



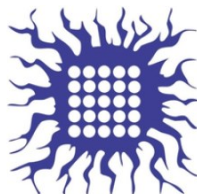
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ICCBIKG_2023



BOOK OF PROCEEDINGS





2nd International Conference on Chemo and BioInformatics
ICCBIKG 2023

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Kragujevac, Serbia

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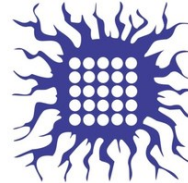
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Table of contents

PLENARY LECTURERS	1
THE IMPORTANCE OF CHEMOMETRICS IN DRUG DISCOVERY FROM MEDICINAL PLANTS	2
A REVIEW OF THE APPLICATION OF THE FINITE ELEMENT SMEARED CONCEPT TO BIOMEDICAL ENGINEERING PROBLEMS	6
IS DEUTERIUM BIOLOGICALLY SIGNIFICANT? SOME UNEXPECTED DEUTERIUM SPECTROSCOPIC DATA	7
TARGETING DEPRESSION VIA COMPUTATIONAL APPROACHES TO DESIGN NEW COUMARIN-BASED SEROTONIN RECEPTOR	
ANTAGONISTS/AGONISTS AND DEVELOP RELIABLE MODELS OF G PROTEIN-COUPLED RECEPTORS.....	10
ALGORITHMS AND WEB SERVERS FOR PROTEIN BINDING SITES DETECTION IN DRUG DISCOVERY	14
TOWARD QUANTITATIVE RAMAN SPECTROSCOPY.....	22
SYNTHETIC DATA GENERATION FOR BIOMEDICAL DEEP LEARNING: METHODS, CHALLENGES, AND OPPORTUNITIES	26
SECTION LECTURERS.....	34
BENZENE AND WATER – DIFFERENT OR SIMILAR?	35
THE HYDROGEN ECONOMY: CHALLENGES AND PROSPECTIVES	39
MULTIPARAMETER MONITORING OF CARDIOVASCULAR FUNCTION	43
DB.3D-QSAR.COM. THE FIRST 3D QSAR MODELS DATABASE.....	51
IRM@Be ²⁺ - QUANTUM CHEMISTRY BETWEEN BAVARIA AND ŠUMADIJA.....	53
APPLICATION OF CARBON-BASED NANOCOMPOSITE SYSTEMS AS PHOTOSENSITIZERS FOR PHOTODYNAMIC THERAPY.....	61
CONFUSION ABOUT THE CHOICE OF EVALUATION METRICS FOR MODEL PERFORMANCE ASSESMENT IN CHEMOINFORMATICS,	
BIOINFORMATICS AND IN GENERAL	67
HISTORY OF RADIOLOGICAL PROTECTION AND EVOLUTION OF DOSIMETRIC QUANTITIES	73
APPLIED SCIENCE AND TECHNOLOGY.....	81
ENTROPY DYNAMICS FOR A PROPELLER-SHAPED QUANTUM BROWNIAN MOLECULAR ROTATOR	82
BIOCORROSION, BIOFOULING AND HEALTH RISK: BIOLOGICAL ACTIVITY REACTION TESTS OF SELECTED BRACKISH GROUNDWATER	
OCCURRENCES IN SERBIA.....	86
BACTERIA IN DRINKING AND BATHING MINERAL WATERS OF SERBIA WITH POLYMER-DEGRADING POTENTIAL	91
MODELING AND SIMULATION OF A POLYMER OPTICAL FIBER HUMIDITY SENSOR FOR THE SKIN MICROENVIRONMENT	96
COMPARISON OF ORGANIC SUBSTANCE CONTENT IN PELOIDS FROM SUTOMORE AND IGALO (MONTENEGRO)	100
DRIFT SPECTROSCOPY AND PERMUTATION IMPORTANCE ALGORITHM IN QUANTITATIVE ANALYSIS OF ORGANIC MATTER IN SOIL MODEL	
SYSTEMS	104
THE INFLUENCE OF PYROCATECHOL ADDED IN PRE-OSCILLATORY PERIOD ON THE DYNAMICS OF THE BRAY-LIEBHAFSKY REACTION.....	108
ENVIRONMENTAL IMPLICATIONS OF FINANCIAL DEVELOPMENT IN CEE COUNTRIES.....	112
GREENHOUSE GAS EMISSIONS AND DIGITAL COMPETITIVENESS IN CEE COUNTRIES	116
ANTIFREEZE WITH COFFEE TASTE	120
THE HYDRATION AND ANTIMICROBIAL PROPERTIES OF SELECTED IMIDAZOLE-BASED IONIC LIQUIDS WITH A HOMOLOGOUS SERIES OF	
CHLORIDE OXYANIONS	124
INFLUENCE OF THE IONIC LIQUIDS-BASED ELECTROLYTES ON THE TOMATO (SOLANUM LYCOPERSICUM L.) AND CUCUMBER (CUCUMIS	
SATIVUS L.) GROWTH, DEVELOPMENT AND OXIDATIVE STRESS	128
SOLUBILITY AND STRUCTURAL ORGANIZATION OF TAURINE MOLECULES IN WATER	132
SELECTING CRITICAL FEATURES FOR BIOMEDICAL DATA CLASSIFICATION	136
THROMBOPHILIA PREDICTION USING MACHINE LEARNING ALGORITHMS	140
SIMULATION OF DNA DAMAGE USING THE “MOLECULARDNA” EXAMPLE APPLICATION OF GEANT4-DNA.....	144
DEVELOPMENT OF NANOMATERIALS FOR SUSTAINABLE FOOD PACKAGING APPLICATIONS.....	148
BIOACCUMULATION POTENTIAL OF 'MEEKER' AND 'WILLAMETTE' RASPBERRY (RUBUS IDAEUS L.) FRUITS TOWARDS MACRO- AND	
MICROELEMENTS AND THEIR NUTRITIONAL EVALUATION	152
IN VITRO AND IN SILICO ASSESSMENT OF ANTI-INFLAMMATORY ACTIVITY OF COCOA POWDERS	156

