

Assoc. Prof. BURAK TÜZÜN

Personal Information

Office Phone: [+90 346 487 0000](tel:+903464870000) Extension: 5467

Email: btuzun@cumhuriyet.edu.tr

Other Email: theburaktuzun@yahoo.com

Web: <https://avesis.cumhuriyet.edu.tr/btuzun>

International Researcher IDs

ScholarID: [qjszf8wAAAAJ&view_op=list_works&sortby=pubdate](https://scholar.google.com/citations?user=qjszf8wAAAAJ&view_op=list_works&sortby=pubdate)

ORCID: 0000-0002-0420-2043

ScopusID: 56699974000

Yoksis Researcher ID: 56581

Education Information

Doctorate, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, Turkey 2010 - 2018

Postgraduate, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, Turkey 2007 - 2010

Undergraduate, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, Turkey 2002 - 2007

Dissertations

Doctorate, Elektron Konformasyonel-Genetik algoritma 4d-qsar Metodu ile Piridin karboksilik Asit, Oksadiazol, Pirimidin ve Oksazol türevlerine ait farmakofor gruplarının belirlenmesi ve biyoaktivite hesabı, Sivas Cumhuriyet Üniversitesi, Fen Fakültesi, Kimya Bölümü, 2018

Postgraduate, Karbamatların flotasyon kolektörleri olarak etkinlikleri, Sivas Cumhuriyet Üniversitesi, Fen Fakültesi, Kimya Bölümü, 2010

Research Areas

Natural Sciences

Academic Titles / Tasks

Associate Professor, Sivas Cumhuriyet University, Sivas Teknik Bilimler Meslek Yüksekokulu, Bitkisel Ve Hayvansal Üretim, 2020 - Continues

Research Assistant, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, 2010 - 2020

Courses

Genel Kimya II, Undergraduate, 2018 - 2019

Genel Kimya, Undergraduate, 2018 - 2019

Genel Kimya, Undergraduate, 2018 - 2019

Published journal articles indexed by SCI, SSCI, and AHCI

- I. **Chemical composition, cytotoxicity, and molecular docking analyses of Thuja orientalis extracts**
KAPANCIK S., Çelik M. S., DEMİRALP M., Ünal K., ÇETİNKAYA S., TÜZÜN B.
Journal of Molecular Structure, vol.1318, 2024 (SCI-Expanded)
- II. **A cadmium-thiocyanate coordination polymer with bridging 2-aminopyridine: Synthesis, characterization DFT studies, Hirshfeld Surface analysis and docking studies**
MbomYufanyi D., TÜZÜN B., Nono J. H., Jong Y. C., Wirsiy J.
Journal of Molecular Structure, vol.1318, 2024 (SCI-Expanded)
- III. **A study on insecticidal activity of the fennel (Foeniculum vulgare) essential oil and its nanoemulsion against stored product pests and molecular docking evaluation**
Çiçek S., Korkmaz Y. B., TÜZÜN B., Işık S., Yılmaz M. T., ÖZOĞUL F.
Industrial Crops and Products, vol.222, 2024 (SCI-Expanded)
- IV. **Molecular descriptors and in silico studies of 4-((5-(decylthio)-4-methyl-4n-1,2,4-triazol-3-yl)methyl)morpholine as a potential drug for the treatment of fungal pathologies**
Myroslava O., Poustforoosh A., Inna B., Parchenko V., TÜZÜN B., Gutyj B.
Computational Biology and Chemistry, vol.113, 2024 (SCI-Expanded)
- V. **Synthesis biological evaluation and molecular docking of isatin hybrids as anti-cancer and anti-microbial agents**
Altamimi M., Syed S. A., TÜZÜN B., Alhazani M. R., Alnemer O., Bari A.
Journal of enzyme inhibition and medicinal chemistry, vol.39, no.1, pp.2288548, 2024 (SCI-Expanded)
- VI. **Morphology studies, optic proprieties, hirschfeld electrostatic potential mapping, docking molecular anti-inflammatory, and dynamic molecular approaches of hybrid phosphate**
Rafik A., TÜZÜN B., Zouihri H., Poustforoosh A., Hsissou R., Elhenaey A. A., Guedira T.
Journal of the Indian Chemical Society, vol.101, no.11, 2024 (SCI-Expanded)
- VII. **Enhanced Corrosion-Inhibition performance of amino Gossypol: A comprehensive theoretical study**
Berdimuradov K., Berdimurodov E., El Ibrahimy B., Demir M., Gokhan Colak S., TÜZÜN B., Rakhmatullaeva M., Diyorova M., Axtamov D., Husenov Q.
Computational and Theoretical Chemistry, vol.1241, 2024 (SCI-Expanded)
- VIII. **Exploring Benzo[b][1,4]Thiazine Derivatives: Multitarget Inhibition, Structure–Activity Relationship, Molecular Docking, and ADMET Analysis**
Alishba A., Ali I., Hameed S., Khan K. M., Salar U., Taha M., Sadeghian N., Taslimi P., TÜZÜN B., Özerkan D., et al.
ChemistrySelect, vol.9, no.38, 2024 (SCI-Expanded)
- IX. **Novel 1,2,4-triazole-maleamic acid derivatives: synthesis and evaluation as anticancer agents with carbonic anhydrase inhibitory activity**
Tapera M., Kekeçmuhammed H., TÜZÜN B., DURNA DAŞTAN S., Safa Çelik M., Taslimi P., DAŞTAN T., Topcu K. S. B., Cacan E., Şahin O., et al.
Journal of Molecular Structure, vol.1313, 2024 (SCI-Expanded)
- X. **Synthesis, crystal structure, Hirshfeld surface analyses, and DFT studies of (S)-2-(3,5-di-tert-butyl-4-hydroxyphenyl)-3,3-diethoxy-1-phenylpropan-1-one**
Khalilov A. N., Cisterna J., Cárdenas A., TÜZÜN B., ERKAN S., Gurbanov A. V., Brito I.
Journal of Molecular Structure, vol.1313, 2024 (SCI-Expanded)
- XI. **Advanced evaluation of novel quinoline derivatives for corrosion inhibition of mild steel in acidic environments: A comprehensive electrochemical, computational, and surface study**
Belkheiri A., Dahmani K., Mzioud K., Rbaa M., Galai M., Hmada A., Erdoğan Ş., TÜZÜN B., Touhami M. E., El-Serehy H. A., et al.
International Journal of Electrochemical Science, vol.19, no.10, 2024 (SCI-Expanded)
- XII. **Removal of safranin O from wastewater using Streptomyces griseobrunneus dead biomass and in silico calculations**
Çelik M. S., KÜTÜK N., YENİDÜNYA A. F., ÇETİNKAYA S., TÜZÜN B.
Biomass Conversion and Biorefinery, vol.14, no.20, pp.25873-25884, 2024 (SCI-Expanded)
- XIII. **The synthesis of novel unnatural amino acid by intramolecular aza-Michael addition reaction as**

multitarget enzyme inhibitors

Abul N., TÜZÜN B., GÜLÇİN İ., ATMACA U.

Journal of Biochemical and Molecular Toxicology, vol.38, no.9, 2024 (SCI-Expanded)

- XIV. **Hydrazone-flavonol based oxidovanadium(V) complexes: Synthesis, characterization and antihyperglycemic activity of chloro derivative in vivo**
Zahirović A., Fočak M., Fetahović S., TÜZÜN B., Višnjevac A., Muzika V., Brulić M. M., Žero S., Čustović S., Crans D. C., et al.
Journal of Inorganic Biochemistry, vol.258, 2024 (SCI-Expanded)
- XV. **Peripheral (E)-2-[(4-hydroxybenzylidene)-3,4-dihydronaphthalen-1(2H)-one]-coordinated phthalocyanines with improved enzyme inhibition properties and photophysicochemical behaviors**
Güleç Ö., Bilgiçli A. T., TÜZÜN B., Taslimi P., Günsel A., GÜLÇİN İ., Arslan M., Yarasir M. N.
Archiv der Pharmazie, vol.357, no.9, 2024 (SCI-Expanded)
- XVI. **8-Aminoquinoline derived two Schiff base platforms: Synthesis, characterization, DFT insights, corrosion inhibitor, molecular docking, and pH-dependent antibacterial study**
Majumdar D., Chatterjee A., Feizi-Dehnyebi M., Kiran N. S., TÜZÜN B., Mishra D.
Heliyon, vol.10, no.15, 2024 (SCI-Expanded)
- XVII. **Bioactivity, crystal and molecular structure of vanadyl(III) complex with N-salicyloyl – N'(3,5-ditertbutyl-2-hydroxy)benzylidene hydrazine**
Amrulla Fatullayeva P., Akper Medjidov A., Gennadievna Safronenko M., Nikolaevic Khrustalev V., Huseyn Ismayilov R., Allahverdi Bayramov M., YALÇIN B., Sadeghian N., Taslimi P., TÜZÜN B.
Polyhedron, vol.257, 2024 (SCI-Expanded)
- XVIII. **Evaluation of antioxidant, antimicrobial, enzyme inhibition activity, and cell viability capacity of Hypericum heterophyllum vent., an endemic species in Turkey's Flora**
Erurygur N., Uçar E., TÜZÜN B., ATAŞ M., İnanır M., DEMİRBAŞ A., BAL H., Şenkal B. C., Uskutoğlu T.
Journal of Molecular Structure, vol.1307, 2024 (SCI-Expanded)
- XIX. **Trinuclear nickel (II) string complexes and copper (II) coordination polymer with pyrazine modulated unsymmetrical dipyridylamino ligand: Synthesis, structure and bioactivity properties with molecular docking**
Ismayilov R. H., Valiyev F. F., Tagiyev D. B., Song Y., Medjidov A. A., Fatullayeva P. A., TÜZÜN B., Taslimi P., Peng C., Chien S., et al.
Journal of Molecular Structure, vol.1307, 2024 (SCI-Expanded)
- XX. **Synthesis, biological activities, and molecular docking studies of triazolo[4,3-b]triazine derivatives as a novel class of α -glucosidase and α -amylase inhibitors**
Seyfi S., Salarinejad S., Moghimi S., Toolabi M., Sadeghian N., TÜZÜN B., Firoozpour L., Ketabforoosh S. H. M. E., Taslimi P., Foroumadi A.
Archiv der Pharmazie, vol.357, no.7, 2024 (SCI-Expanded)
- XXI. **Synthesis, Biological Properties, and Molecular Docking Study of Novel 1,2,3-Triazole-8-quinolinol Hybrids**
El Faydy M., Lakhrissi L., Dahaieh N., Ounine K., TÜZÜN B., Chahboun N., Boshala A., Alobaid A., Warad I., Lakhrissi B., et al.
ACS Omega, vol.9, no.23, pp.25395-25409, 2024 (SCI-Expanded)
- XXII. **Synthesis of 1,3-Disubstituted Tetrahydropyrimidinium Salts and Determination of Their Biological Properties and Molecular Docking**
KARACA E. Ö., GÜRBÜZ N., Demir Y., TÜZÜN B., ÖZDEMİR İ., GÜLÇİN İ.
ChemistrySelect, vol.9, no.19, 2024 (SCI-Expanded)
- XXIII. **Supramolecular clumps of μ_2 -1,3-acetate bridges of Cd(II)-Salen complex: Synthesis, spectroscopic characterization, crystal structure, DFT quantization's, and antifungal photodynamic therapy**
Majumdar D., Philip J. E., Gassoumi B., Ayachi S., Abdelaziz B., TÜZÜN B., Roy S.
Heliyon, vol.10, no.9, 2024 (SCI-Expanded)
- XXIV. **The pharmacological properties of Gypsophila ericalyx: The endemic medicinal plant of northern central Turkey**

