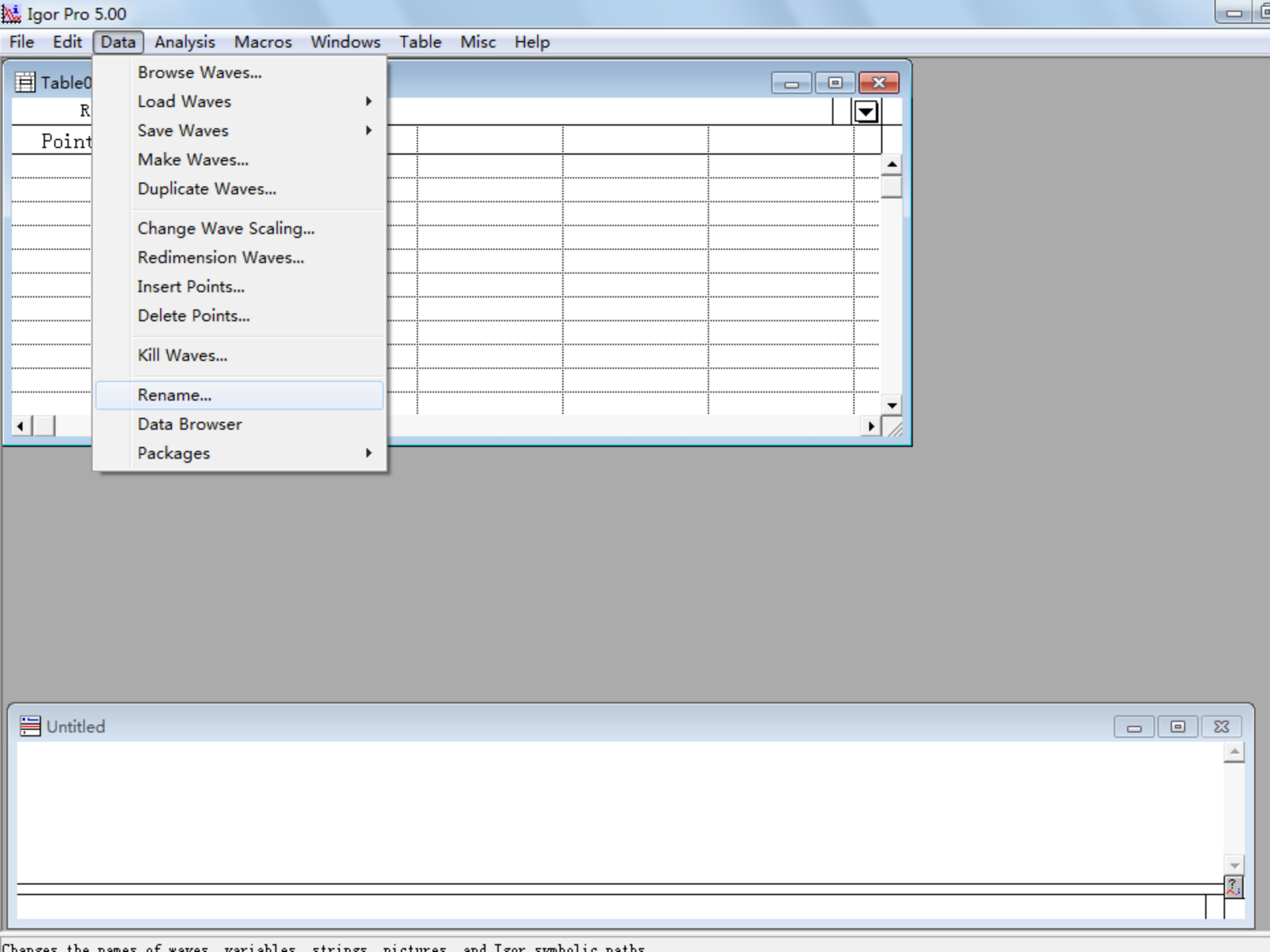
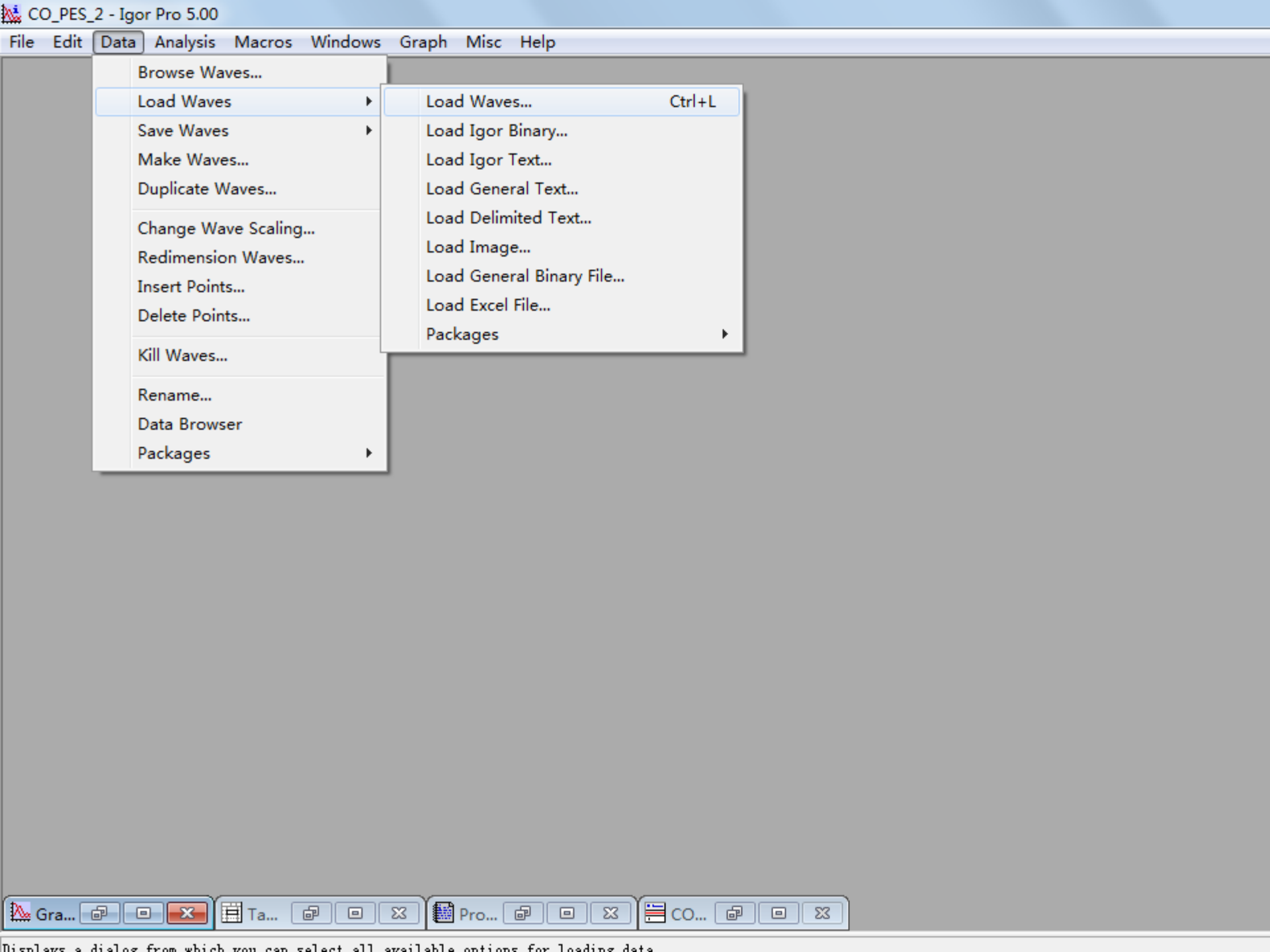