COMPARISON OF THE LUMINESCENCE PROPERTIES OF PHOSPHATE-TUNGSTEN BRONZE AND CERIU DOPED PHOSPHATE-TUNGSTEN BRONZE	160
THE COMPARISON OF TWO METHODS USED TO OBSERVE A NONLINEAR SYSTEM: POTENTIOMETRY AND HOLOGRAPHY	164
RADIOACTIVITY LEVELS AND HEALTH RISKS ASSOCIATED WITH HIMALAYAN SALT CONSUMPTION	168
PREVALENCE OF RADON AND METALS IN NATURAL SPRINGS IN THE SOKOBANJA AREA	172
INVESTIGATION OF THE POSSIBILITY OF INTERACTION BETWEEN LITHIUM FLUORIDE CLUSTERS AND BORON USING LDI MS.....	176
<i>IN VITRO</i> BIOLOGICAL EFFECTS OF CLONAL RED WINES	180
APPLIED MACHINE LEARNING IN EXPLORING KEY FEATURES OF CRAYFISH POPULATIONS	184
DOSE COMPENSATION ALGORITHM IN RADIOTHERAPY PLANNING.....	188
A PROTOCOL FOR THORACIC RADIATION THERAPY IN PATIENTS WITH CARDIAC IMPLANTABLE ELECTRONIC DEVICES.....	193
DISTRIBUTION OF DOSES TO ORGANS AT RISK IN CERVICAL CANCER HIGH DOSE RATE BRACHYTHERAPY USING TANDEM AND OVOIDS OR VAGINAL CYLINDER.....	197
ASSESSMENT OF RADIOACTIVITY LEVELS IN SOIL SAMPLES ON ZLATIBOR MOUNTAIN.....	201
INFLUENCE OF DIFFERENT PRODUCTION SYSTEMS AND TOMATO GENOTYPES ON THE	205
CHALLENGES IN RADIOTHERAPY PLANNING IN PATIENTS WITH SYNCHRONOUS RECTAL AND PROSTATE CANCER AND HIP PROSTHESIS..	209
EXPLORING THE PHARMACOKINETIC PROPERTIES OF (NH ₄) ₄ [Fe(IDADTC) ₂]: <i>IN SILICO</i> BIOLOGICAL SCREENING AND ADMET ANALYSIS	213
THE INFLUENCE OF DIFFERENT PLASTICIZERS ON THE MECHANICAL PROPERTIES OF ACTIVE EDIBLE BILAYER FILMS	217
PATCH CLAMP PIPETTE GIGA SEAL FORMING SUCCESS ON THE NANOSURGERY-OBTAINED FILAMENTOUS FUNGI PROTOPLASTS.....	221
ANALYSIS OF HEAVY METALS IN THE SOIL IN THE IBAR RIVER VALLEY IN THE DISTRICT OF KOSOVSKA MITROVICA	225
WATER QUALITY ANALYSIS IN THE DISTRICT OF KOSOVSKA MITROVICA.....	229
THE EFFECT OF CONSUMER ETHNOCENTRISM ON THE COMPETITIVENESS OF THE ECONOMY OF THE REPUBLIC OF SERBIA.....	232
THE ROLE OF SOCIALLY RESPONSIBLE BUSINESS IN IMPROVING THE COMPANY'S MARKET POSITIONING	236
CHEMOMETRIC APPROACH TO THE INVESTIGATION OF MICROELEMENTS AND POTENTIALLY TOXIC ELEMENTS IN THE SOIL.....	241
APPLICATION OF CHEMOMETRICS IN MONITORING OF SPATIAL AND TEMPORAL VARIATIONS IN RIVER WATER QUALITY AND WATER CLASSIFICATION	245
MECHANOCHEMISTRY: OPTIMIZATION OF THE SYNTHESIS OF DITHIOCARBAMATE DERIVATIVES.....	249
CAPACITIVE BEHAVIOUR OF BIOMASS-DERIVED ACTIVATED CARBON IN AL-ION-CONTAINING ELECTROLYTES	253
THE INTERDEPENDENCE OF STRUCTURAL PROPERTIES AND PSEUDOCAPACITIVE BEHAVIOR OF BIOMASS-DERIVED ACTIVATED CARBON	257
ELUCIDATING HEALTH-ENHANCING PROPERTIES OF NATURAL PRODUCTS: A JOURNEY FROM EXTRACT ISOLATION TO QUANTUM MECHANICS (QM) CALCULATIONS.....	261
A COMPUTATIONAL MODEL OF THE LEFT VENTRICLE – APPLICATION IN CARDIOMYOPATHY DISEASE	265
STATUS AND QUALITY OF LIFE OF PEOPLE WITH CELIAC AND PEOPLE ON A GLUTEN-FREE DIET	269
MODELING OF CIRCULATING TUMOR CELL (CTC) AND PLATELET INTERACTION IN CAPILLARIES.....	274
BIOINFORMATICS AND APPLIED BIOLOGY	279
ABUNDANCE, SPECIES RICHNESS AND DIVERSITY OF EARTHWORMS (LUMBRICIDAE) IN SEVERAL HABITATS OF THE NORTHERN PART OF JASTREBAC MOUNTAIN	280
A NEW RECORD OF <i>DENDROBAENA SERBICA</i> KARAMAN, 1973 (CLITELLATA; LUMBRICIDAE) FROM SERBIA.....	284
POTENTIALLY TOXIC ELEMENTS IN THE EDIBLE PART OF TROUT (<i>SALMO TRUTTA</i> L.) FROM THE UPPER REACHES OF THE RAŠKA AND STUDENICA RIVERS	288
DIET COMPOSITION AND FEEDING HABITS OF COMMON BLEAK (<i>ALBURNUS ALBURNUS</i> L.) IN THE GRUŽA AND GAZIVODE RESERVOIRS	292
IDENTIFICATION OF PROTEIN TARGET MOLECULES FOR [Pd(DACH)Cl ₂] COMPLEX IN HeLa CERVICAL CARCINOMA CELLS	296
EDIBLE MUSHROOMS AS PROMISING ANTIOXIDANTS	300
ANTIMICROBIAL POTENTIAL OF MUSHROOMS <i>MACROLEPIOTA PROCERA</i> AND <i>CHLOROPHYLLUM RHACODES</i>	304
OBESITY AS A RISK FACTOR FOR COVID- 19 MORTALITY: AN OVERVIEW OF PUBLISHED META-ANALYSES	308
CLASSIFICATION AND ANALYSIS OF KEY PARAMETERS IN PREDICTING THE STATE OF FACULTATIVE OLIGOTROPHS IN TWO DIFFERENT RESERVOIRS	312

