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Program Documentation for the Gas Chromatography Automation System

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February 1980

PROGRAM DOCUMENTATION FOR THE GAS CHROMATOGRAPHY AUTOMATION SYSTEM

by

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FOREWORD

Environmental measurements are required to determine the quality of ambient waters and the character of waste effluents. The Environmental Monitoring and Support Laboratory - Cincinnati, conducts research to:

- Develop and evaluate techniques to measure the presence and concentration of physical, chemical, and radiological pollutants in water, wastewater, bottom sediments, and solid waste.

- Investigate methods for the concentration, recovery, and identification of viruses, bacteria and other microbiological organisms in water, and to determine the responses of aquatic organisms to water quality.

- Develop and operate an Agency-wide quality assurance program to assure standardization and quality control of systems for monitoring water and wastewater.

- Develop and operate a computerized system for instrument automation leading to improved data collection, analysis, and quality control.

This report was developed in the Advanced Instrumentation Section of the Environmental Monitoring and Support Laboratory in the interest of advancing laboratory techniques and quality control through computerization.

Dwight G. Ballinger
Director
Environmental Monitoring and Support
Laboratory - Cincinnati

ABSTRACT

This book contains complete documentation for the 22 programs of the EPA Gas Chromatography Automation System (GCAS). The GCAS is a system which accepts information from a commercially available chromatography data system and performs multi-point calibration, calculation of concentrations, identification of compounds, calculation of relative retention times or capacity ratios, calculation of EPA standard quality control statistics, calculation of replicate statistics, dissimilar analysis confirmation, and reporting of results to the Sample File Control System.

The programs of the GCAS are written in Data General Extended BASIC, Revision 4.3, under the operating system RDOS, Revision 6.2. In this document, there is a functional description, a functional flowchart, a symbol definition table, a program listing, and a symbol cross reference table for each of the programs. The structure of all data files is also completely described.

This report was submitted in partial fulfillment of Task No. 79-219 by the SouthWestern Ohio Regional Computer Center of the University of Cincinnati. It covers work done between January 10, 1979, and May 31, 1979, and work was completed as of May 31, 1979.

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SECTION 1

INTRODUCTION

The Gas Chromatography Automation System (GCAS) is a set of 22 computer programs which perform extensive processing of data from a commercially available chromatography data system. This book contains complete technical documentation for the programs. Two other related publications contain the functional specifications and user's guide for the GCAS.

The GCAS is written in Data General Extended BASIC, Revision 4.3, under the operating system RDOS, Revision 6.2. The 22 programs are named GC00 through GC21. The chaining relationships and functions of these programs are shown in Figure 1.

One special consideration which adds significant bulk to the GCAS is that the system handles all errors and escapes without reverting to BASIC command level. This protects the integrity of the system by not allowing any user to perform any unauthorized functions. It also makes the system easy to use by catching human errors, explaining them, and repeating the relevant questions.

The GCAS is designed to be enhanced as more advanced techniques are developed. For example, although the system accepts data only from a Varian 220L Chromatography Data System, a carefully designed replacement for program GC21 would allow the GCAS to be used with a different commercial system. Furthermore, the internal standards calibration method can be added to the GCAS by implementing programs GC03 and GC08. This document contains all information necessary for the maintenance and enhancement of the GCAC.

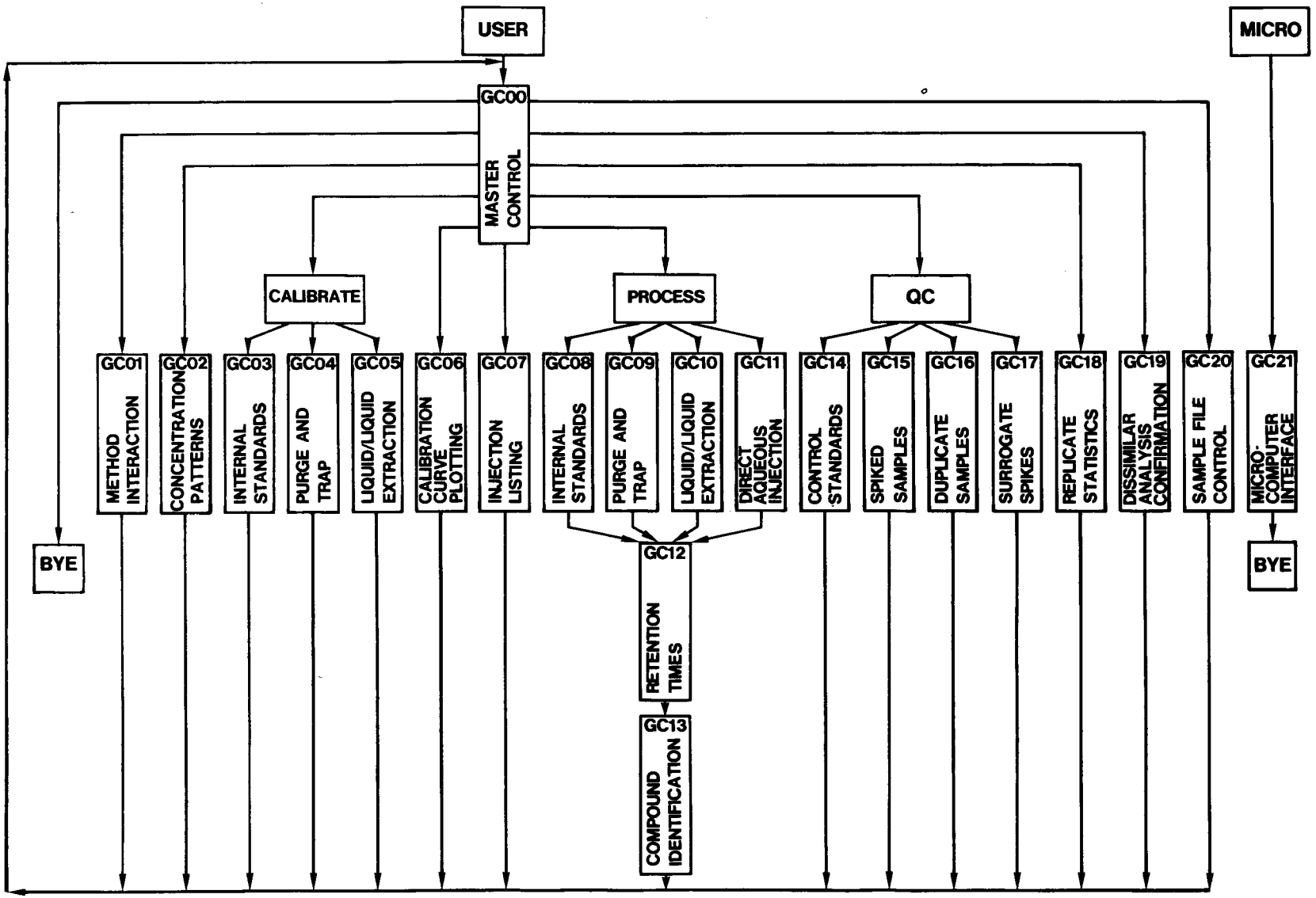

Figure 1. Program modules and their chaining relationships.

SECTION 2

PROGRAM GC00 - MASTER CONTROL

GC00 is the master control program of the Gas Chromatography Automation System. It is entered by chaining from INITIALIZE or any of the other GC programs.

The main function of GC00 is to invoke the other programs at the option of the user. For most of the options, GC00 chains directly to the appropriate program. For calibration or processing, the program reads the type of method (internal standards, purge and trap, etc.) from the method file and then chains to the appropriate program. For quality control statistics, the program gives the user a choice of four types of quality control and then branches to the appropriate program.

GC00 also opens the method file and leaves it open when it chains to another program. Furthermore, the method file remains open when the other programs chain back to GC00. More precisely, GC00 opens the method file when it is first entered from INITIALIZE, GC01, or GC19, but not chaining to GC01 or GC19. It closes the method file when it 1) chains to GC01 or GC19, 2) chains to the Sample File Control programs RUNEDIT or SEND, or 3) logs off from the Nova.

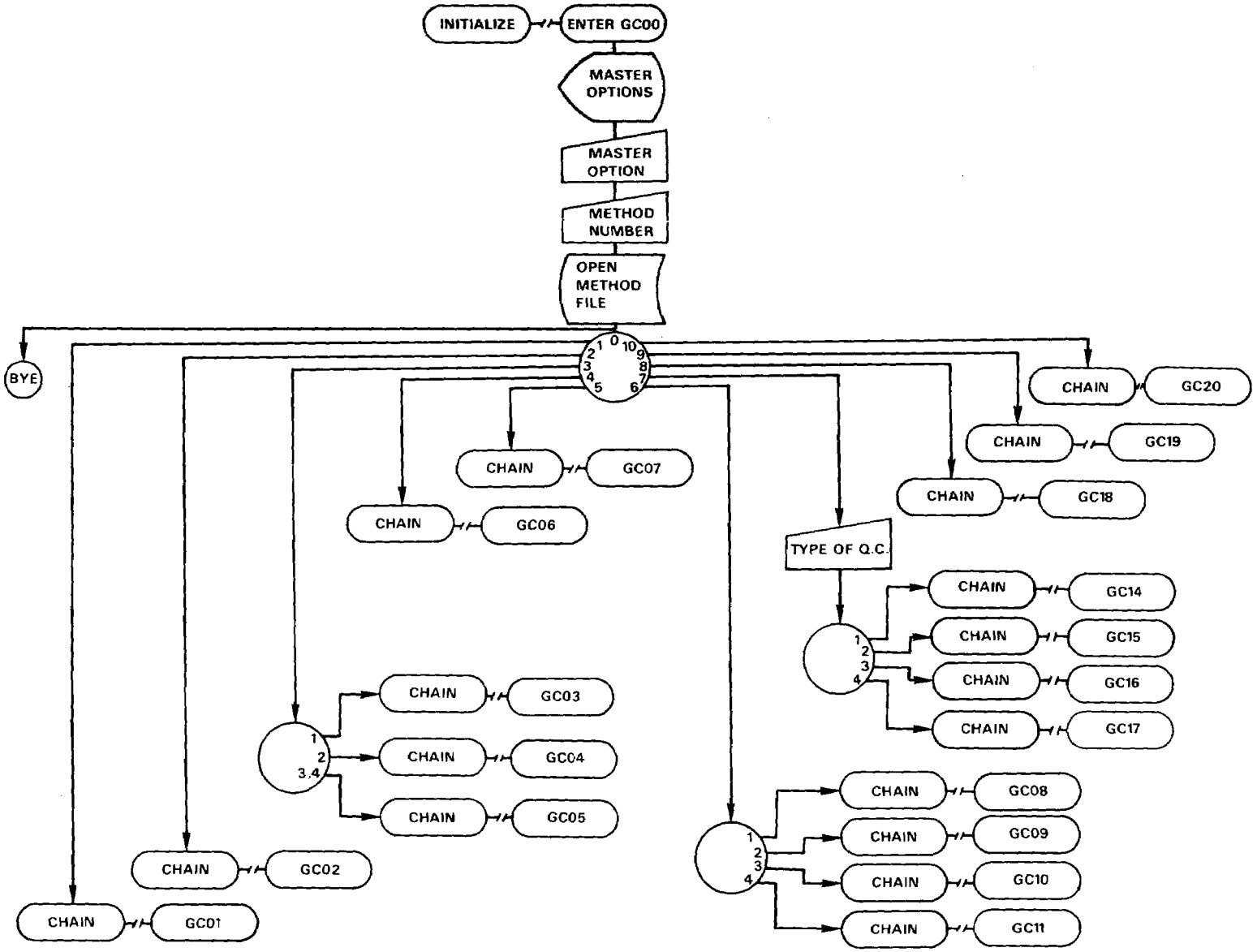

Figure 2. Flowchart of Program GC00.

TABLE 1. SYMBOL DEFINITIONS FOR PROGRAM GCOO

N1	the type of calibration and processing N1=1 internal standards N1=2 purge and trap N1=3 liquid/liquid extraction N1=4 direct aqueous injection
T	the number of the method
T$	the name of the method file
U$	the name of the user
V	a flag for keeping track of the method file V=0 a method file is open V=1 no method file is open
X	the user's answer to multiple choice questions
X$	the user's answer to a Y or N question

PROGRAM LISTING FOR GC00

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                      +
0030 REM   +   PROGRAM GC00, MASTER CONTROL                             +
0040 REM   +   BY:  J. KOPKE (SWORCC), JANUARY 10, 1979                 +
0050 REM   +   MOST RECENT REVISION:  APRIL 16, 1979                    +
0060 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0070 REM
0080 LET V=0
0090 GOTO 0110
0100 LET V=1
0110 ON ESC THEN GOTO 0280
0120 ESC
0125 PAGE =74
0126 GOTO 0280
0130 PRINT
0140 PRINT
0150 PRINT "THESE ARE THE MASTER OPTIONS:"
0160 PRINT
0170 PRINT "     0.  SIGN OFF"
0180 PRINT "     1.  METHOD INTERACTION"
0190 PRINT "     2.  CONCENTRATION PATTERN INTERACTION"
0200 PRINT "     3.  CALIBRATION"
0210 PRINT "     4.  CALIBRATION CURVE PLOTTING"
0220 PRINT "     5.  INJECTION LISTING"
0230 PRINT "     6.  PROCESSING"
0240 PRINT "     7.  QUALITY CONTROL"
0250 PRINT "     8.  REPLICATE STATISTICS"
0260 PRINT "     9.  DISSIMILAR ANALYSIS CONFIRMATION"
0270 PRINT "    10.  SAMPLE FILE CONTROL"
0275 GOTO 0285
0280 PRINT
0285 PRINT
0290 TIME =120
0300 ON ERR THEN GOTO 0340
0310 TINPUT "WHICH MASTER OPTION DO YOU WANT TO USE?  (0-10, OR 'RETUR
*    N' FOR HELP)  ",X$
0320 ON ERR THEN STOP
0325 IF LEN(X$)=0 THEN GOTO 0140
0326 ON ERR THEN GOTO 0405
0327 LET X=VAL(X$)
0328 ON ERR THEN STOP
0330 GOTO 0360

12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```


PROGRAM LISTING FOR GC00

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0340 ON ERR THEN STOP
0350 IF SYS(7)=60 THEN GOTO 0370
0360 IF X<>0 THEN GOTO 0400
0370 PRINT
0380 PRINT "YOU ARE BEING SIGNED OFF FROM THE NOVA BY THIS PROGAM."
0385 CLOSE
0390 BYE
0400 IF X=INT(X) THEN IF X>0 THEN IF X<11 THEN GOTO 0460
0405 ON ERR THEN STOP
0410 PRINT
0420 PRINT "<7><7>";X$;" IS NOT A VALID OPTION NUMBER."
0430 GOTO 0140
0440 REM  ------------------------------------------------------------
0450 REM          OPEN THE METHOD FILE
0460 IF V<>1 THEN GOTO 0770
0470 IF X=1 THEN GOTO 0770
0480 IF X=9 THEN GOTO 0770
0490 PRINT
0500 ON ERR THEN GOTO 0520
0510 INPUT "WHAT IS THE NUMBER OF THE METHOD YOU WANT TO USE?  ",T
0520 ON ERR THEN STOP
0530 IF T=ABS(INT(T)) THEN IF T<=9999 THEN GOTO 0570
0540 PRINT
0550 PRINT "<7><7>";T;"IS NOT A VALID METHOD NUMBER."
0560 GOTO 0490
0570 LET T$="GC0000"
0580 LET T$[7-LEN(STR$(T)),6]=STR$(T)
0590 ON ERR THEN GOTO 0610
0600 RENAME T$,T$
0610 ON ERR THEN STOP
0620 IF SYS(7)<>-48 THEN GOTO 0650
0630 DELAY =1
0640 GOTO 0590
0650 IF SYS(7)=-9 THEN GOTO 0690
0660 PRINT
0670 PRINT "<7><7>THERE IS NO EXISTING METHOD WITH THE NUMBER ";T$[3,6
*    ];"."
0680 GOTO 0490
0690 ON ERR THEN GOTO 0730
0700 OPEN FILE[4,0],T$,200
0710 ON ERR THEN STOP
0720 GOTO 0770

12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

PROGRAM LISTING FOR GC00

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0730 ON ERR THEN STOP
0740 DELAY =1
0750 GOTO 0690
0770 ON X THEN GOTO 0800, 0850, 0890, 0960, 1000, 1040, 1120, 1350, 13
#    90, 1440
0780 REM  ------------------------------------------------------------
0790 REM          INTERACT WITH METHOD
0800 CLOSE
0810 NOESC
0820 CHAIN "GC01"
0830 REM  ------------------------------------------------------------
0840 REM          INTERACT WITH CONCENTRATION PATTERNS
0850 NOESC
0860 CHAIN "GC02"
0870 REM  ------------------------------------------------------------
0880 REM          CALIBRATE
0890 NOESC
0895 READ FILE[4,1],T$,U$,N1
0900 ON N1 THEN GOTO 0910, 0920, 0930, 0930
0910 CHAIN "GC03"
0920 CHAIN "GC04"
0930 CHAIN "GC05"
0940 REM  ------------------------------------------------------------
0950 REM          EXAMINE CALIBRATION CURVES
0960 NOESC
0970 CHAIN "GC06"
0980 REM  ------------------------------------------------------------
0990 REM          LIST EXTANT INJECTIONS
1000 NOESC
1010 CHAIN "GC07"
1020 REM  ------------------------------------------------------------
1030 REM          PROCESS INJECTIONS
1040 NOESC
1045 READ FILE[4,1],T$,U$,N1
1050 ON N1 THEN GOTO 1060, 1070, 1080, 1090
1060 CHAIN "GC08"
1070 CHAIN "GC09"
1080 CHAIN "GC10"
1090 CHAIN "GC11"
1100 REM  ------------------------------------------------------------
1110 REM          CALCULATE QUALITY CONTROL STATISTICS
1120 PRINT
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```


PROGRAM LISTING FOR GC00

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
1130 PRINT "THESE ARE THE TYPES OF QUALITY CONTROL STATISTICS:"
1140 PRINT
1150 PRINT "     1.  CONTROL (CHECK) STANDARDS"
1160 PRINT "     2.  SPIKED SAMPLES"
1170 PRINT "     3.  DUPLICATE SAMPLES"
1180 PRINT "     4.  SURROGATE SPIKES"
1190 PRINT
1200 ON ERR THEN GOTO 1220
1210 INPUT "WHICH TYPE DO YOU WANT TO USE?  (1, 2, 3, OR 4)  ",X
1220 ON ERR THEN STOP
1230 IF X=INT(X) THEN IF X>0 THEN IF X<5 THEN GOTO 1270
1240 PRINT
1250 PRINT "<7><7>";X;"IS NOT A VALID TYPE NUMBER."
1260 GOTO 1120
1270 NOESC
1280 ON X THEN GOTO 1290, 1300, 1310, 1320
1290 CHAIN "GC14"
1300 CHAIN "GC15"
1310 CHAIN "GC16"
1320 CHAIN "GC17"
1330 REM  ------------------------------------------------------------
1340 REM          CALCULATE REPLICATE STATISTICS
1350 NOESC
1360 CHAIN "GC18"
1370 REM  ------------------------------------------------------------
1380 REM          PERFORM DISSIMILAR ANALYSIS CONFIRMATION
1390 CLOSE
1400 NOESC
1410 CHAIN "GC19"
1420 REM  ------------------------------------------------------------
1430 REM          REPORT RESULTS TO SAMPLE FILE CONTROL
1440 NOESC
1450 CHAIN "GC20"
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

SYMBOL TABLE FOR GC00

SYMBOL	REFERENCES			
0110	0090			
0140	0325	0430		
0280	0110	0126		
0285	0275			
0340	0300			
0360	0330			
0370	0350			
0400	0360			
0405	0326			
0460	0400			
0490	0560	0680		
0520	0500			
0570	0530			
0590	0640			
0610	0590			
0650	0620			
0690	0650	0750		
0730	0690			
0770	0460	0470	0480	0720
0800	0770			
0850	0770			
0890	0770			
0910	0900			
0920	0900			
0930	0900			
0960	0770			
1000	0770			
1040	0770			
1060	1050			
1070	1050			
1080	1050			
1090	1050			
1120	0770	1260		
1220	1200			
1270	1230			
1290	1280			
1300	1280			
1310	1280			
1320	1280			
1350	0770			
1390	0770			
1440	0770			
FL#4	0700	0895	1045	
N1	0895	0900	1045	1050
T	0510	0530	0550	0580

SYMBOL TABLE FOR GC00

SYMBOL	REFERENCES									
T$	0570	0580	0600	0670	0700	0895	1045			
U$	0895	1045								
V	0080	0100	0460							
X	0327	0360	0400	0470	0480	0770	1210	1230	1250	1280
X$	0310	0325	0327	0420						

SECTION 3

PROGRAM GC01 - METHOD INTERACTION

GC01 is the program which generates, modifies, deletes, and displays GCAS method files. This program is entered by chaining from GC00 (the master control program), and it chains back to that program if the escape key is pressed.

As GC01 begins, it displays the four types of method interactions which are possible, inputs the user's choice, and then branches to the appropriate section of code.

GENERATE A NEW METHOD

To generate a new method, GC01 first inputs the method number. If the specified method number is not a positive integer of four or fewer digits, a message is printed telling the user that the method number is invalid. The program then creates the name of the method file and attempts to rename that file with its own name. This step always causes an error which is trapped. If the error number is -9, there is already a method file in existence with the specified number. The user is informed of this fact, and the program branches back to the original four choices.

If the specified method number is usable, the program inputs the name of the user, the type of calibration and processing, the type of retention time calculations, and either the relative retention time reference identifier or the dead volume time. These items are written into the first record of the method file. The program then inputs the identifiers, the true names of compounds, and CAS Registry numbers for the method and writes these into the method file. When the user types the word "END" as an identifier, the program closes the method file and asks if the method should be displayed. If the user wants to have the method displayed, the program branches to that routine. Otherwise, it chains back to GC00.

MODIFY AN EXISTING METHOD

If a user wants to modify a method, this program asks for the method number. It checks whether the method number is reasonable and whether the method file already exists, as described above. It then presents four types of modifications, inputs the user's choice, and branches to the appropriate section of code.

Add Another Identifier

If the user wants to modify the method by adding another identifier, the program simply locates the end of the method file and then branches to the section for generating a new method. That section then appends additional identifiers to the method file. All of the concentration pattern files for the method are deleted.

Delete an Identifier

If the user wants to delete an identifier, the program inputs the identifier and searches through the method file for it. If the specified identifier is not in the method file, a message to that effect is printed. If the specified identifier is found in the method file, it is replaced by the dummy entry "99999." After either circumstance, the program asks whether the user wants to deal further with any method, and then either branches back to the original four choices in this program or chains back to GC00.

Add Another Compound to an Identifier

If the user wants to add another compound to the list of those associated with an identifier, this program first inputs the identifier and searches for it in the method file. If there is no matching identifier in the method file, or if the specified identifier already has the limit of three compounds associated with it, an appropriate message is printed. Otherwise, the additional compound name and CAS number are input and written into the method file. Then the program asks whether the user wants to deal further with any method, and it branches accordingly.

Change Retention Time Data

If the user wants to change retention time data, this section of code provides the choice of relative retention time or capacity ratio calculations. If the user selects relative retention time, the program asks for the identifier of the compound to whose retention time all others are relative. If the user selects capacity ratio, the program asks for the dead volume time. In either case, the data items are written into the method file.

DELETE AN EXISTING METHOD

If the user wants to delete an existing method, this program inputs the method number and checks whether the number is reasonable and whether the corresponding method file actually exists. If the file does exist, it is deleted and that event is confirmed to the user. Also, all of the concentration pattern files for the method are deleted. The program then asks if the user wants to deal further with any method and branches accordingly.

DISPLAY AN EXISTING METHOD

If the user wants to display an existing method, this program again inputs the method number and checks whether the corresponding method file actually exists. It then prints headings and the compound identification information from the method file. The program then asks if the user wants to deal further with any method and branches accordingly.

SUBROUTINE TO CHECK CAS NUMBERS

Whenever a user enters a CAS Registry number, GC01 branches to this subroutine to check whether the number is reasonable. A carriage return alone is always accepted as a valid CAS number. The subroutine does not check whether the CAS number is the correct number for the compound named; it only checks the form of the number.

CAS Registry numbers are always of the form

$$d_8d_7d_6d_5d_4d_3\text{-}d_2d_1\text{-}d_0$$

where d_n is a numeric digit. Any of the digits d_4 through d_8 may be blanks, although no embedded blanks are allowed. The positions of the hyphens never vary. Digit d_0 is a check digit which is used to verify that the number has been typed correctly. The check digit is the remainder from the following division:

$$\frac{\sum_{i=1}^{8} i\cdot(d_i)}{10}$$

In this subroutine, the CAS number typed by the user is first padded on the left with spaces until it is 11 characters long. Then if the seventh and tenth characters are not hyphens, the number is immediately identified as invalid. If the hyphens are in the correct positions, the subroutine begins the calculation for the check digit. In doing this, the subroutine must convert each digit from a string to a number. If there is any non-numeric character in the CAS number, an error results, and the number is invalid. Finally, if the calculated check digit does not match the input check digit, the CAS number is invalid. Valid CAS numbers are returned to the invoking procedure changed only by having been padded with blanks. Invalid CAS numbers are changed to "99999" before being returned to the invoking procedure. If the main program finds that a returning CAS number is "99999," it prints an error message and asks for another CAS number.

SUBROUTINE TO CHANGE SLASHES TO COMMAS

The names of many chemical compounds have commas in them, but BASIC does not allow commas to be part of an answer to an INPUT statement. Therefore, this program is set up to allow the user to type a slash where a commas is needed in an identifier or in the name of a compound, and this subroutine substitutes a comma for every slash.

SUBROUTINE TO DELETE CONCENTRATION PATTERNS

This subroutine simply loops through the 26 possible concentration pattern file names, and deletes them all.

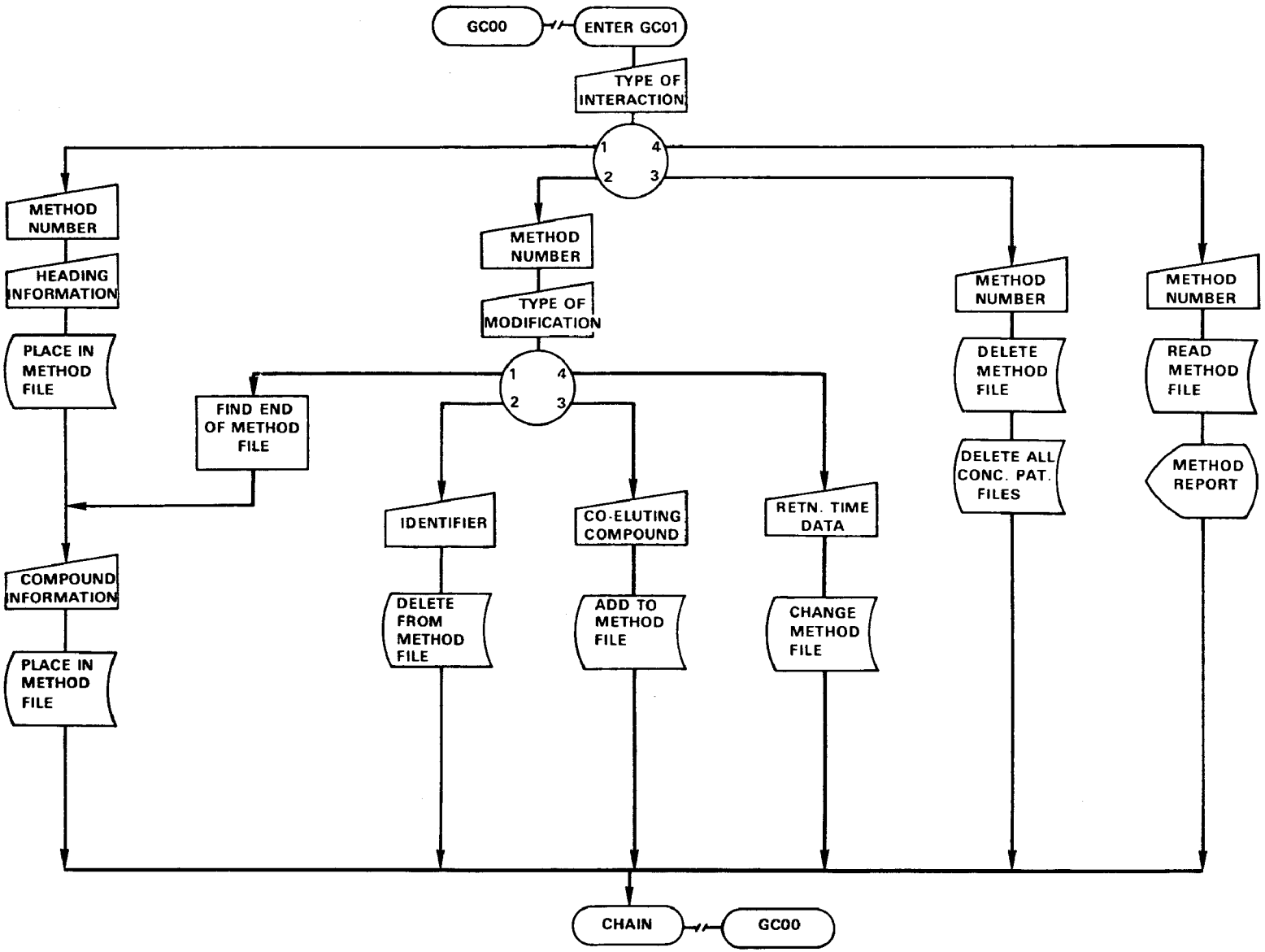

Figure 3. Flowchart of Program GC01.

TABLE 2. SYMBOL DEFINITIONS FOR PROGRAM GC01

A6$	the name of a concentration pattern file
I	a record number counter and control variable for loops
I2	the control variable for loops
I3	the total in check digit calculations
I4	the control variable for a loop
J	the line number in method displays
N$	the identifier for the compound to whose retention time all others are relative, or the dead volume time
N1	the type of method N1=1 internal standards N1=2 purge and trap N1=3 liquid/liquid extraction N1=4 direct aqueous injection
N2	the type of retention time calculations N2=1 relative retention time N2=2 capacity ratio
T	the method number
T$	the name of the method file
U$	the user's name
V	the number of compounds associated with an identifier
V$	an identifier
V1$	the first compound associated with an identifier
V2$	the CAS number for V1$
V3$	the second compound associated with an identifier

TABLE 2. (continued)

V4$	the CAS number for V3$
V5$	the third compound associated with an identifier
V6$	the CAS number for V5$
V7$	the identifier to be modified
V8$	the additional compound to be associated with an identifier
V9$	the CAS number for V8$
W3$	a CAS number being sent to the subroutine
W4$	a CAS number padded with a space
X	the user's answer to a multiple choice question
X$	the user's answer to Y or N questions
X4	a dummy variable
X5	a dummy variable
Z5	the position of a slash in Z5$
Z5$	a string being sent to the subroutine to change slashes to commas

PROGRAM LISTING FOR GC01

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                      +
0030 REM   +   PROGRAM GC01, METHOD GENERATION                          +
0040 REM   +   BY:  J. KOPKE (SWORCC), JANUARY 26, 1979                 +
0045 REM   +   MOST RECENT REVISION:  MARCH 26, 1979                    +
0050 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0060 REM
0070 ESC
0080 ON ESC THEN GOTO 4000
0090 DIM T$[6],U$[30],V$[8],V1$[40],V2$[11],V3$[40],V4$[11],V5$[40]
0100 DIM V6$[11],V7$[8],V8$[40],V9$[11],X$[3],W3$[11],W4$[11],N$[8]
0101 DIM Z5$[40],A6$[9]
0110 PRINT
0120 PRINT "HERE ARE THE TYPES OF METHOD INTERACTIONS:"
0130 PRINT
0140 PRINT "     1.  GENERATE A NEW METHOD"
0150 PRINT "     2.  MODIFY AN EXISTING METHOD"
0160 PRINT "     3.  DELETE AN EXISTING METHOD"
0170 PRINT "     4.  DISPLAY AN EXISTING METHOD"
0180 PRINT
0189 ON ERR THEN GOTO 0191
0190 INPUT "WHICH TYPE DO YOU WANT TO USE?  (1, 2, 3, OR 4)  ",X
0191 ON ERR THEN STOP
0200 ON X THEN GOTO 0260, 1750, 3120, 3370
0210 PRINT
0220 PRINT "<7><7>";X;"IS NOT A VALID TYPE NUMBER."
0230 GOTO 0110
0240 REM   ------------------------------------------------------------
0250 REM          GENERATE A NEW METHOD
0260 PRINT
0269 ON ERR THEN GOTO 0271
0270 INPUT "WHAT SHOULD BE THE NUMBER FOR THE NEW METHOD?  ",T
0271 ON ERR THEN STOP
0280 IF T=INT(ABS(T)) THEN IF T<=9999 THEN GOTO 0320
0290 PRINT
0300 PRINT "<7><7>";T;"IS NOT A VALID METHOD NUMBER."
0310 GOTO 0260
0320 LET T$="GC0000"
0330 LET T$[7-LEN(STR$(T)),6]=STR$(T)
0340 ON ERR THEN GOTO 0360
0350 RENAME T$,T$
0360 ON ERR THEN STOP
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```


PROGRAM LISTING FOR GC01

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0370 IF SYS(7)<>-48 THEN GOTO 0400
0380 DELAY =1
0390 GOTO 0340
0400 IF SYS(7)<>-9 THEN GOTO 0480
0410 PRINT
0420 PRINT "<7><7>THERE IS AN EXISTING METHOD WITH THE NUMBER ";T$[3,6
*    ];"."
0430 PRINT "YOU MAY MODIFY METHOD ";T$[3,6];", OR YOU MAY DELETE IT AN
*    D THEN"
0440 PRINT "     GENERATE A NEW METHOD USING ";T$[3,6];" AS THE METHOD
*     NUMBER."
0450 PRINT "     HOWEVER, YOU MAY NOT GENERATE A SECOND METHOD WITH TH
*    E"
0460 PRINT "     SAME METHOD NUMBER."
0470 GOTO 0110
0480 OPEN FILE[4,0],T$,200
0490 ON ESC THEN GOTO 0510
0500 GOTO 0560
0510 CLOSE FILE[4]
0520 PRINT
0530 PRINT "<7><7>METHOD ";T$[3,6];" HAS BEEN DELETED BECAUSE IT WAS I
*    NCOMPLETE."
0540 DELETE T$
0550 GOTO 4000
0560 PRINT
0570 ON ERR THEN GOTO 0590
0580 INPUT "WHAT IS YOUR NAME?  ",U$
0581 ON ERR THEN STOP
0582 LET Z5$=U$
0583 GOSUB 4370
0584 LET U$=Z5$
0585 GOTO 0600
0590 ON ERR THEN STOP
0591 PRINT
0592 PRINT "<7><7>USE A SLASH (/) WHERE YOU WANT A COMMA."
0593 GOTO 0560
0600 PRINT
0610 PRINT "HERE ARE THE TYPES OF METHODS:"
0620 PRINT
0630 PRINT "     1.  INTERNAL STANDARDS"
0640 PRINT "     2.  PURGE AND TRAP"
0650 PRINT "     3.  LIQUID/LIQUID EXTRACTION"
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

PROGRAM LISTING FOR GC01

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0660 PRINT "     4.  DIRECT AQUEOUS INJECTION"
0670 PRINT
0679 ON ERR THEN GOTO 0681
0680 INPUT "WHICH TYPE DO YOU WANT TO USE?  (1, 2, 3, OR 4)  ",N1
0681 ON ERR THEN STOP
0690 IF INT(ABS(N1))=N1 THEN IF N1>0 THEN IF N1<5 THEN GOTO 0730
0700 PRINT
0710 PRINT "<7><7>";N1;"IS NOT A VALID TYPE NUMBER."
0720 GOTO 0600
0730 PRINT
0740 PRINT "HERE ARE THE TYPES OF RETENTION TIME CALCULATIONS:"
0750 PRINT
0760 PRINT "     1.  RELATIVE RETENTION TIME"
0770 PRINT "     2.  CAPACITY RATIO"
0780 PRINT
0789 ON ERR THEN GOTO 0791
0790 INPUT "WHICH TYPE DO YOU WANT TO USE?  (1 OR 2)  ",N2
0791 ON ERR THEN STOP
0800 PRINT
0810 IF N2=1 THEN GOTO 0850
0820 IF N2=2 THEN GOTO 0880
0830 PRINT "<7><7>";N2;"IS NOT A VALID TYPE NUMBER."
0840 GOTO 0730
0850 PRINT "WHAT IS THE IDENTIFIER FOR THE REFERENCE COMPOUND FOR"
0851 ON ERR THEN GOTO 0860
0852 INPUT "     RELATIVE RETENTION TIMES?  ",N$
0853 ON ERR THEN STOP
0854 LET Z5$=N$
0855 GOSUB 4370
0856 LET N$=Z5$
0857 GOTO 0890
0860 ON ERR THEN STOP
0861 PRINT
0862 PRINT "<7><7>USE A SLASH (/) WHERE YOU WANT A COMMA."
0863 PRINT
0864 GOTO 0850
0880 ON ERR THEN GOTO 0882
0881 INPUT "WHAT IS THE DEAD VOLUME TIME, IN SECONDS?  ",N$
0882 ON ERR THEN GOTO 0886
0883 LET X4=VAL(N$)
0884 ON ERR THEN STOP
0885 GOTO 0890
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```


PROGRAM LISTING FOR GC01

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0886 ON ERR THEN STOP
0887 PRINT
0888 PRINT "<7><7>";N$;" IS NOT A VALID DEAD VOLUME TIME."
0889 GOTO 0800
0890 WRITE FILE[4,1],T$,U$,N1,N2,N$
0900 GOTO 0910
0910 LET I=1
0920 PRINT
0930 PRINT "ENTER THE FOLLOWING COMPOUND IDENTIFICATION INFORMATION."
0940 PRINT "USE A SLASH (/) WHERE YOU WANT A COMMA."
0950 PRINT "TYPE 'END' AS AN IDENTIFIER TO TERMINATE THE LIST."
0960 IF I<=60 THEN GOTO 1010
0970 PRINT
0980 PRINT "<7><7>YOU HAVE ENTERED 60 IDENTIFIERS, WHICH IS THE LIMIT"
0990 PRINT "     FOR THIS PROGRAM."
1000 GOTO 1660
1010 LET V3$="99999"
1020 LET V4$="99999"
1030 LET V5$="99999"
1040 LET V6$="99999"
1050 PRINT
1060 ON ERR THEN GOTO 1080
1070 INPUT "IDENTIFIER?  ",V$
1071 ON ERR THEN STOP
1072 LET Z5$=V$
1073 GOSUB 4370
1074 LET V$=Z5$
1075 GOTO 1090
1080 PRINT
1082 PRINT "<7><7>USE A SLASH (/) WHERE YOU WANT A COMMA."
1083 GOTO 1050
1090 IF V$="END" THEN GOTO 1660
1099 ON ERR THEN GOTO 1101
1100 INPUT "     NUMBER OF COMPOUNDS?  (1, 2, OR 3)  ",V
1101 ON ERR THEN STOP
1110 IF V=INT(ABS(V)) THEN IF V>0 THEN IF V<4 THEN GOTO 1170
1130 PRINT "<7><7>     ";V;"IS NOT A VALID NUMBER OF COMPOUNDS."
1150 GOTO 1100
1170 PRINT "     NAME OF ";
1180 IF V<>1 THEN PRINT "FIRST ";
1189 ON ERR THEN GOTO 1200
1190 INPUT "COMPOUND?  ",V1$
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
1191 ON ERR THEN STOP
1192 LET Z5$=V1$
1193 GOSUB 4370
1194 LET V1$=Z5$
1195 GOTO 1210
1200 ON ERR THEN STOP
1201 PRINT
1202 PRINT "<7><7>     USE A SLASH (/) WHERE YOU WANT A COMMA."
1204 GOTO 1170
1210 ON ERR THEN GOTO 1230
1220 INPUT "          CAS NUMBER?  ",V2$
1230 ON ERR THEN STOP
1240 IF LEN(V2$)=0 THEN GOTO 1320
1250 LET W3$=V2$
1260 GOSUB 4050
1270 IF W3$<>"99999" THEN GOTO 1310
1290 PRINT "<7><7>          ";V2$;" IS NOT A VALID CAS NUMBER."
1300 GOTO 1210
1310 LET V2$=W3$
1320 IF V<2 THEN GOTO 1620
1330 ON ERR THEN GOTO 1350
1340 INPUT "     NAME OF SECOND COMPOUND?  ",V3$
1341 ON ERR THEN STOP
1342 LET Z5$=V3$
1343 GOSUB 4370
1344 LET V3$=Z5$
1345 GOTO 1360
1350 ON ERR THEN STOP
1351 PRINT
1352 PRINT "<7><7>     USE A SLASH (/) WHERE YOU WANT A COMMA."
1354 GOTO 1330
1360 ON ERR THEN GOTO 1380
1370 INPUT "          CAS NUMBER?  ",V4$
1380 ON ERR THEN STOP
1390 IF LEN(V4$)=0 THEN GOTO 1470
1400 LET W3$=V4$
1410 GOSUB 4050
1420 IF W3$<>"99999" THEN GOTO 1460
1440 PRINT "<7><7>          ";V4$;" IS NOT A VALID CAS NUMBER."
1450 GOTO 1360
1460 LET V4$=W3$
1470 IF V<3 THEN GOTO 1620
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```



```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
1480 ON ERR THEN GOTO 1500
1490 INPUT "     NAME OF THIRD COMPOUND?  ",V5$
1491 ON ERR THEN STOP
1492 LET Z5$=V5$
1493 GOSUB 4370
1494 LET V5$=Z5$
1495 GOTO 1510
1500 ON ERR THEN STOP
1501 PRINT
1502 PRINT "<7><7>     USE A SLASH (/) WHERE YOU WANT A COMMA."
1504 GOTO 1480
1510 ON ERR THEN GOTO 1530
1520 INPUT "          CAS NUMBER?  ",V6$
1530 ON ERR THEN STOP
1540 IF LEN(V6$)=0 THEN GOTO 1620
1550 LET W3$=V6$
1560 GOSUB 4050
1570 IF W3$<>"99999" THEN GOTO 1610
1590 PRINT "<7><7>          ";V6$;" IS NOT A VALID CAS NUMBER."
1600 GOTO 1510
1610 LET V6$=W3$
1620 WRITE FILE[4,3*I-1],V$,V1$,V2$,V3$,V4$,V5$,V6$
1630 WRITE FILE[4,3*I],"99/99/99","",99999,99999,99999,99999,99999
1640 LET I=I+1
1650 GOTO 0960
1660 CLOSE FILE[4]
1670 PRINT
1680 ON ERR THEN GOTO 1700
1690 INPUT "DO YOU WANT TO DISPLAY THIS METHOD?  (Y OR N)  ",X$
1700 ON ERR THEN STOP
1710 IF X$[1,1]="Y" THEN GOTO 3550
1720 GOTO 4000
1730 REM  ------------------------------------------------------------
1740 REM          MODIFY AN EXISTING METHOD
1750 PRINT
1759 ON ERR THEN GOTO 1761
1760 INPUT "WHICH METHOD DO YOU WANT TO MODIFY?  ",T
1761 ON ERR THEN STOP
1770 IF ABS(INT(T))=T THEN IF T<=9999 THEN GOTO 1810
1780 PRINT
1790 PRINT "<7><7>";T;"IS NOT A VALID METHOD NUMBER."
1800 GOTO 1750
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
 1810 LET T$="GC0000"
 1820 LET T$[7-LEN(STR$(T)),6]=STR$(T)
 1830 ON ERR THEN GOTO 1850
 1840 RENAME T$,T$
 1850 ON ERR THEN STOP
 1860 IF SYS(7)<>-48 THEN GOTO 1890
 1870 DELAY =1
 1880 GOTO 1830
 1890 IF SYS(7)=-9 THEN GOTO 1950
 1900 PRINT
 1910 PRINT "<7><7>THERE IS NO EXISTING METHOD WITH THE NUMBER ";T$[3,6
*     ];"."
 1920 PRINT "NO METHOD HAS BEEN MODIFIED."
 1930 GOTO 3950
 1940 PRINT
 1950 ON ERR THEN GOTO 1990
 1960 OPEN FILE[4,0],T$,200
 1970 ON ERR THEN STOP
 1980 GOTO 2020
 1990 ON ERR THEN STOP
 2000 DELAY =1
 2010 GOTO 1950
 2020 PRINT
 2030 PRINT "HERE ARE THE TYPES OF METHOD MODIFICATION:"
 2040 PRINT
 2050 PRINT "     1.  ADD AN IDENTIFIER"
 2060 PRINT "     2.  DELETE AN IDENTIFIER"
 2070 PRINT "     3.  ADD ANOTHER CO-ELUTING COMPOUND TO THE LIST FOR A
*     N IDENTIFIER"
 2080 PRINT "     4.  CHANGE RETENTION TIME DATA"
 2090 PRINT
 2099 ON ERR THEN GOTO 2101
 2100 INPUT "WHICH TYPE TO YOU WANT TO USE?  (1, 2, 3, OR 4)  ",X
 2101 ON ERR THEN STOP
 2110 ON X THEN GOTO 2170, 2270, 2460, 2910
 2120 PRINT
 2130 PRINT "<7><7>";X;"IS NOT A VALID TYPE NUMBER."
 2140 GOTO 2020
 2150 REM  ------------------------------------
 2160 REM     ADD ANOTHER IDENTIFIER
 2170 NOESC
 2171 GOSUB 4430
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```



```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
 2172 ESC
 2173 PRINT
 2174 PRINT "ALL CONCENTRATION PATTERNS FOR METHOD ";T$[3,6];" HAVE BEE
*     N DELETED."
 2175 LET I=1
 2180 READ FILE[4,3*I-1],V$
 2190 IF EOF(4) THEN GOTO 2220
 2200 LET I=I+1
 2210 GOTO 2180
 2220 PRINT
 2230 PRINT "ENTER THE COMPOUND IDENTIFICATION INFORMATION FOR THE NEW
*     IDENTIFIER."
 2240 GOTO 0940
 2250 REM  ------------------------------------
 2260 REM     DELETE AN IDENTIFIER
 2270 PRINT
 2280 ON ERR THEN GOTO 2300
 2290 INPUT "WHICH IDENTIFIER DO YOU WANT TO DELETE?  ",V7$
 2291 ON ERR THEN STOP
 2292 LET Z5$=V7$
 2293 GOSUB 4370
 2294 LET V7$=Z5$
 2295 GOTO 2310
 2300 ON ERR THEN STOP
 2301 PRINT
 2302 PRINT "<7><7>USE A SLASH (/) WHERE YOU WANT A COMMA."
 2303 GOTO 2270
 2310 LET I=1
 2320 READ FILE[4,3*I-1],V$
 2330 IF EOF(4) THEN GOTO 2370
 2340 IF V$=V7$ THEN GOTO 2400
 2350 LET I=I+1
 2360 GOTO 2320
 2370 PRINT
 2380 PRINT "<7><7>THERE IS NO IDENTIFIER ";V7$;" IN METHOD ";T$[3,6];"
*     ."
 2390 GOTO 3930
 2400 WRITE FILE[4,3*I-1],"99999","99999","99999","99999","99999","9999
*     9","99999"
 2410 PRINT
 2420 PRINT "IDENTIFIER ";V7$;" HAS BEEN DELETED FROM METHOD ";T$[3,6]
 2430 GOTO 3930
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
2440 REM   ------------------------------------
2450 REM     ADD ANOTHER COMPOUND TO AN IDENTIFIER
2460 PRINT
2470 ON ERR THEN GOTO 2490
2480 INPUT "WHICH IDENTIFIER DO YOU WANT TO ADD TO?  ",V7$
2481 ON ERR THEN STOP
2482 LET Z5$=V7$
2483 GOSUB 4370
2484 LET V7$=Z5$
2485 GOTO 2500
2490 ON ERR THEN STOP
2491 PRINT
2492 PRINT "<7><7>USE A SLASH (/) WHERE YOU WANT A COMMA."
2493 GOTO 2460
2500 LET I=1
2510 READ FILE[4,3*I-1],V$,V1$,V2$,V3$,V4$,V5$,V6$
2520 IF EOF(4) THEN GOTO 2560
2530 IF V$=V7$ THEN GOTO 2600
2540 LET I=I+1
2550 GOTO 2510
2560 PRINT
2570 PRINT "<7><7>THERE IS NO IDENTIFIER ";V7$;" IN METHOD ";T$[3,6];"
*    ."
2580 PRINT "NO IDENTIFIER HAS BEEN CHANGED."
2590 GOTO 3930
2600 IF V5$="99999" THEN GOTO 2640
2610 PRINT
2620 PRINT "<7><7>";V7$;" ALREADY HAS THE LIMIT OF THREE CO-ELUTING CO
*    MPOUNDS."
2630 GOTO 3930
2640 PRINT
2650 ON ERR THEN GOTO 2670
2660 INPUT "WHAT IS THE NAME OF THE ADDITIONAL CO-ELUTING COMPOUND?  "
*    ,V8$
2661 ON ERR THEN STOP
2662 LET Z5$=V8$
2663 GOSUB 4370
2664 LET V8$=Z5$
2665 GOTO 2680
2670 ON ERR THEN STOP
2671 PRINT
2672 PRINT "<7><7>USE A SLASH (/) WHERE YOU WANT A COMMA."
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```



```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
2673 GOTO 2640
2680 PRINT
2690 PRINT "WHAT IS THE CAS NUMBER FOR ";V8$;
2700 ON ERR THEN GOTO 2720
2710 INPUT "?  ",V9$
2720 ON ERR THEN STOP
2730 IF LEN(V9$)=0 THEN GOTO 2810
2740 LET W3$=V9$
2750 GOSUB 4050
2760 IF W3$<>"99999" THEN GOTO 2800
2770 PRINT
2780 PRINT "<7><7>";V9$;" IS NOT A VALID CAS NUMBER."
2790 GOTO 2680
2800 LET V9$=W3$
2810 IF V3$<>"99999" THEN GOTO 2850
2820 LET V3$=V8$
2830 LET V4$=V9$
2840 GOTO 2870
2850 LET V5$=V8$
2860 LET V6$=V9$
2870 WRITE FILE[4,3*I-1],V$,V1$,V2$,V3$,V4$,V5$,V6$
2880 GOTO 3930
2890 REM   ------------------------------------
2900 REM     CHANGE RETENTION TIME DATA
2910 PRINT
2920 PRINT "HERE ARE THE TYPES OF RETENTION TIME CALCULATIONS:"
2930 PRINT
2940 PRINT "     1. RELATIVE RETENTION TIME"
2950 PRINT "     2. CAPACITY RATIO"
2960 PRINT
2969 ON ERR THEN GOTO 2971
2970 INPUT "WHICH TYPE DO YOU WANT TO USE?  (1 OR 2)  ",N2
2971 ON ERR THEN STOP
2980 PRINT
2990 IF N2=1 THEN GOTO 3030
3000 IF N2=2 THEN GOTO 3060
3010 PRINT "<7><7>";N2;"IS NOT A VALID TYPE NUMBER."
3020 GOTO 2910
3030 PRINT "WHAT IS THE IDENTIFIER FOR THE REFERENCE COMPOUND FOR"
3031 ON ERR THEN GOTO 3040
3032 INPUT "     RELATIVE RETENTION TIMES?  ",N$
3033 ON ERR THEN STOP
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

```
12345678911234567892123456789312345678941234567895123456789612345678 97
        0         0         0         0         0         0         0
3034 LET Z5$=N$
3035 GOSUB 4370
3036 LET N$=Z5$
3037 GOTO 3070
3040 ON ERR THEN STOP
3041 PRINT
3042 PRINT "<7><7>USE A SLASH (/) WHERE YOU WANT A COMMA."
3043 PRINT
3044 GOTO 3030
3060 ON ERR THEN GOTO 3062
3061 INPUT "WHAT IS THE DEAD VOLUME TIME, IN SECONDS?  ",N$
3062 ON ERR THEN GOTO 3066
3063 LET X5=VAL(N$)
3064 ON ERR THEN STOP
3065 GOTO 3070
3066 ON ERR THEN STOP
3067 PRINT
3068 PRINT "<7><7>";N$;" IS NOT A VALID DEAD VOLUME TIME."
3069 GOTO 2980
3070 READ FILE[4,1],T$,U$,N1
3080 WRITE FILE[4,1],T$,U$,N1,N2,N$
3090 GOTO 3930
3100 REM  ------------------------------------------------------------
3110 REM          DELETE AN EXISTING METHOD
3120 PRINT
3129 ON ERR THEN GOTO 3131
3130 INPUT "WHICH METHOD DO YOU WANT TO DELETE?  ",T
3131 ON ERR THEN STOP
3140 IF T=INT(ABS(T)) THEN IF T<=9999 THEN GOTO 3180
3150 PRINT
3160 PRINT "<7><7>";T;"IS NOT A VALID METHOD NUMBER."
3170 GOTO 3120
3180 LET T$="GC0000"
3190 LET T$[7-LEN(STR$(T)),6]=STR$(T)
3200 ON ERR THEN GOTO 3220
3210 RENAME T$,T$
3220 ON ERR THEN STOP
3230 IF SYS(7)<>-48 THEN GOTO 3260
3240 DELAY =1
3250 GOTO 3200
3260 IF SYS(7)=-9 THEN GOTO 3310
3270 PRINT
12345678911234567892123456789312345678941234567895123456789612345678 97
        0         0         0         0         0         0         0
```



