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Serbian Chemical Society

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Sadržaj / Contents

PLENARNA PREDAVANJA / PLENARY LECTURES ***1***

Спектроскопско испитивање реакција и структурна карактеризација комплекса злата(III) са пептидима

Милош И. Ђуран, Биљана Ђ. Глишић, Уршула Рихлевска *2*

Spectroscopic investigation of reactions and structural characterization of gold(III) complexes with peptides

SAOPŠTENJA / CONTRIBUTIONS ***7***

ANALITIČKA HEMIJA / ANALYTICAL CHEMISTRY ***8***

Mikroekstrakcija pesticida iz vodenih uzoraka sa jonskim tečnostima kao ekstragensom ***8***

Tatjana M. Trtić-Petrović

Ionic liquid based microextraction of the pesticides from selected water samples

Uticaj matriksa jabuke, višnje i breskve na određivanje ostataka pesticida ***12***

Gorica Lj. Vuković, Vojislava P. Bursić, Sanja D. Lazić, Bojana D. Špirović

Effect of apple, sour cherry and peach matrices on the determination of pesticide residues

Influence of different carbonization and activation parameters on pesticide adsorption on carbon monolith ***16***

Marija M. Vukčević, Ana Kalijadis, Biljana Babić, Zoran Laušević, Mila D. Laušević

Uticaj parametara karbonizacije i aktivacije na adsorpciju pesticida na površini karbon monolita

ELEKTROHEMIJA / ELECTROCHEMISTRY ***20***

Cyclic voltammetric detection of epinephrine, ascorbic acid and uric acid using TX-100 modified carbon paste electrode ***20***

Bahadurgatta E. Kumara Swamy and Bananakere N. Chandrashekar

HEMIJSKO INŽENJERSTVO / CHEMICAL ENGINEERING ***25***

Preparation and characterization of hot-melt extruded solid dispersions of carbamazepine ***25***

Jelena Đuriš, Ioannis Nikolakakis, Svetlana Ibrić, Zorica Đurić, Kyriakos Kachrimanis

Karakterizacija čvrstih disperzija karbamazepina izrađenih metodom ekstruzije topljenjem

Controlled release of carbamazepine from tablets with self – emulsifying pellets ***30***

Mladen R. Milović, Svetlana R. Ibrić

Modifikovano oslobađanje karbamazepina iz tableta sa samolemulgijućim peletama

Experimental measurements of volumetric properties, refractive index and viscosity of the ternary system dimethyladipate + 2-butanone + 2-butanol ***36***

Andjela B. Knežević Stevanović, Sofija P. Miškov, Divna M. Bajić, Dušan K. Grozdanić, Mirjana Lj. Kijevčanin

Eksperimentalno određivanje volumetrijskih svojstava, indeksa refrakcije i viskoznosti ternernog sistema dimetiladipat + 2-butanon + 2-butanol

Determination of viscosity of aqueous alkanolamine solutions as potential carbon dioxide removal reagents ***41***

Vuk D. Spasojević, Slobodan S. Šerbanović, Bojan D. Djordjević, Mirjana Lj. Kijevčanin

Određivanje viskoznosti vodenih rastvora alkanolamina – potencijalnih agensa za uklanjanje ugljen-dioksida

Analiza i modelovanje razmenjivača toplote gas-gas ***46***

Tatjana Kaluđerović Radoičić, Zorana Arsenijević, Mirjana Munćan, Mirjana Kijevčanin, Željko Grbavčić

Mathematical modeling and analysis of gas-gas heat exchanger

Kretanje čestica u fluidizovanom sloju tečnost-čestice 51

Mihal Đuriš, Zorana Arsenijević, Tatjana Kaluđerović Radoičić, Radmila Garić-Grulović,

Particle movement in liquid fluidized beds

Ispitivanje fluidizacionih karakteristika filtracionog peska 56

Mihal M. Đuriš, Zorana Lj. Arsenijević, Rada V. Garić-Grulović, Darko R. Jaćimovski, Željko B. Grbavčić

Analysis of filtration sand fluidization characteristics

Correlation of Liquid-liquid Equilibria by NRTL Model 61

Nikola D. Grozdanić, Gorica R. Ivaniš, Zoran P. Višak, Slobodan P. Šerbanović, Mirjana Lj. Kijevčanin

Korelisanje podataka za ravnotežu tečnost-tečnost pomoću NRTL modela

Forced Path Mechanical Calibration method establishment for high pressure density measurements 65

Lazar Drašković, Aleksandar Tasić, Jelena Vuksanović, Ivona Radović, Mirjana Kijevčanin

Uspostavljanje „Forced Path Mechanical Calibration" metodologije za merenja gustine na visokim pritiscima

Analogija prenosa količine kretanja, toplote i mase u vertikalnom toku pseudofluida 70

Radmila V. Garić-Grulović, Željko B. Grbavčić, Nevenka M. Bošković-Vragolović, Darko R. Jaćimovski, Zorana Lj. Arsenijević, Mihal M. Đuriš

The analogy among momentum, heat and mass transfer in vertical flow of a pseudofluid

METALURGIJA / METALLURGY 75

Tehnološke mogućnosti za smanjenje sadržaja arsena u nestandardnim koncentratima bakra 75

Aleksandra Mitovski, Nada Štrbac, Ivan Mihajlović, Velibor Andrić, Miroslav Sokić

Technological options for the reduction of arsenic content in the nonstandard copper concentrates

NAUKA O MATERIJALIMA / MATERIAL SCIENCE 80

Novel long-chain alkyl polyglucoside as a prospective stabilizer for dermal delivery systems 80

Milica Lukić, Ivana Pantelić, Rolf Daniels, Gordana Vuleta, Snežana Savić

Alkil poliglukozidni emulgator dugog lanca: nova generacija stabilizatora sistema za dermalnu isporuku

Radijaciono-hemijska sinteza termoosetljivih srebro/poli(N-izopropilakrilamid) hidrogel nanokompozita 86

Jelena P. Spasojević, Jelena I. Krstić, Aleksandra N. Radosavljević, Melina T. Kalagasidis-Krušić, Zorica M. Kačarević-Popović

