

STUDY OF THE STRUCTURE AND POLARITY OF AMINO ACIDS IN HIGH-SCHOOL TEACHING WITH THE HELP OF COMPUTER PROGRAMS

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Abstract. The protein amino acid structure and polarity can be studied also from the aspect of acid-base balance, in correspondence with the number of atoms and nucleons, making use of computers and computer programs within biochemistry teaching. Beside a conventional approach, which is used for the classification of amino acids (the high school level), a new approach can be presented considering their polarity and structure. It has been proved in a school experiment that students acquire better knowledge if the topic is interpreted from this new aspect, based on an utterly innovative and interdisciplinary approach.

Keywords: amino acid structure and polarity, high-school chemistry, computers, computer programs, students

Introduction

The study of protein amino acids within the curriculum of chemistry (biochemistry) at Serbian vocational (medical) schools is based on the investigation of basic characteristics of amino acids as the carriers of structural and functional characteristics of proteins (primary structural units of proteins), the function of which is: forming proteins, without, however, any deeper analysis of their interrelations.

Various pedagogical researches [1] and questionnaires (TIMSS, 2003) [2] conducted on the territory of the Republic of Serbia have shown that chemistry teaching is based on mere transfer of knowledge, where frontal approach dominates and which does not leave sufficient room for research and innovative work, which include the engagement of both the students and the teacher [3].

The principal aim to increase students' motivation and interest in the matter of the area of chemistry may be achieved by introducing innovations in the teaching process. For example, practical experience derived from a German concept of chemistry teaching (project Leonardo¹) at FSU of Jena, through the teachers' professional development program within MNT², daily oriented chemistry teaching) points to the need of constant work in the laboratory accompanied with the use of groceries in simple experiments (milk, meat, flour, juice, sweets, liquor) [4]. The aim of this is to bring closer the content of chemistry to students through its practical usage, which is reflected in making beverages, complimentary toiletries, sweets, dairy products, paints, building material.

Of course, ideas on innovations in chemistry have not been strange to Serbian didactics and teaching (in the late 19th and early 20th century) from historical point [5,6]. Rather, it has always been marked by a bad financial status and poor equipment of schools, caused by unfavourable economical state and pursuing bad policy of education, almost constant (annual) reforms of educational system in the last 50 years [7,8].

The utilization of modern electronic aids in chemistry teaching, caused by a strong influence of IT revolution [9], which has derived from a long practical work within chemistry and computer science in primary schools in the area of the city of Niš, represents an alternative and innovative model in chemistry teaching, as well as a methodical and didactic means in presenting certain topics in chemistry (structure and polarity of amino acids), without digressing from the curriculum and basic aims of general education [10].

Understanding the relation between the structure and biochemical function of amino acids is based on an approach which deals with the polarity of amino acids from the point of a so-called acid-base balance in correspondence with the balance of the number of atoms and nucleons in amino acid molecules (Popov [11], Dlyasin [12], Shcherbak [13,14], Verhovod [15], Rakočević [16-18]). It can be achieved with the use of modern electronic teaching aids (computers and simple computer programs: WORD, Corel Draw, Paint and Power Point) [9].

Amino acid charge

Russian scientist Evgenii Popov divided 20 protein amino acids into four stereochemical types. Such a division results from stereochemical characteristics of amino acids. Having analyzed the structure (stereochemistry) of the side chains of amino acids, Popov showed that only one amino acid, glycine (Gly; G) belongs to the stereochemical type of glycine. Another amino acid, proline (Pro; P) belongs to the stereochemical type of proline. Amino acid pair valine and isoleucine (Val-Ile; V-I) belongs to the type of valine. The remaining 16 amino acids belong to the alanina type. This classification derives from the conformation of the side chains of amino acids [11].

