Списък на участия в научни конференции

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2001_4ta Nacionalna conferencia po himia_poster

2002_3 Bulgarski Peptiden Simposium_lecture1 and lecture2

2002_Humboldt Research Conference on Computational Chemistry_poster

2004_2 Humboldt Conference on Computational Chemistry_poster

2004_Nauchna Konferencia 115 Godini Uni Neorganichna Himia_poster

2006_2nd Nationalna Konferencia po Elektronno Obuchenie_lecture

2006_3rd Humboldt Conference on Computational Chemistry_poster1 and poster2

2008_5th Bulgarian Peptide Symposium_poster1 and poster2 and poster3

2008_12 th International Conference on Theoretical Aspects of Catalysis_poster

2009_2nd Humboldt Conference on Noncovalent Interactions_lecture and poster

2010_3rd International Symposium of Organic Chemistry_poster

2010_4th Humboldt Conference of Computational Chemistry_poster

2010_11th International Chemistry Conference and Exhibition in Africa_poster

2010_13th International Conference on Theoretical Aspects of Catalysis_poster

2010_Frontiers of Chemistry form Molecules to Systems_poster

2010_ICTAC 13_poster

2013_Beijing Computational Science Research Center_lecture

2014_2nd International Conference Advanced Functional Materials_poster

2014_33rd European Peptide Symposium_lecture

2014_HPS_lecture

2014_Suranaree University of Technology_lecture

2014_University Sains_lecture

2016_7th BPS with IP_poster

2016_24th MPCE_poster

2016_CEUM_poster

2016_DBEIC_poster

2016_ESCA_poster

2017_Conference Razgrad_lecture

2017_EkoKonferencija_lecture1 and lecture 2

2017_Klimentovi dni_poster

2017_Saratov Fall Meeting 2017_Biospectra_lecture

2018_5th National Congress of Immunology_lecture

2018_6th European Biopharma Congress_poster

2018_11th CC_lecture

2018_11th Internation Congress of Autoimmunity_lecture

2018_20th International Conference and School on Quantum Electronics_poster

2018_LALS_poster

2018_Student Scientific Session_poster

2018_Summer School Albena_poster

2019_ICE_lecture

СХБ
1901

100 години
СЪЮЗ НА ХИМИЦИТЕ В БЪЛГАРИЯ

ЧЕТВЪРТА НАЦИОНАЛНА КОНФЕРЕНЦИЯ ПО ХИМИЯ

27–29 СЕПТЕМВРИ 2001 ГОДИНА
ЦЕНТРАЛНО УПРАВЛЕНИЕ НА БАН
ДОМ НА ТЕХНИКАТА – СОФИЯ

ПРОГРАМА И РЕЗЮМЕТА

ВЛИЯНИЕ НА ЦИС-ВИЦИНАЛНА ХИДРОКСИЛНА ГРУПА ВЪРХУ АМИНОЛИЗАТА НА АРОМАТНИ ЕСТЕРИ

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Аминолизата е най-фундаменталният химически процес в живата клетка и неговото изучаване е от голямо значение за разбирането на процесите, протичащи при функционирането й. При биосинтеза на пептидна връзка в клетъчната рибозома нарастващата полипептидна верига, както и атакуващата аминокиселина са свързани с 3'-хидроксилните групи на 3'-крайния аденозин на транспортните РНК-и, което обуславя наличието на вицинални цис разположени хидроксилни групи около реакционния център.

В настоящото изследване се изучава влиянието на цис-вицинална хидроксилна група върху аминолизата на ацетилиран катехол, който е избран като биоорганичен модел при изучаването на влиянието на хидроксилните групи поради конформационната стабилност на цис разположената хидроксилната група и наличието на кинетични експериментални резултати за подобни реакции [1]. Изчисленията са направени на ниво MP2/6-311++G**//HF/6-311++G** посредством GAMESS [2]. Изследвана е възможността за образуване на вътрешномолекулни водородни връзки в реактантите, интермедиатите и преходните състояния и е оценено влиянието им върху енергетичният профил на реакцията. Намерена е каталитична активност на цис разположената вицинална хидроксилна група при изследваните механизми на аминолиза. За различните изследвани механизми, активиращата енергия на реакцията при ацетилкатехол е с 10 kcal/mol по-ниска от активиращата енергия на съответния реакционен път при ацетилфенол.

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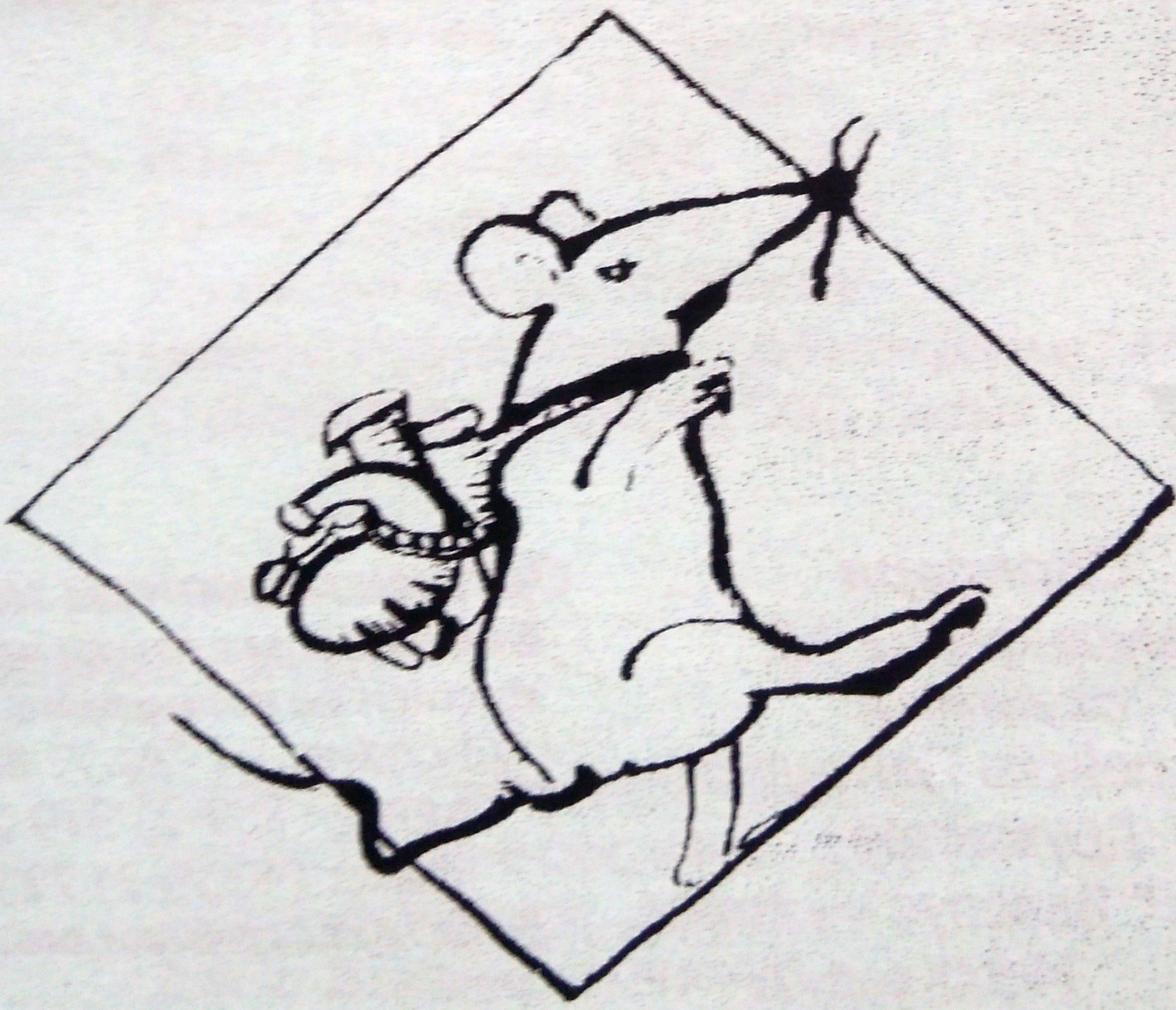
Благодарност: Авторите благодарят на фондация Александър фон Хумболт за дарената компютърна техника.

БЪЛГАРСКО ПЕПТИДНО ДРУЖЕСТВО

3ри БЪЛГАРСКИ ПЕПТИДЕН СИМПОЗИУМ

17-19 Май 2002, Паничище
Северозападна Рила

НАУЧНА ПРОГРАМА И РЕЗЮМЕТА



L-3

СЪУЧАСТИЕ НА ПЕПТИДИЛ-тРНК В КАТАЛИЗА ОТ РИБОЗОМАТА

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***Университет на Упсала, Упсала, Швеция

Структурните изследвания недвусмислено показаха, че рибозомата е рибозим, но дали той само позиционира субстратите или участва с каталитични групи остава неясно. Предположеният киселинно-основен катализ от аденилов остатък A2451 в 23S рибозомалната РНК не беше подкрепен от мутации на този и други нуклеотиди. Съвременната химична биология обаче позволява редуцирането на комплексността на рибозомата и установяване на химичните основи на каталитичния й механизъм. Тук ние предлагаме субстрат-асистиран рибозомен каталитичен механизъм, който е в съгласие както със структуктурните, така и с генетичните данни. Чрез корелация между рибозомната пептидил транферазна активност към модифицирани в 3'-края пептидил-тРНК и реактивоспособността на също така модифицирани пептидил-тРНК мимики при трансестерификация в органична среда, ние установихме съучастие на пептидил-тРНК в катализа от рибозомата. Такъв субстрат-асистиран рибозомен каталитичен механизъм е възможен само в нискодиелектрична апротна среда, тъй като тя сваля "израждането" на реактивоспособността във водна среда чрез промотиране на анхимерно подпомагане от 2'/3'-OH и нуклеобазата. Съучастието на пептидил-тРНК в катализа от рибозомата е най-ефективно при аденозин на 3'-края на пептидил-тРНК, което обяснява защо Природата е избрала аденозина като инвариантен 3'-краен нуклеозид в тРНК.

L-8

ВЛИЯНИЕ НА ВИЦИНАЛНТА ХИДРОКСИЛНА ГРУПА ВЪРХУ АМОНОЛИЗАТА НА ФЕНИЛНИ ЕСТЕРИ

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[2]Химически факултет, СУ "Св. Кл. Охридски

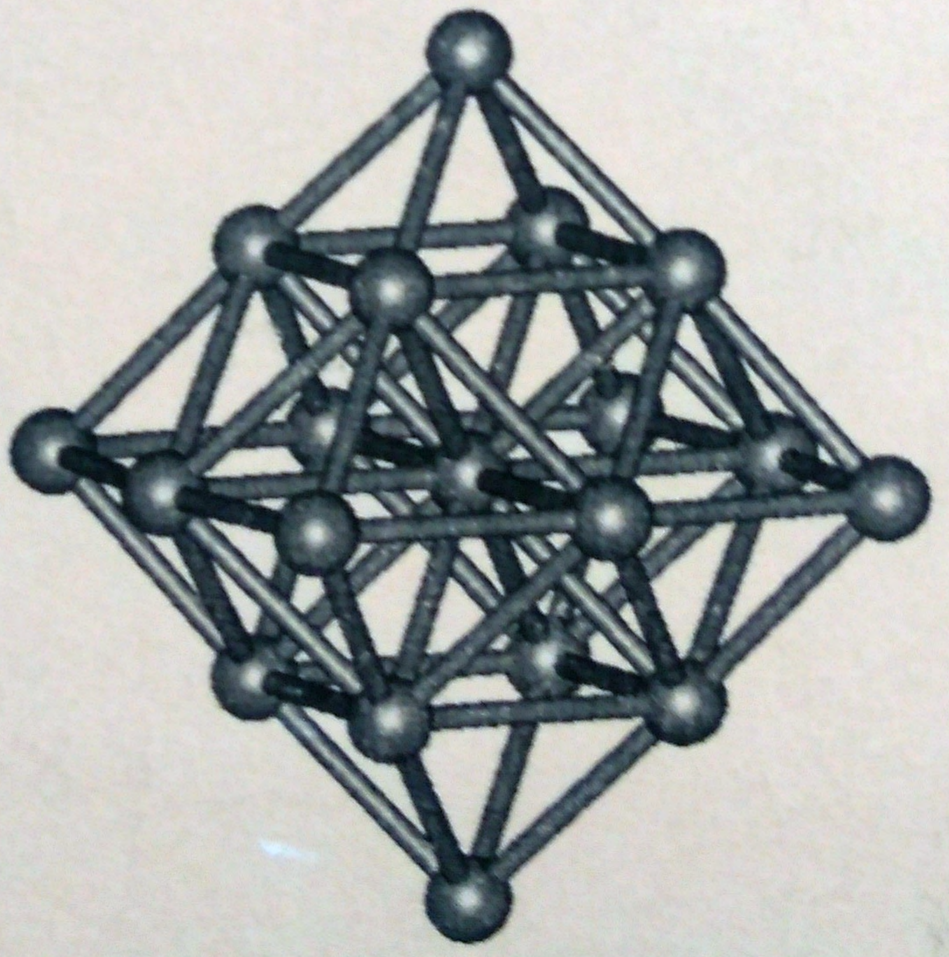
Експерименталното и теоретично изучаване на механизма на аминолизата на естери е от съществено значение за разбирането на процесите, протичащи при функционирането на живата клетката. При биосинтеза на пептидна връзка нарастващата полипептидна верига, естерно свързана с цис-1,2-диолната цистема на 3'-крайния аденилов остатък на транспортната РНК, се атакува от поредната аминокиселина в рибозомата. Пептидният синтез в присъствие на 1,2-дихидроксибензен (катехол) добре имитира биосинтеза на пептиди и белтъци .

В настоящото изследване теоретично се изучава механизма на моделна реакция на биосинтеза на пептидна връзка-аминолиза на ацетилиран катехол. Изчисленията са направени на ниво MP2/6-311++G**//HF/6-311++G** посредством GAMESS . Изследвана е възможността за образуване на вътрешномолекулни водородни връзки в реактантите, интермедиатите и преходните състояния и е оценено влиянието им върху енергетичният профил на реакцията. Намерена е каталитична активност на цис разположената вицинална хидроксилна група при изследваните механизми на аминолиза. За различните изследвани механизми, активиращата енергия на реакцията при ацетилкатехол е с 10 kcal/mol по-ниска от активиращата енергия на съответния реакционен път при ацетилфенол.

HUMBOLTD RESEARCH CONFERENCE ON COMPUTATIONAL CHEMISTRY

Veliko Turnovo, Bulgaria

30 October - 3 November 2002



BOOK OF ABSTRACTS

Sofia, 2002

Catalysis by Vicinal Hydroxyl in Diol Esters Ammonolysis

Miroslav Rangelov,[a] Gabriela Ivanova,[a] Georgi Vayssilov,[b] and Dimiter Petkov[a]

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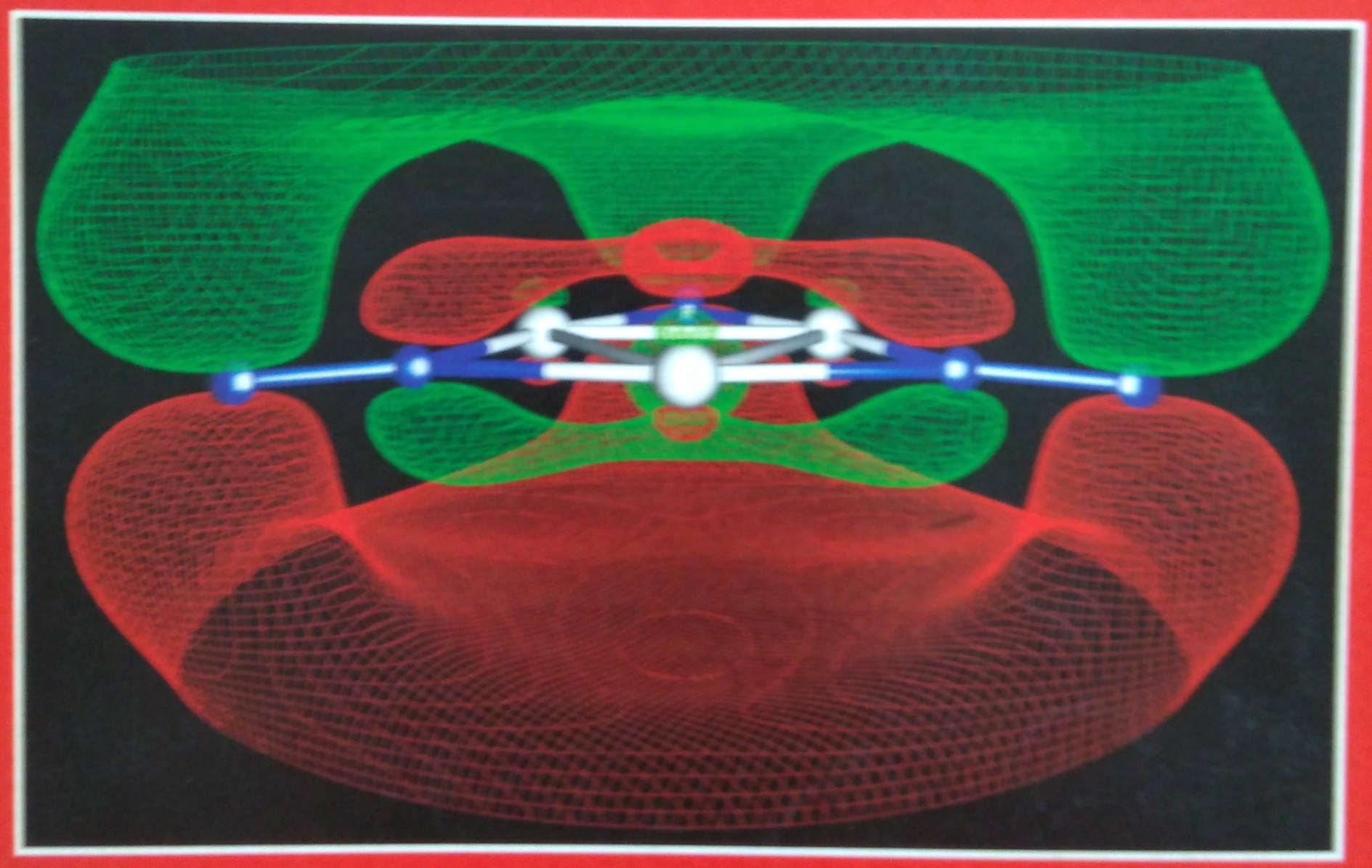
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The key reaction of protein synthesis, peptide bond formation, is catalysed in all living organisms by the ribosome. The complete atomic structure of the large ribosomal subunit at 2.4Å resolution showed no proteins within 18Å from the active site, revealing peptidyl transferase as an RNA enzyme. Reported structural and biochemical features of the universally conserved adenine residue A2486 (A2451 in *Escherichia coli*) in 23S ribosomal RNA led to the proposal of a mechanism of peptidyl transfer rRNA catalysis that implicates this nucleotide as the principal catalytic species. But *in vivo* and *in vitro* investigations carried out later showed that the large ribosomal subunit with mutated A2451 has significant peptidyl transferase activity. Thus the mechanism of peptide bond formation in the ribosome remains unclear. In protein synthesis, the nucleophile is the amino group of the amino acid in the ribosome A-site, and the carbonyl belongs to the P-site amino acid esterified by the 3'-ribose of tRNA. Actually it is an aminolysis reaction. Thus the aminolysis of esters can be studied experimentally as well as theoretically as a model reaction for the formation of peptide bonds during translation. The medum in the ribosome active site could be modeled by aprotic organic solvents in the experimental research as well as by calculations in vacuum in theoretical studies.

Here we report the *ab initio* investigations in vacuum of the mechanism of peptide bond formation model reaction. Our chosen model is the ammonolysis of diol esters as peptidyl-tRNA mimics. The results suggest a participation of peptidyl-tRNA vicinal hydroxyl in the peptide bond formation, catalyzed by the ribosome.

SECOND HUMBOLDT CONFERENCE ON COMPUTATIONAL CHEMISTRY

Nessebar, Bulgaria
1 - 5 September 2004



BOOK OF ABSTRACTS

Mechanism of acyl group migration in nucleosides

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The acyl migration in acylated diols or carbohydrates is very important reaction for both the biological processes in the living cells and for the organic chemistry. One of the most important acyl migration reactions is acyl migration in the aminoacylated t-RNA, which is substrate for the peptide bond synthesis in ribosome. Experimental kinetic investigations 1,2 show that acyl equilibration between these two forms is very fast, exceeding the rate of hydrolysis by four orders of magnitude in neutral pH. Here we report the results of quantum chemical study of the mechanism of the acyl group migration. One of the smallest but still reasonable model systems for the aminoacylated t-RNA is mono formylated tetrahydrofuran-3,4-diol. Molecular orbital calculations at B3LYP/6-31+G* level were carried out using GAUSSIAN98 program. Analytical gradient optimization methods were used to locate the minima, corresponding to reactant, intermediate and product, and saddle points corresponding to transition states.

Both stepwise and concerted pathways were found possible in formyl group migration between vicinal hydroxyl groups in tetrahydrofuran-3,4-diol. According to our theoretical investigations the stepwise mechanism is preferred by 11.6 kcal/mol over concerted. The transition state energy varies by 6-9 kcal/mol in different conformation of each type of transition state due to steric hindrance caused by the high conformational constrains in the tetrahydrofurane ring. The obtained activation energy of the reaction 45.3 kcal/mol is, however, rather high that suggests additional acceleration in the real systems by possible catalytic influence of the nucleobases or initial deprotonation of the 3'-OH group.

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Софийски Университет "Св. Климент Охридски"

ХИМИЧЕСКИ ФАКУЛТЕТ

НАУЧНА КОНФЕРЕНЦИЯ

115 ГОДИНИ УНИВЕРСИТЕТСКА НЕОРГАНИЧНА ХИМИЯ

ЧЕТВЪРТИ НАУЧНО-ПРИЛОЖЕН СЕМИНАР

НОВИ МАТЕРИАЛИ ЗА ИНДУСТРИЯТА

23 НОЕМВРИ 2004 г.

P63

МОДЕЛНО ИЗСЛЕДВАНЕ НА УЧАСТИЕТО НА НУКЛЕОБАЗИТЕ ВЪВ ВЪТРЕШНОМОЛЕКУЛНИ ВОДОРОДНИ ВРЪЗКИ В НУКЛЕОЗИДИ

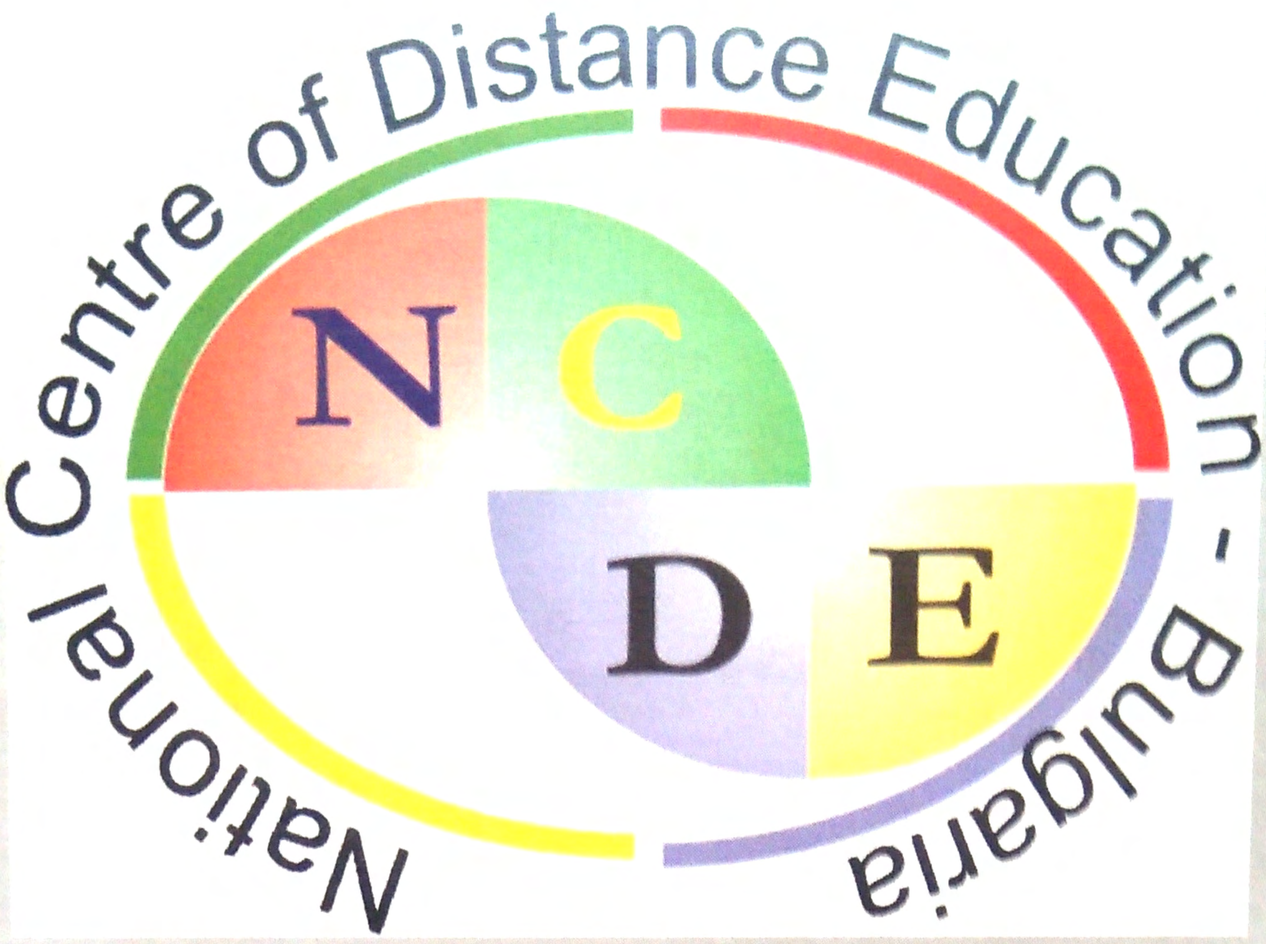
A MODEL INVESTIGATION OF NUCLEOBASE PARTICIPATION INTO NUCLEOSIDES INTERMOLECULAR HYDROGEN BONDS

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During the protein biosynthesis peptide bond formation in the ribosome interior is a key reaction for all living organisms. So far the mechanism of the process catalysed by ribosome remains non-revealed and our goal is to help in its understanding by computational model study of the hydrogen bond formation between nucleobases and methanol. In this way we investigate the possibility for general acid-base catalysis that could be important in the real system where proton-donor and proton-acceptor groups are positioned close to reaction centre. The obtained results lead to the conclusion that the hydrogen transfer occurs easiest in adenine.



ВТОРА НАЦИОНАЛНА КОНФЕРЕНЦИЯ ПО ЕЛЕКТРОННО ОБУЧЕНИЕ ВЪВ ВИСШЕТО ОБРАЗОВАНИЕ

14-16 септември 2006 г.
Китен

ДОКЛАДИ

MOLRAN

Мирослав А. Рангелов

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MolRan е софтуерен продукт, позволявящ визуализация, генериране и обработка на молекулни структури и анализ на техните свойства. Програмата може да работи директно с изходните файлове, получени от други програми като GAUSSIAN, GAMESS, MOPAC, PARAGAUSS, HYPERCHEM, и други. Поддържат се различни файлови формати, а възможността за пренастройка на модула за извличане на структури от текстови файлове позволява MolRan да ползва почти всички текстови файлови формати. MolRan работи с OpenGL графична машина, която позволява генерирането на различни типове висококачествени графични модели на молекулните структури, като получените графични структури могат да се обработят допълнително чрез използването на различни геометрични примитиви. Нови молекулни структури лесно могат да се генерират чрез 2D изчертаване, а приложените емпирични конструктори на молекулни модели и молекулната механика позволяват автоматичното им конвертиране в 3D-структури, които могат да бъдат записани в голям набор файлови формати и да бъдат използвани като входни файлове за други програми. Тази програма притежава голям набор от вградени инструменти, като инструментите за визуализация на траектории, изоконтурни повърхности, молекулни орбитали, електронна плътност, vdW повърхности, срязващи равнини, генератор на къси филмчета и др. Включеният в програмата вътрешен език може да помогне при конструирането на сложни структури. Програмата MolRan дава възможност за бърза обработка на големи набори от различни структури, клъстерен анализ на избрани геометрични свойства, сортиране на структурите по указани геометрични свойства и пр. MolRan може да изчислява положението на нови геометрични примитиви спрямо съществуващи обекти, да конвертира съществуващите примитиви едни в други и чрез пресметнатите геометрични примитиви дава възможност за разнообразни геометрични модификации на молекулните структури.

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Catalysis by Vicinal Hydroxyl in Formylribose Ammonolysis

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#Faculty of Chemistry, University of Sofia " Kliment Ohridski"; 1 James Bourchier Ave., Sofia 1126,Bulgaria; e-mail: gnv@chem.uni-sofia.bg

1,2-Diol monoester aminolysis is a fundamental chemical reaction, the iteration of which on the living cell ribosome results in protein biosynthesis. During elementary act of this peptide bond formation in the ribosome interior the growing polypeptide chain, esterified to cis-1,2-diol of tRNA 3'-terminal adenosine, reacts with the next amino acid in the ribosome peptidyltransfer center. In this hydrophobic ribosome interior the 2`-OH of tRNA the 3'-terminal adenosine is close to the bonds being cleaved and formed and can essentially influence the reaction rate. In order to clarify reaction mechanism and energetics it is necessary to check possible intermediates and transition states along different reaction paths but also to take into account the conformations of the transition states with lowest energy of each path. To complete this task we use the GAUSSIAN98W suite of programs, performing calculations on B3LYP level with 6-31++G** basis set, similarly to our previous study of monoacylated glycol ammonolysis [1].

We check two different types of concerted and stepwise mechanisms (Fig.1) and found that while TSc is not so sensitive to vicinal hydroxyl participation in proton transfer, energy decrease in TS1 and TS2 is capable to provide a very strong catalytic effect.

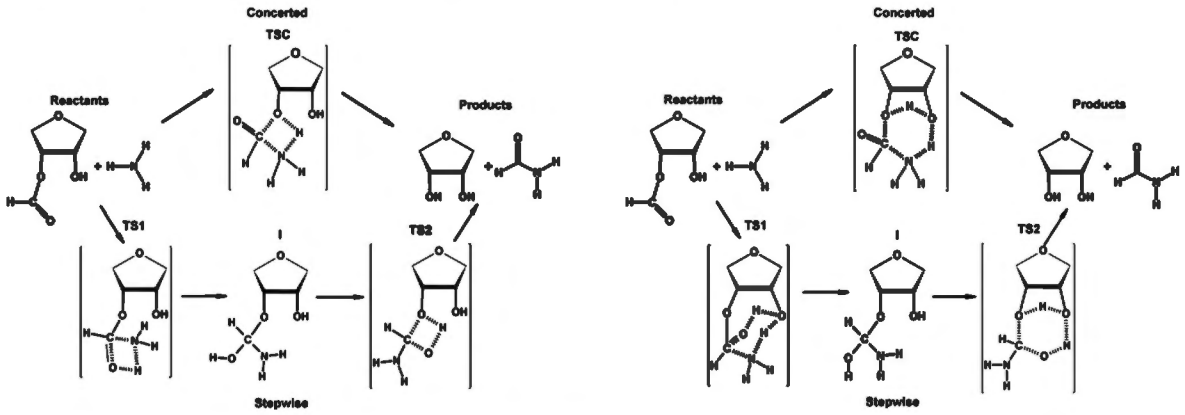


Fig.1 Mechanisms of formylribose ammonolysis

The work is partially supported by VUH-17/05 project of the Bulgarian National Science Fund.

1. M.A. Rangelov, G.N. Vayssilov, V.M. Yomtova, and D.D. Petkov *J.Am.Chem.Soc.* **128**, 4964 (2006).

MolRan program suite

Miroslav A. Rangelov

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MolRan is a tool for the visualization, generation and analysis of molecular structures and their chemical properties. This program can be used for display and analysis of molecular structures, and properties calculated with external programs, like GAUSSIAN, GAMESS, MOPAC, PARAGAUSS, HYPERCHEM, etc. Various predefined Z-matrix, Cartesian and Fractional file formats are supported and the file reader can be easily customized to read structural data from text files with other formats. MolRan has OpenGL graphic engine, which can produce different types of high quality graphic molecule representations and provides a lot of additional geometric primitives that can enrich the produced graphic. New structures can be generated simply by 2D drawing, then the implemented empirical model builder and molecular mechanics can produce a 3D structure that can be saved in wide variety of file types or input files for other programs.

The program has a lot of implemented tools which can plot molecular dynamics trajectories, isocontour surfaces of grid data, molecular orbitals, electron densities, vdW surfaces, cut planes through grid data sets as well as can be used to make short animations, etc.

