A Computerized Metabolic Map

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We have developed a computer representation of metabolic pathways that incorporates metabolic reactive spaces, species distinctions, and reversibility considerations. Furthermore, the distinction is made between pathway substrates and cosubstrates. Reactions are represented as entries in a database; the code was developed under dBASE III+. Two views onto the database have been developed: a spanning tree which performs a depth search and a stepwise navigational approach which offers reaction possibilities one at a time. In addition, metabolic pathways of any desired starting point are output as a Warnier diagram.

INTRODUCTION

The enzymatic reactions that comprise metabolic pathways are the foundation of biochemistry. Much of this fundamental information is at present difficult to tabulate, and to correlate to associated facts about enzymes and their substrates. Wall charts present an overwhelming amount of information, which is nonetheless incomplete and outdated. Moreover, due to display limitations, information such as species, cellular location, and reaction chemistry are difficult to portray.

The primary research literature on metabolic pathways is not easily consulted either; data is scattered, and it is not always easy to reconcile discrepancies between different sources. The most thorough treatise of metabolic reactions is two decades old.[1] Some more recent specialized monographs have appeared which cover specific aspects of metabolic regulation, from which several of the major reactions of biochemistry can be abstracted,[2,3] and at least one modern textbook has attempted to be thorough in its coverage.[4] Yet none of these are encyclopedic nor free frrom errors which are difficult to erase even from new texts.[5]

The essence of the problem is the representation of a large network of chemical reactions, which suggests the use of a computer database. Some efforts in this direction have recently appeared for the specialized purpose of bioengineering[6] and a cataloging program for biochemical reactions has also been published.[7] These programs begin to address much of the problem of representing biochemical reactions but do not provide for users to explore and query the database easily. As they are not written to be based on a relational database, the programs are difficult to maintain and expand to accommodate new data types. Moreover, the viewpoint of how reactions are structured into pathways and how these are regulated has not been expressed in a computer representation. These are the goals that have shaped our development of a computerized metabolic map. We report here a prototyptic system for computer navigation along metabolic pathways.

GENERAL FEATURES

Our metabolic map is a series of programs written in dBASE III+, with an underlying database that currently represents glycolysis, gluconeogenesis, the pentose pathway, the tricarboxylic acid cycle, and urea synthesis. Enzymes and membrane transporters are given equivalent status in this representation, the distinction being that enzymes catalyze a chemical transformation, while transporters catalyze a translocation. In its present form, cytosolic and mitochondrial spaces of cells are represented. Different species presenting availability of different reactions are also represented in the database and supporting programs; in the present case, man, rat, and bird. Reactions are characterized as *near equilibrium* or *nonequilibrium* in accordance with the definitions discussed by Newsholme and Leech.[8] Finally, a distinction is made between pathway substrates and cosubstrates by relegating the latter to separate fields.

Table I. Structure of the Main Database, METABRXN

field	type	len	description
ENZYME_NO	C	8	enzyme number or transporter ID
ENZYME_NAM	C	31	enzyme name
SUBSTRATE	C	36	pathway substrate
PRODUCT	C	36	pathway product
COSUB_	C	9	cosubstrate
COPROD_	C	9	coproduct
SBRANCH	L	1	substrate branch
SAVAIL	L	1	substrate availability
PBRANCH	L	1	product branch
MULTRXNS	L	1	multiple reactions
PAVAIL	L	1	product availability
REVERSIBLE	C	1	near-equilibrium status
VISITED	L	1	node has been traversed
GLOSS	M	10	(unpopulated)
SUBS_MASK	C	3	substrate mask
PROD_MASK	C	3	product mask
SPECIES	C	5	species mask

Two views onto the database are provided in the programs SPANNER and TABLENAV. SPANNER produces a spanning tree over the metabolic graph, beginning with a user-specified starting point and number of steps. Screen or printer output shows the existing pathways, with indentations to represent different levels of the pathways. SPANNER also outputs reactions in the form of a Warnier diagram. A complementary viewpoint is provided by TABLENAV, which is an interactive navigation program, displaying all possible connecting points from a single starting point and allowing navigation from there. Ancillary features of TABLENAV include a trip log (display of all steps to that point) and changing direction.

