

**FROM THE CHAIR--
Don Rosenthal**

The Committee on Computers in Chemical Education (C.C.C.E.) seeks to promote the use of computers and computing in chemical education. We do this by means of this Newsletter, by helping to organize symposia at National Meetings, by sponsoring new initiatives like the Computer Conference to be held this summer (described elsewhere in this Newsletter), by organizing workshops and by holding open meetings at the Biennial Conferences on Chemical Education. Let me describe some future activities and then indicate how you can help.

Symposia at National Meetings: A symposium entitle "Computers in Chemical Education" has been organized for the fall 1993 National Meeting in Chicago. Three half-day sessions will be held - "Computer Molecular Modelling" organized by James Beatty of Ripon College, "Interfacing in the Laboratory" organized by Robert Megargle of Cleveland State University, and "Personal Computers in Chemical Engineering Education" organized by Richard McCluskey of Clarkson University.

I am organizing a symposium on the use of computers in high school chemistry, undergraduate general chemistry, undergraduate organic chemistry and undergraduate analytical chemistry courses for the 13th Biennial Conference on Chemical Education being held at Bucknell University from July 31 to August 4, 1994. There will be a one and a half hour session devoted to each of the four topics. In each session there will be two invited speakers and a half hour devoted to discussion, questions and brief comments on the topic by member of the audience.

A symposium on "Computers in

Chemical Education" is planned for the fall 1994 National Meeting in Washington, D. C. Thomas O'Haver (University of Maryland) is organizing a session on the use of Internet. Harry Pence is organizing a session on integrating computers into the undergraduate chemistry curriculum. A session on "What Chemists Need to Know About Computers and Computing" is being organized jointly with the Division of Computers in Chemistry.

How You Can Help:

We are always looking for material for this Newsletter. Send articles, paragraphs or suggestions to Editor Brian Pankuch. (His address is on the back cover.)

If you are interested in participating in any of our symposia, please contact the session chair. If you have suggestions for symposium topics, please send them to me.

If you have access to Bitnet or Internet, participate in our summer computer conference. If you are unable to participate in all sessions, select a paper or two to read and discuss.

If you would like to suggest some computer related activities or new initiatives, contact me.

We'd like to build our circulation. Share this issue with your friends and make the subscription form available to them.

IS ANYONE OUT THERE? LET US HEAR FROM YOU.

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EDITOR

**SPECTRUM--- A review by
Brian Pankuch**

Spectrum-a tool for exploring data analysis.

This set of tools is primarily for use in analytical chemistry. I spent hours exploring and it is really interesting to use. Having done many of the operations by hand, well with a calculator point by point, it is a great feeling of power to run an absorption or NMR spectra through the many available operations and transformations. If you've done it by hand and haven't tried it by computer you are in for a treat.

By transferring the files on the program diskette to your hard drive and double clicking on the program icon you are up and running. I'd suggest going through a few pages of the instruction manual to get a feel for the program. The program is straight forward to use. It is very intuitive. The 97 page manual is excellent-mostly screen shots showing the before and after using a transformation or operation. The manual is very easy to read and follow.

Despite playing 'what happens if I do this?', I only got Spectrum to crash twice. Considering that I can do this with every program I've ever used without trying, this means that the program is quite stable and robust. Although primarily for those handling data from any type of spectra or graph it is easy enough to use that I'm considering using it for data manipulation and teaching some basics. Of course it would help if we had computers to use in the lab.

The program is designed for advanced and graduate level analytical courses. Strong organic students using gas chromatography, etc., would find parts of the tutorial quite worthwhile. If the data could be transferred directly from the instrument to Spectrum it would be worth spending sometime showing students some of the rudiments of cleaning up a signal. Although using and understanding all the features would

certainly take a lot of expertise, just using some of the basics shown in the following figures (from signals supplied with the program) with less advanced students would seem worthwhile.

The tutorial has a variety of signals and suggested operations to demonstrate signal processing. The tutorial is informative. Having done some of these techniques by hand I can really appreciate the power at my fingertips. I'd recommend getting this program even if you don't have an immediate application. It is good enough and easy enough to use that you will minimally learn a bit and probably find some uses that I

haven't thought of. Data files may be prepared in a text editor, spreadsheet, telecommunications programs, plotting or data acquisition program, and saved in ASCII (text only) format. You can also use the New command under File in the menu to generate synthetic signals. The signals can have optional noise on Gaussian, Lorentzian or sine waves.

