

The term vegetables is generic in the term lima beans.

The results of the first search in each example would answer a specific request, whereas the second would give possible helpful information which would not require examination of the information already found in the specific search.

Search time is scheduled for 2 P. M. each day. Searches received in the morning get "same day" answers. Those received after 1:45 P. M. are held until the next day unless there is an emergency. The search cards are punched by the literature chemist assigned to do the search. The card

is verified, manually, by another literature chemist. The cards are delivered to the computer room, and when the run is completed the results are delivered by hand. The computer print-out of the search results has the following format: the header "The following documents satisfy the conditions of search . . ." This is followed by a list of document numbers along with the title identification of the documents. The documents are screened by the literature chemist for pertinency, and all documents containing the requested information are given to the requestor for his evaluation.

A Working System for Retrieval of Chemical Structures, Adaptable to Pesticidal Screening Data*

By JOE R. WILLARD and EDWARD J. MALKIEWICH

Research and Development Department,
Niagara Chemical Division, FMC Corporation, Middleport, New York
Received April 2, 1964

The need for access to test data from past pesticidal screening, using as the basis for access the chemical structures of the compounds involved, led us several years ago to develop a structure retrieval system based upon a combination of empirical formula and functional group classification.

Because IBM data processing equipment was available to us, it was appropriate that any machine-sorting system devised be adaptable to this equipment. Further, every compound in our screening program is assigned a number at the time of its introduction into the program. This number, designated the NIA number, becomes an integral part of all the chemical and biological records and serves as an excellent "handle" for retrieval of information.

The Basic Worksheet.—The 80 columns of the IBM cards were divided into five areas:

Acquisition number (columns 1–6)
Elemental content (columns 7–13)
Structure classification (columns 14–68)
Company source (columns 69–70)
Biological data (columns 71–80)

Three pages make up the worksheet for coding a compound. The first two relate to chemical and source information and the third to biological information. For convenience, the 11-position of the column has been designated as X and the 12 or highest position as Y.

No 9-position appears in any column of our worksheet. When the cards are processed, the 9-position is punched in all columns where no other position is to be punched. This was originally intended as a quick means of checking the accuracy of punching. Other applications for this 9-position will be illustrated later.

Our worksheet is designed for direct coding in all areas except the company source area where reference is made to lists of companies corresponding to the numbers.

The acquisition number, or NIA number, is written on the code sheet (Fig. 1) and punched by direct reference. The numbers of carbon and hydrogen atoms in the molecule are also written directly on the code sheet. For elements other than carbon and hydrogen, the presence or absence is sufficient evidence to permit retrieval and is coded by circling the appropriate position of columns 11, 12, or 13.

NIA No.	OTHER ELEMENTS					
	1	2	3	4	5	6
	11	12	13			
C	Y Ag	Y F	Y			
	X Al	X Fe	X O			
	0 As	0 Hg	0 P			
7 8	1 B	1 I	1 Pb			
	2 Bi	2 K	2 S			
	3 Br	3 Li	3 Sb			
	4 Ca	4 Mn	4 Se			
H	5 Cl	5 Mo	5 Si			
	6 Co	6 N	6 Sn			
	7 Cr	7 Na	7 Zn			
9 10	8 Cu	8 Ni	8 Other			

Figure 1.

* Presented before the Divisions of Chemical Literature and Agricultural and Food Chemistry, Pesticides Subdivision. Joint Symposium on "Problems of the Pesticide Literature and Some Solutions." 147th National Meeting of the American Chemical Society, Philadelphia, Pa., April 9, 1964.

A major portion of the coding worksheet relates to functional group classification (columns 14-68). This portion will be discussed in detail below.

Columns 69 and 70 are used to designate the source of a particular compound. Each company from whom we have obtained compounds is assigned a code number. For convenience of coding, we have assigned the double numbers (00, 11, 22, etc.) to those companies from whom we receive the greatest number of compounds.