- İnanir M., Uçar E., TÜZÜN B., Eruygur N., ATAŞ M., AKPULAT H. A.
International Journal of Biological Macromolecules, vol.266, 2024 (SCI-Expanded)
- XXV. **Surface adsorption and corrosion resistance performance of modified chitosan: Gravimetric, electrochemical, and computational studies**
Haldhar R., Raorane C. J., Mishra V., TÜZÜN B., Berdimurodov E., Kim S.
International Journal of Biological Macromolecules, vol.264, 2024 (SCI-Expanded)
- XXVI. **The impact of some metals, molecular docking and molecular dynamic calculations on glucose 6-phosphate dehydrogenase activity in *Capoeta trutta* (Heckel, 1843) tissue**
Kırıcı M., TÜZÜN B., Kırıcı M., ATAMANALP M., Poustforoosh A., BEYDEMİR Ş., Reşit Taysı M.
Journal of Molecular Liquids, vol.399, 2024 (SCI-Expanded)
- XXVII. **Biosorption of dye crystal violet on *Tragopogon* sp. leaf powder: Equilibrium, kinetics, thermodynamics, and DFT calculations**
Eyupoglu V., Aksu A., Çetinkaya H. F., ÇETİNTAŞ H. İ., ÇETİNKAYA S., TÜZÜN B.
Journal of Molecular Liquids, vol.398, 2024 (SCI-Expanded)
- XXVIII. **Novel supramolecular co-crystal of 8-hydroxyquinoline with acetone-(2,4-dinitrophenyl)hydrazone: One pot synthesis, structural characterization, Hirshfeld surface and energy framework analysis, computational investigation and molecular docking study**
Zerrouki K., Bouchene R., TÜZÜN B., Retailleau P.
Journal of Molecular Structure, vol.1300, 2024 (SCI-Expanded)
- XXIX. **A Simple and Efficient Procedure Toward 2-Thioxoquinazolin-4(1H)-One Derivatives**
Ahmadi Shourkaei F., Rashidi Ranjbar P., Mahdavi M., TÜZÜN B., Taslimi P.
Iranian Journal of Chemistry and Chemical Engineering, vol.43, no.3, pp.1103-1114, 2024 (SCI-Expanded)
- XXX. **Synthesis, Enzyme Inhibition, and in Silico Studies of Amino Acid Schiff Bases**
Akkuş Taş N., Şenocak A., Taslimi P., TÜZÜN B., KARADAĞ A.
Iranian Journal of Chemistry and Chemical Engineering, vol.43, no.3, pp.1083-1093, 2024 (SCI-Expanded)
- XXXI. **Schiff base derivatives against monkeypox virus: Synthesis, in silico, MM-GBSA and SAR properties**
KARATAŞ H., Kiliç H. K., TÜZÜN B., KÖKBUDAK Z.
Journal of Molecular Structure, vol.1298, 2024 (SCI-Expanded)
- XXXII. **In-situ Salen-type ligand formation-driven of a heterometallic Cu(II)-Hg(II) complex: Synthetic update, crystallographic features, DFT calculations, and unveil antimicrobial profiles**
Majumdar D., Roy S., Elizabeth Philip J., TÜZÜN B., Hazra S.
Inorganic Chemistry Communications, vol.160, 2024 (SCI-Expanded)
- XXXIII. **Crystal growth, morphological, mechanical, spectroscopic studies, optical properties, molecular docking, ADME/T, Hirshfeld surfaces analysis and theoretical calculations of hybrid organic-inorganic phosphate compound**
Rafik A., TÜZÜN B., Zouihri H., EL Ammari L., Safi Z. S., Wazzan N. A., Guedira T.
Inorganic Chemistry Communications, vol.160, 2024 (SCI-Expanded)
- XXXIV. **Schiff base compounds constructed from pyrazole-acetamide: Synthesis, spectroscopic characterization, crystal structure, DFT, molecular docking and antioxidant activity**
Al Ati G., Chkirate K., El-Guourrami O., Chakchak H., TÜZÜN B., Mague J. T., Benzeid H., Achour R., Essassi E. M.
Journal of Molecular Structure, vol.1295, 2024 (SCI-Expanded)
- XXXV. **Antioxidant enzyme activities, molecular docking studies, MM-GBSA, and molecular dynamic of chlorpyrifos in freshwater fish *Capoeta umbla***
Taysı M. R., Kirici M., Kirici M., TÜZÜN B., Poustforoosh A.
Journal of Biomolecular Structure and Dynamics, vol.42, no.1, pp.163-176, 2024 (SCI-Expanded)
- XXXVI. **Investigation on the mechanisms by which the herbal remedies induce anti-prostate cancer activity: uncovering the most practical natural compound**
Poustforoosh A., Faramarz S., Negahdaripour M., TÜZÜN B., Hashemipour H.
Journal of Biomolecular Structure and Dynamics, vol.42, no.7, pp.3349-3362, 2024 (SCI-Expanded)
- XXXVII. **Tracing the pathways and mechanisms involved in the anti-breast cancer activity of glycyrrhizin using bioinformatics tools and computational methods**

- Poustforoosh A, Faramarz S, Negahdaripour M, TÜZÜN B, Hashemipour H.
Journal of Biomolecular Structure and Dynamics, vol.42, no.2, pp.819-833, 2024 (SCI-Expanded)
- XXXVIII. **Response Surface Methodology (RSM) Design to Optimize the Cathode of Li-Ions Batteries Recycling in Deep Eutectic Solvent and DFT Simulation**
Karimi S, Mafton-Azad L, Behnajady B, TÜZÜN B.
Korean Journal of Chemical Engineering, 2024 (SCI-Expanded)
- XXXIX. **Comparative study of experimental and DFT calculations for 3-cinnamoyl 4-hydroxycoumarin derivatives**
Bečić E, Salihović M, TÜZÜN B, Omeragić E, Imamović B, Dedić M, Roca S, Špirtović-Halilović S.
Technology and health care : official journal of the European Society for Engineering and Medicine, vol.32, no.4, pp.2673-2684, 2024 (SCI-Expanded)
- XL. **Novel Schiff Bases: Synthesis, Characterization, Bioactivity, Cytotoxicity, and Computational Evaluations**
Medetalibeyoğlu H, Manap S, Alkan M, Beytur M, Barlak N, Karatas O. F, TÜZÜN B, Yüksek H, Taslimi P.
Polycyclic Aromatic Compounds, 2024 (SCI-Expanded)
- XLI. **SYNTHESIS, MOLECULAR MODELLING AND CHOLINE ESTERASE ENZYME INHIBITORY ACTIVITY OF NOVEL ENAMINONE DERIVATIVES OF SULFONAMIDES**
Bhat M. A, TÜZÜN B, Koyuncu I, Temiz E, Taslimi P, Naglah A. M, Al-Omar M. A, Džudžević-Čančar H.
Bulletin of the Chemical Society of Ethiopia, vol.38, no.5, pp.1351-1368, 2024 (SCI-Expanded)
- XLII. **Synthesis methods and description for new derivatives associated with 8-hydroxyquinoline and their use as acidic corrosion inhibitors for steel and other alloys: A review**
Rbaa M, Berdimurodov E, TÜZÜN B, Berdimuradov K, Zarrouk A.
Corrosion Reviews, 2024 (SCI-Expanded)
- XLIII. **A biochemistry-oriented drug design: synthesis, anticancer activity, enzymes inhibition, molecular docking studies of novel 1,2,4-triazole derivatives**
Yuriy K, Kusdemir G, Volodymyr P, TÜZÜN B, Taslimi P, Karatas O. F, Anastasia K, Maryna P, SAYIN K.
Journal of Biomolecular Structure and Dynamics, vol.42, no.3, pp.1220-1236, 2024 (SCI-Expanded)
- XLIV. **Integrative in silico evaluation of the antiviral potential of terpenoids and its metal complexes derived from Homalomena aromatica based on main protease of SARS-CoV-2**
Goswami A. K, Aboul-Soud M. A, Gogoi N, El-Shazly M, Giesy J. P, TÜZÜN B, Aziz I. M, Almajhdi F. N, Sharma H. K.
Open Chemistry, vol.22, no.1, 2024 (SCI-Expanded)
- XLV. **In vitro and in silico evaluation of the antimicrobial and antioxidant activities of spiropyrazoline oxindole congeners**
Chalkha M, Chebbac K, Nour H, Nakkabi A, El Moussaoui A, TÜZÜN B, Bourhia M, Chtita S, Bakhouch M, Laaroussi H, et al.
Arabian Journal of Chemistry, vol.17, no.1, 2024 (SCI-Expanded)
- XLVI. **Moderate DNA and high SARS-CoV-2 spike protein affinity of oxidovanadium(IV) complexes of 2-furoic acid hydrazones: In silico and in vitro approach**
Zahirović A, TÜZÜN B, Hadžalić S, Osmanković I, Roca S, Begić S, Fočak M.
Journal of Molecular Structure, vol.1294, 2023 (SCI-Expanded)
- XLVII. **Design, synthesis, in-vitro and in-silico studies of chromone-isoxazoline conjugates as anti-bacterial agents**
Kanzouai Y, Chalkha M, Hadni H, Laghmari M, Bouzammit R, Nakkabi A, Benali T, TÜZÜN B, Akhazzane M, Yazidi M. E, et al.
Journal of Molecular Structure, vol.1293, 2023 (SCI-Expanded)
- XLVIII. **Molecular hybrids integrated with imidazole and hydrazone structural motifs: Design, synthesis, biological evaluation, and molecular docking studies**
Tapera M, Kekeçmuhammed H, SARIPINAR E, DOĞAN M, TÜZÜN B, KOÇYİĞİT Ü. M, Çetin F. N.
Journal of Molecular Liquids, vol.391, 2023 (SCI-Expanded)
- XLIX. **Immobilization of pectinase on chitosan-alginate-clay composite beads: Experimental, DFT and molecular docking studies**

Aksu A., Çetinkaya S., Fazıl Yenidünya A. F., Akkuş Çetinus Ş., Gezegen H., Tüzün B.

Journal of Molecular Liquids, vol.390, 2023 (SCI-Expanded)

