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Der Pharmacia Lettre, 2015, 7 (8):135-142
(http://scholarsresearchlibrary.com/archive.html)

Der Pharmacia Lettre
Scholars Research Library
ISSN 0975-5071
USA CODEN: DPLEB4

Periodic table in medical molecular formula safe transfer

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ABSTRACT

Creating a new medicine is a long and rigorous process. Much of what is investigated never makes it to patients because in any search for new medicines, primary concern is always patient safety. It can take years to progress from a promising idea in the research laboratory to receiving approval from regulators. Thousands of different chemicals are investigated to identify the one that can be tested in humans. Developing a new treatment typically goes through several stages from laboratory to patient. These new drugs are patented because these can be easily copied or imitated. So protection of the details of new drugs is of primary importance. In this article we propose a method for encrypting the molecular formula of any medicine.

Key words: Decryption, Encryption, Periodic Table, Binary String, Level – order.

INTRODUCTION

Over the past 30 to 40 years there have been drastic changes in the way new medicines are developed. Before the 1970s drug development was based on phenotypic assays and 'accidental findings', with an approval process that would often take two to three years to complete. Scientists now have a better understanding of the mechanisms leading to disease development, allowing the selection of 'targets' - regulators which are dysfunctional in the disease - allowing scientists to develop new drugs, which inhibit these cellular targets [1].

Scientists spend their life for the benefit of human life. Medicines are discovered to make life less painful. Transmission of the details of any new drug is always a challenge. Many new methods are discovered for safe transmission of these details. The security of a system is essential nowadays. With the growth of the information technology power, and with the emergence of new technologies, the number of threats a user is supposed to deal with grew exponentially [2]. Behnam Bazli et.al., proposed a DNA encryption schemes and use of biological alphabets to manipulate information by employing the DNA sequence reaction, to autonomously make a copy of its threads as an extended encryption key [3] W. Puech and J.M. Rodrigues presented a new method that combines medical image encryption and watermarking technique for safe transmission purpose [4]. In this paper we propose a method of encrypting the molecular formula of a medicine using a new constructed binary periodic table and level tree traversal.

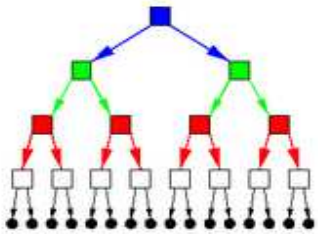
MATERIALS AND METHODS

2.1 Graph

In the most common sense of the term, a graph is an ordered pair G = (V, E) compromising a set V of vertices or nodes together with a set E of edges or links, which are 2 – elements subset of V (that is an edge is related with two vertices, and the relation is represented as an unordered pair of the vertices with respect to the particular edge) [5].

2.2 Tree
Any connected graph without simple cycles is a tree [6].

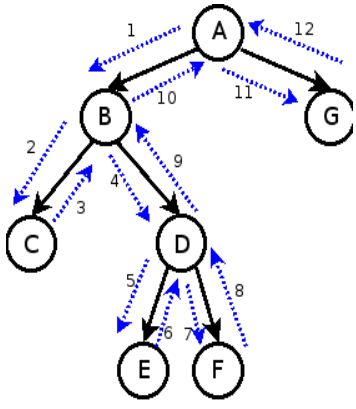
2.3 Rooted Tree
A tree is called a rooted tree if one vertex has been designated the root, in which case the edges have a natural orientation, towards or away from the root. The tree-order is the partial ordering on the vertices of a tree with $u \leq v$ if and only if the unique path from the root to v passes through u. In a rooted tree, the parent of a vertex is the vertex connected to it on the path to the root; every vertex except the root has a unique parent. A child of a vertex v is a vertex of which v is the parent. A descendent of any vertex v is any vertex which is either the child of v or is (recursively) the descendent of any of the children of v. A sibling to a vertex v is any other vertex on the tree which has the same parent as v. [6]. Snapshot – 1 [7] provides an example for rooted tree.



Snapshot – 1

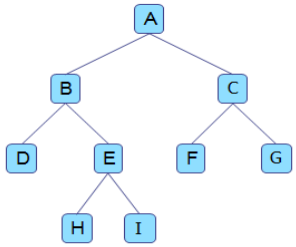
2.4 Tree Traversal
Tree traversal also known as Arkiletian tree search is a form of graph traversal and refers to the process of visiting each node in a tree data structure, exactly once, in a systematic way. Such traversals are classified by the order in which the nodes are visited [8].

2.5 Pre – order
Let T be an ordered rooted tree with root r. If T consists only of r, then r is the preorder traversal of T . Otherwise, suppose that $T_1, T_2, \ldots, T_n$ are the subtrees at r from left to right in T . The preorder traversal begins by visiting r. It continues by traversing T_1 in preorder, then T_2 in preorder, and so on, until T_n is traversed in preorder [9]. Snapshot - 2 [10] provides an example of pre – order tree traversal.