ECOLOGICAL APPLICATIONS BASED ON BACTERIAL COMMUNITY ABUNDANCE IN RESERVOIRS USING AN ARTIFICIAL NEURAL NETWORK APPROACH.....	317
OXIDATIVE DNA DAMAGE PREVENTIVE ACTIVITY OF ESSENTIAL OILS OF THREE <i>PINUS</i> SPECIES: <i>P. MUGO</i> , <i>P. SIBIRICA</i> , AND <i>P. SILVESTRE</i>	321
COMPARATIVE ASSESSMENT OF FISH DIVERSITY INDICES IN PROTECTED VLASINA RESERVOIR AND UNPROTECTED GRUŽA RESERVOIR	326
ASSESSMENT OF DIFFERENT MACHINE LEARNING TOOLS EMPLOYED IN LIPIDOMICS	330
SLIGHT COOLING DURING GROWTH INDUCED CHANGES IN FILAMENTOUS FUNGI HYPHA MITOCHONDRIAL MORPHOLOGY	334
STRUCTURAL SIMULATIONS PREDICTING PROTEIN FOLDING IN ALZHEIMER'S DISEASE	338
A MACHINE LEARNING APPROACH COMBINING OMICS DATA FOR ALZHEIMER'S DISEASE ANALYSIS	342
BIOMEDICAL ENGINEERING	346
NUMERICAL MODELING OF NEW 4,7-DIHYDROXYCOUMARIN DERIVATIVE DIFFUSION WITHIN FINITE ELEMENT LIVER MODEL.....	347
UV-BLOCKING SUSTAINABLE FOOD PACKAGING BASED ON POLYHYDROXYALKANOATE AND BACTERIAL PIGMENT PRODIGIOSIN	351
USING NUMERICAL MODELING TO ANALYZE THE BEHAVIOR OF CANCER CELLS AFTER DIVERSE CO-TREATMENTS.....	355
OVERVIEW OF LEFT VENTRICULAR SEGMENTATION IN ULTRASOUND IMAGES	359
FINITE ELEMENT ANALYSIS OF STRESS DISTRIBUTION IN 3D TOOTH MODEL WITH EXTENSIVE CAVITIES RESTORED WITH DIRECT AND INDIRECT COMPOSITE RESTORATION	363
MULTISCALE MODELLING OF THE EFFECTS OF TEMPERATURE ON CARDIAC TWITCHES	367
ANALYTICALLY COMPUTED FRACTIONAL FLOW RESERVE BASED ON CORONARY CT ANGIOGRAPHY.....	371
A FINITE ELEMENT MODEL FOR STRUCTURAL OPTIMIZATION OF PARAMETRIZED LATTICE SCAFFOLDS	375
APPLICATION OF MACHINE LEARNING ALGORITHMS IN MEDICAL DATA PROCESSING	379
BIOORGANIC, BIOINORGANIC AND MEDICINAL CHEMISTRY.....	382
STRUCTURAL, SPECTROSCOPIC, AND MOLECULAR DOCKING ANALYSIS OF ISOPROTERENOL	383
MOLECULAR DOCKING STUDY OF RUTHENIUM- <i>p</i> -CYMENE COMPLEXES WITH ISOTHIAZOLE DERIVATIVES AS SARS-COV-2 MAIN PROTEASE INHIBITORS	387
SYNTHESIS, SPECTROSCOPIC, AND QUANTUM-CHEMICAL ANALYSIS OF MONONUCLEAR Ru(II)-NAPHTHYLHYDRAZINE COMPLEX	391
SYNTHESIS, SPECTROSCOPIC, AND THEORETICAL ANALYSIS OF Ru(II)-PHENYLHYDRAZINE COMPLEX	395
DNA/BSA BINDING STUDY OF MONONUCLEAR GOLD(III) COMPLEXES WITH CLINICALLY USED AZOLES.....	399
DNA/BSA INTERACTION OF PLATINUM(II) COMPLEXES WITH PHENOTHIAZINE AND <i>N</i> -METHYLPHENOTHIAZINE	403
THE INTERACTION STUDIES OF NOVEL DIAMINOPHENAZINE GOLD(III) COMPLEX AND BOVINE SERUM ALBUMIN (BSA-IBUPROFEN AND BSA-EOZINE Y)	407
THE INFLUENCE OF STRUCTURAL MODIFICATION OF Pd(II) Pincer-TYPE COMPLEXES ON THE KINETICS OF SUBSTITUTION REACTIONS.	411
<i>IN VITRO</i> CYTOTOXIC ACTIVITY OF A MONOLACUNARY WELLS-DAWSON NANOCUSTER AGAINST CERVICAL CARCINOMA HeLa CELLS	415
THE INFLUENCE OF Fe(III) INCORPORATION ON ANTI-CANCER POTENTIAL OF A WELLS-DAWSON NANOCUSTER	419
DFT APPROACH OF THE REDOX PROPERTIES OF BRIMONIDINE AND VARENICLINE.....	423
THEORETICAL AND EXPERIMENTAL STUDY OF BILASTINE IONIZATION	427
NEW VANADIUM COMPLEXES WITH POTENTIAL BIOLOGICAL ACTIVITY.....	431
SYNTHESIS OF SCHIFF BASES BETWEEN SOME FIVE-MEMBERED HETEROCYCLIC ALDEHYDES AND THIOCARBOHYDRAZIDE (TCH) AND OPTIMIZATION OF REACTION CONDITIONS	435
SYNTHESIS, STRUCTURE AND ANTICANCER ACTIVITY OF Zr(IV) COMPLEXES WITH SCHIFF BASES DERIVED FROM 8-HYDROXYQUINOLINE	439
IONIC PALLADIUM(II) COMPLEXES WITH NITRO AND HALOGEN DERIVATIVES OF 8-HYDROXYQUINOLINE	443
A NOVEL SILVER COMPLEX WITH 4-HYDROXYCOUMARIN DERIVATIVE: SYNTHESIS, STRUCTURE, AND BIOLOGICAL ACTIVITY	447
ANTICANCER GALLIUM(III) COMPLEXES WITH HALOGEN- AND NITRODERIVATIVES OF 8-HYDROXYQUINOLINE.....	451
<i>IN SILICO</i> DRUG-LIKENESS, PHARMACOKINETIC AND OTHER ADME PROPERTIES OF 2-(AMINOMETHYL)CYCLOPROPANE-1,1-DICARBOXYLIC ACID.....	455
BSA BINDING OF 2-(AMINOMETHYL)CYCLOPROPANE-1,1-DICARBOXYLIC ACID	459
INVESTIGATION OF BINDING MODE OF NOVEL 2,4-DIKETO ESTERS TO BSA	463

