

Unitary Symmetry of Combinatorial Molecules and Mixtures. Part 2: New Medical Diagnosis as a Combinatorial Tool for Early Prediction of Disease

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Received: March 11, 2017 / Accepted: April 10, 2017 / Published: July 25, 2017

Abstract: The set of chemical entities, each of which retains its general structure for all objects, composition and properties (characteristics), can be regarded as pure objects. All other objects are mixtures. Mixtures of chemical entities, as well as the individual nuclei, atoms and molecules, are classical combinatorial objects, which are practically not been studied in this paradigm.

Abstract organization of combinatorial objects is a system of intersecting true homologous series. In such a homologous series of the combinatorial element a single object is replaced by another single but different element of the selected set of combinable components.

Are not added, but replaced!

Under certain energetic relations between the combinable elements for the two-link homologies in the space of physical and (or) the chemical characteristics can be observed phenomenon with simple unitary symmetry invariants.

Such invariants system allows at very small number of experimental data to find the values of the parameter in question for the entire combinatorial set, i.e. **It has great predictive power**.

As the components of the mixture can be regarded as reactants in chemical processes at any single moment (kinetic embodiment) and fraction compositions of various substances which are in equilibrium (steady) state.

This article will review the basics of combinatorics mixtures and its application in respect of a number of biologically important fluids - blood, lymph and urine. This will in the future not only to construct the taxonomy of these compounds, but also to create an algorithm to determine the "composition of the mixture - pathology" in the very early stages of the disease.

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The main questions that you will find the answers in this article:

- How to identify the patient on the composition the mixture components of sex hormones for a specific age.
- How to identify the "norm" and "Pathology" on the composition the mixtures, hormons in the four environments - venous blood, arterial blood, lymph and urine at the earliest stages of the disease.
- How to construct an algorithm for the selection of pharmacological agents for a particular set of hormones mixture components of a particular patient.

Key words: combinatorics, homology, unitary symmetry, conservation laws, mixtures, hormons.

1. Introduction

Set fraction (n_a, n_b, n_c) of substances A, B, C can be considered as the initial set of a combinatorial operations - combinations with repetitions. In this case, there are two kinds of homologous series:

• one measure of the one substance is replaced by the same proportion of other substance

Here, the amount of shares is constant and equal:

$$\sum n_i(A) + \sum n_i(B) + \sum n_i(C) = 100\%$$

In fact, we are preparing a mixture of the same equity configurations (five measures, each - 20%) for the same starting components A, B, C, but less concentrated with respect to one of the components (A), i.e. we are preparing a new mixture.

• to an existing mixture is added to one or more of the same fractions of one of the substances

In this case, we increase the fractional configuration with 5 shares (each 20%) up to 6 fractions of (each approximately 16.7%). **In fact, we dilute the mixture.**

So, if we choose a finite set of discrete objects **n** (in this case - the number of components A, B, C, equal to 3) and define a finite number of elements **k**, from which the same are composed (on which the object can be divided) components A, B, C (for example, 20% proportion, i.e. elements 5), the total number of components of the combination with repetitions according to formula 1:

$$C_n^k = \frac{(n+k-1)!}{k! (n-1)!}$$

will be equal to 21. All of them are presented in Figure 1.

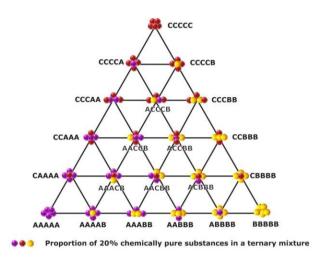


Fig 1. The total number of combinations with a repetitions of the three objects A, B, C up to 5 parts (often read as "n choose k"). True homologous series - three different chemically pure substance (A, B, C) in the same phase state, in the same temperature and under constant pressure. Substances are not chemically interact. Shown a mixture with 20% equity step.

This is - a direct combinatorial problem.

Another case. You already have a set of elements and assume that of these items must be collected a certain number of complex objects. In this case you need to find up the certain combinatorial operations to obtain a strictly defined number of combinatorial objects.

