

Posters

1. NEW TOOL FOR OXIDATIVE CHANGES IMAGING DURING SYSTEMIC ACQUIRED RESISTANCE ESTABLISHMENT IN PLANTS

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Each living cell of a plant constantly produces photons on relatively low level. Under normal physiological conditions, cell photon emission is stationary and minimal. Disturbance in oxidative homeostasis by biotic stress is manifested by increased 'biophoton' production. Such biophoton responses of plants may be used as an integral indicator of the degree of oxidative homeostasis imbalance. In order to gain insight into post-stress regulation mechanisms of the intracellular redox potential connected with defence responses of the plant it should be attempted to maintain natural intracellular parameters instead of using drastic and invasive free radical detection methods. On the other hand, the immense diversity of data obtained so far by researches makes it necessary to find convenient methods of their ordering and presentation. Biophoton generation is thought to represent spontaneous photon emission produced by way of chemical excitation arising from various metabolic processes, particularly from lipid peroxidation. Because ultraweak bioluminescence signal can be measured and visualised using highly sensitive CCD camera this non-destructive technique could be a useful tool in phytopathological studies on plants.

In our study high systemic protection of susceptible potato leaves cv. 'Bintje' – against late blight disease caused by *Phytophthora infestans* was induced by local pre-treatment with inducers such as: 2,6-dichloroisonicotinic acid, β -amino-n-butyric acid, γ -amino-n-butyric acid and laminarine. Biostimulating agents were able to induce resistance in susceptible cultivars what was connected with redox misbalance visualized by highly sensitive equipment of CCD "Night Owl" camera of a Molecular Light Imager LB 981 by EG & G Berthold.

It has been shown by us that imaging of temporal biophoton generation from potato leaves treated with inducers might be a helpful marker in mapping oxidative changes leading to acquired resistance.

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2. A NEW OLFACATORY SYSTEM MODEL BASED ON THE DOCKING EXPERIMENT

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The poster discussed a docking experiment involving vHTS and a human receptor protein which participates in the collection of olfactory sensations for a wide range of aromatic substances used in sensory analysis, such as for the selection and training of evaluation experts and synthetic substances widely used in perfume industry. The proteins designed belong to the 7TM class. Their models were developed based on UNIPROT data, and the 3D structures were designed using MetaServer, based on 2RH1 homologous proteins. Owing to the virtual docking experiment, the binding energy of aromatic compounds to receptor sites of the proteins was theoretically estimated. The results provide a preliminary platform to answer the question in what and how many odour groups a receptor is involved. The present calculations are further steps for the understanding of odour sensing physiology and the relationship between the chemical compound structure, the chemical composition of aromatic substance mixtures and the olfactory sensation collection mechanism. Our studies show that differences in molecule-receptor binding make olfaction one of the most complex senses. It is noted that it is crucial for survival; furthermore, it serves as a warning system against invisible dangers. The mechanism of aromatic substance detection is not perfect, such as for substances with identical odour, but with distinct toxicological properties. The calculation results prove that the odours we consider unpleasant are usually most easily detected.

References

- [1] Pick, H.; Etter, S.; Baud, O.; Schmauder, R.; Bordoli, L.; Schwede, T. & Vogel, H. J Biol Chem, 2009, 284, 30547-30555
- [2] Reisert, J. & Restrepo, D. Chem Senses, Monell Chemical Senses Center, 3500 Market Street, Philadelphia, PA 19104, USA., 2009, 34, 535-545.

3. FGF2-FGFR2 BINDING DOMAIN COMPLEX AS A MODEL SYSTEM FOR STUDIES OF ELECTROMAGNETIC FIELD EFFECTS ON BRAIN CELLS

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The effect of electric fields on proteins has recently become an area of theoretical and practical interest. The possible risks of electric fields for the human body is cause of concern. In vitro experiments have shown that exposure to electromagnetic radiation can cause protein conformational changes [1].

Basic fibroblast growth factor (bFGF or FGF2) is a polypeptide with potent trophic effects on brain cells. bFGF promotes the survival and outgrowth of brain neurons, and protects neurons against toxic processes that are important contributors to cell death after cerebral ischemia. Recent studies in animal models have suggested two potential uses of exogenous bFGF for the treatment of stroke: 1) intra venous bFGF to reduce infarct size in acute stroke, and 2) intracisternal bFGF to enhance neurological recovery in chronic stroke. Human clinical trials of the first of these applications are currently in progress. Basic fibroblast growth factor also induce the proliferation of neural precursor cells isolated from specific regions of the embryonic and adult brain [3]. bFGF shows a local surface concentration of predominately positively charged residues that has been called the "Basic Canyon" (residues Asn-35, Lys 127, Arg-128, Lys-133, Lys-137, Gln-142, and Lys-143) The crystal shows an ordered phosphate ion held by residues Asn-35, Arg-28, and Lys-133 [4].