```
12345678911234567892123456789312345678941234567895123456789612345678 97
        0         0         0         0         0         0         0
3280 PRINT "<7><7>THERE IS NO EXISTING METHOD WITH THE NUMBER ";T$[3,6
*    ];"."
3290 PRINT "NO METHOD HAS BEEN DELETED."
3300 GOTO 3950
3310 NOESC
3311 DELETE T$
3312 GOSUB 4430
3313 ESC
3320 PRINT
3330 PRINT "METHOD ";T$[3,6];" AND ALL OF ITS CONCENTRATION PATTERNS H
*    AVE BEEN DELETED."
3340 GOTO 3950
3350 REM  ------------------------------------------------------------
3360 REM          DISPLAY AN EXISTING METHOD
3370 PRINT
3379 ON ERR THEN GOTO 3381
3380 INPUT "WHAT METHOD DO YOU WANT TO DISPLAY?  ",T
3381 ON ERR THEN STOP
3390 IF T=INT(ABS(T)) THEN IF T<=9999 THEN GOTO 3430
3400 PRINT
3410 PRINT "<7><7>";T;"IS NOT A VALID METHOD NUMBER."
3420 GOTO 3370
3430 LET T$="GC0000"
3440 LET T$[7-LEN(STR$(T)),6]=STR$(T)
3450 ON ERR THEN GOTO 3470
3460 RENAME T$,T$
3470 ON ERR THEN STOP
3480 IF SYS(7)<>-48 THEN GOTO 3510
3490 DELAY =1
3500 GOTO 3450
3510 IF SYS(7)=-9 THEN GOTO 3550
3520 PRINT
3530 PRINT "<7><7>THERE IS NO EXISTING METHOD WITH THE NUMBER ";T$[3,6
*    ];"."
3540 GOTO 3950
3550 ON ERR THEN GOTO 3590
3560 OPEN FILE[4,0],T$,200
3570 ON ERR THEN STOP
3580 GOTO 3620
3590 ON ERR THEN STOP
3600 DELAY =1
3610 GOTO 3550
12345678911234567892123456789312345678941234567895123456789612345678 97
        0         0         0         0         0         0         0
```

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
3620 PRINT
3630 READ FILE[4,1],T$,U$,N1,N2,N$
3635 PRINT
3636 PRINT
3637 PRINT  TAB(24);"M-E-T-H-O-D   R-E-P-O-R-T"
3638 PAGE =74
3640 PRINT "ANALYST:  ";U$; TAB(53);"METHOD NUMBER:  ";T$[3,6]
3660 PRINT "TYPE OF METHOD:  ";
3670 ON N1 THEN GOTO 3680, 3700, 3720, 3740
3680 PRINT "INTERNAL STANDARDS"
3690 GOTO 3750
3700 PRINT "PURGE AND TRAP "
3710 GOTO 3750
3720 PRINT "LIQUID/LIQUID EXTRACTION"
3730 GOTO 3750
3740 PRINT "DIRECT AQUEOUS INJECTION"
3750 ON N2 THEN GOTO 3760, 3780
3760 PRINT "IDENTIFIER FOR RELATIVE RETENTION TIME REFERENCE PEAK:  ";
*     N$
3770 GOTO 3790
3780 PRINT "DEAD VOLUME TIME FOR CAPACITY RATIOS:  ";N$;" SECONDS"
3790 PRINT
3800 PRINT "     IDENTIFIER                NAME OF COMPOUND
*        CAS NUMBER"
3810 PRINT "     ---------  ------------------------------
*      -----------"
3820 LET I=1
3830 LET J=0
3840 READ FILE[4,3*I-1],V$,V1$,V2$,V3$,V4$,V5$,V6$
3850 IF EOF(4) THEN GOTO 3930
3860 IF V$="99999" THEN GOTO 3910
3870 LET J=J+1
3880 PRINT USING "###.  #######    ################################
*     #######  ###########",J,V$,V1$,V2$
3890 IF V3$<>"99999" THEN PRINT USING "                    #############
*     ##########################  ###########",V3$,V4$
3900 IF V5$<>"99999" THEN PRINT USING "                    #############
*     ##########################  ###########",V5$,V6$
3910 LET I=I+1
3920 GOTO 3840
3930 CLOSE FILE[4]
3940 ON ESC THEN GOTO 4000
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```



```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
3950 PRINT
3955 PRINT
3960 ON ERR THEN GOTO 3980
3970 INPUT "DO YOU WANT TO DEAL FURTHER WITH ANY METHOD?  (Y OR N)  ",
*     X$
3980 ON ERR THEN STOP
3990 IF X$[1,1]="Y" THEN GOTO 0110
4000 CLOSE
4010 NOESC
4020 CHAIN "GC00" THEN GOTO 0100
4040 REM
4050 REM   ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
4060 REM          SUBROUTINE TO CHECK VALIDITY OF CAS NUMBERS
4070 IF LEN(W3$)=11 THEN GOTO 4110
4080 LET W4$=" ",W3$
4090 LET W3$=W4$
4100 GOTO 4070
4110 IF W3$[7,7]="-" THEN IF W3$[10,10]="-" THEN GOTO 4130
4120 GOTO 4310
4130 LET I3=0
4140 FOR I4=1 TO 6
4150   IF W3$[I4,I4]<>" " THEN GOTO 4170
4160 NEXT I4
4170 FOR I2=I4 TO 6
4180   ON ERR THEN GOTO 4310
4190   LET I3=I3+VAL(W3$[I2,I2])*(9-I2)
4200   ON ERR THEN STOP
4210 NEXT I2
4220 FOR I2=8 TO 9
4230   ON ERR THEN GOTO 4310
4240   LET I3=I3+VAL(W3$[I2,I2])*(10-I2)
4250   ON ERR THEN STOP
4260 NEXT I2
4270 ON ERR THEN GOTO 4310
4280 IF I3-10*INT(I3/10)<>VAL(W3$[11,11]) THEN GOTO 4310
4290 ON ERR THEN STOP
4300 RETURN
4310 ON ERR THEN STOP
4320 LET W3$="99999"
4330 RETURN
4340 REM
4350 REM   ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

PROGRAM LISTING FOR GC01

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
4360 REM          SUBROUTINE TO CHANGE SLASHES TO COMMAS
4370 LET Z5=POS(Z5$,"/",1)
4380 IF Z5=0 THEN RETURN
4390 LET Z5$[Z5,Z5]=","
4400 GOTO 4370
4405 REM
4410 REM   ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
4420 REM          SUBROUTINE TO DELETE CONCENTRATION PATTERNS
4430 LET A6$=T$,"000"
4440 FOR I=1 TO 26
4450   LET A6$[10-LEN(STR$(I)),9]=STR$(I)
4460   ON ERR THEN GOTO 4480
4470   DELETE A6$
4480   ON ERR THEN STOP
4490 NEXT I
4500 RETURN
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```


SYMBOL TABLE FOR GC01

SYMBOL	REFERENCES		
0100	4020		
0110	0230	0470	3990
0191	0189		
0260	0200	0310	
0271	0269		
0320	0280		
0340	0390		
0360	0340		
0400	0370		
0480	0400		
0510	0490		
0560	0500	0593	
0590	0570		
0600	0585	0720	
0681	0679		
0730	0690	0840	
0791	0789		
0800	0889		
0850	0810	0864	
0860	0851		
0880	0820		
0882	0880		
0886	0882		
0890	0857	0885	
0910	0900		
0940	2240		
0960	1650		
1010	0960		
1050	1083		
1080	1060		
1090	1075		
1100	1150		
1101	1099		
1170	1110	1204	
1200	1189		
1210	1195	1300	
1230	1210		
1310	1270		
1320	1240		
1330	1354		
1350	1330		
1360	1345	1450	
1380	1360		
1460	1420		
1470	1390		

SYMBOL TABLE FOR GC01

SYMBOL	REFERENCES		
1480	1504		
1500	1480		
1510	1495	1600	
1530	1510		
1610	1570		
1620	1320	1470	1540
1660	1000	1090	
1700	1680		
1750	0200	1800	
1761	1759		
1810	1770		
1830	1880		
1850	1830		
1890	1860		
1950	1890	2010	
1990	1950		
2020	1980	2140	
2101	2099		
2170	2110		
2180	2210		
2220	2190		
2270	2110	2303	
2300	2280		
2310	2295		
2320	2360		
2370	2330		
2400	2340		
2460	2110	2493	
2490	2470		
2500	2485		
2510	2550		
2560	2520		
2600	2530		
2640	2600	2673	
2670	2650		
2680	2665	2790	
2720	2700		
2800	2760		
2810	2730		
2850	2810		
2870	2840		
2910	2110	3020	
2971	2969		
2980	3069		
3030	2990	3044	

SYMBOL TABLE FOR GC01

SYMBOL	REFERENCES									
3040	3031									
3060	3000									
3062	3060									
3066	3062									
3070	3037	3065								
3120	0200	3170								
3131	3129									
3180	3140									
3200	3250									
3220	3200									
3260	3230									
3310	3260									
3370	0200	3420								
3381	3379									
3430	3390									
3450	3500									
3470	3450									
3510	3480									
3550	1710	3510	3610							
3590	3550									
3620	3580									
3680	3670									
3700	3670									
3720	3670									
3740	3670									
3750	3690	3710	3730							
3760	3750									
3780	3750									
3790	3770									
3840	3920									
3910	3860									
3930	2390	2430	2590	2630	2880	3090	3850			
3950	1930	3300	3340	3540						
3980	3960									
4000	0080	0550	1720	3940						
4050	1260	1410	1560	2750						
4070	4100									
4110	4070									
4130	4110									
4170	4150									
4310	4120	4180	4230	4270	4280					
4370	0583	0855	1073	1193	1343	1493	2293	2483	2663	3035
	4400									
4430	2171	3312								
4480	4460									

SYMBOL TABLE FOR GC01

SYMBOL	REFERENCES									
A6$	0101	4430	4450	4470						
FL#4	0480	0510	0890	1620	1630	1660	1960	2180	2320	2400
	2510	2870	3070	3080	3560	3630	3840	3930		
I	0910	0960	1620	1630	1640	2175	2180	2200	2310	2320
	2350	2400	2500	2510	2540	2870	3820	3840	3910	4440
	4450	4490								
I2	4170	4190	4210	4220	4240	4260				
I3	4130	4190	4240	4280						
I4	4140	4150	4160	4170						
J	3830	3870	3880							
N$	0100	0852	0854	0856	0881	0883	0888	0890	3032	3034
	3036	3061	3063	3068	3080	3630	3760	3780		
N1	0680	0690	0710	0890	3070	3080	3630	3670		
N2	0790	0810	0820	0830	0890	2970	2990	3000	3010	3080
	3630	3750								
T	0270	0280	0300	0330	1760	1770	1790	1820	3130	3140
	3160	3190	3380	3390	3410	3440				
T$	0090	0320	0330	0350	0420	0430	0440	0480	0530	0540
	0890	1810	1820	1840	1910	1960	2174	2380	2420	2570
	3070	3080	3180	3190	3210	3280	3311	3330	3430	3440
	3460	3530	3560	3630	3640	4430				
U$	0090	0580	0582	0584	0890	3070	3080	3630	3640	
V	1100	1110	1130	1180	1320	1470				
V$	0090	1070	1072	1074	1090	1620	2180	2320	2340	2510
	2530	2870	3840	3860	3880					
V1$	0090	1190	1192	1194	1620	2510	2870	3840	3880	
V2$	0090	1220	1240	1250	1290	1310	1620	2510	2870	3840
	3880									
V3$	0090	1010	1340	1342	1344	1620	2510	2810	2820	2870
	3840	3890								
V4$	0090	1020	1370	1390	1400	1440	1460	1620	2510	2830
	2870	3840	3890							
V5$	0090	1030	1490	1492	1494	1620	2510	2600	2850	2870
	3840	3900								
V6$	0100	1040	1520	1540	1550	1590	1610	1620	2510	2860
	2870	3840	3900							
V7$	0100	2290	2292	2294	2340	2380	2420	2480	2482	2484
	2530	2570	2620							
V8$	0100	2660	2662	2664	2690	2820	2850			
V9$	0100	2710	2730	2740	2780	2800	2830	2860		
W3$	0100	1250	1270	1310	1400	1420	1460	1550	1570	1610
	2740	2760	2800	4070	4080	4090	4110	4150	4190	4240
	4280	4320								
W4$	0100	4080	4090							
X	0190	0200	0220	2100	2110	2130				

SYMBOL TABLE FOR GC01

SYMBOL	REFERENCES									
X$	0100	1690	1710	3970	3990					
X4	0883									
X5	3063									
Z5	4370	4380	4390							
Z5$	0101	0582	0584	0854	0856	1072	1074	1192	1194	1342
	1344	1492	1494	2292	2294	2482	2484	2662	2664	3034
	3036	4370	4390							

SECTION 4

PROGRAM GC02 - CONCENTRATION PATTERN INTERACTION

GC02 is the program which creates, deletes, displays, and lists the names of concentration patterns. It is entered by chaining from the master control program, GC00, and it returns control to that program if the escape key is pressed.

The functions of this program are relatively simple. It first gives the user the choice of the four possible actions and then branches to the appropriate routine.

To create a concentration pattern file, the program loops through the method file and asks the user for the prepared concentration for each identifier. It places these concentrations in the concentration pattern file named by the user.

To delete an existing pattern, the program simply asks the user for the name of the pattern and deletes that file.

To display an existing pattern, the program loops through the method file and the concentration pattern file simultaneously and prints the identifiers and their associated concentrations.

To list the names of the existing concentration patterns, the program checks each of the 26 possible concentration pattern file names to see if such a file exists. It prints the names of those which do exist.

At the end of this program, it chains back to GC00.

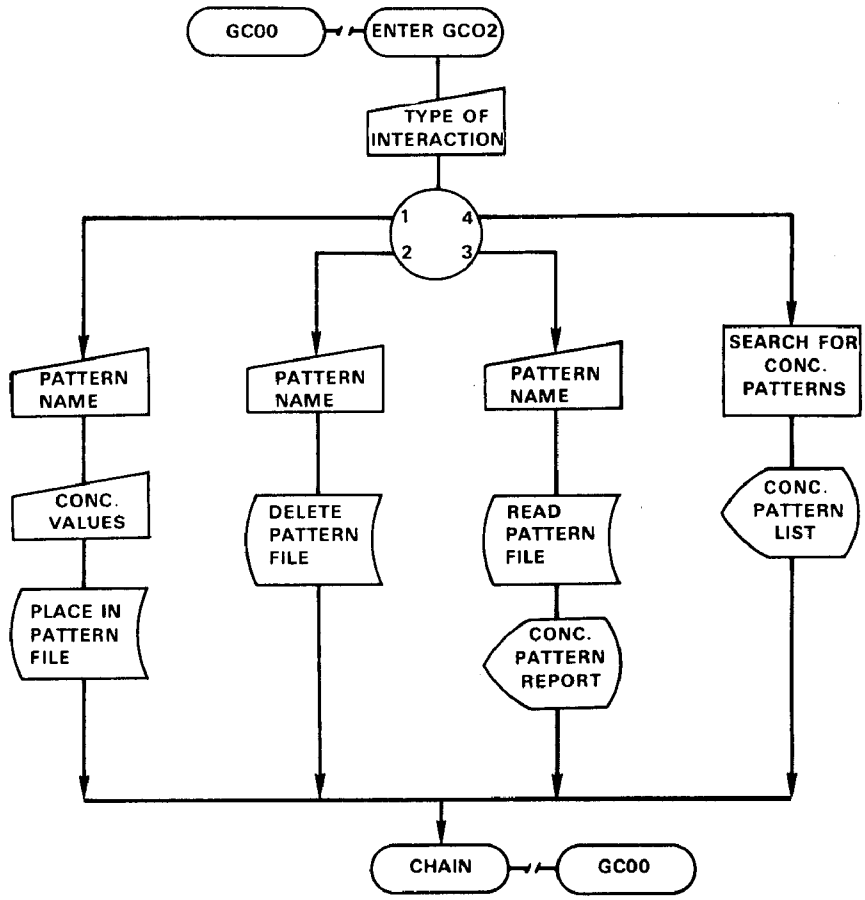

Figure 4. Flowchart of Program GC02.

TABLE 3. SYMBOL DEFINITIONS FOR PROGRAM GCO2

A5	the prepared concentration input by the user
A6$	the name of the concentration pattern file
A7	the position of A8$ in A9$
A8$	the single letter name of a concentration pattern
A9$	the alphabet
I	the control variable for loops
I2	a counter for the number of concentration patterns associated with a method
T$	the name of the method file
V$	an identifier from the method file
X	the user's answer to multiple choice questions
X$	the user's answer to Y or N questions

PROGRAM LISTING FOR GC02

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                    +
0030 REM   +   PROGRAM GC02, CONCENTRATION PATTERN INTERACTION        +
0040 REM   +   BY:  J. KOPKE (SWORCC), MARCH 23, 1979                 +
0050 REM   +   MOST RECENT REVISION:  MAY 18, 1979                    +
0060 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0070 REM
0080 ON ESC THEN GOTO 1830
0090 ESC
0100 DIM A6$[9],A8$[1],A9$[26],T$[6],V$[8],X$[3]
0110 LET A9$="ABCDEFGHIJKLMNOPQRSTUVWXYZ"
0120 READ FILE[4,1],T$
0130 REM   ------------------------------------------------------------
0140 REM          DISPLAY CHOICES
0150 PRINT
0160 PRINT "HERE ARE THE TYPES OF CONCENTRATION PATTERN INTERACTION FO
*     R METHOD ";T$[3,6];":"
0170 PRINT
0180 PRINT "     1.  CREATE A NEW CONCENTRATION PATTERN"
0190 PRINT "     2.  DELETE AN EXISTING PATTERN"
0200 PRINT "     3.  DISPLAY AN EXISTING PATTERN"
0210 PRINT "     4.  LIST THE EXISTING PATTERNS FOR METHOD ";T$[3,6]
0220 PRINT
0230 ON ERR THEN GOTO 0250
0240 INPUT "WHAT TYPE DO YOU WANT TO USE?  (1, 2, 3, OR 4)  ",X
0250 ON ERR THEN STOP
0260 IF X=INT(X) THEN IF X>0 THEN IF X<5 THEN GOTO 0300
0270 PRINT
0280 PRINT "<7><7>";X;"IS NOT A VALID TYPE NUMBER."
0290 GOTO 0150
0300 ON X THEN GOTO 0330, 0820, 1050, 1530
0310 REM   ------------------------------------------------------------
0320 REM          CREATE A NEW CONCENTRATION PATTERN FILE
0330 PRINT
0340 ON ERR THEN GOTO 0360
0350 INPUT "WHAT SHOULD BE THE LETTER NAME FOR THE NEW PATTERN?  (A, B
*     , C, . . . , OR Z)  ",A8$
0360 ON ERR THEN STOP
0370 LET A7=POS(A9$,A8$,1)
0380 IF A7<>0 THEN GOTO 0420
0390 PRINT
0400 PRINT "<7><7>'";A8$;"' IS NOT A VALID LETTER."
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```


PROGRAM LISTING FOR GC02

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0410 GOTO 0330
0420 LET A6$=T$,"000"
0430 LET A6$[10-LEN(STR$(A7)),9]=STR$(A7)
0440 ON ERR THEN GOTO 0460
0450 RENAME A6$,A6$
0460 ON ERR THEN STOP
0470 IF SYS(7)=-10 THEN GOTO 0510
0480 PRINT
0490 PRINT "<7><7>THERE IS ALREADY A PATTERN NAMED '";A8$;"' FOR METHO
*     D ";T$[3,6];"."
0500 GOTO 0330
0510 OPEN FILE[7,0],A6$,4
0520 ON ESC THEN GOTO 0540
0530 GOTO 0590
0540 CLOSE FILE[7]
0550 DELETE A6$
0560 PRINT
0570 PRINT "<7><7>PATTERN '";A8$;"' HAS BEEN DELETED BECAUSE IT WAS IN
*     COMPLETE."
0580 GOTO 1860
0590 CLOSE FILE[4]
0600 OPEN FILE[4,0],T$,200
0602 PRINT
0604 PRINT "HERE ARE THE ALLOWABLE UNITS OF CONCENTRATION:"
0606 PRINT
0608 PRINT "     1.  NANOGRAMS PER MICROLITER"
0610 PRINT "     2.  MICROGRAMS PER LITER"
0612 PRINT
0614 ON ERR THEN GOTO 0618
0616 INPUT "WHICH UNIT DO YOU WANT TO USE? (1 OR 2)  ",X
0618 ON ERR THEN STOP
0620 IF X=INT(X) THEN IF X>0 THEN IF X<3 THEN GOTO 0630
0622 PRINT
0624 PRINT "<7><7>";X;"IS NOT A VALID UNIT NUMBER."
0626 GOTO 0602
0630 PRINT
0640 FOR I=1 TO 60
0650   READ FILE[4,3*I-1],V$
0660   IF EOF(4) THEN GOTO 0770
0670   IF V$<>"99999" THEN GOTO 0700
0680   LET A5=9.99999E-07
0690   GOTO 0750
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

PROGRAM LISTING FOR GC02

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0700   IF I=1 THEN PRINT "CONCENTRATION OF ";
0710   PRINT  TAB(17);V$;"?"; TAB(28);
0720   ON ERR THEN GOTO 0740
0730   INPUT "",A5
0740   ON ERR THEN STOP
0741   IF A5>0 THEN GOTO 0745
0742   PRINT "<7><7>";A5;"IS NOT A VALID CONCENTRATION VALUE."
0743   GOTO 0700
0745   IF X=1 THEN LET A5=1000*A5
0750   WRITE FILE[7,I],A5
0760 NEXT I
0770 CLOSE FILE[7]
0780 ON ESC THEN GOTO 1830
0790 GOTO 1780
0800 REM  ------------------------------------------------------------
0810 REM          DELETE A CONCENTRATION PATTERN FILE
0820 PRINT
0830 ON ERR THEN GOTO 0850
0840 INPUT "WHAT IS THE NAME OF THE PATTERN TO BE DELETED?  (A, B, C,
*     . . . , OR Z)  ",A8$
0850 ON ERR THEN STOP
0860 LET A7=POS(A9$,A8$,1)
0870 IF A7<>0 THEN GOTO 0910
0880 PRINT
0890 PRINT "<7><7>'";A8$;"' IS NOT A VALID LETTER."
0900 GOTO 0820
0910 LET A6$=T$,"000"
0920 LET A6$[10-LEN(STR$(A7)),9]=STR$(A7)
0930 ON ERR THEN GOTO 0985
0940 DELETE A6$
0950 ON ERR THEN STOP
0960 PRINT
0970 PRINT "PATTERN '";A8$;"' HAS BEEN DELETED."
0980 GOTO 1780
0985 ON ERR THEN STOP
0990 PRINT
1000 PRINT "<7><7>THERE IS NO EXISTING PATTERN NAMED '";A8$;"'."
1010 PRINT "NO PATTERN HAS BEEN DELETED."
1020 GOTO 1780
1030 REM  ------------------------------------------------------------
1040 REM          DISPLAY A CONCENTRATION PATTERN
1050 PRINT
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```


PROGRAM LISTING FOR GC02

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
1060 ON ERR THEN GOTO 1080
1070 INPUT "WHAT IS THE NAME OF THE PATTERN TO BE DISPLAYED?  (A, B, C
*     , . . . , OR Z)  ",A8$
1080 ON ERR THEN STOP
1090 LET A7=POS(A9$,A8$,1)
1100 IF A7<>0 THEN GOTO 1140
1110 PRINT
1120 PRINT "<7><7>'";A8$;"' IS NOT A VALID LETTER."
1130 GOTO 1050
1140 LET A6$=T$,"000"
1150 LET A6$[10-LEN(STR$(A7)),9]=STR$(A7)
1160 ON ERR THEN GOTO 1180
1170 RENAME A6$,A6$
1180 ON ERR THEN STOP
1190 IF SYS(7)=-9 THEN GOTO 1230
1200 PRINT
1210 PRINT "<7><7>THERE IS NO EXISTING PATTERN NAMED '";A8$;"'."
1220 GOTO 1050
1230 ON ERR THEN GOTO 1270
1240 OPEN FILE[7,0],A6$,4
1250 ON ERR THEN STOP
1260 GOTO 1300
1270 ON ERR THEN STOP
1280 DELAY =1
1290 GOTO 1230
1300 CLOSE FILE[4]
1310 OPEN FILE[4,0],T$,200
1320 PRINT
1330 PRINT
1340 PAGE =74
1350 PRINT  TAB(9);"C-O-N-C-E-N-T-R-A-T-I-O-N   P-A-T-T-E-R-N   R-E-P-
*     O-R-T"
1360 PRINT "CONCENTRATION PATTERN:  ";A8$; TAB(53);"METHOD NUMBER:  ";
*     T$[3,6]
1370 PRINT
1380 PRINT "     IDENTIFIER     CONCENTRATION"
1390 PRINT "     ----------     -------------"
1400 FOR I=1 TO 60
1410   READ FILE[4,3*I-1],V$
1420   IF EOF(4) THEN GOTO 1470
1430   IF V$="99999" THEN GOTO 1460
1440   READ FILE[7,I],A5
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
1450   PRINT USING "      ########          ####.###",V$,A5
1460 NEXT I
1470 PRINT
1480 PRINT
1490 CLOSE FILE[7]
1500 GOTO 1780
1510 REM   ------------------------------------------------------------
1520 REM          LIST EXTANT CONCENTRATION PATTERN FILES
1530 PRINT
1540 PRINT
1550 PRINT  TAB(8);"C-O-N-C-E-N-T-R-A-T-I-O-N   P-A-T-T-E-R-N   L-I-S-
*     T"
1560 PAGE =72
1570 PRINT "CONCENTRATION PATTERNS FOR METHOD ";T$[3,6];":  ";
1580 LET A6$=T$,"000"
1590 LET I2=0
1600 FOR I=1 TO 26
1610   LET A6$[10-LEN(STR$(I)),9]=STR$(I)
1620   ON ERR THEN GOTO 1640
1630   RENAME A6$,A6$
1640   ON ERR THEN STOP
1650   IF SYS(7)<>-9 THEN GOTO 1720
1660   LET I2=I2+1
1670   IF I2<>1 THEN PRINT ", ";
1680   IF I2<>11 THEN GOTO 1710
1690   PRINT
1700   PRINT "     ";
1710   PRINT A9$[I,I];
1720 NEXT I
1730 IF I2=0 THEN PRINT "NONE"
1740 PRINT
1750 PRINT
1760 REM   ------------------------------------------------------------
1770 REM          WRAP-UP PROCEDURE
1780 PRINT
1790 ON ERR THEN GOTO 1810
1800 INPUT "DO YOU WANT TO DEAL FURTHER WITH ANY CONCENTRATION PATTERN
*     ?  (Y OR N)  ",X$
1810 ON ERR THEN STOP
1820 IF X$[1,1]="Y" THEN GOTO 0150
1830 ON ERR THEN GOTO 1850
1840 CLOSE FILE[7]
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```



```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
1850 ON ERR THEN STOP
1860 NOESC
1870 CHAIN "GC00"
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

SYMBOL TABLE FOR GC02

SYMBOL	REFERENCES									
0150	0290	1820								
0250	0230									
0300	0260									
0330	0300	0410	0500							
0360	0340									
0420	0380									
0460	0440									
0510	0470									
0540	0520									
0590	0530									
0602	0626									
0618	0614									
0630	0620									
0700	0670	0743								
0740	0720									
0745	0741									
0750	0690									
0770	0660									
0820	0300	0900								
0850	0830									
0910	0870									
0985	0930									
1050	0300	1130	1220							
1080	1060									
1140	1100									
1180	1160									
1230	1190	1290								
1270	1230									
1300	1260									
1460	1430									
1470	1420									
1530	0300									
1640	1620									
1710	1680									
1720	1650									
1780	0790	0980	1020	1500						
1810	1790									
1830	0080	0780								
1850	1830									
1860	0580									
A5	0680	0730	0741	0742	0745	0750	1440	1450		
A6$	0100	0420	0430	0450	0510	0550	0910	0920	0940	1140
	1150	1170	1240	1580	1610	1630				
A7	0370	0380	0430	0860	0870	0920	1090	1100	1150	
A8$	0100	0350	0370	0400	0490	0570	0840	0860	0890	0970

SYMBOL TABLE FOR GC02

SYMBOL	REFERENCES									
	1000	1070	1090	1120	1210	1360				
A9$	0100	0110	0370	0860	1090	1710				
FL#4	0120	0590	0600	0650	1300	1310	1410			
FL#7	0510	0540	0750	0770	1240	1440	1490	1840		
I	0640	0650	0700	0750	0760	1400	1410	1440	1460	1600
	1610	1710	1720							
I2	1590	1660	1670	1680	1730					
T$	0100	0120	0160	0210	0420	0490	0600	0910	1140	1310
	1360	1570	1580							
V$	0100	0650	0670	0710	1410	1430	1450			
X	0240	0260	0280	0300	0616	0620	0624	0745		
X$	0100	1800	1820							

SECTION 5

PROGRAM GC03 - INTERNAL STANDARDS CALIBRATION

The internal standards calibration method is a planned future enhancement of the GCAS, but it has not been implemented in Version I.

PROGRAM LISTING FOR GC03

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                    +
0030 REM   +   PROGRAM GC03, INTERNAL STANDARDS CALIBRATION           +
0040 REM   +   BY:  J. KOPKE (SWORCC), JANUARY 10, 1979               +
0045 REM   +   MOST RECENT REVISION:  MARCH 21, 1979                  +
0050 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0060 REM
0070 ESC
0080 ON ESC THEN GOTO 0120
0090 PRINT
0110 PRINT "<7><7>INTERNAL STANDARDS CALIBRATION IS NOT OPERATIONAL AT
*      THIS TIME."
0120 NOESC
0130 CHAIN "GC00"
```


SYMBOL TABLE FOR GC03

SYMBOL	REFERENCES
0120	0080

12345678911234567892123456789312345678941234567895123456789612345678 97
         0   0   0   0   0   0   0

SECTION 6

PROGRAM GC04 - PURGE AND TRAP CALIBRATION

GC04 is the program which performs external standards calibration for the purge and trap method. It is entered by chaining from the master control program, GC00, and it chains back to that program when it has been completed or when the escape key is pressed.

The first task of GC04 is to flag the compounds to be calibrated. Array F is a one-dimensional array of flags, as shown in Figure 5. The nth identifier in array F corresponds to the nth identifier in the method file. A "1" in array F indicates that the corresponding identifier is to be calibrated; a zero implies the opposite. The user is asked if all of the compounds are to be calibrated. If so, all of the flags in array F are set to 1. If not all of the identifiers are to be calibrated, the user is asked about each identifier separately, and only the appropriate positions in array F are set to 1.

Next, GC04 asks for the injection ID for a standard, The program checks whether the ID is reasonable and whether the data file exists. It then opens the injection data file and checks the data file useability flag in the first record to see if the data file can be used. It also looks for any error messages in the injection data file and displays them in case they are important to the user.

GC04 then asks the user for the concentration pattern and opens the concentration pattern file. For each flagged identifier, the program searches the injection data file for the peak area and the concentration pattern file for the prepared concentrations. These data elements are placed in the array G, as shown in Figure 5. Each row of array G contains calibration data corresponding to one identifier. Odd numbered columns contain prepared concentrations, and even numbered columns contain peak areas. If the injection data file does not have a peak area for one of the identifiers, the program refuses to use that data file and asks for another. The injection ID for each good data file is concatenated to the superstring I$.

The program continues to ask for more calibration standards until the user types "END" or until the limit of 15 is reached. Then it gives the user the choice of linear regression, quadratic regression, linear interpolation, and linear regression forced through the origin. The program requires at least three standards for linear regression, since three standards are necessary to confirm that the curve is linear. Similarly, at

least four standards are required for quadratic regression, since four are necessary to confirm that the curve is parabolic.

The program then branches to one of three curve fitting routines. If the user has selected linear or quadratic regression, the program branches to the normal regression routine. This least squares regression algorithm is documented in great detail in Statistical Methods for Business Decisions by Charles Clark and Lawrence Schkade (South-Western Publishing Company, Cincinnati, Ohio, 1969).

If the user has selected linear interpolation, the program simply puts the calibration standards into ascending order by peak area and writes them into the method file. Array G2, shown in Figure 5, is used to hold one row of array G simply so that it can be placed into the method file by a MAT WRITE FILE statement.

If the user has selected linear regression forced through the origin, the program calculates the equation of a line in the form y=bx, where b is determined by the formula:

$$b = \frac{\sum(\text{Signal} \cdot \text{Concentration})}{\sum(\text{Signal}^2)}$$

For all three types of curve fitting, this program also calculates a "fitting error" which is actually a percent, relative, standard error of estimate, calculated by the formula:

$$\text{Fitting Error} = \frac{100\sqrt{\dfrac{\sum(\text{Known Conc.} - \text{Calculated Conc.})^2}{\text{Number of Standards} - 2}}}{\text{Mean Concentration}}$$

When the regression calculations are complete, the calibration data items are written into the method file, and the program chains back to GC00.

TABLE 4. SYMBOL DEFINITIONS FOR PROGRAM GC04.

A6$	the name of a concentration pattern file
A7	the position of A8$ in A9$
A8$	the name of a concentration pattern
A9$	the alphabet
A()	an array used in regression calculations
B	the retention time of a compound
C	the peak area of a compound
D	a holding variable used in a sorting process
D2	a holding variable used in a sorting process
D2$	the injection ID number
D3	a holding variable used in a sorting process
D3$	the name of the data file
D4$	the date of calibration
F	the number of identifiers in the method
F()	the array of flags used to indicate which identifiers are to be calibrated
G$	an identifier read from the data file
G2()	an array consisiting of one row from array G
G()	the array of calibration information (concentrations and peak areas)
H$	the peak type
I	the control variable for several loops
I$	the superstring of injection IDs for the calibration standards

TABLE 4. (continued)

I2$	the superstring of injection IDs in order for linear interpolation purposes
I2	the control variable for several loops
I3	the control variable for several loops
I4	the control variable for several loops
I5	a counter for the number of calibration standards
I6	the control variable for several loops
J	the data file useability flag
J3	the fitting error
J4	the calculated concentration of a standard
J5	the sum of the squares of the differences between the prepared and calculated concentrations of standards
J6	the sum of the concentrations of the standards
J7	used in calculating linear regression forced through the origin
J8	used in calculating linear regression forced through the origin
J9	used in calculating linear regression forced through the origin
P9	the record number of the first record in a data file which describes a peak
R2	the coefficient of the linear term of a regression equation in a linear regression forced through the origin
R()	an array used in regression calculations
T	the method number
T$	the name of the method file
T()	an array used in regression calculations
V$	an identifier from a method file
VO$	an error message from the data file
X	the user's answer to a multiple choice question

TABLE 4 (continued)

X$	the user's answer to a Y or N question
Z3	a variable used in regression calculations

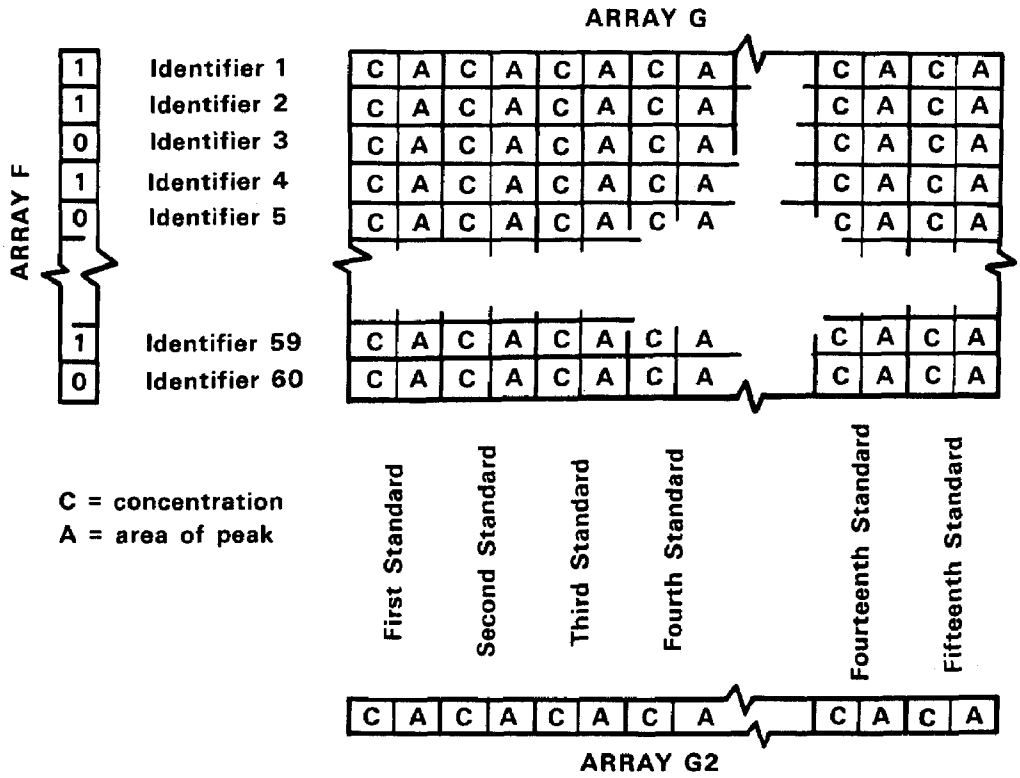

Figure 5. Arrays used in Program GC04.

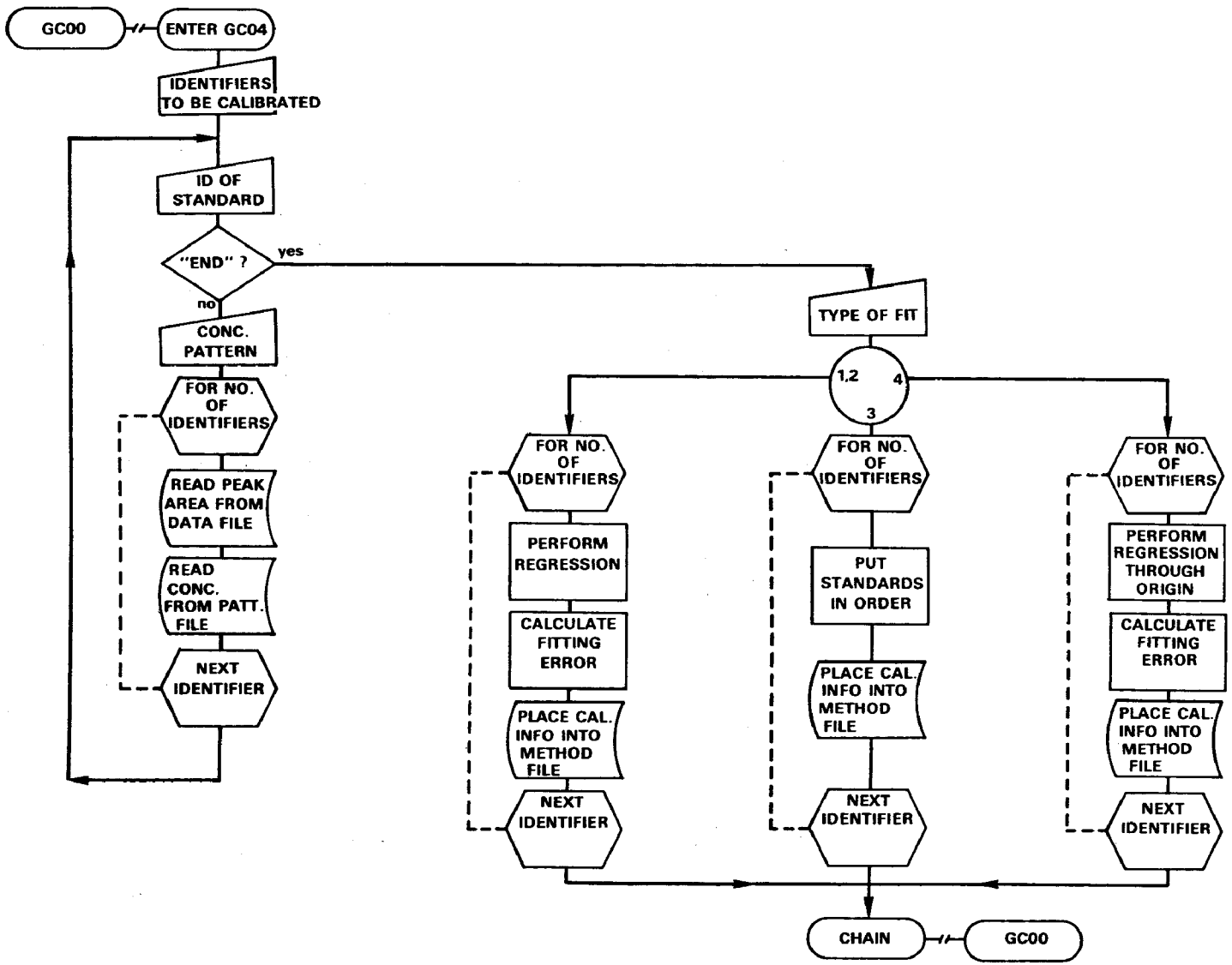

Figure 6. Flowchart of Program GC04.

PROGRAM LISTING FOR GC04

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                      +
0030 REM   +   PROGRAM GC04, EXTERNAL STANDARDS CALIBRATION, P&T         +
0040 REM   +   BY:  J. KOPKE (SWORCC), FEBRUARY 7, 1979                 +
0045 REM   +   MOST RECENT REVISION:  APRIL 17, 1979                    +
0050 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0060 REM
0070 ESC
0080 ON ESC THEN GOTO 3000
0090 DIM A[5],R[3,4],T[4],V0$[20]
0100 DIM F[60],G[60,30],I$[160],T$[6],X$[3],V$[8],D2$[8],D3$[10],D4$[8
*     ],G$[8],H$[2],G2[30],I2$[160]
0105 DIM A9$[26],A8$[1],A6$[9]
0106 LET A9$="ABCDEFGHIJKLMNOPQRSTUVWXYZ"
0110 MAT G=ZER
0120 MAT F=ZER
0130 REM   ------------------------------------------------------------
0140 REM          COUNT NUMBER OF IDENTIFIERS IN METHOD FILE
0150 LET F=0
0160 READ FILE[4,1],T$
0165 CLOSE FILE[4]
0166 OPEN FILE[4,0],T$,200
0170 READ FILE[4,3*(F+1)-1],V$
0180 IF EOF(4) THEN GOTO 0230
0190 LET F=F+1
0200 GOTO 0170
0210 REM   ------------------------------------------------------------
0220 REM          FLAG THE IDENTIFIERS TO BE CALIBRATED
0230 PRINT
0235 PRINT "DO YOU WANT TO CALIBRATE ALL IDENTIFIERS OF METHOD ";T$[3,
*     6];
0237 ON ERR THEN GOTO 0242
0240 INPUT " AT ONCE?  (Y OR N)  ",X$
0242 ON ERR THEN STOP
0250 IF X$[1,1]<>"Y" THEN GOTO 0300
0260 FOR I=1 TO F
0270   LET F[I]=1
0280 NEXT I
0290 GOTO 0410
0300 PRINT
0310 PRINT "DO YOU WANT TO CALIBRATE ";
0320 FOR I=1 TO F
```


PROGRAM LISTING FOR GC04

```
0330   READ FILE[4,3*I-1],V$
0340   IF V$="99999" THEN GOTO 0380
0350   PRINT  TAB(25);V$;"?"; TAB(37);"  (Y OR N)";
0355   ON ERR THEN GOTO 0365
0360   INPUT "  ",X$
0365   ON ERR THEN STOP
0370   IF X$[1,1]="Y" THEN LET F[I]=1
0380 NEXT I
0390 REM   ------------------------------------------------------------
0400 REM          PRINT INSTRUCTIONS FOR ENTERING DATA
0410 PRINT
0420 PRINT "ENTER THE FOLLOWING CALIBRATION INFORMATION."
0440 PRINT "TYPE 'END' AS AN INJECTION ID TO TERMINATE THE LIST."
0450 LET I5=0
0460 REM   ------------------------------------------------------------
0470 REM          OPEN SELECTED DATA FILE
0480 LET I5=I5+1
0490 IF I5<16 THEN GOTO 0540
0500 PRINT
0510 PRINT "<7><7>YOU HAVE USED FIFTEEN CALIBRATION STANDARDS, WHICH I
*     S THE LIMIT"
0520 PRINT "     FOR THIS PROGRAM."
0530 GOTO 1230
0540 PRINT
0545 ON ERR THEN GOTO 0555
0550 INPUT "INJECTION ID FOR CALIBRATION STANDARD?  ",D2$
0555 ON ERR THEN STOP
0560 IF D2$="END" THEN GOTO 1230
0570 IF LEN(D2$)=8 THEN GOTO 0610
0580 PRINT
0590 PRINT "<7><7>";D2$;" IS NOT A VALID INJECTION ID NUMBER."
0600 GOTO 0540
0610 LET D3$="GC",D2$
0620 ON ERR THEN GOTO 0640
0630 RENAME D3$,D3$
0640 ON ERR THEN STOP
0650 IF SYS(7)<>-48 THEN GOTO 0680
0660 DELAY =1
0670 GOTO 0620
0680 IF SYS(7)=-9 THEN GOTO 0720
0690 PRINT
0700 PRINT "<7><7>THERE IS NO EXISTING DATA FOR INJECTION ID ";D2$;"."
```

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0710 GOTO 0540
0720 ON ERR THEN GOTO 0760
0730 OPEN FILE[3,0],D3$,31
0740 ON ERR THEN STOP
0750 GOTO 0810
0760 ON ERR THEN STOP
0770 DELAY =1
0780 GOTO 0720
0790 REM  ------------------------------------------------------------
0800 REM          CHECK DATA FILE USABILITY FLAG
0810 READ FILE[3,1],J
0820 IF J=1 THEN GOTO 0900
0830 PRINT
0840 IF J=2 THEN PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPOR
*    T DID NOT HAVE A TOTAL AREA."
0850 IF J=3 THEN PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPOR
*    T WAS IN THE WRONG FORMAT."
0860 CLOSE FILE[3]
0870 GOTO 0540
0880 REM  ------------------------------------------------------------
0890 REM          PRINT ANY ERROR MESSAGES FOUND IN THE DATA FILE
0900 LET P9=2
0910 READ FILE[3,P9],V0$
0920 IF V0$[1,7]<>"MESSAGE" THEN GOTO 1001
0930 PRINT
0940 PRINT "THE FOLLOWING MESSAGE WAS PART OF THE REPORT FOR"
0950 PRINT "     INJECTION ";D2$;":  ";V0$;"."
0960 PRINT
0970 LET P9=P9+1
0980 GOTO 0910
0990 REM  ------------------------------------------------------------
1000 REM          OPEN CONCENTRATION PATTERN FILE
1001 ON ERR THEN GOTO 1003
1002 INPUT "     CONCENTRATION PATTERN FOR STANDARD?  ",A8$
1003 ON ERR THEN STOP
1004 LET A7=POS(A9$,A8$,1)
1005 IF A7<>0 THEN GOTO 1008
1006 PRINT "<7><7>     '";A8$;"' IS NOT A VALID LETTER."
1007 GOTO 1001
1008 LET A6$=T$,"000"
1009 LET A6$[10-LEN(STR$(A7)),9]=STR$(A7)
1010 ON ERR THEN GOTO 1012
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```



```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
1011 RENAME A6$,A6$
1012 ON ERR THEN STOP
1013 IF SYS(7)=-9 THEN GOTO 1016
1014 PRINT "<7><7>     THERE IS NO EXISTING PATTERN NAMED '";A8$;"'."
1015 GOTO 1001
1016 ON ERR THEN GOTO 1020
1017 OPEN FILE[7,0],A6$,4
1018 ON ERR THEN STOP
1019 GOTO 1026
1020 ON ERR THEN STOP
1021 DELAY =1
1022 GOTO 1016
1024 REM  ------------------------------------------------------------
1025 REM          GATHER CALIBRATION DATA
1026 LET P9=P9+2
1027 FOR I=1 TO F
1030   IF F[I]<>1 THEN GOTO 1190
1040   READ FILE[4,3*I-1],V$
1041   IF V$<>"99999" THEN GOTO 1060
1042   LET F[I]=0
1043   GOTO 1190
1060   READ FILE[7,I],G[I,2*I5-1]
1070   LET I2=P9
1080   READ FILE[3,I2],G$,H$,B,C
1090   IF EOF(3) THEN GOTO 1130
1100   IF G$=V$ THEN IF C<>-9999 THEN GOTO 1180
1110   LET I2=I2+1
1120   GOTO 1080
1130   PRINT
1140   PRINT "<7><7>THE REPORT FOR INJECTION ";D2$;" DOES NOT INCLUDE
*    AN AREA FOR ";V$;"."
1150   PRINT "THEREFORE, ";D2$;" CANNOT BE USED IN THIS CALIBRATION."
1160   CLOSE FILE[3]
1165   CLOSE FILE[7]
1170   GOTO 0540
1180   LET G[I,2*I5]=C
1190 NEXT I
1200 CLOSE FILE[3]
1201 CLOSE FILE[7]
1210 LET I$=I$,D2$
1220 GOTO 0480
1230 LET I5=I5-1
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
1240 IF I5>0 THEN GOTO 1310
1260 PRINT
1270 PRINT "<7><7>BECAUSE NO STANDARDS WERE PROVIDED, NO CALIBRATION H
*    AS BEEN DONE."
1280 GOTO 3000
1290 REM   ------------------------------------------------------------
1300 REM          CREATE DATE OF CALIBRATION
1310 LET D4$="00/00/00"
1320 LET D4$[3-LEN(STR$(SYS(2))),2]=STR$(SYS(2))
1330 LET D4$[6-LEN(STR$(SYS(1))),5]=STR$(SYS(1))
1340 LET D4$[9-LEN(STR$(SYS(3)-1900)),8]=STR$(SYS(3)-1900)
1350 REM   ------------------------------------------------------------
1360 REM          SELECT TYPE OF FIT
1370 PRINT
1380 PRINT "HERE ARE THE TYPES OF CALIBRATION CURVE FITTING:"
1390 PRINT
1400 PRINT "     1.  LINEAR REGRESSION"
1410 PRINT "     2.  QUADRATIC REGRESSION"
1420 PRINT "     3.  LINEAR INTERPOLATION EXTENDED TO THE ORIGIN"
1430 PRINT "     4.  LINEAR REGRESSION FORCED THROUGH THE ORIGIN"
1440 PRINT
1445 ON ERR THEN GOTO 1455
1450 INPUT "WHICH TYPE DO YOU WANT TO USE?  (1, 2, 3, OR 4)  ",X
1455 ON ERR THEN STOP
1460 IF X=1 THEN IF I5>2 THEN GOTO 1500
1465 IF X=2 THEN IF I5>3 THEN GOTO 1500
1470 IF X=3 THEN GOTO 1500
1475 IF X=4 THEN IF I5>2 THEN GOTO 1500
1480 PRINT "<7><7>YOU HAVE NOT USED ENOUGH STANDARDS FOR THIS FIT."
1490 GOTO 1370
1500 ON X THEN GOTO 1890, 1890, 1560, 2650
1510 PRINT
1520 PRINT "<7><7>";X;"IS NOT A VALID TYPE NUMBER."
1530 GOTO 1370
1540 REM   ------------------------------------------------------------
1550 REM          LINEAR INTERPOLATION
1560 FOR I=1 TO F
1570   IF F[I]<>1 THEN GOTO 1830
1580   REM   ------------------------------
1590   REM     COPY STANDARDS TO SMALLER ARRAY
1600   FOR I2=1 TO 30
1610     LET G2[I2]=G[I,I2]
```



```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
1620   NEXT I2
1630   REM   ------------------------------
1640   REM     PUT STANDARDS IN ORDER BY AREA
1645   LET I2$=I$
1650   FOR I3=I5-1 TO 1 STEP -1
1660     FOR I2=1 TO I3
1670       IF G2[2*I2]<G2[2*(I2+1)] THEN GOTO 1770
1680       LET D2=G2[2*I2-1]
1690       LET D3=G2[2*I2]
1700       LET D2$=I2$[8*I2-7,8*I2]
1710       LET G2[2*I2-1]=G2[2*I2+1]
1720       LET G2[2*I2]=G2[2*I2+2]
1730       LET I2$[8*I2-7,8*I2]=I2$[8*(I2+1)-7,8*(I2+1)]
1740       LET G2[2*I2+1]=D2
1750       LET G2[2*I2+2]=D3
1760       LET I2$[8*(I2+1)-7,8*(I2+1)]=D2$
1770     NEXT I2
1780   NEXT I3
1790   REM   ------------------------------
1800   REM     PUT STANDARDS INTO METHOD FILE
1810   MAT WRITE FILE[4,3*I+1],G2
1820   WRITE FILE[4,3*I],D4$,I2$,X,99999,99999,99999,0
1830 NEXT I
1840 PRINT
1850 PRINT "METHOD ";T$[3,6];" HAS BEEN CALIBRATED."
1860 GOTO 3000
1870 REM   ------------------------------------------------------------
1880 REM          NORMAL FIRST AND SECOND DEGREE REGESSION
1890 FOR I=1 TO F
1900   IF F[I]<>1 THEN GOTO 2590
1910   REM   ------------------------------
1920   REM     PERFORM REGRESSION
1930   MAT R=ZER
1940   MAT T=ZER
1950   MAT A=ZER
1960   LET A[1]=I5
1970   FOR I2=1 TO I5
1980     FOR I3=2 TO 2*X+1
1990       LET A[I3]=A[I3]+G[I,I2*2]^(I3-1)
2000     NEXT I3
2010     FOR I3=1 TO X+1
2020       LET R[I3,X+2]=T[I3]+G[I,I2*2-1]*G[I,I2*2]^(I3-1)
```

