

## Prof. Dr. KORAY SAYIN

### Kişisel Bilgiler

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### Uluslararası Araştırmacı ID'leri

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Publons / Web Of Science ResearcherID: V-3704-2017

Yoksis Araştırmacı ID: 25762

### Eğitim Bilgileri

Doktora, Sivas Cumhuriyet Üniversitesi, Fen Bilimleri Enstitüsü, Kimya (Dr), Türkiye 2014 - 2017

Yüksek Lisans, Sivas Cumhuriyet Üniversitesi, Fen Bilimleri Enstitüsü, Kimya (YI) (Tezli), Türkiye 2012 - 2014

Lisans, Çukurova Üniversitesi, Fen-Edebiyat Fakültesi, Kimya Bölümü, Türkiye 2005 - 2009

### Yaptığı Tezler

Doktora, Hesaplamalı kimya yöntemleriyle bazı bor komplekslerinin yapısal ve elektronik özelliklerinin incelenmesi, Sivas Cumhuriyet Üniversitesi, Fen Bilimleri Enstitüsü, Kimya (Dr), 2017

Yüksek Lisans, Hesaplamalı kimya yöntemleri ile bazı platin(II) oksim komplekslerinin moleküler yapısının ve moleküler özelliklerinin araştırılması, Sivas Cumhuriyet Üniversitesi, Fen Bilimleri Enstitüsü, Kimya (YI) (Tezli), 2014

### Araştırma Alanları

İnorganik Kimya

### Akademik Unvanlar / Görevler

Doç. Dr., Sivas Cumhuriyet Üniversitesi, Fen Fakültesi, Kimya Bölümü, 2018 - Devam Ediyor

Dr. Öğr. Üyesi, Sivas Cumhuriyet Üniversitesi, Fen Fakültesi, Kimya Bölümü, 2018 - 2018

Araştırma Görevlisi, Sivas Cumhuriyet Üniversitesi, Fen Fakültesi, Kimya Bölümü, 2017 - 2018

Araştırma Görevlisi, Sivas Cumhuriyet Üniversitesi, Fen Bilimleri Enstitüsü, 2011 - 2017

### Akademik İdari Deneyim

Sivas Cumhuriyet Üniversitesi, Yeni Ve Yenilenebilir Enerji Kaynakları Uygulama Ve Araştırma Merkezi, 2019 - Devam Ediyor

Sivas Cumhuriyet Üniversitesi, Fen Fakültesi, Kimya Bölümü, 2018 - Devam Ediyor

### Verdiği Dersler

Organometalik Kimya, Lisans, 2019 - 2020  
Kimya, Lisans, 2019 - 2020  
Seminer Dersi, Yüksek Lisans, 2019 - 2020  
Genel Kimya, Lisans, 2019 - 2020  
Hesaplamalı Kimya Yöntemleri ve Uygulamaları II, Yüksek Lisans, 2018 - 2019  
Genel Kimya II, Lisans, 2018 - 2019  
Genel Kimya, Lisans, 2019 - 2020  
Koordinasyon Kimyası, Yüksek Lisans, 2019 - 2020  
Genel Kimya Laboratuvarı I, Lisans, 2019 - 2020  
Genel Kimya I, Lisans, 2019 - 2020  
Genel Kimya, Ön Lisans, 2019 - 2020  
Hesaplamalı Kimya Yöntemleri ve Uygulamaları I, Yüksek Lisans, 2019 - 2020  
GENEL KİMYA 2, Lisans, 2017 - 2018  
GENEL KİMYA, Lisans, 2017 - 2018