Snapshot - 2

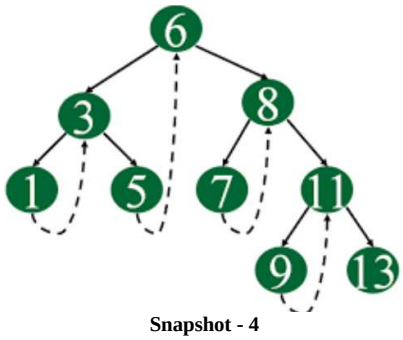
2.6 Post – order
Let T be an ordered rooted tree with root r. If T consists only of r, then r is the post order traversal of T. Otherwise, suppose that $T_1, T_2, \ldots, T_n$ are the sub trees at r from left to right. The postorder traversal begins by traversing T_1 in post order, then T_2 in post order, . . ., then T_n in postorder, and ends by visiting r [9]. Snapshot – 3 [11] provides an example of post – order tree traversal.



Post-order Traversal:
D,H,I,E,B,F,G,C,A
Snapshot – 3

2.7 In – order

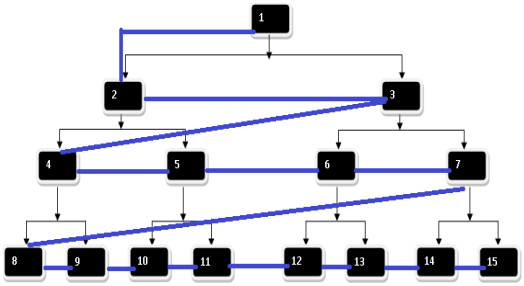
Let T be an ordered rooted tree with root r. If T consists only of r, then r is the inorder traversal of T . Otherwise, suppose that T_1, T_2, . . . , T_n are the subtrees at r from left to right. The inorder traversal begins by traversing T_1 in inorder, then visiting r. It continues by traversing T_2 in inorder, then T_3 in inorder, . . . , and finally T_n in inorder [9]. Snapshot - 4 [12] provides an example of In – order tree traversal.



Snapshot - 4

2.8 Level - Order

It starts at the tree root and explores the neighbor nodes first, before moving to the next level neighbors [13]. Snapshot - 5 [14] provides an example of level – order tree traversal.



Snapshot - 5

Proposed Method

Numerous medicines are available for various diseases in market. Aspirin is used to reduce fever and relieve mild to moderate pain from conditions such as muscle aches, toothaches, common cold, and headaches. It may also be used to reduce pain and swelling in conditions such as arthritis. Aspirin is known as a salicylate and a nonsteroidal anti-inflammatory drug [15]. Paracetamol is used to treat many conditions such as headache, muscle aches, arthritis, backache, toothaches, colds, and fevers. It relieves pain in mild arthritis but has no effect on the underlying inflammation and swelling of the joint [16]. Cocaine also known as benzoylmethylecgonine, is a strong stimulant mostly used as a recreational drug [17]. Methadone is classified as an opioid (an analgesic that is used for severe pain). In the United States, methadone treatment is associated with a significant reduction in predatory crime, improvement in socially acceptable behavior, and psychological well-being [18]. Every medicine has a molecular formula. A molecular formula is a combination of the chemical elements involved in their discovery and the

proportions in which they are used. We create a binary periodic table and hence use it for molecular formula encryption using level tree traversal.

Construction of Binary Periodic Table

Chemical elements are best represented using periodic table. There are lots of information available in the table, like atomic radius, ionization energy (ionization potential), electron affinity, electro negativity, metallic character. Any of these properties can be used for encryption. But most of the chemist are too familiar with these data. So use of this may lead to easy decryption. In a general periodic table there are 114 cells with each cell representing an element. There are 128 distinct binary strings of length 7. We randomly assign distinct binary string of length seven to represent the elements in the periodic table. A sample binary periodic table is seen in Table – 1.

3. ENCRYPTION ALGORITHM

Step 1 Consider the molecular formula of the medicine.
For example the molecular formula of Aspirin is $C_9H_8O_4$.

Step 2 Convert the elements in the molecular formula to a binary string of length 7 using Table – 1. From Table – 1
C = 0000110, H = 0000001, O = 0001000.

Step 3 Convert the numbers in the molecular formula to a binary string of length 7.
9 = 0001001, 8 = 0001000, 4 = 0000100.

Step 4 Concatenating the binary string we generate a binary sequence say M. Let the length of M = k.
For Aspirin the binary string generated is M = 0000110000100100000010001000000100000
000100.

Step 5 Choose a tree with k vertices.

