tration, they are actually printed on separate pages, so that the report can be submitted directly to management.

Figure 8c illustrates a query for all compounds distributed to outside investigators in 1970 for testing "erythrocyte ghosts." Again, INQUIRE formatting instructions produce a custom report.

The inventory history file report is printed after each update and is used, as are the INQUIRE data base reports, as a desktop search tool and computer backup. An example of the report is given in Figure 9, which also shows the provision for including handling precautions within the file.

CHEMICAL NAME Data Base. This date base, which is a module of the Squibb Chemical Structure/Biological Data System, will not be discussed here, because its only use in the CHAUD System is to provide input of standardized chemical names.

FUTURE DEVELOPMENTS

It is planned that the CHAUD System will eventually function as one module of Squibb's Research and Development Information System (RADIS). RADIS was conceived as a "total" scientific information system for Squibb, and is being implemented stepwise as a series of modular data bases containing chemical, biological, and textual information for all Squibb compounds. These modules will eventually be linked via the standardized Squibb compound number, and queries will have access to all necessary data bases for providing answers.

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A Computer-Based Comprehensive Bio-Data Information Retrieval System*

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A card-oriented biological data information system, programmed for a UNIVAC 1050 computer, suffered from a lack of flexibility. When IBM 360 equipment was acquired, it became both necessary and desirable to convert to the new equipment. Initial evaluation of requirements estimated that 3 to 4 man-years would be required to develop new systems and write necessary programs. To reach our goals at substantially less expense and at a more rapid pace, a decision was made to purchase a commercially available data management system called INQUIRE. Problems encountered in conversion from one system to the other are discussed. Data formats, input-output procedures, search strategies, etc., are described.

The Technical Information Service Group (TIS) of the Science Information Services Department at Warner-Lambert Research Institute is responsible for processing internally generated research information. The assignment is far greater than mere storage and retrieval of proprietary data. Personnel in TIS are required to coordinate and correlate various bits and pieces of intelligence received from many local and distant research facilities in all permutations and combinations that can be imagined. Such a task is impossible without the aid of a staff endowed with phenomenal memories or a most complete set of storage, search, and retrieval tools.

An early system developed for retrieval of biological data at TIS used McBee edge-notched card.[1] By its nature, the card limited the number of test procedures that could be recorded. Absolute numbers for dose and resulting raw data were not possible; card format restricted evaluative information to arbitrary ranges. Once a series of compounds meeting the requirements of a search were located, a somewhat similar card system was available for finding additional related compounds.[2] A next step was implementation of a system based on internally punched cards—the Hollerith-coded IBM card.[3]

In this system, basic 80-column tabulating cards were formatted with fixed-fields to handle three types of data. The first format handled measured animal dose-response data from fixed testing procedures. A second type of card layout rated subjective observations or scored data for behavioral effects from standard score sheets. Evaluation data from nonroutine testing procedures, devised or modified to bring out the particular properties of a compound in advanced development, were reported in technical reports.

These cards were used in and by themselves with card sorting equipment and an IBM 026 or 870 document writer. At a later stage in developing our systems approach to

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information retrieval, these cards were imaged on magnetic tape for searching in a UNIVAC 1050 environment.

The UNIVAC system, however, had become inadequate and was frustrating to use. At the time of its inception, the initial computer system was most adequate. Already-existing punched cards were on magnetic tape with added information for output editing and formatting. At that time, by preparing the data base in this manner, an extremely rapid input of existing information was achieved. It was limited in scope, however, because data were arranged with all the limitations of the 80-column punched card. With passage of time and use, the system—cards and tape—became complicated by unconventional use of card columns. For example, suppose that although cc 38–42 were reserved for specific information—animal species—but one test procedure has no species entry, then this space, cc 38–42, would be "borrowed" for some entirely different type of information. It was no longer possible to state unequivocally that a given area in a printout was dedicated to a single class of information. Each test procedure printout developed its own set of peculiarities. Add to these complexities the ministrations of an itinerant programmer who departed before he could document his efforts and you can readily understand how the system became most frustrating to use.