```
12345678911234567892123456789312345678941234567895123456789612345678 97
        0         0         0         0         0         0         0
2030      LET T[I3]=T[I3]+G[I,I2*2-1]*G[I,I2*2]^(I3-1)
2040    NEXT I3
2050    LET T[X+2]=T[X+2]+G[I,I2*2-1]^2
2060  NEXT I2
2070  FOR I2=1 TO X+1
2080    FOR I3=1 TO X+1
2090      LET R[I2,I3]=A[I2+I3-1]
2100    NEXT I3
2110  NEXT I2
2120  FOR I2=1 TO X+1
2130    FOR I3=I2 TO X+1
2140      IF R[I3,I2]<>0 THEN GOTO 2210
2150    NEXT I3
2160    READ FILE[4,3*I-1],V$
2170    PRINT
2180    PRINT "<7><7>THERE IS NO UNIQUE SOLUTION FOR THE CALIBRATION
*     EQUATION FOR ";V$;"."
2190    PRINT "THEREFORE, ";V$;" HAS NOT BEEN CALIBRATED."
2200    GOTO 2590
2210    FOR I4=1 TO X+1
2220      LET D=R[I2,I4]
2230      LET R[I2,I4]=R[I3,I4]
2240      LET R[I3,I4]=D
2250    NEXT I4
2260    LET Z3=1/R[I2,I2]
2270    FOR I4=1 TO X+2
2280      LET R[I2,I4]=Z3*R[I2,I4]
2290    NEXT I4
2300    FOR I4=1 TO X+1
2310      IF I4=I2 THEN GOTO 2360
2320      LET Z3=-1*R[I4,I2]
2330      FOR I6=1 TO X+2
2340        LET R[I4,I6]=R[I4,I6]+Z3*R[I2,I6]
2350      NEXT I6
2360    NEXT I4
2370  NEXT I2
2380  REM  ------------------------------------
2390  REM     CALCULATE FITTING ERROR
2400  LET J5=0
2410  LET J6=0
2420  FOR I2=1 TO I5
2430    LET J4=R[1,X+2]+G[I,I2*2]*R[2,X+2]
12345678911234567892123456789312345678941234567895123456789612345678 97
        0         0         0         0         0         0         0
```



```
12345678911234567892123456789312345678941234567895123456789612345678 97
        0         0         0         0         0         0         0
2440    IF X=2 THEN LET J4=J4+R[3,X+2]*G[I,I2*2]^2
2450    LET J5=J5+(G[I,I2*2-1]-J4)^2
2460    LET J6=J6+G[I,I2*2-1]
2470  NEXT I2
2480  LET J3=SQR(J5/(I5-2))/(J6/I5)
2490  LET J3=J3*100
2500  REM  ------------------------------------
2510  REM     COPY STANDARDS INTO SMALLER ARRAY
2520  FOR I2=1 TO 30
2530    LET G2[I2]=G[I,I2]
2540  NEXT I2
2550  REM  ------------------------------------
2560  REM     PUT STANDARDS INTO METHOD FILE
2570  MAT WRITE FILE[4,3*I+1],G2
2580  WRITE FILE[4,3*I],D4$,I$,X,R[1,X+2],R[2,X+2],R[3,X+2],J3
2590 NEXT I
2600 PRINT
2610 PRINT "METHOD ";T$[3,6];" HAS BEEN CALIBRATED."
2620 GOTO 3000
2630 REM  ------------------------------------------------------------
2640 REM          LINEAR REGRESSION FORCED THROUGH THE ORIGIN
2650 FOR I=1 TO F
2660  LET J7=0
2670  LET J8=0
2680  LET J9=0
2690  IF F[I]<>1 THEN GOTO 2950
2700  FOR I2=1 TO I5
2710    LET J7=J7+G[I,I2*2-1]*G[I,I2*2]
2720    LET J8=J8+G[I,I2*2]^2
2730    LET J9=J9+G[I,I2*2-1]
2740  NEXT I2
2750  LET R2=J7/J8
2760  REM  ------------------------------------
2770  REM     CALCULATE FITTING ERROR
2780  LET J5=0
2790  LET J6=0
2800  FOR I2=1 TO I5
2810    LET J5=J5+(G[I,I2*2-1]-G[I,I2*2]*R2)^2
2820    LET J6=J6+G[I,I2*2-1]
2830  NEXT I2
2840  LET J3=SQR(J5/(I5-2))/(J6/I5)
2850  LET J3=J3*100
12345678911234567892123456789312345678941234567895123456789612345678 97
        0         0         0         0         0         0         0
```

PROGRAM LISTING FOR GC04

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
2860   REM   ------------------------------------
2870   REM     COPY STANDARDS INTO SMALLER ARRAY
2880   FOR I2=1 TO 30
2890     LET G2[I2]=G[I,I2]
2900   NEXT I2
2910   REM   ------------------------------------
2920   REM     PUT DATA INTO METHOD FILE
2930   MAT WRITE FILE[4,3*I+1],G2
2940   WRITE FILE[4,3*I],D4$,I$,X,0,R2,0,J3
2950 NEXT I
2960 PRINT
2970 PRINT "METHOD ";T$[3,6];" HAS BEEN CALIBRATED."
2980 REM   ------------------------------------------------------
2990 REM          RETURN TO MASTER CONTROL
3000 ON ERR THEN GOTO 3020
3010 CLOSE FILE[3]
3020 ON ERR THEN GOTO 3040
3030 CLOSE FILE[7]
3040 ON ERR THEN STOP
3050 NOESC
3060 CHAIN "GC00"
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```


SYMBOL TABLE FOR GC04

SYMBOL	REFERENCES				
0170	0200				
0230	0180				
0242	0237				
0300	0250				
0365	0355				
0380	0340				
0410	0290				
0480	1220				
0540	0490	0600	0710	0870	1170
0555	0545				
0610	0570				
0620	0670				
0640	0620				
0680	0650				
0720	0680	0780			
0760	0720				
0810	0750				
0900	0820				
0910	0980				
1001	0920	1007	1015		
1003	1001				
1008	1005				
1012	1010				
1016	1013	1022			
1020	1016				
1026	1019				
1060	1041				
1080	1120				
1130	1090				
1180	1100				
1190	1030	1043			
1230	0530	0560			
1310	1240				
1370	1490	1530			
1455	1445				
1500	1460	1465	1470	1475	
1560	1500				
1770	1670				
1830	1570				
1890	1500				
2210	2140				
2360	2310				
2590	1900	2200			
2650	1500				
2950	2690				

SYMBOL TABLE FOR GC04

SYMBOL	REFERENCES									
3000	0080	1280	1860	2620						
3020	3000									
3040	3020									
A	1950									
A6$	0105	1008	1009	1011	1017					
A7	1004	1005	1009							
A8$	0105	1002	1004	1006	1014					
A9$	0105	0106	1004							
A[	0090	1960	1990	2090						
B	1080									
C	1080	1100	1180							
D	2220	2240								
D2	1680	1740								
D2$	0100	0550	0560	0570	0590	0610	0700	0840	0850	0950
	1140	1150	1210	1700	1760					
D3	1690	1750								
D3$	0100	0610	0630	0730						
D4$	0100	1310	1320	1330	1340	1820	2580	2940		
F	0120	0150	0170	0190	0260	0320	1027	1560	1890	2650
FL#3	0730	0810	0860	0910	1080	1160	1200	3010		
FL#4	0160	0165	0166	0170	0330	1040	1810	1820	2160	2570
	2580	2930	2940							
FL#7	1017	1060	1165	1201	3030					
F[	0100	0270	0370	1030	1042	1570	1900	2690		
G	0110									
G$	0100	1080	1100							
G2	1810	2570	2930							
G2[	0100	1610	1670	1680	1690	1710	1720	1740	1750	2530
	2890									
G[	0100	1060	1180	1610	1990	2020	2030	2050	2430	2440
	2450	2460	2530	2710	2720	2730	2810	2820	2890	
H$	0100	1080								
I	0260	0270	0280	0320	0330	0370	0380	1027	1030	1040
	1042	1060	1180	1190	1560	1570	1610	1810	1820	1830
	1890	1900	1990	2020	2030	2050	2160	2430	2440	2450
	2460	2530	2570	2580	2590	2650	2690	2710	2720	2730
	2810	2820	2890	2930	2940	2950				
I$	0100	1210	1645	2580	2940					
I2	1070	1080	1110	1600	1610	1620	1660	1670	1680	1690
	1700	1710	1720	1730	1740	1750	1760	1770	1970	1990
	2020	2030	2050	2060	2070	2090	2110	2120	2130	2140
	2220	2230	2260	2280	2310	2320	2340	2370	2420	2430
	2440	2450	2460	2470	2520	2530	2540	2700	2710	2720
	2730	2740	2800	2810	2820	2830	2880	2890	2900	
I2$	0100	1645	1700	1730	1760	1820				

SYMBOL TABLE FOR GC04

SYMBOL	REFERENCES									
I3	1650	1660	1780	1980	1990	2000	2010	2020	2030	2040
	2080	2090	2100	2130	2140	2150	2230	2240		
I4	2210	2220	2230	2240	2250	2270	2280	2290	2300	2310
	2320	2340	2360							
I5	0450	0480	0490	1060	1180	1230	1240	1460	1465	1475
	1650	1960	1970	2420	2480	2700	2800	2840		
I6	2330	2340	2350							
J	0810	0820	0840	0850						
J3	2480	2490	2580	2840	2850	2940				
J4	2430	2440	2450							
J5	2400	2450	2480	2780	2810	2840				
J6	2410	2460	2480	2790	2820	2840				
J7	2660	2710	2750							
J8	2670	2720	2750							
J9	2680	2730								
P9	0900	0910	0970	1026	1070					
R	1930									
R2	2750	2810	2940							
R[	0090	2020	2090	2140	2220	2230	2240	2260	2280	2320
	2340	2430	2440	2580						
T	1940									
T$	0100	0160	0166	0235	1008	1850	2610	2970		
T[	0090	2020	2030	2050						
V$	0100	0170	0330	0340	0350	1040	1041	1100	1140	2160
	2180	2190								
V0$	0090	0910	0920	0950						
X	1450	1460	1465	1470	1475	1500	1520	1820	1980	2010
	2020	2050	2070	2080	2120	2130	2210	2270	2300	2330
	2430	2440	2580	2940						
X$	0100	0240	0250	0360	0370					
Z3	2260	2280	2320	2340						

SECTION 7

PROGRAM GC05 - LIQUID/LIQUID EXTRACTION AND DIRECT AQUEOUS INJECTION CALIBRATION

GC05 is the program which performs calibration for standards prepared by the liquid/liquid extraction and direct aqueous injection methods. It is essentially the same as program GC04. The only difference is that in addition to asking the user for the concentration of each compound, this program also asks for the injection volume of each standard. It then multiplies the prepared concentration (in micrograms per liter) times the injection volume (in microliters) times 1000 to get the mass (in nanograms) of each compound. Calibration is then done on the basis of mass.

One additional symbol is used in GC05. It is Z, the volume of the injection.

PROGRAM LISTING FOR GC05

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                    +
0030 REM   +   PROGRAM GC05, EXTERNAL STANDARDS CALIBRATION, L/L, DAI+
0040 REM   +   BY:  J. KOPKE (SWORCC), MARCH 19, 1979                 +
0045 REM   +   MOST RECENT REVISION:  APRIL 17, 1979                  +
0050 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0060 REM
0070 ESC
0080 ON ESC THEN GOTO 3000
0090 DIM A[5],R[3,4],T[4],V0$[20]
0100 DIM F[60],G[60,30],I$[160],T$[6],X$[3],V$[8],D2$[8],D3$[10],D4$[8
*    ],G$[8],H$[2],G2[30],I2$[160]
0105 DIM A9$[26],A8$[1],A6$[9]
0106 LET A9$="ABCDEFGHIJKLMNOPQRSTUVWXYZ"
0110 MAT G=ZER
0120 MAT F=ZER
0130 REM   ------------------------------------------------------------
0140 REM          COUNT NUMBER OF IDENTIFIERS IN METHOD FILE
0150 LET F=0
0160 READ FILE[4,1],T$
0165 CLOSE FILE[4]
0166 OPEN FILE[4,0],T$,200
0170 READ FILE[4,3*(F+1)-1],V$
0180 IF EOF(4) THEN GOTO 0230
0190 LET F=F+1
0200 GOTO 0170
0210 REM   ------------------------------------------------------------
0220 REM          FLAG THE IDENTIFIERS TO BE CALIBRATED
0230 PRINT
0235 PRINT "DO YOU WANT TO CALIBRATE ALL IDENTIFIERS OF METHOD ";T$[3,
*    6];
0237 ON ERR THEN GOTO 0242
0240 INPUT " AT ONCE?  (Y OR N)  ",X$
0242 ON ERR THEN STOP
0250 IF X$[1,1]<>"Y" THEN GOTO 0300
0260 FOR I=1 TO F
0270   LET F[I]=1
0280 NEXT I
0290 GOTO 0410
0300 PRINT
0310 PRINT "DO YOU WANT TO CALIBRATE ";
0320 FOR I=1 TO F
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```


PROGRAM LISTING FOR GC05

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0330   READ FILE[4,3*I-1],V$
0340   IF V$="99999" THEN GOTO 0380
0350   PRINT  TAB(25);V$;"?"; TAB(37);"  (Y OR N)";
0355   ON ERR THEN GOTO 0365
0360   INPUT "  ",X$
0365   ON ERR THEN STOP
0370   IF X$[1,1]="Y" THEN LET F[I]=1
0380 NEXT I
0390 REM   ------------------------------------------------------------
0400 REM          PRINT INSTRUCTIONS FOR ENTERING DATA
0410 PRINT
0420 PRINT "ENTER THE FOLLOWING CALIBRATION INFORMATION."
0440 PRINT "TYPE 'END' AS AN INJECTION ID TO TERMINATE THE LIST."
0450 LET I5=0
0460 REM   ------------------------------------------------------------
0470 REM          OPEN SELECTED DATA FILE
0480 LET I5=I5+1
0490 IF I5<16 THEN GOTO 0540
0500 PRINT
0510 PRINT "<7><7>YOU HAVE USED FIFTEEN CALIBRATION STANDARDS, WHICH I
*    S THE LIMIT"
0520 PRINT "     FOR THIS PROGRAM."
0530 GOTO 1230
0540 PRINT
0545 ON ERR THEN GOTO 0555
0550 INPUT "INJECTION ID FOR CALIBRATION STANDARD?  ",D2$
0555 ON ERR THEN STOP
0560 IF D2$="END" THEN GOTO 1230
0570 IF LEN(D2$)=8 THEN GOTO 0610
0580 PRINT
0590 PRINT "<7><7>";D2$;" IS NOT A VALID INJECTION ID NUMBER."
0600 GOTO 0540
0610 LET D3$="GC",D2$
0620 ON ERR THEN GOTO 0640
0630 RENAME D3$,D3$
0640 ON ERR THEN STOP
0650 IF SYS(7)<>-48 THEN GOTO 0680
0660 DELAY =1
0670 GOTO 0620
0680 IF SYS(7)=-9 THEN GOTO 0720
0690 PRINT
0700 PRINT "<7><7>THERE IS NO EXISTING DATA FOR INJECTION ID ";D2$;"."
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0710 GOTO 0540
0720 ON ERR THEN GOTO 0760
0730 OPEN FILE[3,0],D3$,31
0740 ON ERR THEN STOP
0750 GOTO 0810
0760 ON ERR THEN STOP
0770 DELAY =1
0780 GOTO 0720
0790 REM  ------------------------------------------------------------
0800 REM          CHECK DATA FILE USABILITY FLAG
0810 READ FILE[3,1],J
0820 IF J=1 THEN GOTO 0900
0830 PRINT
0840 IF J=2 THEN PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPOR
*    T DID NOT HAVE A TOTAL AREA."
0850 IF J=3 THEN PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPOR
*    T WAS IN THE WRONG FORMAT."
0860 CLOSE FILE[3]
0870 GOTO 0540
0880 REM  ------------------------------------------------------------
0890 REM          PRINT ANY ERROR MESSAGES FOUND IN THE DATA FILE
0900 LET P9=2
0910 READ FILE[3,P9],V0$
0920 IF V0$[1,7]<>"MESSAGE" THEN GOTO 0992
0930 PRINT
0940 PRINT "THE FOLLOWING MESSAGE WAS PART OF THE REPORT FOR"
0950 PRINT "     INJECTION ";D2$;":  ";V0$;"."
0960 PRINT
0970 LET P9=P9+1
0980 GOTO 0910
0990 REM  ------------------------------------------------------------
0991 REM          OPEN CONCENTRATION PATTERN FILE
0992 ON ERR THEN GOTO 0994
0993 INPUT "     CONCENTRATION PATTERN FOR STANDARD?  ",A8$
0994 ON ERR THEN STOP
0995 LET A7=POS(A9$,A8$,1)
0996 IF A7<>0 THEN GOTO 0999
0997 PRINT "<7><7>     '";A8$;"' IS NOT A VALID LETTER."
0998 GOTO 0992
0999 LET A6$=T$,"000"
1000 LET A6$[10-LEN(STR$(A7)),9]=STR$(A7)
1001 ON ERR THEN GOTO 1003
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```



```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
1002 RENAME A6$,A6$
1003 ON ERR THEN STOP
1004 IF SYS(7)=-9 THEN GOTO 1007
1005 PRINT "<7><7>     THERE IS NO EXISTING PATTERN NAMED '";A8$;"'."
1006 GOTO 0992
1007 ON ERR THEN GOTO 1011
1008 OPEN FILE[7,0],A6$,4
1009 ON ERR THEN STOP
1010 GOTO 1020
1011 ON ERR THEN STOP
1012 DELAY =1
1013 GOTO 1007
1015 REM  ------------------------------------------------------------
1016 REM          GATHER CALIBRATION DATA
1020 ON ERR THEN GOTO 1022
1021 INPUT "     INJECTION VOLUME IN MICROLITERS?  ",Z
1022 ON ERR THEN STOP
1023 LET P9=P9+2
1024 FOR I=1 TO F
1030   IF F[I]<>1 THEN GOTO 1190
1040   READ FILE[4,3*I-1],V$
1041   IF V$<>"99999" THEN GOTO 1060
1042   LET F[I]=0
1043   GOTO 1190
1060   READ FILE[7,I],G[I,2*I5-1]
1065   LET G[I,2*I5-1]=G[I,2*I5-1]*Z*1000
1070   LET I2=P9
1080   READ FILE[3,I2],G$,H$,B,C
1090   IF EOF(3) THEN GOTO 1130
1100   IF G$=V$ THEN IF C<>-9999 THEN GOTO 1180
1110   LET I2=I2+1
1120   GOTO 1080
1130   PRINT
1140   PRINT "<7><7>THE REPORT FOR INJECTION ";D2$;" DOES NOT INCLUDE
*    AN AREA FOR ";V$;"."
1150   PRINT "THEREFORE, ";D2$;" CANNOT BE USED IN THIS CALIBRATION."
1160   CLOSE FILE[3]
1165   CLOSE FILE[7]
1170   GOTO 0540
1180   LET G[I,2*I5]=C
1190 NEXT I
1200 CLOSE FILE[3]
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

```
12345678911234567892123456789312345678941234567895123456789612345678971
         0         0         0         0         0         0         0
1201 CLOSE FILE[7]
1210 LET I$=I$,D2$
1220 GOTO 0480
1230 LET I5=I5-1
1240 IF I5>0 THEN GOTO 1310
1260 PRINT
1270 PRINT "<7><7>BECAUSE NO STANDARDS WERE PROVIDED, NO CALIBRATION H
*     AS BEEN DONE."
1280 GOTO 3000
1290 REM   ------------------------------------------------------------
1300 REM          CREATE DATE OF CALIBRATION
1310 LET D4$="00/00/00"
1320 LET D4$[3-LEN(STR$(SYS(2))),2]=STR$(SYS(2))
1330 LET D4$[6-LEN(STR$(SYS(1))),5]=STR$(SYS(1))
1340 LET D4$[9-LEN(STR$(SYS(3)-1900)),8]=STR$(SYS(3)-1900)
1350 REM   ------------------------------------------------------------
1360 REM          SELECT TYPE OF FIT
1370 PRINT
1380 PRINT "HERE ARE THE TYPES OF CALIBRATION CURVE FITTING:"
1390 PRINT
1400 PRINT "     1.  LINEAR REGRESSION"
1410 PRINT "     2.  QUADRATIC REGRESSION"
1420 PRINT "     3.  LINEAR INTERPOLATION EXTENDED TO THE ORIGIN"
1430 PRINT "     4.  LINEAR REGRESSION FORCED THROUGH THE ORIGIN"
1440 PRINT
1445 ON ERR THEN GOTO 1455
1450 INPUT "WHICH TYPE DO YOU WANT TO USE?  (1, 2, 3, OR 4)  ",X
1455 ON ERR THEN STOP
1460 IF X=1 THEN IF I5>2 THEN GOTO 1500
1465 IF X=2 THEN IF I5>3 THEN GOTO 1500
1470 IF X=3 THEN GOTO 1500
1475 IF X=4 THEN IF I5>2 THEN GOTO 1500
1480 PRINT "<7><7>YOU HAVE NOT USED ENOUGH STANDARDS FOR THIS FIT."
1490 GOTO 1370
1500 ON X THEN GOTO 1890, 1890, 1560, 2650
1510 PRINT
1520 PRINT "<7><7>";X;"IS NOT A VALID TYPE NUMBER."
1530 GOTO 1370
1540 REM   ------------------------------------------------------------
1550 REM          LINEAR INTERPOLATION
1560 FOR I=1 TO F
1570   IF F[I]<>1 THEN GOTO 1830
```

12345678911234567892123456789312345678941234567895123456789612345678971
         0   0   0   0   0   0   0

12345678911234567892123456789312345678941234567895123456789612345678971
         0   0   0   0   0   0   0

```
1580   REM   ----------------------------------------
1590   REM      COPY STANDARDS TO SMALLER ARRAY
1600   FOR I2=1 TO 30
1610     LET G2[I2]=G[I,I2]
1620   NEXT I2
1630   REM   ----------------------------------------
1640   REM      PUT STANDARDS IN ORDER BY AREA
1645   LET I2$=I$
1650   FOR I3=I5-1 TO 1 STEP -1
1660     FOR I2=1 TO I3
1670       IF G2[2*I2]<G2[2*(I2+1)] THEN GOTO 1770
1680       LET D2=G2[2*I2-1]
1690       LET D3=G2[2*I2]
1700       LET D2$=I2$[8*I2-7,8*I2]
1710       LET G2[2*I2-1]=G2[2*I2+1]
1720       LET G2[2*I2]=G2[2*I2+2]
1730       LET I2$[8*I2-7,8*I2]=I2$[8*(I2+1)-7,8*(I2+1)]
1740       LET G2[2*I2+1]=D2
1750       LET G2[2*I2+2]=D3
1760       LET I2$[8*(I2+1)-7,8*(I2+1)]=D2$
1770     NEXT I2
1780   NEXT I3
1790   REM   ----------------------------------------
1800   REM      PUT STANDARDS INTO METHOD FILE
1810   MAT WRITE FILE[4,3*I+1],G2
1820   WRITE FILE[4,3*I],D4$,I2$,X,99999,99999,99999,0
1830 NEXT I
1840 PRINT
1850 PRINT "METHOD ";T$[3,6];" HAS BEEN CALIBRATED."
1860 GOTO 3000
1870 REM   ------------------------------------------------------------
1880 REM          NORMAL FIRST AND SECOND DEGREE REGESSION
1890 FOR I=1 TO F
1900   IF F[I]<>1 THEN GOTO 2590
1910   REM   ----------------------------------------
1920   REM      PERFORM REGRESSION
1930   MAT R=ZER
1940   MAT T=ZER
1950   MAT A=ZER
1960   LET A[1]=I5
1970   FOR I2=1 TO I5
1980     FOR I3=2 TO 2*X+1
```

12345678911234567892123456789312345678941234567895123456789612345678971
         0   0   0   0   0   0   0

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
1990      LET A[I3]=A[I3]+G[I,I2*2]^(I3-1)
2000    NEXT I3
2010    FOR I3=1 TO X+1
2020      LET R[I3,X+2]=T[I3]+G[I,I2*2-1]*G[I,I2*2]^(I3-1)
2030      LET T[I3]=T[I3]+G[I,I2*2-1]*G[I,I2*2]^(I3-1)
2040    NEXT I3
2050    LET T[X+2]=T[X+2]+G[I,I2*2-1]^2
2060  NEXT I2
2070  FOR I2=1 TO X+1
2080    FOR I3=1 TO X+1
2090      LET R[I2,I3]=A[I2+I3-1]
2100    NEXT I3
2110  NEXT I2
2120  FOR I2=1 TO X+1
2130    FOR I3=I2 TO X+1
2140      IF R[I3,I2]<>0 THEN GOTO 2210
2150    NEXT I3
2160    READ FILE[4,3*I-1],V$
2170    PRINT
2180    PRINT "<7><7>THERE IS NO UNIQUE SOLUTION FOR THE CALIBRATION
*     EQUATION FOR ";V$;"."
2190    PRINT "THEREFORE, ";V$;" HAS NOT BEEN CALIBRATED."
2200    GOTO 2590
2210    FOR I4=1 TO X+1
2220      LET D=R[I2,I4]
2230      LET R[I2,I4]=R[I3,I4]
2240      LET R[I3,I4]=D
2250    NEXT I4
2260    LET Z3=1/R[I2,I2]
2270    FOR I4=1 TO X+2
2280      LET R[I2,I4]=Z3*R[I2,I4]
2290    NEXT I4
2300    FOR I4=1 TO X+1
2310      IF I4=I2 THEN GOTO 2360
2320      LET Z3=-1*R[I4,I2]
2330      FOR I6=1 TO X+2
2340        LET R[I4,I6]=R[I4,I6]+Z3*R[I2,I6]
2350      NEXT I6
2360    NEXT I4
2370  NEXT I2
2380  REM  ------------------------------------
2390  REM    CALCULATE FITTING ERROR
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```



```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
2400  LET J5=0
2410  LET J6=0
2420  FOR I2=1 TO I5
2430    LET J4=R[1,X+2]+G[I,I2*2]*R[2,X+2]
2440    IF X=2 THEN LET J4=J4+R[3,X+2]*G[I,I2*2]^2
2450    LET J5=J5+(G[I,I2*2-1]-J4)^2
2460    LET J6=J6+G[I,I2*2-1]
2470  NEXT I2
2480  LET J3=SQR(J5/(I5-2))/(J6/I5)
2490  LET J3=J3*100
2500  REM  ------------------------------------
2510  REM     COPY STANDARDS INTO SMALLER ARRAY
2520  FOR I2=1 TO 30
2530    LET G2[I2]=G[I,I2]
2540  NEXT I2
2550  REM  ------------------------------------
2560  REM     PUT STANDARDS INTO METHOD FILE
2570  MAT WRITE FILE[4,3*I+1],G2
2580  WRITE FILE[4,3*I],D4$,I$,X,R[1,X+2],R[2,X+2],R[3,X+2],J3
2590 NEXT I
2600 PRINT
2610 PRINT "METHOD ";T$[3,6];" HAS BEEN CALIBRATED."
2620 GOTO 3000
2630 REM  ------------------------------------------------------------
2640 REM          LINEAR REGRESSION FORCED THROUGH THE ORIGIN
2650 FOR I=1 TO F
2660  LET J7=0
2670  LET J8=0
2680  LET J9=0
2690  IF F[I]<>1 THEN GOTO 2950
2700  FOR I2=1 TO I5
2710    LET J7=J7+G[I,I2*2-1]*G[I,I2*2]
2720    LET J8=J8+G[I,I2*2]^2
2730    LET J9=J9+G[I,I2*2-1]
2740  NEXT I2
2750  LET R2=J7/J8
2760  REM  ------------------------------------
2770  REM     CALCULATE FITTING ERROR
2780  LET J5=0
2790  LET J6=0
2800  FOR I2=1 TO I5
2810    LET J5=J5+(G[I,I2*2-1]-G[I,I2*2]*R2)^2
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

PROGRAM LISTING FOR GC05

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0
2820      LET J6=J6+G[I,I2*2-1]
2830    NEXT I2
2840    LET J3=SQR(J5/(I5-2))/(J6/I5)
2850    LET J3=J3*100
2860    REM   ------------------------------------
2870    REM      COPY STANDARDS INTO SMALLER ARRAY
2880    FOR I2=1 TO 30
2890      LET G2[I2]=G[I,I2]
2900    NEXT I2
2910    REM   ------------------------------------
2920    REM      PUT DATA INTO METHOD FILE
2930    MAT WRITE FILE[4,3*I+1],G2
2940    WRITE FILE[4,3*I],D4$,I$,X,0,R2,0,J3
2950 NEXT I
2960 PRINT
2970 PRINT "METHOD ";T$[3,6];" HAS BEEN CALIBRATED."
2980 REM   ------------------------------------------------
2990 REM          RETURN TO MASTER CONTROL
3000 ON ERR THEN GOTO 3020
3010 CLOSE FILE[3]
3020 ON ERR THEN GOTO 3040
3030 CLOSE FILE[7]
3040 ON ERR THEN STOP
3050 NOESC
3060 CHAIN "GC00"
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0
```


SYMBOL TABLE FOR GC05

SYMBOL	REFERENCES				
0170	0200				
0230	0180				
0242	0237				
0300	0250				
0365	0355				
0380	0340				
0410	0290				
0480	1220				
0540	0490	0600	0710	0870	1170
0555	0545				
0610	0570				
0620	0670				
0640	0620				
0680	0650				
0720	0680	0780			
0760	0720				
0810	0750				
0900	0820				
0910	0980				
0992	0920	0998	1006		
0994	0992				
0999	0996				
1003	1001				
1007	1004	1013			
1011	1007				
1020	1010				
1022	1020				
1060	1041				
1080	1120				
1130	1090				
1180	1100				
1190	1030	1043			
1230	0530	0560			
1310	1240				
1370	1490	1530			
1455	1445				
1500	1460	1465	1470	1475	
1560	1500				
1770	1670				
1830	1570				
1890	1500				
2210	2140				
2360	2310				
2590	1900	2200			
2650	1500				

SYMBOL TABLE FOR GC05

SYMBOL	REFERENCES									
2950	2690									
3000	0080	1280	1860	2620						
3020	3000									
3040	3020									
A	1950									
A6$	0105	0999	1000	1002	1008					
A7	0995	0996	1000							
A8$	0105	0993	0995	0997	1005					
A9$	0105	0106	0995							
A[	0090	1960	1990	2090						
B	1080									
C	1080	1100	1180							
D	2220	2240								
D2	1680	1740								
D2$	0100	0550	0560	0570	0590	0610	0700	0840	0850	0950
	1140	1150	1210	1700	1760					
D3	1690	1750								
D3$	0100	0610	0630	0730						
D4$	0100	1310	1320	1330	1340	1820	2580	2940		
F	0120	0150	0170	0190	0260	0320	1024	1560	1890	2650
FL#3	0730	0810	0860	0910	1080	1160	1200	3010		
FL#4	0160	0165	0166	0170	0330	1040	1810	1820	2160	2570
	2580	2930	2940							
FL#7	1008	1060	1165	1201	3030					
F[	0100	0270	0370	1030	1042	1570	1900	2690		
G	0110									
G$	0100	1080	1100							
G2	1810	2570	2930							
G2[	0100	1610	1670	1680	1690	1710	1720	1740	1750	2530
	2890									
G[	0100	1060	1065	1180	1610	1990	2020	2030	2050	2430
	2440	2450	2460	2530	2710	2720	2730	2810	2820	2890
H$	0100	1080								
I	0260	0270	0280	0320	0330	0370	0380	1024	1030	1040
	1042	1060	1065	1180	1190	1560	1570	1610	1810	1820
	1830	1890	1900	1990	2020	2030	2050	2160	2430	2440
	2450	2460	2530	2570	2580	2590	2650	2690	2710	2720
	2730	2810	2820	2890	2930	2940	2950			
I$	0100	1210	1645	2580	2940					
I2	1070	1080	1110	1600	1610	1620	1660	1670	1680	1690
	1700	1710	1720	1730	1740	1750	1760	1770	1970	1990
	2020	2030	2050	2060	2070	2090	2110	2120	2130	2140
	2220	2230	2260	2280	2310	2320	2340	2370	2420	2430
	2440	2450	2460	2470	2520	2530	2540	2700	2710	2720
	2730	2740	2800	2810	2820	2830	2880	2890	2900	

SYMBOL TABLE FOR GC05

SYMBOL	REFERENCES									
I2$	0100	1645	1700	1730	1760	1820				
I3	1650	1660	1780	1980	1990	2000	2010	2020	2030	2040
	2080	2090	2100	2130	2140	2150	2230	2240		
I4	2210	2220	2230	2240	2250	2270	2280	2290	2300	2310
	2320	2340	2360							
I5	0450	0480	0490	1060	1065	1180	1230	1240	1460	1465
	1475	1650	1960	1970	2420	2480	2700	2800	2840	
I6	2330	2340	2350							
J	0810	0820	0840	0850						
J3	2480	2490	2580	2840	2850	2940				
J4	2430	2440	2450							
J5	2400	2450	2480	2780	2810	2840				
J6	2410	2460	2480	2790	2820	2840				
J7	2660	2710	2750							
J8	2670	2720	2750							
J9	2680	2730								
P9	0900	0910	0970	1023	1070					
R	1930									
R2	2750	2810	2940							
R[	0090	2020	2090	2140	2220	2230	2240	2260	2280	2320
	2340	2430	2440	2580						
T	1940									
T$	0100	0160	0166	0235	0999	1850	2610	2970		
T[	0090	2020	2030	2050						
V$	0100	0170	0330	0340	0350	1040	1041	1100	1140	2160
	2180	2190								
V0$	0090	0910	0920	0950						
X	1450	1460	1465	1470	1475	1500	1520	1820	1980	2010
	2020	2050	2070	2080	2120	2130	2210	2270	2300	2330
	2430	2440	2580	2940						
X$	0100	0240	0250	0360	0370					
Z	1021	1065								
Z3	2260	2280	2320	2340						

SECTION 8

PROGRAM GC06 - CALIBRATION CURVE PLOTTING

GC06 is the program which draws a calibration curve and prints a table of residuals. It is entered by chaining from the master control program, GC00, and it chains back to that program if the escape key is pressed. The plotting features of this program are written exclusively for a Tektronix 4000 Series Computer Display Terminal, or a Hewlett-Packard 2647 or 2648 terminal in Tektronix compatability mode. However, the program is designed so that it can print all of the calibration information except the plot itself on a non-Tektronix terminal.

This program uses a set of general purpose BASIC Tektronix plotting subroutines which were developed by the Advanced Instrumentation Section. Complete documentation for those subroutines is available from that office.

As GC06 begins, it asks the analyst what type of terminal is being used. It then asks the user for the number of the method. It checks whether any such method file exists. The program then opens the method file and counts the number of identifiers in that file.

Next, the program asks the user for the identifier whose calibration curve is to be plotted, and it searches the method file for that identifier. When it finds the appropriate identifier, it reads all of the calibration data for that identifier from the method file.

Then, on a Tektronix-type terminal, the program clears the screen by printing "<27><12>" and DELAYing one second to allow the screen to physically clear. Then it prints the headings for the calibration curve plot. The program uses subroutine BSCPLT.SR to establish the origin at a random location within five addressable points of the lower left corner of the screen. This causes each graph to be drawn in a slightly different location so that the screen will wear more evenly.

Next, the program uses subroutine BSCAXS.SR four times to draw the four sides of the box. The axes are then identified.

The subroutine BSCSCL.SR is then used to generate numbers which scale the horizontal and vertical axes.

Next, the subroutine BSCMKR.SR is used to mark the calibration standards on the chart. If the type of curve fitting is linear interpolation, BSCMKR.SR also connects the points with straight line segments. For any of

the other types of curve fitting, GC06 uses subroutine BSCLIN.SR to draw the curve. The bell is then sounded five times to tell the user that the drawing is complete. A TINPUT statement then causes GC06 to wait while the user makes a hard copy of the calibration curve. The program continues when the user presses the RETURN key or when the sixty seconds allowed for the TINPUT are over.

Next, the program prints the table of residuals, and it again sounds the bell five times and waits while the user makes a hard copy.

Finally, if the user wants to produce another graph, the program branches back to begin again. Otherwise, the program disables the escape feature and chains back to GC00.

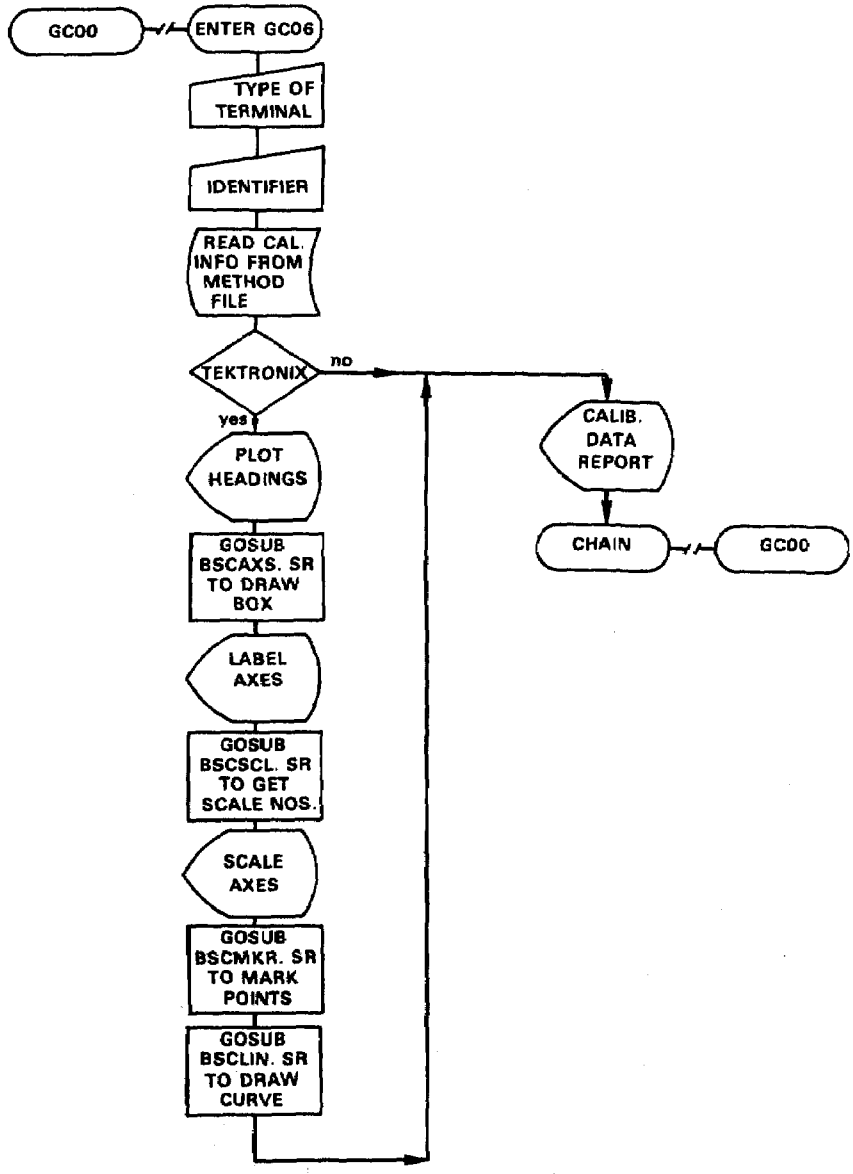

Figure 7. Flowchart of Program GC06.

TABLE 5. SYMBOL DEFINITIONS FOR PROGRAM GC06

D4$	the date of calibration
G2()	the array of prepared concentrations and peak areas
I	the control variable for loops
I$	the superstring of injection IDs of standards used
I5	the number of identifiers in the method file
J3	the fitting error
K	the type of fit K=1 linear regression K=2 quadratic regression K=3 linear interpolation K=4 linear regression forced through the origin
L2	the calculated concentration of a standard
N1	the type of processing and calibration
P1	see BSCPLT.SR
P1$	see BSCPLT.SR
P2	see BSCPLT.SR
P2$	see BSCPLT.SR
P3	see BSCPLT.SR
P3$	see BSCPLT.SR
P4	see BSCPLT.SR
P4$	see BSCPLT.SR
P5	see BSCPLT.SR
P5$	see BSCMKR.SR

TABLE 5. (continued)

P6	see BSCPLT.SR
P7	see BSCPLT.SR
P8	see BSCPLT.SR
P9	see BSCPLT.SR
P()	see BSCLIN.SR
Q1	see BSCAXS.SR
Q2	see BSCAXS.SR
Q3	see BSCAXS.SR and BSCLIN.SR
Q4	see BSCAXS.SR
Q5	see BSCAXS.SR
Q5$	the format of a PRINT USING statement
Q6	see BSCAXS.SR
Q7	see BSCLIN.SR
Q8	see BSCLIN.SR
Q9	see BSCLIN.SR
Q()	see BSCLIN.SR
R1	the constant term of the regression equation
R2	the coefficient of the linear term of the regression equation
R3	the coefficient of the quadratic term of the regression equation
S$	the axis identification string
S1	see BSCSCL.SR
S2	see BSCSCL.SR
S3	see BSCSCL.SR
S4	see BSCSCL.SR

TABLE 5. (continued)

S5	see BSCSCL.SR
S6	see BSCSCL.SR
S7	see BSCSCL.SR
S()	see BSCSCL.SR
T$	the name of the method file
U$	the name of the analyst
U1	see BSCMKR.SR
U2	see BSCMKR.SR
U3	see BSCMKR.SR
V$	an identifier in a method file
V7$	the identifier to be plotted
X$	the user's answer to a Y or N question
X7	the x-coordinate of a point of the curve
X8	the x-coordinate of the left side of the box
X9	the x-coordinate of the right side of the box
Y8	the y-coordinate of the bottom of the box
Y9	the y-coordinate of the top of the box
Z5	the position of a slash in a string

PROGRAM LISTING FOR GC06

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                      +
0030 REM   +   PROGRAM GC06, CALIBRATION CURVE PLOTTING                 +
0040 REM   +   BY:  J. KOPKE (SWORCC), MARCH 6, 1979                    +
0045 REM   +   MOST RECENT REVISION:  MAY 8, 1979                       +
0050 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0060 REM
0070 DIM D4$[8],G2[30],I$[160],P[100],Q5$[75],Q[100],S$[40],T$[6]
0080 DIM U$[20],V$[8],V7$[8],X$[3]
0090 PAGE =132
0100 ON ESC THEN GOTO 3130
0110 ESC
0120 PRINT
0121 PRINT "HERE ARE THE TYPES OF TERMINALS:"
0122 PRINT
0123 PRINT "     1.  TEKTRONIX 4000 SERIES"
0124 PRINT "     2.  HEWLETT-PACKARD 2647 OR 2648"
0125 PRINT "     3.  ALL OTHER TERMINALS"
0126 PRINT
0130 ON ERR THEN GOTO 0150
0140 INPUT "WHICH TYPE OF TERMINAL ARE YOU USING?  (1, 2, OR 3)  ",X
0150 ON ERR THEN STOP
0151 IF X=ABS(INT(X)) THEN IF X>0 THEN IF X<4 THEN GOTO 0160
0152 PRINT
0153 PRINT "<7><7>";X;"IS NOT A VALID TYPE NUMBER."
0154 GOTO 0120
0160 IF X<>3 THEN GOTO 0210
0170 PRINT
0180 PRINT "THE PLOTTING FEATURES OF THIS OPTION WILL BE SKIPPED."
0200 GOTO 0260
0210 GOSUB 9905
0220 REM   ---------------------------------------------------------
0230 REM          OPEN METHOD FILE
0260 READ FILE[4,1],T$
0270 CLOSE FILE[4]
0280 OPEN FILE[4,0],T$,200
0540 REM   ---------------------------------------------------------
0550 REM          COUNT IDENTIFIERS IN METHOD FILE
0560 LET I5=1
0570 READ FILE[4,3*I5-1],V$
0580 IF EOF(4) THEN GOTO 0610
0590 LET I5=I5+1
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```


PROGRAM LISTING FOR GC06

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0600 GOTO 0570
0610 LET I5=I5-1
0620 REM   ---------------------------------------------------------
0630 REM          INPUT IDENTIFIER TO BE PLOTTED
0640 PRINT
0645 PRINT "WHAT IDENTIFIER FROM METHOD ";T$[3,6];
0650 ON ERR THEN GOTO 0720
0660 INPUT " DO YOU WANT CALIBRATION DATA FOR?  ",V7$
0670 ON ERR THEN STOP
0680 LET Z5=POS(V7$,"/",1)
0690 IF Z5=0 THEN GOTO 0780
0700 LET V7$[Z5,Z5]=","
0710 GOTO 0680
0720 ON ERR THEN STOP
0730 PRINT
0740 PRINT "<7><7>USE A SLASH (/) WHERE YOU WANT A COMMA."
0750 GOTO 0640
0760 REM   ---------------------------------------------------------
0770 REM          CHECK IF IDENTIFIER IS IN METHOD FILE
0780 FOR I=1 TO I5
0800   READ FILE[4,3*I-1],V$
0810   IF V$=V7$ THEN GOTO 0880
0820 NEXT I
0830 PRINT
0840 PRINT "<7><7>THERE IS NO IDENTIFIER '";V7$;"' IN METHOD ";T$[3,6]
*    ;"."
0850 GOTO 0640
0860 REM   ---------------------------------------------------------
0870 REM          READ DATA FROM METHOD FILE
0880 READ FILE[4,3*I],D4$,I$,K,R1,R2,R3,J3
0890 IF D4$<>"99/99/99" THEN GOTO 0930
0900 PRINT
0910 PRINT "<7><7>IDENTIFIER ";V7$;" HAS NEVER BEEN CALIBRATED."
0920 GOTO 0640
0930 MAT READ FILE[4,3*I+1],G2
0940 READ FILE[4,1],T$,U$,N1
0950 REM   ---------------------------------------------------------
0960 REM          CLEAR SCREEN, PRINT HEADINGS
0970 IF X=3 THEN GOTO 2530
0971 IF X<>2 THEN GOTO 0980
0972 PRINT "<27>*DF"
0973 PRINT "<27>&S1P0Q"
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

PROGRAM LISTING FOR GC06

```
0980 PRINT "<27><12>";
0990 DELAY =1
1000 PRINT  TAB(22);"GAS CHROMATOGRAPHY AUTOMATION SYSTEM"
1010 PRINT  TAB(20);" C-A-L-I-B-R-A-T-I-O-N    C-U-R-V-E"
1020 PRINT "ANALYST:  ";U$; TAB(60);"METHOD:  ";T$[3,6]
1030 PRINT "IDENTIFIER:  ";V7$; TAB(43);"DATE OF CALIBRATION:  ";D4$
1040 PRINT "TYPE OF FIT:  ";
1050 ON K THEN GOTO 1060, 1080, 1100, 1120
1060 PRINT "LINEAR REGRESSION";
1070 GOTO 1130
1080 PRINT "QUADRATIC REGRESSION";
1090 GOTO 1130
1100 PRINT "LINEAR INTERPOLATION";
1110 GOTO 1130
1120 PRINT "LINEAR REGRESSION THROUGH ORIGIN";
1130 PRINT  TAB(51);
1140 PRINT USING "FITTING ERROR: ###.##Z",J3
1150 REM  ------------------------------------------------------------
1160 REM          DRAW BOX
1170 RANDOMIZE
1180 LET P1=RND(1)*5
1190 LET P2=RND(2)*5
1200 LET P3=0
1210 GOSUB 9968
1220 LET Q1=147
1230 LET Q2=70
1240 LET Q3=11
1250 LET Q4=78
1260 LET Q5=2
1270 GOSUB 9924
1280 LET Q4=54
1290 LET Q5=1
1300 GOSUB 9924
1310 LET Q2=664
1320 LET Q4=78
1330 LET Q5=-2
1340 GOSUB 9924
1350 LET Q1=1005
1360 LET Q2=70
1370 LET Q4=54
1380 LET Q5=-1
1390 GOSUB 9924
```


PROGRAM LISTING FOR GC06

```
1400 REM  ------------------------------------------------------------
1410 REM          LABEL AXES
1420 LET P1=0
1430 LET P2=500
1440 LET P3=3
1450 GOSUB 9968
1460 LET S$="PEAK AREA"
1470 FOR I=1 TO LEN(S$)
1480   PRINT S$[I,I];"<13>";
1490 NEXT I
1500 LET P1=0
1510 LET P2=0
1520 LET P3=3
1530 GOSUB 9968
1540 LET S$="CONCENTRATION IN MICROGRAMS PER LITER"
1550 IF N1>2 THEN LET S$="          MASS IN NANOGRAMS"
1560 PRINT "<29>";P4$;"<31>"; TAB(28);S$
1570 REM  ------------------------------------------------------------
1580 REM          SCALE VERTICAL AXIS
1590 LET S1=0
1600 LET S2=0
1610 FOR I=1 TO LEN(I$)/8
1620   IF G2[2*I]>S2 THEN LET S2=G2[2*I]
1630 NEXT I
1640 GOSUB 9805
1650 LET Y8=S[1]
1660 LET Y9=S[12]
1670 LET P1=0
1680 LET P3=3
1690 FOR I=1 TO 12
1700   LET P2=58+(I-1)*54
1710   GOSUB 9968
1720   PRINT "<29>";P4$;"<31>";
1730   PRINT USING "##########",S[I]
1740 NEXT I
1750 REM  ------------------------------------------------------------
1760 REM          SCALE HORIZONTAL AXIS
1770 LET S1=0
1780 LET S2=0
1790 FOR I=1 TO LEN(I$)/8
1800   IF G2[2*I-1]>S2 THEN LET S2=G2[2*I-1]
1810 NEXT I
```

PROGRAM LISTING FOR GC06

```
1820 GOSUB 9805
1830 LET X8=S[1]
1840 LET X9=S[12]
1850 IF S[12]>=10 THEN GOTO 1880
1860 LET Q5$=" #.##"
1870 GOTO 1920
1880 IF S[12]>=100 THEN GOTO 1910
1890 LET Q5$=" ##.#"
1900 GOTO 1920
1910 LET Q5$="#####"
1920 LET P2=30
1930 FOR I=1 TO 12
1940   LET P1=105+(I-1)*78
1950   GOSUB 9968
1960   PRINT "<29>";P4$;"<31>";
1970   PRINT USING Q5$,S[I]
1980 NEXT I
1990 REM  ------------------------------------------------------
2000 REM          DRAW MARKERS
2010 LET P4=P4+147
2020 LET P5=P5+70
2030 LET P5$="*"
2040 FOR I=1 TO LEN(I$)/8
2050   LET P[I]=858*(G2[2*I-1]-X8)/(X9-X8)
2060   LET Q[I]=594*(G2[2*I]-Y8)/(Y9-Y8)
2070 NEXT I
2080 LET Q3=LEN(I$)/8
2090 LET Q7=-1
2100 IF K<>3 THEN GOTO 2160
2110 LET Q7=1
2120 LET P1=0
2130 LET P2=0
2140 LET P3=3
2150 GOSUB 9968
2160 GOSUB 9881
2170 REM  ------------------------------------------------------
2180 REM          DRAW CURVE
2190 IF K=3 THEN GOTO 2390
2200 LET Q3=1
2210 FOR I=Y8 TO .99*Y9 STEP (Y9-Y8)/100
2220   LET Q[Q3]=594*(I-Y8)/(Y9-Y8)
2230   LET X7=R1+R2*I
```


