

3rd International Conference on Chemo and BioInformatics

Kragujevac, September 25-26, 2025, Serbia



International Conference
on Chemo and BioInformatics

ORGANIZERS AND SPONSORS



Republic of Serbia

MINISTRY OF SCIENCE,
TECHNOLOGICAL DEVELOPMENT AND INNOVATION

MC LABOR
LABORATORIJSKA I PROCESNA OPREMA

Anton Paar
Authorized Distributor

KPM
ANALYTICS
Authorized Distributor

EQUILAB

Hitachi High-Tech

SUPERLAB®
Your lab - Our passion

ANALYSIS
LABORATORY EQUIPMENT



3rd International Conference on Chemo and BioInformatics
ICCBIKG 2025

BOOK OF PROCEEDINGS

September 25-26, 2025
Kragujevac, Serbia

Sponsored by



Anton Paar

Hitachi High-Tech



EQUILAB



SUPERLAB®
Your lab – Our passion



3rd International Conference on Chemo and BioInformatics, Kragujevac, September 25-26, 2025, Serbia.

Editors:

Dr. Igor Saveljić

Prof. Dr. Nenad Filipović

Technical Editors:

Dr. Vladimir Simić

Dr. Marko Antonijević

Proofreading:

Kristina Milisavljević

Press:

„Grafo Ink“, Kragujevac

Impression:

10 copies

Publisher:

Institute for Information Technologies, University of Kragujevac, Serbia, Jovana Cvijića bb, 2025

CIP - Каталогизација у публикацији Народна библиотека Србије, Београд

54:004(048)(0.034.2)

57+61]:004(082)(0.034.2)

INTERNATIONAL Conference on Chemo and BioInformatics (3 ; 2025 ; Kragujevac)
Book of Proceedings [Elektronski izvor] / 3rd International Conference on Chemo and
BioInformatics, ICCBIKG 2025, September 25-26, 2025, Kragujevac, Serbia ; [editors Igor Saveljić,
Nenad Filipović]. - Kragujevac : University, Institute for Information Technologies, 2025
(Kragujevac : Grafo Ink). - 1 USB fleš memorija ; 1 x 2 x 3 cm

Sistemske zahteve: Nisu navedeni. - Nasl. sa naslovne strane dokumenta. - Tiraž 10. - Bibliografija
uz svaki rad.

ISBN 978-86-82172-05-5

a) Хемија -- Информациона технологија -- Зборници b) Биомедицина -- Информациона
технологија -- Зборници

COBISS.SR-ID 176312073

Organized by:

Institute for Information Technologies, University of Kragujevac, **Organizer**



The Ministry of Science, Technological
Development and Innovation of The
Republic of Serbia, *Supporting organization*



University of Kragujevac,
Suborganizer



Faculty of Medicinal Sciences, University of
Kragujevac, *Suborganizer*



Faculty of Science, University of
Kragujevac, *Suborganizer*



Institute for Biological Research "Siniša
Stanković" - National Institute of Republic of
Serbia, University of Belgrade, *Supporting
organization*



Serbian Chemical Society, *Supporting
organization*



Committees

International Organizing Committee:

General Chairman:

Dr. Igor Saveljić (Serbia)

Vice-chairmans:

Dr. Nenad Janković (Serbia)

Prof. Dr. Urban Bren (Slovenia)

Members:

Dr Dejan Milenković (Serbia), Dr. Marijana Petković (Serbia), Dr. Marija Stanić (Serbia), Dr. Melina Kalagasidis Krušić (Serbia), Dr. Suzana Jovanović-Šanta (Serbia), Prof. Dr. Vladimir Ranković (Serbia), Dr. Marina Soković (Serbia), Dr. Mirjana Mihailović (Serbia), Prof. Dr. Vladimir Janjić (Serbia)

International Scientific Committee:

Chairman:

Prof. Dr Nenad Filipović (Serbia)

Vice-chairmans:

Academician Miloš Kojić (Serbia)

Academician Miloš Đuran (Serbia)

Prof. Dr. Zoran Marković (Serbia)

Prof. Dr. Xiaoping Chen (China)

Members:

Prof. Dr. Iztok Turel (Slovenia), Prof. Dr. Bakhtiyor Rasulev (USA), Prof. Dr. Ivan Gutman (Serbia), Prof. Nenad Kostić (USA), Prof. Dr. Demetrio Milea (Italy), Prof. Dr. Quan Yuan (China), Prof. Caroline Da Ros Montes D'Oca (Brazil), Dr. Danijela Bakarić (Croatia), Prof. Dr. Carlos Silva Lopez (Spain), Prof. Dr. Ferda Ari (Turkey), Prof. Dr. Miljan Milošević (Serbia), Dr. Edina Avdović (Serbia), Prof. Dr. Snežana Zarić (Serbia), Prof. Dr. Suzana Jovanović Šanta (Serbia), Dr. Željko Čupić (Serbia), Aleksandar Nešović (Serbia), Dr. Ana Rilak Simović (Serbia), Dr. Marko Živanović (Serbia), Dr. Jelena Katanić Stanković (Serbia), Dr. Milica Nikolić (Serbia), Dr. Dušica Simijonović (Serbia), Dr. Aleksandar Radaković (Serbia), Dr. Jasmina Obradović (Serbia), Dr. Dalibor Nikolić (Serbia), Dr. Jelena Đorović Jovanović (Serbia), Dr. Žiko Milanović (Serbia), Dr. Dejan Milenković (Serbia), Dr. Sonia Morya (India), Dr. Snežana Papović (Serbia), Prof. Dr. Biljana Ljujić (Serbia)

Local Executive Committee:

Chairman:

Dr. Darko Ašanin (Serbia)

Vice-chairmans:

Dr. Marko Antonijević (Serbia)

Dr. Vladimir Simić (Serbia)

Members:

Jelena Živković (Serbia), Bogdan Milićević (Serbia), Lazar Kostić (Serbia), Petar Stanić (Serbia), Aleksandra Marković (Serbia), Tamara Mladenović (Serbia), Aleksandar Nešović (Serbia), Emilija Milović (Serbia), Jovana Matić (Serbia), Nevena Milivojević (Serbia), Danijela Stojković (Serbia), Marija Branković (Serbia), Jana Bašcarević (Serbia), Aleksandar Nikolić (Serbia), Lazar Milović (Serbia), Dr. Mirjana Grujović (Serbia), Dr. Katarina Marković (Serbia).