Both traversals of the database are restricted by the availability of a reaction in the selected species and cellular location. Furthermore, if a reaction is considered to be nonequilibrium in the cell, it cannot be traveled in the reverse direction, as is possible with near-equilibrium reactions. In general, these two views of chemical reactions provide an altogether new vantage point on the chemical reactions of cells that brings out the continuity of the reaction and makes the branch points of intermediary metabolism readily understandable.

THE DATABASE METABRXN AND ITS ASSOCIATED FILES

The metabolic information is stored in the database METABRXN.DBF (metabolic reactions). The structure of this database file is shown in Table I. The table shows the field name, field type, field length, and a short description of each field. A more detailed description of each is given below.

0095-2338/91/1631-0132$02.50/0

```
c  From GLUCOSE-6-P, the following feasible steps appear:
glucose-6-P              <-> fructose-6-P          c  c
RECNO==>   2             Glucose P-Isomerase                BRANCH

glucose-6-P              -> 6-P-gluconolactone      c  c
RECNO==>  28             Glucose 6-P DH                     BRANCH

glucose-6-P              -> glucose                 c  r
RECNO==>  71             Glucose-6-phosphatase       Pi     BRANCH

Enter (+-) the record number of the reaction to pursue.    71
Use minus (-) to see details and reach options.
```

Figure 1. First screen in TABLENAV showing possible routes available from glucose-6-P. The letter "c" in the upper left corner indicates the current metabolic space is the cytosol. Double-headed arrows indicate reactions that can likely be reversed in the cell (near-equilibrium); single-headed arrows indicate nonequilibrium reactions. All are branch points, as indicated at the right.

ENZYME_NO is the official enzyme commission number for each enzyme[9] modified by the addition of an eighth character which is used to represent separate reactions of the same enzyme. This field is also used to identify transporters, for which we have arbitrarily created a nomenclature which includes mnemonic identification.

The ENZYME_NAM field contains a descriptive rather than official name for each enzyme or transporter. SUBSTRATE and PRODUCT fields contain the names of the metabolic pathway intermediates of each record. COSUB_ and COPROD_ are the nonpathway intermediates that potentially connect large numbers of reactions and thus are kept segregated in these separate fields.

SBRANCH and PBRANCH are logical fields used to indicate substrates and products that are shared by different reactions. These branch flags are not essential to the programs but serve to avoid unnecessary searching for a branch point when none exists in the database.

SAVAIL and PAVAIL are logical fields that are not used by either of the main programs, but by a third called SETAVAIL. The purpose of SETAVAIL is to produce a tailored subset of reactions from the main database. Its use is mainly directed for future development, but at present it is possible to run SETAVAIL, select the subpopulation desired, and copy this new abbreviated database for use by the main programs.

MULTRXNS is true when an enzyme requires more than one entry in the database to represent its entire set of pathway metabolites. Since each entry is limited to a single substrate and product, an enzyme which has more than one of either of these occupies more than one entry, with identical ENZYME_NO fields and MULTRXNS set to true.

REVERSIBLE is set to 'E' if the reaction is near equilibrium, to 'F' if it is nonequilibrium in the direction entered in the database, or to 'B' if it is nonequilibrium in the direction opposite to that entered into the database. This preserves flexibility for data entry that is not an issue with the present size but will be with future versions containing a large number of entries. Moreover, reversibility may depend upon the cell type, so this flexibility is more a necessity than a luxury of data entry.

VISITED is used by SPANNER to mark nodes already included in the spanning tree. This prevents SPANNER from retracing its steps.

GLOSS is a memo field that will hold ancillary information. At present, this field is not populated.

SUBSMASK, PRODMASK, and SPECIES hold information concerning the metabolic space of substrate and product, and the species for the enzyme or transporter.

