THE MATHEMATICAL AND LOGICAL APPROACHES TO R&D WORK OF COMPILING CURRICULA FOR CHEMISTRY EDUCATION

Abstract. *The aim of this study was to show how combine qualitative and quantitative approaches in the framework of R&D activities for compiling balanced curricula for chemistry education. The mathematical model based on graph theory was built up. This model allowed us to calculate two kinds of parameters to characterize the structure and composition of a given teaching material:*
- parameters characterizing every single structural element of the teaching material in the selected content;
- parameters describing the teaching material as a whole.
Two important educational concepts of selection and structuring of teaching material was derived from mathematical model represented by directed graph – continuity and compactness.
As an example of using mathematical and logical approaches for compiling curricula of chemistry education these theoretical concepts were applied to organic chemistry courses for basic and high schools. Results showed that the mergering of curriculum design with chemical epistemology, personal and social relevance of teaching material and mathematical and logical models creates a new forum where constraints to educational reforms can be reviewed and resolved.
Key words: *curriculum design and structuring, mathematical models of teaching subject, relevance, organic chemistry.*

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Introduction

There is not any doubt that curriculum design and implementation have been, and continue to be, at the forefront of science education reforms. We consider as the initial position of good learning and good teaching any field of sciences including chemistry a balanced curriculum. According to our paradigm the ideal model of science education today as well as in future is the teaching balanced science in accordance with balanced curricula in strongly social context based on logical, psychological and didactical treatment (Tõldsepp & Toots, 2003). About half of century ago famous Russian psychologist P. Galperin has emphasized that is impossible to teach in sensible way when teaching subject is structured insensible way (Galperin, 1965). The guiding role of teaching subject in the formation of scientific research activity abilities in comprehensive school was supported by V. Lamanauskas too. He has mentioned that teaching subjects become the means of realization of learners´ demands and interests (Lamanauskas, 2008, 132). Conventional approaches in curriculum design have typically included emphases on content knowledge (e.g. problem-solving in the context of substances and chemical reactions) or societal aspects of chemistry (e.g. effects of chemical pollution on the environment). The history of paradigms of chemistry education confirms entirely an above mentioned statement:

1950	Garrett Report
1960	CHEM Study / Chemical Bond Approach (CBA)
1970	Interdisciplinary Approaches in Chemistry (IAC)
1980	Chemistry in the Community (ChemCom)
1990	Global Issues
2000	Science for everybody

The passing over content oriented approaches to societal oriented ones has changed the relationships between content and context knowledge. To enlarge the personal and social oriented

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knowledge (context knowledge) suffer scientific content of teaching subject. It is logical inverse ratio lawfulness. Wider context causes always narrower content.

Unlike chemistry education V. Paškevičs cannot see any changes in educational content of natural sciences. "It has been almost 40 years since my class graduated from the secondary school, but the science curriculum in schools and higher educational establishments hasn´t changed much, especially with regard to physics. Metaphorically speaking, the content of sciences could be compared to the content of a wardrobe containing the clothes of our grandparents and our parents, as well as our own contemporary clothing items which we traditionally try to save until we have worn down the older clothes. In most cases the final result is that there is no time left for the contemporary." (V. Paškevičs, 2006, 4).

Our approach to R&D work of curriculum design and structuring in this paper consists of the declaration that quality and quantity occurs in surrounding us world always together. To avoid the using only of "soft" methodology and strategies for design and structuring of the teaching subjects (or any part of teaching materials) we offer to practice beside of scientific concepts and epistemology mathematical and logical models of teaching materials (Tõldsepp, 2009). The aim of this study was to show how to combine qualitative and quantitative methods in R&D work of curriculum design and structuring. The mathematical models based on directed graphs of teaching subjects were built up and analyzed for different approaches to organic chemistry courses in comprehensive schools.