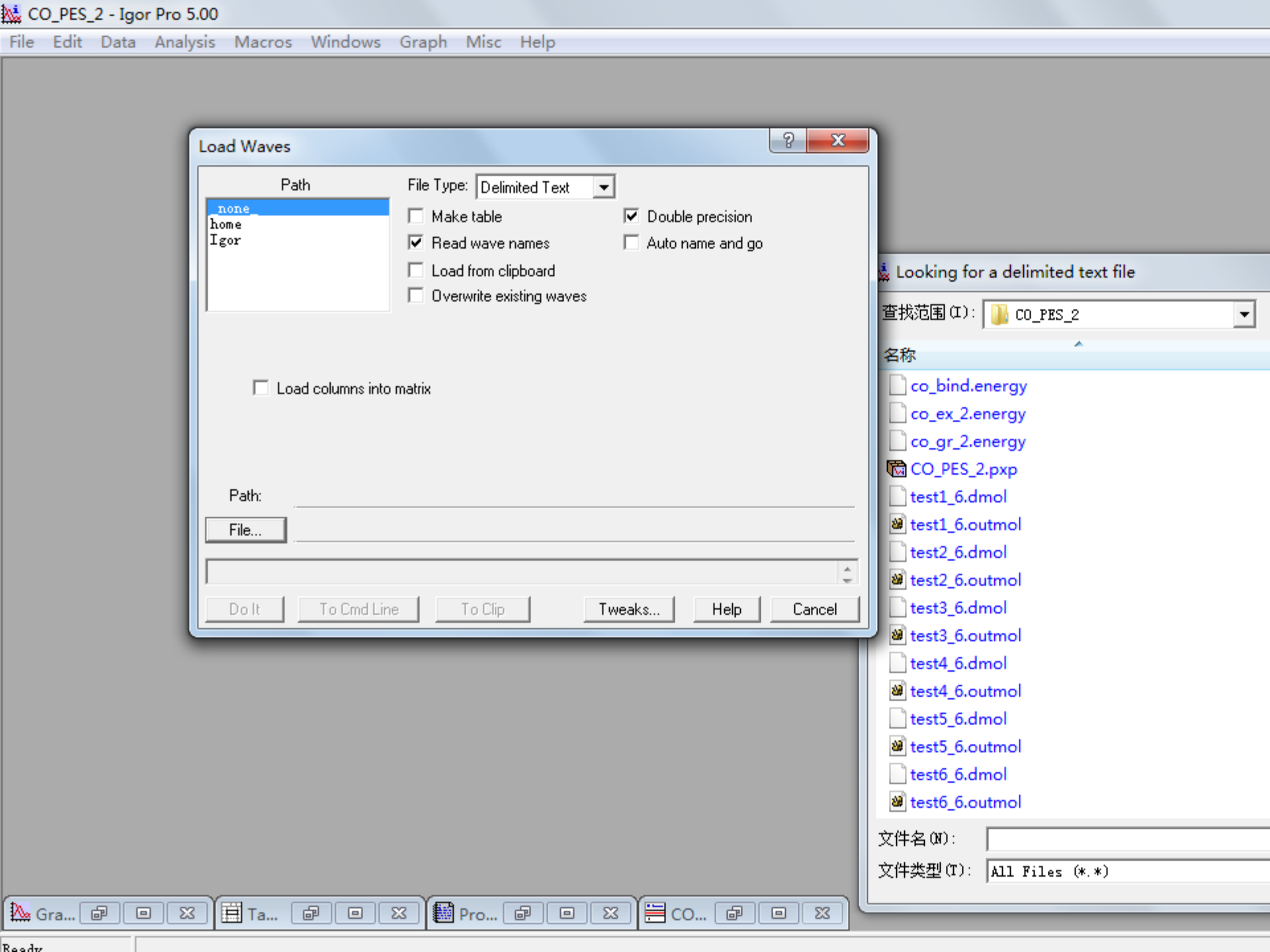
# Loading data into Igor
# Standard method

