5-1987

Program Development for Computer Simulation and Analysis for Multiplex Chromatography

Barbara Pawliszyn
Utah State University

PROGRAM DEVELOPMENT FOR COMPUTER SIMULATION AND ANALYSIS FOR MULTIPLEX CHROMATOGRAPHY

by

Barbara Pawliszyn, Master of Science

A report submitted in partial fulfillment
of the requirements for the degree
of
MASTER OF SCIENCE
in
Computer Science

(Plan B)

Approved:

____________________________ Major Professor	____________________________ Committee Member
____________________________ Committee Member	____________________________ Dean of Graduate Studies

UTAH STATE UNIVERSITY
Logan, Utah

1987

This work is dedicated to

my husband, Janusz

ACKNOWLEDGEMENTS

The preparation of a report at the masters level is a challenging and exacting task. The support of my husband, Janusz was invaluable both for the encouragement he gave me and for his guidance in research methodology. His never failing optimism and insightful comments provided a solid foundation for the work I had to do.

I would like to thank Dr. Greg Jones particularly for his overall direction and helpfulness. For Dr. Bob Campbell's assistance in solving problems of research design, I express my great appreciation. I would also like to thank Dr. Rex Hurst for bring an outside viewpoint to my research.

Barbara Pawliszyn

TABLE OF CONTENTS

LIST OF FIGURES

FIGURE PAGE

ABSTRACT

Program Development for
Computer Simulation and Analysis
for Multiplex Chromatography

by

Barbara Pawliszyn, Master of Science
Utah State University, 1987

Major Professor: Dr. Gregory Jones
Department: Computer Science

In this report, the programs developed for the analysis of simulated data in multiplex chromatography are written in the ASYST language. The integration of the program modules into a menu-driven, user-friendly prototype program is outlined. The program is developed to allow for flexibility and easy upgrading of the code.

This report examines the calculation procedures potentially useful in multiplex chromatography. Analysis of the mutliplex chromatograms is done by three mathematical methods, Cross-Correlation, Hadamard Transform and Fast Fourier Transform. The effects of experimental length/chromatogram length and decision sequences on correlation noise present in a single chromatogram, are discussed. As the number of data points increases, n, the improvement of the signal-to-noise ratio in the resulting single chromatograms is found to be a little less than the theoretical rate of $(n)^{0.5}$. A non-random decision sequence is discovered to introduce drift and noise into the multiplex chromatogram. The influence of electronic white noise and electronic drift in the experimental data (multiplex chromatogram) on the resulting single chromatograms is explored. As electronic white noise increases, the signal-to-noise ratio in the resulting single chromatogram decreases. Electronic drift also introduces noise.

Discussion of the best methods for given experimental conditions is based upon the signal-to-noise ratio in the resulting single chromatograms. Cross-Correlation is theoretically the fastest method but is greatly influenced by drift. Hadamard Transform is slower than Cross-Correlation but is not effected by drift. Fast Fourier Transform has the best signal-to noise ratio in the resulting single chromatogram but the peak magnitudes are not always reflective of the real heights. Fast Fourier Transform is slow but if written in machine language, is faster than Cross-Correlation or Hadamard Transform written in the ASYST language.

CHAPTER I

INTRODUCTION

Overview

Gas, liquid and supercritical fluid chromatographies are very inefficient in terms of the information content of the signal. A single injection of the sample mixture is followed by a long time period during which the chromatogram is developed. Each of the chromatographic peaks corresponds to one component of a sample mixture. The retention time, the time necessary for elution of this component, gives qualitative information. The height of the peak corresponds to quantity of the given component in the mixture.

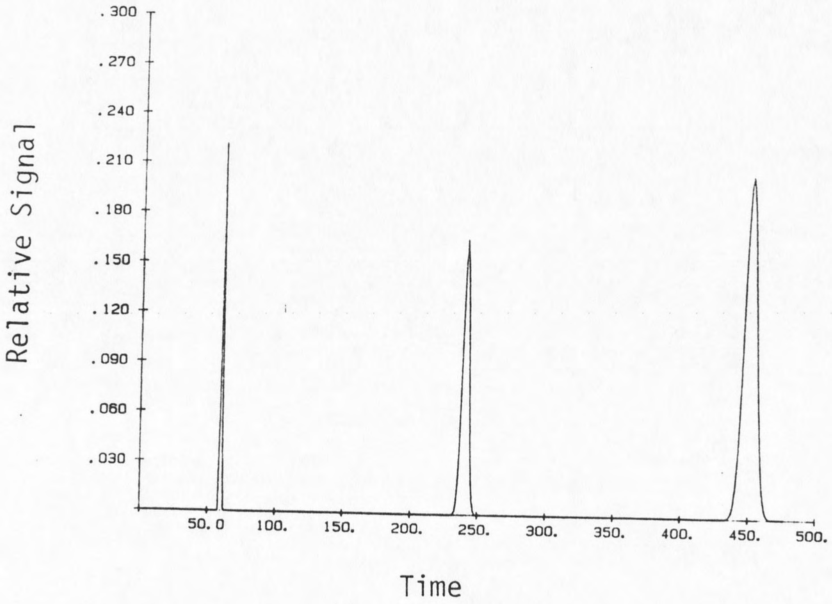
In this report, signal-to-noise ratio (S/N) (see Appendix A for all abbreviations used in this report) or signal magnitude compared to noise magnitude, is defined to be the height of the tallest peak in the single chromatogram divided by two times one standard deviation of noise. Improvement in detection techniques, by increasing the signal or lowering the noise, can enhance the S/N so that the single chromatogram peaks are detectable.

Another method is to generate more time efficient signals and still use the same detector. For example, instead of a single injection of the sample, a random sequence of injections may be input to the column. The average time between the injections is much shorter than the chromatogram length. Therefore, the output signal from the chromatograph corresponds to the sum of the same single chromatogram delayed in time. The time interval between each chromatogram is given by the injection sequence (decision sequence). The detector output (multiplex chromatogram) resembles noise, but, infact, it carries the information about the single chromatogram.

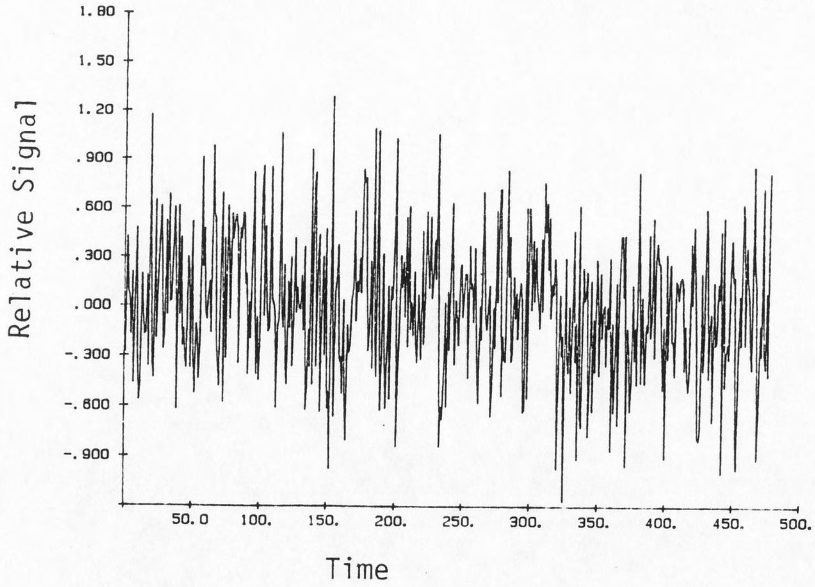
Figure 1.A illustrates a single chromatogram that results from a sample containing three major components. An example of electrical white noise issuing from an instrument is in Figure 1.B. The actual chromatogram recorded is a sum of these two graphs and can be found in Figure 1.C. Notice that in this case the single chromatogram is undetectable due to the low S/N or small signal magnitude compared to noise. Figure 2.A is a multiplex chromatogram resulting from the single chromatogram in Figure 1.A.

The single chromatogram can be calculated from the multiplex chromatogram by using correlation methods. Figure 2.B shows an example of the resulting single chromatograms calculated from the mutliplex chromatogram. Now signals are larger than the noise though the orignal

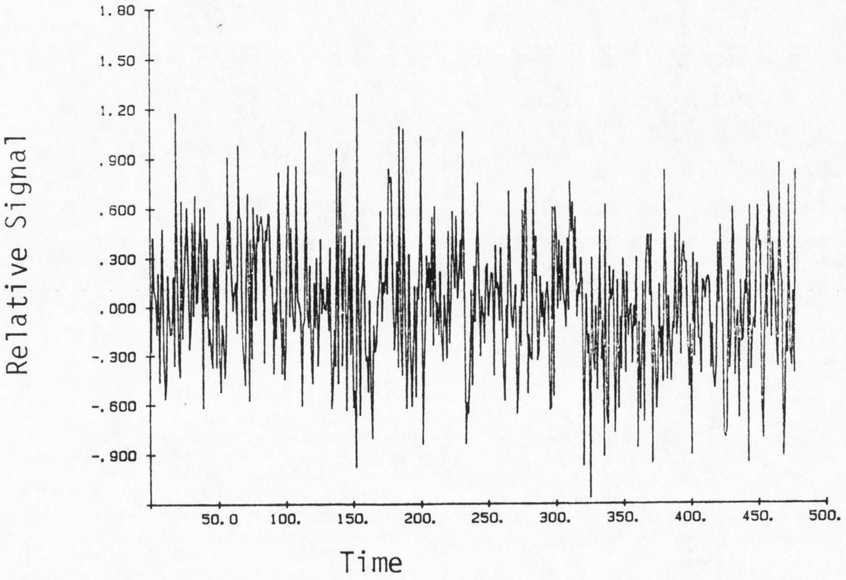
Figure 1. Single Injection Chromatogram Graphs



1.A Single Chromatogram used for Decision Sequences: 2,3,4,5,6 and 7; Defaults Parameters used

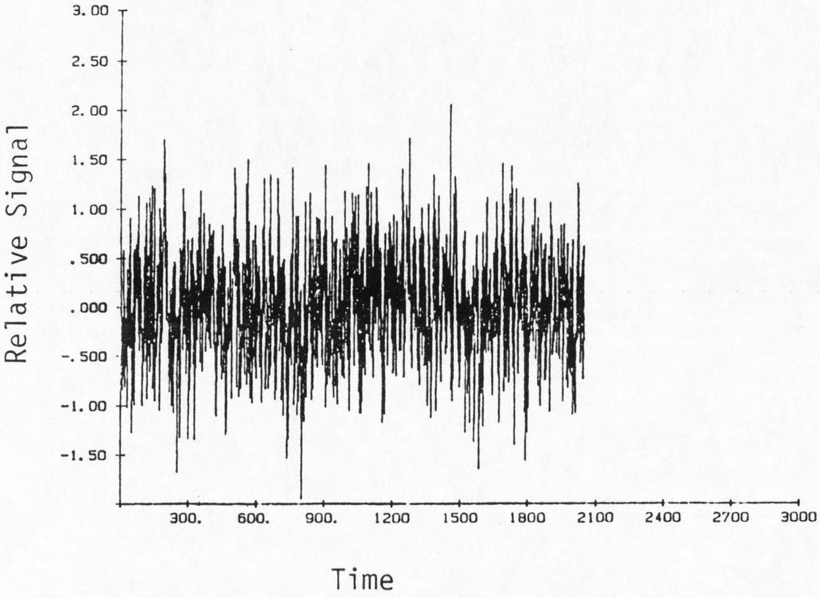


1.B Chromatogram of White Noise only; Noise Magnitude: 2; No other data present

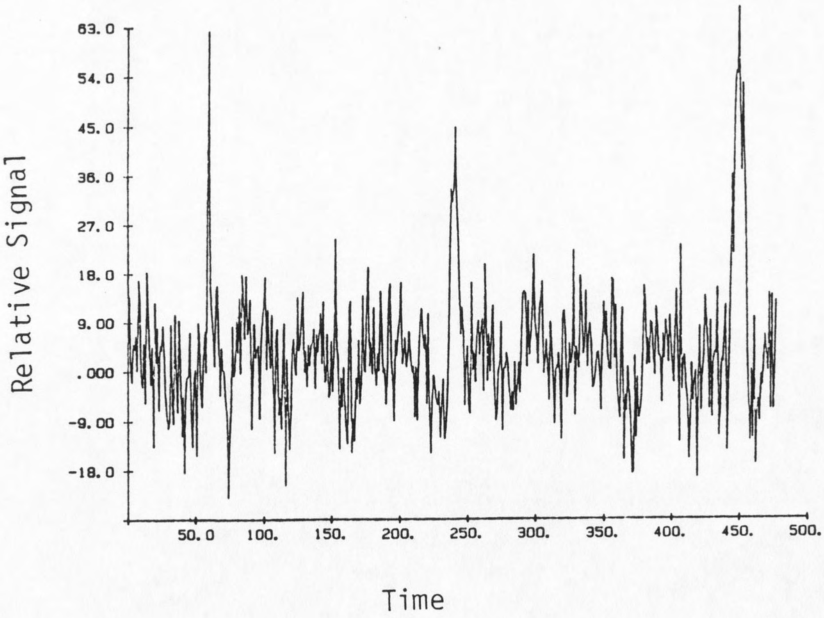


1.C Chromatogram of a Single Injection with White Noise; Noise Magnitude: 2; Figures 1.A and 1.B added together

Figure 2. Multiplex Chromatogram Graphs



2.A Multiplex Chromatogram with White Noise; Noise Magnitude: 2



2.B Single Chromatogram calculated from Figure 2.A single chromatogram was smaller. This is due to the throughput and multiplex advantages. The throughput advantage is the increase in the amount of sample introduced to the column per unit of time. The multiplex advantage exists since a single value from the detector output or multiplex chromatogram, carries information about many points for the single chromatogram (Ref. 1).

A major application of multiplex chromatography is the potential to continuously characterize components in the sample mixtures with high resolution and sensitivity. This method can be applied to on-line optimization of chemical industrial processing conditions, warning against excessive amounts of hazardous chemical wastes or perhaps even a physician monitoring in-vivo, chosen components in the blood stream (drugs, hormones, etc.) of a critically injured or sick patient. This approach eliminates the preconcentration of the sample components required with conventional chromatography. This approach results not only in faster determinations but will prevent confusion caused by sample alterations on catalytic surfaces such as activated carbon, commonly used to preconcentrate polutants.

Signal detection methods, such as Cross-Correlation (CC), Hadamard Transform (HT) and Fast Fourier Transform (FFT) can be applied to calculate the single chromatogram from the chromatographic output (multiplex chromatogram), and the random input (decision sequence). In short, these computational methods' main task is to shift mathematically, the time delay between consecutive chromatograms to zero and then average the chromatogram (Ref. 2).

Correlation

The mathematical definition of correlation is:

$$\text{(A)} \qquad R(T) = \lim_{N \to \infty} \; 1/2N \sum_{-N}^{N} \; x(t)\; y(t + T)\; dt$$

where R(T) is the correlation function formed by summing the lagged products of 2 waveforms, x(t) and y(t), and T is the time lag between x(t) and y(t). Functionally, correlation can be thought of as a matching up of waveform components or a similarity test between waveforms (Ref. 3).

Cross-Correlation

The single chromatogram using CC is computed using:

$$\text{(B)} \qquad R(T) = 1/N \sum_{t=1}^{N} \text{INPUT}(t-T) * \text{OUTPUT}(t)$$

where N is the number of data points in the input and output signals, t is discrete time and T is a delay. For a linear and statistically stationary chromatographic system with a properly chosen input signal, the single chromatogram resulting from CC is identical to the original single chromatogram, with a S/N advantage. Equation (B) would be very tedious to compute manually, but is easily programed for a computer (Ref. 1).

Hadamard Transform

The equation N = WT + E describes a multiplex chromatogram using HT, where W is the mask, T is the original signal (single chromatogram) and E is experimental measurement error (Ref. 4):

$$(C)\qquad \begin{bmatrix} \\ Ni \\ \\ \end{bmatrix} = \begin{bmatrix} & & & \\ W1 & W2 & \dots & Wn \\ & & & \end{bmatrix} \begin{bmatrix} T1 \\ T2 \\ \vdots \\ Tn \end{bmatrix} + \begin{bmatrix} \\ Ei \\ \\ \end{bmatrix}$$

where the i^{th} row of W specifies the mask configuration or decision sequence, used in the i^{th} measurement. If the measurements were perfect then E = 0 and T could be solved by (Ref. 4) :

$$(D)\qquad T = W^{-1} N$$

Fast Fourier Transform

Fourier Transform (FT) takes a very long time to compute if coded naively. In general, FT takes n^2 units of time while Fast Fourier Transform (FFT) takes $nlog_2n$, where n is the number of data points (Ref. 3). This time improvement is due to FFT taking orthagonality of the data into consideration. For example, when n=1024, this amounts to a FFT execution speed 100 times faster than FT. The only disadvantage of FFT is that it can only be applied to data arrays that are a power of 2 in length (Ref. 5).

FFT interpolates a sum of trigometric functions through n data points. Suppose F = (f0 . . . fn-1) is a data array. The functions that actually appear in the F expression are imaginary exponentials but by Euler's formula:

$$\text{(E)} \quad exp(ix) = cos(x) + isin(x)$$

These exponentials are really just the sum of two trigometric functions. From the equations below, notice that the F array consists of complex numbers even when the original data is real (Ref. 5).

FFT is defined to be (Ref. 5):

$$\text{(F)} \quad Fm = 1/n \sum_{m=0}^{n-1} fk \; exp \left\{ \frac{-2*pi*i}{n} \; m*k \right\}$$

The inverse FFT is (Ref. 5):

$$(G)\quad fk = 1/n \sum_{k=0}^{n-1} Fm \exp\left\{\frac{2*pi*i}{n} m*k\right\}$$

From the Fourier Transform correlation property, correlation is greatly simplified by using FFT. The two waveforms to be correlated, x(t) and y(t) are transformed to the frequency domain by FFT giving X(t) and Y(t). Following this, one term is conjugated and then the complex product is formed to give:

$$(H)\qquad S(f) - X^{*}(f)\ Y(f)$$

where (*) denotes conjugation. The final step is inverse tranforming S(f) back to the time domain to give the single chromatogram (Ref. 3).

The conjugate of a complex number is obtained by simply negating the imaginary part of the number. Graphically this can interpreted as reflecting the (x,y) vector around the x axis (Ref. 5).

CHAPTER II

PROBLEM STATEMENT

The main objective for this report is to write and test software to investigate multiplex chromatography by simulating data and calculating resulting single chromatograms. The effects of varying experimental conditions such as white noise and electronic drift, on resulting single chromatograms will be examined. The ability of different calculation methods (CC, HT and FFT) to produce good quality single chromatograms resulting from multiplex data will be explored. Since the inception of multiplex chromatography, only on a limited theoretical study has been conducted (Ref. 6) which investigated the effect of the sample composition and baseline drift on S/N in the calculated single chromatogram.

A menu-driven, prototype program will be written on an IBM compatible microcomputer. The package should be flexible so that later it can be expanded and used to test other less significant parameters such as laser jitter and be able to collect experimental data directly in a form that can later be analyzed by the calculation methods (eg. CC). The program should be user-friendly with clear prompts, error messages and recovery, have a simple and logical call structure and easy to operate.

The user should feel in control yet not be burdened with repetitive data entry.

Appropriate software must be chosen. Since good quality of random numbers will be needed for some calculations, the random number generator used should produce random numbers that pass a 0.05 level of significance. The software should be able to do calculations using complex and double precision operations. In addition, it should be easy to aquire experimental data using direct memory access.

The simulation consists of 5 parts: first, parameters are entered, either default or user determined. Second, a single chromatogram is calculated. Third, a random decision sequence is determined, to be used to calculate the fourth step which is producing a multiplex chromatogram. The multiplex chromatogram is calculated by the following steps: initialize the multiplex chromatogram array to zeros; add the single chromatogram to the array starting at the time intervals where the decision sequence array is true. Finally, random (white) noise is optionally added to the multiplex chromatogram.

The multiplex chromatogram is then analyzed using three mathematical methods: CC, HT and FFT. The resulting single chromatograms are then compared to each other and to the original single chromatogram to see the effects of changing simulation parameters on sensitivity (S/N) and reproducibility of the calculated results. This procedure should lead to a better understanding of such complicated concepts as correlation noise.

Correlation noise is noise in the resulting single chromatogram due simply to the correlation method. The effect of the experimental length/chromatogram length ratio or length proportion (LP) and different decision sequences on correlation noise, in the resulting single chromatogram is to be investigated. In addition, the influence of electrical white noise on resulting single chromatograms is to be explored. The effect of electrical drift in the multiplex chromatogram is to be considered. This approach allows the determination of the best analysis method for a given set of conditions prior to an experiment.

CHAPTER III

PROBLEM SOLUTION

Program Solution

Program and Menu Development and Testing

The major program modules developed for the following sections are integrated into a menu-driven program. Dataflow diagrams, menu hierarchy diagrams and menu screens are in Appendices B, C and D. These diagrams include future anticipated enhancements as well as the core for the prototype. A user's manual and system configuration specifications for the prototype are found in Appendices E and F. Appendix G has a listing of parameter definitions. Function keys, prompts and error messages are used to ensure that the system is easy to use. Consistency in menu display and windows encourage easy learning of the prototype.

Testing of the modules is done by entering in maximum and minimum parameter values and ensuring that the program does not crash. If it does, an error check is put in or acceptable limits are changed. The graph calculations are tested by comparing what is produced to what is expected or desired.

The Program Language ASYST

When personal computers were beginning to appear on the market, it was commonly believed that any business software had to be specially created by expensive consultants using Basic, Fortran, Pascal or Cobol. Then the appearance of Lotus' 1-2-3 and Ashton-Tate's dBASE II showed that general purpose business software could be written. ASYST provides the same type of general purpose software but is designed for scientific and engineering needs (Ref. 5).

ASYST has been developed by Adaptable Laboratory Software, Inc. based upon their experience in scientific and engineering applications. ASYST incorporates many features of well-known computer languages such as APL and Forth. However, like dBASE II and 1-2-3, it is more than a language, it is an application environment. Asyst contains many pre-written software tools such as interactive graphics which can be used by themselves or incorporated into a custom application program (Ref. 5).

ASYST's data acquisition and data analysis modules supply prewritten tools such as the ability to simply input analog information from instruments, the ability to find the local minima on a waveform, or a highly optimized FFT. Direct memory access is supported by ASYST and is easy to configure. This allows for experimental data to be acquired directly into memory (Ref. 5).

Because ASYST has been designed for science and engineering, all of its operations can be used with both real and complex numbers. ASYST supports high precision calculations. Using the 8087 coprocessor, most functions are calculated with a precision of 80 bits. Its automatic plotting supports linear, logarithmic and polar plotting (Ref. 5). The random number generator used is well respected and considered one of the best (Ref. 7).

ASYST can be used interactively or prewritten "templates" or modules can be compiled. Complex computer language is avoided by providing meaningful names for commands. Therefore, for example, FFT can be simply invoked by typing the letters "FFT". New commands can be interactively created or assigned to function keys. All these functions allow the user to focus on the application rather than how to write a complex program (Ref. 5).

ASYST can be used to generate a turnkey, menu-driven program. It supports multiple text and graphics windows. The ability to use function keys reduces keystrokes by the operator and all templates loaded are compiled so they execute at top speed (Ref. 5).

ASYST Random Number Generator Validation

ASYST has several different random number functions, such as RAND.UNIF and RAND.NRML, that are based on one random integer generator. These functions can be utilized in multiplex chromatography, provided that the random numbers they produce are sufficiently random and the number generator pases tests for randomness. The integer sequence of the generator is initialized by assigning a value to the (double precision integer) scalar SEED. SEED is defaulted to the value 1 when the system is loaded. Each time one of the random number functions is executed, the value of SEED is updated to the next term of the random sequence. The sequence does not repeat itself until all 2^{23} double precision integers have been encountered (Ref. 5). The particular generator used in ASYST is the one described in Reference 7. The function RAND.UNIF produces numbers that are distributed like a uniform continuous (0,1) random variable. The function RAND.NRML produces random Gaussian numbers with a mean of 0 and standard deviation of 1.

A Chi-Square test is done for RAND.UNIF on 300 numbers using 10 groups (9 degrees of freedom). A one-sided t-test for RAND.NRML is used on 300 numbers. The Chi-Square test on RAND.UNIF and a two-sided t-test on RAND.NRML are run 100 times and compared to their appropriate distributions (eg. compare the t-test values with a t distribution). The results show that the number generator passes a frequency test.

Data Simulation Solution

Introduction

To generate the multiplex chromatogram, the following steps must be done: first, a single chromatogram is generated; second, a decision sequence is produced; third, the multiplex chromatogram is calculated; and the optional fourth step is the addition of white noise to the multiplex chromatogram.

Single Chromatogram Calculations

The original single chromatogram is made up of a number of Gaussian peaks. Each of the peaks corresponds to a particular component of the sample. The position of the peak (retention time) characterizes the component (qualitative information) and its height is proportional to the amount of this component in the sample (quantitative information). Each peak, i, in the single chromatogram can be described by:

$$\text{(I)} \quad SPi(t) = \frac{VFi * RFi}{Si(2pi)^{0.5}} \; EXP \left\{ \frac{-(t - RTi)^2}{2Si^2} \right\}$$

where SPi(t) is the height of the peak i at time t, defined by the standard deviation of the peak (Si), retention time (RTi) at the maximum SPi(t), volume fraction injected (VFi) and analyte detection response factor (RFi) (Ref. 8). Si is defined to be:

$$(J) \qquad Si = \frac{RTi}{(CE)^{0.5}}$$

where CE is the column efficiency (Ref. 8). Therefore the original single chromatogram is defined to be:

$$(K) \quad SC = \sum_{i=1}^{No.Pk} SPi$$

where No.Pk is the number of peaks in the single chromatogram.

Decision Sequence Calculation

The decision sequence is an array that indicates, by the contents of its elements, when in time a single chromatogram is to be added into the multiplex chromatogram. Random numbers are generated and compared to the average frequency parameter. This parameter determines the average frequency a decision is made. If the random number is less than or equal to this constant then the decision is positive (1), else it is negative (0). Under experimental conditions, a positive decision would indicate the injection of a sample.

Multiplex Chromatogram Calculation

For every decision sequence point that is positive, the single chromatogram is added to the multiplex chromatogram (MC). That is:

$$(L) \quad MC(t \ldots t+CL-1) = MC(t \ldots t+CL-1) + SC(1 \ldots CL) * DS(t)$$

where SC is the single chromatogram, CL is the chromatogram length of the single chromatogram, DS is the decision sequence and t is time. However, since the first values of the multiplex chromatogram will not store much information until the time equal to the length of one single chromatogram length (CL) has passed, the first CL of the multiplex chromatogram is not stored. This satisfies actual experimental procedures, that is, the multiplex chromatogram is not recorded until the output has stabilized.

Calculating Electrical White Noise

Electrical white noise or fundamental noise, arises from the motion of discrete charges in electrical circuits and cannot be completely eliminated (Ref 9). Electrical instruments always produce a signal distribution which is typically Gaussian in nature. The amount of white noise or noise magnitude, must be flexible so that different signal-to-white-noise ratios

(S/WN) can be used when determining the best analysis method (CC, HT, and FFT). White noise values are determined by generating Gaussian random numbers with a mean of zero and a standard deviation of:

(M) SD = (MaxSC) * NM

where MaxSC is the height of the tallest peak in the single chromatogram and NM is the noise magnitude parameter. The white noise values are then added to the multiplex chromatogram. For exactly how noise magnitude relates S/WN see Appendix H.

Calculating Electronic Drift

Electronic drift or flicker noise (1/frequency) arises from imperfect instrumentation or non-ideal component behavior and can in principle be reduced to insignificant levels by careful practice and instrument design. The sources of electrical drift include long-term power-supply fluctuations, changes in component values and temperature drifts (Ref. 9). This results in baseline drifting. The actual characteristics of electrical drift are not really known. Before this topic can be thoroughtly investigated, real experimental data should first be acquired. For this report, a simple case of linear drift is used with its slope being dependent upon the multiplex chromatogram's experimental length (EL) and the maximum value of the multiplex chromatogram.

The multiplex chromatogram with drift (MCD) is calculated as:

$$(N) \quad MCD(t) = MC(t) + (t * MaxMC / EL * DF)$$

where MC(t) is the original multiplex chromatogram, t is time, MaxMC is the mutliplex chromatogram's maximum value, and DF is the drift factor. Note, from equation (N) that the rate of drift for an EL of X and DF of Y is the same as for an EL of 2X and DF of Y/2. Therefore, drift rate is proportional to (EL*DF). Since EL is proportional to EL/CL or LP, and for ease of analysis, drift rate in this report will be defined as (LP*DF).

The three analyis methods (CC, HT and FFT) are tested upon the MCD and upon the MCD which has had its drift reduced. The drift reduction is done as follows. The mean of 20 points before and 20 points after a point in the MCD is calculated. This mean is then subtracted from the MCD point and stored in a new multiplex chromatogram array. The resulting multiplex chromatogram is therefore 40 points shorter than the original MCD since the first and last 20 points cannot have drift reductions, that is, the means can not be calculated.

Data Calculation Solution

Introduction

Since ASYST does array/vector calculations directly and quickly, this feature is utilized wherever possible in the calculations. Internal functions such as FFT (Fast Fourier Transform), IFFT (Inverse Fast Fourier Transform) and CONJ (Conjugation) are available and used where appropriate. The averaging of the resulting single chromatograms is omitted (1/N), to avoid computer rounding errors. The ratios or proportions are more meaningful than absolute magnitude.