Confirmation of such a classification may be found in the study by Miloje Rakočević and Ana Jokić. The authors state that the four stereochemical types (2+2; G, A i V, P)

demand a different approach regarding the stereochemistry of the side chains of amino acids (2). This means that Gly (with the side chain H) has the shortest possible H chain (H-H) and none of the other amino acids possesses a side chain of this kind (Fig. 1). The side chain (CH_3) of alanine (Ala; A), in relation to Gly ($\text{CH}_2\text{-H}$), comes from the shortest possible non-cyclic hydrocarbon chain (CH_4), while the other 15 amino acids contain the side chain analogous to Ala in the form of ($\text{CH}_2\text{-R}$) (Fig. 1). Val, or its side chain, follows from the shortest possible cyclic hydrocarbon, from cyclopropane, with a permanently open chain and a link to the "head" of the amino acid, through a single vertex of the cyclopropane triangle ($\text{CH}_3\text{-CH-CH}_2$) (Fig. 1). Ile belongs to this type with the side chain ($\text{H}_3\text{C-CH}_2\text{-CH}_2\text{-CH}_3$). The proline type (with proline only), follows from cyclopropane, with, however, a constant non-openness and a linkage to the „head“ through two vertices of the cyclopropane triangle (Fig. 1) [17].

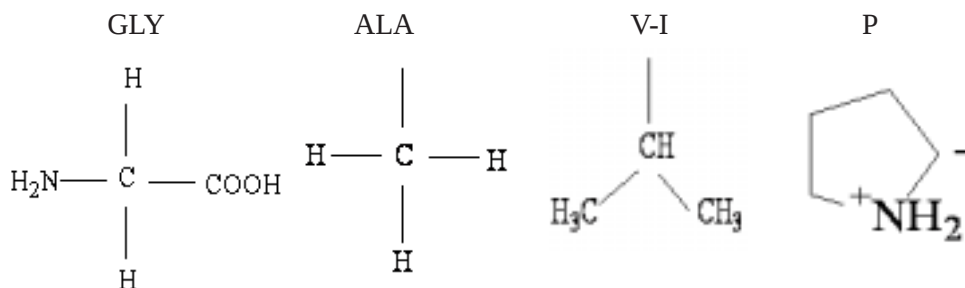


Fig. 1. Four stereochemical types of amino acids which 20 standard amino acids belong to (the basis of their side chains is presented)

Eight pairs of alanine type are classified into two classes: 5 pairs of the alanine type of amino acids belong to the first (inner) class with the presence of O, N and S atoms within a non-cyclic side chain, in the form of functional groups: 1. with the -OH group (Ser-Thr; S-T); 2. with the S atom (Cys-Met; C-T); 3. with the -COOH group (Asp-Glu; D-E); 4. with the amide group (Asn-Gln; N-Q); 5. with the -NH₂ group (Lys-Arg; K-R).

The remaining three pairs belong to the other (outer) class: 1. with a hydrocarbon non-cyclic chain without a heteroatom (Ala-Leu; A-L); 2. with an aromatic chain without a heteroatom (Phe-Tyr; F-Y); 3. with an aromatic chain, without a heteroatom (His-Trp; H-W) [17].

Moreover, it is also shown that one stereochemical type (Ala type) serves as a "measurement subject", while the remaining three types serve as measurement etalons and measurement subjects simultaneously [17].

Stereochemical types of amino acids

A starting point for a new classification of amino acids follows from the works of Miloje Rakočević. One can easily notice that here polar charged amino acids (four aliphatic and one aromatic-heterocyclic) are aligned continuously and are also in contact with two amides and the remaining three aromatic acids (which appear as complements of charged amino acids): D-E-R-K-H/W-Y-F; N-Q-F-Y-W (where D, E are acid; R, K, H alkaline; W, F non-polar amino acids; Y, N, Q polar uncharged amino acids) [18].