Columns 71-80 cover our five major biological programs. Figure 2 presents the details of columns 71-72 which define our fungicide screening program. The columns are used in pairs, with the odd-numbered columns (71, 73, 75, 77, and 79) indicating the biological programs, and the even-numbered columns (72, 74, 76, 78, and 80) indicating the activity of the compound in the corresponding program. No attempt is made to incorporate an absolute quantitative indication of the degree of activity of the compound, but only an indication that the activity was greater than an established minimum.

FUNGICIDE	
71	72
Y	Y
X	X
0 Fol. fung.	0 Active
1 Fol. mild.	1 Active
2 Fol. bact.	2 Active
3 Systemic	3 Active
4 Soil fung.	4 Active
5 Viricide	5 Active
6 Soil drench.	6 Active
7	7
8	8

Figure 2.

Structure Classification.—To ensure specificity in retrieval, our system provides for classification both by functional group and by ring system. The subdivisions in these categories are:

A. Functional groups

1. Hydrocarbons, their halogen and their metal derivatives—columns 14-16 (Fig. 3)
2. Oxygen and sulfur derivatives—columns 17-21 (Fig. 4)
3. Nitrogen derivatives—columns 23-29 (Fig. 5)
4. Organic acids and their derivatives—columns 30-32 (Fig. 6)
5. Oxyacids having central atoms of valence 2, 4, and 6—columns 34-39 (Fig. 7)
6. Oxyacids having central atoms of valence 3, 5, and 7—columns 40-47 (Fig. 8)

B. Ring systems

1. General description—columns 50-51 (Fig. 9)
2. Nonheterocyclic rings—columns 52-55 (Fig. 10)
3. Heterocyclic rings—columns 57-65 (Fig. 11)

Columns 22, 33, 48, 49, 56, 66, 67, and 68, not used at present, are reserved for expansion.

From this brief outline, it can be seen that our functional group classification is based upon the classical approach to organic chemistry with a particular attempt being made to keep like functions together.

Our handling of the standard organic functional groups (Fig. 3-6) involve no radical departure from other systems. The distinctive features of our system are the handling of the oxyacids and the handling of the ring systems.

CHX FUNCTIONAL

14	15	16
Y	Y	Y
X Sat. carb.	X RM	X
0 Olefin	0 R ₂ M	0 M-M
1 Alkyne	1 R ₃ M	1 R ₂ MX _n
2 Alk. hal.	2 RMO	2 Chelates
3 Act. hal.	3 R ₂ MO	3 Metal salts
4 Aryl hal.	4 R ₃ MO	4
5 (C:C) _n conj.	5 RMX _n	5
6 (C:C) _n unconj.	6 R ₂ MX _n	6
7 Straight chain	7 R ₃ MX _n	7
8 Branched chain	8 Other	8

Figure 3.

HYDROXY	ETHER	CARBONYL	ACETAL	C. O. S. N
17	18	19	20	21
Y	Y	Y	Y	Y
X 1° ROH	X	X	X Acetal	X RC(OR)
0 2° ROH	0 ROR	0 RCHO	0 1/2 Acetal	0 RC(O)SR
1 3° ROH	1 ROOR	1 RC(O)R	1 Ketal	1 RC(S)OR
2 Diol	2 RC(O)O ₂ R	2 (CH ₂) _n C=O	2 1/2 Ketal	2 RC(S)SR
3 Polyol	3 RSR	3 -C=C-C=O	3 Thioacetal	3 RC(S)NH ₂
4 1° Thiol	4 RSSR	4 R ₂ -C=C:O	4 1/2 Thioacetal	4 RC(S)NHR
5 2° Thiol	5 RS ₂ R	5 Thio der.	5 Thioketal	5 RC(S)NR ₂
6 3° Thiol	6 -S-R-S-	6 Enol der.	6 1/2 Thioketal	6 RSC:N
7 Phenol	7 RS(O)R	7 Diketone	7 Dithioacetal	7 R-N:C:S
8 ArSH	8 RS(O) ₂ R	8	8 Dithioketal	8 R-N:S:O

Figure 4.

