นิพนธ์ต้นฉบับ

Vitamin and derivative structures : self study computer program.

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   Knowing the chemical structures of vitamins and derivatives leads to a better understanding of both properties and functions. Acquaintance of these difficult structures can be achieved through frequent visualization on the computer screen. Using the Harvard graphic program, the authors constructed the chemical structures of fat soluble vitamins, water soluble vitamins and their derivatives. Notes on the physical, chemical properties and medical importance were included for each structure and catagorized. Any person who knows how to switch on and boot the computer can easily choose to view and study the compound of choice by just pressing one number on the menu, the printing out of the desired structure is immediate on pressing the (Alt) key once.

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       การเรียนรู้โครงสร้างของวิตะมินและอนุพันธ์จะช่วยให้เข้าใจ   ถึงคุณสมบัติและหน้าที่การทำงานของสารกลุ่มนี้ได้ดียิ่งขึ้น ความคุ้นเคยต่อสูตรโครงสร้างที่ซับซ้อนของวิตะมินจะเกิดได้หากได้ดูสังเกตุ หรือเห็นบ่อย ๆ บนจอคอมพิวเตอร์ คณะผู้วิจัยจึงนำ Harvard graphic ซึ่งเป็นโปรแกรมกราฟฟิคสำเร็จรูปมาใช้ในการสร้างภาพโครงสร้างของวิตะมินทั้งกลุ่ม วิตะมินละลายน้ำ และละลายไขมัน พร้อมทั้งบรรจุเนื้อหา ข้อมูลเกี่ยวกับคุณสมบัติทางกายภาพเคมี ความสำคัญทางการแพทย์ของสารแต่ละตัว อีกทั้งจัดแยกกลุ่มอนุพันธ์ โปรแกรมประมวลโครงสร้างของวิตะมินและอนุพันธ์ได้จัดทำขึ้นเพื่อความสะดวกและง่ายต่อการใช้   ผู้ใช้เพียงแต่ทราบวิธีเปิดเครื่องคอมพิวเตอร์   เรียกโปรแกรมออกมาปรากฏบนจอได้ จะมีเมนูให้เลือก เพียงกดตัวเลขหน้าชื่อสารที่ต้องการศึกษา ข้อมูลและโครงสร้างของสารดังกล่าวจะปรากฏบนจอทันที และสามารถพิมพ์สิ่งที่ต้องการโดยกด (Alt) ครั้งเดียว

The sophisticated and complicated chemical structures of biologically active substances including carbohydrates, proteins, vitamins and their derivatives are extremely difficult for students to write or memorise. However, the visualisation and knowledge of chemical structures helps a great deal in the understanding of both physical and chemical natures of these substances. The authors therefore felt that a computerised collection of the chemical structures of vitamins and derivatives as well as a brief note on the physical and chemical properties together with their medical importance, and pharmacological effects would benefit in terms of a self-study program.

The Harvard Graphic is a known commercialised computer software suitable for drawing a line, circle, curve or mixed components found in chemical structures. Simultaneously, information concerning the chemical name, physical and chemical properties, as well as their medical importance can be added as a label to each structure. Print out of the structure and information is a simple process.

Objectives of the project

By using the Harvard Graphic software, the chemical structures of both fat soluble vitamins and water soluble vitamins are constructed. Brief information on the properties and medical importance are later added. The vitamins and their derivatives are catagorized to provide simple searching and printing.

Material and Method

1. Computer hardware specifications :

    1.1 Type of computer : IBM XT, AT or compatible

    1.2 Disk driver : 1.2 Mbyte or 360 Kbyte

    1.3 Hard disk : containing more than 2 Mbyte space.

    1.4 Printer : Dot Matrix

    1.5 Monitor : CGA, EGA or Monochrome

2. The Harvard Graphic software program.

3. Double sided, Double density diskettes sized 5 1/4 inches.

4. The collection of structures

    4.1 The authors had sorted out all the chemical structures of vitamins and derivatives published in the standard text books covering biochemistry, nutrition[1-4] as well as the Merck Index.[5] Double checking and cross checking of all the structures had been done and only those appeared correctly in at least two standard texts were accepted.

