TURKISH CHEMISTS' SOCIETY

12. INTERNATIONAL DRUG CHEMISTRY CONFERENCE

MARCH 07 – MARCH 10, 2024

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Dear colleagues,

We cordially invite you to attend the The Drug Chemistry Congress on March 7-10, 2024 in Antalya, Turkey.

The Drug Chemistry Congress, organized annually by The Turkish Chemists Society for over a decade, has established itself as an institutional event that has been held in person every year without interruption.

With an increasing number of attendees each year and our international format, the conference has become a highly sought after premier event in the scientific community in Turkey and has been rapidly progressing towards becoming an international brand.

In collaboration with The Turkish Chemists Society, Atatürk University, and Gebze Technical University, the "12th International Drug Chemistry Congress" will be held from March 7 to 10, 2024, in Antalya, Turkey.

The scientific program includes invited talks, oral presentations, short oral presentations, poster presentations, and workshop sessions. Short oral presentations will also be displayed as posters, fostering extended discussions with a larger number of participants over an extended period.

Poster presentations will be showcased for a total of four hours over two days during the congress, with the top 10 posters receiving awards. Participants will have the opportunity to publish their work as "Full Text" after the evaluation by the Scientific Committee.

The conference aims to:

1. Bring together all stakeholders in the pharmaceutical field
2. Facilitate collaborations between industry, the public sector, and academia
3. Strengthen university-industry partnerships
4. Create an environment conducive to establish collaboration platforms

Recognizing the importance of the supply chain in R&D and production, we welcome vendors offering materials, devices, and equipment services to academic institutions and companies. Vendors can be part of the conference by setting up booths in the foyer area and opportunities will be provided for conducting workshops.

The 12th International Drug Chemistry Congress will be held at the Mirage Park Resort Hotel in Antalya-Kemer from March 7 to 10, 2024. We look forward to your participation and hope that the conference will make significant contributions to researchers in academia and industry alike.

Join us and participate in sharing knowledge, exploring collaboration opportunites and building long-lasting relations with the larger scientific community.

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CONFERENCE PROGRAMME	
Thursday March 07, 2024	
10:00 – 14:00	Registration
Opening Ceremony	
14:00 – 14:40	Prof. Dr. Ramazan **ALTUNDAŞ**, Chair İkram **CENGİZ**, Chair of The Turkish Chemists` Society, Prof. Dr. Hacı Ali **MANTAR**, Rector, Gebze Technical University
14:40 – 17:30	İlaçta Yerelleşme Raporunun Katılımcılar ile Paylaşılması Yetim İlaçlar TİTCK T.C. Sağlık Bakanlığı
17:30 – 18:00	**Crystal Mortar Awards Ceremony**
Session 1	Session Chair: Dr. Mutlu **TOPAL**
18:00 – 18:40	Dr. Yavuz Gökalp **YILDIZ** *What should be the Development Parameters of the Pharmaceutical Industry in the 21st Century?*
18:40 – 20:30	Dinner

Friday March 08, 2024	
Session 2	Session Chair: Prof. Christa E. **MULLER**
09:00 – 09:40	Prof. Vittorio **PACE**, University of Turin *Designing New Synthetic Concepts in Medicinal Chemistry with C-1 Sources*
09:40 – 10:10	Assoc. Prof. Serhan **TURKYILMAZ**, METU *Cellulose Microspheres Decorated with Zn(II)-Bis(dipicolylamine) Complexes for the Removal of Bacterial Cells from Aqueous Liquids*
10:10 – 11:00	**Coffee Break**
Session 3	Session Chair: Assoc. Prof. Esen **BELLUR ATICI**
11:00 – 11:40	Dr. Joerg **SCHLINGEMANN**, Global Quality Control Principal Expert *The Nitrosamine Saga*
11:40 – 12:10	Assoc. Prof. Ömer Faruk **KARATAS**, Erzurum Technical University *From molecular pathogenesis to drug design; POFUT1 as a novel therapeutic target for head and neck cancers*
12:10 – 12:30	Asst. Prof. Shirin **TARBIAT**, Uskudar University