Using the Data/Load Waves options

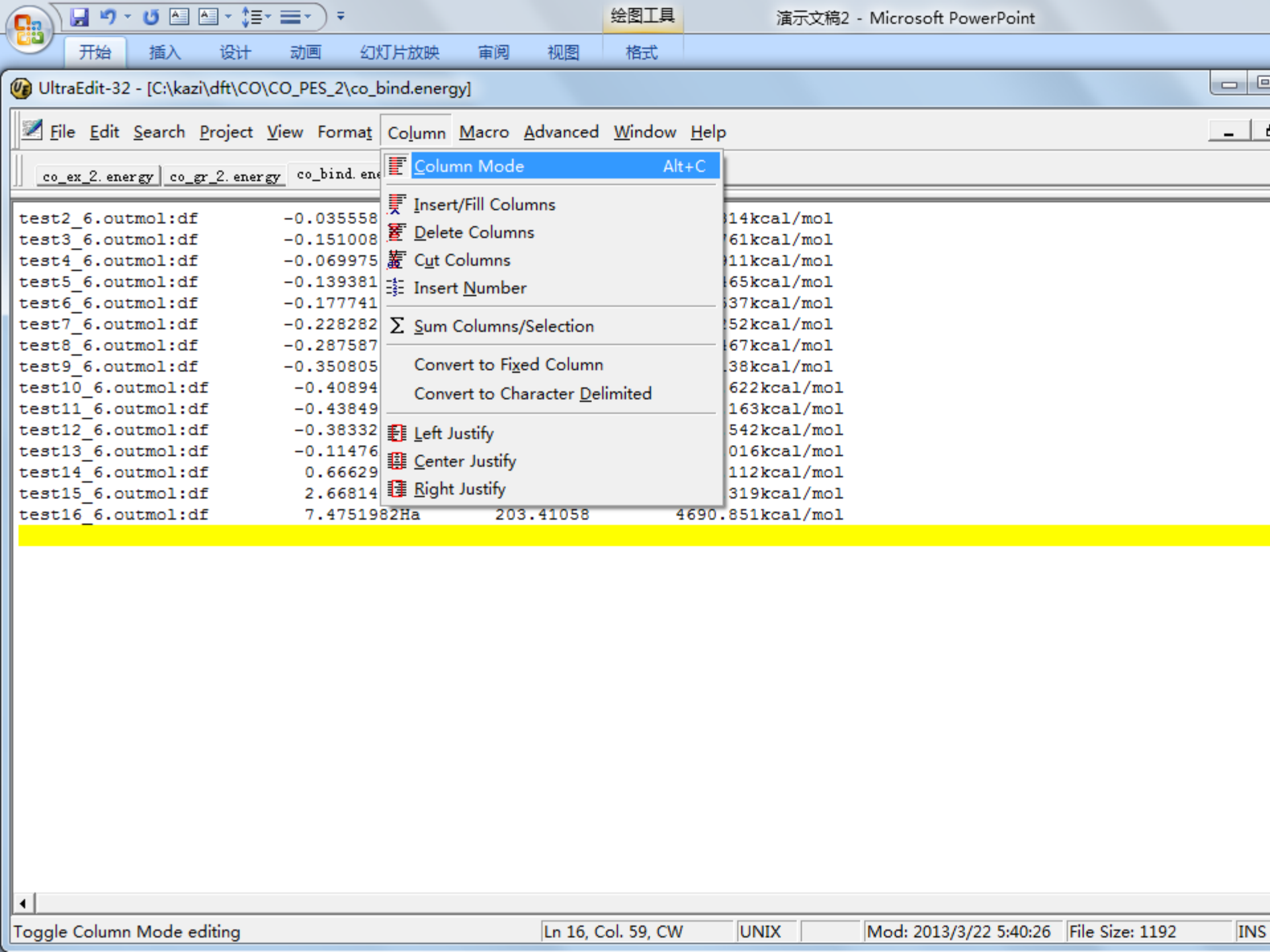

Igor Pro 5.00
File
Edit
Data
Analysis
Macros
Windows
Table
Misc
Help
Table0
Point
Browse Waves...
Load Waves
Save Waves
Make Waves...
Duplicate Waves...
Change Wave Scaling...
Redimension Waves...
Insert Points...
Delete Points...
Kill Waves...
Rename...
Data Browser
Packages
Untitled
Changes the names of waves, variables, strings, pictures, and Igor symbolic paths


CO_PES_2 - Igor Pro 5.00
File
Edit
Data
Analysis
Macros
Windows
Graph
Misc
Help
Browse Waves...
Load Waves
Save Waves
Make Waves...
Duplicate Waves...
Change Wave Scaling...
Redimension Waves...
Insert Points...
Delete Points...
Kill Waves...
Rename...
Data Browser
Packages
Load Waves... Ctrl+L
Load Igor Binary...
Load Igor Text...
Load General Text...
Load Delimited Text...
Load Image...
Load General Binary File...
Load Excel File...
Packages
Gra...
Ta...
Pro...
CO...
Displays a dialog from which you can select all available options for loading data


CO_PES_2 - Igor Pro 5.00
File Edit Data Analysis Macros Windows Graph Misc Help
Load Waves
Path
_none_
home
Igor
File Type: Delimited Text
Make table
Read wave names
Load from clipboard
Overwrite existing waves
Double precision
Auto name and go
Load columns into matrix
Path:
File...
Do It
To Cmd Line
To Clip
Tweaks...
Help
Cancel
Looking for a delimited text file
查找范围(I): CO_PES_2
名称
co_bind.energy
co_ex_2.energy
co_gr_2.energy
CO_PES_2.pxp
test1_6.dmol
test1_6.outmol
test2_6.dmol
test2_6.outmol
test3_6.dmol
test3_6.outmol
test4_6.dmol
test4_6.outmol
test5_6.dmol
test5_6.outmol
test6_6.dmol
test6_6.outmol
文件名(N):
文件类型(T): All Files (*.*)
Gra...
Ta...
Pro...
CO...
Ready

# Loading data into Igor
# Useful Method

Cut and paste columns of data using UltraEdit Column Mode


绘图工具
演示文稿2 - Microsoft PowerPoint
开始
插入
设计
动画
幻灯片放映
审阅
视图
格式
UltraEdit-32 - [C:\kazi\dft\CO\CO_PES_2\co_bind.energy]
File Edit Search Project View Format Column Macro Advanced Window Help
co_ex_2.energy
co_gr_2.energy
co_bind.ene
Column Mode Alt+C
Insert/Fill Columns
Delete Columns
Cut Columns
Insert Number
Sum Columns/Selection
Convert to Fixed Column
Convert to Character Delimited
Left Justify
Center Justify
Right Justify
test2_6.outmol:df -0.035558 314kcal/mol
test3_6.outmol:df -0.151008 761kcal/mol
test4_6.outmol:df -0.069975 911kcal/mol
test5_6.outmol:df -0.139381 465kcal/mol
test6_6.outmol:df -0.177741 537kcal/mol
test7_6.outmol:df -0.228282 252kcal/mol
test8_6.outmol:df -0.287587 467kcal/mol
test9_6.outmol:df -0.350805 138kcal/mol
test10_6.outmol:df -0.40894 622kcal/mol
test11_6.outmol:df -0.43849 163kcal/mol
test12_6.outmol:df -0.38332 542kcal/mol
test13_6.outmol:df -0.11476 016kcal/mol
test14_6.outmol:df 0.66629 112kcal/mol
test15_6.outmol:df 2.66814 319kcal/mol
test16_6.outmol:df 7.4751982Ha 203.41058 4690.851kcal/mol
Toggle Column Mode editing
Ln 16, Col. 59, CW
UNIX
Mod: 2013/3/22 5:40:26
File Size: 1192
INS

Igor Pro 5.00

File Edit Data Analysis Macros Windows Table Misc Help

UltraEdit-32 - [C:\ytmp\abs]