    4.2 The classification of vitamins and related compounds

        The vitamins are classified into 2 classes namely : fat soluble vitamins consisting of vitamin A,D,E,K, and water soluble vitamins which are composed of the B complex group and Ascorbic acid or vitamin C. The related compounds are categorized as Essential nutrients shown in Figure 1.
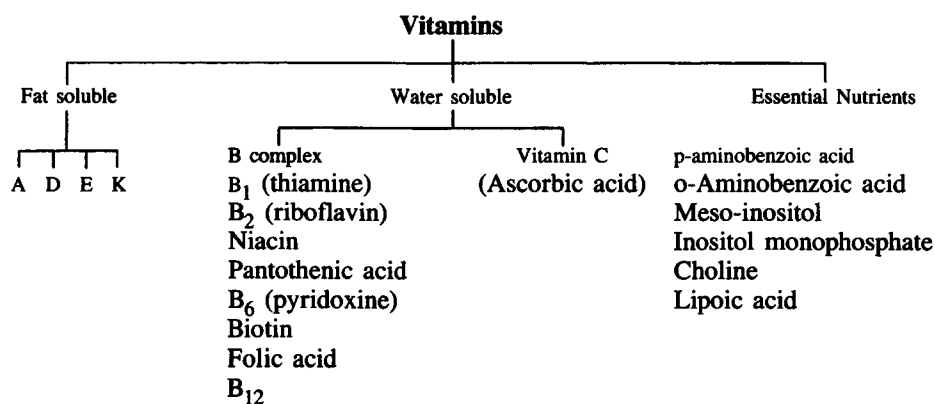
Vitamins

Fat soluble	Water soluble	Essential Nutrients
A D E K	B complex	p-aminobenzoic acid
	B_1 (thiamine) Vitamin C	o-Aminobenzoic acid
	B_2 (riboflavin) (Ascorbic acid)	Meso-inositol
	Niacin	Inositol monophosphate
	Pantothenic acid	Choline
	B_6 (pyridoxine)	Lipoic acid
	Biotin	
	Folic acid	
	B_{12}	

Figure 1. Classification of vitamins.

4.3 The subdivision of individual vitamin. Each vitamin is subclassified as follows :
4.3.1 Vitamin compounds
4.3.2 Vitamin precursors
4.3.3 Vitamin related compound
4.3.4 Vitamin active metabolites or Co-enzyme intermediates
4.3.5 Vitamin intermediates
4.3.6 Vitamin excretory products
4.3.7 Vitamin antagonists

However, some of the structures of vitamin derivatives mentioned in the above subclasses may not be included in this data.

5. Constructing vitamin structures by Harvard Graphic

5.1 Constructing the chemical structures

The Harvard Graphic software is used to draw all the chemical structures of vitamins, all active intermediates, metabolites and derivatives. Details concerning the physical, chemical properties and medical importance are later added. Printout of the structures and information was done several times for proofreads and corrections.

5.2 Menu and "Screenshow"

The authors had designed the menu and worked out the screenshow which is user - friendly. The user can easily select to study any chemical structure by pressing a number once. Apart from the chemical structure and information, the menu also helps the users to understand the biochemical role of the structure set in front them. There are 18 files of "screenshow" as shown in Table 1.

Table 1. The eighteen files of "screenshow"

File number	Heading	Details
1	VITAMI.SHW	Main menu
2	FATVIT.SHW	Main menu on Fat Soluble Vitamins
3	WATERV.SHW	Main menu on Water Soluble Vitamins
4	ESSVIT.SHW	Main menu on Essential nutrients
5	VIT-A-.SHW	Sub-menu of Fat Soluble Vitamins exhibiting Vitamin A
6	VIT-D-.SHW	Sub-menu of Fat Soluble Vitamins exhibiting Vitamin D
7	VIT-E-.SHW	Sub-menu of Fat Soluble Vitamins exhibiting Vitamin E
8	VIT-K-.SHW	Sub-menu of Fat Soluble Vitamins exhibiting Vitamin K
9	VIT-B-.SHW	Sub-menu of Water Soluble Vitamins exhibiting vitamin B
10	VIT-C-.SHW	Sub-menu of Water Soluble Vitamins exhibiting Vitamin C
11	VIT-B_1-.SHW	Sub-menu of Vitamin B showing Vitamin B_1
12	VIT-B_2-.SHW	Sub-menu of Vitamin B showing Vitamin B_2
13	NIACI-.SHW	Sub-menu of Vitamin B showing Niacin
14	PANTO-.SHW	Sub-menu of Vitamin B showing Pantothenic acid
15	PYRID-.SHW	Sub-menu of Vitamin B showing Pyridoxine
16	BIOTI-.SHW	Sub-menu of Vitamin B showing Biotin
17	FOLIC-.SHW	Sub-menu of Vitamin B showing Folic acid
18	VIT-B_{12}.SHW	Sub-menu of Vitamin B showing Vitamin B_{12}

The "screenshow" file of any Sub-menu is consisted of a chart exhibiting the chemical structure of a specific vitamin or derivative. The chart title is always correlated with the heading of screenshow file. For example, VIT-K-13.CHT is the chart title showing the structure of vitamin K with the item number 3 for sorting out on the first screen of VIT-K-.SHW. And VIT-D-1.CHT is the first screen under VIT-D-SHW title. There are 144 charts covering the chemical structures of vitamins and their derivatives.