## SCI, SSCI ve AHCI İndekslerine Giren Dergilerde Yayınlanan Makaleler

- I. **Synthesis of novel isostere analogues of naphthyridines using CuI catalyst: DFT computations (FMO, MEP), molecular docking and ADME analysis**  
Prabha K., Rajendran S., Gnanamangai B. M., Mohan J B., SAYIN K., Prasad K. R., Tüzün G.  
Tetrahedron, cilt.168, 2024 (SCI-Expanded)
- II. **Enhanced Method for the Synthesis and Comprehensive Characterization of 1-(4-Phenylquinolin-2-yl)propan-1-one**  
Rajendran S., Montecinos R., Cisterna J., Prabha K., Rajendra Prasad K. J., Palakurthi S. S., Aljabali A. A. A., Naikoo G. A., Mishra V., Acevedo R., et al.  
ACS Omega, cilt.8, sa.46, ss.43573-43585, 2023 (SCI-Expanded)
- III. **New azo-azomethine based copper(II) and zinc(II) complexes: Synthesis, electrochemistry, photoluminescence properties, density functional theory calculations and molecular docking**  
Purtaş F., SAYIN K., Ceyhan G., Kose M., Kurtoglu M.  
Journal of Molecular Structure, cilt.1291, 2023 (SCI-Expanded)
- IV. **Optimization, spectral characterization, QSAR, and molecular docking analyses of newly designed boron compounds**  
Çetiner E., SAYIN K., ÜNAL Y.  
Structural Chemistry, cilt.34, sa.5, ss.1731-1742, 2023 (SCI-Expanded)
- V. **Synthesis, nanostructuring and in silico studies of a new imine bond containing a macroheterocycle as a promising PBP-2a non-β-lactam inhibitor**  
Huseynzada A., Aghayev M., Hajiyeva S., Israyilova A., SAYIN K., Gasimov E., Rzayev F., Hasanova U., Eyvazova G., Abbasov V., et al.  
Journal of Materials Chemistry B, cilt.11, sa.34, ss.8271-8280, 2023 (SCI-Expanded)
- VI. **[Cu<sub>2</sub>(ox)(dien)<sub>2</sub>](NO<sub>3</sub>)<sub>3</sub>, a precursor for preparation of CuO nanoparticles: Synthesis, structural, Hirshfeld surface analyses, and physico-chemical investigations**  
Akouibaa M., Lakkab I., Direm A., Lachkar M., Ouarsal R., Rakib S., Nasif V., SAYIN K., Morley N., Bali B. E.  
Journal of Molecular Structure, cilt.1282, 2023 (SCI-Expanded)
- VII. **Improved carbon steel corrosion characteristics in static and hydrodynamic HCl media by two novel N<sub>2</sub>O<sub>2</sub> ligands: Experimental and theoretical studies**  
Karimi S., Rezaeivala M., Mokhtare M., Tuzun G., SAYIN K.  
Journal of the Taiwan Institute of Chemical Engineers, cilt.147, 2023 (SCI-Expanded)
- VIII. **Eaton's reagent is an alternative of PPA: Solvent free synthesis, molecular docking and ADME studies of new angular and linear carbazole based naphtho naphthyridines**  
Prabha K., Satheeshkumar R., Aathi M. S., Chandrasekar C., Sukantha T. A., Gnanamangai B. M., Acevedo R., SAYIN K.,

Prasad K. J. R.

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- IX. **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, cilt.148, 2023 (SCI-Expanded)
- X. **Crystal structure, Hirshfeld surface analysis, computational and antifungal studies of dihydropyrimidines on the basis of salicylaldehyde derivatives**  
Huseynzada A., Jelsch C., Akhundzada H. V., Soudani S., Ben Nasr C., SAYIN K., DEMİRALP M., Hasanova U., Eyvazova G., Gakhramanova Z., et al.  
JOURNAL OF THE IRANIAN CHEMICAL SOCIETY, cilt.20, sa.1, ss.109-123, 2023 (SCI-Expanded)
- XI. **Crystal Structure, Hirshfeld Surface Analysis, In-Silico and Antimycotic Investigations of Methyl 6-methyl-4-(4-nitrophenyl)-2-oxo-1,2-dihydropyrimidine-5-carboxylate**  
Huseynzada A., Mori M., Meneghetti F., Israyilova A., Guney E., SAYIN K., Chiarelli L. R., DEMİRALP M., Hasanova U., Abbasov V.  
Crystals, cilt.13, sa.1, 2023 (SCI-Expanded)
- XII. **Spectroscopic (FT-IR, NMR, single crystal XRD) and DFT studies including FMO, Mulliken charges, and Hirshfeld surface analysis, molecular docking and ADME analyses of 2-amino-4'-fluorobenzophenone (FAB)**  
Satheeshkumar R., Prabha K., Vennila K. N., SAYIN K., Güney E., Kaminsky W., Acevedo R.  
Journal of Molecular Structure, cilt.1267, 2022 (SCI-Expanded)
- XIII. **Synthesis, crystal structure, Hirshfeld surface, computational and antibacterial studies of a 9-phenanthrenecarboxaldehyde-based thiodihydropyrimidine derivative**  
Huseynzada A., Mori M., Meneghetti F., Israyilova A., Tuzun G., SAYIN K., Chiarelli L. R., Mutlu C., DEMİRALP M., Hasanova U., et al.  
JOURNAL OF MOLECULAR STRUCTURE, cilt.1267, 2022 (SCI-Expanded)
- XIV. **Synthesis, in silico and investigation of anti-breast cancer activity of new diphenyl urea derivatives: Experimental and computational study**  
GÖMEÇ M., SAYIN K., ÖZKARACA M., ÖZDEN H.  
JOURNAL OF MOLECULAR STRUCTURE, cilt.1265, 2022 (SCI-Expanded)
- XV. **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, cilt.33, ss.1189-1197, 2022 (SCI-Expanded)
- XVI. **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, cilt.287, 2022 (SCI-Expanded)
- XVII. **Revealing the new structure of B8N8 nanocage and comparison of hydrogen storage capacity**  
Nasif V., SAYIN K.  
CHEMICAL PHYSICS, cilt.559, 2022 (SCI-Expanded)
- XVIII. **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-PHYSCOCHEMICAL AND ENGINEERING ASPECTS, cilt.641, 2022 (SCI-Expanded)
- XIX. **Determination of structural, spectral, computational and OLED properties of Ex2.2Box2+ Cyclophane and its derivatives: Experimental and computational study**  
SAYIN K., Rezaeivala M., ERKAN S., Güney E.  
Journal of Molecular Structure, cilt.1253, 2022 (SCI-Expanded)
- XX. **Synthesis, In Vitro Cytotoxicity, and DFT Studies of Novel 2-Amino Substituted Benzonaphthyridines**

