PILOT COMPUTERIZED INFRARED DATA FILE FOR FORENSIC SCIENCE LABORATORIES

F. G. Madrazo
New York State
Identification and Intelligence System
Albany, New York
R. Ellis
New York State Police
Scientific Laboratory
Albany, New York

and

Dr. E. Bungaro
New York City
Medical Examiner's Office
New York, New York

Summary: A computerized infrared data search system is described with emphasis on its application to forensic science problems.

NOTE: The work described in this paper was initiated by the New York State Identification and Intelligence System. This agency, effective September 1, 1972, has become part of the New York State Division of Criminal Justice Services.

INTRODUCTION

Modern forensic science laboratories, in fulfilling their roles as the scientific arm of law enforcement, are increasingly taking advantage of modern analytical instruments to aid in the identification and individualization of common evidence materials. As the types of substances requiring analysis proliferate and as sample sizes diminish, laboratories must use such instruments as gas chromatographs, infrared spectrophotometers, and mass spectrometers to obtain data necessary for sophisticated investigations. These instruments produce great quantities of data in relatively short periods of time even when only small amounts of evidence material are available. However, the interpretation of the data is not always an easy task. Data analysis frequently takes far longer than the time required to obtain the data.

Reports prepared for the Office of Law Enforcement Assistance by John Jay College of Criminal Justice,[1] for the New York State Office of Crime Control Planning by Cornell Aeronautical Laboratory, Inc.,[2] and for the New York State Identification and Intelligence System by Arthur D. Little, Inc.,[3] have identified the current crises in the forensic science laboratories of the country with respect to volume of work, shortage of trained personnel, inadequate instrumentation and data analysis capabilities.

Recognizing the needs in the areas of data handling and analysis, the New York State Identification and Intelligence System (NYSIIS) has pursued a program to provide computerized scientific data files for the forensic science laboratories of New York State. In outlining this program, we identified the following types of files that should considerably aid these laboratories in the previously mentioned areas of data analysis.

The first type of file is designed to aid laboratories in the identification of unknown substances. Modern analytical techniques such as those mentioned above are powerful aids in the analysis of unknown materials.

Due to the data analysis requirements brought about by sophisticated analytical techniques, commercial firms have produced computerized files of reference data. The data for the files are obtained from the analysis of pure chemical compounds. The data resulting from an analysis of an unknown compound is searched against data stored in the files to obtain a list of possible identifications.

Another potential computerized file would aid laboratories in determining the origin of common evidence materials. These files would contain data on the physical properties of materials frequently encountered as evidence. After statistical relationships were derived for the occurrence of these properties, the data could be used to evaluate the probability of a direct relationship between a piece of evidence material and a suspected source or origin.

A third type of file would aid in relating evidence found in connection with one crime to evidence on file from another crime. This is a routine procedure with latent fingerprints, and is occasionally attempted with firearms. Utilizing central computer files, this process can potentially be of value in connection with a large variety of evidence materials.

Because of funding limitations and the desire to develop a service which would immediately assist forensic scientists, we chose to limit our current project to data from a single analytical technique and concentrate on the type of file used for identification of unknown chemical substances.

This paper describes NYSIIS' experience with the implementation and operation of a commercially supplied computerized infrared data file system as applied to typical analytical problems in two of the major forensic science laboratories of

New York State. The following section provides background information on the theory and use of the infrared spectrophotometer as related to forensic problems.

THEORY AND USE OF THE INFRARED SPECTROPHOTOMETER

The infrared spectrophotometer, a highly sophisticated analytical instrument, presents very extensive, specific and complex data to the analyst.

The instrument measures the wavelengths in the infrared region of the light energy spectrum that a chemical compound absorbs. Each compound will absorb at different wavelengths in the IR region and therefore provide a unique spectrum. The IR spectrophotometer measures this and records the absorption on graph paper. (See Figure No. 1.) An analyst can then identify a compound by the shape of the absorption bands, their wavelengths and their intensities.

The samples to be analyzed can be in the gas, liquid or solid state. However, the IR spectrum will vary depending on the physical state of the sample. Due to the fact that glass absorbs IR radiation, the sample holder must be sodium chloride, potassium bromide or a similar salt. Most forensic samples are analyzed in potassium bromide pellets or between sodium chloride plates.

The instrument consists of an infrared radiation source, a sample holder, monochrometer, detector, amplifier and recorder. The instrument is a double beam spectrophotometer. That is, the detector compares the sample and reference beam and then amplifies the signal to drive a pen motor on the recorder. (See Figure 2.)

The IR spectrophotometer is one of the most useful analytical tools in a forensic laboratory. It is used in the analysis of pharmaceuticals, narcotics, dyes, pigments, polymers, explosives, inks and poisons.

The fact that no two compounds have the same IR curve makes the technique one of the most definitive ways to identify a substance. The sample preparation is simple and the data is presented immediately to the analyst. While other methods such as thin layer chromatography (TLC) or gas chromatography (GC) may be quicker and simpler, they rely on physical properties of the compounds and are subject to ambiguities in the interpretation of the data. The IR measures the actual types of chemical bonding in the molecule. Thus the IR is a very specific method to identify a substance. As stated above, the data presented to the analyst by the IR spectrophotometer consists of band shapes, band intensities and band wavelength. Both the intensity and wavelength can be represented as numbers. However, the band shape is subjective. Therefore, computerized treatment of the IR data can only be in terms of band wavelength and intensity.

The practical aspects of handling IR data has almost eliminated the use of band intensity except as a criterion in determining which bands to code. This criterion is somewhat flexible, but usually is 10% of the maximum band size. There is no coding of the absolute or relative intensities of the bands. The only data that is useful to a computer search program then is the actual wavelengths.

The amount of data involved in just using the wavelengths is enormous and if one is presented with an IR spectrum of an unknown compound there are only a few laborious methods of identification open to the analyst. One is to try to make a determination as to what types of bands are present in the IR spectrum by the use of group frequency correlation. Certain chemical groups have characteristic IR absorption frequencies and will be familiar to the analyst. Groups such as benzene ring, carbonyl, OH, N-H and methoxy have bands which are very common and easily recognized. This provides the analyst with information about certain substructures present in the molecule, but does not indicate its total structure.

Another option left open to the analyst is to compare manually his unknown spectrum with a known spectrum. This is an almost impossible task considering there are hundreds of thousands of possible IR curves or different chemical compounds open to comparison. In certain cases when an analyst is presented with a somewhat limited variety of compounds, manual comparisons can be done successfully in a relatively short period of time. An example of this occurs in the identification of some of the common barbiturates and derivatives.