	The Impact of Lignan Fractions of Piper Cubeba Fruit on Alzheimer's Disease
12:30 – 14:00	**Lunch**
Session 4	Session Chair: Assoc. Prof. Ömer Faruk **KARATAS**
14:00 – 14:40	Prof. Christa E. **MULLER**, University of Bonn *Medicinal Chemistry of Purinergic Signaling: Targets and Drugs for Cancer Immunotherapy*
14:40 – 15:10	Prof. Yusuf **TUTAR**, University of Health Sciences *Drug Designing Against Cellular Mechanics*
15:10 – 15:30	Prof. Nurettin **MENGEŞ**, Necmettin Erbakan University *A New Lead Compound for Glioblastoma and Details of Molecular Mechanism*
15:30 – 16:00	**Coffee Break**
Session 5	Session Chair: Assoc. Prof. Safacan **KOLEMEN**
16:00 – 16:40	Prof. Engin **ULUKAYA**, Istinye University *Palladium (II) Based-Anticancer Compounds: A New Hope?*
16:40 – 17:10	Prof. Serdar **DURDAGI**, Bahçeşehir University *MOL2DRUG: Developing and Pretesting of a Mobile Application Utilizing Deep Learning QSAR for Predicting Biological Activity and Toxicity of a Molecule from Hand Drawn or Uploaded Images*
17:10 – 17:30	Assoc. Prof. Hina **SIDDIQUI**, University of Karachi *Privileged-substructure-based Diversity Oriented Synthesis: Examples of Our Work in the Syntheses of New Chemical Entities and their Biological Studies*
17:30 – 17:50	Assoc. Prof. Pınar **ŞEN**, Yeditepe University *Improvement of in Vitro Antimicrobial Activities of Boronic Acid-Functionalized Benzimidazole Derivatives When Conjugated to The Graphene Quantum Dots*
17:50 – 18:10	Dr. Emrah **KAVAK**, Necmettin Erbakan University *Synthesis and Characterization of Artesunate-Indole Hybrid Molecules*
Session 6	**Short Oral Presentations**
18:30 – 19:30	Session Chair: (Mirage I-II) Prof. Aliye **ALTUNDAŞ** Session Chair: (Odeon) Prof. Nermin **SIMSEK KUS** Session Chair: (Phoenix I) Prof. Yunus **KARA** Session Chair: (Phoenix II) Dr. Emine **YURTOĞLU**

19:30 – 20:30	**Dinner**
20:30 – 22:30	**Poster Presentations, Mirage I-II**

Saturday March 09, 2024	
Session 7	Session Chair: Prof. Engin **ULUKAYA**
09:00 – 09:40	Prof. Elia **PSILLAKIS**, Technical University of Crete Towards Circular Analytical Chemistry
09:40 – 10:10	Andrea **SILVESTRI**, *Analytical Research Manager – Sterling SpA* *Challenges in Manufacturing of APIs for Inhalation*
10:10 – 10:30	Assoc. Prof. Safacan **KOLEMEN**, Koç University *Hemicyanine Derivatives as Effective Type I Photosensitizers*
10:30 – 11:00	**Coffee Break**
Session 8	Session Chair: Assoc. Prof. Serhan **TURKYILMAZ**
11:00 – 11:40	Prof. Dr. Bezhan **CHANKVETADZE**, Tbilisi State University *The Role of Enantioselective Liquid Chromatography in Analysis of Chiral Drugs of Abuse*
11:40 – 12:10	Prof. Dr. Sibel **AYŞIL ÖZKAN**, Ankara University *Modern Designs of Molecularly Imprinted Polymers for Electrochemical Sensing and Analysis of Pharmaceuticals*
12:10 – 12:30	Asst. Prof. Faika **BAŞOĞLU ÜNAL**, European University of Lefke *Exploring Apoptosis-Inducing Thiosemicarbazides: Novel Synthesis and Anti-Proliferative Evaluation in HEPG2 Cells*
12:30 – 14:00	**Lunch**
Young Researcher Session 9	Session Chair: Prof. Nurettin **MENGEŞ**
14:00 – 14:15	Iwona **KWIATKOWSKA,** Medical University of Bialystok *Proapoptotic activity of MM-129 and indoximod in experimental colon cancer model*
14:15 – 14:30	Dr. Toghrul **ALMAMMADOV**, Koç University *Activity-based molecular sensors for visualization of cancer cells with an improved selectivity*
14:30 – 14:45	Tuğçe **CİNEK**, Istanbul Health and Technology University *Synthesis and anticancer activities of 5-nonsubstituted/methyl-2-indolinone derivatives*
14:45 – 15:00	Pharm. Yaren Nur **ZENNİ**, Inonu University *Selective MAO-B Inhibitors Bearing Heterocyclic Moieties*
15:00 – 16:00	**Coffee Break**