The electrical field, a component of EM field, may affect on the activity of brain cells. In particular, the strength of interactions between signal molecules could be modulated, especially if highly charged residues are involved in the recognition process. Here we propose to use a complex of bFGF2 - FGF2 receptor (1EVT) as a model for studies of EM field effects on the brain. So far we prepared all-atom model of this complex and performed steered molecular dynamics computer simulations of ligand-receptor mechanical unbinding process. This process has been analyzed in atomic detail. The maximum force of over 2 nanoN has been calculated. Within the proposed model the effects of an external electric field may be simply included, using an appropriate continuous solvent model and additional electrostatic forces attached to charged atoms. The EM field should result in a modified FGF2-FGR2 forced unbinding curve. Systematic studies of such curves may help to elucidate quantitatively the role of EM on nanomechanics of ligand-protein interactions and signalling processes in the brain.

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References

- [1] de Pomerai D.I., Smith B., Dawe A., North K., Smith T., Archer D.B., Duce I.R., Jones D., Candido E.P. (2003) FEBS Lett. 22;543(1-3):93-7
- [2] Rottlaender A., Villwock H., Addicks K., Kuersten S. (2011). Immunology. 13,1365-2567
- [3] Gritti A., Frolichsthal-Schoeller P., Galli R., Parati E.A., Cova L., Pagano S.F., Bjornson C.R., and Vecovi A.L.(1999) J Neurosci 19: 3287-3297
- [4] Plotnikov A. N., Hubbard S. R., Schlessinger J., Mohammadi M. (2000) Cell 12, 413-424

4. STUDIES OF CURRENT-VOLTAGE RELATIONSHIP IN FISH COLLAGEN

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Among the applied research methods, temperature dependence of conductivity can be used for exploration of composite materials, polymers, biological materials such as bone, skin, elastin and collagen, ie. materials with properties of semiconductor or dielectric.

Studies of temperature dependence of conductivity inform us about changes of the conformation of molecule such as denaturation, glass transition and water release. Therefore studies concern phase transitions, which carried out in the heated biological material.

Measurements of temperature dependence of conductivity was carried out in the temperature range 320K-485K. As the studied material collagen obtained from fish skins (FSC-Fish Skin Collagen) was used. As a control material bovine Achilles tendon (BAT) collagen (Sigma) was utilized. It was found, that in the applied voltage range i.e. from 1V to 3V the dependence $I = f(U)$ was linear, fulfilling the Ohm relationship. The voltage $U = 1V$ was used for further studies. The geometrical dimensions of studied samples were kept constant.

In the case of FS collagen at the temperature of 425K, the dependence $I = f(U)$, was approximated as the linear function. Extrapolating this to the value $U = 0V$, the line passes through the origin of coordinates. For temperatures higher than 425K, this condition was not met, which can be explained by the phase transition (denaturation) occurring in collagen heated above 380 K.

5. INVESTIGATION OF THE APPLICABILITY RANGE OF PROTEIN THREADING SOFTWARE

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Number of known protein sequences (more than 14 millions), still significantly exceeds the number of known structures (approximately 70,000). Experimental methods such as NMR and crystallography, are too time consuming to make up the difference. Computer prediction of protein structure and, in particular the methods of comparative modeling, such as threading, are still less accurate (typically) from the experience, but their speed and convenience offer an opportunity to create a universal set of tools for predicting tertiary and quaternary shape of unknown proteins.

Threading is to match the sequence of target to known protein structures, selected from a library of known structures. Energy function, allows us to assess which match are better than others, and keep those with "low energy". After checking the whole library and using new (you can also use the old one) scoring function, we are able to choose the best initial models. These, after further processing (eg. modeling by CABS or UNRES), are becoming the predicted structures of protein.

The whole process, proposed by various research groups, usually looks like a simplified, the above-mentioned schema. The main differences are:

- The appropriate selection of a representative library: The more different structures, the better, but every new structure, increases the computing time.
- Setting up an appropriate scoring function: selection of an appropriate force field (the problem in itself, but generally uses a simplified force fields), the inclusion of secondary or tertiary information (2D and 3D threading), use of the assignment (alignment) sequences (the choice of appropriate matrices and similarities include penalties for a break, a problem becomes extremely important in the case of taking into account tertiary information).

- Creation of threading methods: dynamic programming, Monte Carlo or genetic algorithms.

- Application of various approximations (eg. frozen approximation) in order to either speed up the calculations, or the possibility of providing more information (eg. include Long-term interactions). Proteins structure is strictly related (conserved) with its function.

6. THE RESEARCH ON INFRARED RADIATION FLUCTUATION OF BREAST CANCER PATIENTS WITH THE METHOD OF REGULATION THERMOGRAPHY

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The research on the human electromagnetic radiation fluctuation in region of the infrared light is a precious and underestimated diagnostic method of the study of the human vegetative system and emotional state.

The scientific basis of the thermoregulation diagnosis was created from 1977 to 1989 in the Institute of Social and Occupational Medicine in Heidelberg under prof. G Heima and prof. M. Blomkhe's leadership.

Methods: The temperature of the selected body points being grouped along 10 body lines was measured by the measurement of the infrared radiation intensity. 3 series of measurements at 30 second intervals were taken. The first series was a pattern of the temperature distribution and the next two were considered as a reaction to a sudden drop in temperature after taking clothes off. The first series was the basis for the calculation of the difference in temperature between the given points and the reference point 'Glabella' situated on the forehead (dT_g). It provided a graph of distribution of the body temperature. Next, the differences between second and third series in comparison to the first one (dT_2 and dT_3) were calculated. They depicted the thermal reaction of the points to the cooling. Next, the correlation coefficients were calculated (ρ): dT_2 vs. dT_g and dT_3 vs. dT_g - they correspond to the general tendency of the body to present the given kind of the reaction to the thermal stimulus. The 'regulation coefficients' were calculated from ρ 's: $W_R=50-50\rho$. Finally, the value of $dW_R=W_{R3}-W_{R2}$ was received.