The program is extendible, i.e., you can add your own functions. On the Mac you would need Borland's, Turbo Pascal 1.1 and Turbo Pascal Numeric Methods Toolbox. Since I have neither of the above nor a copy of the source code (the actual line by line code for the program as op-

posed to the compiled code that is what we usually use) for Spectrum, I was not able to actually check the actual procedure. You would also need ResEdit from Apple. Suggestions for making changes looked straight forward if you are a Pascal programmer.

SPECTRUM was the 1990 NCRIPTAL winner. It is priced at \$49.95 for a single copy, \$249 for a department, \$395 for all campus sites. It is available from: Academic Software Development Group, Computer Science Center, Room 3357, University of Maryland, College Park, MD 20742. Phone: 301-405-7600.

Math	
Add constant	⌘A
Multiply by constant	⌘M

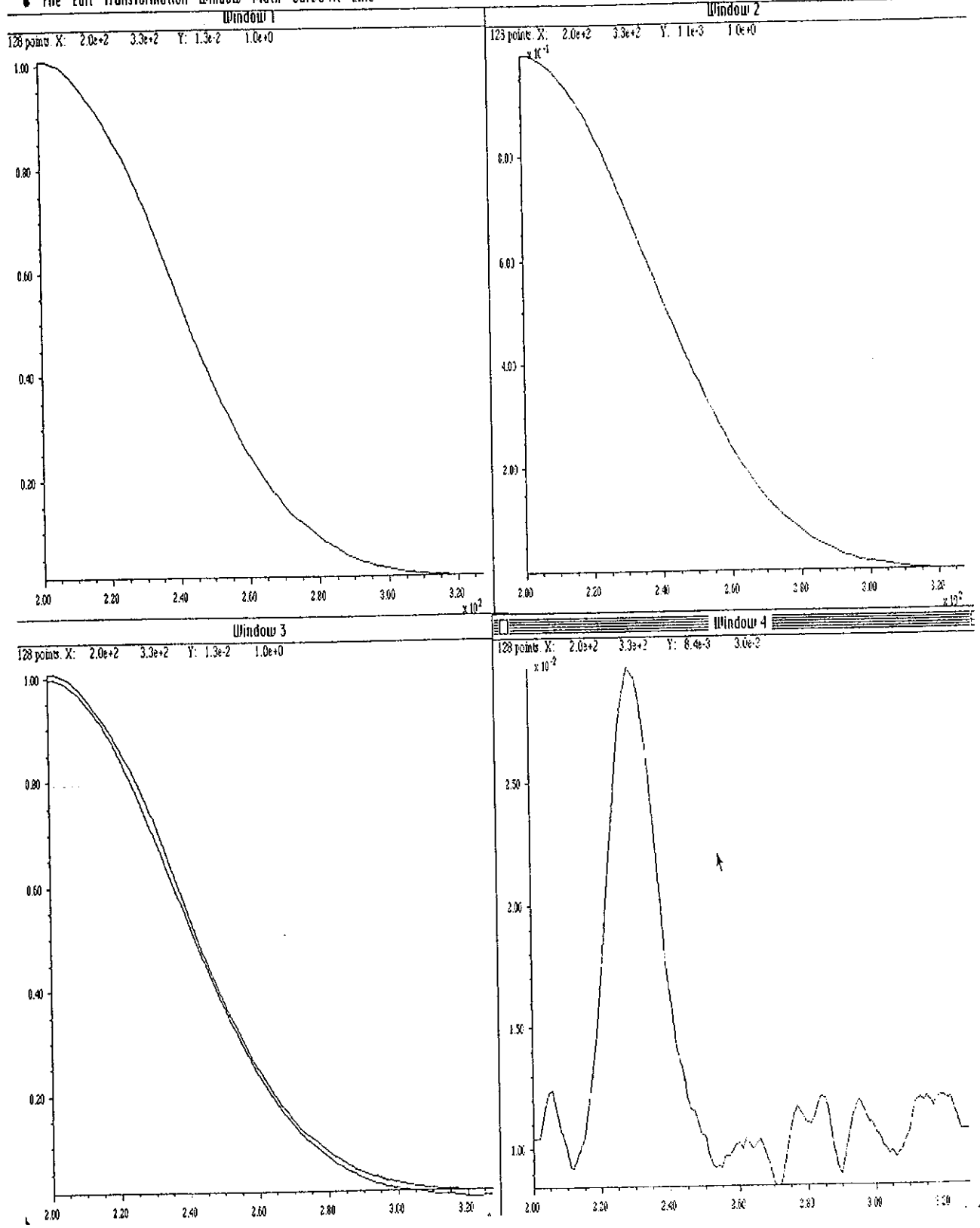
Add clipboard signal	⌘=
Subtract clipboard signal	⌘-
Multiply by clipboard signal	⌘B
Divide by clipboard signal	⌘/