SR FTIR SPECTROSCOPY INVESTIGATION OF Pd@S-CD NANOCOMPOSITE SYSTEM EFFECTS ON BIOMOLECULES IN CERVICAL CARCINOMA CELLS	467
THE EFFECTS OF A SELECTED METHOXY SUBSTITUTED CHALCONE IN HUMAN MELANOMA CELLS IRRADIATED WITH γ -RAYS	471
<i>IN SILICO</i> ESTIMATION OF COX-2 AND 5-LOX INHIBITORY POTENTIAL OF SOME NOVEL THIOUREA DERIVATIVES OF NAPROXEN	475
MOLECULAR DOCKING STUDY OF DESIGNED N-MYRISTOYL TRANSFERASE INHIBITORS.....	479
PLATINUM(II) COMPLEXES WITH EPOXIDE DERIVATIVE OF 1,10-PHENANTHROLINE IN INTERACTION WITH HUMAN SERUM ALBUMIN ..	483
ANALYTICAL VALUES OF BEESWAX FROM MONTENEGRO AND DETECTION OF ADULTERATION	487
PHENOLIC <i>N</i> -ACYL HYDRAZONE DERIVATIVES: <i>IN SILICO</i> ASSESSMENT OF POTENTIAL ANTIBACTERIAL ACTIVITY AGAINST SELECTED G ⁺ AND G ⁻ STRAINS	491
<i>IN SILICO</i> ANTIBIOFILM POTENCY OF PHENOLIC <i>N</i> -ACYL HYDRAZONES AGAINST SELECTED BACTERIAL STRAINS	495
TiO ₂ NANOPARTICLES AND TiO ₂ NANOPARTICLES SURFACE MODIFIED WITH SALICYLIC ACID AFFECT NEUROLOGICAL FUNCTIONS AND OXIDATIVE STRESS MARKERS IN THE EYES OF ADULT RATS	499
SYNTHESIS AND CYTOTOXIC ACTIVITY OF SELECTED DUAL COX-2 AND 5-LOX INHIBITORS IN HELA AND MIA PaCa-2 HUMAN CANCER CELL LINES	503
SYNTHESIS, CHARACTERIZATION AND HSA INTERACTIONS OF A NEW PIANO-STOOL RUTHENIUM(II) COMPLEX CONTAINING A THIOAMIDE-TYPE LIGAND	507
HPLC/UV PROFILE AND DETERMINATION OF TOTAL PHENOLIC AND FLAVONOID CONTENTS OF LICHEN <i>UMBILICARIA CRUSTULOSA</i> GROWING IN SERBIA	511
LICHENO-CHEMICAL ANALYSIS AND <i>IN VITRO</i> ANTIOXIDANT ACTIVITY OF EXTRACTS AND GYROPHORIC ACID FROM LICHEN <i>UMBILICARIA GRISEA</i>	515
BIOLOGICAL ACTIVITY OF THIENYL-TERPYRIDINE Ru(II) COMPLEX IN THE PRESENCE OF BIOCOMPATIBLE IONIC LIQUIDS	519
KINETIC STUDIES OF THE Ru(II) POLYPYRIDYL COMPLEX WITH BIOLOGICALLY RELEVANT LIGANDS	523
SYNTHESIS AND PHYSICO-CHEMICAL CHARACTERISATION OF THE Ni(II) COMPLEX WITH 3-(4-CHLOROPHENYL)-1H-PYRAZOLE LIGAND ..	527