5.3 The command program

The commercially available Harvard Graphic software is quite difficult and complicated for the common user. The authors has modified the Harvard graphic (HG.EXE) by omitting the display of Harvard graphic menu from the screen. Besides, the VITAMIN. COM, a new command which was written using the ASSEMBLY language had been installed to control the display of "screenshow". The users are then provided with an easier way to work on.
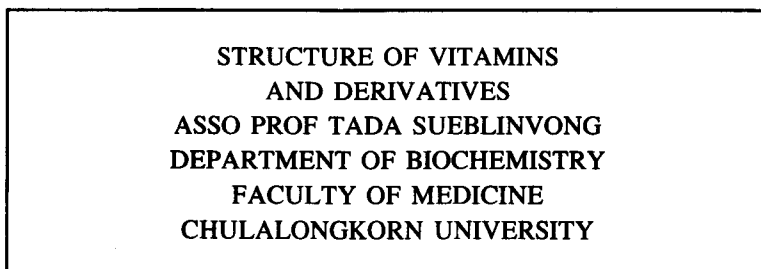
Operation steps and examples

1. Preparation of the computer hardware as previously recommended and the program on the cumulative chemical structures of vitamins and derivatives which are kept in 5 floppy 5 1/4″ diskettes namely : VITAMIN 1-5

2. Switch on the CPU of the hardware and boot with PC-DOS or MS-DOS version 3.0 or newer.

3. Make a new Sub-directory in the hard disk, name it C : \ VITAMIN, then copy the cumulative chemical structures of vitamins and derivatives onto the hard disk starting from VITAMIN 1 to VITAMIN 5.

4. Program the computer to sort out the Sub-directory (CD \ VITAMIN), then key the VITAMIN and press <ENTER> key as follows :

     C > CD \ VITAMIN   <ENTER>
     C > VITAMIN   <ENTER>
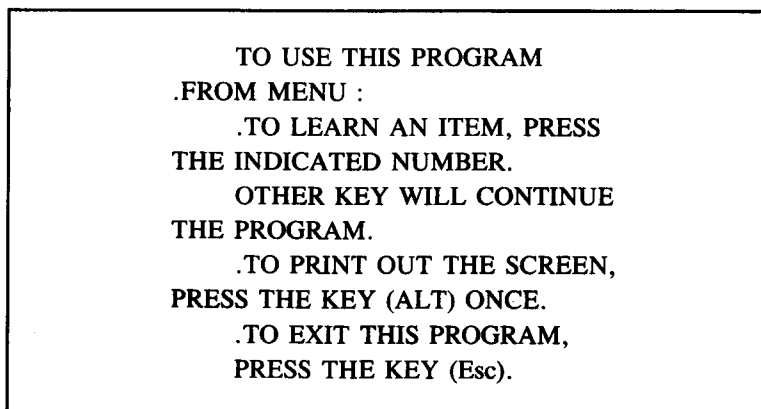
The title page will appear on the screen as shown in Figure 2.

5. After the title page, there is a brief instruction manual as shown in Figure 3.

STRUCTURE OF VITAMINS
AND DERIVATIVES
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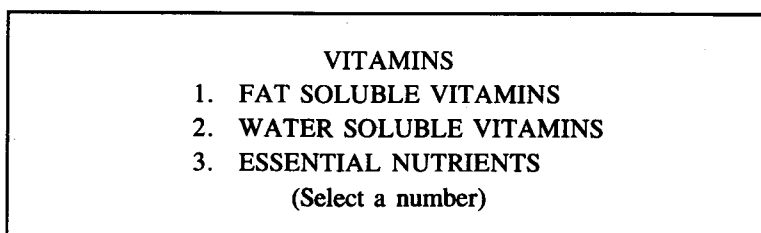
Figure 2. The title page.

TO USE THIS PROGRAM
.FROM MENU :
    .TO LEARN AN ITEM, PRESS
THE INDICATED NUMBER.
    OTHER KEY WILL CONTINUE
THE PROGRAM.
    .TO PRINT OUT THE SCREEN,
PRESS THE KEY (ALT) ONCE.
    .TO EXIT THIS PROGRAM,
PRESS THE KEY (Esc).
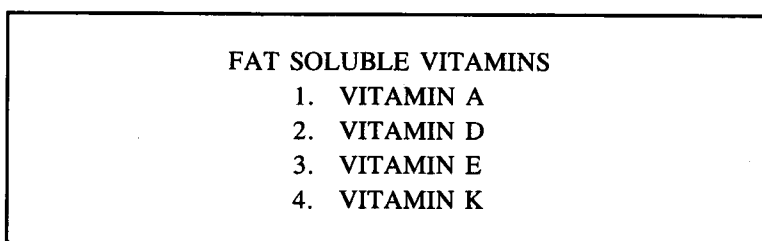
Figure 3. Brief instruction manual.