Radiation-chemical synthesis of thermosensitive silver/poly(N-isopropylacrilamide) hydrogel nanocomposites

The crystallization of glass powders from the system Li_2O-Al_2O_3-GeO_2-P_2O_5 91

Mihajlo B. Tošić, Srđan D. Matijašević, Snežana R. Grujić, Vladimir D. Živanović, Jovica N. Stojanović, Jelena D. Nikolić and Sonja V. Ždrale

Kristalizacija praha stakla iz sistema $Li_2O{\cdot}Al_2O_3{\cdot}GeO_2{\cdot}P_2O_5$

Annel hardening effect in thermomechanically treated a cast copper-gold alloy 95

Svetlana Nestorović, Ivana Marković, Dragoslav Gusković, Desimir Marković

Efekat ojačavanja žarenjem u termomehanički obrađenoj bakar-zlato livenoj leguri

Sintering of glasses in the ternary system La_2O_3-SrO-B_2O_3 studied by hot-stage microscopy 99

Sonja V. Ždrale, Snežana R. Grujić, Mihajlo B. Tošić, Vladimir D. Živanović, Anđelika Z. Bjelajac, Srđan D. Matijašević, Jelena D. Nikolić, Snežana N. Zildžović

Ispitivanje sinterovanja trokomponentnog sistema stakla La_2O_3-SrO-B_2O_3 primenom termomikroskopa

Polimerni kompleksi na bazi amidovanog pektina i montmorilonita za uklanjanje Basic Yellow 28 boje iz vodenih rastvora 102

Aleksandra R. Nešić, Sava J. Veličković, Dušan G. Antonović

Polymer complexes based on amidated pectin and montmorillonite for removal the Basic Yellow 28 dye from aqueous solutions

Sinteza i karakterizacija kompozitnih hidrogelova PMAA/zeolit A 107

Vesna V. Panić, Jelena G. Momić, Sava J. Veličković

The synthesis and characterization of PMMA/zeolite a composite hydrogels

HEMIJA ŽIVOTNE SREDINE / ENVIRONMENTAL CHEMISTRY 112

Determination of pesticide residues in working clothes 112

Nenad Andrić, Dragan Marković

Total VOCs emissions from screen printing 116

Jelena Kiurski, Savka Adamović, Ivana Oros, Dragan Adamović and Jelena Krstić

Emisija ukupnih VOC-ova u sito štampi

Проводљивост, pH и температура воде у акумулацији Врутци 120

Миленија Ј. Марковић, Драган Веселиновић

Conductivity, pH and temperature of water in the accumulation Vrutci

Sadržaj teških metala u reci Pek 124

Nada V. Babović, Tijana S. Čoporda-Mastilović, Mirjana B. Bartula, Dejan P. Marković

Heavy metals content in the Pek River

Ekstrakcija pesticida linurona i tebufenozida u membranskom kontaktoru na bazi poroznih kapilara 128

Jelena S. Đorđević, Tatjana M. Trtić-Petrović

Extraction of pesticides linuron and tebufenozid in a hollow fiber contactor

Determination of the natural zeolite capacity for the adsorptive removal of crystal violet dye from aqueous solution using response surface methods 132

Suzana I. Dimitrijević-Branković, Marija D. Pavlović, Aneta V. Buntić, Milica M. Ranđelović, Katarina R. Mihajlovski, Nevenka Z. Rajić, Dušan G. Antonović, Slavica S. Šiler-Marinković

Određivanje kapaciteta prirodnog zeolita u adsorptivnom uklanjanju boje kristal violet iz vodenog rastvora primenom metode površine odziva

Analiza tragova lekova i pesticida u komunalnoj otpadnoj vodi Beograda 137

Nikolina N. Antić, Marina M. Radišić, Svetlana D. Grujić, Tatjana M. Vasiljević, Mila D. Laušević

Determination of Pharmaceutical and Pesticide Residues in Belgrade Urban Wastewater

Biodegradacija kalemljenih kopolimera polistirena i skroba u rečnoj vodi 141

Vladimir B. Nikolić, Sava J. Veličković, Dušan G. Antonović, Aleksandar R. Popović

Biodegradation of polystyrene-graft-starch copolymers in river water

TEORIJSKA HEMIJA / THEORETICAL CHEMISTRY 146

CompChem (RS) aplikacija u okviru projekta HP-SEE. Dostupni računarski resursi, programi, prednosti i nedostaci 146

Branko J. Drakulić, Ivan O. Juranić

CompChem (RS) aplikacija u okviru projekta HP-SEE. Dostupni računarski resursi, programi, prednosti i nedostaci

BIOHEMIJA / BIOCHEMISTRY 150

Nanoscale Membrane Dynamics in Exocytosis: fine-tuning by PIP2 and Ca(II) 150

Dragomir D. Milovanovic , Alf Honigmann, Geert van den Bogaart

Nanonoskopski pregled dinamike membrane u egzocitozi: suptilna regulacija fosfatidil-inozitolom i Ca^{2+}

Uticaj aktinidina - cistein proteaze iz kivija (Actinidia deliciosa) na ekspresiju proinflamatornih citokina u T84 epitelnim ćelijama humanog kolona 157

Milena Čavić, Milica Grozdanović, Radmila Janković, Marija Gavrović-Jankulović

The effect of actinidin – a kiwifruit (Actinidia deliciosa) cysteine protease on the expression of proinflammatory cytokines in T84 human colonic epithelial cells

Metal based photosensitizers of tetradentate Schiff base: Promising role in anti-tumor activity through singlet oxygen generation mechanism 161

Halehatty S. Bhojya Naik, Sirabadige M. Pradeepa, Atanu Barik, Indira K. Priyadarsini

Ispitivanje reakcije paracetamola sa Fentonovim reagensom i određivanje radical scavenging aktivnost DPPH metodom 165

Slavica M. Sunarić, Milica M. Radić

Investigation of the reaction of paracetamol with Fenton reagent and determination of DPPH radical scavenging activity