Step 6 Assign the sequence M as vertex labels to the tree T using level – order labeling. For the sequence in our example the level order tree is as seen in Fig. 1

Binary Periodic Table of the Elements

												C	Br	He	Tc		
H 0000001												solid	liquid	gas	synthetic		He 0000010
Li 0000011	Be 0000100								KEY	Symbol Binary Conversion		B 0000101	C 0000110	N 0000111	O 0001000	F 0001001	Ne 0001010
Na 0001011	Mg 0001100											Al 0001101	Si 0001110	P 0001111	S 0010000	Cl 0010001	Ar 0010010
K 0010011	Ca 0010100	Sc 0010101	Ti 0010110	V 0010111	Cr 0011000	Mn 0011001	Fe 0011010	Co 0011011	Ni 0011100	Cu 0011101	Zn 0011110	Ga 0011111	Ge 0100000	As 0100001	Se 0100010	Br 0100011	Kr 0100100
Rb 0100101	Sr 0100110	Y 0100111	Zr 0101000	Nb 0101001	Mo 0101010	Tc 0101011	Ru 0101100	Rh 0101101	Pd 0101110	Ag 0101111	Cd 0110000	In 0110001	Sn 0110010	Sb 0110011	Te 0110100	I 0110101	Xe 0110110
Cs 0110111	Ba 0111000	Lu 0111001	Hf 0111010	Ta 0111011	W 0111100	Re 0111101	Os 0111110	Ir 0111111	Pt 1000001	Au 1000010	Hg 1000011	Tl 1000100	Pb 1000101	Bi 1000110	Po 1000111	At 1001000	Rn 1001001
Fr 1001010	Ra 1001011	Lr 1001100	Rf 1001101	Db 1001110	Sg 1001111	Bh 1010000	Hs 1010001	Mt 1010010	Ds 1010011	Rg 1010100	Uub 1010101		Uuq 1010110				
		La 1010111	Ce 1011000	Pr 1011001	Nd 1011010	Pm 1011011	Sm 1011100	Eu 1011101	Gd 1011110	Tb 1011111	Dy 1100000	Ho 1100001	Er 1100010	Tm 1100011	Yb 1100100		
		Ac 1100101	Th 1100110	Pa 1100111	U 1101000	Np 1101001	Pu 1101010	Am 1101011	Cm 1101100	Bk 1101101	Cf 1101111	Es 1110000	Fm 1110001	Md 1110010	No 1110011		

Table – 1

Step 7 Send this tree to the receiver**.**

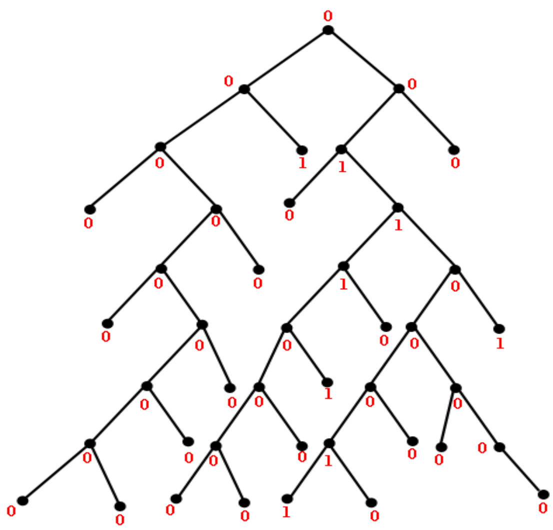
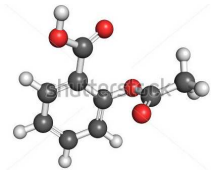
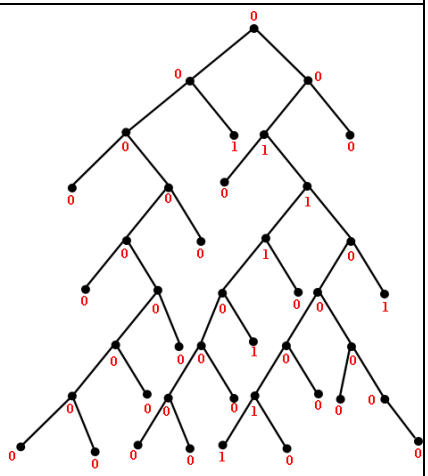
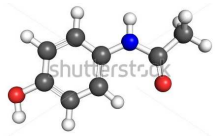
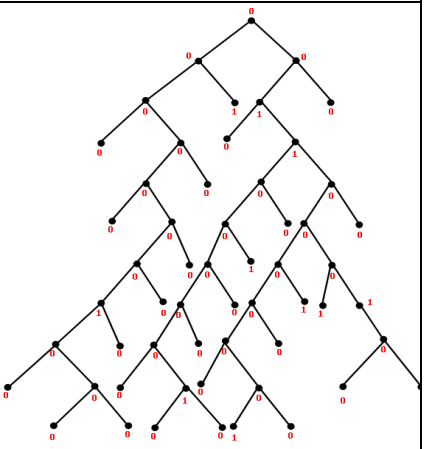
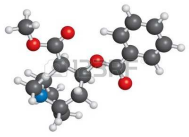
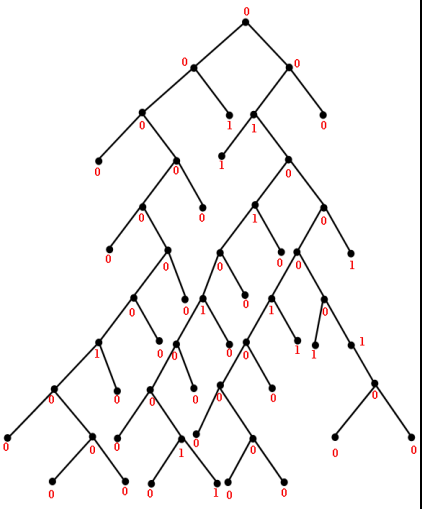