PROGRAM LISTING FOR GC06

```
2240   IF K=2 THEN LET X7=X7+R3*I^2
2250   LET P[Q3]=858*(X7-X8)/(X9-X8)
2260   IF P[Q3]<0 THEN GOTO 2290
2270   IF P[Q3]>858 THEN GOTO 2290
2280   LET Q3=Q3+1
2290 NEXT I
2300 LET Q3=Q3-1
2310 LET P1=P[1]
2320 LET P2=Q[1]
2330 LET P3=3
2340 GOSUB 9968
2350 LET Q7=0
2360 GOSUB 9881
2370 REM  ------------------------------------------------------
2380 REM          SOUND THE BELL; ALLOW TIME FOR HARD COPY
2390 FOR I=1 TO 5
2400   PRINT "<7>"
2410   DELAY =.3
2420 NEXT I
2430 TIME =60
2440 ON ERR THEN GOTO 2460
2450 TINPUT "",X$
2460 ON ERR THEN STOP
2470 PRINT "<27><12>";
2480 DELAY =1
2482 IF X<>2 THEN GOTO 2490
2483 PRINT "<27>E"
2484 PRINT "<27>H<27>J"
2485 PRINT "<27>*DE"
2490 PRINT  TAB(15);"C-A-L-I-B-R-A-T-I-O-N   D-A-T-A   R-E-P-O-R-T"
2500 GOTO 2690
2510 REM  ------------------------------------------------------
2520 REM          PRINT TABLE OF RESIDUALS
2530 PRINT
2540 PRINT
2550 PRINT  TAB(15);"C-A-L-I-B-R-A-T-I-O-N   D-A-T-A   R-E-P-O-R-T"
2560 PRINT "ANALYST:  ";U$; TAB(60);"METHOD:  ";T$[3,6]
2570 PRINT "IDENTIFIER:  ";V7$; TAB(43);"DATE OF CALIBRATION:  ";D4$
2580 PRINT "TYPE OF FIT:  ";
2590 ON K THEN GOTO 2600, 2620, 2640, 2660
2600 PRINT "LINEAR REGRESSION";
2610 GOTO 2670
```

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
2620 PRINT "QUADRATIC REGRESSION";
2630 GOTO 2670
2640 PRINT "LINEAR INTERPOLATION";
2650 GOTO 2670
2660 PRINT "LINEAR REGRESSION THROUGH ORIGIN";
2670 PRINT  TAB(51);
2680 PRINT USING "FITTING ERROR: ###.##%",J3
2690 PRINT
2700 PRINT "INJECTION ID  PEAK AREA   PREPARED   CALCULATED  DIFFERENC
*    E"
2710 PRINT "------------  --------  ---------  ---------  --------
*    -"
2720 LET Q5$="  #######   ######### ----#.###  -----#.###    +++#.#
*    ##"
2730 FOR I=1 TO LEN(I$)/8
2740   ON K THEN GOTO 2750, 2770, 2790, 2750
2750   LET L2=R1+G2[I*2]*R2
2760   GOTO 2800
2770   LET L2=R1+G2[I*2]*R2+R3*G2[I*2]^2
2780   GOTO 2800
2790   LET L2=G2[I*2-1]
2800   PRINT USING Q5$,I$[8*I-7,8*I],G2[I*2],G2[I*2-1],L2,G2[I*2-1]-L2
2810 NEXT I
2820 IF K=3 THEN GOTO 3060
2830 PRINT
2840 PRINT "EQUATION:  CONCENTRATION = ";
2850 ON K THEN GOTO 2860, 2880, 3060, 2900
2860 PRINT USING "+#.##^^^^(A) +#.##^^^^",R2,R1
2870 GOTO 3060
2880 PRINT USING "+#.##^^^^(A^2) +#.##^^^^(A) +#.##^^^^",R3,R2,R1
2890 GOTO 3060
2900 PRINT USING "+#.##^^^^(A)",R2
3040 REM  ------------------------------------------------------------
3050 REM          RETURN TO MASTER CONTROL
3060 PRINT
3065 PRINT
3070 PRINT "DO YOU WANT CALIBRATION INFORMATION FOR ANOTHER IDENTIFIER
*    "
3080 PRINT "     IN METHOD ";T$[3,6];
3090 ON ERR THEN GOTO 3110
3100 INPUT "?  (Y OR N)  ",X$
3110 ON ERR THEN STOP
```

12345678911234567892123456789312345678941234567895123456789612345678 97
         0   0   0   0   0   0   0

12345678911234567892123456789312345678941234567895123456789612345678 97
         0   0   0   0   0   0   0

```
3120 IF X$[1,1]="Y" THEN GOTO 0640
3130 NOESC
3140 CHAIN "GC00"
9800 REM  ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
9801 REM          SUBROUTINE TO PERFORM SCALING (BSCSCL.SR)
9805 DIM S[12]
9806 LET S7=0
9808 LET S3=S2-S1
9809 IF S3>=100 THEN GOTO 9815
9810 LET S1=S1*10
9811 LET S2=S2*10
9812 LET S7=S7+1
9813 GOTO 9808
9815 LET S4=0
9816 IF S3<100 THEN GOTO 9820
9817 LET S3=S3/10
9818 LET S4=S4+1
9819 GOTO 9816
9820 IF S1=0 THEN IF S3-10*INT(S3/10)<=INT(S3/10) THEN LET S3=10*INT(S
*    3/10)
9821 LET S3=INT(S3+.5)
9823 IF S3-10*INT(S3/10)=0 THEN GOTO 9828
9824 IF S3-10*INT(S3/10)=5 THEN GOTO 9828
9825 LET S3=S3+1
9826 GOTO 9823
9828 LET S5=S3*10^(S4-1)
9830 LET S1=INT(S1/10^(S4-1))*10^(S4-1)
9831 IF S1/S5=INT(S1/S5) THEN GOTO 9835
9832 LET S1=S1-10^(S4-1)
9833 GOTO 9831
9835 FOR S6=1 TO 12
9836   LET S[S6]=(S1+(S6-1)*S5)/10^(S7)
9837 NEXT S6
9838 RETURN
9875 REM  ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
9876 REM          SUBROUTINE TO DRAW LINES AND CURVES (BSCLIN.SR)
9881 LET Q8=0
9882 LET P3=3
9885 IF Q7>=0 THEN LET P3=2
9886 FOR Q9=1 TO Q3
9887   LET P1=P[Q9]
9888   LET P2=Q[Q9]
```

12345678911234567892123456789312345678941234567895123456789612345678 97
         0   0   0   0   0   0   0

```
123456789112345678921234567893123456789412345678951234567896123456789 7
         0         0         0         0         0         0         0
9889   GOSUB 9968
9890   LET Q8=Q8+1
9891   IF Q8<>ABS(Q7) THEN GOTO 9896
9892   LET U1=P[Q9]
9893   LET U2=Q[Q9]
9894   GOSUB 9908
9895   LET Q8=0
9896 NEXT Q9
9897 RETURN
9900 REM   ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
9901 REM          SUBROUTINE TO PLACE MARKERS (BSCMKR.SR)
9905 DIM P5$[10]
9906 GOSUB 9958
9907 RETURN
9908 LET P1=U1-5
9909 LET P2=U2-8
9910 LET U3=P3
9911 LET P3=3
9912 GOSUB 9968
9913 PRINT "<29>";P4$;
9914 PRINT "<31>";P5$[1,LEN(P5$)]
9915 LET P1=U1
9916 LET P2=U2
9917 GOSUB 9968
9918 LET P3=U3
9919 RETURN
9920 REM   ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
9921 REM          SUBROUTINE TO DRAW AXES (BSCAXS.SR)
9924 LET P1=Q1
9925 LET P2=Q2
9926 LET P3=3
9927 GOSUB 9968
9928 LET P3=2
9929 IF ABS(Q5)=1 THEN GOTO 9939
9930 FOR Q6=1 TO Q3+1
9931   GOSUB 9968
9932   LET P2=P2+10*Q5/ABS(Q5)
9933   GOSUB 9968
9934   LET P2=P2-10*Q5/ABS(Q5)
9935   GOSUB 9968
9936   LET P1=P1+Q4
9937 NEXT Q6
123456789112345678921234567893123456789412345678951234567896123456789 7
         0         0         0         0         0         0         0
```



```
123456789112345678921234567893123456789412345678951234567896123456789 7
         0         0         0         0         0         0         0
9938 RETURN
9939 FOR Q6=1 TO Q3+1
9940   GOSUB 9968
9941   LET P1=P1+10*Q5/ABS(Q5)
9942   GOSUB 9968
9943   LET P1=P1-10*Q5/ABS(Q5)
9944   GOSUB 9968
9945.  LET P2=P2+Q4
9946 NEXT Q6
9947 RETURN
9950 REM   ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
9951 REM          SUBROUTINE TO PLOT INDIVIDUAL POINTS (BSCPLT.SR)
9958 DIM P1$[32],P2$[32],P3$[32],P4$[4]
9959 LET P4=0
9960 LET P5=0
9961 LET P6=0
9962 LET P1$=" !<34>#$%&'()*+,-./0123456789:;<=>?"
9963 LET P2$="@ABCDEFGHIJKLMNOPQRSTUVWXYZ[\]^_"
9964 LET P3$="`ABCDEFGHIJKLM"
9965 LET P3$=P3$,"NOPQRSTUVWXY"
9966 LET P3$=P3$,"Z[\]^"
9967 RETURN
9968 IF P3<>0 THEN GOTO 9972
9969 LET P4=P1
9970 LET P5=P2
9971 RETURN
9972 PRINT "<29>";
9973 IF LEN(P4$)<>0 THEN PRINT P4$[4,4];
9974 LET P7=INT(P1+P4)
9975 LET P8=INT(P2+P5)
9976 IF P7>1023 THEN LET P7=1023
9977 IF P7<0 THEN LET P7=0
9978 IF P8>780 THEN LET P8=780
9979 IF P8<0 THEN LET P8=0
9980 IF P3=2 THEN LET P6=1
9981 IF P3=3 THEN LET P6=0
9982 LET P9=INT(P8/32)
9983 LET P8=P8-(P9*32)+1
9984 LET P9=P9+1
9985 LET P4$=P1$[P9,P9],P3$[P8,P8]
9986 LET P9=INT(P7/32)
9987 LET P7=P7-(P9*32)+1
123456789112345678921234567893123456789412345678951234567896123456789 7
         0         0         0         0         0         0         0
```

PROGRAM LISTING FOR GC06

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
9988 LET P9=P9+1
9989 LET P4$=P4$,P1$[P9,P9],P2$[P7,P7]
9990 IF P6<>0 THEN GOTO 9992
9991 PRINT "<29>";
9992 PRINT P4$
9993 RETURN
```

12345678911234567892123456789312345678941234567895123456789612345678 97
         0   0   0   0   0   0   0

SYMBOL TABLE FOR GC06

SYMBOL	REFERENCES			
0120	0154			
0150	0130			
0160	0151			
0210	0160			
0260	0200			
0570	0600			
0610	0580			
0640	0750	0850	0920	3120
0680	0710			
0720	0650			
0780	0690			
0880	0810			
0930	0890			
0980	0971			
1060	1050			
1080	1050			
1100	1050			
1120	1050			
1130	1070	1090	1110	
1880	1850			
1910	1880			
1920	1870	1900		
2160	2100			
2290	2260	2270		
2390	2190			
2460	2440			
2490	2482			
2530	0970			
2600	2590			
2620	2590			
2640	2590			
2660	2590			
2670	2610	2630	2650	
2690	2500			
2750	2740			
2770	2740			
2790	2740			
2800	2760	2780		
2860	2850			
2880	2850			
2900	2850			
3060	2820	2850	2870	2890
3110	3090			
3130	0100			
9805	1640	1820		

SYMBOL TABLE FOR GC06

SYMBOL	REFERENCES									
9808	9813									
9815	9809									
9816	9819									
9820	9816									
9823	9826									
9828	9823	9824								
9831	9833									
9835	9831									
9881	2160	2360								
9896	9891									
9905	0210									
9908	9894									
9924	1270	1300	1340	1390						
9939	9929									
9958	9906									
9968	1210	1450	1530	1710	1950	2150	2340	9889	9912	9917
	9927	9931	9933	9935	9940	9942	9944			
9972	9968									
9992	9990									
D4$	0070	0880	0890	1030	2570					
FL#4	0260	0270	0280	0570	0800	0880	0930	0940		
G2	0930									
G2[	0070	1620	1800	2050	2060	2750	2770	2790	2800	
I	0780	0800	0820	0880	0930	1470	1480	1490	1610	1620
	1630	1690	1700	1730	1740	1790	1800	1810	1930	1940
	1970	1980	2040	2050	2060	2070	2210	2220	2230	2240
	2290	2390	2420	2730	2750	2770	2790	2800	2810	
I$	0070	0880	1610	1790	2040	2080	2730	2800		
I5	0560	0570	0590	0610	0780					
J3	0880	1140	2680							
K	0880	1050	2100	2190	2240	2590	2740	2820	2850	
L2	2750	2770	2790	2800						
N1	0940	1550								
P1	1180	1420	1500	1670	1940	2120	2310	9887	9908	9915
	9924	9936	9941	9943	9969	9974				
P1$	9958	9962	9985	9989						
P2	1190	1430	1510	1700	1920	2130	2320	9888	9909	9916
	9925	9932	9934	9945	9970	9975				
P2$	9958	9963	9989							
P3	1200	1440	1520	1680	2140	2330	9882	9885	9910	9911
	9918	9926	9928	9968	9980	9981				
P3$	9958	9964	9965	9966	9985					
P4	2010	9959	9969	9974						
P4$	1560	1720	1960	9913	9958	9973	9985	9989	9992	
P5	2020	9960	9970	9975						

SYMBOL TABLE FOR GC06

SYMBOL	REFERENCES									
P5$	2030	9905	9914							
P6	9961	9980	9981	9990						
P7	9974	9976	9977	9986	9987	9989				
P8	9975	9978	9979	9982	9983	9985				
P9	9982	9983	9984	9985	9986	9987	9988	9989		
P[	0070	2050	2250	2260	2270	2310	9887	9892		
Q1	1220	1350	9924							
Q2	1230	1310	1360	9925						
Q3	1240	2080	2200	2220	2250	2260	2270	2280	2300	9886
	9930	9939								
Q4	1250	1280	1320	1370	9936	9945				
Q5	1260	1290	1330	1380	9929	9932	9934	9941	9943	
Q5$	0070	1860	1890	1910	1970	2720	2800			
Q6	9930	9937	9939	9946						
Q7	2090	2110	2350	9885	9891					
Q8	9881	9890	9891	9895						
Q9	9886	9887	9888	9892	9893	9896				
Q[	0070	2060	2220	2320	9888	9893				
R1	0880	2230	2750	2770	2860	2880				
R2	0880	2230	2750	2770	2860	2880	2900			
R3	0880	2240	2770	2880						
S$	0070	1460	1470	1480	1540	1550	1560			
S1	1590	1770	9808	9810	9820	9830	9831	9832	9836	
S2	1600	1620	1780	1800	9808	9811				
S3	9808	9809	9816	9817	9820	9821	9823	9824	9825	9828
S4	9815	9818	9828	9830	9832					
S5	9828	9831	9836							
S6	9835	9836	9837							
S7	9806	9812	9836							
S[	1650	1660	1730	1830	1840	1850	1880	1970	9805	9836
T$	0070	0260	0280	0645	0840	0940	1020	2560	3080	
U$	0080	0940	1020	2560						
U1	9892	9908	9915							
U2	9893	9909	9916							
U3	9910	9918								
V$	0080	0570	0800	0810						
V7$	0080	0660	0680	0700	0810	0840	0910	1030	2570	
X	0140	0151	0153	0160	0970	0971	2482			
X$	0080	2450	3100	3120						
X7	2230	2240	2250							
X8	1830	2050	2250							
X9	1840	2050	2250							
Y8	1650	2060	2210	2220						
Y9	1660	2060	2210	2220						
Z5	0680	0690	0700							

SECTION 9

PROGRAM GC07 - EXTANT INJECTION LISTING

GC07 is the program which lists the injection ID numbers and report titles for the data files that are currently in existence. This program is entered by chaining from the master control program, GC00, and it chains back to that program if the escape key is pressed.

As GC07 begins, it gives the user three choices: 1) print all extant ID numbers for one instrument, 2) print ID numbers for a specific date for one instrument, or 3) print the report title for any ID from any instrument. The program then branches to the appropriate routine.

The first two choices involve reading ID numbers from an ID list file. GC07 asks the user for the number of the instrument, and uses this number to generate the name of the appropriate ID list file. It then checks whether the ID list file exists. The ID list file must be opened carefully since the microcomputer may be running GC21 which also opens ID list files. Therefore, GC07 establishes an OR ERR THEN GOTO condition, opens the ID list file, copies the entire file into a superstring, and promptly closes the file to avoid making the microcomputer wait.

Then, if the user has selected the first type of report, GC07 prints all of the ID numbers, except dummy ID numbers. If the user has selected the second type of report, GC07 asks for a month and date, and prints only those ID numbers which match the specified month and date. If none of the ID numbers match, the user is informed of that fact.

The third type of report is different from the other two in that it gets the report title from an injection data file. The user is asked for the ID number of interest, and GC07 opens the appropriate data file. It finds the report title and prints it. The program then gives the user a chance to examine another file.

After any of these types of reports, the escape feature is disabled, and the program chains back to GC00.

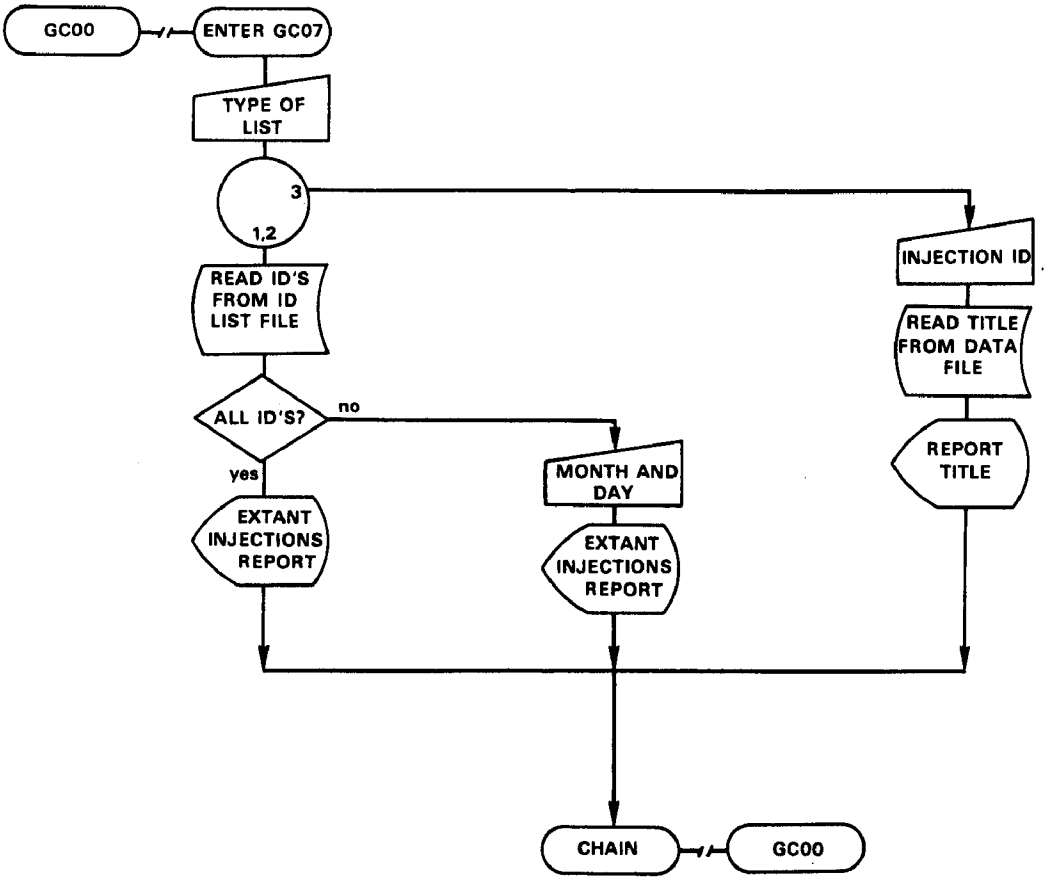

Figure 8. Flowchart of Program GC07.

TABLE 6. SYMBOL DEFINITIONS FOR PROGRAM GC07

C$	the name of the ID list file
D2$	an injection ID Number
D3$	a data file name
E	a counter for the number of ID Numbers which match the specified date
F$	a report title
I	the control variable for loops
I$	the superstring of extant ID numbers
J	the data file useability flag
J$	the date of an injection, in the form MMDD
X	the user's answer to a multiple choice question
X$	a Y or N answer input by the user
X2	the instrument number input by the user
X3	the month and date numbers input by the user

PROGRAM LISTING FOR GC07

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                    +
0030 REM   +   PROGRAM GC07, DATA FILE LISTING                        +
0040 REM   +   BY:  J. KOPKE (SWORCC), JANUARY 23, 1979               +
0045 REM   +   MOST RECENT REVISION:  MAY 1, 1979                     +
0050 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0060 REM
0070 ESC
0080 ON ESC THEN GOTO 1460
0090 DIM C$[8],D2$[8],D3$[10],F$[30],I$[1000],J$[4],X$[3]
0120 REM   ---------------------------------------------------------
0130 REM          DEFINE SEARCH
0140 PRINT
0150 PRINT "HERE ARE THE TYPES OF LISTS:"
0160 PRINT
0170 PRINT "     1.  ALL EXTANT ID NUMBERS FROM ONE INSTRUMENT"
0180 PRINT "     2.  ID NUMBERS FOR A SPECIFIC DATE FROM ONE INSTRUMEN
*    T"
0190 PRINT "     3.  TITLE OF REPORT FOR ANY ID FROM ANY INSTRUMENT"
0200 PRINT
0205 ON ERR THEN GOTO 0215
0210 INPUT "WHICH TYPE DO YOU WANT TO USE?  (1, 2, OR 3)  ",X
0215 ON ERR THEN STOP
0220 ON X THEN GOTO 0260, 0260, 0920
0230 PRINT
0240 PRINT "<7><7>";X;"IS NOT A VALID TYPE NUMBER."
0250 GOTO 0140
0255 REM   ---------------------------------------------------------
0256 REM          COPY ID LIST FILE INTO SUPERSTRING
0260 PRINT
0265 ON ERR THEN GOTO 0271
0270 INPUT "WHAT INSTRUMENT NUMBER?  ",X2
0271 ON ERR THEN STOP
0272 IF X2=ABS(INT(X2)) THEN IF X2<=99 THEN GOTO 0280
0273 PRINT
0274 PRINT "<7><7>";X2;"IS NOT A VALID INSTRUMENT NUMBER."
0275 GOTO 0260
0280 LET C$="GC000000"
0290 LET C$[9-LEN(STR$(X2)),8]=STR$(X2)
0300 ON ERR THEN GOTO 0320
0310 RENAME C$,C$
0320 ON ERR THEN STOP

12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```


PROGRAM LISTING FOR GC07

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0330 IF SYS(7)<>-48 THEN GOTO 0360
0340 DELAY =1
0350 GOTO 0300
0360 IF SYS(7)=-9 THEN GOTO 0400
0370 PRINT
0380 PRINT "THERE HAVE NOT BEEN ANY INJECTIONS INTO INSTRUMENT ";C$[7,
*    8];"."
0390 GOTO 1460
0400 ON ERR THEN GOTO 0460
0410 OPEN FILE[2,0],C$,11
0420 ON ESC THEN GOTO 0500
0430 ON ERR THEN STOP
0440 GOTO 0530
0460 ON ERR THEN STOP
0470 DELAY =1
0480 GOTO 0400
0500 CLOSE FILE[2]
0510 GOTO 1460
0530 FOR I=1 TO 100
0540   READ FILE[2,I],I$[10*I-9,10*I]
0550 NEXT I
0560 CLOSE FILE[2]
0570 ON ESC THEN GOTO 1460
0580 IF X=2 THEN GOTO 0700
0590 REM   ---------------------------------------------------------
0600 REM          PRINT ALL ID NUMBERS
0610 PRINT
0611 PRINT
0612 PRINT  TAB(14);"E-X-T-A-N-T   I-N-J-E-C-T-I-O-N-S   R-E-P-O-R-T"
0613 PRINT "INSTRUMENT NUMBER:  ";C$[7,8]; TAB(59);"ALL INJECTIONS"
0614 PRINT
0620 FOR I=1 TO 100
0630   IF I$[10*I-9,10*I]="GC99999999" THEN GOTO 0670
0640   PRINT I$[10*I-7,10*I];
0645   IF I/6<>INT(I/6) THEN PRINT "     ";
0650   IF I/6=INT(I/6) THEN PRINT
0660 NEXT I
0670 GOTO 1460
0680 REM   ---------------------------------------------------------
0690 REM          PRINT ID NUMBERS MATCHING A DATE
0700 PRINT
0705 ON ERR THEN GOTO 0711

12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0710 INPUT "WHAT MONTH?  (1, 2, 3, . . . , OR 12)  ",X3
0711 ON ERR THEN STOP
0712 IF X3=ABS(INT(X3)) THEN IF X3<=12 THEN GOTO 0720
0713 PRINT
0714 PRINT "<7><7>";X3;"IS NOT A VALID MONTH."
0715 GOTO 0700
0720 LET J$="0000"
0730 LET J$[3-LEN(STR$(X3)),2]=STR$(X3)
0740 PRINT
0745 ON ERR THEN GOTO 0751
0750 INPUT "WHAT DATE?  (1, 2, 3, . . . , OR 31)  ",X3
0751 ON ERR THEN STOP
0752 IF X3=ABS(INT(X3)) THEN IF X3<=31 THEN GOTO 0760
0753 PRINT
0754 PRINT "<7><7>";X3;"IS NOT A VALID DATE."
0755 GOTO 0740
0760 LET J$[5-LEN(STR$(X3)),4]=STR$(X3)
0770 PRINT
0771 PRINT
0772 PRINT  TAB(14);"E-X-T-A-N-T   I-N-J-E-C-T-I-O-N-S   R-E-P-O-R-T"
0773 PRINT "INSTRUMENT NUMBER:  ";C$[7,8];"                MONTH:  ";J
*     $[1,2];"                DAY:  ";J$[3,4]
0775 PRINT
0780 LET E=0
0790 FOR I=1 TO 100
0800   IF I$[10*I-5,10*I-2]<>J$ THEN GOTO 0840
0810   PRINT I$[10*I-7,10*I];
0820   LET E=E+1
0825   IF E/6<>INT(E/6) THEN PRINT "     ";
0830   IF E/6=INT(E/6) THEN PRINT
0840 NEXT I
0850 IF E<>0 THEN GOTO 1460
0870 PRINT "NONE"
0890 GOTO 1460
0900 REM  ------------------------------------------------------------
0910 REM          PRINT VARIAN REPORT TITLE FOR A SPECIFIC ID
0920 PRINT
0925 ON ERR THEN GOTO 0935
0930 INPUT "WHAT ID?  ",D2$
0935 ON ERR THEN STOP
0940 IF LEN(D2$)<>8 THEN GOTO 1030
0945 IF D2$="00000000" THEN GOTO 1030

12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```



```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0950 LET D3$="GC",D2$
0960 ON ERR THEN GOTO 0980
0970 RENAME D3$,D3$
0980 ON ERR THEN STOP
0990 IF SYS(7)<>-48 THEN GOTO 1020
1000 DELAY =1
1010 GOTO 0960
1020 IF SYS(7)=-9 THEN GOTO 1090
1030 PRINT
1040 PRINT "THERE IS NO EXISTING DATA FOR INJECTION ";D2$;"."
1050 GOTO 1410
1090 ON ERR THEN GOTO 1150
1100 OPEN FILE[3,0],D3$,31
1110 ON ESC THEN GOTO 1190
1120 ON ERR THEN STOP
1130 GOTO 1220
1150 ON ERR THEN STOP
1160 DELAY =1
1170 GOTO 1090
1190 CLOSE FILE[3]
1200 GOTO 1460
1220 READ FILE[3,1],J
1230 IF J=1 THEN GOTO 1300
1240 PRINT
1250 IF J=2 THEN PRINT D2$;" CANNOT BE USED BECAUSE THE REPORT DID NOT
*     HAVE A TOTAL AREA."
1260 IF J=3 THEN PRINT D2$;" CANNOT BE USED BECAUSE THE REPORT WAS IN
*     THE WRONG FORMAT."
1270 CLOSE FILE[3]
1280 ON ESC THEN GOTO 1460
1290 GOTO 1410
1300 LET I=2
1310 READ FILE[3,I],F$
1320 IF F$[1,7]<>"MESSAGE" THEN GOTO 1350
1330 LET I=I+1
1340 GOTO 1310
1350 LET I=I+1
1360 READ FILE[3,I],F$
1370 CLOSE FILE[3]
1380 ON ESC THEN GOTO 1460
1390 PRINT
1400 PRINT "FOR ID ";D2$;", THE REPORT TITLE IS '";F$;"."

12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

PROGRAM LISTING FOR GC07

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
1410 PRINT
1415 ON ERR THEN GOTO 1425
1420 INPUT "DO YOU WANT TO PRINT THE TITLE FOR ANOTHER ID?  (Y OR N)
*     ",X$
1425 ON ERR THEN STOP
1430 IF X$[1,1]="Y" THEN GOTO 0920
1440 REM ------------------------------------------------------------
1450 REM          CHAIN BACK TO GC00
1460 PRINT
1461 PRINT
1462 NOESC
1470 CHAIN "GC00"
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```


SYMBOL TABLE FOR GC07

SYMBOL	REFERENCES									
0140	0250									
0215	0205									
0260	0220	0275								
0271	0265									
0280	0272									
0300	0350									
0320	0300									
0360	0330									
0400	0360	0480								
0460	0400									
0500	0420									
0530	0440									
0670	0630									
0700	0580	0715								
0711	0705									
0720	0712									
0740	0755									
0751	0745									
0760	0752									
0840	0800									
0920	0220	1430								
0935	0925									
0960	1010									
0980	0960									
1020	0990									
1030	0940	0945								
1090	1020	1170								
1150	1090									
1190	1110									
1220	1130									
1300	1230									
1310	1340									
1350	1320									
1410	1050	1290								
1425	1415									
1460	0080	0390	0510	0570	0670	0850	0890	1200	1280	1380
C$	0090	0280	0290	0310	0380	0410	0613	0773		
D2$	0090	0930	0940	0945	0950	1040	1250	1260	1400	
D3$	0090	0950	0970	1100						
E	0780	0820	0825	0830	0850					
F$	0090	1310	1320	1360	1400					
FL#2	0410	0500	0540	0560						
FL#3	1100	1190	1220	1270	1310	1360	1370			
I	0530	0540	0550	0620	0630	0640	0645	0650	0660	0790
	0800	0810	0840	1300	1310	1330	1350	1360		

SYMBOL TABLE FOR GC07

SYMBOL	REFERENCES							
I$	0090	0540	0630	0640	0800	0810		
J	1220	1230	1250	1260				
J$	0090	0720	0730	0760	0773	0800		
X	0210	0220	0240	0580				
X$	0090	1420	1430					
X2	0270	0272	0274	0290				
X3	0710	0712	0714	0730	0750	0752	0754	0760

SECTION 10

PROGRAM GC08 - INTERNAL STANDARDS CONCENTRATION CALCULATION

The internal standards calibration method is a planned future enhancement of the GCAS, but it has not been implemented in Version I.

PROGRAM LISTING FOR GC08

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                    +
0030 REM   +   PROGRAM GC08, INTERNAL CALIBRATION PROCESSING          +
0040 REM   +   BY:  J. KOPKE (SWORCC), JANUARY 10, 1979               +
0045 REM   +   MOST RECENT REVISION:  MARCH 21, 1979                  +
0050 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0060 REM
0070 ESC
0080 ON ESC THEN GOTO 9998
0090 PRINT
0110 PRINT "<7><7>INTERNAL STANDARDS PROCESSING IS NOT OPERATIONAL AT
*    THIS TIME."
9998 NOESC
9999 CHAIN "GC00"
```

12345678911234567892123456789312345678941234567895123456789612345678 97
         0   0   0   0   0   0   0

SYMBOL TABLE FOR GC08

SYMBOL	REFERENCES
9998	0080

SECTION 11

PROGRAM GC09 - PURGE AND TRAP CONCENTRATION CALCULATION

GC09 is the program which calculates concentrations of compounds in samples prepared by the purge and trap method. It is entered by chaining from the master control program, GC00, and it chains back to that program if the escape key is pressed.

As the execution of GC09 begins, the method file is already open. The program asks the user for the injection ID of the injection which is to be processed, and it opens the corresponding data file. The program checks the data file useability flag, and informs the user if the data file is unusable. It then displays any error messages which were in the original report.

Next, the program reads the data for a single peak from the data file. If the peak is an unexplained peak, a dummy concentration of -9999 is written into the data file, and the program goes on to the next peak.

For named peaks, the program searches the method file for a matching identifier. If there is no matching identifier, the user is informed that the concentration cannot be calculated, and a dummy concentration of -9999 is written into the data file.

If a matching identifier is found, the program checks whether the identifier has been calibrated. If it has not, the user is informed that the concentration cannot be calculated, and a dummy concentration of -9999 is written into the data file.

If the matching identifier has been calibrated, the program checks the type of calibration and branches to the appropriate section of code. If the type of calibration is linear regression or quadratic regression, the program uses the regression equations developed during calibration to calculate the concentration, which is written into the data file.

If the type of calibration is linear interpolation, the program finds the two calibration standards whose peak areas bracket the peak area of the unknown. If the peak area of the unknown is lower than that of the lowest calibration standard, the program uses the origin and the lowest calibration standard as the basis for the interpolation. If the peak area of the unknown is higher than that of the highest calibration standard, the program extrapolates through the two highest calibration standards. In any case, the concentration of the unknown is calculated by the formula

$$\text{Conc.} = \left(\frac{\text{Conc}_2 - \text{Conc}_1}{\text{Area}_2 - \text{Area}_1}\right)\left(\text{Area} - \text{Area}_1\right) + \left(\text{Conc}_1\right)$$

and written into the data file.

When all of the peaks in the data file have been processed, this program chains to the retention time calculation program, GC12, leaving the method file and the injection data file open.

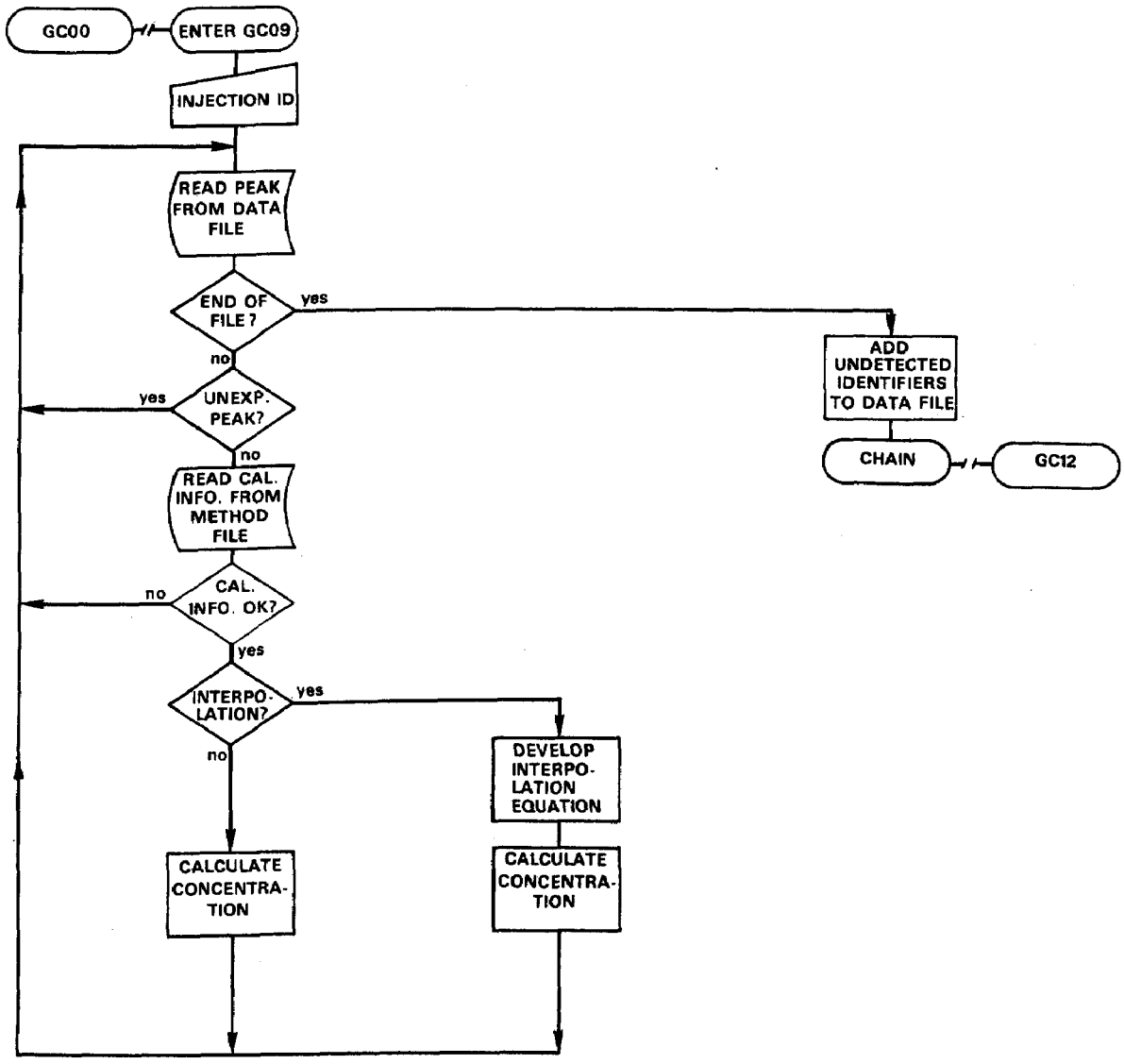

Figure 9. Flowchart of Program GC09.

TABLE 7. SYMBOL DEFINITIONS FOR PROGRAM GC09

B	the absolute retention time of a peak
C	the area of a peak
D2$	an injection ID
D3$	the name of a data file
D4$	the date of calibration
F	the number of identifiers in the method file
F()	the array of flags used to record which identifiers are found in the data file
G$	the identifier from the data file
G2()	the array of concentrations and areas of standards
H$	the peak type
I	a counter used in interpolation to locate the standards between which the unknown lies
I$	the superstring of ID's of standards
I5	the number of standards used to calibrate an identifier
I7	a counter used to locate an identifier in a method file
J	the data file useability flag J=1 the data is useable J=2 the report did not have a TOTAL AREA J=3 the report was in the wrong format
J3	the fitting error of the regression
K	the type of fit K=1 linear regression K=2 quadratic regression K=3 linear interpolation K=4 linear regression forced through the origin

TABLE 7. (Continued)

L	the calculated relative retention time or capacity ratio
M1	the concentration of the standard below the unknown
M2	the area of the standard below the unknown
M3	the concentration of the standard above the unknown
M4	the area of the standard above the unknown
P9	a counter for the position in the data file of the peak being processed
R1	the constant term in the regression equation
R2	the linear term in the regression equation
R3	the quadratic term in the regression equation
T$	the name of the method file
V$	an identifier from the method file
VO$	a MESSAGE read from the data file

PROGRAM LISTING FOR GC09

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                    +
0030 REM   +   PROGRAM GC09, PURGE AND TRAP PROCESSING                +
0040 REM   +   BY:  J. KOPKE (SWORCC), FEBRUARY 13, 1979              +
0045 REM   +   MOST RECENT REVISION:  APRIL 2, 1979                   +
0050 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0060 REM
0070 ESC
0080 ON ESC THEN GOTO 0110
0090 DIM D2$[8],D3$[10],D4$[8],G$[8],G2[30],H$[2],I$[160],T$[6],V$[8],
*    V0$[20]
0095 DIM F[60]
0096 MAT F=ZER
0100 GOTO 0160
0110 ON ERR THEN GOTO 0112
0111 CLOSE FILE[3]
0112 ON ERR THEN STOP
0120 NOESC
0130 CHAIN "GC00"
0140 REM   ---------------------------------------------------------
0150 REM          COUNT IDENTIFIERS IN METHOD FILE
0160 LET F=0
0170 READ FILE[4,1],T$
0175 CLOSE FILE[4]
0176 OPEN FILE[4,0],T$,200
0180 READ FILE[4,3*(F+1)-1],V$
0190 IF EOF(4) THEN GOTO 0240
0200 LET F=F+1
0210 GOTO 0180
0220 REM   ---------------------------------------------------------
0230 REM          OPEN DATA FILE
0240 PRINT
0245 ON ERR THEN GOTO 0255
0248 PRINT "WHAT IS THE ID FOR THE INJECTION TO BE PROCESSED BY METHOD
*     ";T$[3,6];
0250 INPUT "?  ",D2$
0255 ON ERR THEN STOP
0260 IF LEN(D2$)=8 THEN GOTO 0300
0270 PRINT
0280 PRINT "<7><7>";D2$;" IS NOT A VALID INJECTION ID."
0290 GOTO 0240
0300 LET D3$="GC",D2$
```

12345678911234567892123456789312345678941234567895123456789612345678 97
         0   0   0   0   0   0   0

PROGRAM LISTING FOR GC09

12345678911234567892123456789312345678941234567895123456789612345678 97
         0   0   0   0   0   0   0

```
0310 ON ERR THEN GOTO 0330
0320 RENAME D3$,D3$
0330 ON ERR THEN STOP
0340 IF SYS(7)<>-48 THEN GOTO 0370
0350 DELAY =1
0360 GOTO 0310
0370 IF SYS(7)=-9 THEN GOTO 0410
0380 PRINT
0390 PRINT "<7><7>THERE IS NO EXISTING DATA FOR INJECTION ID ";D2$;"."
0400 GOTO 0240
0410 ON ERR THEN GOTO 0450
0420 OPEN FILE[3,0],D3$,31
0430 ON ERR THEN STOP
0440 GOTO 0500
0450 ON ERR THEN STOP
0460 DELAY =1
0470 GOTO 0410
0480 REM   ---------------------------------------------------------
0490 REM          CHECK DATA FILE USARILITY FLAG
0500 PRINT
0510 PRINT "PLEASE BE PATIENT."
0520 READ FILE[3,1],J
0530 IF J=1 THEN GOTO 0610
0540 PRINT
0550 IF J=2 THEN PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPOR
*    T DID NOT HAVE A TOTAL AREA."
0560 IF J=3 THEN PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPOR
*    T WAS IN THE WRONG FORMAT."
0570 CLOSE FILE[3]
0580 GOTO 0240
0590 REM   ---------------------------------------------------------
0600 REM          DISPLAY ANY ERROR MESSAGES
0610 LET P9=2
0620 READ FILE[3,P9],V0$
0630 IF V0$[1,7]<>"MESSAGE" THEN GOTO 0710
0640 PRINT
0650 PRINT "THE FOLLOWING MESSAGE WAS PART OF THE REPORT FOR"
0660 PRINT "     INJECTION ";D2$;":  ";V0$
0670 LET P9=P9+1
0680 GOTO 0620
0690 REM   ---------------------------------------------------------
0700 REM          MATCH IDENTIFIER WITH CALIBRATION DATA
```

12345678911234567892123456789312345678941234567895123456789612345678 97
         0   0   0   0   0   0   0

PROGRAM LISTING FOR GC09

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0710 LET P9=P9+2
0720 READ FILE[3,P9],G$,H$,B,C
0730 IF EOF(3) THEN GOTO 1430
0740 REM   ------------------------------------
0750 REM     SKIP UNEXPLAINED PEAKS
0760 IF G$<>"XXXXXXXX" THEN GOTO 0820
0770 WRITE FILE[3,P9],G$,H$,B,C,-9999
0780 LET P9=P9+1
0790 GOTO 0720
0800 REM   ------------------------------------
0810 REM     LOCATE MATCHING IDENTIFIER IN METHOD FILE
0820 FOR I7=1 TO F
0830   READ FILE[4,3*I7-1],V$
0840   IF G$=V$ THEN GOTO 0960
0850 NEXT I7
0860 PRINT
0870 PRINT "<7><7>THE REPORT FOR INJECTION ";D2$;" CONTAINS A NAMED PE
*     AK WITH THE"
0880 PRINT "     IDENTIFIER '";G$;"',' BUT METHOD ";T$[3,6];" DOES NOT
*     INCLUDE"
0890 PRINT "     THAT IDENTIFIER."
0900 PRINT "THEREFORE, THE CONCENTRATION OF ";G$;" CANNOT BE CALCULATE
*     D."
0910 WRITE FILE[3,P9],G$,H$,B,C,-9999
0920 LET P9=P9+1
0930 GOTO 0720
0940 REM   ------------------------------------
0950 REM     CHECK WHETHER IDENTIFIER HAS BEEN CALIBRATED
0960 READ FILE[4,3*I7],D4$,I$,K,R1,R2,R3,J3
0965 LET F[I7]=1
0966 IF C=-9999 THEN GOTO 1410
0970 IF D4$<>"99/99/99" THEN GOTO 1080
0980 PRINT
0990 PRINT "<7><7>THE REPORT FOR INJECTION ";D2$;" CONTAINS A NAMED PE
*     AK WITH THE"
1000 PRINT "     IDENTIFIER '";G$;"',' BUT THAT IDENTIFIER HAS NEVER BE
*     EN"
1010 PRINT "     CALIBRATED IN METHOD ";T$[3,6];"."
1020 PRINT "THEREFORE, THE CONCENTRATION OF ";G$;" CANNOT BE CALCULATE
*     D."
1030 WRITE FILE[3,P9],G$,H$,B,C,-9999
1040 LET P9=P9+1
```


PROGRAM LISTING FOR GC09

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
1050 GOTO 0720
1060 REM   ------------------------------------------------------------
1070 REM          CALCULATE CONCENTRATION USING REGRESSION EQUATION
1080 IF K=3 THEN GOTO 1160
1090 LET L=R1+R2*C
1100 IF K=2 THEN LET L=L+R3*C
1110 WRITE FILE[3,P9],G$,H$,B,C,L
1120 LET P9=P9+1
1130 GOTO 0720
1140 REM   ------------------------------------------------------------
1150 REM          CALCULATE CONCENTRATION USING INTERPOLATION
1160 LET I5=LEN(I$)/8
1170 MAT READ FILE[4,3*I7+1],G2
1180 IF I5=1 THEN GOTO 1200
1190 IF C>G2[2] THEN GOTO 1250
1200 LET M1=0
1210 LET M2=0
1220 LET M3=G2[1]
1230 LET M4=G2[2]
1240 GOTO 1390
1250 IF C<G2[2*I5] THEN GOTO 1310
1260 LET M1=G2[2*(I5-1)-1]
1270 LET M2=G2[2*(I5-1)]
1280 LET M3=G2[2*I5-1]
1290 LET M4=G2[2*I5]
1300 GOTO 1390
1310 LET I=2
1320 IF G2[2*I]>C THEN GOTO 1350
1330 LET I=I+1
1340 GOTO 1320
1350 LET M1=G2[2*(I-1)-1]
1360 LET M2=G2[2*(I-1)]
1370 LET M3=G2[2*I-1]
1380 LET M4=G2[2*I]
1390 LET L=((M3-M1)/(M4-M2))*(C-M2)+M1
1400 WRITE FILE[3,P9],G$,H$,B,C,L
1410 LET P9=P9+1
1420 GOTO 0720
1430 REM   ------------------------------------------------------------
1440 REM          ADD UNDETECTED COMPOUNDS TO DATA FILE
1450 FOR I=1 TO F
1460   IF F[I]=1 THEN GOTO 1500
```

PROGRAM LISTING FOR GC09

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
1470   READ FILE[4,3*I-1],G$
1475   IF G$="99999" THEN GOTO 1500
1480   WRITE FILE[3,P9],G$," ",-9999,-9999,-9999,-9999
1490   LET P9=P9+1
1500 NEXT I
1510 REM  ------------------------------------------------------
1520 REM          CONTINUE INTO PROGRAM GC18
1530 NOESC
1540 CHAIN "GC12"
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```


SYMBOL TABLE FOR GC09

SYMBOL	REFERENCES									
0110	0080									
0112	0110									
0160	0100									
0180	0210									
0240	0190	0290	0400	0580						
0255	0245									
0300	0260									
0310	0360									
0330	0310									
0370	0340									
0410	0370	0470								
0450	0410									
0500	0440									
0610	0530									
0620	0680									
0710	0630									
0720	0790	0930	1050	1130	1420					
0820	0760									
0960	0840									
1080	0970									
1160	1080									
1200	1180									
1250	1190									
1310	1250									
1320	1340									
1350	1320									
1390	1240	1300								
1410	0966									
1430	0730									
1500	1460	1475								
B	0720	0770	0910	1030	1110	1400				
C	0720	0770	0910	0966	1030	1090	1100	1110	1190	1250
	1320	1390	1400							
D2$	0090	0250	0260	0280	0300	0390	0550	0560	0660	0870
	0990									
D3$	0090	0300	0320	0420						
D4$	0090	0960	0970							
F	0096	0160	0180	0200	0820	1450				
FL#3	0111	0420	0520	0570	0620	0720	0770	0910	1030	1110
	1400	1480								
FL#4	0170	0175	0176	0180	0830	0960	1170	1470		
F[	0095	0965	1460							
G$	0090	0770	0760	0770	0840	0880	0900	0910	1000	1020
	1030	1110	1400	1470	1475	1480				
G2	1170									

SYMBOL TABLE FOR GC09

SYMBOL	REFERENCES									
G2[	0090	1190	1220	1230	1250	1260	1270	1280	1290	1320
	1350	1360	1370	1380						
H$	0090	0720	0770	0910	1030	1110	1400			
I	1310	1320	1330	1350	1360	1370	1380	1450	1460	1470
	1500									
I$	0090	0960	1160							
I5	1160	1180	1250	1260	1270	1280	1290			
I7	0820	0830	0850	0960	0965	1170				
J	0520	0530	0550	0560						
J3	0960									
K	0960	1080	1100							
L	1090	1100	1110	1390	1400					
M1	1200	1260	1350	1390						
M2	1210	1270	1360	1390						
M3	1220	1280	1370	1390						
M4	1230	1290	1380	1390						
P9	0610	0620	0670	0710	0720	0770	0780	0910	0920	1030
	1040	1110	1120	1400	1410	1480	1490			
R1	0960	1090								
R2	0960	1090								
R3	0960	1100								
T$	0090	0170	0176	0248	0880	1010				
V$	0090	0180	0830	0840						
V0$	0090	0620	0630	0660						

SECTION 12

PROGRAM GC10 - LIQUID/LIQUID EXTRACTION CONCENTRATION CALCULATION

GC10 is the program which calculates concentrations of samples prepared by the liquid/liquid extraction method. It is essentially the same as program GC09. The only difference is that this program asks the user for the volume of the injection, the volume of the extract, and the volume of the water extracted. Using the calibration equations, this program calculates the mass in nanograms of each compound. It multiplies this mass by the volume of the extract (in milliliters) and divides by the product of the volume of the injection (in microliters) and the volume of the water extracted (in liters). This produces the concentration in micrograms per liter.

There are three additional symbols used in GC10. They are:

Q the volume of the injection
R the volume of the extract
S the volume of the water extracted

PROGRAM LISTING FOR GC10

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                     +
0030 REM   +   PROGRAM GC10, LIQUID/LIQUID EXTRACTION PROCESSING       +
0040 REM   +   BY:  J. KOPKE (SWORCC), MARCH 19, 1979                  +
0045 REM   +   MOST RECENT REVISION:  APRIL 2, 1979                    +
0050 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0060 REM
0070 ESC
0080 ON ESC THEN GOTO 0110
0090 DIM D2$[8],D3$[10],D4$[8],G$[8],G2[30],H$[2],I$[160],T$[6],V$[8],
*    V0$[20]
0095 DIM F[60]
0096 MAT F=ZER
0100 GOTO 0160
0110 ON ERR THEN GOTO 0112
0111 CLOSE FILE[3]
0112 ON ERR THEN STOP
0120 NOESC
0130 CHAIN "GC00"
0140 REM   ---------------------------------------------------------
0150 REM          COUNT IDENTIFIERS IN METHOD FILE
0160 LET F=0
0170 READ FILE[4,1],T$
0175 CLOSE FILE[4]
0176 OPEN FILE[4,0],T$,200
0180 READ FILE[4,3*(F+1)-1],V$
0190 IF EOF(4) THEN GOTO 0240
0200 LET F=F+1
0210 GOTO 0180
0220 REM   ---------------------------------------------------------
0230 REM          OPEN DATA FILE
0240 PRINT
0245 ON ERR THEN GOTO 0255
0248 PRINT "WHAT IS THE ID FOR THE INJECTION TO BE PROCESSED BY METHOD
*     ";T$[3,6];
0250 INPUT "?  ",D2$
0255 ON ERR THEN STOP
0260 IF LEN(D2$)=8 THEN GOTO 0300
0270 PRINT
0280 PRINT "<7><7>";D2$;" IS NOT A VALID INJECTION ID."
0290 GOTO 0240
0300 LET D3$="GC",D2$
```

12345678911234567892123456789312345678941234567895123456789612345678 97
0 0 0 0 0 0 0

