Laminariales and Fucales just slightly differ by content of protein. At the time the whole tendency of changing protein content – maximum in June and minimum in September – still traced. The content of Iodine in seaweeds is an indicator of value of this raw material as a natural source of iodine for normal functioning of human organism (Podkorytova et al., 2005). Content of Iodine in Laminariales is 2–3 times higher compared to *Fucales* and equals 0.23% in *L. digitata* at the middle of June. In *F. vesiculosus* maximum takes place at July and in *A. nodosum* at August.

Thus, system knowledge about of seaweed chemical composition, maximums of accumulation of important biocomponents and the biotechnological approach to their processing allows to carry out consecutive extraction of biologically active substances with receiving not only them in the allocated condition, but also drinks, the foodstuff possessing treatment-and-prophylactic properties and well influencing a human body.

On the basis of the researches certain patterns in accumulation of biologically active substances by brown seaweed of Arctic Seas in the process of their growth are determined and the new complex technology of brown seaweed processing of *Fucales* and *Laminariales* species with receiving of functional foodstuff (Repina et al., 2004) and probiotics to nutrition is developed (Usov et al., 2001).

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PROPERTIES AND FUNCTIONS OF VERY LONG POLYENOIC FATTY ACID CHAINS OF MEMBRANE LIPIDS (COMPUTER SIMULATION STUDY)

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Biological membranes are heterogeneous: they consist of various lipid molecules with various head groups and fatty acid (FA) chains, biomembranes include proteins as well as other molecules. Membrane lipids, being organized into a bilayer structure, serve as a basic matrix for other constituents. The most commonly occurring biomembrane FA chains have 12 – 22 carbons; they may contain 1 to 6 *cis* double bonds in various positions, i.e., the chains may be saturated, unsaturated or polyunsaturated (PU). As a rule, the double bonds of natural FAs are methylene-interrupted. Phospholipids (in particular phosphatidylcholine, PC) of some tissues were found to contain a series of unusial FAs with a chain longer than 22 carbon atoms, the so-called 'very long chain' (VLC) FAs. These chains (VLC FAs or VLC PUFAs) are important components of different classes of lipids in all organisms from bacteria to man (Řezanka, Sigler, 2009), in spite of the fact that VLC PUFAs are rare, they represent a minor component of the total fatty acids (~1 – 5%). For instance, marine sponges contain VLC PUFAs 26:3(n-7)*cis*, 28:3(n-9)*cis*, 30:3(n-7)*cis*, 30:4(n-6)*cis* and 30:5(n-3)*cis* (Litchfield et.al., 1979); see also data of the other authors (Joseph, 1979; Řezanka, 1989; Djerassi, Lam, 1991; Řezanka, Sigler, 2009). Marine dinoflagellates

Prorocentrum mexicanum, P. micans, Scrippsiella sp., Symbiodinium microadriaticum, Gymnodinium sp., G. sanguineum, Fragilidium sp. were found to contain VLC PUFAs 28:7(n-6)*cis*, 28:8(n-3)*cis* (Mansour et. al., 1999), dinoflagellates *Cryptecodinium cohnii* were found to contain 28:8(n-3)*cis* (Van Pelt et. al., 1999). A set of VLC PUFAs including 36:8(n-3)*cis* was identified in *Amphidinium carterae* (Řezanka et.al., 2008; Řezanka et.al., 2008a) and other cells (Řezanka, Sigler, 2009). More than 50 VLC PUFAs were identified in freshwater crustacean species *Bathynella natans*, *B. baicalensis*, *Baicalobathynella magna*, predominantly 26:5(n-6)*cis*, 28:7(n-6)*cis*, 30:7(n-3)*cis* and 40:7(n-6)*cis* (Řezanka, 2000).