Theoretical Background

Any teaching subject or its subcomponent can be presented as a directed graph $G = (X, U)$ where $X = \{x_1, \ldots, x_n\}$ denotes the vertexes of G – structural elements of a teaching material -- and $U = \{u_1, \ldots, u_n\}$ is a set of ordered pairs $u_a = (x_i, x_j)$ between the structural elements of a teaching material. This definition of the model of a teaching subject implies that $(x_i, x_j) \neq (x_j, x_i)$. In order to simplify the analysis of the model of a teaching subject, let $A = (a_{ij})$ be the adjacency matrix of our directed graph G, where $i, j \in \{1, 2, \ldots, n\}$. We also define the elements of the adjacency matrix as follows:

$$a_{ij} = \begin{cases} 1, & (x_i, x_j) \in U \\ 0, & (x_i, x_j) \notin U \end{cases}$$

This representation of the model of a teaching material allows us to calculate two kinds of parameters to characterize the structure and composition of a given teaching material:
- parameters characterizing every single structural element of the teaching material in the selected content;
- parameters describing the teaching material as a whole. The following characteristics belong to the former category:
- the number of relations with structural elements which provide information needed to teach the structural element in question

$$S_j = \sum_{i=1}^{n} a_j \, ; \qquad (1)$$

i.e the sum of every column
- the number of relations with structural elements which use the information provided by the given structural element

$$S_i = \sum_{j=1}^{n} a_j \, ; \qquad (2)$$

i.e the sum of every row
- the overall connectedness of the specified structural element in a teaching material

$$S = \sum_{i=1}^{n} a_j + \sum_{j=1}^{n} a_j \, . \qquad (3)$$

A large number of our research papers indicate that the quality and durability of students' knowledge acquired from the given structural element depends heavily on its connectedness with other elements of teaching materials (Rannikmäe & Tõldsepp, 1981).

The parameters characterizing every single structural element of the teaching material help us to precise the notion relevance for every element of teaching subject. If S_j (1) has a maximal value we can suppose that structural element j has a great value for the formation of new knowledge in framework of this subject. Consequently, it has structural or/and functional relevance in teaching subject. If S_i (2) has a very small value or it is even nought, means that this structural element has not any scientific relevance. However, it could be of personal or/and social relevance for students. Maybe some structural elements of teaching subjects have no relevance (scientific, personal, social). This problem already belongs to criteria of selection of the teaching material. Why do we need such irrelevant material?

The average distance from the main diagonal of the adjacency matrix

$$\overline{d} = \frac{d}{N} \qquad (4)$$

has proved to be the defining characteristic to describe the teaching material as a whole. Here N is the maximal number ones above the main diagonal of our matrix and d indicates the summary distance from the main diagonal

$$d = \sum_{i=1}^{n-1}\sum_{j=1}^{n-1} a_j \, (j-i)$$

and d_i is the distance of the iith row from the main diagonal

$$d_i = \sum_{j=1}^{n} a_j \, (j-i)$$

The represented model is only valid for directed graphs, i.e. all elements of the adjacency matrix $A = (a_{ij})$ that are below the main diagonal are equal to nought. The average distance from the main diagonal ought to be regarded as an indicator of compactness of the composition of a teaching material. Furthermore, it can also be considered as an indicator which allows us to determine whether a teaching material is ordered optimally. The smaller the parameter's value, the shorter the time lag between learning different parts of a teaching material. We call this rule as the concept of compactness of structuring a teaching material.

The second indicator that characterizes a teaching material as a whole is the sum of the elements on the diagonal adjacent to the main diagonal:

$$K = \sum_{i=1}^{n-1} a_{i,i+1} \qquad \text{where } a_{i,i+1} = 1 \qquad (5)$$

If we presume that ideally every new structural element builds on the previous one, then the value of K has to be maximal for a given matrix. We call this the principle of continuity of a teaching material.

Following the concepts of compactness and continuity help us to minimize the students' working memory. A number of studies have shown (Johnstone, 1991) that the difficulties by learning chemistry are related to the limitations of students' working memory, the active system of memory in which information is assembled and organized prior to recall. Limitations of working memory determine how many items can be stored and rehearsed before they are lost owing to competition from new information (Ellis & Hunt, 1989). The structuring of teaching material according to concepts of compactness and continuity always help to recall previous teaching material.

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Curriculum Implementation

The modern definition of organic chemistry is the chemistry of carbon compounds or sometimes the chemistry of functional groups. In this case we can see harmony among all authorities. However, by design and structuring of organic chemistry as the teaching subject in different textbooks appear different approaches and paradigms. To clear selection criteria of teaching material and paradigms of structuring school organic chemistry we need a model of organic chemistry represented for example as a directed graph.