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Prabha K., Satheeshkumar R., Nasif V., Saranya J., SAYIN K., Natarajan J., Chandrasekar C., Prasad K. J. R.  
CHEMISTRYSELECT, cilt.7, sa.13, 2022 (SCI-Expanded)

- XXI. **Synthesis of diaryl urea derivatives and evaluation of their antiproliferative activities in colon adenocarcinoma**  
GÖMEÇ M., YULAK F., GEZEĞEN H., ÖZKARACA M., SAYIN K., ATASEVEN H.  
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- XXII. **Design and in silico study of the novel coumarin derivatives against SARS-CoV-2 main enzymes**  
ÖZDEMİR M., Köksoy B., Ceyhan D., SAYIN K., Erçağ E., Bulut M., YALÇIN B.  
Journal of Biomolecular Structure and Dynamics, cilt.40, sa.11, ss.4905-4920, 2022 (SCI-Expanded)
- XXIII. **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, cilt.741, 2022 (SCI-Expanded)
- XXIV. **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, cilt.39, sa.18, ss.7263-7273, 2021 (SCI-Expanded)
- XXV. **Synthesis and competitive Li-7 NMR studies of two morpholine-based ligands**  
Rezaeivala M., Zebarjadian M. H., SAYIN K.  
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- XXVI. **Experimental and in silico studies of dichloro-tetrakis (1H-pyrazole)-cobalt(II): Structural description, photoluminescent behavior and molecular docking**  
Direm A., El Bali B., SAYIN K., Abdelbakyd M. S. M., Garcia-Granda S.  
JOURNAL OF MOLECULAR STRUCTURE, cilt.1235, 2021 (SCI-Expanded)
- XXVII. **Experimental and theoretical investigation of inhibition behavior of 2-((4-(dimethylamino)benzylidene)amino)benzenethiol for carbon steel in HCl solution**  
KELEŞ H., KELEŞ M., SAYIN K.  
CORROSION SCIENCE, cilt.184, 2021 (SCI-Expanded)
- XXVIII. **Investigations of structural, spectral (IR, H-1-, F-9-, B-11-, C-13-, (15) N-, O-17-NMR) and anticancer properties of 5FU@B12N12 complexes**  
AKTAŞ A., Nassif W., SAYIN K.  
CHEMICAL PAPERS, cilt.75, sa.4, ss.1727-1737, 2021 (SCI-Expanded)
- XXIX. **Experimental and Computational Investigation for (E)-2-hydroxy-5-(2-benzylidene) Aminobenzoic Acid Schiff Base as a Corrosion Inhibitor for Copper in Acidic Media**  
KILINÇEKER G., Bas M., Zarifi F., SAYIN K.  
IRANIAN JOURNAL OF SCIENCE AND TECHNOLOGY TRANSACTION A-SCIENCE, cilt.45, sa.2, ss.515-527, 2021 (SCI-Expanded)
- XXX. **Investigations substituent effect on structural, spectral and optical properties of phenylboronic acids**  
Çöpçü B., SAYIN K., KARAKAŞ D.  
Journal of Molecular Structure, cilt.1227, 2021 (SCI-Expanded)
- XXXI. **Experimental and computational studies of di-mu-chlorido-bis[chlorido(1,10-phenanthroline-(KN)-N-2,N ')nickel(II)] NiCl2(H2O)(C12N2H8): Crystal structure, quantitative analysis of the intermolecular interactions and electronic properties**  
El Bali B., Lachkar M., Direm A., Cetiner E., SAYIN K., Dusek M.  
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- XXXII. **The highly protective natural medical agents against COVID-19**  
Gokalp F., Sayin K.  