Considering that a forensic laboratory handles evidence associated with drugs, narcotics, arson, hit and run, murder, etc., the types of possible samples are enormous. It would be impossible to identify routinely these samples using a manual search method. Thus, a rapid method of comparing thousands of IR spectra to the unknown curve is an essential tool for a forensic laboratory. A schematic diagram of the possible identification procedures using IR data is given in Figure No. 3.

The availability of a computerized data file aids a forensic operation in two ways. First of all, it increases the overall efficiency of an individual IR

analysis. Secondly, it allows the identification of compounds which were previously unidentifiable within the framework of an individual laboratory's operation. The overall time for analysis may increase because at the same time the speed of IR comparison is increasing, the use of IR by the laboratory increases. The analyst now knows he can identify the unknown with the help of the computer file. In other words, the laboratory can now spend more time in providing a definite answer on a case because there is a reasonable chance for success.

The information provided above indicates why a computerized infrared data file would be an asset to a forensic science operation. The following section describes the system currently operated by NYSIIS.

SYSTEM CHARACTERISTICS

A. General Background

The infrared data file system components in their current configuration are depicted in Figure No. 4.

The data file and search program were obtained from the Dow Chemical Company through a license agreement. Under the terms of this agreement, the NYSIIS Criminalistics Research Bureau has a non-exclusive license to store the data file and permit searches of the file by any governmental forensic science laboratory within the State of New York.

This type of arrangement was necessary because Dow Chemical Company retained the rights to the search program and the data file rights resided with the American Society for Testing and Materials. The fee for this license was negotiated by the Dow legal department and NYSIIS.

The Dow-ASTM system was chosen for evaluation because it offered several features which appeared to be particularly advantageous for use in the forensic science environment.

1. The program is designed to be used by a chemist in his own laboratory through use of a remote terminal. This on-line feature would provide rapid turnaround time.
2. The program is highly interactive. That is, it is easy to operate, is designed in accordance with bench chemist needs, and it provides the capability to perform many searches or alter input data in a specific search within a short period of time. This is in contrast with other search systems which have complex input requirements, are card oriented and require lengthy search times.
3. The search program was available for the Burroughs B6500 computer system and therefore required only minor modification to become operational on the NYSIIS system.

Both the New York State Police Scientific Laboratory and the New York City Medical Examiner's Laboratory agreed to participate in the pilot operation of the file.

Both these laboratories have large caseloads that are potentially amenable to IR analysis. Each of the laboratories expressed the desire to increase the utility of their IR instruments.

As Figure 4 indicates, we have utilized several methods (direct wire, dial data set, direct wire data set) of attaching the computer terminals to the B6500 system. Each of these methods provides the laboratory with access to the file any time the NYSIIS computer is operating. The communications aspects of the system are flexible and have been implemented with the advice of the New York State Office of General Services which operates a statewide telephone network for state agencies through Bell System facilities.

B. Operational Features

Figure 5 is a sample of typical input and output for a computer search of infrared data.

Duncan Erley of the Dow Chemical Company describes the philosophy and details of the search program in an article published in *Analytical Chemistry* in May, 1968, "Fast Searching System for the ASTM Infrared Data File." Modifications of the program for this pilot project have not been in the technical aspects of the search, but in the area of making the search more convenient for use in the forensic application. For instance, the NYSIIS system outputs not only the serial number of the potential "hit," but also the chemical name of the compound. This eliminates a previously tedious chore of manual lookup in an index.

Currently, the program cannot be utilized by more than one laboratory at a time. This has been no problem with only two users, but could potentially be a problem when additional laboratories are added to the system. We are currently working on the necessary programming changes to allow simultaneous use by more than one laboratory.

All file editing functions are performed by Criminalistics Research Bureau personnel through its terminal. A major addition to the file has been the inclusion of forensic laboratory IR standards. Both cooperating laboratories have provided their own standards which have been entered into the file by NYSIIS.

C. System Cost

1. File and Program

The initial file and program fee was $2,500. This provided the basic ASTM data file as used by Dow and the search program. A subsequent purchase was made of a tape of

compound names and molecular formulas for $1,100. As stated previously, the initial fee was negotiated. The name tape was provided by ASTM for their standard rate. Additional file update tapes may be purchased as they are produced by ASTM for approximately $200.

2. Computer Terminal

The Dow-ASTM system was written to accommodate model 33 teletypewriters. However, we were able to substitute the Burroughs TC500 terminal computer under the terms of the NYSIIS contract for the Burroughs B6500 computer system. This enabled us to provide a reliable terminal with potential off-line laboratory uses for approximately $160 per month. The TC500 prints at double the character speed of the TTY and provides buffered input and output registers. This helps to conserve main computer processing time and provides rapid printout for long lists of chemical names.

3. Communications

a. State Police Terminal

	Cost/Mo.
Burroughs Data Sets – 2 at $16/mo.	$ 32.00
Telephone Line	8.00
Adaptor for B6500	45.00
Total/Mo.	$ 85.00

b. New York City Medical Examiner's Terminal

	Cost/Mo.
Bell System Data Sets – 2 at $48/mo.	$ 96.00
Telephone Line (NYS Tie Line)	44.00
Adaptor for B6500	45.00
Total/Mo.	$185.00

Currently, the cost of operating the system is shared between NYSIIS and the user agencies. NYSIIS provides file storage, search and update while the laboratories reimburse NYSIIS for terminal and communication costs.

One of the major goals of the pilot project is to document laboratory experience in using the data file system. Section IV provides an evaluation of the system from the viewpoint of each of the cooperating laboratories.

LABORATORY EVALUATION OF THE SYSTEM

A. State Police Laboratory*

During the period of the pilot project, NYSIIS has provided the State Police Laboratory with a Burroughs TC500 computer terminal, telephone communications lines, a search program, access to the infrared data file and computing time on the Burroughs B6500 computer system. Training in the use of the equipment and other technical services were also provided by the CRB and NYSIIS programming staff.

The State Police Laboratory provided technical personnel to perform file searches in both test and production modes. These personnel were asked to evaluate systems from the viewpoint of the operating forensic science lab and to provide input to NYSIIS Criminalistics Research Bureau personnel so that appropriate systems modifications could be designed.

An initial test series of 100 tests, conducted by two Senior Chemists with considerable infrared experience, soon established that the search program could, in fact, make "hits" on samples commonly encountered by forensic laboratories. This test series also served to furnish a genuine sense of confidence to all of the program participants.