Considering the next stage of system development, the information we had to work with existed in three forms. First, there were original laboratory report forms and documents; next were punched cards prepared from original laboratory reports and finally, a set of UNIVAC 1050 computer magnetic tapes. If we were to create a new system and new programs, how would we generate the new data base? We refused to consider repunching cards from original reports; there were hundreds of thousands of cards already punched. Further, rekeying information was anathema because a new and different card layout would depend on software considerations which, in turn, would impose further manpower effort and consequent delay in implementing a new system. We hoped, therefore, that whatever was planned could use our punched cards, arranged in test number order or our existing magnetic tapes, the latter consisting of an arrangement of punched card images in compound number order.

A preliminary examination of our needs with an outside consultant indicated a requirement of at least 18 calendar months of work before we could be operational—and then only with an expenditure of some 3 to 4 man years of effort and costs. The most dismal aspect, however, was the prospect of continuing frustration from the current inadequate system.

Management considered a number of proprietary programs; one of these was INQUIRE, a data management system produced, marketed, and supported by Infodata Systems, Inc., of Rochester, N. Y. The User's Guide describes the system as:

> ". . .a question-oriented information storage and retrieval system which allows the user to maintain and make effective use of a large body of information."[4]

The user of INQUIRE asks questions in his own language; he has no need to concern himself with computer or program. The system itself consists of programs for locating and retrieving specific items of information; organizing and formatting information; adding, deleting, or changing information in the file; and administratively controlling and monitoring the use of the file. Another way of describing the INQUIRE System would be that it consists of a set of programs which create, maintain, and access data files. The system is written in PL/1 and runs in an IBM OS/360 or 370 environment, model 40 or larger. For details on the operation of the INQUIRE system, see the recent paper by Starker *et al.*[5]

Conversations with Infodata personnel, as well as other users of INQUIRE, indicated that INQUIRE might very well do what we hoped for; store information in random fashion, retrieve it in various combinations and print it in any desired format. Text searching, too, was possible, albeit relatively slowly, for specific words and parts of words. Detailed examination of our biological records by Infodata systems personnel indicated that our bio data could be input to INQUIRE from our magnetic tapes once they had been translated from UNIVAC language into IBM/360 language. It was admitted by Infodata that conversion of our Biological Data file from UNIVAC to INQUIRE would be one of the most difficult tasks that had been attempted to date. Because of the complexity of our data base, Infodata would have to allocate double the amount of time normally devoted to getting a customer's initial data base on line and functioning. Two weeks would be allowed!

Preliminary analysis on the part of TIS professional staff was devoted to individual biological test procedures. It was imperative that each information scientist be thoroughly familiar with all procedures performed in laboratories compared to written instructions for the test, how results were recorded on report forms and how test records appear on punched cards on magnetic tape files. Biological test protocols existed where route of administration of test material was specified as oral; punched-card records indicate that many were done parenterally. Because of space borrowing mentioned earlier, many unusual entries had to be reconciled. We found idiosyncrasies related to chronology. During one time period, test results were recorded in one manner, and, at another time, results were recorded in an entirely different manner on a different type of form. In general, all inconsistencies in data recording had to be pinpointed for each test so that all ambiguities in old UNIVAC records could be clarified. Only in this way could we hope to prepare for a smooth data conversion.

Next was the design of the INQUIRE record. INQUIRE processes and stores information in units called items. It was up to us to define an item by stating what it would contain and to determine when a second or even a third item would be created from a single UNIVAC record. An item was established as a record describing a single compound in a test procedure, administered by a particular route to a single animal species on a particular date, at a reported dose where the results are observed at some given time. A change in the value of any one of the above attributes would cause a new item to be generated.

In designing the new system, we had to remember that in addition to a great variety of biological test results in machine-readable form, there were also test data not yet converted into punched cards. We had also to provide for new procedures in the future. This added up to a requirement for an extremely flexible item format. No matter what type of initial design was conceived, we realized that it might need alteration during the course of our experience working with it. In any event, we hoped our design would be able to handle all data input, past, present, and future. To ensure this complete flexibility, we wanted a maximum number of descriptors. At the same time, we did not want printouts containing a vast number of descriptive names without value entries. We now feel that we have accomplished most of our basic design criteria.