BIOTEHNOLOGIJA / BIOTECHNOLOGY 169

Yeast surface display expression and purification of chimera glucose oxidase construct with Aga2 protein 169

Marija Blazic, Gordana Kovacevic, Nevena Zelenovic, Raluca Ostafe, Marija Gavrovic-Jankulovic, Rainer Fischer, Radivoje Prodanovic

Prečišćavanje himere Aga2 proteina i glukoza oksidaze eksprimirane na površini ćelija kvasca

Cloning, heterologous expression and characterization of glucose oxidase mutants from Aspergillus niger in yeast Pichia pastoris 173

Gordana N. Kovačević, Marija Blažić, Bojana Draganić, Raluca Ostafe, Marija Gavrović-Jankulović, Rainer Fischer, Radivoje Prodanović

Kloniranje, heterologna ekspresija i karakterizacija mutanata glukoza oksidaze iz Aspegillus niger u kvascu Pichia pastoris

Zeolite/apatite system - nature mineral fertilizers 177

Marija L. Mihajlović, Mirjana Stojanović, Zorica Lopičić, Mirko Grubišić, Marija Petrović, Jelena Milojković, Dragan Radulović

Zeolit / apatit sistem – prirodna mineralna đubriva

Determination of exopolysaccharides production by lactic acid bacteria of water kefir grains 181

Miona G. Miljković, Sladjana Z. Davidović, Slavica S. Šiler-Marinković, Suzana I. Dimitrijević-Branković

Ispitivanje proizvodnje egzopolisaharida kod bakterija mlečne kiseline iz vodenog kefira

Enzymatic production of bioactive protein hydrolysates from egg white: effects of ultrasound on egg white proteins 186

Andrea B. Stefanović, Milena G. Žuža, Ana D. Gluvić, Verica B. Manojlović, Dejan I. Bezbradica, Branko M. Bugarski, Zorica D. Knežević-Jugović

Enzimska proizvodnja bioaktivnih hidrolizata proteina belanceta: uticaj ultrazvuka na proteine belanceta

Poređenje imobilizacije peroksidaze iz soje na različite glicidil metakrilat polimere 191

Miloš Prokopijević, Olivera Prodanović, Dragica Spasojević, Željko Stojanović, Ksenija Radotić, Radivoje Prodanović

Comparison of soybean hull peroxidase immobilized on different glycidyl methacrylate polymers

Covalent immobilization of horseradish peroxidase on macroporous glycidyl methacrylate based copolymer 195

Olivera Prodanović, Miloš M. Prokopijević, Dragica R. Spasojević, Željko P. Stojanović, Ksenija D. Radotić, Zorica D. Knežević-Jugović, Radivoje Prodanović

Kovalentna imobilizacija peroksidaze rena na makroporozni glicidil metakrilatni kopolimer

Poređenje četiri metode za imobilizaciju HRP u alginatu radi potencijalne primene u prečišćavanju otpadnih voda 199

Dragica Spasojević, Miloš Prokopijević, Olivera Prodanović, Ksenija Radotić, Radivoje Prodanović

Comparison of four methods for the immobilization of HRP in alginate for potential application in wastewater treatment

Immobilization of Candida antarctica lipase B on supports with epoxy groups via covalent attachment 203

Sonja M. Jakovetić, Rafel Picazo-Espinosa, Maximino Manzanera, Željko P. Stojanović, Radivoje M. Prodanović, Ružica Đ. Miladinović, Zorica D. Knežević-Jugović

Kovalentna imobilizacija lipaze B iz Candida antarctica na nosače sa epoksidnim grupama

Uklanjanje vodonik-sulfida iz efluenta anaerobno prečišćene otpadne vode 208

Dragana V. Kukić, Marina B. Šćiban, Mile T. Klašnja, Jelena M. Prodanović, Vesna M. Vasić

Removal of hydogen sulfide from efluent of anaerobic treated wastewater

HEMIJA I TEHNOLOGIJA MAKROMOLEKULA / CHEMISTRY AND TECHNOLOGY OF MACROMOLECULES 212

Mehanička i termička svojstva nanokompozita na bazi epoksidne smole i nanoglina 212

Miloš D. Tomić, Branko Dunjić, Violeta Likić, Jelena Rogan, Nevenka Rajić, Jasna Đonlagić

Mechanical and thermal properties of epoxy-nanoclay nanocomposites

Mehanička i termička svojstva umreženih poli(uretan-estar-siloksana) 218

Jasna V. Džunuzović, Marija V. Pergal, Rafał Poręba, Sanja Ostojić, Enis S. Džunuzović, Milena Špírková, Slobodan Jovanović

Mechanical and Thermal Properties of Poly(urethane-ester-siloxane) Networks

Termoosetljivi mikrogelovi na bazi poli(N-izopropilakrilamida) i alginata namenjeni kontrolisanom otpuštanju lekova 222

Stojanka M. Petrušić, Petar Jovančić, Branko Bugarski, Svetlana Grujić, Smilja Marković, Jasna Đonlagić

Thermosensitive microgels based on poly(N-isopropylacrylamide) and alginate intended for controlled drug release

Biokompatibilni termoplastični poliuretani na bazi poli(dimetilsiloksana) 227

Marija V. Pergal, Vesna V. Antić, Gordana, Tovilović, Jelena Nestorov, Jasna Đonlagić

Biocompatible thermoplastic polyurethanes based on poly(dimethylsiloxane)

ORGANSKA HEMIJA / ORGANIC CHEMISTRY 232

Aryldiketoacids. Synthesis, high resolution mass spectra, and pharmacophoric similarity with floxacins 232

Ilija N. Cvijetić, Tatjana Ž. Verbić, Ivan O. Juranić, Branko J. Drakulić

Арилдикетокиселине. Синтеза, масени спектри високе резолуције и фармакофорна сличност са антибиотицима из класе флоксацина

Molecular modeling and SAR between phenyl-piperazine-acetamides, phenyl-piperazine-ureas and D2, 5HT1A receptors 236

Vladimir B. Sukalovic, Vukic Soskic, Deana Andric, Goran Roglic, Sladana Kostic-Rajacic