PROGRAM LISTING FOR GC10

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0310 ON ERR THEN GOTO 0330
0320 RENAME D3$,D3$
0330 ON ERR THEN STOP
0340 IF SYS(7)<>-48 THEN GOTO 0370
0350 DELAY =1
0360 GOTO 0310
0370 IF SYS(7)=-9 THEN GOTO 0410
0380 PRINT
0390 PRINT "<7><7>THERE IS NO EXISTING DATA FOR INJECTION ID ";D2$;"."
0400 GOTO 0240
0410 ON ERR THEN GOTO 0450
0420 OPEN FILE[3,0],D3$,31
0430 ON ERR THEN STOP
0440 GOTO 0520
0450 ON ERR THEN STOP
0460 DELAY =1
0470 GOTO 0410
0480 REM   ---------------------------------------------------------
0490 REM          CHECK DATA FILE USABILITY FLAG
0520 READ FILE[3,1],J
0530 IF J=1 THEN GOTO 0610
0540 PRINT
0550 IF J=2 THEN PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPOR
*    T DID NOT HAVE A TOTAL AREA."
0560 IF J=3 THEN PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPOR
*    T WAS IN THE WRONG FORMAT."
0570 CLOSE FILE[3]
0580 GOTO 0240
0590 REM   ---------------------------------------------------------
0600 REM          DISPLAY ANY ERROR MESSAGES
0610 LET P9=2
0620 READ FILE[3,P9],V0$
0630 IF V0$[1,7]<>"MESSAGE" THEN GOTO 0702
0640 PRINT
0650 PRINT "THE FOLLOWING MESSAGE WAS PART OF THE REPORT FOR"
0660 PRINT "     INJECTION ";D2$;":  ";V0$
0670 LET P9=P9+1
0680 GOTO 0620
0690 REM   ---------------------------------------------------------
0700 REM          MATCH IDENTIFIER WITH CALIBRATION DATA
0702 INPUT "     VOLUME OF THE INJECTION, IN MICROLITERS?  ",Q
0704 INPUT "     VOLUME OF THE EXTRACT, IN MILLILITERS?  ",R
```

12345678911234567892123456789312345678941234567895123456789612345678 97
0 0 0 0 0 0 0

PROGRAM LISTING FOR GC10

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0706 INPUT "     VOLUME OF THE WATER EXTRACTED, IN LITERS?  ",S
0708 PRINT
0709 PRINT "PLEASE BE PATIENT."
0710 LET P9=P9+2
0720 READ FILE[3,P9],G$,H$,B,C
0730 IF EOF(3) THEN GOTO 1430
0740 REM   ------------------------------------
0750 REM     SKIP UNEXPLAINED PEAKS
0760 IF G$<>"XXXXXXXX" THEN GOTO 0820
0770 WRITE FILE[3,P9],G$,H$,B,C,-9999
0780 LET P9=P9+1
0790 GOTO 0720
0800 REM   ------------------------------------
0810 REM     LOCATE MATCHING IDENTIFIER IN METHOD FILE
0820 FOR I7=1 TO F
0830   READ FILE[4,3*I7-1],V$
0840   IF G$=V$ THEN GOTO 0960
0850 NEXT I7
0860 PRINT
0870 PRINT "<7><7>THE REPORT FOR INJECTION ";D2$;" CONTAINS A NAMED PE
*     AK WITH THE"
0880 PRINT "     IDENTIFIER '";G$;",' BUT METHOD ";T$[3,6];" DOES NOT
*     INCLUDE"
0890 PRINT "     THAT IDENTIFIER."
0900 PRINT "THEREFORE, THE CONCENTRATION OF ";G$;" CANNOT BE CALCULATE
*     D."
0910 WRITE FILE[3,P9],G$,H$,B,C,-9999
0920 LET P9=P9+1
0930 GOTO 0720
0940 REM   ------------------------------------
0950 REM     CHECK WHETHER IDENTIFIER HAS BEEN CALIBRATED
0960 READ FILE[4,3*I7],D4$,I$,K,R1,R2,R3,J3
0965 LET F[I7]=1
0966 IF C=-9999 THEN GOTO 1410
0970 IF D4$<>"99/99/99" THEN GOTO 1080
0980 PRINT
0990 PRINT "<7><7>THE REPORT FOR INJECTION ";D2$;" CONTAINS A NAMED PE
*     AK WITH THE"
1000 PRINT "     IDENTIFIER '";G$;",' BUT THAT IDENTIFIER HAS NEVER BE
*     EN"
1010 PRINT "     CALIBRATED IN METHOD ";T$[3,6];"."
1020 PRINT "THEREFORE, THE CONCENTRATION OF ";G$;" CANNOT BE CALCULATE
*     D."

12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```


PROGRAM LISTING FOR GC10

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
1030 WRITE FILE[3,P9],G$,H$,B,C,-9999
1040 LET P9=P9+1
1050 GOTO 0720
1060 REM   ------------------------------------------------------------
1070 REM          CALCULATE CONCENTRATION USING REGRESSION EQUATION
1080 IF K=3 THEN GOTO 1160
1090 LET L=R1+R2*C
1100 IF K=2 THEN LET L=L+R3*C
1105 LET L=(L*R)/(Q*S)
1110 WRITE FILE[3,P9],G$,H$,B,C,L
1120 LET P9=P9+1
1130 GOTO 0720
1140 REM   ------------------------------------------------------------
1150 REM          CALCULATE CONCENTRATION USING INTERPOLATION
1160 LET I5=LEN(I$)/8
1170 MAT READ FILE[4,3*I7+1],G2
1180 IF I5=1 THEN GOTO 1200
1190 IF C>G2[2] THEN GOTO 1250
1200 LET M1=0
1210 LET M2=0
1220 LET M3=G2[1]
1230 LET M4=G2[2]
1240 GOTO 1390
1250 IF C<G2[2*I5] THEN GOTO 1310
1260 LET M1=G2[2*(I5-1)-1]
1270 LET M2=G2[2*(I5-1)]
1280 LET M3=G2[2*I5-1]
1290 LET M4=G2[2*I5]
1300 GOTO 1390
1310 LET I=2
1320 IF G2[2*I]>C THEN GOTO 1350
1330 LET I=I+1
1340 GOTO 1320
1350 LET M1=G2[2*(I-1)-1]
1360 LET M2=G2[2*(I-1)]
1370 LET M3=G2[2*I-1]
1380 LET M4=G2[2*I]
1390 LET L=((M3-M1)/(M4-M2))*(C-M2)+M1
1395 LET L=(L*R)/(Q*S)
1400 WRITE FILE[3,P9],G$,H$,B,C,L
1410 LET P9=P9+1
1420 GOTO 0720

12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

PROGRAM LISTING FOR GC10

```
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
1430 REM  ------------------------------------------------------------
1440 REM          ADD UNDETECTED COMPOUNDS TO DATA FILE
1450 FOR I=1 TO F
1460   IF F[I]=1 THEN GOTO 1500
1470   READ FILE[4,3*I-1],G$
1475   IF G$="99999" THEN GOTO 1500
1480   WRITE FILE[3,P9],G$," ",-9999,-9999,-9999,-9999
1490   LET P9=P9+1
1500 NEXT I
1510 REM  ------------------------------------------------------------
1520 REM          CONTINUE INTO PROGRAM GC18
1530 NOESC
1540 CHAIN "GC12"
```

1234567891123456789212345678931234567894123456789512345678961234567897
         0   0   0   0   0   0   0

SYMBOL TABLE FOR GC10

SYMBOL	REFERENCES									
0110	0080									
0112	0110									
0160	0100									
0180	0210									
0240	0190	0290	0400	0580						
0255	0245									
0300	0260									
0310	0360									
0330	0310									
0370	0340									
0410	0370	0470								
0450	0410									
0520	0440									
0610	0530									
0620	0680									
0702	0630									
0720	0790	0930	1050	1130	1420					
0820	0760									
0960	0840									
1080	0970									
1160	1080									
1200	1180									
1250	1190									
1310	1250									
1320	1340									
1350	1320									
1390	1240	1300								
1410	0966									
1430	0730									
1500	1460	1475								
B	0720	0770	0910	1030	1110	1400				
C	0720	0770	0910	0966	1030	1090	1100	1110	1190	1250
	1320	1390	1400							
D2$	0090	0250	0260	0280	0300	0390	0550	0560	0660	0870
	0990									
D3$	0090	0300	0320	0420						
D4$	0090	0960	0970							
F	0096	0160	0180	0200	0820	1450				
FL#3	0111	0420	0520	0570	0620	0720	0770	0910	1030	1110
	1400	1480								
FL#4	0170	0175	0176	0180	0830	0960	1170	1470		
F[	0095	0965	1460							
G$	0090	0720	0760	0770	0840	0880	0900	0910	1000	1020
	1030	1110	1400	1470	1475	1480				
G2	1170									

SYMBOL TABLE FOR GC10

SYMBOL	REFERENCES									
G2[	0090	1190	1220	1230	1250	1260	1270	1280	1290	1320
	1350	1360	1370	1380						
H$	0090	0720	0770	0910	1030	1110	1400			
I	1310	1320	1330	1350	1360	1370	1380	1450	1460	1470
	1500									
I$	0090	0960	1160							
I5	1160	1180	1250	1260	1270	1280	1290			
I7	0820	0830	0850	0960	0965	1170				
J	0520	0530	0550	0560						
J3	0960									
K	0960	1080	1100							
L	1090	1100	1105	1110	1390	1395	1400			
M1	1200	1260	1350	1390						
M2	1210	1270	1360	1390						
M3	1220	1280	1370	1390						
M4	1230	1290	1380	1390						
P9	0610	0620	0670	0710	0720	0770	0780	0910	0920	1030
	1040	1110	1120	1400	1410	1480	1490			
Q	0702	1105	1395							
R	0704	1105	1395							
R1	0960	1090								
R2	0960	1090								
R3	0960	1100								
S	0706	1105	1395							
T$	0090	0170	0176	0248	0880	1010				
V$	0090	0180	0830	0840						
V0$	0090	0620	0630	0660						

SECTION 13

PROGRAM GC11 - DIRECT AQUEOUS INJECTION CONCENTRATION CALCULATION

GC11 is the program which calculates concentrations of samples prepared by the direct aqueous injection method. It is essentially the same as program GC09. The only difference is that this program asks the user for the volume of the injection. Using the calibration equations, this program calculates the mass in nanograms of each compound. It divides this mass by the injection volume (in microliters) and then divides by 1000 to produce the concentration in micrograms per liter.

There is one additional symbol used in GC11. It is Q, the volume of the injection.

PROGRAM LISTING FOR GC11

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                    +
0030 REM   +   PROGRAM GC11, DIRECT AQUEOUS INJECTION PROCESSING      +
0040 REM   +   BY:  J. KOPKE (SWORCC), MARCH 20, 1979                 +
0045 REM   +   MOST RECENT REVISION:  APRIL 2, 1979                   +
0050 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0060 REM
0070 ESC
0080 ON ESC THEN GOTO 0110
0090 DIM D2$[8],D3$[10],D4$[8],G$[8],G2[30],H$[2],I$[160],T$[6],V$[8],
*    V0$[20]
0095 DIM F[60]
0096 MAT F=ZER
0100 GOTO 0160
0110 ON ERR THEN GOTO 0112
0111 CLOSE FILE[3]
0112 ON ERR THEN STOP
0120 NOESC
0130 CHAIN "GC00"
0140 REM   ---------------------------------------------------------
0150 REM          COUNT IDENTIFIERS IN METHOD FILE
0160 LET F=0
0170 READ FILE[4,1],T$
0175 CLOSE FILE[4]
0176 OPEN FILE[4,0],T$,200
0180 READ FILE[4,3*(F+1)-1],V$
0190 IF EOF(4) THEN GOTO 0240
0200 LET F=F+1
0210 GOTO 0180
0220 REM   ---------------------------------------------------------
0230 REM          OPEN DATA FILE
0240 PRINT
0245 ON ERR THEN GOTO 0255
0248 PRINT "WHAT IS THE ID FOR THE INJECTION TO BE PROCESSED BY METHOD
*     ";T$[3,6];
0250 INPUT "?  ",D2$
0255 ON ERR THEN STOP
0260 IF LEN(D2$)=8 THEN GOTO 0300
0270 PRINT
0280 PRINT "<7><7>";D2$;" IS NOT A VALID INJECTION ID."
0290 GOTO 0240
0300 LET D3$="GC",D2$
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```


PROGRAM LISTING FOR GC11

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0310 ON ERR THEN GOTO 0330
0320 RENAME D3$,D3$
0330 ON ERR THEN STOP
0340 IF SYS(7)<>-48 THEN GOTO 0370
0350 DELAY =1
0360 GOTO 0310
0370 IF SYS(7)=-9 THEN GOTO 0410
0380 PRINT
0390 PRINT "<7><7>THERE IS NO EXISTING DATA FOR INJECTION ID ";D2$;"."
0400 GOTO 0240
0410 ON ERR THEN GOTO 0450
0420 OPEN FILE[3,0],D3$,31
0430 ON ERR THEN STOP
0440 GOTO 0520
0450 ON ERR THEN STOP
0460 DELAY =1
0470 GOTO 0410
0480 REM   ---------------------------------------------------------
0490 REM          CHECK DATA FILE USABILITY FLAG
0520 READ FILE[3,1],J
0530 IF J=1 THEN GOTO 0610
0540 PRINT
0550 IF J=2 THEN PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPOR
*    T DID NOT HAVE A TOTAL AREA."
0560 IF J=3 THEN PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPOR
*    T WAS IN THE WRONG FORMAT."
0570 CLOSE FILE[3]
0580 GOTO 0240
0590 REM   ---------------------------------------------------------
0600 REM          DISPLAY ANY ERROR MESSAGES
0610 LET P9=2
0620 READ FILE[3,P9],V0$
0630 IF V0$[1,7]<>"MESSAGE" THEN GOTO 0702
0640 PRINT
0650 PRINT "THE FOLLOWING MESSAGE WAS PART OF THE REPORT FOR"
0660 PRINT "     INJECTION ";D2$;":  ";V0$
0670 LET P9=P9+1
0680 GOTO 0620
0690 REM   ---------------------------------------------------------
0700 REM          MATCH IDENTIFIER WITH CALIBRATION DATA
0702 INPUT "     VOLUME OF THE INJECTION, IN MICROLITERS?  ",Q
0708 PRINT
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

PROGRAM LISTING FOR GC11

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0709 PRINT "PLEASE BE PATIENT."
0710 LET P9=P9+2
0720 READ FILE[3,P9],G$,H$,B,C
0730 IF EOF(3) THEN GOTO 1430
0740 REM  ------------------------------------
0750 REM     SKIP UNEXPLAINED PEAKS
0760 IF G$<>"XXXXXXXX" THEN GOTO 0820
0770 WRITE FILE[3,P9],G$,H$,B,C,-9999
0780 LET P9=P9+1
0790 GOTO 0720
0800 REM  ------------------------------------
0810 REM     LOCATE MATCHING IDENTIFIER IN METHOD FILE
0820 FOR I7=1 TO F
0830   READ FILE[4,3*I7-1],V$
0840   IF G$=V$ THEN GOTO 0960
0850 NEXT I7
0860 PRINT
0870 PRINT "<7><7>THE REPORT FOR INJECTION ";D2$;" CONTAINS A NAMED PE
*    AK WITH THE"
0880 PRINT "     IDENTIFIER '";G$;",' BUT METHOD ";T$[3,6];" DOES NOT
*    INCLUDE"
0890 PRINT "     THAT IDENTIFIER."
0900 PRINT "THEREFORE, THE CONCENTRATION OF ";G$;" CANNOT BE CALCULATE
*    D."
0910 WRITE FILE[3,P9],G$,H$,B,C,-9999
0920 LET P9=P9+1
0930 GOTO 0720
0940 REM  ------------------------------------
0950 REM     CHECK WHETHER IDENTIFIER HAS BEEN CALIBRATED
0960 READ FILE[4,3*I7],D4$,I$,K,R1,R2,R3,J3
0965 LET F[I7]=1
0966 IF C=-9999 THEN GOTO 1410
0970 IF D4$<>"99/99/99" THEN GOTO 1080
0980 PRINT
0990 PRINT "<7><7>THE REPORT FOR INJECTION ";D2$;" CONTAINS A NAMED PE
*    AK WITH THE"
1000 PRINT "     IDENTIFIER '";G$;",' BUT THAT IDENTIFIER HAS NEVER BE
*    EN"
1010 PRINT "     CALIBRATED IN METHOD ";T$[3,6];"."
1020 PRINT "THEREFORE, THE CONCENTRATION OF ";G$;" CANNOT BE CALCULATE
*    D."
1030 WRITE FILE[3,P9],G$,H$,B,C,-9999
```

12345678911234567892123456789312345678941234567895123456789612345678 97
0 0 0 0 0 0 0

PROGRAM LISTING FOR GC11

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
1040 LET P9=P9+1
1050 GOTO 0720
1060 REM  ------------------------------------------------------------
1070 REM          CALCULATE CONCENTRATION USING REGRESSION EQUATION
1080 IF K=3 THEN GOTO 1160
1090 LET L=R1+R2*C
1100 IF K=2 THEN LET L=L+R3*C
1105 LET L=L/Q/1000
1110 WRITE FILE[3,P9],G$,H$,B,C,L
1120 LET P9=P9+1
1130 GOTO 0720
1140 REM  ------------------------------------------------------------
1150 REM          CALCULATE CONCENTRATION USING INTERPOLATION
1160 LET I5=LEN(I$)/8
1170 MAT READ FILE[4,3*I7+1],G2
1180 IF I5=1 THEN GOTO 1200
1190 IF C>G2[2] THEN GOTO 1250
1200 LET M1=0
1210 LET M2=0
1220 LET M3=G2[1]
1230 LET M4=G2[2]
1240 GOTO 1390
1250 IF C<G2[2*I5] THEN GOTO 1310
1260 LET M1=G2[2*(I5-1)-1]
1270 LET M2=G2[2*(I5-1)]
1280 LET M3=G2[2*I5-1]
1290 LET M4=G2[2*I5]
1300 GOTO 1390
1310 LET I=2
1320 IF G2[2*I]>C THEN GOTO 1350
1330 LET I=I+1
1340 GOTO 1320
1350 LET M1=G2[2*(I-1)-1]
1360 LET M2=G2[2*(I-1)]
1370 LET M3=G2[2*I-1]
1380 LET M4=G2[2*I]
1390 LET L=((M3-M1)/(M4-M2))*(C-M2)+M1
1395 LET L=L/Q/1000
1400 WRITE FILE[3,P9],G$,H$,B,C,L
1410 LET P9=P9+1
1420 GOTO 0720
1430 REM  ------------------------------------------------------------
```

12345678911234567892123456789312345678941234567895123456789612345678 97
0 0 0 0 0 0 0

PROGRAM LISTING FOR GC11

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
1440 REM          ADD UNDETECTED COMPOUNDS TO DATA FILE
1450 FOR I=1 TO F
1460   IF F[I]=1 THEN GOTO 1500
1470   READ FILE[4,3*I-1],G$
1475   IF G$="99999" THEN GOTO 1500
1480   WRITE FILE[3,P9],G$," ",-9999,-9999,-9999,-9999
1490   LET P9=P9+1
1500 NEXT I
1510 REM   ------------------------------------------------------
1520 REM          CONTINUE INTO PROGRAM GC18
1530 NOESC
1540 CHAIN "GC12"
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```


SYMBOL TABLE FOR GC11

SYMBOL	REFERENCES									
0110	0080									
0112	0110									
0160	0100									
0180	0210									
0240	0190	0290	0400	0580						
0255	0245									
0300	0260									
0310	0360									
0330	0310									
0370	0340									
0410	0370	0470								
0450	0410									
0520	0440									
0610	0530									
0620	0680									
0702	0630									
0720	0790	0930	1050	1130	1420					
0820	0760									
0960	0840									
1080	0970									
1160	1080									
1200	1180									
1250	1190									
1310	1250									
1320	1340									
1350	1320									
1390	1240	1300								
1410	0966									
1430	0730									
1500	1460	1475								
B	0720	0770	0910	1030	1110	1400				
C	0720	0770	0910	0966	1030	1090	1100	1110	1190	1250
	1320	1390	1400							
D2$	0090	0250	0260	0280	0300	0390	0550	0560	0660	0870
	0990									
D3$	0090	0300	0320	0420						
D4$	0090	0960	0970							
F	0096	0160	0180	0200	0820	1450				
FL#3	0111	0420	0520	0570	0620	0720	0770	0910	1030	1110
	1400	1480								
FL#4	0170	0175	0176	0180	0830	0960	1170	1470		
FI	0095	0965	1460							
G$	0090	0720	0760	0770	0840	0880	0900	0910	1000	1020
	1030	1110	1400	1470	1475	1480				
G2	1170									

SYMBOL TABLE FOR GC11

SYMBOL	REFERENCES									
G2[	0090	1190	1220	1230	1250	1260	1270	1280	1290	1320
	1350	1360	1370	1380						
H$	0090	0720	0770	0910	1030	1110	1400			
I	1310	1320	1330	1350	1360	1370	1380	1450	1460	1470
	1500									
I$	0090	0960	1160							
I5	1160	1180	1250	1260	1270	1280	1290			
I7	0820	0830	0850	0960	0965	1170				
J	0520	0530	0550	0560						
J3	0960									
K	0960	1080	1100							
L	1090	1100	1105	1110	1390	1395	1400			
M1	1200	1260	1350	1390						
M2	1210	1270	1360	1390						
M3	1220	1280	1370	1390						
M4	1230	1290	1380	1390						
P9	0610	0620	0670	0710	0720	0770	0780	0910	0920	1030
	1040	1110	1120	1400	1410	1480	1490			
Q	0702	1105	1395							
R1	0960	1090								
R2	0960	1090								
R3	0960	1100								
T$	0090	0170	0176	0248	0880	1010				
V$	0090	0180	0830	0840						
V0$	0090	0620	0630	0660						

SECTION 14

PROGRAM GC12 - RETENTION TIME CALCULATION

GC12 is the program which calculates relative retention times or capacity ratios. It is entered by chaining from any of the concentration calculation programs (GC08, GC09, GC10, or GC11).

As the program begins, the method file and the injection data file are already open, although at several places in the program, the data file is closed and reopened to set the EOF function for that file back to zero.

The program reads from the method file the flag for the type of retention time calculations and either the relative retention time reference identifier or the capacity ratio dead time. It then branches to the appropriate section of code.

To calculate relative retention times, this program first searches the data file for the identifier of the relative retention time reference peak. If that identifier does not appear in the data file, the program informs the user that relative retention times cannot be calculated, and puts -9999 into the injection data file as the relative retention time of every peak. Conversely, if the program does find the relative retention time reference peak in the data file, it uses its retention time to calculate the relative retention time of every peak in the data file and places those calculated values into the data file. The formula for relative retention time is:

$$\text{Rel. Retn. Time} = \frac{\text{Retn. Time}}{\text{Retn. Time of Reference}} \cdot 100.$$

The formula for capacity ratio is:

$$\text{Capacity Ratio} = \frac{\text{Retn. Time}}{\text{Dead Volume Time}} - 1.$$

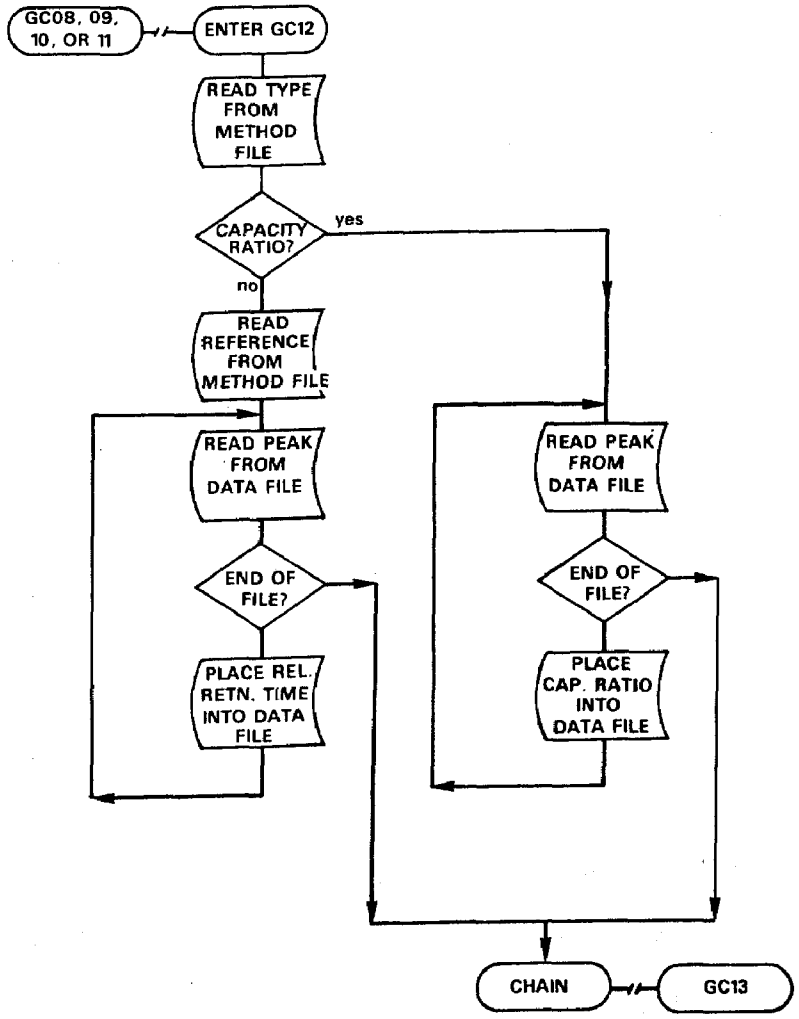

Figure 10. Flowchart of Program GC12.

TABLE 8. SYMBOL DEFINITIONS FOR PROGRAM GC12

B	the absolute retention time of a peak
C	the area of a peak
D3$	the name of the data file
G$	an identifier from a data file
H$	the peak type
I2	the data file record number of the peak being processed
J	the data file useability flag
L	the calculated concentration
L2	the calculated relative retention time or capacity ratio
N$	the relative retention time reference peak or the capacity ratio dead time as a string
N1	the type of method
N2	the type of retention time calculations N2=1 relative retention time N2=2 capacity ratio
N3	retention time of a peak
N4	capacity ratio dead time
P9	the record number of the first peak in the data file
T$	the name of the method file
U$	the name of the user
VO$	a MESSAGE from the data file

PROGRAM LISTING FOR GC12

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                       +
0030 REM   +   PROGRAM GC12, RETENTION TIME CALCULATIONS                 +
0040 REM   +   BY:  J. KOPKE (SWORCC), FEBRUARY 14, 1979                 +
0045 REM   +   MOST RECENT REVISION:  MARCH 21, 1979                     +
0050 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0060 REM
0070 ESC
0080 ON ESC THEN GOTO 0100
0090 GOTO 0130
0100 ON ERR THEN GOTO 0102
0101 CLOSE FILE[3]
0102 ON ERR THEN STOP
0110 NOESC
0120 CHAIN "GC00"
0130 DIM D3$[10],G$[8],H$[2],N$[8],T$[6],U$[30],V0$[20]
0140 REM   ------------------------------------------------------------
0150 REM          DETERMINE TYPE; FIND WHERE TO START
0160 READ FILE[3,1],J,D3$
0170 READ FILE[4,1],T$,U$,N1,N2,N$
0180 LET P9=2
0190 READ FILE[3,P9],V0$
0200 IF V0$[1,7]<>"MESSAGE" THEN GOTO 0230
0210 LET P9=P9+1
0220 GOTO 0190
0230 LET P9=P9+2
0240 IF N2=2 THEN GOTO 0640
0250 REM   ------------------------------------------------------------
0260 REM          RELATIVE RETENTION TIME
0270 LET I2=P9
0280 CLOSE FILE[3]
0290 OPEN FILE[3,0],D3$,31
0300 READ FILE[3,I2],G$,H$,B,C,L
0310 IF EOF(3) THEN GOTO 0370
0320 IF G$=N$ THEN GOTO 0520
0330 LET I2=I2+1
0340 GOTO 0300
0350 REM   ------------------------------------------
0360 REM     CANNOT CALCULATE RELATIVE RETENTION TIMES
0370 PRINT
0380 PRINT "<7><7>METHOD ";T$[3,6];" SPECIFIES THAT THE REFERENCE PEAK
#      FOR RELATIVE"
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```


PROGRAM LISTING FOR GC12

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0390 PRINT "     RETENTION TIME IS ";N$;", BUT THE REPORT FOR INJECTIO
#     N ";D3$[3]
0400 PRINT "     DOES NOT INCLUDE A PEAK WITH THAT IDENTIFIER."
0410 PRINT "THEREFORE, NO RELATIVE RETENTION TIMES CAN BE CALCULATED."
0420 LET I2=P9
0430 CLOSE FILE[3]
0440 OPEN FILE[3,0],D3$,31
0450 READ FILE[3,I2],G$,H$,B,C,L
0460 IF EOF(3) THEN GOTO 0760
0470 WRITE FILE[3,I2],G$,H$,B,C,L,-9999
0480 LET I2=I2+1
0490 GOTO 0450
0500 REM   ------------------------------------------
0510 REM     PUT RELATIVE RETENTION TIME IN DATA FILE
0520 LET N3=B
0530 LET I2=P9
0540 CLOSE FILE[3]
0550 OPEN FILE[3,0],D3$,31
0560 READ FILE[3,I2],G$,H$,B,C,L
0570 IF EOF(3) THEN GOTO 0760
0580 LET L2=(B/N3)*100
0590 WRITE FILE[3,I2],G$,H$,B,C,L,L2
0600 LET I2=I2+1
0610 GOTO 0560
0620 REM   ------------------------------------------------------------
0630 REM          CAPACITY RATIO
0640 LET N4=VAL(N$)
0650 LET I2=P9
0660 CLOSE FILE[3]
0670 OPEN FILE[3,0],D3$,31
0680 READ FILE[3,I2],G$,H$,B,C,L
0690 IF EOF(3) THEN GOTO 0760
0700 LET L2=(B/N4)-1
0710 WRITE FILE[3,I2],G$,H$,B,C,L,L2
0720 LET I2=I2+1
0730 GOTO 0680
0740 REM   ------------------------------------------------------------
0750 REM          FLAG DATA FILE AS BEING PROCESSED
0760 READ FILE[3,1],J,D3$
0770 WRITE FILE[3,1],J,D3$,1
0780 REM   ------------------------------------------------------------
0790 REM          CONTINUE INTO PROGRAM GC19
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

PROGRAM LISTING FOR GC12

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0800 NOESC
0810 CHAIN "GC13"
```


SYMBOL TABLE FOR GC12

SYMBOL	REFERENCES									
0100	0080									
0102	0100									
0130	0090									
0190	0220									
0230	0200									
0300	0340									
0370	0310									
0450	0490									
0520	0320									
0560	0610									
0640	0240									
0680	0730									
0760	0460	0570	0690							
B	0300	0450	0470	0520	0560	0580	0590	0680	0700	0710
C	0300	0450	0470	0560	0590	0680	0710			
T3$	0130	0160	0290	0390	0440	0550	0670	0760	0770	
FL#3	0101	0160	0190	0280	0290	0300	0430	0440	0450	0470
	0540	0550	0560	0590	0660	0670	0680	0710	0760	0770
FL#4	0170									
G$	0130	0300	0320	0450	0470	0560	0590	0680	0710	
H$	0130	0300	0450	0470	0560	0590	0680	0710		
I2	0270	0300	0330	0420	0450	0470	0480	0530	0560	0590
	0600	0650	0680	0710	0720					
J	0160	0760	0770							
L	0300	0450	0470	0560	0590	0680	0710			
L2	0580	0590	0700	0710						
N$	0130	0170	0320	0390	0640					
N1	0170									
N2	0170	0240								
N3	0520	0580								
N4	0640	0700								
P9	0180	0190	0210	0230	0270	0420	0530	0650		
T$	0130	0170	0380							
U$	0130	0170								
V0$	0130	0190	0200							

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

SECTION 15

PROGRAM GC13 - COMPOUND IDENTIFICATION AND DATA PROCESSING REPORT

GC13 is the program which prints the injection data processing report. In doing so, it must also locate the true chemical name and CAS Registry number for each of the named peaks. This program is entered by chaining from the retention time calculation program, GC12. If the escape key is pressed during the execution of GC13, the program chains back to the master control program, GC00.

As GC13 begins, both the injection data file and the method file are already open, although in the program both of these files are closed and promptly reopened to set the EOF functions for them back to zero. This program also opens a temporary formatted output file where it places the lines of the report as they are generated. This avoids having the program monopolize the lineprinter while it searches other files for data.

The first section of this program fills the temporary formatted output file. A record of information is read from the data file, and if that record represents an unexplained peak, this program uses "UNEXPLAINED PEAK" as the name of the compound and a null string as the CAS number. If the record from the data file is a named peak, this program uses the compound name(s) and CAS number(s) from the method file. If there is no matching identifier in the method file, the program uses the string "(identifier - NOT IN METHOD XXXX)" as the name of the compound and a null string as the CAS number. The rest of the numeric items are also written into the temporary file, although if the relative retention time is -9999 (indicating that the item could not be calculated), the corresponding space is left blank.

After all of the records of the data file have been transformed into lines in the temporary file, the program copies the temporary file to the lineprinter. Headings are printed and paging occurs.

When the entire temporary file has been transferred to the lineprinter, all files except the method file are closed and the temporary file is deleted. The program then asks if the user wants to process another injection. If the answer is no, this program disables the escape key and chains back to GC00. If the answer is yes, this program disables the escape key and chains back to the appropriate concentration calculation program, as determined by the type of method flag in the method file.

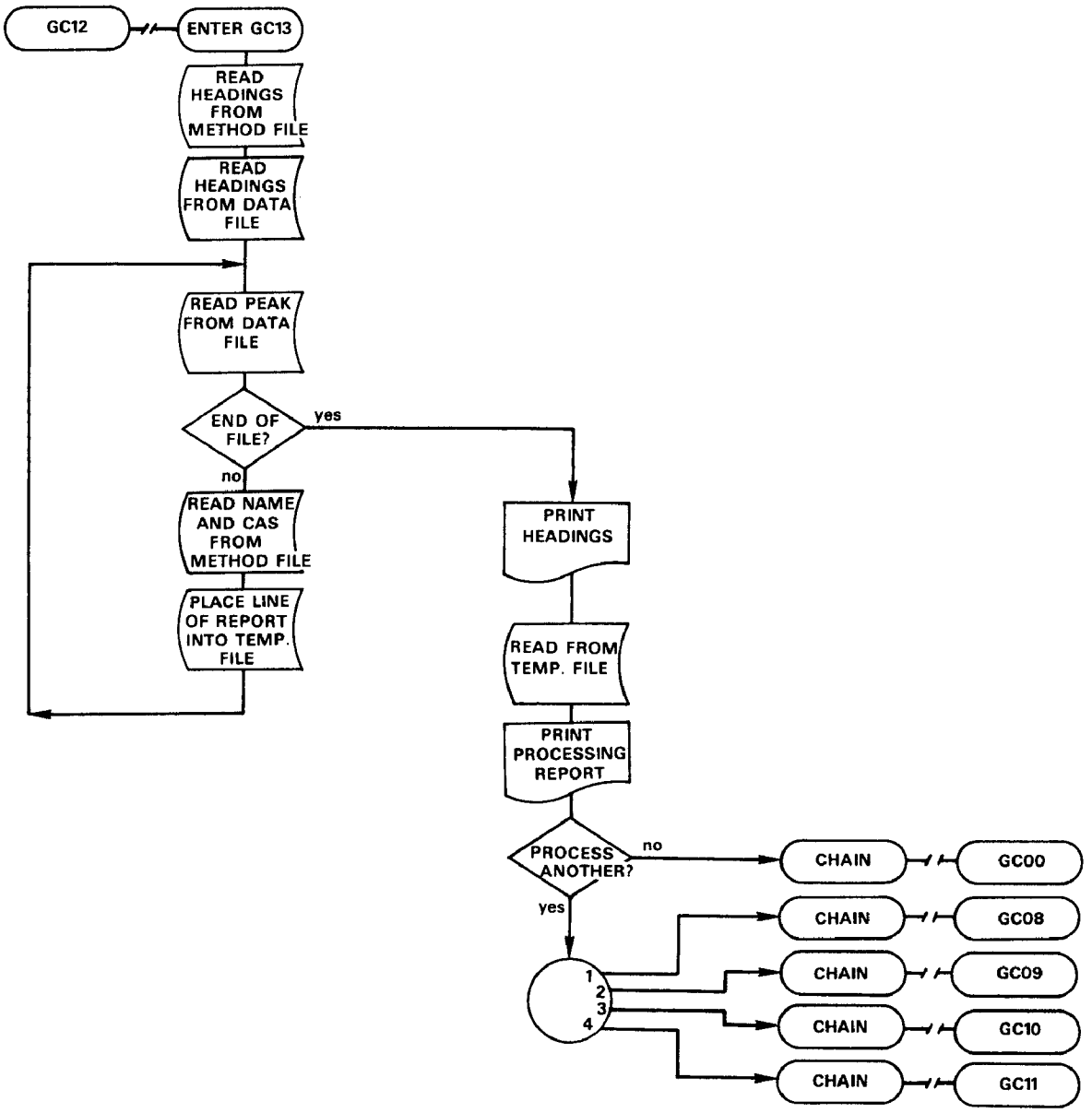

Figure 11. Flowchart of Program GC13.

TABLE 9. SYMBOL DEFINITIONS FOR PROGRAM GC13

B	the absolute retention time of a peak
C	the area of a peak
D3$	the name of the data file
F$	the report title
G$	an identifier from a data file
H$	the peak type
I	the control variable for a loop
I5	the number of identifiers in the method file
I6	the data file position of the peak being processed
I7	the page number of the printed report
J	the data file useability flag
L	the calculated concentration
L2	the calculated relative retention time or capacity ratio
N1	the type of method N1=1 internal standards N1=2 purge and trap N1=3 liquid/liquid extraction N1=4 direct aqueous injection
N2	the type of retention time calculations N2=1 relative retention time N2=2 capacity ratio
P9	the data file record number for the report title
Q$	the name of the temporary formatted output file
Q5$	a format for a PRINT USING statement

TABLE 9. (Continued)

Q6$	a format for a PRINT USING statement
Q7$	the type of method
Q8$	a line being transferred from the temporary formatted output file to the lineprinter
Q9$	the carriage return for Q8$
T$	the name of the method file
U$	the name of the user
V$	an identifier from the method file
V0$	a MESSAGE from the data file
V1$	the name of the first compound associated with an identifier
V2$	the CAS number for V1$
V3$	the name of the second compound associated with an identifier
V4$	the CAS number for V3$
V5$	the name of the third compound associated with an identifier
V6$	the CAS number for V5$
X$	the user's answer to a Y or N question

PROGRAM LISTING FOR GC13

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                      +
0030 REM   +   PROGRAM GC13, COMPOUND IDENTIFICATION AND REPORT         +
0040 REM   +   BY:  J. KOPKE (SWORCC), FEBRUARY 15, 1979                +
0045 REM   +   MOST RECENT REVISION:  APRIL 12, 1979                    +
0050 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0060 REM
0070 ESC
0080 ON ESC THEN GOTO 1640
0090 DIM D3$[10],F$[30],G$[8],H$[2],Q$[13],Q5$[132],Q6$[60],Q7$[30],Q8
*    $[133]
0100 DIM Q9$[2],T$[6],U$[30],V$[8],V0$[20],V1$[40],V2$[11],V3$[40],V4$
*    [11],V5$[40],V6$[11],X$[3]
0110 PAGE =132
0120 LET Q6$="      ######################################  ########
*    ###"
0130 REM   ------------------------------------------------------------
0140 REM          DETERMINE TYPE OF PROCESSING
0150 READ FILE[4,1],T$,U$,N1,N2
0160 ON N1 THEN GOTO 0170, 0190, 0210, 0230
0170 LET Q7$="INTERNAL STANDARDS"
0180 GOTO 0260
0190 LET Q7$="PURGE AND TRAP"
0200 GOTO 0260
0210 LET Q7$="LIQUID/LIQUID EXTRACTION"
0220 GOTO 0260
0230 LET Q7$="DIRECT AQUEOUS INJECTION"
0240 REM   ------------------------------------------------------------
0250 REM          SET EOF(3) AND EOF(4) BACK TO ZERO
0260 CLOSE FILE[4]
0270 OPEN FILE[4,0],T$,200
0280 READ FILE[3,1],J,D3$
0290 CLOSE FILE[3]
0300 OPEN FILE[3,0],D3$,31
0310 REM   ------------------------------------------------------------
0320 REM          COUNT IDENTIFIERS IN METHOD FILE
0330 LET I5=0
0340 READ FILE[4,3*(I5+1)-1],V$
0350 IF EOF(4) THEN GOTO 0400
0360 LET I5=I5+1
0370 GOTO 0340
0380 REM   ------------------------------------------------------------

12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```


PROGRAM LISTING FOR GC13

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0390 REM          OPEN TEMPORARY FORMATTED OUTPUT FILE
0400 LET Q$="GCO",T$[3,6]
0410 OPEN FILE[5,1],Q$
0420 REM   ------------------------------------------------------------
0430 REM          SKIP OVER ANY MESSAGES
0440 LET P9=2
0450 READ FILE[3,P9],V0$
0460 IF V0$[1,7]<>"MESSAGE" THEN GOTO 0510
0470 LET P9=P9+1
0480 GOTO 0450
0490 REM   ------------------------------------------------------------
0500 REM          READ REPORT TITLE
0510 LET P9=P9+1
0520 READ FILE[3,P9],F$
0530 REM   ------------------------------------------------------------
0540 REM          MATCH IDENTIFIER WITH NAME AND CAS NUMBFR
0550 LET I6=1
0560 READ FILE[3,I6+P9],G$,H$,B,C,L,L2
0570 IF EOF(3) THEN GOTO 0960
0580 IF G$="XXXXXXXX" THEN GOTO 0670
0590 FOR I=1 TO I5
0600   READ FILE[4,3*I-1],V$,V1$,V2$,V3$,V4$,V5$,V6$
0610   IF V$=G$ THEN GOTO 0700
0620 NEXT I
0630 LET V1$="(",G$," - NOT IN METHOD ",T$[3,6],")"
0640 LET V2$=""
0650 LET V3$="99999"
0660 GOTO 0700
0670 LET V1$="     UNEXPLAINED PEAK"
0680 LET V2$=""
0690 LET V3$="99999"
0700 LET Q5$="###.  ######################################  ########
*    ###   ##      ######      "
0702 IF C<>-9999 THEN GOTO 0710
0704 LET Q5$=Q5$[1,60],"
*                NOT DETECTED"
0706 PRINT FILE[5],USING Q5$,I6,V1$,V2$
0708 GOTO 0870
0710 IF L2=-9999 THEN GOTO 0740
0720 LET Q5$=Q5$,"  #####.##      "
0730 GOTO 0750
0740 LET Q5$=Q5$,"                "

12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

```
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
0750 LET Q5$=Q5$,"#########.#     "
0760 IF L○-9999 THEN GOTO 0765
0762 IF G$○"XXXXXXXX" THEN LET Q5$=Q5$," NOT CALCULATED"
0763 GOTO 0770
0765 LET Q5$=Q5$,"  -----#.###"
0770 IF L=-9999 THEN IF L2=-9999 THEN GOTO 0820
0780 IF L=-9999 THEN GOTO 0840
0790 IF L2=-9999 THEN GOTO 0860
0800 PRINT FILE[5],USING Q5$,I6,V1$,V2$,H$,B,L2,C,L
0810 GOTO 0870
0820 PRINT FILE[5],USING Q5$,I6,V1$,V2$,H$,B,C
0830 GOTO 0870
0840 PRINT FILE[5],USING Q5$,I6,V1$,V2$,H$,B,L2,C
0850 GOTO 0870
0860 PRINT FILE[5],USING Q5$,I6,V1$,V2$,H$,B,C,L
0870 IF V3$="99999" THEN GOTO 0910
0880 PRINT FILE[5],USING Q6$,V3$,V4$
0890 IF V5$="99999" THEN GOTO 0910
0900 PRINT FILE[5],USING Q6$,V5$,V6$
0910 PRINT FILE[5]," "
0920 LET I6=I6+1
0930 GOTO 0560
0940 REM  ------------------------------------------------------------
0950 REM          PRINT HEADINGS ON LINEPRINTER
0960 ON ERR THEN GOTO 0962
0961 CLOSE FILE[3]
0962 ON ERR THEN GOTO 0964
0963 CLOSE FILE[5]
0964 ON ERR THEN GOTO 0966
0965 CLOSE FILE[6]
0966 ON ERR THEN STOP
0970 OPEN FILE[5,3],Q$
0980 ON ERR THEN GOTO 1020
0990 OPEN FILE[6,1],"$LPT"
1000 ON ERR THEN STOP
1010 GOTO 1050
1020 ON ERR THEN STOP
1030 DELAY =3
1040 GOTO 0980
1050 LET I7=1
1060 PRINT FILE[6], TAB(49);"GAS CHROMATOGRAPHY AUTOMATION SYSTEM"
1070 PRINT FILE[6]
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```



```
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
1080 PRINT FILE[6], TAB(34);"I-N-J-E-C-T-I-O-N   D-A-T-A   P-R-O-C-E-S
*     -S-I-N-G   R-E-P-O-R-T"
1090 PRINT FILE[6]
1100 PRINT FILE[6], TAB(29);
1110 PRINT FILE[6],USING "ANALYST:  ############################   I
*     NJECTION ID NUMBER:  ########",U$,D3$[3]
1120 PRINT FILE[6], TAB(29);
1130 PRINT FILE[6],USING "METHOD NUMBER:  ####                      R
*     EPORT TITLE:  ##########################",T$[3,6],F$
1140 PRINT FILE[6], TAB(29);
1150 PRINT FILE[6],USING "METHOD TYPE:  ########################## D
*     ATE:  ##/##/##",Q7$,SYS(2),SYS(1),SYS(3)-1900
1160 PRINT FILE[6]
1165 PRINT FILE[6]
1170 GOSUB 1730
1180 LET I6=12
1190 REM  ------------------------------------------------------------
1200 REM          COPY LINES FROM TEMPORARY FILE TO LINEPRINTER
1210 LREAD FILE[5],Q8$,Q9$
1220 IF EOF(5) THEN GOTO 1370
1230 LET Q8$=Q8$,Q9$
1240 PRINT FILE[6],Q8$
1250 LET I6=I6+1
1260 IF I6>58 THEN IF LEN(Q8$)<5 THEN GOTO 1280
1270 GOTO 1210
1280 LET I7=I7+1
1281 LREAD FILE[5],Q8$,Q9$
1282 IF EOF(5) THEN GOTO 1370
1290 PRINT FILE[6],"<12>";
1295 PRINT FILE[6], TAB(126);
1300 PRINT FILE[6],USING "PAGE #",I7
1310 PRINT FILE[6]
1320 GOSUB 1730
1330 LET I6=5
1340 GOTO 1230
1350 REM  ------------------------------------------------------------
1360 REM          CONFIRM PROCESSING COMPLETION
1370 PRINT
1380 PRINT "INJECTION ";D3$[3];" HAS BEEN PROCESSED, AND A REPORT IS B
*     EING"
1390 PRINT "     PRINTED BY THE LINEPRINTER."
1400 ON ERR THEN GOTO 1402
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
1401 CLOSE FILE[3]
1402 ON ERR THEN GOTO 1404
1403 CLOSE FILE[5]
1404 ON ERR THEN GOTO 1410
1405 CLOSE FILE[6]
1410 ON ERR THEN GOTO 1430
1420 DELETE Q$
1430 ON ERR THEN STOP
1440 PRINT
1445 ON ERR THEN GOTO 1455
1450 INPUT "DO YOU WANT TO PROCESS ANOTHER INJECTION USING THE SAME ME
*     THOD?  (Y OR N)  ",X$
1455 ON ERR THEN STOP
1460 IF X$[1,1]<>"Y" THEN GOTO 1680
1540 REM  ------------------------------------------------------------
1550 REM          PROCESS ANOTHER INJECTION
1560 NOESC
1570 ON N1 THEN GOTO 1580, 1590, 1600, 1610
1580 CHAIN "GC08"
1590 CHAIN "GC09"
1600 CHAIN "GC10"
1610 CHAIN "GC11"
1620 REM  ------------------------------------------------------------
1630 REM          RETURN TO MASTER CONTROL
1640 ON ERR THEN GOTO 1642
1641 CLOSE FILE[3]
1642 ON ERR THEN GOTO 1644
1643 CLOSE FILE[5]
1644 ON ERR THEN GOTO 1650
1645 CLOSE FILE[6]
1650 ON ERR THEN GOTO 1670
1660 DELETE Q$
1670 ON ESC THEN STOP
1680 NOESC
1690 CHAIN "GC00"
1700 REM
1710 REM  ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
1720 REM          SUBROUTINE TO PRINT COLUMN HEADINGS
1730 PRINT FILE[6], TAB(51);"C.A.S.    PEAK     RETENTION    ";
1740 IF N2<>1 THEN GOTO 1770
1750 PRINT FILE[6],"  RELATIVE     ";
1760 GOTO 1780
```