It is through the various descriptors that we have been able to break up our data into a series of discrete compartments, or fields. An INQUIRE field may be either fixed or variable in length. Because a variable length field has an "overhead" of 8 positions, we limit its use to those fields longer than 8 positions and only for occasional use. Fixed-length fields have no "overhead" and are fields of choice for shorter, constant-use fields. We eventually decided on 21 major information fields, some of which were

sub-fielded. From our experience, these fields have served exceedingly well for both storage and search purposes.

Each of our major descriptive terms is a field name, and the datum that answers this description is the field value. In some instances, we have made these field names into keywords so that they may be retrieved more rapidly. Following are various field names that serve for input and retrieval.

ITEM is a number assigned to each record by INQUIRE that enables an individual record—an item—to be manipulated. No special input effort is required; it is automatic.

INDATE is a six-position fixed field containing the date a record was entered into the system. By searching from one INDATE to another, information can be supplied on a regular update basis.

TESTNO stands for test number. The five-position field is specially keyed for rapid search. Our tests are numbered with three digits and an optional letter. It would look like: TESTNO = 542G.

TESTNAME, or test name, is a 16-position fixed field containing an acronym or abbreviated name of the procedure. For many of our most active tests this name is inserted automatically. BRONCHODIL SCRN is our abbreviated name for bronchodilator screen.

COMPOUND, a 14-position fixed, keyed field, contains characters used to describe test materials. The over-all field is subdivided into various divisions, some of which are keywords for rapid, direct access.

SORTKEY is a 13-position required fixed field that is filled by the program without additional input effort. In this field, characters of COMPOUND are rearranged when items are being sorted into compound number order.

CHEMINIT is a 3-position fixed field that contains the initials of the chemist who first prepared a material. Through the use of this special field we can locate all information that has been gathered on a specific person's compounds.

RDATE—report date—is an 11-position fixed field that contains year, month, day, and sequence number of a report. Each unit of time is a subfield, enabling us to find, for example, all reports from a department from January through June of a given year. Sequence number is used to separate and identify multiple test reports on one compound done on the same day.

BATCH is a 16-position variable length field designed to hold the large string of characters used to identify some experimental formulations.

VEHICLE, a 12-position fixed field, contains a translation of the abbreviation for solvent. For example, TRAG is the input symbol for gum tragacanth, stored in the computer and printed out as TRAGACANTH.

DIET is an 8-position fixed field containing a description of the ration fed to the test animals.

TIME is allocated to 6 fixed positions that indicate when an observation or report was made. Positions 1–3 are numeric, while positions 4–6 represent an abbreviation of the units. It could look like: 003MIN for 3 minutes

AGENTORG is a 12-position fixed field that contains the name of the chemical agent or micro-organism with which the test compound must interact.

SPECIES is an 8-position fixed, keyed field containing the name of the test animal. Input is by abbreviation, translated internally by the preprocessor for storage and output.

ROUTE, another 8-position fixed, keyed field, contains route of administration. Here, too, input is an abbreviation, translated for storage and output.

DOSEU, units of dose, is an 8-position fixed field filled from a table after input of an abbreviation. For a number of tests these units are constant and specified, and can be input automatically by the preprocessor program.

ACTIVITY is a 16-position fixed field containing an over-all evaluation of experimental material as determined by the biologist. Although keypunched input may be an abbreviation, the entry will be translated for storage and later output.

DOSER, or reported dose, is an 8-position fixed field. It is right justified, with decimal in position 6 and any symbol for "greater than" or "less than" in position one. This field is not an arithmetic field; it is merely a character string and as such may not be used for comparison purposes.

An example would look like:

1 2 3 4 5 6 7 8	Field Positions
G 5 0 0 . 0 0	Data Entry

DOSES, or Dose S, is a 12-position fixed, numeric field, preprocessor-prepared by converting the character string in field DOSER into a number representing 10^{10} grams.

An example: DOSER = 511.00
DOSEU = MG/KG
DOSES = 00511000000

The field was designed to permit searches for ranges of doses or specific dose values. DOSER may be expressed as 0.5 mg./kg. or 500 mcg./kg., identical numerically. A search of field DOSER for the 500 mcg. dose would not find the 0.5 mg. one; hence, the DOSES, field.