Session 10	Session Chair: Assoc. Dr. Azim Ziyaei **HALIMEHJANI**
16:00 – 16:30	Prof. Raid J. **ABDEL-JALIL**, Sultan Qaboos University *Design and synthesis of novel Positron Emission Tomography (PET) markers*
16:30 – 17:00	Prof. Erdal **BEDIR**, IZTECH *Expected a small compound yet encountered supramolecular particles with promising anticancer activity*
17:00 – 17:20	Asst. Prof. Hande **GÜNDÜZ**, Koç University *Hydrogen Peroxide Activatable Chemiluminescent Probe for the Detection of Oxidative Stress*
17:20 – 17:40	Asst. Prof. Nigâr **KANTARCI ÇARŞIBAŞI**, Üsküdar University *Queuine as a Potential Multi-Target Drug for Alzheimer's Disease*
17:40 – 18:00	Asad **RIZVI**, Abdi İbrahim *Recent advances in Design of Amorphous Solid Dispersions*
18:30 – 19:30	**Dinner**
19:30 – 21:30	**Poster Presentations, Mirage I-II**

Sunday March 10, 2024	
Session 11	Session Chair: Prof. Raid J. **ABDEL-JALIL**
09:00 – 09:30	Assoc. Prof. Azim Ziyaei **HALIMEHJANI**, Sharif University of Technology *Nitroepoxides as efficient intermediates in Organic Synthesis*
09:30 – 10:00	Prof. Mükerrem Betül **AYCAN YERER**, Erciyes University *Current biotechnological approaches in the development of targeted cancer drug candidates*
10:00 – 10:20	Kadir **ALUÇ**, Abdi İbrahim *Elucidation of an Impurity After Terminal Sterilization in Sugammadex Sodium Iv By Lc-Ms*
10:20 – 10:40	Dr. Ümit **BABACAN**, Akdeniz University *Purification Of Ferulic Acid From Agricultural Wastes Using Feruloyl Esterase Enzyme*
10:40 – 12:00	**Closing Ceremony and Poster Awards**

OP62	Behiye Büşra TAŞBAŞI	Synthesis of a Fluorescent Probe Based on ESIPT Molecules and Evaluation as a Cell Imaging Agent
OP63	Elif Esma GÖNÜL	Ionized Tetracyclic Skeletones for ESIPT-emitted Fluorescent Probes
OP64	Elif GÖKÇAY BİLİCİ	Synthesis of Aromatic Lactones via Keten Addition Reactions and Investigation of their Antioxidant Capacities
OP65	Lale Beril SUBAY	Rapamycin and Niacin Combination Exerts Anti-Cancer Effect Through Activation of Autophagy on Acute Myeloid Leukemia Cells
OP66	İbrahim PINAR	Immunotherapy Approach for Cancer Treatment: Designing of Small Molecules for PD-1/PD-L1 Interaction Inhibition
OP67	Gözde ÇINAR	Design, Synthesis and Anti-coronavirus Evaluation of New Spirothiazolidinone Compounds
OP68	Gözde ÇINAR	Synthesis, Characterization and Antiviral Activity of New Spirothiazolidinone Derivatives Carrying Indole Moiety
OP69	Bilgesu Onur SUCU	Design and Synthesis of Benzofuran/Heterocylic Hybrids as Potential Bioactive Agents
OP70	Efsun KOLATAN	The Importance of Standardization in Laboratory Animal Research
OP71	Esra GÜREL	Synthesis of New Curcumin Compounds Containing O-Alkyl Groups at Phenyl Rings
OP72	Ronak Haj ERSAN	Synthesis and Anticancer Activity of Benzimidazole Derivatives Containing 2-Amide and Ether Bonds