AMINE	N-H	R-C:N	R-N-O
23	24	25	26
Y	Y	Y R-N:C	Y RONO ₂
X	X -N:N(O)-	X R-C:N	X R N:O
0 1° RNH ₂	0 -N:N-	0 RHC:NR	0 R-NO ₂
1 2° RNH ₂	1 =N-N=	1 R ₂ -C:NH	1 R-N:C:O
2 3° RNH ₂	2 -N ₃	2 Monoamid.	2 ROC:N
3 NH ₂ OR	3 -NH-NH-	3 Guanidine	3 RC:N:O
4 RNHOR	4 -NH-NH ₂	4 Monosubst.	4 RCH:NOH
5 R ₂ NOR	5 :N-NH ₂	5 Disubst.	5 R ₂ C:NOH
6 Thio der.	6 -N:N-NH-	6 Tri+ subst.	6 R ₂ C:NOOH
7 Arylamine	7	7 N:C:N	7 RC(NOH)OR
8	8	8 RC(NH)OR	8 RC(NOH)NH ₂

UREA ONIUM SALT

27	28	29
Y Cyanamide	Y	Y
X Cyclic	X Other	X
0 Acyl	0 Ammonium	0 Coord. compd.
1 Monosubst.	1 Monoammon.	1 Isouronium
2 Disubst.	2 Diammon.	2 Isothiuronium
3 Unsym. subst.	3 Triammon.	3 Amidinium
4 Trisubst.	4 Quarterammon.	4
5 Tetrasubst.	5 Sulfonium	5
6 Thiourea	6 Hydrazoneum	6
7 Isourea	7 Oxonium	7
8 Isothiourea	8 Diazonium	8

Figure 5.

CARBOXYLIC	CARBAMIC	CARBONIC
30	31	32
Y Aryl ester	Y Anhydride	Y
X Acid	X Acid	X Acid
0 Acid hal.	0 Acid hal.	0 Acid hal.
1 Int. ester	1 Int. ester	1 Int. ester
2 Ester	2 Ester	2 Ester
3 Amide	3 N-Unsubst.	3 Monothiol
4 Monosubst. amide	4 N-Monosubst.	4 Dithiol
5 Disubst. amide	5 N-Disubst.	5 Trithiol
6 Imide	6 Thiono	6 Thiono
7 RC(O)NHOH	7 Thiolo	7 XC(N)X
8 Anhydride	8 Dithio	8 Anhydride

Figure 6.

SULFENIC	SULFINIC	SULFONIC
34	35	36
Y	Y	Y
X	X	X
0 Acid	0 Acid	0 Acid
1 Acid hal.	1 Acid hal.	1 Acid hal.
2 Int. ester	2 Int. ester	2 Int. ester
3 Ester	3 Ester	3 Ester
4 Amide	4 Amide	4 Amide
5 Monosubst.	5 Monosubst.	5 Monosubst.
6 Disubst. amide	6 Disubst. amide	6 Disubst. amide
7 Imide	7 Imide	7 Imide
8	8 Anhydride	8 Anhydride

SULFUROUS	SULFURIC
37	38
Y Acid hal.	Y Acid hal.
X Acid	X Acid
0 Monoester	0 Monoester
1 Diester	1 Diester
2 Monoamide	2 Monoamide
3 Monosubst. monoamide	3 Monosubst. monoamide
4 Disubst. monoamide	4 Disubst. monoamide
5 Diamide	5 Diamide
6 Monosubst. diamide	6 Monosubst. diamide
7 Disubst. diamide	7 Disubst. diamide
8 Anhydride	8 Anhydride

Figure 7.