Table of contents

PLENARY LECTURERS	1
SLEEP AND THE GUT.....	2
CLINICAL SCIENCES AND TRANSLATIONAL MEDICINE RESEARCH THEME AT COVENTRY UNIVERSITY.....	4
NEXT-GENERATION HYDRAULIC FLUIDS: THE ROLE AND POTENTIAL OF PROTIC IONIC LIQUIDS.....	13
DEVELOPMENT OF EXPERIMENTAL SET UP FOR FUNCTIONAL CHARACTERIZATION OF MATERIALS OF INTEREST IN BIOMEDICAL IMAGING AND/OR PHOTODYNAMIC THERAPY AND/OR DRUG DELIVERY BY FREQUENCY PHOTOACOUSTICS	20
APPLICATION OF HYDROGEL IN DISEASE THERAPY AND TISSUE ENGINEERING	27
PIONEERING SESQUITERPENOID CHEMODIVERSITY IN <i>ARTEMISIA HEDINII</i>	31
COMPUTER SIMULATIONS AS AN IMPORTANT TOOL TO DEVELOP NEW DRUGS AGAINST SARS-CoV-2 ..	35
A MULTI-ORGAN-ON-A-CHIP PLATFORM FOR MODELING CANCER METASTASIS	38
SECTION LECTURERS.....	43
WHEN AZOLES MEET SILVER: A CHEMISTRY POWER DUO AGAINST FUNGI.....	44
MODULATION OF THERMOTROPIC PROPERTIES OF CHOLESTEROL-FREE MODEL MYELIN MEMBRANES BY MYELIN BASIC PROTEIN	48
EFFECT OF STRUCTURAL ELEMENTS OF TANNINS ON THEIR REACTIVITY WITH METAL IONS – EXPERIMENTAL STUDY WITH QM SUPPORT	53
TRANSLATIONAL RESEARCH: CONNECTING THE LABORATORY AND THE CLINIC.....	58
CHANGES IN PROTEIN EXPRESSION IN HeLa CERVICAL CANCER CELLS INDUCED BY [Pd(DACH)Cl ₂] COMPLEX.....	61
EVALUATION OF THE CARCINOGEN-SCAVENGING ACTIVITY OF POLYPHENOLIC COMPOUNDS BY USING QUANTUM MECHANICS-BASED PROTOCOL QM-CSA.....	66
GRAPH-BASED MODELING OF DIABETIC PATIENT DATA FOR READMISSION RISK AND CARE PATTERN ANALYSIS	71
INVERSE MOLECULAR DOCKING FINGERPRINTS FOR TARGET IDENTIFICATION	75
ANTIOXIDANT AND LIPOXYGENASE INHIBITION ACTIVITIES OF ULTRASOUND-ASSISTED EXTRACTS FROM PROKUPAC GRAPE SKINS	81
BIOLOGICAL POTENTIAL OF GRAPE SKIN EXTRACTS: A COMPARATIVE STUDY OF GRAPE VARIETIES FROM THE ŠUMADIJA REGION	85
APPLIED SCIENCE AND TECHNOLOGY	89
PRELIMINARY INVESTIGATION OF NATURAL RADIOACTIVITY (GROSS ALPHA/BETA) IN RURAL WATER SUPPLIES OF BAGERHAT DISTRICT, BANGLADESH.....	90
INVESTIGATION OF BRIGGS-RAUSCHER OSCILLOGRAMS VIA PEAK AREA INTEGRATION	95
ECONOMIC GROWTH, RENEWABLE ENERGY, TRADE OPENNESS AND CO ₂ EMISSIONS: A CAUSALITY ANALYSIS	99
SUSTAINABLE ACTIVATED CARBON: TRANSFORMING SAWDUST WITH ZINC CHLORIDE ACTIVATION TREATMENT	103