Various lipid membranes are extensively studied by a variety of experimental and theoretical methods. Nevertheless experimental data concerning physical-chemical properties of VLC PUFAs are scarce. On the theoretical side, atomic-scale computer simulations have become nowadays a standard tool for studying biomolecular systems. The study of molecular models of various lipids and lipid chains by computer simulation methods can well complement experimental techniques. Analysing the properties of such molecules is of great importance both from the scientific and technological points of view. Namely, besides leading to a deep understanding one of the fundamental properties of natural membranes and their constituents (which are surface active substances), it can also help in designing new, potentially environmentally friendly or even biodegradable but effective materials for the chemical, biotechnological, medical (and, perhaps, washing, cosmetic, pharmaceutical) industry.

In this paper, Monte Carlo computer simulations of VLC PUFAs (more correctly, hydrocarbon chains) with methylene-interrupted cis double bonds, N:4(n-6)*cis*, N:4(n-3)*cis*, N:5(n-6)*cis*, N:5(n-3)*cis*, N:6(n-6)*cis*, N:6(n-3)*cis* have been carried out. Here N is carbon atom number, N = 24, 26, 28, …, 38. This computer simulation method was described earlier (Rabinovich, 1991). Variations of all torsion angles of the chains were considered to be continuous from 0 to 360 deg. The conformational energy of a chain was represented as a sum of the structural unit energies. A scheme of pairwise interdependence of torsions was used. The units reproduce precisely the chain structure. The energy of nonbonded interactions, torsional and electrostatic terms were taken into account. The method is applied to an investigation of the flexibility and other characteristics of the FA chains.

According to statistical averaging formulas of classical statistical physics, thermodynamic averages of any observables of a chain molecule are given by mathematical expressions with multidimensional definite integrals (Flory, 1969). Unfortunately, these integrals cannot be evaluated analytically for more than a handful of nontrivial models of the molecule, and conventional methods of integration are also not feasible. The basic idea of the Monte Carlo method is to calculate the integrals numerically: to generate a large number of trial conformations and replace the integrations by summations over a finite number of conformations of the molecule. In this work, 300000 – 1000000 conformations at temperature 298 K (25 ºC) were generated for each of the above-mentioned FA chains. Mean end-to-end (carbon – carbon) distance $\langle h_0 \rangle$ and mean-square end-to-end distance $\langle h^2_0 \rangle$ of each chain were calculated in theta-conditions (Flory, 1969). Then values of $\langle h_0 \rangle / L$ and $\langle h^2_0 \rangle / L^2$ were obtained, where L is contour length of the chain. It is clear that the smaller ratio $\langle h_0 \rangle / L$ (or $\langle h^2_0 \rangle / L^2$) of a chain, the more flexible the chain is.

The calculated values of $\langle h^2_0 \rangle / L^2$ are shown in Fig.1. To compare the calculated ratio $\langle h^2_0 \rangle / L^2$ of hydrocarbon chains of different unsaturation the value X should be used; X is the arithmetical mean of the numbers of carbon atoms of the double bonds (location of the "center" of the double bonds of the given molecule), see Table 1.

Fig.1 shows that chain flexibility depends on (*i*) the number N of carbons, (*ii*) the number of double bonds in the chain, and (*iii*) their locations in the chain. In other words, the number of double bonds and their position in the chain determine the flexibility, other things (N) being equal. Let us compare also the values of $\langle h_0 \rangle / L$ of the chains (Table 2). It is seen from Fig.1 and Table 2 that flexibilities of (n-3)-hexaenes coincide with flexibilities of corresponding (n-6)-pentaenes (pentaenes of equal length N). The same rule is obtained for (n-3)-pentaenes and (n-6)-tetraenes. As a matter of fact, the general rule for modification of VLC PUFA structures is **saturation** of one double bond located in the third carbon of the chain: in that case there is no difference in flexibility between initial and final chains at N=Const. Two different chains of equal length N have the same flexibility, therefore contributions of both chains to membrane fluidity coincide very closely.