Reciprocal	
Log	⌘G
Peak area...	
Standard Deviation	⌘;
Absolute value	
Square	
Square root	
User 1	
User 2	

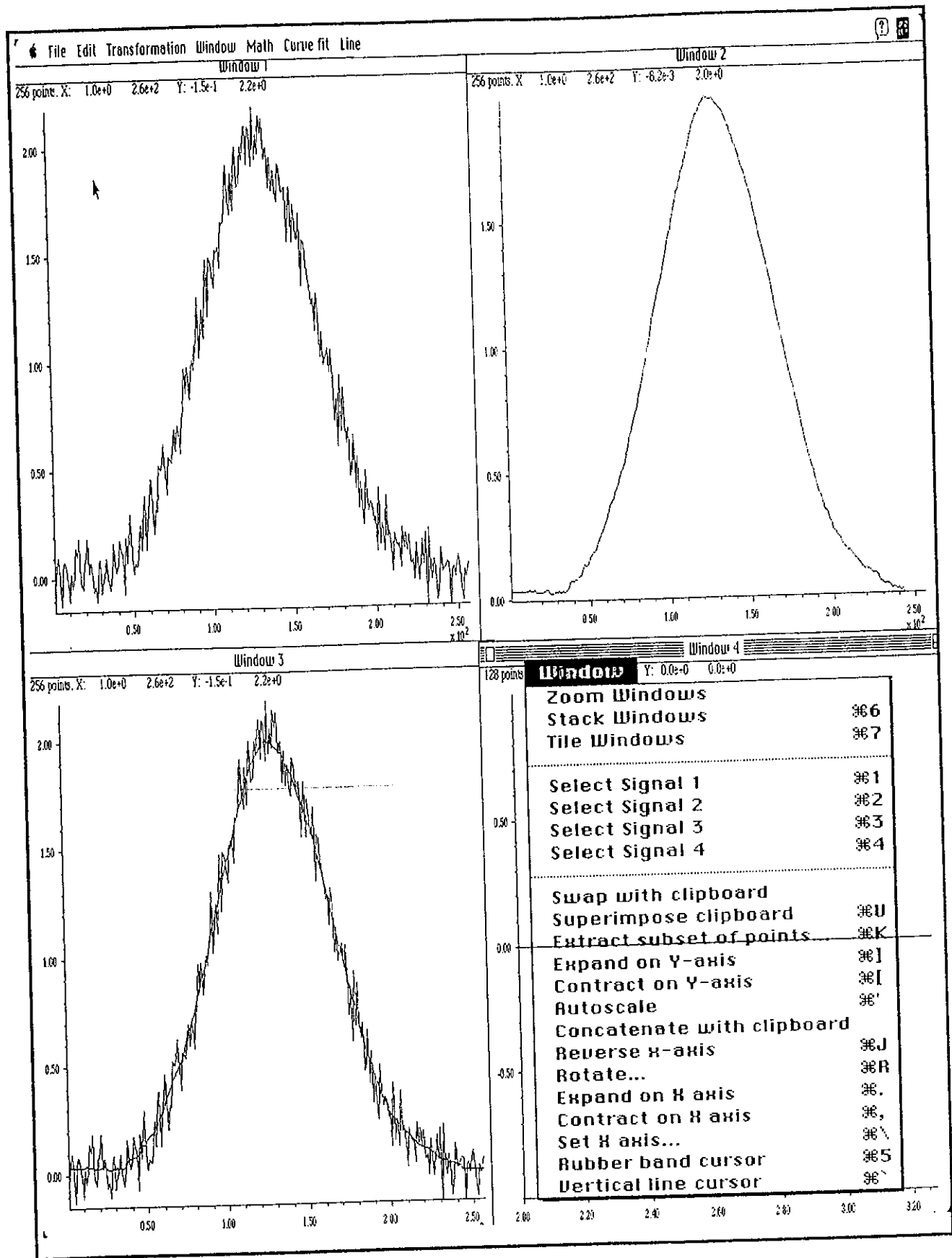
Transformation	
Normalize	⌘B
First Derivative	⌘D
Second Derivative	
Rectangular Smooth...	⌘F
Triangular smooth...	⌘T
Smoothed second derivative...	
Integrate	⌘I
Resolution Enhancement...	
Histogram...	
Interpolate...	⌘L
Forward Fourier Transform	
Inverse Fourier Transform	
Power Spectrum	⌘W
Convolute with clipboard	
Deconvolute clipboard	
Cross correlate with clipboard	
Auto correlate	
Fourier filter...	⌘H
Zero fill...	⌘O