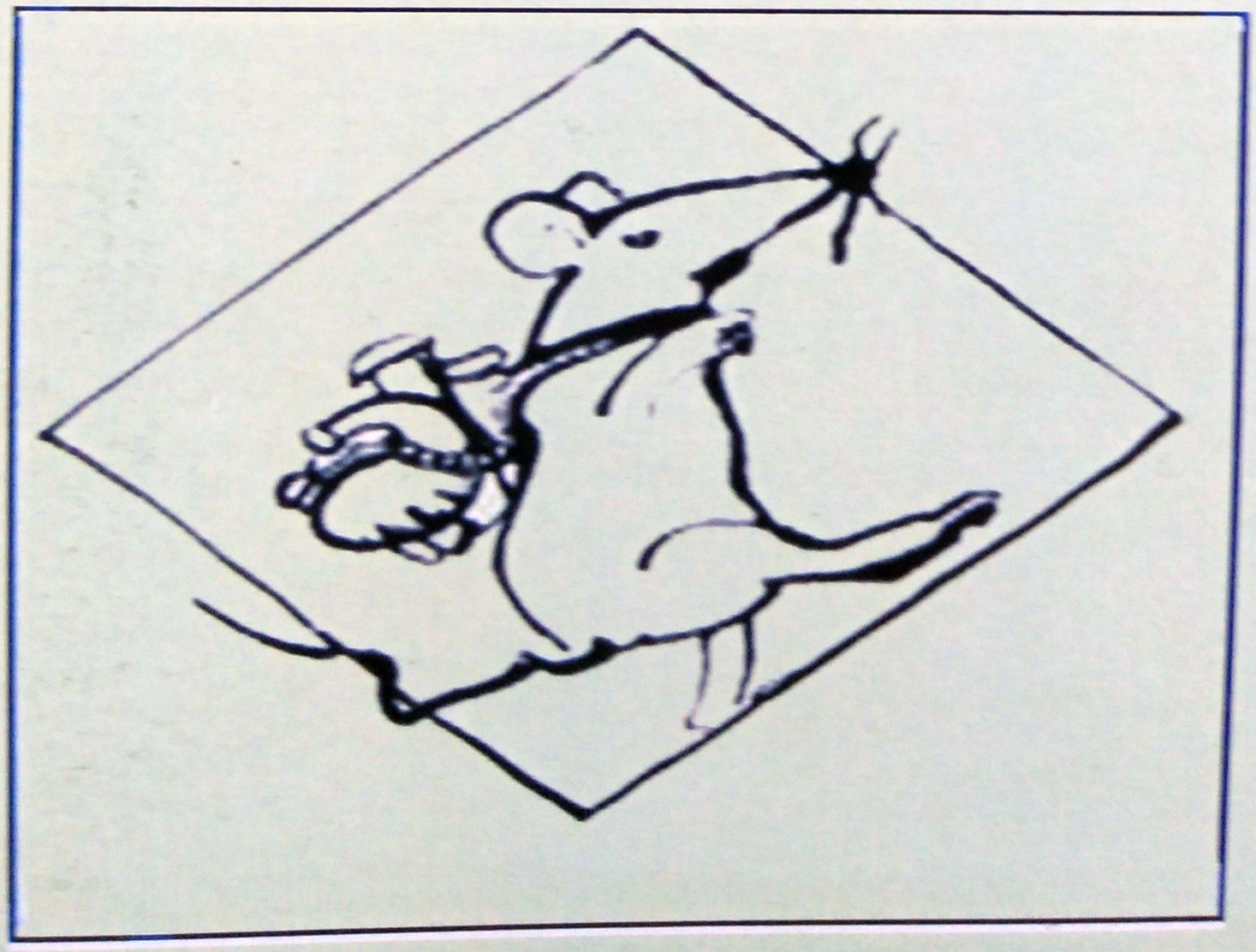
Implemented internal language interpreter can help in job file construction for conformational analysis and manipulations with periodic structures. The program MolRan has tools for fast multiple job file processing as similarity of structures calculation, cluster analysis of selected geometric properties, sorting by selected property, etc. It can calculate and draw as geometric primitives a lot of geometric properties of structures and can use calculated primitives for structure modification.

БЪЛГАРСКО ПЕПТИДНО ДРУЖЕСТВО

5ти БЪЛГАРСКИ ПЕПТИДЕН СИМПОЗИУМ

28-30 Май'08, Бачиново

НАУЧНА ПРОГРАМА И РЕЗЮМЕТА



P1

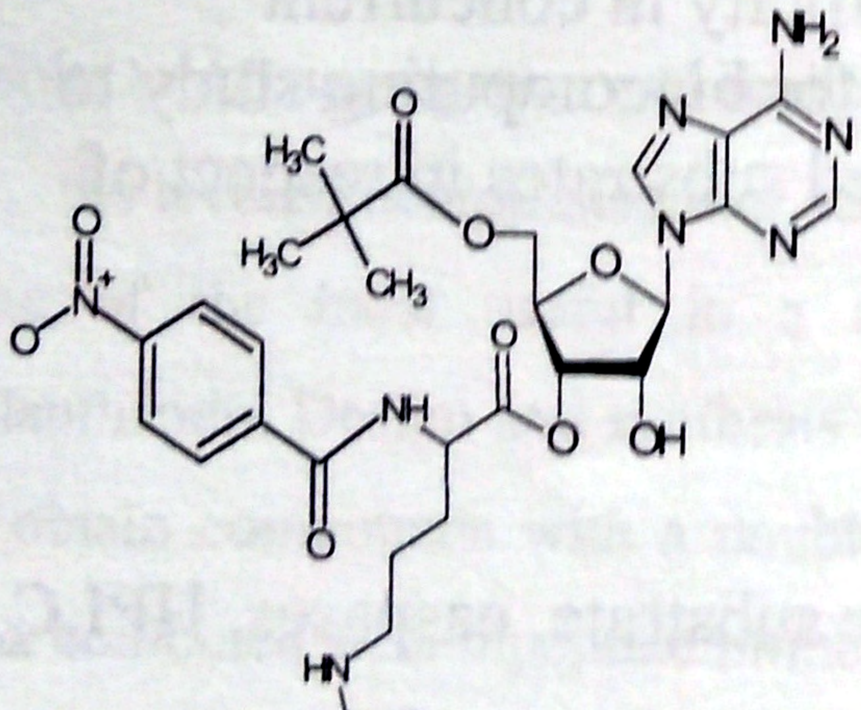
Design and Synthesis of Substrates for Model Ribosomal Reactions

Stanislav G . Bayryamov*, Nikolay G.Vassilev, Miroslav A. Rangelov, Aneta P.Mladjova and Dimiter D. Petkov

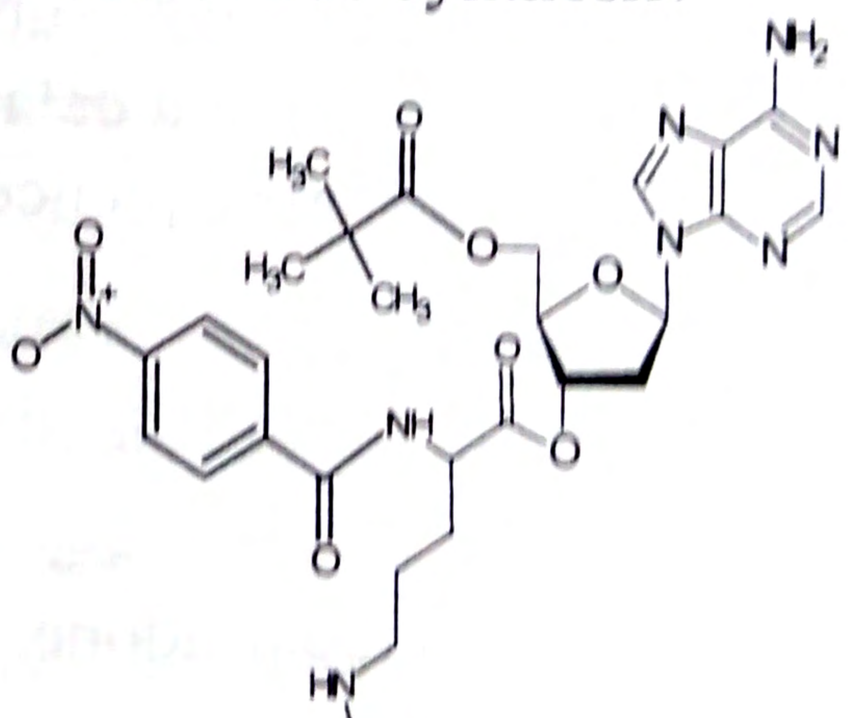
Laboratory of BioCatalysis, Institute of Organic Chemistry, Bulgarian Academy of Sciences, Sofia 1113, Bulgaria

Laboratory forNuclear Magnethic Resonance , Institute of Organic Chemistry, Bulgarian Academy of Sciences, Sofia 1113, Bulgaria

2'/3'-O-[2-N-p-nitrobenzoyl, 5-N-tert-butyloxycarbonyl-L-ornithinyl] 5'-O-pivaloyl adenosine: (2'/3'-O-[Bz(NO_2)-Orn(Boc)]-5'-O-Piv-Ado) [1] and its deoxy analog - 3'-O-[2-N-p-nitrobenzoyl, 5-N-tert-butyloxycarbonyl-L-ornithinyl] 5'-O-pivaloyl 2'-deoxy adenosine: (3'-O-[Bz(NO_2)-Orn(Boc)]-5'-O-Piv-2'-dAdo) [2] were synthesized as substrates for the model ribosome reaction we used to demonstrate the crucial role of A76 2'-OH of peptidyl-tRNA in the rate acceleration of peptide bond formation during protein biosynthesis (J.Amer.Chem. Soc. 129(2007)5790-5791). These ornithinyl nucleosides/adenosines were synthesized using suitable combinations of the methods of peptide, nucleoside and nucleotide synthesis.



[1]



[2]

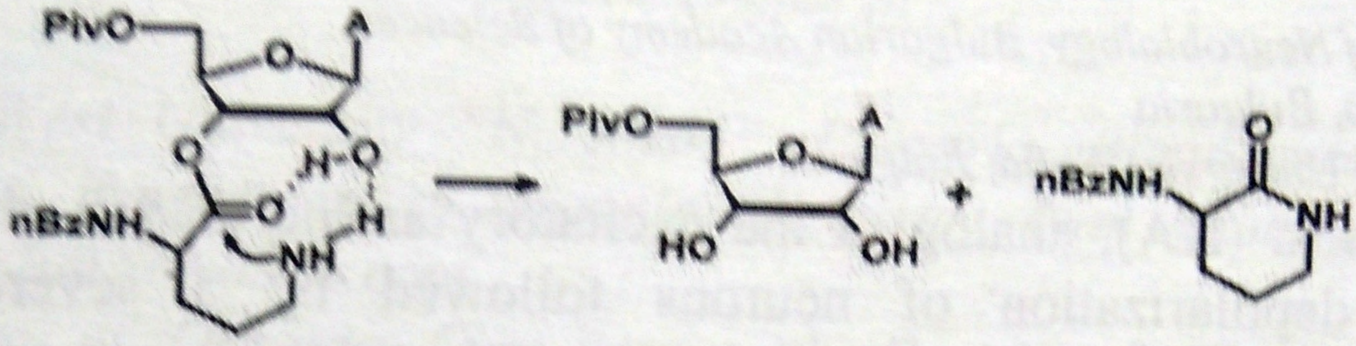
Further study using this model compounds was the first unambiguous experimental demonstration of chemical catalysis of the 1,2-diol monoester aminolysis by its vicinal 2-OH group – the reaction naturally catalyzed by ribosome.

P4

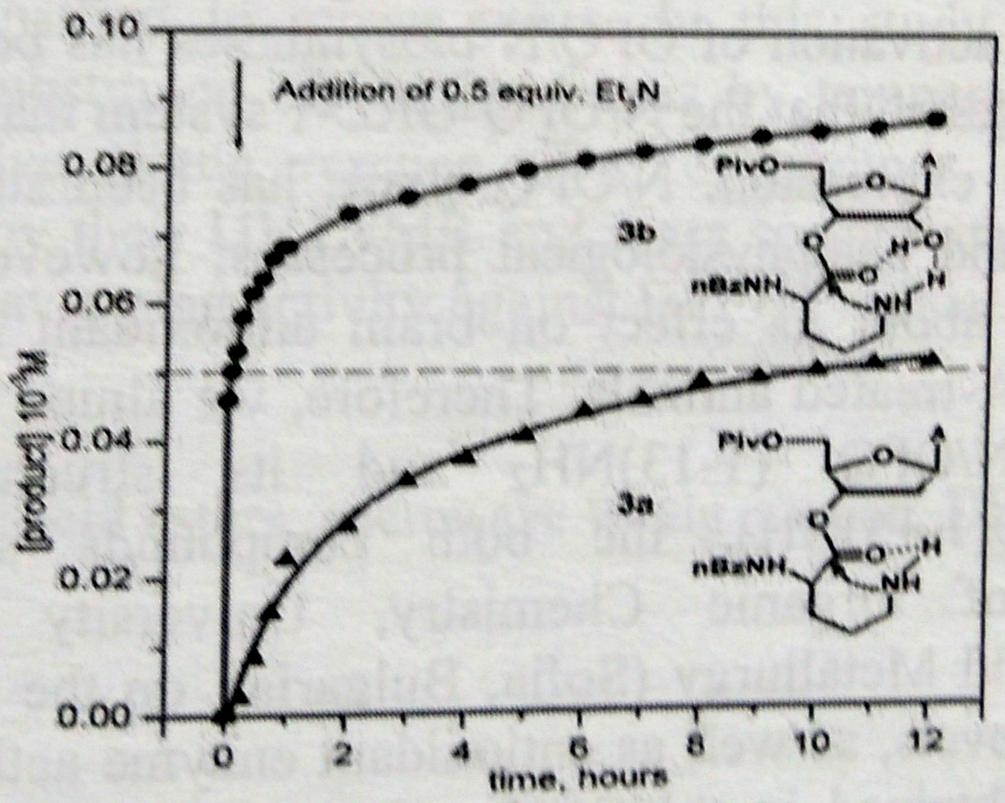
Unambiguous Evidence for Efficient Chemical Catalysis of Adenosine Ester Aminolysis by Its 2'/3'-OH

Stanislav G . Bayryamov, Miroslav A.Rangelov, Aneta P. Mladjova, Vihra Yomtova, and Dimiter D. Petkov*

Laboratory of BioCatalysis, Institute of Organic Chemistry, Bulgarian Academy of Sciences, Sofia 1113, Bulgaria



Intramolecular aminolysis reactions, catalyzed by vicinal OH group, were studied computationally as model reactions of ribosome-catalyzed intracomplex aminolysis. The results predicts 2-6-fold higher enthalpic than entropic contribution to the reduction of the activation free energy, caused by the combined proximity effect of the attacking syn-NH_2 group and the catalytic syn-OH group. The acceleration predicted by the theory is supported by the observed instantaneous lactamization of ornithinyl adenosine as compared to the much slower lactamization of ornithinyl 2'-deoxyadenosine. This observation is the first unambiguous experimental demonstration of chemical catalysis of the 1,2-diol monoester aminolysis by its vicinal 2-OH group – the reaction naturally catalyzed by ribosome.



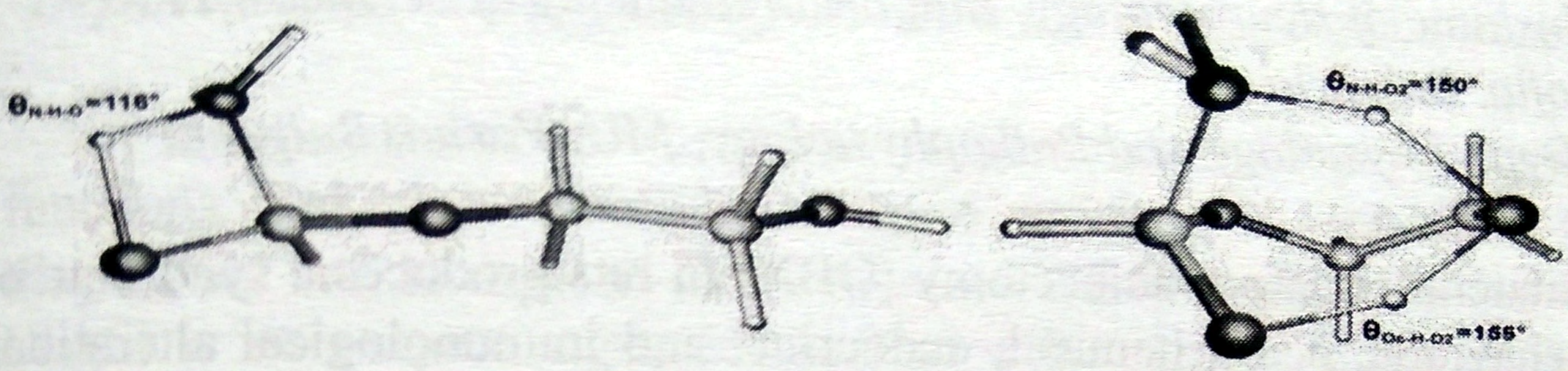
Time course of the intramolecular aminolysis (lactamization) in acetonitrile at 25 °C of 0.1 mmole trifluoroacetate of 2'/3'-O-(α-N-p-nitrobenzoyl ornithinyl) 5'-O-pivaloyl adenosine 3b and deoxyadenosine 3a to α-N-p-nitrobenzoyl cyclic ornithine-after addition of ½ eqv of Et_3N.

P8

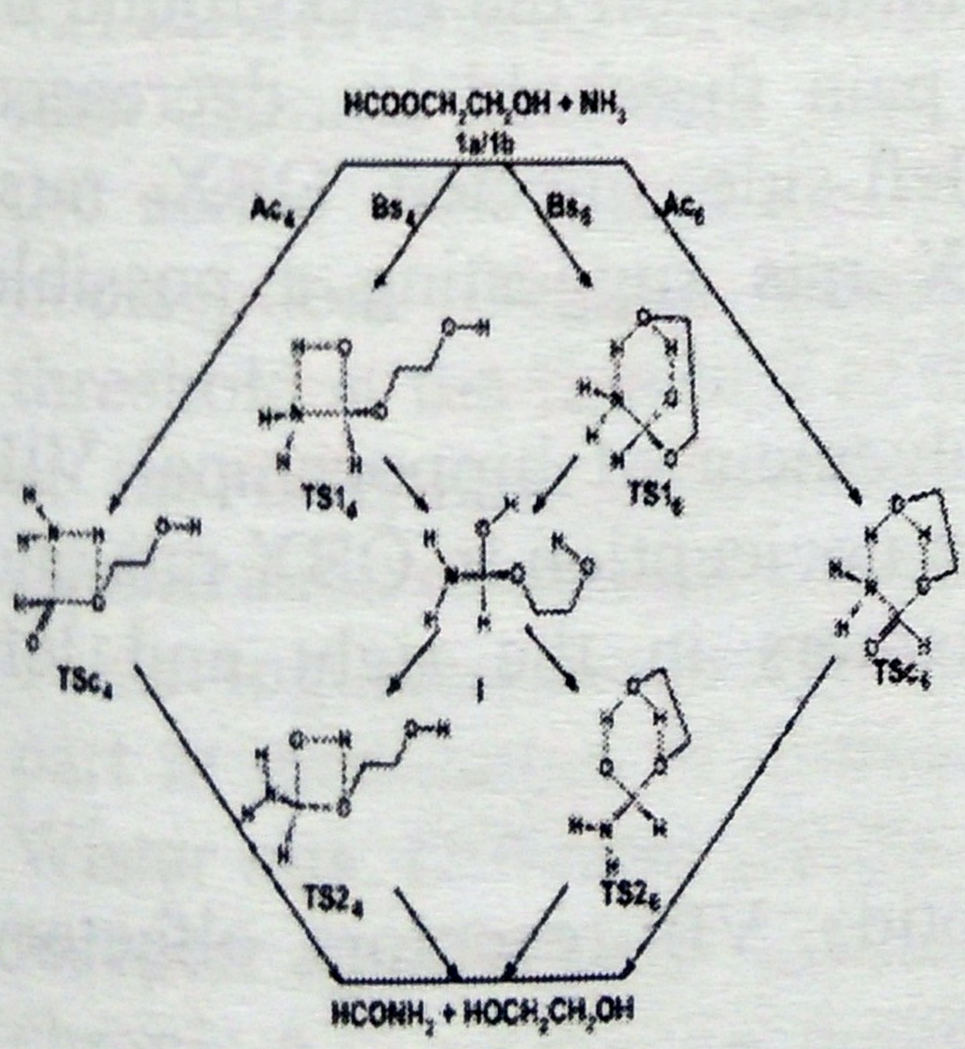
Catalysis of the proton transfer by a vicinal hydroxyl group

Miroslav A. Rangelov, Georgi N. Vayssilov, Vihra M. Yomtova and Dimiter D. Petkov*

Laboratory of BioCatalysis, Institute of Organic Chemistry, Bulgarian Academy of Sciences, 1113 Sofia and Faculty of Chemistry, University of Sofia "St Kliment Ohridsky". 1126 Sofia, Bulgaria



A computational study of 1-formyl 1,2-ethanediol aminolysis predicts a step-wise mechanism involving syn 2-OH-assisted proton transfer. The syn-oriented-2-OH takes over the catalytic role of the external water or amine molecule previously observed in 2-deoxy ester aminolysis. It provides more favorable, that is more linear proton transfer geometry for the rate-limiting transition state resulting in an almost billion-fold rate acceleration of the overall reaction. The findings provide structural basis for the explanation of the efficiency of the proton shuttling mechanism and implies double proton transfer catalysis by peptidyl tRNA A76 2'-OH as a possible catalytic strategy used by ribosome.



Sheme 1. Proposed mechanisms of aminolysis of 1- O-formyl 1,2-ethanediol with anti- (**Ac_4** and **Bs_4**) and syn- (**Ac_6** and **Bs_6**) oriented 2-OH.

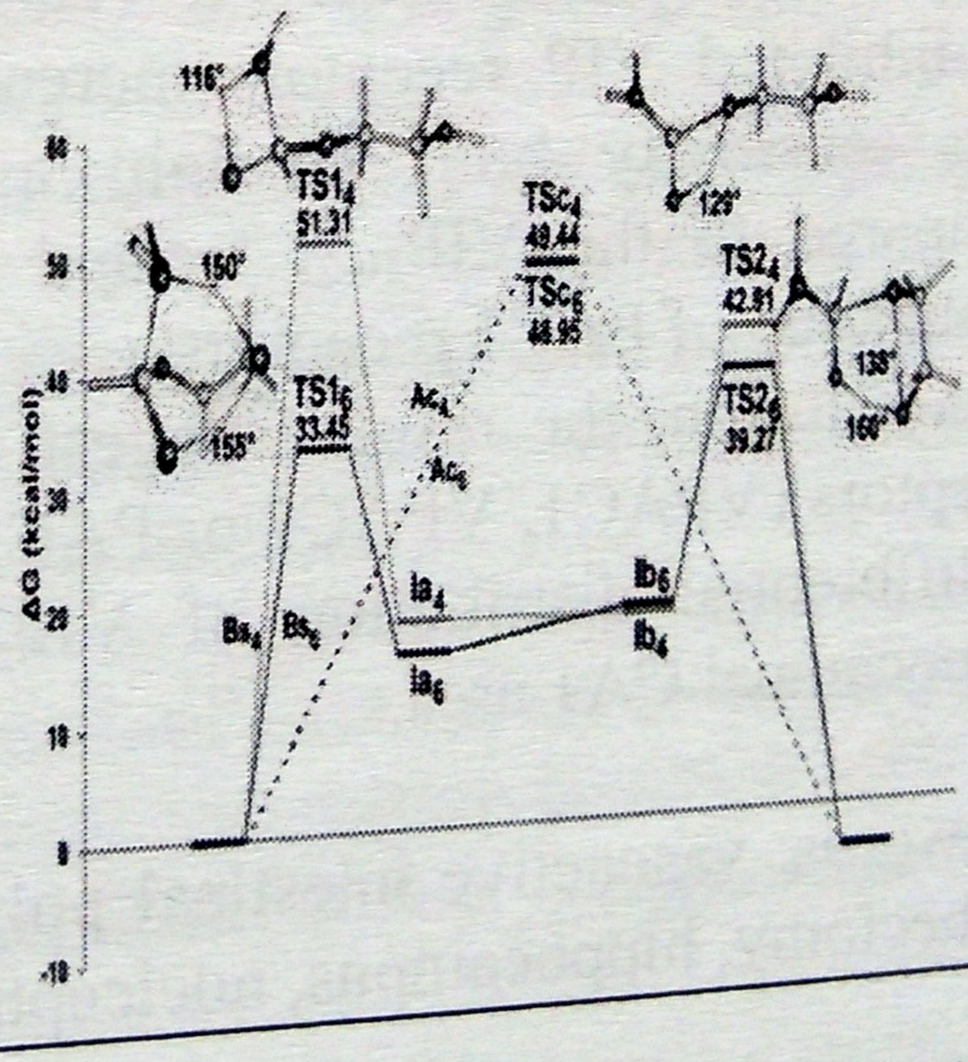


Figure 1. Energy profiles and transition state structures for concerted (dotted line) and stepwise (solid line) mechanisms of the aminolysis of conformers of 1-O-formyl 1,2-ethanediol with an anti- (light line) and syn- (heavy line) oriented 2-OH.

12TH INTERNATIONAL CONFERENCE ON THEORETICAL ASPECTS OF CATALYSIS

ICTAC-12

Varna, Bulgaria

25 – 29 June 2008

BOOK OF ABSTRACTS

PROGRAM

LIST OF PARTICIPANTS

Sofia, 2008

Construction of Catalytic Maps

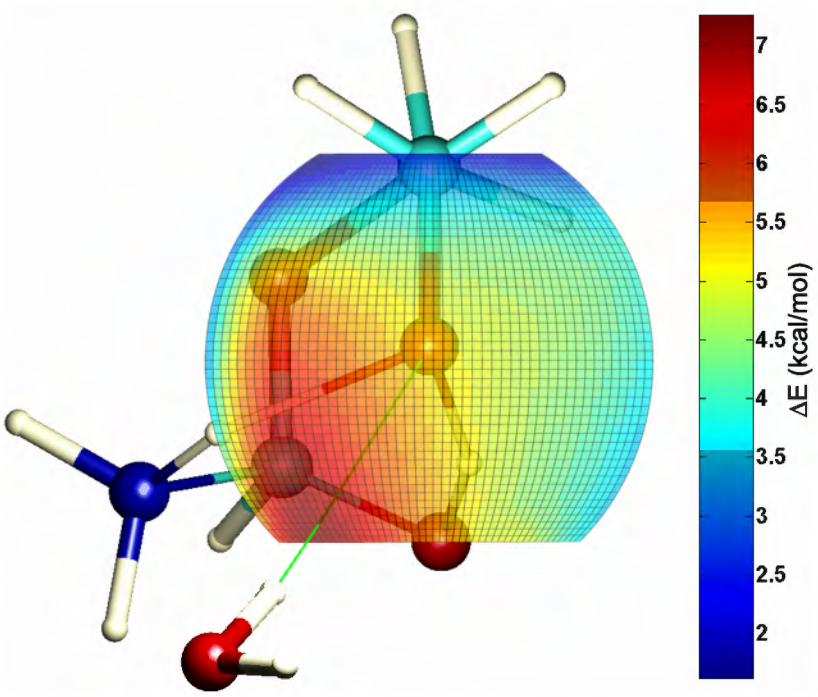
Miroslav A. Rangelov[1], Georgi N. Vayssilov[2]

[1] *Bulgarian Academy of Sciences, Institute of Organic Chemistry, 1113 Sofia, Bulgaria*

[2] *University of Sofia, Faculty of Chemistry, 1126 Sofia, Bulgaria*

One of significant challenges in biocatalysts is to estimate noncovalent influence of chemical groups placed in adjacent position to atoms that participate in bond forming and breaking at the active sites in enzymes or ribozymes. One possible approach for elucidating of this effect is to calculate the energy for the noncovalent interactions of such adjacent group with the atoms involved in bond breaking and forming in the transition states with respect to the reactant. Graphical representation of such energy difference (shown below) can be considered as "a catalytic map" since it shows from which position the side group will have the highest stabilization effect on the transition state and can be used in interpretation of influence of groups in vicinity of the active site as well as in construction of teozymes and compuzymes[1].

Here we report the results obtained by this approach on formylethanediole ammonolysis. In this reaction effect of the vicinal hydroxyl group is approximated with an water molecule.



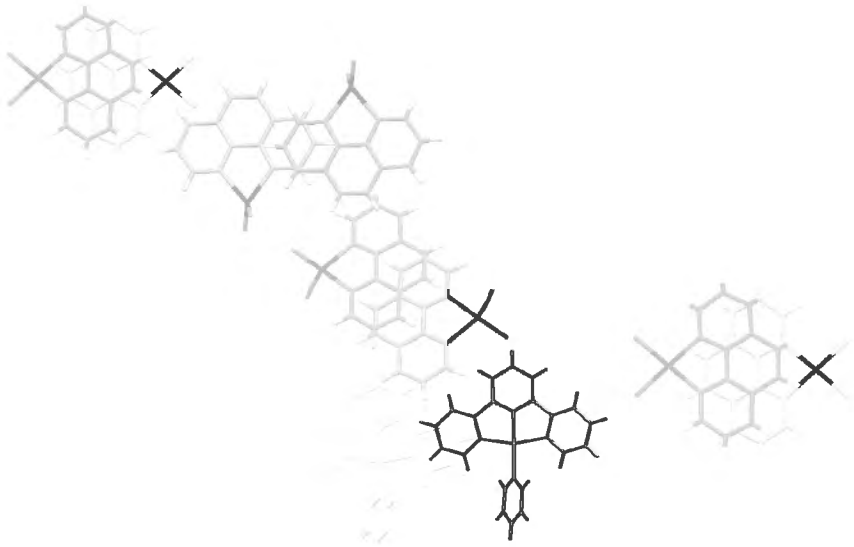
$$E_{cat} = (E_{TS+H2O} - (E_{TS} + E_{H2O})) - (E_{initial+H2O} - (E_{initial} + E_{H2O}))$$

Catalytic map of one of the transition states for formylethanediole ammonolysis.

[1] Tantillo, D.J., Chen, J., Houk, K.N *Current Opinion in Chemical Biology* **2** 743-750

SECOND HUMBOLDT CONFERENCE ON NONCOVALENT INTERACTIONS

Vršac, Serbia
October 22-25, 2009



BOOK OF ABSTRACTS

Computational modeling of the influence of hydrogen bonding and proton transfer on protein biosynthesis in ribosome

Miroslav A. Rangelov[a] and Georgi N. Vayssilov[b]

[a] *Laboratory of BioCatalysis, Institute of Organic Chemistry, Bulgarian Academy of Sciences, Sofia 1113, Bulgaria e-mail: mran@orgchm.bas.bg*

[b] *Faculty of Chemistry, University of Sofia "St. Kliment Ohridski"; 1, James Bourchier Ave., Sofia 1126, Bulgaria; e-mail: gnv@chem.uni-sofia.bg*

The aim of the study is elucidation of the influence of different types of hydrogen bonds and proton transfer processes on the mechanisms of protein biosynthesis in ribosome by studying congruent model systems. Initially, we used formylethanediol model as the obtained results showed its applicability to the studied processes.[1] Due to its small size and the ease of handling, the model allows numerous computational experiments for specifying small effects on the reaction rate. However, the most substantial disadvantage of this model is the exclusion of the ribosomal ring at 3' end adenosine from it. Thus, in order to define the influence of the vicinal hydroxyl in the reaction of ammonolysis in a system closer to the real one, the monoformylated tetrahydrofurane-3,4-diol is a felicitous choice for a substrate in a more precise model system (Fig. 1).

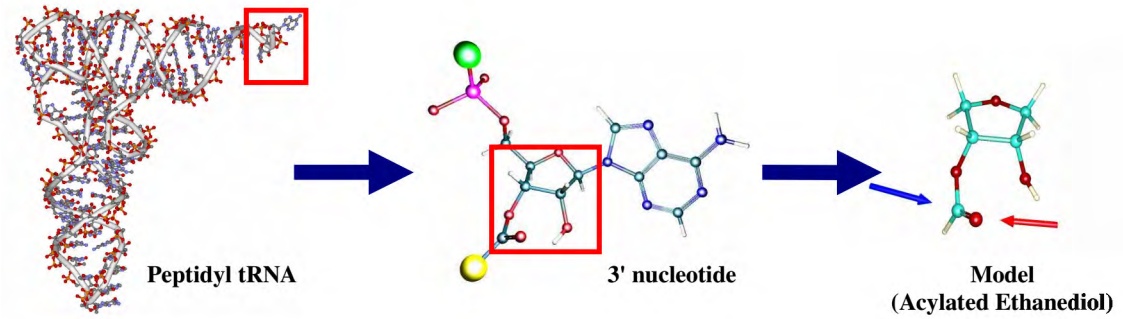


Figure 1. Defining the model system that will be applied in the simulation of the ammonolysis process.

The investigation is supported by project DVU-191 with Bulgarian National Science Fund.

1.Rangelov, M.A., Vayssilov, G.N., Yomtova, V.M., Petkov, D.D, *J. Am. Chem. Soc.* (2006), **128,** 4964 .

A MODEL INVESTIGATION OF NUCLEOBASE PARTICIPATION INTO NUCLEOSIDES INTERMOLECULAR HYDROGEN BONDS

Miroslav A. Rangelov,[a] Petko St. Petkov,[b] Galina P. Petrova,[b] and Georgi N. Vayssilov[b]

[a] *Laboratory of BioCatalysis, Institute of Organic Chemistry, Bulgarian Academy of Sciences, Sofia 1113, Bulgaria e-mail: mran@orgchm.bas.bg*

[b] *Faculty of Chemistry, University of Sofia "St. Kliment Ohridski"; 1, James Bourchier Ave., Sofia 1126, Bulgaria; e-mail: gnv@chem.uni-sofia.bg*

During the protein biosynthesis peptide bond formation in the ribosome interior is a key reaction for all living organisms. So far the mechanism of the process catalysed by ribosome remains non-revealed. It is mainly due to obscurity in the chemical processes mechanism and the ways for catalysis of that reaction in the ribosome interior. Because of proton donor and proton acceptor positioned close to reaction centre. Because of the possibility for general acid base catalysis it is important to know their ability for hydrogen bonding. In this study we calculate lengths and energies of hydrogen bonds between nucleobases and methanol or water.

