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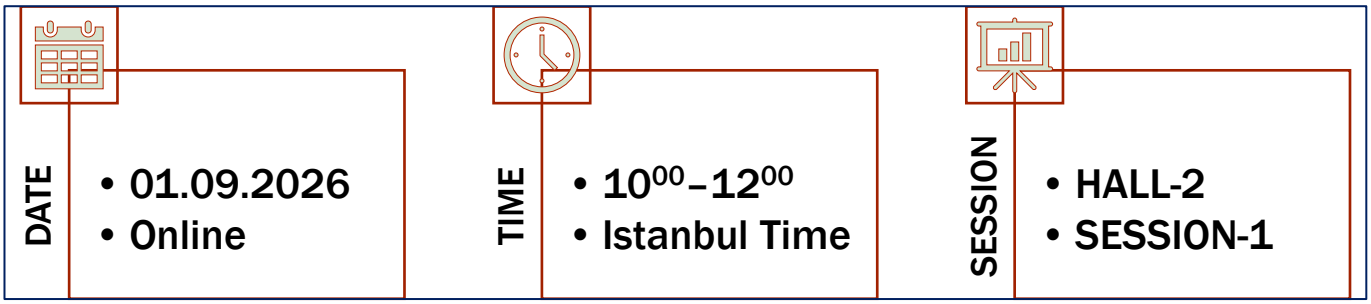
CLASS IMBALANCE IN TOXICITY PREDICTION: THE EFFECT OF PERFORMANCE METRIC AND DECISION THRESHOLD SELECTION ON MODEL RANKING IN THE TOX21 DATASET

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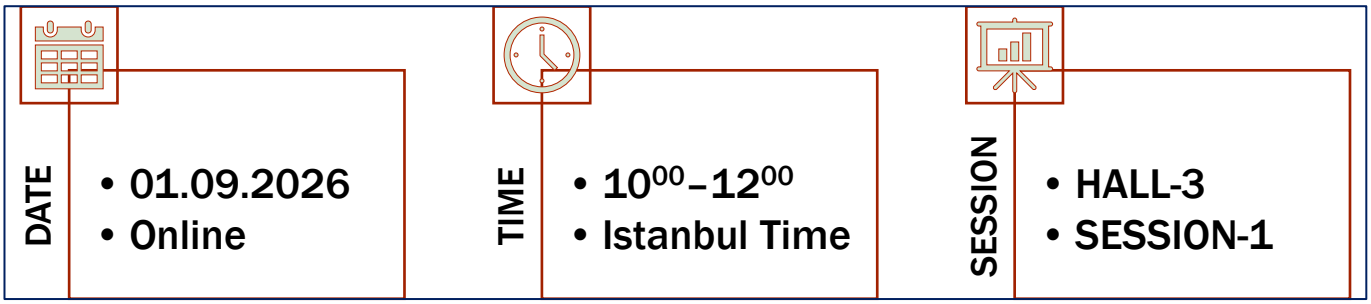
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HEAD OF SESSION: Asst. Prof. Dr. Utku Bulut SIMSEK		
Asst. Prof. Dr. Utku Bulut SIMSEK Assoc. Prof. Dr. Erkan Caner OZKAT	Istanbul Aydin University, Anadolu BIL Vocational School Recep Tayyip Erdogan University	ENGINEERING MICRO SIZED NH2 FUNCTIONALIZED BIMETALLIC MOFS VIA SUPERCRITICAL CO_2 FOR EFFICIENT CARBON CAPTURE
Dr. Girne Gül ÇELEBİ ULUÇAY Prof. Dr. Güzin KAYA	---	VAN GÖLÜ HAVZASI'NDA NÜFUS YOĞUNLUĞU ARTIŞININ MEKÂNSAL ÖRÜNTÜSÜ: EDREMİT, İPEKYOLU VE TUŞBA ÖRNEĞİ
Asst. Prof. Dr. Seda ERDOĞAN	İstanbul Galata University	GENERATIVE ARTIFICIAL INTELLIGENCE FOR THE SPATIAL IMPROVEMENT OF PUBLIC SPACES: THE CASE OF MAÇKA DEMOCRACY PARK
Asst. Prof. Dr. Sinan KEYİNCİ	Çukurova University	EFFECT OF TESLA VALVE DISTRIBUTION ON THE THERMO-HYDRAULIC PERFORMANCE OF A LIQUID-COOLED BATTERY THERMAL MANAGEMENT SYSTEM
Dr. Barış ERKUŞ Doğukan AYHAN	Bursa Uludağ University	A REVIEW OF VIBRATION-BASED FAULT DIAGNOSIS METHODS FOR INTERNAL COMBUSTION ENGINES: SIGNAL PROCESSING TECHNIQUES AND MACHINE LEARNING APPROACHES
Aslıhan Hatun ÇAÇAN	Tokat Gaziosmanpasa University	LINKING MOLECULAR INTERACTIONS TO THE ACOUSTIC AND CALORIC BEHAVIOR OF REAL GASES
İREM KESKİN DR. BURCU ARSLAN AYLİN RAZLIKLI ÖZGE KARATAŞ	VIKING CLEANING AND COSMETICS CO.	SYNTHESIS AND CHARACTERIZATION OF SODIUM BENZOATE AND POTASSIUM SORBATE AND EVALUATION OF THEIR PRESERVATIVE EFFICACY IN A LIQUID SOAP FORMULATION
Gozde YALCIN OZKAT Assoc. Prof. Dr. Erkan Caner OZKAT	Recep Tayyip Erdogan University	CLASS IMBALANCE IN TOXICITY PREDICTION: THE EFFECT OF PERFORMANCE METRIC AND DECISION THRESHOLD SELECTION ON MODEL RANKING IN THE TOX21 DATASET

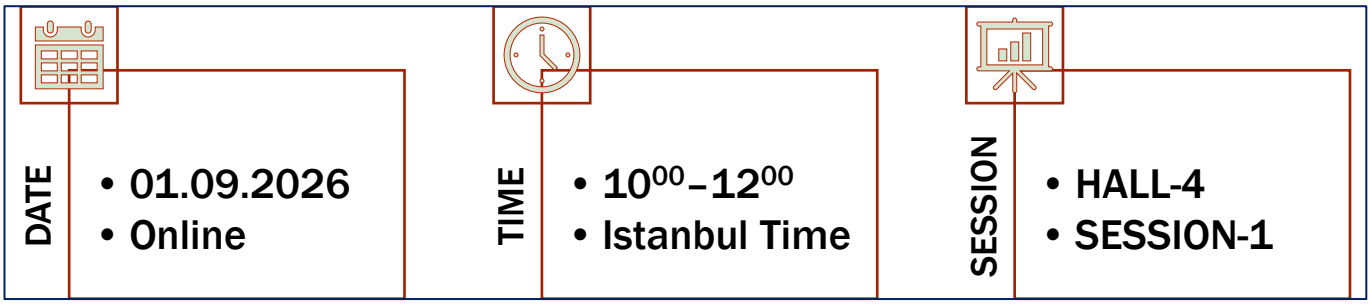


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Banu BAŞ Dilara USTA	Ankara Yıldırım Beyazıt University	EFFECTS OF VESTIBULAR REHABILITATION ON SPATIAL ORIENTATION, SPATIAL COGNITION, AND BALANCE PERFORMANCE: A SYSTEMATIC REVIEW
Dr. Mürşit AKSOY	Hakkari University	THE ROLE OF CORRECTIVE EXERCISES IN PREVENTING SPORTS INJURIES AND EXAMPLES OF POPULAR EXERCISE PRACTICES
Dr. Batuhan DELEN Dr. Gündüz Ercan KUTLUAY	Tekirdağ Namık Kemal University COIZ Kapaklı State Hospital	SCOPE, READABILITY, AND EMERGENCY WARNING INFORMATION IN TURKISH ONLINE PATIENT EDUCATION CONTENT ON PEDIATRIC SUPRACONDYLAR HUMERUS AND ELBOW FRACTURES
Mustafa KAHRAMAN Murat BEĞENIK	TUSEB Türkiye Institute of Public Health and Chronic Diseases Istanbul Medipol University	ACUTE CARDIOVASCULAR RESPONSES TO SOLEUS PUSH-UP EXERCISE DURING AN ORAL GLUCOSE TOLERANCE TEST
Nalan CAVLAK ADSIZ İlhami ADSIZ	Elazığ Fethi Sekin City Hospital	INVESTIGATION OF E-SCOOTER ACCIDENTS ADMITTED TO THE EMERGENCY DEPARTMENT
Assoc. Prof. Dr. Ahmet DINÇ Prof. Dr. Ahmet Nusret BULGURCUOĞLU	Iğdır University	MANAGEMENT OF DUAL CAREER AND ATHLETIC CAREER TRANSITIONS: A WEB OF SCIENCE-BASED BIBLIOMETRIC NETWORK ANALYSIS
Canan BAGCI-TAN Ozden OZGUN-ACAR Asli KIRIKBAKAN	Pamukkale University	PYRROLOQUINOLINE QUINONE MODULATES ALZHEIMER'S DISEASE- RELATED GENE EXPRESSION IN SH-SY5Y CELLS
Pharmacist Elif AKSEN Prof. Dr. Gülbin ÖZÇELİKAY	Ankara University	THE EFFECT OF MERCHANDISING OF NON-PHARMACEUTICAL PRODUCTS ON EFFICIENCY IN COMMUNITY PHARMACIES



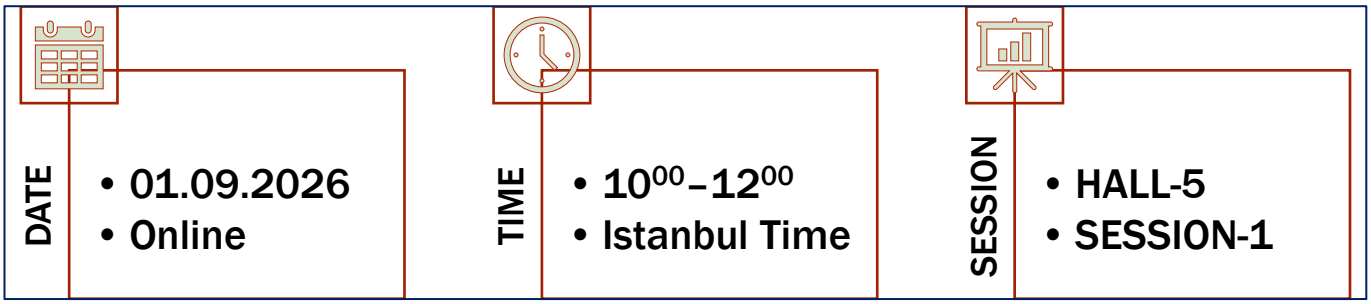
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Assistant Professor Halim YAR	Sirnak University	GULSHENĪ-I SARUKHĀNĪ'S WORK TITLED SAʿDNĀME [ATTRIBUTED TO KHAYĀLĪ-I GULSHENĪ IN THE LIBRARY RECORD]
Dr.Şakir DENİZ	Presidency of Religious Affairs	AN ANALYSIS OF THE METHODOLOGY OF COMMENTING ON A SINGLE HADITH, FOCUSING ON ABU SHAMA AL-MAKDİSİ'S WORK TITLED "SHARH AL-HADITH AL-MUKHTAFA Fİ MAB'AS AL-NABİY AL-MUSTAFA"
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Asst. Prof. Dr. Doğan Barış KILINÇ	Dicle University	SOCRATES' DEATH AS AN EXAMPLE OF TRAGEDY



HEAD OF SESSION: Dr. Makarova-Korobeynikova Ekaterina Petrovna

KOCHUBEY Alexander MAKAROVA-KOROBEYNIKOVA Ekaterina Petrovna	Russian Customs Academy, Russia	INNOVATIVE APPROACHES TO AUTOMATING BUSINESS PROCESSES OF CUSTOMS AUTHORITIES BASED ON ADVANCED TECHNOLOGIES
Kristal Hykaj Ardita Hykaj	Mediterranean University, Albania	THE IMPACT OF THE COVID-19 PANDEMIC ON THE ALBANIAN BANKING SECTOR PERFORMANCE: AN ECONOMETRIC ANALYSIS (2015–2020)
Fatematuz Zohora	University of Barishal, Bangladesh	CARBON ACCOUNTING, CORPORATE GOVERNANCE AND CORPORATE CARBON PERFORMANCE: EVIDENCE FROM BANGLADESH
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Makarova-Korobeynikova Ekaterina Petrovna Sulaimanova Sabina	Russian Customs Academy, Russia	POSSIBILITIES OF INCLUDING A NEURAL NETWORK IN THE WORK OF THE CUSTOMS SERVICE WHEN INSURING INTELLECTUAL PROPERTY ASSETS
Rusli Sri Mulyani	Institut ‘Aisyiyah Sulawesi Selatan, İndonesia	THE ROLE OF HUMAN RESOURCE COMPETENCIES IN SUPPORTING UNIVERSITY QUALITY ASSURANCE AND ACCREDITATION
TETEREV Daniil MAKAROVA-KOROBEYNIKOVA Ekaterina Petrovna	Russian Customs Academy, Russia	THE CURRENT STATE OF INTERACTION BETWEEN CUSTOMS AUTHORITIES AND BUSINESS STRUCTURES
Oluwafunmilayo Caroline OYENIYI	KolaDaisi University, Nigeria	DIGITAL FINANCIAL INCLUSION AND TAX REVENUE PERFORMANCE IN NIGERIA
M.A. Nguyen Thanh Tuan	Vinh Nhuan Middle and High School, Vietnam	BANQUE DE L’INDOCHINE AND CURRENCY ISSUANCE IN FRENCH INDOCHINA (1875 - 1930)



HEAD OF SESSION: Dr. Muhammad Imran		
Orji, Jephter Ebuka	Alex Ekwueme Federal University, Nigeria	SOIL MANAGEMENT PRACTICES FOR MITIGATION OF THE EFFECT CLIMATE CHANGE IN THE TROPICS
Ekanem, Moses Columba	Akwa Ibom State Polytechnic, Nigeria	QUALITY AND NUTRITIONAL CONTENTS OF WATER YAM-COCOYAM COMPOSITE FLOUR SUPPLEMENTED WITH COWPEA FLOUR FOR THE PREPARATION OF EKPANG NKUKWO PREPARATION
Arous Ali KACI Zakia DAHMENE Thoraya	University Djillali Bounaama, Algeria M'hamed Bouguera Boumerdès University, Algeria	IMPACT OF FARMING SYSTEMS AND PRACTICES ON THE CULTIVATION OF DURUM WHEAT (TRITICUM DURUM DESF) UNDER SEMI-ARID CONDITIONS IN ALGERIA
Dr. Muhammad Imran	Government College University, Pakistan	BIOACTIVE COMPOUNDS AND HEALTH BENEFITS OF PEACH FRUIT (PRUNUS PERSICA)
EWETOLA Esther. A. ADEKUNLE Adebola B.	Ladoke Akintola University of Technology, Nigeria	EFFECT OF SELECTED WEED AND SOIL PHYSICAL AND CHEMICAL PROPERTIES ON CARBON SEQUESTRATION
Dr. Farrukh Mahfooz Dr. Riaz Ahmed Dr. Ali Imtiaz	Bahria University, Pakistan	IMPACT OF RECURRING FLOODS ON ENVIRONMENT, HUMAN HEALTH, AND SUPPLY CHAIN DISRUPTION: EVIDENCE FROM PAKISTAN
Said ELANZAOUI	University IBN ZOHR, Morocco	A GREEN MAGNETIC ACTIVATED CARBON FOR EFFICIENT CRYSTAL VIOLET REMOVAL
Shoaib Ahsan Shah	Tianjin University, China	UAV-BASED ODOR SOURCE LOCALIZATION USING DEEP REINFORCEMENT LEARNING IN OUTDOOR ENVIRONMENT



HEAD OF SESSION: Assoc. Prof. Dr. Cemal BUDAĞ		
Dr. Yasemin MÜMİNOĞLU	Muş Alparslan University	THE USE OF PLANTS IN PRIMARY SCHOOL GARDENS AND THEIR IMPORTANCE IN CHILD DEVELOPMENT
Assoc. Prof. Dr. Cemal BUDAĞ	Van Yüzüncü Yıl University	DOG POPULATION IN URBAN ECOSYSTEM: CONTROL STRATEGIES AND FEEDING
Lec. Dr. Elvan KOÇ Bünyamin ÇATALCA Sibel KAYA	Artvin Çoruh University	AN ALTERNATIVE TO TRADITIONAL HERBARIUM TECHNIQUES: PRESERVING WILD PLANTS WITH EPOXY RESIN
Gökberk GÖKÇEK Yusuf Tuna BİRER Veysel Karani YILMAZ Sezer SAĞLAM Rıfat AKGÜL	Mercedes-Benz Türk A.Ş. Aksaray University Selçuk University KTO Karatay University	DEVELOPMENT OF A SIMULATION PLATFORM FOR VEHICLE-INDEPENDENT ECU VALIDATION
Ramazan KARA Assoc. Prof. Dr. Volkan YAMAÇLI	Mersin University	COMPARATIVE PERFORMANCE ANALYSIS OF CURRENT YOLO ARCHITECTURES FOR HUMAN DETECTION IN POST-DISASTER UAV IMAGERY
Dr. Yener TOP	Gümüşhane University	AN ANALYSIS OF THE TURKISH FURNITURE SECTOR REGARDING GREENWASHING: A CASE STUDY OF LARGE-SCALE ENTERPRISES
Asst. Prof. Dr. Derya Buluç	Mimar Sinan Fine Arts University	ANALYSIS OF THE FORMAL AND DECORATIVE CHARACTERISTICS OF OTTOMAN COMMEMORATIVE HANDKERCHIEFS
Dr. Emrah GÖKKAYA Dr. Fatih DENİZLİ Dr. Ömer DEMIRBILEK	Kayseri University Bünyan Vocational School Ministry of Health, Kayseri, Türkiye Malatya Turgut Özal University	LEADERSHIP COMPETENCIES IN DISASTER AND CRISIS MANAGEMENT: CURRENT TRENDS AND FUTURE PERSPECTIVES