```
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
1770 PRINT FILE[6],"  CAPACITY     ";
1780 PRINT FILE[6],"   AREA OF     CONCENTRATION IN"
1790 PRINT FILE[6], TAB(21);"COMPOUND(S)                    NUMBER    T
*     YPE       TIME       ";
1800 IF N2<>1 THEN GOTO 1830
1810 PRINT FILE[6],"RETENTION TIME  ";
1820 GOTO 1840
1830 PRINT FILE[6],"    RATIO       ";
1840 PRINT FILE[6],"     PEAK       MICROGRAMS/LITER"
1850 PRINT FILE[6],"     ------------------------------------------ --
*     -------- ---";
1860 PRINT FILE[6]," ------------  ------------  ------------
*     -------------"
1870 RETURN
```

SYMBOL TABLE FOR GC13

SYMBOL	REFERENCES			
0170	0160			
0190	0160			
0210	0160			
0230	0160			
0260	0180	0200	0220	
0340	0370			
0400	0350			
0450	0480			
0510	0460			
0560	0930			
0670	0580			
0700	0610	0660		
0710	0702			
0740	0710			
0750	0730			
0765	0760			
0770	0763			
0820	0770			
0840	0780			
0860	0790			
0870	0708	0810	0830	0850
0910	0870	0890		
0960	0570			
0962	0960			
0964	0962			
0966	0964			
0980	1040			
1020	0980			
1050	1010			
1210	1270			
1230	1340			
1280	1260			
1370	1220	1282		
1402	1400			
1404	1402			
1410	1404			
1430	1410			
1455	1445			
1580	1570			
1590	1570			
1600	1570			
1610	1570			
1640	0080			
1642	1640			
1644	1642			

SYMBOL TABLE FOR GC13

SYMBOL	REFERENCES									
1650	1644									
1670	1650									
1680	1460									
1730	1170	1320								
1770	1740									
1780	1760									
1830	1800									
1840	1820									
B	0560	0800	0820	0840	0860					
C	0560	0702	0800	0820	0840	0860				
D3$	0090	0280	0300	1110	1380					
F$	0090	0520	1130							
FL#3	0280	0290	0300	0450	0520	0560	0961	1401	1641	
FL#4	0150	0260	0270	0340	0600					
FL#5	0410	0706	0800	0820	0840	0860	0880	0900	0910	0963
	0970	1210	1281	1403	1643					
FL#6	0965	0990	1060	1070	1080	1090	1100	1110	1120	1130
	1140	1150	1160	1165	1240	1290	1295	1300	1310	1405
	1645	1730	1750	1770	1780	1790	1810	1830	1840	1850
	1860									
G$	0090	0560	0580	0610	0630	0762				
H$	0090	0560	0800	0820	0840	0860				
I	0590	0600	0620							
I5	0330	0340	0360	0590						
I6	0550	0560	0706	0800	0820	0840	0860	0920	1180	1250
	1260	1330								
I7	1050	1280	1300							
J	0280									
L	0560	0760	0770	0780	0800	0860				
L2	0560	0710	0770	0790	0800	0840				
N1	0150	0160	1570							
N2	0150	1740	1800							
P9	0440	0450	0470	0510	0520	0560				
Q$	0090	0400	0410	0970	1420	1660				
Q5$	0090	0700	0704	0706	0720	0740	0750	0762	0765	0800
	0820	0840	0860							
Q6$	0090	0120	0880	0900						
Q7$	0090	0170	0190	0210	0230	1150				
Q8$	0090	1210	1230	1240	1260	1281				
Q9$	0100	1210	1230	1281						
T$	0100	0150	0270	0400	0630	1130				
U$	0100	0150	1110							
V$	0100	0340	0600	0610						
VO$	0100	0450	0460							
V1$	0100	0600	0630	0670	0706	0800	0820	0840	0860	

SYMBOL TABLE FOR GC13

SYMBOL	REFERENCES								
V2$	0100	0600	0640	0680	0706	0800	0820	0840	0860
V3$	0100	0600	0650	0690	0870	0880			
V4$	0100	0600	0880						
V5$	0100	0600	0890	0900					
V6$	0100	0600	0900						
X$	0100	1450	1460						

SECTION 16

PROGRAM GC14 - CONTROL STANDARDS CALCULATION

GC14 is the program which calculates percent recoveries for control standards and prints the control standard report. It is entered by chaining from the master control program, GC00, and it returns control to that program if the escape key is pressed.

As GC14 begins, a method file is already open, having been opened by GC00. GC14 first counts the identifiers in the method file. It then asks the user for the injection ID of the control standard and opens the corresponding injection data file. It also asks the user for the letter name of the concentration pattern and opens the concentration pattern file.

Next, GC14 prints the headings for the control standard report. It then loops through the method file. For each identifier in the method file, GC14 reads the prepared concentration from the concentration pattern file and searches the data file for the calculated concentration. It then prints the identifier, the prepared concentration, the calculated concentration, and the percent recovery on the control standard report. Percent recovery is calculated by the formula:

$$\text{Percent Recovery} = 100 \cdot \frac{\text{Measured Concentration}}{\text{Prepared Concentration}}$$

When all of the identifiers have been covered, the program closes the concentration pattern file and the data file, and it asks if the user wants to examine another control standard. It then either branches back to the beginning or chains back to GC00.

TABLE 10. SYMBOL DEFINITIONS FOR PROGRAM GC14

A5	the prepared concentration
A6$	the name of the concentration pattern file
A7	the position of A8$ in A9$
A8$	the letter name of the concentration pattern
A9$	the alphabet
B	the absolute retention time
C	the peak area
D2$	the injection ID
D3$	the name of the data file
F	the number of identifiers in the method file
G$	the identifier from the data file
H$	the peak type
I	the control variable for loops
I2	the control variable for a loop
J	the data file useability flag J=1 good data J=2 no TOTAL AREA J=3 wrong format
J2	the data file processing status flag J2=1 has been processed J2=2 never processed
L	the calculated concentration
L2	the relative retention time or capacity ratio

TABLE 10. (Continued)

P8	the record number of the last record in the data file
P9	the record number of the first record in the data file which represents a peak
Q5$	the format for a PRINT USING statement
T$	the name of the method file
V$	an identifier from the method file
VO$	an error message
X$	the user's answer to Y or N questions

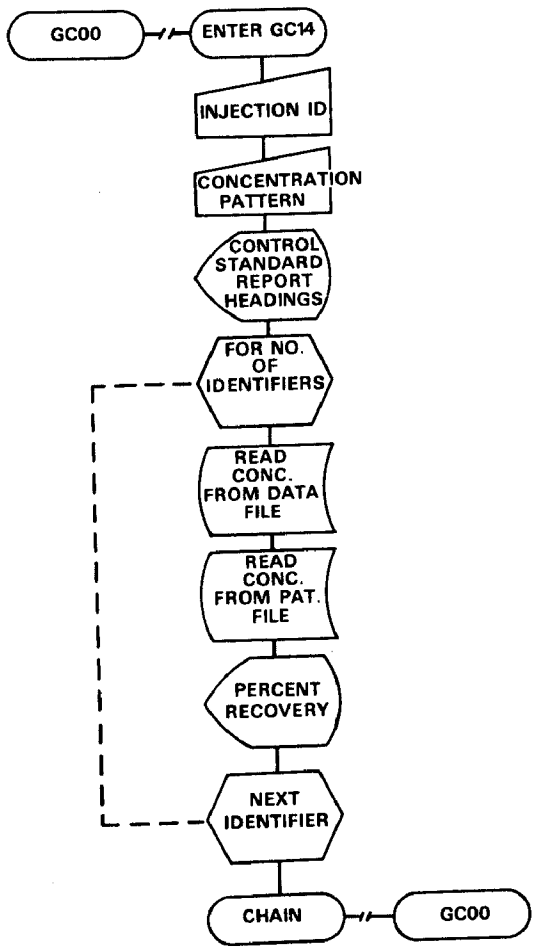

Figure 12. Flowchart of Program GC14.

PROGRAM LISTING FOR GC14

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                      +
0030 REM   +   PROGRAM GC14, CONTROL STANDARDS CALCULATIONS             +
0040 REM   +   BY:  J. KOPKE (SWORCC), APRIL 3, 1979                    +
0050 REM   +   MOST RECENT REVISION:  APRIL 12, 1979                    +
0060 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0070 REM
0080 DIM A6$[9],A8$[1],A9$[26],D2$[8],D3$[10],G$[8],H$[2],Q5$[80],T$[6
*    ],V$[8],V0$[30],X$[3]
0090 LET A9$="ABCDEFGHIJKLMNOPQRSTUVWXYZ"
0100 ON ESC THEN GOTO 0130
0110 ESC
0120 GOTO 0220
0130 ON ERR THEN GOTO 0150
0140 CLOSE FILE[3]
0150 ON ERR THEN GOTO 0170
0160 CLOSE FILE[7]
0170 ON ERR THEN STOP
0180 NOESC
0190 CHAIN "GC00"
0200 REM   ------------------------------------------------------------
0210 REM          COUNT IDENTIFIERS IN METHOD FILE
0220 READ FILE[4,1],T$
0230 CLOSE FILE[4]
0240 OPEN FILE[4],T$,200
0250 LET F=0
0260 READ FILE[4,3*(F+1)-1],V$
0270 IF EOF(4) THEN GOTO 0320
0280 LET F=F+1
0290 GOTO 0260
0300 REM   ------------------------------------------------------------
0310 REM          OPEN DATA FILE
0320 PRINT
0330 ON ERR THEN GOTO 0350
0340 INPUT "WHAT IS THE INJECTION ID FOR THE CONTROL STANDARD?  ",D2$
0350 ON ERR THEN STOP
0360 IF LEN(D2$)=8 THEN GOTO 0400
0370 PRINT
0380 PRINT "<7><7>";D2$;" IS NOT A VALID INJECTION ID."
0390 GOTO 0320
0400 LET D3$="GC",D2$
0410 ON ERR THEN GOTO 0430
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```


PROGRAM LISTING FOR GC14

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0420 RENAME D3$,D3$
0430 ON ERR THEN STOP
0440 IF SYS(7)=-9 THEN GOTO 0480
0450 PRINT
0460 PRINT "<7><7>THERE IS NO EXISTING DATA FOR INJECTION ID ";D2$;"."
0470 GOTO 0320
0480 ON ERR THEN GOTO 0520
0490 OPEN FILE[3,0],D3$,31
0500 ON ERR THEN STOP
0510 GOTO 0570
0520 ON ERR THEN STOP
0530 DELAY =1
0540 GOTO 0480
0550 REM   ------------------------------------------------------------
0560 REM          CHECK DATA FILE USABILITY AND PROCESSING FLAGS
0570 READ FILE[3,1],J,D3$,J2
0580 IF J=1 THEN GOTO 0630
0590 PRINT
0600 IF J<>2 THEN GOTO 0610
0602 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT DID NOT"
0604 PRINT "     HAVE A TOTAL AREA"
0606 GOTO 1420
0610 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT WAS"
0612 PRINT "     IN THE WRONG FORMAT."
0620 GOTO 1420
0630 IF J2=1 THEN GOTO 0690
0640 PRINT
0650 PRINT "<7><7>";D2$;" CANNOT BE USED FOR CONTROL STANDARD CALCULAT
*    IONS UNTIL"
0652 PRINT "     AFTER IT IS PROCESSED."
0660 GOTO 0130
0670 REM   ------------------------------------------------------------
0680 REM          FIND FIRST AND LAST ENTRIES IN DATA FILE
0690 LET P9=2
0700 READ FILE[3,P9],V0$
0710 IF V0$[1,7]<>"MESSAGE" THEN GOTO 0740
0720 LET P9=P9+1
0730 GOTO 0700
0740 LET P9=P9+2
0750 LET P8=P9
0760 READ FILE[3,P8],G$
0770 IF EOF(3) THEN GOTO 0800
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0780 LET P8=P8+1
0790 GOTO 0760
0800 LET P8=P8-1
0810 REM   ------------------------------------------------------------
0820 REM          OPEN CONCENTRATION PATTERN FILE
0830 PRINT
0840 ON ERR THEN GOTO 0860
0850 INPUT "WHAT IS THE CONCENTRATION PATTERN FOR THIS STANDARD?  ",A8
*    $
0860 ON ERR THEN STOP
0870 LET A7=POS(A9$,A8$,1)
0880 IF A7<>0 THEN GOTO 0920
0890 PRINT
0900 PRINT "<7><7>'";A8$;"' IS NOT A VALID LETTER."
0910 GOTO 0830
0920 LET A6$=T$,"000"
0930 LET A6$[10-LEN(STR$(A7)),9]=STR$(A7)
0940 ON ERR THEN GOTO 0960
0950 RENAME A6$,A6$
0960 ON ERR THEN STOP
0970 IF SYS(7)=-9 THEN GOTO 1010
0980 PRINT
0990 PRINT "<7><7>THERE IS NO EXISTING PATTERN NAMED '";A8$;"'."
1000 GOTO 0830
1010 ON ERR THEN GOTO 1050
1020 OPEN FILE[7,0],A6$,4
1030 ON ERR THEN STOP
1040 GOTO 1100
1050 ON ERR THEN STOP
1060 DELAY =1
1070 GOTO 1010
1080 REM   ------------------------------------------------------------
1090 REM          PRINT HEADINGS
1100 PRINT
1110 PRINT
1120 PRINT  TAB(15);"C-O-N-T-R-O-L   S-T-A-N-D-A-R-D   R-E-P-O-R-T"
1130 PRINT "INJECTION ID:  ";D2$; TAB(53);"METHOD NUMBER:  ";T$[3,6]
1140 PRINT "CONCENTRATION PATTERN:  ";A8$; TAB(39);"CONCENTRATIONS IN
*    MICROGRAMS/LITER"
1150 PRINT
1160 PRINT "                PREPARED       MEASURED      PERCENT"
1170 PRINT "IDENTIFIER  CONCENTRATION  CONCENTRATION  RECOVERED"
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```



```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
1180 PRINT "--------  ----------  ----------  --------"
1190 LET Q5$=" #######   -----#.###    -----#.###     ---#.#%"
1195 REM   ------------------------------------------------------------
1196 REM          FILL IN TABLE
1200 FOR I=1 TO F
1210   READ FILE[4,3*I-1],V$
1215   IF V$="99999" THEN GOTO 1360
1220   READ FILE[7,I],A5
1230   FOR I2=P9 TO P8 STEP 1
1240     READ FILE[3,I2],G$,H$,B,C,L,L2
1250     IF G$=V$ THEN GOTO 1270
1260   NEXT I2
1265   LET C=-9999
1266   LET L=-9999
1270   IF C<>-9999 THEN GOTO 1310
1280   PRINT USING Q5$[1,27],V$,A5;
1290   PRINT "NOT DETECTED"
1300   GOTO 1360
1310   IF L<>-9999 THEN GOTO 1350
1320   PRINT USING Q5$[1,27],V$,A5;
1330   PRINT "NOT CALCULATED"
1340   GOTO 1360
1350   PRINT USING Q5$,V$,A5,L,L/A5*100
1360 NEXT I
1370 PRINT
1380 PRINT
1390 REM   ------------------------------------------------------------
1400 REM          WRAP-UP PROCEDURE
1410 CLOSE FILE[7]
1420 CLOSE FILE[3]
1430 PRINT
1440 ON ERR THEN GOTO 1460
1450 INPUT "DO YOU WANT A REPORT ON ANOTHER CONTROL STANDARD?  (Y OR N
*    )  ",X$
1460 ON ERR THEN STOP
1470 IF X$[1,1]="Y" THEN GOTO 0320
1480 NOESC
1490 CHAIN "GC00"
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

SYMBOL TABLE FOR GC14

SYMBOL	REFERENCES									
0130	0100	0660								
0150	0130									
0170	0150									
0220	0120									
0260	0290									
0320	0270	0390	0470	1470						
0350	0330									
0400	0360									
0430	0410									
0480	0440	0540								
0520	0480									
0570	0510									
0610	0600									
0630	0580									
0690	0630									
0700	0730									
0740	0710									
0760	0790									
0800	0770									
0830	0910	1000								
0860	0840									
0920	0880									
0960	0940									
1010	0970	1070								
1050	1010									
1100	1040									
1270	1250									
1310	1270									
1350	1310									
1360	1215	1300	1340							
1420	0606	0620								
1460	1440									
A5	1220	1280	1320	1350						
A6$	0080	0920	0930	0950	1020					
A7	0870	0880	0930							
A8$	0080	0850	0870	0900	0990	1140				
A9$	0080	0090	0870							
B	1240									
C	1240	1265	1270							
D2$	0080	0340	0360	0380	0400	0460	0602	0610	0650	1130
D3$	0080	0400	0420	0490	0570					
F	0250	0260	0280	1200						
FL#3	0140	0490	0570	0700	0760	1240	1420			
FL#4	0220	0230	0240	0260	1210					
FL#7	0160	1020	1220	1410						

SYMBOL TABLE FOR GC14

SYMBOL	REFERENCES							
G$	0080	0760	1240	1250				
H$	0080	1240						
I	1200	1210	1220	1360				
I2	1230	1240	1260					
J	0570	0580	0600					
J2	0570	0630						
L	1240	1266	1310	1350				
L2	1240							
P8	0750	0760	0780	0800	1230			
P9	0690	0700	0720	0740	0750	1230		
Q5$	0080	1190	1280	1320	1350			
T$	0080	0220	0240	0920	1130			
V$	0080	0260	1210	1215	1250	1280	1320	1350
V0$	0080	0700	0710					
X$	0080	1450	1470					

SECTION 17

PROGRAM GC15 - SPIKED SAMPLES CALCULATION

GC15 is the program which calculates the percent recovery of spiked samples and prints a report on those statistics. It is entered by chaining from the master control program, GC00, and it chains back to that program if the escape key is pressed.

As GC15 begins, a method file is already open, having been opened by GC00. GC15 first counts the identifiers in the method file. Then it asks the user for the injection ID of the spike original, the letter name of the concentration pattern for the spike added value, and the injection ID of the spike final, and it opens the three corresponding files.

Next, the program prints the headings for the spiked sample report. It then loops through the method file. It reads an identifier from the method file and reads the spike added value from the concentration pattern file. It loops through the first injection data file, finds the matching identifier and reads its calculated concentration, and then loops through the second injection data file, finds the matching identifier there, and reads its calculated concentration. The percent recovery is calculated as the line of data is printed. Percent recovery of spikes is calculated by the formula:

$$\text{Percent Recovery} = \frac{\text{Final Concentration} - \text{Original Concentration}}{\text{Added Concentration}}$$

When all of the identifiers in the method file have been handled, the program either starts over or chains back to GC00, at the option of the user.

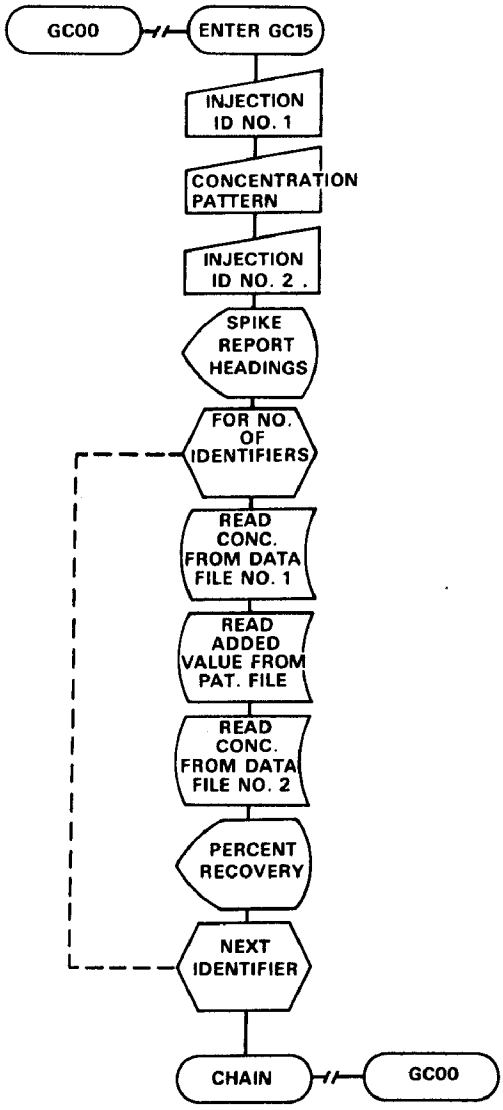

Figure 13. Flowchart of Program GC15.

TABLE 11. SYMBOL DEFINITIONS FOR PROGRAM GC15

A5	the spike added concentration
A6$	the name of the concentration pattern file
A7	the position of A8$ in A9$
A8$	the letter name of the concentration pattern
A9$	the alphabet
B	the absolute retention time
C	the peak area of the spike original
C2	the peak area of the spike final
D2$	the injection ID
D3$	the name of the data file
F	the number of identifiers in the method file
G$	the identifier from the data file
H$	the peak type
I	the control variable for loops
I2	the control variable for loops
J	the data file useability flag J=1 good data J=2 no TOTAL AREA J=3 wrong format
J2	the data file processing status flag J2=1 has been processed J2=2 never processed
L	the relative retention time

TABLE 11. (Continued)

L2	the calculated concentration of the spike original
L3	the calculated concentration of the spike final
P6	the record number of the last record in the spike final data file
P7	the record number of the first record which describes a peak in the spike final data file
P8	the record number of the last record in the spike original data file
P9	the record number of the first record which describes a peak in the spike original data file
T$	the name of the method file
V$	the identifier from the method file
VO$	an error MESSAGE
X$	the user's response to Y or N questions

PROGRAM LISTING FOR GC15

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                    +
0030 REM   +   PROGRAM GC15, SPIKED SAMPLE CALCULATIONS               +
0040 REM   +   BY:  J. KOPKE (SWORCC), APRIL 5, 1979                  +
0050 REM   +   MOST RECENT REVISION:  MAY 2, 1979                     +
0060 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0070 REM
0080 DIM A6$[9],A8$[1],A9$[26],D2$[8],D3$[10],G$[8],H$[2],T$[6],V$[8],
*    V0$[30],X$[3]
0090 LET A9$="ABCDEFGHIJKLMNOPQRSTUVWXYZ"
0100 ON ESC THEN GOTO 0130
0110 ESC
0120 GOTO 0240
0130 ON ERR THEN GOTO 0150
0140 CLOSE FILE[3]
0150 ON ERR THEN GOTO 0170
0160 CLOSE FILE[7]
0170 ON ERR THEN GOTO 0190
0180 CLOSE FILE[0]
0190 ON ERR THEN STOP
0200 NOESC
0210 CHAIN "GC00"
0220 REM   ------------------------------------------------------------
0230 REM          COUNT IDENTIFIERS IN METHOD FILE
0240 READ FILE[4,1],T$
0250 CLOSE FILE[4]
0260 OPEN FILE[4],T$,200
0270 LET F=0
0280 READ FILE[4,3*(F+1)-1],V$
0290 IF EOF(4) THEN GOTO 0340
0300 LET F=F+1
0310 GOTO 0280
0320 REM   ------------------------------------------------------------
0330 REM          OPEN SPIKE ORIGINAL DATA FILE
0340 PRINT
0350 ON ERR THEN GOTO 0370
0360 INPUT "WHAT IS THE INJECTION ID FOR THE UNSPIKED SAMPLE?  ",D2$
0370 ON ERR THEN STOP
0380 IF LEN(D2$)=8 THEN GOTO 0420
0390 PRINT
0400 PRINT "<7><7>";D2$;" IS NOT A VALID INJECTION ID."
0410 GOTO 0340
```

12345678911234567892123456789312345678941234567895123456789612345678 97
         0   0   0   0   0   0   0

PROGRAM LISTING FOR GC15

12345678911234567892123456789312345678941234567895123456789612345678 97
         0   0   0   0   0   0   0

```
0420 LET D3$="GC",D2$
0430 ON ERR THEN GOTO 0450
0440 RENAME D3$,D3$
0450 ON ERR THEN STOP
0460 IF SYS(7)=-9 THEN GOTO 0500
0470 PRINT
0480 PRINT "<7><7>THERE IS NO EXISTING DATA FOR INJECTION ID ";D2$;"."
0490 GOTO 0340
0500 ON ERR THEN GOTO 0540
0510 OPEN FILE[3,0],D3$,31
0520 ON ERR THEN STOP
0530 GOTO 0590
0540 ON ERR THEN STOP
0550 DELAY =1
0560 GOTO 0500
0570 REM   ------------------------------------------------------------
0580 REM          CHECK DATA FILE USABILITY AND PROCESSING FLAGS
0590 READ FILE[3,1],J,D3$,J2
0600 IF J=1 THEN GOTO 0690
0610 PRINT
0620 IF J<>2 THEN GOTO 0660
0630 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT DID NOT"
0640 PRINT "     HAVE A TOTAL AREA"
0650 GOTO 2250
0660 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT WAS"
0670 PRINT "     IN THE WRONG FORMAT."
0680 GOTO 2250
0690 IF J2=1 THEN GOTO 0760
0700 PRINT
0710 PRINT "<7><7>";D2$;" CANNOT BE USED FOR SPIKED SAMPLE CALCULATION
*    S UNTIL"
0720 PRINT "     AFTER IT IS PROCESSED."
0730 GOTO 0130
0740 REM   ------------------------------------------------------------
0750 REM          FIND FIRST AND LAST ENTRIES IN DATA FILE
0760 LET P9=2
0770 READ FILE[3,P9],V0$
0780 IF V0$[1,7]<>"MESSAGE" THEN GOTO 0810
0790 LET P9=P9+1
0800 GOTO 0770
0810 LET P9=P9+2
0820 LET P8=P9
```

12345678911234567892123456789312345678941234567895123456789612345678 97
         0   0   0   0   0   0   0

```
123456789112345678921234567893123456789412345678951234567896123456789 7
         0         0         0         0         0         0         0
0830 READ FILE[3,P8],G$
0840 IF EOF(3) THEN GOTO 0870
0850 LET P8=P8+1
0860 GOTO 0830
0870 LET P8=P8-1
0880 REM  ------------------------------------------------------------
0890 REM          OPEN CONCENTRATION PATTERN FILE
0900 PRINT
0910 ON ERR THEN GOTO 0930
0920 INPUT "WHAT IS THE CONCENTRATION PATTERN FOR THE SPIKE ADDED VALU
*    ES?  ",A8$
0930 ON ERR THEN STOP
0940 LET A7=POS(A9$,A8$,1)
0950 IF A7<>0 THEN GOTO 0990
0960 PRINT
0970 PRINT "<7><7>'";A8$;"' IS NOT A VALID LETTER."
0980 GOTO 0900
0990 LET A6$=T$,"000"
1000 LET A6$[10-LEN(STR$(A7)),9]=STR$(A7)
1010 ON ERR THEN GOTO 1030
1020 RENAME A6$,A6$
1030 ON ERR THEN STOP
1040 IF SYS(7)=-9 THEN GOTO 1080
1050 PRINT
1060 PRINT "<7><7>THERE IS NO EXISTING PATTERN NAMED '";A8$;"'."
1070 GOTO 0900
1080 ON ERR THEN GOTO 1120
1090 OPEN FILE[7,0],A6$,4
1100 ON ERR THEN STOP
1110 GOTO 1170
1120 ON ERR THEN STOP
1130 DELAY =1
1140 GOTO 1080
1150 REM  ------------------------------------------------------------
1160 REM          OPEN SPIKE FINAL DATA FILE
1170 PRINT
1180 ON ERR THEN GOTO 1200
1190 INPUT "WHAT IS THE INJECTION ID FOR THE SPIKED SAMPLE?  ",D2$
1200 ON ERR THEN STOP
1210 IF LEN(D2$)=8 THEN GOTO 1250
1220 PRINT
1230 PRINT "<7><7>";D2$;" IS NOT A VALID INJECTION ID."
123456789112345678921234567893123456789412345678951234567896123456789 7
         0         0         0         0         0         0         0
```



```
123456789112345678921234567893123456789412345678951234567896123456789 7
         0         0         0         0         0         0         0
1240 GOTO 1170
1250 LET D3$="GC",D2$
1260 ON ERR THEN GOTO 1280
1270 RENAME D3$,D3$
1280 ON ERR THEN STOP
1290 IF SYS(7)=-9 THEN GOTO 1330
1300 PRINT
1310 PRINT "<7><7>THERE IS NO EXISTING DATA FOR INJECTION ID ";D2$;"."
1320 GOTO 1170
1330 ON ERR THEN GOTO 1370
1340 OPEN FILE[0,0],D3$,31
1350 ON ERR THEN STOP
1360 GOTO 1420
1370 ON ERR THEN STOP
1380 DELAY =1
1390 GOTO 1330
1400 REM  ------------------------------------------------------------
1410 REM          CHECK DATA FILE USABILITY AND PROCESSING FLAGS
1420 READ FILE[0,1],J,D3$,J2
1430 IF J=1 THEN GOTO 1520
1440 PRINT
1450 IF J<>2 THEN GOTO 1490
1460 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT DID NOT"
1470 PRINT "     HAVE A TOTAL AREA"
1480 GOTO 2250
1490 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT WAS"
1500 PRINT "     IN THE WRONG FORMAT."
1510 GOTO 2250
1520 IF J2=1 THEN GOTO 1590
1530 PRINT
1540 PRINT "<7><7>";D2$;" CANNOT BE USED FOR SPIKED SAMPLE CALCULATION
*    S UNTIL"
1550 PRINT "     AFTER IT IS PROCESSED."
1560 GOTO 0130
1570 REM  ------------------------------------------------------------
1580 REM          FIND FIRST AND LAST ENTRIES IN DATA FILE
1590 LET P7=2
1600 READ FILE[0,P7],V0$
1610 IF V0$[1,7]<>"MESSAGE" THEN GOTO 1640
1620 LET P7=P7+1
1630 GOTO 1600
1640 LET P7=P7+2
123456789112345678921234567893123456789412345678951234567896123456789 7
         0         0         0         0         0         0         0
```

```
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
1650 LET P6=P7
1660 READ FILE[0,P6],G$
1670 IF EOF(0) THEN GOTO 1700
1680 LET P6=P6+1
1690 GOTO 1660
1700 LET P6=P6-1
1710 REM  ------------------------------------------------------------
1720 REM          PRINT HEADINGS
1730 PRINT
1740 PRINT
1750 PRINT  TAB(17);"S-P-I-K-E-D   S-A-M-P-L-E   R-E-P-O-R-T"
1760 READ FILE[3,1],J,D3$,J2
1770 PRINT "INJECTION ID FOR SPIKE ORIGINAL:  ";D3$[3,10]; TAB(53);"ME
*    THOD NUMBER:  ";T$[3,6]
1780 PRINT "CONCENTRATION PATTERN FOR SPIKE ADDED VALUE:  ";A8$
1790 READ FILE[0,1],J,D3$,J2
1800 PRINT "INJECTION ID FOR SPIKE FINAL:  ";D3$[3,10]
1810 PRINT "CONCENTRATIONS IN MICROGRAMS/LITER"
1820 PRINT
1830 PRINT "              ORIGINAL         ADDED          FINAL
*    PERCENT"
1840 PRINT "IDENTIFIER  CONCENTRATION  CONCENTRATION  CONCENTRATION  R
*    ECOVERED"
1850 PRINT "--------- ------------ ------------ ------------ -
*    -------"
1860 REM  ------------------------------------------------------------
1870 REM          FILL IN CHART
1880 FOR I=1 TO F
1890   READ FILE[4,3*I-1],V$
1900   IF V$="99999" THEN GOTO 2200
1910   READ FILE[7,I],A5
1920   FOR I2=P9 TO P8
1930     READ FILE[3,I2],G$,H$,B,C,L,L2
1940     IF G$=V$ THEN GOTO 1960
1950   NEXT I2
1955   LET C=-9999
1956   LET L=-9999
1960   FOR I2=P7 TO P6
1970     READ FILE[0,I2],G$,H$,B,C2,L3,L2
1980     IF G$=V$ THEN GOTO 2000
1990   NEXT I2
1995   LET C2=-9999
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```



```
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
1996   LET L3=-9999
2000   PRINT USING " #######   ",V$;
2010   IF C<>-9999 THEN GOTO 2040
2020   PRINT " NOT DETECTED  ";
2030   GOTO 2080
2040   IF L<>-9999 THEN GOTO 2070
2050   PRINT "NOT CALCULATED ";
2060   GOTO 2080
2070   PRINT USING "-----#.###     ",L;
2080   PRINT USING "-----#.###     ",A5;
2090   IF C2<>-9999 THEN GOTO 2120
2100   PRINT " NOT DETECTED  ";
2110   GOTO 2160
2120   IF L3<>-9999 THEN GOTO 2150
2130   PRINT "NOT CALCULATED ";
2140   GOTO 2160
2150   PRINT USING "-----#.###     ",L3;
2160   IF C<>-9999 THEN IF L<>-9999 THEN IF C2<>-9999 THEN IF L3<>-999
*    9 THEN GOTO 2190
2170   PRINT
2180   GOTO 2200
2190   PRINT USING "---#.#%",(L3-L)/A5*100
2200 NEXT I
2210 PRINT
2220 PRINT
2230 REM  ------------------------------------------------------------
2240 REM          WRAP-UP PROCEDURE
2250 ON ERR THEN GOTO 2270
2260 CLOSE FILE[0]
2270 ON ERR THEN GOTO 2290
2280 CLOSE FILE[3]
2290 ON ERR THEN GOTO 2310
2300 CLOSE FILE[7]
2310 ON ERR THEN STOP
2320 PRINT
2330 ON ERR THEN GOTO 2350
2340 INPUT "DO YOU WANT A REPORT FOR ANOTHER SPIKED SAMPLE?  (Y OR N)
*     ",X$
2350 ON ERR THEN STOP
2360 IF X$[1,1]="Y" THEN GOTO 0340
2370 NOESC
2380 CHAIN "GC00"
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

SYMBOL TABLE FOR GC15

SYMBOL	REFERENCES				
0130	0100	0730	1560		
0150	0130				
0170	0150				
0190	0170				
0240	0120				
0280	0310				
0340	0290	0410	0490	2360	
0370	0350				
0420	0380				
0450	0430				
0500	0460	0560			
0540	0500				
0590	0530				
0660	0620				
0690	0600				
0760	0690				
0770	0800				
0810	0780				
0830	0860				
0870	0840				
0900	0980	1070			
0930	0910				
0990	0950				
1030	1010				
1080	1040	1140			
1120	1080				
1170	1110	1240	1320		
1200	1180				
1250	1210				
1280	1260				
1330	1290	1390			
1370	1330				
1420	1360				
1490	1450				
1520	1430				
1590	1520				
1600	1630				
1640	1610				
1660	1690				
1700	1670				
1960	1940				
2000	1980				
2040	2010				
2070	2040				
2080	2030	2060			

SYMBOL TABLE FOR GC15

SYMBOL	REFERENCES									
2120	2090									
2150	2120									
2160	2110	2140								
2190	2160									
2200	1900	2180								
2250	0650	0680	1480	1510						
2270	2250									
2290	2270									
2310	2290									
2350	2330									
A5	1910	2080	2190							
A6$	0080	0990	1000	1020	1090					
A7	0940	0950	1000							
A8$	0080	0920	0940	0970	1060	1780				
A9$	0080	0090	0940							
B	1930	1970								
C	1930	1955	2010	2160						
C2	1970	1995	2090	2160						
D2$	0080	0360	0380	0400	0420	0480	0630	0660	0710	1190
	1210	1230	1250	1310	1460	1490	1540			
D3$	0080	0420	0440	0510	0590	1250	1270	1340	1420	1760
	1770	1790	1800							
F	0270	0280	0300	1880						
FL#0	0180	1340	1420	1600	1660	1790	1970	2260		
FL#3	0140	0510	0590	0770	0830	1760	1930	2280		
FL#4	0240	0250	0260	0280	1890					
FL#7	0160	1090	1910	2300						
G$	0080	0830	1660	1930	1940	1970	1980			
H$	0080	1930	1970							
I	1880	1890	1910	2200						
I2	1920	1930	1950	1960	1970	1990				
J	0590	0600	0620	1420	1430	1450	1760	1790		
J2	0590	0690	1420	1520	1760	1790				
L	1930	1956	2040	2070	2160	2190				
L2	1930	1970								
L3	1970	1996	2120	2150	2160	2190				
P6	1650	1660	1680	1700	1960					
P7	1590	1600	1620	1640	1650	1960				
P8	0820	0830	0850	0870	1920					
P9	0760	0770	0790	0810	0820	1920				
T$	0080	0240	0260	0990	1770					
V$	0080	0280	1890	1900	1940	1980	2000			
VO$	0080	0770	0780	1600	1610					
X$	0080	2340	2360							

SECTION 18

PROGRAM GC16 - DUPLICATE SAMPLES CALCULATION

GC16 is the program which calculates the difference between duplicate samples and prints a report on those statistics. It is entered by chaining from the master control program, GC00, and it chains back to that program if the escape key is pressed.

When GC16 begins, the method file is already open, and GC16 first counts the number of identifiers in that method file. Then the program asks the user for the injection ID numbers for the two members of the duplicate pair, and it opens the two corresponding injection data files.

After the headings have been printed, the program begins to loop through the method file. It reads an identifier from the method file and searches the two data files for that identifier. It reads the concentrations from the data files, and prints them and their absolute difference.

When all of the identifiers have been accounted for, the program asks the user if it should start over. It then either branches back to the beginning or chains back to GC00.

TABLE 12. SYMBOL DEFINITIONS FOR PROGRAM GC16

B	the absolute retention time
C	the peak area of the first member
C2	the peak area of the second member
D2$	the injection ID
D3$	the name of the data file
F	the number of identifiers in the method file
G$	the identifier from the data file
H$	the peak type
I	the control variable for loops
I2	the control variable for loops
J	the data file useability flag J=1 good data J=2 no TOTAL AREA J=3 wrong format
J2	the data file processing status flag J2=1 has been processed J2=2 never processed
L	the relative retention time
L2	the calculated concentration of the first member
L3	the calculated concentration of the second member

TABLE 12. (Continued)

P6	the record number of the last record in the second member data file
P7	the record number of the first record which describes a peak in the second member data file
P8	the record number of the last record in the first member data file
P9	the record number of the first record which describes a peak in the first member data file
T$	the name of the method file
V$	the identifier from the method file
VO$	an error MESSAGE
X$	the user's response to Y or N questions

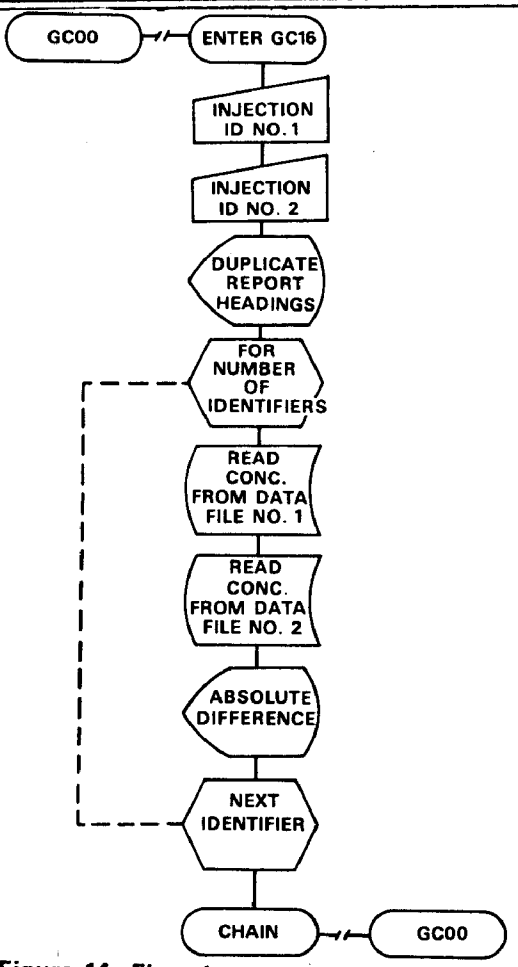

Figure 14. Flowchart of Program GC16.

PROGRAM LISTING FOR GC16

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                      +
0030 REM   +   PROGRAM GC16, DUPLICATE SAMPLES CALCULATIONS             +
0040 REM   +   BY:  J. KOPKE (SWORCC), APRIL 9, 1979                    +
0050 REM   +   MOST RECENT REVISION:  APRIL 12, 1979                    +
0060 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0070 REM
0080 DIM D2$[8],D3$[10],G$[8],H$[2],T$[6],V$[8],V0$[30],X$[3]
0090 ON ESC THEN GOTO 0120
0100 ESC
0110 GOTO 0210
0120 ON ERR THEN GOTO 0140
0130 CLOSE FILE[3]
0140 ON ERR THEN GOTO 0160
0150 CLOSE FILE[0]
0160 ON ERR THEN STOP
0170 NOESC
0180 CHAIN "GC00"
0190 REM   ------------------------------------------------------------
0200 REM          COUNT IDENTIFIERS IN METHOD FILE
0210 READ FILE[4,1],T$
0220 CLOSE FILE[4]
0230 OPEN FILE[4],T$,200
0240 LET F=0
0250 READ FILE[4,3*(F+1)-1],V$
0260 IF EOF(4) THEN GOTO 0310
0270 LET F=F+1
0280 GOTO 0250
0290 REM   ------------------------------------------------------------
0300 REM          OPEN DATA FILE FOR DUPLICATE FIRST MEMBER
0310 PRINT
0320 ON ERR THEN GOTO 0340
0330 INPUT "WHAT IS THE INJECTION ID FOR THE FIRST MEMBER?  ",D2$
0340 ON ERR THEN STOP
0350 IF LEN(D2$)=8 THEN GOTO 0390
0360 PRINT
0370 PRINT "<7><7>";D2$;" IS NOT A VALID INJECTION ID."
0380 GOTO 0310
0390 LET D3$="GC",D2$
0400 ON ERR THEN GOTO 0420
0410 RENAME D3$,D3$
0420 ON ERR THEN STOP
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```


PROGRAM LISTING FOR GC16

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0430 IF SYS(7)=-9 THEN GOTO 0470
0440 PRINT
0450 PRINT "<7><7>THERE IS NO EXISTING DATA FOR INJECTION ID ";D2$;"."
0460 GOTO 0310
0470 ON ERR THEN GOTO 0510
0480 OPEN FILE[3,0],D3$,31
0490 ON ERR THEN STOP
0500 GOTO 0560
0510 ON ERR THEN STOP
0520 DELAY =1
0530 GOTO 0470
0540 REM   ------------------------------------------------------------
0550 REM          CHECK DATA FILE USABILITY AND PROCESSING FLAGS
0560 READ FILE[3,1],J,D3$,J2
0570 IF J=1 THEN GOTO 0660
0580 PRINT
0590 IF J<>2 THEN GOTO 0630
0600 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT DID NOT"
0610 PRINT "     HAVE A TOTAL AREA"
0620 GOTO 1960
0630 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT WAS"
0640 PRINT "     IN THE WRONG FORMAT."
0650 GOTO 1960
0660 IF J2=1 THEN GOTO 0730
0670 PRINT
0680 PRINT "<7><7>";D2$;" CANNOT BE USED FOR SPIKED SAMPLE CALCULATION
*    S UNTIL"
0690 PRINT "     AFTER IT IS PROCESSED."
0700 GOTO 0120
0710 REM   ------------------------------------------------------------
0720 REM          FIND FIRST AND LAST ENTRIES IN DATA FILE
0730 LET P9=2
0740 READ FILE[3,P9],V0$
0750 IF V0$[1,7]<>"MESSAGE" THEN GOTO 0780
0760 LET P9=P9+1
0770 GOTO 0740
0780 LET P9=P9+2
0790 LET P8=P9
0800 READ FILE[3,P8],G$
0810 IF EOF(3) THEN GOTO 0840
0820 LET P8=P8+1
0830 GOTO 0800
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0840 LET P8=P8-1
0850 REM  ------------------------------------------------------------
0860 REM          OPEN DATA FILE FOR DUPLICATE SECOND MEMBER
0870 PRINT
0880 ON ERR THEN GOTO 0900
0890 INPUT "WHAT IS THE INJECTION ID FOR THE SECOND MEMBER?  ",D2$
0900 ON ERR THEN STOP
0910 IF LEN(D2$)=8 THEN GOTO 0950
0920 PRINT
0930 PRINT "<7><7>";D2$;" IS NOT A VALID INJECTION ID."
0940 GOTO 0870
0950 LET D3$="GC",D2$
0960 ON ERR THEN GOTO 0980
0970 RENAME D3$,D3$
0980 ON ERR THEN STOP
0990 IF SYS(7)=-9 THEN GOTO 1030
1000 PRINT
1010 PRINT "<7><7>THERE IS NO EXISTING DATA FOR INJECTION ID ";D2$;"."
1020 GOTO 0870
1030 ON ERR THEN GOTO 1070
1040 OPEN FILE[0,0],D3$,31
1050 ON ERR THEN STOP
1060 GOTO 1120
1070 ON ERR THEN STOP
1080 DELAY =1
1090 GOTO 1030
1100 REM  ------------------------------------------------------------
1110 REM          CHECK DATA FILE USABILITY AND PROCESSING FLAGS
1120 READ FILE[0,1],J,D3$,J2
1130 IF J=1 THEN GOTO 1220
1140 PRINT
1150 IF J<>2 THEN GOTO 1190
1160 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT DID NOT"
1170 PRINT "     HAVE A TOTAL AREA"
1180 GOTO 1960
1190 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT WAS"
1200 PRINT "     IN THE WRONG FORMAT."
1210 GOTO 1960
1220 IF J2=1 THEN GOTO 1290
1230 PRINT
1240 PRINT "<7><7>";D2$;" CANNOT BE USED FOR SPIKED SAMPLE CALCULATION
*    S UNTIL"
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```



```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
1250 PRINT "     AFTER IT IS PROCESSED."
1260 GOTO 0120
1270 REM  ------------------------------------------------------------
1280 REM          FIND FIRST AND LAST ENTRIES IN DATA FILE
1290 LET P7=2
1300 READ FILE[0,P7],V0$
1310 IF V0$[1,7]<>"MESSAGE" THEN GOTO 1340
1320 LET P7=P7+1
1330 GOTO 1300
1340 LET P7=P7+2
1350 LET P6=P7
1360 READ FILE[0,P6],G$
1370 IF EOF(0) THEN GOTO 1400
1380 LET P6=P6+1
1390 GOTO 1360
1400 LET P6=P6-1
1410 REM  ------------------------------------------------------------
1420 REM          PRINT HEADINGS
1430 PRINT
1440 PRINT
1450 PRINT  TAB(13);"D-U-P-L-I-C-A-T-E   S-A-M-P-L-E-S   R-E-P-O-R-T"
1460 READ FILE[3,1],J,D3$,J2
1470 PRINT "INJECTION ID FOR FIRST MEMBER:  ";D3$[3,10]; TAB(53);"METH
*    OD NUMBER:  ";T$[3,6]
1480 READ FILE[0,1],J,D3$,J2
1490 PRINT "INJECTION ID FOR SECOND MEMBER:  ";D3$[3,10]
1500 PRINT "CONCENTRATIONS IN MICROGRAMS/LITER"
1510 PRINT
1520 PRINT "                FIRST        SECOND       ABSOLUTE"
1530 PRINT "IDENTIFIER  CONCENTRATION  CONCENTRATION  DIFFERENCE"
1540 PRINT "--------  -------------  -------------  ----------"
1550 REM  ------------------------------------------------------------
1560 REM          FILL IN CHART
1570 FOR I=1 TO F
1580   READ FILE[4,3*I-1],V$
1590   IF V$="99999" THEN GOTO 1910
1600   FOR I2=P9 TO P8
1610     READ FILE[3,I2],G$,H$,B,C,L,L2
1620     IF G$=V$ THEN GOTO 1660
1630   NEXT I2
1640   LET C=-9999
1650   LET L=-9999
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

PROGRAM LISTING FOR GC16

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
1660   FOR I2=P7 TO P6
1670     READ FILE[0,I2],G$,H$,B,C2,L3,L2
1680     IF G$=V$ THEN GOTO 1720
1690   NEXT I2
1700   LET C2=-9999
1710   LET L3=-9999
1720   PRINT USING " ########   ",V$;
1730   IF C<-9999 THEN GOTO 1760
1740   PRINT " NOT DETECTED  ";
1750   GOTO 1800
1760   IF L<-9999 THEN GOTO 1790
1770   PRINT "NOT CALCULATED ";
1780   GOTO 1800
1790   PRINT USING "-----#.###     ",L;
1800   IF C2<-9999 THEN GOTO 1830
1810   PRINT " NOT DETECTED  ";
1820   GOTO 1870
1830   IF L3<-9999 THEN GOTO 1860
1840   PRINT "NOT CALCULATED ";
1850   GOTO 1870
1860   PRINT USING "-----#.###     ",L3;
1870   IF C<-9999 THEN IF L<-9999 THEN IF C2<-9999 THEN IF L3<-999
*     9 THEN GOTO 1900
1880   PRINT
1890   GOTO 1910
1900   PRINT USING " ++++#.###",L-L3
1910 NEXT I
1920 PRINT
1930 PRINT
1940 REM   ------------------------------------------------------
1950 REM          WRAP-UP PROCEDURE
1960 ON ERR THEN GOTO 1980
1970 CLOSE FILE[3]
1980 ON ERR THEN GOTO 2000
1990 CLOSE FILE[0]
2000 ON ERR THEN STOP
2010 PRINT
2020 ON ERR THEN GOTO 2040
2030 INPUT "DO YOU WANT A REPORT FOR ANOTHER DUPLICATE PAIR?  (Y OR N)
*      ",X$
2040 ON ERR THEN STOP
2050 IF X$[1,1]="Y" THEN GOTO 0310
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```


PROGRAM LISTING FOR GC16

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
2060 NOESC
2070 CHAIN "GC00"
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

SYMBOL TABLE FOR GC16

SYMBOL	REFERENCES				
0120	0090	0700	1260		
0140	0120				
0160	0140				
0210	0110				
0250	0280				
0310	0260	0380	0460	2050	
0340	0320				
0390	0350				
0420	0400				
0470	0430	0530			
0510	0470				
0560	0500				
0630	0590				
0660	0570				
0730	0660				
0740	0770				
0780	0750				
0800	0830				
0840	0810				
0870	0940	1020			
0900	0880				
0950	0910				
0980	0960				
1030	0990	1090			
1070	1030				
1120	1060				
1190	1150				
1220	1130				
1290	1220				
1300	1330				
1340	1310				
1360	1390				
1400	1370				
1660	1620				
1720	1680				
1760	1730				
1790	1760				
1800	1750	1780			
1830	1800				
1860	1830				
1870	1820	1850			
1900	1870				
1910	1590	1890			
1960	0620	0650	1180	1210	
1980	1960				

SYMBOL TABLE FOR GC16

SYMBOL	REFERENCES									
2000	1980									
2040	2020									
B	1610	1670								
C	1610	1640	1730	1870						
C2	1670	1700	1800	1870						
D2$	0080	0330	0350	0370	0390	0450	0600	0630	0680	0890
	0910	0930	0950	1010	1160	1190	1240			
D3$	0080	0390	0410	0480	0560	0950	0970	1040	1120	1460
	1470	1480	1490							
F	0240	0250	0270	1570						
FL#0	0150	1040	1120	1300	1360	1480	1670	1990		
FL#3	0130	0480	0560	0740	0800	1460	1610	1970		
FL#4	0210	0220	0230	0250	1580					
G$	0080	0800	1360	1610	1620	1670	1680			
H$	0080	1610	1670							
I	1570	1580	1910							
I2	1600	1610	1630	1660	1670	1690				
J	0560	0570	0590	1120	1130	1150	1460	1480		
J2	0560	0660	1120	1220	1460	1480				
L	1610	1650	1760	1790	1870	1900				
L2	1610	1670								
L3	1670	1710	1830	1860	1870	1900				
P6	1350	1360	1380	1400	1660					
P7	1290	1300	1320	1340	1350	1660				
P8	0790	0800	0820	0840	1600					
P9	0730	0740	0760	0780	0790	1600				
T$	0080	0210	0230	1470						
V$	0080	0250	1580	1590	1620	1680	1720			
V0$	0080	0740	0750	1300	1310					
X$	0080	2030	2050							

SECTION 19

PROGRAM GC17 - SURROGATE SPIKES CALCULATION

GC17 is the program which calculates the percent recovery of surrogate spikes and prints a report. It is entered by chaining from the master control program, GC00, and it chains back to that program if the escape key is pressed.

As GC27 begins, the method file is already open, and the program counts the number of identifiers in that file. It then asks the user for the injection ID for the sample containing the surrogate spike and opens the corresponding injection data file. The program then asks for the identifier of the surrogate spike compound. It searches the method file to be sure that the identifier is in the method, and then searches the data file to see if the compound was detected. It then asks the user for the prepared concentration of the surrogate spike, and prints the report.

Finally, the program closes the data file and asks the user if it should start over. It then either branches back to the beginning or chains back to GC00. The percent recovery of surrogate spikes is calculated by the formula:

$$\text{Percent Recovery} = 100 \cdot \frac{\text{Measured Concentration}}{\text{Prepared Concentration}}$$

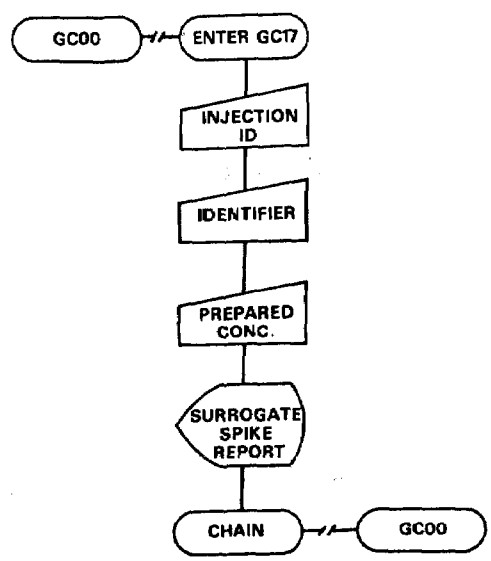

Figure 15. Flowchart of Program GC17.