File Edit Search Project View Format Column Macro Advanced Window Help

U_L_opt.pdb | Energy-UXrib | co.energy | co_ex.energy | abs | rep1

```
    Absorption
         400      2
8000.0000    ,0.11187107
8010.0000    ,0.11696653
8020.0000    ,0.12212091
8030.0000    ,0.12732606
8040.0000    ,0.13257391
8050.0000    ,0.13785647
8060.0000    ,0.14316598
8070.0000    ,0.14849492
8080.0000    ,0.15383608
8090.0000    ,0.15918264
8100.0000    ,0.16452822
8110.0000    ,0.16986691
8120.0000    ,0.17519333
8130.0000    ,0.18050267
8140.0000    ,0.18579073
8150.0000    ,0.19105392
8160.0000    ,0.19628929
8170.0000    ,0.20149457
8180.0000    ,0.20666814
8190.0000    ,0.21180904
8200.0000    ,0.21691699
8210.0000    ,0.22199233
8220.0000    ,0.22703607
8230.0000    ,0.23204981
8240.0000    ,0.23703573
8250.0000    ,0.24199659
8260.0000    ,0.24693568
8270.0000    ,0.25185677
8280.0000    ,0.25676411
8290.0000    ,0.26166235
```

For Help, press F1 | Ln 3, Col. 16, CW | UNIX | Mod: 2013/3/21 2:31:09 | Col Sel: 10 | INS

Igor Pro 5.00

File Edit Data Analysis Macros Windows Table Misc Help

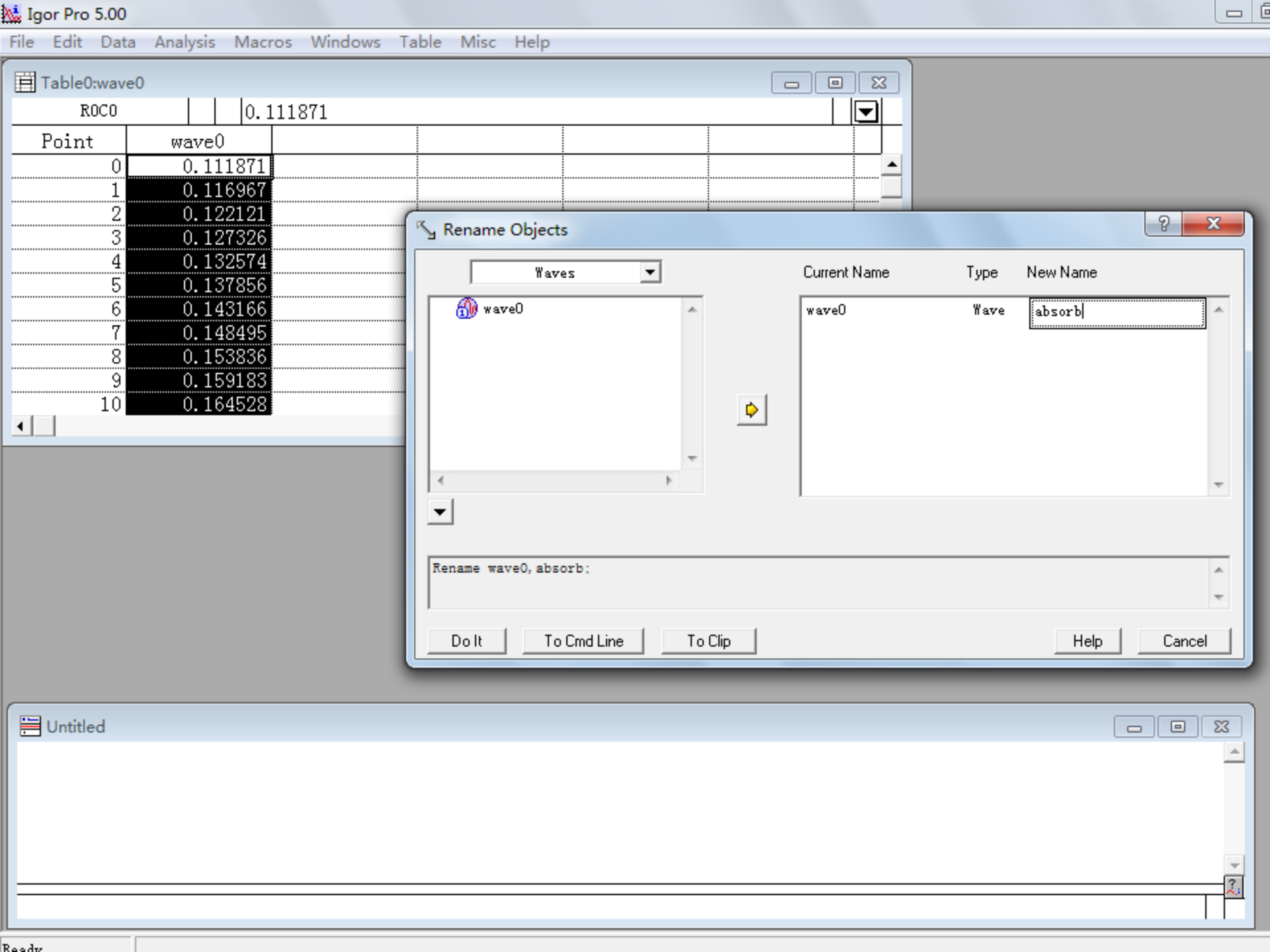
Table0:wave0

| R0C0 | | | 0.111871 | | | | |
|---|---|---|---|---|---|---|---|
| Point | wave0 | | | | | | |
| 0 | 0.111871 | | | | | | |
| 1 | 0.116967 | | | | | | |
| 2 | 0.122121 | | | | | | |
| 3 | 0.127326 | | | | | | |
| 4 | 0.132574 | | | | | | |
| 5 | 0.137856 | | | | | | |
| 6 | 0.143166 | | | | | | |
| 7 | 0.148495 | | | | | | |
| 8 | 0.153836 | | | | | | |
| 9 | 0.159183 | | | | | | |
| 10 | 0.164528 | | | | | | |

Untitled

```
rename wave0 absorb
```

Ready


Igor Pro 5.00
File Edit Data Analysis Macros Windows Table Misc Help
Table0:wave0
R0C0
0.111871
Point
wave0
0 0.111871
1 0.116967
2 0.122121
3 0.127326
4 0.132574
5 0.137856
6 0.143166
7 0.148495
8 0.153836
9 0.159183
10 0.164528
Rename Objects
Waves
wave0
Current Name
Type
New Name
wave0
Wave
absorb
Rename wave0, absorb;
Do It
To Cmd Line
To Clip
Help
Cancel
Untitled
Ready