- L. **Cationic resin polymer A@IRC-50 as an effective adsorbent for the removal of Cr(III), Cu(II), and Ag(I) from aqueous solutions: A kinetic, mathematical, thermodynamic and modeling study**
Bensalah J., Ouaddari H., Erdoğan Ş., TÜZÜN B., Gaafar A. Z., Nafidi H., Bourhia M., Habsaoui A.
Inorganic Chemistry Communications, vol.157, 2023 (SCI-Expanded)
- LI. **Synthesis and characterization of some benzidine-based azomethine derivatives with molecular docking studies and anticancer activities**
Erdoğan M., Yeşildağ A., Yıldız B., TÜZÜN B., Özden Ö.
Chemical Papers, vol.77, no.11, pp.6829-6847, 2023 (SCI-Expanded)
- LII. **Synthesis of new carboxylates and sulfonates containing thiazolidin-4-one ring and evaluation of inhibitory properties against some metabolic enzymes**
Tokalı F. S., Taslimi P., TÜZÜN B., Karakuş A., Sadeghian N., GÜLÇİN İ.
Journal of the Iranian Chemical Society, vol.20, no.10, pp.2631-2642, 2023 (SCI-Expanded)
- LIII. **Novel Quinazolinone Derivatives: Potential Synthetic Analogs for the Treatment of Glaucoma, Alzheimer's Disease and Diabetes Mellitus**
Tokalı F. S., Taslimi P., TÜZÜN B., Karakuş A., Sadeghian N., GÜLÇİN İ.
Chemistry and Biodiversity, vol.20, no.10, 2023 (SCI-Expanded)
- LIV. **Synthesis of novel Cu(II) complexes with N2O2 ligands: Characterization, theoretical calculations, antimicrobial, antioxidant, DNA binding, and in vitro anticancer activity studies**
Mermer A., TÜZÜN B., DURNA DAŞTAN S., Çevik Ö.
Polyhedron, vol.242, 2023 (SCI-Expanded)
- LV. **Isofraxidin: Antioxidant, Anti-carbonic Anhydrase, Anti-cholinesterase, Anti-diabetic, and in Silico Properties**
DURMAZ L., GÜLÇİN İ., Taslimi P., TÜZÜN B.
ChemistrySelect, vol.8, no.34, 2023 (SCI-Expanded)
- LVI. **A new 1-D polymeric chains of (C5H6ClN2)[CdCl3H2O].H2O perovskite: Synthesis, Structure, Physico-Chemical Characteristics, theoretical calculations, and biological effects**
Hermi S., Habib Mrad M., Alotaibi A. A., TÜZÜN B., Böhme U., Alotaibi K. M., Othmani A., Hassan H. A., Ben Nasr C.
Inorganic Chemistry Communications, vol.155, 2023 (SCI-Expanded)
- LVII. **Synthesis, characterization, crystallographic aspects, Fukui function, and photodynamic antifungal chemotherapy investigation of Cd(II)-tricyanomethanide coordination polymer: Insights from DFT**
Majumdar D., Philip J. E., TÜZÜN B., Roy S.
Inorganic Chemistry Communications, vol.155, 2023 (SCI-Expanded)
- LVIII. **Eco-friendly and potential colin esterase enzyme inhibitor agent sulfonyl hydrazone series: Synthesis, Bioactivity Screening, DFT, ADME properties, and Molecular Docking study**
ÖZDEMİR ÖZMEN Ü., TÜZÜN B., Ayan E. B., ÇEVİRİMLİ B. S.
Journal of Molecular Structure, vol.1286, 2023 (SCI-Expanded)
- LIX. **Anticorrosion properties of the epoxy polymer TGETBAU for mild steel in a solution of HCl (1.0 M): Experimental and computational approaches**
Ech-chebab A., Dahmani K., Hsissou R., Khouja O. E., Verma D. K., Berdimurodov E., Erdoğan S., TÜZÜN B., Lachhab R., Ejbouh A., et al.
Journal of Molecular Structure, vol.1284, 2023 (SCI-Expanded)
- LX. **Piperazin incorporated Schiff Base derivatives: Assessment of in vitro biological activities, metabolic enzyme inhibition properties, and molecular docking calculations**
Mermer A., Tüzün B., Durna Daştan S., Koçyiğit Ü. M., Çetin F. N., Çevik Ö.
JOURNAL OF BIOCHEMICAL AND MOLECULAR TOXICOLOGY, vol.1, no.1, pp.1-18, 2023 (SCI-Expanded)
- LXI. **Vanadium(IV) complexes of salicylaldehyde-based furoic acid hydrazones: Synthesis, BSA binding and in vivo antidiabetic potential**
Zahirović A., Hadžalić S., Višnjevac A., Fočak M., TÜZÜN B., Žilić D., Roca S., Jurec J., Topčagić A., Osmanković I.
Journal of Inorganic Biochemistry, vol.244, 2023 (SCI-Expanded)

- LXII. **In Silico Development of Novel Benzofuran-1,3,4-Oxadiazoles as Lead Inhibitors of M. tuberculosis Polyketide Synthase 13**
Irfan A, Faisal S, Zahoor A. F., Noreen R., Al-Hussain S. A., TÜZÜN B., Javaid R., Elhenawy A. A., Zaki M. E. A., Ahmad S., et al.
Pharmaceuticals, vol.16, no.6, 2023 (SCI-Expanded)
- LXIII. **Synthesis, Biological Activity Evaluation and Molecular Docking of Imidazole Derivatives Possessing Hydrazone Moiety**
Kekeçmuhammed H., Tapera M., Aydoğdu E., SARIPINAR E., Aydin Karatas E., Mehtap Uc E., Akyuz M., TÜZÜN B., GÜLÇİN İ., Emin Bora R., et al.
Chemistry and Biodiversity, vol.20, no.6, 2023 (SCI-Expanded)
- LXIV. **Promising Insecticidal Properties of Essential Oils from Artemisia aragonensis Lam. and Artemisia negrei L. (Asteraceae) by Targeting Gamma-Aminobutyric Acid and Ryanodine Receptor Proteins: In Vitro and In Silico Approaches**
Chebbac K., Benziane Ouaritini Z., Allali A., TÜZÜN B., Zouirech O., Chalkha M., El Moussaoui A., Lafraxo S., Nafidi H., Bin Jordan Y. A., et al.
Separations, vol.10, no.6, 2023 (SCI-Expanded)
- LXV. **Crystal structure, Hirshfeld surface and DFT computations, along with molecular docking investigations of a new pyrazole as a tyrosine kinase inhibitor**
Chalkha M., Ameziane el Hassani A., Nakkabi A., TÜZÜN B., Bakhouch M., Benjelloun A. T., Sfaira M., Saadi M., Ammari L. E., Yazidi M. E.
Journal of Molecular Structure, vol.1273, 2023 (SCI-Expanded)
- LXVI. **In vitro cytotoxic effects, in silico studies, some metabolic enzymes inhibition, and vibrational spectral analysis of novel β -amino alcohol compounds**
TAŞ A., TÜZÜN B., Khalilov A. N., Taslimi P., AĞBEKTAŞ T., Cakmak N. K.
Journal of Molecular Structure, vol.1273, 2023 (SCI-Expanded)
- LXVII. **Corrosion inhibition of Carbon Steel using a new morpholine-based ligand during acid pickling: Experimental and theoretical studies**
Rezaeivala M., Bozorg M., Rafiee N., SAYIN K., TÜZÜN B.
Inorganic Chemistry Communications, vol.148, 2023 (SCI-Expanded)
- LXVIII. **Synthesis, characterization, chemical and biological activities of 4-(4-methoxyphenethyl)-5- benzyl-2-hydroxy-2H-1,2,4-triazole-3(4H)-one phthalocyanine derivatives**
Sarkı G., TÜZÜN B., Ünlüer D., KANTEKİN H.
Inorganica Chimica Acta, vol.545, 2023 (SCI-Expanded)
- LXIX. **Biosorption of Rhodamine B dye from aqueous solution by Rhus coriaria L. plant: Equilibrium, kinetic, thermodynamic and DFT calculations**
Çelik M. S., Çetinus Ş., Yenidünya A. F., Çetinkaya S., Tüzün B.
Journal of Molecular Structure, vol.1272, 2023 (SCI-Expanded)
- LXX. **Synthesis, molecular modeling investigation, molecular dynamic and ADME prediction of some novel Mannich bases derived from 1,2,4-triazole, and assessment of their anticancer activity**
Manap S., Medetalibeyoğlu H., Kılıç A., Karataş O. F., TÜZÜN B., Alkan M., Ortaakarsu A. B., Atalay A., Beytur M., Yüksek H.
Journal of Biomolecular Structure and Dynamics, 2023 (SCI-Expanded)
- LXXI. **Sertraline: Theoretical Studies and a New Potentiometric PVC Membrane Sensor for its Determination**
Saber A. L., TÜZÜN B., Alessa H., Althakafy J. T.
Current Analytical Chemistry, vol.19, no.3, pp.262-271, 2023 (SCI-Expanded)
- LXXII. **EXPERIMENTAL AND THEORETICAL INVESTIGATION OF ANTIOXIDANT ACTIVITY OF SOME DERIVATIVES WITH COUMARIN SCAFFOLD**
Tătăringă G., TÜZÜN B., Zbancioc A.
Farmacia, vol.71, no.2, pp.359-366, 2023 (SCI-Expanded)
- LXXIII. **Design, syntheses, theoretical calculations, MM-GBSA, potential anti-cancer and enzyme activities of**

novel Schiff base compounds

Yalazan H., Koç D., Aydın Kose F., Fandaklı S., TÜZÜN B., Akgül M. İ., Sadeghian N., Taslimi P., KANTEKİN H.
Journal of Biomolecular Structure and Dynamics, 2023 (SCI-Expanded)

- LXXIV. **Synthesis, Spectroscopic Characterization, Antibacterial Activity, and Computational Studies of Novel Pyridazinone Derivatives**
Daoui S., Direkel Ş., Ibrahim M. M., TÜZÜN B., Chelfi T., Al-Ghorbani M., Bouatia M., Karbane M. E., Doukkali A., Benchat N., et al.
Molecules, vol.28, no.2, 2023 (SCI-Expanded)
- LXXV. **Removal of Erythrosine B dye from wastewater by Penicillium italicum: experimental, DFT, and molecular docking studies**
ÇETİNKAYA S., Eyupoglu V., ÇETİNTAŞ H. İ., YENİDÜNYA A. F., KEBABCI Ö., TÜZÜN B.
Journal of Biomolecular Structure and Dynamics, vol.41, no.23, pp.14212-14223, 2023 (SCI-Expanded)
- LXXVI. **In vitro anticancer, antioxidant and enzyme inhibitory potentials of endemic Cephalaria elazigensis var. purpurea with in silico studies**
Erdogan M. K., Gundogdu R., Yapar Y., Gecibesler I. H., Kirici M., Behcet L., TÜZÜN B., Taskin-Tok T., Taslimi P.
Journal of Biomolecular Structure and Dynamics, vol.41, no.21, pp.11832-11844, 2023 (SCI-Expanded)
- LXXVII. **Synthesis, carbonic anhydrase inhibitory activity, anticancer activity and molecular docking studies of new imidazolyl hydrazone derivatives**
Tapera M., Kekeçmuhammed H., TÜZÜN B., SARIPINAR E., KOÇYİĞİT Ü. M., Yıldırım E., DOĞAN M., Zorlu Y.
Journal of Molecular Structure, vol.1269, 2022 (SCI-Expanded)
- LXXVIII. **Repositioning of acefylline as anti-cancer drug: Synthesis, anticancer and computational studies of azomethines derived from acefylline tethered 4-amino-3- mercapto-1,2,4-triazole**
Shahzadi I., Zahoor A. F., TÜZÜN B., Mansha A., Anjum M. N., Rasul A., Irfan A., Kotwica-Mojzych K., Mojzych M.
PLoS ONE, vol.17, no.12 December, 2022 (SCI-Expanded)
- LXXIX. **Unravelling the Synthetic Mimic, Spectroscopic Insights, and Supramolecular Crystal Engineering of an Innovative Heteronuclear Pb(II)-Salen Cocrystal: An Integrated DFT, QTAIM/NCI Plot, NLO, Molecular Docking/PLIP, and Antibacterial Appraisal**
Majumdar D., Philip J. E., TÜZÜN B., Frontera A., Gomila R. M., Roy S., Bankura K.
JOURNAL OF INORGANIC AND ORGANOMETALLIC POLYMERS AND MATERIALS, vol.32, no.11, pp.4320-4339, 2022 (SCI-Expanded)
- LXXX. **Determination of biological studies and molecular docking calculations of isatin-thiosemicarbazone hybrid compounds**
Koçyiğit Ü. M., Doğan M., Muğlu H., Taslimi P., Tüzün B., Yakan H., Bal H., Güzel E., Gülçin İ.
Journal of Molecular Structure, vol.1264, 2022 (SCI-Expanded)
- LXXXI. **Experimental and computational investigation of 3,5-di-tert-butyl-2-(((3-((2-morpholinoethyl) (pyridin-2-ylmethyl) amino) propyl)imino) methyl)phenol and related reduced form as an inhibitor for C-steel**
Karimi S., Rezaeivala M., SAYIN K., TÜZÜN B.
MATERIALS CHEMISTRY AND PHYSICS, vol.287, 2022 (SCI-Expanded)
- LXXXII. **The Impact of D614G Mutation of SARS-COV-2 on the Efficacy of Anti-viral Drugs: A Comparative Molecular Docking and Molecular Dynamics Study**
Poustforoosh A., Hashemipour H., TÜZÜN B., Azadpour M., Faramarz S., Pardakhty A., Mehrabani M., Nematollahi M. H.
CURRENT MICROBIOLOGY, vol.79, no.8, 2022 (SCI-Expanded)
- LXXXIII. **Benzotriazole-oxadiazole hybrid Compounds: Synthesis, anticancer Activity, molecular docking and ADME profiling studies**
Mermer A., Bulbul M. V., Kalender S. M., Keskin I., TÜZÜN B., Eyupoglu O. E.
JOURNAL OF MOLECULAR LIQUIDS, vol.359, 2022 (SCI-Expanded)
- LXXXIV. **Synthesis, computational analyses, antibacterial and antibiofilm properties of nicotinamide derivatives**
Taşkın Kafa A. H., Tuzun G., Guney E., Aslan R., Sayin K., Tüzün B., Ataseven H.