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- XXXIII. **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, cilt.122, sa.2, ss.101-110, 2021 (SCI-Expanded)
- XXXIV. **Scale factor database for the vibration frequencies calculated in M06-2X, one of the DFT methods**  
ÜNAL Y., Nassif W., Özeydin B. C., SAYIN K.  
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- XXXV. **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, cilt.122, sa.9, ss.670-679, 2021 (SCI-Expanded)
- XXXVI. **Determination of inhibitor activity of drugs against the COVID-19**  
Gedikli M. A., Tuzun B., Sayin K., ATASEVEN H.  
BRATISLAVA MEDICAL JOURNAL-BRATISLAVSKE LEKARSKE LISTY, cilt.122, sa.7, ss.497-506, 2021 (SCI-Expanded)
- XXXVII. **Could boron compounds be effective against SARS-CoV-2?**  
ATASEVEN H., SAYIN K., TÜZÜN B., GEDİKLİ M. A.  
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- XXXVIII. **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, cilt.122, sa.4, ss.263-269, 2021 (SCI-Expanded)
- XXXIX. **Experimental and computational investigation of variamine blue as an inhibitor for copper in chloride solution**  
KILINÇÇEKER G., ÇELİK S., Zarifi F., SAYIN K.  
JOURNAL OF DISPERSION SCIENCE AND TECHNOLOGY, 2020 (SCI-Expanded)
- XL. **Research on structural, spectral (IR, UV-Vis, H-1- and C-13-NMR) and light emitting properties of triisocyano-based trinuclear Au(I) complexes**  
Ozkan N., ERKAN S., SAYIN K., KARAKAŞ D.  
CHEMICAL PAPERS, cilt.74, sa.8, ss.2415-2425, 2020 (SCI-Expanded)
- XLI. **Evaluation of structural, spectral characterization and in vitro cytotoxic activity studies of some polycyclic aromatic compounds**  
Rezaeivala M., SAYIN K., Şahin-Bölükbaşı S., Tandoğan D., Kose M., Kose A.  
ARABIAN JOURNAL OF CHEMISTRY, cilt.13, sa.6, ss.5593-5604, 2020 (SCI-Expanded)
- XLII. **Crystal structure, Hirshfeld surface analysis and theoretical calculations of an oxalato-bridged copper(II) complex: mu-oxalato-bis[(2,2'-bipyridine) hydrate copper(II) nitrate]**  
Boutobba Z., Direm A., SAYIN K., El Bali B., Lachkar M., Benali-Cherif N.  
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- XLIII. **Water mediated synthesis of 6-amino-5-cyano-2-oxo-N-(pyridin-2-yl)-4-(p-tolyl)-2H-[1,2'-bipyridine]-3-carboxamide and 6-amino-5-cyano-4-(4-fluorophenyl)-2-oxo-N-(pyridin-2-yl)-2H-[1,2'-bipyridine]-3-carboxamide - An experimental and computational studies with non-linear optical (NLO) and molecular docking analyses**  
Jayarajan R., Satheeshkumar R., Kottha T., Subbaramanian S., SAYIN K., Vasuki G.  
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, cilt.229, 2020 (SCI-Expanded)
- XLIV. **Pt-Ni@PC900 Hybrid Derived from Layered-Structure Cd-MOF for Fuel Cell ORR Activity**  
Nadeem M., Yasin G., Arif M., Bhatti M. H., SAYIN K., Mehmood M., Yunus U., Mehboob S., Ahmed I., Floerke U.  
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- XLV. **How do arbidol and its analogs inhibit the SARS-CoV-2?**  
Aktas A., Tuzun B., Kafa T. A. H., Sayin K., Ataseven H.