Since the initial test period, the file has been used on about 150 actual forensic cases, representing approximately 400 searches. Fifty-five unknown samples were identified which would not have been identifiable without the aid of the program.

The types of compounds that have been identified have varied greatly. It has been successful in identifying many narcotics and dangerous drugs and has been used in toxicology for the identification of poisons. Success has also been achieved in the area of paints, dyes, pigments and polymers. It has also been useful in the identification of components of bombs and various high explosives. The system has, in fact, been used in practically every area of the laboratory.

The following illustrative examples serve to document the program's usefulness.

Case 1: A 50 year old chemistry professor was found dead in his car. Found with him was a glass containing what appeared to be some type of whiskey. An acid extraction and a subsequent IR analysis was performed on the liquid. A computer search on the IR spectrum identified the unknown as Chloral Alcoholate. Extraction of stomach contents of the deceased and subsequent IR spectrum computer search identified the unknown to be chloral. A visual comparison of the unknown curves with curves of chloral alcoholate and chloral confirmed the computer identification. Thus, the cause of death was determined by the search program and would not have been possible without it.

Case 2: An unknown white colored substance was turned over to the State Police as being a suspected explosive. An IR analysis and computer search were performed. The substance was identified by the program as being TNT. Subsequent visual comparison with a spectrum of TNT confirmed the identification.

Case 3: A suspected clandestine drug laboratory was raided by local police. The program helped identify eight chemicals used in the synthesis of illicit drugs.

The program has assisted many times in giving an indication that the unknown is of a particular type or class of compounds. While there is no positive identification, the type or class of the compound may offer investigative leads in solution of a case.

One of the most important outcomes of the pilot project has been the development of a

* Extracted from Interim Evaluation Report provided by New York State Police Scientific Laboratory.

systematic approach to performing a search on an unknown spectrum. It has been found that if an analyst starts with a minimum of IR data and adds additional data gradually he can carefully and accurately narrow down to a positive identification. This approach will help minimize discrepancies in two different IR curves of the same compound produced by different people on a different instrument.

Techniques of sorting out suspicious peaks, which may be due to solvents, have proven to be successful. The calling up of stored data on potential "hits" can lead to finding file errors due to coding or instrumental problems. This may lead to an identification by eliminating erroneous bands.

The success of the search also can depend on the operator's experience and knowledge of IR spectroscopy. An experienced operator can recognize any suspicious bands and can interpret group frequencies to aid in the search.

Thus, with a reasonable amount of training to familiarize the operators with the program, a very sophisticated searching procedure can be used which greatly increases the effectiveness of the IR search program.

B. Medical Examiner's Laboratory*

The concept of central files is not only invaluable in toxicology, but also in all scientific work involving criminal investigations. In the limited time the tie line between our laboratories has been in operation, we have had positive computer findings on many samples of material whose identity was unknown to us at the time. Computer data provided confirmation of suspected identity and, of equal importance, ruled out substances which our previous testing had indicated. Information that a chemical substance is not what is suspected can sometimes be just as important as positive identification.

With regard to IR in combination with gas chromatography, I would estimate that the overall effectiveness of IR would be increased by a factor of three to four. The major problem in identifying chemicals isolated from tissue and body fluids with IR is purity of the sample. With IR following gas chromatography, much better specimens would be analyzed. The limits would depend on the limiting sensitivity of the micro-technique employed.

In view of the success of the pilot program and the potential for further development of the central file concept, I incorporated $3,000 into the laboratory budget which becomes available in July 1972 for maintaining the TC500 terminal and associated telephone lines.

The present system for file maintenance works very efficiently. In my opinion, laboratory programming is a highly specialized science and could not be justified as a function for our laboratory. Nor do I see the need for other than a centrally operated location available to a number of laboratories. Our laboratory doesn't have time nor the personnel to maintain even a rudimentary cabinet filing system. The problems of work overload and limited personnel is universal in all technical organizations that I know of neither our staff, which is the largest, nor the staffs of any of the others in this field, has the time for programming even if they had the expertise.

As previously discussed, computerized data for toxicology should be expanded to include ultraviolet spectrophotometry, gas chromatography, thin layer chromatography and micro-color reactions.

Based on the operational experiences accrued over ten months' operation of the pilot system, certain conclusions have been drawn by the participants. These are presented below.

CONCLUSIONS BASED ON OPERATIONAL DATA

1. The system, as it presently exists, is of definite assistance in forensic infrared data interpretation. Its real value has not been to speed up routine cases, but rather to provide an extended capability in those cases which involve new or unfamiliar problems.
2. The program is easy to use and usually leads to a meaningful answer within ten minutes after the unknown data is obtained from an infrared spectrophotometer.
3. The nature of forensic laboratory work requires ready access to the infrared file, thus the central computer system must be available for searching when the analyst requires it.
4. The State Police indicate that their estimated normal use of the infrared search system will be from 30 to 40 cases per month, requiring from 100 to 120 actual searches of the file per month.
5. One of the key issues in development of this program was to determine if an efficient and effective working relationship could be developed and maintained between NYSIIS and the cooperating laboratories. Since the development and maintenance of this type of system requires considerable systems design and programming efforts, a close liaison must be maintained between the user and central service. This liaison is also important because troubleshooting systems problems and their solution is one of the important functions of the central agency. All operational experience attests to the close working relationship that has been developed and the desirability of maintaining this relationship.
6. Modifications should be made in the search program to make it more "forgiving" when erroneous search data is entered. As the program is constructed now, fifteen correct items and one incorrect piece of data will result in a miss. If the program were more flexible, our "hit" rate would be increased.*

* Extracted from Interim Evaluation Report provided by New York State Police Scientific Laboratory.

*An improved version of the original search program is currently commercially available.

7. To confirm an identification, the examiner should have available a "hard copy" of the standard infrared curve for use in a visual comparison with the unknown curve.
   There is no access to such a hard copy with the present system. Although our laboratory maintains some hard copies of selected infrared spectra, the retrieval operation for those curves is cumbersome and represents the greatest time loss in the system. Thus, a major improvement in the system would be for laboratories to have access to hard copies of all the standards in the file through an automatic or semi-automatic retrieval system. With such a system, the actual copy of the known infrared spectrum could be rapidly compared with the unknown spectrum -- making confirmation of identification a simple matter.
8. The concept of storing scientific data relevant to the forensic sciences in a computer and retrieving it when needed is certainly feasible. File effectiveness would be greatly enhanced if additional files could be created to store additional data such as: ultra-violet data, gas-liquid and thin-layer chromatography data, color and crystal test data. These different types of data could then be correlated into a complete cross-referenced master search and retrieval program.