The aim of the research was to evaluate the fluctuation of infrared radiation emitted by healthy patients and those with breast cancer. The emission was mainly connected with autonomic nervous system's functioning in specific parts of the body.

It was observed that dW_R was statistically significantly lower for left nipple line in the group of people with left breast cancer in relation to the healthy women and for right nipple line in the group of people with right breast cancer than in relation to a group of the healthy. The differences between the values of dW_R for left and right breast with breast cancer were significantly asymmetrical in comparison to the control group which was reported to have no asymmetry. It proves that the vegetative system does not work properly on the side where the cancer exists.

Conclusions: The patients suffering from breast cancer are found to show considerable asymmetry in fluctuation of the infrared radiation in relation to the control group. It was also statistically stated that there is a characteristic difference of the fluctuations of the infrared radiation in relation to the control group that depend on a location of cancer in a breast - from left

to right and both together. Healthy women had slight differences in the fluctuations of infrared radiation.

7. THE HYPOTHETICAL ROLE OF EXTERNAL STATIC MAGNETIC FIELDS IN CHIRAL SYMMETRY BREAKING PHENOMENA OBSERVED IN LIVING ORGANISMS

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For simple model proteins, possibilities of creating protein conformations of given handedness are discussed. We analyze how L- and D- stereoisomers of amino acids as well as negatively and positively charged amino acids can affect handedness of a protein chain. The influence of protein synthesis and its direction on protein handedness is stressed. [1,2]

For purely right- or left-handed protein molecules, we analyze possibilities of their spatial separation in the presence of a static external magnetic field [3]. The presented model, qualitative and preliminary, follows the general idea expressed by L.D. Barron: "a magnetic field alone might induce asymmetric synthesis if the prochiral reactant molecules are prealigned, as in a crystal..." [4], and the experimental fact that proteins having tertiary structures composed of parallel or antiparallel helices can be oriented in high static magnetic fields with helices parallel or antiparallel to the field [5].

The proposed model stresses the role of protein conformations and protein synthesis in the separation process. As the effect of aligning helices in magnetic fields is stronger for longer helices, the structure (handedness) - dependent spatial separation should be stronger for bigger, well-shaped helical molecules.

Right- and left-handed protein molecules may be composed of L- and D-amino acids, respectively. Therefore, spatial separation of the molecules of different handedness may lead to spatial separation of L- and D- stereoisomers of amino acids. The question about the level of organic matter organization that might be the most favorable for the occurrence of chiral symmetry breaking phenomena observed in living organisms should be then asked.

References

- [1] I. Mróz, *J Theor Biol* **157** (1995) 245-255.
- [2] I. Mróz, Z. Latajka, *J Theor Biol* **189** (1997) 151-158.
- [3] I. Mróz, *WSEAS Transactions on Biology and Biomedicine* **2** (2005) 381-385.
- [4] L.D. Barron, *Science* **266** (1994) 1491-1492.
- [5] F. Arnesano, L. Banci, I. Bertini, K. van der Wetering, M. Czisch, R. Kaptein, *J Biomol NMR* **17** (2000) 295-304.

8. EFFECT OF MAGNETIC FIELD, THE RED LIGHT AND THEIR COMBINATION ON THE OXYGEN-DEPENDENT MECHANISM OF KILLING OF NEUTROPHILS

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Neutrophils are phagocyte cells. Besides lymphocytes and macrophages neutrophils are involved in the effector's immune response, they are part of the first rapid response. The oxygen-dependent mechanism of killing pathogens by neutrophils is the respiratory burst. It consists in tens of times increase of oxygen consumption and production, and releasing large amounts of the superoxide anion outside the cell. Dismutation of this radical gives the hydrogen peroxide which was the object of interest of this research. Detection of this reactive oxygen species is made by the analysis of fluorescence of DCFH-DA (2',7'-dichlorofluorescein diacetate) probe. The fluorescent dye diffuses into the cell and is converted in the presence of e.g. H₂O₂ to the DCF (2',7'-dichlorofluorescein). This compound emits a fluorescent signal analyzed by the flow cytometer. DCF is linearly dependent on the quantity of the respiratory burst. Blood coming from healthy blood donors (10 people for each physical factor) was the experimental material. It was observed that the variable magnetic field of ELF range of the induction equals 89 μ T, the red light at the energy density of 1.23 J/cm² and a combination of these factors caused a statistically significant reduction of DCF fluorescence of neutrophils at rest and neutrophils after respiratory burst stimulation by PMA (phorbol 12-myristate 13-acetate). These physical factors were applied for 30 min each. The level of the magnetic induction and the density of light remained constant throughout all the time of the application, the pulses however, (pulses of the fundamental frequency are 180 \div 195 Hz) were administered in the form of packets of pulses (12.5 \div 29 Hz), groups of packages (2.8 \div 7.6 Hz) and series (0.08 \div 0.3 Hz). The magnetic field caused a 37.5% statistically significant reduction of DCF fluorescence of unstimulated neutrophils, whereas in PMA-stimulated neutrophils a 28.5% decrease of fluorescence was observed. The red light and the combined effect of the magnetic field and the red light caused a statistically significant reduction of fluorescence, respectively 27.2% and 19.9% only in stimulated neutrophils. The magnetic field application caused the biggest influence on the hydrogen peroxide production. The red light influences only the stimulated neutrophils and to a lesser level. However, a combination of the red light and the magnetic field does not strengthen the effect of the reduction of H₂O₂ production, as it is suggested by the synergy effect. This causes the least influence on the cells. Each of these physical factors affects the cell differently,

