DATELINES:

Philadelphia, Pa.—Association of Clinical Scientists

The 48th Annual Applied Seminar of the Association of Clinical Scientists will be held this year on November 7, 8 and 9 at the Bellevue-Stratford Hotel. Finnigan Corporation will participate in a workshop concerned with applications of computer-assisted GC/MS to the identification and measurement of drugs in body fluids. For further information contact Dr. F. William Sunderman, 14301 New College, Hahnemann Medical College, 230 N. Broad St., Philadelphia, Pa. 19102.

Mexico City, Mexico—
Chemical Congress of the North American Continent

The First Chemical Congress of the North American Continent will convene this year from November 30 to December 5. Dr. Robert Finnigan and Mr. Victor DaGragnano of Finnigan Corporation will give papers. Dr. Finnigan's paper will describe the use of GC/MS in the Analysis of Hazardous Environmental Chemicals. Mr. DaGragnano will discuss the hardware and software aspects of a real time interactive GC/MS data system.

Atlanta Georgia—
Water Quality Technology Conference

The 1975 American Water Works Association Water Quality Technology Conference is being held on December 7, 8 and 9 at the Sheraton Biltmore. Finnigan Corporation will present one of its instruments during the "Exotic Instrumentation Session" and will participate in the discussion of laboratory tools for safe water. For further information contact the American Water Works Association, 6666 Quincy Avenue, Denver, Colorado, 80235. (303) 988-1426.

Oak Brook, Illinois—
2nd International Conference on Stable Isotopes

"Meeting Human Needs" is the theme of the 2nd International Conference of Stable Isotopes to be held at the Oak Brook Hyatt House in Oak Brook, Illinois on October 20–23. The conference will stress pharmacological, clinical and environmental applications, as well as methodological developments. Dr. E.J. Heron, of Finnigan, will present a paper entitled, "Analysis of Uniformity of ^{13}C Incorporation in Compounds of Biological Interest."

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finnigan spectra

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Sunnyvale, California—XRF Workshops

Early in November, Finnigan will continue with a series of four workshops on Trace Element analysis with Energy Dispersive X-Ray Fluorescence. Techniques of analysis down to sub-microgram levels will be discussed and your samples will be analyzed with the fully automated Model 900 X-Ray System. Make your reservation at the site of your choice by calling Mr. Art Pace, X-ray Marketing Manager, (408) 732-0940.

• Atlanta November 5, 1975	Holiday Inn 1380 Virginia Ave. Atlanta, Ga.
• Baton Rouge November 7, 1975	Holiday Inn 9940 Airline Junction US 61 and I-12 Baton Rouge, La.
• Houston November 10, 1975	Marriott Motor Hotel 2100 S. Braeswood Blvd. Houston, Texas
• Dallas November 12, 1975	Holiday Inn Stemmons and Regal Row 1575 Regal Row Dallas, Texas

so complex? What are the sources of these hydrocarbons and their natural distribution pathways? Can we predict the biological effect of such complex PAH mixtures?

Probe distillation and low voltage mass spectrometry will be a valuable tool, when we attempt to answer these questions.

REFERENCES

1. W. Giger and M. Blumer, Anal. Chem. **46**, 1663 (1974).
2. J. Franzen, H. Küper and W. Riepe, Anal. Chem. **46**, 1683 (1974).
3. M. Blumer and W. W. Youngblood, Science **188**, 53 (1975).
4. W. W. Youngblood and M. Blumer, Geochim. et Cosmochim. Acta, **39**, 1303–1314 (1975).
5. M. Blumer, Chem. Geol., in press.

Biographical Note:

M. Blumer, Senior Scientist at the Woods Hole Oceanographic Institution received his Ph.D. at the University of Basel, Switzerland in 1949. He worked in several academic and industrial laboratories in Europe and the U. S. before coming to Woods Hole in 1959. His principal interest lies in the origin and fate of organic compounds in nature. This work is supported by the Office of Naval Research (NOO-14-66 contract CO-241) and the National Science Foundation (grant DES 74-22781).