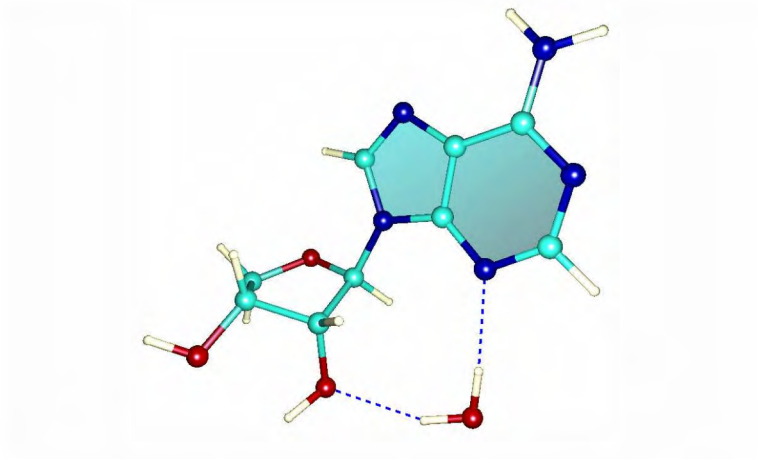


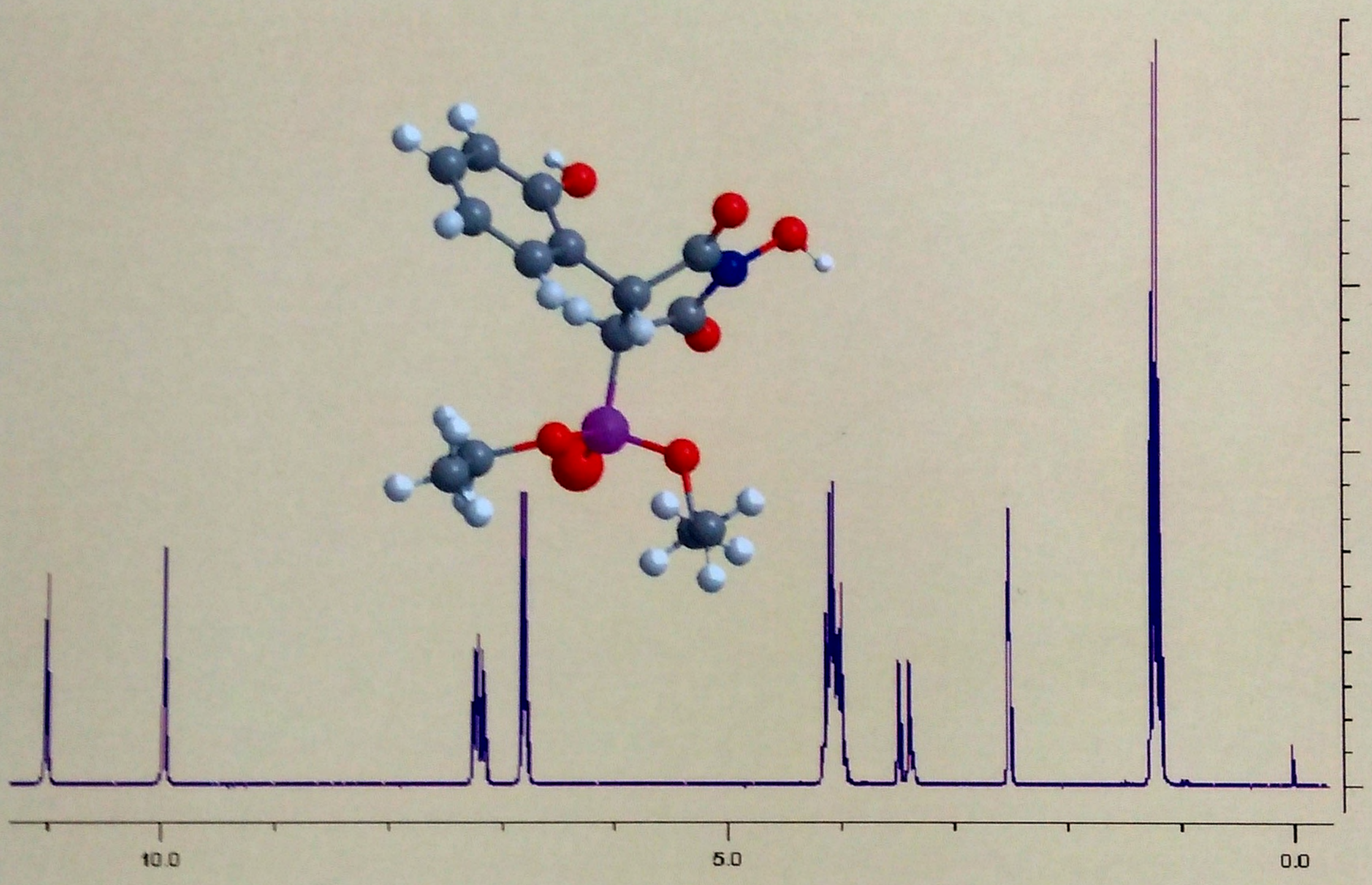
Fig. 1. Optimised structure for formation of hydrogen bonds of water molecule with nucleoside.

The investigation is supported by project DVU-191 with Bulgarian National Science Fund.

THIRD INTERNATIONAL SYMPOSIUM ON ORGANIC CHEMISTRY

WITH SATELLITE MEETING ON

NMR IN LIFE SCIENCES



Sofia, Bulgaria
30 October – 2 November 2010

BOOK OF ABSTRACTS

Avangard Prima
Sofia, 2010

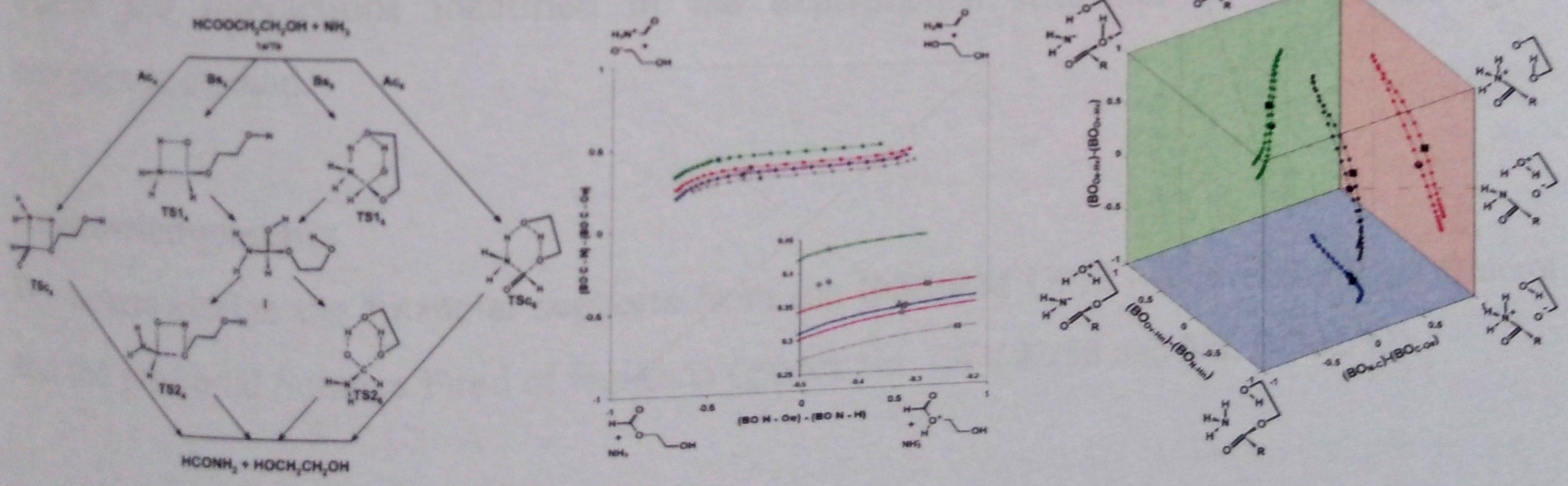
Hydrogen Bond σ-Cooperativity in the Ribosome Proton Shuttling Catalysis

Miroslav A. Rangelov[(a)], Georgi N. Vaissilov[(b)]

(a) Laboratory of BioCatalysis, Institute of Organic Chemistry, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria e-mail: mran@orgchm.bas.bg

(b) Faculty of Chemistry, University of Sofia, 1126 Sofia, Bulgaria

Understanding of the nature of the ribosome catalysis is still a challenge of both chemists and chemical/molecular biologists.[1] This high catalytic proficiency of the ribosome has been recently attributed to the proton shuttling role of the crucial peptidyl tRNA A76 2'-OH. In recent computational studies[2] of the proton shuttle mechanism we predicted that syn-oriented 2-OH provided a favourable proton transfer geometry in 2-hydroxyalkyl ester aminolysis, a reaction naturally catalyzed by the ribosome. There we come to the conclusion this is a necessary but not sufficient condition that can account for the ribosome catalytic efficiency. Here we show that the two hydrogen bonds of the proton shuttling system are charge assisted and act cooperatively to provide transition state stabilization and dramatic rate acceleration of the aminolysis reaction. The last can be seen from computed More-O'Ferral-Jencks diagrams of these reactions.



References

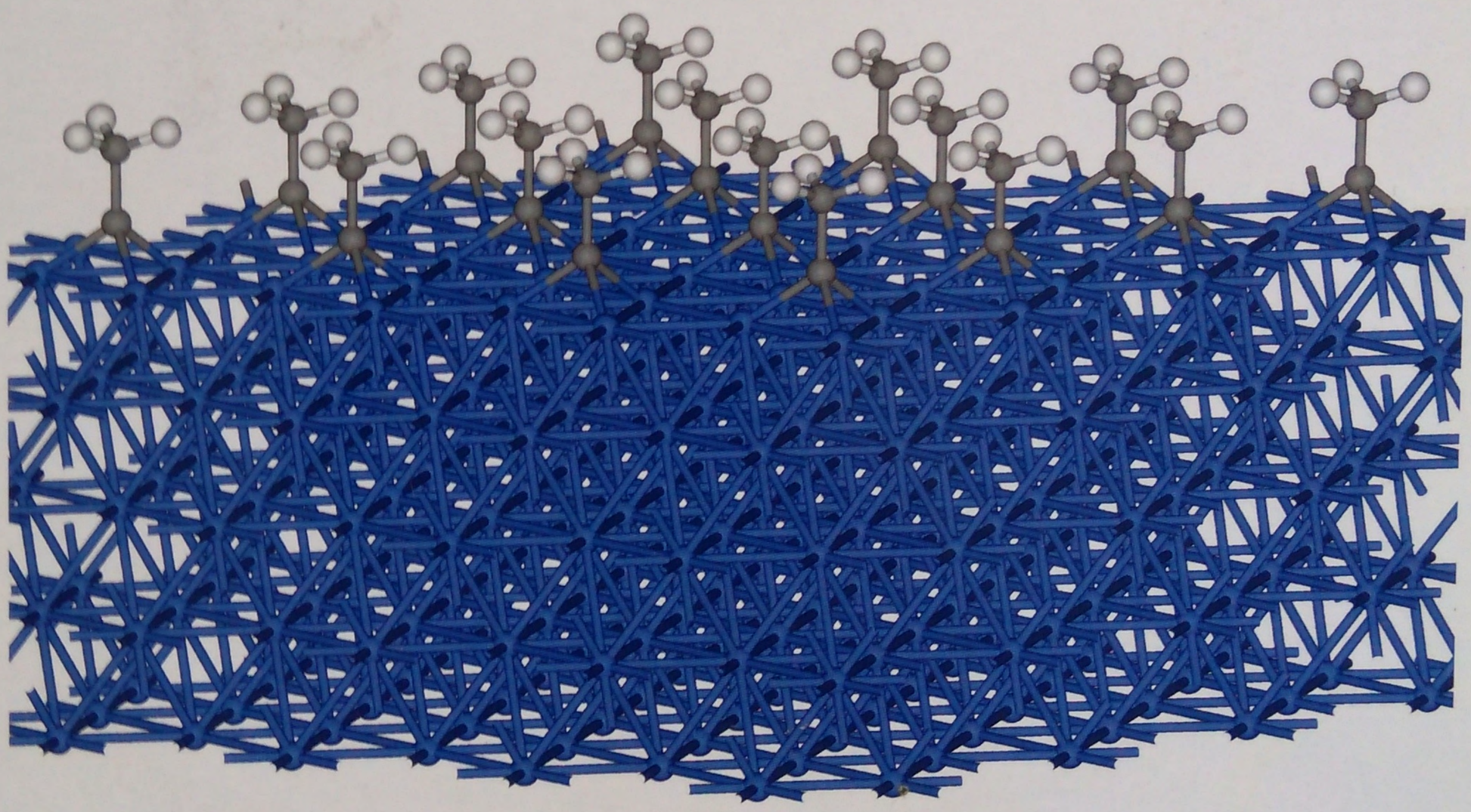
[1] M. Beringer M.V. Rodnina, *Mol. Cell* **2007**, *26*, .311-321

[2] a) M. A. Rangelov, G. N. Vayssilov, V. M. Yomtova, D. D. Petkov,, *J. Am. Chem. Soc.* **2006**, *128*, 4964-4965; b) S. G. Bayryamov, M. A. Rangelov, A. P. Mladjova, V. M. Yomtova, D. D. Petkov, *J. Am. Chem.Soc.* **2007**, *129*, 5790-5791

Fourth Humboldt Conference on

Computational Chemistry

Varna, Bulgaria
12–15 July 2010



BOOK OF ABSTRACTS
PROGRAM
LIST OF PARTICIPANTS

Varna, 2010

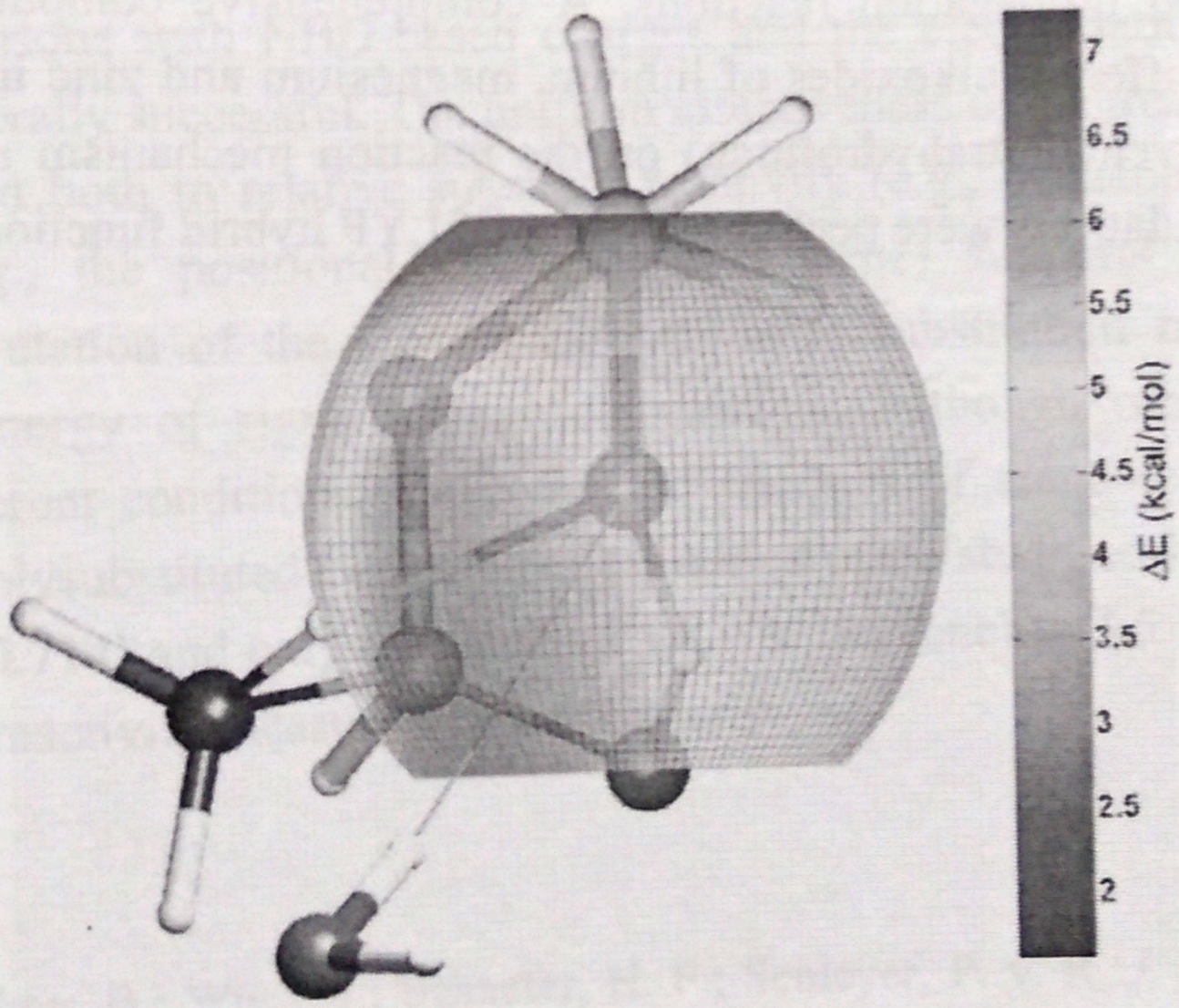
Alexander von Humboldt
Stiftung/Foundation

CONSTRUCTION OF CATALYTIC MAPS

Miroslav A. Rangelov[1], Georgi N. Vayssilov[2]

[1] *Bulgarian Academy of Sciences, Institute of Organic Chemistry, 1113 Sofia, Bulgaria*
[2] *University of Sofia, Faculty of Chemistry, 1126 Sofia, Bulgaria*

One of significant challenges in biocatalysts is to estimate noncovalent influence of chemical groups placed in adjacent position to atoms that participate in bond forming and breaking at the active sites in enzymes or ribozymes. One possible approach for elucidating of this effect is to calculate the energy for the noncovalent interactions of such adjacent group with the atoms involved in bond breaking and forming in the transition states with respect to the reactant. Graphical representation of such energy difference (shown below) can be considered as "a catalytic map" since it shows from which position the side group will have the highest stabilization effect on the transition state and can be used in interpretation of influence of groups in vicinity of the active site as well as in construction of teozymes and compuzymes[1]. Here we report the results obtained by this approach on formylethanediole ammonolysis. In this reaction effect of the vicinal hydroxyl group is approximated with an water molecule.



$$E_{cat} = (E_{TS+H2O} - (E_{TS} + E_{H2O})) - (E_{initial+H2O} - (E_{initial} + E_{H2O}))$$

Catalytic map of one of the transition states for formylethanediole ammonolysis

Acknowledgements

The work was supported by Bulgarian National Fund for Scientific Research (contracts DOO2-133 and DOO2-210).

References:

[1] Tantillo, D.J., Chen, J., Houk, K.N *Current Opinion in Chemical Biology* 2 743-750.

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The 11th International Chemistry Conference and Exhibition in Africa

(11 ICCA)



Luxor, Egypt

Organized by

Chemistry Department, Faculty of Science, Sohag University

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African Association of Pure and Applied Chemistry

P67-III

Computational modeling of the catalytic role of the vicinal hydroxyl in ribose as proton mediator in protein biosynthesis

Miroslav A. Rangelov[1], Hristiyan A. Aleksandrov[2], Petko St. Petkov[2], Galina P. Petrova[2], Vihra M. Yomtova[1], Georgi N. Vayssilov[2]

Laboratory of BioCatalysis, Institute of Organic Chemistry, Bulgarian Academy of Sciences, Sofia 1113, Bulgaria

mran@orgchm.bas.bg

Faculty of Chemistry, University of Sofia "St. Kliment Ohridski" 1, James Bourchier Ave., Sofia 1126, Bulgaria

gnv@chem.uni-sofia.bg

Abstract:

In extension of our previous investigations[1], the present computational model study evaluates the influence of the vicinal OH group in acylated 2'-acylated THF-2',3'-diol on the reaction paths for ester ammonolysis. Two alternative approaches for this influence were considered – stabilization of the (tetragonal) transition states along the reaction path via hydrogen bonds and participation of the vicinal hydroxyl in proton transfer (proton shuttle mechanism). The calculations are performed with the hybrid B3LYP functional with 6-31++G** basis set. The catalytic activation of the ester ammonolysis by a hydrogen bond from the vicinal hydroxyl via tetragonal transition states, occurring preferably via concerted mechanism, was found to be rather modest, the free energy of activation is reduced by less than 6 kcal/mol. The reason for this weak catalytic effect is the rather small proton transfer angles in the transition states, below 130°, much smaller than the optimal angle of 180°. The other mechanism of catalytic activation of the process - by participation of the vicinal hydroxyl in the proton transfer via hexagonal transition states stabilizes considerably the first transition state of the stepwise mechanism, the Gibbs free energy of activation is reduced by 18.2 kcal/mol with respect to the referent value without vicinal OH group. The main reason for this effect is the replacement of single unfavorable proton transfer in $TS1^4$ by two favorable proton transfers in $TS1^6$ that decreases the angular distortions for the proton transfers. The decrease of the free energy of activation due to the more favorable structure of the transition states corresponds to about 10^{10}-fold acceleration of the reaction with respect to the non-catalyzed process, in agreement with the experimental estimate.

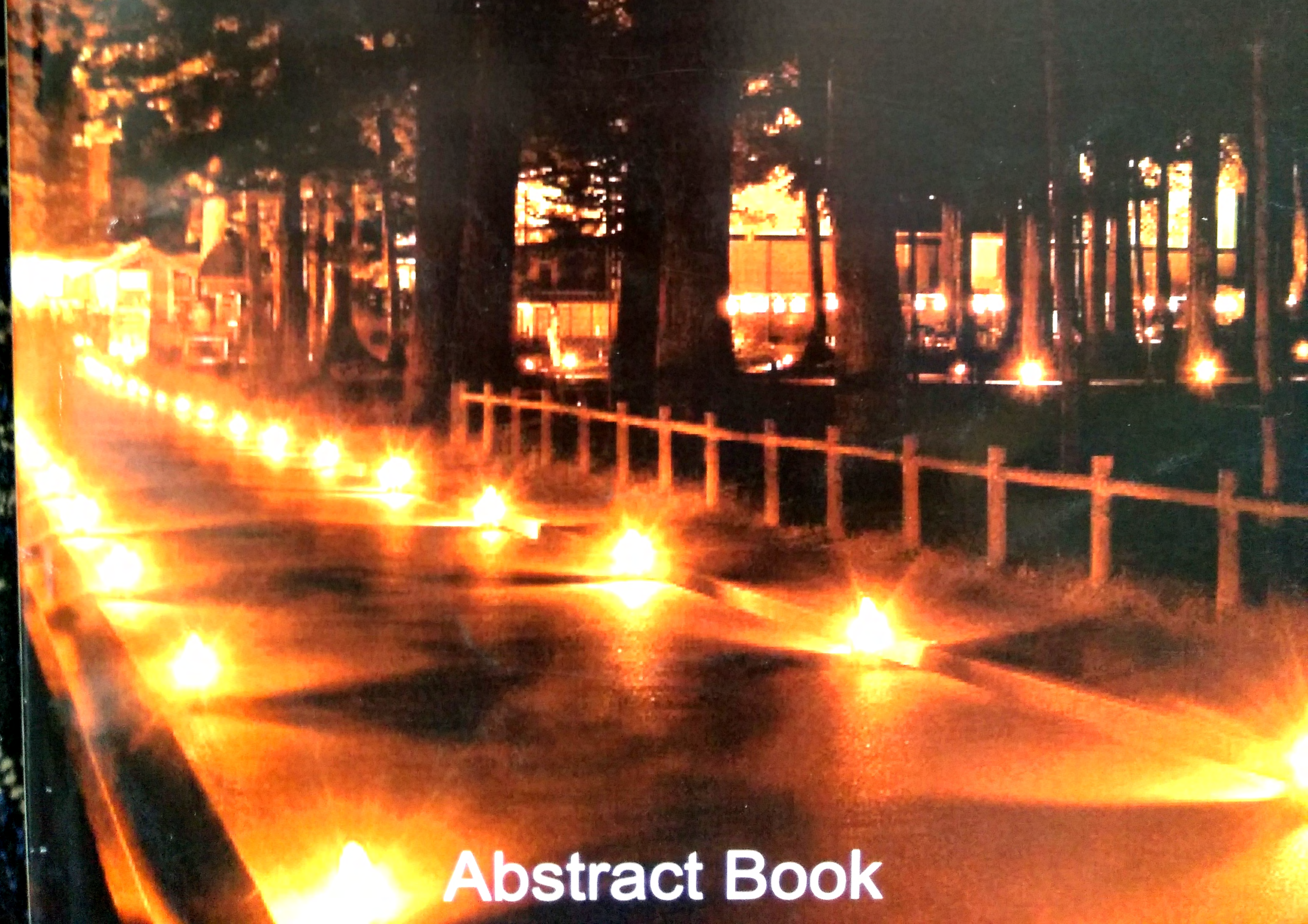
The financial support from NSF-Bulgaria (DO 02-133/2008 and SuperCA+ projects) is gratefully acknowledged.

Reference:

1. Rangelov, M. A.; Vayssilov, G. N.; Yomtova, V. M.; Petkov, D. D. J. Am. Chem. Soc. 2006, 128, 4964.

13th International Conference on Theoretical Aspects of Catalysis

Matsushima Ichinobo Hotel, Japan
June 21 - 25, 2010



Abstract Book

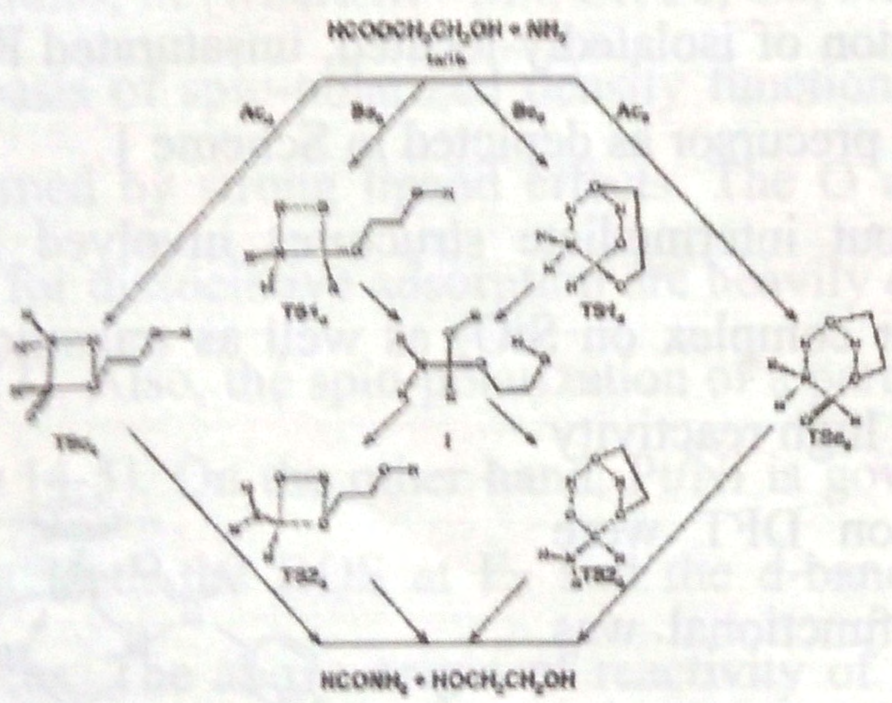
3P24

Hydrogen Bond σ-Cooperativity in the Proton Shuttling Catalysis Used by the Ribosome

Miroslav A. Rangelov[(a)], **Georgi N. Vaissilov**[(b)]

(a) Laboratory of BioCatalysis, Institute of Organic Chemistry, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria
(b) Faculty of Chemistry, University of Sofia, 1126 Sofia, Bulgaria; e–mail: gnv@chem.uni–sofia.bg

The high catalytic proficiency of the ribosome has been attributed to the H^+ shuttling role of the crucial peptidyl tRNA A76 2'-OH [1]. Recently, we predicted computationally [2] that 2-OH provided a favourable H^+ transfer geometry in 2-hydroxyalkyl ester aminolysis (Fig. 1), a reaction naturally catalyzed by the ribosome. This was found a necessary but not sufficient condition that can account for the ribosome catalytic efficiency. Here we show that the two hydrogen bonds of the H^+ shuttling system are charge assisted and act cooperatively to provide transition state stabilization and dramatic acceleration of the reaction.



The strongest ever known hydrogen bonds are the charge-assisted ones like A+-H…B and A-H…B-. A large increase of the hydrogen bond energy is also reported when a bridging OH group simultaneously donates and accepts hydrogen bonds. We extended these ideas towards the mechanism of the ribosome catalysis. As the attack of the amine group towards the carboxyl Cc progresses, the amine N acquires an increasing positive charge and the carbonyl oxygen Oc - an increasing negative charge. This charging strengthens the existing hydrogen bonds between amine, vicinal OH, and Oc. As a consequence, the geometry of the reaction ring changes to a structure facilitating the proton transfer via spontaneous H^+ transfers which driving force is generated charge during amine attack. Thus, the mechanism of the 2-hydroxyalkyl ester aminolysis can be considered as enforced concerted mechanism.

The financial support from NSF Bulgaria (DOO2-133, DOO2-210) and the Center of excellence for supercomputer applications is gratefully acknowledged.

[1] M. M. Changalov et al. *ChemBioChem* **2005**, *6*, 972-977.

[2] M. A. Rangelov et al. *J. Am. Chem. Soc.* **2006**, *128*, 4964-4965.

Tetra-Alkoxy Substituted PPV Derivatives: A New Class of Highly Soluble Liquid-Crystalline Conjugated Polymers

J. Vandenbergh[1], I. Van Severen[1], L. Lutsen[2], P.J. Adriaensens[1], H.J. Bolink[3], T.J. Cleij[1] and D.J.M. Vanderzande[1,2]

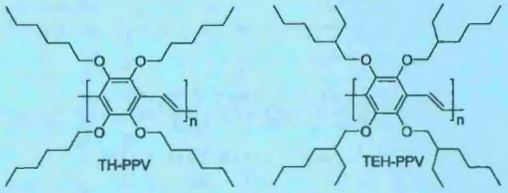
[1]Institute for Materials Research (IMO), Hasselt University, Universitaire Campus, Agoralaan Building D, B-3590 Diepenbeek, Belgium
[2]Division IMOMEC, IMEC, Universitaire Campus, Wetenschapspark 1, B-3590 Diepenbeek, Belgium
[3]Instituto de Ciencia Molecular (ICMol), Universidad de Valencia, P.O. Box 22085, 46071 Valencia, Spain

Poly(*p*-phenylene vinylene) (PPV) and related polymers exhibit numerous attractive optical and electronic properties, which make them interesting candidates for applications, such as organic light emitting diodes (OLEDs), organic field effect transistors (OFETs), (bio)sensors and photovoltaic cells. Considerable interest exists in the development of novel PPV-type polymers, which combine good luminescence properties with improved charge carrier densities. To this end, various approaches have been presented in the literature, which in most cases focus on the development of materials with increased stacking and ordering phenomena. Many of these research efforts focus on a large variety of 2,5-alkoxy substituted PPV-derivatives.

We became interested in the synthesis and optoelectronic properties of tetra-alkoxy substituted PPV derivatives, since they have an inherently regioregular nature and potentially have a favorable geometry for intra- and intermolecular ordering phenomena. Our attention focused on the development of a versatile route towards soluble tetra-alkoxy substituted PPV-derivatives.

Here we present such a route as well as the synthesis and full characterization of the first two examples of highly soluble tetra-alkoxy substituted PPV-derivatives, *i.e.* poly(2,3,5,6-tetrahexyloxy-1,4-phenylene vinylene) (TH-PPV) and poly[2,3,5,6-tetra(2'-ethyl-hexyloxy)-1,4-phenylene vinylene] (TEH-PPV). Furthermore, the solubility and UV-Vis absorption characteristics of TH-PPV and TEH-PPV in various solvents with different polarities have been studied. Observations from polarized light microscopy (PLM) and differential scanning calorimetry (DSC) indicate that TH-PPV exhibits thermally induced order, resulting in an ordered liquid-crystalline mesophase. This confirms our assumption that the tetra-alkoxy substitution pattern indeed can give rise to desirable ordering phenomena. However, due to steric hindrance of the branched alkyl side chains, the second polymer, *i.e.* TEH-PPV, remains rather disordered. Finally, the first data on the application and optoelectronic characterization of TH-PPV in a P-LED device will be presented.

The authors gratefully acknowledge The Fund for Scientific Research-Flanders (FWO) for the financial support. This work has been supported by the European Science Foundation (ESF) under the EUROCORES Programme SONS II.



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Estimation the Effect of Hydrogen Bonds in Stabilization of Transition States in Ester Ammonolysis via Catalytic Maps

Miroslav A. Rangelov1, Georgi N. Vayssilov[2]

[1] Bulgarian Academy of Sciences, Institute of Organic Chemistry, 1113 Sofia, Bulgaria
[2] University of Sofia, Faculty of Chemistry, 1126 Sofia, Bulgaria; e-mail: gnv@chem.uni-sofia.bg

One of significant challenges in biocatalysts is to estimate noncovalent influence of chemical groups placed in adjacent position to atoms that participate in bond forming and breaking at the active sites in enzymes or ribozymes. One possible approach for elucidating of this effect is to calculate the energy for the noncovalent interactions of such adjacent group with the atoms involved in bond breaking and forming in the transition states with respect to the reactant:

$$E_{cat} = (E_{TS+H2O} - (E_{TS} + E_{H2O})) - (E_{initial+H2O} - (E_{initial} + E_{H2O}))$$

Graphical representation of such energy difference (shown below) can be considered as "a catalytic map" since it shows from which position the side group will have the highest stabilization effect on the transition state. Thus, the obtained information can be used in interpretation of influence of groups in vicinity of the active site as well as in construction of teozymes and compuzymes.
Here we report the results obtained by this approach on formylethanediole ammonolysis [1]. In this reaction effect of the vicinal hydroxyl group is approximated with an water molecule.

The work is supported by Bulgarian National Science Fund via project DOO2-133/08.

