IDENTIFICATION

Product Code:	DEC-12-SQ2A-DN1
Product Name:	MASH - Phase II Supplement to MASH User's Manual
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PREFACE

It is suggested that the reader refer to the MASH User's Manual: Version I [DEC-12-SQ2A-D] for which this document is essentially a supplement. This document supersedes DEC-12-SQ2A-DN.

When MASH Phase III is developed, a new MASH User's Manual will be published which will include all previously published MASH documents.

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CONTENTS

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1.0 INTRODUCTION

Phase II of the Mass Spectrometer Handler (MASH) greatly expands the data reporting facilities of Phase I, which was essentially a data acquisition system with minimum report capability. The expansion has been made in the following three major areas:

A. NEW REPORT GENERATOR FEATURES

1. Printed mass tables
2. Chaining facility for examining consecutive files
3. Normalizing to sum of intensities
4. Ordered printout of highest peaks
5. Ability to examine mass chromatographs [see below].
6. Ability to generate hard copy plotter output [see below].

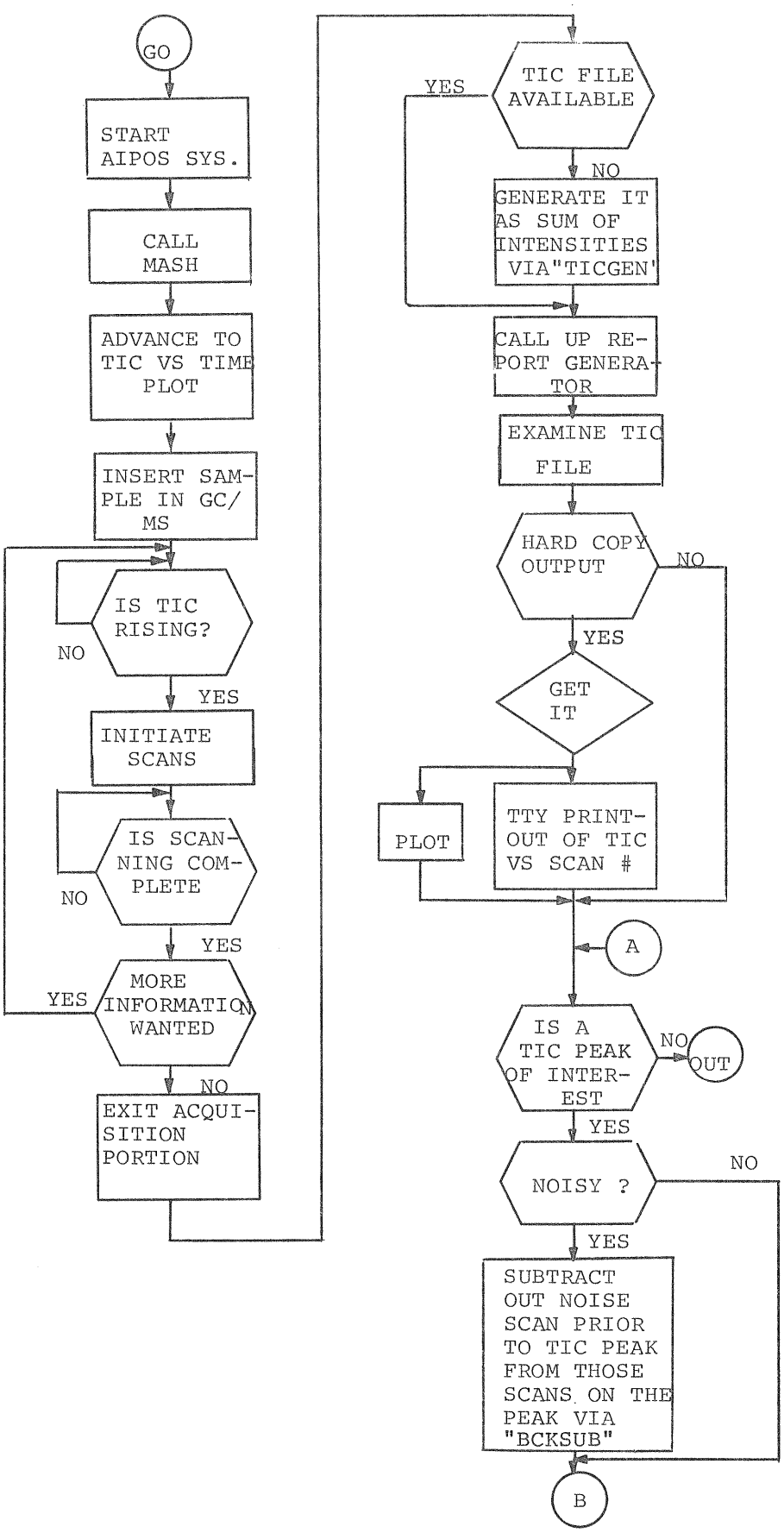
B. PLOTTER CAPABILITY

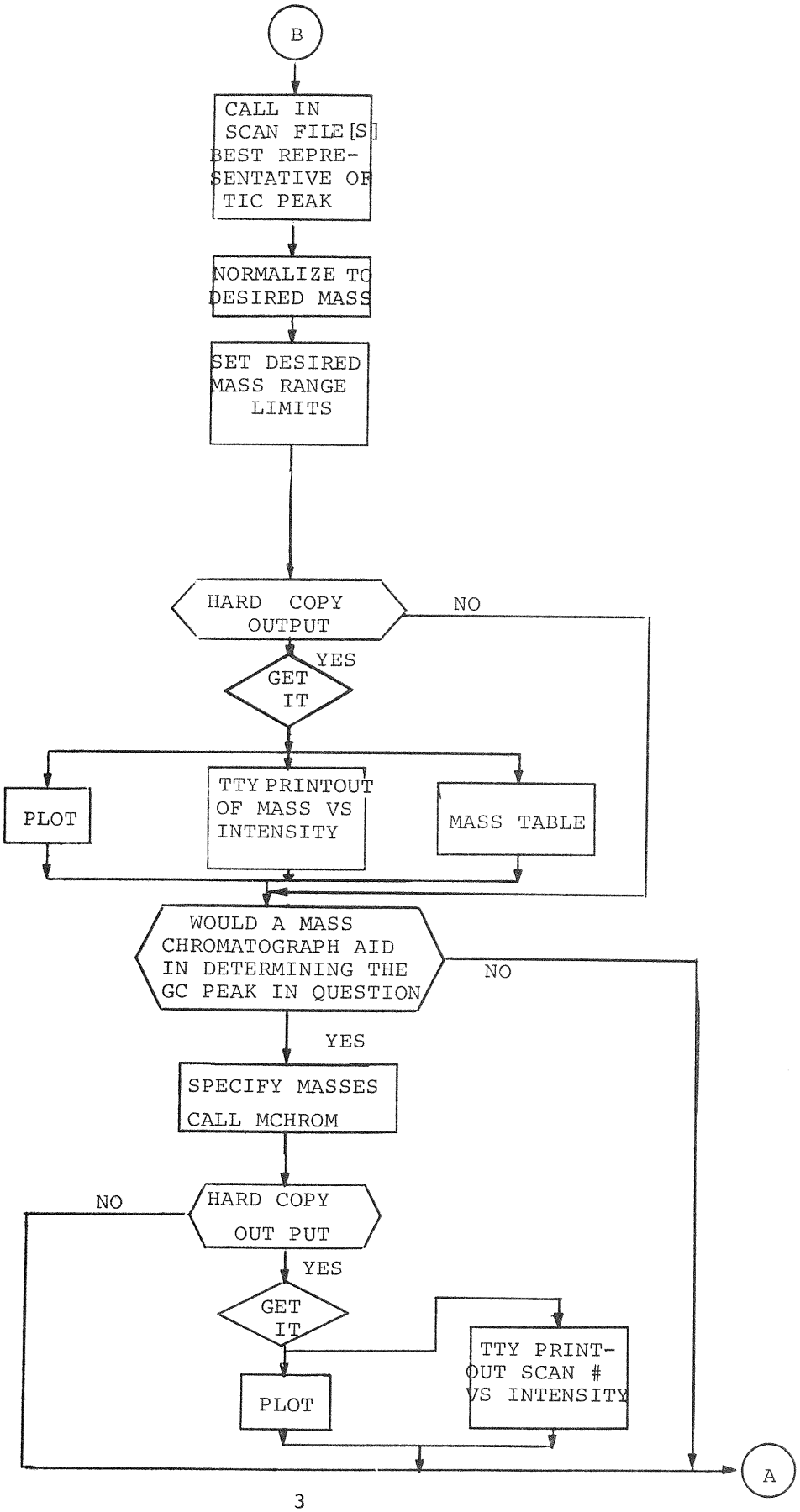
1. CALCOMP or Houston Plotter
2. Electrostatic Printer/Plotter

C. NEW FILE CREATIONS

1. Mass chromatographs [intensity vs. scan for given masses].