EFFECTS OF THE SUSTAINABLE TOURISM CONCEPT, ENVIRONMENTAL BELIEFS, AND SOCIAL MEDIA INFLUENCERS ON THE CHOICE OF GREEN HOTELS WHEN TRAVELING.....	107
CHEMICAL ANALYSIS OF SOIL AND DETERMINATION OF ITS FERTILITY.....	111
CONTENT OF AIR POLLUTANTS IN KRALJEVO	115
SYNTHESIS AND CHARACTERIZATION OF CERIUM SALT OF 12-TUNGSTOPHOSPHORIC HETEROPOLY ACID – CE-PWA	119
SMOOTHED PARTICLE HYDRODYNAMICS (SPH) FOR MODELLING MICROFLUIDIC FLOW THROUGH 3D PRINTED COPPER FILTERS.....	123
CORRELATION ANALYSIS OF HEAVY METALS, RADIONUCLIDES, AND PHYSICOCHEMICAL PROPERTIES IN SOIL FROM SERBIA	127
BENDING ANALYSIS OF FGM PLATES ON A KERR FOUNDATION USING AN HSDT SHAPE FUNCTION	132
THE NEW IONIC ADDITIVES FOR SAFER AND DURABLE ELECTROLYTES IN LITHIUM-ION BATTERIES	137
FROM WASTE TO RESOURCE: SAWDUST-BASED ACTIVATED CARBONS FOR CADMIUM-ION ADSORPTION	141
INTRACELLULAR EFFECT OF SYNERGISTIC ACTION OF N-TiO₂ NANOPARTICLES AND BLUE LIGHT ON HELA CERVICAL CANCER CELLS: RAMAN SPECTROSCOPIC STUDY.....	145
MRI-ONLY RADIOTHERAPY DOSE PLANNING VIA CYCLEGAN-GENERATED SYNTHETIC CT.....	149
ALGAL-DERIVED CHROMOPEPTIDES: ALTERNATIVES TO FETAL BOVINE SERUM IN CELLULAR AGRICULTURE	153
REUSABILITY POTENTIAL OF AMBROSIA-BASED BIOSORBENTS FOR CRYSTAL VIOLET DYE REMOVAL	157
NIOBIMUM ELECTRODEPOSITION FROM CHLOROALUMINATE BASED MOLTEN SALTS CONTAINING NIOBIUM IONS	161
WHEN DOES TRADE BECOME GREEN?	165
KINETIC STUDY OF Re(VII) REMOVAL FROM AQUEOUS SOLUTIONS BY MACROPOROUS MAGNETIC NANOCOMPOSITE	169
ELECTROSPUN POLYSACCHARIDE FIBER STABILIZATION: AN IN-SITU GREEN CROSSLINKING APPROACH	173
INFLUENCE OF METHYL SALICYLATE ON THE SOLUBILITY AND SELF-ASSOCIATION OF CAFFEINE: A THERMODYNAMIC AND SIMULATION STUDY	177
CHARACTERIZATION OF COPPER ELECTRODEPOSITED ONTO PALLADIUM FROM ETHALINE.....	181
TRANSFORMING THE AUTOMOTIVE INDUSTRY: THE ROLE OF ARTIFICIAL INTELLIGENCE IN AUTONOMOUS VEHICLES, MANUFACTURING, AND URBAN MOBILITY	186
REFLECTION-MODE FREQUENCY MODULATED PHOTOACOUSTICS OF THIN TUNGSTEN-BASED FILMS BY NOVEL FUNCTIONAL CHARACTERIZATION EXPERIMENTAL SETUP	194
A SURVEY OF REINFORCEMENT LEARNING APPROACHES FOR TUNING PARTICLE SWARM OPTIMIZATION	199
MERCURY REMOVAL FROM ACID MINE DRAINAGE BY NATURAL PYROPHYLLITE SCHIST MATERIAL.....	203
EXPERIMENTAL STUDY ON A PHASE-CHANGE-MATERIAL-BASED THERMAL MANAGEMENT SCHEME COUPLED WITH EXTERNAL FINS FOR LITHIUM-ION BATTERY	207
COMPREHENSIVE STUDY ON THE IMPACT OF LOW-TEMPERATURE ENVIRONMENTS ON THE PERFORMANCE AND SAFETY OF LITHIUM-ION BATTERIES	212
PROTIC IONIC LIQUID–WATER INTERACTIONS: A COMBINED EXPERIMENTAL AND SIMULATION STUDY ON 2-HYDROXYPROPYLAMMONIUM FORMATE.....	220

RESEARCH ON THE PERFORMANCE OF POWER BATTERIES IN HIGH - TEMPERATURE AND HIGH - HUMIDITY ENVIRONMENTS	224
THE POTENTIAL OF TARTARATES AS A COMPATIBILIZERS AND PLASTICIZERS IN BIODEGRADABLE FILMS..	240
PETROGRAPHY OF HIGH-PH FLUIDS SEDIMENTARY ASSEMBLAGES AND BIOTECHNOLOGICAL POTENTIAL OF SEDIMENT <i>BACILLUS</i>	244
BIOINFORMATICS AND APPLIED BIOLOGY	249
ENHANCED POLYPHENOLIC EXTRACTION EFFICIENCY AND ANTIOXIDANT ACTIVITY OF SAGE USING A DEEP EUTECTIC SOLVENT BASED ON CHOLINE CHLORIDE AND UREA	250
CHROMOSOMAL INSTABILITY IN PERIPHERAL BLOOD LYMPHOCYTES OF ENDOMETRIAL CANCER PATIENTS: IMPACT OF CLINICAL AND REPRODUCTIVE FACTORS.....	254
POTPEĆ RESERVOIR ECOSYSTEM HEALTH: AN ANALYSIS BASED ON THE INDEX OF BIOTIC INTEGRITY (IBI)	258
TRANSCRIPTOMIC AND NETWORK-BASED ANALYSIS OF AUTOPHAGY SIGNALING PATHWAYS IN BORTEZOMIB RESISTANCE IN MULTIPLE MYELOMA.....	262
REVERSING DEATH IN LUNG CANCER: EPIGENETIC CONTROL MECHANISMS UNDERLYING ANASTASIS	266
THE IMPACT OF AGE ON NON-SMALL CELL LUNG CANCER: A COMPREHENSIVE OVERVIEW	270
IDENTIFICATION OF ADARB1 NON-CODING TRANSCRIPTS AS POTENTIAL DIAGNOSTIC BIOMARKERS FOR COLON ADENOCARCINOMA	274
EVALUATION OF THE ANTICANCER AND ANTIBIOFILM PROPERTIES OF <i>AGRIMONIA EUPATORIA</i> L. SILVER NANOPARTICLES	277
EVALUATION OF GENOTOXIC POTENTIAL OF ETHYL METHANESULFONATE IN HUMAN PERIPHERAL BLOOD MONONUCLEAR CELLS <i>IN SILICO</i> AND <i>IN VITRO</i>	281
ASSESSMENT OF ANTIBIOTIC RESISTANCE IN WATERBORNE PATHOGENS	285
IDENTIFICATION OF POTENTIAL MICRORNA BIOMARKERS FOR EARLY DIAGNOSIS OF HEPATOCELLULAR CARCINOMA APPLYING BIOINFORMATICS APPROACHES.....	289
BIOINFORMATICS ANALYSIS OF MICRORNAs DERIVED FROM HTR-8/SVNEO POTENTIALLY TARGETING <i>BCL2</i> IN OVARIAN CANCER CELL LINE A2780	294
BIOINFORMATICS ANALYSIS OF PROSTATE CANCER-RELATED MICRORNA PANEL miR-141-3p, miR-21-5p AND miR-375-3p	298
UNVEILING THE MULTI-TARGET THERAPEUTIC POTENTIAL OF RESVERATROL AGAINST ALZHEIMER'S DISEASE: AN INTEGRATIVE NETWORK PHARMACOLOGY AND MOLECULAR SIMULATION APPROACH.....	302
CHEMOINFORMATICS ANALYSIS OF PROTEIN SURFACE AMINO ACID COMPOSITION.....	307
COMPUTATIONAL EXAMINATION OF THE PHENOLIC COMPOUNDS BINDING TO THE CARBON QUANTUM DOTS MODEL	313
TRANSCRIPTOMIC INSIGHTS INTO GENE AND miRNA DYNAMICS SHAPING EMT IN MULTIPLE MYELOMA	317
INVESTIGATING PROTEIN FOLDING AS A TARGET FOR NEURODEGENERATIVE DISORDERS USING A BIOLOGICAL ACTIVITY PREDICTION MODEL BASED ON DEEP LEARNING	321
BIOINFORMATICS TOOLS IN MOLECULAR ONCOLOGY	325
A MULTI-OMICS BIOINFORMATIC PROFILING OF EPITHELIAL-TO-MESENCHYMAL TRANSITION FOLLOWING ANASTASIS IN LUNG ADENOCARCINOMA CELLS.....	329
EFFECT OF AMYLOID-BETA EXPOSURE ON PHOSPHOLIPID DYNAMICS: A COMPUTATIONAL AND CELLULAR PERSPECTIVE	333