NORMAL AND REVERSED PHASES THIN-LAYER CHROMATOGRAPHY OF ARYLIDENE 2-THIOHYDANTOIN DERIVATIVES	531
INVESTIGATION OF THE ANTICANCER ACTIVITY OF 2-AMINO-6-METHYLBENZOTHAZOLE AND CORRESPONDING Pd(II) COMPLEX USING MOLECULAR DOCKING SIMULATIONS	535
DNA BINDING AND MOLECULAR DOCKING OF FOUR PALLADIUM(II) COMPLEXES WITH <i>O,O'</i> -DIALKYL ESTERS OF (<i>S,S</i>)-PROPYLENEDIAMINE- <i>N,N'</i> -DI-2-(2-BENZYL) ACETIC ACID	539
MACRO AND MICROELEMENTS IN THE LEAF AND EXTRACT OF NETTLE FROM DIFFERENT LOCALITIES OF MONTENEGRO	543
SYNTHESIS AND ANTIOXIDANT ACTIVITY OF NOVEL VANILLIN-BASED FERROCENYL CHALCONES	547
A CONTRIBUTION TO THE KNOWLEDGE OF THE SPECIES <i>DIPSACUS SYLVESTRIS</i> HUDS.	551
QUALITATIVE CONTENT OF SELECTED PHENOLIC COMPOUNDS IN DIFFERENT EXTRACTS OF PLANT SPECIES <i>IRIS PUMILA</i> L.	555
BUILDING A 3D QSAR MODEL WITH ISOPROPYLIDENE ANALOGS OF CYTOTOXIC STYRYL-LACTONES	559
VALIDATION OF GRAVIMETRIC METHOD FOR DETERMINATION OF CLAY IN SOIL	563
PYRAZOLE/TACRINE DERIVATIVES AS POTENTIAL CHOLINESTERASE INHIBITORS.....	567
THE INFLUENCE OF THE METHANOL EXTRACT OF <i>GALIUM VERUM</i> ON CARDIAC OXIDATIVE DAMAGE IN HYPERTENSIVE RATS IN A MODEL OF GLOBAL ISCHEMIA	571
CAN A THREE-WEEK ADMINISTRATION OF METHANOL EXTRACT OF WILD GARLIC MODULATE SYSTEMIC REDOX STATE IN HYPERTENSIVE RATS?	575
CHEMOINFORMATICS, CHEMOGENOMICS AND MOLECULAR DESIGN	579
HIGH-THROUGHPUT SCREENING OF NOVEL HYDROGEN STORAGE MATERIALS – ML APPROACH	580
3D-QUANTITATIVE STRUCTURE-ACTIVITY RELATIONSHIP AND DESIGN OF NOVEL RHO-ASSOCIATED PROTEIN KINASES-1 (ROCK1) INHIBITORS	584
VIRTUAL DOCKING, DESIGN AND <i>IN SILICO</i> ADMET PROFILING OF NOVEL RHO-ASSOCIATED PROTEIN KINASES-1 (ROCK1) INHIBITORS	589
A METRIC FOR PAIRWISE SIMILARITY ANALYSIS OF BINARY CHEMINFORMATICS DATA	593
COUMARINS AS PROMISING PPAR α AGONISTS. NOVEL <i>IN SILICO</i> INSIGHTS	597
COMBINED <i>IN SILICO</i> APPROACH TO IDENTIFY NEW TERPENOID PPAR α AGONISTS.....	601