Molekulsko modelovanje i SAR analiza fenil-piperazin-acetamida, fenil-piperazin-urea i D2, 5HT1A receptora

NASTAVA HEMIJE / CHEMISTRY EDUCATION 243

Примена иконичне репрезентације у провери знања студената хемије 243

Игор М. Мартиновић и Јасминка Н. Королија

Application of iconic representation in student assessment of chemistry knowledge

Евалуација репрезентација у уџбеницима хемије 248

Игор М. Мартиновић, Милена Благојевић и Јасминка Н. Королија

Evaluation of chemical representations in chemistry textbooks

Hemijska pismenost studenata hemije 252

Jasna Adamov, Stanislava Olić, Mirjana Segedinac

Chemical literacy of chemistry students

KERAMIKA / CERAMICS 256

Prikaz metoda za izračunavanje efektivnog koeficijenta difuzije pri sušenju glinenih proizvoda 256

Miloš Vasić

Presentation of methods for determination of effective diffusion coefficient during convective drying of clay masonry units

TEKSTILNO INŽENJERSTVO / TEXTILE ENGINEERING **261**

Полисахаридни влакнасти биополимери као супстрат за добијање вештачког депоа инсулина ***261***

Адела Х. Медовић Баралић, Петар Д. Шкундрић, Љиљана М. Срећковић, Мирјана М. Костић

Polysaccharide fibrous biopolymers as a substrate for obtaining artificial insulin depot

Primena GPC/MALLS metode sa fluorescentnim FDAM markerima za određivanje sadržaja funkcionalnih grupa selektivno oksidisanih celuloznih vlakana ***266***

Jovana Ž. Milanović, Antje Potthast, Sonja Schiehser, Predrag Milanović, Mirjana Kostić

Application of GPC/MALLS method with fluorescence FDAM labeling for determination of functional groups in selectively oxidized cellulose fibers

Uticaj parametara neselektivne oksidacije na sadržaj funkcionalnih grupa u celuloznim vlaknima ***270***

Ana D. Kramar, Matea Korica, Jovana Ž. Milanović, Mirjana M. Kostić

Influence of the nonselective oxidation conditions onto functional groups content in cellulose fibers

Netkani materijal na bazi vune sekundarnog porekla modifikovan nanočesticama TiO_2 za uklanjanje direktnih boja iz vode ***275***

Darka D. Marković, Bojan M. Jokić, Zoran V. Šaponjić, Petar M. Jovančić i Maja M. Radetić

Recycled wool-based nonwoven material modified with TiO_2 nanoparticles for removal of direct dyes from water

Ekološki i ekonomski prihvatljiv biosorbent na bazi kratkih vlakana konoplje: Uticaj strukture na parametre procesa sorpcije jona cinka ***279***

Biljana M. Pejić, Marija M. Vukčević, Ivana Pajić-Lijaković, Mila D. Laušević, Mirjana M. Kostić

Environmentally and economically acceptable biosorbent based on short hemp fibers: Influence of fibers structure parameters on the sorption process of zinc ions

INDEX AUTORA / AUTHOR INDEX **283**

CompChem (RS) aplikacija u okviru projekta HP-SEE. Dostupni računarski resursi, programi, prednosti i nedostaci

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Introduction

High-Performance Computing (HPC) Infrastructure for South East Europe's Research Communities (HP-SEE), supported by the European Commission through seventh framework project (FP7), link existing and upcoming HPC facilities in South East Europe in a common infrastructure, and offer operational solution for it. The initiative open the South East European HPC infrastructure to a wide range of new user communities, including those of less-resourced countries, fostering collaboration and providing advanced capabilities to researchers.[1] The three strategic groups, named as the virtual communities (VC), in computational physics, computational chemistry, and computational life sciences are included in the project.

Project offers computational resources and ported software applications on existing HPC infrastructure from Hungary to Azerbaijan. Along with this regular training and dissemination events were performed, aimed to introduce users in the basic of programming, usage of HPC recourses and software ported. The strong management of the project aim to obtain unified prerequisites on all HPC centers to facilitate porting of the software and their usage. In the same frame younger researcher should be trained to use ported software, perform basic programming and, consequently, be able to use similar HPC facilities in their further work.

Our group is the active participant of the project within Computational Chemistry virtual community. The aim of our application, named 'Quantum Mechanical, Molecular Mechanics, and Molecular Dynamics computation in chemistry' (CompChem(RS)),[2] is to use HPC resources, available in our country (mainly on the Institute of Physics, Belgrade), and resources of other partners, to improve and facilitate ongoing projects that use molecular-dynamics simulations, DFT and *ab initio* calculations. The other aim is the education in this field of postgraduate students.

In this communication we want to address a few points. The first is brief presentation of the software ported, including some examples of usage by our group, as well as the aim for recruitment of other researchers in Republic of Serbia that can become the users. The next is the presentation of HPC resources available by the other partners (Hungary, Romania, and Bulgaria offer BluGene/P super-computers, as an example). The last is the problem, lasting from the very beginning of the project, in the consent and recognition of the usefulness of available resources among different research groups that we met (means, among our colleagues that have a need for the similar resources, but did not use it, even if available). Such problem is, unfortunately, inherent to the area of the South-Eastern Europe, as well as to our scientific community in general.

Software ported

On the so far unique HPC facility in Serbia, PARADOX cluster on the Institute of Physics, Belgrade,[3] we ported source codes (programs) that are instantly ready-to-use, as is shown in Table 1. Scripts for the execution of the programs are available to users that have account on the cluster. The requisites to get access to HP-SEE infrastructure are given on the project Wiki page.[4] Any other software recognized as the useful for the users within VC Computational Chemistry, or the new ones, after registration, can be ported to the cluster. The prerequisite (generally within the project) is that software that should be ported is distributed for free for the academic community. For commercial software, user must provide the proof of license of the software version made for execution on more than one node (parallel execution).