The foregoing has described the operation of a pilot computerized infrared data file system as applied to the needs of two forensic science laboratories in New York State. Future development of the system will be to provide the service for all laboratories that express a need and can share in the cost. The central file concept will also be further developed using the conclusions reached during the pilot project as a guide.

NOTICE

The work described in this paper has been assisted in part by the Law Enforcement Assistance Administration's National Institute of Law Enforcement and Criminal Justice. Grant Number NI 70-065-PG-17, *"Pilot Computerized Infrared Data File,"* authorized by the Omnibus Crime Control and Safe Streets Act of 1968 supported purchase of the data file and implementation of the current system. The conclusions expressed herein do not necessarily represent the opinions of the government of the State of New York nor the government of the United States of America.

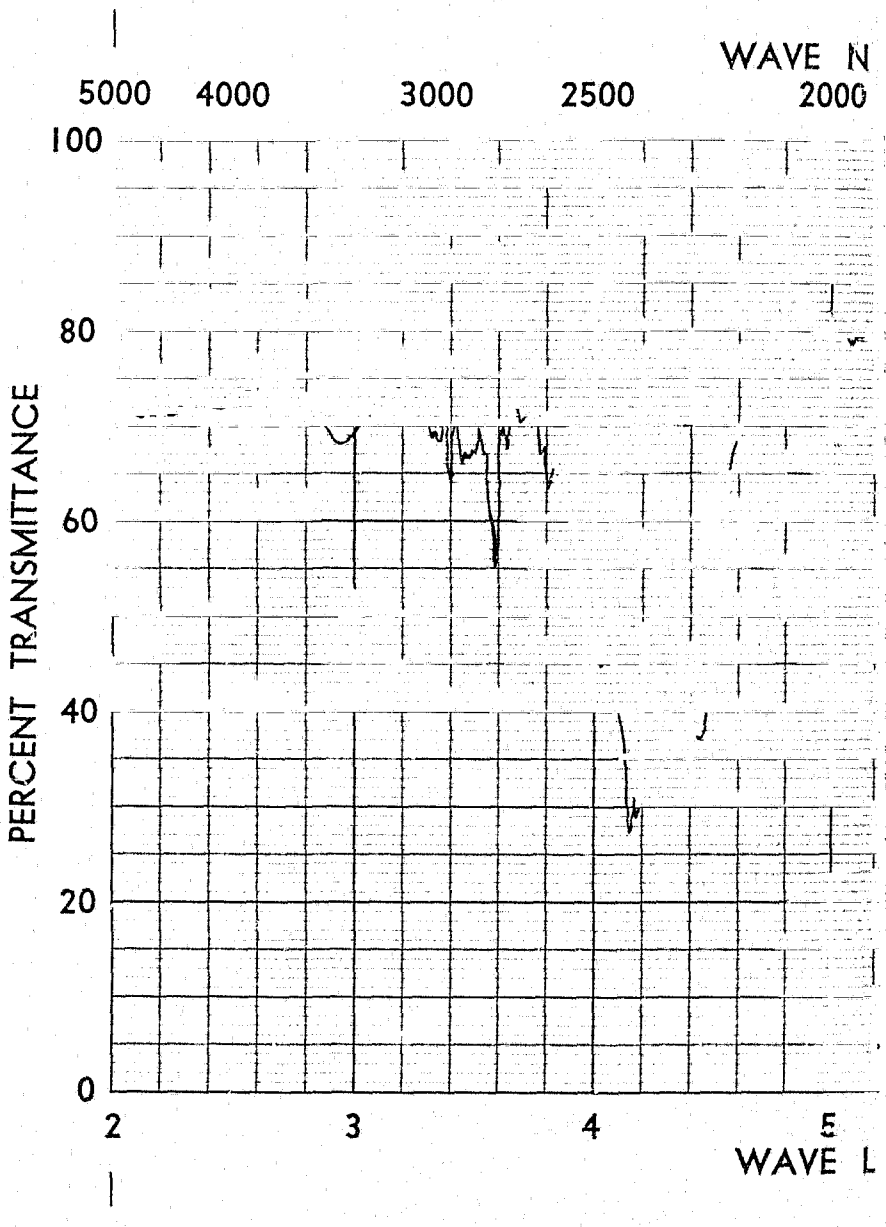
REFERENCES

1 O.L.E.A. Project No. 013, "Study of Needs and the Development of Curricula in the Field of Forensic Science," Dr. Alexander Joseph, John Jay College of Criminal Justice, the City University of New York.
2 "Planning Study for Evaluation of Forensic Laboratory Services in Erie, Niagara and Wyoming Counties, New York," Cornell Aeronautical Laboratory, Inc., Grant from the New York State Office of Crime Control Planning.
3 "Computerized Data Files for Forensic Science Laboratories: A Utility Study," Arthur D. Little, Inc., under contract to the New York State Identification and Intelligence System.

I. R. SPECTROPHOTOMETER
NaCl PRISM

NO. E. BUNGARO				
DATE 6/30/71		INDEX		
SAMPLE CHLORCYCLIZINE HCL (43574) (BURROUGHS WELLCOME)				
FROM ST.				
SAMP. CELL# KB/ MM			CMS.	
REF. CELL NaCl MM			CMS.	
CHEM.		MG.		MG.
SOLV.			1,2 dichloroethane	
VOL.	C.C.	%	C.C.	%
F.S.	SOLID	°C.	GAS	MM

