



# SULTAN ERKAN

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International Researcher IDs

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### Learning Knowledge

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Doctorate 2013 - 2016	Turkey
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Postgraduate 2010 - 2013	Turkey
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### Supported Projects

1. Karakaş D., Erkan S., Project Supported by Higher Education Institutions, Anti-kanser özelliği taşıyan siklometalat iridyum(III) kompleksleri üzerine yapısal, spektroskopik ve kuantum kimyasal hesaplamalar, 2016 - 2020
2. Erkan S., Project Supported by Higher Education Institutions, anti kanser özelliği taşıyan siklometalat iridyum III kompleksleri üzerine yapısal spektroskopik ve kuantum kimyasal hesaplamalar, 2016 - 2020
3. Erkan S., Project Supported by Higher Education Institutions, Thiosemikarbazan türevli organik bileşiklerin ve onların metal komplekslerinin yapısal, spektroskopik ve biyolojik aktivitelerinin hesaplamalı kimya metodları ile incelenmesi, 2018 - 2019
4. Karakaş D., Erkan S., Sayın K., Project Supported by Higher Education Institutions, Mer-[Ru(Cl-Ph-tpy)(N-N)(X)] Tipi Rutenyum (II) Komplekslerinin Yapısal, Elektronik ve Antikanser Özelliklerinin Hesaplamalı Kimya Yöntemleriyle Araştırılması, 2017 - 2019
5. Karakaş D., Sayın K., Erkan S., Sayın T., Project Supported by Higher Education Institutions, Mono- ve Bis-N-Heterosiklik Karbenli Ag(I) ve Pd(II) Komplekslerinin Yapısal, Spektral ve Antikanser Özelliklerinin Hesaplamalı Kimya Yöntemleriyle İncelenmesi, 2017 - 2018
6. Karakaş D., Sayın K., Erkan S., Project Supported by Higher Education Institutions, 2-pridil 2-primidin-4-karboksilik asit ligantlarını içeren Ru II komplekslerinin antitümör özellikleri üzerine teorik çalışma, 2014 - 2015

### Awards

1. Erkan S., üniversite birincilik ödülü, Cumhuriyet Üniversitesi, June 2010

### Jury Memberships

Doctoral Examination, Doctoral Examination, Fırat Üniversitesi, May, 2021

Doctoral Examination, Doctoral Examination, Firat Üniversitesi, May, 2021

Doctoral Examination, Doctoral Examination, Firat Üniversitesi, May, 2021

Doctoral Examination, Doctoral Examination, Kahramanmaraş Sütçü İmam Üniversitesi, October, 2019