influencing different pathways of chemical transformation. For example, the red light acts upon mitochondria, the magnetic field influences the ions in the protein channel and cell membranes. However, the electromagnetic nature of the applied physical factors can cause a similar effect on the mechanisms closely related to the regulation of neutrophil functions.

9. INFLUENCE OF NEAR INFRARED RADIATION (NIR) ON STRUCTURE OF PHENYLALANINE

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The aim of present study is to explain the mechanism of Near Infrared (NIR) light action, the character of changes of phenylalanine at the molecular level. A specially constructed system of NIR radiation of 700–2000 nm has been used in the experiments. ATR-FTIR spectroscopy has been chosen as an experimental technique, because it is one of the most promising methods for diagnostic studies at the molecular level, simultaneously allowing us to understand global processes.

NIR radiation is used in both therapy and medical diagnostics. Many research centres carry out studies into the effects of electromagnetic radiation (i.e. from infrared region) on biological systems. It is known that NIR radiation have following effects: analgesic and anti-inflammatory, healing and strengthening of the immune system, it delays aging of skin and accelerates healing of wounds, protects fibroblasts against the toxicity of UV radiation, and increases microcirculation of blood. Infrared radiation is used, *inter alia*, at different diseases: chronic inflammations and rheumatic diseases, neuralgia and pain syndromes, and mechanical damages of bones.

It should be emphasized that the interaction at the level of tissue or whole organism is the result of the reaction at the cellular and molecular level. Therefore, it becomes important to study the effects of radiation, including NIR, at the molecular level. Although sophisticated laboratory tests and clinical primary mechanism of action of radiation from the NIR is not fully explained, and the results are often controversial. Our results and literature data suggest that the molecular mechanism of action of the NIR is associated with the modification of water and hydrogen bonds. This mechanism relates to so many biological structures, starting from the tissues and ending on simple molecules [1].

Therefore aqueous solutions of phenylalanine amino acid were irradiated by Near Infrared Radiation (NIR). Phenylalanine is amphiphilic molecule and can be a simple model of protein. The ATR-FTIR spectra of phenylalanine after NIR radiation demonstrate modifications due to intermolecular interactions and water solvation. The results of our research show clearly that modifications of water structures as a result of their exposure to NIR weaken interactions between polar groups of phenylalanine amino acid, which is also confirmed by our previous studies [2–6]. After NIR irradiation an intramolecular proton transfer reaction occurs and the concentration of neutral groups increases, resulting in the formation of strong hydrogen bond between the carboxylic (–COOH) and carboxylate (–CO₂[–]) groups. In these conditions, dimerization can appear. This was confirmed by quantum chemical calculations of phenylalanine [7]. The interaction between two identical molecules of the amino acid involves hydrogen bonding – C=O···HOOC–, forming cyclic dimers analogous to dimers formed by carboxylic acids. As a consequence of the aggregation process pK_a values of the amino acid are evidently shifted [8]. The presence of hydrophobic groups can influence these effects. The increase of hydrophobic interactions after NIR radiation favours the aggregation in biological systems, what can modify metabolic processes at the molecular level.

References

- [1] Olsztyńska-Janus S., Gąsior-Głogowska M., Szymborska K., Czarnik-Matusiewicz B., Komorowska M., *Biomedical Engineering, trends, research and Technologies*, ed. by M. Komorowska and S. Olsztyńska-Janus S., Intech, Rijeka, Croatia, 2011, 91-120.
- [2] Olsztyńska S., Thesis, 2004, Wrocław.
- [3] Olsztyńska S., Dziamska A., Komorowska M. *Acta Bioeng. Biomech.*, 1999, 1, 129–133.
- [4] Olsztyńska S., Domagalska B.W., Komorowska M., *Surfactants and dispersed systems in theory and practice*, ed. by K.A. Wilk, Oficyna Wydawnicza Politechniki Wrocławskiej, Wrocław, 2003, 405–409.
- [5] Olsztyńska S., Vrielynck L., Komorowska M., Dupuy N., *Acta Bioeng. Biomech.*, 2001, 3, Suppl. 2, 387–391.
- [6] Olsztyńska S., Dupuy N., Vrielynck L., Komorowska M., *Appl. Spectrosc.*, 2006, 60(9), 1040–1053.
- [7] Olsztyńska-Janus S., Szymborska K., Komorowska M., Lipinski J., *J. Mol. Struct. (THEOCHEM)*, 2009, 911, 1–7.
- [8] Olsztyńska S., Komorowska M., Dupuy N., *Appl. Spectrosc.*, 2006, 60(6), 648–652.