2. Total ion current [as a sum of intensities] vs. scan #.
3. Background subtraction of noise from scan data.

A flowchart of a typical chemist's usage of the MASH Subsystems is on page 2. This chart assumes that calibration has previously been done.


GO
START AIPOS SYS.
CALL MASH
ADVANCE TO TIC VS TIME PLOT
INSERT SAMPLE IN GC/MS
IS TIC RISING?
NO
YES
INITIATE SCANS
IS SCANNING COMPLETE
NO
YES
MORE INFORMATION WANTED
YES
NO
EXIT ACQUISITION PORTION
TIC FILE AVAILABLE
YES
NO
GENERATE IT AS SUM OF INTENSITIES VIA"TICGEN'
CALL UP REPORT GENERATOR
EXAMINE TIC FILE
HARD COPY OUTPUT
NO
YES
GET IT
PLOT
TTY PRINTOUT OF TIC VS SCAN #
A
IS A TIC PEAK OF INTEREST
NO
OUT
YES
NOISY ?
NO
YES
SUBTRACT OUT NOISE SCAN PRIOR TO TIC PEAK FROM THOSE SCANS ON THE PEAK VIA "BCKSUB"
B


B
CALL IN SCAN FILE[S] BEST REPRE-SENTATIVE OF TIC PEAK
NORMALIZE TO DESIRED MASS
SET DESIRED MASS RANGE LIMITS
HARD COPY OUTPUT
NO
YES
GET IT
PLOT
TTY PRINTOUT OF MASS VS INTENSITY
MASS TABLE
WOULD A MASS CHROMATOGRAPH AID IN DETERMINING THE GC PEAK IN QUESTION
NO
YES
SPECIFY MASSES
CALL MCHROM
NO
HARD COPY OUT PUT
YES
GET IT
PLOT
TTY PRINT-OUT SCAN # VS INTENSITY
A

2.0 NEW REPORT GENERATOR FEATURES

2.1 General Description

All options explained in this Section assume that Report Generator [LOOK] has been correctly loaded and is examining a file of interest. Refer to Section 5.0 of the MASH User's Manual, Version 1 for both the loading procedure and the command list of Report Generator.