For compiling optimally structured and psychologically based course of organic chemistry for high school we divided all teaching subject into 14 structural elements (see matrix A and figure 2) and found all links between separate structural elements. Currently, we built up the mathematical model as a directed graph $G = (X, U)$. To simplify the calculation of the parameters characterized the teaching material a directed graph G was represented as the adjacency matrix $A = (a_{ij})$. From matrix A was calculated the parameters for every single structural elements of teaching material (see table 1). Initiated from calculated parameters was found the type of relevance for every structural element of teaching material. We have based on the concept of relevance set up by J. Holbrook. It is intrinsic usefulness, intrinsic meaningfulness, or intrinsic importance (Holbrook, 2008, 258). According to structure of any educational process that consists of teaching and learning, we can differ relevance of two types – it is intrinsic usefulness from point of view of teaching subject (scientific relevance) and intrinsic usefulness and importance from point of view of students (personal and social relevance).

Table 1.   The parameters characterizing the single elements of organic chemistry and type of their relevance.

Structural elements	Sum of columns (S_j)	Sum of rows (S_i)	Sum of all links $(S_j + S_i)$	Type of relevance
1	0	13	13	Scientific
2	1	12	13	Scientific
3	2	11	13	scientific mainly, social
4	3	2	5	socio-economical
5	3	1	4	socio-economical
6	5	5	10	scientific, personal, social
7	4	2	6	Scientific
8	5	5	10	scientific, personal, social
9	5	1	6	scientific mainly
10	6	0	6	personal, social
11	6	0	6	personal, social
12	4	2	6	scientific mainly
13	5	1	6	scientific, personal
14	6	0	6	personal, social

The high values of the sum of rows mean that this structural element of teaching material has an importance for formation knowledge about following material (structure of organic molecules, hydrocarbons). The low values of the sun of rows mean that we can consider this structural element as an outcome (result) of teaching and learning process. Usually this element has social or personal importance (alkyl halides, carbohydrates, fats, proteins). For instance, alkyl halides are used as industrial and household solvents, as anesthetics, as pesticides and as reagents for synthesis of other compounds.
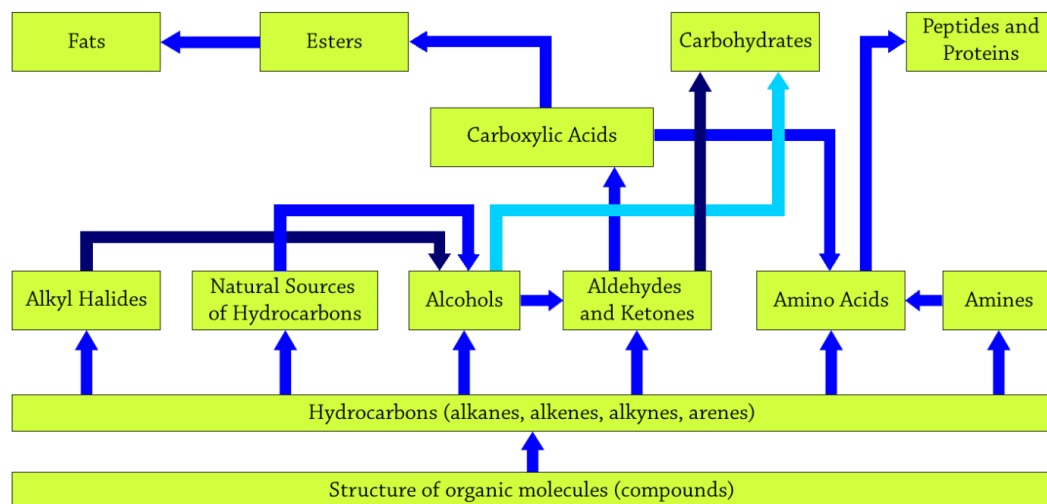
Figure 1.   The general structure of school organic chemistry.

$$
A = \begin{array}{c} \\ 1\\2\\3\\4\\5\\6\\7\\8\\9\\10\\11\\12\\13\\14 \end{array}
\begin{array}{cccccccccccccc}
1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 & 13 & 14 \\
\left(\begin{array}{cccccccccccccc}
0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 1 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{array}\right)
\end{array}
$$

Learning of chemical composition, chemical and physical properties of carbohydrates, fats, proteins and vitamins in chemistry education is important because it provides insight into:
- their role in living organisms,
- relation between structure and function of those molecules i.e. how their interactions enable life to be created, maintained and sustained, and
- their role in consumption of energy necessary for synthesis of their own biomolecules, mechanical work and membrane transport (Korolija, Rajic&Mandic, 2008, 66).