PHOSPHORIC	PHOSPHOROUS	PHOSPHONIC	PHOSPHONOUS
40	41	42	43
Y Imide	Y Imide	Y Imide	Y Imide
X Acid	X Acid	X Acid	X Acid
0 Acid hal.	0 Acid hal.	0 Acid hal.	0 Acid hal.
1 Monoester	1 Monoester	1 Monoester	1 Monoester
2 Diester	2 Diester	2 Diester	2 Diester
3 Triester	3 Triester	3 Monoamide	3 Monoamide
4 Monoamide	4 Monoamide	4 Diamide	4 Diamide
5 Diamide	5 Diamide	5	5
6 Triamide	6 Triamide	6	6
7 Subst. amide	7 Subst. amide	7 Subst. amide	7 Subst. amide
8 Anhydride	8 Anhydride	8 Anhydride	8 Anhydride

PHOSPHINIC	PHOSPHINOUS	NO. AMIDE SUBST.
44	45	46
Y Imide	Y	Y
X	X	X
0 Acid	0 Acid	0 Monosubst.
1 Acid hal.	1 Acid hal.	1 Disubst.
2 Ester	2 Ester	2 Trisubst.
3 Amide	3 Amide	3 Tetrasubst.
4	4	4 Pentasubst.
5	5	5 Hexasubst.
6	6	6 Sym. subst.
7 Subst. amide	7 Subst. amide	7 Unsym. subst.
8 Anhydride	8	8

Figure 8.

TOTAL RINGS	TYPE OF RINGS
50	51
Y	Y
X One	X Sat. alicyclic
0 Two	0 One unsat. alicyclic
1 Three	1 Two unsat. alicyclic
2 Four	2 Spiro
3 Five	3 Bicyclo
4 Six	4 Heterobicyclo
5 Seven	5 Aromatic
6 Eight	6 Fused (benzoid)
7 Nine	7 Fused (benz.-het.)
8 Ten+	8 Hetero

Figure 9.

ALICYCLIC	BICYCLIC	AROMATIC
52	53	54
Y Aryl-bicyclo	Y Sat.	Y
X Aryl-alicyclic	X Unsat.	X
0 Three-C's	0 Zero in (0)	0 Zero in (3)
1 Four	1 One in (0)	1 One in (3)
2 Five	2 Two+ in (0)	2
3 Six	3 Two in (1)	3 Zero in (4)
4 Seven	4 Three in (1)	4 One in (4)
5 Eight	5 Four+ in (1)	5 Five in (1)
6 Nine	6 Two in (2)	6 Six in (1)
7 Ten+	7 Three in (2)	7 Seven in (1)
8	8 Four in (2)	8 Eight in (1)

Figure 10.

TOTAL NO. OF HETERO ATOMS	PRIMARY HETERO RING
57	58
Y One S	Y 4-Membered
X Two S	X 5-Membered
0 Three+ S	0 6-Membered
1 One N	1 7+-Membered
2 Two N	2 O
3 Three N	3 N
4 Four+ N	4 S
5 One O	5 Other
6 Two O	6 O+N
7 Three O	7 O+S
8 Four+ O	8 S+N

Figure 11.

The oxyacids having central atoms of valence 2, 4, or 6 are covered by columns 34-39 (Fig. 7). We have designated the various categories on the basis of the corresponding sulfur acids, *viz.*, sulfenic, sulfinic, sulfonic, sulfurous, sulfuric. By combining a search for the appropriate derivative in the oxyacid section with a search for the particular element involved and the analog punch (X position in 39), retrieval of selenium oxyacids and their distinction from the corresponding sulfur acids are relatively simple.

Columns 40-47 (Fig. 8) treat in the same manner the oxyacids having central atoms of valence 3, 5, and 7. In this, the categories are defined on the basis of the corresponding phosphorus acids. Again multiple searching by combination punches allows distinction between phosphorus acids and other acids having the same central atom valence, such as those of arsenic, antimony, or boron. In our experience, derivatives of these other acids occur with insufficient frequency to require an ability to distinguish a boric acid ester of a hydroxyalkylarsine from an arsenic acid ester of a hydroxyalkylborane.

The handling of ring systems is without doubt the most difficult aspect of organic compound coding. We have approached the problem by the total number of rings present in the molecule (column 50) and the types of rings involved (column 51) (Fig. 9) and by the character of the ring (Fig. 10 and 11).

The handling of the total number of rings and the types of rings (Fig. 9) is relatively self-explanatory. Our problem arose in attempting to devise means for classifying bicyclic, heterocyclic, and heterobicyclic compounds. In the case of bicyclic or polycyclic ring systems, we elected to do this on the basis of the length of the chains joining the bridgehead atoms of the bicyclic structure.