On the other hand, fluidity of the lipid bilayer (which is affected by flexibility of the lipid chains) is a necessary but not sufficient condition for biomembrane functionality, especially because the temperatures of the lamellar gel – liquid crystalline phase transition in fully hydrated PCs of different *sn-2* chain

unsaturation (Koynova, Caffrey, 1998) show that increased chain unsaturation above a certain number of double bonds does not necessarily translate into increased membrane fluidity. It is easily seen from the experimental data collected by Koynova and Caffrey that at physiological temperatures, a fluid lipid bilayer could be attained by lipids having less unsaturated fatty acids than VLC PUFAs (for instance, only 18:1 and 18:2 chains).

Hence the influence of usual PUFA chains and unusual VLC PUFA chains of lipids is much more than the simple 'fluidization' of the matrix of lipid membrane. Another data seem to be essential in that case. Namely, it is known that an increase in the number of methylene-interrupted *cis* double bonds to the maximum in a linear hydrocarbon chain, results in a sharp decline of the absolute magnitude of the chain temperature coefficient | $d \ln\langle h_0\rangle/dT$ | (Rabinovich, Ripatti, 1994; Rabinovich, 2008). For instance, the size temperature sensitivity coefficient $|d \ln\langle h_0\rangle/dT|$ of PU molecule 22:6(n-3)*cis* is ten times lower than that of saturated 22:0 molecule.