Cross-Correlation

Rather than directly applying equation (B) to calculate the resulting single chromatogram, a more efficient algorithm is used. It entails traversing the decision sequence searching for a positive decision. One CL of the mutliplex chromatogram is then extracted at the appropriate location and added to the resulting single chromatogram. This reduces the number of additions since where the decision is negative, the addition to the single chromatogram would just be zeros, a zero operation.

Written in terms of this report, equation (B) is:

$$\text{(O)} \qquad SC(T) = 1/(EL-CL) \sum_{t=1}^{EL-CL} DS(t-T) * MC(t)$$

where SC is the resulting single chromatogram, MC is the multiplex chromatogram, DS is the decision sequence, EL is the experimental length of the multiplex chromatogram and CL is chromatogram length of the single chromatogram. However as mentioned above, averaging is to be ignored, giving:

$$\text{(P)} \qquad SC(T) = \sum_{t=1}^{EL-CL} DS(t-T) * MC(t)$$

<u>Hadamard Transform</u>

In terms of the report, the multiplex chromatogram produced by equation (C) is:

$$\text{(Q)} \qquad \begin{bmatrix} MC_1 & MC_2 & \cdots & MC_{EL} \end{bmatrix} = \begin{bmatrix} DS_{CL} & DS_{CL-1} & \cdots & DS_1 \\ DS_{CL+1} & DS_{CL} & \cdots & DS_2 \\ \vdots & \vdots & & \vdots \\ DS_{CL+EL-1} & DS_{CL+EL-2} & \cdots & DS_{EL} \end{bmatrix} \begin{bmatrix} SC_1 \\ SC_2 \\ \vdots \\ SC_{CL} \end{bmatrix}$$

therefore the HT to produce the resulting single chromatogram, from equation (D), is (Ref. 2):

$$\begin{bmatrix} SC_1 & SC_2 & \dots & SC_{CL} \end{bmatrix} = \begin{bmatrix} DS_{CL} & DS_{CL+1} & \dots & DS_{CL+EL-1} \\ DS_{CL-1} & DS_{CL} & \dots & DS_{CL+EL-2} \\ . & . & & . \\ . & . & & . \\ . & . & & . \\ DS_1 & DS_2 & \dots & DS_{EL} \end{bmatrix} \begin{bmatrix} MC_1 \\ MC_2 \\ . \\ . \\ . \\ MC_{EL} \end{bmatrix} \quad (R)$$

The array/vector operations of ASYST are used to implement this equation. Although this means that there will be many additions with zeros, it is faster and more efficient than using loops and tests for zero additions.

Fast Fourier Transform

The built-in ASYST functions FFT, IFFT and CONJ are used to quickly calculate the SC in equation (H). The multiplex chromatogram and decision sequence arrays used, are truncated so that their lengths are a power of 2. This improves the efficiency of the FFT calcuations.

Best Analysis Method Determination

CC, HT and FFT are used on a number of multiplex chromatograms with different simulation parameters (App. I). Specifically, the following conditions are considered: a basic mutliplex chromatogram to test correlation noise; a multiplex chromatogram with different CL's; multiplex chromatograms with different decision sequences; a multiplex chromatogram with white noise; and a multiplex chromatogram with electrical drift.

The determination of the best analysis method is based upon the accuracy of the resulting single chromatograms. This is determined by comparing the peak retention times and magnitudes of the resulting single chromatograms with that of the original single chromatogram which was used to generate the multiplex chromatogram. In addition, the overall S/N of the single chromatograms resulting from the different methods, is used. S/N is defined as:

$$(S) \quad S/N = \frac{\text{(Height of tallest peak in resulting SC)}}{2 * \text{Standard Deviation of the noise}}$$

where SC is the single chromatogram.

CHAPTER IV

RESULTS AND DISCUSSION

ASYST

ASYST was used very much like a toolbox, piecing appropriate parts together. As a result, programs ran fast due to many of the components being highly optimized (eg. FFT). Menus were quick to develop, pleasing to the eye and display time was fast. In addition, the task of integrating the programs was not too burdensome due to the fact that the author could work at a high-level, that is, concentrate on the the task, not on the coding.

The author had to keep reconfiguring ASYST so that all arrays and program modules could be stored in memory. ASYST was not good at diagnosing when memory ran out, it just "hung" the system. The whole system had to be rebooted and ASYST and the prototype program reloaded. This took about 15 minutes.

The FFT and IFFT functions in ASYST required that the number of data points be a power of 2 for the best and most efficient calculations. The maximum number of points that could be utilized was 2048. This created a constraint on the simulation portion of this report since it limited EL and therefore LP as well. As a result, the single chromatogram resulting from FFT never had a LP greater than 4. However, its optimized code provided fast calculations.

Random Number Generator

The results for evaluating the randomness of RAND.UNIF and RAND.NRML can be found in Appendix J. Both functions appear to have passed the 0.05 level of significance with each having only 1 out of 15 runs not passing. However, when these tests were run 100 times each and tested against their appropriate distributions at the 0.05 level of significance, they passed very well. The Chi-Square calculated from the total observed values for RAND.UNIF was 1.17, well below the value 7.81 for 3 degrees of freedom with a significance level of 0.05 (Ref. 10). The Chi-Square calculated from the total observed values for RAND.NRML was 7.9, below the value 14.1 for 7 degrees of freedom with a significance level of 0.05 (Ref.10). In addition, for the two-sided t-test of RAND.NRML, the average means were close to zero. Therefore, modules that used these functions could be sure of utilizing good quality random numbers though no generator can ever be truly random. From the literature it appears that it is one of the best algorithms available (Ref. 7).

Coding and Testing of Programs and Menus

It was found that when resolution of the original single chromatogram became too coarse, peaks were lost due to rounding errors. Therefore, to ensure that a peak was always present in the original SC, a round adjustment was added (see code: Calculate.Single.Chrom in App. K).

At first the author used loops to enter information into arrays. The processing time of some programs using these loops was very long. As a result, ASYST's array/vector operations were utilized, speeding up computational time as much as 7 times!

CC was found to be a faster calculation method than HT, probably due to HT taking time to do many multiplications by zero. FFT was the fastest but could not be compared to the other two methods since it utilized optimized functions internal to the system. The literature indicates that it would actually be the slowest since its speed is a function of $n\log_2 n$ while CC and HT speeds are linear.

Correlation Noise

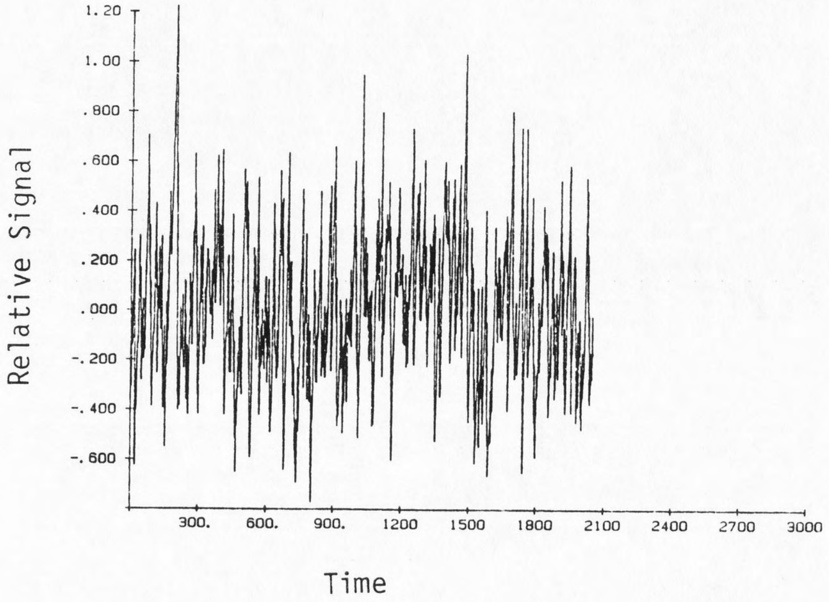
Independent of which calculation method was used, there was certain amount of noise present even when no electrical noise was added to the multiplex chromatogram

(Fig.3). This is called correlation noise. It is due to the non-ideal random number generator and limited number of injections. Correlation noise in the single chromatograms was proportional to the largest peak present in the resulting single chromatograms. The single chromatogram resulting from FFT had less correlation noise than either CC or HT. From Appendix L, it can be observed that for any set of given conditions, FFT consistently had a S/N about twice as high (less correlation noise) as the S/N for either CC or HT.

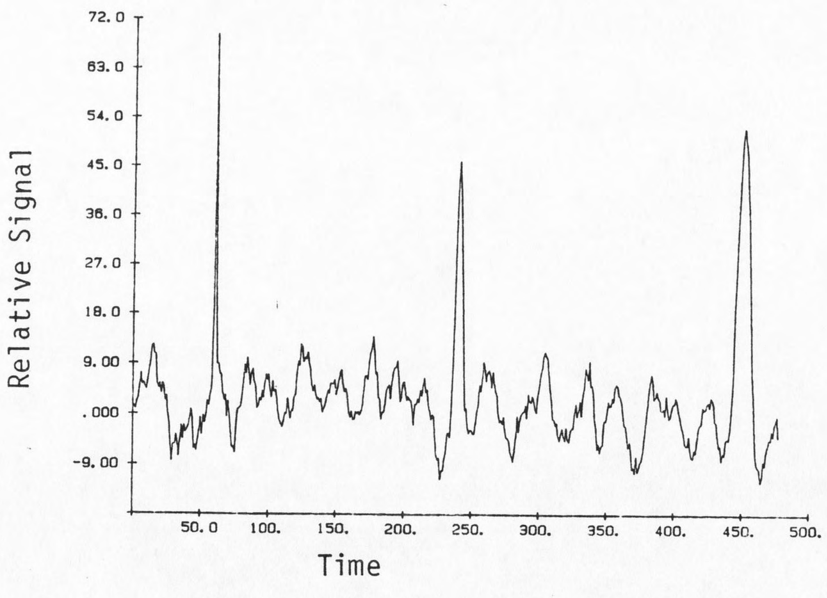
When compared to the original single chromatogram, all three methods produced single chromatogram peaks at the correct retention times and with appropriate width (Fig. 1.A, 3.B, 3.C, 3.D). However, the single chromatograms resulting from FFT did not always have similar peak magnitude compared to the original single chromatogram, while CC and HT did (Fig. 1.A, 4, 5).

From Appendix M, a CC single chromatogram with a LP of 4, CL of 128 and EL of 512, had a S/N of 2.4; a CC single chromatogram with a LP of 16, CL of 32, and EL of 512 had a S/N of 3.0; and a CC single chromatogram with a LP of 4, CL of 477 and EL 1908, had a S/N of 4.5. That is, two CC single chromatograms with an EL of 512 had S/N's of 2.4 and 3.0 while two CC single chromatograms with a LP of 4 had S/N of 2.4 and 4.5. Therefore, the

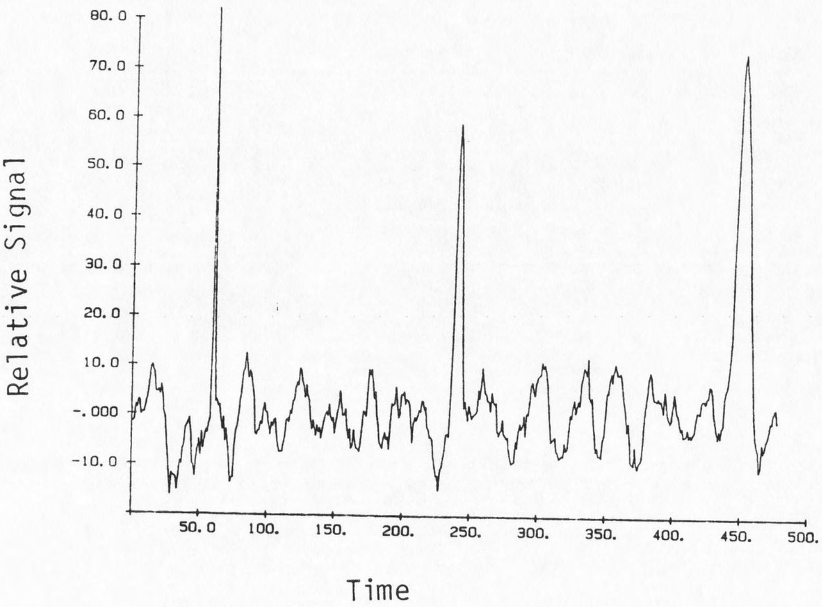
Figure 3. Graphs for Decision Sequence 8 Using Default Values



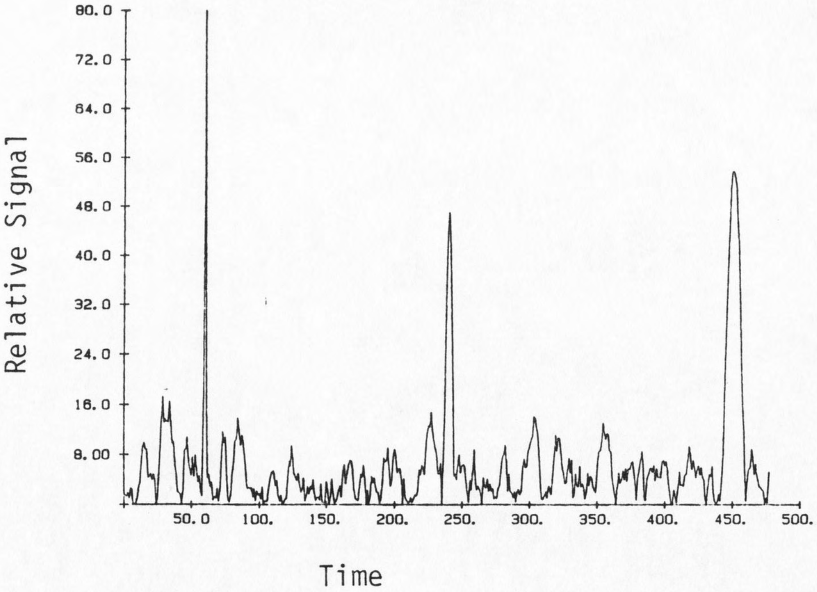
3.A Multiplex Chromatogram; LP: 4



3.B Cross-Correlation Single Chromatogram calculated from Figure 3.A

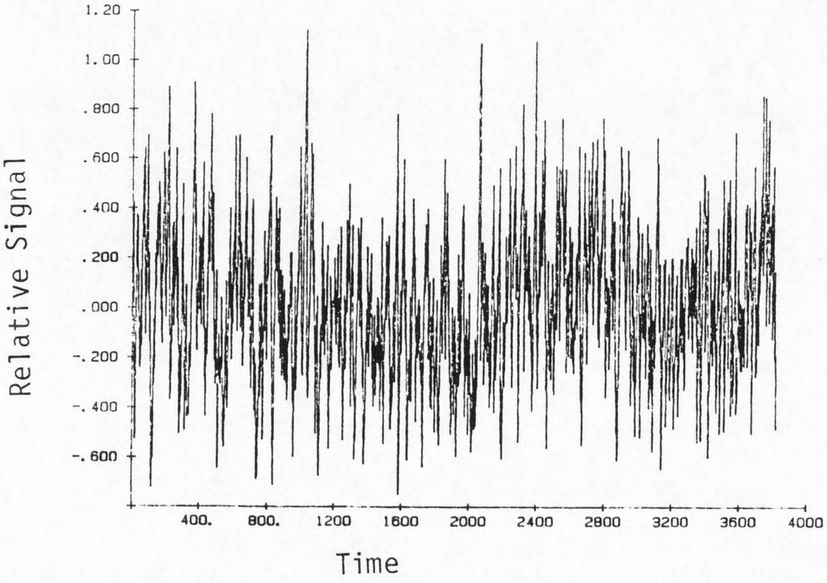


3.C Hadamard Transform Single Chromatogram calculated from Figure 3.A

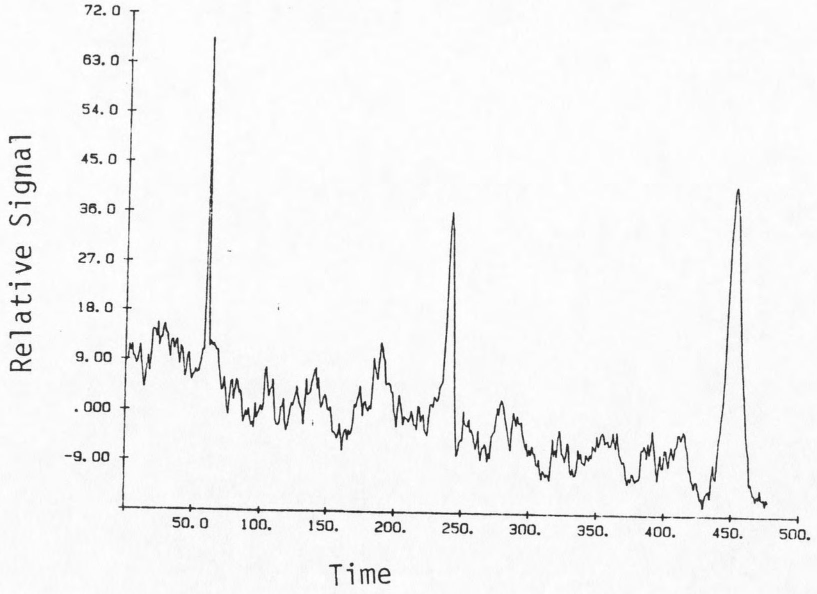


3.D Fast Fourier Transform Single Chromatogram calculated from Figure 3.A

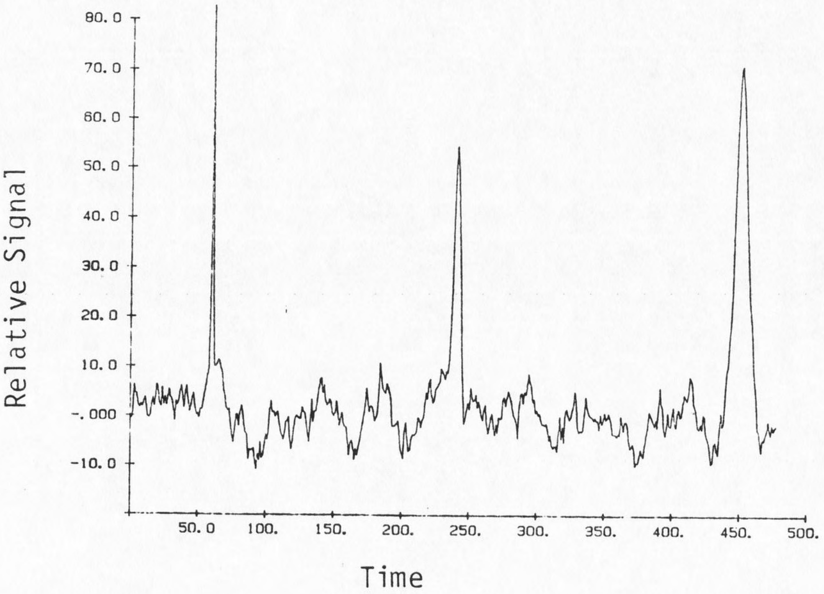
Figure 4. Graphs for Decision Sequence 3 Using Default Values



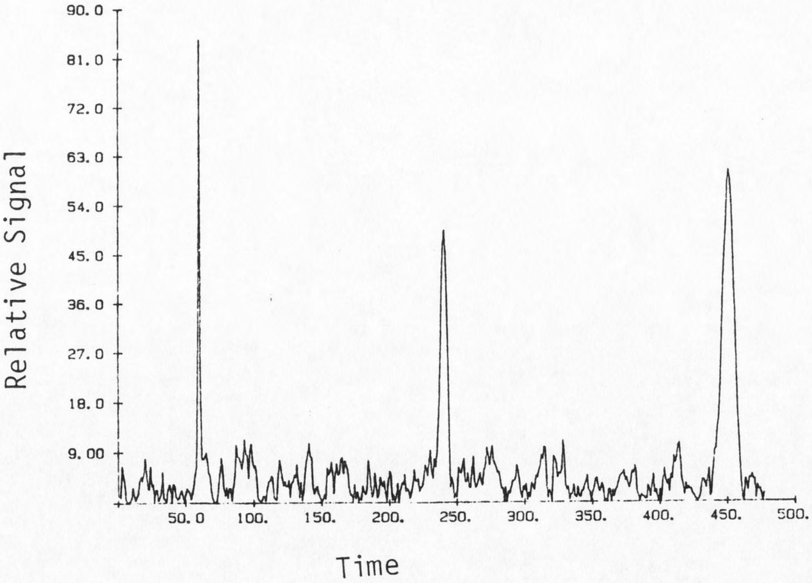
4.A Multiplex Chromatogram; LP: 4



4.B Cross-Correlation Single Chromatogram calculated from Figure 4.A

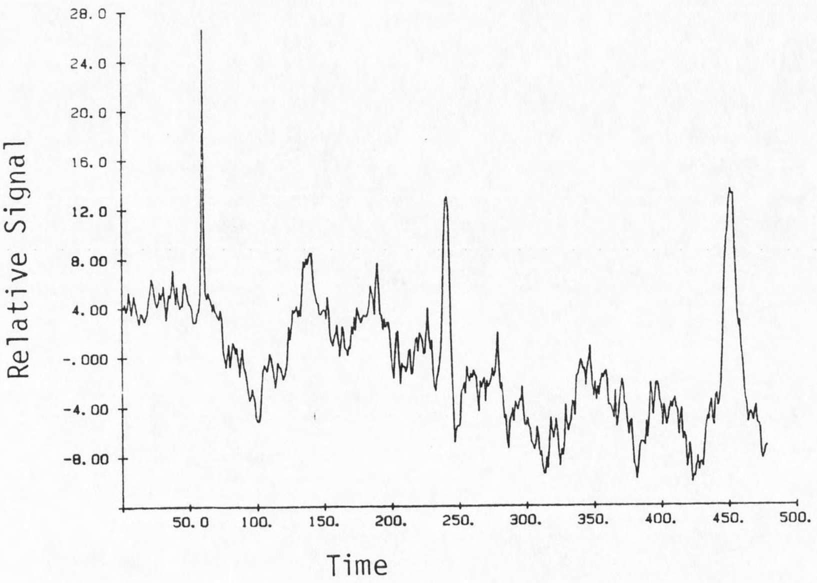


4.C Hadamard Transform Single Chromatogram calculated from Figure 4.A

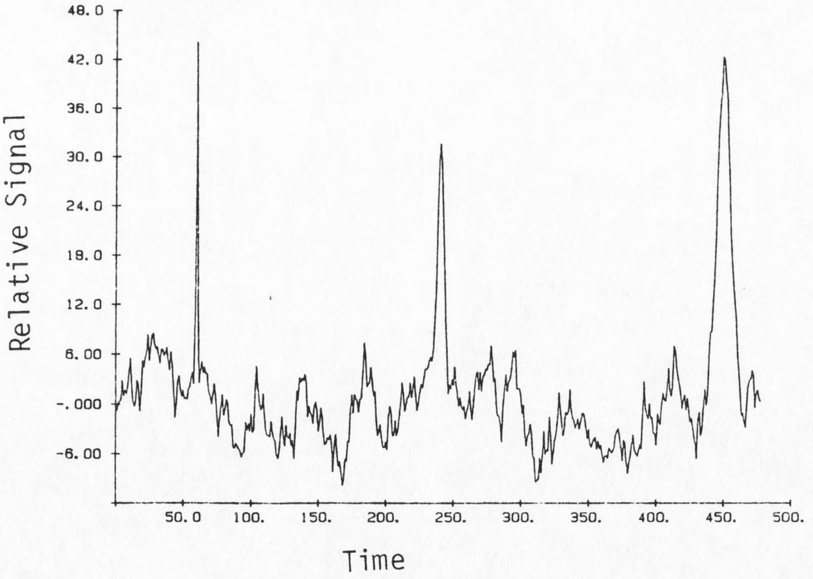


4.D Fast Fourier Transform Single Chromatogram calculated from Figure 4.A

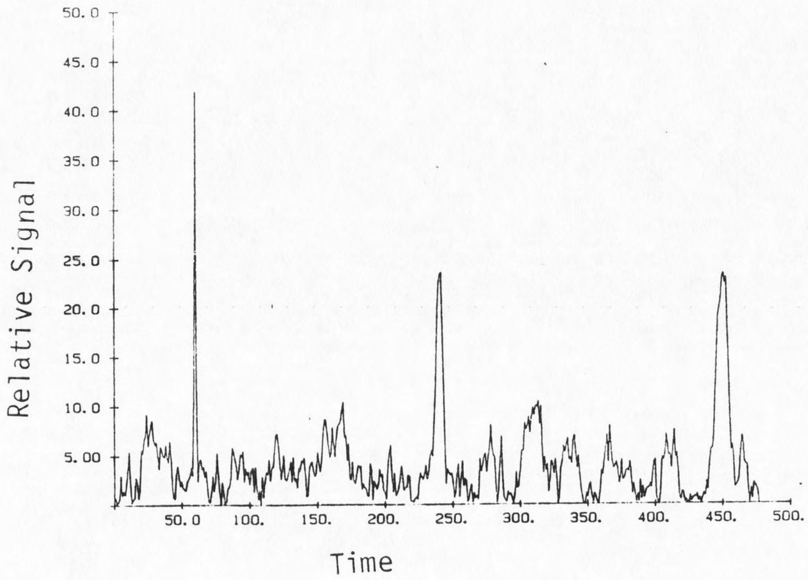
Figure 5. Graphs for Decision Sequence 3 Using Default Values and LP of 2 and 1



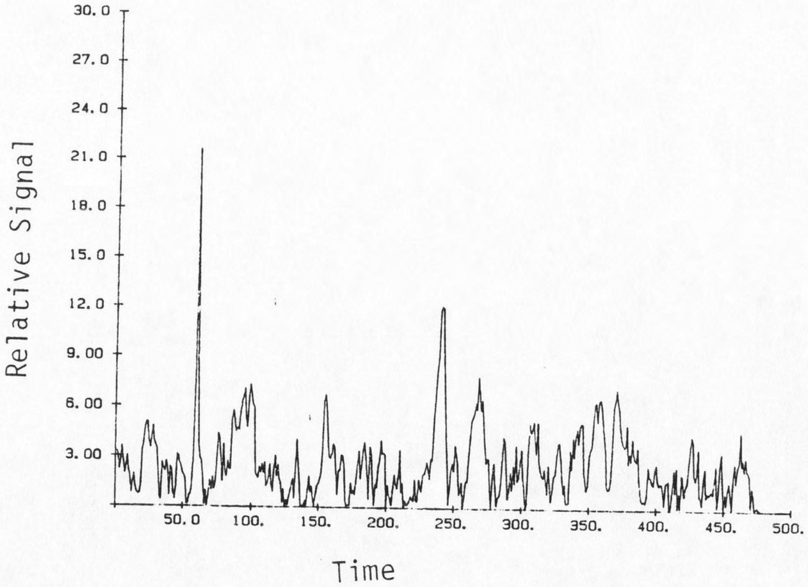
5.A Cross-Correlation Single Chromatogram calculated from Figure 4.A with LP: 2



5.B Hadamard Transform Single Chromatogram calculated from Figure 4.A with LP: 2



5.C Fast Fourier Transform Single Chromatogram calculated from Figure 4.A with LP: 2



5.D Fast Fourier Transform Single Chromatogram calculated from Figure 4.A with LP: 1

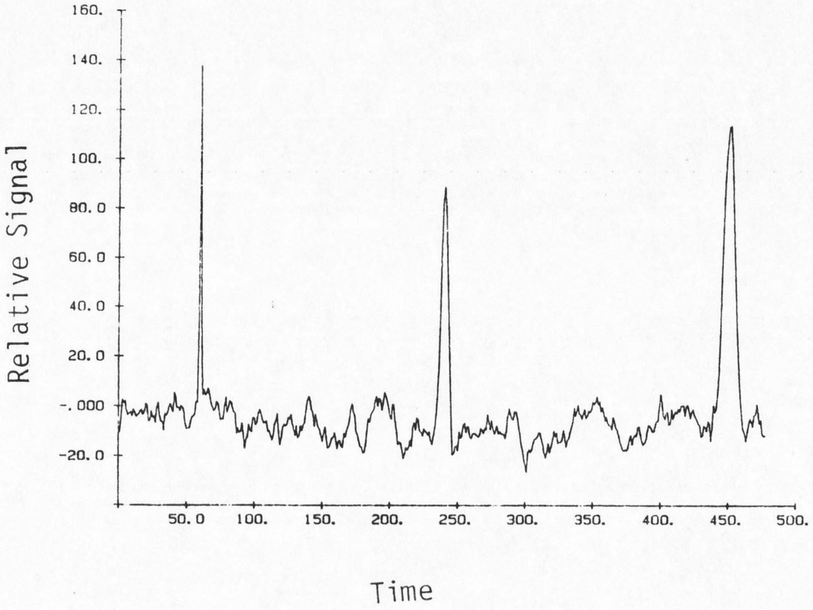
total number of points used in the calculations, rather than LP, affected the value S/N. It can also be observed that as the number of data points increased (EL), the S/N improved a little less than $(EL)^{0.5}$ which is the theoretical rate (Ref. 1).

Single chromatograms from CC and HT appear to have had about the same S/N given the same data, but were significantly lower than that for FFT. For example from Appendix N, the S/N averages were 4.00 for CC, 4.43 for HT and 6.59 for FFT.

The use of different decision sequences influenced the S/N of the resulting single chromatogram to some extent. For example in Appendix N, CC varied from 3.1 to 5.5, HT from 3.7 to 5.5 and FFT from 5.5 to 8.0.