The upper (first) row of amino acids arranged in this way contains the amino acids D-E-R-K-H with 60 atoms; then follow their complements: N-F-Y-W-Q with 66 atoms (Table 1). System pairs that follow in Table 2. add up naturally and appear as the following two columns (Table 1); they can be regarded as two columns of non-complements: A-P-T-S-G; L-I-M-C-V [18]

Table 1. Atom number within two systems-complements and non-complements

D 07	N 08	A 04	L 13	→	32
R 17	P 08	F 14	I 13	→	52
K 15	Y 15	T 08	M 11	→	49
H 11	W 18	S 05	C 05	→	39
E 10	Q 11	G 01	V 10	→	32
↓	↓	↓	↓		
60	66	26	52		
		78			

As we can see, the same logic of the distribution of the number of atoms as specific quantum (60, 66 and 78), which we had when classifying into golden amino acids, their complements and non-complements, appears here as well [18].

Furthermore, a specific situation occurs when proline and phenylalanine exchange places (Table 2: the more strongly crosshatched fields represent non-polar, while the less strongly crosshatched - polar amino acids).

Table 2. Arrangement of non-polar amino acid pairs resulting from the place exchange of Pro and Phe

					a1	a2	n
D 07	N 08	A 04	L 13	→	32		189
						84	
R 17	P 08	F 14	I 13	→	52		289
K 15	Y 15	T 08	M 11	→	49		299
H 11	W 18	S 05	C 05	→	39	120	289
E 10	Q 11	G 01	V 10	→	32		189
↓	↓	↓	↓				
60	60	32	52				
120		84					
					a1	a2	n
D 07	N 08	A 04	L 13	→	32		189
						84	
R 17	P 08	F 14	I 13	→	52		289
K 15	Y 15	T 08	M 11	→	49		299
H 11	W 18	S 05	C 05	→	39	120	289
E 10	Q 11	G 01	V 10	→	32		189
↓	↓	↓	↓				
60	60	32	52				
120		84					

Thus, the result is a completely organized system, harmonious structure of amino acid constituents of the genetic code. In the first column are polar charged, in the second polar uncharged and in the fourth column uncharged amino acids, whereas in the third column there is a combination of polar and non-polar amino acids. On the other hand, this strict physical and chemical determination is followed by the balance of atom number (columns a1 and a2), as well as nucleon number (column *n*) [18].

Planning and conducting a didactic-methodical experiment

The experimental lesson was realized in one of the vocational schools in Niš, Medical School "Dr Milenko Hadžić" (in the school year 2003/04), Republic of Serbia. Grammar schools were not taken into consideration exactly because of the curriculum of chemistry. The lesson was conducted in two 4th grade classes of vocational profiles: charge nurse (*cn*) and obstetric nurse (*on*). The number of students in the experimental lesson was 60 (representative sample). Another important issue was to maintain an objective school environment without any artificial group equality (according to IQ, intellectual abilities, previous knowledge, interests). The classes were randomly chosen. Furthermore, it was also important that both classes (IV *cn* and IV *on*) have the biochemistry lesson in the same day and in duration of four school hours (two double hours or one double hour per class).

Having taken into consideration the specific curriculum of chemistry at vocational schools (biochemistry), 4th grade classes were chosen, since there is a unit on amino acids within the curriculum of chemistry, and, within the unit, the topic: the structure and polarity of amino acids. Although the aim of learning chemistry at 4th grade is rounding off the knowledge of chemistry and preparing for further education on university level, this can be achieved by increasing and expanding teaching contents [1], introducing innovations, using computer aids [9] in combination with new views of the structure and polarity of acids [16-18].

Due to the complexity of new concepts of the structure of amino acids and their classification according to polarity, they were reduced and adopted to the features of secondary school teaching: curriculum, teaching and educational aims, the use of informational/communicational technology, multimedia sources of symbolic and mathematical forms, age, intellectual abilities and interests of students [10].