IS THE KEY TO THE DISEASE IN ANTIOXIDANTS, IMMUNITY OR SOMETHING ELSE?	337
PREDICTION OF THE BIOLOGICAL ACTIVITY OF COMPOUNDS ON THE 11B-HSD2 ENZYME USING DIFFERENT MACHINE LEARNING APPROACHES.....	342
INSPECTION OF MEAT FOR TRICHINELLOSIS. CLASSIFICATION OF <i>TRICHINELLA SPIRALIS</i> USING A CONVOLUTIONAL NEURAL NETWORK	357
LENGTH–WEIGHT RELATIONSHIP OF BROWN TROUT IN SELECTED RIVERS OF THE WEST MORAVA RIVER SYSTEM (SERBIA).....	366
AN ENHANCED METHOD FOR QUANTIFYING ENERGY LOSS DUE TO DIFFUSION IN CORONARY ARTERIES WITH STENOSIS.....	370
BIOMEDICAL ENGINEERING	379
NUMERICAL MODELING OF TUMOR GROWTH USING SOLID MURINE 3D FINITE ELEMENT MODEL	380
TIME-DEPENDENT APOPTOTIC RESPONSES TO VITAMIN E IN PRECANCEROUS LESIONS-ON-CHIP MODELS.....	384
INTEGRATION OF 3D PRINTING TECHNOLOGIES WITH DEUTERATED POLYUNSATURATED FATTY ACIDS (D- PUFAs).....	388
LIMITATIONS OF COARSE GRAIN MODELS OF ACTIN FILAMENT ON PREDICTION OF X-RAY DIFFRACTION PATTERNS IN CONTRACTING SKELETAL MUSCLE	392
THE EFFECT OF DULBECCO’S ‘EAGLE’ MEDIUM ON THE MASS AND TRIBOLOGICAL CHARACTERISTICS OF PLA SAMPLES: A PRELIMINARY STUDY	396
SEMANTIC SEGMENTATION OF CHEST COMPUTED TOMOGRAPHY SCANS FOR QUANTIFYING PATHOLOGICALLY ALTERED LUNG PARENCHYMA IN PATIENTS WITH POST-COVID SYNDROME	400
AI BASED PREDICTION MODEL AND INFLUENTIAL FACTORS FOR HYPERSENSITIVITY IN DENTAL IMPLANTS MADE OF Ti ALLOYS.....	405
DEVELOPMENT OF BIOCOMPATIBLE POLYURETHANES AS FUNCTIONAL BIOMATERIALS FOR ADVANCED WOUND HEALING APPLICATIONS	409
FOTELP-VOX-GA: INTEGRATING GENETIC ALGORITHMS INTO MONTE CARLO DOSE CALCULATION FOR PROSTATE CANCER	414
HARNESSING HYDROLIZED SILK FIBROIN IN ELECTROSPUN NANOFIBERS FOR BIOMEDICAL APPLICATIONS	418
<i>IN VIVO</i> MODELS FOR SPINAL DISC REGENERATION.....	422
EFFECT OF GRADIENT MAGNETIC FIELDS ON MOLECULAR DIFFUSION THROUGH CELL MEMBRANES: A THEORETICAL AND NUMERICAL STUDY.....	426
COUPLED AGENT-BASED AND FINITE ELEMENT MODELLING OF CANCER CELL BEHAVIOUR	430
STRUCTURAL VULNERABILITY OF J-J STENTS TO RADIOTHERAPY IN CERVICAL CANCER PATIENTS: IMPLICATIONS FOR TREATMENT PLANNING	434
SIMULATING THE BEHAVIOUR OF CANCER CELLS IN THE MICROFLUIDIC CHIP	438
EXPLORING (ALKYL-Ω-OL)TRIPHENYLTIN(IV) COMPOUNDS AS RENIN INHIBITORS: NUMERICAL MODELLING OF DIFFUSION PROCESS WITHIN FINITE ELEMENT LIVER MODEL	442
BIOORGANIC, BIOINORGANIC, AND MEDICINAL CHEMISTRY	446
SELENIUM-RELATED GENE ACTIVATION IN FETAL GROWTH RESTRICTION PLACENTAS: A BIOINFORMATICS ANALYSIS	447
BIOAVAILABILITY OF SELENIUM SUPPLEMENTATION: RELEVANCE TO MATERNAL HEALTH AND PRODUCT QUALITY ASSESSMENT.....	451