10. CHANGES IN DISTORTION PRODUCT OF OTOACOUSTIC EMISSION IN TINNITUS PATIENTS STIMULATED BY THE ELF MAGNETIC STIMULATION

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Approximately 17% of the population in the world experience tinnitus. This is the conscious experience of sound that originates in the head, without the external source. There are many complementary and alternative therapies used to tame tinnitus. Awareness about its causes and ways to reduce its effects are improving, but for some it remains incurable.

The purpose of this study was to determine if magnetostimulation suppresses tinnitus. The magnetostimulation involves treating the body with extremely low-frequency magnetic fields of low magnetic induction value (ELF- MF) using Viofor JPS System.

Since previous results imply that tinnitus may be evaluated objectively by DPOAE's, before and after magnetostimulation patients were examined using the audiometer and DPOAE (distortion product otoacoustic emission) to find changes in the DPOA's amplitudes.

However any significant changes were found among patients with tinnitus, for the control group statistically important changes in DPOAE levels were observed.

11. HYDROXYL RADICAL PRODUCTION IN POTATO TUBER DURING THE HYPERSENSITIVE RESPONSE TO FUNGUS *PHYTOPHTHORA INFESTANS*.

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Late bright disease of potato is considered to be one of the most dangerous diseases in agriculture. The causative agent for it is oomycete *Phytophthora infestans*. The disease has been intensively studied in past few decades but still is the cause of the major loss in potato cultivation. Using electron paramagnetic resonance spectroscopy we observed the formation of hydroxyl radical in oomycete infected potato tuber. To confirm that hydroxyl radical is formed by one electron reduction of molecular oxygen, superoxide anion radical and hydrogen peroxide was measured by

using nitroblue tetrazolium (NBT) and 3,3-diaminobenzidine tetrahydrochloride (DAB) imaging technique, respectively. To study the deleterious effect of hydroxyl radical on lipids and proteins we observed the enhancement in ultra-weak photon emission from oomycete infected tuber. The data presented in this study reveals that hypersensitive response of the oomyceteous fungus *Phytophthora infestans* on potato tuber is associated with the formation of hydroxyl radical. The study also shows ultra-weak photon emission can be use as the measure of oxidative processes and can be use in quality control at food industry.

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12. THE IP VS. VDE COMPETITION AS A KEY FACTOR DETERMINING THE STABILITY OF THE $MgBX_3$ (X = F, Cl) COMPOUNDS

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The kinetical and thermodynamical stability of a molecule is one of the most important issues while designing novel compounds possessing desired properties. In our preceding paper [1] we provided (on the basis of theoretical considerations supported by *ab initio* calculations) the explanation of the hypothetical $HAiCl_4$ acid instability. The existence of the corresponding salts (i.e., $LiAlCl_4$, $NaAlCl_4$, and $KAlCl_4$) was confirmed whereas their parent acid ($HAiCl_4$) was identified as an $HCl \cdots AlCl_3$ adduct with the hydrogen chloride tethered weakly to the quasi-planar aluminum chloride molecule. As we concluded, the electron affinity of the neutral $AlCl_4$ molecule was the most important factor determining the ability to form a stable $MAiCl_4$ compound ($M=Li, Na, K$). Since forming the chemical bonds exhibiting primarily ionic character (as observed in $MAiCl_4$ species) usually requires utilizing strong electron acceptors, we naturally focus our attention on the species termed *superhalogens* by Boldyrev and Gutsev in the early 80's [2]. Superhalogens (e.g., $AlCl_4$, BF_4 , BCl_4) are extraordinary inorganic compounds exhibiting extremely large electron affinities exceeding the electron affinity of the chlorine atom [3]. One of the reasons why superhalogen species attract the attention of the experimental chemists is the role they can play in synthesis (e.g., in oxidation of counterpart systems with high ionization potentials) [4-6] Our goal was to follow this idea while verifying the stability of some novel compounds, however, we decided to investigate more carefully the factors determining their geometrical and thermodynamical stability (i.e., the susceptibility to fragmentations).

In this contribution we discuss the possible existence and stability of novel molecules defined by the $MgBX_5$ ($X=F, Cl$) formula. We propose to use the values of ionization potential (IP) and electron binding energy of the radical fragments MgX and BX_4 (i.e., the subunits the $MgBX_5$ molecules are assembled of) to estimate the expected stability of the compound. We believe that introducing such simple models is important for general chemistry because it allows to predict the stability of molecules before they are actually synthesized. In addition, it is our hope to encourage the experimental chemists to use more extensively basic physicochemical parameters (such as ionization potentials and electron affinities) characterizing the substrates to anticipate the properties (e.g., thermodynamical stability) of the novel compounds.

References

- [1] C. Sikorska, S. Freza, P. Skurski, J. Phys. Chem. A 114 (2010) 2235.
- [2] G. L. Gutsev, A. I. Boldyrev, Chem. Phys. 56 (1981) 277.
- [3] C. Sikorska, S. Smuczyńska, P. Skurski, I. Anusiewicz, Inorg. Chem. 47 (2008) 7348.
- [4] N. Bartlett, Proc. Chem. Soc. (1962) 218.
- [5] F. Wudl, Acc. Chem. Res. 17 (1984) 227.
- [6] D. F. Hunt, G. C. Stafford, Jr., F. W. Crow, J. W. Russell, Anal. Chem. 48 (1976) 2098.