The handling of heterocyclic rings is further complicated by the need to distinguish between the various heterocyclic

rings in a particular compound. We classify first on the basis of the number of oxygen, nitrogen, or sulfur atoms in the ring (Fig. 11). The heterocyclic rings within the molecule are further classified starting with the largest ring. When two or more rings in a molecule are the same size, that ring having the greatest number of hetero atoms is given priority, and so on in descending order. Provision is made for four heterocyclic rings with columns 60-65 duplicating columns 58 and 59 for the second, third, and fourth hetero rings.

Coding of Structures.—Since the manner of handling the functional group classification and the emphasis to be placed on the various groups can vary according to the requirement of the individual program, we would demonstrate our procedure by coding a series of compounds rather than by giving great detail as to the manner in which we define the individual groupings.

The soil fungicide Lanstan, obtained for testing from Commercial Solvents Corporation, is coded as shown in Fig. 12.

The coding of the miticide Tedion is shown in Fig. 13.

The compound solan (Fig. 14) introduces a complication over those previously presented in that there is both a

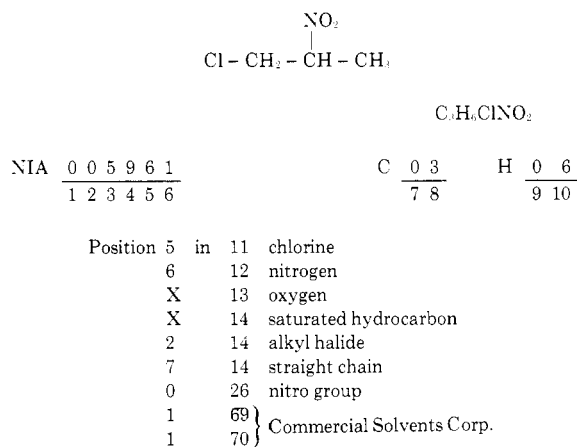


Figure 12.

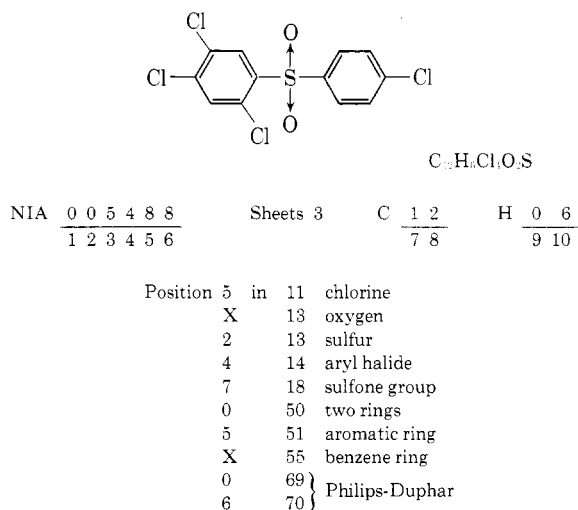


Figure 13.

branched chain (the chain of the carboxylic acid involved) and a straight chain (the methyl group on the ring). While methyl might be considered as no chain, we have, for convenience, designated it a straight chain. Also to be noted is the arylamine grouping. It might be argued that this compound is an amide since the arylamine grouping is no longer present; however, we have found this a most important classification for recovery of analogs.

The herbicide dicryl, which is related to solan, illustrates an important feature of our system which allows us to distinguish α,β -unsaturated carbonyl groupings from compounds containing unsaturated groups which are not conjugated with either another olefinic grouping or a carbonyl (Fig. 15).