HEAD OF SESSION: Assoc. Prof. Dr. Azime ARISOY

Dr. Özge DEMİRDELEN	Çağ University	THE CONCEPT OF "JUDGMENT" IN EXTRAJUDICIAL FOREIGN DIVORCES IN LIGHT OF THE CJEU's JUDGMENT IN CASE C-646/20: THE BRUSSELS II BIS AND BRUSSELS II TER REGULATIONS AND ARTICLE 27/A OF THE CIVIL REGISTRATION SERVICES ACT
Assoc. Prof. Dr. Azime ARISOY	Burdur Mehmet Akif Ersoy University	THE GREYING OF POVERTY AND THE RISK OF SOCIAL EXCLUSION: A COMPARATIVE ANALYSIS OF THE POPULATION AGED 65 AND OVER IN THE EUROPEAN UNION AND TÜRKIYE
Asst. Prof. Dr. Mehmet BİLGE	Burdur Mehmet Akif Ersoy University	AN EVALUATION OF THE NEW CHILD PROTECTION LAW REGULATION FROM A SOCIAL WORK PERSPECTIVE
Asst. Prof. Dr. Vildan MEYDAN	Hitit University	RECOGNITION AND LEGITIMACY IN TÜRKIYE'S AFRICA POLICY: THE CASE OF THE SOMALIA–ETHIOPIA CRISIS
Lec. Büşra Özdemir	Beykoz University	DARK PATTERN USE ON E-COMMERCE PLATFORMS: A QUALITATIVE CONTENT ANALYSIS FROM A DIGITAL MARKETING PERSPECTIVE
Dr. Sevinç Zeynep KAVRUK	Aydın Adnan Menderes University	SENSORY PROCESSING AND SENSORY SENSITIVITY IN GIFTED INDIVIDUALS: A SYSTEMATIC REVIEW
Research Assistant Dr. Müge PEŞTERE AKÇAY	Pamukkale University	TÜRKIYE İÇIN ZAMANLA DEĞIŞEN BIR PARASAL KOŞULLAR ENDEKSI: PARASAL AKTARIM MEKANIZMASININ DÖNÜŞÜMÜ VE DIŞ TICARET ÜZERINDEKI ETKILERI



HEAD OF SESSION: Prof. Dr. Ananda Majumdar		
Prof. Dr. Ananda Majumdar	Harvard University, USA	THE MOTHER/DAUGHTER DILEMMA: THE FAILURE OF MOTHERHOOD IN WILKIE COLLINS' THE WOMAN IN WHITE
Research Scholar, Mohd Shahbaz Khan Prof. Sameena	Aligarh Muslim University, INDIA	UNDERSTANDING AGEING IN INDIA: SOCIAL CHALLENGES AND CARE NEEDS
Mina Mohammadi	Ahlul Bayt International University, Iran	MATERNAL DISCRIMINATION AND POLICY FRAMEWORKS: A CRITICAL EXAMINATION OF THE MOTHERHOOD PENALTY
Pamilerin Ogundare Julius Ekem Rotimi Samuel Ogundare	Federal University Oye Ekiti, Nigeria Obafemi Awolowo University, Nigeria	SOCIETAL REINTEGRATION OF BRAZILIAN DEPORTEES: OBSTACLES, RESOURCES, AND PATHWAYS TO SUSTAINABLE RETURN
Dr. Ahmadu Sani Gurjiya Emen Essien Udofia	Federal University Gusau, Nigeria	RELATIONSHIP BETWEEN SELF-CONCEPT AND ACADEMIC PERFROMANCE AMONG SECONDARY SCHOOL STUDENTS IN GUSAU LGA, ZAMFARA STATE
Dr. Kehinde AYODELE Prof. P.A. AMOSUN	University of Ibadan, Nigeria	DIAGNO-PRESCRIPTIVE APPROACH IN SOLVING PERCEIVED DIFFICULT CONCEPTS IN GEOGRAPHY: AN EXPERIENCE IN PROBLEM-BASED LEARNING STRATEGY
Hassan BENTALEB	Ibn Tofail University, Morocco	FROM CURRICULUM TO CLASSROOM: IMPLEMENTING ECOLOGICAL CONCEPTS IN LIFE AND EARTH SCIENCES EDUCATION IN MOROCCAN MIDDLE SCHOOLS
Dr. Collens Ikechuwu Odo	Michael Okpara University of Agriculture, Nigeria	EVALUATING PARENTING STYLE INDICATORS AS PREDICTORS OF UNETHICAL BEHAVIOUR AMONG SECONDARY SCHOOL BIOLOGY STUDENTS



HEAD OF SESSION: Moses Adeolu AGOI		
Oluwakemi Racheal OSHINOWO Moses Adeolu AGOI Olayemi Grace ABIMBOLA Emmanuel Taiwo AGOI	Lagos State University of Education, Nigeria Loughborough University, Nigeria	SUSTAINABLE SMART UNIVERSITIES: AN INTERDISCIPLINARY PERSPECTIVE ON ARTIFICIAL INTELLIGENCE, DIGITAL ARCHITECTURE, AND EDUCATIONAL MANAGEMENT
IGE, David Dele Akanbi, Bello Muhammed PhD	University of Abuja, Nigeria	ENHANCEMENT OF THE EXISTING PUBLIC TRANSPORT SYSTEM FOR REAL-TIME BUS SCHEDULING AND PASSENGER DEMAND PREDICTION AT THE UNIVERSITY OF ABUJA
EKENE ERIC NNAEMEKA AKANBI BELLO MUHAMMED PhD	University of Abuja, Nigeria	ENHANCING GENERAL SECURITY AND MINIMIZING PROXY THROUGH RFID EMBEDDED ID CARD IN THE UNIVERSITY OF ABUJA
Akanbi, Bello Muhammed PhD Itua Omonoheromon Precious	University of Abuja, Nigeria	DIGITAL TRANSFORMATION OF RESEARCH JOURNAL MANAGEMENT: DESIGN AND IMPLEMENTATION OF A WEB-BASED JOURNAL MANAGEMENT AND PUBLICATION SYSTEM FOR THE FACULTY OF SCIENCE, UNIVERSITY OF ABUJA
OUKKAS Mebarek	Center University Nour Bachir of El Bayadh, Algeria	INVESTIGATION AND SIMULATION OF INTERFACE DAMAGE IN A HYBRID NANOCOMPOSITE
Joan S. Muñoz Roberto E. Martinez	National University of Colombia, Colombia	HEAVY NEUTRINO PRODUCTION AND LEPTON FLAVOR VIOLATION AT FUTURE e+e− COLLIDERS IN A NON-UNIVERSAL U(1)' MODEL
Mohammed NAJI	Hassan II University, Morocco	METAL HYDRIDES AS PROMISING MATERIALS FOR SAFE AND EFFICIENT HYDROGEN STORAGE: A COMPREHENSIVE REVIEW

DATE	TIME	SESSION
• 01.09.2026 • Online	• 12^{30}–14^{30} • Istanbul Time	• HALL-5 • SESSION-2

HEAD OF SESSION: Major Gheorghe GIURGIU		
Hafiz Moahid Ali Imran Hafeez	University of Engineering and Technology, Pakistan	FATIGUE RESPONSE OF HOT MIX ASPHALT (HMA) MODIFIED WITH THE COMBINATION OF STONE DUST AND NANO-CLAY
Salihu SULEIMAN Adamu M. BABAYO	Federal University Birnin Kebbi, Nigeria Abubakar Tafawa Balewa University Bauchi, Nigeria	NATURE-INSPIRED THERMAL ADAPTATION FOR RESIDENTIAL BUILDING ENVELOPES IN NORTH WESTERN NIGERIA: A BIOMIMETIC DESIGN FRAMEWORK
Bendahmane Hasna	Mohammed V University, Morocco	ENSURING CONSISTENCY BETWEEN RASTER MAPS AND DESCRIPTIVE STATISTICS IN REMOTE SENSING: A CONCEPTUAL FRAMEWORK USING INSAR LAND SUBSIDENCE
Olusegun Olukayode Olaleye Emmanuel Okon Wilson	Maritime Academy of Nigeria Akwa Ibom State Polytechnic, Nigeria	AI-DRIVEN QUALITY CONTROL IN MODERN MANUFACTURING SYSTEMS
Olusegun Olukayode Olaleye Emmanuel Okon Wilson	Maritime Academy of Nigeria Akwa Ibom State Polytechnic, Nigeria	SUSTAINABLE MANUFACTURING PRACTICES FOR IMPROVING PRODUCTIVITY AND RESOURCE EFFICIENCY IN DEVELOPING COUNTRIES
Major Gheorghe GIURGIU Prof. dr. med. Manole COJOCARU	Deniplant-Aide Sante Medical Center, Romania Titu Maiorescu University, Romania	WHAT WE KNOW ABOUT PSORIASIS SO FAR?
Sehrish Firyal Bareerah Sohail	University of Veterinary and Animal Sciences, Pakistan	MOLECULAR CHARACTERIZATION OF STAPHYLOCOCCUS AUREUS RECOVERED FROM RAW MEAT
Ph.D. Tran Le Nhat Quang MSc. Le Trong De	University of Danang, Vietnam Vinh Medical University, Vietnam	CURRENT STATUS AND DEVELOPMENT SOLUTIONS FOR ESPORTS AND PHYGITAL SPORTS IN VIETNAM: TOWARD A PROFESSIONAL AND SUSTAINABLE DIGITAL SPORTS ECOSYSTEM

2nd ISTINYE INTERNATIONAL INTERDISCIPLINARY ACADEMIC STUDIES CONGRESS

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PROCEEDINGS BOOK



EDITED BY

Prof. Dr. Osman ERKMEN

Assoc. Prof. Dr. E. İlhan ŞAHIN

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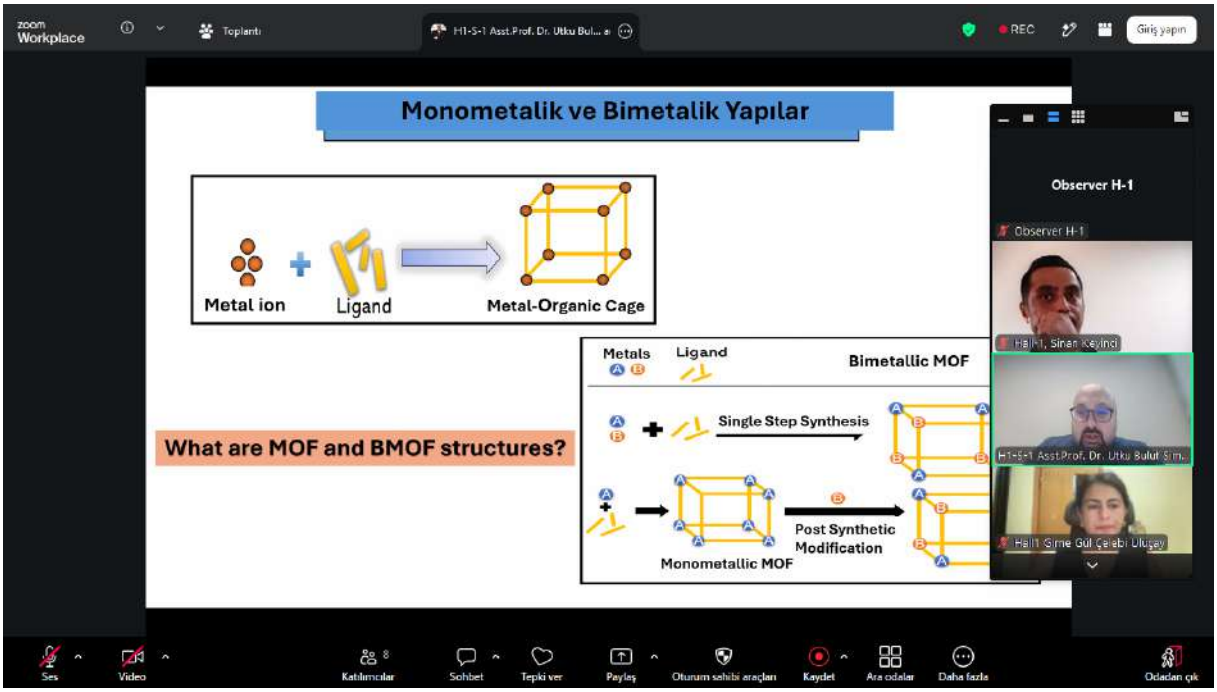
İLGİLİ MAKAMA

2. İstinye Uluslararası Disiplinlerarası Akademik Çalışmalar Kongresi 1-2 Eylül, 2026 tarihinde İstanbul, Türkiye'de (çevrimiçi) 15 farklı ülkenin (Türkiye, USA, Nigeria, Romania, China, Russia, Albania, Bangladesh, India, İndonesia, Vietnam, Algeria, Pakistan, Morocco, Colombia) akademisyen/araştırmacılarının katılımıyla gerçekleşmiştir. Kongre 16 Ocak 2020 Akademik Teşvik Ödeneği Yönetmeliğine getirilen "Tebliğlerin sunulduğu yurt içinde veya yurt dışındaki etkinliğin uluslararası olarak nitelendirilebilmesi için Türkiye dışında en az beş farklı ülkeden sözlü tebliğ sunan konuşmacının katılım sağlaması ve tebliğlerin yarıdan fazlasının Türkiye dışından katılımcılar tarafından sunulması esastır." değişikliğine uygun düzenlenmiştir.
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Saygılarımla

Assoc. Prof. Dr. E. İlhan Şahin
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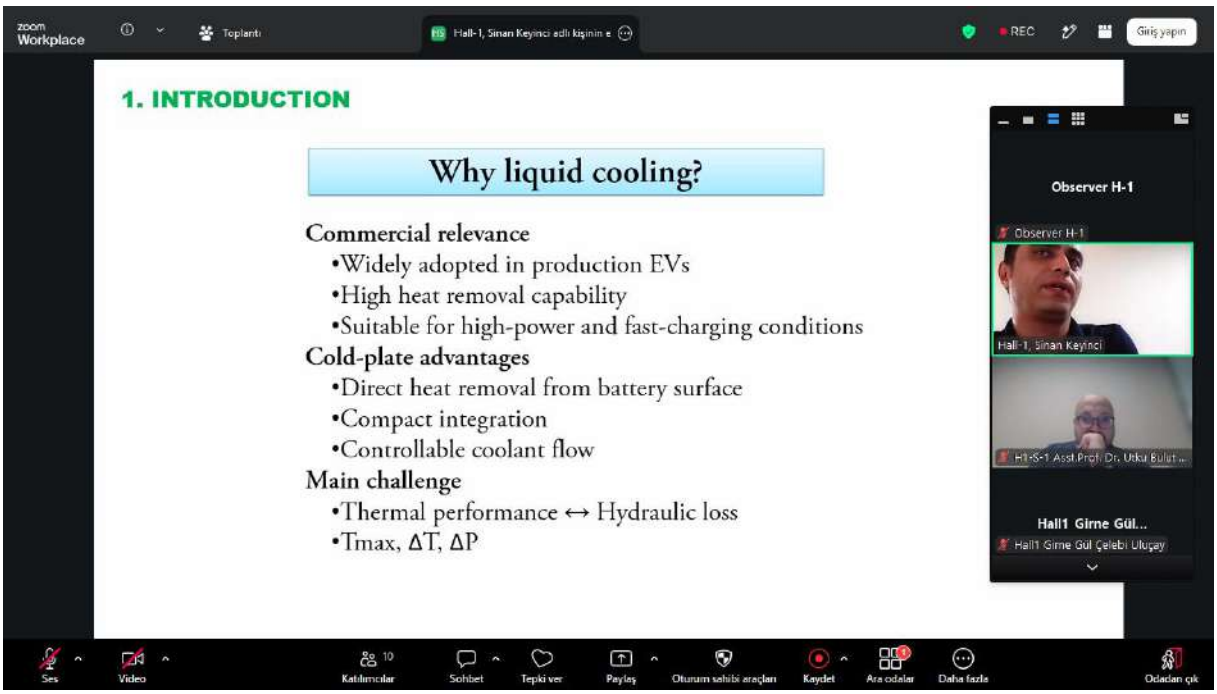
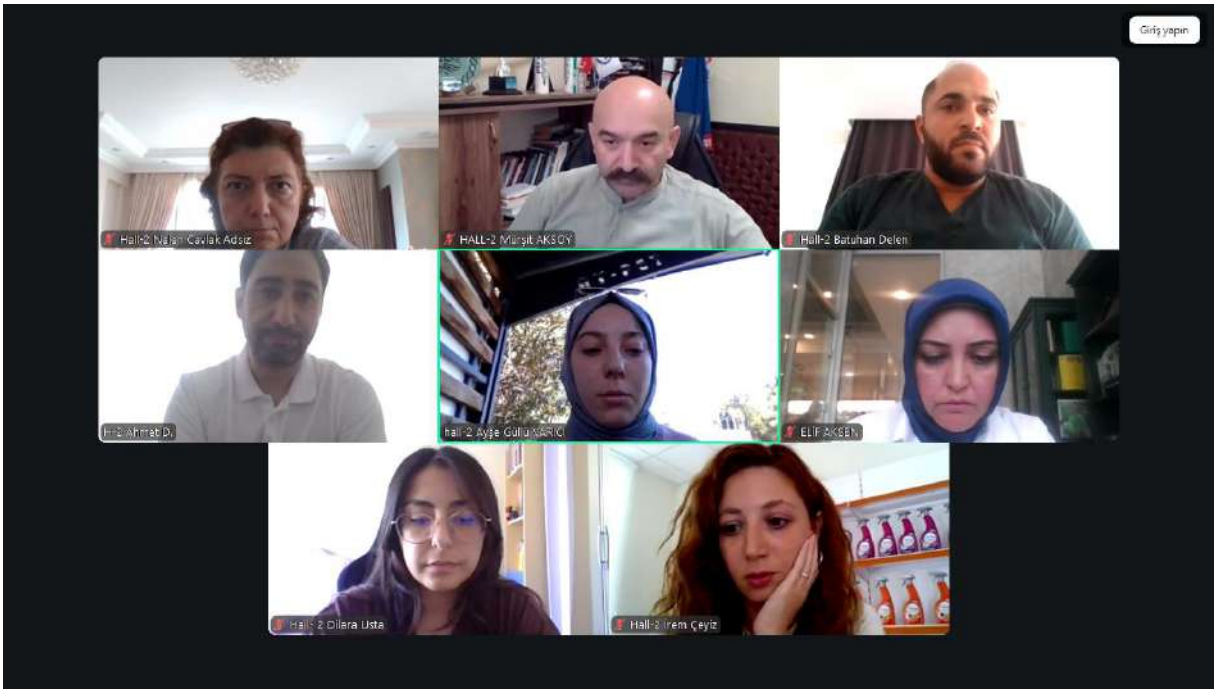