13. THE INFLUENCE OF UV IRRADIATION ON COLLAGEN FROM THE FISH SCALES

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Collagen is the most abundant protein representing nearly 30% of total proteins in the animal body. At present, the main sources of type I collagen are bovine or porcine dermis. Non-denatured collagens from these sources can be applied in cosmetics, biomedical, and pharmaceutical industries. Denatured collagen, known as gelatin, is widely applied in the food and biomedical industries. However, due to outbreak of Bovine Spongiform Encephalopathy (BSE), Foot and Mouth Disease (FMD) in pigs, cattle, the applications of collagen and collagen derived products from these sources have been limited. Type I collagen has also been extracted from skin, bone, fins, and scales of fresh water and marine fishes. Collagens from these sources were evaluated for their potential application as an alternative to mammalian collagen. However, the properties of such collagen markedly vary with the habitat, species and part of fish it is isolated from, demanding a need for characterization of this protein from different sources. The use of fish collagen, instead of mammalian collagen, has numerous rewards. During food processing, fish solids waste constitute 50–70% of the original raw material,

depending on the processes used and types of products. Also fish collagen could be used by the Islamic and Hindu nations, which cannot use mammalian collagen, owing to religious constraints.

Present study focuses on characterization of collagen from scales of *Esox lucius* and influence of UV irradiation on the surface properties of fish collagen films. Collagen was isolated from fish scale, a calcified tissue, through demineralization following acetic acid treatment. The isolated and purified collagen was characterized by FTIR, SDS–PAGE analysis and amino acid analysis. Denaturation temperature of collagen was estimated by thermally induced changes in viscosity.

Air-dried collagen films were submitted to treatment with UV irradiation for different time intervals, in air at room temperature using a mercury lamp, Philips TUV-30, which emits light of mainly 254 nm wavelength. The surface properties of collagen films before and after UV-irradiation were investigated using the technique of Atomic Force Microscopy (AFM) and by contact angle measurements. AFM was performed by using a MultiMode Scanning Probe Microscope Nanoscope IIIa (Digital Instruments Veeco Metrology Group, Santa Barbara, CA) operating in the tapping mode in air. The contact angles of two liquids: diiodometan and glycerol on the surface of studied films were measured using a goniometer equipped with the system of drop-shape analysis (G 10/DSA, Krüss, Germany). The surface free energy was calculated using Owen Wendt method.

AFM images of fish collagen films show collagen fibers. The size of fibrils in irradiated collagen films is bigger than in nonirradiated ones. The surface roughness of these films decreases after 2 and 12 h of UV irradiation.

The values of surface free energy and the polar component of surface free energy increased after exposure to UV radiation. The increase of polarity of collagen films indicates that photooxidation reactions take place on the surface.

14. EFFECTS OF ELECTROMAGNETIC RADIATION ON BIOLOGICAL MATERIAL PRODUCED BY INSECTS

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Silks are biological materials which are produced by more than 30,000 known species of spider, and by most of the 113,000 species in the insect order *Lepidoptera* (butterfly, caterpillars, silkworms). Moreover, silks are produced by members of several other animals like mussels, bees, scorpions, mites and fleas. A large number of silk because of the long-established process of silkworm rearing (400 000

tones per year of dry cocoons) is available worldwide for the textile industry. It is well known that the fabrics made from silk exposed to prolonged sunlight lose their mechanical properties.

The aim of our work was to study the photochemical behaviour of silk fibroin. To explain the quantum phenomena occurring in silk fibroin under the action of the electromagnetic field from UV-Vis range, we used a soluble form of silk and examined it by UV-Vis, FTIR and fluorescence spectroscopy.

Silk is widely used not only in the textile industry but also it is a valuable material in medicine, thanks to its extraordinary mechanical properties and biocompatibility. Silk fibroin - a main component of silk, can form a variety of morphological forms, such as scaffolds for cell growth, hydrogels, membranes, films, fibers and capsules. Regarding the requirement of UV sterilization of biomaterials before implantation there is a need to investigate the properties of materials after UV-irradiation and to understand photochemical processes occurring. Moreover, silk hydrolysates are recently commonly used as additives to hair conditioners or body creams, therefore it is desirable to know how this substance can interact with skin after the absorption of ultraviolet radiation.

It was found that the absorption of silk fibroin in solution increased during UV-irradiation of the sample, most notably between 250 and 400 nm. Moreover, after UV-irradiation a wide peak emerged between 290 and 340 nm with maximum at about 305 nm. The new peak suggests that new photoproducts are formed during UV-irradiation of regenerated silk fibroin. The results will be presented and discussed in a poster.