User Written Software Extends The Use Of GC-MS Data Systems

by **Joseph E. Evans**
Finnigan

Over the past few years, we have seen a dramatic increase in the popularity of the combined gas chromatograph-mass spectrometer (GC-MS). This is due, in part, to recent governmental regulations requiring definitive identification of environmental pollutants. Another factor that has contributed to this increase in popularity is the minicomputer-based dedicated data system. The advent of these systems introduced an efficient method for collection, reduction, and analysis of the large volume of data associated with the combined GC-MS. Due to the realization of greater through-put efficiency, an increasing number of laboratories can now profitably use an instrument that was once considered only a tool of research.

Since a GC-MS data system represents a substantial investment for any laboratory, it must be made cost-effective by utilizing it to the fullest extent possible. When used to further analyze mass spectral data, they cannot only help justify the large initial expenditure, but also increase analysis reliability by performing some of the mundane and time-comsuming tasks often neglected by the inexperienced mass spectrometrist.

Almost all data systems offer the user the option of writing his own programs in BASIC. This high level language is extremely powerful yet little practice is required for one to become proficient in its use. Relatively unsophisticated programs, writtin in BASIC, allow the user almost unlimited manipulation of his chromatographic and mass spectral data. The advent of Finnegan BASIC has taken this capability one step further. Now the mass spectroscopist can not only write his own programs but also use them to automatically access and process his stored chromatographic and mass spectral data. Two programs that illustrate the usefulness of user written software are Program ELAL[1] and Program FINL[2].

Program ELAL

Program ELAL will compute an elemental analysis on low and medium resolution mass spectra for C, H, N, Cl, Br, F, S, Si, O, and P. It is written in both Dartmouth and Finnigan BASIC and is based upon a modification of the manual method of elemental analysis described by McLafferty[3]. The program requires only five items of information. These are the mass and intensity of the (A) peak and the intensities of the (A+1), (A+2), and (A+4) peaks. ELAL normalizes and displays the input data, computes the analysis, and then outputs a tabular listing of the elements encountered. Other pertinent information concerning the analysis is also presented, thus allowing the user to evaluate the accuracy of ELAL's computations. Some of these include the (A+1) remainder after carbon calculation, the (A+2) remainder after calculation of any (A+2) element, a Cl/Br fit factor, and a rings + double bonds calculation. After listing the elements, the program enters a subroutine that allows operator interaction. This allows the user to correct any mistake he feels ELAL may have made. The entire analysis is then recomputed based upon these corrections. A typical elemental analysis appears in Figure 19.

```
PROGRAM ELAL
AN ELEMENTAL ANALYSIS OF MASS SPECTRA

INPUT AM,A,A+1,A+2,A+4
?72,100,3.5,.48,0

INPUT NORMALIZED
A= 100
A+1= 3.5
A+2= .48
A+4= 0

A+1 REMAINDER = .349999
A+2 CORRECTED = .4437
A+2 REMAINDER (O) = 6.37001E-02
MASS OF A REMAINING =  4
MASS OF A REMAINING =  4

C 3    H 4    N 0    CL 0    BR 0    F 0
S 0    SI 0    O 2    P 0

R+DB=  2
AM= 72
MW= 72

INTERACTION?  TYPE 1 IF YES, 2 IF NO
?2
```

Figure 19: An Elemental Analysis of Acrylic Acid, CH_2=CHCOOH.

Program FINL

Program FINL performs a fragment ion and neutral loss analysis on low resolution mass spectra. Although quite simple in nature, FINL can be very useful when interpreting unknown spectra. To use the program, one simply