So far we have a ported tools for massive classical molecular dynamics studies (NAMD), *ab initio* molecular dynamics (CPMD), classical DFT and *ab initio* calculations (Gaussian, Firefly). The last programs listed can be used for calculations on the semiempirical level of theory, too. For the molecular docking, AutoDock Vina is installed. For the modelling of the large set of compounds, including ligand-

based and structure-based virtual screening, we ported OpenEye applications. OMEGA is fast conformer generation tool, able to process tens of thousands of compounds per day. ROCS is shape comparison tool that can be used for virtual screening. EON compare electrostatic potentials of pre-aligned molecules, and often is used for the refinement of the ROCS results. FRED is docking program that performs fast exhaustive docking, and also can be used for virtual screening. To make comparison with other HPC centers in the project, we offer the list of programs related to chemistry, available on Bulgarian Supercomputer Center (BGSC), hosting IBM BlueGene/P.

Table 1. Software ported to PARADOX cluster.

Software/version[a)]	Mode of execution[b)]	Home Page
NAMD 2.8	P	www.ks.uiuc.edu/Research/namd/
Firefly 7.1G	P	classic.chem.msu.su/gran/firefly/index.html
CPMD 3.1	P	cpmd.org
Gaussian03	P	www.gaussian.com/
AutoDock Vina 1.0	P/S	vina.scripps.edu/
OpenEye Software OMEGA, EON, ROCS, FRED	P/S	www.eyesopen.com/products

a) The last stable version ported on the day of the submission of this communication; b) P – parallel, S – sequential.

BGSC offer NAMD, GROMACS, LAMMPS, and DL POLY for the molecular dynamics; CPMD, NW Chem, Quantum Espresso, and CP2K for the *ab initio* molecular dynamics simulation; GAMESS for the DFT and *ab initio* calculations.

Resources

Our home cluster PARADOX offer 89 worker nodes (2 x quad core Intel Xeon E5345 @ 2.33 GHz with 8GB of RAM) and 15 service nodes (Xeon-based nodes). About 80 nodes are always available for computation. Jobs are submitted using PBS queuing system. Number of nodes and number of processors per node can be chosen in the input script, as well as needed time of computation. Rare advantage is that there is no limitation on time of the computation. Such limitation is frequent on the big clusters. Paradox also offers large space for the permanent storage of the input/output data. Other resources within HP-SEE project is listed in Table 2.

Table 2. Illustration of the computing power offered within the HP-SEE project.

Name	Configuration	Processors*/ Threads**
Bulgarian Supercomputing Centre (BGSC) / BG	IBM Blue Gene/P	8192
HPCG at IICT-BAS / BG	Express 7000	576
HPCG at IICT-BAS / BG	NVIDIA GTX 295 (GPU)	1920
IFIN-HH / RO	Intel Xeon / AMD opteron	704
NCIT – UV / RO	IBM Blue Gene/P	4096
NCIT – UV / RO	Intel Xeon	400
NIIFI - SC / HU	AMD Opteron	798
Pecs - SC / HU	Intel Xeon	1152
Szeged - SC / HU	AMD Opteron	2304
Debrecen - SC / HU	Silicon Graphics (SGI)	1536

* Processors 850 MHz – 3.2 GHz; ** Threads reported for the Graphics processing units (GPU).

Usage examples

The one of the main aims of the project is to allow to participants to perform modelling of interest to their research in a full scale. So far we have been limited by the computational power, and able to perform very short simulations, or just to try the software of interest to us. Now we are able to use programs in their full power. As an example, molecular dynamics simulation, using biasing forces to map free-energy landscapes of compounds examined, were performed on the set of ~ 20 congeners in different explicit or implicit isotropic, or explicit anisotropic solvents, during 20-30 ns each. Small part of the results is published so far.[5,6] For such calculations about 10000 cpu hours were used on PARADOX, and the lot of the storage space. A bit (1/20), of the each run of such simulations, on the author lab computer (~ 5 GHz in two processors), takes about three days. For the different project we have need to perform docking of about 120 small organic molecules to acetylcholinesterase active site to obtain conformations suitable to be used in three-dimensional QSAR.[7] By using AutoDock Vina, which is very fast, on PARADOX this took half of the day. On the user lab computer few days will be spent for such calculation, using full processors power, and the lot of memory. Consequently, no other tasks could be done on that computer. As the last example, we examined dynamic behaviour of the protein isolated in the department of biochemistry of the Faculty of Chemistry.[8] Even protein is not big (140 amino-acid residues) large solvent cluster have been added, along with counter ions, to simulate ionic strength comparable with experimental conditions. Due to memory issues such calculation cannot be even started at the lab computer.

Number of users

So far, our part of the project counts eleven users, including two technical staff that did not use CPUs (also did not perform planed tasks at all). For the technical side of view we have high quality support from the researchers of Scientific Computing Laboratory – Institute of Physics, Belgrade. In Serbia, research community count much more users that devote their research time to computational chemistry (in the broadest sense). Many attempts to involve number of our colleagues, from the very beginning of the project, did not trigger their interest. Arguments for non-interest span range from asking 'Is it possible to use my terminal, and graphical user interface to submit and monitor my job, as that I perform computations in my own computer', to the inability to port software of interest in a way to be executed in parallel mode. There are many other subjective points of view, which are not suitable to be described in communication for the scientific conference. Number of training events so far, that instruct the users in using of HPC, from console commands, to non-trivial programming; as well as many information on usage of resources, in a cook-book way, on the project Wiki web site, freely available to all interested should be mentioned. There are a lot of researchers that did not give any comment, just cover their knowledge and skills (Figure 1).

Figure 1. The corresponding author view on the possible subjective attitude, that triggers non-interest to project in our scientific community.