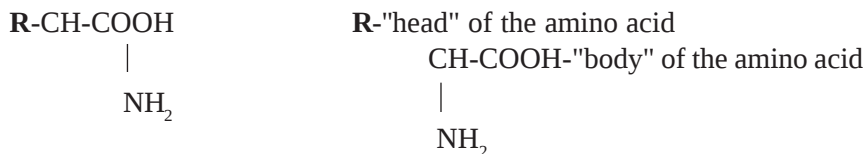
Organization and realization of the lesson plan

In the experimental lesson, when explaining the characteristics, structure and polarity of amino acids (traditional approach, scheduled by secondary school curriculum of chemistry), the classification of amino acids was presented from the aspect of the so-called acid-base balance in correspondence with the balance of the number of atoms and nucleons of the four stereochemical types of amino acids, where 20 standard amino acids belong. The classification by M. Rakočević, derived from the struc-

ture of amino acid side chains, was taken due to the simplicity of the display of hydrocarbon side chains and calculation of the nuclide number, when compared with the system with aromatic chain without the heteroatom (Phe-Tyr, F-Y) and with the heteroatom (His-Trp, H-W), plus the amino acid with the -OH group (Ser, S). Serine (S) with the OH-group in the side chain comes from the alanine hydrocarbon side chain and represents the simplest example of an amino acid with the heteroatom in the side chain. Also the amino acid Alanine (Ala, A) was used as the basic measurement standard instead of Glycine (Gly), since it contains only the H atom in the side chain.

Simplifying the calculation of the nuclide number in the heads of amino acids is used only for discovering and determining the position of the two systems of complementary and non-complementary amino acids, which in turn determine their polarity. Instead of complex schemes resulting from the balance of the number of atoms determined by the direction of the golden section on the binary-code tree of I, II and DT (doublet-triplet) systems and the class of 2 enzymes of aminoacyl-tRNA synthase, rational structural formulas of amino acids with hydrocarbon chains and hydroxyl group are used [16-18]. For the sake of the correspondence of side chain structures, the students were also presented with the other standard-20 standard amino acids, derived from the function they have when forming proteins, according to Peter Carson³⁾ (comparison standard) [19].

The general formula of amino acids was taken as the basic model of structure (when calculating the number of nuclides in the head of an amino acid):

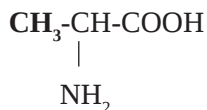


First, the students were given the task to (with the help of computers and appropriate computer programs) construct the structure of the side chains of the following amino acids: Ala, Ser, Val and Gly along with the "body" of the amino acid. They were also supposed to highlight the "head" of the amino acid by bolding. They were given a possibility to choose and combine among the following computer programs: Paint, Word, Power Point and Corel Draw, while constructing the head and side chains of the amino acids [9], or to find the suitable structures on certain web pages on the Internet (e.g. Wikipedia) [20].

The next step was to calculate the number of nuclides in each of the heads of the above mentioned amino acids according to the following model, with the help of the table of natural isotopes of the elements in the Periodic table (nucleon number in the amino acid body was used as a standard) [13-15].

Information on the first most significant nuclide

For **CH₃-group** in *Alanine* (information on the first most significant nuclide): The numeric value A (mass or atomic number) of the first most significant nuclide of Hydrogen is taken (the table of natural isotopes of the elements in the Periodic table), which equals one (1) for Hydrogen (¹H); it is multiplied by the number of atoms of H in the methyl group (03). The procedure is repeated for C (Carbon), by multiplying the numeric value A of the first most significant nuclide of carbon (¹²C), which equals (12), by one, since CH₃-group contains only one C atom. The total amount (of the number) for the first most significant nuclide in the head of **Alanine** equals **15**.



Alanine: Nucleon number. in the "head" (15)

$$(\text{H}) = 01 \text{ (}^1\text{H nuclide)}$$

$$(\text{H}) = 01 \times 03 = 03$$

$$(\text{C}) = 12 \text{ (}^{12}\text{C nuclide)}$$

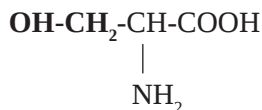
$$(\text{C}) = 01 \times 12 = \underline{12}$$
$$15$$

Information on the most complex nuclide

The procedure is the same as in the first case (for the first most significant nuclide).