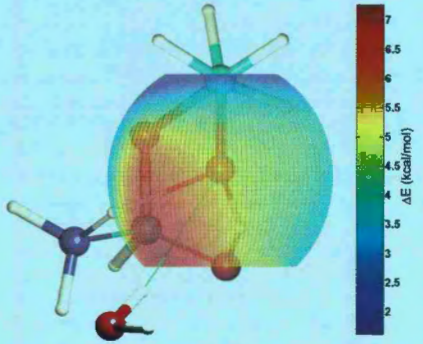


Fig. 1. Catalytic map of one of the transition states for formylethanediole ammonolysis.

References

1. M. A. Rangelov, G. N. Vayssilov, V. M. Yomtova, D. D. Petkov, *J. Am. Chem. Soc.* **128** (2006) 4964.

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Aug 9th, 2013

Assoc. Prof. Dr. Miroslav Rangelov
Institut of Organic Chemistry
Bulgarian Academy of Sciences
1113 Sofia
Bulgaria
passport number: 367620141

Dear Prof. Miroslav Rangelov,

It gives me much pleasure to invite you to visit Beijing Computational Science Research Center (CSRC) starting from September 19 to 25, 2012. Your detailed schedule is arranged as follows:

1. Sep 19, leaving Bulgaria and take a flight to Beijing, which arrives in Beijing on Sep 19;
2. During your stay in Beijing, we will arrange accommodation according to your schedule, the hotel is Run Ze Jia Ye Hotel, #3, Heqing Road, Haidian District, Beijing, ZIP: 100084, telephone: (86)10-62520066 (北京市海淀区荷清路三号，润泽嘉业大酒店，邮编：100084，电话：(86)10-62520066);
3. When you visit CSRC (located in the building next to the Run Ze Jia Ye Hotel). Your host, Prof. Hai-Qing Lin (telephone: (86)10-82687022), will make all related arrangements, including a seminar. Your office is room 621, telephone (86)10-82687091;
4. Sep 25, departure from Beijing to Xi'an.

CSRC will provide the following financial support to cover your accommodation at the Run Ze Jia Ye Hotel.

We are looking forward to seeing you in Beijing. Had there been any question, please don't hesitate to contact me at 86-10-82687022 or Miss Zheng Yang at 86-10-82687001.

With my best wishes!

BEIJING COMPUTATIONAL SCIENCE RESEARCH CENTER 北京计算科学研究中心

Sincerely yours,

Hai-Qing Lin

Director, CSRC
haiqing0@csrc.ac.cn

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BOOK OF ABSTRACTS

Algorithm for the ribosome structure neutralization and development of force field for drug candidates

Miroslav A. Rangelov[1], Peicho P. Petkov[2], Georgi N. Vayssilov[3], Stoyan Markov[4]

[1]*Institute of Organic Chemistry, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria*
[2]*University of Sofia, Faculty of Physics, 1126 Sofia, Bulgaria*
[3]*University of Sofia, Faculty of Chemistry and Pharmacy, 1126 Sofia, Bulgaria*
[4]*Institute of Parallel Processing, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria*

More than 80% of antibiotics used nowadays target the ribosome. For this reason full and precise atomistic model is necessary for development of the next generation of antibiotics. One of major problems in molecular dynamics (MD) simulation of large nucleoproteins is uncompensated charge of phosphate groups. We developed heuristic method for their neutralization which is applied on the ribosome. The resulting full ribosome structure is still unsuitable for all atoms MD because of the many charged groups it contains. This is because the ribosome is mainly composed of RNA chains leading to a huge amount of negatively charged phosphate groups in the PDB X-Ray Structures. In nature they are neutralized by Na^+, Mg^{2+} ions and a limited amount of positively charged amino acid residues incorporated in the polypeptide chains. For neutralization of these groups a heuristic algorithm for adding counter ions in big nucleoproteins as the ribosome unit has been developed and the charged groups in the ribosome structure were effectively neutralized using mono and divalent ions according to their environment. The neutralized structure equilibrates with all atom MD within several ns.

Several program modules for fast and user friendly testing of drug like molecules inside ribosome using GROMACS are developed. The most important module reads hessian matrix, masses, optimized structure and created by g_x2top topology of drug candidate and calculates all necessary force field constants necessary for molecular dynamics simulation of drug candidate inside ribosome.

The work on these topics was supported by Bulgarian Science Fund and computer time is provided by Bulgarian Supercomputer Center.

1. M.A. Rangelov, G.N. Vayssilov, V.M. Yomtova, D.D. Petkov, J.Am.Chem.Soc. 128, 4964 (2006).
2. M.A. Rangelov, G.P. Petrova, V.M. Yomtova, G.N. Vayssilov, J.Org.Chem. 75, 6782 (2010).
3. S. Kolev, P.St. Petkov, M. Rangelov, G.N. Vayssilov, ACS Chem. Biol. 8, 1576 (2013).

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PROGRAMME

O15	**Novel bicyclic peptide selectively inhibits matrix metalloproteinase-2 activity in vivo** *A. Mäkelä, M. Blanco, J. Tolvanen, O. Heikkilä*
16.40 – 17.10	**COFFEE BREAK**
	SESSION 4
	Chairpersons: *B. Rijkers (Netherlands)* *M. Teixidó (Spain)*
	O16 – O20
17.10 – 18.50	
O16	**Pharmacological investigations ofnew galantamine Peptide derivatives** *N. Danchev, I. Nikolova, I. Vasenkov, Ich. Ivanov, M. Georgieva, D. Danalev*
O17	**Matrix assisted peptide synthesis on nanoparticles** *Victoria Machley, Ilias Kharlamtash, Aryeh Weiss and Gerardo Byk*
O18	**Orally active peptidomimetics based on branched 2,5-diketopiperazines; structure functional studies.** *V. Dolgin*
O19	**Development of elmyelin in the treatment of multiple sclerosis; Preparation of IND file towards Phase I clinical investigation** *J. Matsoukas*
O20	**Pushing the limits of peptide synthesis further** *J.M. Collins, S.K. Singh, K.A. Porter, M.J. Kamey*
18.50 – 19.20	**WORKSHOP CEM**

TUESDAY, SEPTEMBER 2ND 2014

	SESSION 5
	Chairpersons: *P. Cordopatis (Greece)* *E. Naydenova (Bulgaria)*
08.30 – 9.10	**PL02**
PL02	**What was first, the genetic code or its products?** *Ada Yonath* (Department of Structural Biology, Weizmann Institute, Rehovot, Israel)
09.10 – 10.30	**O21 – O24**
O21	**Algorithm for the ribosome structure neutralisation and development of force field for drug candidates** *M.A. Rangelov, P. Petkov, S. Markov, G. N. Vayssilov, L. Litov*
O22	**Discovery of a selective lysosomal alpha-mannosidase inhibitor from an imino-sugar library** *Y.-P. Chang, M. Muckeen, D. S. Alonzi, R. Sagar, A. Dickens, T. M. Chapman, T. D. Butters, D. C. Anthony, B. G. Davis*
O23	**New easy and efficient methods for peptide cyclization and acetylation** *A. Friedler*

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Computing Centre of the Slovak Academy of Sciences
in cooperation with IBM

Ing. Tomáš Lacko, director

AGENDA

Day 1 / Tuesday / 18.11.2014 / Computing Centre of SAS

10:00 – 13:00 **Ceremonial opening of the Aurel supercomputer extension**
and other computing resources in the administration of CC of SAS within SIVVP.
-Invited guests only

13:00 – 13:05 **Presentations Begin**
Participation allowed without registration.

13:05– 13:40 **Dr. Jane Ignatius**
Project Director, Computing Research Infrastructures
„Finland Case in Supercomputing“

13:40 - 14:00 **Prof. RNDr. Karol Marhold, CSc.**
Mgr. Anna Guttová, PhD.
RNDr. Dušan Senko, PhD.
Institute of Botany of SAS
„Evolutionary Hypotheses Testing using DNA Sequences and Climate Data“

14:00 - 14:30 **Dr. Miroslav Rangelov**
Institute of Organic Chemistry with Centre of Phytochemistry, BAS
„HPC for Modeling of Large Biomolecules“

14:30 – 15:00 **Dr. Maciej Remiszewski**
Director of Development & Collaboration, ICM Warsaw University
-Video call /SKYPE/
„From the lab to the Road - Commercializing HPC driven research”

9 Dúbravská cesta, 845 35 Bratislava, Slovakia, Tel.: +421 2 322 93 112, e-mail: tomas.lacko@savba.sk

Invited Speakers

Name	Institution
Dr. Lukáš Demovič	Computing Centre, SAS
Dr. Jozef Federič	Computing Centre, SAS
Dr. Anna Guttová	Institute of Botany, SAS
Dr. Jane Ignatius	Project Director, Computing Research Infrastructures
Ing. Tomas Lacko	Computing Centre Director, SAS
Cristiano Malossi	Research Specialist, IBM Rueschlikon Research Lab, Zuerich
Prof. Karol Marhold	Institute of Botany, SAS
Prof. Roman Martoňák	Faculty of Mathematics, Physics and Informatics, Comenius University
Rick Newman	Director of Server Solution Sales, IBM Central & Eastern Europe
Dr. Michal Pitoňák	Computing Centre, SAS
Dr. Miroslav Rangelov	Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of sciences
Dr. Maciej Remiszewski	Director of Development & Collaboration, ICM Warsaw University

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Nakhon Ratchasima 30000 THAILAND
Tel. +66 44 224193 Fax. +66 44224185
Email: jatuporn@g.sut.ac.th

January 6, 2014

Dr. Miroslav Rangelov

Institute of Organic Chemistry – BAS,

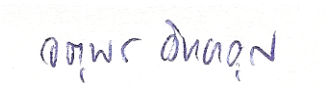
Sofia, Bulgaria

Dear Dr. Miroslav Rangelov:

It is my pleasure to offer this invitation letter for your visit to Suranaree University of Technology (SUT), Thailand from the 2nd to the 8rd of February, 2014 to discuss common research interest to see possibility in collaboration between our universities.

I am looking forward to welcoming you in Thailand.

Sincerely yours,



Jatuporn Wittayakun, Ph. D.

Associate Professor in Chemistry

Chair of School of Chemistry and

Acting Chair of School of Biochemistry

Algorithm for the ribosome structure neutralisation and development of force field for drug candidates

Miroslav A. Rangelov[1]. Georgi N. Vayssilov[2]
[1]*Institute of Organic Chemistry, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria*
[2]*University of Sofia, Faculty of Chemistry , 1126 Sofia, Bulgaria*

More than 80% of antibiotics used nowadays targets the ribosome. They target the ribosomes at precise locations within functionally significant sites. They exert their inhibitory action by diverse modes, including competing with substrate binding, interfering with ribosomal dynamics, minimizing ribosomal mobility, facilitating miscoding, hampering the progression of the mRNA chain, and blocking the nascent protein exit tunnel. For this reason full and precise atomistic model is necessary for development of the next generation of antibiotics. One of major problems in molecular dynamics (MD) simulation of large nucleoproteins is uncompensated charge of phosphate groups. We developed heuristic method for ther neutralisation wich is applied on the ribosome. Ribosomes, the universal cellular nano-machines, act as polymerases that translate the genetic code into proteins with high efficiency. It is a complex molecular machine translated the genetic code of its provisional form - information RNA to proteins. The key role of the bacterial ribosome makes it an important target for antibacterial agents. The resulting full ribosome structure is still unsuitable for all atoms MD because of the many charged groups it contains. This is because the ribosome is mainly composed of RNA chains leading to a huge amount of negatively charged phosphate groups in the PDB X-Ray Structures. In nature they are neutralized by Na^+, Mg^{2+} ions and a limited amount of positively charged amino acid residues incorporated in the polypeptide chains. For neutralization of these groups a heuristic algorithm for adding counter ions in big nucleoproteins as the ribosome unit has been developed and the charged groups in the ribosome structure were effectively neutralized using mono and divalent ions according to their environment. The neutralized structure equilibrates with all atom MD within several ns.

Several program modules for fast and user friendly testing of drug like molecules inside ribosome using GROMACS are developed. The most important module reads hessian matrix, masses, optimized structure and created by g_x2top topology of drug candidate and calculates all necessary force field constants necessary for molecular dynamics simulation of drug candidate inside ribosome.

Due to necessary expertise from different research fields the method was developed in cooperation between several groups within the frame of the National Center of Supercomputer Applications, Sofia, Bulgaria: M. Rangelov and S. Markov from Bulgarian Academy of Sciences, and P. Petkov, P. Petkov, L. Litov and G. Vayssilov from University of Sofia, Bulgaria.

The work on these topics was supported by Bulgarian Science Fund and computer time is provided by Bulgarian Supercomputer Center.

1. M.A. Rangelov, G.N. Vayssilov, V.M. Yomtova, D.D. Petkov, J.Am.Chem.Soc. 128, 4964 (2006).
2. M.A. Rangelov, G.P. Petrova, V.M. Yomtova, G.N. Vayssilov, J.Org.Chem. 75, 6782 (2010).
3. S. Kolev, P.St. Petkov, M. Rangelov, G.N. Vayssilov, ACS Chem. Biol. 8, 1576 (2013).

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8th January 2014

Dear Prof. DSc. Georgi N. Vayssilov, Prof. Rositca Nikolova and Dr. Miroslav Rangelov,

On behalf of the School of Chemical Sciences, Universiti Sains Malaysia, it is my great pleasure to invite you to visit our school for the period from 10–12 Feb. 2014. While at Universiti Sains Malaysia, we would be delighted if you could give a seminar during your visit. In addition, we welcome your visit to meet some members of our school for round table discussion on problems of common interest, and of course to know a little bit of the surrounding.

I very much hope that you are able to accept the invitation, and we are looking forward to welcoming you in Penang.

Yours sincerely,

Dr. Eng-Poh NG

Senior Lecturer

Cc. Dean,

School of Chemical Sciences

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VISITING PROFESSOR SEMINAR

Development of algorithm for charge compensation of the large nucleoproteins

Speaker

CHIEF ASSIST. PROF. MIROSLAV RANGELOV

Laboratory of Biocatalysis

Institute of Organic Chemistry, Bulgarian Academic of Science,

Sofia, Bulgaria

Chairperson

DR. NG ENG POH

ABSTRACTS

One of major problems in molecular dynamics (MD) simulation of large nucleoproteins is uncompensated charge of phosphate groups. We developed heuristic method for the neutralisation which is applied on the ribosome. Ribosomes, the universal cellular nano-machines, act as polymerases that translate the genetic code into proteins with high efficiency. It is a complex molecular machine translated the genetic code of its provisional form - information RNA to proteins. The key role of the bacterial ribosome makes it an important target for antibacterial agents.

Due to limitations of X-ray methodology all available ribosome structures contain a lot of missing monomers and are unsuitable for molecular dynamics. For this reason a new whole ribosome structure (E.Coli) was constructed. Starting from most completed available PDB structures we constructed our initial Ribosome model. To obtain a full ribosome structure a new heuristic algorithm is developed. According to this algorithm if there is even a low intensity X-ray map available for the missing monomers it has been used for its placement and positioning. If there is no X-ray map with good enough quality the KEM map is used. When KEM and X-ray maps are of insufficient resolution for positioning of the monomers they are placed by hand and are optimized by Coot FF according to Ramachandran plot minima. After the process of addition of missing monomers the ribosome structure were relaxed by MD.

The resulting full ribosome structure is still unsuitable for all atoms MD because of the many charged groups it contains. This is because the ribosome is mainly composed of RNA chains leading to a huge amount of negatively charged phosphate groups in the PDB X-Ray Structures. In nature they are neutralized by Na^{+}, Mg^{2+} ions and a limited amount of positively charged amino acid residues incorporated in the polypeptide chains. For neutralization of these groups a heuristic algorithm for adding counter ions in big nucleoproteins as the ribosome unit has been developed and the charged groups in the ribosome structure were effectively neutralized using mono and divalent ions according to their environment. The neutralized structure equilibrates with all atom MD within several ns.

UNIVERSITI SAINS MALAYSIA

Monday

February 10, 2014

11:00 - 12:00 p.m.

Conference Room, School of Chemical Sciences, USM

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7TH Bulgarian Peptide Symposium

with international participation

JUNE 10 – 12, 2016, BLAGOEVGRAD, BULGARIA



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biological activity between the three models of DOR and a series of delta-opioid selective enkephalin analogues.

Keywords: QSAR, Docking, Ligand-receptor interaction, GOLD, Delta opioid receptor

Acknowledgments:

This work is partially supported by the project of the Bulgarian National Science Fund, entitled: Bioinformatics research: protein folding, docking and prediction of biological activity, NSF I02/16, 12.12.14.

References:

[1]N. Pencheva, P. Milanov, L. Vezenkov, T. Pajpanova, E. Naydenova. (2004). *Eur. J. Pharmacol.*,498, 249-256.

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[5] F.Sapundzhi, T.Dzimbova, P. Milanov, N. Pencheva. (2015). Proceedings of the Sixth International Scientific Conference - FMNS2015, 1, 104-112.

P 53

In silico investigation of immunological mimicry of single-chain variable fragment (scFv) antibody and natural C1q globular heads

Miroslav Rangelov[1], Nadezhda Todorova[2], Ivanka Tsacheva[3]

[1] Institute of Organic Chemistry with Centre of Phytochemistry (IOCCP), Bulgarian Academy of Sciences

[2] Institute of Biodiversity and Ecosystem Research (IBER), Bulgarian Academy of Sciences

[3] Biology Faculty, Sofia University "St. Kliment Ohridski"

C1q is a crucial recognizing first subcomponent of the classical

complement pathway and as such is also involved in pathological conditions, such as autoimmune disorders like systemic lupus erythematosus (SLE). Molecular events that lead to generation of autoantibodies against C1q (anti-C1q) are still unknown, although some hypothesis, concerning the exact timing and mechanism exist. C1q is thought to undergo a conformational transition exposing neo-epitopes that lead to recognition of the molecule as immunogenic. Naive phage library was used to search for single-chain variable fragments (scFv) that mimic the globular head regions of natural C1q (ghC1q), thus inhibiting its recognition from autoantibodies. After several panning rounds, a promising clone was isolated and sequenced.
Based on its nucleotide sequence, a structural 3D model of resulting polypeptide chain was generated, as homology model according to alignment on the deposited crystallized scFv PDBs. The resulting structure was used to find conformational and electrostatic similar regions between homology structure and natural C1q globular heads. This similarity helps to clarify regions from C1q molecule crucial for generation of SLE autoantibodies. The model will be further helpful for SLE patogenesis-assossiated conformational or sequential neo-epitopes search in the three ghC1q chains.

P 54
Mass spectrometry analysis of immunoglobulin at different conditions

Velikova R, Dolashka P, Dolashki A, Vasilev Tch, Pashov A

The immune system is capable of producing a large repertoire of antibodies that can recognize a wide variety of different molecular structures and conformations. Polyspecific antibodies represent a first line of defense against infection and regulate inflammation, properties hypothesized to rely on their ability to interact with multiple antigens.

The specific binding portion of the antibody (paratope) binds very specific to a particular part of the antigen (epitope) that led to the formation of the antibody. Through this connection immunoglobulin

24th Congress of Chemists and Technologists of Macedonia

BOOK of ABSTRACTS

11-14 September 2016

Ohrid, Republic of Macedonia

MPCE 021

MOLECULAR DOCKING STUDY ON BINDING MODES OF ISOXAZOLO- AND THIAZOLOHYDRAZILIDENE-CHROMANE-2,4-ONES WITH B-RAF KINASE

Denitsa Yancheva[1], Bozhanka Mikhova[1], Lulzime Ballazhi[2], Miroslav Rangelov[1], Faik Imeri[3], Emil Popovski[4], Ahmed Jashari[5], Goran Stojkovikj[4], Kristina Mladenovska[2]

e-mail: krml@ff.ukim.edu.mk

1- Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences, Acad. G. Bonchev Str., build. 9, 1113 Sofia, Bulgaria

2- Faculty of Pharmacy, Center of Biomolecular Pharmaceutical Analyses, University "Ss Cyril and Methodius", Mother Theresa 47, 1000 Skopje, Republic of Macedonia

3- Institute of Physiology, University of Zürich, CH-8057, Zürich, Switzerland

4- Institute of Chemistry, Faculty of Natural Sciences and Mathematics, University "Ss. Cyril and Methodius", Arhimedova Str. No. 3, PO Box 162, 1000 Skopje, Republic of Macedonia

5- Faculty of Natural Sciences & Mathematics, State University of Tetovo, Pashe Deralla bb, 1200 Tetovo, Republic of Macedonia

Recently a series of novel isoxazolo- and thiazolohydrazilidene-chromane-2,4-ones was synthesized and shown to exhibit cytotoxicity on human breast cancer cell line MDA-MB-231 [1]. MDA-MB-231 cells are very sensitive to treatment with B-Raf kinase inhibitors blocking the RAF/MEK/ERK signaling pathway and affecting the tumor growth. Among the three RAF isoforms in humans (A-Raf, B-Raf, and C-Raf), B-Raf is the most critical to mediate Ras activity. A significant fraction of melanoma, colorectal, thyroid and breast cancers have activating B-Raf mutations, particularly at valine 599 [2].

The results of a molecular docking study conducted in effort to throw more light on the possible interaction of the synthesized isoxazolo- and thiazolohydrazilidene-chromane-2,4-ones with B-Raf are presented. The compounds were docked into the crystal structure of human oncogenic ^{V599E}B-Raf in complex with the inhibitor sorafenib. All of them occupied an internal pocket formed by the activation segment and the P-loop of ^{V599E}B-Raf. The ligand-pocket binding was driven by hydrogen bonding to amino acid residues Lys482, Glu500, Thr528 and Asp593 and hydrophobic interactions with Leu504, Leu513, Gly592 and Phe594. In this way, the ligands connected simultaneously to the activation segment and the catalytic loop of ^{V599E}B-Raf, were being able to promote an inactive conformation of the enzyme and hinder its phosphorylation.

Key words: hydrazinyldiene-chroman-2,4-diones, molecular docking, B-Raf kinase

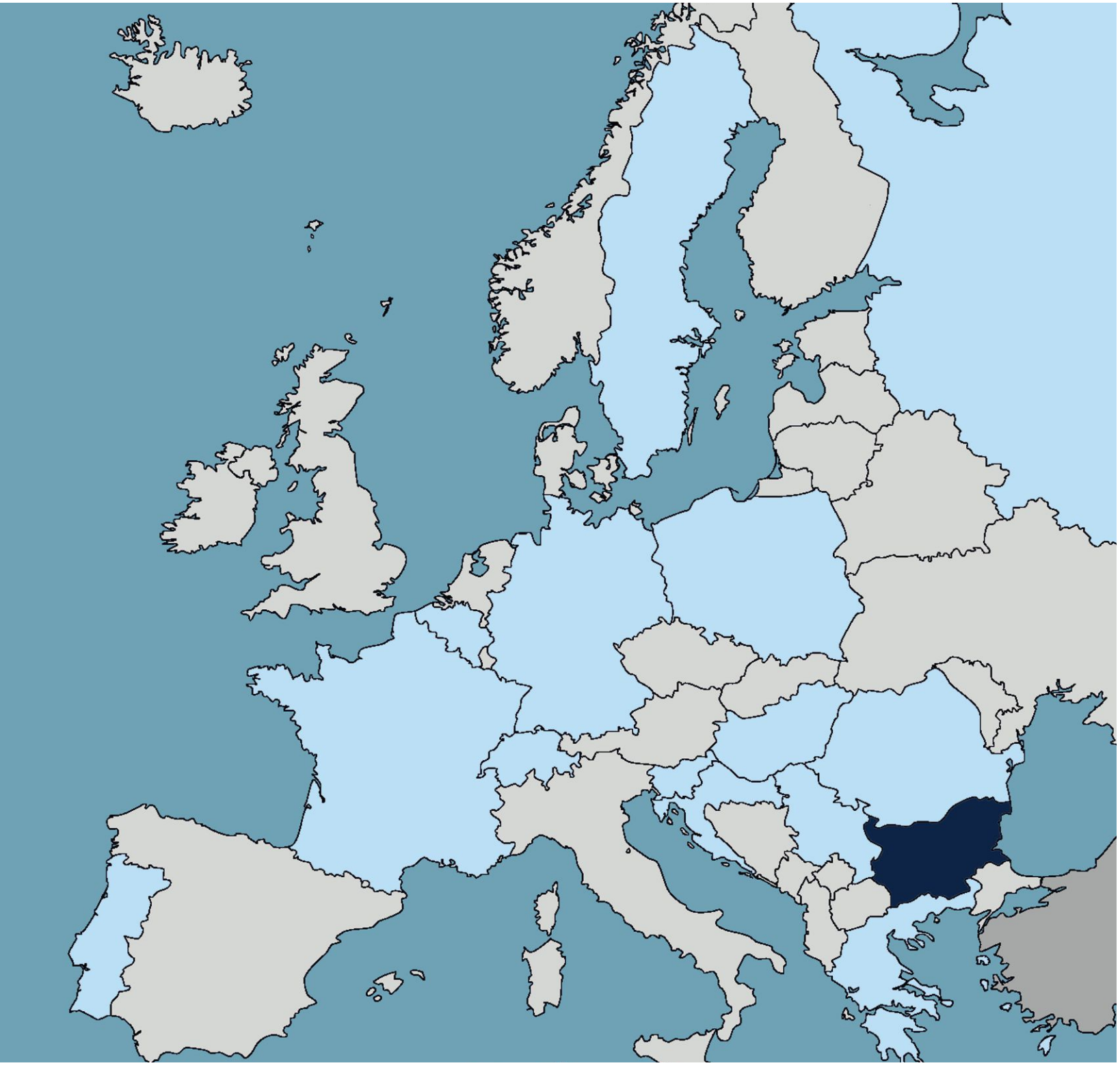
References:

[1] Jashari A, Imeri F, Ballazhi L, Shabani A, Mikhova B, Dräger G, Popovski E, Huwiler A (2014) Synthesis and cellular characterization of novel isoxazolo- and thiazolohydrazinyldiene-chroman-2,4-diones on cancer and non-cancer cell growth and death. Bioorg Med Chem 22:2655-2661.

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18th Central and Eastern European NMR Symposium and Bruker Users' Meeting

CEUM 2016 Sofia



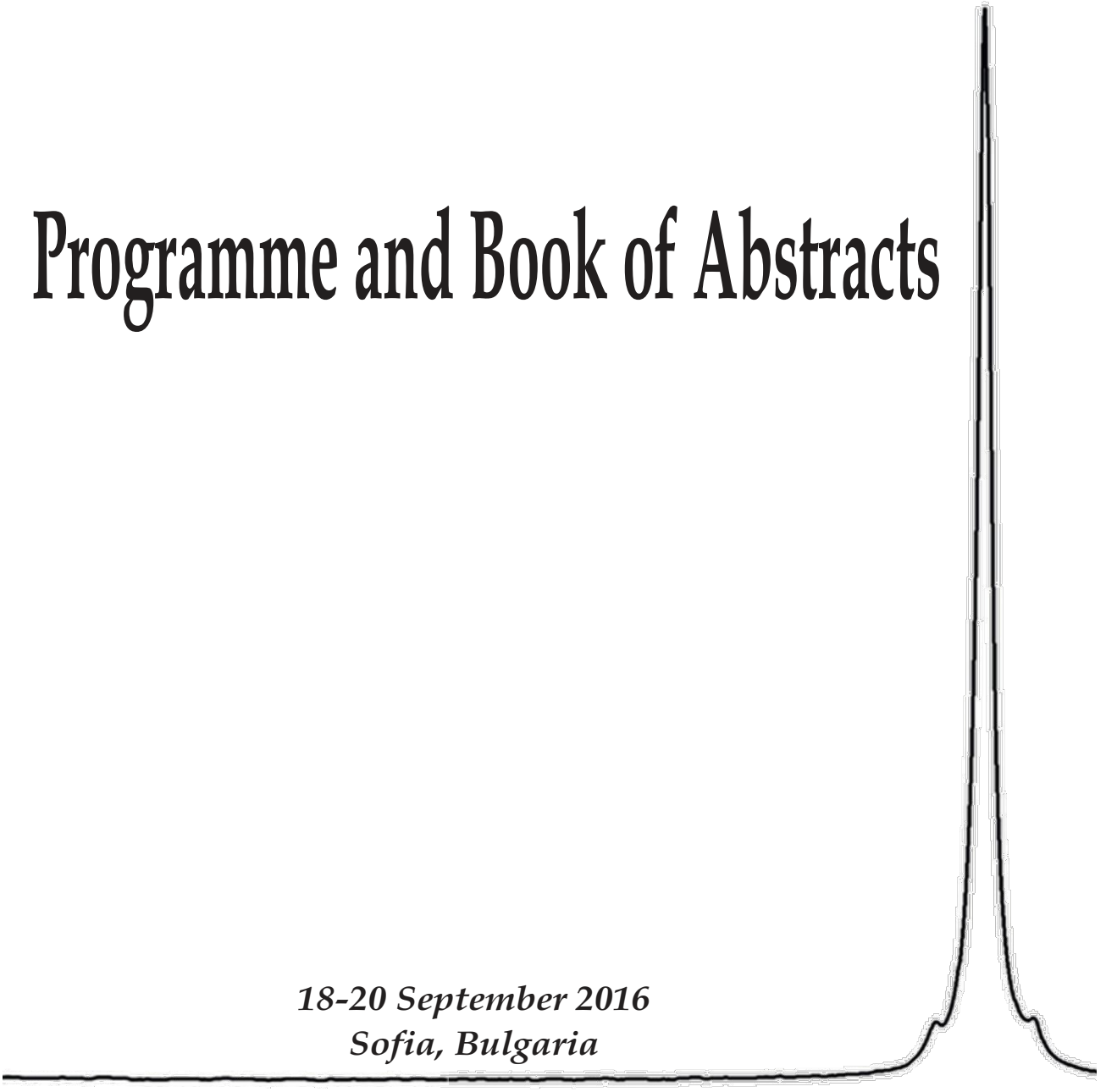
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18th Central and Eastern European NMR Symposium & Bruker Users' Meeting

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A ^{31}P NMR Probe of Intracellular Volume in *E.coli* DH 5-alpha Cell Cultures: Is it possible to count these cells by NMR?

Nadezhda Todorova [b], Miroslav Rangelov [a], Nikolay G. Vassilev [a]

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Dimethyl methylphosphonate (DMMP), when added to a suspension of erythrocytes, has been reported to have a lower frequency chemical shift inside of cells than outside [1]. This work further investigates the same phenomenon in bacterial cells and describes the application of DMMP as a measure of intra- versus extracellular volumes in Gram-negative cell culture. Longitudinal relaxation (T1) values for intra- and extracellular DMMP were estimated so that partially saturated DMMP peaks in ^{31}P NMR spectra of *E.coli* DH 5-alpha cell cultures can be corrected to give the relative volumes of the intra- and extracellular compartments; this information provides a relative measure of culture growth.

Diffusion NMR spectroscopy [2] was also used to study intracellular volume and apparent water diffusion constants in cell culture of the same laboratory strain. The attenuation of the water signal versus the squared gradient strength was fitted by the sum of two decaying exponentials. The fractional volume of the slow component as determined from the biexponential diffusion curve didn't correlate well with the relative intracellular volume, as obtained from the ^{31}P NMR spectra of the sample.

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Acknowledgements: *The financial support by the Bulgarian Science Fund (Projects UNA-17/2005 and DRNF-02/13) is gratefully acknowledged.*



DIVERSITY AND BIOTECHNOLOGICAL POTENTIAL OF EXTREMOPHILES

International Conference held in Sofia,

26-28 September 2016

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2. Encheva-Malinova, M., L. Yocheva, B. Gocheva, P. Hristova, N. Bogatzevska, M. Stoyanova, S. Tishkov, P. Moncheva. ANTARCTIC ACTINOMYCETES AND THEIR ANTIBACTERIAL POTENTIAL
3. Todorova, N., M. Rangelov, B. Duarte, I. Caçador, V. Karamfilov. MICROBIAL DIVERSITY IN OIL CONTAMINATED BLACK SEA COASTAL ENVIRONMENTS
4. Rusinova-Videva, S., A. Adamov, S. Nachkova. REMOVAL OF METAL IONS FROM AQUEOUS SOLUTIONS BY BIOSORPTION ONTO ANTARCTIC YEASTS *CRYPTOCOCCUS LAURENTII* AL_{65}
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6. Miteva-Staleva, J., E. Krumova, M. Angelova. LOW TEMPERATURE STRESS AND AGING IN FUNGI
7. Kalcheva, H., M. Dinka, E. Ágoston-Szabó. THE IMPACT OF PSYCHROTOLERANT BACTERIA FROM THE DANUBE RIVER ON TWO WETLANDS (BÉDA-KARAPANCSA, DANUBE-DRAVA NATIONAL PARK, HUNGARY) AND RELATIONS OF PLANKTONIC BACTERIA TO ENVIRONMENTAL FACTORS

Social Program

26.09.2016, 17 h - Guide Tour around Sofia

27.09.2016 – 9.30 h –Visit of the Laboratory of Biotechnology, Institute of Microbiology, BAS, Plovdiv

28.09.2016, 19 h – Official dinner for all participants

Diversity and Biotechnology of Extremophiles
International Conference 26-28 September, 2016, Sofia

MICROBIAL DIVERSITY IN OIL CONTAMINATED BLACK SEA COASTAL ENVIRONMENTS

Nadezhda Todorova[1], Miroslav Rangelov[2], Bernardo Duarte[3], Isabel Caçador[3], Ventzislav Karamfilov[1]

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[2] Institute of Organic Chemistry with Centre of Phytochemistry (IOCCP-BAS), Bulgaria

[3] Marine and Environmental Sciences Centre (MARE), Faculty of Sciences of the University of Lisbon, Portugal

South-Western (SW) part of the Black Sea is characterized by a persistence of oil and oil derivatives due to the intensive maritime transport, summer recreational activities and commercial fishing. As only microorganisms are capable of oil degradation, their role in remediation of impacted habitats is significant. On the other hand, salinity and temperature are considered the major environmental determinants of microbial community composition. Based on the Black Sea unique environmental conditions (average salinity 17.5‰ and temperature with a marked yearly periodicity) and in combination with pollution, the development of specific bacterial consortia is expected.