Igor Pro 5.00

File Edit Data Analysis Macros Windows Table Misc Help

Table0:absorb,rr

| R0C1 | | | 8000 | | | |
|---|---|---|---|---|---|---|
| Point | absorb | rr | | | | |
| 0 | 0.111871 | 8000 | | | | |
| 1 | 0.116967 | 8010 | | | | |
| 2 | 0.122121 | 8020 | | | | |
| 3 | 0.127326 | 8030 | | | | |
| 4 | 0.132574 | 8040 | | | | |
| 5 | 0.137856 | 8050 | | | | |
| 6 | 0.143166 | 8060 | | | | |
| 7 | 0.148495 | 8070 | | | | |
| 8 | 0.153836 | 8080 | | | | |
| 9 | 0.159183 | 8090 | | | | |
| 10 | 0.164528 | 8100 | | | | |

Untitled

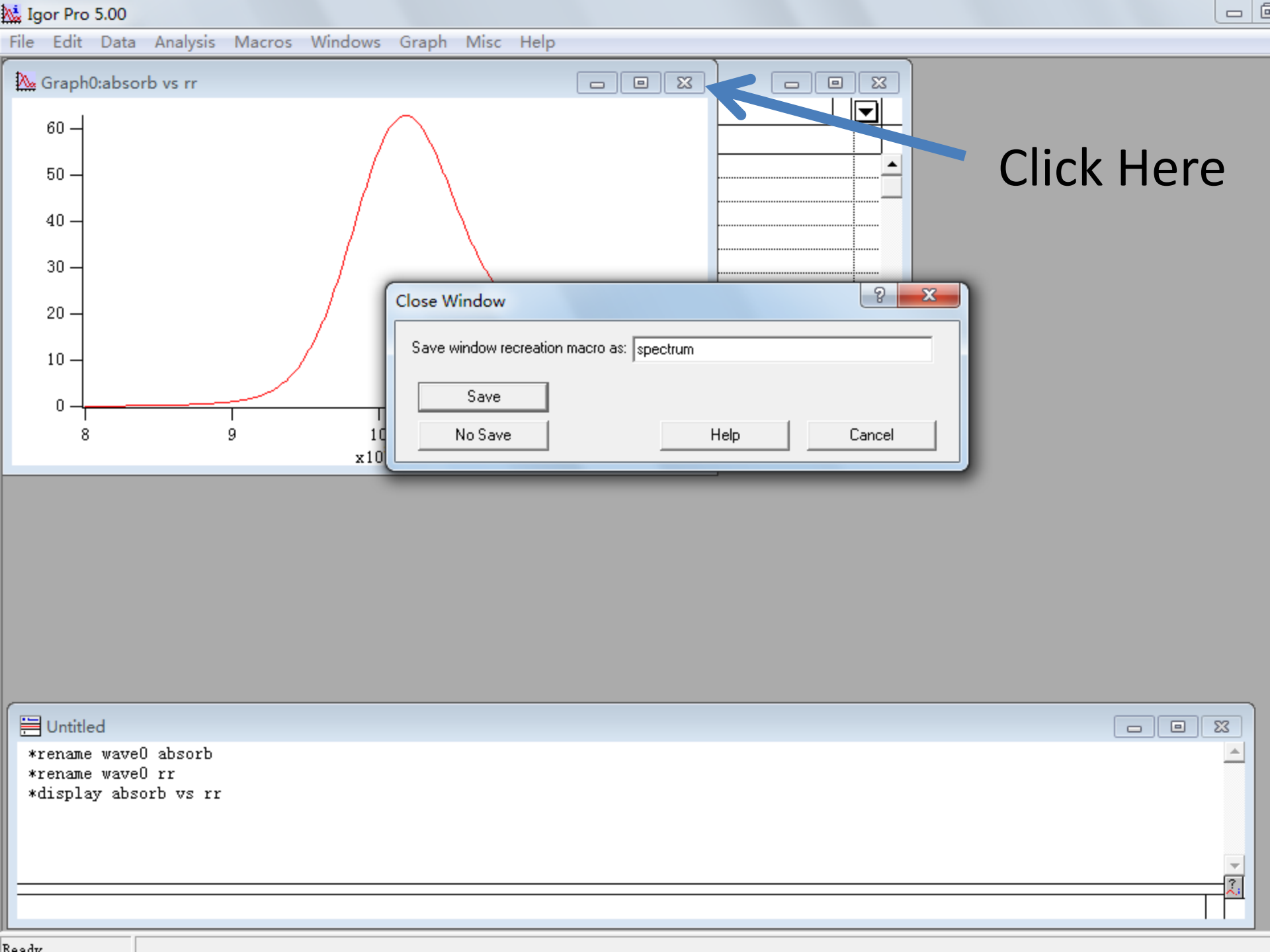
```
*rename wave0 absorb
*rename wave0 rr
```