2.2 Mass Table

LOREM .001

MASS TABLE

STARTING MASS : 100

	0	1	2	3	4	5	6	7	8	9
0-	23.2	4.5	.0	.0	.0	.6	.0	.0	.0	.6
1-	.0	.0	3.4	10.9	.4	.5	.0	2.1	.0	****
2-	2.2	.0	.0	.0	3.1	.6	.6	.9	.0	.0
3-	.0	****	3.5	3.5	.0	.0	.4	.8	.0	.4
4-	.0	.0	.0	9.4	1.5	2.7	.0	.3	.4	.0
5-	4.8	7.2	.0	.0	.0	6.6	.4	.7	.0	.0
6-	.0	.0	11.1	6.2	.4	.0	.0	1.1	.6	60.6
7-	2.0	.0	.0	.0	1.4	1.6	.0	.5	.0	.8
8-	.0	72.4	3.3	1.7	.0	.0	3.4	1.1	.0	.0
9-	.0	.0	.0	12.2	1.2	1.4	.6	1.2	1.0	.9

	0	1	2	3	4	5	6	7	8	9
0-	1.1	2.2	.0	.0	.0	9.0	.8	.8	.0	.0
1-	.6	.0	4.8	3.1	.0	.0	.0	4.0	.8	23.9
2-	1.1	.0	.6	.4	1.9	1.8	.0	.0	.0	.9
3-	.0	34.0	1.9	.9	.0	.0	3.5	1.3	.4	.4
4-	3.5	1.7	.5	19.9	1.4	.8	.0	.0	1.0	.8
5-	.5	1.3	.0	.0	1.5	8.4	.9	.7	.0	.0
6-	.6	.0	1.2	1.8	.0	.2	.0	5.0	.7	10.7
7-	.7	.0	.4	.2	1.2	1.4	.0	.0	.0	1.2
8-	.0	21.9	1.4	.7	.0	.0	2.0	1.0	.0	.0
9-	.0	.9	.0	15.1	1.2	.5	.0	.0	.9	.6

Figure 1 - Mass Table

The following conditions must be met before a mass table for a given scan can be printed.

A. The file being examined must be a scan file [i.e., Mass vs. Intensity].

B. The file must be normalized to the desired peak [since all intensity values print out in normalized form if lower than 100%, or as *** if greater than or equal to 100%].

C. The Mass Table range desired for printout must be the range currently shown on the scope [set via the L and R commands].

D. If the Report Generator was loaded from LINCtape, the WRITE ENABLE switch must be enabled on the loading unit.

The sequence of steps to generate a Mass Table from the scope image is:

1. Type "M". The display vanishes, and a ":" is printed. [No ":" probably means that the WRITE ENABLE switch is off. Turn it on, and the ":" should follow.]

2. Type the number of columns desired (2-14), where the number is the atomic weight of the group suspected of forming the basic building block of the unknown compound. [For example, 14 would imply CH_2 was suspect.] If the number is correctly chosen, the Mass Table shows the concentration of all ions differing only by such building blocks, as the elements of a given column.

3. Type carriage return to generate the Mass Table. To find the normalized intensity of any given mass, subtract the starting mass of the table [as typed], from the given mass, and divide the difference by the number typed for the column length. The quotient is the row # [on the extreme left of the typeout], and the remainder is the column number [on the top of the typeout] of the intensity "element". [For example, if the starting mass is 100, the desired mass is 131, and the number of columns is 10, look in Row 3, Column 1. Note that for the PFK mass table peak 131 is saturated.] The intensity value output for mass "M" will be the highest value between mass M-.3 and M+.3.

4. To stop printout at any point after the Mass Table header is printed, type CTRL/R[1]. The program returns to the scope display.

5. When printout is completed, the program, as in the CTRL/R case, returns to the scope display, and awaits new command.

[1]CTRL/R is typed by holding down the CTRL key while typing R.

2.3 The Y Command

The Y command allows the operator to chain MASH files, normalize or print stored data. When Y command is typed, the display vanishes and a ":" is printed (for LINCtape loaded programs, the WRITE ENABLE switch must be ON). The operator now has five choices:

2.3.1 Type S [for "SHOW ME"] to print a list of the other four options in the form:

```
TYPE 1      for chaining facility
TYPE 2      for normalization to sum of intensities
TYPE 3      for normalization to highest sum of intensities
TYPE 4      for printout of ten highest peaks
TYPE S      for SHOW ME
```

Type CTRL/R to stop typeout and return to the display. Upon completion of the typeout another colon is printed.

2.3.2 Type 1 to call the chaining facility.

Previously, when the information in a given scan was exhausted, the operator was forced to exit, return to job control, type a new "load" line of the form:

```
LTa: LOOK  LTb:OUTPUT = LTc:INPUT
```

and wait for the tape to stop shuffling before he could see the next MASH file.

The chaining facility allows the operator to type 1 , to go directly to the next MASH file.

Before 1 is typed, the following condition must be met:

a. The next file after the current input file must be a MASH file,exclusive of the ".SAM" variety. If not, an error message occurs and the program returns to job control.

If this condition is met, type Y and then 1 to go from MASH file to MASH file. Example - to go from PFK.ØØ5 to PFK.ØØ6, type Y↵,1↵.

2.3.3 Type 2 to call for a normalization to the sum of the intensities in the current scan. In this case, the file being examined must be a MASH scan file, or the program returns to the display. Such normalization is useful in providing a measure of the extent of distribution of ions throughout a given spectrum. All intensities will, until a renormalization or exit is taken, be effectively reported as a percent of total ion current.

2.3.4 Type 3 to call for a normalization to the highest sum of intensities in the current scan provided the following conditions are met:

a. The file being examined is a MASH scan file
b. At the time Report Generator was called, the T.I.C. file associated with this scan file [same first six characters, followed by .TIC] was given as a second input file.