Some decision sequences produced a drift in the single chromatogram resulting from CC, though not for HT or FFT (Fig. 5.A, 5.B, 5.C). This drift was due to the decision sequence having been less than random. In this situation, the decision sequence was such that more single chromatograms were added to the begining of the multiplex chromatograms than to the end or visa vera. This drift effect was less noticable as LP increased (Fig. 5.A, 4.B, 6). This is due to the fact that as the LP increased (EL increased), the decision sequence became more random. In Figure 4.A, this drift in the multiplex

Figure 6. Cross-Correlation Single Chromatogram Graph for Decision Sequence 3 Using Default Values and LP of 8



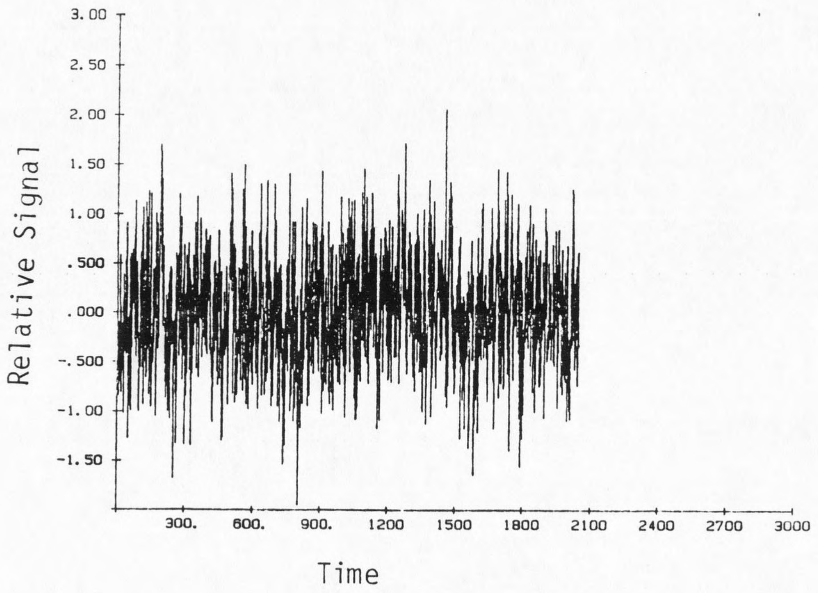
chromatogram is visible. The reason that CC is affected and not HT or FFT, can be explained by the different ways CC, HT and FFT are calculated. That is, in CC, the first points of the resulting single chromatogram are more influenced by the first portion of the multiplex chromatogram and last points of the single chromatogram more influenced by the latter portion of the multiplex chromatogram. In HT and FFT, all points in the single chromatogram are affected equally.

Electrical White Noise

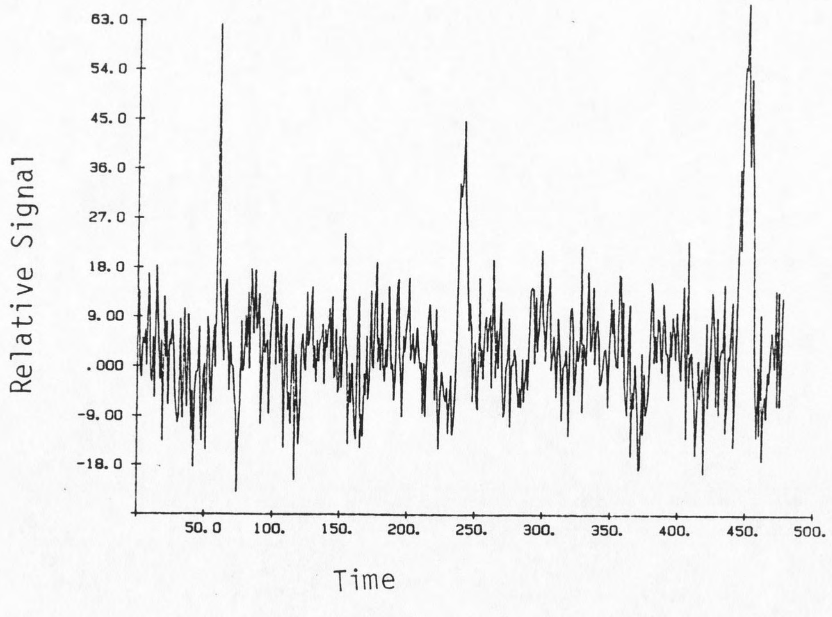
When white noise was present, the multiplex method improved S/N about 10 times. For example from Appendix O, the S/N went from 0.25 to 2.8 for CC, to 2.8 for HT and to 3.7 for FFT. The improvement can be seen by comparing Figure 1.C, a single injection chromatogram which has no detectable peaks, with Figures 7.B, 7.C and 7.D which have detectable peaks in the single chromatograms calculated from the multiplex chromatogram (Fig. 7.A).

The effects of adding white noise to multiplex chromatograms, on S/N in single chromatograms resulting from CC, HT and FFT, can be seen by comparing Figure 3 with Figure 7. For all three analysis methods, as more white noise was added (ie. noise magnitude increased or

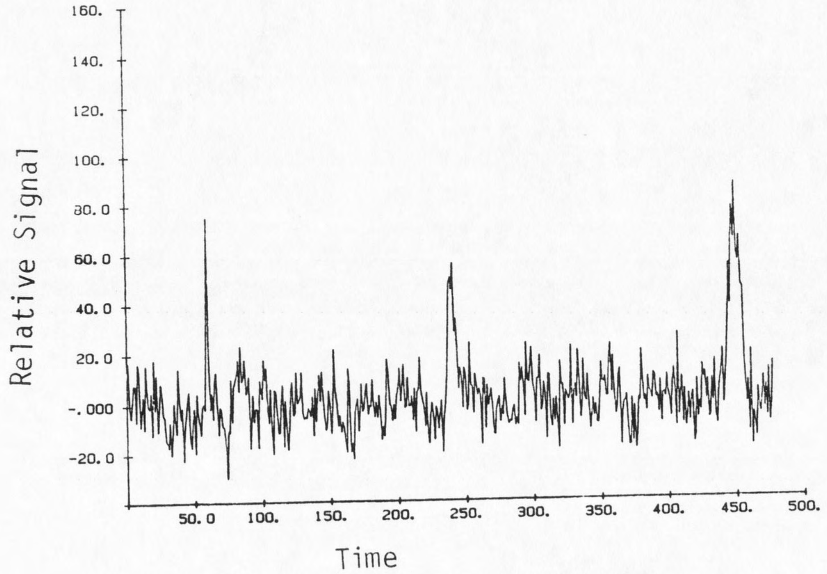
Figure 7. Graphs for Decision Sequence 8 Using Default Values with White Noise



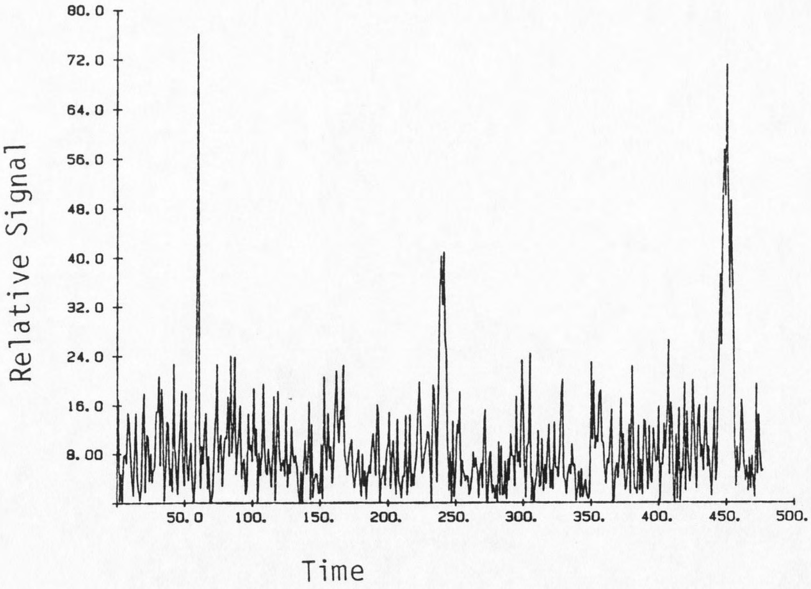
7.A Multiplex Chromatogram; LP: 4; Noise Magnitude: 2



7.B Cross-Correlation Single Chromatogram calculated from Figure 7.A



7.C Hadamard Transform Single Chromatogram calculated from Figure 7.A



7.D Fast Fourier Transform Single Chromatogram calculated from Figure 7.A

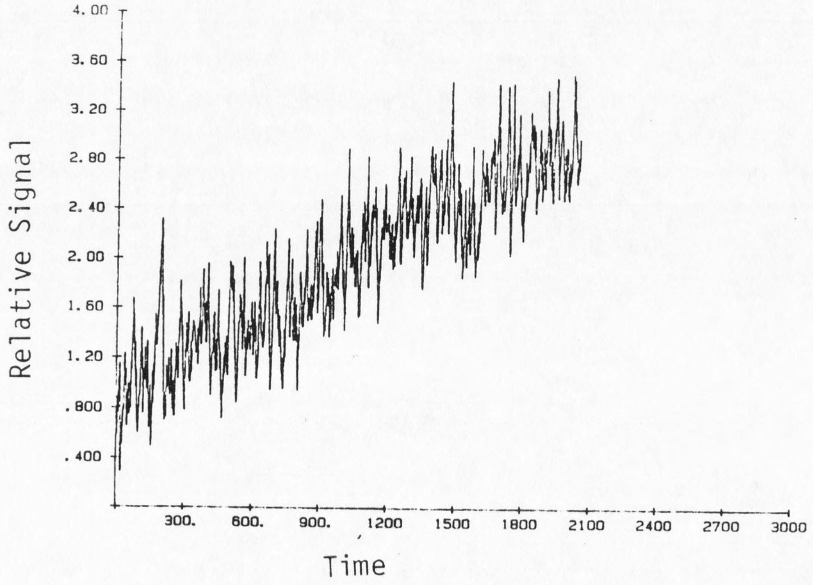
S/N ratio decreased), the S/N of the resulting single chromatograms decreased. For example, from Appendix O, for noise magnitudes of 0, 1, 2 and 4, the S/N of the single chromatograms resulting from CC was 5.5, 4.0, 2.8 and 1.3 respectively. However, given the same noise magnitude, the S/N of the resulting single chromatogram improved with a larger LP. For example, for a noise magnitude of 1 and a LP of 4 and 16, the S/N for CC was 4.0 and 5.0 respectively. That is, as the number of points in the multiplex chromatogram (EL) increased, S/N of the resulting single chromatogram increased as well.

It is important to remember that the S/N in calculated single chromatograms is a result of both correlation noise and white noise. Therefore as white noise magnitude increases, the total contribution of correlation noise to S/N in the resulting single chromatogram diminishes.

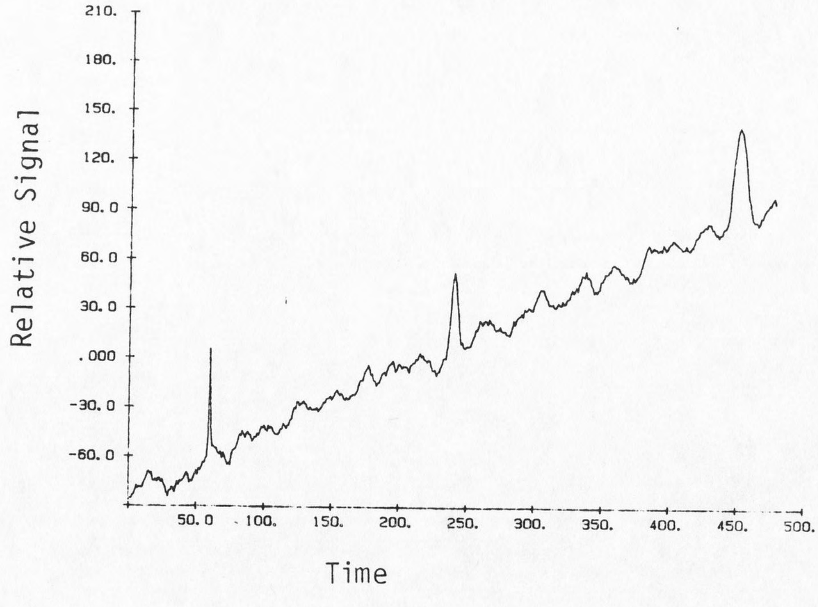
Electrical Drift

When the multiplex chromatogram had linear drift present, the single chromatogram resulting from CC, but not from HT or FFT, was affected (Fig. 8). The explanation for this can be found in the correlation noise section above. However unlike drift produced by a specific decision sequence, an increase in LP did not diminish the CC single chromatogram's electrical drift

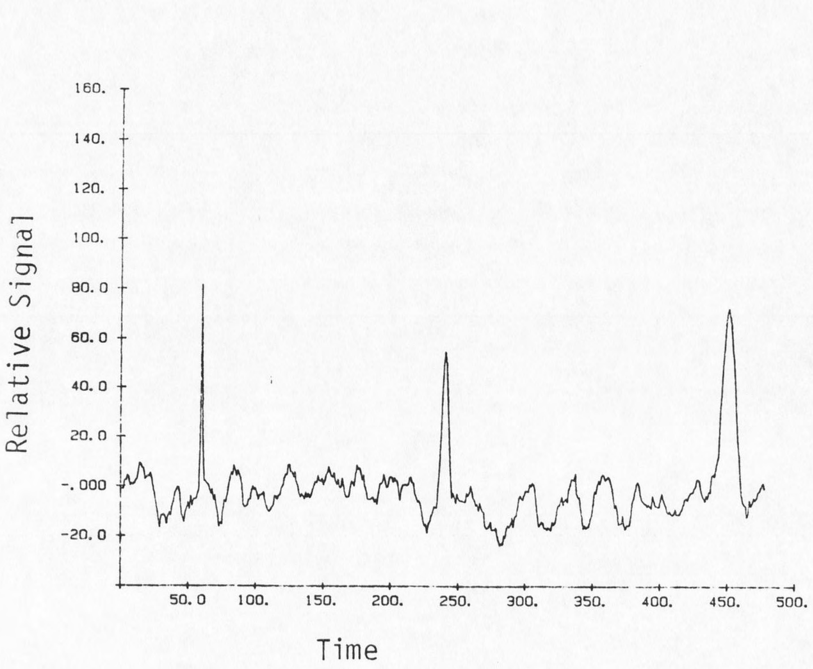
Figure 8. Graphs for Decision Sequence 8 Using Default Values with Drift Rate of 4 and LP of 4



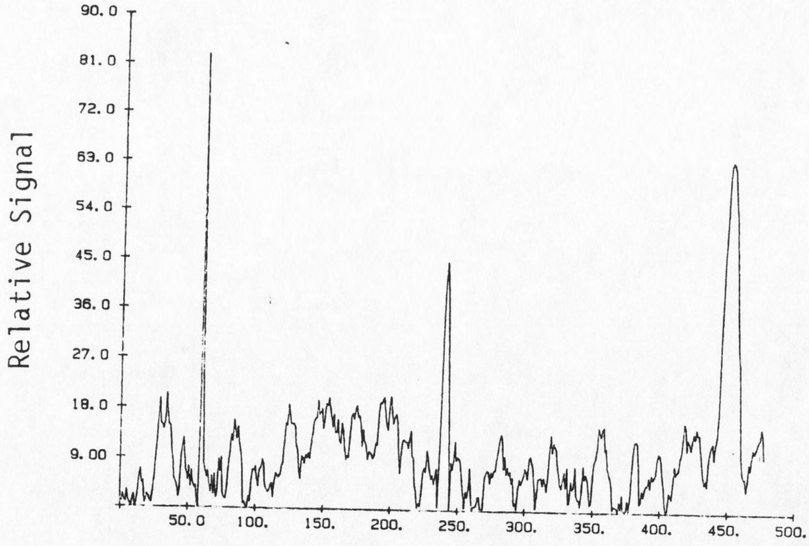
8.A Multiplex Chromatogram



8.B Cross-Correlation Single Chromatogram calculated from Figure 8.A

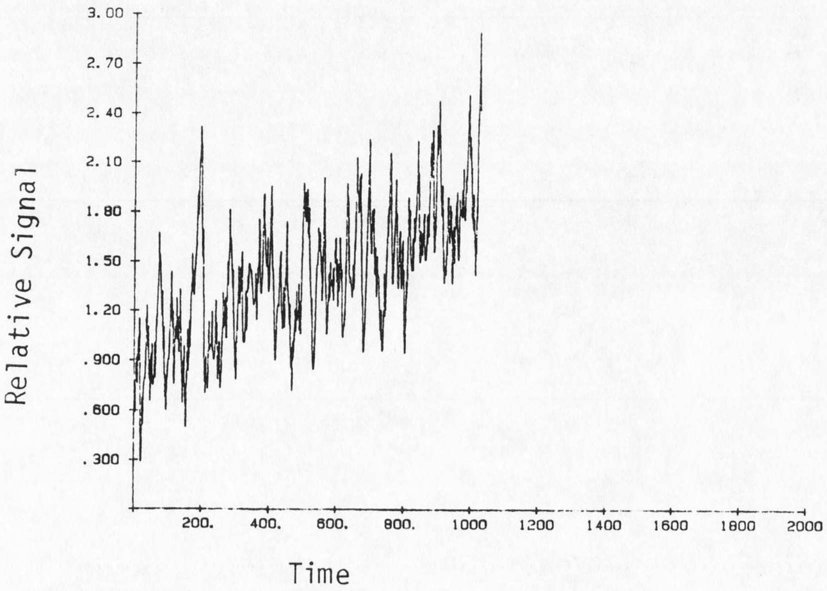


8.C Hadamard Transform Single Chromatogram calculated from Figure 8.A

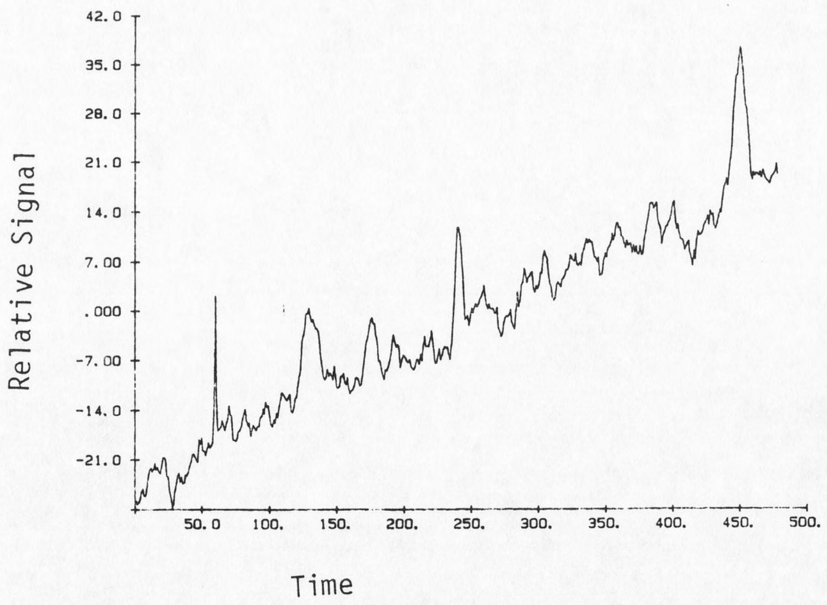


8.D Fast Fourier Transform Single Chromatogram calculated from Figure 8.A

Figure 9. Graphs for Decision Sequence 8 Using Default Values with Drift Rate of 4 and LP of 2



9.A Multiplex Chromatogram



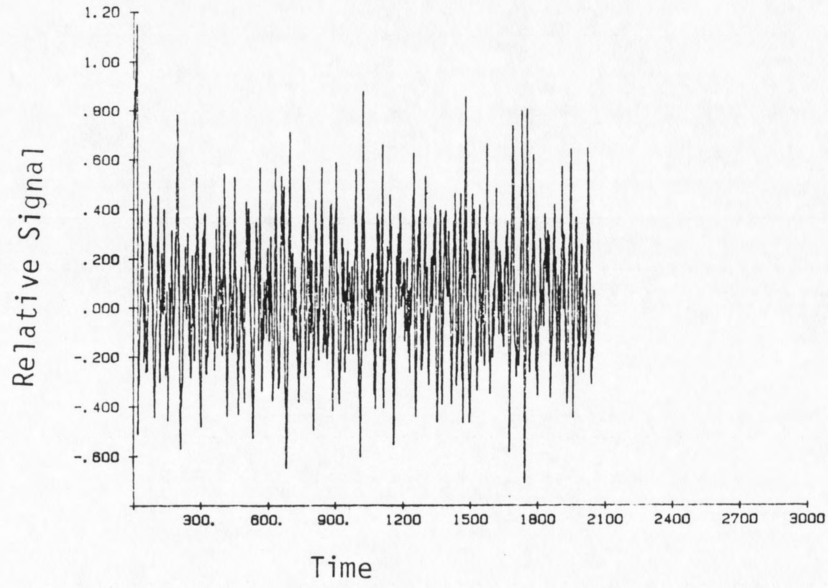
9.B Cross-Correlation Single Chromatogram calculated from Figure 9.A

since the electrical drift in this report was linear and not a function of random numbers that should average to zero (Fig. 9.A, 9.B, 8.A, 8.B). Although the single chromatograms of HT and FFT might not exhibit a drift, they were still affected by it. That is, as more drift was added (drift rate increased), the S/N of the single chromatograms decreased (ie. noise increased). Drift also decreased the S/N for CC. For example, from Appendix P, for an LP of 4 and drift rate of 0, 2 and 4, the S/N for FFT was 6.5, 4.8 and 4.1 respectively.

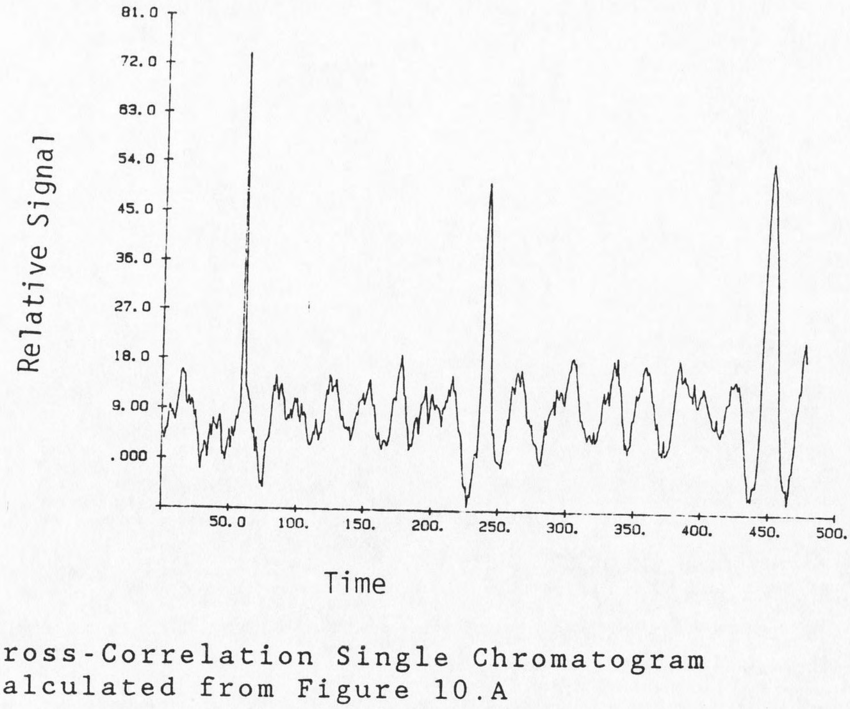
When an attempt was made to reduce the electrical drift, the S/N was still lower than in the single chromatograms calculated from a multiplex chromatogram with no initial electronic drift (Fig. 3, 10). For example from Appendix P, when there was no drift, the S/N for CC was 5.5, HT was 5.3 and FFT was 6.5, but when electrical drift was added and then reduced, CC was 4.0, HT was 3.7 and FFT was 3.5.

When comparing single chromatograms calculated from a multiplex chromatogram with electrical drift, to single chromatograms calculated from a multiplex chromatogram with the electronic drift reduced, only CC showed an improvement. The S/N for CC went from 3.0 to 4.0, while HT went from 4.0 to 3.7 and FFT from 4.1 to 3.5. It is apparent that the reduction introduced more noise and

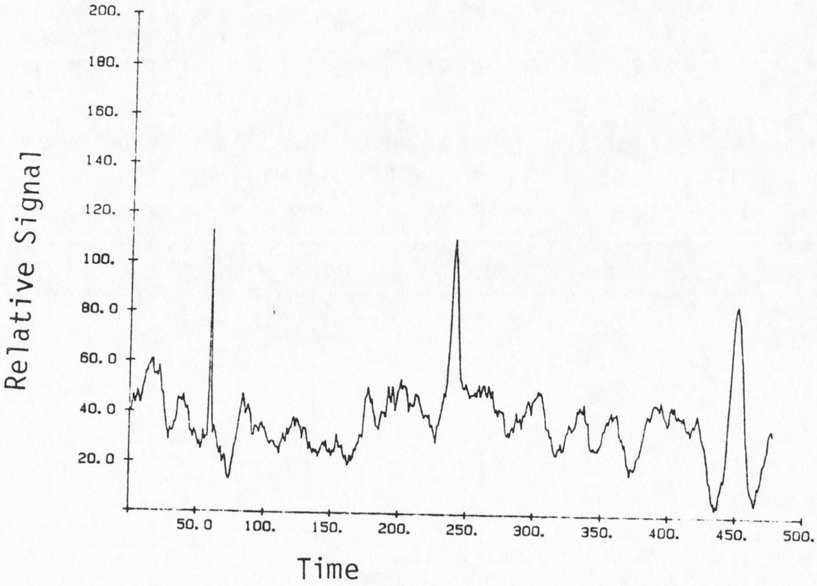
Figure 10. Graphs for Decision Sequence 8 Using Default Values with Drift Rate of 4



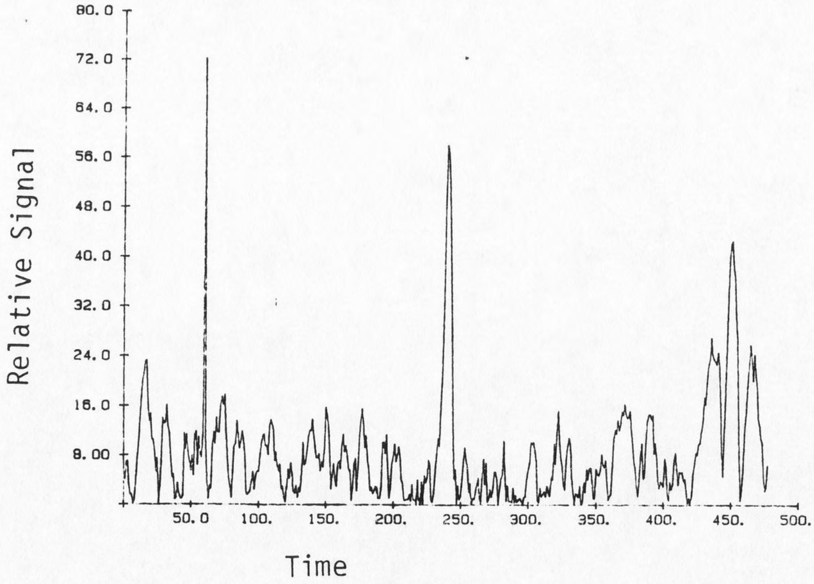
10.A Multiplex Chromatogram



10.B Cross-Correlation Single Chromatogram calculated from Figure 10.A



10.C Hadamard Transform Single Chromatogram calculated from Figure 10.A



10.D Fast Fourier Transform Single Chromatogram calculated from Figure 10.A

since HT and FFT were not affected by the electronic drift, their S/N's fell. However, since CC was affected by drift, the addition of noise by the drift reduction was compensated by the improvement in electronic drift.

CHAPTER V

FUTURE ENHANCEMENTS

Decision Sequence

When generating the decision sequence, rejection of close calls may be required. That is, a second positive decision can not be made until a certain period of time has passed. This period of time is called the "rejection period". In real experiments, one method of the "injection" can be a laser shot (Ref. 11). There is a limit to how often a laser can be fired at a sample. This is due to a recharge time required by the laser before it is able to fire again.

Multiplex Chromatogram

Presently the single chromatogram is added in precisely the same way each time. It would be interesting to see the effects if the single chromatogram is added slightly earlier or later than the actual positive decision sequence times. The term for such offsetting is called "jitter". The jitter can be generated purposely as a way of experiment or it can be due to imprecisions in the timing of the injection.

Another aspect that should be investigated, is the effect of varying injected amounts or magnitudes of the single chromatogram. That is, sometimes the full single chromatogram would be added but other times, only a smaller magnitude of the single chromatogram would be used. For example, in laser injection, laser intensity varies which means that the laser is unable to fire at a sample at exactly the same intensity each time. This is called a "laser intensity" factor. Therefore the magnitude of the single chromatogram produced and added to the multiplex chromatogram would vary from firing to firing.

Different methods of adding and reducing drift should also be investigated. To accomplish this, experimental data is first required to determine the optimum method.

CHAPTER VI

CONCLUSIONS

ASYST has been a satisfying language to work with. Its toolbox approach reduced coding time and gave professional looking results. The fact that the functions (eg. FFT) were highly optimized and that array operations were available, resulted in a prototype program that ran quickly. Double precision and complex operations allowed for the level of accuracy and type of computations needed for this report. ASYST provided many error checking systems but was not good at determining and preventing total filling up of memory. When memory was completely utilized, the whole system had to be rebooted.

The random number functions RAND.UNIF and RAND.NRML utilized a good random number generator. This was confirmed by the results of tests in this report as well as in the literature.