R0 to R9, where R stands for response, is a series of ten 28-position fields, subfielded into label, value, and units position. The layout of this field is:

	1 12	1 8	1 8	Subfield Positions
Subfield Names	LABEL	VALUE	UNITS	
	1 12	13 20	21 28	Field Positions

For example, if R5 were to contain the ALD 50 dose of 670.00 mg./kg., it would look like:

R5	ALD50	670.00MG/KG
R51	ALD50	
R52	670.00	
R53	MG/KG	

The subfield VALUE can be further subfielded so that a symbol for "greater than" or "less than" can be entered.

TALLY is a 600-position variable-length field designed to contain a series of specific observations and responses, peculiar to a given test procedure. The value of this field to laboratory scientists is based, not on any single finding, but rather on over-all pattern or trend indicated by *all* observations and responses.

In some test procedures the biologist observes treated test animals for certain signs and symptoms or behavior patterns as listed on a check list. Observed responses are coded next to an observation name—the TALLY parameter.

A tally parameter name is never more than 12 positions in length; name is followed by a series of single alphameric characters that evaluate this parameter. Evaluation responses, in INQUIRE entry order, are:

Dose
Direction of Response
Onset
Duration
Degree

Although various combinations and arrangements of these five evaluations are found in a number of test procedures, no single test ever has used more than four of them. Regardless of order used on report forms, response evaluations must be in the above order for input to INQUIRE.

COMMENTS is another 600-position variable-length field that contains the text of the biologist's remarks. It may be searched for a particular word or phrase or a portion of a word. A COMMENTS field for a typical blood

pressure lowering experiment:

NO ACUTE B P LOWERING EFFECT IN THE NORMAL RAT. SEE RESEARCH REPORT 1234

These fields have proved adequate for all forms of biological data. If a DATUM cannot go into a RESPONSE field and is not in TALLY format, then it is entered as free text in COMMENTS.

The process for introducing biological data into INQUIRE begins with the protocol for the test. As each new protocol manuscript is received, it is processed according to the flow diagram (Figure 1). The manuscript is checked to ensure that instructions are complete and capable of being followed by a person knowledgeable in laboratory techniques. From the protocol, a report form is designed, and once details of both protocol and form are resolved, system input documentation is written. Concurrently, an abstract of the procedure is prepared to enable recipients of report forms to understand what was done and the meaning of reporting terms. Once documentation is accepted by Research Systems for preparation of a preprocessor program, keypunch instructions are prepared.

Preprocessors (PP) may be either test-dependent or test independent. If a particular test will have considerable activity—large numbers of reports each month—a program is prepared that will automatically input all constantly recurring information without keypunch effort. When test number (TESTNO) is read on input, the PP program will automatically insert certain information peculiar to that test in appropriate fields. These automatic

INQUIRE	INPUT NOTES
SPECIES (12) A prefix-keyed, 8-position fixed field containing the name of the test animal. Positions 1 - 3 = D O G	DOG is printed on the report form and is not keypunched. Input into this field is automatic via the preprocessor. In the event that DOG is crossed out and another species name entered, the override procedure is used. The test no. is keypunched in cc 01-05; the accession no. in cc 06-09 and the field no. (for SPECIES this number is 12) in cc 10-11. The name of the other species is then keypunched in cc 12 on as required.
ROUTE (13) Prefix-keyed, 8-position fixed field that indicates the route of administration. Positions 1 - 2 = P O	ORAL is pre-printed on the report form. No keypunching is required unless the override procedure is used.
D O S E U (14) An 8-position fixed field containing units of dose. Positions 1 - 8 = alpha	Keypunch the abbreviation as entered in the report. Preprocessor will translate on input as required. cc 12 - 19 = alpha