If successful, all intensities in the scan are normalized to the highest sum of intensities for the experiment. If used consistently in the reporting of each scan, it means that the intensity percentage reported for every mass is directly proportional to the number of ions having that mass at the time the scan was taken. As an example, scans taken when the gas chromatograph was at or near a peak will report higher intensity percentages than other scans further away from a peak. This would apply even if the compound involved was the same, simply because the quantity of the compound was different.

If this feature is to be used consistently, a suggestion to speed up reporting would be to move the TIC file to a new tape unit prior to calling Report Generator. This would save "tape spinning" each time this type of normalization was called for a new scan file.

Assuming the scan data was on unit 1, and the name of the experiment was called "sample", the procedure might be to use the job control commands:

a) LTØ:MOVE SAMPLE.TIC = LT1:SAMPLE.TIC

to move the file and:

b) LTØ: LOOK OUTPUT=LT1:SAMPLE.ØØ1,SAMPLE.TIC

to call Report Generator with this normalization feature enabled.

2.3.5 Type 4 to call for an ordered printout of the ten largest peaks in the file [which may be stopped by ↑R causing a return to the display], which is identical to the form of printouts generated by the "P" and "V" commands -- for many purposes [such as library identification], the ten highest peaks are of major importance. Also, the highest peak can thus be quickly identified for normalization purposes.

2.4 Examining Mass Chromatographs

A Mass Chromatograph file created via MCHROM (see below) can be examined via Report Generator. Use the Mass Chromatograph file name and unit as the input file name and unit when issuing the call to the AIPOS Monitor, as, for example:

LTa: LOOK LTb:OUTPUT=LTc:M69

where M69 is a Mass Chromatographic file.

A Mass Chromatograph file can also be examined using the "Y" command if it is the next file in a sequence of MASH files.

2.5 Generating Hard Copy Plotter Output

The Plot option in Report Generator is an exceedingly powerful one because of the extent of control the operator maintains over what is plotted. The operator can take a basic file and, before plotting:

1. Delete specific peaks
2. Perform thresholding to retain only significant peaks
3. Set the range of X [masses, scan numbers] through which the plot is desired via the "L" and "R" commands.
4. Set the range of Y [intensities, T.I.C.'s] by normalizing to a peak which will cause most peaks of interest to be in mid-range via the "N" command.

When the Q command is given to the Report Generator program (assuming conditions B, C, and D, of Section 2.2 are met) the scope image is plotted out. The plotter may be on or off at this point.

The Teletype prints:

```
TYPE

SPACING:
HEADER:

:
```

The operator types the spacing desired: 2-20 for the electrostatic plotter and 0-9 for the X-Y plotter. The spacing is proportional to the X-axis length. If a wide range of X is being examined in an overview [see Figure 2], spacing should be small. If a small range is being studied closely, spacing should be wider [see Figures 3 and 4]. If a number out of limits or a non-number is typed, it is equivalent to hitting CTRL/R.

Upon receiving the spacing, the program prints another ":". The operator types in the one line "HEADER" (up to 68 characters) to appear on the plot. For example:

"HIGH BOILING PFK NORMALIZED TO MASS 131 - MARCH 1971"

Be sure the plotter is turned on before typing carriage return.

When carriage return is typed, the scope goes dark and plotting commences. The routine returns to display the scope image of the file being plotted only if:

1. the plotter was initially off;
2. ↑R is typed (in which case, the plot is incomplete);
3. the plot is completed.

Examples of Mass vs. Intensity plots are given in Figures 2, 3, and 4. Another type of possible plot is shown in Figure 5. Note that all X values are rounded to unity. The Y value plotted at X value "m", for example, is the highest Y value for any X between m-.3 and m+.3.