enters the mass of the molecular ion and the masses of up to eight fragment ions. FINL then calculates the neutral losses and displays them along with the general formulas for the loss and the types of compounds generally associated with them. After this is complete, a similar table is generated for the fragment ions. All output data necessary for the analysis are stored in core thus eliminating the need for peripheral storage devices and complex operating systems. The data are quite extensive and include both common and unusual fragment ions and neutral losses. Figure 20 illustrates the results of a FINL analysis.

```
PROGRAM FINL
A FRAGMENT ION AND NEUTRAL LOSS ANALYSIS

ENTER THE MOLECULAR ION
?72

ENTER UP TO 8 FRAGMENT IONS
?55,45,27,0,0,0,0,0

NEUTRAL LOSSES

MASS   FORMULA          COMPOUND TYPE

 17    NH3              AMINES
 17    OH               ACIDS,OXIMES
 27    HCN              N-HETERO,CYANIDES,ARYL-NH2
 27    C(N)H(2N-1)      RCOOR'
 45    C(N)H(2N+1)O     R*OR',RCO*OR'

FRAGMENT IONS

MASS   FORMULA          COMPOUND TYPE

 55    C(N)H(2N-1)CO    ALKENYL/ACYALKYL CARBONYL,CYC ALC/ETH
 55    C(N)H(2N-1)      ALKENES,CYCALKANES
 55    C(N)H(2N-1)N     ALKYL CYANIDES
 45    C(N)H(2N-1)S     THIACYCALKANES,UNSAT SUB S-CPDS
 45    C(N)H(2N+1)O     ALIPHAT ALC/ETH
 45    C(N)H(2N+3)SI    ALK SILANES

OTHER IONS? ENTER 1 IF YES, 2 IF NO
?2

ABBREVIATIONS

R--H OR ALKYL GROUP; X--ANY HALOGEN; Y--FUNCTIONAL GROUP
Z--H REARRANGEMENT, COMMON EXAMPLES ARE
-CH2CH2-,-CH2O-,-OCH2-,-COCH2-,-COOR
```

Figure 20: A Fragment Ion and Neutral Loss Analysis of Acrylic Acid, CH_2=CHCOOH.

Both ELAL and FINL were designed as identification aids, not as replacements for other procedures such as use of reference spectra and confirmation by analysis of standards. When used routinely, however, they can contribute much to the identification process. An example of their usefulness is the case of computerized mass spectral library searches, especially those which are performed off-line on a time-shared basis. When using a time-shared library, one should perform the search as efficiently as possible. This reduces CPU time, the main factor influencing the cost of the search. By using elemental analysis data, one can restrict the search to those compounds having a specific elemental composition, thereby saving the time and money involved in a search of the entire library. When used with a dedicated library, both ELAL and FINL can assist the mass spectrometrist in determining which of the "N" best fits, selected by the computer, has the greatest probability of being correct. This helps to alleviate the identification problems which arise when two or more compounds of differing elemental composition give rise to similar spectra.

Although ELAL, FINL, and similar user written programs can be utilized quite succesfully with any data system offering BASIC programming, their ultimate usefulness can be realized only when under an advanced system such as Finnigan BASIC. With conventional systems, the user must have the data listed in tabular form, manually locate the parent ion, and then enter the data in the BASIC program via the keyboard. These steps must be repeated for each set of data. Finnigan BASIC, on the other hand, can retrieve the stored data from the disc and by means of a subroutine, written in BASIC, locate the parent ion and each prominent ion series. The system will then automatically perform an elemental and fragment ion analysis on the stored data. The data can even be chained for analysis overnight.

Both ELAL and FINL illustrate how dedicated data systems can be used to further analyze mass spectral data. Although both are relatively unsophisticated and require little programming experience, they can be quite useful when analyzing unknown mass spectra. Hopefully they will encourage GC-MS users to explore the possibility of designing and writing their own software and then sharing through the Finnigan BASIC Users Group.

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Biographical Note:

Joseph E. Evans comes to Finnigan Corporation from the U.S. Army Environmental Hygiene Agency where he was Chief of the Special Chemistry Branch and in charge of the Mass Spectrometry Laboratory. He received a B.S. in Microbiology from Clemson University and a M.S. and Ph.D. in Biophysics from the University of Houston. His interests include environmental and biomedical applications of GC-MS and the use of portable mass spectrometers in environmental monitoring. Dr. Evans is currently Finnigans east-coast GC-MS specialist and is charged with establishing our new D.C. area applications facility.