Information on the least complex nuclides

For **OH-CH₂-** group in *Serine* for the least complex nuclide: The procedure of calculation is the same as in case **Alanine**, the only difference being the fact that the values of A are now taken for the least complex nuclide of Hydrogen (²H), Carbon (¹³C) and Oxygen (¹⁷O) in the natural mixture of the isotope.



Serine: Nucleon number in the "head" (36)

$$(\text{H}) = 02 \text{ (}^2\text{H nuclide)}$$

$$(\text{H}) = 03 \times 02 = 06$$

$$(\text{C}) = 13 \text{ (}^{13}\text{C nuclide)}$$

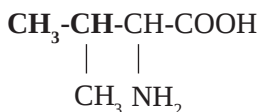
$$(\text{C}) = 01 \times 13 = 13$$

$$(\text{O}) = 17 \text{ (}^{17}\text{O nuclide)}$$

$$(\text{O}) = 01 \times 17 = \underline{17}$$
$$36$$

Information on the nuclides with the minimum content of the most significant

For $(\text{CH}_3)_2\text{-CH-}$ group in *Valine* for the nuclide with the minimum content of the most significant: The procedure is the same as in case **Serine**, the difference being the fact that now the values of A are taken for the nuclides of Hydrogen (^2H), Carbon (^{13}C) with the minimum content of the most significant in the natural mixture of the isotope.



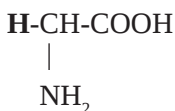
Valine: Nucleon number in the "head" (53)

$$\begin{aligned} (\text{H}) &= 02 \text{ } (^2\text{H} \text{ nuclide}) \\ (\text{C}) &= 13 \text{ } (^{13}\text{C} \text{ nuclide}) \end{aligned}$$

$$\begin{aligned} (\text{H}) &= 07 \times 02 = 14 \\ (\text{C}) &= 03 \times 13 = \underline{39} \\ &53 \end{aligned}$$

Information on all nuclides

For **H-** in *Glycine* for all nuclides: in this case, when the content of all nuclides of an element is calculated, the example of **Glycine** is taken, which contains only H atom in the side chain. This is done for two reasons: because of the simplicity of the structure and the value of A for the nucleotides (^1H) i (^2H), which simplifies the calculation.



Glycine: Nucleon number in the "head" (03)

$$\begin{aligned} (\text{H}) &= 01 \text{ } (^1\text{H} \text{ nuclide}) \\ (\text{H}) &= 02 \text{ } (^2\text{H} \text{ nuclide}) \end{aligned}$$

$$\begin{aligned} (\text{H}) &= 01 + 02 = \underline{03} \\ &03 \end{aligned}$$

The use of the programs Power Point, Paint, Power Point or Corel Draw when constructing amino acid molecules provides clarity of the displayed models, which in turn corresponds with the levels of abstraction. The level of pictures (the third level) is more accessible and graspable to most students than the abstract level (the fourth level, characteristic of numbers). However, calculating the nucleon number (mathematical model) would correspond to the fourth level (the level of numbers) [21]. Both third and fourth levels of abstraction could be applied to the programs, since geometry (spatial layout of atoms in a molecule) and the image (structure) of molecules are interrelated [9]. The balance of the atom and nucleon number would correspond in this case to the fourth mathematical level [21].

In the case of using and processing information in order to achieve real models (in the case of amino acids-model of pictures and language), the question of implementing Bruner's theory of teaching is posed. According to American psychologist Jerome Seymour Bruner, there are three modes of information representation: enactive, iconic, and symbolic [22]. The enactive representation would correspond to actions, the iconic-to concrete or abstract images, and the symbolic-to words and charts. Applying Bruner's approach when explaining the structure and polarity of amino acids, the iconic representation (of abstract images) would correspond to the structure of amino acid side chains, while the nucleic acid number in molecules of amino acids would correspond to the symbolic representation as long as numbers were viewed as part of the mathematical (universal) language.