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- XLVI. **Structural, spectral characterization and molecular docking analyses of mer-ruthenium (II) complexes containing the bidentate chelating ligands**  
Erkan S., Kaya S., Sayin K., Karakaş D.  
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, cilt.224, 2020 (SCI-Expanded)
- XLVII. **Quantum chemical calculations on sparfloxacin and boron complexes**  
ÜNGÖRDÜ A., SAYIN K.  
CHEMICAL PHYSICS LETTERS, cilt.733, 2019 (SCI-Expanded)
- XLVIII. **Synthesis of novel 1,10-phenanthroline derivatives and it used as probes for sensitive detection of Zn<sup>2+</sup> and Cd<sup>2+</sup> metal ions - Spectroscopic and theoretical approach**  
Satheeshkumar R., Rajamanikandan R., Ilanchelian M., Sayin K., Prasad K. J. R.  
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, cilt.221, 2019 (SCI-Expanded)
- XLIX. **Investigations of structural, spectral and electronic properties of enrofloxacin and boron complexes via quantumchemical calculation and molecular docking**  
SAYIN K., ÜNGÖRDÜ A.  
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, cilt.220, 2019 (SCI-Expanded)
- L. **Research of the substituent effect on non-linear optical properties of bis (difluoroboron)-1,2-bis((1H-pyrrol-2-yl)methylene)hydrazine (BOPHY) derivatives: Molecular simulation analyses**  
SAYIN K.  
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, cilt.212, ss.380-387, 2019 (SCI-Expanded)
- LI. **The Different Effects of Metal Ions on the Synthesis of Macroacyclic Compounds: X-ray Crystal Structure, Theoretical Studies, Antibacterial and Antifungal Activities**  
Rezaeiylala M., Golbedaghi R., Khalili M., Ahmad M., Sayin K., Chalabian F.  
RUSSIAN JOURNAL OF COORDINATION CHEMISTRY, cilt.45, sa.2, ss.142-153, 2019 (SCI-Expanded)
- LII. **Investigations over optical properties of boron complexes of benzothiazolines**  
TÜZÜN B., SAYIN K.  
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, cilt.208, ss.48-56, 2019 (SCI-Expanded)
- LIII. **New diazo-containing phenolic oximes: structural characterization, computational studies, and solvent extraction of Cu(II), Ni(II), and Zn(II) ions**  
KARABÖRK M., Kirpik H., SAYIN K., KÖSE M.  
TURKISH JOURNAL OF CHEMISTRY, cilt.43, sa.1, ss.197-212, 2019 (SCI-Expanded)
- LIV. **Investigations of structural, spectral, electronic and biological properties of N-heterocyclic carbene Ag(I) and Pd(II) complexes**  
Sayin K., Kariper S. E., Tastan M., Sayin T. A., Karakaş D.  
JOURNAL OF MOLECULAR STRUCTURE, cilt.1176, ss.478-487, 2019 (SCI-Expanded)
- LV. **Investigation of structural and biological properties of N-heterocyclic carbene silver(I) and palladium(II) complexes**  
SAYIN K.  
JOURNAL OF COORDINATION CHEMISTRY, cilt.71, sa.20, ss.3292-3303, 2018 (SCI-Expanded)
- LVI. **Crystal structure, thermal, luminescent and terahertz time domain spectroscopy of magnesium N-phthaloyl-beta-alaninate: A combined experimental and theoretical study**  
Nadeem M., Bhatti M. H., SAYIN K., Yunus U., Mehmood M., Mehboob S., Floerke U.  
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- LVII. **Investigation of structural, electronic properties and docking calculations of some boron complexes with norfloxacin: A computational research**  
SAYIN K., KARAKAŞ D.

- SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, cilt.202, ss.276-283, 2018 (SCI-Expanded)
- LVIII. **Half-sandwich Ruthenium(II) arene complexes bearing the azo-azomethine ligands: Electrochemical, computational, antiproliferative and antioxidant properties**  
Inan A., Sunbul A. B., İkiz M., Tayhan S. E., BİLGİN S., Elmastas M., SAYIN K., CEYHAN G., KÖSE M., İSPİR E.  
JOURNAL OF ORGANOMETALLIC CHEMISTRY, cilt.870, ss.76-89, 2018 (SCI-Expanded)
- LIX. **Sev and pcu topological nets in one-pot newly synthesized mixed-ligand imidazole-containing Cu(II) coordination frameworks: Crystal structure, intermolecular interactions, theoretical calculations, magnetic behavior and biological activity**  
Direm A., Abdelbaky M. S. M., SAYIN K., Cornia A., Abosede O., Garcia-Granda S.  
INORGANICA CHIMICA ACTA, cilt.478, ss.59-70, 2018 (SCI-Expanded)
- LX. **Quantum chemical investigation of levofloxacin-boron complexes: A computational approach**  
SAYIN K., KARAKAŞ D.  
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- LXI. **Unsymmetrical tripodal amines containing one pyridine-armed with N3O2-donor set: Coordination chemistry with zinc(II) and theoretical studies**  
Keypour H., Shayesteh M., Rezaeivala M., Dhers S., SAYIN K.  
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- LXII. **Computational study of some fluoroquinolones: Structural, spectral and docking investigations**  
SAYIN K., KARAKAŞ D., ERKAN KARİPER S., Sayin T. A.  
JOURNAL OF MOLECULAR STRUCTURE, cilt.1156, ss.172-181, 2018 (SCI-Expanded)
- LXIII. **Investigation of anticancer properties of caffeinated complexes via computational chemistry methods**  
SAYIN K., ÜNGÖRDÜ A.  
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- LXIV. **Antiproliferative, antioxidant, computational and electrochemical studies of new azo-containing Schiff base ruthenium(II) complexes**  
Inan A., İkiz M., Tayhan S. E., BİLGİN S., GENÇ N., SAYIN K., CEYHAN G., KÖSE M., Dag A., İSPİR E.  
NEW JOURNAL OF CHEMISTRY, cilt.42, sa.4, ss.2952-2963, 2018 (SCI-Expanded)
- LXV. **Computational investigations of trans platinum(II) oxime complexes used as anticancer drug**  
SAYIN K., KARAKAŞ D.  
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, cilt.188, ss.537-546, 2018 (SCI-Expanded)
- LXVI. **Synthesis, spectroscopic, in vitro cytotoxicity and crystal structures of novel fluorinated dispiroheterocycles: DFT approach**  
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- LXXVIII. **Pd(II) complexes of novel phosphine ligands: Synthesis, characterization, and catalytic activities on Heck reaction**  
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## **Kitap & Kitap Bölümleri**

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### **Hakemli Kongre / Sempozyum Bildiri Kitaplarında Yer Alan Yayınlar**

- I. **A comparative theoretical and spectroscopic study of aminomethylbenzoic acid derivatives as potential NLO candidates**  
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- II. **Quantum Chemical Calculations on Manganese Complexes with Penta-Amine Macrocyclic Schiff Base Ligand: Computational and Molecular Docking**  
ERKAN S., SAYIN K., KARAKAŞ D.  
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- III. **MOLECULAR DOCKING ANALYSES BETWEEN SAUCHINONE AND QUERCETIN AGAINST EPIDERMAL GROWTH FACTOR RECEPTOR IN LUNG CANCER**  
Özaydın B. C., SAYIN K., ATASEVEN H.  
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- IV. **INVESTIGATIONS OF ANTICANCER PROPERTIES OF TWO ANTIOXIDANT COMPOUNDS, (2R)-3-(3,4-DIHYDROXYPHENYL)-2-[(E)-3-(3,4-DIHYDROXYPHENYL)PROP-2-ENOYL]OXYPROPANOIC ACID AND 6-HYDROXY-2,2-DIMETHYL-3-CHROMEN**  
Nassif W., SAYIN K., ATASEVEN H.  
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- V. **MORPHOLINE-BASED SCHIFF BASE COMPLEXES SYNTHESIS, CHARACTERIZATION AND CYTOTOXIC ACTIVITY**  
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- VI. **INVESTIGATION OF EFFICIENCY OF CARMUSTINE AND LOMUSTINE AGAINST MELANOMA CANCER (PDB ID: 5IXB)**  
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- VII. **Can B12N12 nanomaterial effective in the inhibiting of Vascular Endothelial Growth Factor Receptor 2 (VEGFR2)?**  
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- VIII. **Determination of Biological Reactivity against Lung Cancer Cell and Investigations of NLO Properties of Ciprofloxacin-Boron Complexes**