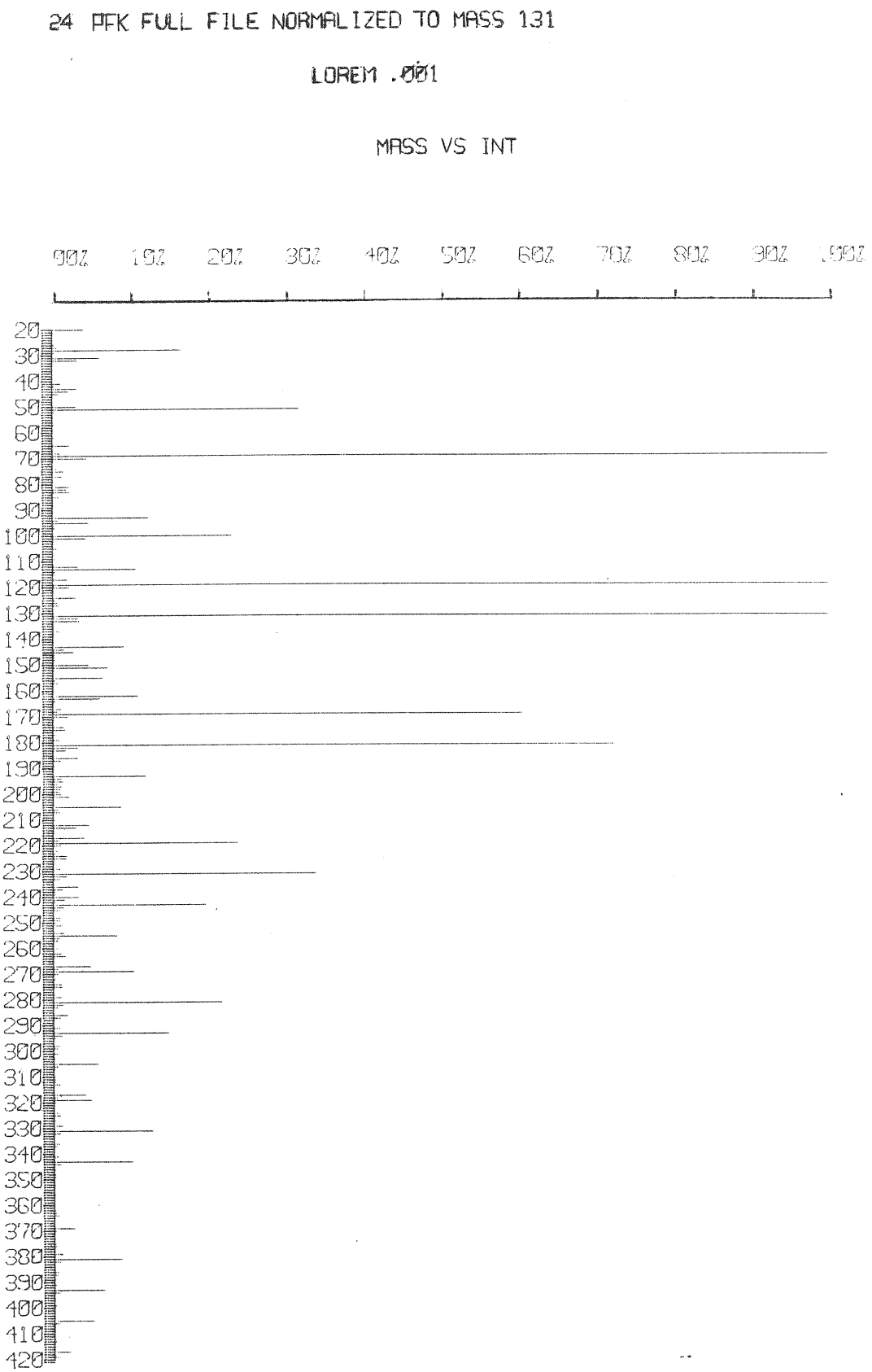


Figure 2 - Plot of Entire File (Spacing = Ø)

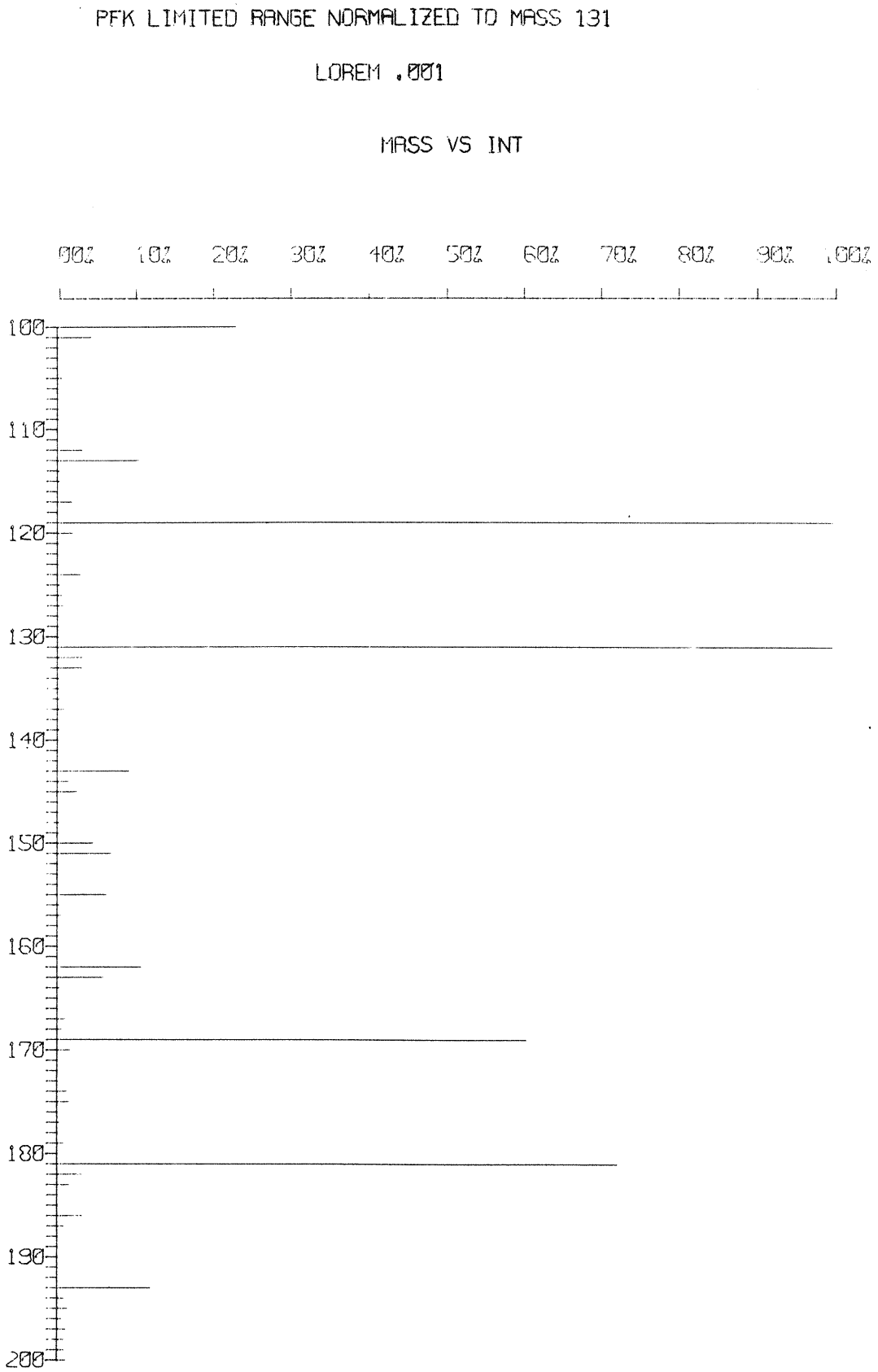


Figure 3 - Plot of Mass Region of Interest (Spacing = 3).