16. QUANTUM PHYSICS SHEDS SOME LIGHT ON HADO SHIATSU

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Quantum effects are present in human organisms on a macroscopic scale. The living organism can be considered a macroscopic quantum system, where the fluctuations of the elementary components are tuned together in a global macroscopic fluctuation. This property is named "coherence". Matter therefore is not inert, is in perennial fluctuation. Vacuum fluctuates too, being full of fluctuating fields. Coherence establishes a dynamic order which is fundamental for equilibrium in living beings. In the coherent state, an electromagnetic field, produced by the common fluctuation of molecules, is trapped within the fluid (matter). The wave becomes the prisoner of matter. The electromagnetic field cannot be irradiated outwards, but the potential of the field can leak out, (the so called Aharonov-Bohm effect). This originates different phenomena:

"Intriguingly, recent work has documented that light-absorbing molecules in some photosynthetic proteins capture and transfer energy according to quantum-mechanical probability laws instead of classical laws at temperatures up to 180 K." [1]

In coherence domains of living matter, atoms and molecules share a dialogue because the various coherence domains are in phase one with another, or rather they are correlated. We can consider the degree of coherence in a living system as a measurement parameter for health, it being related to the efficiency of energy transfer and use of the system's resources to carry out its vital functions. Given the particular properties of coherent domain chains, strongly linked with the special nature of biological water, energy can travel through them and is available for the body's vital activities. A human being is in a healthy condition when this flow occurs consistently. To be healthy does not require much energy, given that an excess would extinguish the system's coherence, its dynamics passing rapidly from one of ordered movement to chaos. Illness may ensue when, on losing coherence in the system, energy fails to move and becomes blocked.

Let us consider the basic equations :

$$\varphi = \frac{q}{\hbar} \int_P \vec{A} \cdot d\vec{x},$$

$$\varphi_t - \varphi_0 = -\frac{qVt}{\hbar}.$$

The phase, connected with these travelling excitations, is characterized by spatial and temporal derivatives. So potentials are generated and they create themselves phase variations. Therefore, there is a possibility of interactions among organisms based on the phase, so without significant energy exchanges.

The development of a system called Hado Shiatsu has grown out of the aforementioned concepts.

In the Japanese tradition Hado is the innate transforming power of each thing and each living being. The literal translation of its ideogram is "wave-like movement, vibration". The word "Shiatsu" means "finger pressure". It is a discipline developed in Japan and connected with Traditional Chinese Medicine, martial art and meditation.

Hado Shiatsu is a therapeutic approach based on "empathic connections", that means phase resonance not energy exchange. A sort of "meditative state", where phase is no more chaotic, will allow both givers and receivers to be in phase with healthy environments. A better life quality will be supported, enhancing the coherence of the system.

In accordance with Weber and Fechner law, which applies to all living beings, slighter the stimulus bigger the inner reaction of a system. In Hado the approach is a "whisper": a light, gentle touch to relate to the field trapped into the matter, supporting the creation of

solitons and leaving a sort of informed print into the biological water.

Hado Shiatsu uses a new meridian model inspired by Quantum Physics: "Here we suggest that self-organization of the living organism implies the appearance of an array of quasi-one-dimensional coherent domains that behave as the pathways where a flow of matter, energy and information is self-confined... This array can be linked with functioning of energetic channels known as meridians in the Eastern medicine." [2]

"Moreover, the organism can be represented as a liquid crystalline continuum, which can carry the signals for intercommunication in a way, similar to liquid crystals. Such systems are highly nonlinear optical media and can support the existence of specific pathways for the propagation of electromagnetic signals." [3]

In this context, the network of connections takes on relevant importance. When we envisage the meridians as a particular form of coherence domain in the connective tissue they are a sort of watery sheath encasing molecular chains. It is here where energy captured by the molecules arrives. Energy is brought to the molecule by a soliton, a localized wave packet that does not dissipate energy in its movement. When it encounters a "metabolic situation" requiring just the amount of energy it holds, the soliton gives up its own and ceases to exist.

Several scientific studies support the hypothesis that a "therapeutic" touch on the human body produces electricity that goes into ideal transmission pathways, the aforementioned Meridian-like channels. The stimulated meridian "lights up" and produces "coherent photons" [4-6].

References

- [1] Collini E, Wong CY, et al. Vol 463 | 4 February 2010 | doi:10.1038/nature08811
- [2] Brizhik LS, Del Giudice E, et al. *Electromagnetic Biology and Medicine* 28(1): 28-40
- [3] Brizhik LS, Popp FA, Schlebusch K-P 2008 Abstracts, *Acupuncture, Auriculo-Acupuncture, Sciences et Neurosciences: Des laboratoires à nos consultations médicales. Echanges Soulié de Morant. Les Invalides, Paris, 8 March 2008*
- [4] Chien C H, Tsuei J J, Lee S C et al. 1991, *American journal of Chinese Medicine* 19(3-4):285-292
- [5] Schwartz S A, De Mattei R J, Brame E G Jr. et al. 1990, *Subtle Energies* 1(1): 43-72
- [6] Zimmerman J 1990, *BEMI Currents, Journal of the Bio-Electro-Magnetics Institute* 2: 8-17

17. DOES THE NEAR-INFRARED RADIATION (NIR) DESTABILIZE THE DNA MOLECULE?

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The structure of water bonded determines the conformation of biological macromolecules and controls their metabolic activity. In the further layer such molecules are surrounded by global water. Structure modification of water bonded and global water caused by physical or chemical factors induces structural changes in biological systems. The structure of water which surrounds the molecule can be changed by magnetic field, pressure, temperature, presence of ions or organic solvents [1,2]. Another efficient structural modification factor is also a near infrared radiation (NIR). Our recent research focused on amino-acids, proteins and erythrocytes show, that the only common object activated by NIR radiation are structures of water bonded and global water. Modifications in adjacent water structures caused by NIR radiation take effects on polar group protonation and on secondary processes consist in aggregation and conformational changes in biological molecules [3,4].