Line
Plain line
Dots
Connected dots

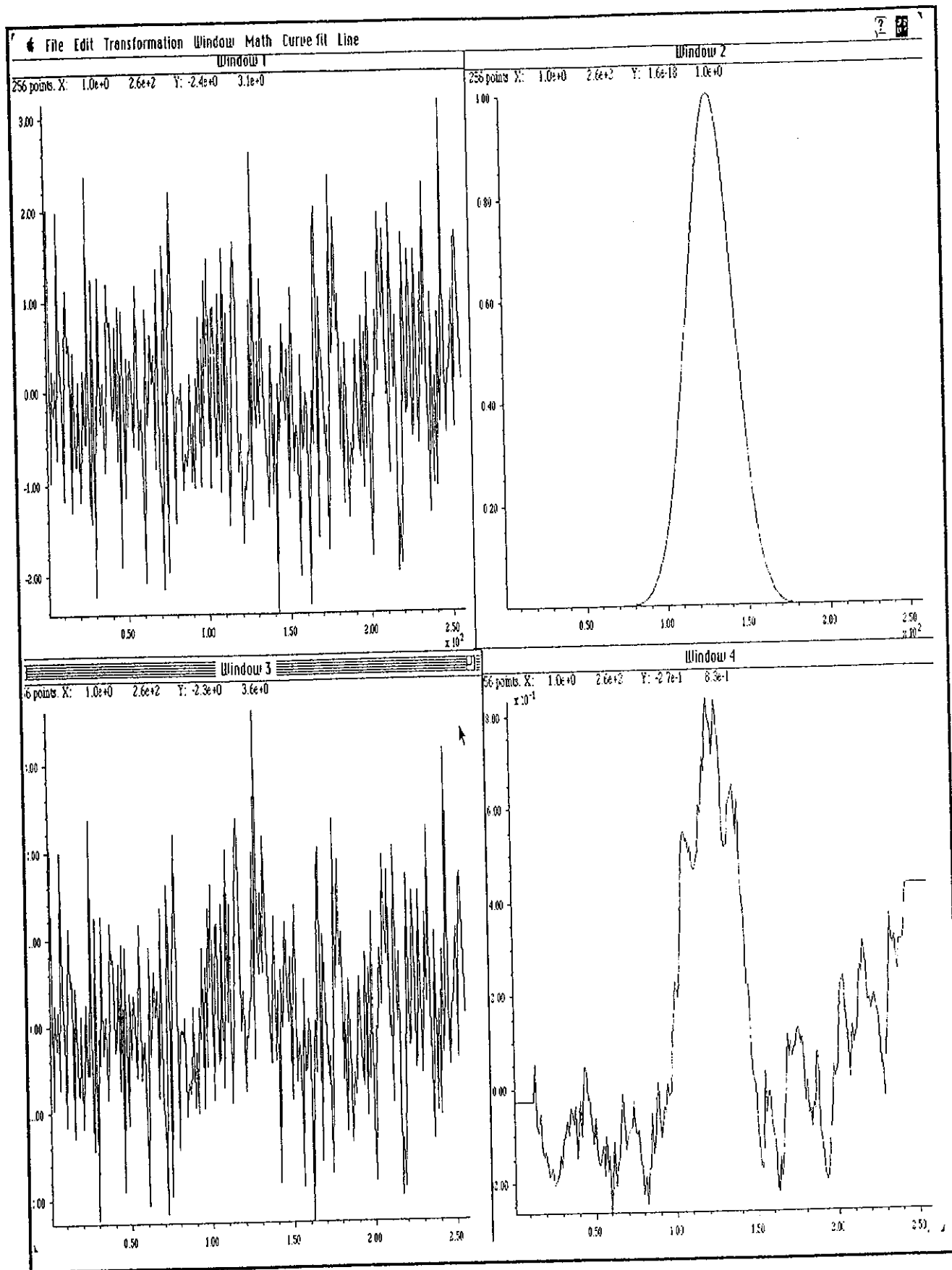
These are screen shots showing the wide diversity of functions available from the menus. Many other capabilities are available.