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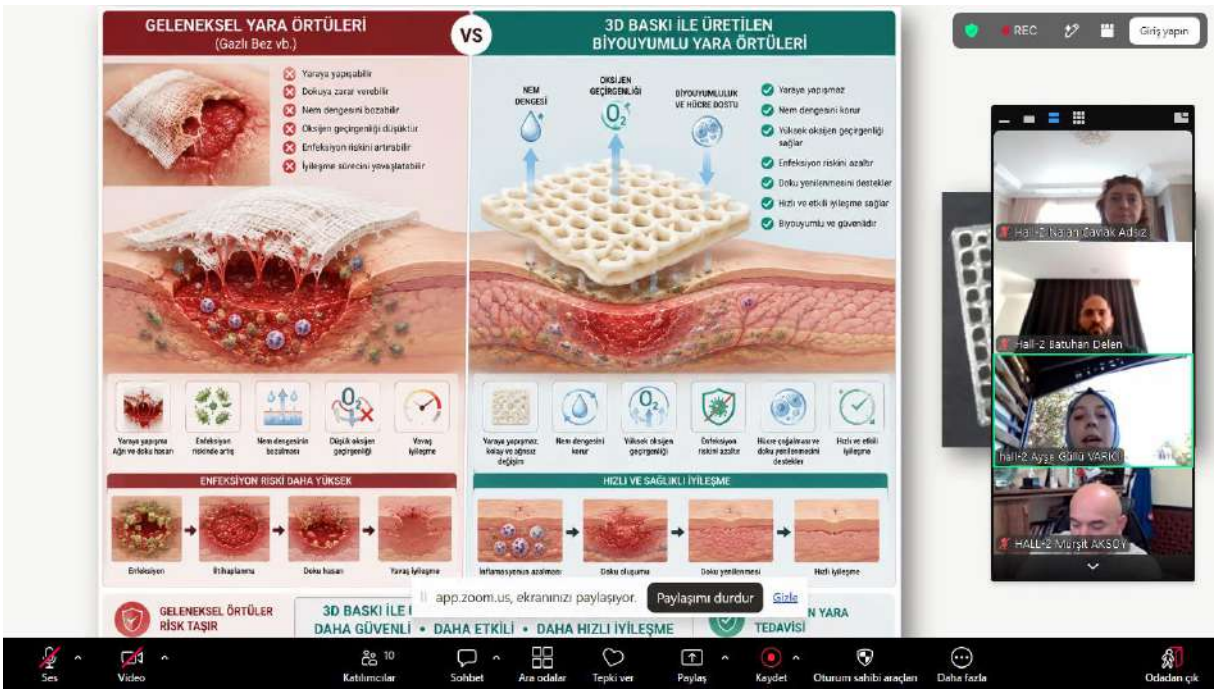


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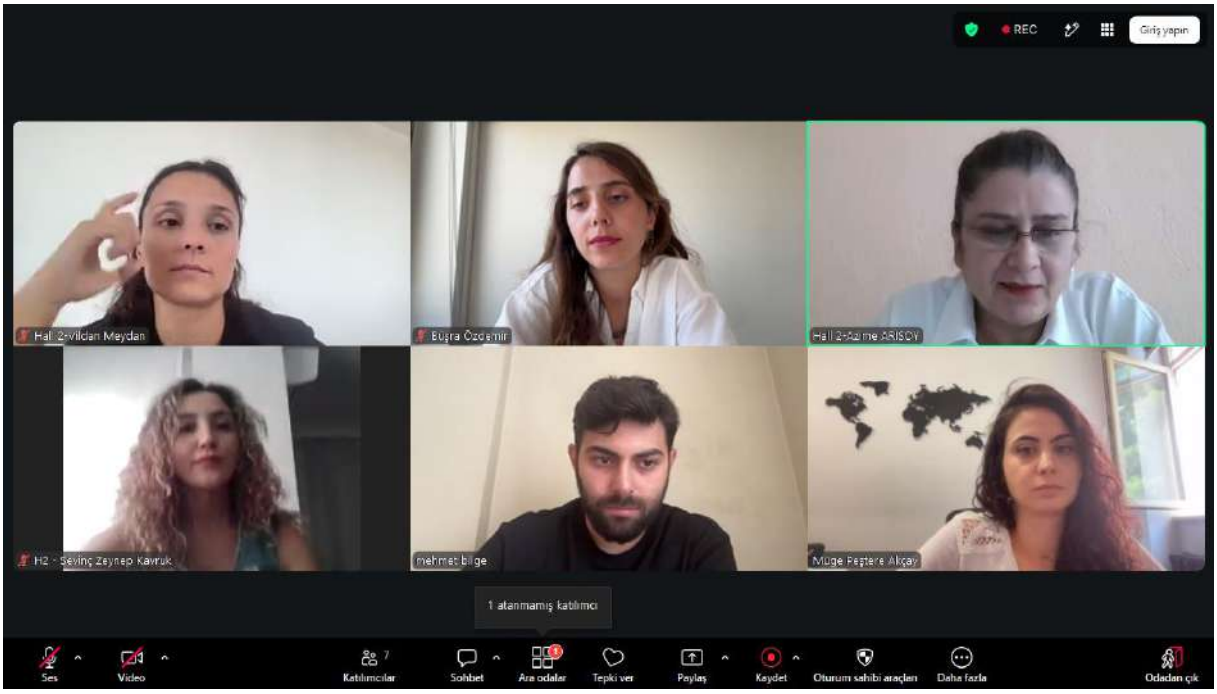
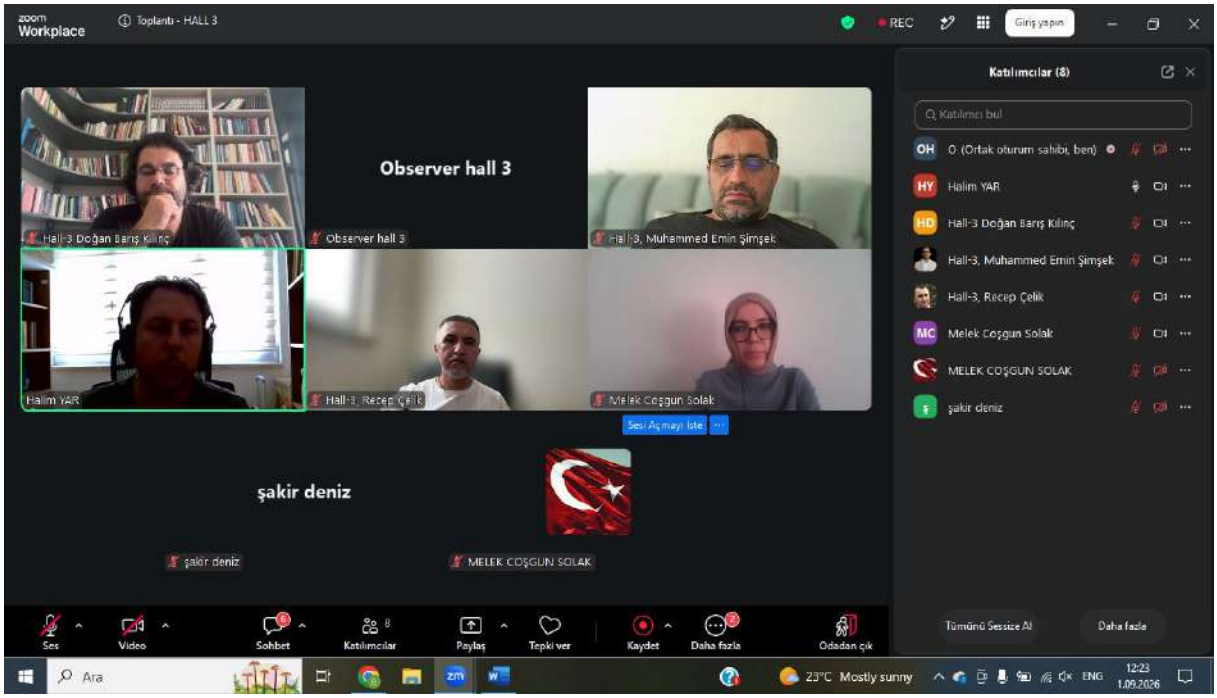




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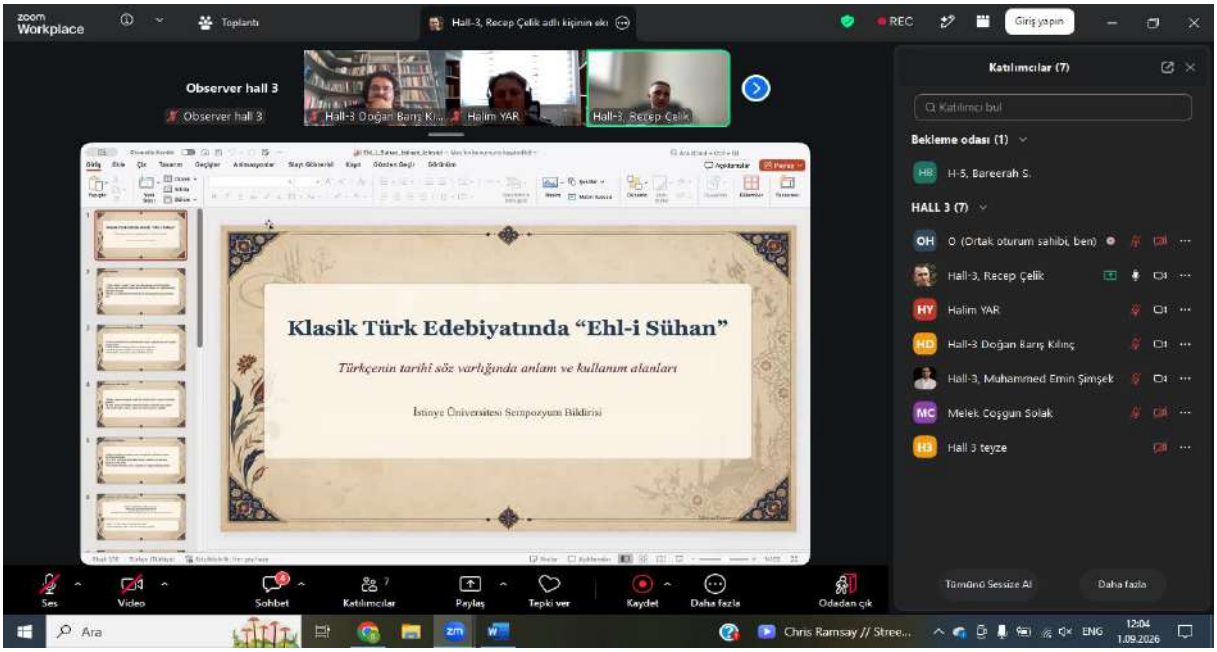
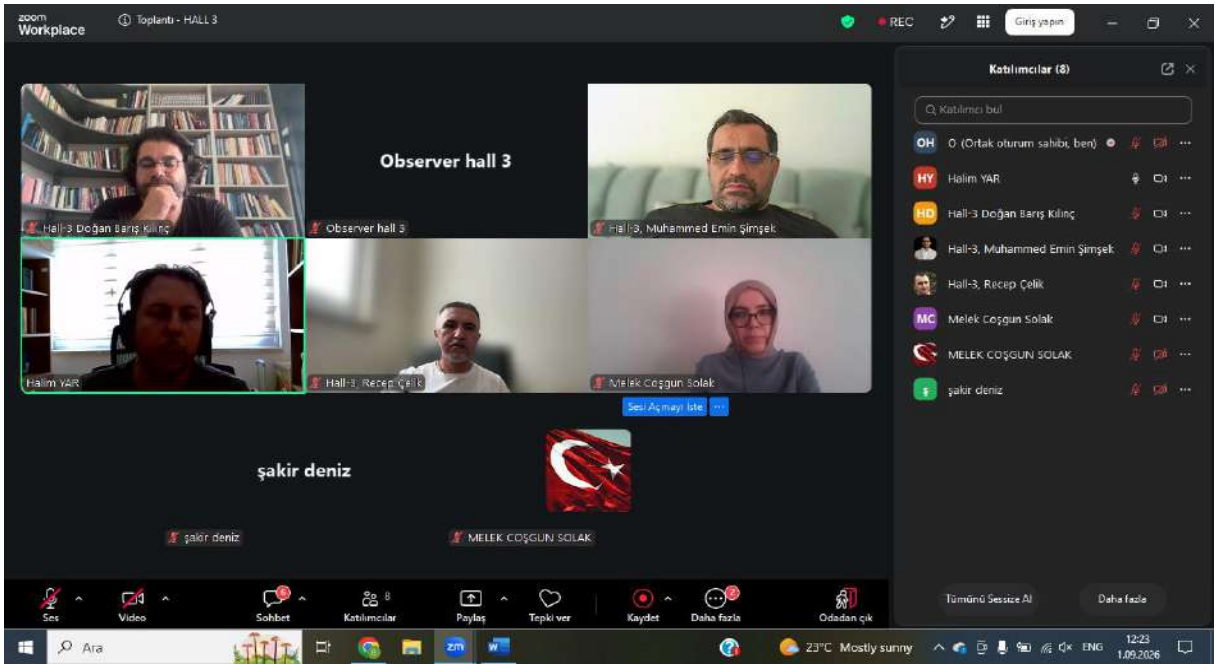


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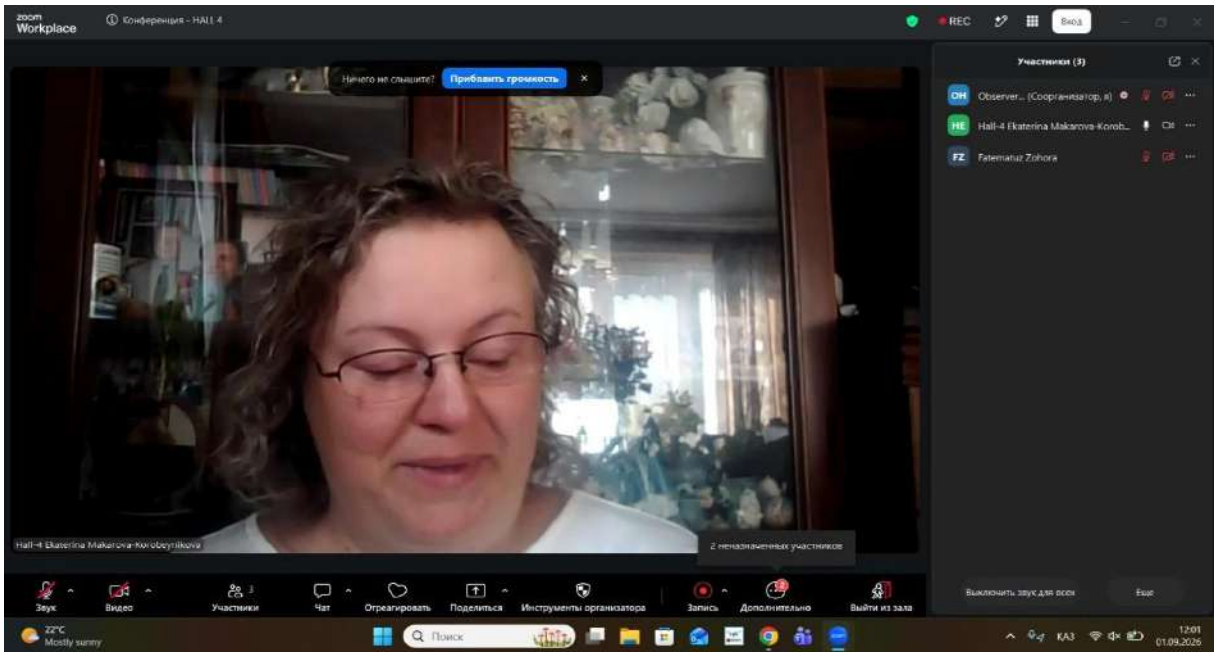


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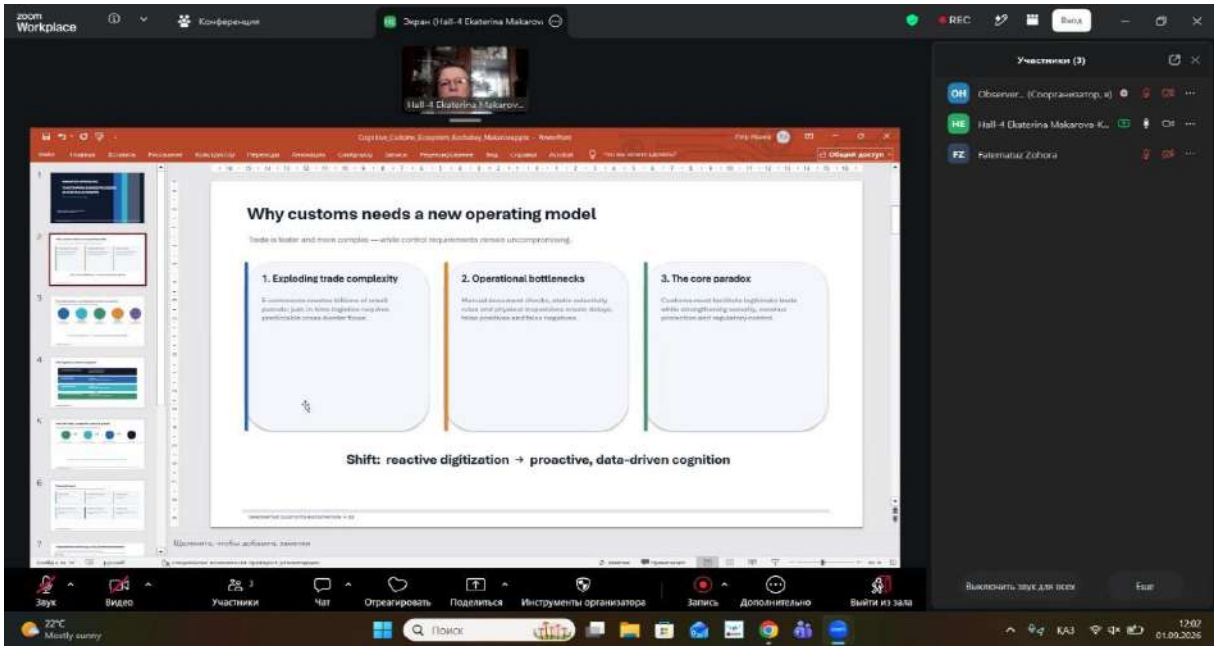