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In the figure 1 is given a general structure of school organic chemistry independently of the para-digms, concepts and strategies of teaching and learning. However it should be taken into account by design and implementation of teaching subject to save peculiarities of organic chemistry as a field of science. Looking at the figure 1 we can see that we do not need more classes of organic compounds (ethers, carboxylic acid derivates, heterocyclic compounds etc.) for comprehensive school, because they have not relevance for achieving the most important outcomes – fats, carbohydrates, proteins. To teach all hydrocarbons together corresponds entirely to definition of organic chemistry declared by Carl Schorlemmer in 1889 – organic chemistry is the chemistry of hydrocarbons and their derivates. Keeping the classical paradigms, epistemology and structure of organic chemistry (structure of organic molecules → hydrocarbons → alcohols → carbonyl compounds → carboxylic compounds → carbo-hydrates → amino compounds), following the psychological concepts of continuity and compactness as well as taking into account the relevance of every structural element we achieve an optimal design and order of the school organic chemistry (see figure 2)[1]. The parameter of continuity is very closed to maximum value $d\bar{d} = 0.77$ ($d\bar{d}_{max} = 1$) and lack of long intervals between the structural elements that have logical relationships.

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1   In the figures 2-4 are given only the most important links between the structural elements of teaching subject.
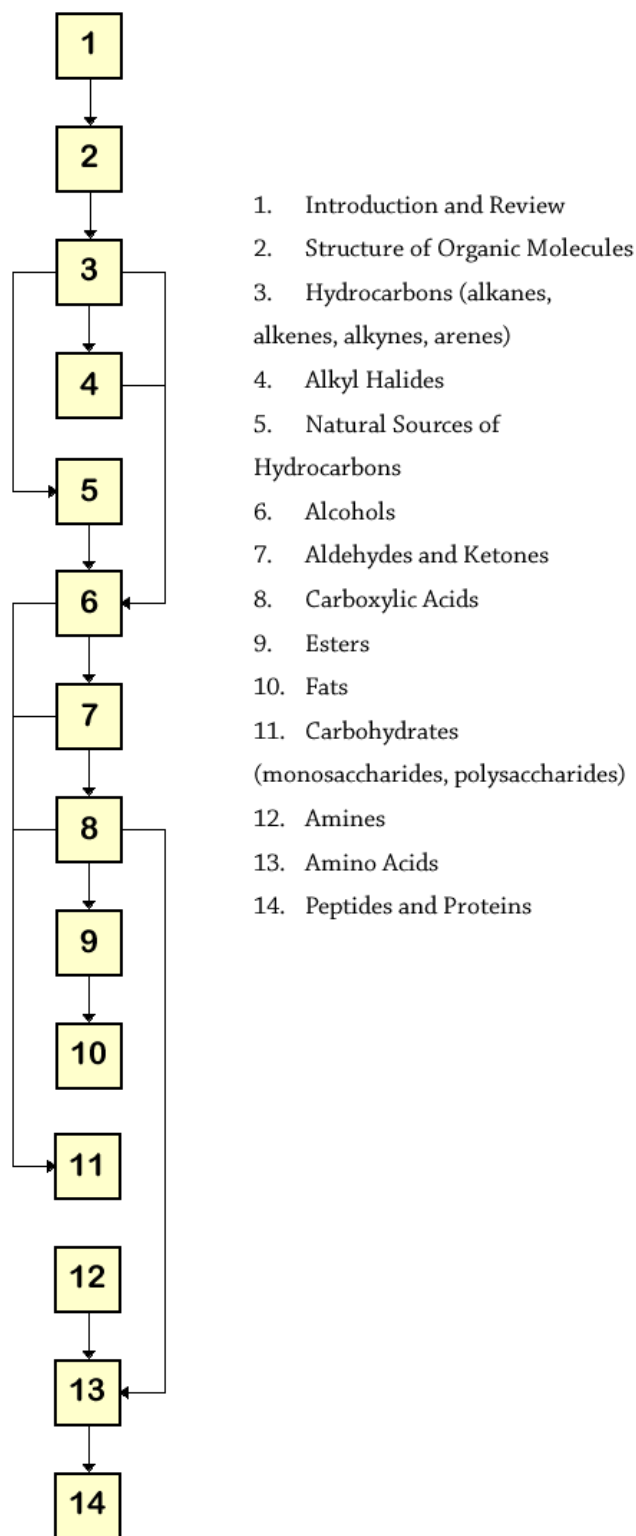
1. Introduction and Review
2. Structure of Organic Molecules
3. Hydrocarbons (alkanes, alkenes, alkynes, arenes)
4. Alkyl Halides
5. Natural Sources of Hydrocarbons
6. Alcohols
7. Aldehydes and Ketones
8. Carboxylic Acids
9. Esters
10. Fats
11. Carbohydrates (monosaccharides, polysaccharides)
12. Amines
13. Amino Acids
14. Peptides and Proteins