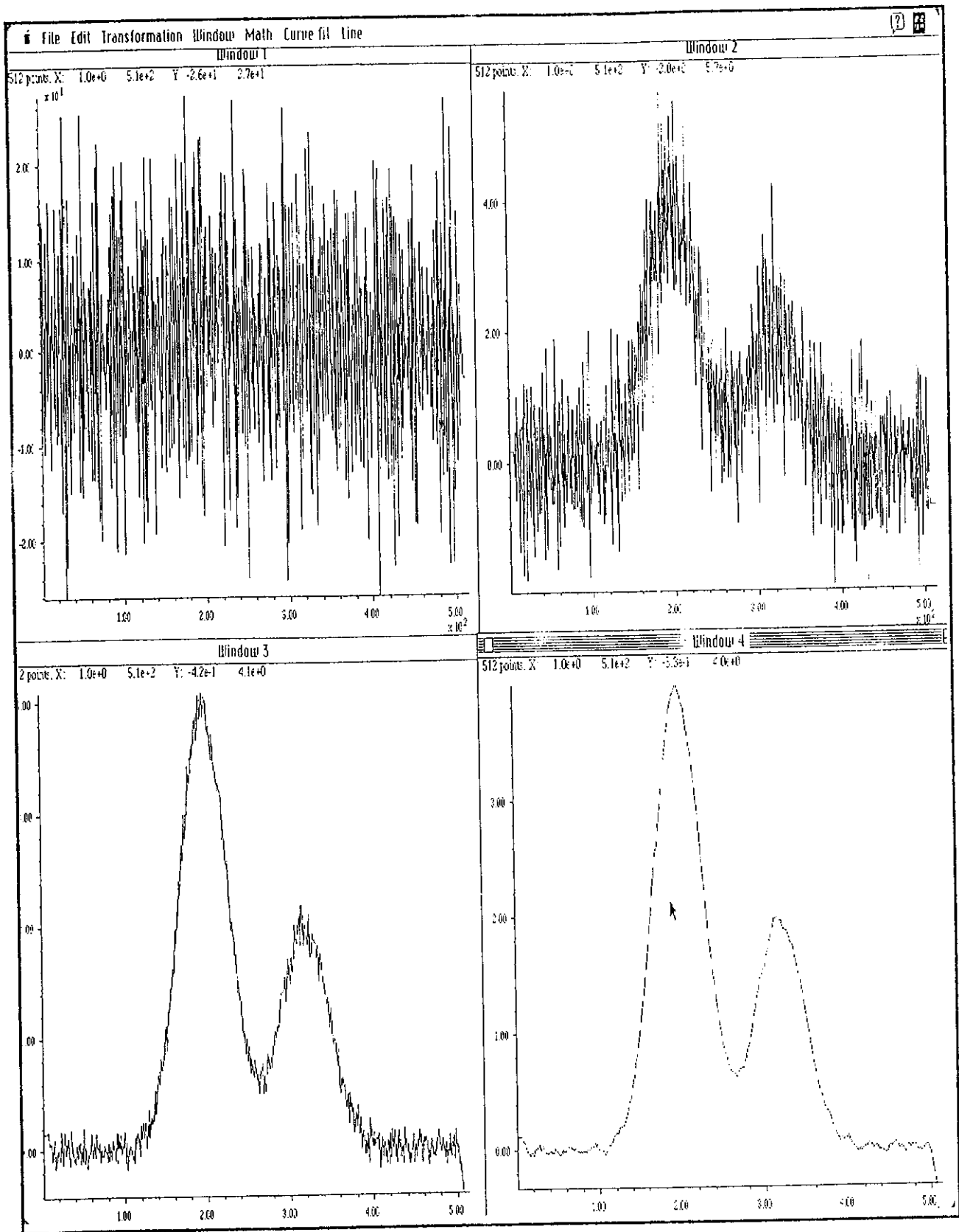
Window 1 is a signal, Window2-background, Window3- both signal and background, Window4-subtract background to get the actual signal that was buried under the background. Amazing!