The user has to wait for a moment, then the main menu will appear on the monitor screen as shown in Figure 4. The user then choose to learn the interested item by pressing the item number once. If the number 1 is pressed; then the menu for Fat soluble vitamins will appear on the screen as shown in Figure 5.

VITAMINS
1. FAT SOLUBLE VITAMINS
2. WATER SOLUBLE VITAMINS
3. ESSENTIAL NUTRIENTS
(Select a number)

Figure 4. Main menu.

```
┌─────────────────────────────────────────┐
│           FAT SOLUBLE VITAMINS          │
│            1.   VITAMIN A               │
│            2.   VITAMIN D               │
│            3.   VITAMIN E               │
│            4.   VITAMIN K               │
└─────────────────────────────────────────┘
```
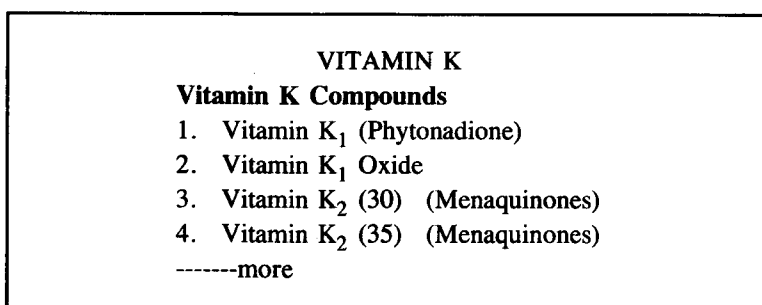
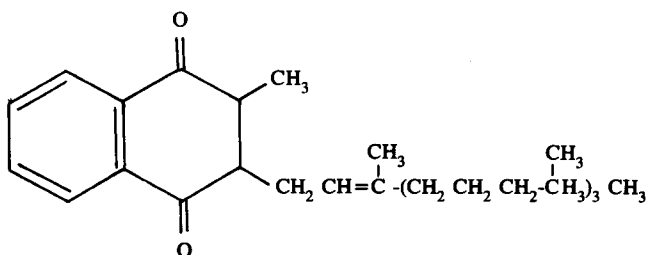**Figure 5.** Menu on Fat soluble vitamins.

If item number 4 is chosen by the user, then the menu for Vitamin K will appear on the monitor screen, as presented in Figure 6. Further pressing on item number 1 (Figure 6.) ; then, the chemical structure of Vitamin K_1 together with the information covering physical, chemical properties and medical importance will be seen on the monitor screen as shown in Figure 7.

Printing of the chemical structure which appeared on the monitor screen can be done easily by setting the printer ready and pressing the key <ALT> once. Once the printing is finished, the program will return to where it was before being interrupted and the user can continue further study. At any time the user want to interrupt the printing process, the key <Esc> should be pressed, and the program will return to where it was before printing. To exit the program, <Esc> key should be pressed.

```
┌─────────────────────────────────────────────┐
│                  VITAMIN K                  │
│  Vitamin K Compounds                        │
│    1.   Vitamin K₁ (Phytonadione)           │
│    2.   Vitamin K₁ Oxide                    │
│    3.   Vitamin K₂ (30)   (Menaquinones)    │
│    4.   Vitamin K₂ (35)   (Menaquinones)    │
│  -------more                                │
└─────────────────────────────────────────────┘
```

Figure 6. Menu on Vitamin K.

VITAMIN K1

λ_{MAX} (IN PETR ETHER) = 242,248,260,269,325 nm.
$E_{1cm}^{1\%}$ = 396,419,383,387,68
FORMULA : $C_{31}H_{46}O_2$
MOL.WT. = 450.68
MEDICAL IMPORTANCE : PROTHROMBOGENIC VITAMIN

Figure 7. : The chemical structure of Vitamin K_1

Discussion

There is a commercially available program software linked to the Apple Macintosh for the application on creating the chemical structure of chemical compounds. However the price is beyond that affordable by the official budget. Another problem encountered by the authors is that the computer hardware available in the office is an IBM. These are the reasons which forced the authors to use only the available resources to produce this program. Besides, the commercially available software named "Chem Write" provides the user with parts of structures for examples; the hexagonal structure of either benzene ring, cyclohexane or pyran, or the pentagonal form of furan or cyclopentane, the double bond part, the triple bond part, etcetera; Such things are similar to the jigsaw parts, and the user has to assemble these jigsaw parts into the desired structures. This commercially available software would therefore provide users with less limitation in terms of application if only its price is less expensive.

The software on the cumulative chemical structures of vitamins and derivatives which is developed by the authors will provide the user with a complete and whole structure of individual compounds existed on the menu as well as information as presented in Figure 7. within minutes. The printout process is simple. Therefore this software should be very useful for any interested user. Free copying of this software is possible upon request, but kindly bring your own floppy diskettes.

Acknowledgement

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