The insecticide Morocide also illustrates two characteristics of our system (Fig. 16). Note that a straight chain is indicated for the 2-butyl group on the benzene ring. We use the character of the chain, irrespective of position of substitution, in determining whether the chain shall be indicated as a straight or branched chain. Y position in 30

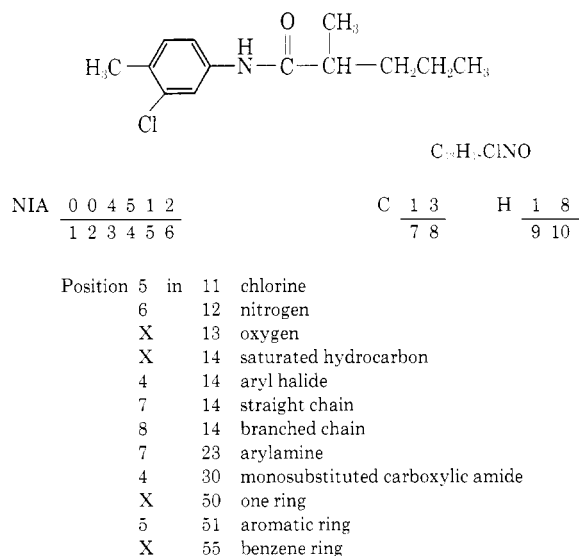


Figure 14.

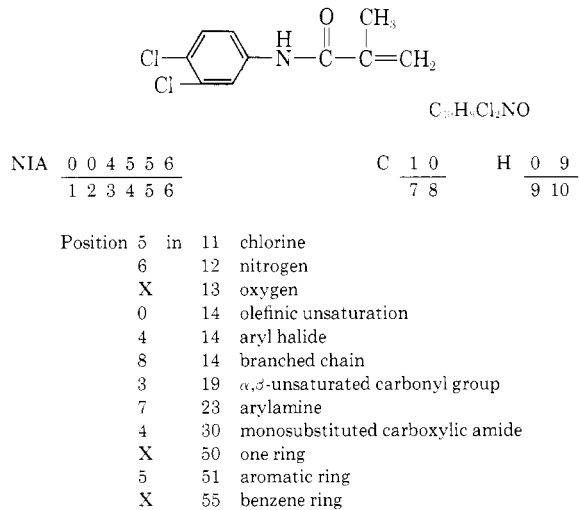
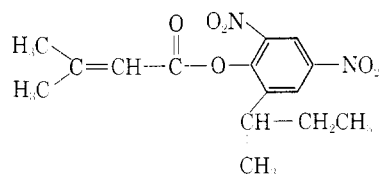


Figure 15.



NIA $\frac{0\ 0\ 9\ 0\ 4\ 4}{1\ 2\ 3\ 4\ 5\ 6}$

C $\frac{1\ 5}{7\ 8}$ H $\frac{1\ 8}{9\ 10}$

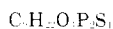
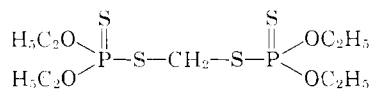
Position	6	in	12	nitrogen
	X		13	oxygen
	X		14	saturated hydrocarbon
	0		14	olefinic unsaturation
	7		14	straight chain
	8		14	branched chain
	3		19	α,β -unsaturated carbonyl group
	0		26	nitro group
	Y		30	aryl ester of carboxylic acid
	2		30	carboxylic ester group
	X		50	one ring
	5		51	aromatic ring
	X		55	benzene ring
	0		69	Farbwerke Hoechst
	4		70	

Figure 16.

also indicates a most useful functional group, namely, the aryl ester grouping.

The coding of ethion (Fig. 17) demonstrates our handling of phosphoric acid esters. This is a relatively simple phosphoric acid ester containing two identical phosphorodithioate groups. Further, the compound contains a -S-R-S- linkage. Note that the -S-R-S- classification in our interpretation does not include the -S-R-S- linkage found in dithioacetals and dithioketals. The structure of ethion may be considered a dithioacetal; however, in our interpretation this is not the case since the hydrolysis products are not mercaptans.

The insecticide Thiodan illustrates one of the more complicated compounds in our coding system (Fig. 18). Note that this compound contains a heterocyclic ring fused to a bicyclic ring. Further, it includes an internal ester of a sulfurous acid. As demonstrated in Fig. 18, all these characteristics are readily handled by the coding indicated.