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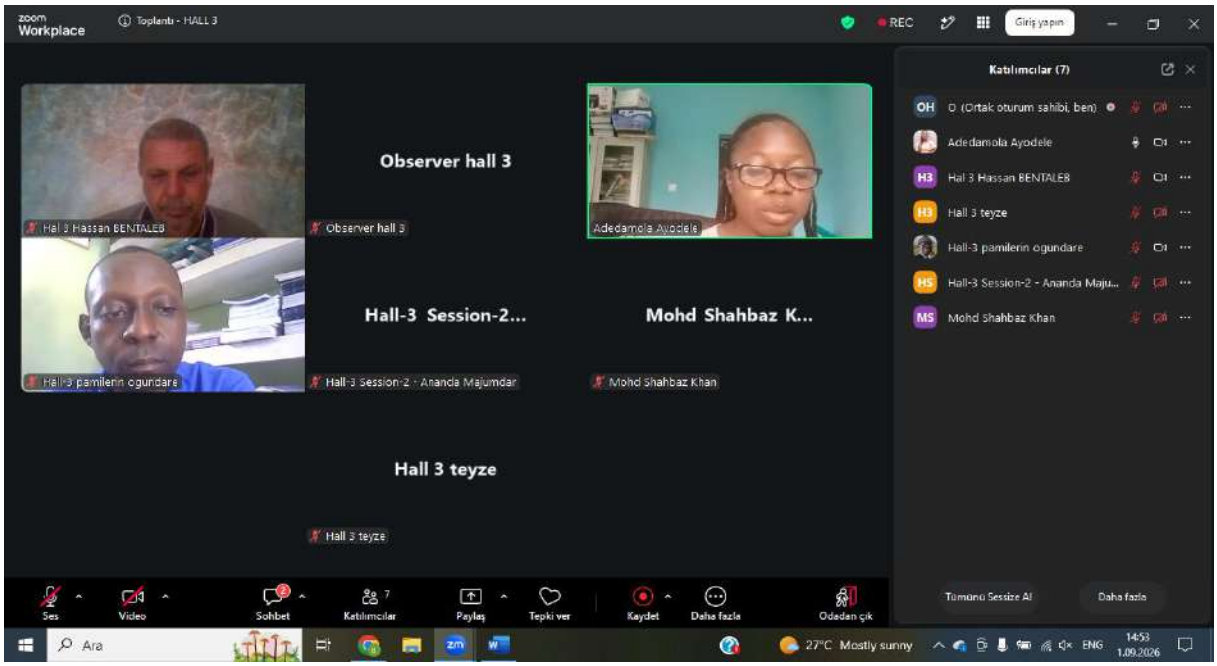
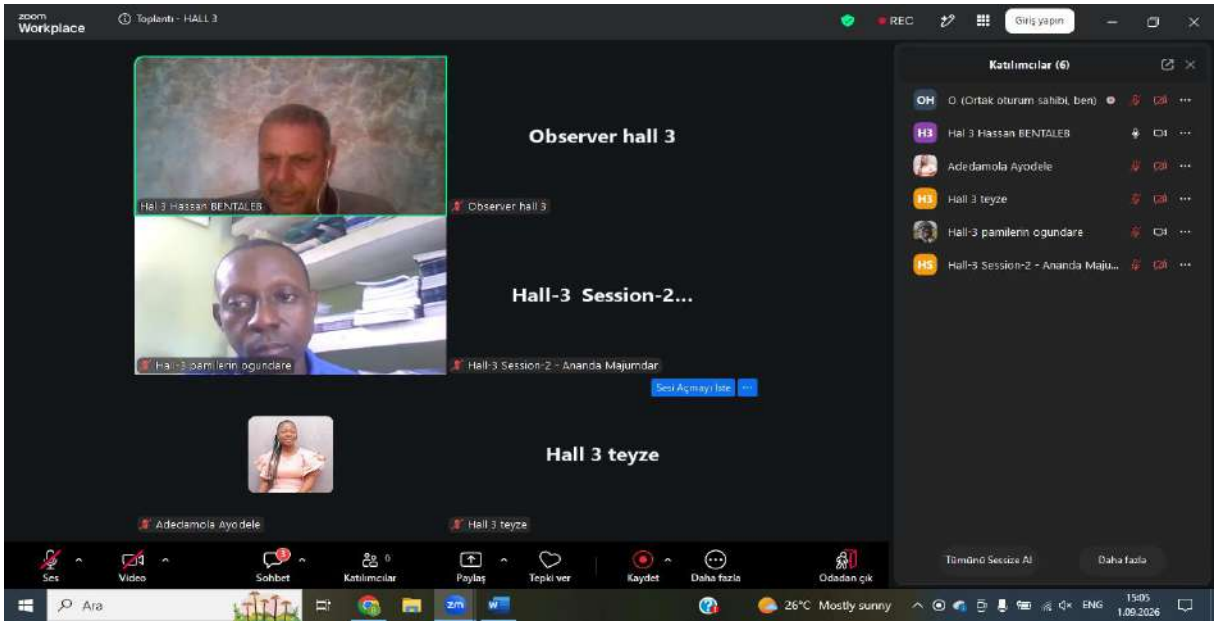


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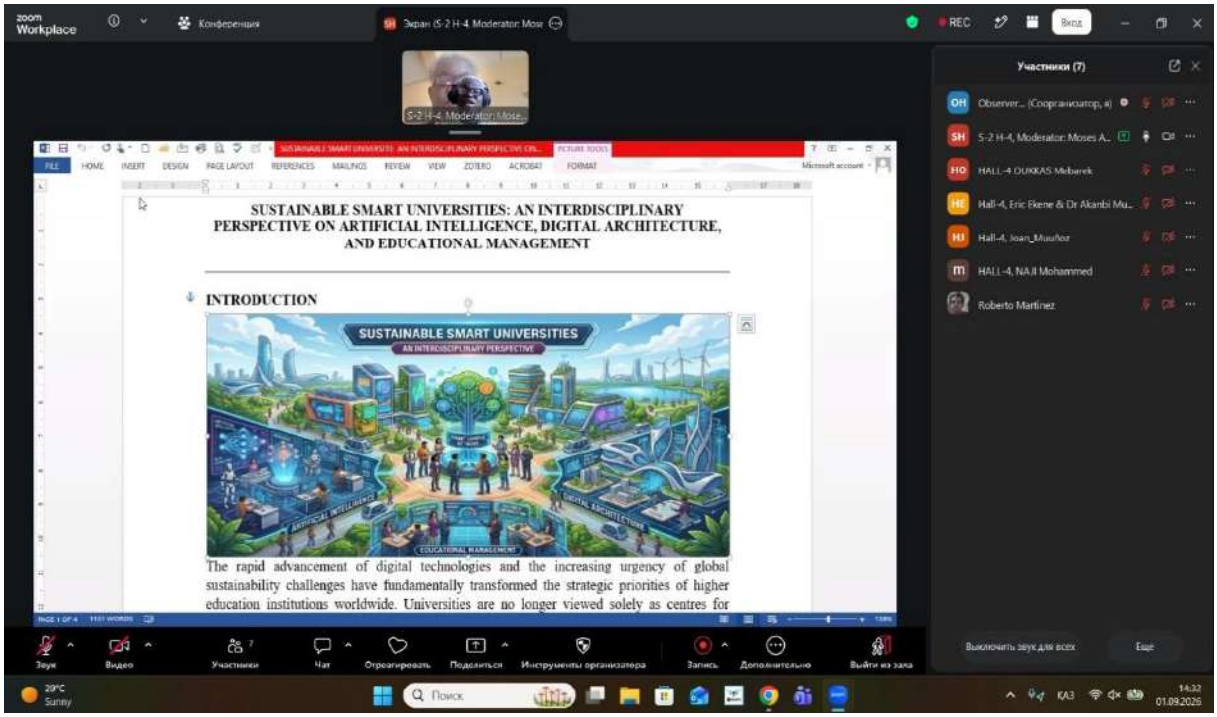
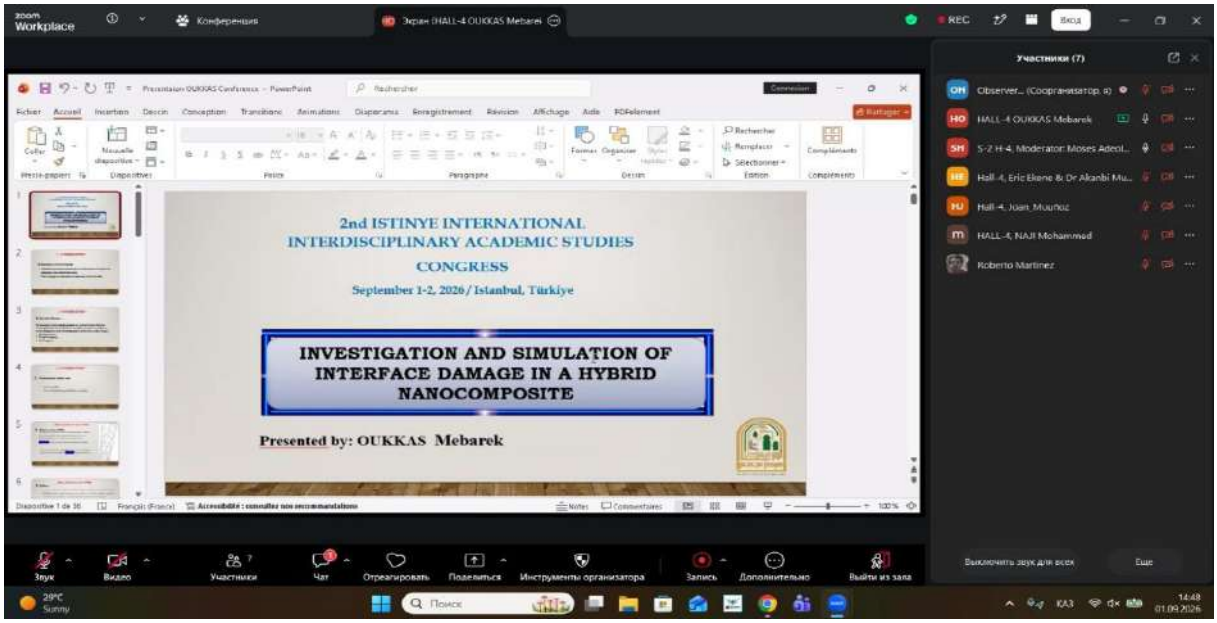


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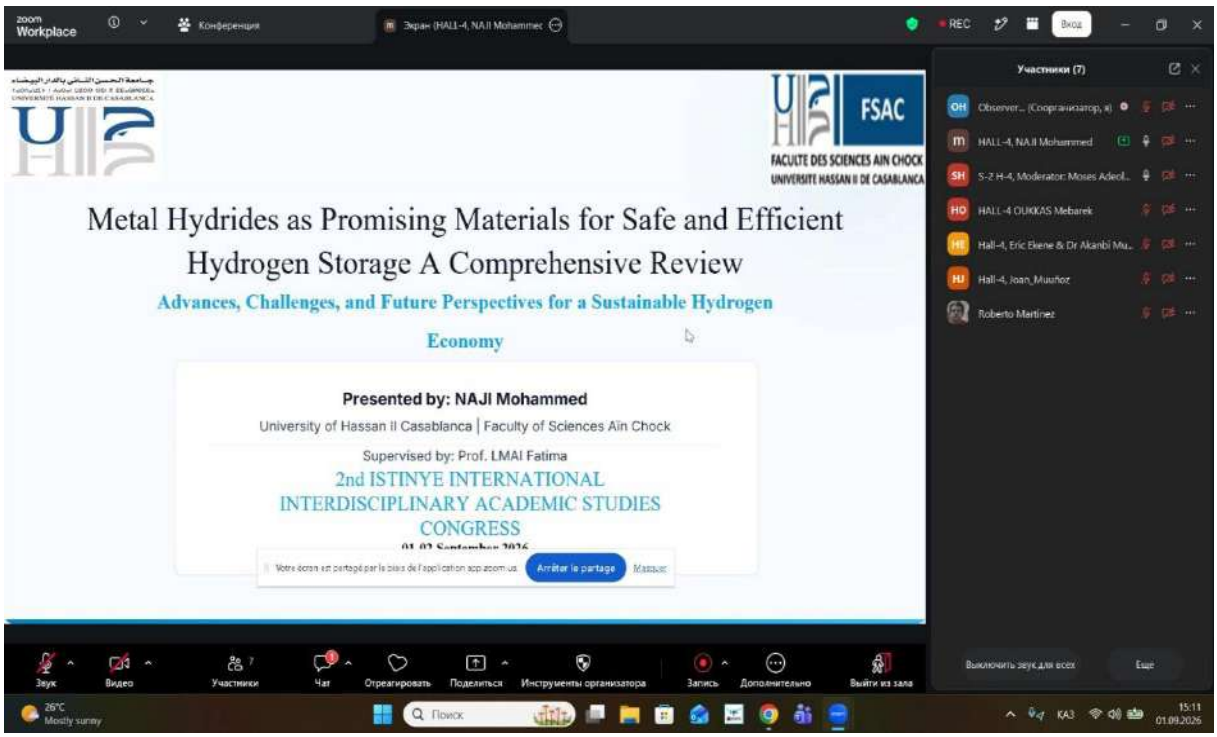


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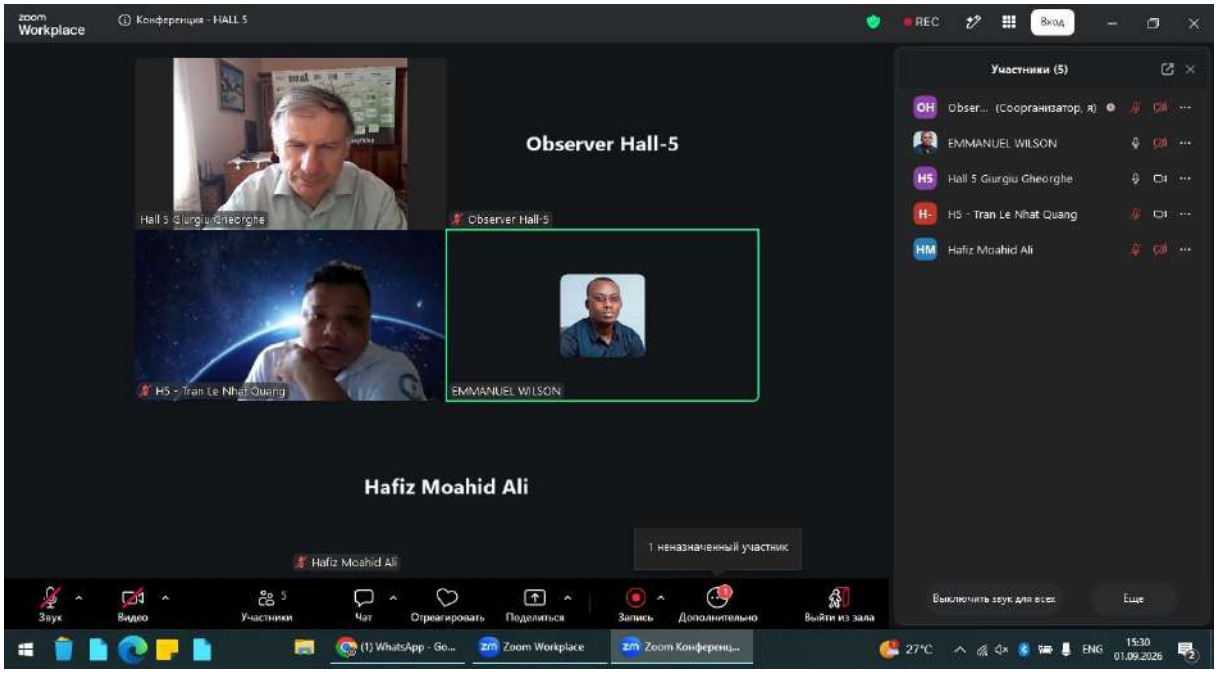
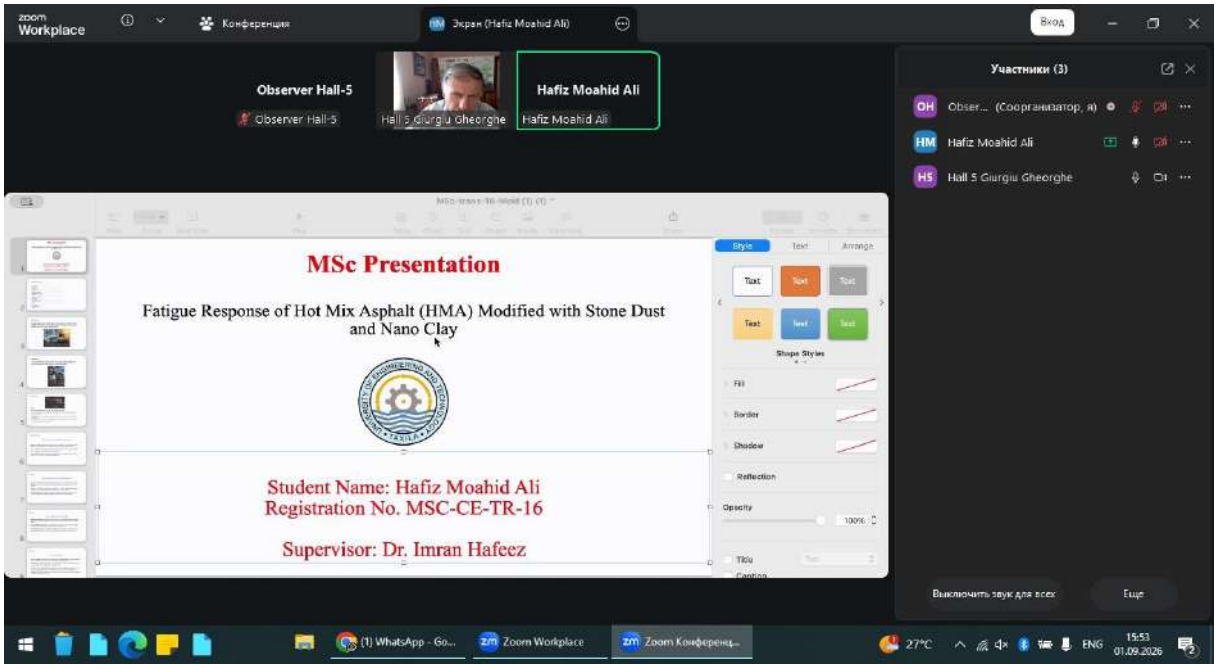
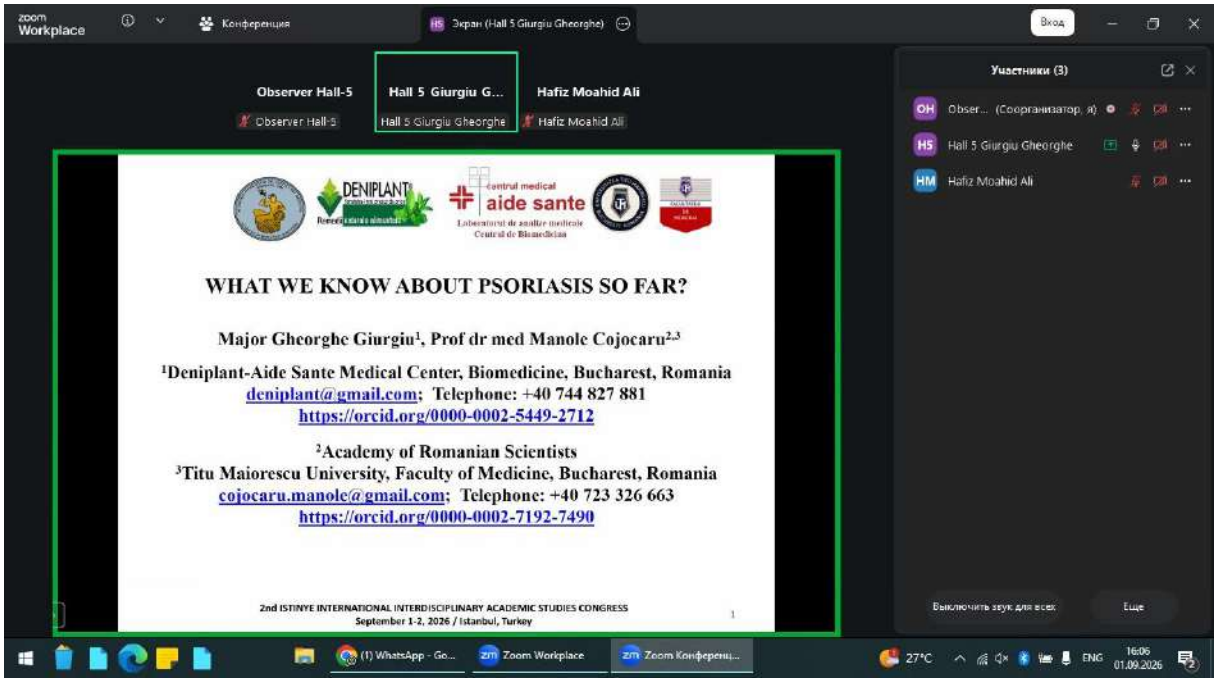