Example: It was known that RNA is composed of nitrogenous bases - adenine (A), guanine (G), cytosine (C), uracil (U). It was also known that the genetic code must consist of combinations of these bases that fully overlap required for protein synthesis needs of the 20 amino acids. Such combinatorial operations was a combination of 4 to 3, with repetitions and permutations - a total of 64 combinatorial object called codons later.

This is a reverse combinatorial problem.

Here formal graphical interpretation is presented in Figure 2.

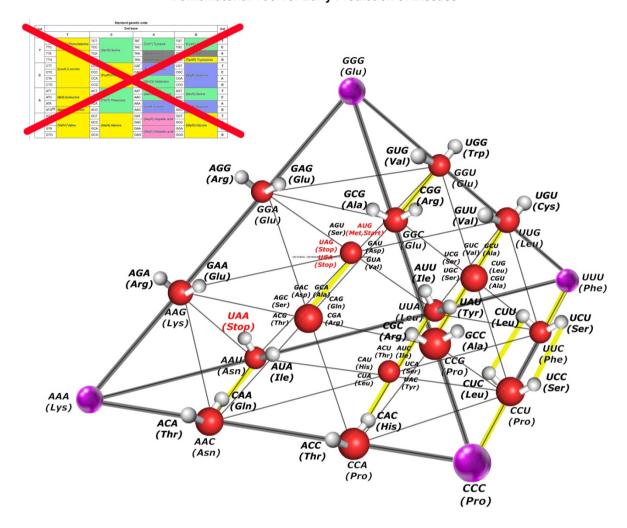


Fig 2. The formal structure of homologous series of codons. Codons, specify which amino acid (in brackets) will be added next during protein synthesis. Yellow lines show the "related" transitions from one codon to another codon while replacing (C - U). In order not to overload the graphic not all combinations shown here.

This structure should replace the archaic table of the genetic code and other nonsense codons finding illustrations in textbooks and Wikipedia [1].

The main advantage of such structures of homologous series is a combinatorial Paradigms visibility and ease of finding "related" two-link homologies, which under certain conditions can be regarded as invariants of certain values of physical parameters.

1.1. Unitary symmetry of molecules and mixtures

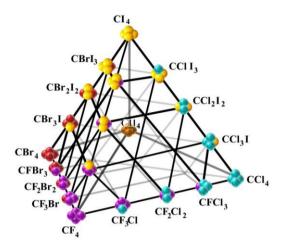
In nuclear physics and elementary particle theory, on understanding of symmetry and associated concepts of the hierarchy of interactions play a fundamental role [2]. Thus the relative insignificance of electromagnetic and weak interactions as compared with the strong interaction of nucleons in the nucleus enables a model of the nucleus to be examined in the limit of precise symmetry of strong interactions. In such a model, the, protons and neutrons become physically indistinguishable states of a nucleon, while the properties of the nucleus become invariant relative to isotopic transformations.

It is also possible to speak of the hierarchy of interactions participating in the formation of molecules. The energy of chemical bonds, which is 1-2 orders of magnitude greater than the energy of non-valent interactions, can be given as on example of "strong" interaction. Another example relates to the case when the energy of the valence interactions is much higher than the energy of intermolecular bonds in a condensed medium.

Weak interactions in chemistry are normally taken into account by introducing different perturbations into physical models. These perturbations are generally unmeasured parameters that are basically the adjustable magnitudes.

However, in the chosen class of molecules an attempt can be made to find the ratios of values of the examined parameter in which the contributions of "weak" interactions are compensated.

Previously [3, 4, 5, 6, 7], it was shown that, for example, the halogen substituted methanes can be represented as a combination with repeatitions and the corresponding system of homologous series (irreducible representations of the group SU (5)) will look as shown in Figure 3).



Five "ligands" (H,F,Br,I) with the same outer electron shell located around some unchangeable "molecular core"

Fig 3. The structure of the homologous series of molecules with the general formula $Y_0H_jF_kCl_mBr_nI_p$, where Y_0 are the atoms of carbon subgroup or other complex atomic structure. The structure of the homologous series turned out to be the weight diagram that corresponds to the irreducible representations of the group SU (5).