- STRUCTURAL CHEMISTRY, vol.33, pp.1189-1197, 2022 (SCI-Expanded)
- LXXXV. **Synthesis, Molecular Docking and Antiproliferative Activity Studies of a Thiazole-Based Compound Linked to Hydrazone Moiety**
Kekecmammed H., Tapera M., TÜZÜN B., AKKOÇ S., ZORLU Y., SARIPINAR E.
CHEMISTRYSELECT, vol.7, no.26, 2022 (SCI-Expanded)
- LXXXVI. **Synthesis, structural confirmation, antibacterial properties and bio-informatics computational analyses of new pyrrole based on 8-hydroxyquinoline**
Lakhrissi Y., Rbaa M., TÜZÜN B., Hichar A., Anouar E. H., Ounine K., Almalki F., Ben Hadda T., Zarrouk A., Lakhrissi B.
JOURNAL OF MOLECULAR STRUCTURE, vol.1259, 2022 (SCI-Expanded)
- LXXXVII. **Quinoline-fused both non-peripheral and peripheral Zn-II and Mg-II phthalocyanines: Anti-cholinesterase, anti-alpha-glucosidase, DNA nuclease, antioxidant activities, and in silico studies**
Yalazan H., TÜZÜN B., AKKAYA D., BARUT B., KANTEKİN H., YILDIRMIŞ S.
APPLIED ORGANOMETALLIC CHEMISTRY, vol.36, no.7, 2022 (SCI-Expanded)
- LXXXVIII. **Synthesis, characterization, molecular modeling against EGFR target and ADME/T analysis of novel purine derivatives of sulfonamides**
Bhat M. A. A., TÜZÜN B., Alsaif N. A. A., Khan A. A. M., Naglah A. M.
JOURNAL OF MOLECULAR STRUCTURE, vol.1257, 2022 (SCI-Expanded)
- LXXXIX. **Alkyl chain modified metalophthalocyanines with enhanced antioxidant-antimicrobial properties by doping Ag⁺ and Pd²⁺ ions**
ALICI E. H., BİLGİÇLİ A. T., Tuezuen B., Guensel A., ARABACI G., Yarasir M. N.
JOURNAL OF MOLECULAR STRUCTURE, vol.1257, 2022 (SCI-Expanded)
- XC. **Antiproliferative activity and molecular docking studies of new 4-oxothiazolidin-5-ylidene acetate derivatives containing guanylhydrazone moiety**
Al-Janabi I. A. S., Yavuz S. C., KÖPRÜ S., Tapera M., Kekecmammed H., AKKOÇ S., TÜZÜN B., Patat A., SARIPINAR E.
JOURNAL OF MOLECULAR STRUCTURE, vol.1258, 2022 (SCI-Expanded)
- XCII. **Synthesis, characterization and bioactivity of novel 8-hydroxyquinoline derivatives: Experimental, molecular docking, DFT and POM analyses**
Rbaa M., Haida S., TÜZÜN B., Hichar A., El Hassane A., Kribii A., Lakhrissi Y., Ben Hadda T., Zarrouk A., Lakhrissi B., et al.
JOURNAL OF MOLECULAR STRUCTURE, vol.1258, 2022 (SCI-Expanded)
- XCIII. **Synthesis, Characterization, Molecular Docking, Acetylcholinesterase and alpha-Glycosidase Inhibition Profiles of Nitrogen-Based Novel Heterocyclic Compounds**
GÜLÇİN İ., Petrova O., Taslimi P., Malysheva S. F., Schmidt E. Y., Sobenina L. N., Gusarova N. K., Trofimov B. A., TÜZÜN B., Farzaliyev V. M., et al.
CHEMISTRYSELECT, vol.7, no.19, 2022 (SCI-Expanded)
- XCIV. **Experimental and theoretical investigation of corrosion inhibition effect of two piperazine-based ligands on carbon steel in acidic media**
Rezaeivala M., Karimi S., SAYIN K., TÜZÜN B.
COLLOIDS AND SURFACES A-PHYSICO-CHEMICAL AND ENGINEERING ASPECTS, vol.641, 2022 (SCI-Expanded)
- XCV. **The Evaluation of Anticancer, Antioxidant, Antidiabetic and Anticholinergic Potentials of Endemic Rhabdosciadium microcalycinum Supported by Molecular Docking Study**
Erdogan M. K., Gundogdu R., Yapar Y., Gecibesler I. H., Kirici M., Behcet L., TÜZÜN B., Taslimi P.
CHEMISTRYSELECT, vol.7, no.17, 2022 (SCI-Expanded)
- XCVI. **Architectural View of Flexible Aliphatic -OH Group Coordinated Hemi-Directed Pb(II)-Salen Coordination Polymer: Synthesis, Crystal Structure, Spectroscopic Insights, Supramolecular Topographies, and DFT Perspective**
Majumdar D., TÜZÜN B., Pal T. K., Das S., Bankura K.
JOURNAL OF INORGANIC AND ORGANOMETALLIC POLYMERS AND MATERIALS, vol.32, no.3, pp.1159-1176, 2022 (SCI-Expanded)
- XCVI. **Novel amino acid Schiff base Zn(II) complexes as new therapeutic approaches in diabetes and Alzheimer's disease: Synthesis, characterization, biological evaluation, and molecular docking**

studies

ŞENOCAK A., Tas N. A., Taslimi P., TÜZÜN B., AYDIN A., KARADAĞ A.

JOURNAL OF BIOCHEMICAL AND MOLECULAR TOXICOLOGY, vol.36, no.3, 2022 (SCI-Expanded)

- XCVII. **Novel phenolic Mannich base derivatives: synthesis, bioactivity, molecular docking, and ADME-Tox Studies**
TOKALI F. S., Taslimi P., Demirciolu I. H., Sendil K., TÜZÜN B., GÜLÇİN İ.
JOURNAL OF THE IRANIAN CHEMICAL SOCIETY, vol.19, no.2, pp.563-577, 2022 (SCI-Expanded)
- XCVIII. **3D-QSAR, molecular docking, molecular dynamics, and ADME/T analysis of marketed and newly designed flavonoids as inhibitors of Bcl-2 family proteins for targeting U-87 glioblastoma**
Poustforoosh A., Faramarz S., Nematollahi M. H., Hashemipour H., TÜZÜN B., Pardakhty A., Mehrabani M.
JOURNAL OF CELLULAR BIOCHEMISTRY, vol.123, no.2, pp.390-405, 2022 (SCI-Expanded)
- XCIX. **Could pyrimidine derivative be effective against Omicron of SARS-CoV-2?**
KARATAŞ H., TÜZÜN B., KÖKBUDAK Z.
BRATISLAVA MEDICAL JOURNAL-BRATISLAVSKE LEKARSKE LISTY, vol.123, no.7, pp.505-513, 2022 (SCI-Expanded)
- C. **In Silico and In Vitro Antiproliferative Activity Assessment of New Schiff Bases**
KÖKBUDAK Z., AKKOÇ S., Karata H., TÜZÜN B., Aslan G.
CHEMISTRYSELECT, vol.7, no.3, 2022 (SCI-Expanded)
- CI. **Biological effects and molecular docking studies of Catechin 5-O-gallate: antioxidant, anticholinergics, antiepileptic and antidiabetic potentials**
Taslimi P., KOÇYIĞIT Ü. M., TÜZÜN B., KIRICI M.
JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS, vol.40, no.6, pp.2489-2497, 2022 (SCI-Expanded)
- CII. **Design, synthesis, characterization, biological evaluation, and molecular docking studies of novel 1,2-aminopropanthiols substituted derivatives as selective carbonic anhydrase, acetylcholinesterase and alpha-glycosidase enzymes inhibitors**
Huseynova A., Kaya R., Taslimi P., Farzaliyev V., Mammadyarova X., Sujayev A., TÜZÜN B., KOÇYIĞIT Ü. M., Alwasel S., GÜLÇİN İ.
JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS, vol.40, no.1, pp.236-248, 2022 (SCI-Expanded)
- CIII. **Anti-corrosion behavior of 2-((3-(2-morpholino ethylamino)-N3-((pyridine-2-yl)methyl)propylimino)methyl)pyridine and its reduced form on Carbon Steel in Hydrochloric Acid solution: Experimental and theoretical studies**
Rezaeivala M., Karimi S., TÜZÜN B., SAYIN K.
THIN SOLID FILMS, vol.741, 2022 (SCI-Expanded)
- CIV. **Design, synthesis, characterization, biological evaluation, and molecular docking studies of novel 1,2-aminopropanthiols substituted derivatives as selective carbonic anhydrase, acetylcholinesterase and α -glycosidase enzymes inhibitors**
Huseynova A., Kaya R., Taslimi P., Farzaliyev V., Mammadyarova X., Sujayev A., TÜZÜN B., KOÇYIĞIT Ü. M., Alwasel S., GÜLÇİN İ.
Journal Of Biomolecular Structure & Dynamics, vol.40, no.1, pp.236-248, 2022 (SCI-Expanded)
- CV. **Biological Activity and Molecular Docking Study of Some Bicyclic Structures: Antidiabetic and Anticholinergic Potentials**
Taslimi P., Akhundova F., Kurbanova M., TÜRKAN F., TÜZÜN B., Sujayev A., Sadeghian N., Maharramov A., Farzaliyev V., GÜLÇİN İ.
POLYCYCLIC AROMATIC COMPOUNDS, vol.42, no.9, pp.6003-6016, 2022 (SCI-Expanded)
- CVI. **1,2,3-Triazole substituted phthalocyanine metal complexes as potential inhibitors for anticholinesterase and antidiabetic enzymes with molecular docking studies**
KOÇYIĞIT Ü. M., TASLİMİ P., TÜZÜN B., YAKAN H., MUĞLU H., GÜZEL E.
Journal Of Biomolecular Structure & Dynamics, vol.40, no.10, pp.4429-4439, 2022 (SCI-Expanded)
- CVII. **Anti-quorum sensing activity in Pseudomonas aeruginosa PA01 of benzimidazolium salts: electronic, spectral and structural investigations as theoretical approach**
ÖNEM E., TÜZÜN B., AKKOÇ S.

- JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS, vol.40, no.15, pp.6845-6856, 2022 (SCI-Expanded)
- CVIII. Metal contained Phthalocyanines with 3,4-Dimethoxyphenethoxy substituents: their anticancer, antibacterial activities and their inhibitory effects on some metabolic enzymes with molecular docking studies**
Taslimi P., TÜRKAN F., Gungordu Solgun D., Aras A., ERDEN Y., ÇELEBİOĞLU H. U., TÜZÜN B., Ağırtaş M. S., Gunay S., GÜLÇİN İ.
JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS, vol.40, no.7, pp.2991-3002, 2022 (SCI-Expanded)
- CIX. Co and Zn Metal Phthalocyanines with Bulky Substituents: Anticancer, Antibacterial Activities and Their Inhibitory Effects on Some Metabolic Enzymes with Molecular Docking Studies**
TÜRKAN F., Taslimi P., Cabir B., Ağırtaş M. S., ERDEN Y., ÇELEBİOĞLU H. U., TÜZÜN B., BURSAL E., GÜLÇİN İ.
POLYCYCLIC AROMATIC COMPOUNDS, vol.42, no.7, pp.4475-4486, 2022 (SCI-Expanded)
- CX. Synthesis, crystal structure, DFT, alpha-glucosidase and alpha-amylase inhibition and molecular docking studies of (E)-N'-(4-chlorobenzylidene)-5-phenyl-1H-pyrazole-3-carbohydrazide**
Karrouchi K., Fettach S., Anouar E. H., TÜZÜN B., Radi S., Alharthi A. I., Ghabbour H. A., Mabkhot Y. N., Faouzi M. E. A., Ansar M., et al.
JOURNAL OF MOLECULAR STRUCTURE, vol.1245, 2021 (SCI-Expanded)
- CXI. Investigation of structural, electronical and in vitro cytotoxic activity properties of some heterocyclic compounds**
AKKOÇ S., TÜZÜN B., Ozalp A., KÖKBUDAK Z.
JOURNAL OF MOLECULAR STRUCTURE, vol.1246, 2021 (SCI-Expanded)
- CXII. Structurally diverse heterobimetallic Pb(II)-Salen complexes mechanistic notion of cytotoxic activity against neuroblastoma cancer cell: Synthesis, characterization, protein-ligand interaction profiler, and intuitions from DFT**
Majumdar D., TÜZÜN B., Pal T. K., Saini R., Bankura K., Mishra D.
POLYHEDRON, vol.210, 2021 (SCI-Expanded)
- CXIII. Cytotoxic effect, spectroscopy, DFT, enzyme inhibition, and molecular docking studies of some novel mesitylamino propanols: Antidiabetic and anticholinergics and anticancer potentials**
Khalilov A. N., TÜZÜN B., Taslimi P., TAŞ A., TUNÇBİLEK Z., Cakmak N. K.
JOURNAL OF MOLECULAR LIQUIDS, vol.344, 2021 (SCI-Expanded)
- CXIV. New anti-viral drugs for the treatment of COVID-19 instead of favipiravir**
Aktaş A., Tüzün B., Aslan R., Sayın K., Ataseven H.
JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS, vol.39, no.18, pp.7263-7273, 2021 (SCI-Expanded)
- CXV. Synthesis, bioinformatics and biological evaluation of novel pyridine based on 8-hydroxyquinoline derivatives as antibacterial agents: DFT, molecular docking and ADME/T studies**
Rbaa M., Oubihi A., Hajji H., TÜZÜN B., Hichar A., Anouar E. H., Berdimurodov E., Ajana M. A., Zarrouk A., Lakhrissi B.
JOURNAL OF MOLECULAR STRUCTURE, vol.1244, 2021 (SCI-Expanded)
- CXVI. Tetra-substituted phthalocyanines bearing thiazolidine derivatives: synthesis, anticancer activity on different cancer cell lines, and molecular docking studies**
BİLGİÇLİ A. T., Hepokur C., Bilgili H. G., TÜZÜN B., GÜNSEL A., MISİR S., ZENGİN M., YARAŞIR M. N.
DALTON TRANSACTIONS, vol.50, no.43, pp.15778-15792, 2021 (SCI-Expanded)
- CXVII. Octa-substituted Zinc(II), Cu(II), and Co(II) phthalocyanines with 1-(4-hydroxyphenyl)propane-1-one: Synthesis, sensitive protonation behaviors, Ag(I) induced H-type aggregation properties, antibacterial-antioxidant activity, and molecular docking studies**
BİLGİÇLİ A. T., Kandemir T., TÜZÜN B., Ariduru R., GÜNSEL A., Abak C., YARAŞIR M. N., ARABACI G.
APPLIED ORGANOMETALLIC CHEMISTRY, vol.35, 2021 (SCI-Expanded)
- CXVIII. Synthesis, biological activity and docking calculations of bis-naphthoquinone derivatives from Lawsone**
Riaz M. T., Yaqub M., Shafiq Z., Ashraf A., Khalid M., Taslimi P., TAŞ R., TÜZÜN B., GÜLÇİN İ.
BIOORGANIC CHEMISTRY, vol.114, 2021 (SCI-Expanded)
- CXIX. Cytotoxic effects, carbonic anhydrase isoenzymes, alpha-glycosidase and acetylcholinesterase inhibitory properties, and molecular docking studies of heteroatom-containing sulfonyl hydrazones**

derivatives

- Celebioglu H. U., Erden Y., Hamurcu F., Taslimi P., Şentürk O. S., Ozmen U. O., TÜZÜN B., GÜLÇİN İ.
JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS, vol.39, no.15, pp.5539-5550, 2021 (SCI-Expanded)
- CXX. **Synthesis of (4R)-2-(3-hydroxyphenyl)thiazolidine-4-carboxylic acid substituted phthalocyanines: Anticancer activity on different cancer cell lines and molecular docking studies**
BİLGIÇLİ A. T., Genc Bilgili H., Hepokur C., TÜZÜN B., GÜNSEL A., ZENGİN M., YARAŞIR M. N.
APPLIED ORGANOMETALLIC CHEMISTRY, vol.35, no.7, 2021 (SCI-Expanded)
- CXXI. **Synthesis and docking calculations of tetrafluoronaphthalene derivatives and their inhibition profiles against some metabolic enzymes**
Erdogan M., Taslimi P., TÜZÜN B.
ARCHIV DER PHARMAZIE, vol.354, no.6, 2021 (SCI-Expanded)
- CXXII. **Evaluation of potential anti-RNA-dependent RNA polymerase (RdRP) drugs against the newly emerged model of COVID-19 RdRP using computational methods**
Poustforoosh A., Hashemipour H., TÜZÜN B., Pardakhty A., Mehrabani M., Nematollahi M. H.
BIOPHYSICAL CHEMISTRY, vol.272, 2021 (SCI-Expanded)
- CXXIII. **Synthesis, molecular docking, and biological activities of new cyanopyridine derivatives containing phenylurea**
GEZEĞEN H., Gurdere M. B., Dincer A., Ozbek O., KOÇYİĞİT Ü. M., Taslimi P., TÜZÜN B., Budak Y., Ceylan M.
ARCHIV DER PHARMAZIE, vol.354, no.4, 2021 (SCI-Expanded)
- CXXIV. **Quantum chemical study of thiazole derivatives as corrosion inhibitors based on density functional theory**
TÜZÜN B., Bhawsar J.
ARABIAN JOURNAL OF CHEMISTRY, vol.14, no.2, 2021 (SCI-Expanded)
- CXXV. **Are clarithromycin, azithromycin and their analogues effective in the treatment of COVID19**
Gedikli M. A., Tuzun B., Aktas A., Sayin K., Ataseven H.
BRATISLAVA MEDICAL JOURNAL-BRATISLAVSKE LEKARSKE LISTY, vol.122, no.2, pp.101-110, 2021 (SCI-Expanded)
- CXXVI. **Efficient synthesis and molecular docking studies of new pyrimidine-chromeno hybrid derivatives as potential antiproliferative agents**
Yavuz S. C., AKKOÇ S., TÜZÜN B., ŞAHİN O., SARIPINAR E.
SYNTHETIC COMMUNICATIONS, vol.51, no.14, pp.2135-2159, 2021 (SCI-Expanded)
- CXXVII. **The biological activities, molecular docking studies, and anticancer effects of 1-arylsulphonylpyrazole derivatives**
Taslimi P., ERDEN Y., Mamedov S., Zeynalova L., Ladokhina N., TAŞ R., TÜZÜN B., Sujayev A., Sadeghian N., Alwasel S. H., et al.
JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS, vol.39, no.9, pp.3336-3346, 2021 (SCI-Expanded)
- CXXVIII. **Could boron-containing compounds (BCCs) be effective against SARS-CoV-2 as anti-viral agent?**
Cetiner E., Sayin K., Tuzun B., ATASEVEN H.
BRATISLAVA MEDICAL JOURNAL-BRATISLAVSKE LEKARSKE LISTY, vol.122, no.4, pp.263-269, 2021 (SCI-Expanded)
- CXXIX. **Could Peganum harmala be effective in the treatment of COVID-19?**
Tuzun B., Nasibova T., Garaev E., Sayin K., ATASEVEN H.
BRATISLAVA MEDICAL JOURNAL-BRATISLAVSKE LEKARSKE LISTY, vol.122, no.9, pp.670-679, 2021 (SCI-Expanded)
- CXXX. **Determination of anticancer properties and inhibitory effects of some metabolic enzymes including acetylcholinesterase, butyrylcholinesterase, alpha-glycosidase of some compounds with molecular docking study**
Turkan F., Taslimi P., Abdalrazaq S. M., Aras A., Erden Y., Celebioglu H. U., TÜZÜN B., Ağırtaş M. S., GÜLÇİN İ.
JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS, vol.39, no.10, pp.3693-3702, 2021 (SCI-Expanded)
- CXXXI. **Could boron compounds be effective against SARS-CoV-2?**
ATASEVEN H., SAYIN K., TÜZÜN B., GEDİKLİ M. A.

- BRATISLAVA MEDICAL JOURNAL-BRATISLAVSKE LEKARSKE LISTY, vol.122, no.10, pp.753-758, 2021 (SCI-Expanded)
- CXXXII. **Determination of the inhibition profiles of pyrazolyl-thiazole derivatives against aldose reductase and alpha-glycosidase and molecular docking studies**
Demir Y., Taslimi P., KOÇYİĞİT Ü. M., Akkus M., Ozaslan M. S., Duran H. E., Budak Y., TÜZÜN B., Gurdere M. B., CEYLAN M., et al.
ARCHIV DER PHARMAZIE, vol.353, no.12, 2020 (SCI-Expanded)
- CXXXIII. **Investigation of structural, spectral, electronic, and biological properties of 1,3-disubstituted benzimidazole derivatives**
AKKOÇ S., TÜZÜN B., İLHAN İ. Ö., AKKURT M.
JOURNAL OF MOLECULAR STRUCTURE, vol.1219, 2020 (SCI-Expanded)
- CXXXIV. **Bioactivity and molecular docking studies of some nickel complexes: New analogues for the treatment of Alzheimer, glaucoma and epileptic diseases**
Kisa D., Korkmaz N., Taslimi P., TÜZÜN B., Tekin S., Karadag A., Sen F.
BIOORGANIC CHEMISTRY, vol.101, 2020 (SCI-Expanded)
- CXXXV. **Novel propanolamine derivatives attached to 2-metoxifenol moiety: Synthesis, characterization, biological properties, and molecular docking studies**
Bilgicli H. G., Ergon D., Taslimi P., TÜZÜN B., Kuru I. A., Zengin M., GÜLÇİN İ.
BIOORGANIC CHEMISTRY, vol.101, 2020 (SCI-Expanded)
- CXXXVI. **Anti-corrosion performance of 8-hydroxyquinoline derivatives for mild steel in acidic medium: Gravimetric, electrochemical, DFT and molecular dynamics simulation investigations**
Douche D., Elmsellem H., Anouar E. H., Guo L., Hafez B., TÜZÜN B., El Louzi A., Bougrin K., Karrouchi K., Himmi B.
JOURNAL OF MOLECULAR LIQUIDS, vol.308, 2020 (SCI-Expanded)
- CXXXVII. **Turn-on fluorescent probe for Zn²⁺ ions based on thiazolidine derivative**
Bilgicli H., Bilgicli A. T., Günsel A., TÜZÜN B., Ergon D., Yarasir M. N., Zengin M.
APPLIED ORGANOMETALLIC CHEMISTRY, vol.34, no.6, 2020 (SCI-Expanded)
- CXXXVIII. **Molecular docking and 4D-QSAR model of methanone derivatives by electron conformational-genetic algorithm method**
TÜZÜN B., SARIPINAR E.
JOURNAL OF THE IRANIAN CHEMICAL SOCIETY, vol.17, no.5, pp.985-1000, 2020 (SCI-Expanded)
- CXXXIX. **The Water-Soluble Peripheral Substituted Phthalocyanines as Corrosion Inhibitors for Copper in 0.1 N HCl: Gravimetric, Electrochemical, SEM-EDS, and Quantum Chemical Calculations**
Akin M., Günsel A., Bilgicli A. T., TÜZÜN B., Arabaci G., ŞAKI N., Yarasir M. N.
PROTECTION OF METALS AND PHYSICAL CHEMISTRY OF SURFACES, vol.56, no.3, pp.609-618, 2020 (SCI-Expanded)
- CXL. **Novel carvacrol based new oxypropanolamine derivatives: Design, synthesis, characterization, biological evaluation, and molecular docking studies**
Bytyqi-Damoni A., Kestane A., Taslimi P., TÜZÜN B., Zengin M., Bilgicli H. G., GÜLÇİN İ.
JOURNAL OF MOLECULAR STRUCTURE, vol.1202, 2020 (SCI-Expanded)
- CXLI. **The new ball-type zinc phthalocyanine with S-S bridge; Synthesis, computational and photophysicochemical properties**
Bilgicli A. T., Bilgicli H. G., Günsel A., Piskin H., TÜZÜN B., Yarasir M. N., Zengin M.
JOURNAL OF PHOTOCHEMISTRY AND PHOTOBIOLOGY A-CHEMISTRY, vol.389, 2020 (SCI-Expanded)
- CXLII. **Investigation of pyrazolyl derivatives schiff base ligands and their metal complexes used as anti-cancer drug**
TÜZÜN B.
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, vol.227, 2020 (SCI-Expanded)
- CXLIII. **Novel biologically active metallophthalocyanines as promising antioxidant-antibacterial agents: Synthesis, characterization and computational properties**
Günsel A., Kobyaoğlu A., Bilgicli A. T., TÜZÜN B., Tosun B., Arabaci G., Yarasir M. N.