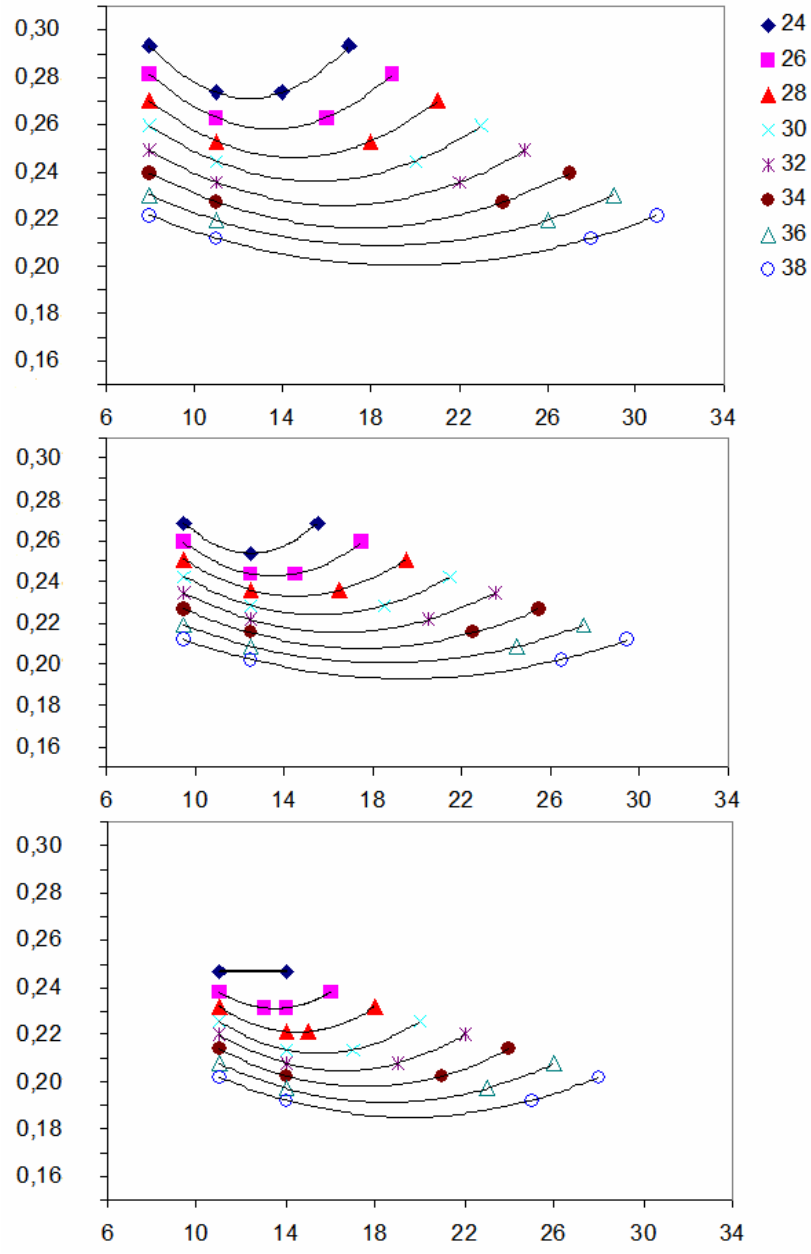

Fig.1. Monte Carlo computer simulation results, T = 25 ºC.
Vertical axes: flexibility $\langle h^2_0\rangle/L^2$ of chains
N:4(n-3)*cis* and N:4(n-6)*cis* (above);
N:5(n-3)*cis* and N:5(n-6)*cis* (in the centre);
N:6(n-3)*cis* and N:6(n-6)*cis* (below).
Each number in the column of symbols is the chain length (it is the number of carbon atoms N).
Horizontal axes:
The arithmetical mean of the numbers of the double bonded carbon atoms, X

Table 1. Correspondence of the X value to the location of methylene-interrupted double bonds in polyunsaturated hydrocarbon chains

Position of double bonds, **tetraenes**	X	Position of double bonds, **pentaenes**	X	Position of double bonds, **hexaenes**	X
3, 6, 9, 12	**8**	3, 6, 9, 12, 15	**9.5**	3, 6, 9, 12, 15, 18	**11**
4, 7, 10, 13	**9**	4, 7, 10, 13, 16	**10.5**	4, 7, 10, 13, 16, 19	**12**
5, 8, 11, 14	**10**	5, 8, 11, 14, 17	**11.5**	5, 8, 11, 14, 17, 20	**13**
6, 9, 12, 15	**11**	6, 9, 12, 15, 18	**12.5**	6, 9, 12, 15, 18, 21	**14**
7, 10, 13, 16	**12**	7, 10, 13, 16, 19	**13.5**	7, 10, 13, 16, 19, 22	**15**
8, 11, 14, 17	**13**	8, 11, 14, 17, 20	**14.5**	8, 11, 14, 17, 20, 23	**16**
9, 12, 15, 18	**14**	9, 12, 15, 18, 21	**15.5**	9, 12, 15, 18, 21, 24	**17**
10, 13, 16, 19	**15**	10, 13, 16, 19, 22	**16.5**	10, 13, 16, 19, 22, 25	**18**
11, 14, 17, 20	**16**	11, 14, 17, 20, 23	**17.5**	11, 14, 17, 20, 23, 26	**19**
12, 15, 18, 21	**17**	12, 15, 18, 21, 24	**18.5**	12, 15, 18, 21, 24, 27	**20**
13, 16, 19, 22	**18**	13, 16, 19, 22, 25	**19.5**	13, 16, 19, 22, 25, 28	**21**
14, 17, 20, 23	**19**	14, 17, 20, 23, 26	**20.5**	14, 17, 20, 23, 26, 29	**22**
15, 18, 21, 24	**20**	15, 18, 21, 24, 27	**21.5**	15, 18, 21, 24, 27, 30	**23**
16, 19, 22, 25	**21**	16, 19, 22, 25, 28	**22.5**	16, 19, 22, 25, 28, 31	**24**
17, 20, 23, 26	**22**	17, 20, 23, 26, 29	**23.5**	17, 20, 23, 26, 29, 32	**25**
18, 21, 24, 27	**23**	18, 21, 24, 27, 30	**24.5**	18, 21, 24, 27, 30, 33	**26**
19, 22, 25, 28	**24**	19, 22, 25, 28, 31	**25.5**	19, 22, 25, 28, 31, 34	**27**
20, 23, 26, 29	**25**	20, 23, 26, 29, 32	**26.5**	20, 23, 26, 29, 32, 35	**28**
21, 24, 27, 30	**26**	21, 24, 27, 30, 33	**27.5**		
22, 25, 28, 31	**27**	22, 25, 28, 31, 34	**28.5**		
23, 26, 29, 32	**28**	23, 26, 29, 32, 35	**29.5**		
24, 27, 30, 33	**29**				
25, 28, 31, 34	**30**				
26, 29, 32, 35	**31**				