All three analysis methods, (CC, HT and FFT) had correlation noise in the resulting single chromatograms. When white noise magnitude was low, correlation noise was the determining factor of S/N in the resulting single chromatograms. Correlation noise and electrical white noise were reduced as the number of data points used increased, at a rate a little less than $(EL)^{0.5}$. By increasing EL, the S/N improved but required more time to do the calculations.

When only correlation noise was present, the best S/N was an average of 10 for the single chromatograms resulting from CC on a multiplex chromatogram with LP of 16, CL of 477, EL of 7632 and no electrical noise. No resulting single chromatagram under these conditions can have a S/N better than this since correlation noise is always present. This experimental length can be considered a reasonable value for on-line acquisition and analysis since further improvement in S/N is approximately $(EL)^{0.5}$ and a larger EL would increase calculation time. With this in mind, when electrical noise is small and a single injection experiment produces a chromatogram with S/N of 10 or more, there is no advantage in using the multiplex method since the method would actually add more noise (correlation noise) to the resulting single chromatogram. Only when electrical noise is significant and therefore S/N is low (much less than 10) in the single injection method, can the mutliplex method effectively reduce the noise and produce a single chromatogram with a better S/N. The multiplex method improves S/N due to white noise by about 10 times.

Since correlation noise is the limiting factor of the S/N in the resulting single chromatograms and is also proportional to the tallest single chromatogram peak, it limits the size of the smallest detectable peak. That is, in a multiplex chromatogram with an EL of 7632, the smallest peak would need to be larger than 1/10 the tallest peak height for it to be distinguishable from noise since the S/N would be 10.

CC is a faster calculation method than HT. If these two analysis methods could be optimized as was the FFT function, the fastest calculations would be CC and then HT, which speeds are proportional to the number of data points, n. FFT would be the slowest since its speed is proportional to $n\log_2 n$. How much CC would be faster than HT would depend on the number of zero operations that could be eliminated. Theoretically then, CC would be the simplest method to choose if speed were important, as is in the case of on-line acquisition and analysis.

One problem with CC is that it is sensitive to drift in the multiplex chromatogram. This drift could be the result of the non-randomness of the decision sequence or due to electronic drift. This presents the problem of finding a method of reducing drift. As initial results indicate, the method of reduction influences S/N by diminishing S/N. This is especially true for HT and FFT which are not effected by drift. Therefore various drift reduction methods must be investigated before valid analysis of drift can be done. This will require the collection of experimental data to first characterize the real nature of electronic drift.

If the number of data points used is limited, HT and FFT methods are better than CC. Both methods produce more detectable peaks, with FFT having the larger S/N. However, HT is better since the single chromatogram peak heights resulting from FFT do not always reflect the original peak magnitudes.

In reflecting back, this has been a challenging and interesting project. It has developed the author's skills in investigating, determining and producing a computer solution to a problem in a field other than computer science.

REFERENCES

[1] Phillips J: Multiplex Gas Chromatography. Anal Chem 52: 468A, 1980

[2] Marshall AG, editor: Fourier, Hadamard and Hilbert Transforms in Chemistry. Plenum Press, NY, 1982

[3] Ramirez RW: The FFT Fundamentals and Concepts. Prentice-Hall Inc, NJ, 1985

[4] Harwit M, Sloan NJA: Hadamard Transform Optics. Academic Press, NY, 1979

[5] ASYST, A Scientific System Manual. MacMillan Software Co, NY, 1985

[6] Kaljurand M, Kullik E: Comparison Between Conventional and Cross-Correlation Gas Chromatography. J Chromatogr 186: 145, 1979

[7] Knuth DE: Seminumerical Algorithms, TheArt of Computer Programming, Vol2. Addison Wesley Pub Co, NJ, 1982

[8] Synovec RE, Yeung ES: Improvement of the Limit of Detection in Chromatography by an Integration Method. Anal Chem 57: 2162, 1985

[9] Malmstadt H, Enke C, Crouch S: Electronics and Instrumentation for Scientists. Benjamin/Cummings Pub Co Inc, Menlo Pk CA, 1981

[10] Banks J, Carson JS: Discrete-Event System Simulation. Prentice-Hall Inc, NJ, 1984

[11] Pawliszyn J, Lui S: Sample Introduction for Capillary Gas Chromatography with Laser Desorption and Optical Fibers. Anal Chem 59: 1475, 1987

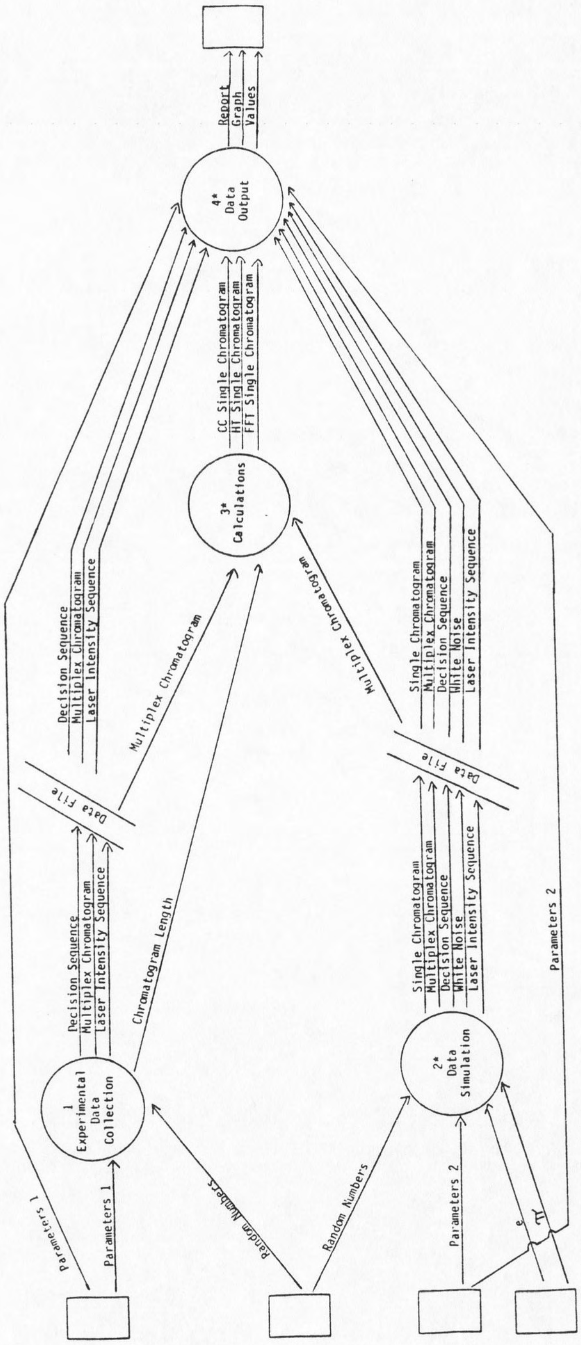
Appendix A

List of Abbreviations Used in this Report

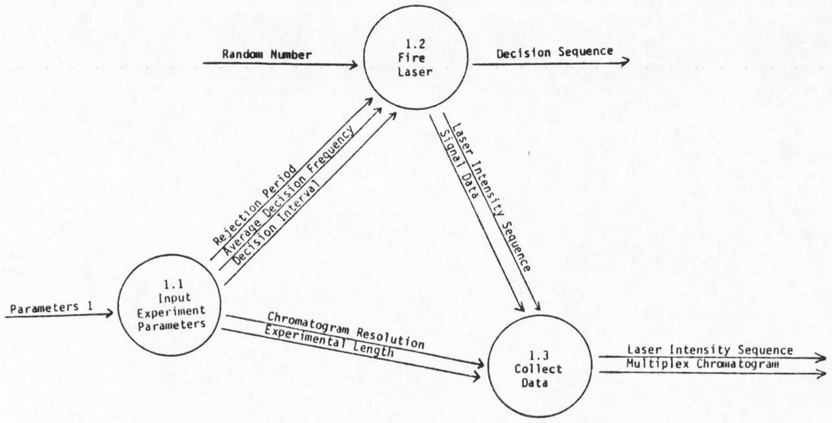
SC	SINGLE CHROMATOGRAM
MC	MULTIPLEX CHROMATOGRAM
MCD	MULTIPLEX CHROMATOGRAM WITH DRIFT
DS	DECISION SEQUENCE
CL	CHROMATOGRAM LENGTH (OF SC)
EL	EXPERIMENTAL LENGTH (OF MC)
LP	LENGTH PROPORTION (CL/EL)
NM	NOISE MAGNITUDE
S/N	SIGNAL-TO-NOISE RATIO
S/WN	SIGNAL--TO-WHITE NOISE RATIO
DF	DRIFT FACTOR
CC	CROSS-CORRELATION
HT	HADAMARD TRANSFORM
FT	FOURIER TRANSFORM
FFT	FAST FOURIER TRANSFORM

Appendix B

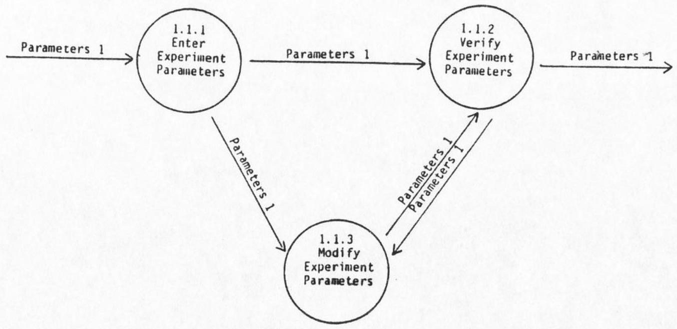
Data Flow Diagrams



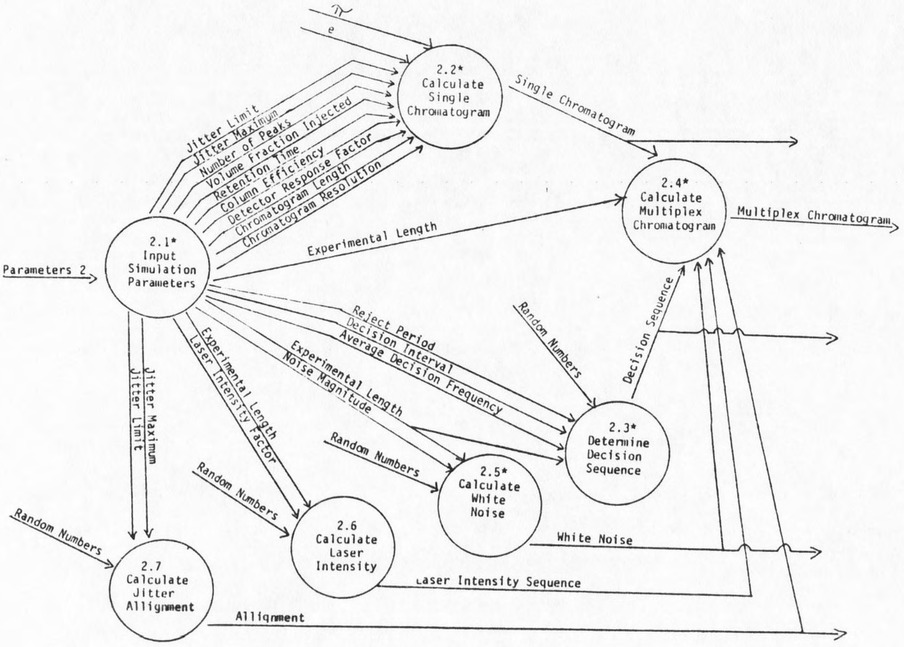
B.1 Data Flow Context Diagram



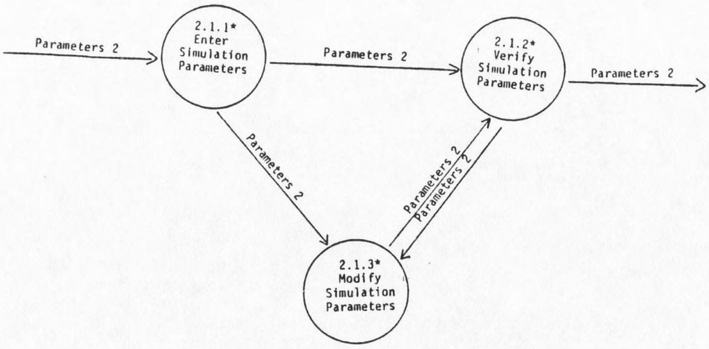
B.2 Diagram 1 - Experimental Data Collection


Parameters 1
1.1.1 Enter Experiment Parameters
Parameters 1
1.1.2 Verify Experiment Parameters
Parameters 1
Parameters 1
Parameters 1
Parameters 1
1.1.3 Modify Experiment Parameters

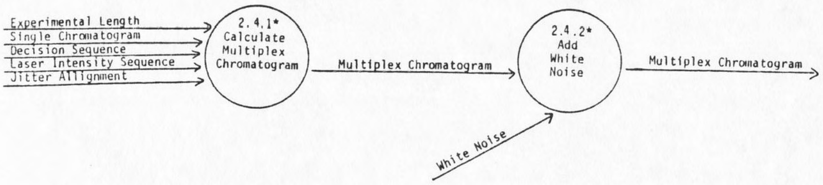
B.3 Diagram 1.1 - Input Experimental Parameters



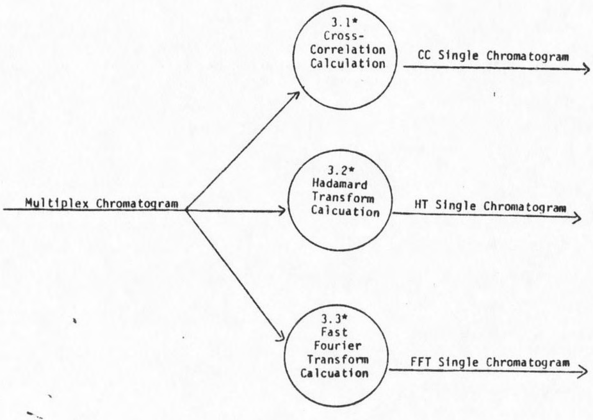
B.4 Diagram 2 - Data Simulation


Parameters 2
2.1.1* Enter Simulation Parameters
Parameters 2
2.1.2* Verify Simulation Parameters
Parameters 2
Parameters 2
Parameters 2
Parameters 2
2.1.3* Modify Simulation Parameters

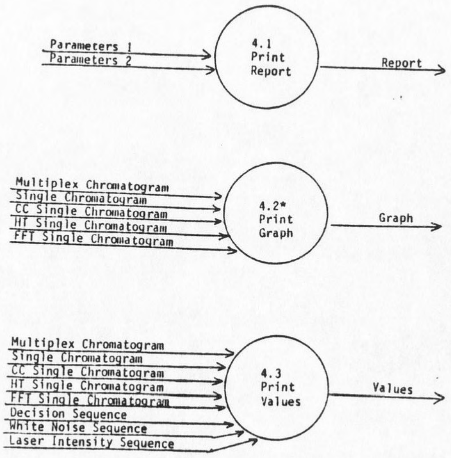
B.5 Diagram 2.1 - Input Simulation Parameters



B.6 Diagram 2.4 - Calculate Multiplex Chromatogram



B.7 Diagram 3 - Calculations



B.8 Diagram 4 - Data Output

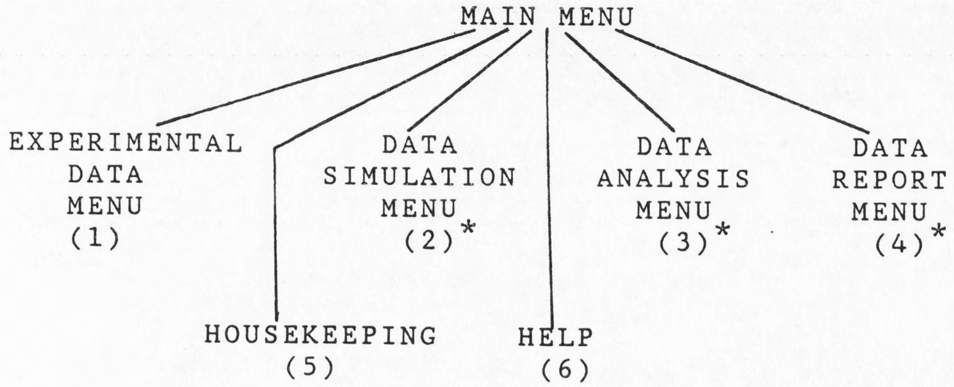
* indicates available

Appendix C

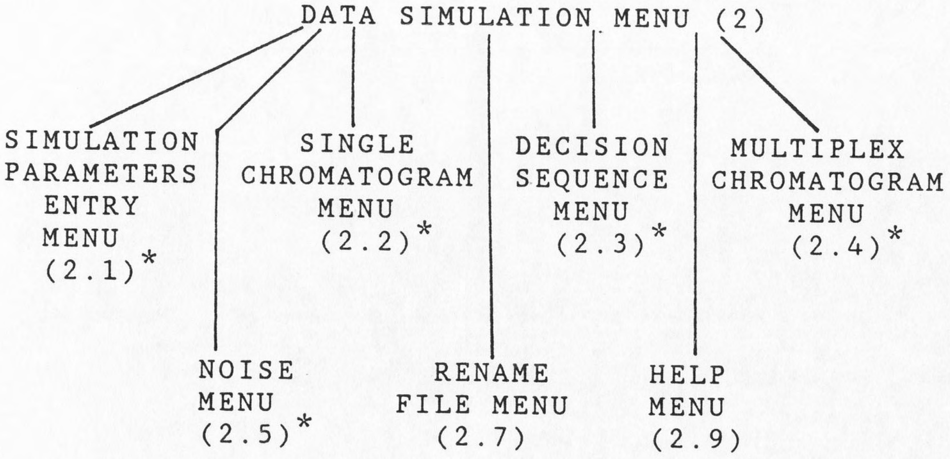
Hierarchy Structure of Prototype Program

Menu Calls

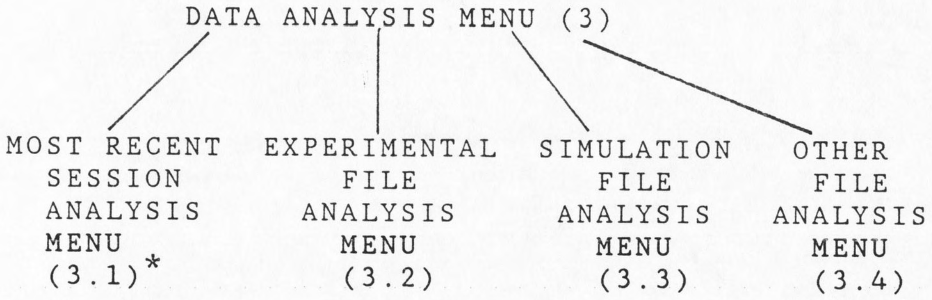
MAIN MENU CALLS:



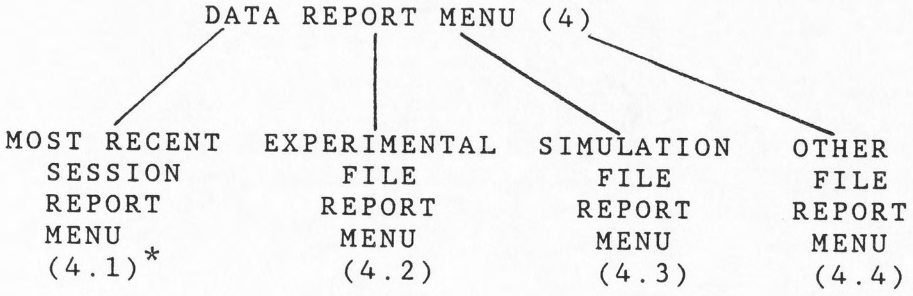
DATA SIMULATION MENU (2) CALLS:


DATA SIMULATION MENU (2)
SIMULATION PARAMETERS ENTRY MENU (2.1)*
SINGLE CHROMATOGRAM MENU (2.2)*
DECISION SEQUENCE MENU (2.3)*
MULTIPLEX CHROMATOGRAM MENU (2.4)*
NOISE MENU (2.5)*
RENAME FILE MENU (2.7)
HELP MENU (2.9)

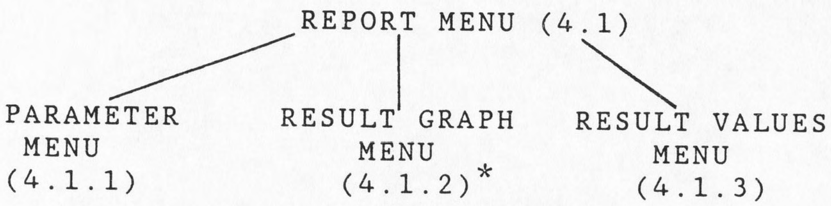
DATA ANALYSIS MENU (3) CALLS:


DATA ANALYSIS MENU (3)
MOST RECENT SESSION ANALYSIS MENU (3.1)*
EXPERIMENTAL FILE ANALYSIS MENU (3.2)
SIMULATION FILE ANALYSIS MENU (3.3)
OTHER FILE ANALYSIS MENU (3.4)

DATA REPORT MENU (4) CALLS:


DATA REPORT MENU (4)
MOST RECENT SESSION REPORT MENU (4.1)*
EXPERIMENTAL FILE REPORT MENU (4.2)
SIMULATION FILE REPORT MENU (4.3)
OTHER FILE REPORT MENU (4.4)

REPORT MENU (4.1) CALLS:



* - indicates menus are available

Appendix D

Prototype Program Menu Screens

D.1 MAIN MENU

```
                  MAIN MENU


                   WELCOME
                  TO   THE
            MULTIPLEX CHROMATOGRAM
                   PROGRAM


<F1>   EXPERIMENTAL DATA COLLECTION
<F2>   DATA SIMULATION
<F3>   DATA ANALYSIS
<F4>   DATA REPORT
<F5>   HOUSEKEEPING
<F6>   HELP
<F10>  EXIT
```

D.2 DATA SIMULATION MENU (2)

```
     DATA SIMULATION MENU


<F1>   PARAMETERS
<F2>   SINGLE CHROMATOGRAM CALCULATION
<F3>   DECISION SEQUENCE CALCULATION
<F4>   MULTIPLEX CHROMATOGRAM CALCULATION
<F5>   NOISE CALCULATION
<F6>   RENAME FILES
<F7>   HELP
<F10>  EXIT


FILE NAME TO BE USED:  BARSIMTP.DAT
```

D.3 SIMULATION PARAMETERS ENTRY MENU (2.1)

```
     SIMULATION PARAMETERS ENTRY MENU


<F1> ENTER PARAMETERS            <F5>  DISPLAY PARAMETERS
<F2> USE DEFAULT PARAMETERS      <F6>  CHANGE PARAMETERS
<F3> USE STORED PARAMETERS       <F7>  FINISH NEXT STEPS
                                       AUTOMATICALLY
<F4> LIST DIRECTORY              <F10> EXIT
```

D.4 SINGLE CHROMATOGRAM MENU (2.2)

```
     SINGLE CHROMATOGRAM MENU


<F1>  DISPLAY ALL PARAMETERS                  <F10> EXIT
<F2>  DISPLAY SINGLE CHROMATOGRAM PARAMETERS
<F3>  CHANGE SINGLE CHROMATOGRAM PARAMETERS
<F4>  CALCULATE SINGLE CHROMATOGRAM
<F5>  USE STORED SINGLE CHROMATOGRAM
<F6>  DISPLAY SINGLE CHROMATOGRAM GRAPH
```

D.5 DECISION SEQUENCE MENU (2.3)

```
     DECISION SEQUENCE MENU


<F1>  DISPLAY ALL PARAMETERS                  <F10> EXIT
<F2>  DISPLAY DECISION SEQUENCE PARAMETERS
<F3>  CHANGE DECISION SEQUENCE PARAMETERS
<F4>  CALCULATE DECISION SEQUENCE
<F5>  USE STORED DECISION SEQUENCE
<F6>  DISPLAY DECISION SEQUENCE GRAPH
```

D.6 MULTIPLEX CHROMATOGRAM MENU (2.4)

```
     MULITPLEX CHROMATOGRAM MENU


<F1>  DISPLAY ALL PARAMETERS                  <F10> EXIT
<F2>  DISPLAY MULTIPLEX CHROMATOGRAM PARAMETERS
<F3>  CHANGE MULTIPLEX CHROMATOGRAM PARAMETERS
<F4>  CALCULATE MULTIPLEX CHROMATOGRAM
<F5>  USE STORED MULTIPLEX CHROMATOGRAM
<F6>  DISPLAY MULTIPLEX CHROMATOGRAM GRAPH
```

D.7 NOISE MENU (2.5)

```
     NOISE MENU


<F1>  DISPLAY ALL PARAMETERS                  <F10> EXIT
<F2>  DISPLAY NOISE PARAMETERS
<F3>  CHANGE NOISE PARAMETERS
<F4>  CALCULATE NOISE
<F5>  USE STORED NOISE
<F6>  DISPLAY NOISE GRAPH
```

D.8 DATA ANALYSIS MENU (3)

```
     DATA ANALYSIS MENU


DATA TO BE ANALYZED :      <F1>  MOST RECENT SESSION
                           <F2>  EXPERIMENTAL FILE
                           <F3>  SIMULATION FILE
                           <F4>  OTHER FILE
                           <F10> EXIT
```

D.9 ANALYSIS MENU (3.1)

```
     ANALYSIS MENU

<F1>  CROSS-CORRELATION
<F2>  HADAMARD TRANSFORM
<F3>  FAST FOURIER TRANSFORM
<F10> EXIT
```

D.10 DATA REPORT MENU (4)

```
     DATA REPORT MENU


REPORT:    <F1>  MOST RECENT SESSION
           <F2>  EXPERIMENTAL FILE
           <F3>  SIMULATION FILE
           <F4>  OTHER FILE
           <F10> EXIT
```

D.11 REPORT MENU (4.1)

```
     REPORT MENU


REPORT:    <F1>  PARAMETERS
           <F2>  RESULT GRAPHS
           <F3>  RESULT VALUES
           <F10> EXIT
```

D.12 REPORT GRAPHS MENU (4.1.2)

```
     REPORT GRAPHS MENU


<F1>  SINGLE CHROMATOGRAM
<F2>  MULTIPLEX.CHROMATOGRAM
<F3>  CROSS CORRELATION CHROMATOGRAM
<F4>  HADAMARD CHROMATOGRAM
<F5>  FAST FOURIER TRANSFORM CHROMATOGRAM
<F10> EXIT
```

Appendix E

User's Manual For Prototype Program

Hardware Specifications

This software requires an IBM compatible PC having a hard disk, graphics monitor, keyboard, printer and 8087 math processor. A minimum of 640 K of memory is needed.

System Configuration

Besure that the copy of ASYST that you use has been configured with the "required memory" listed in Appendix F of this report. These are the minimum values needed to load this program with no other definitions (programs) loaded. If other programs are to co-exist with this program, you must make the appropriate adjustments to the configuration. For more information regarding configuration, refer to the ASYST manual (Ref. 5).

Loading the Prototype Program

Follow the instructions in the ASYST manual (Ref. 5) to boot into ASYST. The files required to run the prototype program are:

```
BARINIT.PRO
BARSIMFL.PRO
BARPAR1.PRO
BARPAR2.PRO
BARSIM.PRO
BARCROSS.PRO
BARHAD.PRO
BARFOUR.PRO
BARMENUS.PRO
```

These files can be automatically loaded and a data storage file called "BARSIMTP.DAT" created by using the file BARLOAD.PRO.

1) Load this loading/initializing program when in ASYST at the OK prompt. Type:

```
LOAD BARLOAD.PRO
```

A series of dots will appear during the loading of this file. The OK prompt will return when it is completed.

2) To load and initialize the prototype program, type:

```
LOAD.PROGRAM
```

Again a series of dots will appear.

Entering and Using the Prototype Program

To enter the program type:

```
START.PROGRAM
```

The main menu will then be displayed. Any menu can be exited by using the functions key F10. To exit from the program and return to ASYST operating system, simply touch F10 until the OK prompt reappears.

The menus are self-directing but only some menu-picks are available at this time. If you happen to choose an option not available, you will receive a prompt in blue stating this. Just touch any key to continue. All menus are labeled in green, so you will know exactly where you are at all times. To see the hierarchy of the menus see Appendix C. If at any time an error is encountered, a bell will sound twice and a red error message describing the error will display at the top of the screen. You will then be given the opportunity to correct the error.

When simulating data, a particular order must be adhered to:

1) Determine the parameters
2) Calculate the single chromatogram and decision sequence
3) Calculate the multiplex chromatogram
4) Calculate and add noise to the multiplex chromatogram (optional)
5) Analyze data
6) Report data

You may always go back to a previous step, however, to get valid results, never skip an item when doing steps 1 to 6.

Appendix F

Memory Configuration and Required Space for Prototype Program

SYSTEM NUCLEUS (fixed at 64 Kbytes)
- Is the part of memory where most of the system code resides. Also where strings and scalars are stored. The system size cannot be changed.

USER DICTIONARY (default 16 Kbytes, range 8 - 64 Kbytes, required 21 Kbytes)
- Where code for colon definitions are compiled.

SYMBOL TABLE (default 24 Kbytes, range 20 -64 Kbytes required 29 Kbytes)
- Where the list of all names ASYST can recognize, is stored.

DATA ACQUISITION BUFFER (default 0 Kbytes, range 0 - 64 Kbytes)
- Reserved for all buffered I/O.

HEAP (default 32 Kbytes, range 6 - 128 Kbytes)
- Where ASYST temporarily stores all unnamed arrays, however with an increase of heap size, the amount of space available for named arrays decreases.

STRING VARIABLE STORAGE (default 0 Kbytes, range 0 - 64 Kbytes, required 6 Kbytes)
- Where contents of strings and string arrays are stored.