SYNERGISTIC ANTIBACTERIAL EFFECT OF COPPER COMPLEX AND <i>LYTHRUM SALICARIA</i> PLANT EXTRACT ...	455
B-CYCLODEXTRIN INCLUSION COMPLEX – <i>IN VITRO</i> ASSESSMENT OF THE ANTIOXIDANT ACTIVITY	459
SYNTHESIS, THEORETICAL ANALYSIS, AND HSA/DNA BINDING ACTIVITY OF THE [RuCl ₂ (H ⁶ -P-CYME)(BPH-KN)] COMPLEX	463
COMBINATION CHEMO-TARGETING OF NSCLC CELLS WITH DOCETAXEL AND NICLOSAMIDE: A MULTIMODAL CELL DEATH	467
NOVEL ISOCHROMENE-FUSED CF ₃ -SUBSTITUTED PYRAZOLE COMPOUNDS INDUCE CYTOTOXICITY THROUGH CASPASE MEDIATED APOPTOSIS	471
COMPARISON BETWEEN MECHANOCHEMICAL AND SOLUTION SYNTHESIS OF AMMONIUM-IMINODIACETATEDITHIOCARBAMATE	475
IN SILICO EVALUATION OF TRYPTAMINE-DERIVED SCHIFF BASES AS MODULATORS OF THE SEROTONIN 5-HT _{2A} RECEPTOR	479
EVALUATING THE ADMET PROPERTIES OF ISOSTERIC SUBSTITUTION IN SCHIFF BASE DERIVATIVES	483
IN SILICO EVALUATION OF DRUG-LIKENESS PROPERTIES OF STEROIDAL SEMICARBAZONES AND STEROIDAL OXAZOLO[4.5-b]QUINOXALINES	487
BIOMOLECULAR INTERACTIONS OF NOVEL RUTHENIUM(II) COMPLEXES WITH HUMAN SERUM ALBUMIN	491
BINDING INTERACTIONS OF BIGINELLI-TYPE COMPOUNDS WITH SERUM ALBUMIN AND DNA	495
TARGETING THYROID CANCER: <i>IN VITRO</i> ANALYSIS OF A BENZOFURAN-SUBSTITUTED CHALCONE COMPOUND	499
CRYSTALLOGRAPHIC, QUANTUM-CHEMICAL, AND BIOMOLECULAR INTERACTION STUDY OF A EUROPIUM(III) COMPLEX WITH PYRIDOXAL-SEMICARBAZONE LIGAND	505
UHPLC-DAD-MS/MS PHYTOCHEMICAL PROFILING OF <i>GERANIUM ROBERTIANUM</i> L. HERBA EXTRACT OBTAINED BY ULTRASOUND-ASSISTED EXTRACTION	509
SYNTHESIS, CHARACTERIZATION AND ANTICANCER POTENTIAL OF THE SELECTED BIGINELLI HYBRIDS AND THEIR NANOCOMPOSITES	514
FLAVONOIDS FROM <i>THYMUS VULGARIS</i> AND <i>THYMUS SERPYLLUM</i> AND THEIR ANTIOXIDATIVE ACTIVITY	518
DNA/BSA INTERACTIONS OF NEW GOLD(III) COMPLEXES WITH SOME PYRIDINE-CONTAINING LIGANDS	523
SYNTHESIS AND STRUCTURAL CHARACTERIZATION OF A NEW SILVER(I) COMPLEX WITH MICONAZOLE	527
SYNTHESIS AND STRUCTURAL CHARACTERISTICS OF SILVER(I) COMPLEX WITH <i>N</i> -BENZYLTHIABENDAZOLE	531
THE AMINO ACID AND FATTY ACID COMPOSITION AND ANTIOXIDANT ACTIVITY OF FUNCTIONAL SNACK PRODUCTS	535
MECHANOCHEMICAL SYNTHESIS OF Ru(II) COMPLEXES WITH ISOTHIAZOLE-TYPE OF LIGAND	539
SYNTHESIS, CHARACTERIZATION, AND ANTIFUNGAL ACTIVITIES OF NOVEL FERROCENYL PYRAZOLINES CONTAINING SULFONAMIDE MOIETY	543
QUANTIFICATION OF PHENOLS, FLAVONOIDS, AND SUGARS IN TWO MEDICINAL FUNGI: <i>FOMES FOMENTARIUS</i> (L.) AND <i>SCHIZOPHYLLUM COMMUNE</i> (FR.)	547
MINERAL CONTENT OF HONEY FROM SERBIA: ANALYSIS OF ESSENTIAL AND TOXIC ELEMENTS	551
SYNTHESIS AND CHARACTERIZATION OF NEW SCHIFF BASES WITH THIOCARBOHYDRAZIDE AND SOME AROMATIC ALDEHYDES AND DETERMINATION OF THEIR ANTIOXIDANT POTENTIAL	555
EPR-BASED EVALUATION OF ANTIOXIDANT PROPERTIES OF NOVEL SCHIFF BASES	559
STUDY OF HOST–GUEST INTERACTION BETWEEN B-CYCLODEXTRIN AND CHROMENO-PYRIMIDINE DERIVATIVE	563
CAFFEINE IN DEUTERO WATER, SOLVENT ISOTOPE EFFECT ON HYDRATION PROPERTIES	567