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CompChem (RS) aplikacija u okviru projekta HP-SEE. Dostupni računarski resursi, programi, prednosti i nedostaci

Projekt 'High-Performance Computing for the south eastern European Communities' (HP-SEE), podržan od strane Evropske komisije, povezuje postojeće resurse u oblasti računara visokih performanci od Mađarske do Azerbejdžana u zajedničku infrastrukturu. U okviru projekta postoje tri strateške grupe (virtuelne zajednice), Računarska fizika, Računarska hemija i Računarske prirodne nauke. Kao deo projekta, u okvru virtuelne zajednice Računarska Hemija, u Republici Srbiji postoji aplikacija 'Kvantno mehanička, molekulsko mehanička izračunavanja i simulacije molekulske dimnamike u hemiji' (skraćenica CompChem). U sopštenju su kratko prikazani dostupni računarski resursi u okviru celog projekta, programi povezamni sa hemijom instalirani na našem nacionalnom centru za izračunavanja visokih performansi, kao i nekim drugim centrima u okviru projekta. Na pristupačan način su opisane prednosti korišćenja dostupnih resursa i dat je kitički osvrt na mali interes naše naučne zajednice za korišćenje dostupnih računarskih kapaciteta/instaliranih programa.

Zahvalnica: Ova komunikacija prikazuje rezultate dobijene radom na projektu 'High-Performance Computing Infrastructure for South East Europe's Research Communities' (HP-SEE), finansiranog od strane Evropske Komisije (ugovor broj 261499), u okviru sedmog okvirnog projekta HP-SEE. Ministarstvo Prosvete i Nauke Republike Srbije, delom, finansira istraživanja u okviru projekta 172035.

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Aryldiketoacids. Synthesis, high resolution mass spectra, and pharmacophoric similarity with floxacins

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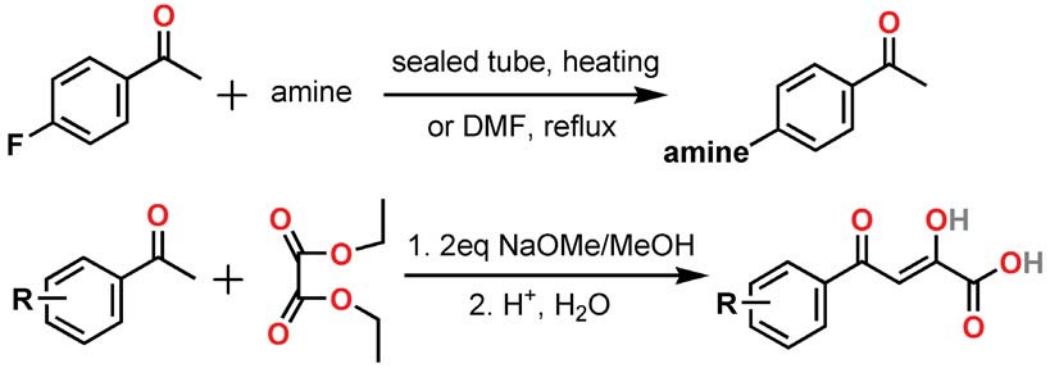
Introduction

Aryldiketoacids (ADKs) are proved as highly biologically active molecules, targeting several important enzymes associated with the life-threatening pathogens. One of the most important is Human imunodeficiency virus (HIV-1) intergase, the enzyme responsible for the integration of viral DNA in host genome.[1] Diketoacids bind to the active site Mg^{2+}/Asp domain in HIV-1 integrase, sequestrate Mg^{2+} ion, and inhibit the enzyme.

There is an urgent need for the new antibacterial drugs, because of the rapid development of bacterial resistant toward wide spectrum of commercially available antibacterial drugs. Methycilin-drug resistant *Staphylococcus aureus* (MDRSA) are one of the most spread bacteria, especially in hospital conditions. Discovery of the new drug targets in bacteria is crucial for overcoming resistance. Inhibition of isoprenoid biosynthesis, involved in lipid biosynthesis, could be accomplished by targeting farnesyl diphosphate synthase (FPPS), or undecaprenyl diphosphate synthase (UPPS). Dehydrosqualene synthase (CrtM) is another prenyl transferase involved in cell wall biosynthesis. UPPS and CrtM posses similar active site Mg^{2+}/Asp domain as HIV-1 intergase. Several well-known HIV-1 intergase inhibitors are proved as very potent inhibitors of prenyl transferases.[2]

Results and discussion

Ciprofloxacin and other floxacins are antibacterial drugs, highly potent against gram-positive and gram-negative strains, and inhibit DNA replication by targeting DNA-topoisomerase complex. We observed structural similarity between floxacins and aryldiketoacids. Biological test showed that several ADK, synthesized by us, act against MDRSA in micromolar range of concentrations.[3] In order to design more potent inhibitors of MDRSA, new series of ADK have been synthesized. Along with this, we showed that *meta*-alkyl substituted ADK have higher affinity toward Mg^{2+} ion, compared to *ortho*- and *para*-substituted congeners, and form complexes with ML_2 stoichiometry ($\log\beta_2$ ~ 10).[4] The indication on different complexation ability within congeneric series of ADK, was initially obtained by analyzing high resolution mass spectra. *Meta*-alkyl substituted ADK show peak corresponding to 2(M-1)+Na of high intensity, where M is a mass of molecular ion.



R = 3-Me-, 2,4-di-Me-, 2,4,5-tri-Me-, 2,3,5,6-tetra-Me-, 2,4,6-tri-*i*-Pr-, 2,5-di-cyclohexyl-, 3-fluorenyl-, 2-tetralinyl-, 3-Br-, 4-Br-2,5-di-Me-, 4-MeO-2,5-di-Me-, 4-OH-3,5-di-Me-, 2-MeO-, 3-MeO-, 3-CF_3-, 4-piperidinyl-, 4-pyrolidinyl-, 4-morpholinyl-, 4-(*N*,*N*-di-Me)-, 4-*N*-Me-piperazinyl-, 4-imidazolyl-, 4-*N*-cyclohexyl-

Figure 1. *Synthesis of compounds reported.*

ADKs were synthesized by Claisen condensation of substituted acetophenones with diethyl-oxalate, followed by *in-situ* base hydrolysis of ethyl ester formed, to give aryldiketoacids (Figure 1). Substituted

acetophenones used were commercially available (3-CH_3, 2-OCH_3, 3-OCH_3, 3-CF_3), or synthesized using different procedures. Alkyl- and halogen- substituted acetophenones were obtained by Friedel-Crafts acylation of corresponding substituted benzenes, using $AlCl_3$ as a catalyst in CH_2Cl_2 as a solvent. The 4-amino-substituted acetophenones were obtained starting from commercially available 4-F acetophenone. Condensation with cyclic secondary amines (piperidine, *N*-methylpiperazine, morpholine, pyrolidine, imidazole) proceeded easily, with yields over 90%, mixing the excess of amine with 4-F acetophenone and heating for 2-3 hours on 130-140 °C in the pressure-resistant steel tube, without any solvent. Similarly, refluxing the mixture of 4-F acetophenone, amine, and K_2CO_3 in DMF on 110-120 °C for 24^h, we obtained the same products in high yields. Synthesized compounds were purified by crystallization or by dry-flash chromatography, and characterized by ^1H and ^{13}C NMR, ESI-MS, IR spectra and melting points.