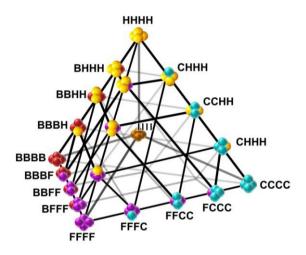
The corresponding system of invariants is presented in Table. 1

Table 1. The system of equations for the replacement F-H. Before each chemical compound in order to save space omitted designations of some physical or chemical parameter of the molecule (A). For some parameters, for which the geometric symmetry does not play a big role, the equation with (*) and without () can be combined.

Replacement: F ←→ H		
1	CF3C1 - CF3Br = CH3C1 - CH3Br	
1*	CHF2C1 - CHF2Br = CH2FC1 - CH2FBr	
2	CF3Br - CF3I = CH3Br - CH3I	
2*	CHF2Br - CHF2I = CH2FBr - CH2FI	
3	CF3C1 - CF3I = CH3C1 - CH3I	
3*	CHF2C1 - CHF2I = CH2FC1 - CH2FI	
4	CF2C12 - CF2Br2 = CHFC12 - CHFBr2 = CH2C12 - CH2Br2	
5	CF2C12 - CF2I2 = CHFC12 - CHFI2 = CH2C12 - CH2I2	
6	CF2Br2 - CF2I2 = CHFBr2 - CHFI2 = CH2Br2 - CH2I2	
7	CFC13 - CFBr3 = CHC13 - CHBr3	
8	CFBr3 - CFI3 = CHBr3 - CHI3	
9	CFI3 - CFC13 = CHI3 - CHC13	

The proposed system of equations can be easily transformed to organic compounds (replacing C - CH3, C2H5 ...) or inorganic set (replacing C - Si, Ge, Sn, Pb).

Mixtures can also be represented in the form of combinations with repetitions and the corresponding system of homologous series (irreducible representations of the group SU (5)) will look as shown in Figure 4).



Five (n) components (H,F,B,I) of 25% fractions (k = 4)

Fig 4. The structure of the homologous series of mixtures The structure of the homologous series turned out to be the weight diagram that corresponds to the irreducible representations of the group SU (5). In order not to overload the graphic not all combinations shown here. Designations of the components - (H, F, B, I) - are chosen specifically to emphasize the commonality with Fig. 3.

The corresponding system of invariants is presented in Table. 2

Table 2. The system of equations for the replacement of 25% fraction of F component on the same fraction of component H. Before each chemical compound in order to save space omitted designations of some physical or chemical parameter of the mixtures.

Replacement F H		
1	FFFC - FFFB = HHHC - HHHB	
2	HFFC - HFFB = HHFC - HHFB	
3	FFFB - FFFI = HHHB - HHHI	
4	HFFB - HFFI = HHFB - HHFI	
5	FFFC - FFFI = HHHC - HHHI	
6	FFCC - FFBB = HFCC - HFBB = HHCC - HHBB	
7	FFCC - FFII = HFCC - HFII = HHCC - HHII	
8	FFCC - FFII = HFBB - HFII = HHBB - HHII	
9	FCCC - FBBB = HCCC - HBBB	
10	FBBB - FIII = HBBB - HIII	
11	FIII - FCCC = HIII - HCCC	

So, if the components are not connected to each other by chemical bonds the molecules in the mixture react with one another only by means of weak forces, the mixture is considered at the same temperature and at a constant pressure, then it is expected that, for example, for a three-component mixture is equality:

$$J(AAACB)t - J(AACCB)t = J(AACBB)t - J(ACCBB)t$$
 (2)

where in parentheses are the equivalent fractions of the components, and J - physical or chemical parameter of a mixture of components at a certain point in time. In this case the equality corresponds to replacing 20% of the component A to the same fraction of the component C (see. Fig. 1)

A unique feature of these systems of homologous series is that their regular arrangement in space of their physical and chemical properties, has a **powerful universal predictive power of certain properties**.

2. The Unitary Symmetry of Molecules. Examples

In [7] it is shown how to use the invariants of the system can detect erroneous values of the Vertical Ionization Energies (VIE - IVIE) and a small number of experimental data to calculate a lot of new VIE values (see Figure 5).