GPIB QUEUE (default 0 Kbytes, range 0 - 64 Kbytes)
- Used to store a list of asynchronous GPIB tasks (IEEE bus).

ARRAY MEMORY (required 141 Kbytes)
- All memory not used by DOS or by any of the above parts of ASYST is available for use by named arrays.

Note: the required Kbytes listed above are the minimum amounts needed to run this report's prototype program.

Appendix G

Parameter Description and Values

CODE NAME	RANGE	DEFAULT	TYPE	DESCRIPTION
EXP.LENG	0 - 10800 SEC.	2048	I	EXPERIMENTAL/ MULTIPLEX CHROM. LENGTH
CHROM. LENG	60 - 2700 SEC.	477	I	SINGLE CHROM. LENGTH
CHROM. RESOL	0.001 - 1.0 SEC.	1	R	TIME BETWEEN DATA POINTS
DEC.INT	0.1 - 10 SEC.	1	R	DECISION INTERVAL: TIME PASSED BEFORE ANOTHER DECISION CAN BE MADE
AVE.DEC. FREQ	0.01 - 4 SEC.	4	R	AVERAGE DECISION FREQUENCY : AVERAGE INTERVAL BETWEEN ADDING IN SINGLE CHROM.
REJ.PER	0 - 10 SEC.	0	R	REJECTION PERIOD: TIME THAT MUST PASS NEXT ADDITION OF SINGLE CHROM.
NO.OF. PEAKS	0 - 100	3	I	NUMBER OF PEAKS IN SINGLE CHROM.
RET.TIME	0 - 360	1 - 60 2 - 240 3 - 450	R[100]	RETENTION TIME: TIME WHEN PEAKS OCCUR
VOL.FRAC. INJ	0 - 1.0	1 - 1/3 2 - 1/3 3 - 1/3	R[100]	VOLUME FRACTION INJECTED: HOW MUCH OF THAT SUBSTANCE THERE IS
DET.RES. FAC	0 - 1000000	1 - 1 2 - 3 3 - 7	R[100]	DETECTOR RESPONCE FACTOR : HOW SENSITIVE INSTRUMENT IS TO THAT SUBSTANCE
COL.EFF	1000 - 1000000	10000	R	COLUMN EFFICIENCY

NOISE.MAG	0 - 10.0	0.01	R	NOISE MAGNITUDE: INFLUENCES AMOUNT OF ELECTRICAL NOISE COMPARED TO HEIGHT OF TALLEST PEAK IN SC. S.D. OF ELECTRICAL NOISE = TALLEST PEAK HEIGHT * NOISE MAGNITUDE
LASER. INT.FAC	0 - 0.5	0	R	LASER INTENSITY FACTOR: AVERAGE LASER INTENSITY
JIT.DET. LIM	0.01 - 1.0 SEC.	0.1	R	JITTER DETECTION LIMIT: SMALLEST DETECTABLE AMOUNT SIGNAL CAN JITTER
JIT.MAX	0 - 0.2 SEC.	0	R	JITTER MAXIMUM: MAXIMUM AMOUNT SIGNAL CAN JITTER

I = INTEGER
R = REAL
R[100] = REAL ARRAY OF 100 ELEMENTS

Appendix H

Relationship of Signal-to-White-Noise Ratio To Noise Magnitude

IF: $$S/N = \frac{(MaxSC)}{2 * SDN}$$

where S/N is signal-to-noise ratio in the single chromatogram, MaxSC is the height of the tallest peak in the single chromatogram, and SDN is the standard deviation of noise;

AND: $$SDN = MaxSC * NM$$

where NM is noise magnitude;

THEN: $$S/WN = 1 / (2*NM)$$

where S/WN is the signal-to-white-noise ratio.

Appendix I

Parameters Used for Different Decision Sequences

DEC.SEQ#	DEFAULT	1	2	3	4	5	6	7	8	9
DEC.INT	1	*	*	*	*	*	*	*	*	*
AVE.DEC. FREQ	4	*	*	*	*	*	*	*	*	*
REJ.PER	0	*	*	*	*	*	*	*	*	*
LP	4	2	1	1	*	*	*	*	2	4
		3	2	2					4	8
		4	3	3					8	
		8	4	4					16	
		16	8	8						
			16	16						
CL	477	32	*	*	*	*	*	*	*	128
NO.OF.PEAKS	3	*	*	*	*	*	*	*	*	*
RET.TIME	60	8	*	*	*	*	*	*	*	40
	240	18	*	*	*	*	*	*	*	80
	450	25	*	*	*	*	*	*	*	120
VOL.FRAC. INJ	1/3	*	*	*	*	*	*	*	*	*
	1/3	*	*	*	*	*	*	*	*	*
	1/3	*	*	*	*	*	*	*	*	*
DET.RES. FAC	1	*	*	*	*	*	*	*	*	*
	3	*	*	*	*	*	*	*	*	*
	7	*	*	*	*	*	*	*	*	*
COL.EFF	10000	*	*	*	*	*	*	*	*	*
NOISE.MAG	.01	*	*	*	*	*	*	*	0-10	*
LASER.INT FAC	0	*	*	*	*	*	*	*	*	*
JIT.DET LIM	0.1	*	*	*	*	*	*	*	*	*
JIT.MAX	0	*	*	*	*	*	*	*	*	*
DRIFT	0	*	*	*	*	*	*	*	0-5	*

* indicates the default values are used.

Appendix J

Random Number Generator Test Results

J.1 - RAND.UNIF Test:

Test A : A Chi-Square value was computed on a set of 300 random uniform numbers using 10 groups:

0.0<=x<.1, .1<=x<.2, .2<=x<.3, .3<=x<.4, .4<=x<.5,
.5<=x<.6, .6<=x<.7, .7<=x<.8, .8<=x<.9, .9<=x<=1.0.

Test A was run 15 times giving the follow values:

10.83	6.40	8.00	11.47	17.47
7.80	7.20	6.53	4.37	10.83
5.10	2.03	13.97	9.60	8.80

The expected Chi-Square of 9 degrees of freedom of a significance level of 0.05 is 16.9 (Ref.8).

J.2 - Chi-Square Value Fit Test for RAND.UNIF

Test B : Test A run 100 times and values tabulated into significance level groups:

x<=.01, .01<x<=.05, .05<x<=.10, x>.10.

Test B was run 5 times giving the following values:

	.01	.05	.10	REM
EXPECTED:	1	4	5	90
OBSERVED:	0	3	4	93
	0	3	3	94
	1	7	4	88
	1	4	6	89
	1	5	6	88
TOTAL EXPECTED:	5	20	25	450
TOTAL OBSERVED:	3	22	23	452

The Chi-Square calculated from the total observed values is 1.17. The expected Chi-Square of 3 degrees of freedom with a significance level of 0.05 is 7.81 (ref.8).

J.3 - RAND.NRML Test:

Test C : A one sided average t value was computed on a set of 300 random normal numbers. Test A was run 15 times giving the follow values:

0.73	1.17	0.29	1.27	0.59
0.82	0.39	0.89	1.52	0.12
1.02	0.64	1.31	1.72	0.50

The expected t-test value for 300 items at a significance level of 0.05 is 1.645 (Ref. 10).

J.4 - Chi-Square Value Fit Test for RAND.NRML

Test D : Test C run 100 times using a two sided t-test and values tabulated into significance level groups:

x<=-.01, -.01<x<=-.05, -.05<x<=-.10, -.10<x<0,
0>=x<.10, .05>x>=.10, .01>x>=.05, x>=.01

Test B was run 10 times giving the following values:

	MEAN	-.01	-.05	-.10	-REM	+REM	.10	.05	.01
EXPECTED:	0.0	1	4	5	40	40	5	4	1
OBSERVED:	-.0024	2	6	6	30	45	6	5	0
	-.0000	1	2	2	46	40	5	1	3
	.0009	1	6	2	45	32	8	4	2
	-.0030	1	5	7	37	41	5	3	1
	-.0105	1	8	2	45	40	2	2	0
	-.0078	1	5	7	39	42	5	1	0
	-.0036	1	5	3	40	46	2	2	1
	.0039	3	4	4	31	49	3	4	2
	-.0011	1	3	5	46	35	5	2	3
	.0161	0	3	3	36	47	4	6	1
TOTAL EXPECTED:		10	40	50	400	400	50	40	10
TOTAL OBSERVED:		12	47	41	395	417	45	30	13

The Chi-Square calculated from the total observed values is 7.9. The expected Chi-Square of 7 degrees of freedom with a significance level of 0.05 is 14.1 (Ref. 10).