## Published journal articles indexed by SCI, SSCI, and AHCI

- 1. 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)
- 2. Mononuclear and binuclear dioxidomolybdenum(VI) chelates derived from a tridentate ONO donor aroylhydrazone: Spectral, structural, DFT and in silico biological investigations**  
Aravindakshan A. A., Mohan N., Kurup M. P., ERKAN S., BATIR G. G., Manoj E.  
Polyhedron, vol.256, 2024 (SCI-Expanded)
- 3. Spectroscopic, crystal structure and DFT-assisted studies of some nickel(II) chelates of a heterocyclic-based NNO donor aroylhydrazone: in vitro DNA binding and docking studies**  
Nair Y., Joy F., Vinod T., Vineetha M., Kurup M. R. P., KAYA S., SERDAROĞLU G., ERKAN S.  
Molecular Diversity, vol.28, no.2, pp.509-530, 2024 (SCI-Expanded)
- 4. The Anticancer Potentials of Substituted Indeno[1,2-b]quinoline Amines against HT29 and SW620: Experimental and In silico Approach**  
Ökten S., AYDIN A., ERKAN S., Tutar A.  
Letters in Drug Design and Discovery, vol.21, no.1, pp.143-151, 2024 (SCI-Expanded)
- 5. Modeling, spectroscopic structural properties of platinum-II complexes of 2-((phenylimino)methyl)phenolate-based ligands and research of nonlinear optical, organic light emitting diode and solar cell performances**  
ERKAN S., KARAKAŞ D.  
Materials Today Communications, vol.37, 2023 (SCI-Expanded)
- 6. Bromination and conversion of tetrahydro-1H-indene to bisoxirane with a new approach: synthesis, structural characterization by spectroscopic and theoretical methods, and biological analysis supported by DFT and docking**  
Yılmaz R. F., Erkan S., Ökten S., Tutar A., Şahin E.  
TURKISH JOURNAL OF CHEMISTRY, vol.47, no.6, pp.1459-1478, 2023 (SCI-Expanded)
- 7. Investigation of Antimicrobial Activities and Molecular Docking Studies of Synthesized Sulfonamide Compounds**  
Ozbey G., Tanriverdi E., Şenkal B. F., Korkmaz B., ERKAN S., Bulut N., Zigo F., OTLU B.  
Pharmaceutical Chemistry Journal, vol.57, no.9, pp.1394-1400, 2023 (SCI-Expanded)
- 8. In Silico and In Vitro Studies of Novel Azomethines on DNA Repair Genes in Gastric Cell Lines.**  
Ozturk A., Agbektas T., Huseynzada A., Guliyev R., Ganbarova R., Hasanova U., Tas A., Erkan S., Zontul C., Inandiklioglu N., et al.  
Life (Basel, Switzerland), vol.13, no.10, 2023 (SCI-Expanded)
- 9. Synthesis, docking studies, in vitro cytotoxicity evaluation and DNA damage mechanism of new tyrosine-based tripeptides**  
Çalışkan E., Kaplan A., Şekerci G., ÇAPAN İ., TEKİN S., ERKAN S., Koran K., SANDAL S., GÖRGÜLÜ A. O.  
Journal of Biochemical and Molecular Toxicology, vol.37, no.8, 2023 (SCI-Expanded)
- 10. Analysis of boronic acids containing amino ferrocene by DFT approach and in silico studies**  
Muhammad U. S., ERKAN S., KAYA S.  
Journal of Molecular Structure, vol.1284, 2023 (SCI-Expanded)
- 11. Investigation of substituent effect on rhenium complexes by DFT methods: Structural analysis, IR spectrum, quantum chemical parameter, NLO and OLED properties, molecular docking**  
Yıldız C. A., Güney E., Nasif V., KARAKAŞ D., ERKAN S.

- Journal of Molecular Structure, vol.1278, 2023 (SCI-Expanded)
12. **Equilibrium and DFT modeling studies for the biosorption of Safranin O dye from water samples using Bacillus subtilis biosorbent**  