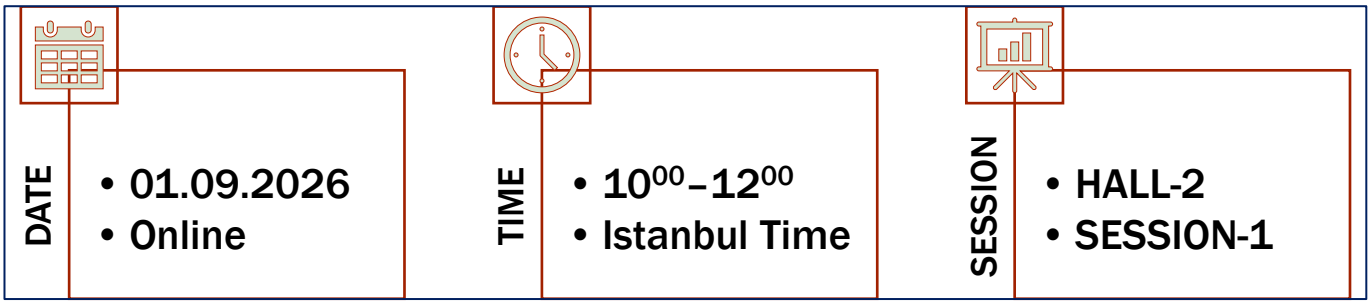
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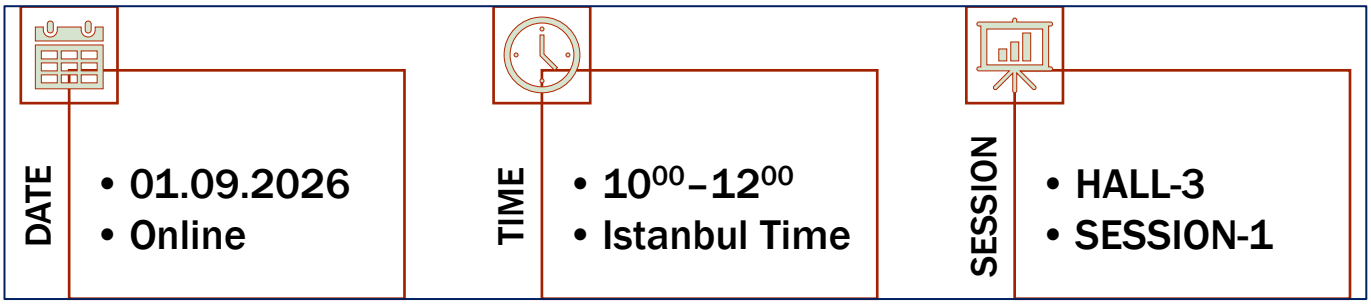




HEAD OF SESSION: Asst. Prof. Dr. Utku Bulut SIMSEK		
Asst. Prof. Dr. Utku Bulut SIMSEK	Istanbul Aydin University, Anadolu BIL Vocational School	ENGINEERING MICRO SIZED NH2 FUNCTIONALIZED BIMETALLIC MOFS VIA SUPERCRITICAL CO_2 FOR EFFICIENT CARBON CAPTURE
Dr. Girne Gül ÇELEBİ ULUÇAY Prof. Dr. Güzin KAYA	---	VAN GÖLÜ HAVZASI'NDA NÜFUS YOĞUNLUĞU ARTIŞININ MEKÂNSAL ÖRÜNTÜSÜ: EDREMİT, İPEKYOLU VE TUŞBA ÖRNEĞİ
Asst. Prof. Dr. Seda ERDOĞAN	İstanbul Galata University	GENERATIVE ARTIFICIAL INTELLIGENCE FOR THE SPATIAL IMPROVEMENT OF PUBLIC SPACES: THE CASE OF MAÇKA DEMOCRACY PARK
Asst. Prof. Dr. Sinan KEYİNCİ	Çukurova University	EFFECT OF TESLA VALVE DISTRIBUTION ON THE THERMO-HYDRAULIC PERFORMANCE OF A LIQUID-COOLED BATTERY THERMAL MANAGEMENT SYSTEM
Dr. Barış ERKUŞ Doğukan AYHAN	Bursa Uludağ University	A REVIEW OF VIBRATION-BASED FAULT DIAGNOSIS METHODS FOR INTERNAL COMBUSTION ENGINES: SIGNAL PROCESSING TECHNIQUES AND MACHINE LEARNING APPROACHES
Aslıhan Hatun ÇAÇAN	Tokat Gaziosmanpasa University	LINKING MOLECULAR INTERACTIONS TO THE ACOUSTIC AND CALORIC BEHAVIOR OF REAL GASES
İREM KESKİN DR. BURCU ARSLAN AYLİN RAZLIKLI ÖZGE KARATAŞ	VIKING CLEANING AND COSMETICS CO.	SYNTHESIS AND CHARACTERIZATION OF SODIUM BENZOATE AND POTASSIUM SORBATE AND EVALUATION OF THEIR PRESERVATIVE EFFICACY IN A LIQUID SOAP FORMULATION
Gozde YALCIN OZKAT Assoc. Prof. Dr. Erkan Caner OZKAT	Recep Tayyip Erdogan University	CLASS IMBALANCE IN TOXICITY PREDICTION: THE EFFECT OF PERFORMANCE METRIC AND DECISION THRESHOLD SELECTION ON MODEL RANKING IN THE TOX21 DATASET

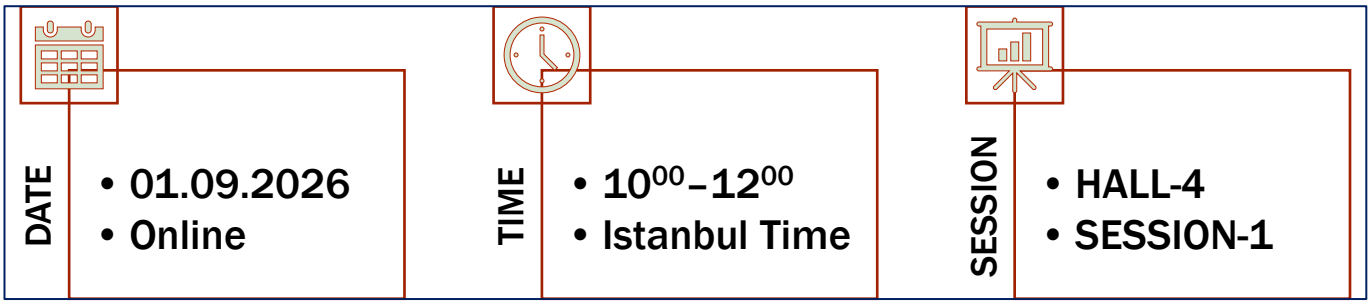


HEAD OF SESSION: Assoc. Prof. Dr. Ahmet DINÇ		
Lec. Ayşe Güllü VARICI	İstinye University	3D BIOPRINTING TECHNOLOGY APPROACH IN WOUND DRESSING PRODUCTION
Banu BAŞ Dilara USTA	Ankara Yıldırım Beyazıt University	EFFECTS OF VESTIBULAR REHABILITATION ON SPATIAL ORIENTATION, SPATIAL COGNITION, AND BALANCE PERFORMANCE: A SYSTEMATIC REVIEW
Dr. Mürşit AKSOY	Hakkari University	THE ROLE OF CORRECTIVE EXERCISES IN PREVENTING SPORTS INJURIES AND EXAMPLES OF POPULAR EXERCISE PRACTICES
Dr. Batuhan DELEN Dr. Gündüz Ercan KUTLUAY	Tekirdağ Namık Kemal University COIZ Kapaklı State Hospital	SCOPE, READABILITY, AND EMERGENCY WARNING INFORMATION IN TURKISH ONLINE PATIENT EDUCATION CONTENT ON PEDIATRIC SUPRACONDYLAR HUMERUS AND ELBOW FRACTURES
Mustafa KAHRAMAN Murat BEĞENIK	TUSEB Türkiye Institute of Public Health and Chronic Diseases Istanbul Medipol University	ACUTE CARDIOVASCULAR RESPONSES TO SOLEUS PUSH-UP EXERCISE DURING AN ORAL GLUCOSE TOLERANCE TEST
Nalan CAVLAK ADSIZ İlhami ADSIZ	Elazığ Fethi Sekin City Hospital	INVESTIGATION OF E-SCOOTER ACCIDENTS ADMITTED TO THE EMERGENCY DEPARTMENT
Assoc. Prof. Dr. Ahmet DINÇ Prof. Dr. Ahmet Nusret BULGURCUOĞLU	Iğdır University	MANAGEMENT OF DUAL CAREER AND ATHLETIC CAREER TRANSITIONS: A WEB OF SCIENCE-BASED BIBLIOMETRIC NETWORK ANALYSIS
M. Sc. Canan BAĞCI TAN Lec. Dr. Ozden OZGUN-ACAR Prof. Dr. Aslı KIRIKBAKAN	Pamukkale University	PYRROLOQUINOLINE QUINONE MODULATES ALZHEIMER'S DISEASE- RELATED GENE EXPRESSION IN SH-SY5Y CELLS
Pharmacist Elif AKSEN Prof. Dr. Gülbin ÖZÇELİKAY	Ankara University	THE EFFECT OF MERCHANDISING OF NON-PHARMACEUTICAL PRODUCTS ON EFFICIENCY IN COMMUNITY PHARMACIES



HEAD OF SESSION: Asst. Prof. Dr. Doğan Barış KILINÇ

Dr. Recep ÇELİK	Aksaray University	"EHL-I SÜHAN" IN CLASSICAL TURKISH LITERATURE: MEANING AND FUNCTION IN THE HISTORICAL VOCABULARY OF TURKISH
Assistant Professor Halim YAR	Sirnak University	GULSHENĪ-I SARUKHĀNĪ'S WORK TITLED SAʿDNĀME [ATTRIBUTED TO KHAYĀLĪ-I GULSHENĪ IN THE LIBRARY RECORD]
Dr.Şakir DENİZ	Presidency of Religious Affairs	AN ANALYSIS OF THE METHODOLOGY OF COMMENTING ON A SINGLE HADITH, FOCUSING ON ABU SHAMA AL-MAKDİSİ'S WORK TITLED "SHARH AL-HADITH AL-MUKHTAFA Fİ MAB'AS AL-NABİY AL-MUSTAFA"
Asst. Prof. Dr. Muhammed Emin ŞIMŞEK	Gaziantep Islamic Science and Technology University	CURRICULUM AND PEDAGOGY IN MUSLIM PRESCHOOL INSTITUTIONS IN ENGLAND: A QUALITATIVE CASE STUDY
Dr. Melek COŞGUN SOLAK	Yozgat Bozok University	RELIGIOUS EXPERIENCE IN THE AGE OF SOCIAL ACCELERATION: A SOCIOLOGICAL INQUIRY INTO TIME AND MEANING
Asst. Prof. Dr. Doğan Barış KILINÇ	Dicle University	SOCRATES' DEATH AS AN EXAMPLE OF TRAGEDY



HEAD OF SESSION: Dr. Makarova-Korobeynikova Ekaterina Petrovna

KOCHUBEY Alexander MAKAROVA-KOROBEYNIKOVA Ekaterina Petrovna	Russian Customs Academy, Russia	INNOVATIVE APPROACHES TO AUTOMATING BUSINESS PROCESSES OF CUSTOMS AUTHORITIES BASED ON ADVANCED TECHNOLOGIES
Kristal Hykaj Ardita Hykaj	Mediterranean University, Albania	THE IMPACT OF THE COVID-19 PANDEMIC ON THE ALBANIAN BANKING SECTOR PERFORMANCE: AN ECONOMETRIC ANALYSIS (2015–2020)
Fatematuz Zohora	University of Barishal, Bangladesh	CARBON ACCOUNTING, CORPORATE GOVERNANCE AND CORPORATE CARBON PERFORMANCE: EVIDENCE FROM BANGLADESH
Mr.S.Praveenkumar Dr.S.Chandrasekar	The Madura College, India	INTEGRATED E-WALLET ACCOUNTING: FORMALIZING INFORMAL BUSINESSES FOR VIKSIT BHARAT 2047
Makarova-Korobeynikova Ekaterina Petrovna Sulaimanova Sabina	Russian Customs Academy, Russia	POSSIBILITIES OF INCLUDING A NEURAL NETWORK IN THE WORK OF THE CUSTOMS SERVICE WHEN INSURING INTELLECTUAL PROPERTY ASSETS
Rusli Sri Mulyani	Institut ‘Aisyiyah Sulawesi Selatan, İndonesia	THE ROLE OF HUMAN RESOURCE COMPETENCIES IN SUPPORTING UNIVERSITY QUALITY ASSURANCE AND ACCREDITATION
TETEREV Daniil MAKAROVA-KOROBEYNIKOVA Ekaterina Petrovna	Russian Customs Academy, Russia	THE CURRENT STATE OF INTERACTION BETWEEN CUSTOMS AUTHORITIES AND BUSINESS STRUCTURES
Oluwafunmilayo Caroline OYENIYI	KolaDaisi University, Nigeria	DIGITAL FINANCIAL INCLUSION AND TAX REVENUE PERFORMANCE IN NIGERIA
M.A. Nguyen Thanh Tuan	Vinh Nhuan Middle and High School, Vietnam	BANQUE DE L’INDOCHINE AND CURRENCY ISSUANCE IN FRENCH INDOCHINA (1875 - 1930)



HEAD OF SESSION: Dr. Muhammad Imran		
Orji, Jephter Ebuka	Alex Ekwueme Federal University, Nigeria	SOIL MANAGEMENT PRACTICES FOR MITIGATION OF THE EFFECT CLIMATE CHANGE IN THE TROPICS
Ekanem, Moses Columba	Akwa Ibom State Polytechnic, Nigeria	QUALITY AND NUTRITIONAL CONTENTS OF WATER YAM-COCOYAM COMPOSITE FLOUR SUPPLEMENTED WITH COWPEA FLOUR FOR THE PREPARATION OF EKPANG NKUKWO PREPARATION
Arous Ali KACI Zakia DAHMENE Thoraya	University Djillali Bounaama, Algeria M'hamed Bouguera Boumerdès University, Algeria	IMPACT OF FARMING SYSTEMS AND PRACTICES ON THE CULTIVATION OF DURUM WHEAT (TRITICUM DURUM DESF) UNDER SEMI-ARID CONDITIONS IN ALGERIA
Dr. Muhammad Imran	Government College University, Pakistan	BIOACTIVE COMPOUNDS AND HEALTH BENEFITS OF PEACH FRUIT (PRUNUS PERSICA)
EWETOLA Esther. A. ADEKUNLE Adebola B.	Ladoke Akintola University of Technology, Nigeria	EFFECT OF SELECTED WEED AND SOIL PHYSICAL AND CHEMICAL PROPERTIES ON CARBON SEQUESTRATION
Dr. Farrukh Mahfooz Dr. Riaz Ahmed Dr. Ali Imtiaz	Bahria University, Pakistan	IMPACT OF RECURRING FLOODS ON ENVIRONMENT, HUMAN HEALTH, AND SUPPLY CHAIN DISRUPTION: EVIDENCE FROM PAKISTAN
Said ELANZAOUI	University IBN ZOHR, Morocco	A GREEN MAGNETIC ACTIVATED CARBON FOR EFFICIENT CRYSTAL VIOLET REMOVAL
Shoaib Ahsan Shah	Tianjin University, China	UAV-BASED ODOR SOURCE LOCALIZATION USING DEEP REINFORCEMENT LEARNING IN OUTDOOR ENVIRONMENT