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- IX. **Comparison of Biological Reactivity of Pantoprazole and Lansoprazole by Computational Chemistry Techniques**  
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- X. **Quantum Chemical Calculations on Ag and Pb Complexes with Penta-Amine Macrocyclic Schiff Base Ligand: Computational and Molecular Docking Analyses**  
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- XI. **Can pantoprazole use in the treatment of ulcerative colitis?**  
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- XII. **Investigation of The Usability of Pantoprazole in Ulcerative Colits**  
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- XIII. **Investigation of Antiplatelet Effects of Pantoprazole**  
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- XIV. **Charge Transfer Property of Tris(3-nitro-8-hydroxyquinolinato) Aluminium**  
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- XV. **Reorganization Energy of Tris(3-amino-8-hydroxyquinolinato) Aluminium Complex**  
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- XVI. **DFT Studies of Heat Shock Protein (HSP) Inhibitors**  
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- XVII. **QUANTUM CHEMICAL CALCULATIONS ON FLAVONOID BAICALIN IN WATER PHASE**  
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- XVIII. **Comparison of structural and electronic properties of B<sub>12</sub>N<sub>12</sub> and Al<sub>12</sub>N<sub>12</sub> nanocages**  
SAYIN K.  
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- XIX. **Quantum Chemical Calculations of A Proton Pump Inhibitor: ADFT Study**  
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- XX. **Flavanoid Baisalin Bileşiğinin Kuantum Kimyasal HesaplamalarYöntemleriyle İncelenmesi**  
SAYIN K., ÜNGÖRDÜ A., KARAKUŞ N.  
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- XXI. **Quantum Chemical Investigations of boron nitride nano-cages(B<sub>3</sub>N<sub>3</sub>, B<sub>4</sub>N<sub>4</sub> and B<sub>6</sub>N<sub>6</sub>)**  
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- XXII. **Anticancer effect of proton pump inhibitor on hepatocellular carcinoma**  
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- XXIII. **Computational Studies on Shrock Type Mo(CO)<sub>5</sub>(Cme<sub>2</sub>) and Mo(CO)<sub>5</sub>(Cmeet) Alkliden Complexes Based on Density Functional Theory**  
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- XXIV. **Quantum Chemical Calculations on [Tp(CO)<sub>2</sub>Mo C-Ph]<sub>2</sub> and[L(CO)<sub>2</sub>Mo C-Ph] Alkylidene Complexes**

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- XXV. **Investigation of 1-Allyl-3-Butylbenzimidazolium-Derived Silver (I) Complexes in Terms of Structure and Biological Activity by Computational Chemistry Methods**  
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- XXVI. **Investigations of Structural, Spectral, Electronic and Biological Properties of N-Heterocyclic Carbene Pd(II) Complex**  
ERKAN KARİPER S., SAYIN K., KARAKAŞ D., TÜZÜN B.  
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- XXVII. **Spectral analysis and molecular docking of metal complexes with bis(pyridine carboxamide) benzene ligand**  
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- XLVIII. **Bazı çinko II komplekslerinin biyolojik aktiflik sıralamasının hesapsal yöntemlerle belirlenmesi**  
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- XLIX. **Metansülfonilhidrazon temelli krompentakarbonil kompleksleri üzerine yapısal spektroskopik ve aktivite hesaplamaları**  
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- L. **Bazı B laktam inhibitörler üzerine kuantum kimyasal çalışmalar**  
ERKAN KARİPER S., SAYIN K., KARAKAŞ D.  
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- LI. **Yoğunluk fonksiyon teori metoduyla MgO<sub>2</sub>Ti<sub>2</sub> OPri 6 MgO<sub>2</sub>Ti<sub>2</sub> OPri 2 Acac 4 ve MgO<sub>2</sub>Ti<sub>2</sub> OPri 2 bzac 4 kompleksleri üzerine hesapsal çalışmalar**

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## **Metrikler**

Yayın: 192

Atıf (WoS): 855

Atıf (Scopus): 934

H-İndeks (WoS): 18

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## **Akademi Dışı Deneyim**

Başergün Boya ve Kimya Sanayi A.Ş.