PHOENİX-II

Poster no	Author	Title
OP73	Aslıhan KARA	Synthesis of Ferrocene-Benzofuran-Artemisinin Derivatives
OP74	Emrah POLAT	Investigation of Anti-Cancer Effects of Enantiomerically Pure (S)-4-Aminokinazoline Derivatives on Human Lung (A-549) Cancer Cell Line
OP75	Salma GHAZY	A Novel Algorithm for Virtual Screening of Extensive Small Molecule Libraries Targeting ERCC1-XPF Interfaces to Identify Therapeutically Non-Resistant Small Anti-Cancer Compounds
OP76	Ciğdem KANBEŞ-DİNDAR	Evaluating the Interaction Between The Antineoplastic Drug Bexarotene and Double-stranded DNA Using Electrochemical and Spectroscopic Methods
OP77	Ioannis PAPAZOGLOU	Computational RNA Aptamer Design: A Pipeline for Precise Targeting of Macromolecular Elements in the Pursuit of Treating Retinal Degeneration within the RETORNA - A HORIZON Europe Initiative
OP78	Tamerlan MAMMADOV	Synthesis Novel Artesunate-Benzothiophene Derivatives
OP79	Khaled A.N. ABUSHARKH	Design, synthesis and antiproliferative activities of new benzothiazole/ benzothiazole thiazolidine-2,4-dione derivatives as potential FOXM1 inhibitors
OP80	Şule EROL GÜNAL	Evaluation of Pharmacokinetic and Drug Likeliness Properties of Thiazolidine-4-one Derivatives

Design, synthesis and antiproliferative activities of new benzothiazole/ benzothiazole thiazolidine-2,4-dione derivatives as potential FOXM1 inhibitors

Khaled A.N. Abusharkh[a-c], Ferah Comert Onder[d], Venhar Cınar[e], Zuhal Hamurcu[e], Bulent Ozpolat[f], Mehmet Ay[b]

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Abstract:

Heterocycles are vital pharmacophores, holding significance in the creation of privileged chemical structures endowed with diverse pharmacological activities[1]. Among them, benzothiazole, a fused benzoheterocycle, is prevalent in numerous naturally occurring products, contributing to their medicinal, pharmacological, and pharmaceutical applications[1]. The benzothiazole scaffold exhibits a broad spectrum of biological activities including antitumor properties. Benzothiazole derivatives exhibit significant and diverse biological and pharmacological activities, demonstrating efficacy against a range of tumors including cervical, colon, liver, ovarian, non-small cell lung, and breast cancers.

FOXM1 overexpression is associated with poor prognosis and shorter patient survival in various malignancies, including breast cancer. Thus, targeting FOXM1 is considered as a promising approach for targeted cancer therapy[4]. Therefore, in this study, we designed and synthesized two series of benzothiazole derivatives and the structures of all the compounds were confirmed on the basis collective use of FTIR, ^{1}H-NMR, ^{13}C-NMR, and LC-MS/MS. The antiproliferative activity was evaluated against triple negative breast cancer cell line (MDA-MB-231). Specifically, compounds KC11, KC23, and KC21 exhibited notable cytotoxic effects, emerging as the most potent derivatives among all tested compounds against MDA-MB-231 cancer cell lines, with IC_{50} values of 10 µM, 10 µM, and 20 µM, respectively. In molecular docking studies, the synthesized compounds exhibited docking scores ranging from -5.8 to -6.8 kcal/mol. Notably, KC21 displayed the highest score of -6.8 kcal/mol. The DNA-binding domain specifically targets crucial amino acids including His287, Asn283, and Arg286, as demonstrated in preclinical studies. As a result, the interactions between the synthesized compounds and the active site residues of FOXM1-DBD were meticulously scrutinized and compared with the positive control, FDI-6. Most of the synthesized compounds exhibited involvement in at least two interactions with critical amino acids, namely His287, Asn283, and Arg286. Next, to test whether these compounds could be used as FOXM1 inhibitors, FOXM1 protein expression level will investigate in treated of breast cancer cells with KC11, KC23, and KC21.

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