Appendix K

Prototype Program Code

```
ECHO.OFF
\ BARINIT.PRO - DEFINES VARIABLES, CONSTANTS AND WINDOWS

\ REMEMBER THAT THIS IS A STACK ORIENTED LANGUAGE
\ THAT IS, IF A DEFINITION WISHES TO CALL ANOTHER
\ DEFINITION, THAT DEFINITION MUST BE DEFINED EARLIER


: INIT.START \ MAKES DELETION OF PROGRAM EASY
;             \ SINCE IT'S THE FIRST DEFINITION

\ SET UP MENU WINDOWS

 0 20  0 59 WINDOW {TITLE}
19  0 24 79 WINDOW {LOWSCREEN}
 2  0  7 79 WINDOW {HIGHSCREEN}
 2  0 24 79 WINDOW {FULLSCREEN}
 2  0 16 79 WINDOW {UPPERSCREEN}
17  0 18 79 WINDOW {PROMPT}
 1  0  1 79 WINDOW {ERROR}


\ SET UP WINDOW COLOR ATTRIBUTES

: ERROR.COLOR.ON {ERROR}
    79 VIDEO.ATTRIBUTE \ YELLOW ON RED INTENSITY ON
    SCREEN.CLEAR
;
: ERROR.COLOR.OFF {ERROR}
    7 VIDEO.ATTRIBUTE \ WHITE ON BLACK
    SCREEN.CLEAR
;
: TITLE.COLOR.ON {TITLE}
    47 VIDEO.ATTRIBUTE \ WHITE ON GREEN INTENSITY ON
    SCREEN.CLEAR
;
: TITLE.COLOR.OFF {TITLE}
    7 VIDEO.ATTRIBUTE \ WHITE ON BLACK
    SCREEN.CLEAR
;
: LOW.SCREEN.COLOR.ON {LOWSCREEN}
    14 VIDEO.ATTRIBUTE \ YELLOW ON BLACK
    SCREEN.CLEAR
;
: LOW.SCREEN.COLOR.OFF {LOWSCREEN}
    7 VIDEO.ATTRIBUTE \ WHITE ON BLACK
    SCREEN.CLEAR
;
: HIGH.SCREEN.COLOR.ON {HIGHSCREEN}
    14 VIDEO.ATTRIBUTE \ YELLOW ON BLACK
```

```
      SCREEN.CLEAR
 ;
 : HIGH.SCREEN.COLOR.OFF {HIGHSCREEN}
      7 VIDEO.ATTRIBUTE \ WHITE ON BLACK
      SCREEN.CLEAR
 ;
 : UPPER.SCREEN.COLOR.ON {UPPERSCREEN}
      14 VIDEO.ATTRIBUTE \ YELLOW ON BLACK
      SCREEN.CLEAR
 ;
 : UPPER.SCREEN.COLOR.OFF {UPPERSCREEN}
      7 VIDEO.ATTRIBUTE \ WHITE ON BLACK
      SCREEN.CLEAR
 ;
 : PROMPT.COLOR.ON {PROMPT}
      23 VIDEO.ATTRIBUTE \ WHITE ON BLUE INTENSITY ON
      SCREEN.CLEAR
 ;
 : PROMPT.COLOR.OFF {PROMPT}
      7 VIDEO.ATTRIBUTE \ WHITE ON BLACK
      SCREEN.CLEAR
 ;
 : FULL.SCREEN.COLOR.OFF {FULLSCREEN}
      7 VIDEO.ATTRIBUTE \ WHITE ON BLACK
      SCREEN.CLEAR
 ;

\ DEFINE CONTROL VARIABLES

  3 STRING MENU.ON
  3 STRING AUTO.COMPLETE
  1 STRING WHICH.MENU
  3 STRING VALID.PARAMETER

\ DEFINE PARAMETER VARIABLES

INTEGER SCALAR EXP.LENG               \ LENGTH OF MULTIPLEX
                                      \ CHROMATOGRAM (SEC)
INTEGER SCALAR CHROM.LENG             \ LENGTH OF SINGLE
                                      \ CHROMATOGRAM (SEC)
INTEGER SCALAR NO.OF.PEAKS            \ IN SINGLE
                                      \ CHROMATOGRAM

REAL DIM[ 100 ] ARRAY RET.TIME        \ (SEC)
REAL DIM[ 100 ] ARRAY VOL.FRAC.INJ
REAL DIM[ 100 ] ARRAY DET.RES.FAC

REAL SCALAR DEC.INT          \ TIME PASSED BEFORE ANOTHER
                             \ DECISION CAN BE MADE (SEC)
REAL SCALAR AVE.DEC.FREQ     \ AVERAGE INTERVAL BETWEEN
                             \ FIRING OF LASER (SEC)
REAL SCALAR REJ.PER          \ TIME PASSED BEFORE NEXT
                             \ PULSE (SEC)
REAL SCALAR PT.RES           \ FREQUENCY DATA
                             \ COLLECTED/SAMPLED (SEC)
```

```
REAL SCALAR COL.EFF
\ THIS MAY NOT BE NEEDED : REAL SCALAR COL.EFF.FACTOR
REAL SCALAR NOISE.MAG
REAL SCALAR CHROM.RESOL    \ TIME BETWEEN DATA
                           \ POINTS (SEC)
REAL SCALAR LASER.INT.FAC  \ AVERAGE CHANGE IN LASER
                           \ BRIGHTNESS
REAL SCALAR JIT.DET.LIM    \ SMALLEST DETECTABLE AMOUNT
                           \ SIGNAL CAN JITTER (SEC)
REAL SCALAR JIT.MAX        \ MAXIMUM AMOUNT SIGNAL CAN
                           \ JITTER (SEC)

\ DEFINE PARAMETER'S CONSTANTS

INTEGER SCALAR EXP.LENG.MIN
INTEGER SCALAR EXP.LENG.MAX
INTEGER SCALAR CHROM.LENG.MIN
DP.INTEGER SCALAR CHROM.LENG.MAX
INTEGER SCALAR MIN.NO.OF.PEAKS
INTEGER SCALAR MAX.NO.OF.PEAKS
REAL SCALAR RET.TIME.MIN
REAL SCALAR RET.TIME.MAX
REAL SCALAR VOL.FRAC.INJ.MIN
REAL SCALAR VOL.FRAC.INJ.MAX
REAL SCALAR DET.RES.FAC.MIN
REAL SCALAR DET.RES.FAC.MAX
REAL SCALAR DEC.INT.MIN
REAL SCALAR DEC.INT.MAX
REAL SCALAR AVE.DEC.FREQ.MIN
REAL SCALAR AVE.DEC.FREQ.MAX
REAL SCALAR REJ.PER.MIN
REAL SCALAR REJ.PER.MAX
REAL SCALAR PT.RES.MIN
REAL SCALAR PT.RES.MAX
REAL SCALAR COL.EFF.MIN
REAL SCALAR COL.EFF.MAX
\ THIS MAY NOT BE NEEDED: REAL SCALAR COL.EFF.FACTOR.MIN
\ THIS MAY NOT BE NEEDED: REAL SCALAR COL.EFF.FACTOR.MAX
REAL SCALAR NOISE.MAG.MIN
REAL SCALAR NOISE.MAG.MAX
REAL SCALAR CHROM.RESOL.MIN
REAL SCALAR CHROM.RESOL.MAX
REAL SCALAR LASER.INT.FAC.MIN
REAL SCALAR LASER.INT.FAC.MAX
REAL SCALAR JIT.DET.LIM.MIN
REAL SCALAR JIT.DET.LIM.MAX
REAL SCALAR JIT.MAX.MIN
REAL SCALAR JIT.MAX.MAX

: INITIATE.FIRST.PARAM.CONSTANTS

0 EXP.LENG.MIN :=
10800 EXP.LENG.MAX :=

60 CHROM.LENG.MIN :=
2700 CHROM.LENG.MAX :=

0.001 CHROM.RESOL.MIN :=
1.0 CHROM.RESOL.MAX :=

0.1 DEC.INT.MIN :=
10.0 DEC.INT.MAX :=

0.01 AVE.DEC.FREQ.MIN :=
4.0 AVE.DEC.FREQ.MAX :=

0.0 REJ.PER.MIN :=
10.0 REJ.PER.MAX :=
;


: INITIATE.EXP.CONSTANTS

INITIATE.FIRST.PARAM.CONSTANTS

0.05 PT.RES.MIN :=
1.0 PT.RES.MAX :=
;


:  INITIATE.SIM.CONSTANTS

INITIATE.FIRST.PARAM.CONSTANTS

0 MIN.NO.OF.PEAKS :=
100 MAX.NO.OF.PEAKS :=

0.0 RET.TIME.MIN :=
3600.0 RET.TIME.MAX :=

0.0 VOL.FRAC.INJ.MIN :=
1.0 VOL.FRAC.INJ.MAX :=

0.0 DET.RES.FAC.MIN :=
1000000.0 DET.RES.FAC.MAX :=

1000.0 COL.EFF.MIN :=
1000000.0 COL.EFF.MAX :=

\ THIS MAY NOT BE NEEDED :REAL SCALAR COL.EFF.FACTOR.MIN
\ THIS MAY NOT BE NEEDED :REAL SCALAR COL.EFF.FACTOR.MAX

0.0 NOISE.MAG.MIN :=
10.0 NOISE.MAG.MAX :=

0.0 LASER.INT.FAC.MIN :=
0.5 LASER.INT.FAC.MAX :=

0.01 JIT.DET.LIM.MIN :=
1.0 JIT.DET.LIM.MAX :=
0.0 JIT.MAX.MIN :=
0.2 JIT.MAX.MAX :=
;

: NO.OPTION
     PROMPT.COLOR.ON
     BELL
     ." THIS OPTION IS NOT AVAILABLE - "
     ." TOUCH ANY KEY TO CONTINUE "
     PCKEY ?DROP DROP
     PROMPT.COLOR.OFF
;
```

```
ECHO.OFF

\ BARSIMFL.PRO - SO CAN WRITE SIMULATION DATA
  EASILY TO A FILE

: SIMFL.START \ FIRST DEFINITION OF FILE BARSIMFL.PRO
;

\ VARIABLES FOR SINGLE CHROMATOGRAM CALCULATIONS
 REAL DIM[ 4096 ] ARRAY SINGLE.CHROM
 INTEGER SCALAR LAST.ELEMENT
 REAL    SCALAR SIGMA
 REAL    SCALAR DENOM
 REAL    SCALAR FRAC
 REAL    SCALAR EXPO.DENOM

\ VARIABLES FOR MULTIPLEX CHROMATOGRAM CALCULATIONS
 REAL DIM[ 16384 ] ARRAY MULTIPLEX.CHROM

\ VARIABLES FOR DECISION SEQUENCE CALCULATIONS
 INTEGER DIM[ 20480 ] ARRAY DEC.SEQ
             \ SINGLE.CHROM + MULTIPLEX.CHROM SIZES
 INTEGER SCALAR LAST.DEC
             \ LAST ELEMENT IN DEC.SEQ WITH VALUE 1
 REAL    SCALAR REJ.FAC
             \ DEC.INT/AVE.DEC.FREQ

\ VARIABLES FOR MULITPLEX CHROMATOGRAM CALCULATIONS
 INTEGER SCALAR START
 INTEGER SCALAR FINISH

\ VARIABLE FOR CALCULATE.NOISE AND ELSEWHERE,
\ WHERE NEED DUMMY VARIABLE
 REAL SCALAR MISC

\ VARIABLES FOR SIMULATION FILE MAINTENANCE
 64 STRING COM.LINE
 14 STRING FILENAME

: DEFAULT.SIM.FILENAME

  " BARSIMTP.DAT" FILENAME ":=
;

: CREATE.SIM.FILE  \ CREATES A FILE FOR SIMULATION DATA

  FILE.TEMPLATE \ SPECIFY THE APPROPRIATE FILE TEMPLATE
     15 COMMENTS
     REAL DIM[ 12 ] SUBFILE \ TO STORE SCALARS
                            \ EXP.LENG, CHROM.LENG,
                            \ CHROM.RESOL, DEC.INT,
                            \ AVE.DEC.FREQ, REJ.PER,
                            \  NO.OF.PEAKS,  COL.EFF,
                            \ NOISE.MAG, LASER.INT.FAC,
                            \ JIT.DET.LIM, JIT.MAX
```

```
      RET.TIME          []FORM.SUBFILE
      VOL.FRAC.INJ      []FORM.SUBFILE
      DET.RES.FAC       []FORM.SUBFILE
      SINGLE.CHROM      []FORM.SUBFILE \ SINGLE.CHROM, CROSS.CHROM
    4 TIMES                           \ FFT.CHROM, HADAMARD.CHROM
    DEC.SEQ           []FORM.SUBFILE
    MULTIPLEX.CHROM []FORM.SUBFILE
  END
\  LATER THESE NEXT 3 LINES CAN BE USED SO USER CAN
\  SPECIFY FILE NAME TO BE CREATED
\  CR ." NAME OF FILE TO CREATE? "
\  "INPUT  FILENAME ":= \ STORE FILENAME IN STRING
\  VARIABLE FILENAME DEFER> FILE.CREATE

  DEFAULT.SIM.FILENAME \ FOR NOW ONLY THE DEFAULT FILE
                       \ NAME USED
  FILENAME FILE.CREATE

;

: WRITE.RET.TIME

  FILENAME DEFER> FILE.OPEN
  2 SUBFILE RET.TIME ARRAY>FILE
  FILE.CLOSE
;

: WRITE.VOL.FRAC.INJ

  FILENAME DEFER> FILE.OPEN
  3 SUBFILE VOL.FRAC.INJ ARRAY>FILE
  FILE.CLOSE
;

: WRITE.DET.RES.FAC

  FILENAME DEFER> FILE.OPEN
  4 SUBFILE DET.RES.FAC ARRAY>FILE
  FILE.CLOSE
;

: WRITE.SINGLE.CHROM

  FILENAME DEFER> FILE.OPEN
  5 SUBFILE SINGLE.CHROM ARRAY>FILE
  FILE.CLOSE
;

: WRITE.CROSS.CHROM

  FILENAME DEFER> FILE.OPEN
  6 SUBFILE SINGLE.CHROM ARRAY>FILE
  FILE.CLOSE
;
```

```
: WRITE.FFT.CHROM

  FILENAME DEFER> FILE.OPEN
  7 SUBFILE SINGLE.CHROM ARRAY>FILE
  FILE.CLOSE
;

: WRITE.HADAMARD.CHROM

  FILENAME DEFER> FILE.OPEN
  8 SUBFILE SINGLE.CHROM ARRAY>FILE
  FILE.CLOSE
;

: WRITE.DEC.SEQ

  FILENAME DEFER> FILE.OPEN
  9 SUBFILE DEC.SEQ ARRAY>FILE
  FILE.CLOSE
;

: WRITE.MULTIPLEX.CHROM

  FILENAME DEFER> FILE.OPEN
  10 SUBFILE MULTIPLEX.CHROM ARRAY>FILE
  FILE.CLOSE
;

: READ.RET.TIME

  FILENAME DEFER> FILE.OPEN
  2 SUBFILE RET.TIME FILE>ARRAY
  FILE.CLOSE
;

: READ.VOL.FRAC.INJ

  FILENAME DEFER> FILE.OPEN
  3 SUBFILE VOL.FRAC.INJ FILE>ARRAY
  FILE.CLOSE
;

: READ.DET.RES.FAC

  FILENAME DEFER> FILE.OPEN
  4 SUBFILE DET.RES.FAC FILE>ARRAY
  FILE.CLOSE
;

: READ.SINGLE.CHROM

  FILENAME DEFER> FILE.OPEN
  5 SUBFILE SINGLE.CHROM FILE>ARRAY
  FILE.CLOSE
;
```

```
: READ.CROSS.CHROM

  FILENAME DEFER> FILE.OPEN
  6 SUBFILE SINGLE.CHROM FILE>ARRAY
  FILE.CLOSE
;

: READ.FFT.CHROM

  FILENAME DEFER> FILE.OPEN
  7 SUBFILE SINGLE.CHROM FILE>ARRAY
  FILE.CLOSE
;

: READ.HADAMARD.CHROM

  FILENAME DEFER> FILE.OPEN
  8 SUBFILE SINGLE.CHROM FILE>ARRAY
  FILE.CLOSE
;

: READ.DEC.SEQ

  FILENAME DEFER> FILE.OPEN
  9 SUBFILE DEC.SEQ FILE>ARRAY
  FILE.CLOSE
;

: READ.MULTIPLEX.CHROM

  FILENAME DEFER> FILE.OPEN
  10 SUBFILE MULTIPLEX.CHROM FILE>ARRAY
  FILE.CLOSE
;

: WRITE.SCALARS

  FILENAME DEFER> FILE.OPEN
  1 SUBFILE
  REAL DIM[ 12 ] UNNAMED.ARRAY
  @[ 1 ] ENTER[ EXP.LENG , CHROM.LENG , CHROM.RESOL ,
                DEC.INT , AVE.DEC.FREQ ,
                REJ.PER , NO.OF.PEAKS , COL.EFF ,
                NOISE.MAG , LASER.INT.FAC ,
                JIT.DET.LIM , JIT.MAX ]
  ARRAY>FILE
  FILE.CLOSE
;

: READ.SCALARS

  FILENAME DEFER> FILE.OPEN
  1 SUBFILE FILE>UNNAMED.ARRAY
  FILE.CLOSE
```

```
   DUP [ 1 ]  EXP.LENG :=
   DUP [ 2 ]  CHROM.LENG :=
   DUP [ 3 ]  CHROM.RESOL :=
   DUP [ 4 ]  DEC.INT :=
   DUP [ 5 ]  AVE.DEC.FREQ :=
   DUP [ 6 ]  REJ.PER :=
   DUP [ 7 ]  NO.OF.PEAKS :=
   DUP [ 8 ]  COL.EFF :=
   DUP [ 9 ]  NOISE.MAG :=
   DUP [ 10 ] LASER.INT.FAC :=
   DUP [ 11 ] JIT.DET.LIM :=
       [ 12 ] JIT.MAX :=
;

: WRITE.ALL.SIM

   WRITE.RET.TIME
   WRITE.VOL.FRAC.INJ
   WRITE.DET.RES.FAC
   WRITE.SINGLE.CHROM
   WRITE.MULTIPLEX.CHROM
   WRITE.DEC.SEQ
   WRITE.SCALARS
;

: READ.ALL.SIM

   READ.RET.TIME
   READ.VOL.FRAC.INJ
   READ.DET.RES.FAC
   READ.SINGLE.CHROM
   READ.MULTIPLEX.CHROM
   READ.DEC.SEQ
   READ.SCALARS
;
```

```
ECHO.OFF

\ BARPAR1.PRO - PART I
\ TO ENTER IN PARAMETERS OF SIMULATION/ EXPEIMENT
\ THE USER IS PROMPTED FOR THE VALUES
\ THE VALUES ARE CHECKED, TO BE SURE THAT THEY ARE IN RANGE
\ THE MORE EXPANDED VERSION IS IN BARPAR1.ORG

: PAR1.START \ THE FIRST DEFINITION
;

: PRINT.EXP.LENG
     ."                            1 : EXPERIMENTAL LENGTH : "
     EXP.LENG .
;

: ENTER.EXP.LENG.VALUE
     PROMPT.COLOR.ON
     " NO " VALID.PARAMETER ":=

     BEGIN
       " NO " VALID.PARAMETER "=
     WHILE
       {PROMPT} CR
       ."  EXPERIMENTAL LENGTH ( 0 - 10,800 SEC) : "
       BEGIN
          #INPUT NOT
       WHILE
          ERROR.COLOR.ON ."                INVALID NUMBER"
          BELL BELL
          {PROMPT} CR
          ."  EXPERIMENTAL LENGTH ( 0 - 10,800 SEC) : "
       REPEAT


       EXP.LENG :=

       EXP.LENG EXP.LENG.MIN >= EXP.LENG EXP.LENG.MAX <= AND
                                  \ TEST IF IN RANGE
       IF
          " YES" VALID.PARAMETER ":=
          {LOWSCREEN} PRINT.EXP.LENG CR
          ERROR.COLOR.OFF
       ELSE
          ERROR.COLOR.ON
          ."             EXPERIMENTAL LENGTH OUT OF RANGE"
          BELL BELL
       THEN
     REPEAT
;

: PRINT.CHROM.LENG
     ."                            2 : CHROMATOGRAM LENGTH : "
      CHROM.LENG .
;
```

```
: CALCULATE.CHROM.LENG.VALUE
     \ LAST RET.TIME + 6 SIGMA
     RET.TIME [ NO.OF.PEAKS ]
     DUP COL.EFF SQRT / 6 * +
     CHROM.LENG :=
;

: ENTER.CHROM.LENG.VALUE
     PROMPT.COLOR.ON
     " NO " VALID.PARAMETER ":=

     BEGIN
       " NO " VALID.PARAMETER "=
     WHILE
       {PROMPT} CR
       ."  CHROMATOGRAM LENGTH ( 60 - 2,700 SEC) : "
       BEGIN
          #INPUT NOT
       WHILE
          ERROR.COLOR.ON ."             INVALID NUMBER"
          BELL BELL
          {PROMPT} CR
          ."  CHROMATOGRAM LENGTH ( 60 - 2,700 SEC) : "
       REPEAT

       CHROM.LENG :=

       CHROM.LENG CHROM.LENG.MIN >=
       CHROM.LENG CHROM.LENG.MAX <= AND
       \ TEST IF IN RANGE
       IF
          " YES" VALID.PARAMETER ":=
          {LOWSCREEN} PRINT.CHROM.LENG CR
          ERROR.COLOR.OFF
       ELSE
          ERROR.COLOR.ON
          ."             CHROMATOGRAM LENGTH OUT OF RANGE"
          BELL BELL
       THEN
     REPEAT
;

: PRINT.CHROM.RESOL
     ."                      3 : CHROMATOGRAM RESOLUTION : "
     CHROM.RESOL .
;

: ENTER.CHROM.RESOL.VALUE
     PROMPT.COLOR.ON
     " NO " VALID.PARAMETER ":=

     BEGIN
       " NO " VALID.PARAMETER "=
     WHILE
```

```
       {PROMPT} CR
       ."   CHROMATOGRAM RESOLUTION ( 0.001 - 1.0 SEC) : "
       BEGIN
          #INPUT NOT
       WHILE
          ERROR.COLOR.ON ."              INVALID NUMBER"
          BELL BELL
          {PROMPT} CR
          ."  CHROMATOGRAM RESOLUTION ( 0.001 - 1.0 SEC) : "
       REPEAT

       CHROM.RESOL :=

       CHROM.RESOL CHROM.RESOL.MIN >=
       CHROM.RESOL CHROM.RESOL.MAX <= AND
       \ TEST IF IN RANGE
       IF
          " YES" VALID.PARAMETER ":=
          {LOWSCREEN} PRINT.CHROM.RESOL CR
          ERROR.COLOR.OFF
       ELSE
          ERROR.COLOR.ON
          ."            CHROMATOGRAM RESOLUTION OUT OF RANGE"
          BELL BELL
       THEN
     REPEAT
;

: PRINT.DEC.INT
     ."                     4 : DECISION INTERVAL : "
     DEC.INT .
;

: ENTER.DEC.INT.VALUE
      CHROM.RESOL DEC.INT :=  \ SO FOR NOW PROGRAM IS
                              \ NOT AS FLEXIBLE
;

: PRINT.AVE.DEC.FREQ
     ."                     5 : AVERAGE DECISION FREQUENCY : "
    AVE.DEC.FREQ .
;

: ENTER.AVE.DEC.FREQ.VALUE
     PROMPT.COLOR.ON
     " NO " VALID.PARAMETER ":=

     BEGIN
       " NO " VALID.PARAMETER "=
     WHILE
       {PROMPT} CR
       ."  AVERAGE DECISION FREQUENCY ( 0.01 - 4.0 SEC) : "
       BEGIN
          #INPUT NOT
       WHILE
```

```
           ERROR.COLOR.ON ."              INVALID NUMBER"
           BELL BELL
           {PROMPT} CR
           ."  AVERAGE DECISION FREQUENCY ( 0.01 - 4.0 SEC) : "
        REPEAT

        AVE.DEC.FREQ :=

        AVE.DEC.FREQ AVE.DEC.FREQ.MIN >=
        AVE.DEC.FREQ AVE.DEC.FREQ.MAX <= AND
        \ TEST IF IN RANGE
        IF
           " YES" VALID.PARAMETER ":=
           {LOWSCREEN} PRINT.AVE.DEC.FREQ CR
           ERROR.COLOR.OFF
        ELSE
           ERROR.COLOR.ON
           ."            AVERAGE DECISION FREQUENCY OUT OF RANGE"
          BELL BELL
       THEN
     REPEAT
;

: PRINT.REJ.PER
      ."                     6 : REJECTION PERIOD : " REJ.PER .
;

: ENTER.REJ.PER.VALUE
     PROMPT.COLOR.ON
     " NO " VALID.PARAMETER ":=

     BEGIN
       " NO " VALID.PARAMETER "=
     WHILE
       {PROMPT} CR
       ."  REJECTION PERIOD ( 0.0 - 10.0 SEC) : "
       BEGIN
          #INPUT NOT
       WHILE
          ERROR.COLOR.ON ."              INVALID NUMBER"
          BELL BELL
          {PROMPT} CR
          ."  REJECTION PERIOD ( 0.0 - 10.0 SEC) : "
       REPEAT

       REJ.PER :=

       REJ.PER REJ.PER.MIN >= REJ.PER REJ.PER.MAX <= AND
       \ TEST IF IN RANGE
       IF
          " YES" VALID.PARAMETER ":=
          {LOWSCREEN} PRINT.REJ.PER CR
          ERROR.COLOR.OFF
       ELSE
          ERROR.COLOR.ON
```

```
           ."             REJECTION PERIOD OUT OF RANGE"
           BELL BELL
        THEN
      REPEAT
 ;

 : PRINT.PT.RES
    ."                    7 : DATA COLLECTION POINT RESOLUTION : "
  PT.RES .
 ;

 : ENTER.PT.RES.VALUE
      PROMPT.COLOR.ON
      " NO " VALID.PARAMETER ":=

      BEGIN
        " NO " VALID.PARAMETER "=
      WHILE
        {PROMPT} CR
    ."  DATA COLLECTION POINT RESOLUTION ( 0.05 - 1.0 SEC) : "
        BEGIN
           #INPUT NOT
        WHILE
           ERROR.COLOR.ON ."              INVALID NUMBER"
           BELL BELL
           {PROMPT} CR
       ."  DATA COLLECTION POINT RESOLUTION ( 0.05 - 1.0 SEC) : "
       REPEAT

       PT.RES :=

       PT.RES PT.RES.MIN >= PT.RES PT.RES.MAX <= AND
       \ TEST IF IN RANGE
       IF
          " YES" VALID.PARAMETER ":=
          {LOWSCREEN} PRINT.PT.RES CR
          ERROR.COLOR.OFF
       ELSE
          ERROR.COLOR.ON
          ."     DATA COLLECTION POINT RESOLUTION OUT OF RANGE"
          BELL BELL
       THEN
     REPEAT
;

: PRINT.NO.OF.PEAKS
 ."                       8 : NUMBER OF PEAKS : " NO.OF.PEAKS .
;

: ENTER.NO.OF.PEAKS.VALUE
     PROMPT.COLOR.ON
     " NO " VALID.PARAMETER ":=

     BEGIN
       " NO " VALID.PARAMETER "=
     WHILE
       {PROMPT} CR ."  NUMBER OF PEAKS ( 0 - 100 SEC) : "
       BEGIN
          #INPUT NOT
       WHILE
          ERROR.COLOR.ON ."              INVALID NUMBER"
          BELL BELL
          {PROMPT} CR ."  NUMBER OF PEAKS ( 0 - 100 SEC) : "
       REPEAT

       NO.OF.PEAKS :=

       NO.OF.PEAKS MIN.NO.OF.PEAKS >=
       NO.OF.PEAKS MAX.NO.OF.PEAKS <= AND
       \ TEST IF IN RANGE
       IF
          " YES" VALID.PARAMETER ":=
          {LOWSCREEN} PRINT.NO.OF.PEAKS CR
          ERROR.COLOR.OFF
       ELSE
          ERROR.COLOR.ON
          ."             NUMBER OF PEAKS OUT OF RANGE"
          BELL BELL
       THEN
     REPEAT
;

: PRINT.RET.TIME
 ."                       9 : PEAK " I . ."  RETENTION TIME : "
     RET.TIME [ I ] .
;

: ENTER.RET.TIME.VALUE
     PROMPT.COLOR.ON
     " NO " VALID.PARAMETER ":=

     BEGIN
       " NO " VALID.PARAMETER "=
     WHILE
       {PROMPT} CR
   ."  PEAK " I . ."  RETENTION TIME ( 0.0 - 3600.0 SEC) : "
       BEGIN
          #INPUT NOT
       WHILE
          ERROR.COLOR.ON ."              INVALID NUMBER"
          BELL BELL
          {PROMPT} CR
      ."  PEAK " I . ."  RETENTION TIME ( 0.0 - 3600.0 SEC) : "
       REPEAT

       RET.TIME [ I ] :=

       RET.TIME [ I ] RET.TIME.MIN >=
       RET.TIME [ I ]  RET.TIME.MAX <= AND
       \ TEST IF IN RANGE
       IF
          " YES" VALID.PARAMETER ":=
          {LOWSCREEN} PRINT.RET.TIME CR
          ERROR.COLOR.OFF
       ELSE
          ERROR.COLOR.ON
     ."         PEAK " I . ."  RETENTION.TIME OUT OF RANGE"
          BELL BELL
       THEN
     REPEAT
;

: PRINT.VOL.FRAC.INJ
 ."      10 : PEAK " I . ."  VOLUME FRACTION INJECTED : "
     VOL.FRAC.INJ [ I ] .
;

: ENTER.VOL.FRAC.INJ.VALUE
     PROMPT.COLOR.ON
     " NO " VALID.PARAMETER ":=

     BEGIN
       " NO " VALID.PARAMETER "=
     WHILE
       {PROMPT} CR
   ."  PEAK " I . ."  VOLUME FRACTION INJECTED (0.0 - 1.0) : "
       BEGIN
          #INPUT NOT
       WHILE
          ERROR.COLOR.ON ."              INVALID NUMBER"
          BELL BELL
          {PROMPT} CR
          ."  PEAK " I . ."  VOLUME FRACTION INJECTED"
                      ."  ( 0.0 - 1.0) : "
       REPEAT

       VOL.FRAC.INJ [ I ] :=

       VOL.FRAC.INJ [ I ]
       VOL.FRAC.INJ.MIN >= VOL.FRAC.INJ [ I ]
       VOL.FRAC.INJ.MAX <= AND
       \ TEST IF IN RANGE
       IF
          " YES" VALID.PARAMETER ":=
          {LOWSCREEN} PRINT.VOL.FRAC.INJ CR
          ERROR.COLOR.OFF
       ELSE
          ERROR.COLOR.ON
          ."        PEAK " I . ."  VOLUME FRACTION INJECTED "
                         ." OUT OF RANGE"
          BELL BELL
       THEN
     REPEAT
;
```

```
: PRINT.DET.RES.FAC
 ."            11 : PEAK " I . ."  DETECTOR RESPONSE FACTOR : "
 .   DET.RES.FAC [ I ] .
;

: ENTER.DET.RES.FAC.VALUE
     PROMPT.COLOR.ON
     " NO " VALID.PARAMETER ":=

     BEGIN
       " NO " VALID.PARAMETER "=
     WHILE
       {PROMPT} CR ."  PEAK " I . ."  DETECTOR RESPONSE FACTOR "
                   ." (0.0 - 1,000,000.0) : "
       BEGIN
          #INPUT NOT
       WHILE
          ERROR.COLOR.ON ."               INVALID NUMBER"
          BELL BELL
          {PROMPT} CR
          ."  PEAK " I . ."  DETECTOR RESPONSE FACTOR"
                      ."  ( 0.0 - 1,000,000.0) : "
       REPEAT

       DET.RES.FAC [ I ] :=

       DET.RES.FAC [ I ] DET.RES.FAC.MIN >= DET.RES.FAC [ I ]
       DET.RES.FAC.MAX <= AND
       \ TEST IF IN RANGE
       IF
          " YES" VALID.PARAMETER ":=
          {LOWSCREEN} PRINT.DET.RES.FAC CR
          ERROR.COLOR.OFF
       ELSE
          ERROR.COLOR.ON
          ."        PEAK " I . ."  DETECTOR RESPONSE FACTOR "
                         ." OUT OF RANGE"
          BELL BELL
       THEN
     REPEAT
;

: PRINT.COL.EFF
     ."                    12 : COLUMN EFFICIENCY : " COL.EFF .
;

: ENTER.COL.EFF.VALUE
     PROMPT.COLOR.ON
     " NO " VALID.PARAMETER ":=

     BEGIN
       " NO " VALID.PARAMETER "=
     WHILE
       {PROMPT} CR
       ."  COLUMN EFFICIENCY (1,000.0 - 1,000,000.0) : "
```

```
         BEGIN
            #INPUT NOT
         WHILE
            ERROR.COLOR.ON ."                    INVALID NUMBER"
            BELL BELL
            {PROMPT} CR
            ."  COLUMN EFFICIENCY (1,000.0 - 1,000,000.0) : "
         REPEAT

         COL.EFF :=

         COL.EFF COL.EFF.MIN >= COL.EFF COL.EFF.MAX <= AND
         \ TEST IF IN RANGE
         IF
            " YES" VALID.PARAMETER ":=
            {LOWSCREEN} PRINT.COL.EFF CR
            ERROR.COLOR.OFF
         ELSE
            ERROR.COLOR.ON
            ."              COLUMN EFFICENCY OUT OF RANGE "
            BELL BELL
         THEN
      REPEAT
;

: PRINT.NOISE.MAG
      ."                      13 : NOISE MAGNITUDE : " NOISE.MAG .
;

: ENTER.NOISE.MAG.VALUE
      PROMPT.COLOR.ON
      " NO " VALID.PARAMETER ":=

      BEGIN
        " NO " VALID.PARAMETER "=
      WHILE
        {PROMPT} CR ."  NOISE MAGNITUDE (0.0 - 1.0) : "
        BEGIN
           #INPUT NOT
        WHILE
           ERROR.COLOR.ON ."                    INVALID NUMBER"
           BELL BELL
           {PROMPT} CR ."  NOISE MAGNITUDE (0.0 - 1.0) : "
        REPEAT

        NOISE.MAG :=

        NOISE.MAG NOISE.MAG.MIN >= NOISE.MAG NOISE.MAG.MAX <= AND
        \ TEST IF IN RANGE
        IF
           " YES" VALID.PARAMETER ":=
           {LOWSCREEN} PRINT.NOISE.MAG CR
           ERROR.COLOR.OFF
        ELSE
           ERROR.COLOR.ON
```

```
          ."            NOISE MAGNITUDE OUT OF RANGE "
          BELL BELL
       THEN
     REPEAT
;

: PRINT.LASER.INT.FAC
     ."                     14 : LASER INTENSITY FACTOR : "
     LASER.INT.FAC .
;

: ENTER.LASER.INT.FAC.VALUE
     PROMPT.COLOR.ON
     " NO " VALID.PARAMETER ":=

     BEGIN
      " NO " VALID.PARAMETER "=
     WHILE
       {PROMPT} CR ."  LASER INTENSITY FACTOR (0.0 - 0.5) : "
       BEGIN
          #INPUT NOT
       WHILE
          ERROR.COLOR.ON ."             INVALID NUMBER"
          BELL BELL
          {PROMPT} CR ."  LASER INTENSITY FACTOR (0.0 - 0.5) : "
       REPEAT

       LASER.INT.FAC :=

       LASER.INT.FAC LASER.INT.FAC.MIN >=
       LASER.INT.FAC LASER.INT.FAC.MAX <= AND
       \ TEST IF IN RANGE
       IF
          " YES" VALID.PARAMETER ":=
          {LOWSCREEN} PRINT.LASER.INT.FAC CR
          ERROR.COLOR.OFF
       ELSE
          ERROR.COLOR.ON
          ."            LASER INTENSITY FACTOR OUT OF RANGE "
          BELL BELL
       THEN
     REPEAT
;

: PRINT.JIT.DET.LIM
     ."                     15 : JITTER DETECTION LIMIT : "
     JIT.DET.LIM .
;

: ENTER.JIT.DET.LIM.VALUE
     PROMPT.COLOR.ON
     " NO " VALID.PARAMETER ":=

     BEGIN
       " NO " VALID.PARAMETER "=
      WHILE
        {PROMPT} CR ."  JITTER DETECTION LIMIT (0.01 - 1.0) : "
        BEGIN
           #INPUT NOT
        WHILE
           ERROR.COLOR.ON ."              INVALID NUMBER"
           BELL BELL
           {PROMPT} CR ."  JITTER DETECTION LIMIT (0.01 - 1.0) : "
       REPEAT

       JIT.DET.LIM :=

       JIT.DET.LIM JIT.DET.LIM.MIN >=
       JIT.DET.LIM JIT.DET.LIM.MAX <= AND
       \ TEST IF IN RANGE
       IF
          " YES" VALID.PARAMETER ":=
          {LOWSCREEN} PRINT.JIT.DET.LIM CR
          ERROR.COLOR.OFF
       ELSE
          ERROR.COLOR.ON
          ."             JITTER DETECTION LIMIT OUT OF RANGE "
          BELL BELL
       THEN
     REPEAT
;

: PRINT.JIT.MAX
     ."                      16 : JITTER MAXIMUM : " JIT.MAX .
;

: ENTER.JIT.MAX.VALUE
     PROMPT.COLOR.ON
     " NO " VALID.PARAMETER ":=

     BEGIN
       " NO " VALID.PARAMETER "=
     WHILE
       {PROMPT} CR ."  JITTER MAXIMUM (0.0 - 0.2) : "
       BEGIN
          #INPUT NOT
       WHILE
          ERROR.COLOR.ON ."              INVALID NUMBER"
          BELL BELL
          {PROMPT} CR ."  JITTER MAXIMUM (0.0 - 0.2) : "
       REPEAT

       JIT.MAX :=

       JIT.MAX JIT.MAX.MIN >= JIT.MAX JIT.MAX.MAX <= AND
       \ TEST IF IN RANGE
       IF
          " YES" VALID.PARAMETER ":=
          {LOWSCREEN} PRINT.JIT.MAX CR
          ERROR.COLOR.OFF
```

```
    ELSE
       ERROR.COLOR.ON
       ."                JITTER MAXIMUM OUT OF RANGE "
       BELL BELL
    THEN
  REPEAT
;
```

```
ECHO.OFF
\ BARPAR2.PRO - PART II
\ TO ENTER PARAMETERS OF SIMULATION/EXPERIMENT
\ THESE DEFINITIONS CALL THE DEFINITIONS IN PART I
\ THE MORE EXPANDED VERSION IS IN BARPAR2.ORG

: BAR2.START \ THIS MAKES HOUSECLEANING EASIER SINCE IT'S
             \ THE FIRST DEFINITION
;

: ENTER.EXP.PARAM
     NO.OPTION
;

: ENTER.SIM.PARAM
  STORE.FUNCTION.KEYS
  CLEAR.FUNCTION.KEYS
  FULL.SCREEN.COLOR.OFF
  LOW.SCREEN.COLOR.OFF
  PROMPT.COLOR.ON
  ENTER.EXP.LENG.VALUE
  ENTER.CHROM.RESOL.VALUE
  ENTER.DEC.INT.VALUE
  ENTER.AVE.DEC.FREQ.VALUE
  ENTER.REJ.PER.VALUE
  ENTER.NO.OF.PEAKS.VALUE

  {LOWSCREEN} CR
  NO.OF.PEAKS 1 + 1 DO
    ENTER.RET.TIME.VALUE
    ENTER.VOL.FRAC.INJ.VALUE
    ENTER.DET.RES.FAC.VALUE
  LOOP

  101 NO.OF.PEAKS 1 + DO  \ TO ZERO OUT THE REMAINING
                          \ OF THE ARRAYS
    0 RET.TIME [ I ] :=
    0 VOL.FRAC.INJ [ I ] :=
    0 DET.RES.FAC [ I ] :=
  LOOP

  ENTER.COL.E]FF.VALUE
  ENTER.NOISE.MAG.VALUE
  ENTER.LASER.INT.FAC.VALUE
  ENTER.JIT.DET.LIM.VALUE
  ENTER.JIT.MAX.VALUE
  CALCULATE.CHROM.LENG.VALUE
  PROMPT.COLOR.OFF

  WRITE.SCALARS
  WRITE.RET.TIME
  WRITE.VOL.FRAC.INJ
  WRITE.DET.RES.FAC

  RESTORE.FUNCTION.KEYS
```

```
 ;

 : DEFAULT.EXP.PARAM
      NO.OPTION
 ;

 : DEFAULT.SIM.PARAM
      STORE.FUNCTION.KEYS
      CLEAR.FUNCTION.KEYS
      1 CHROM.RESOL :=
      1 DEC.INT :=
      4 AVE.DEC.FREQ :=
      0 REJ.PER :=
      3 NO.OF.PEAKS :=

      0 RET.TIME :=
     60 RET.TIME [ 1 ] :=
    240 RET.TIME [ 2 ] :=
    450 RET.TIME [ 3 ] :=

      0 VOL.FRAC.INJ :=
      1.0 3.0 / VOL.FRAC.INJ [ 1 ] :=
      1.0 3.0 / VOL.FRAC.INJ [ 2 ] :=
      1.0 3.0 / VOL.FRAC.INJ [ 3 ] :=

      0 DET.RES.FAC :=
      1 DET.RES.FAC [ 1 ] :=
      3 DET.RES.FAC [ 2 ] :=
      7 DET.RES.FAC [ 3 ] :=

      10000 COL.EFF :=
      0.01 NOISE.MAG :=
      0 LASER.INT.FAC :=
      0.1 JIT.DET.LIM :=
      0 JIT.MAX :=

 \ CALCULATE CHROM.LENG :   LAST RET.TIME + 6 SIGMA
      RET.TIME [ NO.OF.PEAKS ]
      DUP COL.EFF SQRT / 6 * +
      CHROM.LENG :=

      2048 EXP.LENG :=

      WRITE.SCALARS
      WRITE.RET.TIME
      WRITE.VOL.FRAC.INJ
      WRITE.DET.RES.FAC

      RESTORE.FUNCTION.KEYS
 ;

 : DISPLAY.EXP.PARAM
      NO.OPTION
 ;
```

```
: DISPLAY.SIM.PARAM
     STORE.FUNCTION.KEYS
     CLEAR.FUNCTION.KEYS
     PROMPT.COLOR.ON
     ."  TOUCH ANY KEY TO HALT LISTING" CR
     ."  TOUCH A SECOND KEY TO CONTINUE LISTING"
     ."  - 3 KEYS FAST TO STOP LISTING"

     UPPER.SCREEN.COLOR.OFF
     PRINT.EXP.LENG CR      PAUSE
     PRINT.CHROM.LENG CR    PAUSE
     PRINT.CHROM.RESOL CR   PAUSE
     PRINT.DEC.INT CR       PAUSE
     PRINT.AVE.DEC.FREQ CR  PAUSE
     PRINT.REJ.PER CR       PAUSE
     PRINT.NO.OF.PEAKS CR   PAUSE

     NO.OF.PEAKS 1 + 1 DO
       PRINT.RET.TIME CR
       PRINT.VOL.FRAC.INJ CR
       PRINT.DET.RES.FAC CR
       PAUSE
       ?KEY
       IF
         KEY DROP
         LEAVE EXIT
       THEN
     LOOP

     PRINT.COL.EFF CR          PAUSE
     PRINT.NOISE.MAG CR        PAUSE
     PRINT.LASER.INT.FAC CR    PAUSE
     PRINT.JIT.DET.LIM CR      PAUSE
     PRINT.JIT.MAX CR          PAUSE
     PROMPT.COLOR.OFF
     RESTORE.FUNCTION.KEYS
;

: CHANGE.EXP.PARAM
     NO.OPTION
;

: CHANGE.SIM.PARAM
     STORE.FUNCTION.KEYS
     CLEAR.FUNCTION.KEYS
     LOW.SCREEN.COLOR.OFF
     PROMPT.COLOR.ON
     BEGIN
       {PROMPT} CR
       ."  NUMBER CODE OF PARAMETER TO BE CHANGED"
       ."  (99 WILL EXIT) : "
       #INPUT
       LOW.SCREEN.COLOR.ON
       ." PRESENT VALUE : "
       CASE
```

```
 1 OF PRINT.EXP.LENG CR
      ." NEW VALUE : " CR
      ENTER.EXP.LENG.VALUE
      ERROR.COLOR.OFF
   ENDOF
 2 OF PRINT.CHROM.LENG CR
      ." NEW VALUE : " CR
      ENTER.CHROM.LENG.VALUE
      ERROR.COLOR.OFF
   ENDOF
 3 OF PRINT.CHROM.RESOL CR
      ." NEW VALUE : " CR
      ENTER.CHROM.RESOL.VALUE
      ERROR.COLOR.OFF
   ENDOF
 4 OF PRINT.DEC.INT CR
      ." NEW VALUE : " CR
      ENTER.DEC.INT.VALUE
      ERROR.COLOR.OFF
   ENDOF
 5 OF PRINT.AVE.DEC.FREQ CR
      ." NEW VALUE : " CR
      ENTER.AVE.DEC.FREQ.VALUE
      ERROR.COLOR.OFF
   ENDOF
 6 OF PRINT.REJ.PER CR
      ." NEW VALUE : " CR
      ENTER.REJ.PER.VALUE
      ERROR.COLOR.OFF
   ENDOF
 8 OF PRINT.NO.OF.PEAKS CR
      ." NEW VALUE : " CR
      ENTER.NO.OF.PEAKS.VALUE
      ERROR.COLOR.ON
      ."   WARNING - PEAK VALUES FOR THE
      .  FOLLOWING MUST BE ENTERED"
      BELL
      NO.OF.PEAKS 1 + 1 DO
        ENTER.RET.TIME.VALUE
        ENTER.VOL.FRAC.INJ.VALUE
        ENTER.DET.RES.FAC.VALUE
      LOOP

      ERROR.COLOR.OFF
   ENDOF
 9 OF {PROMPT} CR ." WHICH PEAK : " #INPUT
      DUP DO
        {LOWSCREEN} PRINT.RET.TIME CR
        ." NEW VALUE : " CR
        ENTER.RET.TIME.VALUE
        ERROR.COLOR.OFF
      LOOP
   ENDOF
10 OF {PROMPT} CR ." WHICH PEAK : " #INPUT
      DUP DO
```

```
             {LOWSCREEN} PRINT.VOL.FRAC.INJ CR
             ." NEW VALUE : " CR
             ENTER.VOL.FRAC.INJ.VALUE
             ERROR.COLOR.OFF
           LOOP
        ENDOF
     11 OF {PROMPT} CR ." WHICH PEAK : " #INPUT
           DUP DO
             {LOWSCREEN} PRINT.DET.RES.FAC CR
             ." NEW VALUE : " CR
             ENTER.DET.RES.FAC.VALUE
             ERROR.COLOR.OFF
           LOOP
        ENDOF
     12 OF PRINT.COL.EFF CR
           ." NEW VALUE : " CR
           ENTER.COL.EFF.VALUE
           ERROR.COLOR.OFF
        ENDOF
     13 OF PRINT.NOISE.MAG CR
           ." NEW VALUE : " CR
           ENTER.NOISE.MAG.VALUE
           ERROR.COLOR.OFF
        ENDOF
     14 OF PRINT.LASER.INT.FAC CR
           ." NEW VALUE : " CR
           ENTER.LASER.INT.FAC.VALUE
           ERROR.COLOR.OFF
        ENDOF
     15 OF PRINT.JIT.DET.LIM CR
           ." NEW VALUE : " CR
           ENTER.JIT.DET.LIM.VALUE
           ERROR.COLOR.OFF
        ENDOF
     16 OF PRINT.JIT.MAX CR
           ." NEW VALUE : " CR
           ENTER.JIT.MAX.VALUE
           ERROR.COLOR.OFF
        ENDOF
     99 OF FULL.SCREEN.COLOR.OFF
           ERROR.COLOR.OFF
           EXIT
        ENDOF
           ERROR.COLOR.ON
           ."    NOT A VALID NUMBER CODE - TRY AGAIN"
           BELL BELL
      ENDCASE
AGAIN

WRITE.SCALARS
WRITE.RET.TIME
WRITE.VOL.FRAC.INJ
WRITE.DET.RES.FAC

RESTORE.FUNCTION.KEYS
```

```
;

: DISPLAY.SINGLE.CHROM.PARAM
    STORE.FUNCTION.KEYS
    CLEAR.FUNCTION.KEYS
    PROMPT.COLOR.ON
    ."  TOUCH ANY KEY TO HALT LISTING" CR
    ."  TOUCH A SECOND KEY TO CONTINUE LISTING"
    ." - 3 KEYS FAST TO STOP LISTING"

    UPPER.SCREEN.COLOR.OFF
    PRINT.CHROM.LENG CR   PAUSE
    PRINT.CHROM.RESOL CR  PAUSE
    PRINT.NO.OF.PEAKS CR  PAUSE

    NO.OF.PEAKS 1 + 1 DO
      PRINT.RET.TIME CR
      PRINT.VOL.FRAC.INJ CR
      PRINT.DET.RES.FAC CR
      PAUSE
      ?KEY
      IF
        KEY DROP
        LEAVE EXIT
      THEN
    LOOP

    PRINT.COL.EFF CR         PAUSE
    PROMPT.COLOR.OFF
    RESTORE.FUNCTION.KEYS
;

: CHANGE.SINGLE.CHROM.PARAM
    STORE.FUNCTION.KEYS
    CLEAR.FUNCTION.KEYS
    LOW.SCREEN.COLOR.OFF
    PROMPT.COLOR.ON
    BEGIN
      {PROMPT} CR
      ."  NUMBER CODE OF PARAMETER TO BE CHANGED
      ."  (99 WILL EXIT) : "
      #INPUT
      LOW.SCREEN.COLOR.ON
      ." PRESENT VALUE : "
      CASE
          2 OF PRINT.CHROM.LENG CR
               ." NEW VALUE : " CR
               ENTER.CHROM.LENG.VALUE
               ERROR.COLOR.OFF
            ENDOF
          3 OF PRINT.CHROM.RESOL CR
               ." NEW VALUE : " CR
               ENTER.CHROM.RESOL.VALUE
               ERROR.COLOR.OFF
            ENDOF
      8 OF PRINT.NO.OF.PEAKS CR
           ." NEW VALUE : " CR
           ENTER.NO.OF.PEAKS.VALUE
           ERROR.COLOR.ON
           ."   WARNING - PEAK VALUES FOR THE"
           ."  FOLLOWING MUST BE ENTERED"
           BELL
           NO.OF.PEAKS 1 + 1 DO
             ENTER.RET.TIME.VALUE
             ENTER.VOL.FRAC.INJ.VALUE
             ENTER.DET.RES.FAC.VALUE
           LOOP

           ERROR.COLOR.OFF
        ENDOF
      9 OF {PROMPT} CR ." WHICH PEAK : " #INPUT
           DUP DO
             {LOWSCREEN} PRINT.RET.TIME CR
             ." NEW VALUE : " CR
             ENTER.RET.TIME.VALUE
             ERROR.COLOR.OFF
           LOOP
        ENDOF
     10 OF {PROMPT} CR ." WHICH PEAK : " #INPUT
           DUP DO
             {LOWSCREEN} PRINT.VOL.FRAC.INJ CR
             ." NEW VALUE : " CR
             ENTER.VOL.FRAC.INJ.VALUE
             ERROR.COLOR.OFF
           LOOP
        ENDOF
     11 OF {PROMPT} CR ." WHICH PEAK : " #INPUT
           DUP DO
             {LOWSCREEN} PRINT.DET.RES.FAC CR
             ." NEW VALUE : " CR
             ENTER.DET.RES.FAC.VALUE
             ERROR.COLOR.OFF
           LOOP
        ENDOF
     12 OF PRINT.COL.EFF CR
           ." NEW VALUE : " CR
           ENTER.COL.EFF.VALUE
           ERROR.COLOR.OFF
        ENDOF
     99 OF FULL.SCREEN.COLOR.OFF
           ERROR.COLOR.OFF
           EXIT
        ENDOF
           ERROR.COLOR.ON
           ."    NOT A VALID NUMBER CODE - TRY AGAIN"
        BELL BELL
      ENDCASE
AGAIN

WRITE.SCALARS
```

```
     WRITE.RET.TIME
     WRITE.VOL.FRAC.INJ
     WRITE.DET.RES.FAC

     RESTORE.FUNCTION.KEYS
;
: DISPLAY.DEC.INT.PARAM