TABLE 13. SYMBOL DEFINITIONS FOR PROGRAM GC17

A5	the prepared concentration of the surrogate spike
B	the absolute retention time
C	the peak area
D2$	the injection ID
D3$	the name of the data file
F	the number of identifiers in the method file
G$	the identifier from the data file
H$	the peak type
I	the control variable for loops
J	the data file useablility flag J=1 good data J=2 no TOTAL AREA J=3 wrong format
J2	the data file processing status flag J2=1 has been proccessed J2=2 never processed
L	the calculated concentration
L2	the relative retention time or capacity ratio
P9	the record number for the first peak in the data file
T$	the name of the method file
V$	the identifier from the method file
VO$	an error MESSAGE
V1$	the full chemical name of the surrogate spike compound

TABLE 13. (Continued)

V7$	the identifier input by the user
X$	the user's answer to Y or N questions

PROGRAM LISTING FOR GC17

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                    +
0030 REM   +   PROGRAM GC17, SURROGATE SPIKE CALCULATIONS             +
0040 REM   +   BY:  J. KOPKE (SWORCC), APRIL 12, 1979                 +
0050 REM   +   MOST RECENT REVISION:  APRIL 12, 1979                  +
0060 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0070 REM
0080 DIM D2$[8],D3$[10],G$[8],H$[2],T$[6],V$[8],V0$[30],V1$[40],V7$[8]
*     ,X$[3]
0090 ON ESC THEN GOTO 0120
0100 ESC
0110 GOTO 0190
0120 ON ERR THEN GOTO 0140
0130 CLOSE FILE[3]
0140 ON ERR THEN STOP
0150 NOESC
0160 CHAIN "GC00"
0170 REM   ---------------------------------------------------------
0180 REM          COUNT IDENTIFIERS IN METHOD FILE
0190 READ FILE[4,1],T$
0200 CLOSE FILE[4]
0210 OPEN FILE[4],T$,200
0220 LET F=0
0230 READ FILE[4,3*(F+1)-1],V$
0240 IF EOF(4) THEN GOTO 0290
0250 LET F=F+1
0260 GOTO 0230
0270 REM   ---------------------------------------------------------
0280 REM          OPEN DATA FILE
0290 PRINT
0300 ON ERR THEN GOTO 0320
0310 INPUT "WHAT IS THE INJECTION ID FOR THE SURROGATE SPIKE?  ",D2$
0320 ON ERR THEN STOP
0330 IF LEN(D2$)=8 THEN GOTO 0370
0340 PRINT
0350 PRINT "<7><7>";D2$;" IS NOT A VALID INJECTION ID."
0360 GOTO 0290
0370 LET D3$="GC",D2$
0380 ON ERR THEN GOTO 0400
0390 RENAME D3$,D3$
0400 ON ERR THEN STOP
0410 IF SYS(7)=-9 THEN GOTO 0450
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```


PROGRAM LISTING FOR GC17

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0420 PRINT
0430 PRINT "<7><7>THERE IS NO EXISTING DATA FOR INJECTION ID ";D2$;"."
0440 GOTO 0290
0450 ON ERR THEN GOTO 0490
0460 OPEN FILE[3,0],D3$,31
0470 ON ERR THEN STOP
0480 GOTO 0540
0490 ON ERR THEN STOP
0500 DELAY =1
0510 GOTO 0450
0520 REM   ---------------------------------------------------------
0530 REM          CHECK DATA FILE USABILITY AND PROCESSING FLAGS
0540 READ FILE[3,1],J,D3$,J2
0550 IF J=1 THEN GOTO 0640
0560 PRINT
0570 IF J<>2 THEN GOTO 0610
0580 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT DID NOT"
0590 PRINT "     HAVE A TOTAL AREA"
0600 GOTO 1210
0610 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT WAS"
0620 PRINT "     IN THE WRONG FORMAT."
0630 GOTO 1210
0640 IF J2=1 THEN GOTO 0710
0650 PRINT
0660 PRINT "<7><7>";D2$;" CANNOT BE USED FOR SURROGATE SPIKE CALCULATI
*     ONS UNTIL"
0670 PRINT "     AFTER IT IS PROCESSED."
0680 GOTO 0120
0690 REM   ---------------------------------------------------------
0700 REM          LOCATE DATA
0710 PRINT
0720 ON ERR THEN GOTO 0740
0730 INPUT "WHAT IS THE IDENTIFIER FOR THE SURROGATE SPIKE COMPOUND?
*     ",V7$
0740 ON ERR THEN STOP
0750 FOR I=1 TO F
0760   READ FILE[4,3*I-1],V$,V1$
0770   IF V$=V7$ THEN GOTO 0820
0780 NEXT I
0790 PRINT
0800 PRINT "<7><7>THERE IS NO IDENTIFIER ";V7$;" IN METHOD ";T$[3,6];"
*     ."
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

```
123456789112345678921234567893123456789412345678951234567896123456789 7
         0         0         0         0         0         0         0
0810 GOTO 1210
0820 LET P9=2
0830 READ FILE[3,P9],V0$
0840 IF V0$[1,7]<>"MESSAGE" THEN GOTO 0870
0850 LET P9=P9+1
0860 GOTO 0830
0870 LET P9=P9+2
0880 READ FILE[3,P9],G$,H$,B,C,L,L2
0890 IF EOF(3)<>1 THEN GOTO 0930
0900 PRINT
0910 PRINT "<7><7>IDENTIFIER ";V7$;" WAS NOT DETECTED IN INJECTION ";D
*     2$;"."
0920 GOTO 1210
0930 IF G$=V7$ THEN GOTO 0960
0940 LET P9=P9+1
0950 GOTO 0880
0960 IF C=-9999 THEN GOTO 0900
0970 IF L<>-9999 THEN GOTO 1010
0980 PRINT
0990 PRINT "<7><7>THE CONCENTRATION OF ";D2$;" WAS NOT CALCULATED DURI
*     NG PROCESSING."
1000 GOTO 1210
1010 PRINT .
1020 PRINT "WHAT IS THE PREPARED CONCENTRATION OF ";V7$;" IN";
1030 ON ERR THEN GOTO 1050
1040 INPUT " MICROGRAMS/LITER?  ",A5
1050 ON ERR THEN STOP
1060 REM  ------------------------------------------------------
1070 REM          PRINT REPORT
1080 PRINT
1090 PRINT
1100 PRINT  TAB(15);"S-U-R-R-O-G-A-T-E   S-P-I-K-E   R-E-P-O-R-T"
1110 PRINT "INJECTION ID:  ";D2$; TAB(54);"METHOD NUMBER:  ";T$[3,6]
1120 PRINT "PREPARED CONCENTRATION OF ";V1$;":  ";
1130 PRINT USING "-----#.###",A5
1140 PRINT USING "CALCULATED CONCENTRATION:  -----#.###",L
1150 PRINT USING "PERCENT RECOVERED:  ---#.#%",L/A5*100
1160 PRINT "CONCENTRATIONS IN MICROGRAMS/LITER"
1170 PRINT
1180 PRINT
1190 REM  ------------------------------------------------------
1200 REM          WRAP-UP PROCEDURE
123456789112345678921234567893123456789412345678951234567896123456789 7
         0         0         0         0         0         0         0
```



```
123456789112345678921234567893123456789412345678951234567896123456789 7
         0         0         0         0         0         0         0
1210 ON ERR THEN GOTO 1230
1220 CLOSE FILE[3]
1230 ON ERR THEN STOP
1240 PRINT
1250 ON ERR THEN GOTO 1270
1260 INPUT "DO YOU WANT A REPORT ON ANOTHER SURROGATE SPIKE?  (Y OR N)
*       ",X$
1270 ON ERR THEN STOP
1280 IF X$[1,1]="Y" THEN GOTO 0290
1290 NOESC
1300 CHAIN "GC00"
123456789112345678921234567893123456789412345678951234567896123456789 7
         0         0         0         0         0         0         0
```

SYMBOL TABLE FOR GC17

SYMBOL	REFERENCES									
0120	0090	0680								
0140	0120									
0190	0110									
0230	0260									
0290	0240	0360	0440	1280						
0320	0300									
0370	0330									
0400	0380									
0450	0410	0510								
0490	0450									
0540	0480									
0610	0570									
0640	0550									
0710	0640									
0740	0720									
0820	0770									
0830	0860									
0870	0840									
0880	0950									
0900	0960									
0930	0890									
0960	0930									
1010	0970									
1050	1030									
1210	0600	0630	0810	0920	1000					
1230	1210									
1270	1250									
A5	1040	1130	1150							
B	0880									
C	0880	0960								
D2$	0080	0310	0330	0350	0370	0430	0580	0610	0660	0910
	0990	1110								
D3$	0080	0370	0390	0460	0540					
F	0220	0230	0250	0750						
FL#3	0130	0460	0540	0830	0880	1220				
FL#4	0190	0200	0210	0230	0760					
G$	0080	0880	0930							
H$	0080	0880								
I	0750	0760	0780							
J	0540	0550	0570							
J2	0540	0640								
L	0880	0970	1140	1150						
L2	0880									
P9	0820	0830	0850	0870	0880	0940				
T$	0080	0190	0210	0800	1110					

SYMBOL TABLE FOR GC17

SYMBOL	REFERENCES						
V$	0080	0230	0760	0770			
V0$	0080	0830	0840				
V1$	0080	0760	1120				
V7$	0080	0730	0770	0800	0910	0930	1020
X$	0080	1260	1280				

SECTION 20

PROGRAM GC18 - REPLICATE STATISTICS CALCULATION

GC18 is the program which calculates replicate statistics and prints a report. It is entered by chaining from the master control program, GC00, and it chains back to that program if the escape key is pressed.

When GC18 begins, the method file is already open, and the program counts the number of identifiers in that file. The program then asks the user for the injection ID for a sample, and opens the corresponding injection data file. The program then reads each identifier from the method file and locates the calculated concentration of each identifier in the data file. It places the concentration in array 0, and then it closes the data file and goes back to ask the user for another injection ID.

When the user types "END" as an injection ID (or when ten replicates have been entered) the program begins to print the report. It prints the headings first, and then fills in the table. It reads the replicate concentrations for each identifier from array 0, calculates the mean concentration and standard deviation, and prints these statistics.

When all of the identifiers have been dealt with, the program asks the user if it should start over. It then either branches back to the beginning or chains back to GC00.

TABLE 14. SYMBOL DEFINITIONS FOR PROGRAM GC18

B	the absolute retention time
C	the peak area
D2$	the injection ID
D3$	the name of the data file
F	the number of identifiers in the method file
G$	the identifier from the data file
H$	the peak type
I	the control variable for loops
I$	the superstring of injection ID numbers for replicates
I2	the control variable for loops
J	the data file useability flag J=1 good data J=2 no TOTAL AREA J=3 wrong format
J2	the data file processing status flag J2=1 never processed J2=2 processed
L	the calculated concentration
L2	the relative retention time or capacity ratio
O()	the array of calculated concentrations of replicates
P8	the record number for the last peak in the data file
P9	the record number for the first peak in the data file
R4	the standard deviation

TABLE 14. (Continued)

R5	the average concentration (arithmetic mean)
R6	the number of replicate injections
R7	the number of replicates of an individual compound
R8	the sum of the measured concentrations (used in calculating the average and the standard deviation)
R9	the sum of the squares of the measured concentrations (used in calculating the standard deviation)
T$	the name of the method file
V$	the identifier from the method file
VO$	an error MESSAGE
X$	the user's response to a Y or N question

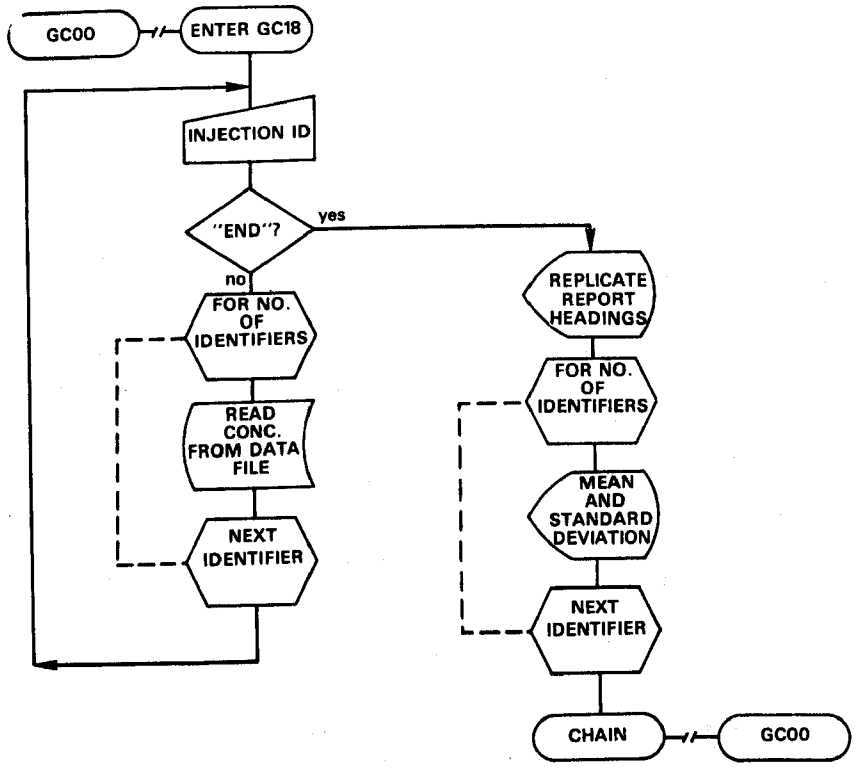

Figure 16. Flowchart of Program GC18.

PROGRAM LISTING FOR GC18

```
123456789112345678921234567893123456789412345678951234567896123456789 7
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                    +
0030 REM   +   PROGRAM GC18, REPLICATE STATISTICS CALCULATIONS        +
0040 REM   +   BY:  J. KOPKE (SWORCC), APRIL 16, 1979                 +
0050 REM   +   MOST RECENT REVISION:  APRIL 16, 1979                  +
0060 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0070 REM
0080 DIM D2$[8],D3$[10],G$[8],H$[2],I$[80],O[60,10],T$[6],V$[8],VO$[30
*    ],X$[3]
0090 ON ESC THEN GOTO 0120
0100 ESC
0110 GOTO 0190
0120 ON ERR THEN GOTO 0140
0130 CLOSE FILE[3]
0140 ON ERR THEN STOP
0150 NOESC
0160 CHAIN "GC00"
0170 REM   ------------------------------------------------------------
0180 REM          COUNT IDENTIFIERS IN METHOD FILE
0190 READ FILE[4,1],T$
0200 CLOSE FILE[4]
0210 OPEN FILE[4],T$,200
0220 LET F=0
0230 READ FILE[4,3*(F+1)-1],V$
0240 IF EOF(4) THEN GOTO 0290
0250 LET F=F+1
0260 GOTO 0230
0270 REM   ------------------------------------------------------------
0280 REM          OPEN DATA FILE
0290 PRINT
0300 PRINT "ENTER THE INJECTION ID NUMBERS FOR THE REPLICATE INJECTION
*    S."
0310 PRINT "TYPE 'END' TO TERMINATE THE LIST."
0320 LET R6=0
0330 LET I$=""
0340 PRINT
0350 IF R6<10 THEN GOTO 0390
0360 PRINT "<7><7>YOU HAVE ENTERED TEN REPLICATES, WHICH IS THE LIMIT
*    "
0370 PRINT "     FOR THIS PROGRAM."
0380 GOTO 1140
0390 ON ERR THEN GOTO 0410
123456789112345678921234567893123456789412345678951234567896123456789 7
         0         0         0         0         0         0         0
```


PROGRAM LISTING FOR GC18

```
123456789112345678921234567893123456789412345678951234567896123456789 7
         0         0         0         0         0         0         0
0400 INPUT "INJECTION ID FOR REPLICATE?  ",D2$
0410 ON ERR THEN STOP
0420 IF D2$="END" THEN GOTO 1140
0430 IF LEN(D2$)=8 THEN GOTO 0470
0440 PRINT
0450 PRINT "<7><7>";D2$;" IS NOT A VALID INJECTION ID."
0460 GOTO 0340
0470 LET D3$="GC",D2$
0480 ON ERR THEN GOTO 0500
0490 RENAME D3$,D3$
0500 ON ERR THEN STOP
0510 IF SYS(7)=-9 THEN GOTO 0550
0520 PRINT
0530 PRINT "<7><7>THERE IS NO EXISTING DATA FOR INJECTION ID ";D2$;"."
0540 GOTO 0340
0550 ON ERR THEN GOTO 0590
0560 OPEN FILE[3,0],D3$,31
0570 ON ERR THEN STOP
0580 GOTO 0640
0590 ON ERR THEN STOP
0600 DELAY =1
0610 GOTO 0550
0620 REM   ------------------------------------------------------------
0630 REM          CHECK DATA FILE USABILITY AND PROCESSING FLAGS
0640 READ FILE[3,1],J,D3$,J2
0650 IF J=1 THEN GOTO 0760
0660 PRINT
0670 IF J<>2 THEN GOTO 0720
0680 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT DID NOT"
0690 PRINT "     HAVE A TOTAL AREA"
0700 CLOSE FILE[3]
0710 GOTO 0340
0720 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT WAS"
0730 PRINT "     IN THE WRONG FORMAT."
0740 CLOSE FILE[3]
0750 GOTO 0340
0760 IF J2=1 THEN GOTO 0840
0770 PRINT
0780 PRINT "<7><7>";D2$;" CANNOT BE USED FOR REPLICATE STATISTICS CALC
*    ULATIONS UNTIL"
0790 PRINT "     AFTER IT IS PROCESSED."
0800 CLOSE FILE[3]
123456789112345678921234567893123456789412345678951234567896123456789 7
         0         0         0         0         0         0         0
```

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0810 GOTO 0340
0820 REM  ------------------------------------------------------------
0830 REM          FIND FIRST AND LAST ENTRIES IN DATA FILE
0840 LET P9=2
0850 READ FILE[3,P9],V0$
0860 IF V0$[1,7]<>"MESSAGE" THEN GOTO 0890
0870 LET P9=P9+1
0880 GOTO 0850
0890 LET P9=P9+2
0900 LET P8=P9
0910 READ FILE[3,P8],G$
0920 IF EOF(3) THEN GOTO 0950
0930 LET P8=P8+1
0940 GOTO 0910
0950 LET P8=P8-1
0960 REM  ------------------------------------------------------------
0970 REM          COPY DATA TO ARRAY
0980 LET R6=R6+1
0990 LET I$=I$,D2$
1000 FOR I=1 TO F
1010   READ FILE[4,3*I-1],V$
1020   FOR I2=P9 TO P8
1030     READ FILE[3,I2],G$,H$,B,C,L,L2
1040     IF G$=V$ THEN GOTO 1080
1050   NEXT I2
1060   LET O[I,R6]=-9999
1070   GOTO 1090
1080   LET O[I,R6]=L
1090 NEXT I
1100 CLOSE FILE[3]
1110 GOTO 0340
1120 REM  ------------------------------------------------------------
1130 REM          PRINT HEADING
1140 IF R6>1 THEN GOTO 1190
1150 PRINT
1160 PRINT "<7><7>REPLICATE STATISTICS CANNOT BE CALCULATED WITH FEWER
*      THAN"
1170 PRINT "     TWO GOOD INJECTIONS."
1180 GOTO 1660
1190 PRINT
1200 PRINT
1210 PRINT  TAB(10);"R-E-P-L-I-C-A-T-E   S-T-A-T-I-S-T-I-C-S   R-E-P-O
*     -R-T"

12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```



```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
1220 PRINT "METHOD NUMBER:  ";T$[3,6]; TAB(39);"CONCENTRATIONS IN MICR
*     OGRAMS/LITER"
1230 PRINT "REPLICATE INJECTION ID NUMBERS:  ";
1240 FOR I=1 TO R6
1250   PRINT I$[8*I-7,8*I];
1260   IF I<>R6 THEN PRINT ", ";
1270   IF I<>4 THEN GOTO 1300
1280   PRINT
1290   PRINT "     ";
1300 NEXT I
1310 PRINT
1320 PRINT
1330 PRINT "                AVERAGE     STANDARD   NUMBER OF"
1340 PRINT "IDENTIFIER  CONCENTRATION  DEVIATION  REPLICATES"
1350 PRINT "---------  -------------  ---------  ----------"
1360 REM  ------------------------------------------------------------
1370 REM          FILL IN CHART
1380 FOR I=1 TO F
1390   READ FILE[4,3*I-1],V$
1400   IF V$="99999" THEN GOTO 1620
1410   LET R8=0
1420   LET R9=0
1430   LET R7=0
1440   FOR I2=1 TO R6
1450     IF O[I,I2]=-9999 THEN GOTO 1490
1460     LET R7=R7+1
1470     LET R8=R8+O[I,I2]
1480     LET R9=R9+O[I,I2]^2
1490   NEXT I2
1500   PRINT USING " ######## ",V$;
1510   IF R7>0 THEN GOTO 1540
1520   PRINT "                                    0"
1530   GOTO 1620
1540   LET R5=R8/R7
1550   PRINT USING "  -----#.###   ",R5;
1560   IF R7>1 THEN GOTO 1590
1570   PRINT "            ";
1580   GOTO 1610
1590   LET R4=SQR((R9-R8^2/R7)/(R7-1))
1600   PRINT USING " -----#.## ",R4;
1610   PRINT USING "     ###",R7
1620 NEXT I

12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

PROGRAM LISTING FOR GC18

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
1630 REM
1640 REM          WRAP-UP PROCEDURE
1650 PRINT
1660 PRINT
1670 ON ERR THEN GOTO 1690
1680 INPUT "DO YOU WANT A REPORT ON ANOTHER SET OF REPLICATES?  (Y OR
*     N)  ",X$
1690 ON ERR THEN STOP
1700 IF X$[1,1]="Y" THEN GOTO 0290
1710 NOESC
1720 CHAIN "GC00"
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```


SYMBOL TABLE FOR GC18

SYMBOL	REFERENCES									
0120	0090									
0140	0120									
0190	0110									
0230	0260									
0290	0240	1700								
0340	0460	0540	0710	0750	0810	1110				
0390	0350									
0410	0390									
0470	0430									
0500	0480									
0550	0510	0610								
0590	0550									
0640	0580									
0720	0670									
0760	0650									
0840	0760									
0850	0880									
0890	0860									
0910	0940									
0950	0920									
1080	1040									
1090	1070									
1140	0380	0420								
1190	1140									
1300	1270									
1490	1450									
1540	1510									
1590	1560									
1610	1580									
1620	1400	1530								
1660	1180									
1690	1670									
B	1030									
C	1030									
D2$	0080	0400	0420	0430	0450	0470	0530	0680	0720	0780
	0990									
D3$	0080	0470	0490	0560	0640					
F	0220	0230	0250	1000	1380					
FL#3	0130	0560	0640	0700	0740	0800	0850	0910	1030	1100
FL#4	0190	0200	0210	0230	1010	1390				
G$	0080	0910	1030	1040						
H$	0080	1030								
I	1000	1010	1060	1080	1090	1240	1250	1260	1270	1300
	1380	1390	1450	1470	1480	1620				
I$	0080	0330	0990	1250						

SYMBOL TABLE FOR GC18

SYMBOL	REFERENCES								
I2	1020	1030	1050	1440	1450	1470	1480	1490	
J	0640	0650	0670						
J2	0640	0760							
L	1030	1080							
L2	1030								
O[	0080	1060	1080	1450	1470	1480			
P8	0900	0910	0930	0950	1020				
P9	0840	0850	0870	0890	0900	1020			
R4	1590	1600							
R5	1540	1550							
R6	0320	0350	0980	1060	1080	1140	1240	1260	1440
R7	1430	1460	1510	1540	1560	1590	1610		
R8	1410	1470	1540	1590					
R9	1420	1480	1590						
T$	0080	0190	0210	1220					
V$	0080	0230	1010	1040	1390	1400	1500		
V0$	0080	0850	0860						
X$	0080	1680	1700						

SECTION 21

PROGRAM GC19 - DISSIMILAR ANALYSIS CONFIRMATION

GC19 is the program which prints a dissimilar analysis confirmation report. It is entered by chaining from the master control program, GC00, and it chains back to that program if the escape key is pressed.

GC19 first asks the user for the method numbers and the injection ID numbers to be used in the confirmation report. The user is forced to input at least two but no more than four method numbers and at least one but no more than four injection ID numbers for each of the methods. The method numbers and injection ID numbers are checked as they are input to ensure that they are valid numbers and that the corresponding data files exist. The names of the method files are placed in superstring S5$, and the names of the data files are placed in superstring S6$.

The program then asks the user for the identifier for which the confirmation report is to be compiled, and it checks to be sure that the identifier does occur in all of the specified methods.

Next, the program prints the headings for the report, and then begins to fill in the report. For each line of the report, the program opens a data file and locates the concentration for the specified identifier.

When the report is complete, the program asks the user whether it should start over. If the user answers YES, the program branches back to the point of asking for the identifier to be used. Otherwise, control is returned to GC00.

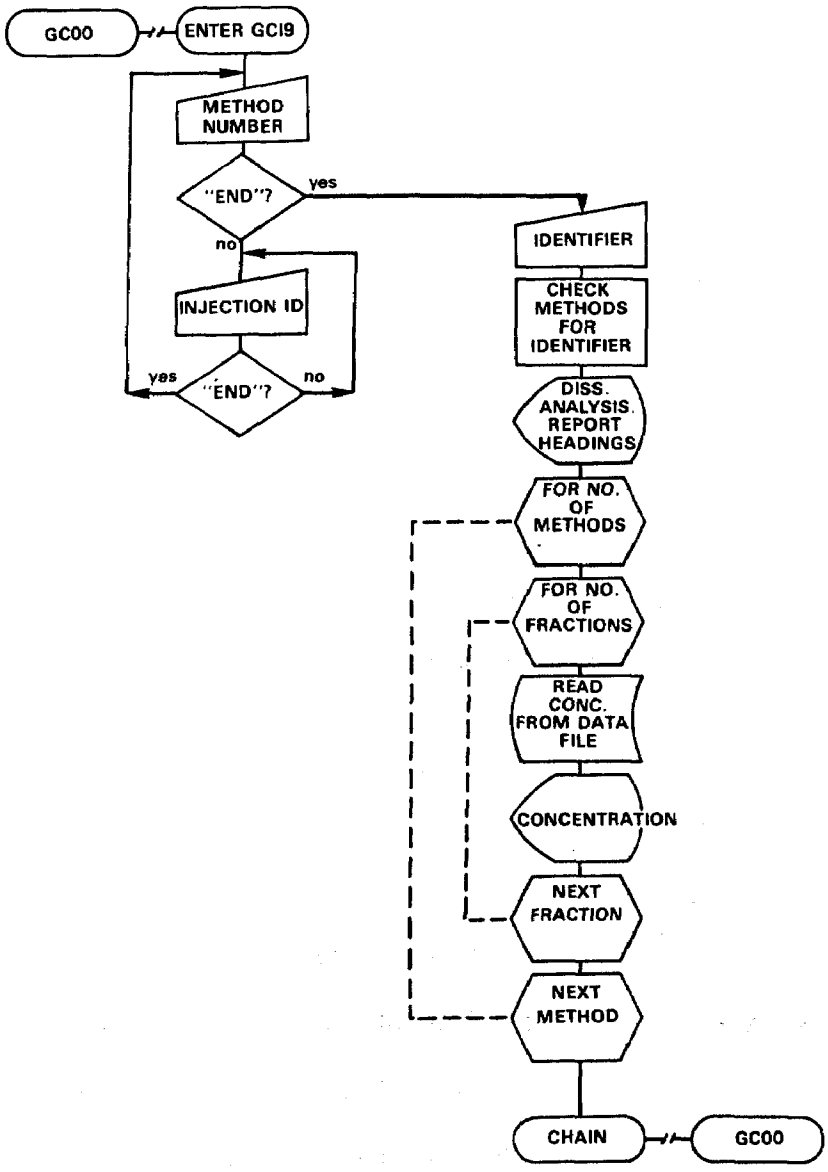

Figure 17. Flowchart of Program GC19.

TABLE 15. SYMBOL DEFINITIONS FOR PROGRAM GC19

B	the absolute retention time
C	the peak area
D2$	the injection ID
D3$	the name of a data file
G$	the identifier from the data file
H$	the peak type
I	the control variable for loops
I2	the control variable for loops
J	the data file useability flag J=1 good data J=2 no TOTAL AREA J=3 wrong format
J2	the data file processing status flag J2=1 processed J2=2 never processed
L	the calculated concentration
P9	the record number being accessed in the data file
S5	the counter for the number of methods
S5$	the superstring of the names of the method files
S6$	the superstring of the names of the data files
S6()	the array of four counters which count the number of data files used with each method
S7	the record number being accessed in the method file
T	the method number

TABLE 15. (Continued)

T$	the name of the method file
T1$	the method number as a string
V$	the identifier from the method file
V0$	an error MESSAGE from the data file
V7$	the identifier for which the report is generated
X$	the user's response to a Y or N question
Z5	the character position of a slash in the identifier

PROGRAM LISTING FOR GC19

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                    +
0030 REM   +   PROGRAM GC19, DISSIMILAR ANALYSIS CONFIRMATION         +
0040 REM   +   BY:  J. KOPKE (SWORCC), APRIL 19, 1979                 +
0050 REM   +   MOST RECENT REVISION:  APRIL 19, 1979                  +
0060 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0070 REM
0080 ON ESC THEN GOTO 2040
0090 ESC
0100 DIM D2$[8],D3$[10],G$[8],H$[2],S5$[24],S6$[160],S6[4],T$[6],T1$[6
*     ],V$[8],V0$[30],V7$[8],X$[3]
0110 REM   ------------------------------------------------------------
0120 REM          INPUT METHOD NUMBERS
0130 LET S5$="                          "
0140 FOR I=1 TO 16
0150   LET S6$=S6$,"          "
0160 NEXT I
0170 LET S5=0
0180 IF S5<>4 THEN GOTO 0190
0182 PRINT
0184 PRINT "<7><7>YOU HAVE ENTERED FOUR METHODS WHICH IS THE LIMIT FOR
*      THIS PROGRAM."
0186 GOTO 0940
0190 PRINT
0200 PRINT "WHAT IS THE NUMBER OF THE ";
0210 ON S5+1 THEN GOTO 0220, 0240, 0260, 0280
0220 PRINT "FIRST ";
0230 GOTO 0290
0240 PRINT "SECOND ";
0250 GOTO 0290
0260 PRINT "THIRD ";
0270 GOTO 0290
0280 PRINT "FOURTH ";
0290 PRINT "METHOD?"
0300 ON ERR THEN GOTO 0320
0310 INPUT "     (TYPE 'END' TO TERMINATE THE LIST OF METHODS)  ",T1$
0320 ON ERR THEN STOP
0330 IF T1$<>"END" THEN GOTO 0380
0340 IF S5>1 THEN GOTO 0940
0350 PRINT
0360 PRINT "<7><7>YOU MUST USE AT LEAST TWO DIFFERENT METHODS."
0370 GOTO 0190
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```


PROGRAM LISTING FOR GC19

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0380 ON ERR THEN GOTO 0420
0390 LET T=VAL(T1$)
0400 ON ERR THEN STOP
0410 IF T=ABS(INT(T)) THEN IF T>0 THEN IF T<10000 THEN GOTO 0460
0420 ON ERR THEN STOP
0430 PRINT
0440 PRINT "<7><7>";T1$;" IS NOT A VALID METHOD NUMBER."
0450 GOTO 0190
0460 LET T$="GC0000"
0470 LET T$[7-LEN(STR$(T)),6]=STR$(T)
0480 ON ERR THEN GOTO 0500
0490 RENAME T$,T$
0500 ON ERR THEN STOP
0510 IF SYS(7)<>-10 THEN GOTO 0550
0520 PRINT
0530 PRINT "<7><7>THERE IS NO EXISTING METHOD WITH THE NUMBER ";T$[3,6
*     ];"."
0540 GOTO 0190
0550 PRINT
0560 LET S5=S5+1
0570 LET S5$[6*S5-5,6*S5]=T$
0580 REM   ------------------------------------------------------------
0590 REM          INPUT INJECTION ID NUMBERS
0600 LET S6[S5]=0
0610 IF S6[S5]<>4 THEN GOTO 0620
0612 PRINT "<7><7>YOU HAVE ENTERED FOUR FRACTIONS WHICH IS THE LIMIT F
*     OR ONE METHOD."
0614 GOTO 0180
0620 PRINT "WHAT IS THE INJECTION ID FOR THE ";
0630 ON S6[S5]+1 THEN GOTO 0640, 0660, 0680, 0700
0640 PRINT "FIRST ";
0650 GOTO 0710
0660 PRINT "SECOND ";
0670 GOTO 0710
0680 PRINT "THIRD ";
0690 GOTO 0710
0700 PRINT "FOURTH ";
0710 PRINT "FRACTION FOR METHOD ";T$[3,6];"?"
0720 ON ERR THEN GOTO 0740
0730 INPUT "     (TYPE 'END' TO TERMINATE THE LIST OF FRACTIONS)  ",D2
*     $
0740 ON ERR THEN STOP
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0750 IF D2$<>"END" THEN GOTO 0790
0760 IF S6[S5]>0 THEN GOTO 0180
0770 PRINT "<7><7>YOU MUST USE AT LEAST ONE FRACTION FOR A METHOD."
0780 GOTO 0620
0790 IF LEN(D2$)=8 THEN GOTO 0820
0800 PRINT "<7><7>";D2$;" IS NOT A VALID INJECTION ID NUMBER."
0810 GOTO 0620
0820 LET D3$="GC",D2$
0830 ON ERR THEN GOTO 0850
0840 RENAME D3$,D3$
0850 ON ERR THEN STOP
0860 IF SYS(7)<>-10 THEN GOTO 0890
0870 PRINT "<7><7>THERE IS NO EXISTING DATA FOR INJECTION ";D2$;"."
0880 GOTO 0620
0890 LET S6[S5]=S6[S5]+1
0900 LET S6$[((S5-1)*40)+S6[S5]*10-9,((S5-1)*40)+S6[S5]*10]=D3$
0910 GOTO 0610
0920 REM  ------------------------------------------------------------
0930 REM          CHECK METHOD FOR PRESENCE OF IDENTIFIER
0940 PRINT
0950 ON ERR THEN GOTO 0990
0960 INPUT "WHAT IS THE IDENTIFIER FOR WHICH YOU WANT A CONFIRMATION R
*    EPORT?  ",V7$
0970 ON ERR THEN STOP
0980 GOTO 1030
0990 ON ERR THEN STOP
1000 PRINT
1010 PRINT "<7><7>USE A SLASH (/) WHERE YOU WANT A COMMA."
1020 GOTO 0940
1030 LET Z5=POS(V7$,"/",1)
1040 IF Z5=0 THEN GOTO 1070
1050 LET V7$[Z5,Z5]=","
1060 GOTO 1030
1070 FOR I=1 TO S5
1080   ON ERR THEN GOTO 1120
1090   OPEN FILE[4,0],S5$[6*I-5,6*I],200
1100   ON ERR THEN STOP
1110   GOTO 1160
1120   PRINT
1130   PRINT "<7><7>METHOD ";S5$[6*I-3,6*I];" IS BEING USED BY ANOTHER
*     USER."
1140   PRINT "     THIS OPTION IS BEING TERMINATED."
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```



```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
1150   GOTO 2040
1160   LET S7=1
1170   READ FILE[4,3*S7-1],V$
1180   IF EOF(4)<>1 THEN GOTO 1230
1190   PRINT
1200   PRINT "<7><7>IDENTIFIER ";V7$;" DOES NOT APPEAR IN METHOD ";S5$
*     [6*I-3,6*I];"."
1210   CLOSE
1220   GOTO 1980
1230   IF V$=V7$ THEN GOTO 1260
1240   LET S7=S7+1
1250   GOTO 1170
1260   CLOSE
1270 NEXT I
1280 REM  ------------------------------------------------------------
1290 REM          PRINT HEADINGS
1300 PRINT
1310 PRINT
1320 PRINT "     D-I-S-S-I-M-I-L-A-R   A-N-A-L-Y-S-I-S   C-O-N-F-I-R-M
*     -A-T-I-O-N"
1330 PRINT "IDENTIFIER:  ";V7$; TAB(39);"CONCENTRATIONS IN MICROGRAMS/
*     LITER"
1340 PRINT
1350 PRINT "METHOD  INJECTION   CALCULATED"
1360 PRINT "NUMBER     ID      CONCENTRATION"
1370 PRINT "------  --------  -------------"
1380 REM  ------------------------------------------------------------
1390 REM          FILL IN CHART
1400 FOR I=1 TO S5
1410   FOR I2=1 TO S6[I]
1420     LET D3$=S6$[((I-1)*40)+I2*10-9,((I-1)*40)+I2*10]
1430     ON ERR THEN GOTO 1470
1440     OPEN FILE[3,0],D3$,31
1450     ON ERR THEN STOP
1460     GOTO 1520
1470     ON ERR THEN STOP
1480     PRINT
1490     PRINT "<7><7>THE DATA FOR INJECTION ";D3$;" IS BEING USED BY
*     ANOTHER USER."
1500     PRINT "     THIS OPTION IS BEING TERMINATED."
1510     GOTO 2040
1520     REM  ------------------------------------
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
1530    REM     CHECK DATA FILE FLAGS
1540    READ FILE[3,1],J,D3$,J2
1550    IF J=1 THEN GOTO 1640
1560    PRINT
1570    IF J<>2 THEN GOTO 1610
1580    PRINT "<7><7>";D3$[3,10];" CANNOT BE USED BECAUSE THE REPORT
*     DID NOT HAVE"
1590    PRINT "     A TOTAL AREA.  ";
1600    GOTO 1670
1610    PRINT "<7><7>";D3$;" CANNOT BE USED BECAUSE THE REPORT WAS IN
*      THE WRONG"
1620    PRINT "     FORMAT.  ";
1630    GOTO 1670
1640    IF J2=1 THEN GOTO 1710
1650    PRINT "<7><7>";D3$[3,10];" CANNOT BE USED FOR DISSIMILAR ANAL
*     YSIS CONFIRMATION"
1660    PRINT "     UNTIL AFTER IT IS PROCESSED.  ";
1670    PRINT "THIS OPTION IS BEING TERMINATED."
1680    GOTO 2040
1690    REM  ------------------------------------
1700    REM     FIND CONCENTRATION
1710    LET P9=2
1720    READ FILE[3,P9],V0$
1730    IF V0$[1,7]<>"MESSAGE" THEN GOTO 1760
1740    LET P9=P9+1
1750    GOTO 1720
1760    LET P9=P9+2
1770    READ FILE[3,P9],G$,H$,B,C,L
1780    IF EOF(3)<>1 THEN GOTO 1800
1790    LET C=-9999
1800    IF G$=V7$ THEN GOTO 1830
1810    LET P9=P9+1
1820    GOTO 1770
1830    CLOSE
1840    PRINT USING " ####    ########",S5$[6*I-3,6*I],D3$[3,10];
1850    IF C<>-9999 THEN GOTO 1880
1860    PRINT "   NOT DETECTED"
1870    GOTO 1920
1880    IF L<>-9999 THEN GOTO 1910
1890    PRINT "  NOT CALCULATED"
1900    GOTO 1920
1910    PRINT USING "  ------#.###",L
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```



```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
1920   NEXT I2
1930   PRINT
1940 NEXT I
1950 REM  ------------------------------------------------------------
1960 REM          WRAP-UP PROCEDURE
1970 PRINT
1980 PRINT
1990 ON ERR THEN GOTO 2020
2000 PRINT "DO YOU WANT A CONFIRMATION REPORT FOR ANOTHER COMPOUND USI
*     NG"
2010 INPUT "     THE SAME METHODS AND FRACTIONS?  (Y OR N)  ",X$
2020 ON ERR THEN STOP
2030 IF X$[1,1]="Y" THEN GOTO 0940
2040 CLOSE
2050 NOESC
2060 CHAIN "GC00" THEN GOTO 0100
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

SYMBOL TABLE FOR GC19

SYMBOL	REFERENCES			
0100	2060			
0180	0614	0760		
0190	0180	0370	0450	0540
0220	0210			
0240	0210			
0260	0210			
0280	0210			
0290	0230	0250	0270	
0320	0300			
0380	0330			
0420	0380			
0460	0410			
0500	0480			
0550	0510			
0610	0910			
0620	0610	0780	0810	0880
0640	0630			
0660	0630			
0680	0630			
0700	0630			
0710	0650	0670	0690	
0740	0720			
0790	0750			
0820	0790			
0850	0830			
0890	0860			
0940	0186	0340	1020	2030
0990	0950			
1030	0980	1060		
1070	1040			
1120	1080			
1160	1110			
1170	1250			
1230	1180			
1260	1230			
1470	1430			
1520	1460			
1610	1570			
1640	1550			
1670	1600	1630		
1710	1640			
1720	1750			
1760	1730			
1770	1820			
1800	1780			

SYMBOL TABLE FOR GC19

SYMBOL	REFERENCES									
1830	1800									
1880	1850									
1910	1880									
1920	1870	1900								
1980	1220									
2020	1990									
2040	0080	1150	1510	1680						
B	1770									
C	1770	1790	1850							
D2$	0100	0730	0750	0790	0800	0820	0870			
D3$	0100	0820	0840	0900	1420	1440	1490	1540	1580	1610
	1650	1840								
FL#3	1440	1540	1720	1770						
FL#4	1090	1170								
G$	0100	1770	1800							
H$	0100	1770								
I	0140	0160	1070	1090	1130	1200	1270	1400	1410	1420
	1840	1940								
I2	1410	1420	1920							
J	1540	1550	1570							
J2	1540	1640								
L	1770	1880	1910							
P9	1710	1720	1740	1760	1770	1810				
S5	0170	0180	0210	0340	0560	0570	0600	0610	0630	0760
	0890	0900	1070	1400						
S5$	0100	0130	0570	1090	1130	1200	1840			
S6$	0100	0150	0900	1420						
S6[	0100	0600	0610	0630	0760	0890	0900	1410		
S7	1160	1170	1240							
T	0390	0410	0470							
T$	0100	0460	0470	0490	0530	0570	0710			
T1$	0100	0310	0330	0390	0440					
V$	0100	1170	1230							
V0$	0100	1720	1730							
V7$	0100	0960	1030	1050	1200	1230	1330	1800		
X$	0100	2010	2030							
Z5	1030	1040	1050							

SECTION 22

PROGRAM GC20 - SAMPLE FILE CONTROL INTERACTION

GC20 is the module of the GCAS which creates run results files for transmission to the Sample File Control (SFC) System. The format of the run results file is defined in the document "EPA Sample File Control Functional Design." The program is entered by chaining from the master control program, GC00, and it chains back to that program if the escape key is pressed. Also, if the escape key is pressed, the run results file being created is deleted.

As GC20 begins, it gives the user the choice of creating a new run results file, editing an existing run results file, or sending an existing run results file to the SFC computer. If the user chooses to edit a file, control is passed to the SFC foreground BASIC program RUNEDIT. Similarly, if the user wants to send a run results file to the SFC computer, control is passed to the program SEND.

If the user chooses to create a new run results file, GC20 asks for the information necessary to name the file and generate its header record.

Next, the program allows the user to report any laboratory control standards. The user must enter the injection ID and concentration pattern letter for each control standard, and the program copies the appropriate data from the injection data file and concentration pattern file into the run results file.

The user is then allowed to report the concentrations of samples to SFC, along with any combination of spikes, duplicates, and surrogate spikes. The user enters the injection ID for the sample, and the calculated concentrations are copied from the injection data file into the run results file. The prepared concentration of any surrogate spike is also placed in the run results file. For a spiked sample, the user enters the injection ID for the sample after spiking and the concentration pattern for the spike added values, and the program copies the appropriate data from the injection data file and concentration pattern file into the run results file. Again, the prepared concentration of any surrogate spike is also placed into the run results file. For a duplicate of a sample, the user enters the injection ID for the duplicate, and the program copies the necessary data from the injection ID file into the run results file. Once again, the prepared concentration of any surrogate spike is also placed into the run results file.

When the user has placed all of the data for a set of samples into the run results file, the program forces the user to use either RUNEDIT or SEND. When either of these programs is completed, control is returned to the GCAS master control program, GC00.

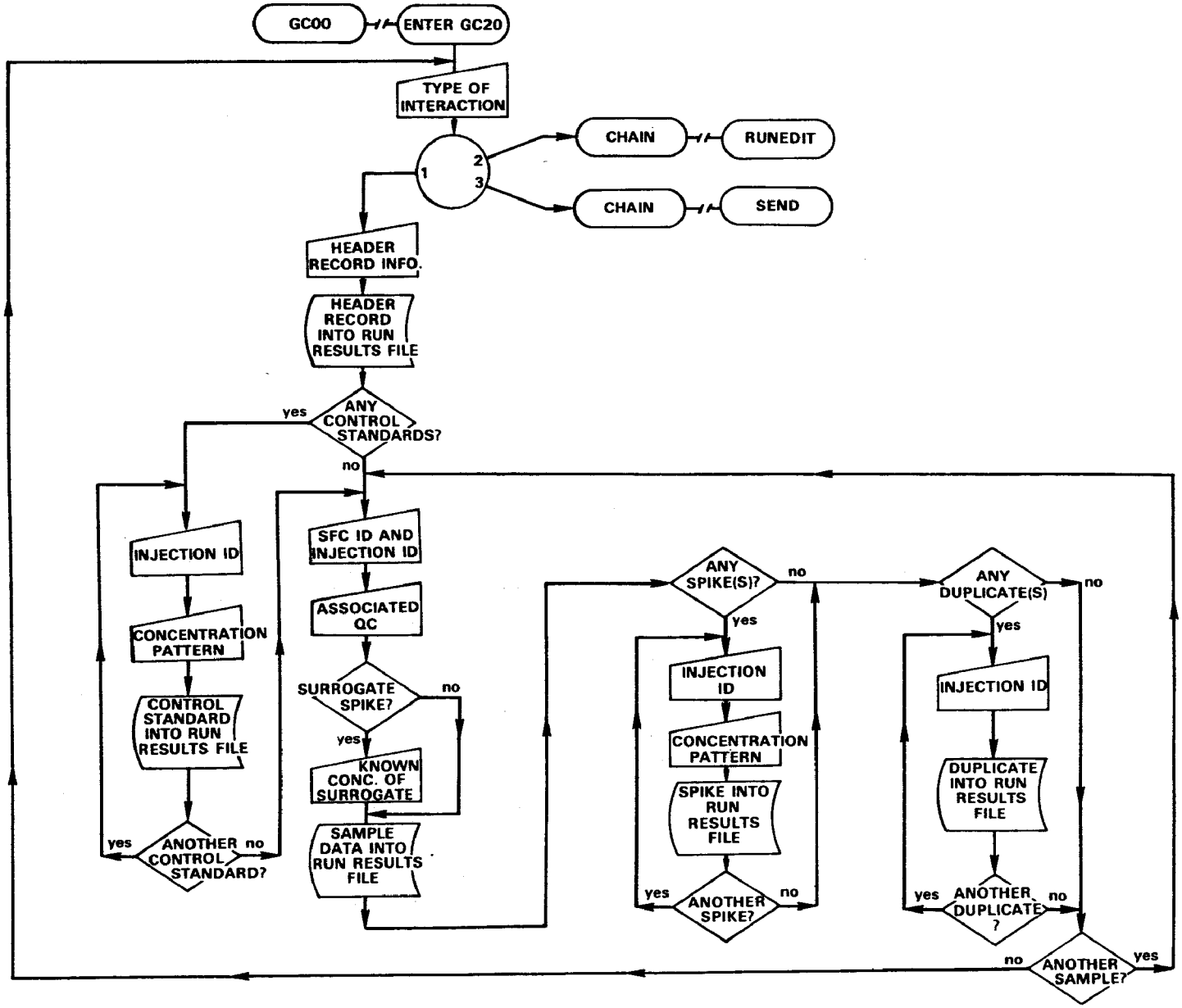

Figure 18. Flowchart of Program GC20.

TABLE 16. SYMBOL DEFINITIONS FOR PROGRAM GC20

A5	the concentration from a concentration pattern file
A6$	the name of a concentration pattern file
A7	the position of A8$ in A9$
A8$	the letter name of a concentration pattern
A9$	the alphabet
B	the absolute retention time
C	the peak area
D2$	an injection ID number
D3$	the name of an injection data file
E9	a flag which is used by subroutines to report to the main program that the current process should be terminated E9=0 continue normally E9=1 terminate process
F	the number of identifiers in the method file
G$	an identifier from an injection data file
H$	the peak type
I	the control variable for loops
I2	the control variable for loops
I8$	the measurement instrument ID
I9$	the initials of the analyst
J	the data file useability flag J=1 good data J=2 no TOTAL AREA J=3 wrong format

TABLE 16. (Continued)

J2	the data file processing flag J2=1 has been processed J2=2 never processed
L	the calculated concentration
N7$	the non-numeric result code
N8$	the QC type code
N9$	the QC type code for duplicates
P8	the record number of the last peak in the injection data file
P9	the record number of the first peak in the injection data file
Q5$	the format for PRINT USING statements
Q6$	the format for PRINT USING statements
R$	the name of the run results file
R1$	the parameter/method code
S9$	the identifier for the surrogate spike compound
T$	the name of the method file
T9$	the SFC sample ID number
V$	an identifier for the surrogate spike compound
VO$	a MESSAGE read from a data file
V1$	the full name of the first compound associated with an identifier
V2$	the CAS number for V1$
V3$	the full name of the second compound associated with an identifier
W3$	a CAS number with the hyphens removed
X	the user's answer to multiple choice questions
X$	the user's answer to most Y OR N questions

TABLE 16. (Continued)

X1$	the user's answer to a Y OR N question
X2$	the user's answer to a Y OR N question
X3$	the user's answer to a Y OR N question
X4	the prepared concentration of a surrogate spike
X4$	the user's answer to a Y OR N question
Z9	a counter for the number of spikes or duplicates of a sample

PROGRAM LISTING FOR GC20

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                    +
0030 REM   +   PROGRAM GC20, SAMPLE FILE CONTROL INTERACTION          +
0040 REM   +   BY:  J. KOPKE (SWORCC), MAY 25, 1979                   +
0050 REM   +   MOST RECENT REVISION:  MAY 29, 1979                    +
0060 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0070 REM
0080 DIM A6$[9],A8$[1],A9$[26],D2$[8],D3$[10],G$[8],H$[2],I8$[5],I9$[3
*    ],N7$[3]
0090 DIM N8$[3],N9$[3],Q5$[80],Q6$[80],R$[11],R1$[7],S9$[8],T$[6],T9$[
*    8],V$[8]
0100 DIM V0$[30],V1$[40],V2$[11],V3$[40],W3$[9],X$[1],X1$[1],X2$[1],X3
*    $[1],X4$[1]
0110 LET Q5$="2 ####### ### C ######## #.####^^^^ UG/L     ###
*                              *
0120 LET A9$="ABCDEFGHIJKLMNOPQRSTUVWXYZ"
0130 ON ESC THEN GOTO 0370
0140 ESC
0150 REM   ------------------------------------------------------------
0160 REM          CHECK VALIDITY OF THE METHOD FOR SFC PURPOSES
0170 READ FILE[4,1],T$
0180 CLOSE FILE[4]
0190 OPEN FILE[4],T$,200
0200 LET F=0
0210 READ FILE[4,3*(F+1)-1],V$,V1$,V2$,V3$
0220 IF EOF(4) THEN GOTO 0520
0230 IF V3$="99999" THEN GOTO 0280
0240 PRINT
0250 PRINT "<7><7>METHOD ";T$[3,6];" CANNOT BE USED FOR SFC PURPOSES B
*    ECAUSE "
0260 PRINT "     IT DEALS WITH CO-ELUTING COMPOUNDS."
0270 GOTO 0370
0280 IF LEN(V2$)<>0 THEN GOTO 0330
0290 PRINT
0300 PRINT "<7><7>METHOD ";T$[3,6];" CANNOT BE USED FOR SFC PURPOSES B
*    ECAUSE"
0310 PRINT "     IT IS MISSING AT LEAST ONE CAS NUMBER."
0320 GOTO 0370
0330 LET F=F+1
0340 GOTO 0210
0350 REM   ------------------------------------------------------------
0360 REM          ABNORMAL ENDING ROUTINE
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```


PROGRAM LISTING FOR GC20

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0370 ON ERR THEN GOTO 0390
0380 CLOSE FILE[0]
0390 ON ERR THEN GOTO 0410
0400 CLOSE FILE[3]
0410 ON ERR THEN GOTO 0430
0420 CLOSE FILE[7]
0430 ON ERR THEN GOTO 0470
0440 DELETE R$
0450 PRINT
0460 PRINT "<7><7>THE RUN RESULTS FILE HAS BEEN DELETED BECAUSE IT WAS
*     INCOMPLETE."
0470 ON ERR THEN STOP
0480 NOESC
0490 CHAIN "GC00"
0500 REM   ------------------------------------------------------------
0510 REM          INPUT TYPE OF INTERACTION
0520 PRINT
0530 PRINT "HERE ARE THE TYPES OF SAMPLE FILE CONTROL INTERACTION:"
0540 PRINT
0550 PRINT "     1.  CREATE A NEW RUN RESULTS FILE"
0560 PRINT "     2.  EDIT OR DELETE AN EXISTING RUN RESULTS FILE"
0570 PRINT "     3.  SEND AN EXISTING RUN RESULTS FILE TO THE SFC COMP
*    UTER"
0580 PRINT
0590 ON ERR THEN GOTO 0610
0600 INPUT "WHICH TYPE DO YOU WANT TO USE?  (1, 2, OR 3)  ",X
0610 ON ERR THEN STOP
0620 IF X=INT(X) THEN IF X>0 THEN IF X<4 THEN GOTO 0660
0630 PRINT
0640 PRINT "<7><7>";X;"IS NOT A VALID TYPE NUMBER."
0650 GOTO 0520
0660 ON X THEN GOTO 0960, 0690, 0830
0670 REM   ------------------------------------------------------------
0680 REM          EDIT A RUN RESULTS FILE
0690 PRINT
0700 PRINT "YOU ARE BEING TRANSFERRED TO THE SFC 'RUNEDIT' PROGRAM WHI
*    CH"
0710 PRINT "     WILL ALLOW YOU TO DELETE OR MODIFY YOUR RUN RESULTS F
*    ILE."
0720 PRINT "AFTER YOU HAVE COMPLETED 'RUNEDIT' YOU WILL BE TRANSFERRED
*     BACK"
0730 PRINT "     TO THIS SYSTEM."
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
 0740 PRINT "THEN, REMEMBER TO SEND THE RUN RESULTS FILE TO THE SFC COM
*     PUTER."
 0750 FOR I=1 TO 10
 0760   PRINT
 0770 NEXT I
 0780 NOESC
 0790 CLOSE
 0800 CHAIN "RUNEDIT"
 0810 REM  ------------------------------------------------------------
 0820 REM          SEND A RUN RESULTS FILE TO THE PDP-11
 0830 PRINT
 0840 PRINT "YOU ARE BEING TRANSFERRED TO THE SFC 'SEND' PROGRAM WHICH
*     WILL"
 0850 PRINT "     ALLOW YOU TO SEND YOUR RUN RESULTS FILE TO THE SFC CO
*     MPUTER."
 0860 PRINT "AFTER YOU HAVE FINISHED 'SEND' YOU WILL BE TRANSFERRED BAC
*     K TO"
 0870 PRINT "     THIS SYSTEM."
 0880 FOR I=1 TO 10
 0890   PRINT
 0900 NEXT I
 0910 NOESC
 0920 CLOSE
 0930 CHAIN "SEND"
 0940 REM  ------------------------------------------------------------
 0950 REM          OPEN RUN RESULTS FILE
 0960 PRINT
 0970 ON ERR THEN GOTO 0990
 0980 INPUT "WHAT IS THE PARAMETER/METHOD CODE FOR THE RUN?  ",R1$
 0990 ON ERR THEN STOP
 1000 LET I2=1
 1010 LET R$=R1$,A9$[I2,I2],".BJ"
 1020 ON ERR THEN GOTO 1040
 1030 RENAME R$,R$
 1040 ON ERR THEN STOP
 1050 IF SYS(7)<>-10 THEN GOTO 1120
 1060 LET R$=R1$,A9$[I2,I2],".RR"
 1070 ON ERR THEN GOTO 1090
 1080 RENAME R$,R$
 1090 ON ERR THEN STOP
 1100 IF SYS(7)<>-10 THEN GOTO 1120
 1110 GOTO 1190
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```