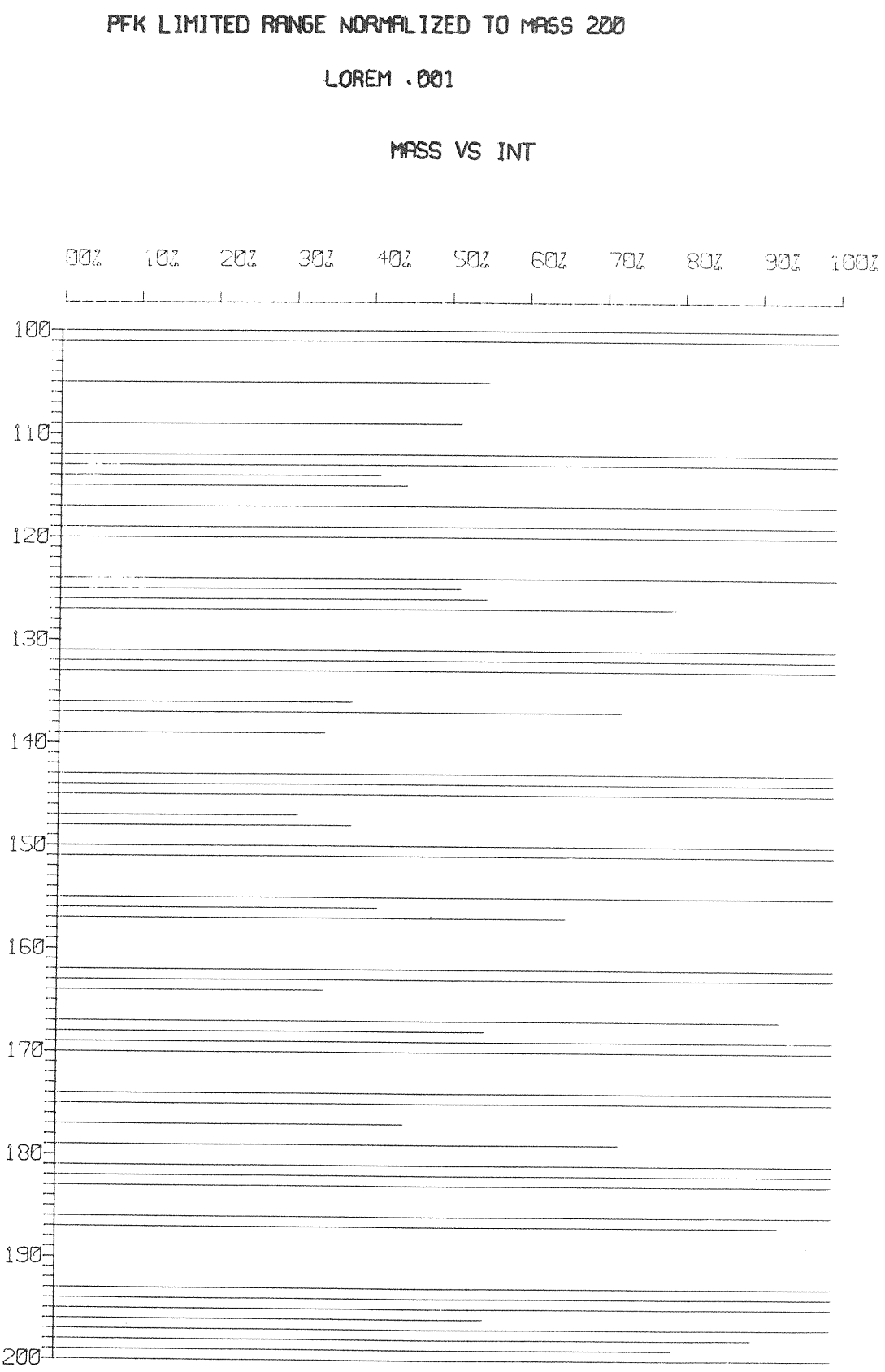


Figure 4 - Plot Emphasizing Small Peaks in the Mass Region of Interest

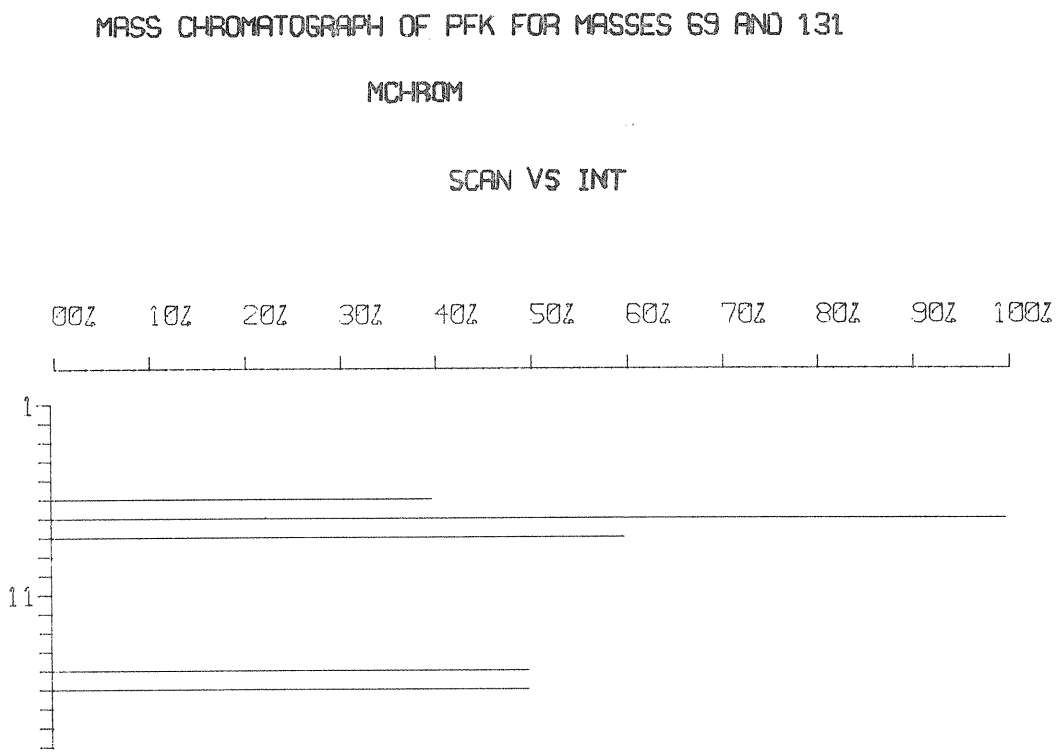


Figure 5 - X-Y Recorder Plot of Mass Chromatograph

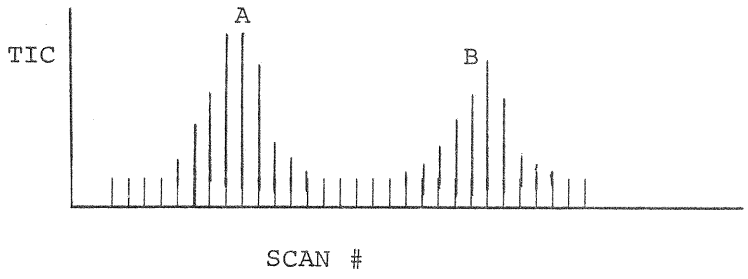
3.0 NEW FILE CREATIONS

In all programs which follow, it is assumed that the order of the MASH acquisition generated files has been left untouched on an AIPOS tape since the experiment involved was run. Violation of this assumption could cause catastrophic error.

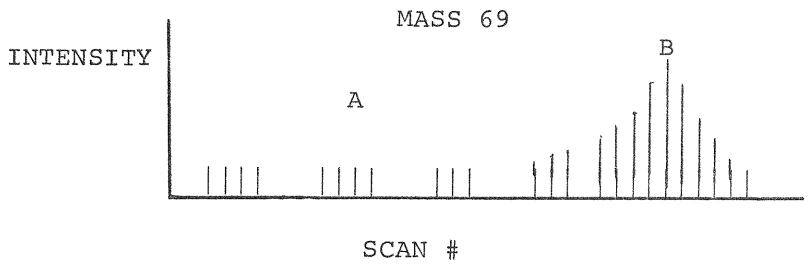
3.1 Mass Chromatographs

MASH uses the program "MCHROM" to process a sequence of mass vs. intensity scans to generate an output file consisting of the averaged intensities [of the specified masses] in a given scan vs. the scan number. The output file created can be examined by Report Generator.

Such files of intensity vs. scan number for given mass[es] have proved to be of value in determining the compounds involved in GC peaks. For example, in a given experiment, if the TIC vs. scan number file looked like:



and the intensity vs. scan number plot looked like:



then an ion of Mass 69 did not appear in the compound causing Gas Chromatograph peak A, but was a major component of peak B.

The operator can specify up to five masses whose intensities are to be averaged [of use when a particular grouping is suspected as a prime GC peak component] when the program "MCHROM" is called from the AIPOS Monitor. The calling statement takes the form of:

```
LTa:MCHROM LTb:MA697Ø=LTc:EXPERM.SAM;69,7Ø