MADE-SUPPORTED VIRTUAL SCREENING FOR SMALL-MOLECULE FURIN INHIBITORS	571
HETEROCYCLIC DERIVATIVES OF STEROIDAL THIOSEMICARBAZONES AND THEIR <i>IN SILICO</i> DRUG-LIKENESS PREDICTION AS POTENTIAL ANTICANCER AGENTS	575
INVESTIGATION OF THE CYTOTOXIC AND APOPTOTIC EFFECTS OF THE NEWLY SYNTHESIZED BENZOFURAN-LINKED CHALCONE COMPOUNDS IN BREAST CANCER	579
CHEMOINFORMATICS, CHEMOGENOMICS, AND MOLECULAR DESIGN	588
COMPUTER-AIDED DRUG DESIGN OF NOVEL DUAL HISTONE DEACETYLASE INHIBITORS	589
THEORETICAL INSIGHT INTO REDOX PROPERTIES OF 9-ACRIDINYL AMINO ACID DERIVATIVES	593
PHYSICOCHEMICAL AND PHARMACOLOGICAL PROPERTIES OF FUSED BICYCLIC HYDANTOINS	597
COMPUTER-AIDED DESIGN AND ANALYSIS OF MULTIFUNCTIONAL TETRAHYDROCANNABINOL DERIVATIVES TARGETING ACETYLCHOLINESTERASE AS POTENTIAL ANTIOXIDANT NEUROPROTECTORS FOR ALZHEIMER'S DISEASE	601
MULTIFUNCTIONAL TETRAHYDROCANNABINOL DERIVATIVES AS POTENTIAL ANTIOXIDANT NEUROPROTECTORS: <i>IN SILICO</i> TARGETING OF MONOAMINE OXIDASE B AND CATECHOL-O-METHYLTRANSFERASE IN PARKINSON'S DISEASE THERAPY.....	605
A SYSTEMATIC ANALYSIS OF INTERMOLECULAR INTERACTIONS OF CYTOCHROME P450S WITH THEIR LIGANDS	610
CONSIDERATION OF ELECTROPHORETIC BEHAVIOR OF SOME IMIDAZOLINE AND A-ADRENERGIC RECEPTORS LIGANDS USING DFT APPROACH.....	614
A NEW 2-BENZOFURAN-LINKED CHALCONE-TAMOXIFEN COMBINATION FOR TARGETING ER+ BREAST CANCER	618
CONTRIBUTION TO ELUCIDATING THE MECHANISM OF ANTIMICROBIAL ACTION OF A DINUCLEAR Pt/Cu COMPLEX AGAINST <i>ENTEROCOCCUS FAECALIS</i> – <i>IN SILICO</i> APPROACH	622
VIRTUAL SCREENING OF POLYPHENOLIC COMPOUNDS FROM EDIBLE PLANTS FOR POTENTIAL APPLICATION IN ALZHEIMER'S THERAPY	626
DATA MINING FROM OSCILLATORY REACTIONS PERTURBED BY USNIC ACID.....	630
CHEMOINFORMATICS APPROACHES FOR AUTHENTICATING CEREAL-BASED FOODS: FROM GRAIN TO BAKERY PRODUCTS	634
EVALUATING THE PHARMACOLOGICAL PROFILE OF ANGULAR TRIQUINANE TYPE HYDANTOINS	638
EXPLORING BETA BLOCKING AS A POSSIBLE MECHANISM OF ANTICANCER ACTION OF 2-THIOHYDANTOINS	642
STRUCTURAL AND ELECTRONIC RESPONSE OF NEW NITROAROMATIC COMPOUNDS TO SOLVENT POLARITY: A DFT STUDY.....	646
APPLICATION OF MOLECULAR MODELING IN PREDICTING PALLIATIVE FEATURES OF HDAC4 PROTACS AGAINST SPINAL MUSCULAR ATROPHY	650
QUANTUM THEORY OF ATOMS IN MOLECULES ANALYSIS OF NH/O HYDROGEN BONDS OF GLYCINE COMPLEXES WITH A WATER MOLECULE.....	654
ANTI-METASTATIC EFFECTS OF CHALCONE COMPLEX ON PROSTATE CANCER AND PROSTATE CANCER STEM CELL-LIKE CELLS.....	658
<i>IN SILICO</i> INVESTIGATION OF SUBSTITUTION MECHANISM AT THE NICKEL CARBONYL COMPLEX	662
CHEMOMETRIC MODELING FOR BLOOD-BRAIN-BARRIER PERMEABILITY PREDICTION OF PROTEIN KINASE INHIBITORS.....	666
STACKING INTERACTIONS BETWEEN TWO HYDROQUINONE MOLECULES IN CRYSTAL STRUCTURES	670

GRASP_MAT WORKSHOP.....	674
GRAPE SKIN EXTRACT–ENRICHED HYDROGELS FOR WOUND HEALING: AN ANTIOXIDANT-BASED APPROACH	675
GRAPE SKIN EXTRACT HYDROGEL RESTORES SYSTEMIC REDOX BALANCE IN DIABETIC RATS.....	679
RATIONAL DESIGN OF APIGENIN DERIVATIVES AS POTENT INFLAMMATORY MODULATORS FOR IMPROVED DIABETIC WOUND HEALING	683
FORMULATION OF ALGINATE–GELATIN HYDROGELS WITHIN A CIRCULAR ECONOMY FRAMEWORK: CONTROLLED RELEASE OF GRAPE SKIN EXTRACT VIA GELATIN CONTENT MODULATION.....	687

Bending Analysis of FGM Plates on a Kerr Foundation Using an HSDT Shape Function

Aleksandar B. Radaković^{1*}, Dragan V. Čukanović², Gordana Bogdanović³, Aleksandar M. Nešović¹, Petar M. Knežević²

¹University of Kragujevac, Institute for information technologies Kragujevac, Jovana Cvijića bb, 34000 Kragujevac, Serbia, e-mail: aradakovic@uni.kg.ac.rs

²University of Priština, Faculty of Technical Sciences, Knjaza Miloša 7, 38220 Kosovska Mitrovica, Serbia, e-mail: dragan.cukanovic@pr.ac.rs, petar.knezevic@pr.ac.rs

³University of Kragujevac, Faculty of Engineering, Sestre Janjić 6, 34000 Kragujevac, Serbia, e-mail: gocab@kg.ac.rs

* *Corresponding author*

DOI: 10.46793/ICCBIKG25.132R

Abstract: This paper presents a novel higher-order shear deformation theory (HSDT) shape function for the bending analysis of functionally graded (FGM) plates resting on a Kerr elastic foundation. The formulation ensures shear stress-free boundary conditions and accurately captures through-thickness variations without the need for shear correction factors. Numerical implementation and comparison with established reference solutions confirm the reliability, accuracy, and improved stability of the proposed function for different foundation parameters and geometric ratios. The findings further demonstrate the critical role of the Kerr model in representing interlayer interactions and enhancing the predictive capability of plate-foundation systems. The proposed approach provides an efficient and versatile framework for advanced analysis and design of FGM structures.