Table 2. Values of $<h_0>/L$ for several FA chains*

chain	$<h_0>/L$	chain	$<h_0>/L$
38:5(n-6)*cis*	**0.423**	**38:6(n-3)*cis***	**0.423**
36:5(n-6)*cis*	**0.430**	**36:6(n-3)*cis***	**0.429**
34:5(n-6)*cis*	**0.436**	**34:6(n-3)*cis***	**0.435**
32:5(n-6)*cis*	**0.442**	**32:6(n-3)*cis***	**0.441**
30:5(n-6)*cis*	**0.449**	**30:6(n-3)*cis***	**0.447**
28:5(n-6)*cis*	**0.456**	**28:6(n-3)*cis***	**0.452**
26:5(n-6)*cis*	**0.463**	**26:6(n-3)*cis***	**0.457**
24:5(n-6)*cis*	**0.472**	**24:6(n-3)*cis***	**0.465**
chain	$<h_0>/L$	chain	$<h_0>/L$
38:4(n-6)*cis*	**0.434**	**38:5(n-3)*cis***	**0.434**
36:4(n-6)*cis*	**0.441**	**36:5(n-3)*cis***	**0.441**
34:4(n-6)*cis*	**0.449**	**34:5(n-3)*cis***	**0.449**
32:4(n-6)*cis*	**0.458**	**32:5(n-3)*cis***	**0.458**
30:4(n-6)*cis*	**0.466**	**30:5(n-3)*cis***	**0.465**
28:4(n-6)*cis*	**0.474**	**28:5(n-3)*cis***	**0.473**
26:4(n-6)*cis*	**0.482**	**26:5(n-3)*cis***	**0.480**
24:4(n-6)*cis*	**0.491**	**24:5(n-3)*cis***	**0.487**

*Errors of the calculations are within ±0,004 value.

It was shown experimentally that VLC PUFAs are concentrated in unusual dipolyunsaturated molecular species of PC and are attached to the *sn-1* position of the glycerol backbone, whereas 22:6(n-3)*cis* is mainly esterified at the *sn-2* position. Dipolyunsaturated boundary lipids with VLC PUFAs seem to provide the proper conditions of the proteins for their optimal functioning at different temperatures, similar to usual PUFAs (Rabinovich, Ripatti, 1994; Rabinovich, 2008). Clearly, further research is necessary to elucidate fully the properties of this unique VLC PUFA lipid tails.

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COMPUTER SIMULATION STUDY OF PROPERTIES OF UNSATURATED LIPID MEMBRANES

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Biomembranes surround cells: a membrane separates the interior of a cell from the outside environment. Being selectively permeable, membranes participate in control of the movement of various compounds (substances) into and out of cells. Biomembranes are very complex heterogeneous systems consisting of many different types of lipids, sterols, proteins, carbohydrates and various membrane associated molecules which are involved in a variety of cellular processes. Consequently, membranes play an active part in the life of the cell, they exist as dynamic structures. Lipid molecules differ with respect to the type of hydrophilic head-group and occur with a wide variety of hydrophobic hydrocarbon chains of fatty acids (FAs). Usually the most abundant phospholipid in animal and plants is phosphatidylcholine (PC), it is the key building block of membrane bilayers. Knowledge of physical-chemical properties of lipid bilayers is a key element of our general understanding of biomembrane functioning, which is one of the greatest challenging problems in biochemical, biophysical and biomedical sciences. This information is also relevant and essential in new biotechnological and biomedical applications.