Three fields—ENZYME_NO, SUBSTRATE, and PRODUCT—are indexed, using a forced uppercase function, i.e., UPPER(substrate), so that searches using these are rapid and case independent. A small series of steps to reindex the database and reset flags such as SBRANCH and PBRANCH is performed by a small program, SETFLAGS.

During the execution of the programs, temporary information relevant to program flow, such as record counts and level of traversal, are stored in a separate database containing 12 fields called WRKPROTO. In SPANNER, this file serves as an auxiliary stack in the spanning tree traversal of the metabolic graph; the values saved must contain fields to resume the tree traversal from the stacked point whenever branches exist. In TABLENAV, WRKPROTO records the entire trip for latter recall of the trip log, or for backing up to a previous step.

TABLENAV USER'S VIEW

TABLENAV is a procedure file in dBASE, which is entered by issuing the commands

```
set procedure to TABLENAV
do TABLENAV
```

In the compiled version of the program (using CLIPPER), the executable file TABLE.EXE is provided instead.

Once the program is initiated, the program requests species and initial metabolic space specification. The starting metabolite is then selected from the BROWSE mode of dBASE. The list can be scrolled (PgUp/PgDown or Up/Down arrow keys) and selection is made, as indicated by a prompt, through the ESC or Ctrl-End key.

Following this selection, a selection table is presented which gives the possible points which can be accessed from the metabolite that was selected. The reactions shown are those which are allowed both by position in the metabolic map, proper metabolic space, species, and direction of reaction. A sample screen is shown in Figure 1. In this example, glucose-6-phosphate was selected, and no preference given for cell space. In the top line of Figure 1, the 'c' indicates that the cytosol is the active space, and each listed reaction possibility is given below the header line. Each possibility occupies two lines. In the first line are the substrate, arrows to indicate direction and reversibility, the product, and letters indicating metabolic space for the reaction substrate and product. Apart from cytosol ('c') and mitochondria ('m'), the third entry in Figure 1 contains an 'r' indicating that the product of glucose-6-phosphatase is actually in the endoplasmic reticulum; while this third space is in the database at present no other records have this indicator. The glucose-6-phosphatase is actually a special case of an enzyme which is also a transporter; this is indicated by the fact that the substrate and product have different metabolic spaces. In most cases of transporters, substrate and product are identical but their metabolic spaces are different. The second line of information for each record is the record number (RECNO), name of the enzyme, co-

```
Substrate direction; Product direction; Onward; Ass.rxn;
Branch now; Gloss display; Display path; Regress; Exit program;
Enter a command letter O
                    P-bound  cytop.
Substrate: glucose-6-P                                  BRANCH


                                                        c  r
Enzyme:   Glucose-6-phosphatase
                    FORWARD
Product: glucose
          +Pi
```

Figure 2. Second screen in TABLENAV. Each option is listed at the top of the screen and selected by typing its first letter. "P-bound" indicates the direction of metabolic flow, in this case "product bound", as entered in the database. The reaction, as shown at right, involves a change in metabolic space from the cytosol (c) to the endoplasmic reticulum (r) as glucose is converted to glucose-6-P. Thus, the program represents the glucose phosphatase translocase system.

```
glucose                          cFc 2070101  glucose-6-P
  glucose-6-P                      cFc 5030109  fructose-6-P
    fructose-6-P                     cFc 2070111  fructose-1,6-bisP
      fructose-1,6-bisP                cFc 4010213  glyceraldehyde-3-P
      fructose-1,6-bisP                cFc 4010213  dihydroxyacetone-P
      fructose-1,6-bisP                cFc 3010311  fructose-6-P
      fructose-1,6-bisP                cFc 4010213  dihydroxyacetone-P
    glyceraldehyde-3-P               cRc 2020102  fructose-6-P
      glyceraldehyde-3-P               cFc 1020112  1,3-bisPglycerate
    erythrose-4-P                    cRc 2020101a fructose-6-P
      sedoheptulose-7-P                cRc 2020102  erythrose-4-P
  glucose-6-P                      cFr 3010309  glucose
No steps from GLUCOSE                              at level  2
  glucose-6-P                    cFc 1010149  6-P-gluconolactone
    6-P-gluconolactone               cFc 3010131  6-P-gluconate
      6-P-gluconate                  cFc 1010144  ribulose-5-P
```

Figure 3. Screen or printer output of SPANNER. Each depth level is represented by increasing indentation of the text line for that reaction. The notation in the middle contains three letters that give the metabolic space of origin in small letters, the direction (F for forward, R for reverse), and the metabolic space of the product of the reaction. The number in the list is the enzyme commission number.

substrates and coproducts (if any), and indication of whether MULTRXNS or BRANCH flags are set.