Keywords: FG plates, higher-order theories, Kerr foundation

1. Introduction

Functionally graded materials (FGMs) are advanced composites with continuously varying properties, reducing interlaminar stress concentrations compared to conventional laminates [1]. Property gradients are defined by functions describing material variation along the desired direction [2].

Stress-strain analysis of FGM plates can use 3D elasticity or equivalent single-layer (ESL) theories. Classical plate theory (CPT) [3] applies to thin plates, including geometric nonlinearity [4] and dynamic problems [5], often with Winkler or Winkler-Pasternak foundations [6]. First-order shear deformation theory (FSDT) includes shear effects but requires correction factors, while higher-order shear deformation theory (HSDT), including Reddy's TSDT [7], allows accurate analysis of moderately thick and thick plates without corrections, under static, dynamic, and thermo-mechanical loadings. Both polynomial and functional HSDT forms (hyperbolic, exponential, parabolic) [8] exist.

This study proposes a novel functional HSDT shape function for improved bending analysis, with Kerr elastic foundation modeling plate–substrate interaction.

2. Methodology

In this study, a higher-order shear deformation theory (HSDT) is applied, wherein the displacement fields are expressed as:

$$\begin{cases} (x, y, z) = u_0(x, y) + z\varphi_x(x, y) + f(z)\psi_x(x, y) \\ v(x, y, z) = v_0(x, y) + z\varphi_y(x, y) + f(z)\psi_y(x, y) \\ w(x, y, z) = w_0(x, y) \end{cases} \quad (1)$$

where the shape function $f(z)$ satisfies the condition of zero transverse shear stresses on the free surfaces.

In this paper, a new shape function is applied:

$$f(z) = z(\cosh(z/h) - 1.388) \quad (2)$$

By integrating the stress–strain relations through the plate thickness, the resultant forces and moments are obtained:

$$\begin{aligned} \begin{bmatrix} N_z & N_y & N_{xy} \end{bmatrix}^T &= \mathbf{A}\boldsymbol{\varepsilon}^0 + \mathbf{B}\boldsymbol{\kappa}^b + \mathbf{C}\boldsymbol{\kappa}^s, \quad \begin{bmatrix} M_x & M_y & M_{xy} \end{bmatrix}^T = \mathbf{B}\boldsymbol{\varepsilon}^0 + \mathbf{D}\boldsymbol{\kappa}^b + \mathbf{T}\boldsymbol{\kappa}^s \\ \begin{bmatrix} P_x & P_y & P_{xy} \end{bmatrix}^T &= \mathbf{C}\boldsymbol{\varepsilon}^0 + \mathbf{T}\boldsymbol{\kappa}^b + \mathbf{G}\boldsymbol{\kappa}^s, \quad \begin{bmatrix} R_x & R_y \end{bmatrix}^T = \mathbf{F}\boldsymbol{\theta} \end{aligned} \quad (3)$$

where $\boldsymbol{\varepsilon}^0$ are the mid-plane strains, $\boldsymbol{\kappa}^b$ the curvatures due to bending, $\boldsymbol{\kappa}^s$ zakrivljenosti the curvatures due to shear deformation, and $\boldsymbol{\theta}$ the rotations of transverse sections. The stiffness matrices $\mathbf{A}, \mathbf{B}, \mathbf{C}, \mathbf{D}, \mathbf{T}, \mathbf{G}$ and $\mathbf{F}$ are defined in [5].

The static problem is formulated by applying Hamilton's principle:

$$\delta \int_{t_1}^{t_2} [U - U_e - W] dt = 0 \quad (4)$$

where U is the strain energy of deformation (stretching, bending, and shear), U_e is the potential energy of the elastic foundation, and W is the work (potential) of the external load.

The bending response of FGM plates strongly depends on the elastic foundation model, which provides additional resistance by reducing deflections and redistributing forces. In practice, Winkler, Pasternak, and Kerr models are commonly used, differing in how they account for local and shear effects through the foundation thickness.

The foundation reaction can be represented by simplified models: the Winkler model ($q = K_o w_o$) the Winkler-Pasternak model ($q = K_o w_o - K_1 \nabla^2 w_o$), , and the Kerr model ($q = w_o K_o K_1 / (K_o + K_1) - (K_2 K_1 / (K_o + K_1)) \nabla^2 w_o$), where K_o , K_1 , and K_2 denote the elastic and shear stiffness parameters of the foundation layers.

3. Results and Discussion

For obtaining numerical results in the macromechanical analysis of simply supported FGM plates, analytical methods based on Taylor series expansions are employed. The plate is subjected to an external sinusoidal transverse load.

For the HSDT theory based on shape functions, a comparative analysis is presented for the normalized values of vertical displacement $\bar{w}$ (deflection), normal stresses $\bar{\sigma}_{xx}$ and $\bar{\sigma}_{yy}$, shear stress $\bar{\tau}_{xy}$, and transverse shear stresses $\bar{\tau}_{xz}$ and $\bar{\tau}_{yz}$. The normalization of these quantities was performed according to [5].

To illustrate the influence of the elastic foundation on the displacements and stresses of FGM plates, results are presented for different combinations of constituent volume fractions in the FGM, i.e., for various combinations of elastic foundation parameter values. In addition to the normalization given in (7.2), it is necessary to apply normalization for:

$$\bar{k}_0 = k_0 a^4 / D, \bar{k}_1 = k_1 a^2 / D \text{ and } \bar{k}_2 = k_2 a^4 / D \quad (5)$$

where the bending stiffness of the plate is $D = E_c h^3 / 12(1 - \nu^2)$.