Figure 2. **The optimal structure of school organic chemistry for grade 11 (Karelson & Tõldsepp, 2007).**

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All attempts to change the classical design and structure of the school organic chemistry lead us farer from optimal order of presentation the teaching material. The social oriented structure of organic chemistry in the Finnish textbook shows some logical contradictions and less value of parameter continuity – $d\bar{d}$ = 0.60. It is logically impossible to teach the industry of organic compounds (alkenes, aromatic hydrocarbons etc.) without the knowledge about hydrocarbons.
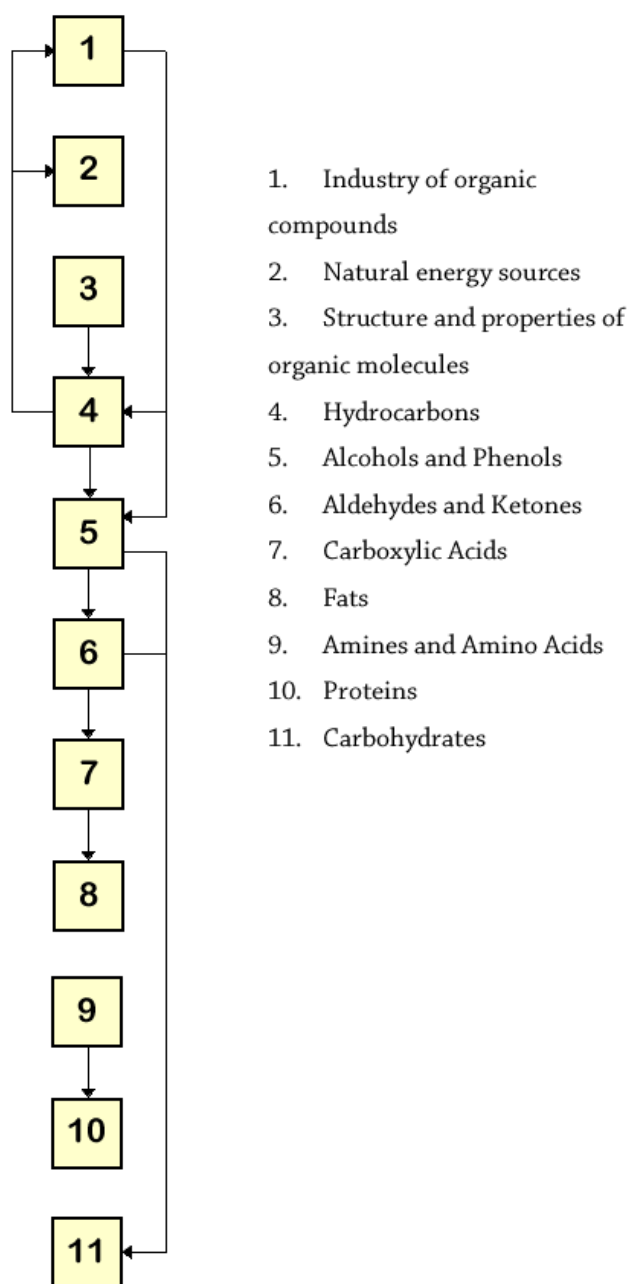

1. Industry of organic compounds
2. Natural energy sources
3. Structure and properties of organic molecules
4. Hydrocarbons
5. Alcohols and Phenols
6. Aldehydes and Ketones
7. Carboxylic Acids
8. Fats
9. Amines and Amino Acids
10. Proteins
11. Carbohydrates

Figure 3.   The non-optimal structure of school organic chemistry (Haavisto, Nikkola & Viljanmaa, 1985).