Conclusion

After numerous reforms introduced in Serbia since World War II, high school curriculums have been filed complaints, primarily because of low achievements of students [7]. At vocational (medical) schools chemistry programs fail to provide a better understanding of the subject and vocation, and necessary skills for working in the chosen profession [1]. The problem of chemistry curriculums is the fact that they are mainly unsuitable for the age of students. This is why students perceive chemistry as a boring, abstract and hard subject [23].

Another major problem of chemistry teaching is bad financial situation in most schools, then poor equipment of schools with necessary laboratory supplies and shortage of laboratory space, without which chemistry curriculum can neither be imagined nor realized.

One of the possibilities and alternatives for overcoming the problems of today's chemistry teaching lies in the utilization of modern electronic teaching aids (computers, computer programs [9]), innovations and interdisciplinary approach of presenting teaching contents (structure and polarity of amino acids [16-18]).

The use of computers and computer programs, according to general objectives of learning chemistry, aims at developing the ability to use information from various sources (traditional and electronic literature, then communication via information-communication technology, the Internet, multimedia sources, symbolic and mathematical forms) [24]. According to general educational aims of chemistry at high schools (foreign educational programs, e.g. Malta-teaching objective: A greater awareness of the role of science and technology in everyday life), students develop the ability to use scientific and technological devices, computers, audio and video resources, and personally use devices of informational technology in order to understand, analyse, classify and connect information and data [10].

Introducing innovations and interdisciplinary approaches when presenting new topics enable students to build their knowledge through their own activities, where the

role of the teacher is to support and guide the student in the process of discovery, develop their ability to satisfy curiosity and interests, and build knowledge [24]. This stimulates creativity of students and their openness for constant changes (application of the model of evaluation and the idea of change).

Another important way of overcoming students' negative attitude towards chemistry is to reinforce and develop students' intellectual abilities through the areas they are interested in or are good at, in case of difficulties in concentration, and understanding lessons (learning chemistry with the help of the computer) [25].

The role of the teacher, as a methodist, motivator, mentor, designer of the learning environment, and above all innovator and researcher, in the innovative and creative field of work would be to pursue new scientific ideas in the teaching process (willingness to change), apply new technical and technological aids, combine teaching methods, cooperate and exchange ideas with their colleagues, in order to modernize and advance teaching [26].

The study of characteristics, structure and polarity of amino acids from the aspect of the so-called acid-base balance in correspondence with the balance of the atom and nucleon number in their molecules is graspable to secondary school students (reduced content presented in the work). It takes place along with the traditional interpretation (comparison standard). With certain necessary corrections, it could be applied when presenting the unit: biological importance of organic compounds, that is the topic: Amino acids within the curriculum at 8th grade primary school.

Introducing innovations, new ideas, integrating and utilizing new technologies, following trends, would lead to modernizing the contents of chemistry curriculum and introducing modern principles of general education, as well as to approaching European school standards.

NOTES

1. Project "Leonardo" aims at presenting the somewhat reduced content of chemistry teaching to pupils at lower grades of primary school (from 1st grade and on), and also to children at pre-school. The main idea is to introduce the study of chemistry as early as possible, already at nursery school.

2. Mensch-Natur-Technik (Man-Nature-Technology) is a subject whose program consists of the contents of biology, physics and technology. It is dealt with at 5th and 6th grades of primary school (grammar school) in Germany. According to the syllabus, MNT corresponds to Science, which exists at schools in England and the USA.

3. Amino acids where the side chain is pure hydrocarbon: Ala, Leu, Ile, Pro and Phe; or only hydrogen: Gly. Amino acids with groups in the side chain which act as polar, without ionizing groups: -SH, -OH, -CO-NH₂; Tyr, Trp, Ser, Thr, Cys, Met, Asn and Gln. Acidic amino acids or monoamino-dicarboxylic: Glu, Asp. Base amino acids or diamino-monocarboxylic: Lys, Arg and His.

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