HEAD OF SESSION: Assoc. Prof. Dr. Cemal BUDAĞ		
Dr. Yasemin MÜMİNOĞLU	Muş Alparslan University	THE USE OF PLANTS IN PRIMARY SCHOOL GARDENS AND THEIR IMPORTANCE IN CHILD DEVELOPMENT
Assoc. Prof. Dr. Cemal BUDAĞ	Van Yüzüncü Yıl University	DOG POPULATION IN URBAN ECOSYSTEM: CONTROL STRATEGIES AND FEEDING
Lec. Dr. Elvan KOÇ Bünyamin ÇATALCA Sibel KAYA	Artvin Çoruh University	AN ALTERNATIVE TO TRADITIONAL HERBARIUM TECHNIQUES: PRESERVING WILD PLANTS WITH EPOXY RESIN
Gökberk GÖKÇEK Yusuf Tuna BİRER Veysel Karani YILMAZ Sezer SAĞLAM Rıfat AKGÜL	Mercedes-Benz Türk A.Ş. Aksaray University Selçuk University KTO Karatay University	DEVELOPMENT OF A SIMULATION PLATFORM FOR VEHICLE-INDEPENDENT ECU VALIDATION
Ramazan KARA Assoc. Prof. Dr. Volkan YAMAÇLI	Mersin University	COMPARATIVE PERFORMANCE ANALYSIS OF CURRENT YOLO ARCHITECTURES FOR HUMAN DETECTION IN POST-DISASTER UAV IMAGERY
Dr. Yener TOP	Gümüşhane University	AN ANALYSIS OF THE TURKISH FURNITURE SECTOR REGARDING GREENWASHING: A CASE STUDY OF LARGE-SCALE ENTERPRISES
Asst. Prof. Dr. Derya Buluç	Mimar Sinan Fine Arts University	ANALYSIS OF THE FORMAL AND DECORATIVE CHARACTERISTICS OF OTTOMAN COMMEMORATIVE HANDKERCHIEFS
Dr. Emrah GÖKKAYA Dr. Fatih DENİZLİ Dr. Ömer DEMIRBILEK	Kayseri University Bünyan Vocational School Ministry of Health, Kayseri, Türkiye Malatya Turgut Özal University	LEADERSHIP COMPETENCIES IN DISASTER AND CRISIS MANAGEMENT: CURRENT TRENDS AND FUTURE PERSPECTIVES



HEAD OF SESSION: Assoc. Prof. Dr. Azime ARISOY		
Dr. Özge DEMİRDELEN	Çağ University	THE CONCEPT OF "JUDGMENT" IN EXTRAJUDICIAL FOREIGN DIVORCES IN LIGHT OF THE CJEU's JUDGMENT IN CASE C-646/20: THE BRUSSELS II BIS AND BRUSSELS II TER REGULATIONS AND ARTICLE 27/A OF THE CIVIL REGISTRATION SERVICES ACT
Assoc. Prof. Dr. Azime ARISOY	Burdur Mehmet Akif Ersoy University	THE GREYING OF POVERTY AND THE RISK OF SOCIAL EXCLUSION: A COMPARATIVE ANALYSIS OF THE POPULATION AGED 65 AND OVER IN THE EUROPEAN UNION AND TÜRKIYE
Asst. Prof. Dr. Mehmet BİLGE	Burdur Mehmet Akif Ersoy University	AN EVALUATION OF THE NEW CHILD PROTECTION LAW REGULATION FROM A SOCIAL WORK PERSPECTIVE
Asst. Prof. Dr. Vildan MEYDAN	Hitit University	RECOGNITION AND LEGITIMACY IN TÜRKIYE'S AFRICA POLICY: THE CASE OF THE SOMALIA–ETHIOPIA CRISIS
Lec. Büşra Özdemir	Beykoz University	DARK PATTERN USE ON E-COMMERCE PLATFORMS: A QUALITATIVE CONTENT ANALYSIS FROM A DIGITAL MARKETING PERSPECTIVE
Dr. Sevinç Zeynep KAVRUK	Aydın Adnan Menderes University	SENSORY PROCESSING AND SENSORY SENSITIVITY IN GIFTED INDIVIDUALS: A SYSTEMATIC REVIEW
Research Assistant Dr. Müge PEŞTERE AKÇAY	Pamukkale University	TÜRKIYE İÇIN ZAMANLA DEĞIŞEN BIR PARASAL KOŞULLAR ENDEKSI



HEAD OF SESSION: Prof. Dr. Ananda Majumdar		
Prof. Dr. Ananda Majumdar	Harvard University, USA	THE MOTHER/DAUGHTER DILEMMA: THE FAILURE OF MOTHERHOOD IN WILKIE COLLINS' THE WOMAN IN WHITE
Research Scholar, Mohd Shahbaz Khan Prof. Sameena	Aligarh Muslim University, INDIA	UNDERSTANDING AGEING IN INDIA: SOCIAL CHALLENGES AND CARE NEEDS
Mina Mohammadi	Ahlul Bayt International University, Iran	MATERNAL DISCRIMINATION AND POLICY FRAMEWORKS: A CRITICAL EXAMINATION OF THE MOTHERHOOD PENALTY
Pamilerin Ogundare Julius Ekem Rotimi Samuel Ogundare	Federal University Oye Ekiti, Nigeria Obafemi Awolowo University, Nigeria	SOCIETAL REINTEGRATION OF BRAZILIAN DEPORTEES: OBSTACLES, RESOURCES, AND PATHWAYS TO SUSTAINABLE RETURN
Dr. Ahmadu Sani Gurjiya Emen Essien Udofia	Federal University Gusau, Nigeria	RELATIONSHIP BETWEEN SELF-CONCEPT AND ACADEMIC PERFROMANCE AMONG SECONDARY SCHOOL STUDENTS IN GUSAU LGA, ZAMFARA STATE
Dr. Kehinde AYODELE Prof. P.A. AMOSUN	University of Ibadan, Nigeria	DIAGNO-PRESCRIPTIVE APPROACH IN SOLVING PERCEIVED DIFFICULT CONCEPTS IN GEOGRAPHY: AN EXPERIENCE IN PROBLEM-BASED LEARNING STRATEGY
Hassan BENTALEB	Ibn Tofail University, Morocco	FROM CURRICULUM TO CLASSROOM: IMPLEMENTING ECOLOGICAL CONCEPTS IN LIFE AND EARTH SCIENCES EDUCATION IN MOROCCAN MIDDLE SCHOOLS
Dr. Collens Ikechuwu Odo	Michael Okpara University of Agriculture, Nigeria	EVALUATING PARENTING STYLE INDICATORS AS PREDICTORS OF UNETHICAL BEHAVIOUR AMONG SECONDARY SCHOOL BIOLOGY STUDENTS



HEAD OF SESSION: Moses Adeolu AGOI		
Oluwakemi Racheal OSHINOWO Moses Adeolu AGOI Olayemi Grace ABIMBOLA Emmanuel Taiwo AGOI	Lagos State University of Education, Nigeria Loughborough University, Nigeria	SUSTAINABLE SMART UNIVERSITIES: AN INTERDISCIPLINARY PERSPECTIVE ON ARTIFICIAL INTELLIGENCE, DIGITAL ARCHITECTURE, AND EDUCATIONAL MANAGEMENT
IGE, David Dele Akanbi, Bello Muhammed PhD	University of Abuja, Nigeria	ENHANCEMENT OF THE EXISTING PUBLIC TRANSPORT SYSTEM FOR REAL-TIME BUS SCHEDULING AND PASSENGER DEMAND PREDICTION AT THE UNIVERSITY OF ABUJA
EKENE ERIC NNAEMEKA AKANBI BELLO MUHAMMED PhD	University of Abuja, Nigeria	ENHANCING GENERAL SECURITY AND MINIMIZING PROXY THROUGH RFID EMBEDDED ID CARD IN THE UNIVERSITY OF ABUJA
Akanbi, Bello Muhammed PhD Itua Omonoheromon Precious	University of Abuja, Nigeria	DIGITAL TRANSFORMATION OF RESEARCH JOURNAL MANAGEMENT: DESIGN AND IMPLEMENTATION OF A WEB-BASED JOURNAL MANAGEMENT AND PUBLICATION SYSTEM FOR THE FACULTY OF SCIENCE, UNIVERSITY OF ABUJA
OUKKAS Mebarek	Center University Nour Bachir of El Bayadh, Algeria	INVESTIGATION AND SIMULATION OF INTERFACE DAMAGE IN A HYBRID NANOCOMPOSITE
Joan S. Muñoz Roberto E. Martinez	National University of Colombia, Colombia	HEAVY NEUTRINO PRODUCTION AND LEPTON FLAVOR VIOLATION AT FUTURE e+e− COLLIDERS IN A NON-UNIVERSAL U(1)' MODEL
Mohammed NAJI	Hassan II University, Morocco	METAL HYDRIDES AS PROMISING MATERIALS FOR SAFE AND EFFICIENT HYDROGEN STORAGE: A COMPREHENSIVE REVIEW

DATE	TIME	SESSION
• 01.09.2026 • Online	• 12^{30}–14^{30} • Istanbul Time	• HALL-5 • SESSION-2

HEAD OF SESSION: Major Gheorghe GIURGIU

Hafiz Moahid Ali Imran Hafeez	University of Engineering and Technology, Pakistan	FATIGUE RESPONSE OF HOT MIX ASPHALT (HMA) MODIFIED WITH THE COMBINATION OF STONE DUST AND NANO-CLAY
Salihu SULEIMAN Adamu M. BABAYO	Federal University Birnin Kebbi, Nigeria Abubakar Tafawa Balewa University Bauchi, Nigeria	NATURE-INSPIRED THERMAL ADAPTATION FOR RESIDENTIAL BUILDING ENVELOPES IN NORTH WESTERN NIGERIA: A BIOMIMETIC DESIGN FRAMEWORK
Bendahmane Hasna	Mohammed V University, Morocco	ENSURING CONSISTENCY BETWEEN RASTER MAPS AND DESCRIPTIVE STATISTICS IN REMOTE SENSING: A CONCEPTUAL FRAMEWORK USING INSAR LAND SUBSIDENCE
Olusegun Olukayode Olaleye Emmanuel Okon Wilson	Maritime Academy of Nigeria Akwa Ibom State Polytechnic, Nigeria	AI-DRIVEN QUALITY CONTROL IN MODERN MANUFACTURING SYSTEMS
Olusegun Olukayode Olaleye Emmanuel Okon Wilson	Maritime Academy of Nigeria Akwa Ibom State Polytechnic, Nigeria	SUSTAINABLE MANUFACTURING PRACTICES FOR IMPROVING PRODUCTIVITY AND RESOURCE EFFICIENCY IN DEVELOPING COUNTRIES
Major Gheorghe GIURGIU Prof. dr. med. Manole COJOCARU	Deniplant-Aide Sante Medical Center, Romania Titu Maiorescu University, Romania	WHAT WE KNOW ABOUT PSORIASIS SO FAR?
Sehrish Firyal Bareerah Sohail	University of Veterinary and Animal Sciences, Pakistan	MOLECULAR CHARACTERIZATION OF STAPHYLOCOCCUS AUREUS RECOVERED FROM RAW MEAT
Ph.D. Tran Le Nhat Quang MSc. Le Trong De	University of Danang, Vietnam Vinh Medical University, Vietnam	CURRENT STATUS AND DEVELOPMENT SOLUTIONS FOR ESPORTS AND PHYGITAL SPORTS IN VIETNAM: TOWARD A PROFESSIONAL AND SUSTAINABLE DIGITAL SPORTS ECOSYSTEM

CONTENTS

CONGRESS ID	I
PHOTO GALLERY	II
PROGRAM	III
CONTENT	IV

AUTHOR	TITLE	No
Akanbi, Bello Muhammed Itua Omonoheromon Precious	DIGITAL TRANSFORMATION OF RESEARCH JOURNAL MANAGEMENT: DESIGN AND IMPLEMENTATION OF A WEB-BASED JOURNAL MANAGEMENT AND PUBLICATION SYSTEM FOR THE FACULTY OF SCIENCE, UNIVERSITY OF ABUJA	1
Arous Ali KACI Zakia DAHMENE Thoraya	IMPACT OF FARMING SYSTEMS AND PRACTICES ON THE CULTIVATION OF DURUM WHEAT (TRITICUM DURUM DESF) UNDER SEMI-ARID CONDITIONS IN ALGERIA	2
Aslıhan Hatun ÇAÇAN	LINKING MOLECULAR INTERACTIONS TO THE ACOUSTIC AND CALORIC BEHAVIOR OF REAL GASES	3
Ayşe Güllü Varıcı	3D BIOPRINTING TECHNOLOGY APPROACH IN WOUND DRESSING PRODUCTION	4
Azime ARISOY	THE GREYING OF POVERTY AND THE RISK OF SOCIAL EXCLUSION: A COMPARATIVE ANALYSIS OF THE POPULATION AGED 65 AND OVER IN THE EUROPEAN UNION AND TÜRKİYE	6
Bendahmane Hasna	ENSURING CONSISTENCY BETWEEN RASTER MAPS AND DESCRIPTIVE STATISTICS IN REMOTE SENSING: A CONCEPTUAL FRAMEWORK USING INSAR LAND SUBSIDENCE	8
Büşra Özdemir	E-TİCARET PLATFORMLARINDA KARANLIK TASARIM KULLANIMI: DİJİTAL PAZARLAMA PERSPEKTİFİNDEN NİTEL BİR İÇERİK ANALİZİ	9
Derya Buluç	OSMANLI HATIRA MENDİLLERİNİN BİÇİMSEL VE SÜSLEME ÖZELLİKLERİNİN ANALİZİ	11
EKANEM, MOSES COLUMBA	QUALITY AND NUTRITIONAL CONTENTS OF WATER YAM-COCOYAM COMPOSITE FLOUR SUPPLEMENTED WITH COWPEA FLOUR FOR THE PREPARATION OF EKPANG NKUKWO PREPARATION	13
Elvan KOÇ Bünyamin Çatalca Sibel KAYA	AN ALTERNATIVE TO TRADITIONAL HERBARIUM TECHNIQUES: PRESERVING WILD PLANTS WITH EPOXY RESIN	14
EWETOLA Esther. A ADEKUNLE Adebola B	EFFECT OF SELECTED WEED AND SOIL PHYSICAL AND CHEMICAL PROPERTIES ON CARBON SEQUESTRATION	16
Farrukh Mahfooz	IMPACT OF RECURRING FLOODS ON ENVIRONMENT, HUMAN HEALTH, AND SUPPLY CHAIN DISRUPTION: EVIDENCE FROM PAKISTAN	17
Fatematuz Zohora	CARBON ACCOUNTING, CORPORATE GOVERNANCE AND CORPORATE CARBON PERFORMANCE: EVIDENCE FROM BANGLADESH	18

Gheorghe GIURGIU Manole COJOCARU	WHAT WE KNOW ABOUT PSORIASIS SO FAR?	19
Hassan BENTALEB	FROM CURRICULUM TO CLASSROOM: IMPLEMENTING ECOLOGICAL CONCEPTS IN LIFE AND EARTH SCIENCES EDUCATION IN MOROCCAN MIDDLE SCHOOLS.	20
IGE, David Dele Akanbi, Bello Muhammed	ENHANCEMENT OF THE EXISTING PUBLIC TRANSPORT SYSTEM FOR REAL-TIME BUS SCHEDULING AND PASSENGER DEMAND PREDICTION AT THE UNIVERSITY OF ABUJA	21
İrem KESKİN Burcu ARSLAN Aylin RAZLIKLI Özge KARATAŞ	SYNTHESIS AND CHARACTERIZATION OF SODIUM BENZOATE AND POTASSIUM SORBATE AND EVALUATION OF THEIR PRESERVATIVE EFFICACY IN A LIQUID SOAP FORMULATION	22
KOCHUBEY Alexander MAKAROVA-KOROBEYNIKOVA Ekaterina Petrovna	INNOVATIVE APPROACHES TO AUTOMATING BUSINESS PROCESSES OF CUSTOMS AUTHORITIES BASED ON ADVANCED TECHNOLOGIES	25
Kristal Hykaj Ardita Hykaj	THE IMPACT OF THE COVID-19 PANDEMIC ON THE ALBANIAN BANKING SECTOR PERFORMANCE: AN ECONOMETRIC ANALYSIS (2015–2020)	26
Makarova-Korobeynikova Ekaterina Petrovna Sulaimanova Sabina	POSSIBILITIES OF INCLUDING A NEURAL NETWORK IN THE WORK OF THE CUSTOMS SERVICE WHEN INSURING INTELLECTUAL PROPERTY ASSETS	27
Mehmet BİLGE	AN EVALUATION OF THE NEW CHILD PROTECTION LAW REGULATION FROM A SOCIAL WORK PERSPECTIVE	28
Mina Mohammadi	MATERNAL DISCRIMINATION AND POLICY FRAMEWORKS: A CRITICAL EXAMINATION OF THE MOTHERHOOD PENALTY	30
Mohammed NAJI	METAL HYDRIDES AS PROMISING MATERIALS FOR SAFE AND EFFICIENT HYDROGEN STORAGE: A COMPREHENSIVE REVIEW	31
Mohd Shahbaz Khan Sameena	UNDERSTANDING AGEING IN INDIA: SOCIAL CHALLENGES AND CARE NEEDS	32
Muhammad Imran	BIOACTIVE COMPOUNDS AND HEALTH BENEFITS OF PEACH FRUIT (PRUNUS PERSICA)	33
Mustafa Kahraman Murat Beğenik	ACUTE CARDIOVASCULAR RESPONSES TO SOLEUS PUSH-UP EXERCISE DURING AN ORAL GLUCOSE TOLERANCE TEST	34
Müge Pestere-Akcay	TÜRKİYE İÇİN ZAMANLA DEĞİŞEN BİR PARASAL KOŞULLAR ENDEKSİ	35
Mürşit AKSOY	THE ROLE OF CORRECTIVE EXERCISES IN PREVENTING SPORTS INJURIES AND EXAMPLES OF POPULAR EXERCISE PRACTICES.	37
Nalan Cavlak Adsız İlhami Adsız	ACİL SERVİSE BAŞVURAN E-SCOOTER KAZALARININ İNCELENMESİ	39
Olusegun Olukayode Olaleye Emmanuel Okon Wilson	SUSTAINABLE MANUFACTURING PRACTICES FOR IMPROVING PRODUCTIVITY AND RESOURCE EFFICIENCY IN DEVELOPING COUNTRIES	41
Oluwafunmilayo Caroline OYENIYI	DIGITAL FINANCIAL INCLUSION AND TAX REVENUE PERFORMANCE IN NIGERIA	42
Orji, Jephter Ebuka	SOIL MANAGEMENT PRACTICES FOR MITIGATION OF THE EFFECT CLIMATE CHANGE IN THE TROPICS	43