BAIRD ASSOCIATES, INC.
CAMBRIDGE, MASS., U.S.A.
1029-9



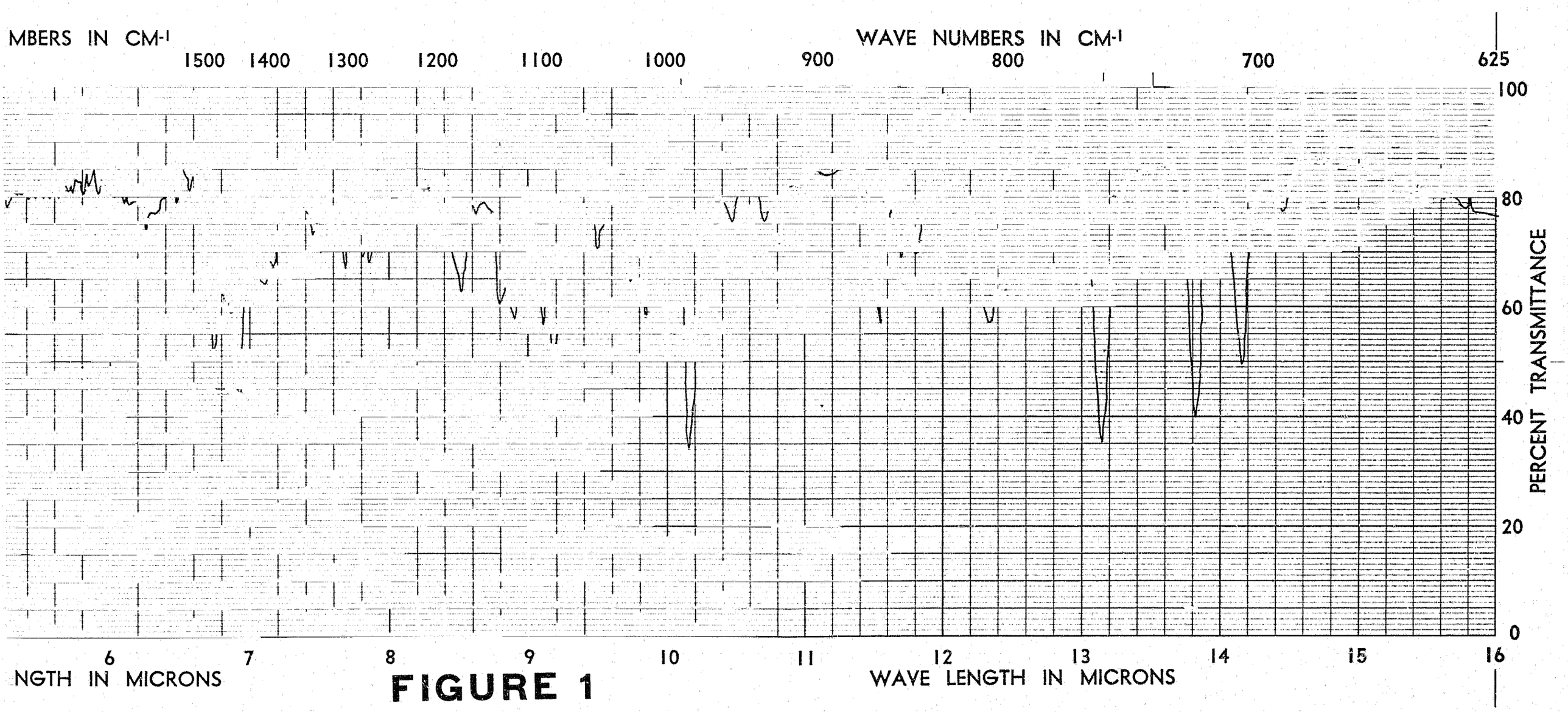

MBERS IN CM-1
1500
1400
1300
1200
1100
1000
900
WAVE NUMBERS IN CM-1
800
700
625
100
80
60
40
20
0
PERCENT TRANSMITTANCE
6
7
8
9
10
11
12
13
14
15
16
NGTH IN MICRONS
WAVE LENGTH IN MICRONS