We applied molecular methods to reveal and compare composition and variety of natural bacterial communities based on 16S rDNA operational taxonomic units (OTUs) in a pristine and an area suffering chronic oil pollution. Dominance of certain associated to oil-degradation alpha-and gamma-Proteobacteria lineages in a functional bacterial community possessing biodegradative potential was found in sediment samples, where PAH levels were above the maximum admissible concentrations of 6.8 mg/kg $\sum PAH_{16}$ (EPA list) (Todorova *et* al, 2014). Real-time PCR was used to assess quantitatively bacterial OTUs, showing two orders of magnitude lower bacterial 16S rDNA in oil polluted sediments. 16S rDNA sequencing snapshot of pristine site (identified under The Ocean Sampling Day initiative) demonstrated presence of major marine bacterial groups. Comparative ARDRA (Amplified Ribosomal DNA Restriction enzyme Analysis) analysis of bacterial communities inhabiting both polluted and enriched in-situ oil-supplemented sediments with pristine environment revealed a difference of <20% in the restriction patterns, being indicative for bacterial complexity there and representation of oil-degraders in rare biosphere. In general, oil pollution resulted in less relative abundance and variety of bacterial community.

Further characterization of microbial diversity in oil contaminated coastal environments was based on *dsr*AB gene, as many oil-degraders proved to be also sulphate reducers. Functional clone libraries, sequencing and phylogenetic analysis clustered clones in two groups, *Desulphobacter* and uncultured marine strain. Isolates from the polluted environment were successfully cultured on oil supplemented media and will be used for degrading gene analysis in the future.

This was the first ECSA conference in which the Abstracts where not in paper but in a mobile App so there is no physical support of it.

Towards the development of a Marine Health Index: a first approach provided by the Ocean Sampling Day (OSD) campaigns

Bernardo Duarte[1], João Canning-Clode[2,3,4], Catarina Magalhães[5], Luís Torgo[6], Nadezhda H. Todorova[7], Miroslav Rangelov[8], Mahrous Kandil[9], Anastasis Oulas[10], Paraskevi N. Polymenakou[10], Kelly D. Goodwin[11], Tim Kahlke[12], Rodrigo Costa[13], Francesca Malfatti[14], João Carlos Marques[15], Isabel Caçador[1]

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[11] National Oceanic and Atmospheric Administration (NOAA) AOML & SWFSC, 8901 La Jolla Shores Drive La Jolla, CA 92037.
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[15] MARE – Marine and Environmental Sciences Centre, c/o Department of Zoology, Faculty of Sciences and Technology, University of Coimbra, 3000 Coimbra, Portugal.

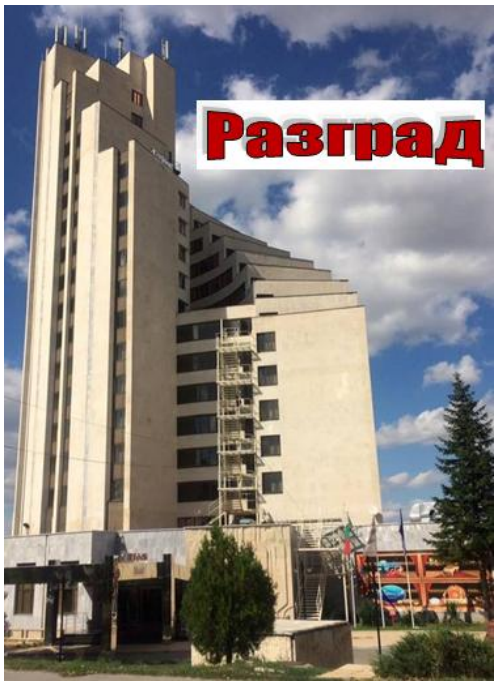
Marine systems play a critical role in supporting human well-being, from providing food, livelihoods and recreational opportunities to regulating global climate.

Indeed, almost 70% of the world population lives nearby coastal and marine water bodies. This leads to inevitable outcomes derived from anthropogenic activity. One of the main questions imposed to marine scientists by policy makers is how to evaluate the health of coastal marine systems and the development of efficient tools to numerically describe the ecological status of these systems.

The MicroB3 project, though the Ocean Sampling Day (OSD) campaigns in 2014 and 2015 provided an unique dataset of the microbial diversity of the oceans around the world. In addition, this dataset provided a metagenomic-based understanding of the roles that microbes may have as key players in these marine ecosystems. The presence and abundance of specific microorganisms as well as their metabolic activity can provide powerful insights on their response to negative anthropogenic inputs.

The present work aims to describe the first insights into the development of a Marine Health Index based on the microbial taxonomic (16S rRNA and 18S rRNA genes) and metagenomic data generated from the global 2014 and 2015 OSD initiatives and relate the diversity and the distribution of those genes with environmental anthropogenic pressure data. A preliminary numerical tool is presented and applied to different marine ecosystems in order to discuss its applicability in future monitoring programs.

РУСЕНСКИ УНИВЕРСИТЕТ "АНГЕЛ КЪНЧЕВ"
ФИЛИАЛ РАЗГРАД
СЪЮЗ НА УЧЕНИТЕ В БЪЛГАРИЯ– КЛОН РАЗГРАД
ДОМ НА НАУКАТА И ТЕХНИКАТА - РАЗГРАД
РЕГИОНАЛЕН АКАДЕМИЧЕН ЦЕНТЪР НА БАН РАЗГРАД
ПОД ПАТРОНАЖА НА КМЕТА НА ОБЩИНА РАЗГРАД



56-ТА ГОДИШНА НАУЧНА КОНФЕРЕНЦИЯ НА РУСЕНСКИ УНИВЕРСИТЕТ ФИЛИАЛ - РАЗГРАД

Индустрия 4.0. Бизнес среда. Качество на живот

03.11. - 04.11.2017 г.
Хотел "Картоон" гр. Разград

П Р О Г Р А М А

03.11.2017 г.

09:30 – 16:00ч.
Хотел ”Картоон” - до рецепция
Регистрация на участниците в конференцията

11:00 ч.
КОНФЕРЕНТНА ЗАЛА LCR

Откриване, Приветствия 11:00 ч.		
ПЛЕНАРНИ ДОКЛАДИ		**Бета-глюкани от гъби в развитието на функционалните храни** ***доц. ктн Марк Шамцян*** Санкт-Петербургски държавен технологически институт, (Технически университет), Санкт Петербург, Русия
11.15-13.00		**Производство на алкохол за горене на база мокро смилане на царевица** ***Светлозар Караджов*** Амилум България ЕАД
14.00-16.30		**Заседание на секция ” Химични технологии” зала LCR**
		Постер сесия: **Секция ”Биотехнологии и хранителни технологии” зала LB**
19:00 ч.		**Вечеря за участниците в конференцията** **Ресторант „Папараци” - вход с куверти**
04.11.2017г.	**9.30-11.30**	**Заседание на секция ” Биотехнологии и хранителни технологии”- зала LCR**
	9.30-11.30	**Постер сесия – секция ”Химични технологии” зала LB**
	11.30	**Награждаване на авторите на най-добрите доклади от двете секции с кристален приз “THE BEST PAPER“** **Закриване на конференцията**

03.11.2017

Section "Chemical Technologies "
Sectional reports: 03.11. 2017 14.00-16.30 – room LCR
Session Chair: Miluvka Stancheva

FRI–LCR-1-CT(R)

01 Porous structure of chars obtained from agro-wastes
Lenia Gonsalvesh, Velyana Georgieva, Mariana Tavlieva, Stancho Pavlov

02 Full assignment of ^{1}H and ^{13}C NMR spectra of (9*H*-fluoren-9-yl)-urea
Maria Frenkeva, Marin Marinov, Plamen Penchev

03 Power consumption reduction by modifying the shape of mixing impellers in chemical reactors
Dobrin Georgiev, Zhivko Ivanov, Mariana Karaivanova

04 Oxidation kinetics of copper slag
Dimitar Georgiev, Dimitar Rusev, Ivan Gradinarov

05 Possibilities for technology to produce biodisel from waste oils
Evgeniy Ganev, Boyan Ivanov, Dragomir Dobrudzhaliev, Yunzile Dzhelil

06 Formamide-based prebiotic chemistry:one-pot synthesis of nucleobases and amino acids
Venelin Enchev, Nadezhda Markova, Nina Stoyanova, Miroslav Rangelov, Ivan Angelov, Ivayla Dincheva

Section " Biotechnologies and Food Technologies "
Poster session: 03.11.2017 14.00-16.30 – room LB
Session Chair: Nastia Ivanova

FRI–LB-P-1-BFT(R)

01. Influence of whole grain cereals on health
Gjore Nakov, Ljupka Necinova, Toni Miteski

02. Dietary habits of a part of the population in the republic of Macedonia
Viktorija Stamatovska, Zora Uzunoska, Tatjana Kalevska, Gjore Nakov, Ana Antovska

03. Application of a document camera for color measurement of dairy products
Zlatin Zlatev

04. Biochemical aspects of walnut dairy free milk
Cristina Popovici, Alexei Baerle, Pavel Tatarov

05. Quality of milk for the production of white brined cheese
Tatjana Kalevska, Zora Uzunoska, Viktorija Stamatovska, Vezirka Jankuloska

06. Determination of fenbuconazole in apples (golden delicious) from different location
Vezirka Jankuloska, Ilija Karov, Gorica Pavlovska, Tatjana Kalevska

07. Application of dietary fiber in raw-smoked sausage type „Petrohan”
Diana Indzhelieva, Katja Valkova-Jorgova, Diliyana Gradinarska

08. Chemical composition of aromatic products from laurel leaves (*Laurus nobilis* L.)
Galina Stefanova, Lubomir Stefanov, Stanka Damyanova, Albena Stoyanova

09. Features of foreign experience of mikro-insurance for insurance market in Ukraine
Mykhailo Arych

10. Substantiation of the heat treatment modes of the cooked sausage in the universal smoking-cooking chamber
Oleksiy Nescuba, Olena Chepeliuk, Oleksandr Chepeliuk

11. Intensification of the extraction process manufacture of bitter tinctures
Natalia Popova, Taras Misyura, Chornyi Valentyn, Rybachok Albina

12. Innovative method of water treatment in hydroponic system
Valeriy Myronchuk, Iryna Dubovkina
13. Development of mechatronic modules for packaging machines on the basis of synergetic integration elements
Liudmyla Kryvoplias-Volodina, Olexandr Gavva, Taras Hnativ
14. Features of a ultra-fine grinding by wet method in bead mills
Kateryna Hrininh, Oleksii Gubenia
15. Investigation of the yeast dough mixing process
Vitalii Rachok, Yuliia Telychkun, Mykola Desyk, Volodymyr Telychkun
16. The research of a one-step and two-step ejector with a compact and dispersed jet of liquid
Vitaly Ponomarenko, Dmitriy Lulka, Tsvetan Dimitrov, Svyatoslav Lementar, **Yaroslav Khitriy, Natali Perekrest**
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18. Effect of influence OF *Bacillus subtilis* TS 01 on the growth of mycotoxigenic fungi
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19. Using relative data in food technology
Mariyka Petrova
20. Use of essential oils in dairy products 2. Essential oil of dill (*Anethum graveolens)*
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21. Thermomechanical characteristics of high elastic vulcanizates used in food machinery
Delian Gospodinov, Vilheln Hadjiiski, Stefan Stefanov

04.11.2017

. **Section " Biotechnologies and Food Technologies "**
Sectional reports: 04.11. 2017 09.30-11.30– room LCR
Session Chair: Iliana Kostova

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01. Physical characteristics of functional biscuits
Gjore Nakov
02. Actuality and importance of the gluten-free baking goods production, choice of raw materials
Ivayla Sopotenska, Valentina Chonova
03. Modeling of mechanical systems by the reodynamic method
Victor Goots, Oleksii Gubenia, Alina Sheina, Myroslav Tarasenko
04. Influence of Pleurotus ostreatus preparations on yogurt cultures
Ekaterina Antontceva, Sergei Sorokin, Mark Shamtsyan
05. Milk-clotting activity of higher fungi Funalia trogii
Ekaterina Gannochka, Boris Kolesnikov, Mark Shamtsyan
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07 Mushroom polysaccharide for fortification of dairy product
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Session Chair: Tsvetan Dimitrov

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02. Aqueous solution properties of diblock copolymers of poly(allyl glycidyl ether) and polyglycidol
Miroslava Valchanova, Stanislav Rangelov, Emilya Ivanova, Sevdalina Turmanova
03. Tautomerism of inosine in water: Is it possible?
Nadezhda Markova, Venelin Enchev
04. High density polyethylene composites containing wood flour
Antoniya Ilieva, Dimitrina Kiryakova, Milica Koleva
05. Theoretical model of development of chemical toxic zone as a result of accident with propene
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06. Low-temperature glass-ceramics based on spodumene
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07. Effect of the coefficient of mass transfer by rectification of tetrachloromethane-toluene mixture
Zhivko Ivanov, Mariana Karaivanova, Dobrin Georgiev
08. The efficiency of protective actions of the borosilicate coatings
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Iliana Nikolova, Marin Marinov

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ECOLOGICAL MOVEMENT OF NOVI SAD

Nadezhda Todorova[1], Alexander Stankov[1], Miroslav Rangelov[2], Gabriele Jovtchev[1]
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HAS ROUNDUP AN IMPACT ON MICROBIAL COMMUNITIES OF AGRICULTURAL SOILS?

Abstract

During the last two decades Roundup has been widely used in agriculture. We started a pilot field study of glyphosate administration on natural bacterial community inhabiting agricultural soil. ARDRA (Amplified Ribosomal DNA Restriction enzyme Analysis) fingerprint technique was used to compare snapshot of ingenious bacterial diversity in glyphosate treated and untreated soil. First results showed, that Roundup applied as a single pre-sowing procedure, do not change dramatic the complexity of the bacteria community on the studied area. Further investigations are planned for several years, in order to determine possible long-term effects.

Key words: *Roundup, agricultural soils, bacterial diversity, fingerprint technique*

INTRODUCTION

The impact of glyphosate (the active form in Rounup), the most widely used worldwide herbicide nowadays, on soil health is rather complex with contrasting results in scientific studies up to date (Soil association document 2016, Myers 2016). Microbial communities in the soil, that form the basis of ecosystem services such as the transformation of man-introduced substances and the nutrient cycling, are also directly affected. Numerous studies are examining the effects of glyphosate on indigenous bacteria, most of them used culture-based methods (Shushkova et al. 2012, Imparato et al. 2016) or targeted specific bacterial gene activities (Lancaster et al. 2009,

Zobiole et al. 2011). Gaining details on the effects of the pesticide on affected group is important step of understanding the functional mechanism, but is too far of getting the broad picture of community reaction (Johnsen et al. 2001). These experiments were done in most cases under controlled laboratory or greenhouse conditions. In our experimental setup, we used field conditions to create a basis for an eco-toxicological, practice-oriented study.

We have used an ARDRA (Amplified Ribosomal DNA Restriction enzyme Analysis) fingerprint technique to compare snapshot of ingenious bacterial diversity in glyphosate treated and untreated soil.

MATERIAL AND METHODS

Natural soil samples in triplicate were collected form the upper surface horizon (1-8 cm depth) at experimental field site in Sofia before and 10 days after a Roundup (RU) treatment. RU is a liquid water-soluble organophosphorus leaf herbicide with contact action, containing glyphosate (360 g/l) as an active ingredient adding 180 g/l surfactant (CAS No. 1071-83-6; > 90% purity). It was used in a concentration of 400 ml/ 1000 m^2, proposed by the supplier for barley and applied as pre-sowing procedure.

A representative part was further used for DNA extraction with Power Soil isolation kit (MoBio, now Qiagen). 16S rRNA gene was amplified with Bacteria-specific primers 8F and 1513R (PCR conditions, Todorova et al. 2014). A combination of two frequently cutting restriction enzymes Msp I and Alu I created gene fragments from total community amplified 16S rDNA, visualized on 5% PAA gel, analyzed with BioNumerics software.

RESULTS

The impact of single Roundup treatment on the natural bacterial communities was assessed by comparative analysis of the total community DNA, which was of high molecular weight and pure (free of humic acids), thus reducing the potential bias in molecular analyses.

Complex restriction patterns were observed in most of the samples. In order to determine the relationship between the community fingerprints, similarities were calculated based on the whole-track densitometric curves (Pearson product-moment correlation coefficient) (Fig.1).

We observed similar pattern of 16S rDNA fragments in all samples, both their richness and relative abundance. According to UPGMA dendrogram the samples were very similar to each other, despite the high number of restriction fragments. Thus fingerprints did not reveal a dramatic change in the complexity of the bacteria affected by single treatment with Roundup. Result is meaningful for dominant community members on the studied area.

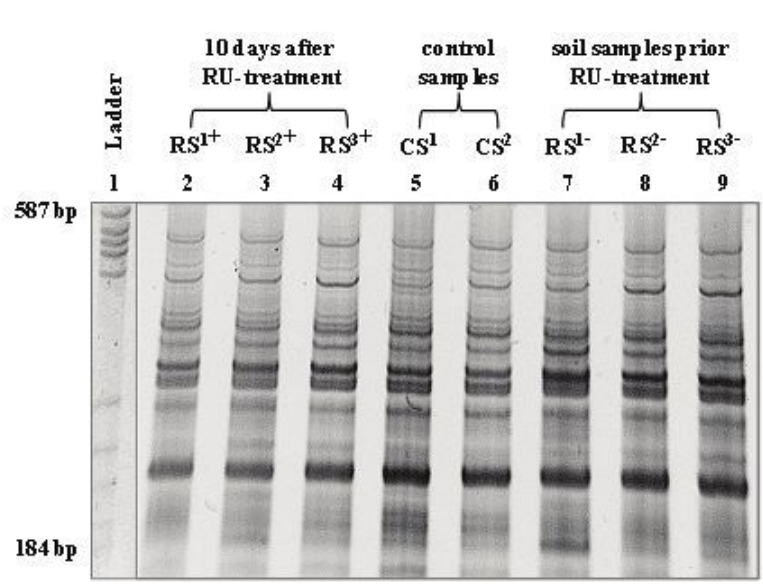


Figure 1. ARDRA profiles of PCR-amplified community 16SrRNA genes (lane 1 Molecular marker: pBR322DNA/BsuRI; lane 2 to 4: restriction patterns from Roundup treated samples; lane 5 to 6: restriction patterns of control untreated samples; lane 7 to 9: restriction patterns before Roundup application) RS – Roundup sample; CS – control sample

DISCUSSION

The composition of the bacterial communities was assessed by molecular approach. Fingerprint techniques have proven to be efficient for screening of spatial and temporal changes in the composition of environmental microbial communities (Osborn et al., 2000; Bowman et al., 2003).

Similar results to our findings were reported by Newman et al. 2016, who demonstrated similarity of alpha diversity estimates of rhizosphere bacteria of the control and glyphosate-treated samples. In their long-term glyphosate treatment only minor changes in relative abundance of bacteria at phylum level were observed. This study and findings of Weaver et al. 2007 are in congruence with the high similarity of bacterial biodiversity assessment of dominant members by our single herbicide application. As recent studies suggested that glyphosate may have an indirect effect on the soil microbial community function and structure in natural ecosystems more studies are needed to further evaluate the most used.

CONCLUSIONS

- Similar ARDRA profiles of soil microbiota were revealed in control and single RU treatment showing no big change in the richness and relative abundance of dominant community members.

OBJECTIVES FOR FURTHER INVESTIGATIONS

- Detailed analysis of the agricultural soil - soil type, pH, total organic carbon (TOC), etc.
- Microbial community reaction on long-term application - impact of RU on soil microorganisms at phylum level, possible shift effects on soil functionality.

ACKNOWLEDGMENTS
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ДА ЛИ ХЕРБИЦИД ROUNDUP ИМА УТИЦАЈ НА МИКРОБИЈАЛНЕ ЗАЈЕДНИЦЕ ПОЉОПРИВРЕДНИХ ЗЕМЉИШТА?

Апстракт

Током последње две деценије хербицид Roundup се масовно користи у пољопривреди. Започели смо теренско пилот истраживање примене глифосата на природну заједницу бактерија која насељава пољопривредно земљиште. ARDRA (Појачана рибозомална ДНК рестриктивна анализа ензима) техника отиска прста је употребљена за упоређивање снимања оригиналних бактеријских различитости код земљишта која јесу и која нису третирана глифосатом. Први резултати показују да хербицид Roundup примењен као појединачни поступак предсетве, није драматично променио комплексност заједнице бактерија на истраживаном подручју. Даља истраживања се планирају за неколико година, како би се утврдили могући дугорочни ефекти.

Кључне речи: *хербицид Roundup, пољопривредна земљишта, бактеријска разноврсност, техника отиска прста*

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CELLRAN: NEW CONCEPTUAL PROGRAM FOR ECOSYSTEM ANALYSIS AND MODELLING

Abstract

CellRan is a de-novo created program for ecology users. It has scripting capabilities but also integrated equations solver that gives to user freedom to define the virtual world resources, objects and events as well as simulated organisms in a more native manner. Program has a user-friendly graphical interface and a lot of representation capabilities. CellRan is an event-driven, turn based program and interactions between simulated species and among them and simulated world are described as quants exchange which is more natural way than by describing them by time derivatives. CellRan is a good prognosis tool for endangered of extinction species or new invasive events, as it works with real countable individuals. This makes really important difference by faith prognosis of small population dynamics and solving complex spatial and temporal population dynamics.

Key words: *computer modeling, user friendly interface, population dynamic simulation, free software*

INTRODUCTION

Ecosystems are defined as a network of interactions among organisms, and between organisms and their environment. Jackson and coauthors (2000) underlined that the process of creating a conceptual model begins with open questions. As consequence thereof, the researcher formulates hypotheses, evaluates available and needed data, and assesses the degree of understanding of the system under

consideration. Thus, the conceptual model converts to a quantitative model.

An understanding of the dynamics of spatial and temporal processes in ecosystems often requires a modeling approach (Pérez et al. 2000). On one site a population is composed of individuals, which are elements on the same hierarchical level that interact with each other. On the other there is the whole plethora of dynamic connections with abiotic and biotic factors.

Due to the complexity of ecosystems, informatics tools are required for system analysis and modeling. The input is wide-ranging information in the form of expert knowledge, applied in mathematical equations, analyzed and modeled with special programming and simulation tools. Great benefit could be the presentation of results by graphical interface in a user friendly way.

One of the biggest limitations of classical equation based modeling is that spatial structure is often ignored. Spatial impressions of single objects can be shown using virtual reality. That way we can often use this approach to study spatial ecological questions: What is the effect of spatial structure on the systems' dynamics? How and when does spatial structure form? What kinds of spatial structures are possible and how are these related to model parameters?

We were searching for a broad spectrum programming tool, allowing nearly universal application in description of population dynamics. Biggest part of present models as pointed by Jorgensen 2015, have rigid structures and a fixed set of parameters meaning that no changes or replacements of the components are possible. Consequently our concept was to implement more freedom directly at the basic level, as a new free program, CellRan.

MATERIALS AND METHODS

CellRan modeling program uses simple event-driven script language for describing interconnections between organisms and organisms and virtual world. The program explores the multi-layer Cellular Automata principle with applied closed-boundary conditions of virtual world. Each individual behavior and its interconnections with other individuals and layers is determined by the user either by script or by adding a simple rule inserted in world through graphical interface. Turn based simulation is performed by index walking or by random walking calculation of enumerated individuals. Simulated organism behavior in virtual world and virtual world itself are described as real number quants exchange which is more natural way than by describing them by time derivatives as in system of differential equations solvers. Data collected by detailed logging of simulation can be used for further mathematical analysis or for various valuable system evolution representations as time dynamic, spatial dynamic, behavioral dynamic or resources dynamic of the whole system or some element or element group.

RESULTS

In our test models birth rate, ecological fitness in means of adaptive evolution and death rate are put in close relation to consumed and available resources. The distribution of a species is spatially auto correlated according to available resources due to implemented locomotory. When first-order neighborhood effects are considered (as in predator-prey relationships) the movement of simulated organisms in world represents adequately real movement of hunting and fleeing. Time behaviors of models are also adequate according to existed table data of similar real systems.

More opportunity to describe a detailed system is implemented in resources, described as multiple data layers attached on every position in the virtual world. Thus non homogeneity in the world could be defined either by explicit mathematical formulas of that layers or manually by mouse click on the raster. Using explicit parametric formulas Initial conditions of world resources could be equally or non-equally distributed or even non-smooth distributed. This non-homogeneity allows studying population dynamics with respect to high or low intraspecies competition giving rise to solution in description of various ecological niches.

We have used event-driven language to realistically describe different organisms, their behavior and their interactions with the environment, including elements of learning by interconnectivity with the world. Thus genetically and evolutionary events could be simulated by the informational flow in the generations. Specific defined features could be made inheritable in that way allowing simulations of shift to long- as well as short-term alterations.

There is the possibility to identify each population member in the model using its coordinates as well as its simulation parameters of life and fitnes

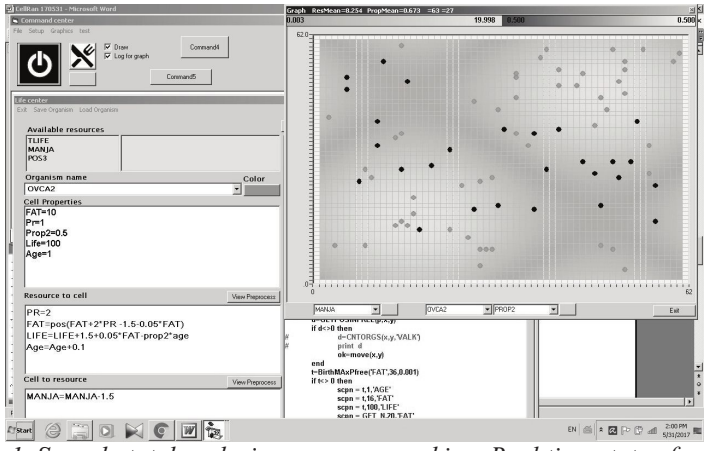


Figure 1. Snapshot, taken during program working. Real time state of system is visualized by section of virtual world in which one resource and one property of organisms can be represented by color coding and spatial position of individuals are clearly visible.

The possibility of changing size of the simulation and its duration is a prerequisite of reaching steady state and analyzing durability of the modeled ecosystem. The rates used for simulation are reasonably applicable to a real-world condition, though fine tuning would be beneficial on each studied population.

One big advantage of CellRan in the possibility to study and simulate the real non homogeneity of the environment, such as spatial components and/or behavioral inconsistency in the species population, but also dynamics of a group of individuals with nonhomogeneous behavior e.g. different sex driven dynamics and their impact on the future of the population.

The model is individuals driven not population driven, and the user works with a defined real number of individuals, whose faith and development in the world could be tracked down. This possibility allows a simulation being a step closer to the real environment then a system of differential equations, which are by definition smooth real functions. Models based on differential equations do not work with individuals rather with the system as a whole e.g. predator – pray dynamics, which is in steady state by statistically medium big groups, but gives unrealistic average results by small populations. CellRan is a good prognosis tool for endangered species as working with real countable individuals.

DISCUSSION

Dynamic deterministic models are valuable in providing important aspect in ecological processes. Dynamics is crucial characteristic regarding time or space changes in variables, stability of the system as seen in pray-predator interactions, uninterrupted time development by succession etc.(Chon et al 2009).

CellRan was developed as a useful tool for non-mathematics or non-programmers. Predominantly users with a biological/ecological education can easy handle it. Unlike software available in this field so far the customer can find answers of some specific questions, *via* input of information regarding cells or organisms, life cycles, predator-prey relations, relevant substrates and/or abiotic factors. Here, the users are not limited to apply completed formulas or modules (Kazancı, 2007), but they can insert own elementary formulas/equations, which fits most suitable for specific case scenarios. Such type of specific information is often ignored in other program products.

As output of the current software, case analyses can be performed - clearly represented as a mathematical model and visualized.

The wide application range coverts various ecological scenarios, short- and long-term ecological processes in ecosystems, prediction of population growth or interference, environmental risk assessment, factors and mechanisms leading to biodiversity loss, in the broader sense - processes of evolution and others. Analyses by means of this new software product could translate ecological hypotheses into predictions that can be evaluated and interpreted in light of existing or new data. In

this respect, researchers of different biological disciplines may be potential users of this software.

CONCLUSIONS

By implemented detailed logging of the system evolution CellRan program could represent and plot time behavior of studied system, similarly to programs based on solving system of differential equations. But in contrast to them CellRan allows to describe simple interactions of organisms in a more natural way. We can thus model behavior in native network, depending on environment, neighbors, organism ingenious properties etc. The most important advantage of CellRan is modeling realistically behavior of small groups. Small population, as that by endangered of extinction species or new invasive event, could be quantized on quantity of individuals - natural numbers. This means that a whole group of that individual will be simulated in virtual resource homogenous or non-homogenous world, and collected data will be represented as time dynamic, spatial dynamic or behavioral dynamic or resources dynamic of the system. Deferential equations are statistically correct by big populations, but because they use smooth real functions its results are also real numbers which bad corresponds with small populations which are by definition real numbers (because of impossibility of existence of living fraction of individual organism), that makes really important difference by faith prognosis of small population dynamics.

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CELLRAN: НОВИ КОНЦЕПТУАЛНИ ПРОГРАМ ЗА АНАЛИЗУ И МОДЕЛИРАЊЕ ЕКОСИСТЕМА

Апстракт

CellRan је новокреирани програм за еколошке кориснике. Има способности скриптирања, али и интегрисани солвер за једначине који даје кориснику слободу да дефинише виртуелне ресурсе света, објекте и догађаје, као и симулиране организме на више начина. Програм има једноставан графички интерфејс и пуно могућности за представљање. CellRan н је програм који се темељи на догађајима, а интеракције између симулираних врста и међу њима и симулираног света описују се као размена квинтова што је природнији начин него што их описује временским дериватима. CellRan је добар алгоритам за прогнозу изумирања угрожених врста или нових инвазивних догађаја јер ради са стварним бројивим јединкама. Ово чини заиста значајну разлику код вероватне прогнозе мале популационе динамике и решавања комплексне просторне и временске динамике популације.

Кључне речи: *компјутерско моделирање, кориснички интерфејс, симулација становништва, слободан софтвер*

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M22	Katerina Stoyanova, Nadezhda Todorova, Miroslav Rangelov, Vishnya Stoyanova, Ginka Nikolova, Safa Mohedin, Anna Yordanova, Lublena Yoncheva, Vanya Bogoeva, Ivanka Tsacheva **THE USE OF ANTI-IDIOTYPE scFv FOR THE LOCALIZATION OF A GLOBULAR AUTOEPITOPE OF C1q**
M23	Nikola Mladenov, Kirilka Mladenova , Pavel Videv, Veselina Moskova-Doumanova, Tanya Topouzova-Hristova, Zdravko Lalchev, Tonya Andreeva, Svetla Petrova, Jordan Doumanov **TENSIOMETRIC INVESTIGATIONS OF HBEST1 AND SM MONOLAYERS**

M22

THE USE OF ANTI-IDIOTYPE scFv FOR THE LOCALIZATION OF A GLOBULAR AUTOEPITOPE OF C1q

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Keywords: C1q, globular autoepitopes, scFv

Anti-C1q autoantibodies are a clinical feature of a few autoimmune disorders in humans diseases like systemic lupus erythematosus (SLE), rheumatoid arthritis (RA), mixed connective tissue disease, Felty's syndrome, rheumatoid vasculitis, polyarteitis nodosa, polychondritis, Sjögren's syndrome, etc. It is now clear that C1q turns into an autoantigen upon immobilization and it is assumed that the process of immobilization brings about the exposure of neo-epitopes which are recognized by the anti-C1q antibodies. Yet the immunogenic stimulus that gives rise to the formation of anti-C1q antibodies is still unknown. Localizing the autoepitopes that are recognized by the polyclonal autoantibodies to C1q might shed light to the structural changes of the protein that render it autoantigenic. Recently, a major linear epitope within the N-terminal domain, designated CLR, was identified. We addressed the issue of C1q autoantigenicity by generating a scFv that is anti-idiotypic to a fraction of anti-C1q autoantibodies, isolated from Lupus Nephritis (LN) sera, which specifically recognized only the intact C1q molecule. We also studied conformational changes of the protein C1q due to the binding of anti-C1q, registered by fluorescence spectroscopy method. The anti-idiotypic scFv was found to have approximately 50 % inhibitory capacity on the recognition of immobilized C1q by the LN autoantibodies. The anti-idiotypic scFv was sequenced and *in silico* folded into a 3D structure which was superimposed on the crystalized 3D structure of the C-terminal domain of C1q thus revealing a structural homology with the globular fragments of all three types of polypeptide chains comprising C1q, designated ghA, ghB and ghC. The scFv was further revealed to inhibit the recognition of immobilized ghA by the LN autoantibodies. In conclusion the generated anti-idiotypic scFv can serve as a structural analogue to a conformational globular autoepitope of C1q and can be further subjected to *in vivo* functional analysis.