1. Introduction
2. Alkanes
3. Petroleum
4. Alkyl Halides
5. Alcohols
6. Amines
7. Alkenes and Arenes
8. Aldehydes and Ketones
9. Carboxylic Acids
10. Amino Acids
11. Esters
12. Fats
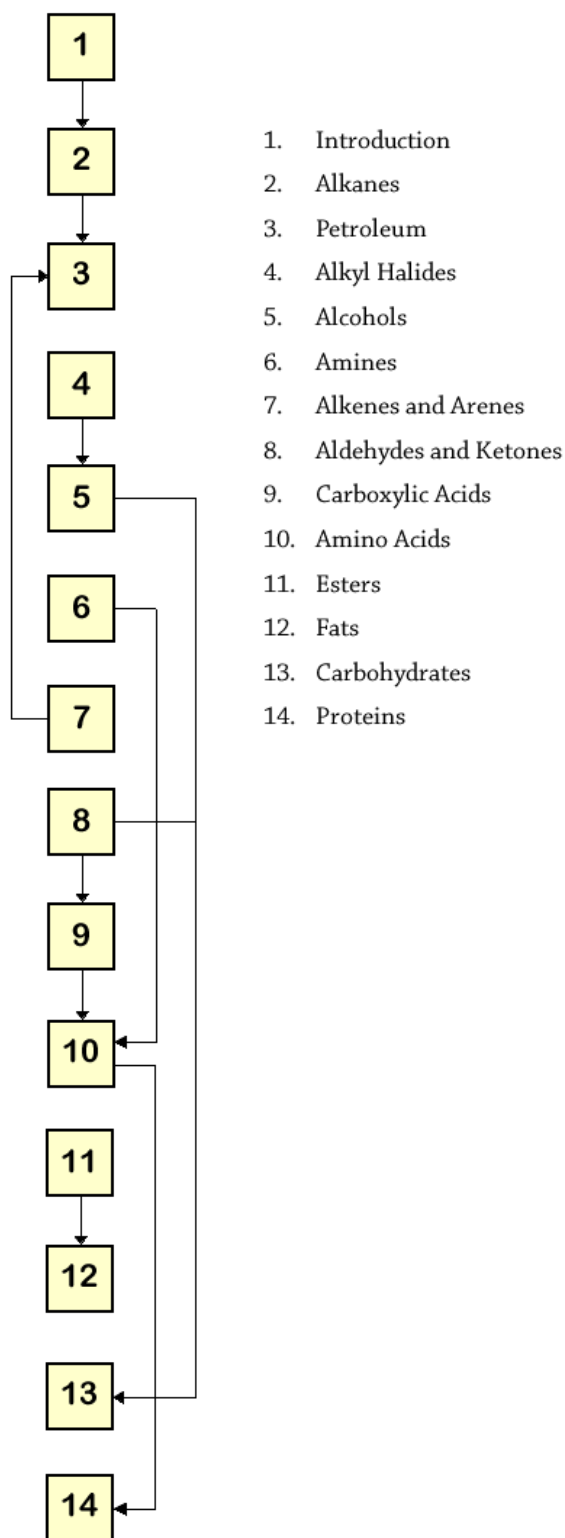13. Carbohydrates
14. Proteins

Figure 4.   The non-optimal structure of school organic chemistry (Tuulmets, 2002).

Another Estonian textbook of organic chemistry ignores the classical concepts of design school organic chemistry and result is a very low value of parameter $\bar{d}\bar{d}$. It is equal to 0.43. In addition we meet the very long intervals between the structural elements that have logical relationships and one important logical contradiction. It is impossible to teach chemical composition and properties of petroleum without any knowledge about alkenes and arenes.

Conclusions

Our conclusions related only to comprehensive school organic chemistry. University organic chemistry has the different aims, different paradigms and design. The school chemistry is not the same as chemistry. As conclusion we would like to suggest the following criteria for selection and structuring school science:

- to take into consideration the relevance (scientific, social, personal) of every element of teaching subject;
- to save the paradigms, structure and epistemology of every field of science;
- to follow the psychological concepts of continuity and compactness by structuring teaching subject.

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