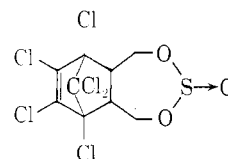


NIA $\frac{0\ 0\ 1\ 2\ 4\ 0}{1\ 2\ 3\ 4\ 5\ 6}$

C $\frac{0\ 9}{7\ 8}$ H $\frac{2\ 2}{9\ 10}$

Position	X	in	13	oxygen
	0		13	phosphorus
	2		13	sulfur
	X		14	saturated hydrocarbon
	7		14	straight chain
	6		18	an -S-R-S- linkage
	3		40	triester of phosphoric acid
	4		47	thionothio group

Figure 17.



Position 2 in 50	four rings
X 51	saturated alicyclic ring
5 51	aromatic ring
7 51	hetero ring fused to aromatic ring
3 52	six-membered alicyclic ring
X 55	benzene ring
2 57	two nitrogens in the hetero rings
5 57	one oxygen in the hetero rings
0 58	largest ring is six-membered
3 58	largest ring contains nitrogen only
0 59	largest ring is fused to an aromatic ring
3 59	largest ring is fused to a hetero ring
X 60	next largest ring is five-membered
6 60	next largest ring contains oxygen and nitrogen
3 61	next largest ring is fused to a hetero ring

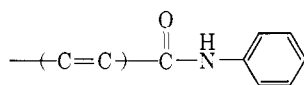
Note that the largest ring is a six-membered ring and the second largest heterocyclic ring is a five-membered ring. Since the six-membered ring takes precedence over the five-membered ring, we need not be concerned with the number of hetero atoms present in each of the two rings. It should be noted that in the classification of the individual rings, we have indicated that the aromatic ring is fused to a heterocyclic ring and that the largest hetero ring is fused to an aromatic system and also to a heterocyclic system. Similarly, the second largest hetero ring is fused to a hetero ring. We can thus define rather explicitly the character of the three-ring system to which the alicyclic ring is linked. There is no means within the system, however, for indicating the positions of substitution of the alicyclic ring. We do not feel that such an indication is essential to the recovery of the needed information.

Illustrative of the biological data is that covering the tests with dicryl (NIA 4556) and with Thiordan (NIA 5462). As seen in Fig. 19, dicryl was tested in seven herbicide screening tests and was found active in three. The testing of Thiordan (NIA 5462) as an insecticide is presented in Fig. 20. Thiordan was tested in all insecticide screening tests (column 77) and showed activity in all (column 78).

Retrieval of Information.—Retrieval of information from our system involves a combination of the IBM search and a critical review of the pertinent structures by the information specialist. In most cases five positions are sufficient to give us the generic group in which we are interested. For example, to search for all analogs of dicryl (NIA 4556), we would ask for five structural groupings.

Position 7 in 23	arylamine
4 30	monosubstituted carboxylic amide
3 19	α,β -unsaturated carbonyl group
X 50	one ring
5 51	aromatic ring

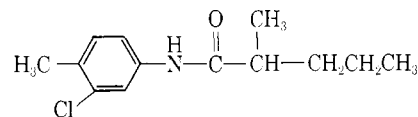
We would obtain a list including all compounds having in common the structure



Were it desirable to have all the arylamides of aliphatic carboxylic acids, slight modification of the question would give this list. Our form of question in this case would be

Position 7 in 23	arylamine
4 30	monosubstituted carboxylic amide
X 50	one ring
(a) 3 19	α,β -unsaturated carbonyl group
(b) 0 14	olefinic unsaturation
(c) 8 14	branched chain
(d) 7 14	straight chain

In response to this question, the cards representing acyl-anilides would be divided into four categories corresponding to those derived from (a) α,β -unsaturated alkenoic acids (with straight and branched chain acids), (b) alkenoic acids in which unsaturation occurs elsewhere in the molecule (this list would also include compounds containing an unsaturated substituent on the benzene ring of the anilide), (c) alkenoic acids in which the chain is not branched (this list would also include those anilides derived from alkynoic acids, α -haloalkanoic, ketoalkanoic acids, etc.). Note that the sequence of the questions is quite important. For example, in the dicryl series, the compound



HERBICIDES	
79	80
Y	Y
X	X
① Pre. mono.	0 Active
① Pre. dicot.	① Active
② Post. mono.	② Active
③ Post. dicot.	③ Active
④ Defoliant	4 Active
⑤ Growth reg.	5 Active
6 Per. spec.	6 Active
⑦ Soil incor.	7 Active
8 Chlorosis	8 Active

Figure 19.