```

where:

MA697Ø = File created, to be examined by Report Generator.

EXPERM = Six character name of series of MASH files created during the Acquisition mode of MASH.

For example, an index of LTc shows:

```
EXPERM.SAM
EXPERM.TIC
EXPERM.ØØ1
      .
      .
EXPERM.nnn
```

and "69" and "7Ø" are the masses whose intensities are to be averaged.

Upon completion of the call statement, MCHROM generates the output file as a Mass Chromatograph, and exits to Job Control with no further operator input required.

Possible errors are:

8Ø = Parameter error [in calling statement]
83 = I/O file error
84 = Error in scan files

All errors cause a return to Job Control. Errors 80 and 83 are terminal. Error 84 allows creation of a partial Mass Chromatograph.

3.2 Total ION Current As a Sum of Intensities vs. Scan Number

The program "TICGEN" is used with those GC-MS systems for which the total ion current [T.I.C] is not available during scanning. Upon identification of the experiment, TICGEN sums all the intensities of a given scan, and saves the sum and the scan number. When all scans in the experiment have been examined, the intensity values are

scaled and saved in the TIC file previously created by Acquisition [and previously filled, if the TIC was available].

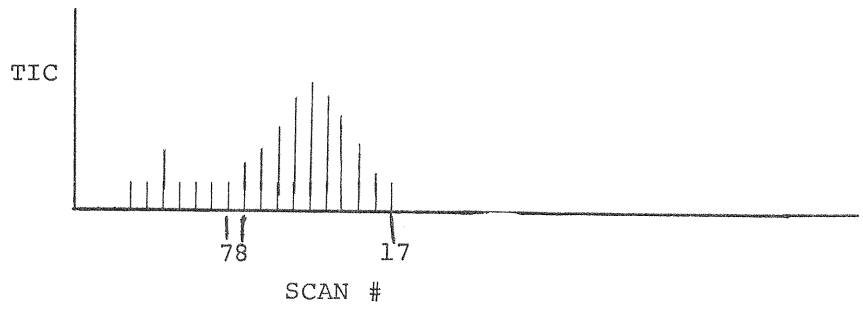
The calling sequence is:

LTa:TICGEN=LTb:EXPERM.SAM

The TIC file is stored in a previously created slot called "EXPERM.TIC". Possible errors are the same as for MCHROM. All errors cause a return to the AIPOS Monitor.