FIGURE 1

SCHEMATIC DIAGRAM OF AN IR SPECTROPHOTOMETER

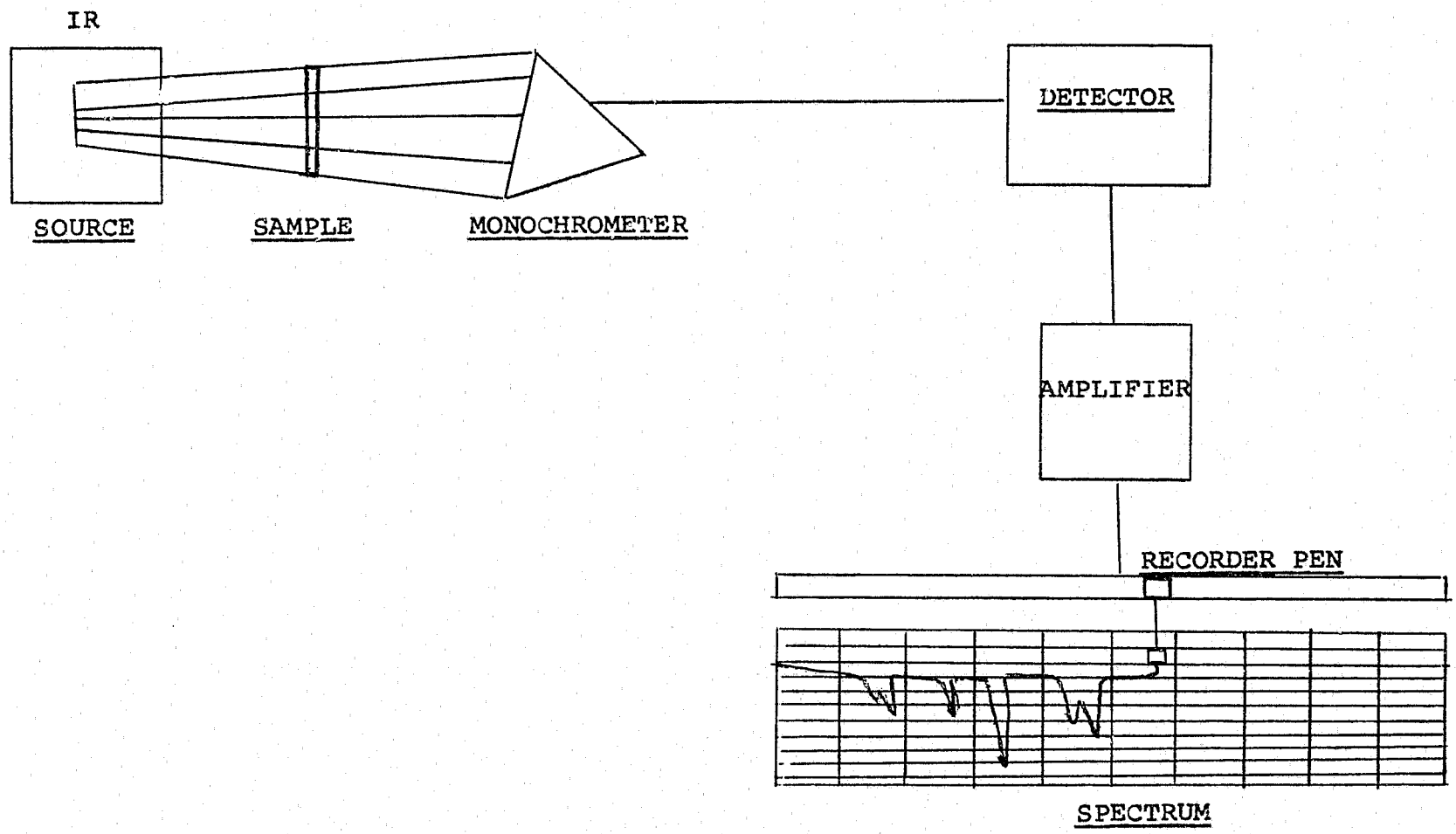
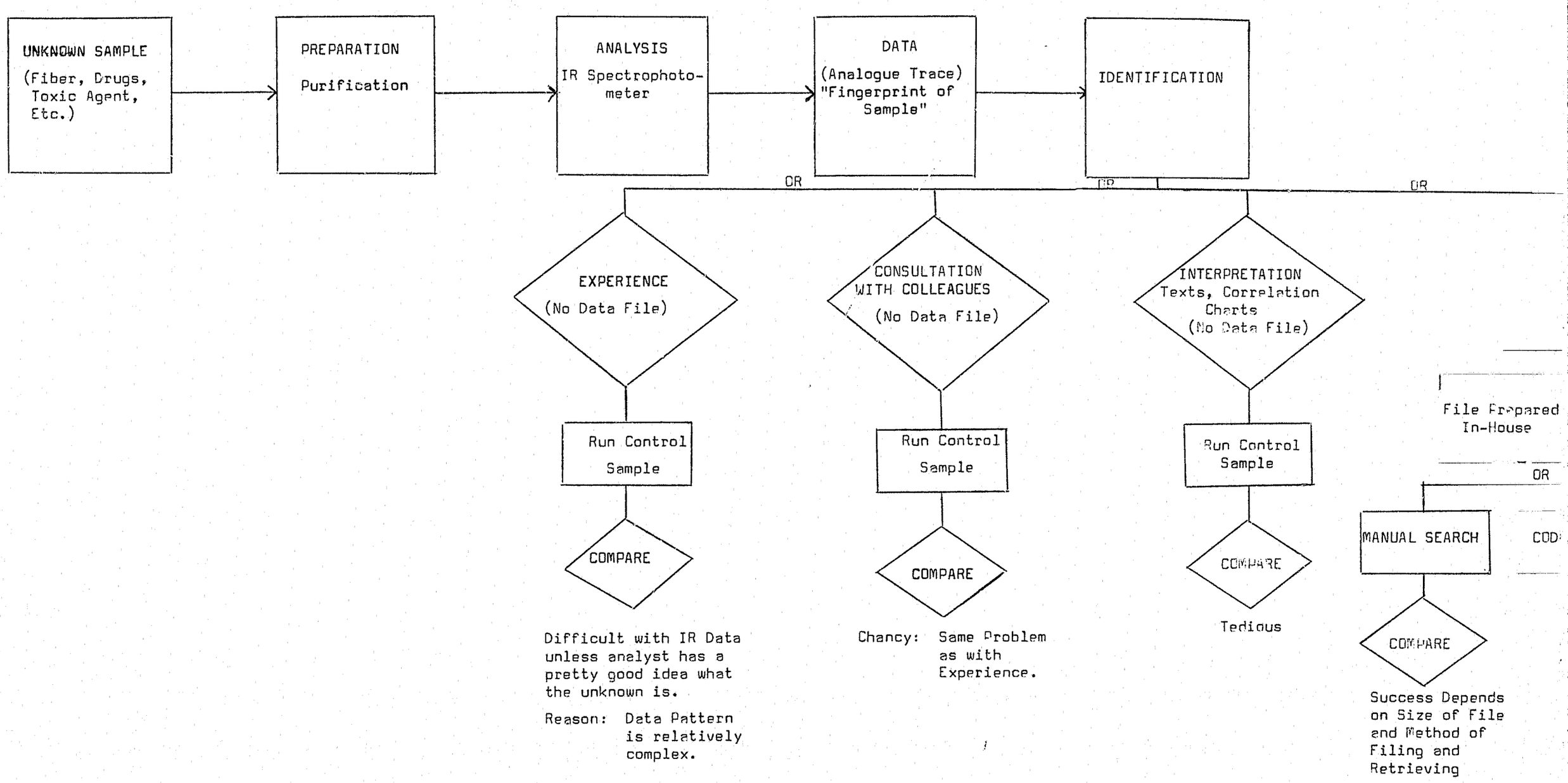
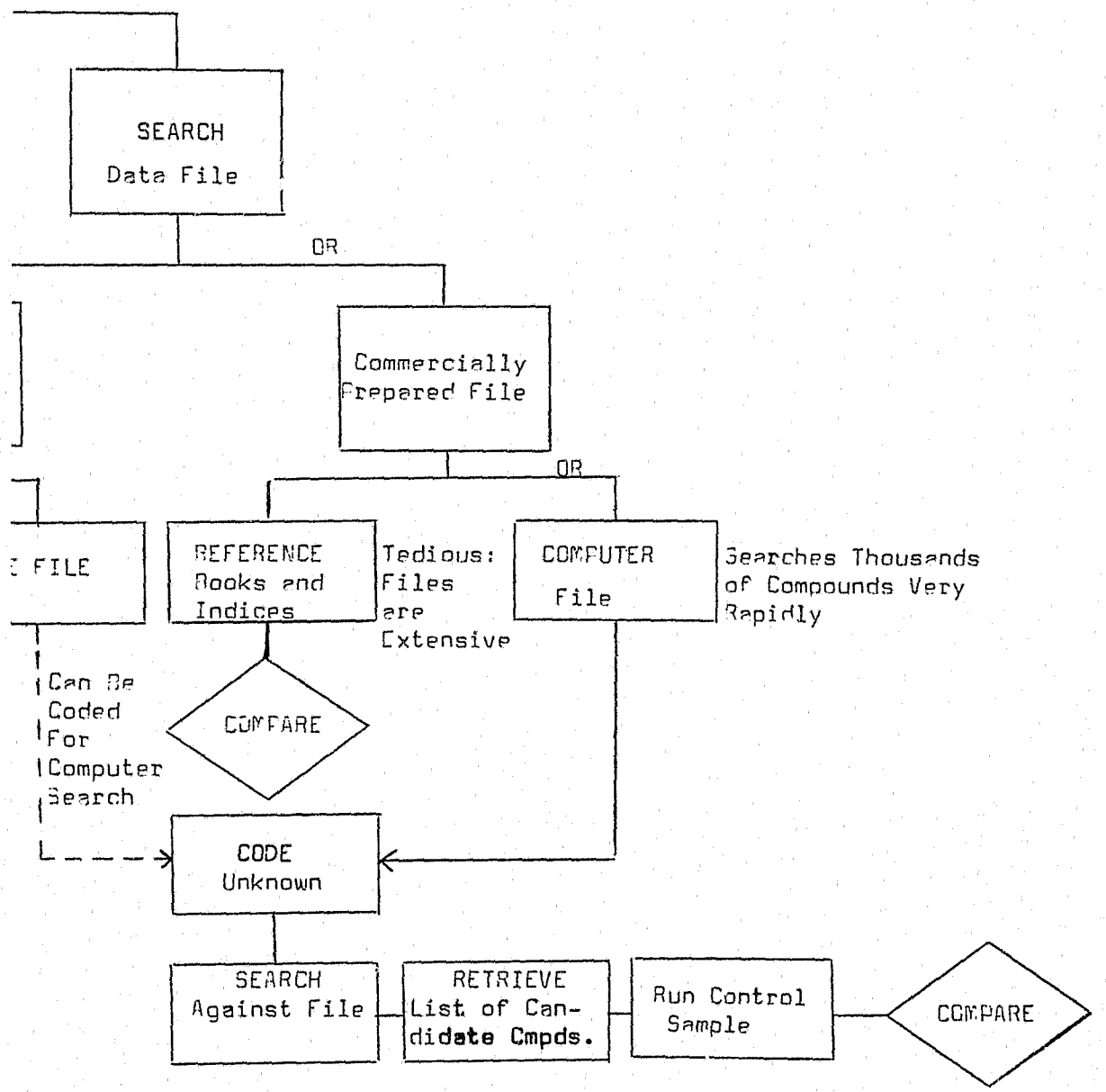