Figure 2. Sample of documentation

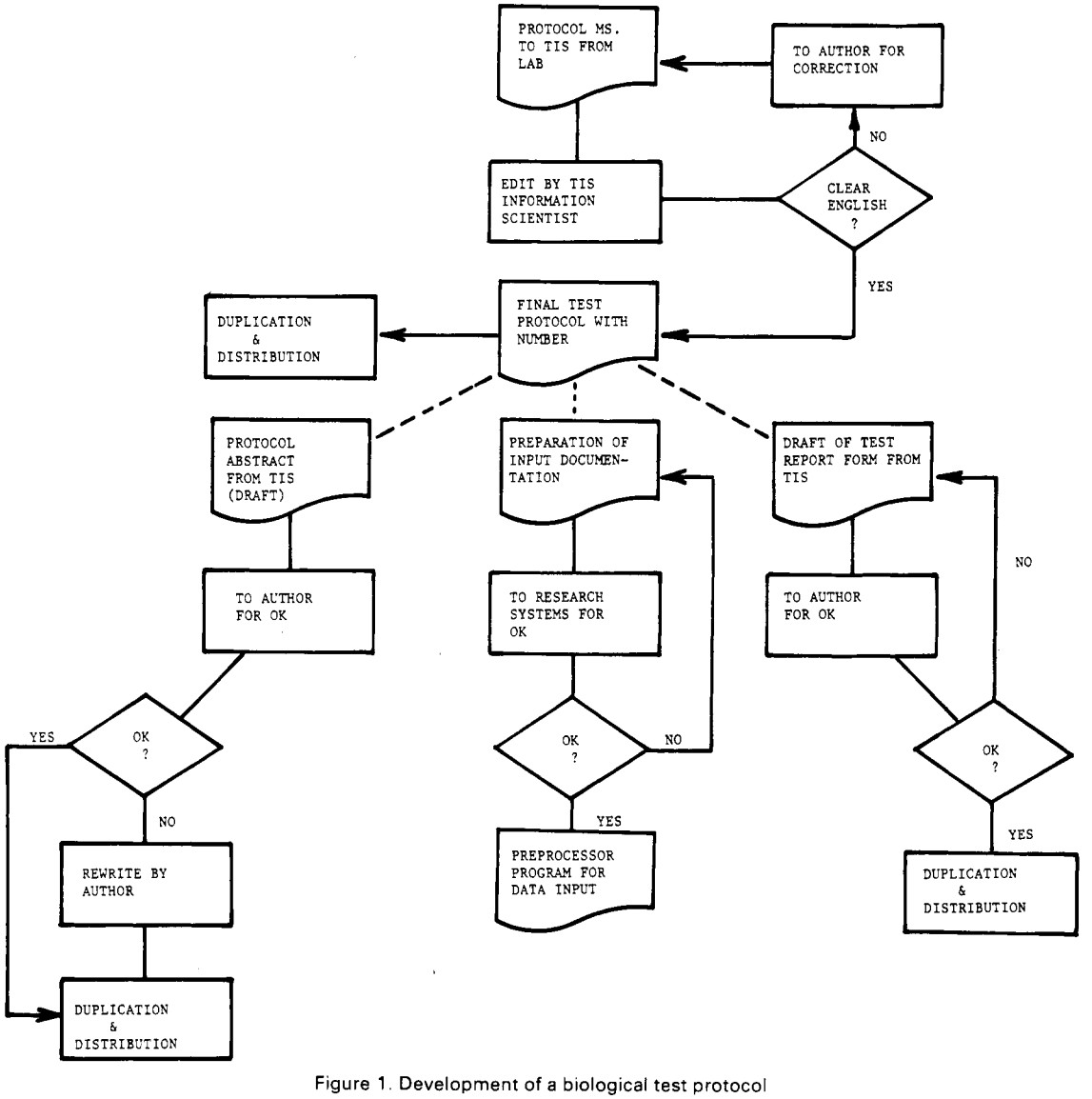

Figure 1. Development of a biological test protocol

RAPID QUALITATIVE
ANTIBACTERIAL-ANTIFUNGAL SCREENING
MICROBIOLOGY

COMPOUND (04): ▲W _____

TEST NO.
ANTIBACTERIAL – ▲500 _____ ACC. NO
ANTIFUNGAL – ▲502 _____ ACC. NO

ROUTE: IN VITRO

DATE (06) ___/___/___

TEST	ACTIVITY (15)	
500	▲ACTIVE ☐	▲INACTIVE ☐
502	▲ACTIVE ☐	▲INACTIVE ☐

N.B. REF _____

CHEMIST _____ (05) _____

COMMENTS (38-47): _____

TESTED BY _____ DATE _____ APPROVED BY _____ DATE _____

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Figure 3. Typical biological test report form