JOURNAL OF MOLECULAR STRUCTURE, vol.1200, 2020 (SCI-Expanded)

- CXLIV. **Optoelectronic parameters of peripherally tetra-substituted copper(ii) phthalocyanines and fabrication of a photoconductive diode for various conditions**
Gunsel A., Bilgicli A. T., Piskin H., Tuzun B., Yarasir M. N., Gunduz B.
NEW JOURNAL OF CHEMISTRY, vol.44, no.2, pp.369-380, 2020 (SCI-Expanded)
- CXLV. **How do arbidol and its analogs inhibit the SARS-CoV-2?**
Aktas A., Tuzun B., Kafa T. A. H., Sayin K., Ataseven H.
Bratislavske lekarske listy, vol.121, no.10, pp.705-711, 2020 (SCI-Expanded)
- CXLVI. **Novel tribenzylaminobenzosulphonylimine based on their pyrazine and pyridazines: Synthesis, characterization, antidiabetic, anticancer, anticholinergic, and molecular docking studies**
Mamedova G., Mahmudova A., Mamedov S., Erden Y., Taslimi P., TÜZÜN B., Tas R., Farzaliyev V., Sujayev A., Alwasel S. H., et al.
BIOORGANIC CHEMISTRY, vol.93, 2019 (SCI-Expanded)
- CXLVII. **Synthesis, characterization, biological evaluation, and molecular docking studies of some piperonyl-based 4-thiazolidinone derivatives**
Bilgicli H. G., Taslimi P., Akyuz B., TÜZÜN B., GÜLÇİN İ.
ARCHIV DER PHARMAZIE, vol.353, no.1, 2019 (SCI-Expanded)
- CXLVIII. **Synthesis of non-peripherally tetra-substituted copper(ii) phthalocyanines: characterization, optical and surface properties, fabrication and photo-electrical properties of a photosensitive diode**
Gunsel A., Bilgicli A. T., Piskin H., TÜZÜN B., Yarasir M. N., Gunduz B.
DALTON TRANSACTIONS, vol.48, no.39, pp.14839-14852, 2019 (SCI-Expanded)
- CXLIX. **Comparison of spectroscopic, electronic, theoretical, optical and surface morphological properties of functional manganese(III) phthalocyanine compounds for various conditions**
Gunsel A., Bilgicli A. T., Piskin H., TÜZÜN B., Delibas N. C., Yarasir M. N., Gunduz B.
JOURNAL OF MOLECULAR STRUCTURE, vol.1193, pp.247-264, 2019 (SCI-Expanded)
- CL. **Synthesis of tetra-substituted phthalocyanines bearing 2-(ethyl(m-tolyl) amino)ethanol: Computational and photophysical studies**
GÜNSEL A., BİLGİÇLİ A. T., TÜZÜN B., PISKIN H., YAŞA ATMACA G., ERDOĞMUŞ A., YARAŞIR M. N.
JOURNAL OF PHOTOCHEMISTRY AND PHOTOBIOLOGY A-CHEMISTRY, vol.373, pp.77-86, 2019 (SCI-Expanded)
- CLI. **Selective chemosensor phthalocyanines for Pd²⁺ ions; synthesis, characterization, quantum chemical calculation, photochemical and photophysical properties**
GÜNSEL A., Kirbac E., TÜZÜN B., ERDOĞMUŞ A., BİLGİÇLİ A. T., YARAŞIR M. N.
JOURNAL OF MOLECULAR STRUCTURE, vol.1180, pp.127-138, 2019 (SCI-Expanded)
- CLII. **Investigations over optical properties of boron complexes of benzothiazolines**
TÜZÜN B., SAYIN K.
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, vol.208, pp.48-56, 2019 (SCI-Expanded)
- CLIII. **Synthesis of tetra-substituted metallophthalocyanines: Spectral, structural, computational studies and investigation of their photophysical and photochemical properties**
Guzel E., GÜNSEL A., TÜZÜN B., YAŞA ATMACA G., BİLGİÇLİ A. T., ERDOĞMUŞ A., YARAŞIR M. N.
POLYHEDRON, vol.158, pp.316-324, 2019 (SCI-Expanded)
- CLIV. **Anticorrosive Effects of Some Thiophene Derivatives Against the Corrosion of Iron: A Computational Study**
Guo L., Safi Z. S., KAYA S., Shi W., TÜZÜN B., ALTUNAY N., KAYA C.
FRONTIERS IN CHEMISTRY, vol.6, 2018 (SCI-Expanded)
- CLV. **4D-QSAR Study of Some Pyrazole Pyridine Carboxylic Acid Derivatives By Electron Conformational-Genetic Algorithm Method**
TÜZÜN B., ÇAĞLAR YAVUZ S., Sabanci N., SARIPINAR E.
CURRENT COMPUTER-AIDED DRUG DESIGN, vol.14, no.4, pp.370-384, 2018 (SCI-Expanded)
- CLVI. **Novel type ketone-substituted metallophthalocyanines: synthesis, spectral, structural, computational and anticancer studies**

- HEPOKUR C., GÜNSEL A., YARAŞIR M. N., BİLGİÇLİ A. T., TÜZÜN B., Tuzun G., Yaylim I.
RSC ADVANCES, vol.7, no.89, pp.56296-56305, 2017 (SCI-Expanded)
- CLVII. **Quantum chemical and molecular dynamic simulation studies for the prediction of inhibition efficiencies of some piperidine derivatives on the corrosion of iron**
KAYA S., Guo L., KAYA C., TÜZÜN B., Obot I. B., Tourir R., Islam N.
JOURNAL OF THE TAIWAN INSTITUTE OF CHEMICAL ENGINEERS, vol.65, pp.522-529, 2016 (SCI-Expanded)
- CLVIII. **Quantum chemical and molecular dynamics simulation studies on inhibition performances of some thiazole and thiadiazole derivatives against corrosion of iron**
KAYA S., KAYA C., Guo L., KANDEMİRLİ F., TÜZÜN B., Ugurlu I., Madkour L. H., SARAÇOĞLU M.
JOURNAL OF MOLECULAR LIQUIDS, vol.219, pp.497-504, 2016 (SCI-Expanded)
- CLIX. **Density Functional Theory (DFT) modeling and Monte Carlo simulation assessment of inhibition performance of some carbonyl Schiff bases for steel corrosion**
Obot I. B., KAYA S., KAYA C., TÜZÜN B.
PHYSICA E-LOW-DIMENSIONAL SYSTEMS & NANOSTRUCTURES, vol.80, pp.82-90, 2016 (SCI-Expanded)
- CLX. **Theoretical evaluation of triazine derivatives as steel corrosion inhibitors: DFT and Monte Carlo simulation approaches**
Obot I. B., KAYA S., KAYA C., TÜZÜN B.
RESEARCH ON CHEMICAL INTERMEDIATES, vol.42, no.5, pp.4963-4983, 2016 (SCI-Expanded)
- CLXI. **Theoretical evaluation of some benzotriazole and phosphono derivatives as aluminum corrosion inhibitors: DFT and molecular dynamics simulation approaches**
KAYA S., Banerjee P., Saha S. K., TÜZÜN B., KAYA C.
RSC ADVANCES, vol.6, no.78, pp.74550-74559, 2016 (SCI-Expanded)
- CLXII. **Determination of corrosion inhibition effects of amino acids: Quantum chemical and molecular dynamic simulation study**
KAYA S., TÜZÜN B., KAYA C., Obot I. B.
JOURNAL OF THE TAIWAN INSTITUTE OF CHEMICAL ENGINEERS, vol.58, pp.528-535, 2016 (SCI-Expanded)

Articles Published in Other Journals

- I. **Influence of ZnO Nanoparticle Size on Barrier Performance and Corrosion Protection of Poly(dimethylsiloxane)-Coated Q235 Steel in Chloride Environment: Bode and Computational Simulation Investigations**
Arukalam I. O., Uzochukwu I. N., TÜZÜN B., Dagdag O., Oguzie E. E.
Chemistry Africa, vol.7, no.2, pp.853-863, 2024 (ESCI)
- II. **Two adamantan-1-amine-based scaffolds: Synthesis, crystallographic synthons, TD/DFT calculations, in-depth molecular docking/ADME/T simulations, and shedding light on antibacterial/fungal activities**
Majumdar D., Elizabeth Philip J., TÜZÜN B., Sutradhar D., Roy S.
Results in Chemistry, vol.6, 2023 (ESCI)
- III. **Mathematical Modeling of the Biological Activity of a New Complex Compound Based on Palladium and Mexidol**
TÜZÜN B., Jafarova R., Bagirov I., Magerramova N., Nasibova T.
JOURNAL OF BIOCHEMICAL TECHNOLOGY, vol.14, 2023 (ESCI)
- IV. **Could Zingiber officinale plant be effective against Omicron BA.2.75 of SARS-CoV-2?**
SARAÇ H., DEMİRBAŞ A., TÜZÜN B.
Turkish Computational and Theoretical Chemistry, vol.7, no.3, pp.42-56, 2023 (Scopus)
- V. **Antioxidant Activity Properties of Extract of Turmeric (Curcuma longa L.) Plant**
SARAÇ H., TÜZÜN B.
Turkish Computational and Theoretical Chemistry, vol.8, no.2, pp.19-27, 2023 (Scopus)
- VI. **Could Momordica Charantia Be Effective In The Treatment of COVID19?**

TÜZÜN B., SAYIN K., ATASEVEN H.