<i>IN SILICO</i> SCREENING OF <i>SOLANUM LYCOPERSICUM</i> CAROTENOIDS FROM CAROTENOIDS DATABASE FOR CANDIDATES PPARA AGONISTS	605
NUMERICAL SIMULATIONS OF THE OSCILLATORY DYNAMICS IN THE BRAY-LIEBHAFSKY REACTION PERTURBED BY L-TYROSINE.....	609
THE ASSESSMENT OF THE ANTIOXIDANT CAPACITY OF THE SELECTED VANILLIN-BASED PYRIDO-DIPYRIMIDINES USING DPPH ASSAY: <i>IN SILICO</i> APPROACH	613
INHIBITORY POTENTIAL OF BARBARIN AND ITS PLATINUM(II) COMPLEX TOWARDS PBP1A PROTEIN	617
MODELING ION- π INTERACTIONS OF TRANSITION METAL COMPLEXES	621
SUBSTITUENT EFFECTS ON STACKING INTERACTIONS OF AROMATIC LIGANDS IN ORGANOMETALLIC COMPOUNDS – CHEMOINFORMATICS AND QUANTUM CHEMICAL STUDY	625
COMPUTATIONAL STUDY ON THE INTERACTIONS OF QUERCETIN 3-O-RUTINOSIDE WITH HUMAN DPP III	629
NONCOVALENT INTERACTIONS OF HALOGEN ATOMS IN HALOGENATED BIPYRIDINES	633
REPULSIVE WATER-WATER CONTACTS FROM CAMBRIDGE STRUCTURAL DATABASE	637
COMPUTER-AIDED DESIGN OF NEW DRUGS AGAINST BREAST CANCER.....	641
STACKING INTERACTIONS AT LARGE HORIZONTAL DISPLACEMENTS—COMPARISON OF VARIOUS RING TYPES.....	645
INFLUENCE OF COORDINATION ON OH/ π AND NH/ π INTERACTIONS	649
RELATIVISTIC DFT CALCULATION AND THEIR EFFECT ON THE ACCURACY OF RESULTS	653
ANALYSIS OF PREDICTION OF WATER SOLUBILITY AND LIPOPHILICITY OF COUMARINS BY FREE CHEMINFORMATICS TOOLS	657
INFLUENCE OF PHTHALIMIDE SUBSTITUTION ON THE INTERACTION WITH CARBON NANOTUBE	662
INTERACTION ENERGY AND DECOMPOSITION OF INTERACTION ENERGY OF HALO-SUBSTITUTED PHTHALIMIDE WITH CARBON NANOTUBE	666
IDENTIFICATION OF SMALL MOLECULE BINDING SITES USING CMDock	670
A COMPREHENSIVE <i>IN SILICO</i> PROTOCOL FOR FAST AUTOMATED MUTAGENESIS AND BINDING AFFINITY SCORING OF PROTEIN-LIGAND COMPLEXES	674
WORKFLOW AUTOMATION OF HIGH-THROUGHPUT INVERSE DOCKING USING PHARMMAPPER	678
INVESTIGATING THE POTENTIAL INHIBITORY EFFECT OF THE MEGAPHONE (MOLECULE) ON NASOPHARYNGEAL CANCER GROWTH FACTOR RECEPTORS	682
GREEN SYNTHESIS OF CHROMENO-PYRIMIDINE DERIVATIVES – PART I.....	686
CHROMENO-PYRIMIDINE-TYPE COMPOUNDS (PART II): <i>IN VITRO</i> EVALUATION OF ANTIOXIDANT POTENTIAL	690