3.3 Background Subtraction of Noise from Scan Data

A common problem in GC-MS analysis is contamination of a peak on a GC by peaks that have occurred previously. A background subtraction program [BCKSUB], was created to handle this problem in the MASH system. For example, in the plot below:



If scan 7 were subtracted from scans 8-17, the resulting scans would be freer of the GC "prehistory", and give truer values for the component causing the G-C peak.

"BCKSUB" is called from the AIPOS Monitor via a calling statement of the form:

LTa:BCKSUB=LTb:EXPERM.ØØ7,EXPERM.ØØ8,EXPERM.Ø17

where:

EXPERM is the name of the experiment.

EXPERM.ØØ7 [the first input file] is the scan to be subtracted.

EXPERM.ØØ8 [the second input file] is the first scan to be "cleaned up".

EXPERM.Ø17 [the third input file], is the last scan to be "cleaned up".

The mass peak heights at the start of the GC peak [SCAN, EXPERM.ØØ7], are subtracted from each scan in the GC peak [SCANS EXPERM.ØØ8 - EXPERM.Ø17], the results becoming the new mass peak heights of the GC peak scans. Error messages are the same as MCHROM. All errors cause a return to AIPOS Job Control.

4.0 MASH ASSEMBLY INSTRUCTIONS

This Section provides the assembly instructions for the six programs which make up the MASH Phase II system.

a. Calibration
b. Acquisition
c. Report Generation
d. Mass Chromatograph
e. TIC As Sum of Intensities
f. Background Subtract

4.1 Assembly Instructions: Calibration and Acquisition

1. Assemble "OVLYC4" via DIAL-MS Assembler[1]. Save Binary with command:

   →SB nameA,unit,P1Ø4ØØ ↵

2. Assemble "PREAC" via FPP Assembler[2]. Save Binary with command:

   →SB nameB,unit ↵

3. Assembler "ACQ27" via FPP Assembler. Save Binary with command:

   →SB nameC,unit ↵

4. Assemble "ACFPPT" via FPP Assembler. Make sure "MASHFPPN" is on the same unit, and that the unit is either "LT1" or "R11". Save Binary with command:

   →SB nameD,unit ↵

5. Assemble "PACPU2" via FPP Assembler. Make sure "PAFPP" is on the same unit, and that the unit is either "LT1" or "R11". Save Binary with command:

   →SB nameE,unit ↵

---

[1]Refer to LAP6-DIAL Programmer's Reference Manual (DEC-12-SE2D-D).

[2]Refer to FPP Assembler User's Guide (DEC-12-AQ2A-D).

6. Assemble "CURFIT4" via FPP Assembler. Save Binary with command:

   →SB nameF,unit ↵

7. Assemble "MASHEC" via FPP Assembler. Save Binary with command:

   →SB nameG,unit ↵

8. Load AIPOS[1]. Order:

   BUILD CALIB ↵

9. Give "nameA" through "nameG" as successive overlays in exactly the order above. No scratch area or working areas are required.

10. Do an ALIAS on CALIB.BIN calling it ACQUI.BIN. Both should be 74_8 blocks long.

4.2 Assembly Instructions: Report Generator

1. Assemble "REPORTC" via FPP Assembler. Make sure that both "MLB1S" and "MLB2S" are on the same unit, and that the unit is either "LT2" or "R12". Save Binary with command:

   →SB name1,unit,P11ØØØ ↵

2. Assemble "MASSTB1Ø" via FPP Assembler. Save Binary with command:

   →SB name2,unit ↵

3. Assemble "YOVLY" via FPP Assembler. Save Binary with command:

   →SB name3,unit ↵

4. Assemble "EPLOT4" via FPP Assembler. Save Binary with command:

   →SB name4A,unit ↵

[1]Refer to AIPOS User's Manual (DEC-12-SQ1A-D).

5. Assemble "XYPLOTI" via FPP Assembler. Save Binary with command:

   →SB name4B1, unit↵

6. Assemble "XYFPPI" via FPP Assembler. Save Binary with command:

   →SB name4B2,unit ↵

7. Load AIPOS. Order:

   BUILD LOOK ↵

8. Give "name1" through "name3" as successive overlays in exactly the order above. If the installation has a Calcomp plotter, a Houston plotter, or no plotter, finish with overlays "name4B1" and "name4B2". If the installation has a digital plotter (Versatic, for example), finish with overlay "name4A."

9. In either case, four blocks of scratch area and one working area are required.

4.3 Assembly Instructions: Mass Chromatograph

1. Assemble "MCHRM5" via FPP Assembler. Save Binary with command:

   →SB name1,unit,P1ØØØØ ↵

2. Load AIPOS. Order:

   BUILD MCHROM ↵

3. Give "name1" as the only overlay. No scratch area or working area is needed.

4.4 Assembly Instructions: TIC As Sum of Intensities

1. Assemble "TICGENC" via FPP Assembler. Save Binary with command:

   →SB namel,unit,P1Ø6ØØ ↵

2. Load AIPOS. Order:

   BUILD TICGEN ↵

3. Give "namel" as the only overlay. No scratch area or working area is required.

4.5 Assembly Instructions: Background Subtract

1. Assemble "BCKSUBC" via FPP Assembler. Save Binary with command:

   →SB namel,unit,P1Ø6ØØ ↵

2. Load AIPOS. Order:

   BUILD BCKSUB ↵

3. Give "namel" as the only overlay. No scratch area or working area is required.