The prompt at the bottom of the screen of Figure 1 allows selection of the next step, by entering the record number. Alternatively, a negative number can be entered, in which case a detailed screen of one reaction is presented. The new screen is shown in Figure 2. Several new options for the single reaction presented are offered; selection is accomplished by typing the first letter of the words listed at the top. Choosing "Substrate" or "Product" allows a change of direction. "Onward" returns to the traversal screen (Figure 1). "Branch" allows a switch to the associated reaction, for cases in which there are two substrates or products. The "Gloss" display brings up the contents of this memo field, which is at present empty. "Display path" shows a trip log of the pathway as traversed so far. The trip log output is a listing of essentially identical form with the SPANNER output shown in Figure 3. "Regress" allows backing up to a user-selected number of steps. Finally, "Exit" allows the user to quit the program. Operation within the framework of the screen of Figure 2 also allows "cheating": it is possible to travel irreversible steps in the reverse direction, and to follow reactions that violate cell space restrictions. This may be of use since many reaction sequences in different organisms may not yet be entered and this represents the only means to traverse such sequences. Furthermore, it is a means to explore theoretical pathways, of possible importance for bioengineering.

There is no printed output provided for TABLENAV, but as the path traversed is saved in the auxiliary database, it can be displayed in the detailed screen (Display path), and the screen can then be printed or saved. The major usefulness of TABLENAV at present is as a pathway exploration. Recording of segments of the database is best performed by SPANNER.

SPANNER USER'S VIEW

SPANNER is also a procedure file and is initiated similarly to TABLENAV

```
set procedure to SPANNER
do SPANNER
```

and the compiled version, SPAN.EXE can be run directly.

After selecting species, metabolic space, and an initial metabolite, SPANNER automatically generates a spanning tree at a depth set at present to a maximum of 13. The spanning diagram is either sent to the screen or printer, and output consists of reactions in which levels are grouped by indentation.