CUMHURİYET SCIENCE JOURNAL, vol.43, no.2, pp.211-220, 2022 (Peer-Reviewed Journal)

- VII. **Exploring the multi-target enzyme inhibition potential of new sulfonamido-thiazoline derivatives; synthesis and computational studies**
Shafique I, Saeed A, Ahmed A, Shabir G, Ul-Hamid A, Khan A, TÜZÜN B., Kirici M., Taslimi P., Latif M.
Results in Chemistry, vol.4, 2022 (Scopus)
- VIII. **Reinvigorate the synthesis, spectroscopic findings, SEM morphology investigation, and antimicrobial silhouette of contemporary Salen ligands: A comprehensive DFT landscape**
Majumdar D., Philip J. E., Roy S., TÜZÜN B.
Results in Chemistry, vol.4, pp.100574, 2022 (Scopus)
- IX. **Some old 2-(4-(Aryl)-thiazole-2-yl)-3a,4,7,7a-tetrahydro-1H-4,7-tethanoisoindole-1,3(2H)-dione derivatives: Synthesis, inhibition effects and molecular docking studies on Aldose reductase and α -Glycosidase**
TASLIMI P., DEMİR Y., DURAN H. E., KOÇYİĞİT Ü. M., TÜZÜN B., ASLAN O. N., CEYLAN M., GÜLÇİN İ.
Cumhuriyet Science Journal, vol.42, 2021 (Peer-Reviewed Journal)
- X. **Examination of anti-oxidant properties and molecular docking parameters of some compounds in human body**
TÜZÜN B.
Turkish Computational and Theoretical Chemistry, vol.4, no.2, pp.76-87, 2020 (Scopus)
- XI. **Experimental and Theoretical Study of Effect of Allium sativum Extracts as Corrosion Inhibitor on Mild Steel in 1 M HCl Medium**
Ojha L. K., TÜZÜN B., Bhawsar J.
Journal of Bio- and Tribo-Corrosion, vol.6, no.2, 2020 (Scopus)
- XII. **Investigation of the Molecules Obtained from Marijuana: Computational Study of Spectral, Structural and Docking**
TÜZÜN B.
Journal of Physical and Theoretical Chemistry, vol.16, pp.59-74, 2020 (Peer-Reviewed Journal)
- XIII. **Investigation of Benzimidazole Derivates as Corrosion Inhibitor by DFT**
TÜZÜN B.
cumhuriyet science journal, vol.40, no.2, pp.396-405, 2019 (Peer-Reviewed Journal)
- XIV. **Investigation of DNA-RNA Molecules for the Efficiency and Activity of Corrosion Inhibition by DFT and Molecular Docking**
TÜZÜN B., KAYA C.
Journal of Bio- and Tribo-Corrosion, vol.4, no.4, 2018 (Scopus)
- XV. **Electrochemical and Computational Studies of Some Triazepine Carboxylate Compounds as Acid Corrosion Inhibitors for Mild Steel**
KA A., tour r., GALAI M., MOUHSINE H., OUAKKI M., KAYA S., TÜZÜN B., Boukhris S., TOUHAMI E., KACIMI E.
Journal of Bio- and Tribo-Corrosion, vol.4, no.3, pp.1-18, 2018 (Scopus)
- XVI. **Theoretical Evaluation of Six Indazole Derivatives as Corrosion Inhibitors Based on DFT**
TÜZÜN B.
Turkish Computational and Theoretical Chemistry, vol.2, no.1, pp.12-22, 2018 (Scopus)
- XVII. **Conceptual Density Functional Theoretical Investigation of the Corrosion Inhibition Efficiencies of Some Molecules Containing Mercapto (-SH) Group**
KAYA S., TÜZÜN B., KAYA C.
Current Physical Chemistry, vol.7, no.2, pp.147-153, 2017 (Peer-Reviewed Journal)
- XVIII. **4D-QSAR analysis and pharmacophore modeling: propoxy methylphenyl oxasiazole derivatives by electron conformatitional-genetic algorithm method**
TÜZÜN B., ÇAĞLAR YAVUZ S., SARIPINAR E.
Journal of Physical and Theoretical Chemistry, vol.14, no.2, pp.149-164, 2017 (Peer-Reviewed Journal)
- XIX. **Selectivity of Salicylaloxime and its Derivatives**
TÜZÜN B.

Books & Book Chapters

- I. **The Evolution of Pyrimidine Bases**
KEBABCİ Ö., TÜZÜN B.
in: The Chemistry of Pyrimidine Derivatives, Schneider Barry, Editor, Nova Science Publishers, New York, pp.47-67, 2024
- II. **Polymeric nanoparticles and their composites in corrosion inhibition**
ÇELİK M. S., ÇETİNKAYA H. F., ÇETİNKAYA S., TÜZÜN G., TÜZÜN B.
in: Corrosion Prevention Nanoscience: Nanoengineering Materials and Technologies, Turhlievich Berdimurodov Elyor, Verma Chandrabhan, Editor, Walter de Gruyter GmbH, pp.135-145, 2023
- III. **MXenes and their composites as corrosion prevention**
AKSU A., ÇETİNKAYA H. F., ÇETİNKAYA S., TÜZÜN G., TÜZÜN B.
in: Corrosion Prevention Nanoscience: Nanoengineering Materials and Technologies, Turhlievich Berdimurodov Elyor, Verma Chandrabhan, Editor, Walter de Gruyter GmbH, pp.53-65, 2023
- IV. **The Potential of Medicinal and Aromatic Plants to Prevent Prostate Cancer**
ÇETİNKAYA S., TÜZÜN B.
in: Horizons in Cancer Research, Watanabe Hiroto S., Editor, Nova Science Publishers, New York, pp.117-142, 2023
- V. **Omicron: Emergence, Detection, and Response**
ÇETİNKAYA S., ÖZBİLÜM ŞAHİN N., YENİDÜNYA A. F., TÜZÜN B.
in: Advances in Health and Disease, Duncan, Lowell T., Editor, Nova Science Publishers, New York, pp.161-197, 2023
- VI. **MİDE KANSERİNE KİMYACI BAKIŞI**
TÜZÜN B., SAYIN K.
in: Mide Kanseri Multidisipliner Bakış, , Editor, cumhuriyet üniversitesi, Sivas, pp.261-276, 2022
- VII. **Applications of the Effectiveness of Corrosion Inhibitors with Computational Methods and Molecular Dynamics Simulation**
ERDOĞAN Ş., TÜZÜN B.
in: Corrosion: Fundamentals and Protection Mechanisms, , Editor, BoD–Books on Demand, pp.51-71, 2022
- VIII. **Development process for eco-friendly corrosion inhibitors**
Rbaa M., Galai M., Dagdag O., Guo L., TÜZÜN B., Berdimurodov E., Zarrouk A., Lakhrici B.
in: Eco-Friendly Corrosion Inhibitors, , Editor, elsevier, pp.27-42, 2022
- IX. **MİDE KANSERİ VE İN SİLİKO ÇALIŞMALAR**
TÜZÜN B., SAYIN K.
in: Mide Kanseri Multidisipliner Bakış, , Editor, cumhuriyet üniversitesi, Sivas, pp.195-216, 2022
- X. **Triazepines Compounds as Novel Synthesized Corrosion Inhibitors: State of Play and Perspectives**
Alaoui K., Abousalem A., TÜZÜN B., Kacimi Y. E.
in: New Challenges and Industrial Applications for Corrosion Prevention and Control, Younes El Kacimi, Savas Kaya, Rachid Touri, Editor, IGI global publisher of times knowledge, -, pp.156-186, 2020

Refereed Congress / Symposium Publications in Proceedings

- I. **Breast cancer Properties of Extract of Ceratonia siliqua**
ÇETİNKAYA S., TÜZÜN B.
3 rd International Conference on Scientific and Academic Research, Konya, Turkey, 25 - 26 December 2023
- II. **Breast cancer Properties of Extract of Artemisia absinthium**
ÇETİNKAYA S., TÜZÜN B.
3 rd International Conference on Scientific and Academic Research, Konya, Turkey, 25 - 26 December 2023

- III. **Antioxidant Properties of *Lycium barbarum* Extracts**
ÇETİNKAYA S., TÜZÜN B.
PROCEEDINGS OF IKSTC 2023 - 2ND INTERNATIONAL KARATEKİN SCIENCE AND TECHNOLOGY CONFERENCE,
Çankırı, Turkey, 21 - 22 December 2023
- IV. **Immobilization of Microbial Pectinase to Chitosan-Based Composite: Experimental, DFT, and Molecular Docking Studies**
AKSU A., ÇETİNKAYA S., YENİDÜNYA A. F., ÇETİNUS Ş., GEZEĞEN H., TÜZÜN B.
2nd International Conference on Engineering, Natural and Social Sciences, Konya, Turkey, 04 April 2023
- V. **Colon cancer Properties of Extract of Saffron (*Crocus sativus* L.) Plant**
ÇETİNKAYA S., TÜZÜN B.
1st International Conference on Engineering, Natural and Social Sciences, Konya, Turkey, 20 December 2022
- VI. **Prostate cancer Properties of Extract of *Olea europaea* Plant**
ÇETİNKAYA S., TÜZÜN B.
1st International Conference on Engineering, Natural and Social Sciences, Konya, Turkey, 20 December 2022
- VII. **Breast cancer Properties of Extract of *Viscum album* Plant**
ÇETİNKAYA S., TÜZÜN B.
1st International Conference on Engineering, Natural and Social Sciences, Konya, Turkey, 20 December 2022
- VIII. **Breast cancer Properties of Extract of *Rosa damascena* Plant**
ÇETİNKAYA S., TÜZÜN B.
1st International Conference on Engineering, Natural and Social Sciences, Konya, Turkey, 20 December 2022
- IX. **EFFECT OF CARBONITRILE-BASED COMPOUND ON OXIDATIVE STRESS RELATED GENES IN LUNG CANCER CELLS**
Tunçbilek Z., Ağbektaş T., Taş A., Tüzün B., Siliğ Y.
3. International Cancer Days, Sivas, Turkey, 15 - 17 September 2022, pp.290
- X. **comparison of the activities of diaryl urea derivatives by in silico and in vitro methods**
karataş ş. n., TÜZÜN B.
3. international cancer days, Sivas, Turkey, 15 September 2022
- XI. **EFFECT OF CARBONITRILE-BASED COMPOUND ON OXIDATIVE STRESS RELATED GENES IN LUNG CANCER CELLS**
TUNÇBİLEK Z., AĞBEKTAŞ T., TAŞ A., TÜZÜN B., SİLİĞ Y.
III. INTERNATIONAL CANCER DAYS, Turkey, 14 - 16 September 2022
- XII. **DETERMINATION OF THE ACTIVITIES OF HORSE CHESTNUT (*Aesculus hippocastanum* L.) EXTRACT AGAINST LIVER CANCER PROTEINS**
SARAÇ H., TÜZÜN B.
International Antalya Scientific Research and Innovative Studies Congress, 18 - 21 December 2021
- XIII. **ACTIVITIES OF DANDELION (*Taraxacum officinale*) EXTRACT AGAINST BREAST CANCER PROTEINS**
DURUKAN H., TÜZÜN B., SARAÇ H., DEMİRBAŞ A.
International Antalya Scientific Research and Innovative Studies Congress, 18 - 21 December 2021
- XIV. **Activities of *Laurus nobilis* L. extract against Liver cancer proteins**
DURUKAN H., TÜZÜN B.
International Anatolian Congress on Medicinal and Aromatic Plants, 16 - 18 November 2021
- XV. **Activities of *Crocus sativus* L. extract against Liver cancer proteins**
DURUKAN H., TÜZÜN B.
1st International Conference on Applied Engineering and Natural Sciences, Konya, Turkey, 1 - 03 November 2021
- XVI. **Activities of *Mentha pulegium* extract against breast cancer proteins**
SARAÇ H., TÜZÜN B.
1st International Conference on Applied Engineering and Natural Sciences, Konya, Turkey, 1 - 03 November 2021
- XVII. **Activities of *Helichrysum arenarium* extract against Lung cancer proteins**
DEMİRBAŞ A., TÜZÜN B.
1st International Conference on Applied Engineering and Natural Sciences, Konya, Turkey, 1 - 03 November 2021
- XVIII. **INVESTIGATION OF ANTI-CANCER PROPERTIES OF NOVEL EUGENOL BEARING OXYPROPANOLAMINES**