     STORE.FUNCTION.KEYS
     CLEAR.FUNCTION.KEYS

     UPPER.SCREEN.COLOR.OFF
     PRINT.DEC.INT CR
     PRINT.AVE.DEC.FREQ CR
     PRINT.REJ.PER CR
     RESTORE.FUNCTION.KEYS
;

: CHANGE.DEC.INT.PARAM
     STORE.FUNCTION.KEYS
     CLEAR.FUNCTION.KEYS
     LOW.SCREEN.COLOR.OFF
     PROMPT.COLOR.ON
     BEGIN
       {PROMPT} CR
       ."  NUMBER CODE OF PARAMETER TO BE CHANGED"
       ."  (99 WILL EXIT) : "
       #INPUT
       LOW.SCREEN.COLOR.ON
       ." PRESENT VALUE : "
       CASE
          4 OF PRINT.DEC.INT CR
               ." NEW VALUE : " CR
               ENTER.DEC.INT.VALUE
               ERROR.COLOR.OFF
            ENDOF
          5 OF PRINT.AVE.DEC.FREQ CR
               ." NEW VALUE : " CR
               ENTER.AVE.DEC.FREQ.VALUE
               ERROR.COLOR.OFF
            ENDOF
          6 OF PRINT.REJ.PER CR
               ." NEW VALUE : " CR
               ENTER.REJ.PER.VALUE
               ERROR.COLOR.OFF
            ENDOF
         99 OF FULL.SCREEN.COLOR.OFF
               ERROR.COLOR.OFF
               EXIT
            ENDOF
               ERROR.COLOR.ON
               ."   NOT A VALID NUMBER CODE - TRY AGAIN"
               BELL BELL
         ENDCASE
    AGAIN
```

```
     WRITE.SCALARS
     WRITE.RET.TIME
     WRITE.VOL.FRAC.INJ
     WRITE.DET.RES.FAC

     RESTORE.FUNCTION.KEYS
;

: DISPLAY.NOISE.PARAM
     STORE.FUNCTION.KEYS
     CLEAR.FUNCTION.KEYS

     UPPER.SCREEN.COLOR.OFF
     PRINT.EXP.LENG CR
     PRINT.NOISE.MAG CR
     RESTORE.FUNCTION.KEYS
;

: CHANGE.NOISE.PARAM
     STORE.FUNCTION.KEYS
     CLEAR.FUNCTION.KEYS
     LOW.SCREEN.COLOR.OFF
     PROMPT.COLOR.ON
     BEGIN
       {PROMPT} CR ."  NUMBER CODE OF PARAMETER TO BE"
                   ."  CHANGED (99 WILL EXIT) : "
       #INPUT
       LOW.SCREEN.COLOR.ON
       ." PRESENT VALUE : "
       CASE
          1 OF PRINT.EXP.LENG CR
               ." NEW VALUE : " CR
               ENTER.EXP.LENG.VALUE
               ERROR.COLOR.OFF
            ENDOF
         13 OF PRINT.NOISE.MAG CR
               ." NEW VALUE : " CR
               ENTER.NOISE.MAG.VALUE
               ERROR.COLOR.OFF
            ENDOF
          6 OF PRINT.REJ.PER CR
               ." NEW VALUE : " CR
               ENTER.REJ.PER.VALUE
               ERROR.COLOR.OFF
            ENDOF
         99 OF FULL.SCREEN.COLOR.OFF
               ERROR.COLOR.OFF
               EXIT
            ENDOF
               ERROR.COLOR.ON
               ."     NOT A VALID NUMBER CODE - TRY AGAIN"
               BELL BELL
          ENDCASE
    AGAIN
```

```
     WRITE.SCALARS
     WRITE.RET.TIME
     WRITE.VOL.FRAC.INJ
     WRITE.DET.RES.FAC

     RESTORE.FUNCTION.KEYS
;

: DISPLAY.MULTIPLEX.CHROM.PARAM
     STORE.FUNCTION.KEYS
     CLEAR.FUNCTION.KEYS

     UPPER.SCREEN.COLOR.OFF
     PRINT.EXP.LENG CR
     PRINT.LASER.INT.FAC CR
     PRINT.JIT.DET.LIM CR
     PRINT.JIT.MAX CR
     RESTORE.FUNCTION.KEYS
;

: CHANGE.MULTIPLEX.CHROM.PARAM
     STORE.FUNCTION.KEYS
     CLEAR.FUNCTION.KEYS
     LOW.SCREEN.COLOR.OFF
     PROMPT.COLOR.ON
     BEGIN
       {PROMPT} CR ."  NUMBER CODE OF PARAMETER TO BE"
                   ."  CHANGED (99 WILL EXIT) : "
       #INPUT
       LOW.SCREEN.COLOR.ON
       ." PRESENT VALUE : "
       CASE
          1 OF PRINT.EXP.LENG CR
               ." NEW VALUE : " CR
               ENTER.EXP.LENG.VALUE
               ERROR.COLOR.OFF
            ENDOF
         14 OF PRINT.LASER.INT.FAC CR
               ." NEW VALUE : " CR
               ENTER.LASER.INT.FAC.VALUE
               ERROR.COLOR.OFF
            ENDOF
         15 OF PRINT.JIT.DET.LIM CR
               ." NEW VALUE : " CR
               ENTER.JIT.DET.LIM.VALUE
               ERROR.COLOR.OFF
            ENDOF
         16 OF PRINT.JIT.MAX CR
               ." NEW VALUE : " CR
               ENTER.JIT.MAX.VALUE
               ERROR.COLOR.OFF
            ENDOF
         99 OF FULL.SCREEN.COLOR.OFF
               ERROR.COLOR.OFF
               EXIT
            ENDOF
               ERROR.COLOR.ON
               ."    NOT A VALID NUMBER CODE - TRY AGAIN"
               BELL BELL
          ENDCASE
     AGAIN

     WRITE.SCALARS
     WRITE.RET.TIME
     WRITE.VOL.FRAC.INJ
     WRITE.DET.RES.FAC
     RESTORE.FUNCTION.KEYS
;
```

```
    'ECHO.OFF

    \ BARSIM.PRO - CALCULATE SINGLE CHROMATOGRAM, DECISION
    \              SEQUENCE, MULTILPLEX CHROMATOGRAM AND
    \              MUTLIPLEX CHROMATOGRAM WITH WHITE NOISE

    : SIM.START \ FIRST DEFINITION
    ;

    : CALCULATE.SINGLE.CHROM  \ CALCULATE SINGLE CHROMATOGRAM

      PROMPT.COLOR.ON
      ." CALCULATING SINGLE CHROMATOGRAM - PLEASE WAIT"
         0 SINGLE.CHROM :=   \ INITIALIZE SINGLE CHROMATOGRAM
         READ.SCALARS

         \ FOR EACH PEAK CALCULATE THE VALUES AND ADD TO
         \ SINGLE CHROMATOGRAM

         NO.OF.PEAKS 1 +   1  DO

              \ CALCULATE SIGMA
              RET.TIME [ I ] COL.EFF SQRT / SIGMA :=

              \ CALCULATE FRACTION DENOMINATOR
              PI 2.0 * SQRT SIGMA * DENOM :=

              \ CALCULATE FRACTION
              VOL.FRAC.INJ [ I ] DET.RES.FAC [ I ] * DENOM /
              FRAC :=

              \ CALCULATE PEAK VALUES +-6 SIGMA
              4096 RAMP DEC.INT *
              SUB[ RET.TIME [ I ] 6 SIGMA * - , 13 SIGMA * 0.5 + ]
   \ THE 0.5 IS ADDED TO PREVENT ROUND TRUNCATION OF THE RANGE

              CHROM.RESOL RET.TIME [ I ] *  -
              SIGMA /


              DUP * NEG 2.0 /
              EXP FRAC *

              SINGLE.CHROM
              SUB[ RET.TIME [ I ] 6 SIGMA * - , 13 SIGMA * 0.5 + ]
              +
              SINGLE.CHROM
              SUB[ RET.TIME [ I ] 6 SIGMA * - , 13 SIGMA * 0.5 + ] :=

     LOOP
  WRITE.SINGLE.CHROM
  PROMPT.COLOR.OFF
  BELL

;
```

```
: DISPLAY.CHROM

   SINGLE.CHROM
   SUB[ 1 , CHROM.LENG CHROM.RESOL * ]
   GRAPHICS.DISPLAY
   Y.AUTO.PLOT
   BELL

;

: DISPLAY.SINGLE.CHROM
   READ.SINGLE.CHROM
   DISPLAY.CHROM
;


: CALCULATE.DEC.SEQ \ CALCULATE DECISION SEQUENCE

   PROMPT.COLOR.ON
   ." CALCULATING DECISION SEQUENCE - PLEASE WAIT"

   0 DEC.SEQ := \ INITIALIZE DEC.SEQ

   \ INITIALIZE LAST SO COULD FIRE AT TIME 0
   REJ.PER DEC.INT * NEG LAST.DEC :=

   DEC.INT AVE.DEC.FREQ / REJ.FAC := \ RANDOM # CUT-OFF

   EXP.LENG CHROM.LENG + DEC.INT * 1 + 1 DO
                         \ DO FOR VALID RANGE OF ARRAY
     RAND.UNIF
     REJ.FAC <=
     IF
       1 DEC.SEQ [ I ] :=
     THEN
   LOOP
   WRITE.DEC.SEQ

   PROMPT.COLOR.OFF
   BELL
;

: DISPLAY.DEC.SEQ
  READ.DEC.SEQ
  DEC.SEQ
  SUB[ 1 , EXP.LENG DEC.INT * ]
  GRAPHICS.DISPLAY
  Y.AUTO.PLOT
  BELL CR ." TOUCH ANY KEY  TO CONTINUE " PCKEY ?DROP DROP
  NORMAL.DISPLAY
;
```

```
: CALCULATE.MULTIPLEX.CHROM \ CALCULATE MULTIPLEX CHROMATOGRAM

  PROMPT.COLOR.ON
  ." CALCULATING MULTIPLEX CHROMATOGRAM - PLEASE WAIT"

  0 MULTIPLEX.CHROM := \ INITIALIZE MULTIPLEX.CHROM
  READ.DEC.SEQ
  READ.SINGLE.CHROM

\ DOES NOT STORE FIRST CHROM.LENG OF CALCULATIONS IN
\ MULTIPLEX.CHROM

  CHROM.LENG EXP.LENG + DEC.INT *    1 DO
    DEC.SEQ [ I ] 1 =
    IF
      I CHROM.LENG DEC.INT * - 1 +       START :=
      START CHROM.LENG DEC.INT * + 1 -   FINISH :=

      START 1 <
      IF
        FINISH EXP.LENG DEC.INT * >
        IF
          MULTIPLEX.CHROM
          SINGLE.CHROM SUB[  I   , EXP.LENG DEC.INT * ]
          + MULTIPLEX.CHROM :=
        ELSE
          MULTIPLEX.CHROM SUB[ 1 , FINISH ]
          SINGLE.CHROM
            SUB[ CHROM.LENG DEC.INT * FINISH - 1 + , FINISH ]
          + MULTIPLEX.CHROM SUB[ 1 , FINISH ] :=
        THEN

      ELSE
        FINISH EXP.LENG DEC.INT * >
        IF
          MULTIPLEX.CHROM
            SUB[ START , EXP.LENG DEC.INT * START - 1 + ]
          SINGLE.CHROM
            SUB[ 1 , EXP.LENG DEC.INT * START - 1 + ]
          + MULTIPLEX.CHROM
              SUB[ START , EXP.LENG DEC.INT * START - 1 + ] :=
        ELSE
          MULTIPLEX.CHROM
            SUB[ START , CHROM.LENG DEC.INT * ]
          SINGLE.CHROM
            SUB[ 1 , CHROM.LENG DEC.INT * ]
          + MULTIPLEX.CHROM
              SUB[ START , CHROM.LENG DEC.INT * ] :=
        THEN

      THEN

    THEN

  LOOP
```

```
   WRITE.MULTIPLEX.CHROM

   PROMPT.COLOR.OFF
   BELL
 ;

 : DISPLAY.MULTIPLEX.CHROM

   READ.MULTIPLEX.CHROM
   MULTIPLEX.CHROM
   SUB[ 1 , EXP.LENG DEC.INT * ]
   GRAPHICS.DISPLAY
   Y.AUTO.PLOT
   BELL
 ;

 : CALCULATE.NOISE \ CALCULATE WHITE NOISE AND ADD TO
                   \ TO MULTIPLEX CHROMATOGRAM

   PROMPT.COLOR.ON
   ." CALCULATING NOISE - PLEASE WAIT"

   READ.MULTIPLEX.CHROM
   READ.SINGLE.CHROM

   SINGLE.CHROM SUB[ 1 , CHROM.LENG DEC.INT * ]
   []MAX  NOISE.MAG *
   MISC :=

   EXP.LENG DEC.INT * 1 +  1 DO
     MISC
     RAND.NRML
     *
     MULTIPLEX.CHROM [ I ] +
     MULTIPLEX.CHROM [ I ] :=
  LOOP
WRITE.MULTIPLEX.CHROM

  PROMPT.COLOR.OFF
  BELL

;
```

```
ECHO.OFF

\ BARCROSS.PRO - DOES CROSS CORRELATION ON MULTIPLEX CHROM

: CROSS.CORRELATE

  PROMPT.COLOR.ON
  ." CALCULATING CROSS CORRELATION - PLEASE WAIT"

  0 SINGLE.CHROM :=

\ NORMALIZE MULTIPLEX.CHROM TO AVERAGE ABOUT 0

  READ.MULTIPLEX.CHROM
  READ.DEC.SEQ
  MULTIPLEX.CHROM SUB[ 1 , EXP.LENG DEC.INT * ]
  MULTIPLEX.CHROM SUB[ 1 , EXP.LENG DEC.INT * ]
  MEAN -
  MULTIPLEX.CHROM SUB[ 1 , EXP.LENG DEC.INT * ] :=

  CHROM.LENG DEC.INT *   START :=

  EXP.LENG CHROM.LENG - DEC.INT *        1 DO


    DEC.SEQ [ START ] 1 =
    IF


      SINGLE.CHROM SUB[ 1 , CHROM.LENG DEC.INT * ]
      MULTIPLEX.CHROM SUB[ I , CHROM.LENG DEC.INT * ] +
      SINGLE.CHROM SUB[ 1 , CHROM.LENG DEC.INT * ] :=
    THEN
    1 START + START :=
  LOOP
  WRITE.CROSS.CHROM

  PROMPT.COLOR.OFF
  BELL
;

: DISPLAY.CROSS.CHROM
  READ.CROSS.CHROM
  DISPLAY.CHROM
;
```

```
 ECHO.OFF

 \ BARHAD.PRO - CALCULATES THE HADAMARD TRANSFORM

 : HADAMARD

   PROMPT.COLOR.ON
   ." CALCULATING HADAMARD TRANSFORM - PLEASE WAIT"

   0 SINGLE.CHROM :=


 \ NORMALIZE MULTIPLEX.CHROM TO AVERAGE ABOUT 0

   READ.MULTIPLEX.CHROM
   READ.DEC.SEQ

   MULTIPLEX.CHROM SUB[ 1 , EXP.LENG DEC.INT * ]
   MULTIPLEX.CHROM SUB[ 1 , EXP.LENG DEC.INT * ]
   MEAN -
   MULTIPLEX.CHROM SUB[ 1 , EXP.LENG DEC.INT * ] :=


   CHROM.LENG DEC.INT * 1 +   1 DO

     DEC.SEQ
     SUB[ CHROM.LENG  DEC.INT * I - 1 +  , EXP.LENG DEC.INT * ]

    MULTIPLEX.CHROM SUB[ 1 , EXP.LENG DEC.INT * ]
    << * | + >>
    SINGLE.CHROM SUB[ I , 1 ] :=
  LOOP
  WRITE.HADAMARD.CHROM

  PROMPT.COLOR.OFF
  BELL
;


: DISPLAY.HADAMARD.CHROM
  READ.HADAMARD.CHROM
  DISPLAY.CHROM
;
```

```
ECHO.OFF

\ BARFOUR.PRO CALCULATES THE FAST FOURIER TRANSFORM
\ CHROMATOGRAM

: FOURIER

  PROMPT.COLOR.ON
  ." CALCULATING FAST FOURIER TRANSFORM - PLEASE WAIT"

\ DETERMINE BEST 2'S POWER SIZE

  EXP.LENG DEC.INT *
  CASE
    2048 MIN 2048 OF 2048 MISC := ENDOF
    1024 MIN 1024 OF 1024 MISC := ENDOF
     512 MIN  512 OF  512 MISC := ENDOF
     256 MIN  256 OF  256 MISC := ENDOF
     128 MIN  128 OF  256 MISC := ENDOF
      64 MIN   64 OF   64 MISC := ENDOF
      32 MIN   32 OF   32 MISC := ENDOF

    0 MISC :=
  ENDCASE


\ CALCULATE FFT CHROM

  MISC 0 <>
  IF

    \ PUT THE 2 ARRAYS INTO THE FREQUENCY DOMAIN VIA FFT
    0 SINGLE.CHROM :=
    READ.MULTIPLEX.CHROM
    MULTIPLEX.CHROM SUB[ 1 , MISC ]
    DUP MEAN -
    FFT

    READ.DEC.SEQ
    DEC.SEQ SUB[ CHROM.LENG DEC.INT * , MISC ]
    DUP MEAN -
    FFT

    \ TAKE CONJUCATION, MULTIPLY AND CONVERT BACK TO
    \ TIME DOMAIN
    CONJ
    *
    IFFT
    ZMAG
    SUB[ 1 , CHROM.LENG ]
    SINGLE.CHROM SUB[ 1 , CHROM.LENG ] :=

    WRITE.FFT.CHROM

  ELSE
```

```
    ERROR.COLOR.ON
    ." EXPERIMENTAL LENGTH TOO SHORT"
  THEN

  PROMPT.COLOR.OFF
  BELL
;


: DISPLAY.FFT.CHROM
  READ.FFT.CHROM
  DISPLAY.CHROM
;
```

```
ECHO.OFF

\ BARMENUS.PRO - MENUS OF THIS MENU DRIVEN PROGRAM

: MENU.START \ FIRST DEFINITION
;

: EXIT.PROCEDURE \ TURNS OFF PRESENT MENU SO TO RETURN
                 \  TO CALLING MENU
  " NO " MENU.ON ":=
;

: DEFAULT.EXP.FILENAME
  " BAREXPTP.DAT" FILENAME ":=
;


\ MENU SCREENS

: DIRECTORY.LISTING
  NO.OPTION
;

: PRINT.EXP.DATA.MENU
     NO.OPTION
;


: PRINT.REPORT.SCREEN
  SCREEN.PRINT
  NORMAL.DISPLAY
;

: DEFINE.ALL.KEYS.NORMAL
  CLEAR.FUNCTION.KEYS
  F1  FUNCTION.KEY.DOES NORMAL.DISPLAY
  F2  FUNCTION.KEY.DOES NORMAL.DISPLAY
  F3  FUNCTION.KEY.DOES NORMAL.DISPLAY
  F4  FUNCTION.KEY.DOES NORMAL.DISPLAY
  F5  FUNCTION.KEY.DOES NORMAL.DISPLAY
  F6  FUNCTION.KEY.DOES NORMAL.DISPLAY
  F7  FUNCTION.KEY.DOES NORMAL.DISPLAY
  F8  FUNCTION.KEY.DOES NORMAL.DISPLAY
  F9  FUNCTION.KEY.DOES NORMAL.DISPLAY
  F10 FUNCTION.KEY.DOES NORMAL.DISPLAY
;

: SAME.REPORT.SCREEN
     ." <F1>  PRINT" CR
     ." <F10> EXIT" CR
     DEFINE.ALL.KEYS.NORMAL
     F1  FUNCTION.KEY.DOES PRINT.REPORT.SCREEN
;
```

```
: PRINT.DISPLAY.SINGLE.CHROM
     DISPLAY.SINGLE.CHROM CR
     ." SINGLE" CR
     ." CHROMATOGRAM" CR CR
     SAME.REPORT.SCREEN
;

: PRINT.DISPLAY.MULTIPLEX.CHROM
     DISPLAY.MULTIPLEX.CHROM CR
     ." MULTIPLEX" CR
     ." CHROMATOGRAM" CR CR
     SAME.REPORT.SCREEN
;

: PRINT.DISPLAY.CROSS.CHROM
     DISPLAY.CROSS.CHROM CR
     ." CROSS" CR
     ." CORRELATION" CR
     ." CHROMATOGRAM" CR CR
     SAME.REPORT.SCREEN
;

: PRINT.DISPLAY.HADAMARD.CHROM
     DISPLAY.HADAMARD.CHROM CR
     ." HADAMARD" CR
     ." TRANSFORM" CR
     ." CHROMATOGRAM" CR CR
     SAME.REPORT.SCREEN
;

: PRINT.DISPLAY.FOURIER.CHROM
     DISPLAY.FFT.CHROM CR
     ." FAST" CR
     ." FOURIER" CR
     ." TRANSFORM" CR
     ." CHROMATOGRAM" CR CR
     SAME.REPORT.SCREEN
;

: GET.STORED.SIM.PARAM
  NO.OPTION
;

: COMPLETE.ALL.STEPS
  NO.OPTION
;

: ENTER.SIM.PARAM.MENU \ MENU 2.1
     TITLE.COLOR.ON  ."      SIMULATION PARAMETERS ENTRY MENU"
     LOW.SCREEN.COLOR.OFF
 ."          <F1> ENTER PARAMETERS       "
             ." <F5>  DISPLAY PARAMETERS" CR
 ."          <F2> USE DEFAULT PARAMETERS  "
             ." <F6>  CHANGE PARAMETERS" CR
 ."          <F3> USE STORED PARAMETER   "
```

```
            ." <F7>  FINISH NEXT STEPS AUTOMATICALLY"
                                                           CR
  ."        <F4> LIST DIRECTORY          <F10> EXIT" CR

     CLEAR.FUNCTION.KEYS
     F1  FUNCTION.KEY.DOES ENTER.SIM.PARAM
     F2  FUNCTION.KEY.DOES DEFAULT.SIM.PARAM
     F3  FUNCTION.KEY.DOES GET.STORED.SIM.PARAM
     F4  FUNCTION.KEY.DOES DIRECTORY.LISTING
     F5  FUNCTION.KEY.DOES DISPLAY.SIM.PARAM
     F6  FUNCTION.KEY.DOES CHANGE.SIM.PARAM
     F7  FUNCTION.KEY.DOES COMPLETE.ALL.STEPS
     F10 FUNCTION.KEY.DOES EXIT.PROCEDURE
;

: PRINT.ENTER.SIM.PARAM.MENU
     {DEF} SCREEN.CLEAR
     BEGIN
       " YES" MENU.ON "=
     WHILE
       ENTER.SIM.PARAM.MENU
       PCKEY INTERPRET.KEY
     REPEAT
     " YES" MENU.ON ":=
               \ SO CALLILNG MENU WILL REPRINT ITSELF
;

: WHICH.SINGLE.CHROM
  NO.OPTION
;

: DO.PRINT.DISPLAY.SINGLE.CHROM
     PRINT.DISPLAY.SINGLE.CHROM
     PCKEY INTERPRET.KEY
;

: SINGLE.CHROM.MENU \ MENU 2.2
     TITLE.COLOR.ON ."       SINGLE CHROMATOGRAM MENU"
     LOW.SCREEN.COLOR.OFF
 ."               <F1> DISPLAY ALL PARAMETERS"
                 ."                  <F10> EXIT" CR
 ."              <F2> DISPLAY SINGLE CHROMATOGRAM PARAMETERS"
                                                            CR
."              <F3> CHANGE SINGLE CHROMATOGRAM PARAMETERS"
                                                            CR
."              <F4> CALCULATE SINGLE CHROMATOGRAM" CR
."              <F5> USE STORED SINGLE CHROMATOGRAM" CR
."              <F6> DISPLAY SINGLE CHROMATOGRAM GRAPH"

    CLEAR.FUNCTION.KEYS
    F1  FUNCTION.KEY.DOES DISPLAY.SIM.PARAM
    F2  FUNCTION.KEY.DOES DISPLAY.SINGLE.CHROM.PARAM
    F3  FUNCTION.KEY.DOES CHANGE.SINGLE.CHROM.PARAM
    F4  FUNCTION.KEY.DOES CALCULATE.SINGLE.CHROM
    F5  FUNCTION.KEY.DOES WHICH.SINGLE.CHROM
```

```
     F6  FUNCTION.KEY.DOES DO.PRINT.DISPLAY.SINGLE.CHROM
     F10 FUNCTION.KEY.DOES EXIT.PROCEDURE
;

: PRINT.SINGLE.CHROM.MENU
     {DEF} SCREEN.CLEAR
     BEGIN
       " YES" MENU.ON "=
     WHILE
       SINGLE.CHROM.MENU
       PCKEY INTERPRET.KEY
     REPEAT
     " YES" MENU.ON ":= \ SO CALLING MENU WILL REPRINT ITSELF
;

: WHICH.DEC.SEQ
  NO.OPTION
;

: DECISION.SEQ.MENU \ MENU 2.3
     TITLE.COLOR.ON ."       DECISION SEQUENCE MENU"
     LOW.SCREEN.COLOR.OFF
 ."                   <F1> DISPLAY ALL PARAMETERS"
                    ."                 <F10> EXIT" CR
 ."                  <F2> DISPLAY DECISION SEQUENCE PARAMETERS"
                                                     CR
 ."                  <F3> CHANGE DECISION SEQUENCE PARAMETERS"
                                                     CR
 ."                  <F4> CALCULATE DECISION SEQUENCE" CR
 ."                  <F5> USE STORED DECISION SEQUENCE" CR
 ."                  <F6> DISPLAY DECSION SEQUENCE GRAPH"

     CLEAR.FUNCTION.KEYS
     F1  FUNCTION.KEY.DOES DISPLAY.SIM.PARAM
     F2  FUNCTION.KEY.DOES DISPLAY.DEC.INT.PARAM
     F3  FUNCTION.KEY.DOES CHANGE.DEC.INT.PARAM
     F4  FUNCTION.KEY.DOES CALCULATE.DEC.SEQ
     F5  FUNCTION.KEY.DOES WHICH.DEC.SEQ
     F6  FUNCTION.KEY.DOES DISPLAY.DEC.SEQ
     F10 FUNCTION.KEY.DOES EXIT.PROCEDURE
;

: PRINT.DECISION.SEQ.MENU
     {DEF} SCREEN.CLEAR
     BEGIN
       " YES" MENU.ON "=
     WHILE
       DECISION.SEQ.MENU
       PCKEY INTERPRET.KEY
     REPEAT
     " YES" MENU.ON ":= \ SO CALLING MENU WILL REPRINT ITSELF
;

: WHICH.NOISE
  NO.OPTION
```

```
;

: DISPLAY.NOISE
  NO.OPTION
;

: NOISE.MENU \ MENU 2.4
     TITLE.COLOR.ON ."                NOISE MENU"
     LOW.SCREEN.COLOR.OFF
."                    <F1> DISPLAY ALL PARAMETERS    "
                     ."  <F10> EXIT" CR
."                   <F2> DISPLAY NOISE PARAMETERS" CR
."                   <F3> CHANGE NOISE PARAMETERS" CR
."                   <F4> CALCULATE NOISE" CR
."                   <F5> USE STORED NOISE" CR
."                   <F6> DISPLAY NOISE GRAPH"

     CLEAR.FUNCTION.KEYS
     F1  FUNCTION.KEY.DOES DISPLAY.SIM.PARAM
     F2  FUNCTION.KEY.DOES DISPLAY.NOISE.PARAM
     F3  FUNCTION.KEY.DOES CHANGE.NOISE.PARAM
     F4  FUNCTION.KEY.DOES CALCULATE.NOISE
     F5  FUNCTION.KEY.DOES WHICH.NOISE
     F6  FUNCTION.KEY.DOES DISPLAY.NOISE
     F10 FUNCTION.KEY.DOES EXIT.PROCEDURE
;

: PRINT.NOISE.MENU
     {DEF} SCREEN.CLEAR
     BEGIN
       " YES" MENU.ON "-
     WHILE
       NOISE.MENU
       PCKEY INTERPRET.KEY
     REPEAT
     " YES" MENU.ON ":= \ SO CALLING MENU WILL REPRINT ITSELF
;

: WHICH.MULTIPLEX.CHROM
  NO.OPTION
;

: DO.PRINT.DISPLAY.MULT.CHROM
     PRINT.DISPLAY.MULTIPLEX.CHROM
     PCKEY INTERPRET.KEY
;

: MULTIPLEX.CHROM.MENU \ MENU 2.5
     TITLE.COLOR.ON ."          MULTIPLEX CHROMATOGRAM MENU"
     LOW.SCREEN.COLOR.OFF
."                 <F1> DISPLAY ALL PARAMETERS
                 ."                    <F10> EXIT" CR
."           <F2> DISPLAY MULTIPLEX CHROMATOGRAM PARAMETERS"
                                                          CR
."           <F3> CHANGE MULTIPLEX CHROMATOGRAM PARAMETERS"
```

```
                                                                   CR
 ."                   <F4> CALCULATE MULTIPLEX CHROMATOGRAM " CR
 ."                  <F5> USE STORED MULTIPLEX CHROMATOGRAM "
                       ." PARAMETERS" CR
 ."                   <F6> DISPLAY MULTIPLEX CHROMATOGRAM GRAPH"

     CLEAR.FUNCTION.KEYS
     F1  FUNCTION.KEY.DOES DISPLAY.SIM.PARAM
     F2  FUNCTION.KEY.DOES DISPLAY.MULTIPLEX.CHROM.PARAM
     F3  FUNCTION.KEY.DOES CHANGE.MULTIPLEX.CHROM.PARAM
     F4  FUNCTION.KEY.DOES CALCULATE.MULTIPLEX.CHROM
     F5  FUNCTION.KEY.DOES WHICH.MULTIPLEX.CHROM
     F6  FUNCTION.KEY.DOES DO.PRINT.DISPLAY.MULT.CHROM
     F10 FUNCTION.KEY.DOES EXIT.PROCEDURE
;

: PRINT.MULTIPLEX.CHROM.MENU
     {DEF} SCREEN.CLEAR
     BEGIN
       " YES" MENU.ON "=
     WHILE
       MULTIPLEX.CHROM.MENU
       PCKEY INTERPRET.KEY
     REPEAT
     " YES" MENU.ON ":= \ SO CALLING MENU WILL REPRINT ITSELF
;

: RENAME.SIM.FILE
  NO.OPTION
;

: PRINT.HELP.SIM.DATA
  NO.OPTION
;

: DATA.SIM.MENU \ MENU 2.0
    TITLE.COLOR.ON ."        DATA SIMULATION MENU"
    UPPER.SCREEN.COLOR.OFF
    CR CR
 ."                    <F1>  PARAMETERS" CR
 ."                    <F2>  SINGLE CHROMATOGRAM CALCULATION" CR
 ."                    <F3>  DECISION SEQUENCE CALCULATION" CR
 ."                    <F4>  MULTIPLEX CHROMATOGRAM CALCULATION" CR
."                    <F5>  NOISE CALCULATION" CR
."                    <F6>  RENAME FILES" CR
."                    <F7>  HELP" CR
."                    <F10> EXIT" CR

   CLEAR.FUNCTION.KEYS
   F1  FUNCTION.KEY.DOES PRINT.ENTER.SIM.PARAM.MENU
   F2  FUNCTION.KEY.DOES PRINT.SINGLE.CHROM.MENU
   F3  FUNCTION.KEY.DOES PRINT.DECISION.SEQ.MENU
   F4  FUNCTION.KEY.DOES PRINT.MULTIPLEX.CHROM.MENU
   F5  FUNCTION.KEY.DOES PRINT.NOISE.MENU
   F6  FUNCTION.KEY.DOES RENAME.SIM.FILE
```

```
      F7  FUNCTION.KEY.DOES PRINT.HELP.SIM.DATA
      F10 FUNCTION.KEY.DOES EXIT.PROCEDURE
 ;

 : PRINT.DATA.SIM.MENU
      {DEF} SCREEN.CLEAR
      " S" WHICH.MENU ":=
      DEFAULT.SIM.FILENAME
      PROMPT.COLOR.ON ." FILE NAME TO BE USED: " FILENAME "TYPE
      BEGIN
        " YES" MENU.ON "=
      WHILE
        LOW.SCREEN.COLOR.OFF
        DATA.SIM.MENU
        PCKEY INTERPRET.KEY
        PROMPT.COLOR.OFF
      REPEAT
      " YES" MENU.ON ":= \ SO CALLING MENU WILL REPRINT ITSELF
 ;

 : ANALYSIS.MENU \ MENU.3.1
      TITLE.COLOR.ON  ."          ANALYSIS MENU"
      LOW.SCREEN.COLOR.OFF
  ."                          <F1>  CROSS-CORRELATION" CR
  ."                          <F2>  HADAMARD TRANSFORM" CR
  ."                          <F3>  FAST FOURIER TRANSFORM" CR
  ."                          <F10> EXIT" CR

      CLEAR.FUNCTION.KEYS
      F1  FUNCTION.KEY.DOES CROSS.CORRELATE
      F2  FUNCTION.KEY.DOES HADAMARD
      F3  FUNCTION.KEY.DOES FOURIER
      F10 FUNCTION.KEY.DOES EXIT.PROCEDURE
 ;

 : GET.RECENT.DATA
   " BARSIMTP.DAT" FILENAME ":=
          \ ***** LATER TEST IF WAS EXP. OR SIM MOST RECENT
 ;

 : ANAL.RECENT.SESSION
      GET.RECENT.DATA
      BEGIN
        " YES" MENU.ON "=
      WHILE
        ANALYSIS.MENU
        PCKEY INTERPRET.KEY
      REPEAT
      " YES" MENU.ON ":= \ SO CALLING MENU WILL REPRINT ITSELF
 ;

 : GET.EXP.FILE
   NO.OPTION
 ;
```

```
: ANAL.EXP.FILE
    NO.OPTION
;

: GET.SIM.FILE
  NO.OPTION
;

: ANAL.SIM.FILE
  NO.OPTION
;

: GET.FILE
  NO.OPTION
;

: ANAL.FILE
  NO.OPTION
;

: DATA.ANAL.MENU    \ MENU 3.0
     TITLE.COLOR.ON ."            DATA ANALYSIS MENU"
     LOW.SCREEN.COLOR.OFF
 ."    DATA TO BE ANALYZED:  <F1>  MOST RECENT SESSION" CR
 ."                          <F2>  EXPERIMENTAL FILE" CR
 ."                          <F3>  SIMULATION FILE" CR
 ."                          <F4>  OTHER FILE" CR
 ."                          <F10> EXIT"

     CLEAR.FUNCTION.KEYS
     F1  FUNCTION.KEY.DOES ANAL.RECENT.SESSION
     F2  FUNCTION.KEY.DOES ANAL.EXP.FILE
     F3  FUNCTION.KEY.DOES ANAL.SIM.FILE
     F4  FUNCTION.KEY.DOES ANAL.FILE
     F10 FUNCTION.KEY.DOES EXIT.PROCEDURE
;

: PRINT.DATA.ANAL.MENU
     {DEF} SCREEN.CLEAR
     BEGIN
       " YES" MENU.ON "=
     WHILE
       DATA.ANAL.MENU
       PCKEY INTERPRET.KEY
     REPEAT
     " YES" MENU.ON ":= \ SO CALLING MENU WILL REPRINT ITSELF
;

: PRINT.REPORT.PARAM.MENU
  NO.OPTION
;


: REPORT.GRAPHS.MENU \ MENU 4.1.2
     TITLE.COLOR.ON ."            REPORT GRAPHS MENU"
```

```
        LOW.SCREEN.COLOR.OFF
  ."          GRAPH:  <F1>  SINGLE CHROMATOGRAM" CR
  ."                  <F2>  MULTIPLEX.CHROMATOGRAM" CR
  ."                  <F3>  CROSS CORRELATION CHROMATOGRAM" CR
  ."                  <F4>  HADAMARD CHROMATOGRAM" CR
  "                   <F5>  FAST FOURIER TRANSFORM CHROMATOGRAM"
                                                   CR
  ."                  <F10> EXIT"

        CLEAR.FUNCTION.KEYS
        F1  FUNCTION.KEY.DOES PRINT.DISPLAY.SINGLE.CHROM
        F2  FUNCTION.KEY.DOES PRINT.DISPLAY.MULTIPLEX.CHROM
        F3  FUNCTION.KEY.DOES PRINT.DISPLAY.CROSS.CHROM
        F4  FUNCTION.KEY.DOES PRINT.DISPLAY.HADAMARD.CHROM
        F5  FUNCTION.KEY.DOES PRINT.DISPLAY.FOURIER.CHROM
        F10 FUNCTION.KEY.DOES EXIT.PROCEDURE

        PCKEY INTERPRET.KEY
;

: PRINT.REPORT.GRAPHS.MENU
  {DEF} SCREEN.CLEAR
  BEGIN
    " YES" MENU.ON "-
  WHILE
    REPORT.GRAPHS.MENU
    PCKEY INTERPRET.KEY
  REPEAT
  " YES" MENU.ON ":- \ SO CALLING MENU WILL REPRINT ITSELF
;

: PRINT.REPORT.VALUES.MENU
  NO.OPTION
;

: WHICH.REPORT.MENU \ MENU 4.1
      TITLE.COLOR.ON  ."             REPORT MENU"
      LOW.SCREEN.COLOR.OFF
 ."            REPORT:        <F1>  PARAMETERS" CR
 ."                           <F2>  RESULT GRAPHS" CR
 ."                           <F3>  RESULT VALUES" CR
 ."                           <F10> EXIT" CR

      CLEAR.FUNCTION.KEYS
      F1  FUNCTION.KEY.DOES PRINT.REPORT.PARAM.MENU
      F2  FUNCTION.KEY.DOES PRINT.REPORT.GRAPHS.MENU
      F3  FUNCTION.KEY.DOES PRINT.REPORT.VALUES.MENU
      F10 FUNCTION.KEY.DOES EXIT.PROCEDURE
;

: REPORT.RECENT.SESSION
  GET.RECENT.DATA
  {DEF} SCREEN.CLEAR
  BEGIN
    " YES" MENU.ON "=
  WHILE
    WHICH.REPORT.MENU
    PCKEY INTERPRET.KEY
  REPEAT
  " YES" MENU.ON ":= \ SO CALLING MENU WILL REPRINT ITSELF
;

: REPORT.EXP.FILE
  NO.OPTION
;

: REPORT.SIM.FILE
  NO.OPTION
;

: REPORT.FILE
  NO.OPTION
;

: DATA.REPORT.MENU  \ MENU 4.0
     TITLE.COLOR.ON ."            DATA REPORT MENU"
     LOW.SCREEN.COLOR.OFF
 ."              REPORT:    <F1>  MOST RECENT SESSION" CR
 ."                         <F2>  EXPERIMENTAL FILE" CR
 ."                         <F3>  SIMULATION FILE" CR
 ."                         <F4>  OTHER FILE" CR
 ."                         <F10> EXIT"

     CLEAR.FUNCTION.KEYS
     F1  FUNCTION.KEY.DOES REPORT.RECENT.SESSION
     F2  FUNCTION.KEY.DOES REPORT.EXP.FILE
     F3  FUNCTION.KEY.DOES REPORT.SIM.FILE
     F4  FUNCTION.KEY.DOES REPORT.FILE
     F10 FUNCTION.KEY.DOES EXIT.PROCEDURE
;

: PRINT.DATA.REPORT.MENU
     {DEF} SCREEN.CLEAR
     BEGIN
       " YES" MENU.ON "=
     WHILE
       DATA.REPORT.MENU
       PCKEY INTERPRET.KEY
     REPEAT
     " YES" MENU.ON ":= \ SO CALLING MENU WILL REPRINT ITSELF
;

: HOUSEKEEPING
  NO.OPTION
;

: PRINT.HELP.MENU
  NO.OPTION
;
```

```
: SYSTEM.RETURN
   {DEF} SCREEN.CLEAR
   ABORT
;

: SYSTEM.EXITING
  CLEAR.FUNCTION.KEYS
  SYSTEM.RETURN
;

: MAIN.MENU  \ INTRODUCTORY MENU - FIRST ONE DISPLAYED
     {DEF} SCREEN.CLEAR
     TITLE.COLOR.ON ."                    MAIN MENU"
     FULL.SCREEN.COLOR.OFF
     CR CR
."                                   WELCOME" CR
."                                  TO     THE" CR
."                            MULTIPLEX CHROMATOGRAM" CR
."                                   PROGRAM" CR CR CR
."                      <F1>  EXPERIMENTAL DATA COLLECTION" CR
."                      <F2>  DATA SIMULATION" CR
."                      <F3>  DATA ANALYSIS" CR
."                      <F4>  DATA REPORT" CR
."                      <F5>  HOUSEKEEPING" CR
."                      <F6>  HELP" CR
."                      <F10> EXIT" CR

     CLEAR.FUNCTION.KEYS
     F1  FUNCTION.KEY.DOES PRINT.EXP.DATA.MENU
     F2  FUNCTION.KEY.DOES PRINT.DATA.SIM.MENU
     F3  FUNCTION.KEY.DOES PRINT.DATA.ANAL.MENU
     F4  FUNCTION.KEY.DOES PRINT.DATA.REPORT.MENU
     F5  FUNCTION.KEY.DOES HOUSEKEEPING
     F6  FUNCTION.KEY.DOES PRINT.HELP.MENU
     F10 FUNCTION.KEY.DOES SYSTEM.EXITING

     INITIATE.EXP.CONSTANTS
     INITIATE.SIM.CONSTANTS
;

: PRINT.MAIN.MENU
     BEGIN
       " YES" MENU.ON "=
     WHILE
       MAIN.MENU
       PCKEY  INTERPRET.KEY
     REPEAT
;

: START.PROGRAM
     " YES" MENU.ON ":=
     PRINT.MAIN.MENU
;
```

```
ECHO.OFF

\ BARDRIFT.PRO - TO ADD DRIFT TO MULTIPLEX.CHROM

: CALCULATE.DRIFT

  READ.MULTIPLEX.CHROM

  MULTIPLEX.CHROM SUB[ 1 , EXP.LENG DEC.INT * ]
  []MAX

  EXP.LENG DEC.INT * /
  MISC * MISC :=

  EXP.LENG DEC.INT *    RAMP
  MISC *
  MULTIPLEX.CHROM SUB[ 1 , EXP.LENG DEC.INT * ] +
  MULTIPLEX.CHROM SUB[ 1 , EXP.LENG DEC.INT * ] :=

  WRITE.MULTIPLEX.CHROM

;
```

```
ECHO.OFF

\ BARCROSS.FIT - DOES CROSS CORRELATION ON MULTIPLEX CHROM


: CROSS.CORRELATE

\ ." BEGIN " CR
  0 SINGLE.CHROM :=

\ NORMALIZE MULTIPLEX.CHROM TO AVERAGE ABOUT 0

  READ.MULTIPLEX.CHROM
  READ.DEC.SEQ
\  MULTIPLEX.CHROM SUB[ 1 , EXP.LENG DEC.INT * ]
\  MULTIPLEX.CHROM SUB[ 1 , EXP.LENG DEC.INT * ]
\  MEAN -
\  MULTIPLEX.CHROM SUB[ 1 , EXP.LENG DEC.INT * ] :=

  CHROM.LENG DEC.INT * 20 +    START :=
\ ." START = " START . CR

  EXP.LENG CHROM.LENG - DEC.INT * 20 -      21 DO

\ ." DEC INDEX" START . CR

    DEC.SEQ [ START ] 1 =
    IF

\ ." MC:" I . CHROM.LENG . ."  SC ALL"

      SINGLE.CHROM SUB[ 1 , CHROM.LENG DEC.INT * ]
\ ." AFTER RESULT " CR
      MULTIPLEX.CHROM SUB[ I , CHROM.LENG DEC.INT * ] +
\ ." AFTER MULTI " CR
      SINGLE.CHROM SUB[ 1 , CHROM.LENG DEC.INT * ] :=
\ ." AFTER CALCULATION " CR
    THEN
    1 START + START :=
\ PAUSE
  LOOP
  WRITE.CROSS.CHROM
;

: DISPLAY.CROSS.CHROM
  READ.CROSS.CHROM
  DISPLAY.CHROM
;
```

```
ECHO.OFF

\ BARHAD.FIT - CALCULATES THE HADAMARD TRANSFORM

: HADAMARD

  0 SINGLE.CHROM :=


\ NORMALIZE MULTIPLEX.CHROM TO AVERAGE ABOUT 0

  READ.MULTIPLEX.CHROM
  READ.DEC.SEQ

\  MULTIPLEX.CHROM SUB[ 1 , EXP.LENG DEC.INT * ]
\  MULTIPLEX.CHROM SUB[ 1 , EXP.LENG DEC.INT * ]
\  MEAN -
\  MULTIPLEX.CHROM SUB[ 1 , EXP.LENG DEC.INT * ] :=


  CHROM.LENG DEC.INT * 1 +   1 DO

    DEC.SEQ
      SUB[ CHROM.LENG  DEC.INT * I - 1 + 20 +   ,
           EXP.LENG DEC.INT * 20 - ]

    MULTIPLEX.CHROM SUB[ 21 , EXP.LENG DEC.INT * 20 - ]
    << * | + >>
    SINGLE.CHROM SUB[ I , 1 ] :=
  LOOP
  WRITE.HADAMARD.CHROM
;


: DISPLAY.HADAMARD.CHROM
  READ.HADAMARD.CHROM
  DISPLAY.CHROM
;
```

```
ECHO.OFF

\ BARFOUR.FIT CALCULATES THE FAST FOURIER TRANSFORM
\ CHROMATOGRAM

: FOURIER

\ DETERMINE BEST 2'S POWER SIZD

 ." A" CR
 EXP.LENG DEC.INT *
 CASE
   2088 MIN 2088 OF 2048 MISC := ENDOF
   1064 MIN 1064 OF 1024 MISC := ENDOF
    552 MIN  552 OF  512 MISC := ENDOF
    296 MIN  296 OF  256 MISC := ENDOF
    168 MIN  168 OF  128 MISC := ENDOF
    104 MIN  104 OF   64 MISC := ENDOF
     72 MIN   72 OF   32 MISC := ENDOF

   0 MISC :=
 ENDCASE

 ." MISC =" MISC .


\ CALCULATE FFT CHROM

 MISC 0 <>
 IF
   0 SINGLE.CHROM :=
   READ.MULTIPLEX.CHROM
   MULTIPLEX.CHROM SUB[ 21 , MISC ]
   DUP MEAN -
   FFT

   READ.DEC.SEQ
   DEC.SEQ SUB[ CHROM.LENG DEC.INT * 20 + , MISC ]
   DUP MEAN -
   FFT

   CONJ
   *
   IFFT
   ZMAG
   SUB[ 1 , CHROM.LENG ]
   SINGLE.CHROM SUB[ 1 , CHROM.LENG ] :=

   WRITE.FFT.CHROM

 ELSE
   ERROR.COLOR.ON
   ." EXPERIMENTAL LENGTH TOO SHORT"
 THEN
;
```

```
: DISPLAY.FFT.CHROM
  READ.FFT.CHROM
  DISPLAY.CHROM
;
```

```
  ECHO.OFF

  \ BARREDD.PRO - REDUCE DRIFT IN MULTIPLEX.CHROM

  : REDUCE.AVE.DRIFT

    READ.MULTIPLEX.CHROM
  \ NOTE WHEN CALCULATING SINGLE.CHROM YOU MUST SKIP
  \ THE FIRST AND LAST 20 POINTS

    20 1 + START :=
    START 20 + FINISH :=

    MULTIPLEX.CHROM SUB[ 1 , FINISH ]
    MEAN  41 * MISC :=

    MULTIPLEX.CHROM SUB[ 1 , EXP.LENG DEC.INT * ]
    []COPY

    EXP.LENG DEC.INT * FINISH - 1 + 1 +       START DO

      MULTIPLEX.CHROM [ I ] MISC 41 /  - MULTIPLEX.CHROM [ I ] :=

    DUP
    [ I 20 - ]
    -1 * MISC + MISC :=
    DUP
    [ I 20 + ]
    MISC + MISC :=

  LOOP
  DROP

 WRITE.MULTIPLEX.CHROM

;
```

```
ECHO.OFF

\ BARRAND.PRO - TO TEST THE RANDOMNESS OF ASYST'S RANDOM
\ NUMBER GENERATOR

: RAND.START \ FIRST DEFINITION
;

REAL DIM[ 300 ] ARRAY RAND.ARRAY
REAL DIM[ 300 ] ARRAY NORM.ARRAY

INTEGER SCALAR INDEX
INTEGER DIM[ 10 ] ARRAY INTERVAL.ARRAY
REAL SCALAR CHI.VAL

REAL SCALAR AVE
REAL SCALAR SD
REAL SCALAR T.VAL

REAL DIM[ 4 ] ARRAY MISC     \ .01, .05, .1 , REST
REAL DIM[ 4 ] ARRAY MISCN    \ -.01, -.05, -.1 , -REST

REAL SCALAR AVE.MEAN
REAL SCALAR AVE.T

: FILL.NORM.TEST

  300 1 +    1 DO
  RAND.NRML NORM.ARRAY [ I ] :=
  LOOP
;

: NORMAL.TEST     \ T-TEST

  FILL.NORM.TEST
  NORM.ARRAY MEAN AVE :=
  NORM.ARRAY VARIANCE SQRT SD :=
  300 SQRT AVE * SD /
  T.VAL :=
  ."    T VALUE:" T.VAL .
;

: FILL.RAND.TEST

  300 1 +    1 DO
  RAND.UNIF RAND.ARRAY [ I ] :=
  LOOP
;

: RAND.TEST           \ CHI-SQUARE TEST

  FILL.RAND.TEST
  0 INTERVAL.ARRAY :=

  301 1 DO
```

```
     RAND.ARRAY [ I ] 0.05 + 10 * INDEX :=
     INTERVAL.ARRAY [ INDEX ] 1 + INTERVAL.ARRAY [ INDEX ] :=
   LOOP


   0 CHI.VAL :=

   10 1 +     1 DO
     INTERVAL.ARRAY [ I ] 30 - DUP * 30.0 /
     CHI.VAL +   CHI.VAL :=
     CHI.VAL . CR
   LOOP

  ."     CHI VALUE:" CHI.VAL .

;

: T.TEST \ RUN  SEVERAL TIMES AND SEE IF THE MEAN IS 0

    0 MISC :=
    0 MISCN :=
    0 AVE.MEAN :=
    0 AVE.T :=

    100 1 +    1 DO
      NORMAL.TEST
      AVE AVE.MEAN + AVE.MEAN :=
      T.VAL AVE.T + AVE.T :=
      T.VAL 0 <
      IF
         T.VAL
         CASE
           -2.33  MAX   -2.33  OF   1 MISCN [ 1 ]
                                + MISCN [ 1 ] :=   ENDOF
           -1.645 MAX   -1.645 OF   1 MISCN [ 2 ]
                                + MISCN [ 2 ] :=   ENDOF
           -1.28  MAX   -1.28  OF   1 MISCN [ 3 ]
                                + MISCN [ 3 ] :=   ENDOF
           1 MISCN [ 4 ] + MISCN [ 4 ] :=
         ENDCASE
      ELSE
         T.VAL
         CASE
           2.33  MIN   2.33  OF   1 MISC [ 1 ]
                              + MISC [ 1 ] :=   ENDOF
           1.645 MIN   1.645 OF   1 MISC [ 2 ]
                              + MISC [ 2 ] :=   ENDOF
           1.28  MIN   1.28  OF   1 MISC [ 3 ]
                              + MISC [ 3 ] :=   ENDOF
           1 MISC [ 4 ] + MISC [ 4 ] :=
         ENDCASE
     THEN
   LOOP

   CR  ." MISCN01 " MISCN [ 1 ] .
```

```
     CR  ." MISCN05 " MISCN [ 2 ] .
     CR  ." MISCN1  " MISCN [ 3 ] .
     CR  ." MISCN   " MISCN [ 4 ] .
     CR  ." MISC    " MISC  [ 4 ] .
     CR  ." MISC1   " MISC  [ 3 ] .
     CR  ." MISC05  " MISC  [ 2 ] .
     CR  ." MISC01  " MISC  [ 1 ] .

     AVE.MEAN 100 / AVE.MEAN :=
     CR  ." MEAN " AVE.MEAN .

     AVE.T 100 / AVE.T :=
     CR  ." AVE.T " AVE.T .
;


: CHI.TEST \ RUN SEVERAL TIMES AND SEE IF THE VALUES
          \ ARE LIKE CHI-SQUARE DISTRIBUTION

    0 MISC :=
    0 MISC01 :=
    0 MISC05 :=
    0 MISC1 :=

    100 1 +     1 DO
      RAND.TEST
      CHI.VAL

      CASE
         21.7 MIN   21.7 OF   1 MISC01 + MISC01 :=    ENDOF
         16.9 MIN   16.9 OF   1 MISC05 + MISC05 :=    ENDOF
         14.7 MIN   14.7 OF   1 MISC1  + MISC1  :=    ENDOF

         1 MISC + MISC :=
      ENDCASE

   LOOP

   CR CR
   CR  ." MISC01 " MISC01 . CR
   CR  ." MISC05 " MISC05 . CR
   CR  ." MISC1  " MISC1 . CR
   CR  ." MISC   " MISC  . CR

;
```