Selecting critical features for biomedical data classification

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Abstract: In this paper, the application of machine learning methods on large data sets with numerous features was investigated, with a focus on the identification of critical features in order to reduce the data and produce more accurate results. The research discusses feature extraction techniques for classifying two biomedical data sets with 62 and 71 features, respectively. The results were compared and presented using four classification techniques. The acquired results demonstrate that the selected important features typically produce more accurate results, or at least the same results while reducing the size of the data set and making data collecting easier.

Keywords: feature selection, machine learning, biomedical data classification, pregnant women

1. Introduction

Prior to applying machine learning techniques to huge datasets with numerous features, it is crucial to prioritize the most significant ones in order to reduce the size of the dataset and produce more accurate results. Choosing good features means choosing only the important features and not leaving out any essential features [1]. High dimension biomedical data usually contains a large number of weak relevant or irrelevant features. Therefore, feature selection is considered to be an essential step in the diagnosis of related diseases using high dimension biomedical data [2]. In classification models for colorectal cancer cases phenotypic [3] as well as for the classification of high-dimensional biomedical data [4], attribute selection produced

positive outcomes. This research deals with the problem of determining diagnostic biomarkers in pregnancy. Thrombophilia in pregnancy, preeclampsia and gestational diabetes are a few of the issues that could occur during pregnancy. This study aims to develop a more accurate method of determining whether a pregnant woman has any of the issues above. For this study, biomedical and demographic information was gathered. The research task is to single out the most significant attributes that provide an equally good model for predicting possible problems in pregnancy as a model built on all available attributes. To check the correctness, the classification of pregnant women was applied based on the available biomedical and demographic data using four classification methods and the obtained models were compared with the classification models obtained on a separate set of attributes.

2. Materials and Methods

Subjects were selected from pregnant women who are accommodated at the Gynecology-Obstetrics Clinic of the University Clinical Center Kragujevac for treatment or labor. Four categories of pregnant women were included in the study: 1) healthy pregnant women (control group); 2) women with preeclampsia; 3) pregnant women with thrombophilia; 4) women with gestational diabetes, controlled by diet. Ethics Committee of the University Clinical Center Kragujevac approved the study protocol, and all patients gave informed consent. For the purposes of this research, two sets of data were selected. The first data set contains information on demographic data for 65 women, of which 27 women have biomedical data. These women are from all four categories. The second set of data consists of demographic and biomedical data of 35 who belong to the group of healthy pregnant women or pregnant women with thrombophilia. Biomedical data consists of clinical data obtained by taking an anamnesis, blood and urine analysis, and via ultrasound examination of pregnant women. Demographic data were collected using a questionnaire on demographic and lifestyle issues. The aim of this study is to enhance the model and categorize pregnant women into one of the four or one of the two groups found in the initial data set. Before applying the modeling, we completed identifying the associated features from a collection of data and removing the irrelevant or less significant features. The SelectKBest class (from the Python scikit-learn library) is used to choose 10 of the best features. The chi-squared (chi2) statistical test was performed to determine the most important categorical features (demographic) and ANOVA for numerical data (biomedical analysis). This study compares the performance of K-nearest neighbors (KNN), Random Forest (RF), Support Vector Machines (SVM), and Naive Bayes (NB) machine learning methods for classification on the described datasets. Comparisons were made between the classification outcomes obtained using the set of attributes chosen through univariate selection and the outcomes of applying the methods to all available attributes. The implementation of the proposed machine learning methods is done using Python and corresponding ML packages (pandas, numpy). To compare classification results, the accuracy measure was used.