Aknowledgement. *The presented experimental work was financed by Grant DN01/9 of the NSF of the Bulgarian Ministry for Education and Science.*

Biospectra, Plenary Lecture

RAMAN SPECTROSCOPY OF METEORITE-CATALYZED SYNTHESIZED PREBIOTIC COMPOUNDS FROM FORMAMIDE AFTER PROTON IRRADIATION

E. Borisova(1), L. Avramov(1), V. Enchev(2), I. Angelov(2), M. Ranglov(2), D. Bratashov(3), D. Gorin(3), M. Kapralov(4), E. Krasavin(4), R. Saladino(5)
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Discussion Live Chat

ABSTRACT

This investigation is a part at answering the central question of the problem of the production of the prebiotic compounds underlying the formation of the living systems. Research is focused on the development of unified theoretical and experimental approaches taking into account the possible influence of the following factors: energy, evolution, protometabolic, and the primordial environment — on the origin of life. We are looking for a sequence of processes that can lead to the formation of a complete, chemically active prebiotic system. Formamide (NH2CHO) is becoming one of the most intensively studied precursors for prebiotic syntheses of compounds potentially relevant for the origin of life. [1] It could be a parental molecule for synthesis of prebiotic molecules under proton irradiation. Different mineral content of meteorites gives variety of possible catalytic actions that would force this synthesis. The products of such processes could be detected by the spectroscopic methods. Therefore liquid formamide has been irradiated by high-energy proton beams in the presence of powdered meteorites, and the products of the catalyzed resulting syntheses were analyzed by Raman spectroscopy technique, which is an extremely sensitive spectral tool for evacuation of organic matter presence. The meteorites tested were representative of the four major classes: iron, stony iron, chondrites, and achondrites. In the irradiated samples were observed Raman signals from amino acids, carboxylic acids, and sugars, which correspond to some earlier investigations, when mass-spectrometry approach was used [3].
Raman spectroscopy could be used as a faster and non-destructive complementary tool for evaluation of synthesized prebiotic molecules in such model system “metheorite+proton irradiation + formamide”. The obtained results will contribute to the general understanding of the origin of life.

Acknowledgements: This work is supported in part by the National Science Fund of

Bulgarian Ministry of Education and Science under grant #DN-09/7/2016 “Modeling of the meteorite-catalyzed processes of prebiotic compounds formation”.

References:
1) Saladino R, Crestini C, Pino S, Costanzo G, Di Mauro E, Formamide and the origin of life. Phys Life Rev 9(1):84–104 (2012).
2) Saladino R, Carota E., Botta G, Kapralov M, Timoshenko G, Rozanov A, Krasavin E, Mauro E, Meteorite-catalyzed syntheses of nucleosides and of other prebiotic compounds from formamide under proton irradiation, PNAS 112(21): E2746-E2755 (2015)

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Raman spectroscopy of meteorite-catalyzed synthesized prebiotic compounds from formamide after proton irradiation

Dr. Ekaterina Georgieva Borisova
Institute of Electronics, Bulgarian Academy of Sciences, Associate Professor

„Immunology for All”

FIFTH NATIONAL CONGRESS OF IMMUNOLOGY

25 – 28 October 2018
Imperial Hotel & SPA, Plovdiv



Bulgarian Society of Immunology
Bulgarian Association of Clinical Immunology

- SESSION 5-
AUTOIMMUNITY I
Chairs: *I. Altankova, A. Tchorbanov*

AUTOANTIGENICITY OF C1Q - THE CONTRIBUTION OF THE GLOBULAR DOMAINS.

Ivanka Tsacheva[1], Nadezhda Todorova[2], Miroslav Rangelov[3], Vishnya Stoyanova[4], Ginka Nikolova[5], Hristo Georgiev[5], Safa Mohedin[1], Vanya Bogoeva [6]

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Aim: To study the structure/autoantigenicity relationship of C1q and the contribution of the globular modules ghA, ghB and ghC of C1q for the formation of C1q autoepitopes.
Methods: Generation of scFv anti-idiotypic to anti-C1q from clinically active and non-active Lupus Nephritis (LN) sera; Selection of inhibitory scFv on the recognition of C1q by the lupus autoantibodies using ELISA and spectrofluorimetric analyses; Sequence analysis of selected scFv and generation of a 3D model by molecular dynamics for localisation of C1q autoepitopes.
Results: Affinity purified LN autoantibodies were used to screen the phage library Griffin.1. Fourteen out of 21 positive clones were found anti-idiotypic and were subjected to inhibitory analysis on the recognition of C1q by the lupus autoantibodies. Four clones were inhibitory and considered structural analogues to C1q autoepitopes – A1, A12, F6 and F9. A1 was sequenced and *in silico* folded into a 3D structure, then superimposed on the crystalized 3D structure of the globular C1q domain thus revealing a structural homology with all three globular modules ghA, ghB and ghC.
Conclusion: The CDRs of A1 showed structural similarity to a globular autoepitope of C1q and structurally mimicked the ghA sequence GSEAD suggested as a cross-epitope between anti-DNA and anti-C1q antibodies.
Acknowledgement. The experimental work was financed by Grant DN01/9 of the Bulgarian NSF.

IMMUNOSUPPRESSIVE CYTOKINES SECRETED BY MESENCHYMAL STEM CELLS

Dobroslav Kyurkchiev

Laboratory of Clinical immunology, University hospital “St. Ivan Rilski”
Department of Clinical laboratory and clinical immunology, MF, Medical university of Sofia

University of Plovdiv "Paisii Hilendarski"
Faculty of Chemistry

11-th Chemistry Conference (11CC)
11 – 13 October 2018, Plovdiv

Book of abstracts

ONE-POT SYNTESIS OF FORMAMIDE-BASED PREBIOTIC COMPOUNDS AFTER HEATING AND PROTON IRRADIATION

V. Enchev[1], I. Angelov[1], N. Markova[1], N. Stoyanova[1], M. Kapralov[2], E. Krasavin[2], M. Rangelov[1], L. Avramov[3]

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Understanding the formation of biogenic molecules in abiotic conditions is a prerequisite in the origin-of-life studies. Determining the conditions allowing an efficient one-pot synthesis of the largest possible panel of biogenic compounds may shed light on the plausible scenario in which the processes that started life might have occurred. We report experiments describing the syntheses taking place from formamide. The warming of formamide at 170°C and 180°C in vacuo yielded large panels of different compounds: purine and nucleobases (adenine, cytosine and uracil), amino acids (glycine, alanine), hypoxanthine, pterine, urea and urocanic acid. After that to model the Solar Wind radiation, these probes were irradiated at 25°C with 170 MeV protons generated by the Phasotron facility of the Joint International Nuclear Institute (Dubna, Russia). The absorbed dose was 6 Gy. New panel of compounds was detected: timine, 2-methylpurine, 6-methylpurine, 4-methylcytosine and one nucleoside – 6-carboxamido-9-β-D-ribofuranosylpurine. Mechanism of reactions affording nucleic bases and amino acids were simulated by high-level (MP2 and SCS-MP2) ab initio quantum chemical methods.

Acknowledgements: Financial support from the grant DN09/7/2016 of the National Science Fund, Bulgaria, is greatly acknowledged.

11th International Congress on Autoimmunity

Lisbon, Portugal, 16-20 May 2018

Program Book



AUTO1-0220
SHORT ORAL DISCUSSION 20 - COMPLEMENT IN AUTOIMMUNITY (STATION 2)

ANTI-IDIOTYPE scFv GENERATED AS STRUCTURAL ANALOGUES OF C1q GLOBULAR AUTOEPITOPES

I. Tsacheva[1], N. Todorova[2], M. Rangelov[3], V. Stoyanova[4], G. Nikolova[5], H. Georgiev[6], S. Mohedin[1], V. Bogoeva[7]
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Background

The serum protein C1q is an autoantigen in several autoimmune disorders in humans, most notably in systemic lupus erythematosus (SLE). Yet the immunogenic stimulus for the development of anti-C1q autoantibodies is still unknown.

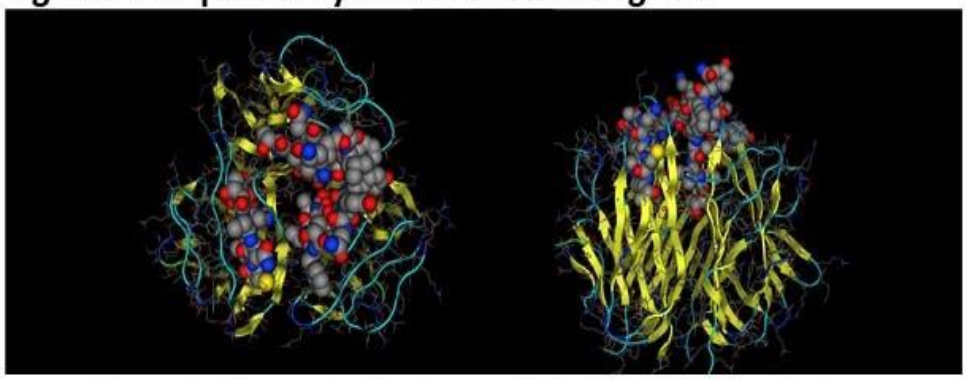
Method

We addressed that issue by studying the structural features of C1q autoepitopes that are recognized by the polyclonal anti-C1q. We used six fractions of anti-C1q with presumed different epitope specificities as antigens for the generation of anti-idiotypic scFv antibodies from the phage library “Griffin1”. The six fractions of anti-C1q were affinity purified from previously characterized Lupus Nephritis (LN) sera.

Results

The monoclonal scFv A1 was found to have approximately 50 % inhibitory capacity on the recognition of C1q by the LN autoantibodies. It was sequenced and *in silico* folded into a 3D structure which was superimposed on the crystalized 3D structure of the globular domain of C1q thus revealing a structural homology with the globular fragments of all three types of polypeptide chains comprising C1q, designated
ghA, ghB and ghC (fig1)

Figure 1. C1q mimicry of scFv A1 CDR regions



Based on the loop similarity model, all of the three CDR regions of scFv V_H have analogs in the apex of native gC1q, which exhibit marked differences in their surface patterns, with respect to both charged and hydrophobic residues.

. The V_H CDR2 of A1 structurally mimicked the ghA sequence GSEAD suggested as a cross-epitope between anti-DNA and anti-C1q antibodies (table1). The scFv A1 was further revealed to inhibit the recognition of ghA by the LN autoantibodies.

Table 1. Loop similarity between scFv A1 and C1q

CDR1	H		G	G	S	F	S	G	Y	Y	
Ac1q		55-60	L	S	Q	W	E	I	C	L	
Bc1q		82-91	D	Y	A	Y	N	T	F	Q	V
Cc1q		79	H	T	S	K	T	N	Q	V	
CDR2	H		I	N	H	S	G	S	T		
Ac1q		121-128	D	A	E	S	G	Q	Y	I	
Bc1q		116-123	G	N	E	G	A	N	S	I	
Cc1q		56-63	A	S	H	T	A	N	L	C	
CDR3	H		A	R	S	H	S	A	A		
Ac1q		81-88	T	T	N	K	G	L	F	Q	
Bc1q		36-43	A	S	S	R	G	N	L	C	
Cc1q		112-119	V	G	I	Q	G	S	D	S	

R,H,K -> positively charged in darker gray; D,E -> negatively charged in dark gray; S,T,N,Q,P,C -> polar uncharged (H-bonds) in gray; G,A,V,I,L,M,F,Y,W -> hydrophobic in light gray.

Conclusion This data suggests that scFv A1 is a structural analogue to a globular autoepitope of C1q and can be further subjected to *in vivo* functional analysis. Other potential inhibitors are the monoclonal scFv F6, F9 and A12.

Acknowledgement. The experimental work was financed by Grant DN01/9 of the Bulgarian NSF.

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LALS

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POSTER 17:

Raman spectroscopy of prebiotic compounds obtained after proton irradiation of formamide used as precursor of meteorite-catalyzed synthesis

E. Borisova[1,3], L. Avramov[1], V. Enchev[2], I. Angelov[2], M. Ranglov[2], D. Bratashov[3], D. Gorin[3], M. Kapralov[4], E. Krasavin[4], R. Saladino[5]

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01100 Viterbo, Italy

Formamide (NH2CHO) is becoming one of the most intensively studied precursors for prebiotic syntheses of compounds potentially relevant for the origin of life. [1] It is discussed as a possible parential molecule for synthesis of prebiotic molecules under proton irradiation, mimicking open space conditions. Different mineral content of meteorites allow variety of possible catalytic actions that would force such synthesis. The products of these processes could be detected using highly sensitive techniques for investigation of trace quantities of compounds, such as Raman spectroscopy method.

A liquid formamide had been irradiated by high-energy proton beams in the presence of powdered meteorites from several different sources with variable properties and mineral content, and the products of the catalyzed resulting syntheses were analyzed by Raman spectroscopy technique, which is an extremely sensitive spectral tool for detection of organic matter. The meteorites tested were representative of the four major classes: iron, stony iron, chondrites, and achondrites. In the irradiated samples were observed Raman signals from amino acids, carboxylic acids, and sugars, which correspond to some earlier investigations, when mass-spectrometry approach was applied [2].

This investigation is a part at answering the central question of the problem of the production of the prebiotic compounds underlying the formation of the living systems. Research is focused on the development of unified theoretical and experimental approaches taking into account the influence of the following factors: energy, evolution, protometabolic, and the primordial environment — on the origin of life. We are looking for a sequence of processes that can lead to the formation of a complete, chemically active prebiotic system. Raman spectroscopy could be used as a fast and non-destructive complementary tool for evaluation of

synthesized prebiotic molecules in such “metheorite+proton irradiation + formamide” model system. The obtained results could contribute to the general understanding of the origin of life.

Acknowledgements:

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Студентска Научна Сесия 2018

АНТИКОНВУЛСИВНА АКТИВНОСТ НА НОВИ МЕЛАТОНИНОВИ АНАЛОЗИ

Надежда Янакиева

Катедра Химия

Виолина Т. Ангелова[1], Мирослав Рангелов[2], Николай Василев[2], Надежда Тодорова[2], Павлина Андреева-Гатева[3], Яна Чекаларова[4]

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Синтезирани са серия нови индолови производни и тяхната антиконвулсивна активност и невротоксичност са определени *in vivo* чрез максимален електрошок тест (MES тест), 6 Hz тест и ротарод тест при мишки.

Базирайки се на проучването, че мелатониновите рецептори MT1 и MT2 са нова потенциална цел за разработването на антиконвиусивни средства, е създаден фармакофорният модел, целящ създаване на потенциални кандидати за лекарства, насочени към този рецептор. Използвана е обширна база данни от лекарствени молекули, взаимодействащи с мелатониновия MT1 рецептор. Полученият модел съдържа 5 фармакофорни региона и дава важна информация за активността на лигандите, както и за формата, местоположението на донора на Н-връзка и акцепторите на Н-връзки. Избрани са 11 съединения с висок афинитет на свързване с рецептора като крайни хитове и са подложени на биологичен скрининг.

Антиконвулсантните ефекти на новосинтезираните съединения бяха по-високи или съизмерими с тези на мелатонина при MES теста. Нито едно съединение не показа невротоксичност при рота-род теста. Съединението с най-висока активност при 6 Hz теста съдържа *p*-Cl-фенилов фрагмент (ED_{50}=13.98 mg.kg^{-1}, PI>21.46). Съединението с 2-тиофенов фрагмент показа високи активности както при MES теста (ED_{50}=108,7 mg.kg^{-1}, PI>2.76), така и при 6 Hz теста (ED_{50}=96.36 mg.kg^{-1}, PI>3.11), а 2-фурановият заместител в ароилхидразоновата част води до висока активност само при 6Hz теста (ED_{50}=38.8 mg.kg^{-1}, PI>7.89).

Тези резултати водят до заключението, че серията индолови производни заслужава по-обширно проучване при различни модели на епилепсия. Необходими са допълнителни изследвания, за да бъдат установявени антиконвулсивните механизми на действие.



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FORMAMIDE-BASED PREBIOTIC CHEMISTRY OF NUCLEOBASES AND AMINO ACIDS

V. Enchev[1], I. Angelov[1], N. Markova[1], N. Stoyanova[1], I. Dimcheva[2] , M. Rangelov[1], L. Avramov[3]

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One of the main challenges in re-establishing the conditions in which life is supposed to have originated is the generation of precursors in an abiotic environment. Understanding the formation of biogenic molecules in abiotic conditions is a prerequisite in the origin-of-life studies. Determining the conditions allowing an efficient one-pot synthesis of the largest possible panel of biogenic compounds may shed light on the plausible scenario in which the processes that started life might have occurred. The formamide-based synthetic system proved to be particularly robust. This idea has been supported by the detection of sufficient amounts of formamide in the interstellar regions with dense molecular clouds and in the process of formation of new stars. We report experiments describing the syntheses taking place from formamide. Large panels of different compounds were observed after standatd and microwave heating – nucleobases (adenine, cytosine, uracil), amino acids (glycine, alanine), hypoxanthine, pterine, purine, urea and urocanic acid. To study the potential mechanisms of the reactions leading to nucleic bases and amino acids high-level ab initio quantum chemical methods (MP2 and SCS-MP2) were used.

Acknowledgements: Funding of this work by the National Science Fund, under Grant DN09/7/2016 is gratefully acknowledged.

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ABSTRACT BOOK

Essays on Ecosystem and Environmental Research



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ABSTRACT BOOK

Essays on Ecosystems and Environmental Research

Editors:

Prof. Hysen Mankolli, Albania, Prof. Sukru Dursun, Turkey,
Prof. Massimo Zuchetti, Italy, Prof. Cezar Kongoli, USA

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092	GEOBOTANIC CHARACTERISTICS OF VEGETATION IN THE BAIKAL STATE BIOSPHERE RESERVE	Elena Martusova[1], Alexander Sizykh[2*], Alexey Shekhovtsov[3]	[1]Baikal State Biosphere Reserve, 671220, st. Tankhoi 34, Buryat Republic, Russia; [2*]Siberian Institute of Plant Physiology, SB RAS, 664033, Irkutsk, Lermontova str., 132, Russia; [3]V.B. Sochava Institute of Geography SB RAS, 664033, Irkutsk, Ulan-Batorskaya str., 1, Russia;	**Russia**
111	SPATIAL-DYNAMIC CHANGES OF FORESTS STRUCTURES IN THE GREEN ZONE OF IRKUTSK CITY FOR LAST DECADES (South -West Pre-Baikal)	Alexander Sizykh[*], Ruslan Moritz	Siberian Institute of Plant Physiology and Biochemistry SB RAS, 664033, Irkutsk, Lermontova str., 132, Russia	**Russia**

INTERNATIONAL CONFERENCE OF ECOSYSTEMS

ICE2019, 8 June 2019

Hello everyone

Dear professors, researchers, and friends, today we hold this international conference with research and studies with focus on ecosystems.
The research centers on the environment components, energy, climate, soil, water, air, physics, biology and chemistry. We study factors of Biodiversity, Forests, Environment protection, health of ecosystems and many more.
I am so happy to see you all here today.
Let me thank all participants from more than 12 universities Turkey, Kosovo, Ukraine, Albania, Germany and USA;

Thank you for your attention and support for this conference.
I hope for a good success of ICE2019.

And now Prof. Vjollca Ibro, from Agricultural Universiy, Albania will speak.
Next Prof. Sukru Dursun, from Turkey;
Next Prof. Cezar Kongoli, from USA;
Next Prof. Altin Dori, from Albania;
Next Prof. Luydmilla Symochko, Uzhhorid National University, Ukraine;
Next Prof. Elez Krasniqi, from University of Prishtina, Kosovo;
Next Prof. Flora Merko, from Alexander Mosiu University, Albania;
Next Prof. Fatma Kunt, from Nexhmedin Erbakan, Turkey;

Now it is time to continue with the first session…

ICE 2018 Organizing Committee
Organizer of the Conference
Prof. Dr. Hysen MANKOLLI,
International Journal of Ecosystems and Ecology Science (IJEES); Health and Environment Association, Tirana Albania;
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https://sites.google.com/site/environmenthealthassociation/7th-international-conference-of-ecosystems-tirana-albania
http://ijees.net/

Good morning everyone,

Honorable members of the Organizing Committee and the Scientific Committee of the International Conference of Ecosystems,

Dear Prof. Mankolli,

Dear colleges and friends,

I feel happy and honored, at the same time, to take the floor to speak at the opening ceremony of the 9-th International Conference of Ecosystems.

The conference has been going on in Tirana for nearly a decade.
This event gathers researchers from several countries, not just the region, but also the wider. They have the possibility to present and to discuss here the results of their scientific works in the very important fields like environment, agriculture, food and so on.
As a participant of several years in this conference, I can say with conviction that its scientific level has come rising year after year.

I'm a professor at Agricultural University of Tirana, one of the oldest and the best universities in Albania. Considering the teaching programs and fields of research, our university in reality is a life sciences university.

I teach Plant Physiology for Study Programs like Agro-environment and Ecology, Plant Production and Agro-mechanization.
I try to aware the students, that we live in a time, when global pollution has become a threat and, Agriculture is a factor and at the same time, a victim of it.
In the age when we live and especially for the future, we have to face the challenges of growing food demand, but also the risk of fall in yields, due to the impact of biotic and a/biotic stresses related with climatic changes.

I appreciate the organizers of the conference very much, for the selected topics. Also, I thank you for choosing Tirana for the development of its works. Among others, this has facilitated the participation of many young researchers, Master & PhD students with limited economic opportunities.

The conference's topics for years have been closely linked to the challenges of time in the region and wider. I believe that, the participants with their works will contribute somehow to their struggle and to improve the lifestyle of humankind in harmony with all ecosystems.

Thank you

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ICE2019 ABSTRACTS

001 NEW ADVANCED MATERIALS FOR ENERGY PRODUCTION WITH FUSION REACTORS

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ABSTRACT

Energy meant as heat and electricity has a crucial role in our every day's life; during the years its demand has increased because of the increase in the average wellness of our modern society. The second half of the XX century saw the birth of the nuclear industry, but after the eighties it did not spread as expected. Reasons dealing with radioactive safety and waste management can be quoted to explain this stagnation. Nuclear fusion is considered a valid option to solve the energy demand permanently. Generally speaking, fusion energy is considered a clean energy source, with no NOx and COx emissions, no risk of core melt, no proliferation and a limited amount of radioactive waste. Moreover, considering the potential energy output downstream the fusion reaction, it looks practically infinite source of energy. The high temperature and the high neutron flux in fusion reactors require the most advanced materials, characterized by good irradiation resistance, enough strength to withstand such extremes conditions, proper thermal conductivity to transfer the heat efficiently, proper compatibility with the coolant and breeders. So far, alloys such as the Reduced Activation Ferritic (RAF) steels, the Reduced Activation Ferritic-Martensitic (RAFM) steels and the Vanadium alloys have been developed with the aim to meet the mentioned criterion. Among the RAFM there is the Oxide Dispersed Strengthened steel, (ODS), a high performances alloy designed in the early eighties in order to dispose, during the decommissioning of a nuclear plant, wastes with lower radioactivity: thus elements with long half life, such as Niobium and Molybdenum have been replaced by elements with way shorter half life such as tungsten, vanadium and titanium. According to some studies, this alloy has a ductile-brittle transition temperature (DBTT) depending on the chromium weight% and apparently the best compromise between strength and toughness is with a Cr weight% from 9 to 10. Its creep strength seems to be sensible to the tungsten content in the alloy, since it increases proportionally for weight% of W up to 2%; beyond this threshold positive variation in the DBTT have been observed. Apart from structural materials, fusion reactors need breeding materials in order to produce by themselves their

own tritium, starting from Li-bearing materials. At the PlasmaScience and Fusion Center (PSFC) of the Massachusetts Institute of Technology (MIT) an innovative design was created: ARC, the Affordable Robust Compact reactor. ARC achieve its compactness partially due to the presence of High Temperature Superconductors (HTS) for the magnetic confinement and the use of molten salt Lithium-Fluoride, Beryllium-Fluoride (FLIBE) as coolant, neutron shield, and tritium breeder. FLIBE has the characteristic of extremely high boiling point (abou t 1700 K) which guarantees a single-phase flow. As an electrical conducting fluid, MHD flows can be encountered in FLiBe.The flow inside breeding blanket channels can be very complex and results in high pressuredrops, especially when the channels are also made by electrically conducting materials. The knowledge of fluid velocity profile, pressure drop and prediction of thermal heat fluxes are of considerable interest for blanket design.

Key words: new advanced materials, energy production, fusion reactors, energy

002 PARTICLE MATTER POLLUTION OF BOSNIA DISTRICT OF KONYA CITY

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ABSTRACT

Rapid population growth, urbanization, plans and industrialization and migration to the city in the recent century. since the beginning of the world is the most important problems. Konya city Turkey during last 2-3-decade, important province pile pollution has increased a median. Air pollution, which started to be effective after 1975 in Konya, is the most important question of the city today. Konya Metropolitan Municipality Environmental Protection and Control Department's regulation on the subject continues air pollution follows: It is important to board of directors with air pollution. The air quality measuring devices of Konya city are monitored on the regularly and are also shared online for the public to follow. In addition, the appearance of polluting sources influences the causes of a pollutant (Industry, Traffic and Domestic Business) in the city. For this purpose, the project of Modelling Air Quality and Creating Clean Air Action Plans was launched in 2017. Air Pollution Monitoring project results, which were prepared and completed in 2009, are aimed to be prepared and already underway. It focusses on reducing airborne levels towards this goal, we evaluate it in every dimension and implement the explanation. Bosnia district of the Konya is the most fast-growing part with parallel to increasing university student in the region. In this study atmospheric particle matter levels were investigated and modelled. Form the results of this study, source of air pollution will be investigated.

Keywords: Air Pollution, Particle Matter, Bosnia District, Konya, Atmosphere, Modelleing

003 SOIL MICROBIOME OF FOREST ECOSYSTEMS: DIVERSITY AND FUNCTIONAL CHARACTERISTICS

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ABSTRACT

Primeval forests are ideal ecosystems to study the interaction of bacteria, fungi, and archaea with their abiotic environment. In the Transcarpathian region of Ukraine exist a unique opportunity for studying the biodiversity and natural processes of primeval forest ecosystems, i.e. forests that have never been significantly modified by human activity. The region covers an area of about 53,650 ha and became part of the World Network of Biospheres Reserves of UNESCO in 1992. However, it should be noted that the attention of researchers focused mainly on studies of flora and fauna biodiversity and almost never directed to the ecological study of soil microbial communities. Due to this fact, the purpose of the research was to study soil microbiome of primeval forest ecosystems. The diversity of soil microorganisms varies with the height of the habitat above sea level and depends on the age and type of wood species. The number of ammonifying bacteria with increasing height decreased, minimum content was at an altitude of 1.100 meters above sea level. Fluctuations of number micromycetes were not as significant as bacteria, but in edaphotops located within 500-800 meters, their biodiversity was higher than at other sampling points. Rebuilding the functional structure of soil microbiome due to the influence of exogenous factors, cause changes in the direction of microbiological processes. Soil of forest ecosystems was characterized by relatively low level of phytotoxic activity. Study of authentic soil microbiota creates the necessary prerequisites for the conservation of microbial diversity and forming the base of the eco-microbiological monitoring.

Key words: microbiome, forest, soil, ecosystem.

004 RELATIONS BETWEEN INDUSTRIAL POLICY AND ENVIRONMENT: CASE STUDY OF NORTH MACEDONIA

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ABSTRACT

Contemporary industrial policy has to be environmentally friendly policy. Industrial policy is complex policy that involves many other spheres such as: environment, transport, economy, energy, agriculture, education, social protection and many other spheres. In this paper the main attention is on relation between industrial policy and the environment. Almost all industrial sectors manufacture products that causes environmental threats and degradation in all phases of their life circulations: projecting, designing, preparation and fitting the raw materials and parts on the final product, energy consumption, manufacturing, assembling, sorting and storage of final products, primary, packaging, transport, loading and unloading, usage and on the end of life cycle of products, reuse, recycling and other forms of recovery and dumping as a least favorable way of waste management. This produces a number of threats for the environment and contributes to the water, air and soil pollution. Industrial policy is closely linked with the integrated product policy which is a relatively new policy. European Union is one of the world leaders in the field on environment and endeavors to environmentally friendly industrial policy policy. The EU adopts legal regulation, strategies and plans that promote this policy but also makes strong efforts its practical implementation.
The Republic North Macedonia is candidate state for the membership of the EU since 2005 and expects to start the negotiation with the EU. North Macedonia started with the implementation of the EU environmental regulation in 2004 and permanently works towards the harmonization of its regulation with the EU regulation. This regulation stipulates the standards which aim to the environmentally friendly industrial policy. Also, there are adopted the strategic documents in the field on the industrial policy. The problems appear in the practical implementation and the industrial sector is still not completely environmentally friendly and seriously contributes to the degradation of the environment, particularly the air quality. The main aims of this paper are to analyze the industrial policy in Macedonia from the aspects of environment and the links between environment and industrial sector and compare it with the EU conditions. Additional aim is to give some recommendations.

Key words: environment, industrial policy, regulation, inspection, European Union.

005 CONCENTRATION OF SOME METALS (PB, ZN, FE, CU, CD, NI) IN THE TOPSOIL AND HAY IN THE THREE VILLAGES OF FORMER LEAD AND ZINC SMELTER "TREPÇA" IN MITROVICË REGION

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ABSTRACT

The aim of this study was the evaluation of concentration of Pb,Zn,Fe,Cu,Ni, and Cd in the topsoil and hay in Kelmend, Boletin and Zhazhë villages situated in different distances (1.0; 2,0; and 5.0 km) from former lead and zinc smelter "Trepça"- contaminated area, and in the Koliq village 40 km fare away from smelter area. For this purpose 60 topsoil samples and 62 samples are collected in Kelmend (15; 15), Boletin (5;5), Zhazhë (20;22) and in Koliq village (20;20). The soil Pb concentration in the villages of contaminated area (Kelmend, Boletin and Zhazhë) was significantly higher ($P < 0.001$) in comparison with the concentration in the soil of Koliq. There was also established significantly higher concentration of Pb in the soil of Kelmend in comparison with Pb concentration in the soil of Zhazhë ($P< 0.001$), and Boletin (**$P< 0.05$**). Zn concentration in the topsoil of Kelmend was significantly higher compared Zn concentration in soil of Boletin and Zhazhë ($P< 0.01$), and Koliq ($P<0.001$). Zn concentration in the soil of Zhazhë is significantly higher ($P<0.001$) compared with Zn concentration in Koliq. Cu concentration in the soil of Kelmend villages is significantly higher in comparison with Cu concentration in the soil of Zhazhë ($P<0.001$), and Boletin ($P<0.02$). Cd concentration in soil of Boletin and Kelmend is significantly higher ($P<0.001$), in comparison with Cd concentration in Koliq and Zhazhë. Ni concentration in the soil in Koliq is significantly higher ($P<0.001$), in comparison with Ni concentration in Zazhë, Boletin and Kelmend. Pb concentration in the hay of Kelmend and Boletin was significantly higher ($P<0.01$) in comparison in Zhazhë and Koliq. Zn concentration in the hay of Kelmend in significantly higher ($P<0.001$), compared with Zn concentration in Koliq, Boletin and Zhazhë. Cu concentration in the hay of Kelmend, Boletin and Zhazhë is significantly higher ($P<0.001$), compared with Cu concentration in Koliq. Cu concentration in the hay of Zhazhë is significantly higher ($P<0.004$), compared with Cu concentration in Kelmend. Cd concentration in the hay of Boletin is significantly higher ($P<0.01$), compared with Cd concentration Boletin. Ni concentration in the hay of all localities was approximately equivalent. Fe concentration was detected only in the hay of all delaminated localities and there **was** no statically a difference of concentration between groups. There was established significantly between Zn concentration in soil on hay ($r=0.738$; $P<0.001$).

Key words: Metals, Concentration, Soil, Hay, Smelter "Trepça"

006 EVALUATION OF A GLOBAL SNOW DEPTH ANALYSIS BASED ON OPTIMAL INTERPOLATION

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ABSTRACT

Assimilation of snowpack observations into Numerical Weather Prediction (NWP) models represents a key component that impacts the accuracy of predicted meteorological parameters. NOAA's National Centers for Environmental Prediction (NCEP) operational NWP models routinely assimilate observations of snow depth and snow cover area to improve snow model initializations. A new snow depth analysis based on optimal interpolation method has been developed with improved spatial resolution compared to the existing analysis and the capability to assimilate both satellite and station snow depth. An essential component and assumption of the analysis are the spatial correlation functions and scales of snow depth distribution with respect to horizontal distance and elevation. Based on these correlation functions and the predetermined data errors, snow depth from the surrounding stations are weighted to compute an analysis snow depth estimate. This study presents an accuracy assessment of the analysis over North America that uses correlation scales currently adopted in operational snow analysis at world's major weather and climate prediction centers: an e-folding scale of 120 km for horizontal distance and an e-folding scale of 800 m for elevation. Snow depth data to drive and evaluate the analysis are obtained from the Global Historical Climatology Network (GHCN) during the 2016-2017 winter season. Snow depth from NOAA's Global Forecast System (GFS) was used as first guess. It was found that a range of 600 km is sufficient for a near complete coverage of analysis over North America in areas with sparse in-situ measurements available for interpolation. The analysis improves first guess estimates substantially over relatively flat areas. However, improvements are smaller, and the accuracy is much lower over high-elevation terrain, mainly attributed to inaccurate e-folding scales used for interpolation.

Key words: evaluation, global snow depth, analysis optimal interpolation, NOAA

007 ENVIRONMENTAL IMPACTS OF OIL ACTIVITIES IN THE FRAGILE VAL D'AGRI ECOSYSTEM, BASILICATA, SOUTHERN ITALY

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ABSTRACT

Since the start in the nineties of oil production in the agricultural Val d'Agri (Basilicata, Southern Italy), one of the most fragile european territories, sector's contribution to the economy of this italian region came at a huge environmental disaster and cost, involving recurrent spills that resulted in the spewing of oil and wastewater into a sensitive ecosystem. Gas emissions in the air from the Val d'Agri Oil Center (COVA) contributed to degradation of the fragile agricultural and water-rich Val d'Agri ecosystem and to damage to the human health. Impacts are related to: 1) a widespread pollution of soil and groundwater due to leakages at the Val d'Agri Oil Center (COVA) from thanks of crude oil flowing towards the nearby Pertusillo freshwater reservoir, that provides water to human use for millions of people. At least 400 tons of crude oil spilled probably since 2009, contaminating 26,000 m^2 of soil, underground and groundwater; 2) contamination by hydrocarbons and metals of the Pertusillo waters and sediments; 3) leakages from underground of red fluids contaminated by hydrocarbons and metals that flow from the margins into the Pertusillo reservoir; 4) gray, warm, saline, aluminum-rich groundwater flowing on agricultural soils at 1,8 km from the Costa Molina 2 oil wastewater injection well, contaminated by hydrocarbons, metals (lead, aluminum, iron, manganese, vanadium, zinc, ecc.), sodium, phenols, surfactants, ecc., typical of oil wastewater; 5) air pollution produced by COVA emissions, that caused an excess of mortality and hospitalization due to cardio-respiratory diseases in the adiacent areas of Grumento Nova and Viggiano; 6) several episodes of water eutrophication in the Pertusillo reservoir, favoured by the huge nitrogen emissions in air at COVA, and by the downwind location of the water reservoir.