The difference of complexation ability of ADK was confirmed in the newly prepared set by ESI-MS spectra. Selected examples are shown on Figure 2 and in Table 1. Obviously, compounds bearing *meta*-alkyl substituents show much more intensive [2(M-1)+Na] ions that the rest in the set. Highest ratio is observed for the 3-Me- derivative. Presence of the both *meta*-alkyl and *ortho*-alkyl substituents, as in 2,4,5-tri-CH_3-, and 2,3,5,6-tetra-CH_3- derivatives, attenuate such effect in some extent, probably because aryl to Ar-C(O)- torsion. *Ortho*- substituents increase this torsion angle, and probably decrease the resonance between diketo moiety and aryl ring. Alkoxy and halogens, as substituents in *meta*-position, did not influence in the same manner as alkyl substituents.

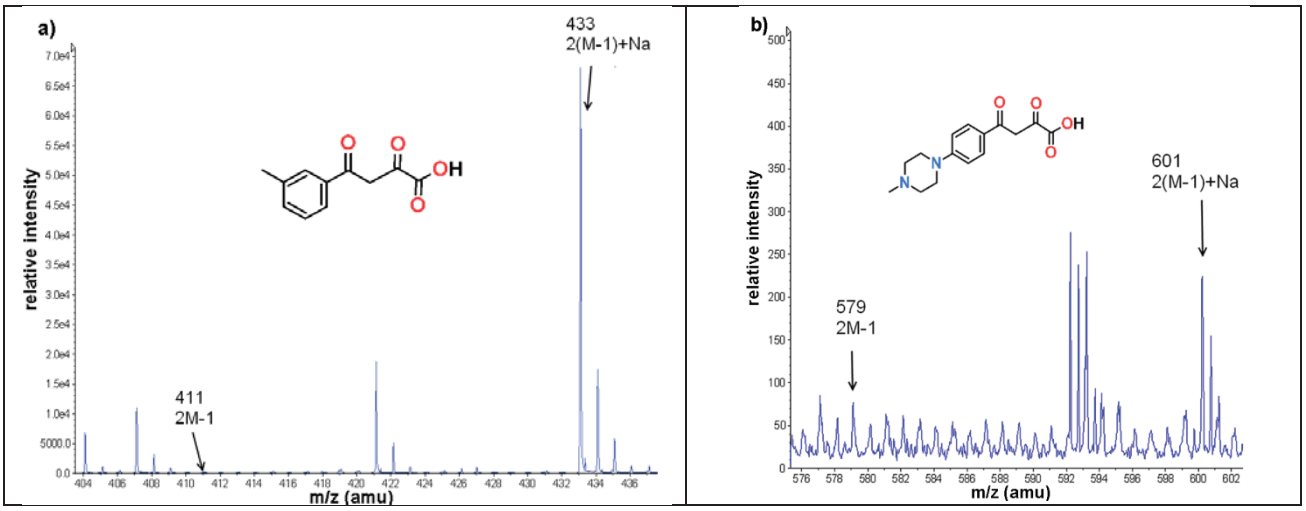


Figure 2. Selected regions of ESI-MS spectra. (a) 3-CH_3ADK, and (b) 4-N-Me-piperazinyl ADK.

Table 1. Intensities of observed peaks in ESI-MS spectra and their relative ratios, displayed for selected compounds.

Compound	Ion intensity		$\frac{2(M-1)+Na}{2M-1}$
	2M-1	2(M-1)+Na	
3-CH_3-	211	57222	271
2,4,5-tri-CH_3-	766	85509	112
3-OCH_3-	227	14011	62
4-OCH_3-2,5-di-CH_3-	1226	102381	84
2,3,5,6-tetra-CH_3-	847	151487	179
3-Br-	707	33065	47
4-(*N*-CH_3-pyperazinyl)-	35	69	2

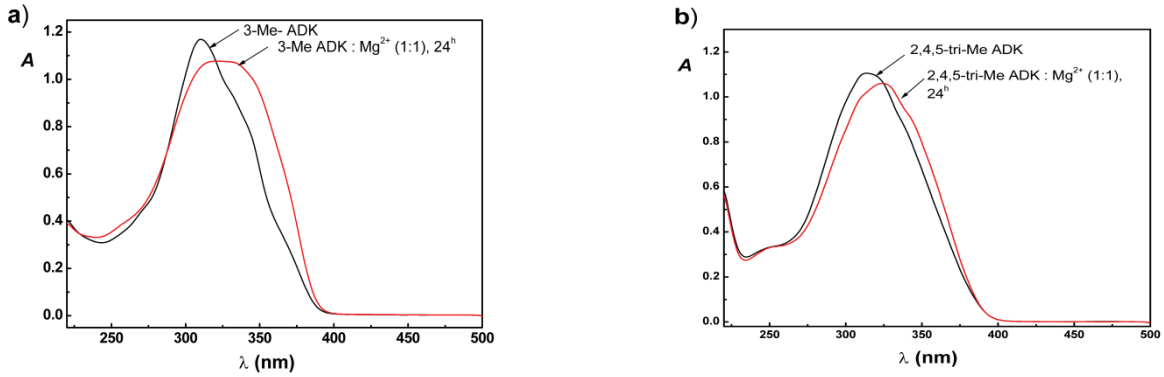


Figure 3. UV/Vis absorption spectra of a) 3-CH_3-, and b) 2,4,5-tri-Me- derivatives; before (black) and after the addition of Mg^{2+} (red).