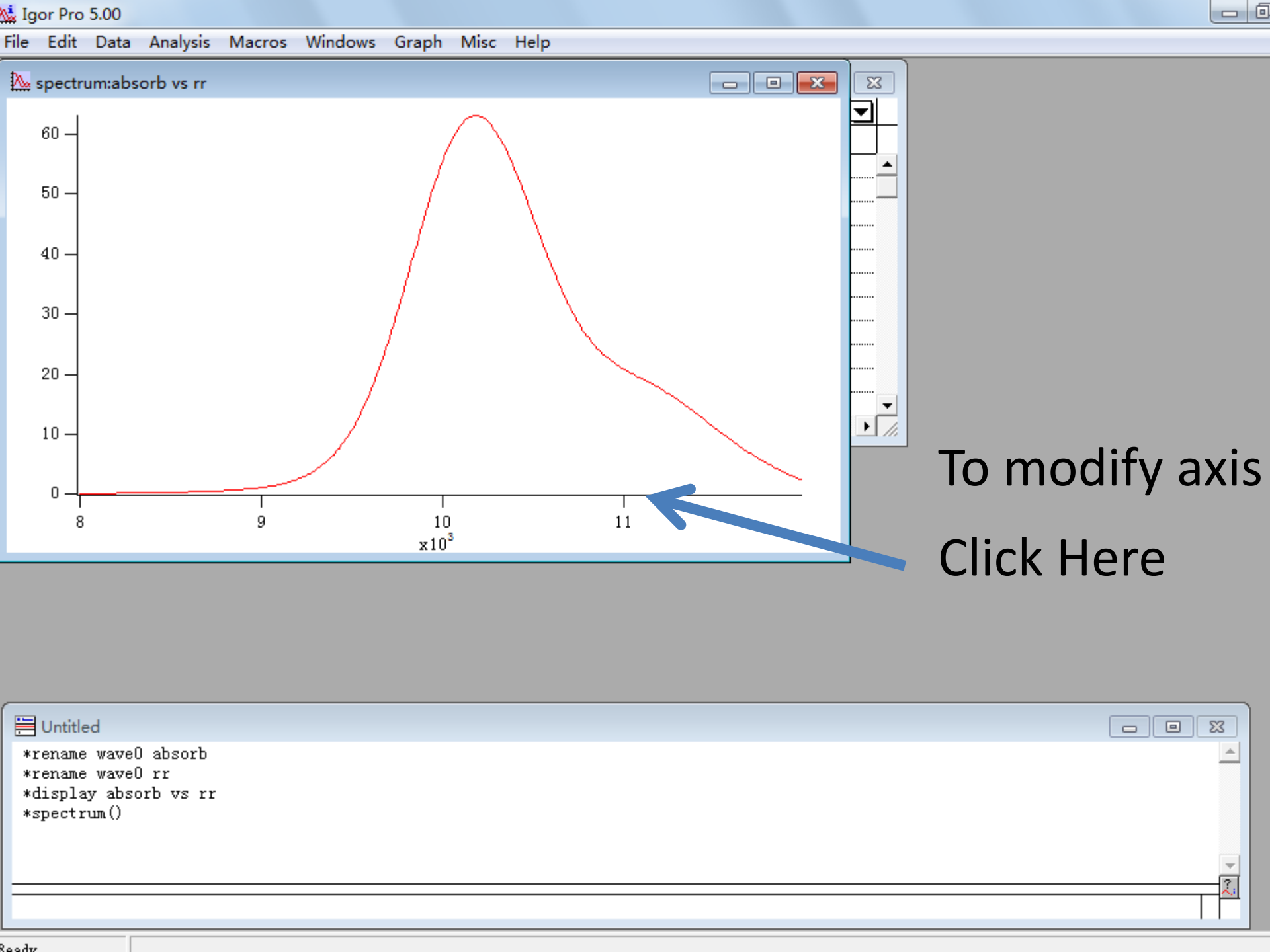
```
display absorb vs rr
```

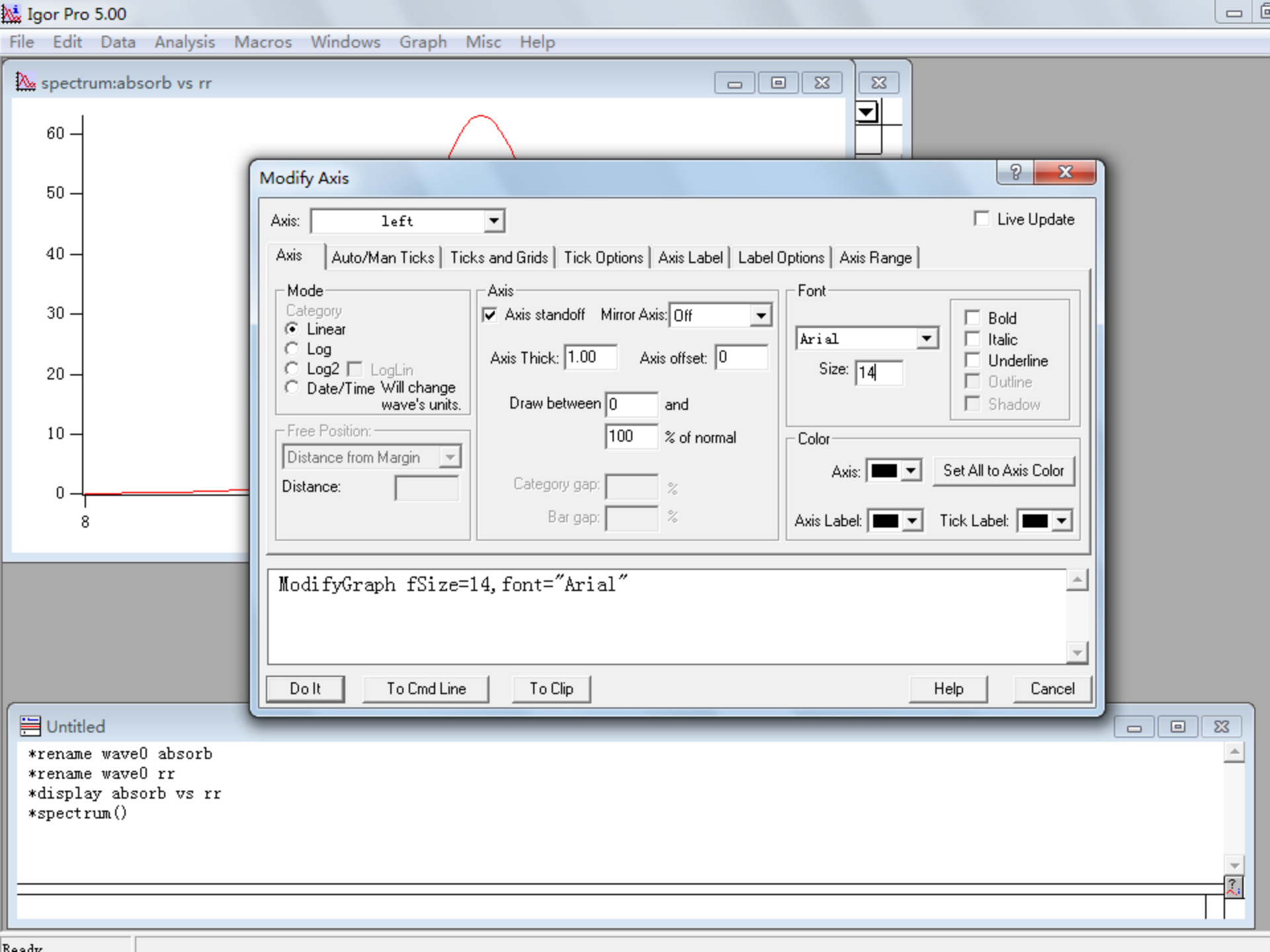
Ready

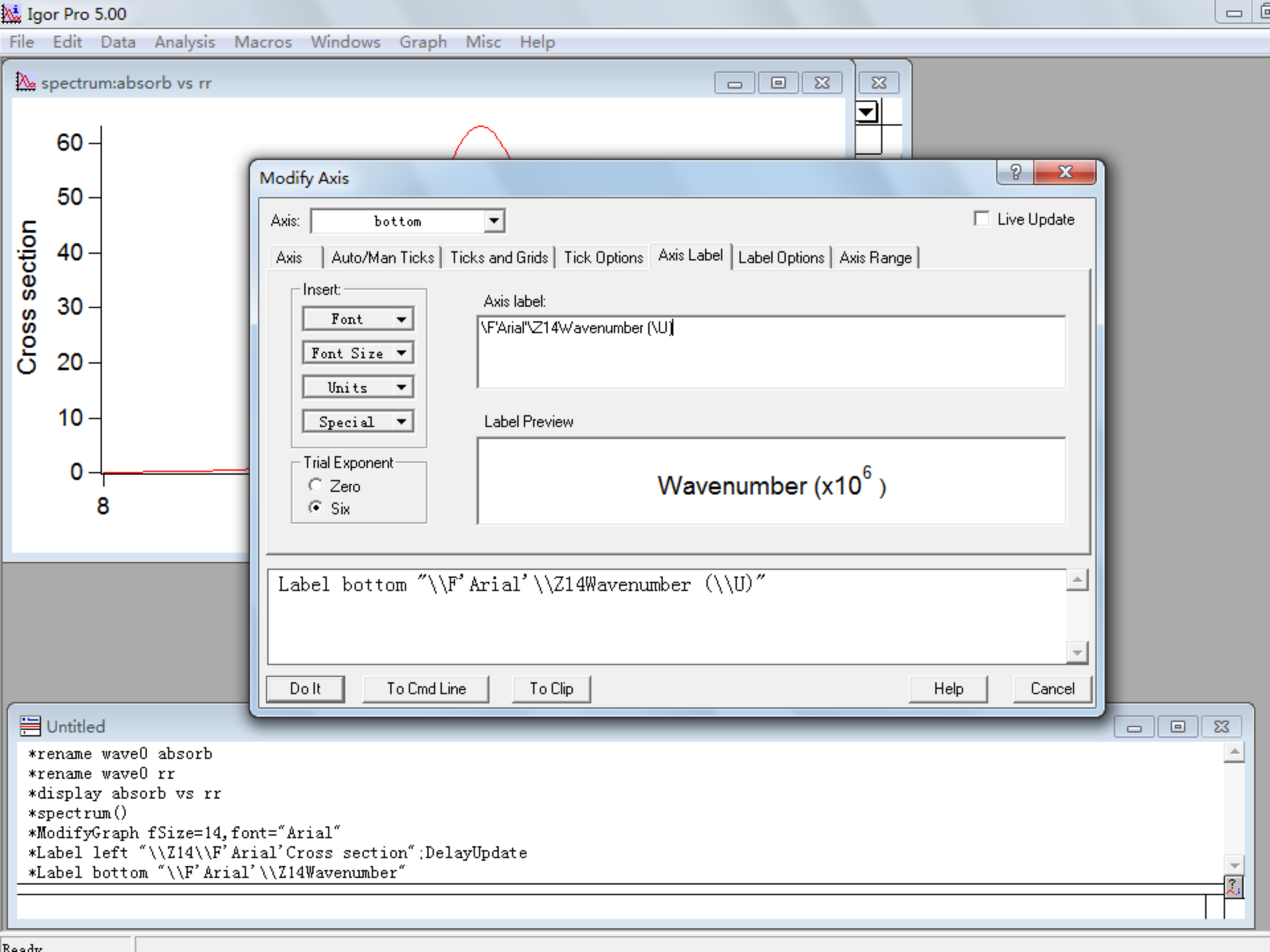
# Saving Graphs

To close the graph and save it, click on the  X in the upper right hand corner


Igor Pro 5.00
File Edit Data Analysis Macros Windows Graph Misc Help
Graph0:absorb vs rr
60
50
40
30
20
10
0
8
9
x10
Click Here
Close Window
Save window recreation macro as:
spectrum
Save
No Save
Help
Cancel
Untitled
*rename wave0 absorb
*rename wave0 rr
*display absorb vs rr
Ready


Igor Pro 5.00
File Edit Data Analysis Macros Windows Graph Misc Help
spectrum:absorb vs rr
60
50
40
30
20
10
0
8
9
10
11
x10^3
To modify axis
Click Here
Untitled
*rename wave0 absorb
*rename wave0 rr
*display absorb vs rr
*spectrum()


Igor Pro 5.00
File Edit Data Analysis Macros Windows Graph Misc Help
spectrum:absorb vs rr
60
50
40
30
20
10
0
8
Modify Axis
Axis: left
Live Update
Axis Auto/Man Ticks Ticks and Grids Tick Options Axis Label Label Options Axis Range
Mode
Category
Linear
Log
Log2 LogLin
Date/Time Will change wave's units.
Free Position:
Distance from Margin
Distance:
Axis
Axis standoff Mirror Axis: Off
Axis Thick: 1.00 Axis offset: 0
Draw between 0 and
100 % of normal
Category gap: %
Bar gap: %
Font
Arial
Size: 14
Bold
Italic
Underline
Outline
Shadow
Color
Axis:
Set All to Axis Color
Axis Label: Tick Label:
ModifyGraph fSize=14,font="Arial"
Do It
To Cmd Line
To Clip
Help
Cancel
Untitled
*rename wave0 absorb
*rename wave0 rr
*display absorb vs rr
*spectrum()
Ready


Igor Pro 5.00
File Edit Data Analysis Macros Windows Graph Misc Help
spectrum:absorb vs rr
Cross section
60
50
40
30
20
10
0
8
Modify Axis
Axis: bottom
Live Update
Axis Auto/Man Ticks Ticks and Grids Tick Options Axis Label Label Options Axis Range
Insert:
Font
Font Size
Units
Special
Trial Exponent
Zero
Six
Axis label:
\F'Arial'\Z14Wavenumber (\U)
Label Preview
Wavenumber (x10^6 )
Label bottom "\\F'Arial'\\Z14Wavenumber (\\U)"
Do It
To Cmd Line
To Clip
Help
Cancel
Untitled
*rename wave0 absorb
*rename wave0 rr
*display absorb vs rr
*spectrum()
*ModifyGraph fSize=14,font="Arial"
*Label left "\\Z14\\F'Arial'Cross section";DelayUpdate
*Label bottom "\\F'Arial'\\Z14Wavenumber"
Ready

# Fitting with Igor

Select Analysis/Curve Fitting

Choose a fitting function

To use cursor type <Ctrl I>

Select [Data Options] to limit the range

CO_PES_2 - Igor Pro 5.00

File Edit Data Analysis Macros Windows Graph Misc Help

Curve Fitting...
Wave Stats...
Fourier Transforms...
Smooth...
Hanning...
Convolve...
Correlate...
Integrate...
Differentiate...
Histogram...
Sort...
Misc Operations
Compose Expression...
Interpolate...
Packages