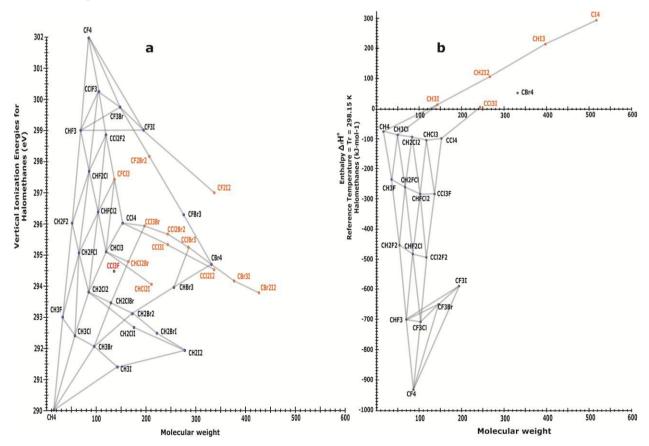


Fig.5a. Vertical Ionization Energies (VIE - I_{VIE}) and Enthalpy ΔH_f^o . of halogenated methanes v.s. on their molecular weight. Black letters and blue dots indicate the compounds listed in [8] (for I_{VIE}) Orange color compounds and their values (VIE), the resulting calculations similar to those of Table 1. Red marked compound CFCl₃, is erroneous in [8] **Fig.5b**. Black letters and blue dots indicate ΔH_f^o for compounds listed in [9]. Orange color compounds and their values is the resulting calculations of ΔH_f^o [10]. The value ΔH_f^o (CCl₃I) is the result of calculations similar to those of Table 1

Unfortunately, the NIST database for ΔH_f^o is in very poor condition and to provide any calculation is not possible.

This way you can solve the problem of "structure - property" is easily and reliably compared to known calculations (see Gaussian 94 [11].).

Such problems are particularly relevant when creating pharmaceuticals. In this case, the prediction of the biochemical activity by analyzing homology invariance pharmacological acquires not only, but also economic sense.

3. Unitary Symmetry of Biological Mixtures. Introduction.

Similar calculations and check on the accuracy can be carried out and for mixtures. Of particular interest, it seems to me, is the problem of finding a relationship "composition of the mixture - a pathology." In this case it is necessary to consider as mixtures the blood, lymph and urine

With respect to our body the blood of plays the role of "materials supplier" to all tissues (arterial) and "waste transporter" to waste outputting organs, which may be collected all over the body (venous).

Lymph acts as a waste collector from all nooks of our body. Function of the lymph - returning proteins, water, salts, metabolites and toxins from the tissues into the blood. Urine is a liquid, by which all water-soluble metabolites derive out of the body.

The most important part in all these processes play (activating, delaying, diverting) the complex molecules - hormones.

On the one hand, it is known [12] that are hormones humoral (blood-borne) regulators of certain processes in various organs and systems: **hormone** is any member of a class of signaling molecules produced by glands in multicellular organisms that are transported by the circulatory system to target distant organs to regulate **physiology and behaviour**, including sexual orientation.

On the other hand, hormones is a mixtures components of plasma, lymph and urine.

The ingredients of these mixtures is determined primarily by the structure of DNA and varies with age and depends on the metabolic processes in the body.

If a set of chemical reactions that occur in a living organism to maintain its operation **correspond to its genetic norm**, the composition of the mixtures of components **slightly changing nevertheless remains** within a certain range. This deviation is called a NORM.

If the metabolism is disturbed due to the dysfunction of the epithelial tissue is a layer cells lining the surface (epidermis) and the body cavity and the mucous membranes of internal organs, digestive tract, respiratory tract, genito-urinary tract, as well as forming a majority of the glands of the body (endocrine glands - suppliers of hormones), the composition of the mixtures of components varies. **This deviation** from the norm is called a PATHOLOGY.

But as the "NORM" and "PATHOLOGY" must somehow be measured! In order to properly manage them and predict their change in one way or another affecting the endocrine glands and thus changing the composition of the components of mixtures in all three major fluids, for example, by acting on the metabolism by a variety of chemical additives.