Appendix L

Signal-to-Noise Ratios for Correlation Noise with Different Decision Sequences (DS) and Length Proportions (LP)

DS	LP	CL	CC	HT	FFT
2	1x	477	-	-	3.4*
2	2x	477	2.0	2.8	4.0
2	3x	477	4.0	3.5	-
2	4x	477	4.5	3.7	5.0
2	8x	477	6.7	4.2	-
2	16x	477	13.3	7.0	-
3	1x	477	-	-	2.6*
3	2x	477	1.8	3.0	4.4
3	3x	477	3.6	5.0	-
3	4x	477	4.5	5.5	8.0
3	8x	477	6.7	11.0	-
3	16x	477	10.5	13.7	-
8	2x	477	2.8	4.0	3.7
8	4x	477	5.5	5.3	6.5
8	8x	477	5.7	5.8	-
8	16x	477	6.7	-	-

* - indicates that not all peaks were distinguishable from noise.

Appendix M

Signal-to-Noise Ratios for Correlation Noise with Different Decision Sequences (DS), Single Chromatogram Lengths (CL) and Length Proportions (LP)

DS	LP	EL	CL	CC	HT	FFT
1	2x	64	32	1.3	1.5	1.6
1	3x	96	32	1.5	1.6	-
1	4x	128	32	2.0	2.0	2.9
1	8x	256	32	2.4	2.8	3.3
1	16x	512	32	3.0	3.7	5.0
9	4x	512	128	2.4	2.5	3.6
9	8x	1024	128	2.8	3.2	4.7
3	1x	477	477	-	-	2.6*
3	2x	954	477	1.8	3.0	4.4
3	3x	1431	477	3.6	5.0	-
3	4x	1908	477	4.5	5.5	8.0
3	8x	3816	477	6.7	11.0	-
3	16x	7632	477	10.5	13.7	-

* - indicates that not all peaks were distinguishable from noise.

Appendix N

Signal-to-Noise Ratios for Correlation Noise with Different Decision Sequences (DS)

DS	LP	CL	CC	HT	FFT
2	4x	477	4.5	3.7	5.0
3	4x	477	4.5	5.5	8.0
4	4x	477	3.1	4.0	6.9
5	4x	477	4.0	4.8	7.7
6	4x	477	4.2	3.7	5.5
7	4x	477	5.0	4.0	6.5
8	4x	477	5.5	5.3	6.5
AVE			4.00	4.43	6.59

Appendix O

Signal-to-Noise Ratios for White Noise with Different Noise Magnitudes (NM)

DS	LP	CL	NM	ADDED S/N	CC	HT	FFT
8	4x	477	0	0.0	5.5	5.3	6.5
8	4x	477	1	0.5	4.0	3.7	4.8
8	4x	477	2	0.25	2.8	2.8	3.7
8	4x	477	4	0.125	1.3	1.6	1.5
8	4x	477	4	0.125	*	1.1*	1.3*
8	4x	477	10	0.05	*	*	*
8	4x	477	2	0.25	3.4	3.5	-
8	4x	477	4	0.125	1.7	2.3	-
8	16x	477	1	0.5	5.0	-	-
8	16x	477	2	0.25	3.6	-	-
8	16x	477	4	0.125	2.0	-	-

* indicates chromatogram looks like noise.
Note: each line represents a different set of random numbers used.

Appendix P

Signal-to-Noise Ratios When Drift Is Added to Multiplex Chromatogram

DS	LP	CL	DF	DRIFT RATE	DRIFT REDUCED	CC	HT	FFT
8	2x	477	0.0	0		2.8	4.0	3.7
8	2x	477	0.5	4		2.8	3.8	3.7
8	2x	477	5.0	10		2.0	3.0	1.3*
8	4x	477	0.0	0		5.5	5.3	6.5
8	4x	477	0.5	2		3.6	4.0	4.8
8	4x	477	1.0	4		3.0	4.0	4.1
8	4x	477	1.0	4	X	4.0	3.7	3.5

* indicates chromatogram looks like noise.

Note: X indicates that the drift was reduced in the MC before CC, HT or FFT were calculated. DF is drift factor parameter.