Table0:pes,rr,

R12C0

| Point |
|---|
| 0 |
| 1 |
| 2 |
| 3 |
| 4 |
| 5 |
| 6 |
| 7 |
| 8 |
| 9 |
| 10 |
| 11 |
| 12 |

ground vs rr

20
0
-20
-0.2
-0.1
0.0
0.1
0.2
0.3

A: excited
B: excited
pnt: 10 X: -0.15 Y: 21.333 dX: 0.3
pnt: 4 X: 0.15 Y: -12.724 dY: -34.056

*SetAxis/A
*SetAxis/A

CurveFit poly 5, excit

Fits a curve (waveform or XY pair) to built-in or user-defined functions

CO_PES_2 - Igor Pro 5.00

File Edit Data Analysis Macros Windows Graph Misc Help

Table0:pes,rr,excited,ground

| R12C0 | |
|---|---|
| Point | pes |
| 0 | -1.90 |
| 1 | -3.79 |
| 2 | -4.83 |
| 3 | -6.21 |
| 4 | -7.82 |
| 5 | -9.54 |
| 6 | -11. |
| 7 | -11.9 |
| 8 | -10.4 |
| 9 | -3.12 |
| 10 | 18.1 |
| 11 | 72.6 |
| 12 | |

*SetAxis/A
*SetAxis/A

Graph0:excited vs rr;ground vs rr

60
40
20
0
-20
-0.2
-0.1
0.0
0.1
0.2
0.3

Curve Fitting

Function and Data | Data Options | Coefficients | Output Options

Function
poly
Polynomial Terms: 5
New Fit Function...
Edit Fit Function...

Y Data
excited
From Target

X Data
If you have only a Y wave, selec
_calculated_
rr

Show:
Equation
Commands

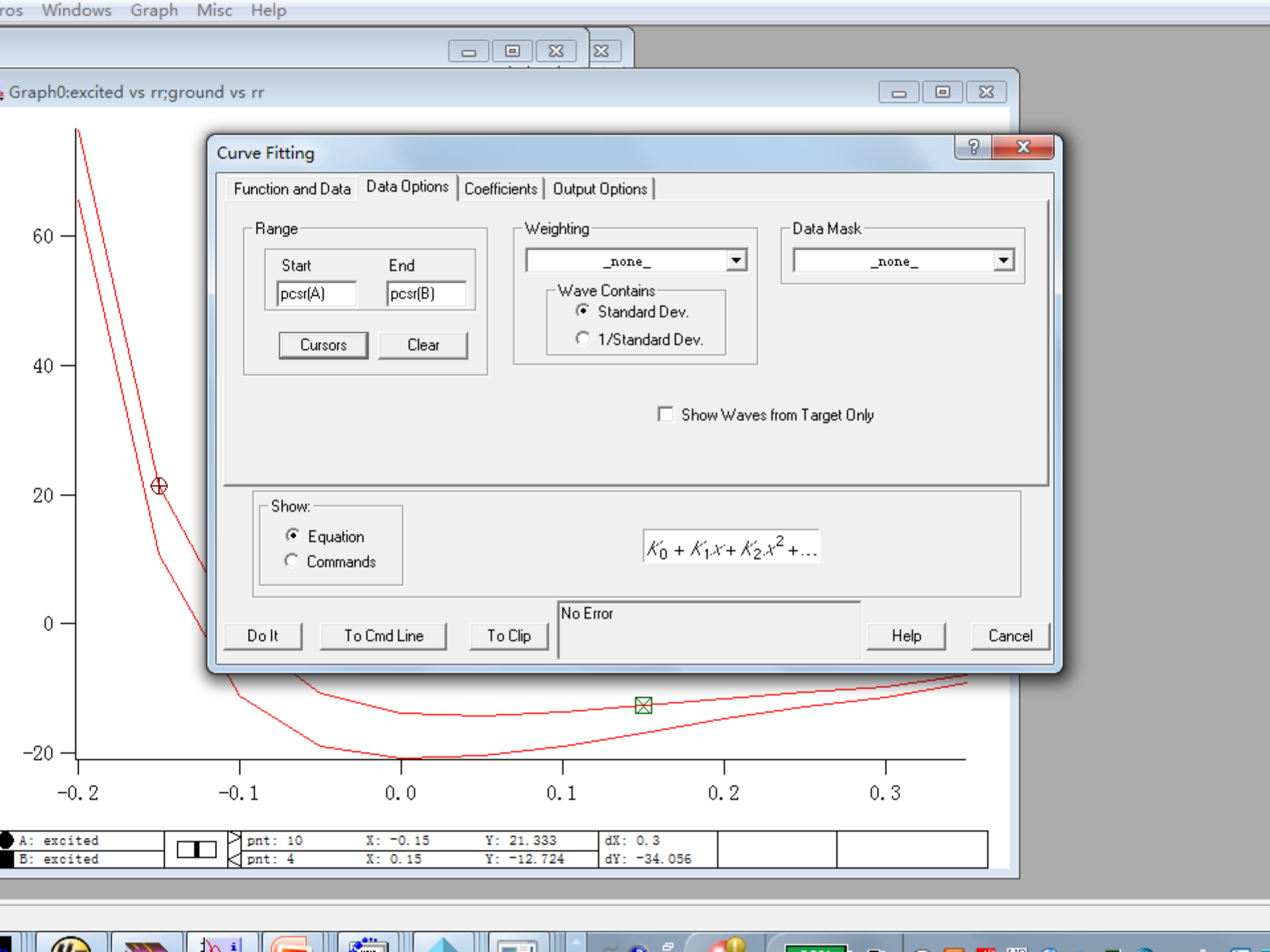
$K_0 + K_1 x + K_2 x^2 + \ldots$

No Error

Do It | To Cmd Line | To Clip | Help

A:
B: ground
pnt:
X:
Y:
dX:
pnt: 3
X: 0.2
Y: -14.785
dY:

Ready


ros Windows Graph Misc Help
Graph0:excited vs rr;ground vs rr
Curve Fitting
Function and Data
Data Options
Coefficients
Output Options
Range
Start
End
pcsr(A)
pcsr(B)
Cursors
Clear
Weighting
_none_
Wave Contains
Standard Dev.
1/Standard Dev.
Data Mask
_none_
Show Waves from Target Only
Show:
Equation
Commands
$K_0 + K_1 x + K_2 x^2 + \ldots$
No Error
Do It
To Cmd Line
To Clip
Help
Cancel
60
40
20
0
-20
-0.2
-0.1
0.0
0.1
0.2
0.3
A: excited
B: excited
pnt: 10
X: -0.15
Y: 21.333
dX: 0.3
pnt: 4
X: 0.15
Y: -12.724
dY: -34.056