Key words: environmental impacts, oil production, agricultural Val d'Agri, Basilicata, Southern Italy

008 BIOETHANOL IN TURKEY

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ABSTRACT

In accordance with the estimates, fossil fuels are decreasing in the world, but these fuels will continue to be the dominant sources until 2040. The share of renewable energy resources in 2040 is expected to be 16.1%. Similarly, it is expected that global electricity demand will increase up to 80%, by 2.3% rate annually, by 2040. In the light of all these considerations, renewable energies stand out for energy solutions all over the world. In this scope, one of the liquid biofuels, bioethanol is a good energy alternative not only for Turkey's energy future and agriculture, but also the world's as well. Sugar beet is the most convenient and efficient agricultural raw material source for bioethanol production. As the use of bioethanol production increases in Turkey, sugar beet production for bioethanol will increase, gradually. The production of biofuels from agricultural products and the energy agriculture that develops in agriculture sector is a rapidly growing in the world. Developed countries produce a significant portion of the energy in their own countries to meet their energy needs from agricultural products at an increasing rate. In this way, it is ensured that fossil fuels with limited reserves, which are known to have negative effects on the environment, will be used in less amounts and the income of the agricultural sector will be increased by producing high value-added products. In this study, one of the significant biofuels, bioethanol has been examined and its potential, technologies, importance and the latest situation in Turkey investigated. Also, it is aimed to support Turkey's one of the most important energy policies, which is to increase the production of domestic and renewable energies.

Keywords: Renewable Energy, Biomass, Biofuel, Bioethanol, Turkey

009 EDUCATION FOR SUSTAINABLE DEVELOPMENT IN THE CURRICULUM OF PRIMARY EDUCATION IN THE NORTH MACEDONIA

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ABSTRACT

The education for sustainable development (ESD) in the curricula affirms to foster students' ability to take part in promoting sustainable development. A number of studies show that the implementation of sustainable development is highly demanding for teachers and requires specific knowledge and abilities. Therefore, it is important to determine what competencies teachers need in order to develop and implement education for sustainable development and to attain specific educational goals with their students. ESD requires a specific and more constructive focus on teaching, which raises the question of building corresponding competencies in teachers' education. In this paper we present the results from a research carried out in primary schools in the Republic of North Macedonia aiming to assess the level of teachers' competencies with respect to ESD (in this research our target were teachers of natural sciences). The objective of the study is to explore the perceptions and views on teachers' competencies in relation to education for sustainable development. For this purpose as research instrument we have designed and applied an online questionnaire on separate samples for teachers and students. We used the results obtained from the empirical analysis to find solutions for raising awareness among teachers to develop competences for ESD in order to be more present in the teaching process, as well as integrating of ESD within the existing curricula. The recommendations given in this paper on the development of competences for education for sustainable development derived from the results of this research relate not only to teachers in natural sciences, but to all teachers involved in primary and secondary education.

Keywords: education for sustainable development (ESD), ESD competencies, science curriculum.

010 MOLDOVA'S CODRY – PRIORITY REGION FOR BIODIVERSITY CONSERVATION

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ABSTRACT

One of the priority regions of biodiversity conservation in the Republic of Moldova is the Central Region of Codry, where unlike other regions, the share of natural ecosystems is satisfactory and their functionality is relatively optimal. In this context, ten protected natural areas, which are part of the Codry Forest District from Moldovan Central Plateau, were included in the researches.These areas belong to the following categories of protection: Monuments of Nature, Forest Natural Reservations and Landscape Reservations. The study is based on field and laboratory researches. The ecosystems were evaluated in the main phenological development phases of vegetation and animal life. The diversity of flora and fauna has been established. The emphasis is placed on assessing the valuable species of flora and fauna protected in these areas and their abundance. As a result of the researches it was found that each of the evaluated areas has its role in preserving certain valuable species. As a component part of the same forest massif, similarly for the researched areas is the protection of the precious sectors with forest vegetation and the conservation the flora and fauna specific for the Codry area. The presence of certain rare species only in some reservations and their absence in others makes the difference between the valuable biological potential of the researched areas. A greater diversity of rare flora and fauna species has been recorded in Landscape Reservations.

Key words: Moldova's forests Codry, biodiversity conservation, natural protected areas, rare species, abundance.

011 INTRODUCING HERBAL MEDICINE INTO CONVENTIONAL HEALTH CARE

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ABSTRACT

Ayurveda, the traditional Indian medicinal system remains the most ancient yet living traditions with sound philosophical and experimental basis. It is a science of life with a holistic approach to health and personalized medicine. It is known to be a complete medical system that comprised physical, psychological, philosophical, ethical, and spiritual health. In Ayurveda, each cell is considered to be inherently an essential expression of pure intelligence hence called self-healing science. In addition, to the self-healing concept, the use of herbal treatment is equally important in this Indian traditional system of medicine. According to the World Health Organization, about 70–80% of the world populations rely on nonconventional medicines mainly of herbal sources in their healthcare. Public interest for the treatment with complementary and alternative medicine is mainly due to increased side effects in synthetic drugs, lack of curative treatment for several chronic diseases, high cost of new drugs, microbial resistance, and emerging diseases, etc Ayurvedic treatment is although highly effective; proper mode of action, pharmacology, pharmacokinetics, and pharmacovigilance of many important Ayurvedic drugs are still not fully explored. Moreover, the comprehensive knowledge of the basic ideologies of Ayurveda is poorly acceptable scientifically due to lack of evidence. In the modern time, when the Western medicinal system is reached almost at the top because of validated research and advanced techniques, there is an urgent need to validate basic principles as well as drugs used in the ayurvedic system of medicine with the help of advanced research methodology. Therefore, advancements in the ongoing research methodology are highly required for the promotion of Ayurveda.

Key words: herbal medicine, conventional health care

012 **THE COMBINATION OF NEURAL THERAPY WITH OZONE THERAPY IN SILENT INFLAMMATION (I.V. / I.A APPLICATIONS)**

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ABSTRACT

Ozone treatment is used in general practice mainly in the "great self-blood therapy." The application as a local treatment method is also established in the bag fumigation. Now, there are recurrent cases of persistent pain in the shoulders, hip joints or bursae, which under a local treatment with injections improve suprisingly. With the help of cases, I show you that the cause of such chronic pain is often the infection with borellia and their coinfections, and how the strategy for sustainable treatment of this germ spectrum can be Neural therapy.

Key words: ozone treatment, ozone therapy, neural therapy

013 EVALUATION OF TOXIC AND GENOTOXIC EFFECTS OF ROUNDUP AFTER DIRECT AND INDIRECT TREATMENT

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ABSTRACT

Roundup (glyphosate) is one of the most widely used systemic, non-selective herbicide in the world. Numerous studies exist about its genotoxic effect both in "*in vivo"* and in "*in vitro"* using various concentrations and endpoints. Based on the contradictory results we decided to investigate the toxic effect of concentrations of roundup used in the agriculture after direct treatment in *Hordeum vulgare* and in human lymphocytes as well as indirect applying S10 fraction from barley seedlings affected by the herbicide. ICP analysis of soil (granulometry and pH also) was performed in order to confirm the lack of harmful substances for plants and for demonstration of equal initial chemical condition of both treated and untreated fields, so manifested effects on test-system could be a result from roundup treatment. Morphometric method was used in barley grown from M1 seedlings treated with the herbicide. Cytogenetic methods were used to test cytotoxic/genotoxic effect of roundup on lymphocytes, where the cells were directly treated with the herbicide and indirectly, using S10 of barley pre-treated with roundup. Morphometric data showed high inhibitory effect in barley leaves and roots after roundup application. The herbicide also induced high cytotoxic/ genotoxic activities after direct treatment of lymphocytes. S10 fraction of barley grown from seedlings affected with the herbicide induced yield of injuries that are close to that detected after direct treatment with roundup, but with lower concentration (0.9 µg/ml). Clearly harmful effect of roundup not only after direct but also after indirect treatment was observed, and its use need to be rethought.

Keywords: Roundup, cytotoxic and genotoxic activities, *H. vulgare*, human lymphocytes *in vitro*

014 VASCULAR FLORA ON THE SERPENTINES OF ZATRIQI SURROUNDINGS (ZATRIQ-DRENOC-RAHOVEC), MUNICIPALITY OF RAHOVEC

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ABSTRACT

In this paper we present the results of research on the vascular flora of the serpentine terrain of Zatriqi surroundings (Zatriq-Drenoc-Rahovec), Rahoveci Municipality in the southwestern part the Republic of Kosovo. Research is conducted in 2015 with some additions until 2019. Based on preliminary phytocenologic data and interesting flora of serpentine terrain of Kosovo we decided to conduct this research which will result in a rather detailed dexcription of vascular flora. The explored area belongs to the hilly-mountainous area, the substratum is on a serpentine rocky base, while the climate is dominated by the continental climate. In the explored space from the floral aspect, although the substrate is unsuitable for growth and development of plant species, there are considerable number of plant species to be found. It is worth mentioning in this case and serpentines express the current state of the flora of the aforementioned space. Vascular flora of Zatriq and its surroundings, characterize flora in particular taxonomic presence of relict and endemic species of Balkan floristic element. Within the vascular flora a particular site has threatened plant species based on the IUCN criteria, presented in the Red Book of Vascular Flora of the Republic of Kosovo. In the syntaxonomic aspect, the researched area is dominated by plant species that form the phytocenoses of the orders *Quercetalia pubescentis* Br. Bl. (1931 n. nud.) 1932 and *Halacsyetalia sendtneri* H. Ritter-Studnicka 1970.

Key words: Natural ecosystems, Zatriq, Vascular flora, Endemic plants, Threatened plants, Republic of Kosovo.

015 PREPARATION OF AG-NI DOPED TIO_2 NANOMATERIALS COATED ON GLASS SURFACE WITH SOL-GEL METHOD

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ABSTRACT

Nowadays nanomaterials gain great importance owing to their broad usage in many fields such as material science, medicine and health, environment, energy, computer, industry and agriculture. Nanomaterials are defined as the structures whose sizes change between 1 to 100 nm. There are several methods developed for producing these materials such as sol-gel, wet impregnation, arc discharge, hydrothermal process, inert gas condensation and aerosol process. Sol-gel, one of the mostly used and easy to apply method that is a wet chemical method to produce both powder and coated nanomaterials. Sol-gel procedure based on the dissolving of metal precursor into a solvent and keeping the mixing for a certain time. Temperature, pH, mixing speed are really important factors affecting the final product materials. After sol is produced, it can be either gelated and dried to produce powder or coated and heated to produce coated nanomaterials. In this recent study, the preparation procedure of Ag-Ni doped TiO_2 nanomaterials coated on glass sheet surface which is a modified photocatalyst material was explained. Production of Ag-Ni doped TiO_2 consists of three main steps such as preparation of sol (Titanium-n-butoxide, Ni $(NO_3)_2$ and $AgNO_3$ used as precursor), coating of glass surface with sol (dip coating), heating of glass in high temperatures (calcination at 600 ^oC). From XRD diffraction and EDX analysis, crystal structure, size of nanoparticles and elemental percentage of doped elements was detected. According to these results, anatase form TiO_2 was produced with 5% of Ag and 0.5% of Ni doping. The average of almost 20 nm size nanomaterials was obtained.

Keywords: Nanomaterials, sol-gel, dip coating, TiO_2, doped TiO_2, Ag, Ni

016 CREDIBILITY OF INFORMATION SOURCES USED BY ARTISANAL FISHERS IN SELECTED COASTAL STATES OF NIGERIA

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ABSTRACT

A study on credibility of information sources used by artisanal fishers in selected coastal states of Nigeria was carried out between January 2018 and December 2018. The study focused on Bayelsa, Rivers and Akwa Ibom states, Nigeria in West Africa. Data was obtained from primary sources using questionnaire. Descriptive and inferential statistical analysis was employed. The result indicates that majority of the artisanal fishers were male (79.90%) and 43% of the fishers falls within the age bracket of between 41 – 50 years. About 5.2% have been engaged in fishing activities for the past 15 years and above, while 88% of the artisanal fishers had one form of education or the other. Majority of artisanal fishers (55%) earn monthly income of between ₦11,000-₦50,000 ($30 – $130). The low income earned by fishers have negative effect on their livelihood. The most credible sources of information were: Fishers groups (75%), credit agencies (66.5%), output buyers (55.2%) and cell phones (50.9%). From the study, it is obvious that artisanal fishers need credible information in nearly all the coastal areas of Nigeria to improve the fishing industry which could eventually improve their livelihood.

Key word: accessibility, artisanal fishers, credibility, dissemination, fishing, information source.

017 STUDY ON MANURE SILKWORMS AND ARBUSCULAR MYCORRHIZAL FUNGI TO PROMOTE GROWTH AND YIELD OF MARIGOLD IN ALKALINE SOILS

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ABSTRACT

Effects of manure from silkworms and arbuscular mycorrhizal fungi (AMF) to promote growth and yield of marigold in alkaline soils was studied. The experimental designed was done into completely randomized design (CRD) consists of four treatments and three replications namely 1) no fertilizer application 2) manure from silkworms applied 3) arbuscular mycorrhizal applied 4) combination of manure from silkworms and arbuscular mycorrhizal applied. The experiment was conducted between August 9th to December 9th 2017 at the Nong-Kwang Higher Education Academic Training Centre, Buriram Rajabhat University, Muang Buriram, Thailand. Anova and mean comparison were analyzed for plant growth namely plant height, number of pairs of leaf, number of shoot tip and yield namely number of flower, size of flower. The result showed that using of combination of manure from silkworms and arbuscular mycorrhizal had highly significant increase plant height ($p<0.01$), number of shoot tip($p<0.01$) and size of flower($p<0.01$). The result indicated that the combination of of manure from silkworms and arbuscular mycorrhizal could promote growth and yield of marigold in alkali soil.

Keywords: AMF, manure, silkworms, marigold

018 IN VIVO USE OF WATERMELON SEEDS

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ABSTRACT

It is possible to evaluate agricultural products from seed to shell. Watermelon (*Citrullus lanatus*) is an important vegetable species made in the world farming watermelon, Cucubitaceae is a plant belonging to the family. It is aimed to determine the effect of watermelon seed which is natural waste on nutrition (directly and indirectly by consumption). For this purpose, the nutrients of the model organism (*Drosophila melanogaster*) were fed by mixing the watermelon seed (0.1-10%). Survival rate and development time of the insect is determined. Besides the use of watermelon seeds as an alternative by-product, the impact on living beings as a waste is discussed.

Keywords: *Drosophila melanogaster*, *Citrullus lanatus*, survival rate, development time

019 CRITICALLY ENDANGERED PLANTS BY IUCN PRESENTS IN PASHTRIK, THE REPUBLIC OF KOSOVO

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ABSTRACT

Based on the research on the Pashtriku Mountain in the period 2000-2019, it results with floristic diversity with great interest for the natural heritage of the Republic of Kosovo. Special floristic values represent the endemic species of the Balkan florist element as well as the presence of threatened species which are protected by law. During the final phase of the detailed analysis of Pashtriku's vascular flora (2016-2019), we have also analyzed the state of the threatened plant species. Within the plant species of vascular flora which are evaluated according to IUCN criteria are also categorized species as Critically endangered species. In this paper we will present results about the threatened condition of the species: *Adonis microcarpa, Berberis vulgaris, Coronilla vaginalis, Fritillaria graeca, Klasea radiata*, *Onosma visianii* and *Solenanthus krasniqii*. These plant species according to the IUCN criteria were previously evaluated in 2013 in the Red Book of Vascular Flora of the Republic of Kosovo.

Key words: Natural Ecosystems, Pashtrik, Vascular Flora, Threatened Plants, Republic of Kosovo.

020 CLIMATE LIMITATIONS OF THE BEECH (*FAGUS SYLVATICA*) WITHIN THE REPUBLIC OF MOLDOVA TERRITORY

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ABSTRACT

Beech forests in the Republic of Moldova represent their East areal in the spatial distribution within Europe and occupy about 400 ha. In the trend of unfavorable changes in the climate conditions (summer mean temperature has increased, while the annual rainfall has shown a decreasing trend in Moldova) beech stands are face to climatic constraints in their distribution and development. Therefore, based on a set of climatic indices (Forest Aridity Index – FAI; DeMartonne Index – IM; Ellenberg Quotient – EQ; and Beech tolerance index - Q_{BTI}) was explain causes of beech surface decreasing in Moldova. The competitiveness of beech is limited by increasing water stress and it is replaced by forests consist of more drought-tolerant species. Per general, beech stands in Moldova, are growing in climatic conditions expressed by FAI values between 5.8-7.5; IM values greater than 32.0; EQ values - 27.0-30.0 and Q_{BTI} values - 15.0-17.0 units. Vitality of beech in "Plaiul Fagului" and "Codrii" Reservations (areas that include almost all beech stands from our country) is negatively affected by the impact of biotic and anthropic factors, and from abiotic factors - climate aridization leaves more and more fingerprints in the compositional structure of the forest ecosystems in the region.

Key words: climate indices, xeric limit, beech stands, distribution area.

021 A COMPARATIVE ACCOUNT OF DETRITUS FOOD CHAIN AROUND VIRGIN AND RECLAIMED ISLANDS OF SUNDARBAN ESTUARINE MANGROVE ECOSYSTEM, INDIA: A MODELLING STUDY

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ABSTRACT

Decomposition and subsequent remineralisation of mangrove detritus is essential in nutrient dynamics within the forest as well as in offshore system. A five-compartment model of detritus food chain dynamics has been developed for surrounding water of both virgin and reclaimed islands of mangrove estuarine creeks of Sundarban. The model simulates concentration of nutrient, biomass of phytoplankton, zooplankton, detritus and detritivorous fishes. Almost 70% of the detritus formed in the soil was being washed in the estuarine water to act as source or sink of nutrient for the primary producers of aquatic food chain. Increased detrital nitrogen values in the post monsoon months, estimated from the field study, denotes probable accumulation of nitrogen due to anthropogenic run-off specially around reclaimed islands. Comparisons of simulated and observed results demonstrated that detritus food chain along with plankton populations in the estuary can be adequately modelled by accounting for plant production, litter decomposition and export to the adjacent estuarine water, and allochthonous input of minerals and organic matter. Model sensitivity analysis shows the most sensitive parameters for the parameters under consideration. The model has been calibrated and validated using field data accordingly. Increased detrital nitrogen values in the post monsoon months, assists the growth and high yield of detritivorous fishes in winter season as found in simulated and field observations. Comparison of simulated and observed results demonstrated the dependence of phytoplankton growth is a function of nutrient concentration and zooplankton grazing. Model results also show the dependence of detritivorous fishes on detritus which is a function of detritus biomass. Inturn, detritus biomass is dependent upon several factors like mortality of phoplankton, zooplankton, and detrivorous fishes; and chiefly on litter biomass and litter decomposition. Comparative study of nutrient cycling around pristine islands demonstrate significant difference in production of population biomass during annual cycles effecting the food chain dynamics.

Key words: food chain, virgin, mangrove ecosystem, mortality, zooplankton, detrivorous fishes, India;

022 CHALLENGES FOR HOSPITAL ENERGY EFFICIENCY IN ALBANIA

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ABSTRACT

This paper aims to make an analysis of energy consumption and energy efficiency for hospitals in Albania. Hospitals represent one of the most complex building typology from the energy consumption point of view. A brief presentation of Albanian health sector is given and then main focus is oriented to regional and municipal hospitals. Energy auditing is made for 10 hospitals selected from all climate zones of Albania. An analysis of building structure, technical systems and thermal comfort is given. Electricity represent the main energy source followed by diesel oil and pellet. Are identified and analysed factors that influence energy consumption. Measures to identify opportunities to improve energy efficiency are presented. Are proposed eligible investments aiming at increasing energy efficiency, reduction of energy losses and, in general, at a more rational production, distribution and/or use of energy. Also are introduced energy management systems and/or automatic controls and measuring systems on energy supply side. Following energy audit, a list of prioritized energy conservation measures requiring further consideration are drawn up, indicating the energy saving for each one, the respective investment required and providing a cost-benefit analysis, showing both economic and financial indicators.

Keywords: energy efficiency, hospitals, energy consumption, heating, cooling.

023 THE IMPACT OF GOVERNMENT DECISIONS ON IMPROVING THE ECOSYSTEM

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ABSTRACT

Many people around the world carry out various activities for environmental protection. But in the meantime, we should not forget that there are others who try to use the environment simply for their private interests. It should be noted that conservation and care for the environment is not merely a social obligation but is also an individual responsibility as the society and individuals care about the management of natural resources, aiming at their inadequate use, so that these resources are useful not only for today's society, but also for future generations. Sustainable environmental development means rational use of natural environmental resources in order to improve people's lives today and tomorrow. This can be achieved by carrying out a good management of renewable natural resources such as water, soil, solar energy, wind energy, etc. For this reason, the Albanian government has undertaken an initiative to realize the project of 100 villages. By improving the water distribution system, it enables farmers to develop areas without water resources. Another government initiative to reduce air pollution is the introduction of ecological cars for state police. But today, the developed and civilized world faces many other environmental issues such as high pollution, erosion of ecosystem balances, uncontrolled use of natural resources, etc. In this paper will be studied by statistical techniques the impact of government decisions regarding preservation of eco-system values.

Keywords: ecosystem, ecological cars, development project, air pollution.

024 SUSTAINABILITY RATINGS IN HIGHER EDUCATIONS

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ABSTRACT

Sustainability and green life concepts have been confused. However, in recent decades, sustainability has been getting better understood and implemented among universities. Sustainability in universities is very similar to cities' which is based on economic, social and environmental foundations. It is obvious that achieving sustainability in these areas will have a wide range of benefits. However, there are also many secondary benefits for the higher education institutions such as prestige and reputation. Physical and mental health of students, academicians and employees increase as well as their success and happiness level. The aim of the study is to reveal expected outcomes of the universities that will compete in the sustainability field. In this study, sustainable practices have been researched, and rewards are discussed in economic, social and environmental aspects for universities. These practices are limited with climate, energy, waste, water, transportation and education since sustainability is a very broad concept. In this context two universities are compared. Michigan State University is the one with the gold rating in the Sustainability Tracking, Assessment and Rating System (STARS) and the other one is new player in the field, Selcuk university. Both universities are similar in size, academic departments and climate. STARS is used as a reference assessment system because of its transparency in assessments and publicly accessible data.

* This study has been derived from first authors MSc Thesis.

Key words: Campus sustainability, sustainability assessment, sustainability rewards, ratings, STARS

025 COASTAL FLORISTIC INVASION IN ALBANIA

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ABSTRACT

Albania is characterized by a rich biological diversity, is particularly vulnerable to the threats posed by alien invasive species. The spread of invasive alien species is creating complex and far-reaching challenges that threaten both the natural biological riches of the earth and the well-being of our people. While the problem is global, the nature and severity of the impacts on society, economic life, health, and natural heritage are distributed unevenly across nations and regions. Some aspects of the global invasive alien species (IAS) problem require solutions tailored to the specific values, needs, and priorities of nations while others call for consolidated action by the larger world community. Preventing the international movement of invasive alien species and coordinating a timely and effective response to invasions requires cooperation and collaboration among governments, economic sectors, non-governmental organizations, and international treaty organizations. Many features have been attributed to invasive species and invaded ecosystems, but none are universal and invasive species tend to have a suite of traits rather than all of them. The large numbers of alien organisms introduced into Albania do not generally endanger the biodiversity on a large scale.

Key-words: alien species, invasive alien species (IAS), introduction, intentional introduction, establishment.

027 CAN WATER OLIGOCHAETES BE USED IN DETERMINATION OF ECOLOGICAL STATUS AND POTENTIAL OF STANDING WATER BODIES?

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ABSTRACT

The aim of the present study is to assess the implementing of the metric "%Oligochaeta" for assessment of the ecological status and potential of standing water bodies. The survey was based on published and unpublished data. Samples were taken during 2003; 2007; 2011; 2012; 2013 and 2017 in the littoral zone of standing water bodies in Bulgaria. Studied sites referred to eco-regions Eastern Balkan and Pontic Province and belong to different types of stagnant water bodies, according to the adopted national typology of freshwater bodies (Ordinance No 4/2013). Qualitative samples of benthic macroinvertebrates were taken according to the standard ISO/EN/BDS methods. An adapted version of the multi-habitat sampling method was applied. The species composition and abundance of the macrozoobenthos were measured and further "%Oligochaeta" was calculated. The index was designed to characterize the abundance of the macrozoobenthic fauna in lakes and reservoirs and it was experimentally tested and standardized for the purpose of developing a classification system for assessment of the ecological status/potential of different types of surface water bodies. The Oligochaeta fauna of the studied stagnant water bodies, both lakes and reservoirs, was composed of tolerant species, easily adaptive to different environmental conditions including anthropogenic impacts. Water oligochaetes and the index itself have a great potential for hydrobiological assessments, but the vast typological diversity of standing water bodies in Bulgaria, that include artificial and highly modified surface water bodies, and their intensive economic use, does not give enough statistically reliable confirmations, so further research is needed to build up more data and conclusions.

Keywords: lakes, %Oligochaeta index, abundance, water quality

028 THE INTEGRATING ECOLOGICAL URBAN ENVIRONMENTAL PERFORMANCE CRITERIA IN URBAN DESIGN STUDIOUS OF UNIVERSITY STUDENTS

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ABSTRACT

Nowadays one of the most important environmental problems of our world is climate change, which is closely related to the urban environment. As to Roaf buildings as a part of habitat are defined fundamental basis ecology and sustainability. Urban plans combine both urban and functional, technical designs and these urban environmental relations. The application knowledge and skills of urban planners that are the ecological environmental performance criteria are too important for setting of environmental quality. Therefore, ecological urban environmental performance criteria and urban planning department's students' sensitive environmental values became the two keys concepts of this research. This paper discusses the applications sustainable design in last grade of undergraduate design studio. Especially it is determined the visual perceptions of university students of urban planning about ecological urban environment and nature related to human and nature relationships. Four students from the 30-person design studio chose the topic of ecological urban growth as a research topic. In the regional and local urban environment scale, students' projects was evaluated as climate analysis, field resources analysis, performance evaluation of form options, solar control and shading, daylight analysis and whole building energy use. In this study the NEP analysis on the sample of 12% of the class and the thematic ideas of the projects were compared in terms of urban environmental design principles. Thus, the effectiveness of urban environmental performance criteria in planning discipline was evaluated.

Keywords: Urban planning, Ecological urban environment performance criteria, New Environmental Paradigm's scale (NEP scales)

029 THE EVALUATION OF PERCEPTIONS' SUSTAINABLE RURAL AND URBAN INTERFACE OF THE URBAN INHABITANTS IN THE PERIPHERY OF KONYA

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ABSTRACT

The continuity of rural and urban space is the main problem area of the urban environment. Ecological based spatial modeling of rural urban continuity defines urban growth strategies. In this context, environmental consciousness of the city living in the periphery is one of the important indicators of the sustainability of the ecological structure of the urban environment in the periphery. In this study, urban land use behaviors and expectations of the inhabitants of Konya city Kayacık and Tatlıcak villages will be evaluated by NEP scale analysis method. In this study, 5-point Likert-scale NEP analysis of nature-centered and human-centered land use approaches to sample size in 10% of both village population is examined and it is examining environmentally sensitive behaviors.

Keywords: Konya peri-urbanisation, Urban environment identity, nature centered perception, human centered environmental perception.

030 GENETIC AREAS OF SHARRI MOUNTAINS (KOSOVA)

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ABSTRACT

Sharri Mountain lies between the Depression of Dukagjin in the north-west, Kosovo field in the north-east, Drenica Depression in the north and Depression of Polog in Macedonia in the South. The Sharri Mountains is 80 km long and 25 km wide. Its morphology is characterized by a high mountain peaks and steep slopes with the minimum quota of 400-500 to the maximum quota of over 2500m. Hydrographic network of Sharr Mountains is characterized by many streams and rivers sources that flow into the basin of River Lepenci and basin of River Lumëbardhi. As regards the climate it is characterized by several types of climate: mountain climate, continental climate, Mediterranean climate and the variable continental climate. The average annual temperatures move from minimum of -1.4 ºC and up to -2.8ºC while higher average temperature 18.1º C - 20.6º C until significant changes are recorded in the change of seasons (in April-May and September-October). An average annual rainfall is 800-900 mm. Sharri area tectonically belongs to Sharr Korab Tectonic zone (SKZ). Geological basement constructed from crystal formation Pz-shale and rock originating from magma deposits Granitic up to the new Quaternary. The total area of the National Park of Sharri Mountains is 227.60 km^2. Genetic areas which include the National Park and its periphery have an area of 577.12 km^2 which is divided into three subzones.
1. Sub-zone I - Lumëbardhi Prizren (192.06km2);
2. Sub-zone II Korish - Mushtisht (111.76km2);
3. Sub-zone II Lepenci (273.29km2);
Forests and bush deemed to cover over 60% of this area. Less surface area of pastures and meadows (30%) and even fewer have the field of gardens (5%) and non-productive land (5%). Based on current research in the Sharr mountains they are inventoried about 1,000 types of flora, since research has not been completed, it is assumed that the number of species expected to be approximately 2,100. Kosovo vegetation is classified in 139 associations, 63 alliances, 35 orders and 20 classes. The richest areas with fauna in Kosovo are in the Sharr where it is estimated that there are 8 species of fish, 13 amphibian, 12 species of elusory 154 species of birds, 37 species of mammals and 147 species of butterflies daily. Conflicts facing this area are: Conservation Park and tourism, exploitation of resources natural resources, monuments-historic geo-monument, inappropriate expansion of infrastructure towards the park, illegal constructions, use of uncontrolled forest, damage to flora and local fauna, etc. Economic development needs of the region through tourism and the preservation of the national park, there are two issues that various specialists should be taken seriously in order to design an integrated management plan of the area taking into account all relevant factors

Key words: Genetic areas, Conservation Park, Natural resources, Tourism, Sharri Mountain.

033 DETERMINATİON OF PARTICULATE MATTER AND NOISE LEVELS OF TRAFFIC IN KONYA

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ABSTRACT

"Air Pollution" is defined as the increase of pollutants in the atmosphere such as dust, gas, smoke, odor and impure water vapor to the amounts that will affect the health of the creatures in a negative way. Measures that can be taken against air pollution are quite different according to pollution source. Various air pollutants in the atmosphere are formed by natural or human sources. Today, air pollution has become a serious problem especially in big cities in countries that are industrialized in the advanced level. Every year, an estimated 3 million people in the world lose their lives because of air pollution. 90% of deaths from air pollution are seen in developing countries. In addition to the air polluting gases, the second major air pollutants are suspended particulate matter. Particulates are substances in the atmosphere or in a gaseous mass that are solid or liquid in size greater than 0,0002 μm and smaller than 500 μm. Atmospheric PM is a complex mixture of elemental and organic carbon, ammonium, nitrate, sulfate, mineral dust, trace elements and water. The types and properties of the particles present in the air vary depending on the source, shape, size, size distribution, shape, density, specific components they contain, and the medium in which they are dispersed. When such pollutants are inhaled by air, they can enter the human body and cause respiratory system diseases. Noise, by definition, is the voice reaching harmful and disturbing levels to the health of man and other living things. Loud music, television sound, loud voice over the phone, noisy traffic, sounds we often hear in everyday life, and sounds that our ears do not tolerate. However, from time to time these voices cause the surge to transcend the state of being voiced. The voices started to bother us. The problems that cause the noise are solitary; difficulty in hearing, lack of coverage. In addition to all these disturbances, sleeping is also affected. In this study, Konya's air pollution and noise pollution will be interpreted by considering PM_{10} and noise values which are taken in Meram, Karatay and Selçuklu districts of Konya.

Keywords: Noise pollution, Particulate matter, Traffic, Soundplan, Konya.

035 DETERMINATION OF THE CHERRY DISEASES WITH A SPECIAL EMPHASIS ON THE STAINING OF THE CHERRY LEAVES *(Blumeriella jaapi)*

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ABSTRACT

In this paper was done a research on cherry diseases Blumeria jappi and the spreading of acro-ecological conditions of Anamorava region during the whole year. In this research was included staining of the leaves in cherry trees–Blumeria japi and some other diseases of the Anamorava region during the whole year. During the research of the varieties of the cherry Obllaqina and Keleris 14 we have achieved these results. The Pathogen Stigmina Carpophila to the two varieties of the cherry tree is presented in the second week of the month of June with a frequences of 1 stain as an average for one sample to the variety Obllaqine and 6 stains to the variery Keleris. The maximum number of leave stains of this pathogen in both varieties was concluded in the last week of the month of August with 21 respectively 57 stains to the varieties Obllaqina and Keleris. The frequency of the occurrence of other diseases in different varieties of the cherry trees was also different throughout the vegetation period Alternaria was present in the first week of June, whereas the highest intensity to the variety Obllaqina, 5 stains in the first and second week of July, respectively in the first week of the month of September to the variety Keleris with 23 stains. From the variance analysis table and LSD testing , it can be seen that statistical differences of the different levels of signification were concluded between two varieties of chery trees included in the experiment, Obllaqina and Keleris.
The largest number of the leaf stains on average is ascertained in the variety Keleris 14.42 whereas the smaller number in the variety Obllaqin 4,39. In this regard we say that the variety Keleris has been mostly affected by the different pathogens, whereas Obllaqina was a variety that has been the least affected by the different pathogens. A considerable number of the authors such as Susuri and Myrta 2012 ,Agrios ,2015 ,Ciancio and Mukerji 2008 in theior works have shown the varying degree of sensitivity of different varieties, not only to a cherry tree but also other types of fruits from the group of seeds and the core, so the staining of cherry leaves but as well as against other diseases. In this regard, our research findings are in line with the research of these authors. Regarding the type of pathogen found, the largest number of stains were found at B .Japi, 559 stains , while the lowest at Monilinia laxa, 47 stains . Number of stains found on the leaves by Alternaria spp and S, Carpophilla was 209 respectively 389 graf 2 ,the average frequency of stains of the diseases caused by different pathogens to the various types of cherry trees was different Tab 2. From the variance analysis table and LSD testing , it can be seen that statistical differences of the different levels of signification were concluded between two varieties of chery trees included in the experiment, Obllaqina and Keleris. The largest number of the leaf stains on average is ascertained in the variety Keleris 14.42 whereas the smaller number in the variety Obllaqin 4,39. In this regard we say that the variety Keleris has been mostly affected by the different pathogens, whereas Obllaqina was a variety that has been the least affected by the different pathogens.