FIGURE 2



UNKNOWN COMPOUND ID PROCESS USING INFRARED

FIGURE 3


SEARCH
Data File
OR
Commercially
Prepared File
OR
FILE
REFERENCE
Books and
Indices
Tedious:
Files
are
Extensive
COMPUTER
File
Searches Thousands
of Compounds Very
Rapidly
Can Be
Coded
For
Computer
Search
COMPARE
CODE
Unknown
SEARCH
Against File
RETRIEVE
List of Can-
didate Cmpds.
Run Control
Sample
COMPARE

```
INFRARED FILE SEARCH PROGRAM          09/11/72
DO YOU WANT PROGRAMMATIC INSTRUCTIONS--YES OR OCK


SAMPLE...
DEMONSTRATION SEARCH                    OPERATOR ENTRIES UNDERLINED
GROUPS AND BANDS PRESENT
6.2 6.5 6.9 7.3 7.4 7.7 7.9 8.0 8.2 8.5 9.2
GROUPS ABSENT. NO BAND REGIONS


INPUT DATA
GROUPS
**** NO DATA ****
BANDS
 6.2  6.5  6.9  7.3- 7.4  7.7  7.9- 8.0  8.2  8.5  9.2
NO GROUPS
**** NO DATA ****
NO BANDS
**** NO DATA ****
OPTION...
1                    SEARCH OPTION
SUBFILES...
CR.
TOTAL MATCHING 11-WORD RECORDS =      17
NUMBER OF UNIQUE SERIAL NUMBERS SAVED FOR REPRINT =      10
OPTION...
2                    HITS RESULTING FROM SEARCH
WHAT STARTING POINT - 3 DIGITS
001
00088CR        METHYLENE-BIS-/4-HYDROXYCOUMARINE/,3,3PR

00101CR        CARBAMATE, 2-HYDROXY-3-O-METHOXY-  PHENOXY-PROPYL

00163CR        CODEINE ALKALOID

00270CR        ESTRATRIEN-3-OL-17-ONE, 1,3,5/10/-

00277CR        PHENOTHIAZINE, 10-/2-DIETHYLAMINO- PROPYL/-, HCL

00311CR   1,2-PROPANEDIOL, 3-/O-METHOXYPHENOXY/-

00324CR        PHTHALAZINE, 1-HYDRAZINO-,  HCL

00555CR        PHENOTHIAZINE, 2-CHLORO-10-/3-/1-  METHYL-4-PIPERAZINYL/PROPYL/

00578CR        PHENOTHIAZINE, 10-/2-/1-PYRROLIDYL/ ETHYL/-,  HCL

00724CR        ETHANOL, 1-/P-BETA-DIETHYLAMINO-    ETHOXYPHENYL/-1-/P-TOLYL/-2-


OPTION...
4                              ALTER DATA OPTION
GROUPS AND BANDS PRESENT
6.2 7.6 10.3                   CHANGED DATA
GROUPS ABSENT. NO BAND REGIONS
8.8-9.0                        CHANGED DATA


INPUT DATA
GROUPS
**** NO DATA ****
BANDS
 6.5  6.9  7.3- 7.4  7.6- 7.7  7.9- 8.0  8.2  8.5  9.2 10.3
NO GROUPS
**** NO DATA ****
NO BANDS
 8.8- 9.0
OPTION...
1                    NEW SEARCH
SUBFILES...
SP.                  DIFFERENT SUBFILE
TOTAL MATCHING 11-WORD RECORDS =       4
NUMBER OF UNIQUE SERIAL NUMBERS SAVED FOR REPRINT =       2
OPTION...
2
WHAT STARTING POINT - 3 DIGITS
001
00128SP  D.B.-AMOBARBITAL(FREE ACID)

00193SP  D.B.-PSILOCYBIN


OPTION...
7
TIME FOR SAMPLE:
DEMONSTRATION SEARCH
006 MIN 08 SEC ELAPSED.  000 MIN 02 SEC PROCESS.  000 MIN 05 SEC I-O.

OPTION...
8

END OF PROGRAM..
```