ÇETİNKAYA S., KAYA S., Aksu A., ÇETİNTAŞ H. İ., Jalbani N. S., ERKAN S., Marzouki R.  
Journal of Molecular Structure, vol.1276, 2023 (SCI-Expanded)
  13. **A series of phenanthroline-imine compounds: Computational, OLED properties and fluorimetric sensing of nitroaromatic compounds**  
Kose A., ERKAN S., Tümer M.  
Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, vol.286, 2023 (SCI-Expanded)
  14. **Chemical composition, antimicrobial activities, and molecular docking studies of Turkish propolis ethanol extract**  
Ozbey G., Muz M. N., Tanriverdi E. S., ERKAN S., Bulut N., OTLU B., Zigo F.  
Czech Journal of Food Sciences, vol.41, no.2, pp.144-154, 2023 (SCI-Expanded)
  15. **Assessing cytotoxic activities, theoretical and in silico molecular docking calculations of phthalocyanines bearing cinnamyloxy-groups**  
Özten Ö., Kuznetsov A. E., GÖKÇE M., ERKAN S., Bulut E., TAŞKIN Ö. S., ZENGİN KURT B., Yıldız M. Z., Sobotta L., Güzel E.  
Journal of Biomolecular Structure and Dynamics, 2023 (SCI-Expanded)
  16. **Equilibrium and Computational Chemical Modelling Studies for the Removal of Methyl Orange and Methyl Red Dyes from Water Using Modified Silica Resin**  
Junejo R., Shams Jalbani N., BATIR G. G., ERKAN S., Marzouki R., Memon S.  
International Journal of Environmental Analytical Chemistry, vol.103, no.19, pp.8000-8016, 2023 (SCI-Expanded)
  17. **Manganese(III) Acetate-Based Radical Cyclization Reactions for Pyranocoumarin and Pyranoquinoline Compounds: Synthesis, DFT and Molecular Docking Studies**  
YAKUT M., YILMAZ M., Pekel T., ERKAN S., Katırcı R., Biçer E.  
ChemistrySelect, vol.7, no.44, 2022 (SCI-Expanded)
  18. **Synthesis, characterization, non-linear optical and DNA binding properties of a Schiff base ligand and its Cu(II) and Zn(II) complexes**  
Kose A., Gungor O., Balli J. N., ERKAN S.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1268, 2022 (SCI-Expanded)
  19. **Computational design and characterization of platinum-II complexes of some Schiff bases and investigation of their anticancer-antibacterial properties**  
Kaya S., ERKAN S., KARAKAŞ D.  
APPLIED ORGANOMETALLIC CHEMISTRY, vol.36, no.9, 2022 (SCI-Expanded)
  20. **Synthesis of New Cinnamoyl-Amino Acid Conjugates and in Vitro Cytotoxicity and Genotoxicity Studies**  
Caliskan E., Ozturk D. A., KORAN K., TEKİN S., SANDAL S., ERKAN S., GÖRGÜLÜ A. O., ÇETİN A.  
CHEMISTRY & BIODIVERSITY, vol.19, no.8, 2022 (SCI-Expanded)
  21. **Potential thiosemicarbazone-based enzyme inhibitors: Assessment of antiproliferative activity, metabolic enzyme inhibition properties, and molecular docking calculations**  
Yakan H., KOÇYİĞİT Ü. M., Muglu H., ERGÜL M., ERKAN S., Guzel E., Taslimi P., GÜLÇİN İ.  
JOURNAL OF BIOCHEMICAL AND MOLECULAR TOXICOLOGY, vol.36, no.5, 2022 (SCI-Expanded)
  22. **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, vol.1253, 2022 (SCI-Expanded)
  23. **Synthesis, spectral characterization, chemical reactivity and anticancer behaviors of some novel hydrazone derivatives: Experimental and theoretical insights**  
ÇAKMAK R., Basaran E., KAYA S., ERKAN S.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1253, 2022 (SCI-Expanded)
  24. **A new 3-substituted BODIPY dye: Synthesis, crystal structure, photophysical, non-linear optic and**