Key words: Diseases ,Pathogen, stains, varieties ,leaves, food, climatic and earth conditions etc.

038 EVALUATION OF BLENDED SNOW DEPTH PRODUCTS: CASE STUDY

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ABSTRACT

Snow information – Snow Cover Area, Snow Depth and Snow Water Equivalent (SWE) - is an important input to numerical weather and climate prediction models. NOAA has a variety of snow products including those based on satellite passive microwave sensors such as JPSS AMSR2 and ATMS. The objective of this project is to evaluate the performance of satellite-based snow products over regions that have sparse in-situ data. Of special interest and mountain regions and remote areas including those over US and elsewhere. To accomplish the goal of the project, the following activities will be carried out: Collect regional historical snow data not available via public networks. Do a quantitative evaluation of the snow products using in-situ data. Ecology is the study of the complex ways that living things interact with their environment Deciduous plants handle the lack of water by shedding their leaves, which tend to evaporate water into the air. During cold winter months, most deciduous plants drop their leaves and go dormant. Evergreen plants keep their foliage, but their leaves and needles have a thick, waxy coatings to reduce water loss. In areas that receive frequent snow and may have cold weather year-round, such as in the Arctic, plants have adapted in other ways. Trees may grow close to the ground or grow in shapes that help them shed heavy snow more easily. Plants may hold onto dead leaves for insulation or use deep snow like a blanket to protect against the cold. Some evergreens also have a special valve in their cells. This valve automatically seals off individual frozen cells to prevent a chain reaction of freezing. Satellites are well suited to the measurement of snow cover because the high albedo of snow presents a good contrast with most other natural surfaces except clouds.

Key words: evaluation, snow depth products, climate prediction models.

041 COMPARISON OF THE AREA AND THE NUMBER OF LEAVES OF SOME CULTIVARS AND ROOTSTOCKS OF APPLES IN ANAMORAVA'S REGION.

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ABSTRACT

In the paper are researched the number and the surface of leaves in some combination of cultivars and rootstocks of apples in six cultivars, three of them new cultivars that are planed for the first time in egro-ecological conditions of the Anamorava's region in the past two years. In the research are involved; Diameter of trunk 20 cm on the grafting place, complete heigh of the tree; heigh of the trunk, height of the crown and width of the crown. During the research: Mondial Gala, Red Chiet, on the rootstock MM 106, Pinova on the rootstocks MM 104, Jonagold, Granny Smith, Golden Deishes on rootstock M 9, we achieved the folloqing results: Based on the variencesanalyses at the difference of trunk diameter between the two measurements were found significant differences only between Granny cultivar and Gala cultivar. The results of our research are not consistent with the results of Trillot at al. 2003, while they partly match with the results of Zajmi 1986. From the data presented in tab. 11 at the total height of the tree it is seen that the combination of greater rage during 2008 is the Pinova cultivar on rootstock MM 104 with an avarage worth 207.3 cm while the smallest is the combination golden Delishesi Clone B on the rootstock M9 worth 181 cm. Regarding to the height of the trunk again appears to be with higher calue the Pinova cultivar 58.1 while the smallest value the Red Chief on MM 106 worth 49.5 cm, while in other combinations is about 51 cm. When it comes to the height of the crown again Pinova combination on MM 1004 has reached higher value of 149.1 cm and smaller Granny Smith combination on M 9 worth 127.1 cm. Regarding the width of the crown both directions north - south and east - west again from tab. it is obvious that Pinova combination on MM 104 has achieved greater width of the crown (north - south 85.68 cm, east - west 82.15 cm) and smaller worth of the crown has achieved combination of Golden Delisher Clone B on rootstock M 9 (63.05 cm north-south and east-west 65.60 cm) which means that have been expressed inherent properties as well as the rootstock cultivar. When these data compared to author Zajmi 1985 data, for the total height of the trunk, are lower maybe because author Zajmi conducted his research in the end of the fifth vegetation and the most sensational rootstock, respectively M 26, while our research belong to the third and fourth vegetation on rootstock M9.

Key words: surface of the leaf, number of leaves, leaf surface per sqm, cultivar, rootstock.

045 WATER QUALITY AND DIVERSITY OF FISHES AND ALGAL MEMBERS IN RIVER SWAT KHYBER PAKHTUN KHWA PAKISTAN

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ABSTRACT

In the present study the extent of heavy metals contamination such as Iron, Copper, Lead, Manganese and Zinc in the water of river Swat has been assessed. Fresh water contaminations pose several serious risks to human health. River Swat serves as a main source of drinking water, agricultural activities and fishing in Swat and adjacent areas. Since there are no formal control measures of wastes into the river Swat, it is important to study the metals contaminant in it, thus assessing its suitability for domestic and agricultural use. In the present study different physio-chemical parameters and heavy metals in water in ten different sites of river Swat, Pakistan were evaluated. For this, the water samples were collected from each sampling station from January 2011 to January 2012.In these samples different Physio-chemical parameter alkalinity, hardness, pH, electrical conductivity and total dissolve solid were studied. Similarly, the heavy metals profile of Pb, Zn, Mn, Cu and Fe were determined in water by using atomic absorption spectrophotometer (AAS). The Food chain of aquatic flora, fauna is clearly disturbed showing impact clearly. The biomass of producers disturb leads to a clear deficiency in weakness of osteoicthyes by reduce fins.

Key words: water quality, diversity of fishes, algal members, river, Pakistan

050 **BLOOD LEAD LEVEL (BLL) AND Δ-AMINOLEVULINIC ACID DEHYDRATASE (Δ -ALAD) ACTIVITY, HEMATOCRIT VALUE (HCT) AND HEMOGLOBIN AMOUNT (HB) OF RESIDENTS LIVING NEAR FORMER LEAD AND ZINC SMELTER "TREPÇA" IN KOSOVO**

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ABSTRACT

The Mitrovica district was the most polluted area with heavy metals caused for decades from lead and zinc smelter "Trepça". The aim of this study was the evaluation of effects of such contamination in the BLL and δ -ALAD activity in residents of Boletin village situated 2 km far from smelter "Trepça" and residents of Koliq village 40 km far from smelter un-contaminated area. BLL in the adult residents (female and male) of Boletin was significantly higher ($P<0.001$; 13.0± 4.7 µg/kg) in comparison with that in the blood (8.0± 2.9 µg/kg) of residents of Koliq. The δ -ALAD activity in the blood of Boletin residents was significantly depressed ($P<0.001$; 32.1±5.8 U/E) compared with δ -ALAD activity in the blood (61.4±17.1 U/E) of Koliq residents. There was established weak relationship between BLL and δ - ALAD activity ($r= -0.443$; $P<0.232$; $r= - 0.123$; $P<0.422$ respectively) in the residents of both localities. Hct value of Boletin residents was significantly higher ($P<0.001$; 51.0±5.6 %) compared with Hct value (39.0±4.2 %) in the residents of Koliq. The amount of Hb in the residence of Boletin is lower in (no significant difference) comparison with amount of Hb of residents of Koliq village. The results of this study suggest that δ -ALAD activity can be used as sensitive marker for evaluation of adverse effects of subclinical blood lead levels in adult persons, and the close vicinity of former "Trepça" smelter, 18 years after closing down still represent threat for health of residents of this area.

Keywords: Lead, Zinc, Blood, δ –ALAD, Hct, Hb, Trepça

055 ANALYSIS OF EMISSIONS FROM DIESEL PASSENGER CARS IN MACEDONIA

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ABSTRACT

The process of sharp increase in the presence of internal combustion diesel engines among passenger cars in the Macedonian fleet of vehicles, significantly increases its share in polluting emissions from the burning of diesel fuel in transport. Therefore, proper analysis and accurate calculation of emission factors from diesel passenger cars and their pollution emissions will be calculated through the Tier 2 method for emission calculations from the European Environmental Agency. This study is based on data obtained from official institutions and their adequate approximation obtained results which give us an approximate figure to the actual situation of pollution from passenger cars with diesel Internal combustion engines.

Key words: Diesel vehicles, Emission factor, Tier 2, Air Pollution

056 THE BIOCLIMATIC CLASSIFICATION OF MICROECOSYSTEM KORCA REGION IN ALBANIA

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ABSTRACT

The bio climate of one zone is considered as a combination between vegetation zone and climatic elements. The bio clime study on Korça - eco zone and the bioclimatic indexes give a view about the conception and using values of bio climate classification indexes. This study based on Emberger and FAO Model of learned Frenchman, which is the most quoted on studies with bioclimatic character on Mediterranean eco-zone for period 30 years. The Emberger Classification is known and applied, because it gives a detailed using about studied zone. The Emberger Classification is based on pluviometric index Q and vegetation index and gives a more detailed classification than others. After mathematic data processing and comparison of bioclimatic indexes according to respective classes is concluded that according to Emberger Korça – eco zone is classificated on three respective bio climates: Micro zone with semiarid bio climate with coefficient Q<60 and annual precipitations 400-600 mm per year, in which take parts: Sheqeras and Gurshqipe; Micro zone with sub humid bio climate with coefficient 60<Q<90 and annual precipitations 600-700 mm per year, in which take parts: Dvorani, Zvirina, Bilishti, Liqenas (Korça); Micro zone with humid bio climate with coefficient 90<Q<150 and annual precipitations over than 700 mm per year, in which take parts: Shtylla, Korita, Gjonbabasi, Vithkuqi, Voskopoja. Using of bioclimatic maps for agro-ecosystems construction on Korça zone; The change of precipitations amounts per every 100 m is oscillated from 40 to 60 mm;

Key words: microecosystem, classification, climatic data, indexes;

058 TOLERANCE OF LICHENS FROM PROTECTED AREAS TO THE CHANGES OF ENVIRONMENTAL FACTORS

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ABSTRACT

In the forest-petrophitic ecosystems of the middle course of the Dniester (right bank) the lichens from 9 protected areas belonging to 34 species were recorded. Of these 12 are rare species, 3 are included in the Moldova's Red Book (2015). It was established that for 10 species the ecological valences to the substrate, illumination and humidity are very narrow, so the ecological spectrum is very narrow. Among the 10 stenoic species 2 are included in the Red Book and 8 are rare, so these will be the first affected in the case of changes in the environmental components.

Keywords: lichens, ecological valences, natural ecosistems.

060 WHEAT PRODUCTION TRENDS IN SOME AREAS OF KOSOVO

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ABSTRACT

Wheat is the most precious herb of wheat cultivated in the Earth's world and meets 30% of the human body's needs with calories. Wheat in the Gjilan region is cultivated with a large area and in Kosovo is grown 80,000-100,000 ha with grain, and the yield is quite large where about every hectare is gained approximately 33.6 / ha. This study analyzes the growing grain production period in different regions of Kosovo such as Gjilan, Peja, Prishtina and Ferizaj. The method used is statistical. The results of the study show that wheat production in the areas studied does not have any statistically verified changes. This shows that ecological conditions in regions studied have a similar role in developing and producing wheat in Kosovo. The changes found are the result of other technical agro-factors.

Key words: tendency, production, wheat, area, Kosovo.

061 **ASSESSMENT OF POTENTIAL PHYTO- ANF GENOTOXICITY INDUCED BY SOME IMIDACLOPRID-BASED INSECTICIDES ON A NON-TARGET CROP AND HIGHER PLANT ASSAY**

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ABSTRACT

Environmental pollution issues due to increased use and often incorrect appliance of pesticides are harmful phenomena constantly encountered in developing countries as Albania. The current study assessed the toxicity induced by short-term exposure of seeds and bulbs of *Allium cepa* L. to commercial formulations of imidacloprid-based insecticides. The biological materials were exposed for 12, 24, 48 and 72 h to three experimental doses (1.5, 3 and 4.5 gr/L) of KOHINOR 200 SL, PULSAR 200 SL MALLET 20 SL and MIDAS. Phytotoxicity was determined through the limitation of seed germination capacity, reduction of longitudinal root growth and mitotic index, while genotoxicity inducement by scoring frequencies of micronuclei and chromosome abnormalities in root meristem. All evaluated parameters obviously varied in insecticide formulation-, concentration- and time exposure-dependent manner. The results detected suppression in seed germination and significant root growth restriction after 48 and 72 hour treatments, having EC_{50} values included into field applications for PULSAR and MIDAS. Additionally, the strongest mito-depressive activity was revealed since at the medium concentrations, incurring sublethal effect to meristematic cells. Excluding the lowest concentrations, the other tested ones could generally induce presence of micronuclei and significant frequencies of chromosomal abnormalities after 72 h exposure, revealing the confident genotoxic effects and potential mutagenicity of imidacloprid-based insecticides under study. This simulating investigation highlighted the capability of a common crop in Albanian agriculture and plant assay as onion in recognizing and predicting insecticides pollution and induction of environmental stress with probable deleterious consequences on food chain consumers and human population health.

Key words: Imidacloprid-based insecticides, *Allium cepa* L. assay, phytotoxiciry, genotoxicity, Albanian agriculture.

065 THE IMPACT OF TEMPERATURE CLIMATE FACTOR ON PRODUCTION OF WHEAT, IN GJILAN AREA, KOSOVO

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ABSTRACT

The influence of the ecological temperature factor on the developmental performance and the yield of wheat is known. The study in the Gjilan area shows us that there is a correlation between the weathering and the vegetative development phases and the wheat plant producer. The grain yield data for the 10-year period and the average temperature for each sub-period of the plant development in Gjilan, eco area indicate that the linkage between the climatic factor and production is apparent especially in the stages of germination and vegetation of the vegetative process. Based on the analytical results it is shown that significant changes in temperature give rise to the impact of the Wheat Plant.

Key words: temperature, production, wheat, area, Gjilan

068 *AEGILOPS* SEEDS GERMINABILITY AND THEIR SEEDLINGS DROUGHT SURVIVAL RATE

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ABSTRACT

Different species of *Aegilops* genus, as wild relatives of wheat, are used as valuable sources of genes for wheat improvement. The actual interest is to improve wheat tolerance to abiotic stresses like drought, heat, salinity and some diseases, too. The recent study compared eight *Aegilop*s accessions for their seeds germinability and their seedlings drought survival rate. The objective is to find out if exist any difference among them related these two traits and how these parameters correlate between them in different ear shape *Aegilops* accessions. The experimental probe was established as a completely randomized desighn with four replicates, at room conditions, in Crop Physiology Laboratory, AUT. Thirty seeds for each of eight Ae. accessions have been moistened with distilled water in Petri dishes (10 cm diameter). Seed germination was characterized by a standard germination test, based on the 1 mm root protrusion. Germinability was determined by counting the number of germinated seeds in a container and their seedling growth ability. The five week-old seedlings were subjected to drought by withholding water for 7 days. After irrigation was resumed, the survival rate was quantified one day later. This study provides that the conical shape ear accessions are superior in all seed parameters, including the seeds germinability, compared the cylindrical ear ones. The conical shape ear accessions seedlings drought survival rate was greater too. There were found positive strong correlations among seeds germinability and their seedlings drought survival rate for all *Aegilops* accessions taken in consideration.

Key words: *Aegilops accessions*, seed germinability, seedlings drought survival rate.

069 VARIATION OF PHYSICAL AND CHEMICAL PARAMETERS OF WASTEWATER POLLUTED OF URBAN WASTE IN MITROVICA, KOSOVO

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ABSTRACT

Any environmental pollution is associated with its effects on the host environment. The surface waters of the Iber River are a challenge that comes from the drainage of the wastewater of the urban waste dump. This paper aims to show the variations of the physical and chemical parameters of the polluted waters of the urban waste landfill in Mitrovica, as well as their impact on the water quality of the Iber River. To achieve the implementation of this survey, three monitoring stations were set up, from which water samples were collected for laboratory analysis at different time periods during 2017 - 2018. The physic - chemical analyzed parameters showed the following results: water temperature ranges from 15.7 °C to 23.3 °C, pH 7.5 to 8.2, electrical conductivity from 315 µS / cm to 5010 µS / cm, dissolved oxygen from 1.33 mg / l to 4.41 mg / l, from 3.3 mg / l to 358 mg / l, nitrates from 0.5 mg / l to 12.7 mg / l, etc. The values obtained through laboratory analyzes were compared to the values AI no. 30/2014, on limiting values for discharge of wastewater in the water body.

Keywords: Polluted water, variation, parameter, surface, physical-chemical etc.

070 THE IMPACT OF MARKETING ON ORNAMENTAL PLANT PRODUCTION BUSINESSES IN KOSOVO

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ABSTRACT

From the research we can conclude that marketing of floriculture is very important but insufficient in Kosovar businesses. The flower market in Kosovo is still not cheap at all, but it has to be said that it has recently made great strides in this direction. In practice, there are cases when individuals and businesses are not widely dedicated after marketing to expand businesses, although almost everyone thinks marketing is very important in this regard, as through marketing, consumers are introduced to the types of flowers that can meet their demands and desires. In general, the factors that have a profound impact on the floricultural market are: marketing and dedication to flowers, improving the different types of flowers, vertical integration of farms and finding new revenue alternatives that would affect profit growth, which is the purpose of any business. The application of advanced marketing, market research, increased assortment, variety differentiation and promotion, is almost incomplete in floricultural businesses. Businesses should be organized to take concrete measures in defense of their interests in the framework of deepening partnership with the Government of the country, to have adequate participation in the country's policy-making institutions. From the results we conclude that 60% of the respondents stated that the information on the sale of flowers is taken from social networks. Kosovar ornamental plant makers devote marketing importance to 27%, respondents think that applying marketing in the flower business brings benefits up to 86%, in the expansion of the flower market the quality is very important factor 92% of respondents were declared.

Keywords: flower, Industry in floricultura, marketing, Kosovo.

071 THE PLACE OF POPS IN THE CURRICULA OF PRIMARY SCHOOL, OUTDOOR LEARNING OF THIS ISSUE

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ABSTRACT

During last 5-years, the environmental education issue in the curricula of primary schools of Albania is increased up to 12 hours per year in the seven class of the primary education cycle. The students of this class do not have enough knowledge about Persistent Organic Pollutants (POPs) and consequently do not understand what they represent and the risks they pose to human health. Their traditional treatment has not been effective compared to their teaching in and through environment. In order to increase the understanding of these themes, we combined their theoretical classroom teaching with practical outdoor observations. During the last two years we applied the practical recognition of organic pollutants (POPs) at high intensity road crossings and the recognition of these substances in shops where the substances contained in these pollutants are sold. After that, the knowledge of the students on POPs was 58% higher than before teaching in and through the environment, making it so effective for students of seven classes.

Keywords: Primary school, curricula, POPs, environmental education

073 THE IMPORTANCE OF CALCULATING GREEN GDP IN ECONOMIC GROWTH OF A COUNTRY – CASE STUDY ALBANIA

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ABSTRACT

Gross domestic product (GDP) or gross national product (GNP), are commonly used to determine the economic performance of a whole country or region, to make international comparisons and to measure the produced output but they ignore the ingredients needed to generate such output like water and air. So, there is a general consensus that these indicators, (especially) according to the concepts of sustainable development and green growth, appear to be poor measurements. Environmental sustainability of economic growth has come to be recognized as one of the most important pillars of sustainable growth and development. Green GDP is an Index, an alternative indicator of economic growth that incorporates environmental consequences of that growth by including the depletion of natural resources and degradation of the environment, so it takes into consideration the environmental impacts on the productivity of the country. Taking in consideration that the main purposes of Green GDP accounting are used to provide a more correct measure of welfare and to examine the sustainability of the economy, we used this indicator to give our opinion for the importance of calculating green GDP in economic growth of Albania. We use the general scheme of calculation where the first deduction in DGP presents the costs of CO2 pollution (as CO2 emissions times carbon market price), second the opportunity costs of one tone of waste that could be used in the production of electrical energy), and a third is the adjusted savings of natural resource depletion as a percentage of the gross national income per country. Hence, we try to build an alternative Green GDP indicator that can give a clearer perspective on the consequences of economic progress by offering a new approach in quantifying the cost of ecological and environmental degradation in Albania. Not only will it evaluate the real costs of environmental damage, but it will also process some opportunity costs in Albania Case.

Keywords: Green GDP, Economic growth, Negative externalities, Environmental damage.

075 IMPACT OF ORNAMENTAL PLANTS IN THE ARCHITECTURE OF GREEN URBAN ENVIRONMENTS IN KOSOVO

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ABSTRACT

The interest and demands of people for ornamental plants in our country grows more and more physical and chemical properties of the earth, has removed man from nature by worsening the health and state of the environment, due to the expansion of urban areas, and especially large cities. Noise or high acoustic pollution from vehicle movements, and noise and other obstacles and its psychic and emotional pollution. Greening can, not meet all the needs of people for the requirements: aesthetic, health, etc., but it is always preferable to plant as many ornamental flowers as possible. In the last decade, the regulation of gardens in Kosovo also took an important step, and as a result, their role increased, especially in big cities such as: Prizren, Peja, Prishtina, etc. From our research we conclude that the impact of ornamental plants in the urban environment architecture in Kosovo is important, as opinion and positive response have been stated by 68% of the respondents stated, and 71% said that the architecture of the green areas in Kosovo. Regarding the survey of which cities of Kosovo devote most importance to ornamental flowers are citizens of Prizren, with 28%, with 44% of respondents think that landscape architecture is important for human health while 56% think it has an impact on the architecture of green urban environments. In our research 34% of respondents think that maintenance of gardens in green urban environments is difficult.

Keywords: Kosovo, ornamental plants, architecture, urban environments, garden.

077 FOOD AND MICROBIOLOGICAL ASSESSMENT

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ABSTRACT

Foods which are used from human, has been conducted on microbiological problems relating to the safety and spoilage of vegetables and fruits in recent years. Fruits and vegetables are among the richest products of vitamins, minerals and fiber. The ever-increasing demand for availability and consumption of these fresh products, along with the health aspect, has led to an increase in global fruit and vegetable trade. Contamination of fresh fruits and vegetables is a particular concern as many of these products are consumed alive without any prior processing, which would eliminate or reduce the biological, microbiological and physical hazards. Fruits and vegetables may be contaminated at any stage of growth, processing, trading, manipulation or preservation. Irregular farmers' practices are recognized as sources of microbiological contamination of vegetables Microbiological contamination can be done directly or indirectly by water, soil, chemicals or even insects. Such a thing would necessarily lead to a potential food security problem. Over the last few years, the presence of fresh fruit and vegetables in the country's various markets and markets has increased considerably. The consumer can find and consume these products regardless of time and season. Thus, the globalization of food products as a whole not only affects the distribution of different food products but also the spread of potential risks to human health from one region to another, thus enabling wider spread of pathogens anywhere in world. As a result, increasing the level of consumption of fruits and vegetables has also become an important tool in statistics on food-borne diseases. During these years, a number of gastrointestinal diseases and poisoning have been observed, related to the consumption of fruits and vegetables contaminated with bacteria pathogens such as *Listeria monocytogenes*, Salmonella, *Shigella sonnei* and Escerichia coli 0157, present in products such as peppers, carrots, cabbage etc. Given the fact that fruits and vegetables are produced in natural environments or in greenhouses, we can say that these products are very fragile to the contamination of human pathogens. The growing level of fruit and vegetable consumption has also led to an increase in the number of poisoning to consumers.

Keywords: foods, microbiological assessment, *Salmonella spp*., *Enterobacteriaceae.*

079 ASSESSMENT OF GENETIC RELATIONSHIPS AMONG MYRTLE POPULATION IN CENTRAL ALBANIA BY CHLOROPLASTIC MARKERS

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ABSTRACT

Myrtus communis L. (myrtle) is a common Mediterranean aromatic and medicinal shrub, well known for its antiseptic, antibacterial properties and as in recent reports, an apoptosis inducing factor in cancer cells. In Albania wild populations of *M. communis* are mainly found in Western and Middle region, where a significantly increased anthropogenic activity was previously reported. The objective of this study was to assess genetic relationships among myrtle populations in five different areas of the Middle area of Albania. Fifteen populations collected in five regions of study were genotyped by six chloroplastic markers (*trn*Y–*trn*D, *trn*L, *psb*C- *trn*S, rpS16– *trn*K, ccmp2, ccssr9). UPGMA cluster (Unweighted Pair Group Method with Arithmetic) analysis differentiated populations in three different groups. High similarity among populations was observed, with similarity values ranging from 50%- 98%. The cluster analysis showed no clear grouping of the most populations by their region of origin, nevertheless the majority of populations coming from the 'Plazh Gjenerali' area were differentiated in one clear subcluster. The preliminary results reported on the genetic relationships among myrtle populations serve the utilization and conservation of wild genetic resources of this medicinal and aromatic plant.

Keywords: chloroplastic markers, genetic relationships, myrtle

080 VARIATION OF PHYSICAL AND CHEMICAL PARAMETERS IN GROUNDWATER IN THE NORTHWESTERN PART OF THE DRINI I BARDHË RIVER BASIN, KOSOVO

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ABSTRACT

Groundwater resources represent one of the safest sources of drinking water supply. In many parts of the world over 70% of drinking water is made up of groundwater. In the Republic of Kosovo, the supply of potable water from groundwater sources is represented by about 40%. Subterranean water resources are among the key components for sustainable socio-economic development, being closely linked to all human activities. Demographic growth, overall economic development, has increased industrial and agro-productive capacities and producers at the country level by posing an increased pressure on the use of groundwater. However, in the last few decades there is a growing concern about the quality of groundwater. Therefore, this paper through the scientific research, laboratory analysis and the obtained and interpreted results aims at highlighting the quality of groundwater in the northwestern area of the watershed of Drini i Bardhë – Kosovë, through physicochemical indicators. In order to determine the quality of the groundwater of this area, a scientific research study was undertaken in the period from March 2018 to January 2019, to analyze the variation of physicochemical parameters in these waters. On this occasion, 50 points for the physicochemical analysis of samples in groundwater were determined. Some of the physicochemical parameters are directly measured in the field, such as: temperature, pH, electrical conductivity, dissolved oxygen in the water, etc., while other parameters are analyzed in the laboratory. Temperature values varies from 5.2 to 14.5º C, with an average value of 11.1º C, electrical conductivity from 267 to 1746 μS / cm, with an average value of 651.5 μS / cm, pH from 6.39-8.65 with an average value of 7.0, Ca^{2+} ranges from 35.4-203.2 mg / l, HCO_3^- from 63-488 mg / l, Na^+ from 0.53-61.6 mg / l, Cl^- from 9.23-192 mg / l, $SO4^{2-}$ from 1.8-288 mg / l, and CO_2 from 0.7-148.4 mg / l.

Key words: Groundwater, Drini i Bardhë, physicochemical, watershed area, variation.

081 LABORATORY SCALE ELIMINATION OF SOME HEAVY METALS WITH HOLLOW ALUMINOSILICATE SPHERES

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ABSTRACT

This examination aims to eliminate venomous heavy metals in wastewater using hollow aluminosilicate spheres. The chemical and physical parameters of hollow aluminosilicate spheres were investigated. The effects of contact time, amount of hollow aluminosilicate spheres and pH on the treatment of heavy metals in the water environment were evaluated by batch experiments. The yield capacities of hollow aluminosilicate spheres were examined for Cd, Ni, and Zn, with amounts of 57.29%, 23.66%, and 45,17% respectively. The following heavy metal removal efficiency of hollow aluminosilicate spheres was determined: Cd > Zn > Ni.

Keywords: Adsorption, Hollow aluminosilicate spheres, Heavy metals, Wastewater

082 PROPAGATION OF *LIBOCEDRUS "DECURRENS"* THROUGH GRAFTING: A CASE STUDY IN ALBANIA

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ABSTRACT

The grafting of ornamental plants is a relatively new practice in Albania aimed at improving both yields and the environment. Although much information is available on the seedling production of *Cupressus* spp., whereas few grafting cases have been recorded. This note reports the first grafting of the *Libocedrus "Decurrens"* (the scion), which is not well known in Albania, on a local ecotype of Mediterranean cypress (the rootstock). The experiment was carried out in a plastic greenhouse in the Laknas area in February 2015 by approach graftage. Five hundred grafted baby plants were grown in controlled conditions (T=22°C e UR 90%). The variation in the development of grafting partners in time can be explained by the fact that after grafting, the root system of the plant experiences a slowdown in growth rate because of the crunch of grafting. It is thought to be caused by both components from different species with genetic variation with each other. This great difference, when all growing conditions are the same, can also be explained by the quality of grafting for each plant. At the end of our study, the percentage of grafting compatibility was 82%.

Keywords: Conifer, Container Production, Vegetative Multiplication, Ornamental Nursery

083 A REVIEW OF THREATENED AND RISKED ENTOMOPHAUNA ON SHKODRA LAKE AREA

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ABSTRACT

In this paper are presented some Shkodra Lake Area Entomophauna species that are endangered in this habitat and have their threatened categories at the national level based on the Red List of IUCN (International Union for the Protection of Nature). There are exactly 39 species with their risked categories. These data are derivative of a several-year monitoring, based on expeditions carried out in different areas in this aea. About 39 species of Insects Order (Odonata 2 species, Mantopera 2 species, Neuroptera 2 species, Lepidoptera 24 species, Coleoptera 9 species) from different regions of Northern Albania. Most of them seem to be threatened on their habitats, belonging to the IUCN red list, where: 30 species belong to the vulnerable category (VU), such as Erynnis Tages; 6 are near threatened species (LR), such as Lestes Dryas; 2 are endangered (EN), such as Gmnopleurus Mopsus; 1 are critically endangered (CR) such as Osmoderma Eremita. Some of threatening aspects we can point out are related with this habitat, like the deterioration or disturbing, especially during reproductive period (i.e. before the egg disposal), pollution of waters and other ecological changes. The quality of water is considered good. [1,2]. We wish to contribute in the further knowledge of Insectophauna of Albania Region, focusing also in preservation and conservation of endangered species and their respective habitats, especially warm field-hilly regions, warm lower grass areas, rich vegetation areas and water heated areas. Most of them have a negative impact on ecological system [3].

Key words: threatened species, endangered species, IUCN category, Red List of Insects, habitat, scientific name, chorology, bio-ecology of species.

086 **BIOGEOGRAPHIC ASPECTS OF THE CHARACTERISTICS OF ZONALITY, HEIGHT BELTS AND EXTRAZONALITY IN THE STRUCTURE OF VEGETATION (LAKE BAIKAL REGION)**

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ABSTRACT

The ideas concerning continuity and discreteness of vegetation cover are always in the basis of numerous classification structures. The development of biogeography and geobotanic mapping as a method allowed to accumulate a huge experience for establishing of classification systems and approaches reflecting these or those peculiarities in territories under definite physical-geographic conditions. It starts with description of communities without ranges determining regional-zonal features of vegetation and results in establishing of formations characterizing historical-genetic links in formation and development of vegetation in concrete territories. Due to this fact, the revealed arealogical (geoelemental) and belt-zonal compositions of plants species in communities are basic criteria for assessment of structural-dynamic organization of vegetation under concrete physical-geographic conditions at any territory.

Key words: vegetation, biogeographic aspects, zonality, height belts, extrazonality, arealogical and belt-zonal compositions of plant species, key sites, Lake Baikal region

092 **GEOBOTANIC CHARACTERISTICS OF VEGETATION IN THE BAIKAL STATE BIOSPHERE RESERVE**

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ABSTRACT

The vegetation was studied along a definite itinerary and was aimed to reveal a detailed structure of the communities at the natural reserve territory. The results the geobotanic descriptions of the vegetation of the Pereyomnaya and Abiduy Rivers basins as key sites for research of the reserve vegetation for all of the reserve were showed. And we added additional information on the structure of the plant communities obtained for last time investigation of the reserve vegetation. The territory of Baikal Biosphere Reserve organized in 1969 represents a unique area of the vegetation structure in Southern Pre-Baikal region.

Key words: geobotanic characteristics of vegetation, southern Pre'Baikal, Baikal state biosphere reserve

111 **SPATIAL-DYNAMIC CHANGES OF FORESTS STRUCTURES IN THE GREEN ZONE OF IRKUTSK CITY FOR LAST DECADES (South -West Pre-Baikal)**

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ABSTRACT

Main properties, which a city green zone must include are environment protection, environment formation, as well as sanitary-hygienic and recreational functions. Due to this fact, provision of such studies with information is one of the most complicated aspects while analyzing the materials obtained and available archival data. There are nowadays several hundreds applied-research methods for analytical examination of geoecological problems including data characterizing biota on the territories surrounding large population aggregates, such as cities, settlements, etc. An important fact is a territorial location of a population aggregate with its physical-geographic conditions, as well as with history of general formation and development of this or that population aggregate. Large population aggregates (cities, settlements) of the East Siberia are located under different natural and climatic conditions, in different natural zones and territories. In this paper, problems of spatial-temporal changes in the structure of forests surrounding Irkutsk City are reported. Irkutsk City is situated in the south of the East Siberia (in Pre-Baikal).

Key words: spatial-dynamics changes of forests, green zone, south-west Pre-Baikal