OUKKAS Mebarek	INVESTIGATION AND SIMULATION OF INTERFACE DAMAGE IN A HYBRID NANOCOMPOSITE	44
Özge DEMİRDELEN	THE CONCEPT OF "JUDGMENT" IN EXTRAJUDICIAL FOREIGN DIVORCES IN LIGHT OF THE CJEU'S JUDGMENT IN CASE C-646/20: THE BRUSSELS II BIS AND BRUSSELS II TER REGULATIONS AND ARTICLE 27/A OF THE CIVIL REGISTRATION SERVICES ACT	45
Pamilerin Ogundare Julius Ekem Rotimi Samuel Ogundare	SOCIETAL REINTEGRATION OF BRAZILIAN DEPORTEES: OBSTACLES, RESOURCES, AND PATHWAYS TO SUSTAINABLE RETURN	47
Rusli Sri Mulyani	THE ROLE OF HUMAN RESOURCE COMPETENCIES IN SUPPORTING UNIVERSITY QUALITY ASSURANCE AND ACCREDITATION	48
Said ELANZAOUI	A GREEN MAGNETIC ACTIVATED CARBON FOR EFFICIENT CRYSTAL VIOLET REMOVAL	49
Seda Erdoğan	ÜRETKEN YAPAY ZEKÂ İLE KAMUSAL MEKÂNLARIN MEKÂNSAL İYİLEŞTİRİLMESİ: MAÇKA DEMOKRASİ PARKI ÖRNEĞİ	50
Sehrish Firyal Bareerah Sohail	MOLECULAR CHARACTERIZATION OF *STAPHYLOCOCCUS AUREUS* RECOVERED FROM RAW MEAT	52
Sevinç Zeynep KAVRUK	SENSORY PROCESSING AND SENSORY SENSITIVITY IN GIFTED INDIVIDUALS: A SYSTEMATIC REVIEW	53
Shoaib Ahsan Shah	UAV-BASED ODOR SOURCE LOCALIZATION USING DEEP REINFORCEMENT LEARNING IN OUTDOOR ENVIRONMENT	55
Sinan Keyinci	EFFECT OF TESLA VALVE DISTRIBUTION ON THE THERMO-HYDRAULIC PERFORMANCE OF A LIQUID-COOLED BATTERY THERMAL MANAGEMENT SYSTEM	56
Şakir DENİZ	AN ANALYSIS OF THE METHODOLOGY OF COMMENTING ON A SINGLE HADITH, FOCUSING ON ABU SHAMA AL-MAKDISI'S WORK TITLED "SHARH AL-HADITH AL-MUKHTAFA FI MAB'AS AL-NABIY AL-MUSTAFA"	58
Ahmadu Sani Gurjiya Emen Essien Udofia	RELATIONSHIP BETWEEN SELF-CONCEPT AND ACADEMIC PERFROMANCE AMONG SECONDARY SCHOOL STUDENTS IN GUSAU LGA, ZAMFARA STATE	60
Ahmet DİNÇ Ahmet Nusret BULGURCUOĞLU	MANAGEMENT OF DUAL CAREER AND ATHLETIC CAREER TRANSITIONS: A WEB OF SCIENCE-BASED BIBLIOMETRIC NETWORK ANALYSIS	69
Ananda Majumdar	THE MOTHER/DAUGHTER DILEMMA: THE FAILURE OF MOTHERHOOD IN WILKIE COLLINS' THE WOMAN IN WHITE	81
Barış ERKUŞ Doğukan AYHAN	A REVIEW OF VIBRATION-BASED FAULT DIAGNOSIS METHODS FOR INTERNAL COMBUSTION ENGINES: SIGNAL PROCESSING TECHNIQUES AND MACHINE LEARNING APPROACHES	91
Batuhan DELEN Gündüz Ercan KUTLUAY	SCOPE, READABILITY, AND EMERGENCY WARNING INFORMATION IN TURKISH ONLINE PATIENT EDUCATION CONTENT ON PEDIATRIC SUPRACONDYLAR HUMERUS AND ELBOW FRACTURES	103

Canan BAĞCI TAN Özden ÖZGÜN ACAR Aslı KIRIKBAKAN	PYRROLOQUINOLINE QUINONE MODULATES ALZHEIMER'S DISEASE-RELATED GENE EXPRESSION IN SH-SY5Y CELLS	112
Cemal BUDAĞ Ömer ATIŞ	KENTSEL EKOSİSTEMDE KÖPEK POPÜLASYONU: KONTROL STRATEJİLERİ VE BESLENME	121
Collens Ikechuwu Odo	EVALUATING PARENTING STYLE INDICATORS AS PREDICTORS OF UNETHICAL BEHAVIOUR AMONG SECONDARY SCHOOL BIOLOGY STUDENTS	137
Doğan Barış KILINÇ	SOCRATES' DEATH AS AN EXAMPLE OF TRAGEDY	148
EKENE ERIC NNAEMEKA AKANBI BELLO MUHAMMED	ENHANCING GENERAL SECURITY AND MINIMIZING PROXY THROUGH RFID EMBEDDED ID CARD IN THE UNIVERSITY OF ABUJA	155
Elif AKSEN Gülbin ÖZÇELİKAY	A STUDY ON THE PRACTİCES OF PRODUCT DİSPLAY AND MERCHANDİSİNG İN COMMUNİTY PHARMACİES	161
Emrah GÖKKAYA Fatih DENİZLİ Ömer DEMİRBİLEK	LEADERSHIP COMPETENCIES IN DISASTER AND CRISIS MANAGEMENT: CURRENT TRENDS AND FUTURE PERSPECTIVES	166
Girne Gül ÇELEBİ ULUÇAY Güzin KAYA	SPATIAL PATTERNS OF POPULATION DENSITY INCREASE IN THE LAKE VAN BASIN: THE CASE OF EDREMİT, İPEKYOLU, AND TUŞBA	189
Gozde YALCIN OZKAT Erkan Caner OZKAT	CLASS IMBALANCE IN TOXICITY PREDICTION: THE EFFECT OF PERFORMANCE METRIC AND DECISION THRESHOLD SELECTION ON MODEL RANKING IN THE TOX21 DATASET	197
Gökberk GÖKÇEK Yusuf Tuna BİRER Veysel Karani YILMAZ Sezer SAĞLAM Rıfat AKGÜL Ahmet AVCI	DEVELOPMENT OF A VEHICLE-INDEPENDENT E/E SIMULATION PLATFORM AND ITS APPLICATION IN ECU VALIDATION PROCESSES	207
Hafiz Moahid Ali Imran Hafeez	FATIGUE RESPONSE OF HOT MIX ASPHALT (HMA) MODIFIED WITH THE COMBINATION OF STONE DUST AND NANO-CLAY	214
Halim YAR	GULSHENĪ-İ SARUKHĀNĪ'S WORK TITLED SA'DNĀME [ATTRIBUTED TO KHAYĀLĪ-İ GULSHENĪ IN THE LIBRARY RECORD	228
Joan S. Muñoz Roberto E. Martinez	HEAVY NEUTRINO PRODUCTION AND LEPTON FLAVOR VIOLATION AT $e+e-$ COLLIDERS IN A NON-UNIVERSAL $U(1)'$ MODEL	248
K.A. Ayodele P.A. Amosun	DIAGNO-PRESCRIPTIVE APPROACH IN SOLVING PERCEIVED DIFFICULT CONCEPTS IN GEOGRAPHY: AN EXPERIENCE IN PROBLEM-BASED LEARNING STRATEGY	254
Melek COŞGUN SOLAK	RELIGIOUS EXPERIENCE IN THE AGE OF SOCIAL ACCELERATION: A SOCIOLOGICAL INQUIRY INTO TIME AND MEANING	264
Muhammed Emin Şimşek	İNGİLTERE'DEKİ MÜSLÜMAN OKUL ÖNCESİ EĞİTİM KURUMLARINDA DİN EĞİTİMİ: AMAÇ, MUHTEVA VE UYGULAMALAR	277
Nguyen Thanh Tuan	BANQUE DE L'INDOCHINE AND CURRENCY ISSUANCE IN FRENCH INDOCHINA (1875–1930)	287
Olusegun Olukayode Olaleye Emmanuel Okon Wilson	AI-DRIVEN QUALITY CONTROL IN MODERN MANUFACTURING SYSTEMS	301

Oluwakemi Racheal OSHINOWO Moses Adeolu AGOI Olayemi Grace ABIMBOLA Emmanuel Taiwo AGOI	SUSTAINABLE SMART UNIVERSITIES: AN INTERDISCIPLINARY PERSPECTIVE ON ARTIFICIAL INTELLIGENCE, DIGITAL ARCHITECTURE, AND EDUCATIONAL MANAGEMENT	309
Ramazan KARA Volkan YAMAÇLI	AFET SONRASI İHA GÖRÜNTÜLERİNDE İNSAN TESPİTİ İÇİN GÜNCEL YOLO MİMARİLERİNİN KARŞILAŞTIRMALI PERFORMANS ANALİZİ	321
Recep ÇELİK	KLASİK TÜRK EDEBİYATINDA "EHL-İ SÜHAN": TÜRKÇENİN TARİHÎ SÖZ VARLIĞINDA ANLAM VE KULLANIM ALANLARI	328
S.Praveenkumar S.Chandrasekar	INTEGRATED E-WALLET ACCOUNTING: FORMALIZING INFORMAL BUSINESSES FOR VIKSIT BHARAT 2047	341
Salihu SULEIMAN Adamu M. BABAYO	NATURE-INSPIRED THERMAL ADAPTATION FOR RESIDENTIAL BUILDING ENVELOPES IN NORTH WESTERN NIGERIA: A BIOMIMETIC DESIGN FRAMEWORK	346
Tran Le Nhat Quang Le Trong De	CURRENT STATUS AND DEVELOPMENT SOLUTIONS FOR ESPORTS AND PHYGITAL SPORTS IN VIETNAM: TOWARD A PROFESSIONAL AND SUSTAINABLE DIGITAL SPORTS ECOSYSTEM	350
Vildan MEYDAN	RECOGNITION AND LEGITIMACY IN TURKIYE'S AFRICA POLICY: THE CASE OF THE SOMALIA–ETHIOPIA CRISIS	358
Yasemin MÜMİNOĞLU	THE USE OF PLANTS IN PRIMARY SCHOOL GARDENS AND THEIR IMPORTANCE IN CHILD DEVELOPMENT	366
Yener TOP	AN ANALYSIS OF THE TURKISH FURNITURE SECTOR REGARDING GREENWASHING: A CASE STUDY OF LARGE-SCALE ENTERPRISES	377
TETEREV Daniil MAKAROVA-KOROBEYNIKOVA Ekaterina Petrovna	THE CURRENT STATE OF INTERACTION BETWEEN CUSTOMS AUTHORITIES AND BUSINESS STRUCTURES	386
Utku Bulut SIMSEK	ENGINEERING MICRO SIZED NH2 FUNCTIONALIZED BIMETALLIC MOFS VIA SUPERCRITICAL CO2 FOR EFFICIENT CARBON CAPTURE	387
Banu Baş Dilara Usta	EFFECTS OF VESTIBULAR REHABILITATION ON SPATIAL ORIENTATION, SPATIAL COGNITION, AND BALANCE PERFORMANCE: A SYSTEMATIC REVIEW	389

CLASS IMBALANCE IN TOXICITY PREDICTION: THE EFFECT OF PERFORMANCE METRIC AND DECISION THRESHOLD SELECTION ON MODEL RANKING IN THE TOX21 DATASET

Gozde YALCIN OZKAT

Recep Tayyip Erdogan University, Faculty of Engineering and Architecture, Department of Bioengineering, Rize, Turkey.

ORCID NO: 0000-0002-9689-2239

Erkan Caner OZKAT

Recep Tayyip Erdogan University, Faculty of Engineering and Architecture, Department of Mechanical Engineering, Rize, Turkey.

ORCID NO: 0000-0003-0530-5439

ABSTRACT

Machine learning models for toxicity prediction are usually reported with a single performance metric, most often the area under the receiver operating characteristic curve (AUROC). Toxicology datasets, however, are severely imbalanced, and as the positive class becomes rarer AUROC reflects the quality of the decisions a model would make in practice ever more weakly. In this study, 12 assays from the Tox21 screening programme, accessed through the Therapeutics Data Commons, were examined across an imbalance range in which the positive class accounts for 2.9% to 16.2% of the molecules. Two split protocols, five random seeds, two molecular representations and four learning algorithms were fully crossed, giving 960 independently trained models, each evaluated both with threshold-free metrics and with a decision threshold selected on a validation partition. The results show that the choice of metric changes the ranking of models: the configuration selected by AUROC is also the best configuration under the prevalence-aware metric in only 61.7% of the blocks. Leaving the decision threshold at its default value of 0.5 costs on average 0.024 units of the Matthews correlation coefficient: that threshold recovers only 52.4% of the positive molecules an assay actually contains. The size of the gain is governed not by the positive class rate but by how far a model's probabilities are displaced relative to the default cut-off. We therefore recommend that toxicity prediction studies report a prevalence-aware metric alongside AUROC, together with a tuned decision threshold and a multi-seed evaluation.

Keywords: Toxicity prediction, class imbalance, model evaluation, decision threshold, Tox21.

INTRODUCTION

Toxicity is one of the principal reasons why drug candidates are withdrawn during development, and because these failures often occur at a late stage they are costly in both time and expenditure. Predicting toxic effects computationally, and early, has therefore been a long-standing objective. The Tox21 screening programme opened this field to data-driven work by releasing the results of screening more than ten thousand compounds against a panel of nuclear receptor and stress response pathways (Huang et al., 2016; Richard et al., 2021). The Tox21 Data Challenge organised within the programme demonstrated the usefulness of deep learning for toxicity prediction (Mayr et al., 2016), and the dataset has since become a

standard benchmark for molecular machine learning (Wu et al., 2018). Comparative studies on these collections have also shown that descriptor-based models remain competitive with graph neural networks on datasets of moderate size (Jiang et al., 2021).

The standardisation of datasets has not been matched by a standardisation of evaluation practice. In the molecular machine learning literature the performance of a model is usually reported from a single split, a single molecular representation and a single metric, and that metric is most often the area under the receiver operating characteristic curve (AUROC). AUROC is a ranking measure that is invariant to class prevalence, and when the positive class is rare it can give a misleadingly favourable impression of the decisions a model would actually make. This limitation has been examined in detail in the statistical learning literature: the precision-recall curve has been shown to be more informative on imbalanced datasets (Davis and Goadrich, 2006; Saito and Rehmsmeier, 2015), and the Matthews correlation coefficient (MCC) has been shown to be preferable to accuracy and to the F1 score in binary classification (Chicco and Jurman, 2020). Reporting such measures alongside AUROC has nevertheless not become common practice in toxicity prediction.

A second problem, closely related to the first, is the choice of the decision threshold. A model reported with threshold-free metrics must still produce a classification decision in practice, and that decision is taken by default at a probability cut-off of 0.5. In an assay where the positive class accounts for a few per cent of the molecules, this cut-off can leave a model flagging almost nothing as positive; such a model may report a high AUROC and still be unusable for screening. Selecting the threshold on a separate validation partition is a well-established remedy (Provost and Fawcett, 2001), but how much difference this step makes in the context of toxicity prediction has not been measured systematically.

The extent to which evaluation practice determines reported results is receiving increasing attention in machine-learning-based science generally (Kapoor and Narayanan, 2023). In the molecular domain the discussion has largely been conducted in terms of the data splitting protocol: splitting by Bemis-Murcko scaffold (Bemis and Murcko, 1996) has been recommended because it yields a more realistic estimate of prospective performance than random splitting (Sheridan, 2013), and evaluations that withhold structurally novel chemistry have been shown to expose weaknesses that random benchmarks conceal (van Tilborg et al., 2022); see also Walters and Barzilay (2021) for a critical assessment of evaluation practice in the field. What has not been measured directly is how far the choice of metric and threshold changes which model 'wins' on one and the same dataset.

This study provides that measurement. Twelve assays from the Tox21 programme were examined in a fully crossed design of two split protocols, five random seeds, two molecular representations and four learning algorithms, giving 960 independently trained models. The design is treated as an experiment rather than as a leaderboard, which allows a variance share and a significance test to be attached to each factor. The contribution can be stated under three headings: (i) measuring how often the choice of metric changes the ranking of models, (ii) showing how the gain from tuning the decision threshold relates to class imbalance, and (iii) comparing both effects with the effect of the splitting protocol, which is more widely discussed in the literature.

MATERIALS AND METHODS

Dataset

Twelve assays from the Tox21 screening programme were used. The data were obtained through the Therapeutics Data Commons, which collects machine learning datasets for therapeutic science behind a single interface (Huang et al., 2022). The assays contain between

5810 and 7265 molecules and are all binary classification tasks. Molecular structures were taken in SMILES form, duplicate structures were removed, and no curation was applied beyond that of the source collection. The sizes, positive class rates and scaffold novelty of the assays are given in Table 1.