CHEMIST (05)

ACUTE TOXICITY – BEHAVIOR SCREEN
PHARMACODYNAMICS DEPARTMENT

TEST NO SPECIES
▲001 MOUSE _____ ACC. NO
▲001A RAT

COMPOUND (04) ▲W _____

DATE (06) ___/___/___

	DOSE (16)	UNITS (14)	ROUTE (13)	ACT (15)	COMMENTS (38-47)
ACC. NO	12 13 14 15 16 17 18 19	MG/KG	IP		
	12 13 14 15 16 17 18 19	MG/KG	IP		
	12 13 14 15 16 17 18 19	MG/KG	IP		
	12 13 14 15 16 17 18 19 ALD50 (18) 12 13 14 15 16 17 18 19	MG/KG	IP		

N.B. REF _____

EXPERIMENT _____

TESTED BY _____ DATE _____ APPROVED BY _____ DATE _____

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Figure 4. Typical biological test report form

options have a default feature; changes may be made. Thus, even though field SPECIES is nominally RAT for a given protocol, if hamsters are used on an occasion, this species can be input without effort.

Once the protocol has been approved and assigned a test number, documentation is written for preparation of the PP program. A portion of typical documentation is shown in Figure 2.

The PP is a special program that formats input material into INQUIRE Standard Input (ISI) so that it can be processed by the Data load program. Test-dependent (PP) are written so that input of test number will automatically cause certain information to be entered, even though it has not been keypunched. The sample of documentation in Figure 2 illustrates this automatic entry of information.

We have in our files considerable data resulting from test procedures that are no longer done. This information is, however, related to our current interests and to procedures now being done. To get this information into INQUIRE, we have a test-independent PP which requires that all fields by keypunched; it does not have the automatic input features of a test-dependent PP. Backlog data will be input to the system once; a special input program for each type of test would be uneconomical. Thus, the general purpose program—test-independent PP—handles all test data, regardless of procedure, that will be processed a single time.

Typical biological test report forms, illustrated in Figures 3 and 4, are processed in accordance with the flow chart (Figure 5). Edited forms are keypunched and key verified; cards are accumulated in the keypunch area. Input to INQUIRE is on a regular schedule. Cards are then transmitted to the computer for preparation of the INQUIRE Standard Input tape and a listing of this file.