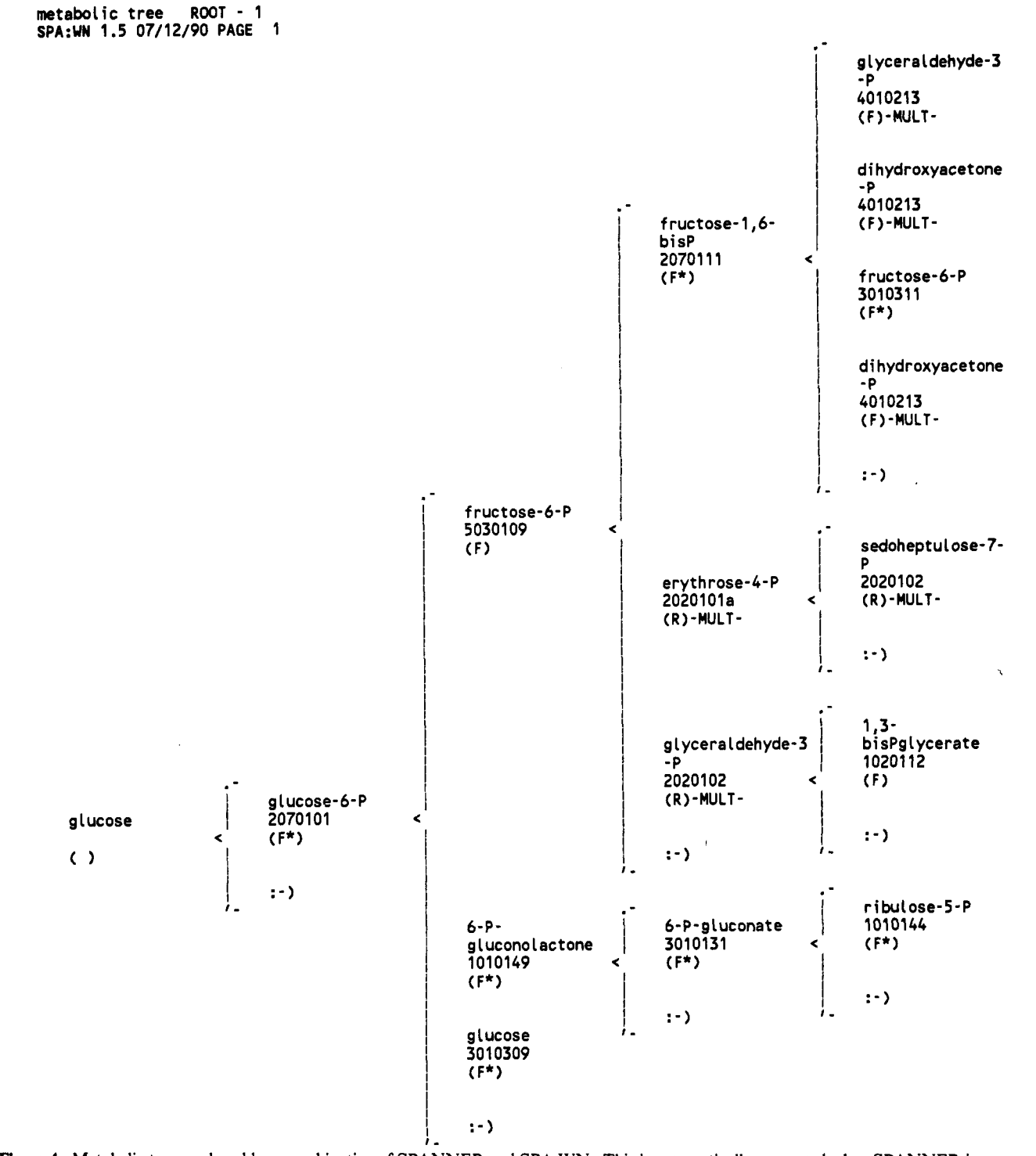

Figure 4. Metabolic tree produced by a combination of SPANNER and SPA:WN. This is automatically generated when SPANNER is executed and stored as an ASCII file. As in all SPA:WN representations, if the number of levels produced is greater than the physical limits of the page, a reference to the page number at the edge is given for the continuation.

In addition to this output, SPANNER also generates another file, SPAWNIN.WAR, and invokes a separate program, SPA:WN, to produce a Warnier diagram of the metabolic tree. The program SPA:WN is a public domain offering[10] that is a programming aid and, in fact, was used to produce and debug code for the programs developed for this project. A Warnier diagram[11] represents hierarchies of a logical structure as a tree. In the case of metabolic pathways, all the products reachable from a substrate are presented as children of the substrate.

An example of initial output from a SPANNER run is shown in Figure 3. This is a short spanning tree set to a depth of 3. Each line lists the metabolite indented to its level in the tree. On the same line, a three-letter code indicating the substrate metabolic space origin, the reaction direction, and the product metabolic space follow. Thus, in line one of Figure 3, the indication "cFc" means that the substrate is cytosolic, the reaction proceeds in the forward direction as written in the database, and the product is cytosolic. The enzyme commission number or transporter name follows. The final entry on the line is the product of the reaction. Dead ends are indicated in this output by the indication "No steps from.." followed by the endpoint metabolite.

The same run of SPANNER that produced Figure 3 also created the Warnier diagram shown in Figure 4. Even with this small spanning tree, the reactions are much more readily

evident in this display. Figure 4 presents the same information as Figure 3, with an additional indicator of MULT to point out those cases of enzymes with multiple substrates and products. The indicators in parentheses refer to the direction of reaction as entered in the database; R indicates a near-equilibrium reaction run in reverse. Metabolically irreversible steps are indicated by the inclusion of an asterisk. For larger searches, SPA:WN automatically creates pages no larger than 123 lines by 132 characters and provides cross references among the continuation pages. Thus even very large spanning trees can be represented in this fashion.