```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
 1120 LET I2=I2+1
 1130 IF I2<27 THEN GOTO 1010
 1140 PRINT
 1150 PRINT "<7><7>THERE ARE ALREADY 26 RUN RESULTS FILES FOR PARAMETER
*     /METHOD"
 1160 PRINT "     CODE ";R1$;"."
 1170 PRINT "REPORT THIS PROBLEM TO THE NOVA SYSTEM MANAGER."
 1180 GOTO 0370
 1190 OPEN FILE[0,1],R$
 1200 PRINT
 1210 ON ERR THEN GOTO 1230
 1220 INPUT "WHAT IS THE MEASUREMENT INSTRUMENT ID?  ",I8$
 1230 ON ERR THEN GOTO 1260
 1240 PRINT
 1250 INPUT "WHAT ARE THE INITIALS OF THE RESPONSIBLE ANALYST?  ",I9$
 1260 ON ERR THEN STOP
 1270 LET Q6$="1 ## ## ## ## ##### ###### ###
*                                          "
 1280 PRINT FILE[0],USING Q6$,SYS(3)-1900,SYS(2),SYS(1),SYS(11),SYS(12)
*     ,I8$,R$,I9$
 1290 REM  ------------------------------------------------------------
 1300 REM          PUT CONTROL STANDARDS INTO RUN RESULTS FILE
 1310 PRINT
 1320 ON ERR THEN GOTO 1340
 1330 INPUT "DO YOU WANT TO REPORT ANY CONTROL STANDARD(S) TO SFC?  (Y
*     OR N)  ",X$
 1340 ON ERR THEN STOP
 1350 IF X$[1,1]<>"Y" THEN GOTO 1780
 1360 PRINT
 1370 ON ERR THEN GOTO 1390
 1380 INPUT "WHAT IS THE INJECTION ID FOR THE CONTROL STANDARD?  ",D2$
 1390 ON ERR THEN STOP
 1400 GOSUB 3820
 1410 IF E9<>0 THEN GOTO 1710
 1420 PRINT
 1430 ON ERR THEN GOTO 1450
 1440 INPUT "WHAT IS THE CONCENTRATION PATTERN FOR THE CONTROL STANDARD
*     ?  ",A8$
 1450 ON ERR THEN STOP
 1460 GOSUB 4440
 1470 IF E9<>0 THEN GOTO 1710
 1480 FOR I=1 TO F
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

```
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
 1490   LET N7$="   "
 1500   READ FILE[4,3*I-1],V$,V1$,V2$
 1510   IF V$="99999" THEN GOTO 1680
 1520   READ FILE[7,I],A5
 1530   FOR I2=P9 TO P8 STEP 1
 1540     READ FILE[3,I2],G$,H$,B,C,L
 1550     IF G$=V$ THEN GOTO 1580
 1560   NEXT I2
 1570   LET C=-9999
 1580   IF C<>-9999 THEN GOTO 1620
 1590   LET L=0
 1600   LET N7$="BDL"
 1610   GOTO 1650
 1620   IF L<>-9999 THEN GOTO 1650
 1630   LET L=0
 1640   LET N7$="NAR"
 1650   LET W3$=V2$[1,6],V2$[8,9],V2$[11]
 1660   PRINT FILE[0],USING Q5$," ","LCM",W3$,L,N7$
 1670   PRINT FILE[0],USING Q5$," ","LCT",W3$,A5," "
 1680 NEXT I
 1690 CLOSE FILE[3]
 1700 CLOSE FILE[7]
 1710 PRINT
 1720 ON ERR THEN GOTO 1740
 1730 INPUT "DO YOU WANT TO REPORT ANOTHER CONTROL STANDARD TO SFC?  ",
*     X$
 1740 ON ERR THEN STOP
 1750 IF X$[1,1]="Y" THEN GOTO 1360
 1760 REM  ------------------------------------------------------------
 1770 REM          INPUT SURROGATE SPIKE IDENTIFIER
 1780 PRINT
 1790 ON ERR THEN GOTO 1810
 1800 INPUT "DO YOU WANT TO REPORT ANY SAMPLE(S) BACK TO SFC?  (Y OR N)
*      ",X$
 1810 ON ERR THEN STOP
 1820 IF X$[1,1]<>"Y" THEN GOTO 3730
 1830 PRINT
 1840 ON ERR THEN GOTO 1860
 1850 INPUT "HAVE YOU USED A SURROGATE SPIKE WITH ANY OF THE SAMPLES?
*     (Y OR N)  ",X1$
 1860 ON ERR THEN STOP
 1870 IF X1$[1,1]<>"Y" THEN GOTO 2010
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```



```
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
 1880 PRINT
 1890 ON ERR THEN GOTO 1910
 1900 INPUT "WHAT IS THE IDENTIFIER FOR THE SURROGATE SPIKE COMPOUND?
*     ",S9$
 1910 ON ERR THEN STOP
 1920 FOR I=1 TO F
 1930   READ FILE[4,3*I-1],V$
 1940   IF V$=S9$ THEN GOTO 2010
 1950 NEXT I
 1960 PRINT
 1970 PRINT "<7><7>THERE IS NO SUCH IDENTIFIER IN METHOD ";T$[3,6];"."
 1980 GOTO 1830
 1990 REM  ------------------------------------------------------------
 2000 REM          INPUT INFORMATION FOR SAMPLE
 2010 PRINT
 2020 ON ERR THEN GOTO 2040
 2030 INPUT "WHAT IS THE SFC SAMPLE ID FOR THE SAMPLE?  ",T9$
 2040 ON ERR THEN GOTO 2070
 2050 PRINT
 2060 INPUT "WHAT IS THE CORRESPONDING INJECTION ID NUMBER?  ",D2$
 2070 ON ERR THEN STOP
 2080 GOSUB 3820
 2090 IF E9<>0 THEN GOTO 3680
 2100 PRINT
 2110 ON ERR THEN GOTO 2130
 2120 INPUT "DO YOU WANT TO REPORT ANY SPIKE(S) FOR THIS SAMPLE?  (Y OR
*      N)  ",X2$
 2130 ON ERR THEN GOTO 2160
 2140 PRINT
 2150 INPUT "DO YOU WANT TO REPORT ANY DUPLICATE(S) FOR THIS SAMPLE?  (
*     Y OR N)  ",X3$
 2160 ON ERR THEN STOP
 2170 IF X1$[1,1]="Y" THEN GOTO 2200
 2180 LET X4$="N"
 2190 GOTO 2320
 2200 PRINT
 2210 PRINT "DID YOU ADD THE SURROGATE SPIKE ";S9$;
 2220 ON ERR THEN GOTO 2240
 2230 INPUT " TO THIS SAMPLE?  (Y OR N)  ",X4$
 2240 ON ERR THEN STOP
 2250 IF X4$[1,1]<>"Y" THEN GOTO 2320
 2260 PRINT
1234567891123456789212345678931234567894123456789512345678961234567897
         0         0         0         0         0         0         0
```

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
2270 ON ERR THEN GOTO 2290
2280 INPUT "WHAT IS THE PREPARED CONCENTRATION OF THE SURROGATE SPIKE?
*      ",X4
2290 ON ERR THEN STOP
2300 REM  ------------------------------------------------------------
2310 REM          PUT UNKNOWN INTO RUN RESULTS FILE
2320 IF X2$[1,1]="Y" THEN GOTO 2380
2330 IF X3$[1,1]="Y" THEN GOTO 2360
2340 LET N8$="   "
2350 GOTO 2420
2360 LET N8$="LD1"
2370 GOTO 2420
2380 IF X3$[1,1]="Y" THEN GOTO 2410
2390 LET N8$="LS0"
2400 GOTO 2420
2410 LET N8$="LDX"
2420 FOR I=1 TO F
2430   LET N7$="   "
2440   READ FILE[4,3*I-1],V$,V1$,V2$
2450   IF V$="99999" THEN GOTO 2650
2460   FOR I2=P9 TO P8 STEP 1
2470     READ FILE[3,I2],G$,H$,B,C,L
2480     IF G$=V$ THEN GOTO 2510
2490   NEXT I2
2500   LET C=-9999
2510   IF C<>-9999 THEN GOTO 2550
2520   LET L=0
2530   LET N7$="BDL"
2540   GOTO 2580
2550   IF L<>-9999 THEN GOTO 2580
2560   LET L=0
2570   LET N7$="NAR"
2580   LET W3$=V2$[1,6],V2$[8,9],V2$[11]
2590   IF X4$[1,1]<>"Y" THEN GOTO 2640
2600   IF V$<>S9$ THEN GOTO 2640
2610   PRINT FILE[0],USING Q5$,T9$,"LS1",W3$,L,N7$
2620   PRINT FILE[0],USING Q5$,T9$,"LS2",W3$,X4," "
2630   GOTO 2650
2640   PRINT FILE[0],USING Q5$,T9$,N8$,W3$,L,N7$
2650 NEXT I
2660 CLOSE FILE[3]
2670 REM  ------------------------------------------------------------
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```



```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
2680 REM          PUT SPIKE INTO RUN RESULTS FILE
2690 IF X2$[1,1]<>"Y" THEN GOTO 3200
2700 LET Z9=0
2710 PRINT
2720 ON ERR THEN GOTO 2740
2730 INPUT "WHAT IS THE INJECTION ID OF THE SAMPLE AFTER SPIKING?  ",D
*    2$
2740 ON ERR THEN STOP
2750 GOSUB 3820
2760 IF E9<>0 THEN GOTO 3120
2770 PRINT
2780 ON ERR THEN GOTO 2800
2790 INPUT "WHAT IS THE CONCENTRATION PATTERN FOR THE SPIKE ADDED VALU
*    ES?  ",A8$
2800 ON ERR THEN STOP
2810 GOSUB 4440
2820 IF E9<>0 THEN GOTO 3120
2830 FOR I=1 TO F
2840   LET N7$="   "
2850   READ FILE[4,3*I-1],V$,V1$,V2$
2860   IF V$="99999" THEN GOTO 3080
2870   READ FILE[7,I],A5
2880   FOR I2=P9 TO P8 STEP 1
2890     READ FILE[3,I2],G$,H$,B,C,L
2900     IF G$=V$ THEN GOTO 2930
2910   NEXT I2
2920   LET C=-9999
2930   IF C<>-9999 THEN GOTO 2970
2940   LET L=0
2950   LET N7$="BDL"
2960   GOTO 3000
2970   IF L<>-9999 THEN GOTO 3000
2980   LET L=0
2990   LET N7$="NAR"
3000   LET W3$=V2$[1,6],V2$[8,9],V2$[11]
3010   IF X4$[1,1]<>"Y" THEN GOTO 3060
3020   IF V$<>S9$ THEN GOTO 3060
3030   PRINT FILE[0],USING Q5$,T9$,"LS1",W3$,L,N7$
3040   PRINT FILE[0],USING Q5$,T9$,"LS2",W3$,X4+A5,"   "
3050   GOTO 3080
3060   PRINT FILE[0],USING Q5$,T9$,"LSF",W3$,L,N7$
3070   PRINT FILE[0],USING Q5$,T9$,"LSA",W3$,A5,"   "
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
 3080 NEXT I
 3090 CLOSE FILE[3]
 3100 CLOSE FILE[7]
 3110 LET Z9=Z9+1
 3120 IF Z9<1 THEN GOTO 2710
 3130 PRINT
 3140 ON ERR THEN GOTO 3160
 3150 INPUT "DO YOU WANT TO REPORT ANOTHER SPIKE OF THE SAME SAMPLE?  (
*     Y OR N)  ",X$
 3160 ON ERR THEN STOP
 3170 IF X$[1,1]="Y" THEN GOTO 2710
 3180 REM  ------------------------------------------------------------
 3190 REM          PUT DUPLICATE INTO RUN RESULTS FILE
 3200 IF X3$[1,1]<>"Y" THEN GOTO 3680
 3210 LET Z9=0
 3220 PRINT
 3230 ON ERR THEN GOTO 3250
 3240 INPUT "WHAT IS THE INJECTION ID FOR THE DUPLICATE OF THE SAMPLE?
*      ",D2$
 3250 ON ERR THEN STOP
 3260 GOSUB 3820
 3270 IF E9<>0 THEN GOTO 3550
 3280 LET N9$="LD",STR$(Z9+2)
 3290 FOR I=1 TO F
 3300   LET N7$="   "
 3310   READ FILE[4,3*I-1],V$,V1$,V2$
 3320   IF V$="99999" THEN GOTO 3520
 3330   FOR I2=P9 TO P8 STEP 1
 3340     READ FILE[3,I2],G$,H$,B,C,L
 3350     IF G$=V$ THEN GOTO 3380
 3360   NEXT I2
 3370   LET C=-9999
 3380   IF C<>-9999 THEN GOTO 3420
 3390   LET L=0
 3400   LET N7$="BDL"
 3410   GOTO 3450
 3420   IF L<>-9999 THEN GOTO 3450
 3430   LET L=0
 3440   LET N7$="NAR"
 3450   LET W3$=V2$[1,6],V2$[8,9],V2$[11]
 3460   IF X4$[1,1]<>"Y" THEN GOTO 3510
 3470   IF V$<>S9$ THEN GOTO 3510
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```



```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
 3480   PRINT FILE[0],USING Q5$,T9$,"LS1",W3$,L,N7$
 3490   PRINT FILE[0],USING Q5$,T9$,"LS2",W3$,X4,"   "
 3500   GOTO 3520
 3510   PRINT FILE[0],USING Q5$,T9$,N9$,W3$,L,N7$
 3520 NEXT I
 3530 CLOSE FILE[3]
 3540 LET Z9=Z9+1
 3550 IF Z9<1 THEN GOTO 3220
 3560 IF Z9<8 THEN GOTO 3610
 3570 PRINT
 3580 PRINT "YOU HAVE REPORTED EIGHT DUPLICATES FOR THIS SAMPLE, WHICH
*     IS"
 3590 PRINT "     THE MAXIMUM ALLOWED BY SFC."
 3600 GOTO 3680
 3610 PRINT
 3620 ON ERR THEN GOTO 3640
 3630 INPUT "DO YOU WANT TO REPORT ANOTHER DUPLICATE OF THE SAME SAMPLE
*     ?  (Y OR N)  ",X$
 3640 ON ERR THEN STOP
 3650 IF X$[1,1]="Y" THEN GOTO 3220
 3660 REM  ------------------------------------------------------------
 3670 REM          WRAP-UP PROCEDURE
 3680 PRINT
 3690 ON ERR THEN GOTO 3710
 3700 INPUT "DO YOU WANT TO REPORT ANOTHER SAMPLE TO SFC?  (Y OR N)  ",
*     X$
 3710 ON ERR THEN STOP
 3720 IF X$[1,1]="Y" THEN GOTO 2010
 3730 CLOSE FILE[0]
 3740 PRINT
 3750 PRINT "THE NAME OF THE RUN RESULTS FILE IS '";R$[1,LEN(R$)-3];"'.
*     "
 3760 LET R$=""
 3770 PRINT
 3780 PRINT "YOU MUST NOW EITHER DELETE THIS FILE OR SEND IT TO THE SFC
*      COMPUTER."
 3790 GOTO 0520
 3800 REM  ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 3810 REM          SUBROUTINE TO OPEN DATA FILE
 3820 IF LEN(D2$)=8 THEN GOTO 3870
 3830 PRINT
 3840 PRINT "<7><7>";D2$;" IS NOT A VALID INJECTION ID."
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
3850 LET E9=1
3860 RETURN
3870 LET D3$="GC",D2$
3880 ON ERR THEN GOTO 3900
3890 RENAME D3$,D3$
3900 ON ERR THEN STOP
3910 IF SYS(7)=-9 THEN GOTO 3960
3920 PRINT
3930 PRINT "<7><7>THERE IS NO EXISTING DATA FOR INJECTION ID ";D2$;"."
3940 LET E9=1
3950 RETURN
3960 ON ERR THEN GOTO 4000
3970 OPEN FILE[3,0],D3$,31
3980 ON ERR THEN STOP
3990 GOTO 4050
4000 ON ERR THEN STOP
4010 DELAY =1
4020 GOTO 3960
4030 REM  ------------------------------------------------------------
4040 REM          CHECK DATA FILE USABILITY AND PROCESSING FLAGS
4050 READ FILE[3,1],J,D3$,J2
4060 IF J=1 THEN GOTO 4190
4070 PRINT
4080 IF J<>2 THEN GOTO 4140
4090 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT DID NOT"
4100 PRINT "     HAVE A TOTAL AREA."
4110 CLOSE FILE[3]
4120 LET E9=1
4130 RETURN
4140 PRINT "<7><7>";D2$;" CANNOT BE USED BECAUSE THE REPORT WAS"
4150 PRINT "     IN THE WRONG FORMAT."
4160 CLOSE FILE[3]
4170 LET E9=1
4180 RETURN
4190 IF J2=1 THEN GOTO 4280
4200 PRINT
4210 PRINT "<7><7>";D2$;" CANNOT BE USED FOR SFC PURPOSES UNTIL"
4220 PRINT "     AFTER IT IS PROCESSED."
4230 CLOSE FILE[3]
4240 LET E9=1
4250 RETURN
4260 REM  ------------------------------------------------------------
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```



```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
4270 REM          FIND FIRST AND LAST ENTRIES IN DATA FILE
4280 LET P9=2
4290 READ FILE[3,P9],V0$
4300 IF V0$[1,7]<>"MESSAGE" THEN GOTO 4330
4310 LET P9=P9+1
4320 GOTO 4290
4330 LET P9=P9+2
4340 LET P8=P9
4350 READ FILE[3,P8],G$
4360 IF EOF(3) THEN GOTO 4390
4370 LET P8=P8+1
4380 GOTO 4350
4390 LET P8=P8-1
4400 LET E9=0
4410 RETURN
4420 REM  ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
4430 REM          SUBROUTINE TO OPEN CONCENTRATION PATTERN FILE
4440 LET A7=POS(A9$,A8$,1)
4450 IF A7<>0 THEN GOTO 4500
4460 PRINT
4470 PRINT "<7><7>'";A8$;"' IS NOT A VALID LETTER."
4480 LET E9=1
4490 RETURN
4500 LET A6$=T$,"000"
4510 LET A6$[10-LEN(STR$(A7)),9]=STR$(A7)
4520 ON ERR THEN GOTO 4540
4530 RENAME A6$,A6$
4540 ON ERR THEN STOP
4550 IF SYS(7)=-9 THEN GOTO 4610
4560 PRINT
4570 PRINT "<7><7>THERE IS NO EXISTING CONCENTRATION PATTERN NAMED '";
*     A8$;"'."
4580 CLOSE FILE[3]
4590 LET E9=1
4600 RETURN
4610 ON ERR THEN GOTO 4660
4620 OPEN FILE[7,0],A6$,4
4630 ON ERR THEN STOP
4640 LET E9=0
4650 RETURN
4660 ON ERR THEN STOP
4670 DELAY =1
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

PROGRAM LISTING FOR GC20

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
4680 GOTO 4610
```

12345678911234567892123456789312345678941234567895123456789612345678 97
0 0 0 0 0 0 0

SYMBOL TABLE FOR GC20

SYMBOL	REFERENCES			
0210	0340			
0280	0230			
0330	0280			
0370	0130	0270	0320	1180
0390	0370			
0410	0390			
0430	0410			
0470	0430			
0520	0220	0650	3790	
0610	0590			
0660	0620			
0690	0660			
0830	0660			
0960	0660			
0990	0970			
1010	1130			
1040	1020			
1090	1070			
1120	1050	1100		
1190	1110			
1230	1210			
1260	1230			
1340	1320			
1360	1750			
1390	1370			
1450	1430			
1580	1550			
1620	1580			
1650	1610	1620		
1680	1510			
1710	1410	1470		
1740	1720			
1780	1350			
1810	1790			
1830	1980			
1860	1840			
1910	1890			
2010	1870	1940	3720	
2040	2020			
2070	2040			
2130	2110			
2160	2130			
2200	2170			
2240	2220			
2290	2270			

SYMBOL TABLE FOR GC20

SYMBOL	REFERENCES			
2320	2190	2250		
2360	2330			
2380	2320			
2410	2380			
2420	2350	2370	2400	
2510	2480			
2550	2510			
2580	2540	2550		
2640	2590	2600		
2650	2450	2630		
2710	3120	3170		
2740	2720			
2800	2780			
2930	2900			
2970	2930			
3000	2960	2970		
3060	3010	3020		
3080	2860	3050		
3120	2760	2820		
3160	3140			
3200	2690			
3220	3550	3650		
3250	3230			
3380	3350			
3420	3380			
3450	3410	3420		
3510	3460	3470		
3520	3320	3500		
3550	3270			
3610	3560			
3640	3620			
3680	2090	3200	3600	
3710	3690			
3730	1820			
3820	1400	2080	2750	3260
3870	3820			
3900	3880			
3960	3910	4020		
4000	3960			
4050	3990			
4140	4080			
4190	4060			
4280	4190			
4290	4320			
4330	4300			

SYMROL TABLE FOR GC20

SYMBOL	REFERENCES									
4350	4380									
4390	4360									
4440	1460	2810								
4500	4450									
4540	4520									
4610	4550	4680								
4660	4610									
A5	1520	1670	2870	3040	3070					
A6$	0080	4500	4510	4530	4620					
A7	4440	4450	4510							
A8$	0080	1440	2790	4440	4470	4570				
A9$	0080	0120	1010	1060	4440					
B	1540	2470	2890	3340						
C	1540	1570	1580	2470	2500	2510	2890	2920	2930	3340
	3370	3380								
D2$	0080	1380	2060	2730	3240	3820	3840	3870	3930	4090
	4140	4210								
D3$	0080	3870	3890	3970	4050					
E9	1410	1470	2090	2760	2820	3270	3850	3940	4120	4170
	4240	4400	4480	4590	4640					
F	0200	0210	0330	1480	1920	2420	2830	3290		
FL#0	0380	1190	1280	1660	1670	2610	2620	2640	3030	3040
	3060	3070	3480	3490	3510	3730				
FL#3	0400	1540	1690	2470	2660	2890	3090	3340	3530	3970
	4050	4110	4160	4230	4290	4350	4580			
FL#4	0170	0180	0190	0210	1500	1930	2440	2850	3310	
FL#7	0420	1520	1700	2870	3100	4620	.			
G$	0080	1540	1550	2470	2480	2890	2900	3340	3350	4350
H$	0080	1540	2470	2890	3340					
I	0750	0770	0880	0900	1480	1500	1520	1680	1920	1930
	1950	2420	2440	2650	2830	2850	2870	3080	3290	3310
	3520									
I2	1000	1010	1060	1120	1130	1530	1540	1560	2460	2470
	2490	2880	2890	2910	3330	3340	3360			
I8$	0080	1220	1280							
I9$	0080	1250	1280							
J	4050	4060	4080							
J2	4050	4190								
L	1540	1590	1620	1630	1660	2470	2520	2550	2560	2610
	2640	2890	2940	2970	2980	3030	3060	3340	3390	3420
	3430	3480	3510							
N7$	0080	1490	1600	1640	1660	2430	2530	2570	2610	2640
	2840	2950	2990	3030	3060	3300	3400	3440	3480	3510
N8$	0090	2340	2360	2390	2410	2640				
N9$	0090	3280	3510							

SYMBOL TABLE FOR GC20

SYMBOL	REFERENCES									
P8	1530	2460	2880	3330	4340	4350	4370	4390		
P9	1530	2460	2880	3330	4280	4290	4310	4330	4340	
Q5$	0090	0110	1660	1670	2610	2620	2640	3030	3040	3060
	3070	3480	3490	3510						
Q6$	0090	1270	1280							
R$	0090	0440	1010	1030	1060	1080	1190	1280	3750	3760
R1$	0090	0980	1010	1060	1160					
S9$	0090	1900	1940	2210	2600	3020	3470			
T$	0090	0170	0190	0250	0300	1970	4500			
T9$	0090	2030	2610	2620	2640	3030	3040	3060	3070	3480
	3490	3510								
V$	0090	0210	1500	1510	1550	1930	1940	2440	2450	2480
	2600	2850	2860	2900	3020	3310	3320	3350	3470	
V0$	0100	4290	4300							
V1$	0100	0210	1500	2440	2850	3310				
V2$	0100	0210	0280	1500	1650	2440	2580	2850	3000	3310
	3450									
V3$	0100	0210	0230							
W3$	0100	1650	1660	1670	2580	2610	2620	2640	3000	3030
	3040	3060	3070	3450	3480	3490	3510			
X	0600	0620	0640	0660						
X$	0100	1330	1350	1730	1750	1800	1820	3150	3170	363C
	3650	3700	3720							
X1$	0100	1850	1870	2170						
X2$	0100	2120	2320	2690						
X3$	0100	2150	2330	2380	3200					
X4	2280	2620	3040	3490						
X4$	0100	2180	2230	2250	2590	3010	3460			
Z9	2700	3110	3120	3210	3280	3540	3550	3560		

SECTION 23

PROGRAM GC21 - MICROCOMPUTER INTERFACE

GC21 is the program to receive data from the microcomputer and compact it into an injection data file. The microcomputer copies a report as it is printed by the Varian. It then sends an escape character to the Nova and waits for the Nova to respond with "ACCOUNT ID." The microcomputer then sends the account ID to the Nova and waits for the Nova to respond with the asterisk prompt. The microcomputer then sends to the Nova the command RUN "GC21". When this program reaches the INPUT statement, it sends a question mark prompt to the microcomputer. The microcomputer then sends to the Nova one line of the Varian report followed by a carriage return, and the program places the line into the arrival file. This continues until the entire report has been transmitted. Then, instead of sending a line of a report, the microcomputer sends an escape character to the Nova. GC21 then generates the name of the data file, enters that name into the ID list file, and compacts the report into the data file. When GC21 terminates, the word STOP is sent by the Nova to the microcomputer, which then sends a BYE command back to the Nova, ending the session. Details for the functions of the microcomputer can be found in the EPA document "Intercomputer Communications Using Microprocessors."

All of the above would be a simple process, except for the fact that Varian reports can vary considerably. GC21 must be prepared to handle any possibility, since the microcomputer is unable to react to Nova error messages. Consequently, GC21 contains a variety of complicated procedures which may never be used. For example, before GC21 opens any file, it always sets the ON ERR THEN GOTO condition in case the file is in use or is being dumped to tape for some reason. If an error does occur in opening a file, GC21 waits one second and tries again.

GC21 is divided into three main sections: 1) a procedure to input the report from the microcomputer and store it in an arrival file, 2) a procedure to compact the report from the arrival file into an injection data file and store that name in the ID list file, and 3) a subroutine to name an injection data file.

FROM MICROCOMPUTER TO ARRIVAL FILE

The first procedure is to input the report from the microcomputer and store it in the arrival file. GC20 simply inputs a line of the report as a string variable. An ON ERR THEN GOTO condition is established for this INPUT statement in case an analyst uses a comma in the Varian report title.

If the line which is input has a length of zero, GC21 immediately returns to the INPUT statement.

Beginning with the second line of the Varian report, GC21 checks each line to see if it begins with the letters GC. Every Varian report should begin with the letters GC and end with the words TOTAL AREA. However, if for some reason a report does not end with TOTAL AREA, the microcomputer will not recognize the end of the report, and it will continue to transmit a second report as if it were a part of the first. For this reason, GC21 checks every line for the letters GC. If the line does not begin with GC, it is written into the arrival file, and the program branches back to the INPUT statement. However, if a line does begin with GC, the program branches to the subroutine to generate the name of the injection data file, and then places into that data file a flag (a "2") to indicate that the report is not useable. GC21 then reopens the arrival file and begins to copy the second report into it.

When an escape character is received instead of a line of a report, GC21 branches to the next routine.

FROM ARRIVAL FILE TO DATA FILE

When the arrival file is complete, GC21 branches to the subroutine to generate the name of the injection data file. Then the arrival file is scanned for the line.

PEAK NAME TYPE COMP RETN CORR AREA FACTOR.

If this line cannot be found, the Varian report is in the wrong format. In such a case, GC21 writes into the data file a flag (a "3") to indicate that the report is not useable, and then GC21 stops.

If the report is in the correct format, GC21 continues to scan the arrival file for the TOTAL AREA line, and records the total area. A flag (a "1") is written into the injection data file to indicate that the report is useable.

Next, GC21 begins to scan the arrival file a third time. It finds the method number and the report title, if any, and writes them into the injection data file.

Continuing its scan through the arrival file, GC21 locates the lines referring to individual peaks. It does this by attempting to convert the first six characters of each line to a number. Lines in which this cannot be done are error messages, second page headings, or total concentrations which should be ignored.

The peak identifier and peak type are recorded from each line of data. The retention time is converted to a number and recorded. The percent area is converted to a number, multiplied by the total area, and divided by 100

to find the actual area of the peak. These four items are then written into the injection data file.

When the entire arrival file has been scanned for the third time, GC21 stops.

SUBROUTINE TO NAME AN INJECTION DATA FILE

Generating the name of an injection data file really involves generating the injection ID number. To do this, the subroutine first scans the arrival file for the instrument number, which it uses to create the name of the appropriate ID list file. It then attempts to RENAME the ID list file with the same name. This always produces an error which is trapped by an ON ERR THEN GOTO statement. If the error number is -10, the ID list file already exists and can be used. If the error number is -9, the ID list file has not been created for the instrument. In this second case, the subroutine creates an ID list file and fills it with 100 dummy entries.

The subroutine then determines the date for the injection ID number. If the analyst has specified a date in the operator identification field of the Varian report, that date is used. (This feature allows the operator of an auto-injector to keep the date from changing at midnight.) Otherwise, the date from the Nova system clock is used.

Next, the subroutine assigns the sequence number for the injection. To do this, it must use the date and sequence number of the previous injection, which it finds in the first injection ID number in the ID list file. If the date of the current injection is the same as the date of the previous injection, the sequence number assigned is 1 greater than the previous sequence number. If the dates are different, the sequence number is reset to 01.

Finally the subroutine deletes the oldest data file in the ID list file. The ON ERR THEN GOTO condition is again set for this DELETE statement because the oldest ID number in the file may be a dummy entry. All of the other ID numbers (data files names) are shifted down one position in the ID list file, and the newest ID is placed at the top of the list. Control is then returned to the invoking procedure.

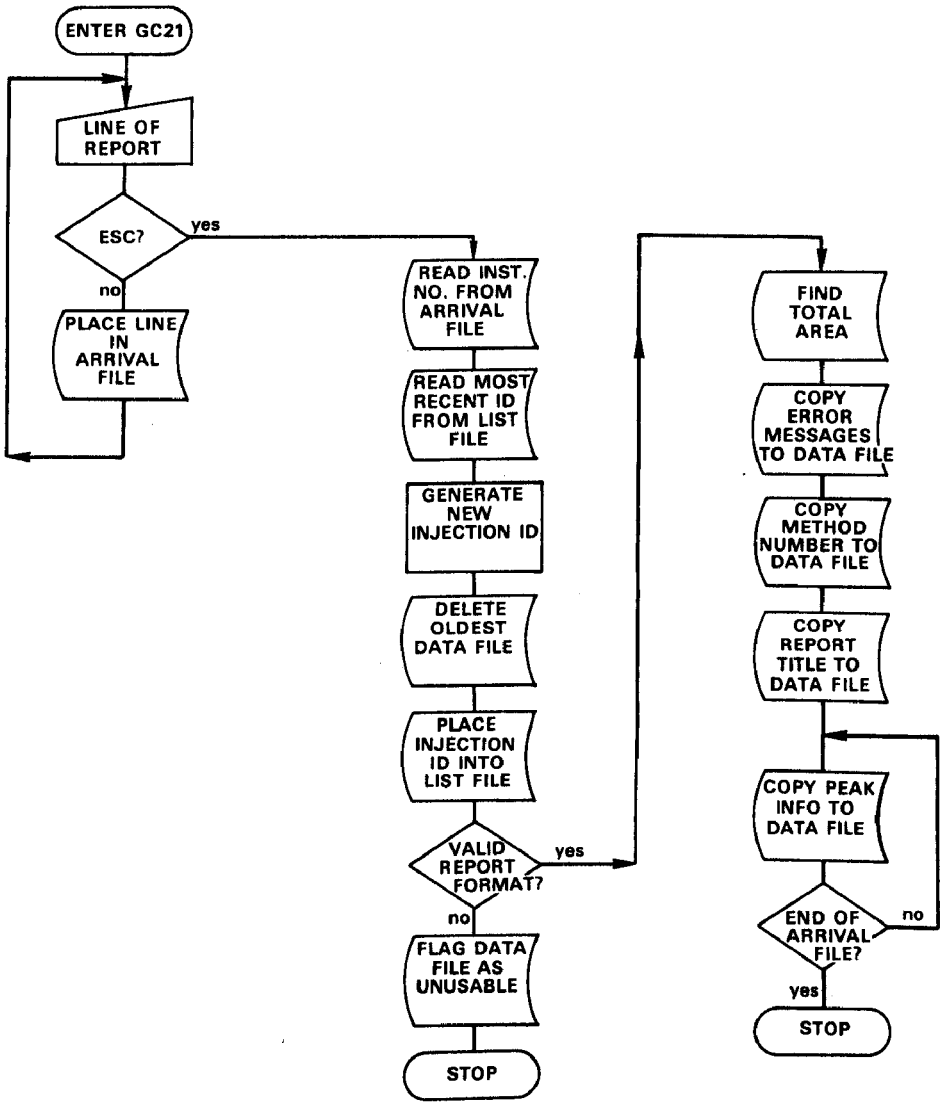

Figure 19. Flowchart of Program GC21.

TABLE 17. SYMBOL DEFINITIONS FOR PROGRAM GC21

A	the total area of all peaks in the report
A$	a line of the report
A2$	a holding variable for the value of A$
B	the retention time of a compound
B$	the instrument number
C	the area of a single peak
C$	the name of the ID list file
D$	the name of the data file created
D2$	the name of a previously created data file
E$	the method number
F$	the report title (or the word NONE)
G$	the identifier of a compound
H$	the peak type
I	the control variable for several loops
T1	the record number of the last record used in the data file
W	the number of lines that have been input
Y	the sequence number

PROGRAM LISTING FOR GC21

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   GAS CHROMATOGRAPHY AUTOMATION SYSTEM                    +
0030 REM   +   PROGRAM GC21, MICROCOMPUTER INTERFACE                  +
0040 REM   +   BY:  J. KOPKE (SWORCC), JANUARY 18, 1979               +
0045 REM   +   MOST RECENT REVISION:  MAY 1, 1979                     +
0050 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0060 REM
0070 ESC
0080 DIM A$[72],A2$[72],B$[2],C$[8],D$[10],E$[10],F$[30],G$[8],H$[2]
0090 REM   ---------------------------------------------------------
0100 REM          INPUT LINES FROM MICRO; STORE IN ARRIVAL FILE
0110 ON ERR THEN GOTO 0150
0120 OPEN FILE[1,1],"GC00000000"
0130 ON ERR THEN STOP
0140 GOTO 0180
0150 ON ERR THEN STOP
0160 DELAY =1
0170 GOTO 0110
0180 LET W=0
0190 ON ESC THEN GOTO 0520
0200 ON ERR THEN GOTO 0220
0210 INPUT "?",A$
0220 ON ERR THEN STOP
0230 ON ESC THEN STOP
0240 IF A$="" THEN GOTO 0190
0250 IF W=0 THEN GOTO 0480
0260 IF A$[1,6]◇"  GC  " THEN GOTO 0480
0270 REM   ---------------------------------
0280 REM     HANDLE FIRST OF TWO MERGED REPORTS
0285 LET A2$=A$
0290 CLOSE FILE[1]
0300 GOSUB 1620
0305 ON ERR THEN GOTO 0310
0308 DELETE D$
0310 ON ERR THEN GOTO 0350
0320 OPEN FILE[3,0],D$,31
0330 ON ERR THEN STOP
0340 GOTO 0380
0350 ON ERR THEN STOP
0360 DELAY =1
0370 GOTO 0310
0380 WRITE FILE[3,1],2,D$,0
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```


PROGRAM LISTING FOR GC21

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
0390 CLOSE FILE[3]
0400 ON ERR THEN GOTO 0440
0410 OPEN FILE[1,1],"GC00000000"
0420 ON ERR THEN STOP
0430 GOTO 0470
0440 ON ERR THEN STOP
0450 DELAY =1
0460 GOTO 0400
0470 LET W=0
0475 LET A$=A2$
0480 LET W=W+1
0490 PRINT FILE[1],A$
0500 GOTO 0190
0510 REM   ---------------------------------------------------------
0520 REM          COMPACT ARRIVAL FILE INTO DATA FILE
0530 ON ESC THEN STOP
0540 CLOSE FILE[1]
0550 GOSUB 1620
0560 REM   ---------------------------------
0570 REM     CHECK FOR VALID REPORT FORMAT
0580 ON ERR THEN GOTO 0620
0590 OPEN FILE[1,3],"GC00000000"
0600 ON ERR THEN STOP
0610 GOTO 0650
0620 ON ERR THEN STOP
0630 DELAY =1
0640 GOTO 0580
0650 LREAD FILE[1],A$
0660 IF EOF(1)◇1 THEN GOTO 0770
0665 ON ERR THEN GOTO 0670
0668 DELETE D$
0670 ON ERR THEN GOTO 0710
0680 OPEN FILE[3,0],D$,31
0690 ON-ERR THEN STOP
0700 GOTO 0740
0710 ON ERR THEN STOP
0720 DELAY =1
0730 GOTO 0670
0740 WRITE FILE[3,1],3,D$,0
0750 CLOSE FILE[3]
0755 CLOSE FILE[1]
0760 STOP
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```

```
12345678911234567892123456789312345678941234567895123456789612345678971
         0         0         0         0         0         0         0
0770 IF A$<>"  PEAK    NAME   TYPE       COMP     RETN    CORR       A
*    REA    FACTOR" THEN GOTO 0650
0780 REM   ------------------------------------
0790 REM     FIND TOTAL AREA OF ALL PEAKS
0800 LREAD FILE[1],A$
0810 IF A$[1,12]<>"  TOTAL AREA" THEN GOTO 0800
0820 LET A=VAL(A$[13,23])
0830 CLOSE FILE[1]
0835 ON ERR THEN GOTO 0840
0838 DELETE D$
0840 ON ERR THEN GOTO 0880
0850 OPEN FILE[3,0],D$,31
0860 ON ERR THEN STOP
0870 GOTO 0910
0880 ON ERR THEN STOP
0890 DELAY =1
0900 GOTO 0840
0910 WRITE FILE[3,1],1,D$,0
0920 LET T1=1
0930 REM   ------------------------------------
0940 REM     SCAN REPORT FOR ERROR MESSAGES
0950 ON ERR THEN GOTO 0990
0960 OPEN FILE[1,3],"GC00000000"
0970 ON ERR THEN STOP
0980 GOTO 1020
0990 ON ERR THEN STOP
1000 DELAY =1
1010 GOTO 0950
1020 LREAD FILE[1],A$
1030 IF EOF(1) THEN GOTO 1080
1040 IF A$[1,7]<>"MESSAGE" THEN GOTO 1020
1050 WRITE FILE[3,T1+1],A$
1060 LET T1=T1+1
1070 GOTO 1020
1080 CLOSE FILE[1]
1090 REM   ------------------------------------
1100 REM     FIND VARIAN METHOD NUMBER
1110 ON ERR THEN GOTO 1150
1120 OPEN FILE[1,3],"GC00000000"
1130 ON ERR THEN STOP
1140 GOTO 1180
1150 ON ERR THEN STOP
12345678911234567892123456789312345678941234567895123456789612345678971
         0         0         0         0         0         0         0
```



```
12345678911234567892123456789312345678941234567895123456789612345678971
         0         0         0         0         0         0         0
1160 DELAY =1
1170 GOTO 1110
1180 LREAD FILE[1],A$
1190 IF A$[1,6]<>"  INST" THEN GOTO 1180
1200 IF LEN(A$)<=39 THEN LET E$=A$[31,LEN(A$)]
1205 IF LEN(A$)>39 THEN LET E$=A$[31,39]
1210 WRITE FILE[3,T1+1],E$
1220 LET T1=T1+1
1230 REM   ------------------------------------
1240 REM     FIND REPORT TITLE, IF ANY
1250 LREAD FILE[1],A$
1260 IF A$[1,7]="MESSAGE" THEN GOTO 1250
1270 IF A$[1,6]="  PEAK" THEN GOTO 1300
1280 LET F$=A$[17,LEN(A$)]
1285 IF F$="                                  " THEN GOTO 1300
1290 GOTO 1310
1300 LET F$="NONE"
1310 IF F$[LEN(F$)]<>" " THEN GOTO 1319
1311 LET F$=F$[1,LEN(F$)-1]
1312 GOTO 1310
1319 WRITE FILE[3,T1+1],F$
1320 LET T1=T1+1
1330 REM   ------------------------------------
1340 REM     IGNORE LINES NOT DESCRIBING PEAKS
1350 ON ERR THEN STOP
1360 LREAD FILE[1],A$
1370 IF EOF(1)<>1 THEN GOTO 1410
1380 CLOSE FILE[1]
1390 CLOSE FILE[3]
1400 STOP
1410 ON ERR THEN GOTO 1350
1420 LET D=VAL(A$[1,6])
1430 ON ERR THEN STOP
1500 REM   ------------------------------------
1510 REM     COPY IDENTIFIER, TYPE, RETENTION TIME, AND AREA
1520 LET G$=A$[9,16]
1521 IF G$[LEN(G$)]<>" " THEN GOTO 1530
1522 LET G$=G$[1,LEN(G$)-1]
1523 GOTO 1521
1530 IF G$="  UNEXP" THEN LET G$="XXXXXXXX"
1535 LET H$=A$[19,20]
1540 LET B=VAL(A$[34,41])
12345678911234567892123456789312345678941234567895123456789612345678971
         0         0         0         0         0         0         0
```

PROGRAM LISTING FOR GC21

```
123456789112345678921234567893123456789412345678951234567896123456789 7
         0         0         0         0         0         0         0
1550 LET C=A*VAL(A$[51,62])/100
1560 WRITE FILE[3,T1+1],G$,H$,B,C,0,0
1570 LET T1=T1+1
1580 GOTO 1350
1590 REM
1600 REM
1610 REM   ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
1620 REM          SUBROUTINE TO CREATE DATA FILE NAME AND
1630 REM               PUSH IT INTO THE LIST FILE GC0000**
1640 REM   ------------------------------------
1650 REM     FIND INSTRUMENT NUMBER
1660 ON ERR THEN GOTO 1700
1670 OPEN FILE[1,3],"GC00000000"
1680 ON ERR THEN STOP
1690 GOTO 1730
1700 ON ERR THEN STOP
1710 DELAY =1
1720 GOTO 1660
1730 LREAD FILE[1],A$
1740 IF EOF(1)<>1 THEN GOTO 1750
1741 LET A$="  INST    99"
1750 IF A$[1,6]<>"  INST" THEN GOTO 1730
1760 CLOSE FILE[1]
1770 LET B$=A$[11,12]
1780 REM   ------------------------------------
1790 REM     OPEN ID LIST FILE; FILL IT WITH
1800 REM          DUMMY ID'S IF IT IS NEW
1810 IF B$[1,1]=" " THEN LET B$[1,1]="0"
1820 LET C$="GC0000",B$
1830 ON ERR THEN GOTO 1850
1840 RENAME C$,C$
1850 ON ERR THEN STOP
1860 IF SYS(7)<>-48 THEN GOTO 1890
1870 DELAY =1
1880 GOTO 1830
1890 IF SYS(7)<>-9 THEN GOTO 1990
1900 ON ERR THEN GOTO 1940
1910 OPEN FILE[2,0],C$,11
1920 ON ERR THEN STOP
1930 GOTO 1970
1940 ON ERR THEN STOP
1950 DELAY =1
```

123456789112345678921234567893123456789412345678951234567896123456789 7
0 0 0 0 0 0 0

PROGRAM LISTING FOR GC21

```
123456789112345678921234567893123456789412345678951234567896123456789 7
         0         0         0         0         0         0         0
1960 GOTO 1900
1970 GOTO 2105
1980 ON ERR THEN GOTO 2020
1990 OPEN FILE[2,0],C$,11
2000 ON ERR THEN STOP
2010 GOTO 2050
2020 ON ERR THEN STOP
2030 DELAY =1
2040 GOTO 1980
2050 FOR I=1 TO 100
2060   WRITE FILE[2,I],"GC99999999"
2070 NEXT I
2090 REM   ------------------------------------
2100 REM     DETERMINE DATE OF INJECTION
2105 IF A$[48,51]<>"DATE" THEN GOTO 2130
2110 LET D$="GC",B$[1,2],A$[52,55]
2120 GOTO 2180
2130 LET D$="GC",B$[1,2],"0000"
2140 LET D$[7-LEN(STR$(SYS(2))),6]=STR$(SYS(2))
2150 LET D$[9-LEN(STR$(SYS(1))),8]=STR$(SYS(1))
2160 REM   ------------------------------------
2170 REM     DETERMINE SEQUENCE NUMBER
2180 READ FILE[2,1],D2$
2190 IF D$[1,8]=D2$[1,8] THEN GOTO 2220
2200 LET D$[9,10]="01"
2210 GOTO 2270
2220 LET Y=VAL(D2$[9,10])+1
2225 IF Y=100 THEN LET Y=0
2230 LET D$[9,10]="00"
2240 LET D$[11-LEN(STR$(Y)),10]=STR$(Y)
2250 REM   ------------------------------------
2260 REM     DELETE OLDEST DATA FILE
2270 READ FILE[2,100],D2$
2280 ON ERR THEN GOTO 2300
2290 DELETE D2$
2300 ON ERR THEN STOP
2310 REM   ------------------------------------
2320 REM     PUSH DATA FILE NAME INTO LIST FILE
2330 FOR I=99 TO 1 STEP -1
2340   READ FILE[2,I],D2$
2350   WRITE FILE[2,I+1],D2$
2360 NEXT I
```

123456789112345678921234567893123456789412345678951234567896123456789 7
0 0 0 0 0 0 0

PROGRAM LISTING FOR GC21

```
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
2370 WRITE FILE[2,1],D$
2380 CLOSE FILE[2]
2390 RETURN
12345678911234567892123456789312345678941234567895123456789612345678 97
         0         0         0         0         0         0         0
```


SYMBOL TABLE FOR GC21

SYMBOL	REFERENCES		
0110	0170		
0150	0110		
0180	0140		
0190	0240	0500	
0220	0200		
0310	0305	0370	
0350	0310		
0380	0340		
0400	0460		
0440	0400		
0470	0430		
0480	0250	0260	
0520	0190		
0580	0640		
0620	0580		
0650	0610	0770	
0670	0665	0730	
0710	0670		
0740	0700		
0770	0660		
0800	0810		
0840	0835	0900	
0880	0840		
0910	0870		
0950	1010		
0990	0950		
1020	0980	1040	1070
1080	1030		
1110	1170		
1150	1110		
1180	1140	1190	
1250	1260		
1300	1270	1285	
1310	1290	1312	
1319	1310		
1350	1410	1580	
1410	1370		
1521	1523		
1530	1521		
1620	0300	0550	
1660	1720		
1700	1660		
1730	1690	1750	
1750	1740		
1830	1880		

SYMBOL TABLE FOR GC21

SYMBOL	REFERENCES									
1850	1830									
1890	1860									
1900	1960									
1940	1900									
1970	1930									
1980	2040									
1990	1890									
2020	1980									
2050	2010									
2105	1970									
2130	2105									
2180	2120									
2220	2190									
2270	2210									
2300	2280									
A	0820	1550								
A$	0080	0210	0240	0260	0285	0475	0490	0650	0770	0800
	0810	0820	1020	1040	1050	1180	1190	1200	1205	1250
	1260	1270	1280	1360	1420	1520	1535	1540	1550	1730
	1741	1750	1770	2105	2110					
A2$	0080	0285	0475							
B	1540	1560								
B$	0080	1770	1810	1820	2110	2130				
C	1550	1560								
C$	0080	1820	1840	1910	1990					
D	1420									
D$	0080	0308	0320	0380	0668	0680	0740	0838	0850	0910
	2110	2130	2140	2150	2190	2200	2230	2240	2370	
D2$	2180	2190	2220	2270	2290	2340	2350			
E$	0080	1200	1205	1210						
F$	0080	1280	1285	1300	1310	1311	1319			
FL#1	0120	0290	0410	0490	0540	0590	0650	0755	0800	0830
	0960	1020	1080	1120	1180	1250	1360	1380	1670	1730
	1760									
FL#2	1910	1990	2060	2180	2270	2340	2350	2370	2380	
FL#3	0320	0380	0390	0680	0740	0750	0850	0910	1050	1210
	1319	1390	1560							
G$	0080	1520	1521	1522	1530	1560				
H$	0080	1535	1560							
I	2050	2060	2070	2330	2340	2350	2360			
T1	0920	1050	1060	1210	1220	1319	1320	1560	1570	
W	0180	0250	0470	0480						
Y	2220	2225	2240							

SECTION 24

FILE STRUCTURES

The following tables detail the structure of the files used in the GCAS.

TABLE 18. STRUCTURE OF THE SAMPLE FILE CONTROL RUN RESULTS FILE

Name of file: PPPPPPPA.RR

where PPPPPPP = parameter/method code
A = a letter of the alphabet

File Number: 0

Contents

This is a sequential file consisting of eighty-byte strings. The format of the strings and their order are defined in the Sample File Control Foreground BASIC Functional Design.

TABLE 19. STRUCTURE OF THE ARRIVAL FILE

Name of file: GC00000000

File Number: 1

Contents

This is a sequential file. The report is placed in this file one line at a time as it is received from the microcomputer. Each line is a string of at most 70 characters.

TABLE 20. STRUCTURE OF THE ID LIST FILE

Name of file: GC0000II where II = instrument number

File Number: 2

Record Length: 11 bytes

Record	Contents
1	most recent D$
2	second most recent D$
3	third most recent D$
.	.
.	.
.	.
100	hundredth most recent D$

where D$ = the name of a data file

TABLE 21. STRUCTURE OF THE INJECTION DATA FILE

Name of file:	GCIIMMDDSS	where II = instrument number MM = month DD = day SS = sequence number
File Number:	3	
Record Length:	31 bytes	

Record	Contents	
1	J, D$, J2	where J = data file useability flag 1. good data 2. no TOTAL AREA 3. wrong format D$ = name of the data file J2 = status flag 1. has been processed 2. never processed
2	VO$	where VO$ = MESSAGE (if any)
n+2	E$	where E$ = method number
n+3	F$	report title
n+4	G$,H$,B,C,L,L2	where G$ = identifier H$ = peak type B = absolute retention time C = peak area L = calculated concentration L2 = calculated relative retention time
n+5	G$,H$,B,C,L,L2	
.	.	
.	.	
.	.	
		where n = number of error messages

TABLE 22. STRUCTURE OF THE METHOD FILE

Name of file: GCMMMM where MMMM = method number

File Number: 4

Record Length: 200 bytes

Record		Contents
1	T$,U$,N1,N2,N$	where T$ = name of method file U$ = name of user N1 = type of method 1. internal standards 2. purge and trap 3. liquid/liquid 4. direct aqueous N2 = type of retention time 1. relative 2. capacity ratio N$ = identifier for relative retention time reference compound, or capacity ratio dead volume time as a string
3i-1	V$,V1$,V2$,V3$,V4$,V5$,V6$	where V$ = identifier V1$ = first compound name V2$ = first CAS number V3$ = second compound name V4$ = second CAS number V5$ = third compound name V6$ = third CAS number
3i	D4$,I$,K,R1,R2,R3,J3	where D4$ = date of calibration I$ = superstring of injection IDs of standards K = type of fit 1. linear regression 2. quadratic regression 3. linear interpolation 4. linear regression forced through origin R1 = constant term of equation R2 = linear term of equation R3 = quadratic term of equation J3 = fitting error

TABLE 22. (Continued)

Record	Contents
3i+1	G(i,1),G(i,2),G(i,3),....,G(i,30) where G(i,odd) = concentration G(i,even) = area
3i-1	V$,V1$,V2$,V3$,V4$,V5$,V6$
3i	D4$,I$,K,R1,R2,R3,J3
3i+1	G(i,1),G(i,2),G(i,3),....,G(i,30)
.	.
.	.
.	.
.	.
.	.
.	.
.	.
.	.
.	.
.	.
	where i = counter for identifiers

TABLE 23. STRUCTURE OF THE TEMPORARY FORMATTED OUTPUT FILE

Name of file:	GCOMMMM	where MMMM = method number
File Number:	5	

Contents

This is a sequential file. The formatted output report is placed into this file line by line as it is generated. Each line is a string of at most 132 characters.

TABLE 24. STRUCTURE OF THE CONCENTRATION PATTERN FILE

Name of file: GGMMMMOSS where MMMM = method number
SS = sequence number matching a letter of the alphabet

File Number: 7

Record Length: 4 bytes

Record	Contents
1	A5 for first identifier
2	A5 for second identifier
3	A5 for third identifier
.	.
.	.
.	.
.	.

where A5 = the known concentration

TECHNICAL REPORT DATA
(Please read Instructions on the reverse before completing)

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16. ABSTRACT

This documentation contains the program listings, program flowcharts, symbols definitions, symbol references and program descriptions of all the Basic language programs which implement the functional specifications for an advanced chromatography automation system (EPA report EPA 60014-79-038). The programs are written in Data General Extended Basic Revision 4.3.

17. KEY WORDS AND DOCUMENT ANALYSIS

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