- TÜZÜN B.
II. INTERNATIONAL CANCER DAYS, Sivas, Turkey, 16 - 18 September 2021
- XIX. INVESTIGATION OF SPECTROSCOPIC, THEORETICAL AND MOLECULAR DOCKING OF IMIDAZOLE DERIVATIVES**
TÜZÜN B.
II. INTERNATIONAL CANCER DAYS, Sivas, Turkey, 16 - 18 September 2021
- XX. INVESTIGATION OF SPECTROSCOPIC AND THEORETICAL OF PYRIDYL-CARBOXYLATE SCHIFF-BASE**
TÜZÜN B.
international journal of mathematics, engineering, natural medical sciences, 14 - 15 December 2019
- XXI. INVESTIGATION OF SPECTROSCOPIC AND THEORETICAL OF CHALCONE DERIVATIVES**
TÜZÜN B.
international journal of mathematics, engineering, natural medical sciences, 14 - 15 December 2019
- XXII. INVESTIGATION OF BIOLOGICAL ACTIVITY PROPERTIES OF DERIVATIVES OF PROPYLIDENEHYDRAZINEYL PYRIDINE**
TÜZÜN B.
Inorganic chemistry congress, 19 - 22 July 2019
- XXIII. INVESTIGATION OF SPECTROSCOPIC AND THEORETICAL OF 1-2 DIAMINOPROPANE DERIVATIVES**
TÜZÜN B.
inorganic chemistry congress, 19 - 22 July 2019
- XXIV. The computational analysis on NLO properties and molecular docking studies for some cyclophosphazenes compounds**
ERKAN KARİPER S., TÜZÜN B.
2nd International Symposium on Innovative Approaches in Scientific Studies, 30 November - 02 December 2018
- XXV. Investigation of Spectroscopic, Theoretical and Molecular Docking of methoxyphenyl derivatives**
TÜZÜN B., ERKAN KARİPER S.
2nd International Symposium on Innovative Approaches in Scientific Studies, 30 November - 02 December 2018
- XXVI. The structural, spectroscopic and molecular docking analysis on phosphorus-nitrogen compounds**
ERKAN KARİPER S., TÜZÜN B.
2nd International Symposium on Innovative Approaches in Scientific Studies, 30 November - 02 December 2018
- XXVII. Investigation of anti-cancer properties of derivatives of 2-benzimidazole**
TÜZÜN B., ERKAN KARİPER S.
2nd International Symposium on Innovative Approaches in Scientific Studies, 30 November - 02 December 2018
- XXVIII. Investigation of Spectroscopic, Theoretical and Molecular Docking of vanillin thiosemicarbazone derivatives**
TÜZÜN B., ERKAN S.
2nd international symposium on innovative approaches in scientific studies, 30 November - 02 December 2018
- XXIX. Investigation of Spectroscopic, Theoretical and Molecular Docking of vanillin thiosemicarbazone derivatives**
TÜZÜN B., ERKAN KARİPER S.
2nd International Symposium on Innovative Approaches in Scientific Studies, 30 November - 02 December 2018
- XXX. Investigations of spectroscopic, theoretical and molecular docking of Benzothiazole based schiff base ligand and its metal complexes**
TÜZÜN B.
4th organic chemistry congress with international participation, 4 - 07 October 2018
- XXXI. Investigations of spectroscopic, theoretical and molecular docking of Pyrimidine Morpholine based schiff base ligand and its metal complexes,**
TÜZÜN B.
4th organic chemistry congress with international participation, 4 - 07 October 2018
- XXXII. Investigation of β -Diketonate Ligand and Metal Complexes: Molecular Docking and Spectroscopic Properties by Computational Chemistry Methods**
ERKAN KARİPER S., TÜZÜN B.

- International Conference on Physical Chemistry and Functional Materials, 19 - 21 June 2018
- XXXIII. **Examination of Vaniline Thiosemicarbazone Ligand and Trace Metal Cop-per Spectroscopic Properties by Computational Chemistry Methods**
ERKAN KARİPER S., TÜZÜN B.
International Trace Analysis Congress(iTAC 2018), Sivas, Turkey, 20 - 23 June 2018
- XXXIV. **Detailed examination of bis-NHC palladium (II) complex by DFT method**
ERKAN KARİPER S., SAYIN K., KARAKAŞ D., TÜZÜN B.
International conference on physical chemistry and functional materials, Elazığ, Turkey, 19 - 21 June 2018, pp.226
- XXXV. **Investigation of structural, spectral, electronic and biological properties of N-heterocyclic carbene Pd(II) complex**
ERKAN KARİPER S., SAYIN K., KARAKAŞ D., TÜZÜN B.
International conference on physical chemistry and functional materials, Elazığ, Turkey, 19 - 21 June 2018, pp.274
- XXXVI. **Investigations of Structural, Spectral, Electronic and Biological Properties of N-Heterocyclic Carbene Pd(II) Complex**
ERKAN KARİPER S., SAYIN K., KARAKAŞ D., TÜZÜN B.
International Conference on Physical Chemistry and Functional Materials, 19 - 21 June 2018
- XXXVII. **Investigation of Schiff Bases and Their Trace Metal (II) Complexes by Computational Chemistry Methods**
TÜZÜN B.
International Trace Analysis Congress, 19 - 21 June 2018
- XXXVIII. **Spectral analysis and molecular docking of metal complexes with bis(pyridine carboxamide) benzene ligand**
ERKAN KARİPER S., TÜZÜN B., SAYIN K.
International Conference on Physical Chemistry and Functional Materials, 19 - 21 June 2018
- XXXIX. **Detailed Examination of Bis-NHC Palladium (II) Complex by DFT Method**
ERKAN KARİPER S., SAYIN K., KARAKAŞ D., TÜZÜN B.
International Conference on Physical Chemistry and Functional Materials, 19 - 21 June 2018
- XL. **Metal complexes with pyrazoly direved: Spectral analysis and biological evaluation**
ERKAN KARİPER S., TÜZÜN B., SAYIN K.
International Conference on Physical Chemistry and Functional Materials, 19 - 21 June 2018
- XLI. **Investigation of Anticancer Properties of Cannabinoid Complexes By Computational Methods**
TÜZÜN B.
Uluslararası Katılımlı 6. İlaç Kimyası: İlaç Etkin MaddesiTasarımı, Sentezi, Üretimi ve Standardizasyonu Kongresi, 22 - 25 March 2018
- XLII. **4D-QSAR Study of Some Pyrimidine Derivatives By Electron Conformational-Genetic Algorithm Method**
TÜZÜN B., SARIPINAR E.
Uluslararası Katılımlı 6. İlaç Kimyası: İlaç Etkin MaddesiTasarımı, Sentezi, Üretimi ve Standardizasyonu Kongresi, 22 - 25 March 2018
- XLIII. **dft modeling and monte carlo simulation assessment of inhibition performance of some carbohydrazide schiff bases for stell corrosion**
TÜZÜN B., KAYA S.
international conference on techonology, engineering and science, 26 - 29 October 2017
- XLIV. **quantum chemical simulation studies on ihbition performances of some thiazole and thiadiazole derivatives against corrosion of iron**
TÜZÜN B., KAYA S., KAYA C.
2nd international gazi symposium series, 11 - 13 October 2017
- XLV. **determination of corrosion inhibition effets of amino acids:quantum chemical and molecular dynamic simulation study**
TÜZÜN B., KAYA S., KAYA C.
2nd international gazi symposium series, 11 - 13 October 2017

- XLVI. **investigations on small molecular dft and molecular dynamic simulation approaches**
TÜZÜN B., Tüzün G.
international congress on chemistry and materials science, 5 - 07 October 2017
- XLVII. **investigation via principal component analysis dft and molecular dynamics simulations approaches on the anticorrosive effect of some thiophene derivatives against the corrosion of iron**
TÜZÜN B., KAYA S.
international congress on chemistry and materials science, 5 - 07 October 2017
- XLVIII. **theoretical evaluation of triazine derivatives as stell corrosion inhibitors:dft**
TÜZÜN B., Tüzün G.
3.international turkish congress on molecular spectroscopy, 26 - 29 August 2017
- XLIX. **theoretical evaluation of triazine derivatives as stell corrosion inhibitors monte carlo simulation approache**
TÜZÜN B., KAYA S., KAYA C.
3. international turkish congress on molecular spectroscopy, 26 - 29 August 2017
- L. **4d-qsar ec-ga metodu ile pirimidin bileşik serisinin farmakofor grubunun belirlenmesi ve biyoaktivite hesabı**
TÜZÜN B., SARIPINAR E.
5. ilaç kimyası kongresi, 30 March - 02 April 2017
- LI. **4d-qsar ec-ga metodu ile oksadiazol bileşik serisinin farmakofor grubunun belirlenmesi ve biyoaktivite hesabı**
TÜZÜN B., SARIPINAR E.
5.ilac kimyası kongresi, 30 March - 02 April 2017
- LII. **4D QSAR EC GA METODU İLE PRİDİN KARBOKSİLİK ASİT BİLEŞİK SERİSİNİN FARMAKOFOR GRUBUNUN BELİRLENMESİ VE BİYOAKTİVİTE HESABI**
TÜZÜN B., SARIPINAR E.
4. ilaç kimyası kongresi, Aydın, Turkey, 17 - 20 March 2016
- LIII. **Efficien of carbamates as flatation collectors**
TÜZÜN B., YEKELER H.
chemical physics congress-IX, Turkey, 14 - 16 October 2010
- LIV. **Karbamatların Flotasyon Kolektörleri Olarak Etkinlikleri**
TÜZÜN B., YEKELER H.
24. ulusal kimya kongresi, Turkey, 29 June - 02 July 2010

Supported Projects

TÜZÜN B., Project Supported by Higher Education Institutions, Birinci seri geçiş metallerinin korozyonun inhibisyonunda yeni sentezlenmiş heterosiklik ligandların kullanılması ve moleküler modellemenin teorik olarak araştırılması, 2017 - Continues

Sayın K., Ataseven H., Taş A., Keklikçioğlu N., Tüzün B., Gezegen H., Özkaraca M., Görgülü A. O., Kanbur M., Keklikcioğlu Çakmak N., TUBITAK Project, Yeni Tıp Benzamidlerin Sentezi İle Histon Deasetilaz (Hdac) İnhibitörü Olarak Mide Kanseri İlaç Tasarımı, 2021 - 2024

Tüzün B., Project Supported by Higher Education Institutions, Thiosemikarbazan türevli organik bileşiklerin ve onların metal komplekslerinin yapısal, spektroskopik ve biyolojik aktivitelerinin hesaplamalı kimya metotları ile incelenmesi, 2018 - 2019

TÜZÜN B., Project Supported by Higher Education Institutions, Elektron Konformasyonel Genetik algoritma 4d qsar Metodu ile Piridin karboksilik Asit Oksadiazol Pirimidin ve Oksazol türevlerine ait farmakofor gruplarının belirlenmesi ve biyoaktivite hesabı, 2014 - 2018

TÜZÜN B., KAYA C., Project Supported by Higher Education Institutions, Fe METALİNİN KOROZYONUNU ENGELLEMEDE İNHİBİSYON ETKİLERİNİN YENİ SENTEZLENMİŞ HETEROSİKLİK BİLEŞİKLERİN KULLANILMASI VE MOLEKÜLER MODELLEME ÇALIŞMALARI, 2017 - 2017

KAYA C., KAYA S., TZN B., Project Supported by Higher Education Institutions, yeni sentezlenmiř heterosiklik bileřiklerin eřitli metallerin korozyonu karřısında inhibisyon etkilerinin teorik yntemler aracığıyla arařtırılması ve molekller modelle alıřmaları, 2016 - 2016

Metrics

Publication: 253

Citation (WoS): 1666

Citation (Scopus): 4126

H-Index (WoS): 21

H-Index (Scopus): 33