DISCUSSION

Relational database features will be of key importance in accessing and storing information in the projected metabolic database. This is a primary advantage of the fact that the program is based upon a relational database environment rather than a general purpose programming language. One significant use of this feature will be the entry of inhibitors for enzymes and transporters. These can be readily entered into a separate file and related to the main one through the unique field of ENZYME_NO. Not only is the coding simple for such additions, there is no need to alter the main database or its associated programs.

The usefulness of the database format of the program can be extended well beyond inhibitors. Any associated information can be stored in a manner that allows retrieval based upon a number of useful criteria: associated reaction, substrate, species or cell type, or class of reaction. The latter information is already implicitly encoded in the use of the enzyme commission numbers. A simple searching algorithm could be readily established to use this information to produce lists of enzymatic reactions by chemical class.

A major change that we foresee is the entry of a large number of reactions into the database. This will take place soon, as presently a group in Switzerland is keying in the set of known enzyme reactions that are given in the listings.[12] A further improvement will be the development of graphics to display chemical structures either sequentially for use in display and output or in overlay mode to demonstrate chemical changes to a pathway substrate as it is metabolized. These enhancements should greatly add to the interest and overall usefulness of the database. Still, the programs already developed allow insight into the structure of metabolic pathways that is not easy to obtain in noncomputer representations.

Other computer representations of metabolism are distinct from our own. Seressiotis and Bailey[6] have written a program in LISP that they consider "artificially intelligent" as it is able to output sequences from its database. The viewpoint of this program is engineering: the authors plan to use the results to select or design (presumably by molecular biology techniques) microorganisms for production of desired byproducts. Whether this program is more useful than our own in contemplating such design plans is difficult to judge. Our program also generates such lists, and our ancillary program SETAVAIL allows marking which reactions can be excluded from a new copy of the database. However, our vantage point and capabilities are unique. Any computer representation of metabolism requires that a number of decisions be made concerning the structure of pathways and their interrelations. In our case, that has led to incorporation of reversibility, pathway substrate ideas, membrane transport, and species specifications.

The species specifications are also found in the FORTRAN program of Goryanin et al.,[7] but the goal of this effort appears to be primarily cataloging. This program essentially produces lists of a coded flat-file database. A major advantage of our effort over the previous codings of metabolic reactions is the use of dBASE itself. This makes extensions extremely simple to incorporate, as building a relational database from scratch in FORTRAN would constitute a major effort. Even in LISP, recoding to include new features is a major undertaking. A second underlying unique feature of the present program is the extensive use of Warnier diagrams. These have been of use both in the coding, debugging, and revision of the program (several versions have been developed in arriving at the present stage), and in the output for SPANNER.

Recently, a similar model of metabolic reactions was published by Barcza et al.[13] This program is based on CHEMBASE, a commercial database specialized for chemical structures. While the pathway presentation features of that program are more rudimentary than those presented here, it is possible to retrieve records based upon chemical structure. Clearly, the incorporation of chemical structure into a metabolic map program is an important attribute; we are currently working to merge this feature with our program.

There are other programs which present enzymatic reactions of metabolism that are not actually metabolic map programs. For example, a commercial program "Animated Pathways in Biochemistry"[14] has recorded screens of several pathways, but none of these are connected to each other, and nothing can be searched or stored. This is essentially a recording that can be replayed indefinitely for purposes of learning a few pathways and the structures of the intermediates, more similar to a textbook than a computerized metabolic map.

Mathematical modeling at present incorporates a much more limited range of reactions. Existing models such as that of Garfinkel[15] allow conclusions about a single or few reactions that are difficult to apply to a large number of reactions. This is the result of two factors. First, it is necessary to provide a platform to at least represent a large number of reactions in an efficient way that is close to metabolic reality. Second, the numbers for the kinetic constants are not generally known for reactions inside cells. Our program contributes to the first goal, and addition of constants can be as readily added as any other information. When the second is realized with further research, our program can serve as a ready repository of new information as it arises.