Complexation ability of *meta*-substituted ADK with Mg^{2+} was determined by UV/Vis spectroscopy (Figure 3); batochromic shift of absorption maximum was recorded upon complexation. Those results are in agreement with our previous findings.[4]

Pharmacophoric similarity of floxacins and reported compounds:

Reported set is prepared as continuation of our work on ADK derivatives that can overcome multidrug resistance in MDRSA.[3] Pharmacophoric similarity with known fluoroquinoline antibiotics (Figure 4) was examined by superimposition in the ROCS program.[5] The crystal structure of the norfloxacin (Figure 4a)[6] is used as a template. Ten conformations of the each compound studied were obtained by OMEGA,[7] from the SMILES notation, and 'rms' keyword was set to 0.15. 100 random starts per molecule were used. Both template and queries are treated in their neutral forms. Tanimoto and Tanimoto combo (include shape and OpenEye 'color' force field (ff)) similarity scores were used for the quantification of results.

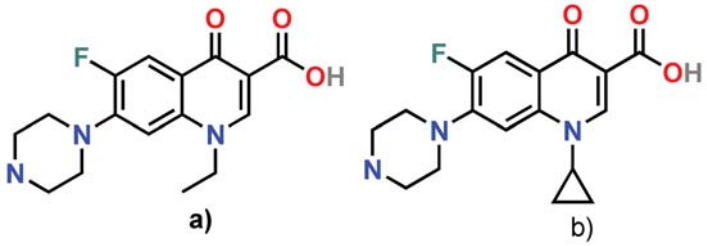


Figure 4. Structures of norfloxacin (a) and ciprofloxacin (b)

The highest similarity between norfloxacin, by both shape and pharmacophore (color ff) similarity, not surprisingly, were observed for derivatives having 4-hetero(ali)cyclic substituents. Best overlap was found for 4-*N*-Me-piperazinyl derivative (Tanimoto Combo 1.074, Shape Tanimoto 0.696, Color Tanimoto 0.378) Figure 5a, followed by 4-pyrolidinyl- derivative (Tanimoto Combo 1.037, Shape Tanimoto 0.733, Color Tanimoto 0.304).

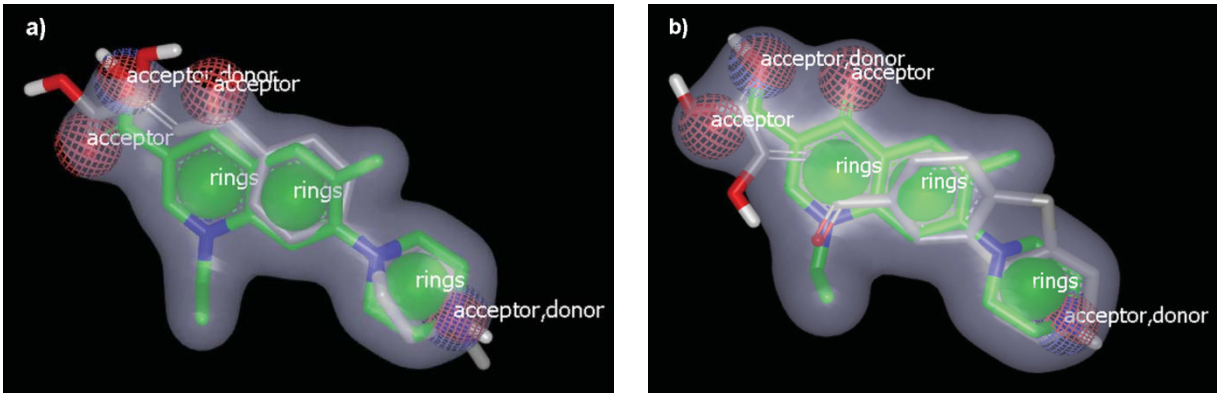


Figure 5. a) 4-N-Me-piperazinyl- and b) 3-fluorenyl derivatives superimposed on norfloxacin.

It should be noted that among highly ranked derivatives we found 3-fluorenyl- derivative (Tanimoto Combo 1.030, Shape Tanimoto 0.742, Color Tanimoto 0.287), that show better shape similarity than previous two, but is positioned with their diketo moiety opposite to the -C(O)-C-COOH moiety of the norfloxacin, Figure 5b. Favored overlap of norfloxacin Ph-piperazinyl moiety with fluorenyl moiety of ADK contributes to relatively high shape score.

Conclusion

We reported preparation and characterization of 22 aryldiketo acids, designed to confirm significant observations obtained by our group on congeners in the same series. High-resolution ESI-MS spectra showed better complexation of monovalent metal ions for *meta*-alkyl substituted derivatives. Introduction of *ortho*-alkyl substituents attenuate such effect in some extent. The same derivatives exert good complexation of Mg^{2+} ion, and this is proved by UV/Vis spectroscopy. This observation has pharmacological relevance, due to significance of Mg^{2+} ion in HIV-1 integrase active site. 4-Hetero(ali)cyclic substituted derivatives show significant pharmacophoric similarity with floxacin antibiotics. Biological tests of prepared compounds against multidrug resistant *Staphylococcus aureus* are in preparation.

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Арилдикетокиселине. Синтеза, масени спектри високе резолуције и фармакофорна сличност са антибиотицима из класе флоксацина

Арилдикетокиселине (АДК) су биолошки активни молекули који делују на ензим интегразу HIV-1 вируса. Наша претходна истраживања су показала већи афинитет мета-супституисаних АДК ка комплексирању Mg^{2+} јона у односу на остале супституционе обрасце. Још важније, АДК показују антибактеријску активност према сојевима бактерија Staphylococcus aureus *резистентним према више антибиотика (MDRSA). Као наставак ових истраживања, синтетисали смо серију од 22 нова конгенера, као потенцијално боље антибактеријске агенсе (MDRSA). У овом саопштењу је укратко описана њихова синтеза, афинитет ка комплексирању једно- и двовалентних металних јона, као и фармакофорна сличност са антибиотицима из класе флоксацина.*

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