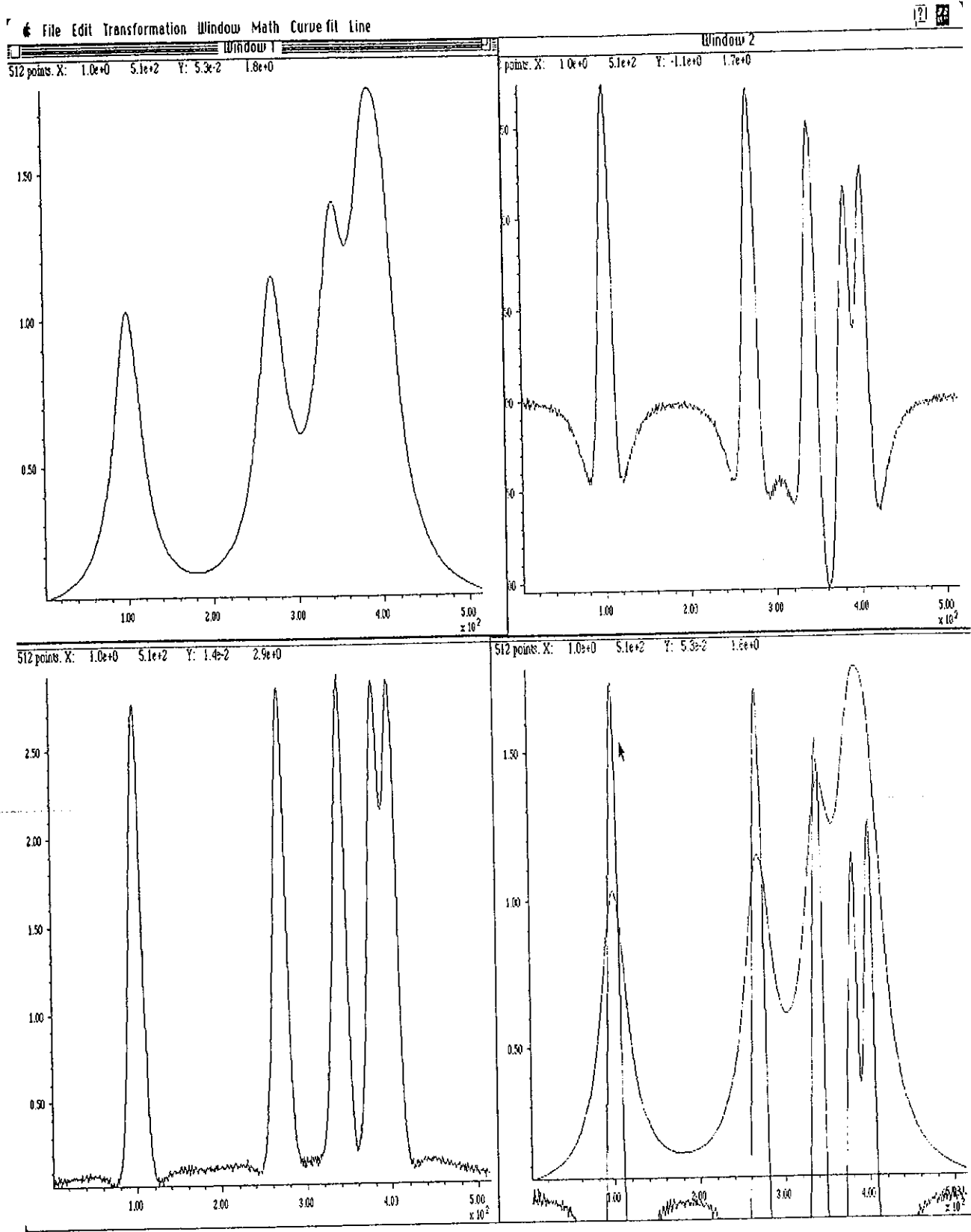
Window 1 shows noise, Window 2 shows gaussian, Window 3 shows both combined, Window 4-some window transformations available from the menu.



Window1 shows noise , Window2 shows gaussian, Window3 shows both combined, Window4 shows the combination -smoothed with rectangular smooth.



Window 1 a very noisy signal, Window 2-rectangular smooth using 11 points, Window 3-two rectangular smooths using 11 points, Window 4-four rectangular smooths using 11 points, notice how each smoothing improves the signal.



Enhancing resolution- Window 1 shows five bands. with low resolution. Window 2 shows the second derivative with a multiplier of -700 notice the extraneous positive lobes around the peaks. Window 3 shows the addition of Windows 1 and 2. Window 4 superimposes Windows 1 and 2.