Molecular Representations and Learning Algorithms

Two fixed molecular representations were compared. ECFP4 is a 1024-bit Morgan fingerprint of radius 2 (Rogers and Hahn, 2010). PHYSCHEM concatenates 209 RDKit two-dimensional descriptors with the 167 MACCS keys, giving a 376-dimensional descriptor block. Non-finite descriptor values were set to zero, and features were standardised on the training partition for the scale-sensitive algorithms. Four algorithms were used: L2-regularised logistic regression (LINEAR), a random forest of 300 trees (RF; Breiman, 2001), gradient-boosted trees with 400 estimators (XGB; Friedman, 2001; Chen and Guestrin, 2016), and a single-hidden-layer network of 256 units with early stopping (MLP). Implementations were scikit-learn (Pedregosa et al., 2011) and XGBoost, and hyperparameters were fixed in advance and were identical across all assays, splits and seeds. This is not a shortcut but a requirement of the design: tuning per cell would confound the factor effects with the tuning budget.

Splitting Protocols

Each assay was partitioned 70% training, 10% validation and 20% test under two protocols. The random protocol assigns molecules uniformly at random; the scaffold protocol keeps molecules sharing a Bemis-Murcko scaffold (Bemis and Murcko, 1996) together, so that no scaffold can occur on both the training and the test side. The validation partition was never used for fitting and was reserved solely for selecting the decision threshold. Every split was repeated with five different random seeds.

Performance Metrics and Decision Threshold

AUROC and average precision were computed as threshold-free metrics. Because the expected average precision of a random classifier equals the positive class rate, a prevalence-normalised form was used so that assays of different prevalence remain comparable: AUPRC_norm = (AP - y) / (1 - y), where y is the positive class rate in the test partition. As threshold-dependent metrics, the Matthews correlation coefficient (Matthews, 1975; Chicco and Jurman, 2020), the F1 score and balanced accuracy were each reported in two forms: at the default cut-off of 0.5, and at the cut-off that maximises MCC on the validation partition. In the second case the threshold is selected from validation data alone and the test partition is never inspected, so the resulting decision rule is out of sample.

Statistical Analysis

The design comprises 12 assays x 2 split protocols x 5 seeds x 2 representations x 4 algorithms = 960 independently trained models. Factor effects were tested over blocks formed by the remaining factors, using the Friedman test for factors with three or more levels and the paired Wilcoxon signed-rank test for the two-level factor; pairwise comparisons were then made with Wilcoxon signed-rank tests and Holm correction. Variance shares were computed within each assay as the between-level sum of squares divided by the total sum of squares, and then averaged over assays. Agreement between metric rankings was assessed with the Spearman rank correlation. The analyses were carried out in Python 3 using RDKit (Landrum, 2024), scikit-learn, XGBoost, SciPy and pandas.

RESEARCH AND FINDINGS

The Imbalance Structure of the Assays

Table 1 summarises the size and imbalance structure of the twelve assays. The positive class rate ranges from 2.9% (NR-PPAR-gamma) to 16.2% (SR-ARE), with a corresponding negative-to-positive ratio of up to 33.7. In the sparsest assay the test partition retains on average only 38 positive molecules, a quantity that directly bounds the sensitivity of any performance estimate. Under the scaffold protocol every test molecule carries a Bemis-Murcko scaffold unseen in training, as intended. Even under the random protocol this fraction lies between 23.2% and 25.9%, because most scaffolds in these datasets occur only once. Random splitting is therefore not the permissive evaluation setting it is often assumed to be.

Table 1. Size and imbalance structure of the Tox21 assays. The last column is the fraction of test molecules whose scaffold is absent from training.

Assay	n	Pos. rate (%)	Imbalance	Test pos.	Unseen scaf. (random, %)
NR-PPAR-gamma	6450	2.9	33.7	38	23.6
NR-AR-LBD	6758	3.5	27.5	45	25.0
SR-ATAD5	7072	3.7	25.8	54	24.6
NR-AR	7265	4.3	22.5	61	25.9
NR-ER-LBD	6955	5.0	18.9	71	24.6
NR-Aromatase	5821	5.2	18.4	59	23.9
SR-HSE	6467	5.8	16.4	75	24.3
SR-p53	6774	6.2	15.0	87	24.9
NR-AhR	6549	11.7	7.5	155	25.0
NR-ER	6193	12.8	6.8	161	24.1
SR-MMP	5810	15.8	5.3	183	24.9
SR-ARE	5832	16.2	5.2	184	23.2

Effect of Metric Choice on Model Ranking

Within every (assay, split protocol, seed) block the eight configurations formed by two representations and four algorithms were ranked by AUROC and by prevalence-normalised average precision, and the two rankings were compared. Across all 120 blocks the two metrics place the same configuration first in only 61.7% of cases. The rankings are not unrelated: the mean Spearman rank correlation is 0.842. What matters in practice, however, is the top of the ranking. The cost of selecting on AUROC, measured against the best configuration under the prevalence-aware metric, averages 0.012 units, but exceeds 0.02 units in 20.0% of blocks and reaches 0.118 units at worst.

Agreement varies strongly between assays (Table 2). It reaches 90% on SR-MMP but falls to 0% on SR-ATAD5, where the two metrics never select the same configuration in any block. The same pattern appears at the level of individual algorithms: the difference between the random forest and gradient boosting is not significant under AUROC ($p = 0.187$) but becomes significant under the prevalence-aware metric ($p = 0.005$). Which algorithm is judged superior therefore depends directly on the metric that is reported.

Table 2. Effect of metric choice on model ranking. Agreement is the fraction of blocks in which the AUROC-best configuration is also best under the prevalence-aware metric; regret is the cost of that choice in AUPRC_norm units.

Assay	Agreement	Spearman	Regret (AUPRC_norm)
SR-ATAD5	0%	0.729	0.048
NR-AR-LBD	20%	0.571	0.045
NR-ER	50%	0.886	0.008
NR-AhR	70%	0.924	0.005
NR-Aromatase	70%	0.795	0.003
NR-ER-LBD	70%	0.774	0.003
NR-PPAR-gamma	70%	0.829	0.016
SR-ARE	70%	0.943	0.001
SR-HSE	70%	0.919	0.010
NR-AR	80%	0.855	0.001
SR-p53	80%	0.933	0.005
SR-MMP	90%	0.952	0.001

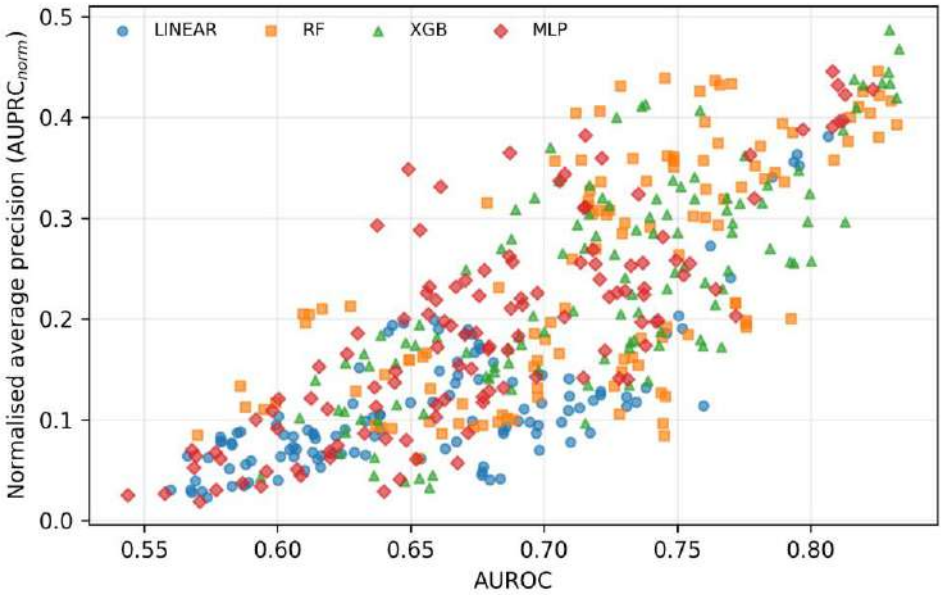


Figure 1. AUROC and normalised average precision for every model under the scaffold split. The wide range of AUPRC_norm values at a given AUROC shows that the two metrics do not carry the same information.

Effect of Decision Threshold Selection

Threshold-dependent metrics improve markedly when the cut-off is selected on the validation partition rather than left at 0.5. Mean MCC rises from 0.296 to 0.320 (0.024 units) and mean F1 from 0.301 to 0.357 (0.056 units); the improvement is significant in a paired test ($p < 0.001$) and is observed in 60.1% of models. The selected thresholds average 0.36, well below the default value.

The source of this gain is that on imbalanced data the default cut-off systematically under-represents the positive class. At a threshold of 0.5 the models flag on average 4.7% of test molecules as positive, whereas the true positive rate is 8.9%; in other words the default cut-off recovers only 52.4% of the expected number of positives. 88.1% of models are biased in this

direction. Tuning the threshold raises this figure to 106.4%, and a significant relationship emerges between the threshold-induced deficit and the gain in MCC (Spearman rho = 0.34, $p < 0.001$).

The magnitude of the gain is not, however, explained by the positive class rate, contrary to intuition: at assay level the rank correlation between MCC gain and positive class rate is not significant (rho = 0.16, p = 0.618). As Figure 2 shows, the largest gains are obtained not in the assays with the rarest positive class but in those where the model's probability outputs are displaced furthest relative to the default cut-off (NR-PPAR-gamma, SR-ATAD5). In some assays the gain is close to zero or even slightly negative, which shows that a threshold chosen on the validation partition does not always transfer equally well to the test partition, and serves as a reminder that with a sparse positive class the threshold selection step is itself a source of uncertainty.

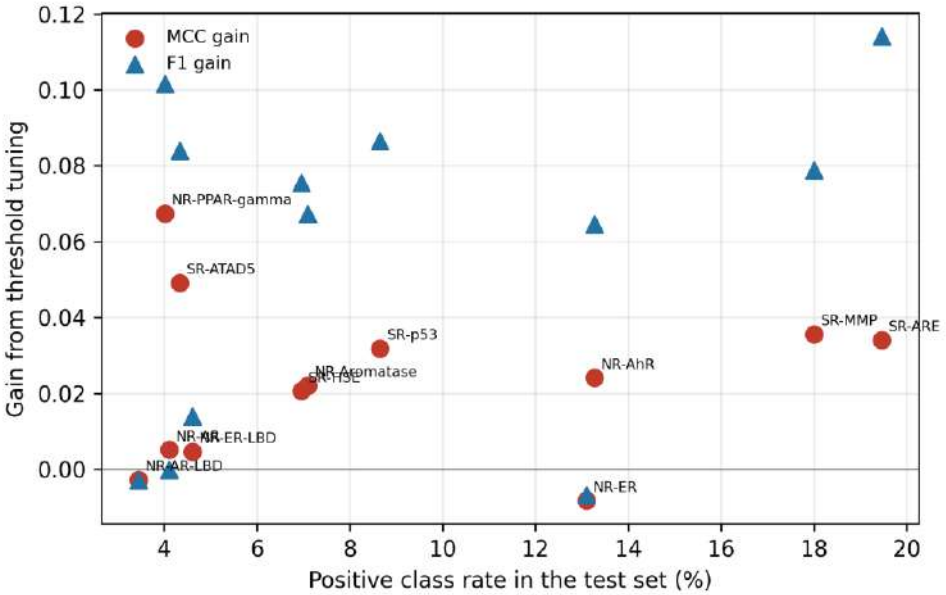


Figure 2. Gain in MCC and F1 from decision threshold tuning, by assay. The gain is not a monotonic function of the positive class rate.

Table 3. Performance at the default and at the tuned decision threshold. The last column is the mean of the thresholds selected on the validation partition.

Assay	Pos. rate (%)	MCC (0.5)	MCC (tuned)	F1 (0.5)	F1 (tuned)	Thr.
NR-AR-LBD	3.5	0.496	0.493	0.491	0.488	0.53
NR-PPAR-gamma	4.0	0.144	0.212	0.121	0.223	0.24
NR-AR	4.1	0.455	0.460	0.446	0.446	0.60
SR-ATAD5	4.3	0.158	0.207	0.137	0.221	0.22
NR-ER-LBD	4.6	0.369	0.373	0.353	0.367	0.47
SR-HSE	7.0	0.187	0.208	0.166	0.242	0.24
NR-Aromatase	7.1	0.224	0.246	0.212	0.280	0.29
SR-p53	8.7	0.218	0.249	0.207	0.293	0.29
NR-ER	13.1	0.275	0.267	0.300	0.294	0.52
NR-AhR	13.3	0.376	0.400	0.406	0.470	0.35
SR-MMP	18.0	0.407	0.443	0.464	0.543	0.31
SR-ARE	19.5	0.249	0.283	0.303	0.418	0.30

Effect of Representation, Algorithm and Splitting Protocol

At the level of molecular representation the descriptor block outperforms the fingerprint under both metrics (Table 4): mean AUROC 0.727 against 0.663, a median difference of 0.067 ($p < 0.001$). Among the algorithms the random forest and gradient boosting are clearly ahead, both beating the linear model and the neural network by significant margins. That the network remains only somewhat above the linear model on these datasets is a consequence of the fixed hyperparameter design, and shows that the advantage of deeper models does not appear of its own accord when no tuning is performed.

Table 4. Marginal effect of representation and algorithm under the scaffold split. Win rate is the fraction of blocks in which a level is best within its factor.

Factor	Level	AUROC	Win rate	AUPRC_norm	Win rate
Representation	ECFP4	0.663	7%	0.161	8%
Representation	PHYSCHEM	0.727	93%	0.235	92%
Algorithm	LINEAR	0.656	4%	0.112	0%
Algorithm	MLP	0.680	3%	0.192	6%
Algorithm	RF	0.722	54%	0.250	62%
Algorithm	XGB	0.721	38%	0.238	32%

The splitting protocol is the single strongest factor on these datasets. Over 480 matched triples the random split yields a median AUROC 0.107 units higher than the scaffold split, an advantage observed in 98.1% of pairs ($p < 0.001$). The penalty is larger still under the prevalence-aware metric (0.190 units), which indicates that what is lost when moving to structurally novel chemistry is the ability to capture the sparse positive class rather than ranking power as such. The distribution of within-assay variance tells the same story: the splitting protocol accounts for 49.9%, the representation 19.0%, the algorithm 17.9% and the random seed 2.1%. The small share of the seed does not, however, mean that results can safely be reported from a single seed: in 70.8% of (assay, protocol) cells the winning configuration changes with the seed, and the seed-to-seed range of the best score reaches a

median of 0.030 units, which is of the same order as differences routinely treated as meaningful in the literature.

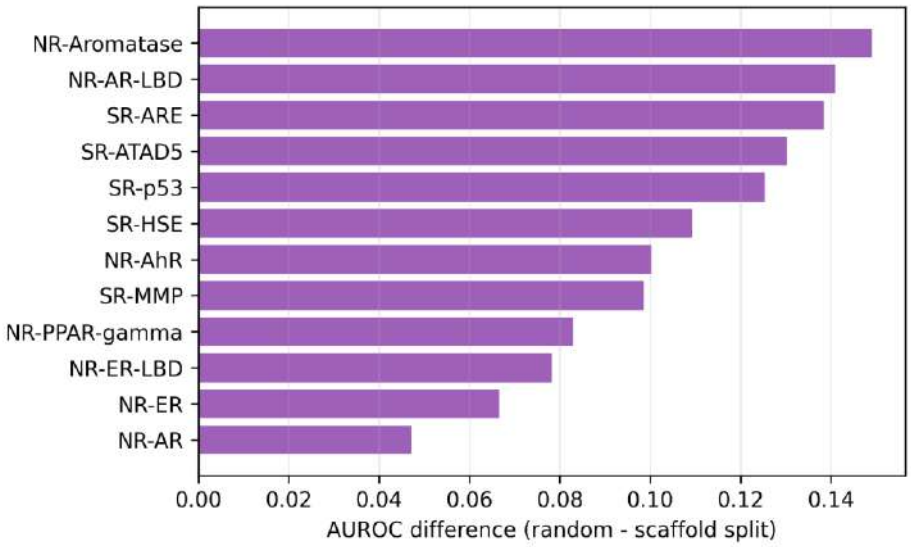


Figure 3. Splitting protocol penalty by assay (random-split AUROC minus scaffold-split AUROC).

CONCLUSION

In this study twelve assays from the Tox21 screening programme were examined through 960 independently trained models in a fully crossed design, in order to measure how far evaluation decisions determine reported results. The findings fall under three headings.

First, the choice of performance metric changes the ranking of models. The configuration selected by AUROC coincides with the best configuration under the prevalence-aware metric in only 61.7% of blocks, and in some assays the two metrics never agree. That the difference between the random forest and gradient boosting is not significant under AUROC yet is significant under the prevalence-aware metric is a concrete instance of this.

Second, leaving the decision threshold at its default value carries a systematic cost on imbalanced data. The default cut-off recovers on average 52.4% of the expected number of positives, whereas a threshold selected on the validation partition gains 0.024 units of MCC and 0.056 units of F1. This gain is not a monotonic function of the positive class rate, however; what governs it is how far the model's probabilities are displaced relative to the default cut-off. Threshold selection is therefore not a setting that can be anticipated from the imbalance level of a dataset, but a step that must be carried out separately for each model.

Third, these two effects are not negligible beside the effect of the splitting protocol, which is more widely discussed in the literature. Moving to a scaffold split costs a median of 0.107 AUROC units, and the protocol explains 49.9% of within-assay variance. The choice of metric and threshold does not remove this effect, but it changes which model is selected within a given split. In addition, the fact that the winning configuration changes with the seed in 70.8% of cells shows that single-seed reporting is not reliable on these datasets.

In the light of these findings, the following are proposed as a minimum reporting standard for toxicity prediction studies: (i) at least one prevalence-aware metric (normalised average

precision or MCC) should be given alongside AUROC; (ii) where a classification decision is reported, the decision threshold should be selected on a separate validation partition and the selected threshold should be stated; (iii) results should be produced with multiple seeds and presented with a dispersion estimate; and (iv) scaffold-split results should be reported alongside random-split results. The limitations of the study include the use of fixed hyperparameters, five seeds and only two molecular representations. These were deliberate choices made to prevent factor effects from becoming confounded; extending the same framework to learned representations such as graph neural networks, and to the tuning budget itself, is a natural continuation of this work.

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