If we choose certain ligands in these chemical additives, then constructing a system of chemical compounds for example halogen methanes (see. Fig. 3) where the ligands are halogen atoms, can be easily using invariant system (see. Table 1) to determine the most active functions, concerning endocrine glands, chemical compounds. At the same chemical additives should not be noticeable to other organs to change their functioning. **This is the main task of Pharmaceutical.**

And it can be easily solved by the invariants of the system, faster and more efficient than the methods currently practiced in the future.

But here again the question arises - how to measure the "NORM" and "PATHOLOGY" by the most effective way - least costly and most accurate method? Physicists know such methods. Whether these methods biochemists know? But the problem lies elsewhere.

It does not quite simple combinatorial case. For halogen methanes, for example, the number of combinations of ligands with low repetitions is small -70. The same number a **n** for combinations shown in Figure 4.

The number of combinations of hormones 57 (n) in the main body fluids with a repetitions to count using the formula 1 has to be count for a long time. Especially not knowing the number of repetitions (k), but simply turning over 1,2,3,4,5,6 But then comes to help with Parallelism of combinatorics of the proton and neutron. Here, (n) = 2 and (k) can iterate indefinitely. But **Homeostasis** in a nascent solar system has allowed to survive only a small number of combinations with repetitions - 2-3. In Figure 6, they are marked with red circles.

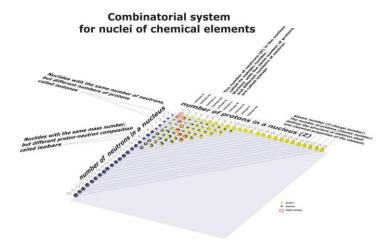


Fig 6. Stable combinations of protons and neutrons with repetitions in a Solar System Homeostasis circled in red And then a combinatorial problem, and at the same time and search for invariants of the unitary symmetry (similar to the system of equations in Table 2) for 57 hormones is simplified considerably. In relation to the nuclei of this simplification can be illustrated by the invariants of mirror nuclei (see. Figure 7).

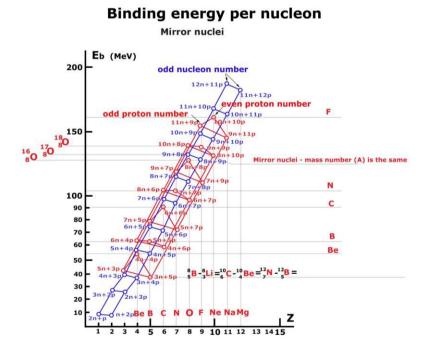


Fig 7. The homology of mirror nuclei and their invariants (In the lower right corner of the figure). [14] The experimental data are taken from [13].

Note the parallel line groups. This means that if two parallel lines, have been constructed by three known points of 4, the fourth easily determined. In practice, often to determine mutually agreed values of a

parameter for the entire combinatorial set of objects is necessary to know a very small number of "reference" values.

The equations in the lower right corner are the invariants for the part of mirror nuclei. They are the result of a special symmetry found in nature - unitary symmetry.

With respect to mixtures of hormones should observe the same situation. Homeostasis of the living organism on Earth was saved (and retained) only a small number of repetitions (k) hormone components to be combined in the "Norma". Small variations of combinatorial numbers of repetitions (k) of these components is to transcend the limits of Homeostasis, i.e. They are PATHOLOGIES.

Acceptable variations of repetitions (k) certainly known to biochemists. It is only necessary to collect the experimental data in the Uniform Bank hormones mixtures (UBHM).

4. Unitary symmetry biological mixtures. From "Norms" to "Pathologies".

It is well known [12] that the combination (composition) in a mixture of hormones for each person is different. It varies with age and depends on a combination (composition) of sex hormones. Therefore, the first step in identifying Pathologies should be to identify the composition of the sex hormones to a certain age (see Fig. 8).