CROP INSECTICIDES	
77	78
Y	Y
X	X
① Bean beet. init.	① Active
① P. aphid init.	① Active
② Mite init.	② Active
③ E & R	③ Hydro
④ Milk. W.B. init.	④ Active
⑤ Army W. init.	⑤ Active
⑥ Plum curc. init.	⑥ Active
⑦ Grain ins. init.	⑦ Active
8	8

Figure 20.

(solan, Fig. 14) contains a methyl group which would be coded as a straight chain, but the compound should be classed as a branched chain alkanolic acid derivative (group c of the acylanilides above). There is, of course, no guarantee that a branched chain grouping may not occur on the phenyl ring of the anilide from a straight chain acid. However, this is a less frequent occurrence in our collections.

As further illustration, assume it is desirable to have a complete listing of noncyclic analogs of ethion, with the analogs categorized between the thiono analogs and the oxo analogs. The question would then be

- Position 3 in 40 triester of phosphoric acid
 6 18 -S-R-S- linkage
 0 47 monothiol ester of phosphoric acid
 9 50 eliminates all ring compounds
 (a) 4 47 thionothiolo group
 (b) remainder

Group a would contain compounds having either one or two P=S linkages. This group could readily be divided further by sorting for the thiono group (position 3 in 47).

The form of report from the Data Processing Group in response to our question is a simple line designation incorporating the compound number, the number of carbons and hydrogens, and a designation for each of the biological activity areas (Fig. 21).

Com- pound number	C	H	CC 71	CC 72	CC 73	CC 74	CC 75	CC 76	CC 77	CC 78	CC 79	CC 80
4550	12	16		9	9	9						
4551	11	14				9			9	9		
4553	13	18		9		9		9	9	9		
4554	14	20		9		9		9	9	9		
4555	11	12		9	9	9				9		
4556	10	9				9				9		
4557	18	28				9		9	9	9		9
4558	17	26				9		9	9	9		9

Figure 21.

On the NIA 4556 line (NIA 4556 contains ten carbons and nine hydrogens), blanks in columns 71 and 72 indicate that NIA 4556 has been tested as a fungicide (column 71) and was sufficiently active in at least one of the screening tests to meet out minimum qualifications (column 72). Similarly, it was tested in our household insecticide program (blank in 73) but was not active in any of the screening tests of that program (9 in 74). It was tested as a nematocide (blank in 75) and found active (blank in 76). It was tested as a crop insecticide (blank in 77), but found inactive (9 in 78). It was tested as an herbicide (blank in 79) and, as one would anticipate, showed activity in at least one of those tests (blank in 80).

A part of the report obtained in response to questions regarding ethion analogs is presented in Figure 22. NIA 1240, which contains 9 carbons and 22 hydrogens, was tested and found to be active as a fungicide, as a household insecticide, as a nematocide, and as a crop insecticide, but was not active in the herbicide test.

Com- pound number	C	H	CC 71	CC 72	CC 73	CC 74	CC 75	CC 76	CC 77	CC 78	CC 79	CC 80
1231	12	28		9		9	9	9			9	9
1239	9	20	9	9		9	9	9			9	9
1240	9	22										9
1241	6	16	9	9			9	9			9	9
1242	14	32	9	9			9	9			9	9

Figure 22.

Experience with the System.—The system has been in operation a little more than one year, during which time more than 1000 searches have been made. This experience has demonstrated the system to be satisfactory, and we are at the present time attempting to modify the system to incorporate data from the literature, with particular emphasis on the patent literature.