Fig. 1

Table – 2 provides examples of some common drugs and the corresponding level trees

S. No	Ball and Stick Representation	Molecular Formula and its Binary Conversion	Tree Representation
1.	 **Aspirin**	$C_9H_8O_4$ 000011000010010000001000100000010000000100	
2.	 **Paracetamol**	$C_8H_9NO_2$ 000011000010000000001000100100001110000000000010000000010	
3.	 **Cocaine**	$C_{17}H_{21}NO_4$ 000011000100010000001001010100001110000000000010000000100	

4. DECRYPTION ALGORITHM

For decrypting the sequence we reverse the procedure.
Suppose the received sequence is as seen in Fig. 2

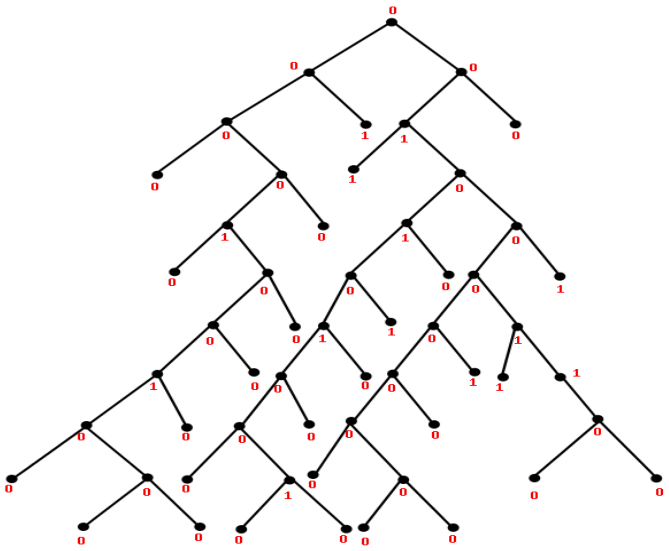
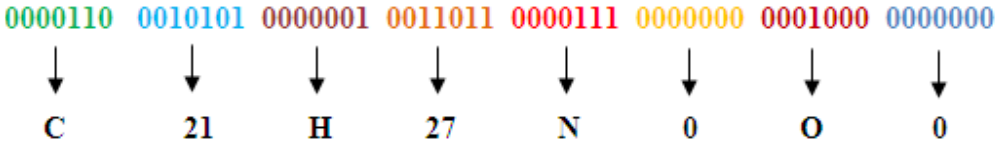


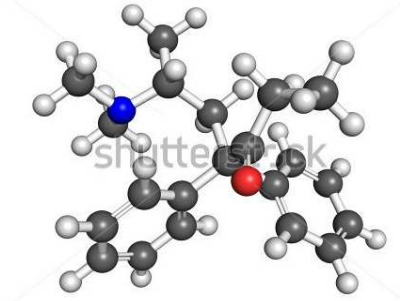
Fig. 2

Step 1 Using level – order traversal the sequence generated from the tree is 0000110001010 1000000100110110000111000000000010000000000.

Step 2 Split the sequence into segments of length 7.



From the Table – 1 and the binary conversion the molecular formula is $C_{21}H_{27}N0$ which represents Methadone.



Snapshot - 6

CONCLUSION

Drug discovery and development is very expensive. Of all compounds investigated for use in humans only a small fraction are eventually approved in most nations by government appointed medical institutions or boards, who have to approve new drugs before they can be marketed in those countries.

Discovering drugs to be a commercial or a public health success, involves a complex interaction between investors, industry, academia, patent laws, regulatory exclusivity, marketing and the need to balance secrecy with communication. The proposed method guarantees for secure transmission and reception of drugs. The method is

seemed to be so secure that it would be very difficult for any intrude to break the encrypted message and retrieve the actual message.

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