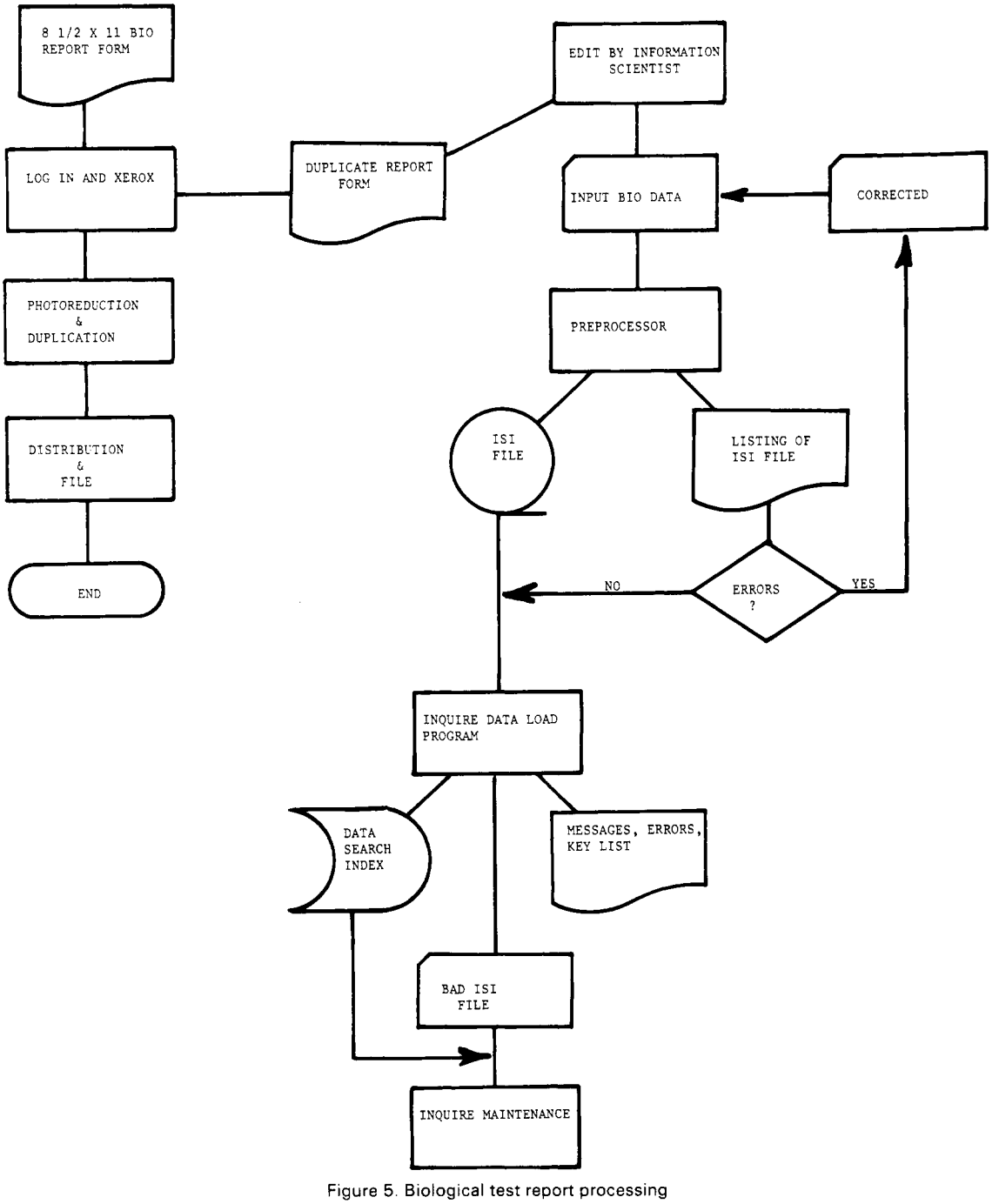

Figure 5. Biological test report processing

TECHNICAL INFORMATION SECTION

BIO-DATA SEARCH

TO: RESEARCH SYSTEMS	DATE REQUESTED:	DATE REQUIRED:	JOB NO.:
NO. CARDS:	NO. ITEMS:	NO. COPIES:	

DATE:	FROM:	DEPT.:
QUERY NO.:	PROCESSED BY:	DELIVER TO:

QUESTION:

Each command - FIND, TAB, TITLE, SORT, HEADER ', SUBHEAD ' - will be KP if it is circled. The last entry in all commands is a comma (,).

FIND

TAB is keypunched as follows: field name, ∅, digits, repeated as required in the full 80 cc; use as many cards as necessary. For TITLE, KP word under the title column heading as written, ∅, and the field name as written on the same line under column TAB, but without digits. Use full 80 cc and as many cards as required. See examples below:

		TITLE	TAB
IF	Appears on the form - (Example only)	Compound 'dose mg'	Compound 1 doser 10
THEN	Keypunch -	TAB COMPOUND 1 DOSER 10 . . . . etc . . . ,	
		TITLE COMPOUND COMPOUND 'DOSE MG' DOSER . . . . etc . . . ,	

TITLE	TAB	TITLE	TAB

SORT

HEADER '

SUBHEAD '

Figure 6. Natural language input form

The printout goes to the Information Scientist who initialed the work request for bio-data input. Obvious errors are indicated on the printout, which is then sent to our senior keypuncher for correction. The ISI Tape file is then entered on to disks as the data, search, and index files.

The input to INQUIRE has been described in some detail; let us now consider output from the system—how to obtain answers to questions.