Figure 5

CURRENT

SYSTEM CONFIGURATION

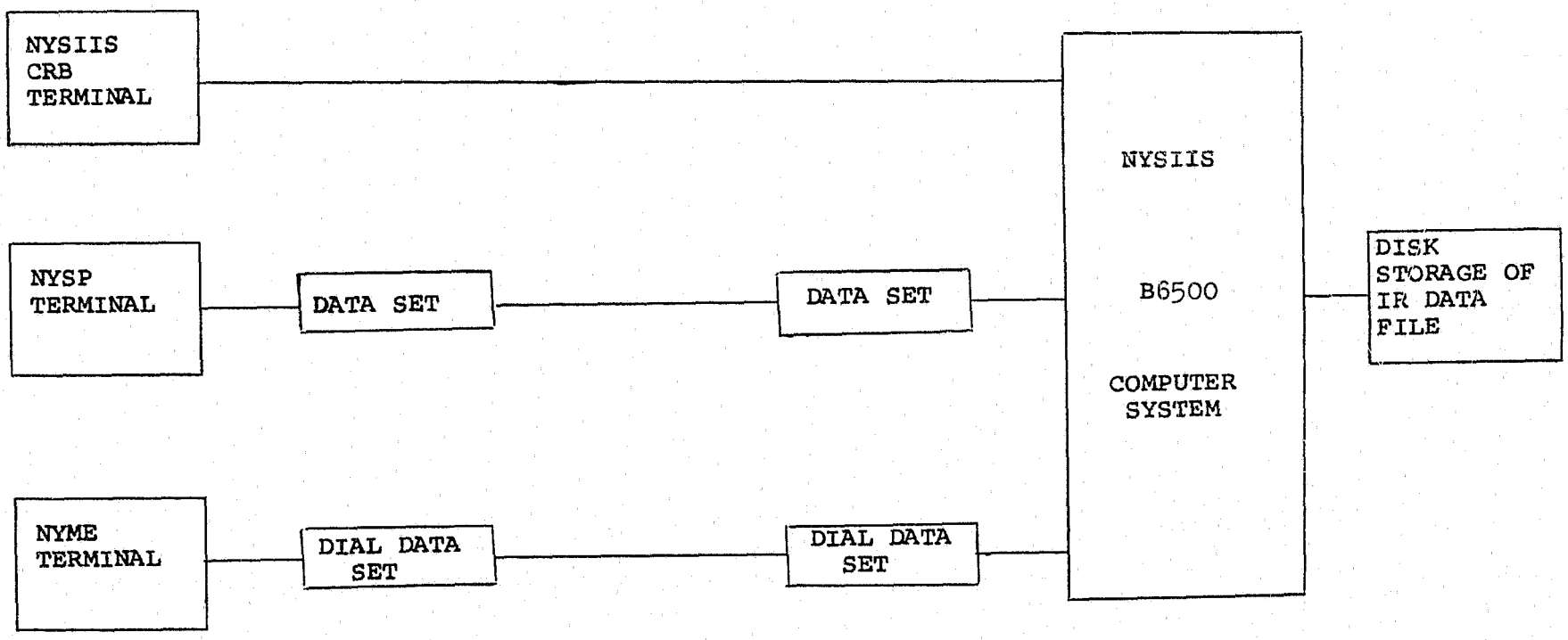


FIGURE 4

```
INFRARED FILE SEARCH PROGRAM          09/11/72
DO YOU WANT PROGRAMMATIC INSTRUCTIONS--YES OR OCK


SAMPLE...
DEMONSTRATION SEARCH                          OPERATOR ENTRIES UNDERLINED
GROUPS AND BANDS PRESENT
6.2 6.5 6.9 7.3 7.4 7.7 7.9 8.0 8.2 8.5 9.2
GROUPS ABSENT. NO BAND REGIONS


INPUT DATA
GROUPS
**** NO DATA ****
BANDS
 6.2  6.5  6.9  7.3- 7.4  7.7  7.9- 8.0  8.2  8.5  9.2
NO GROUPS
**** NO DATA ****
NO BANDS
**** NO DATA ****
OPTION...
1                    SEARCH OPTION
SUBFILES...
CR
TOTAL MATCHING 11-WORD RECORDS =      17
NUMBER OF UNIQUE SERIAL NUMBERS SAVED FOR REPRINT =      10
OPTION...
2                    HITS RESULTING FROM SEARCH
WHAT STARTING POINT - 3 DIGITS
001
00088CR        METHYLENE-BIS-/4-HYDROXYCOUMARINE/,3,3PR

00101CR        CARBAMATE, 2-HYDROXY-3-O-METHOXY-  PHENOXY-PROPYL

00163CR        CODEINE ALKALOID

00270CR        ESTRATRIEN-3-OL-17-ONE, 1,3,5/10/-

00277CR        PHENOTHIAZINE, 10-/2-DIETHYLAMINO- PROPYL/-, HCL

00311CR   1,2-PROPANEDIOL, 3-/O-METHOXYPHENOXY/-

00324CR        PHTHALAZINE, 1-HYDRAZINO-,  HCL

00555CR        PHENOTHIAZINE, 2-CHLORO-10-/3-/1-  METHYL-4-PIPERAZINYL/PROPYL/

00578CR        PHENOTHIAZINE, 10-/2-/1-PYRROLIDYL/ ETHYL/-,  HCL

00724CR        ETHANOL, 1-/P-BETA-DIETHYLAMINO-    ETHOXYPHENYL/-1-/P-TOLYL/-2-


OPTION...
4                    ALTER DATA OPTION
GROUPS AND BANDS PRESENT
6.2 7.6 10.3         CHANGED DATA
GROUPS ABSENT. NO BAND REGIONS
8.8-9.0              CHANGED DATA


INPUT DATA
GROUPS
**** NO DATA ****
BANDS
 6.5  6.9  7.3- 7.4  7.6- 7.7  7.9- 8.0  8.2  8.5  9.2 10.3
NO GROUPS
**** NO DATA ****
NO BANDS
 8.8- 9.0
OPTION...
1                    NEW SEARCH
SUBFILES...
SP                   DIFFERENT SUBFILE
TOTAL MATCHING 11-WORD RECORDS =       4
NUMBER OF UNIQUE SERIAL NUMBERS SAVED FOR REPRINT =       2
OPTION...
2
WHAT STARTING POINT - 3 DIGITS
001
00128SP  D.B.-AMOBARBITAL(FREE ACID)

00193SP  D.B.-PSILOCYBIN


OPTION...
7
TIME FOR SAMPLE:
DEMONSTRATION SEARCH
006 MIN 08 SEC ELAPSED.  000 MIN 02 SEC PROCESS.  000 MIN 05 SEC I-O.

OPTION...
8

END OF PROGRAM..
```

Figure 5

END