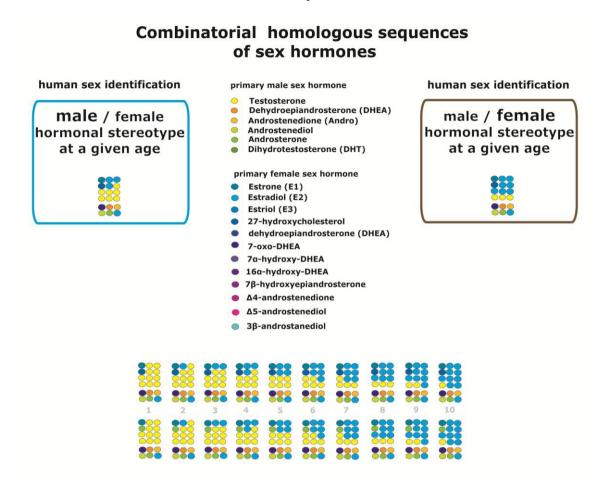


Fig 8. Combinatorial homologous sequences of sex hormones. In the lower part of the figure represented a model version of the two combinatorial homology of sex hormones.

As is known, the composition of of sex hormones to a certain age determines the physiology and behaviour of Human. Thus it is known that the secondary sex characteristics are determined by combinations with repetitions of all of sex hormones. Each combination contributes to the peculiarities of the development of the musculoskeletal system, body proportions, subcutaneous fat and hair, the degree of development of mammary glands, tone of voice, behaviors and many others.

In fact, some combination of sex hormones is "hormonal individual passport", including his tendency to some form homophilia. Therefore, before conducting analysis according to "the hormonal composition of the mixture - pathology" should determine the composition of an individual's sexual hormones.

The first step is to create using the accumulated experimental data Uniform Sex Hormones Mixtures Bank (USHMB). These data will allow to find the boundary values of the number of repetitions (k) for hormone components to be combined in the "Norma" in the real Homeostasis.

By generating a combination of 18 sex hormones with (k) repetitions we can get the homology system similar to the system, which have been shown to Fig 1, 3, 4.

As a result, we get something similar to the combinatorial nuclei system (see. Fig. 6), where from the entire set of combinations with repetitions in the conditions of the nascent solar system "survived" only very few combinations (a manifestation of parallelism, is rarely used in the comparison of laws for different levels organization of matter).

The next step is a composing of those equations that represented in the Table. 2 or similar invariant for mirror nuclei (see. Figure 7). The obtained equations and the existing fragmented experimental data collected in (USHMB).

We can get mutually agreed set of some measured physical parameter for the entire set of combinations of sex hormones with a reasonable number of repetitions of components for a particular age range. This set of data can be graphically represented as the dependence of a measured physical parameter calculated from a certain physical parameter of the mixture, such as the molecular weight of a mixture of hormones (like Figure 5 representation).

After this simple procedure, any individual, have addressed in (USHMB), using the measured physical parameter of a mixture of sex hormones get their specific composition (and vice - versa) of hormonal composition to obtain the value of a physical parameter of the mixture), i.e. to find their point in the sex hormonal scale of heterophile secondary sexual characteristics (see Fig. 9).

> Find yourself in the F-M the range of changes of sex hormones combinations

male / female ormonal stereotype at a given age male / female hormonal stereotype at a given age combinatorial plane sex hormone identification 180g T (years)

Fig 9. Combinatorial sex hormone identification plane.

Determination of sex hormones is not just a "hormonal fingerprinting". This is **the way to the selection of appropriate composition of pharmacological agents for the individual patient** with the appropriate invariants of unitary symmetry.

In addition, the combinatorial structure of sex hormones must be connected via the corresponding invariants of the unitary symmetry with the combinatorial structure of each of the 18 hormone producers as by the scheme shown in Fig. 10.