Table 1 presents the normalized values of displacements and stresses of square FGM plates on a Winkler - Pasternak elastic foundation for different combinations of stiffnesses k_0 and k_1 and aspect ratios a/h . The data clearly show that the results obtained using the proposed shape functions closely follow the reference values [1], confirming the reliability and accuracy of the new formulation in describing vertical displacements and stresses, as well as the model's ability to accurately quantify the plate-foundation interaction.

Table 1. Normalized values of displacement and stresses of square plate on elastic foundation for $p = 5$, different values of the k_0 и k_1 and the ratio a/h ($a/b = 1$)

p	k_0	k_1	Theory	$\bar{w} \ (h = 0)$		$\bar{\sigma}_{xx} (h/2)$		$\bar{\tau}_{xy} (-h/3)$		$\bar{\tau}_{xz} (h = 0)$	
				$a/b = 1$							
				$a/h = 10$	$a/h = 5$	$a/h = 10$	$a/h = 5$	$a/h = 10$	$a/h = 5$	$a/h = 10$	$a/h = 5$
5	0	0	[1]	0.9118	-----	4.2488	-----	0.5754	-----	0.2016	-----
			Present	0.9113	1.0881	4.2441	2.2106	0.5757	0.2840	0.1916	0.1911
100	0		[1]	0.4969	-----	2.3154	-----	0.3136	-----	0.1098	-----
			Present	0.4967	0.5450	2.3135	1.1072	0.3138	0.1422	0.1045	0.0957
0	10		[1]	0.3443	-----	1.6043	-----	0.2173	-----	0.0761	-----
			Present	0.3442	0.3667	1.6032	0.7451	0.2174	0.0957	0.0724	0.0644
100	10		[1]	0.2617	-----	1.2197	-----	0.1652	-----	0.0578	-----
			Present	0.2617	0.2745	1.2190	0.5577	0.1653	0.0716	0.0550	0.0482

Table 2. Normalized values of displacement and stresses of square plate on elastic foundation for $p = 5$, different values of the k_0 , k_1 and k_2 and the ratio a/h ($a/b = 1$)

p	k_0	k_1	k_2	$\bar{w} \ (h = 0)$	$\bar{\sigma}_{xx} \ (h/2)$	$\bar{\tau}_{xy} \ (-h/3)$	$\bar{\tau}_{xz} \ (h = 0)$
				$a/b = 1$			

				$a/h = 10$	$a/h = 5$	$a/h = 10$	$a/h = 5$	$a/h = 10$	$a/h = 5$	$a/h = 10$	$a/h = 5$
5	100	0	0	0.9112	1.0883	4.2443	2.2111	0.5757	0.2840	0.1916	0.1911
	100	100	0	0.4989	0.5557	2.3241	1.1291	0.4996	0.2414	0.1663	0.1624
	0	100	100	0.7824	0.6090	3.6441	1.2373	0.5587	0.2480	0.1860	0.1669
	100	0	100	0.9112	1.0883	4.2443	2.2110	0.5757	0.2841	0.1916	0.1911
	100	100	100	0.4581	0.4008	2.1335	0.8144	0.4870	0.2158	0.1621	0.1452

Table 2 shows the normalized displacements and stresses of square FGM plates on a multilayer Kerr foundation. Increasing the stiffness and shear resistance of the middle layer reduces deformations and stresses, while a lower a/h ratio amplifies this effect, confirming the Kerr model's ability to accurately capture interlayer interactions and the overall mechanical response of the plates.

4. Conclusions

In this study, a novel HSDT shape function was developed and applied to the bending analysis of functionally graded (FGM) plates on a Kerr elastic foundation. Numerical results show that the proposed function provides accurate predictions of transverse displacements and stresses, with stable performance across various foundation parameters and plate thicknesses. The MATLAB implementation enables straightforward application and visualization, supporting further research, design optimization, and experimental validation. Comparison with reference values confirms the high accuracy and reliability of the formulation, while the Kerr foundation analysis clearly demonstrates its ability to capture interlayer interactions and the overall mechanical response of plates. The proposed approach offers an efficient and flexible tool for engineering applications and further studies of FGM structures.

References

- [1] R.M. Mahamood, E.T. Akinlabi, M. Shukla, S. Pityana., Functionally graded material: An overview, *Proceedings of the World Congress on Engineering*, Vol. III, WCE 2012, London, U.K., July 4–6, 2012.
- [2] V. Birman, L.W. Byrd., Modeling and analysis of functionally graded materials and structures, *Applied Mechanics Reviews*, 60(5) (2007) 195–216.
- [3] V.G. Kirchhoff., Über das Gleichgewicht und die Bewegung einer elastischen Scheibe, *Journal für die reine und angewandte Mathematik*, 40 (1850) 51–88.
- [4] J. Yang, H.S. Shen., Non-linear analysis of FGM plates under transverse and in-plane loads, *International Journal of Non-Linear Mechanics*, 38(4) (2003) 467–482.
- [5] Mengzhen Li, C. Guedes Soares, Renjun Yan, Free vibration analysis of FGM plate on Winkler/Pasternak/Kerr foundation by using a simple quasi - 3D HSDT, *Composites Structures* 264 (2021) 113643.
- [6] S. Chakraverty, K.K. Pradhan., Free vibration of functionally graded thin rectangular plates resting on Winkler elastic foundation with general boundary conditions using Rayleigh–Ritz method, *International Journal of Applied Mechanics*, 6(4) (2014) 1450043.
- [7] N.D. Phan, J.N. Reddy., Analysis of laminated composite plates using a higher-order shear deformation theory, *International Journal for Numerical Methods in Engineering*, 21(12) (1985) 2201–2219.

- [8] S.S. Akavci., Two new hyperbolic shear displacement models for orthotropic laminated composite plates, *Mechanics of Composite Materials*, 46(2) (2010) 215–226.