SUMMARY

We described here a computerized representation of metabolism that can trace pathways and serve as a useful source for information retrieval. The program is written in dBASE III+ and has also been compiled. Metabolic spaces, transporters, and reaction reversibility are represented. Two separate views of the database are provided. One allows a search of a user-selected depth and outputs both a listing and a Warnier diagram, a tree-like representation of metabolic pathways. The other allows stepwise navigation of the database. The program is extensible in a number of directions and can serve both as a teaching and research tool in biochemistry.

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HMIMS: Hazardous Materials Incident Management System for Air Force Fire Departments†

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The Hazardous Materials Incident Management System (HMIMS), an integral part of the Air Force comprehensive hazardous material (HAZMAT) program, is a computerized chemical incident response system. It is intended primarily for use by Air Force fire departments to retrieve response information during chemical incidents and as an instrument to collect information on amount, location, and nature of chemicals on the base. Both graphic and nongraphic data are supported by the HMIMS. The graphics include a hierarchy of maps which supports both small-scale (as a regional map) and large-scale (building or room) display. The nongraphics databases incorporate the chemical inventories, Material Safety Data Sheets, Response Data Sheets, and standard operating procedures, and the site characterization and analysis information necessary to generate Superfund Amendments and Reauthorization Title III Tier I and Tier II reports. The HMIMS is installed on two personal computers, one at the fire house and another on a HAZMAT vehicle at the incident site. Communications software enables the two to act in conjunction. The HMIMS assists hazard assessment and response during HAZMAT emergencies, provides incident management guidelines, and functions as a training tool to simulate emergency response.

INTRODUCTION

The Hazardous Materials Incident Management System (HMIMS) is a software product designed to meet the on-scene hazardous material (HAZMAT) management requirements of the Air Force.[1] Emergency response personnel responding to HAZMAT incidents face complex and uncertain situations. In addition to familiar hazards, such as fire and structural instability, HAZMATs pose a threat which cannot be understood until the materials are identified and their characteristics are described. Despite incomplete information regarding the type of HAZMAT, protective clothing requirements, or potentially vulnerable areas, decisions must be made in response to emergency situations. To make a decision during such times, emergency managers need as much information as possible, as rapidly as possible.[2-4]

There is a great deal of environmental awareness and recognition of potential hazards associated with chemical exposures. Congress has proposed and the Environmental Protection Agency and other governmental agencies have promulgated a succession of environmental regulations to protect the public, workers, and environment. The Resource Conservation and Recovery Act, Clean Water Act, Clean Air Act, Occupational Safety and Health Act, and the Transportation Safety Act have generated numerous regulations and guidelines related to chemical spills, HAZMAT management, and worker safety. One highly visible public law, administered by the U.S. Environmental Protection Agency, is the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA), better known as Superfund. In 1986, Superfund was amended through the Superfund Amendments and Reauthorization Act (SARA). One part of SARA, Title III[5] was a new and distinct law separate from CERCLA in intent, scope, and issue. It brought to federal, state, and local governments, as well as to private industries, numerous requirements in the areas of emergency planning, community right-to-know, hazardous emissions reporting, and emergency notification. The objectives of Title III are to improve local chemical emergency response capabilities and to provide citizens access to information about chemical hazards in their localities.

The Air Force has interpreted these laws and regulations for the Air Force community. Each Air Force base, depending on its size and mission, may have many different HAZMATs. Addressing their needs for emergency response can be a challenging task. The Air Force, through regulations and a letter from the Director of Engineering and Services at Headquarters, U.S. Air Force, dated Dec 16, 1985, has determined that the responsibility for initial response and coordination of HAZMAT incidents at each Air Force base resides with the base fire department.[6-8]

To assist fire departments in responding to HAZMAT spills and ongoing installation restoration programs, the Air Force

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