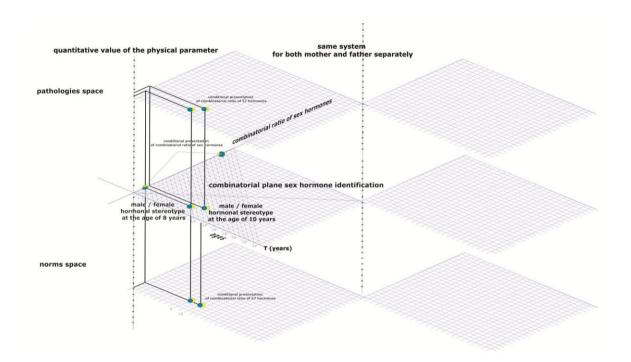


Figure 10. Combinatorial homology diagnostic system "composition of the mixture of sex hormones, the patient's age, the composition of the synthesis of hormones from producer (*L*) - pathology" for one of the 18 hormone producers. To the right is shown the ability to compare the combinatorial structure of the patient with the same combinatorial structure parent hormones.

Tracking hormonal composition over time will allow to predict the development of the pathology in time.

So, what is so attractive combinatorial taxonomy?

If using entire set of 18 combinations of sex hormones with a certain number of repetitions (a mixture of sex hormones):

• identify those that correspond to the homeostasis of the human body

- opt for this kind of mixtures of certain physical parameters (e.g. the dielectric constant (εr), permeability
 (μr) and electrical conductivity (σr)) accurately determines the mix of human hormones (as in fingerprinting)
- calculate the physical parameters for all real mixtures in equations such as those presented in Table. 2
- measure the physical parameters of the particular mixture of hormones, consult your doctor, the patient

We can get the keypoint on the plane, "age - a mixture of hormones" - sexual determinants of the individual patient (see Figure 9.).

I assume that the pathology is born and develops in different gender stereotypes in different ways. If from the entire set of hormones - 57:

- identify and group them on the basis of "the place of the synthesis"
- identify and group them on the basis of possible participation in the formation of pathology
- generate within each group the appropriate number of combinations of hormones with an appropriate number of repetitions
- identify those that correspond to the homeostasis of the human body
- opt for this kind of mixtures of certain physical parameters (e.g. The dielectric constant (εr), permeability (μr) and electrical conductivity (σr)) accurately determines the mix of human hormones (as in fingerprinting)
- calculate the physical parameters for all real mixtures in equations such as those presented in Table.
- measure the physical parameters of the particular mixture of hormones, consult your doctor, the patient

We in the space "the mix of sex hormones, the patient's age, the composition of the synthesis of hormones from the place (L) (the value of a physical parameter of the mixture, corresponding to a given composition and the appropriate attribution of certain pathologies mixture"), can obtain the characteristic point (see. Figure 10).

According to the accumulated experimental data which corresponds age sexual determinant (the patient with the characteristic composition of the sex hormones) in "NORM":

- it is possible to calculate the "mixtures course" (the evolution of the mixture) over time, on relevant invariants (Table 2 type) i.e., predict the emergence and development of disease.
- reaction of the mixture on the pharmacological and physical therapy impact

The prediction accuracy is determined by accuracy of measuring concentrations of components of the mixture.

Note that this analysis be carried out as for a blood hormones mixtures and for mixtures of hormones in urine and lymph. This will significantly improve the diagnostic accuracy of pathological changes and their temporal orientation.

Very interesting is the problem of correlation of hormones mixtures invariants of children and their parents.

5. Conclusions

The paradigm of "a set of elements - a combination of elements - combinatorial homology - homology invariants - the system of equations for the invariants - finding a physical parameter for the entire class combinations for a limited number of experimental values" is the prevailing paradigm of Natural phenomena - from elementary particles through the nucleus, atoms, simple molecules, complex molecules in consideration with their individual and as mixtures.

Moreover the mixture can be regarded as a state of equilibrium and the kinetic embodiment. In the latter case, the mixture passes through the stages, for example by dissociation from the parent molecule through the formation of radicals, and their formation of stable products.

Considered paradigm radically changes both the research itself, and natural science education process [22].

Acknowledgments

The first studies in this direction were published at the beginning of the 80s [15,16, 17,18]. A theoretical analysis of unitary symmetry was first published by me together with Vladimir Lyakhovskii in [19]. I express my deep appreciation all collaborators for a very useful discussion.

The author expresses his gratitude to Prof. R. Hefferlin. [20, 21]. We corresponded and discussed with him over the years. He recently passed away.

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