3. Results and discussion

The proposed method for the selection of attributes for the classification of biomedical data sets was applied to both described sets. The extracted demographic and biomedical features for the two datasets are displayed in Figure 1.

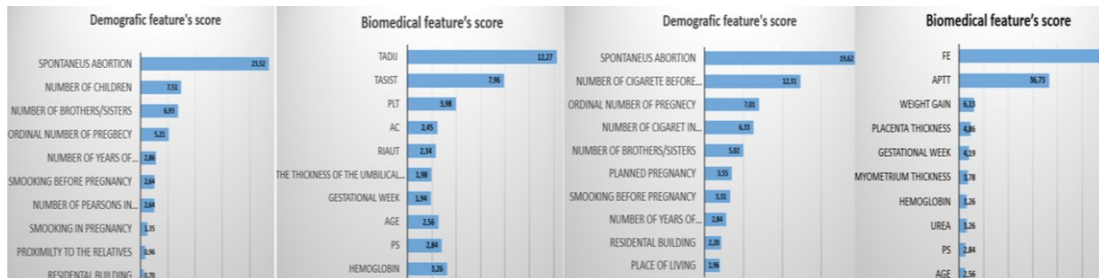


Figure 1. Demographic and biomedical feature's score for the first (left) and the second (right) data set.

A classification using all demographic (biomedical) variables was carried out and the results were compared with those when the classification was carried out just on the basis of 10 selected ones. This was done in order to assess the significance of the selected features on both sets of data. The proposed strategy was evaluated using five-fold cross-validation. The first set of data contains four groups of pregnant women, and the classification of this set was made into 4 classes. Four classification methods were applied, and the obtained results are shown in Table 1.

Table 1. Results of 4-class classification on the first data set when using demographic (left) and biomedical (right) data with all attributes and reduced data.

Demographic features					Biomedical features				
#Features	KNN	RF	SVM	NB	#Features	KNN	RF	SVM	NB
Top 10	0.39	0.39	0.39	0.30	Top 10	0.7	0.63	0.51	0.58
All (25)	0.39	0.29	0.37	0.25	All (37)	0.37	0.45	0.44	0.45

The best classification results for both demographic and biomedical features are obtained using the top 10 extracted features, using the KNN method: 0.39 for demographic and 0.7 for biomedical (Table 1). For all four methods, attribute reduction gave better or at least the same accuracy. The low precision is due to the large number of classes and the small sample. The second set of data shows the results of applying this method when we have only two classes of healthy pregnant women and pregnant women with thrombophilia. Table 2 shows the results obtained by applying the classification to all attributes compared to the classification only to the selected ones. As for demographic attributes, the RF method applied to the selected 10 attributes gave the best results. Again, in all cases, the classification is of the same or better accuracy compared to the reduced attributes.

Table 2. Results of binary classification on the second data set when using demographic (left) and biomedical (right) data with all attributes and reduced data.

Demographic features					Biomedical features				
#Features	KNN	RF	SVM	NB	#Features	KNN	RF	SVM	NB
Top 10	0.80	0.83	0.80	0.63	Top 10	0.83	0.91	0.63	1.00
All (34)	0.66	0.83	0.63	0.57	All (37)	0.46	0.94	0.63	0.97

The classification using biomedical attributes is shown in Table 2, where the best results were given by the NB method using 10 selected attributes. Only in the case of the RF method, less precise results were obtained on the reduced data set compared to the whole set. In all other and global classification methods when applied over 10 attributes give the same or better precision. These results justify the application of the attribute extraction method before creating the classification model. The selection of attributes that are correlated with one disease gave much better results.

4. Conclusions

Based on the presented results, it can be concluded that the application of attribute extraction on biomedical data improves classification results. It has been shown that binary classification gives better results and that, in general, it is necessary to expand the data set. Future studies will focus on data preparation and training set enlargement in order to obtain more precise results.

References

- [1] Y. Lyu, Y. Feng, K. Sakurai., *A survey on feature selection techniques based on filtering methods for cyber attack detection*, Information, 14.3 (2023) 191.
- [2] J. Tao, Y. Kang., *Features importance analysis for emotional speech classification*, Lecture Notes Comput Sci, 3784 (2015) 449–57.
- [3] T. W. Cenggoro, B. Mahesworo, A. Budiarto, J. Baurley, T. Suparyanto, B.Pardamean *Features importance in classification models for colorectal cancer cases phenotype in Indonesia*, Procedia Comput Science, 157 (2019) 313–320.
- [4] B. Zhang, C. Peng., *Classification of high dimensional biomedical data based on feature selection using redundant removal*, PloS one, 14.4 (2019) e0214406.