It has been our practice to have our customers—users—submit their questions in natural language, completely unstructured. We do not burden then with restrictions or limitations of INQUIRE or with the details of what specific information is currently on line. Rather, we let them tell us what they want to know, and the information scientist then asks questions to ensure that there is complete understanding. The information scientist converts the user's questions into a plan for action.

Routinely, queries are transmitted to the system in late afternoon and responses returned next morning. Since operations are not on a real-time basis, any error in interpretation or coding will result in a 24-hour delay, we use the form shown in Figure 6. Questions are first written out in natural language on this form. Queries are coded by an information scientist to ensure proper logic, format, and punctuation and then keypunched.

Before keypunching, coded forms are checked by another information scientist for technical errors. With our 12-hour turn around, it would be unfortunate to have a rush question fail because of an omitted comma. The keypunched question, together with Job Control Language cards, are transmitted to the computer via our telecommunications terminal. Our question is received on scratch tape which is physically transferred to a different machine for actual search. The formatted answer, too, is placed on a scratch tape which is later transferred to a different machine for transmittal back to our terminal.

All questions are not put to the computer. Many questions can be answered faster by manual search methods. For example, if we are asked for the toxicity of a small series of specific compounds in terms of the LD_{50} (the dose that induces death in 50% of the animals tested), we can look it up in a printout of all LD_{50}s, arranged in compound number order. In anticipation of this type of question, we maintain a current listing of toxicity data.

Now, to indicate in a practical manner what the system can do, let us follow a question from genesis to answer. Someone would like to know:

> "What is the activity judgment of all compounds tested in the anti-hypertensive evaluation procedure and the anti-hypertensive screen that have been tested at a dose less than 60 mg./kg.?"

The information scientist knows that this information is contained in reports from tests 414A and 416H. When the natural language question is coded and prepared for the computer, the question takes the following form:

```
1) FIND TESTNO = 414A OR
   TESTNO = 416H AND
2) DOSER LT ' 60.00',
3) SORT SORTKEY (A 13) DOSER
   (A 8),
4) TAB COMPOUND 1 DOSER 32
   DOSEU 44 JUDGEMENT 62,
5) HEADER 'TESTS 414A AND 416H
   WITH DOSE LESS THAN 60
   MG/KG'
6) TITLE COMPOUND COMPOUND
   DOSE DOSER UNITS DOSEU
   JUDGMENT JUDGEMENT.
```

In practice these statements would be keypunched on a series of cards with punctuation as above. These could be prepared as a continuous series, but for checking purposes, each part of the question is placed on its own card. The numbers are used only for identification.

Line 1 tells the system to search for either of two test files, test 414A or 416H. Line 2 states that, in addition, we are interested only if dose is less than 60 units. Single quote marks surrounding three blank spaces and digits in Line 2 define the 8-position field, the one referred to as Reported Dose. Line 3 is an instruction to sort the 13 positions of compound number, as stored in the special SORTKEY field, and to sort also the 8 positions of dose, both in an ascending order.

At line 4 is a printing instruction indicating at which print positions various fields are to be printed. Line 5, beginning with "HEADER," is the title to appear centered at the top of the printout. The final line in the sample question indicates how printed column titles are to be spelled. This command, TITLE is necessary if any one of these words is to be spelled in different manner from the way it is stored in the computer. Then all words must be mentioned in the comand. Note that we use DOSE rather than DOSER, UNITS instead of DOSEU, and we have inserted an E in the spelling of JUDGEMENT.

A portion of the answer to the above question would appear as follows:

TESTS 414A AND 416H WITH DOSE LESS THAN 60 MG/KG

COMPOUND		DOSE	UNITS	JUDGEMENT
W	989	20.00	MG/KG	INACTIVE
W	1273	10.00	MG/KG	INACTIVE
W	2019	2.00	MG/KG	ACTIVE
WX	2197 L002	30.00	MG/KG	INACTIVE
W	4468A	50.00	MG/KG	SLIGHT
W	5610	25.00	MG/KG	INACTIVE
W	5624	48.00	MG/KG	SLIGHT

Response to searches may be printed in formats that best meet needs of users. One of the most valuable features of INQUIRE is its output flexibility, limited only by paper width and line printer capability.

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