DNA molecule has been investigated in order to clarify processes that take place under the influence of NIR. Such choice is motivated by the DNA hydration layer that has a first-rate influence on this molecule stabilization. UV-VIS spectroscopy results obtained for water DNA solutions show that melting process of the macromolecules has three stages. Stage sensitive to NIR radiation is a dissociation of bases of molecule. Studies have shown that all used doses of radiation destabilize the system [5]. Opposite results can be obtained after introduction of modifiers to the solution of DNA.

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References

- [1] O. D. Boner, C. F. Jumper, *Infrared Phys.* 13 (1973) 233
- [2] W. J. Lamb, D. R. Brown, J. Jonas, *J. Phys. Chem.* 85 (1981) 3883
- [3] M. Komorowska, A. Cuissot, A. Czarnoleski, W. Bialas, *J. Photochem. Photobiol. B: Biol.* 68 (2002) 93
- [4] S. Olsztynska-Janus, K. Szymborska, M. Komorowska, J. Lipinski, *J. Mol. Str. (Theochem)* 911(2009) 1
- [5] K. Szymborska, *Interdyscyplinarność badań naukowych, Oficyna PWR, Wrocław 2009*, 52.

18. MOLECULAR DYNAMICS OF CONTACT LENS HYDROGELS BY ^1H NMR METHODS

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The solid-state ^1H NMR on-resonance and off-resonance techniques have been used to study molecular dynamics of selected soft contact lenses. The measurements were carried out using a home made pulse spectrometer operating at the frequency of 30.2 MHz. The shape of the ^1H NMR line (first derivative) was measured by the continuous wave method. The spin-lattice T_1 and spin-spin T_2 relaxation times in the laboratory frame as well as the second moment M_2 of absorption line and the slope line width were analyzed as a function of temperature. The study applies poly(2-hydroxyethyl methacrylate) pHEMA hydrogels with different content of the water. The thermal properties of hydrogels were characterized using differential scanning calorimetry.

19. IN SEARCH OF IONIZING RADIATION EFFECT ON NUCLEOSIDES: RADIOLYSIS OF CYTYDINE

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DNA is considered as the crucial target for biological effects of ionizing radiations, such as cell death, chromosomal aberrations, mutagenesis and carcinogenesis. Extensive work has been devoted to the processes underlying the damages of the constituents of DNA. It is known that the DNA lesions are induced mainly due to the attack by the hydroxyl radicals (OH^\cdot) formed from the radiolysis of water. The lesions occur at every nucleotides along the DNA molecule. So the influence of radiation on the nucleic acids components has been intensively investigated [1-3].

In our studies gamma radiation initiated processes occurring in aqueous solutions of cytydine were examined by means of UV spectrometry and chromatography methods. Kinetic study of cytydine disappearance and formation of radiolysis products were investigated by HPLC in the concentration range of 100 – 1750 mmol/l. It was found that irradiation of aqueous solutions of cytydine ($c = 100 \mu\text{mol/l}$) leads to its complete disappearance at dose above 1,5 kGy. Chromatographic analysis showed that four

main products detectable by UV are formed during irradiation in the dose range of 0,2 – 1,5 kGy. Reaction rate constants were calculated. It was proved that cytydine disappearance follows the pseudo-first-order rate kinetics.

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References

- [1] C.von Sonntag, Free-Radical-Induced DNA Damage and Its Repair, Springer, Hiedelberg, 2006.
- [2] J. Cadet, T. Douki, D. Gasparutto, Radiat. Phys.Chem., 72 (2005) 293.
- [3] M. D. Evans, M. Dizdaroglu, M. S. Cooke. Mutation Res., 567 (2004) 1.

20. RAPID DNA SEQUENCING VIA TRANSVERSE ELECTRONIC TRANSPORT

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A rapid and low-cost DNA sequencing method would revolutionize medicine: a person could have their full genome sequenced so that treatments could be tailored to their specific conditions; doctors could know in advance a patient's likelihood to develop a given ailment; cures to major diseases could be developed faster. These goals of "personalized medicine" are hampered today by the high cost and slow speed of DNA sequencing methods. We will discuss a sequencing protocol we suggest that is based on the measurement of transverse electronic currents during the translocation of single-stranded DNA through nanopores. We have performed molecular dynamics simulations coupled to quantum mechanical calculations of the tunneling current in experimentally realizable systems in order to understand the operating principles behind this sequencing method. Several recent experiments also support our theoretical predictions. In addition to their possible impact in medicine and biology, the above methods offer ideal test beds to study open scientific issues in the relatively unexplored area at the interface between solids, liquids, and biomolecules at the nanometer length scale [1].

References

- [1] M. Zwolak and M. Di Ventura, "Physical Approaches to DNA Sequencing and Detection", Rev. Mod. Phys. 80, 141 (2008).