## **OLED properties**

Kirpik H., ERKAN S., KÖSE M.

JOURNAL OF MOLECULAR STRUCTURE, vol.1252, 2022 (SCI-Expanded)

25. **Synthesis, photophysical, electrochemical, and DFT examinations of two new organic dye molecules based on phenothiazine and dibenzofuran**  
Periyasamy K., Sakthivel P., Venkatesh G., Anbarasan P. M., Vennila P., Mary Y. S., Kaya S., ERKAN S.  
JOURNAL OF MOLECULAR MODELING, vol.28, no.2, 2022 (SCI-Expanded)
26. **Phthalocyanine complexes with (4-isopropylbenzyl)oxy substituents: preparation and evaluation of anti-carbonic anhydrase, anticholinesterase enzymes and molecular docking studies**  
Guzel E., KOÇYİĞİT Ü. M., Taslimi P., GÜLÇİN İ., ERKAN S., NEBİOĞLU M., Arslan B. S., ŞİŞMAN İ.  
JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS, vol.40, no.2, pp.733-741, 2022 (SCI-Expanded)
27. **N-substituted benzenesulfonamide compounds: DNA binding properties and molecular docking studies**  
Gungor S. A., TÜMER M., KÖSE M., ERKAN S.  
JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS, vol.40, no.16, pp.7424-7438, 2022 (SCI-Expanded)
28. **Effect of hydrocarbon chain length for acid corrosion inhibition of mild steel by three 8-(n-bromo-R-alkoxy)quinoline derivatives: Experimental and theoretical investigations**  
Erkan S., Tazouti A., Errahmany N., Rbaa M., Galai M.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1244, pp.130976-130997, 2021 (SCI-Expanded)
29. **Halogens effect on spectroscopy, anticancer and molecular docking studies for platinum complexes**  
Khalid H. H., ERKAN S., BULUT N.  
OPTIK, vol.244, 2021 (SCI-Expanded)
30. **Application of pyrrolidinomethylcalix[4]arene coated silica adsorbent for the removal of Chicago sky blue 6B dye from water samples: Equilibrium and computational modelling studies**  
Junejo R., Jalbani N. S., KAYA S., ERKAN S., Ebenso E. E.  
SUPRAMOLECULAR CHEMISTRY, vol.33, no.10, pp.586-597, 2021 (SCI-Expanded)
31. **Biologically active phthalocyanine metal complexes: Preparation, evaluation of alpha-glycosidase and anticholinesterase enzyme inhibition activities, and molecular docking studies**  
Guzel E., KOÇYİĞİT Ü. M., Taslimi P., ERKAN S., Taskin O. S.  
JOURNAL OF BIOCHEMICAL AND MOLECULAR TOXICOLOGY, vol.35, no.6, pp.1-9, 2021 (SCI-Expanded)
32. **In-Vitro Anticancer and Antibacterial Activities of Brominated Indeno[1,2-b]quinoline Amines Supported with Molecular Docking and MCDM\*\***  
Aydin A., Okten S., ERKAN S., Bulut M., ÖZCAN E., TUTAR A., EREN T.  
CHEMISTRYSELECT, vol.6, no.13, pp.3286-3295, 2021 (SCI-Expanded)
33. **Quantum chemical and molecular dynamic simulation studies for the identification of the extracted cinnamon essential oil constituent responsible for copper corrosion inhibition in acidified 3.0 wt% NaCl medium**  
Dahmani K., Galai M., Ouakki M., Cherkaoui M., Touir R., Erkan S., Kaya S., El Ibrahim B.  
INORGANIC CHEMISTRY COMMUNICATIONS, vol.124, 2021 (SCI-Expanded)
34. **Experimental and theoretical study of new Schiff bases based on imidazo(1,2-a)pyridine as corrosion inhibitor of mild steel in 1M HCl**  
El Aatiaoui A., Koudad M., Chelfi T., ERKAN S., Azzouzi M., Aouniti A., Savas K., Kaddouri M., Benchat N., Oussaid A.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1226, 2021 (SCI-Expanded)
35. **Chemically modified guar gum and ethyl acrylate composite as a new corrosion inhibitor for reduction in hydrogen evolution and tubular steel corrosion protection in acidic environment**  
Singh A., Ansari K. R., Quraishi M. A., KAYA S., ERKAN S.  
INTERNATIONAL JOURNAL OF HYDROGEN ENERGY, vol.46, no.14, pp.9452-9465, 2021 (SCI-Expanded)
36. **Equilibrium, thermodynamic, and density functional theory modeling studies for the removal of dichromate ions from wastewater using calix[4]arene modified silica resin**  
Junejo R., Jalbani N. S., Memon S., KAYA S., ERKAN S., SERDAROĞLU G., Palabiyik I. M.  
Journal of Chemical and Engineering Data, vol.66, pp.379-388, 2021 (SCI-Expanded)

37. **Computational investigation of molecular structures, spectroscopic properties and antitumor-antibacterial activities of some Schiff bases**  
Kaya S., ERKAN S., KARAKAŞ D.  
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, vol.244, 2021 (SCI-Expanded)
38. **Spectral analysis and DFT investigation of some benzopyran analogues and their self-assemblies with graphene**  
Al-Otaibi J. S., Mary Y. S., Mary Y. S., KAYA S., ERKAN S.  
JOURNAL OF MOLECULAR LIQUIDS, vol.317, 2020 (SCI-Expanded)
39. **Quinoline-based promising anticancer and antibacterial agents, and some metabolic enzyme inhibitors**  
Okten S., Aydin A., KOÇYİĞİT Ü. M., Cakmak O., ERKAN S., Andac C. A., Taslimi P., GÜLÇİN İ.  
ARCHIV DER PHARMAZIE, vol.353, no.9, 2020 (SCI-Expanded)
40. **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, vol.74, no.8, pp.2415-2425, 2020 (SCI-Expanded)
41. **Synthesis, Antiproliferative and Cytotoxic Activities, DNA Binding Features and Molecular Docking Study of Novel Enamine Derivatives**  
Gurdere M. B., Aydin A., Yencilek B., Erturk F., Ozbek O., ERKAN S., Budak Y., CEYLAN M.  
CHEMISTRY & BIODIVERSITY, vol.17, no.7, 2020 (SCI-Expanded)
42. **Benzaldehyde derivatives with functional propargyl groups as alpha-glucosidase inhibitors**  
Gungor S. A., TÜMER M., KÖSE M., ERKAN S.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1206, 2020 (SCI-Expanded)
43. **Antiproliferative Evaluation of Some 2-[2-(2-Phenylethenyl)-cyclopent-3-en-1-yl]-1,3-benzothiazoles: DFT and Molecular Docking Study**  
Ceylan M., ERKAN S., YAĞLIOĞLU A. Ş., Uremis N. A., Koc E.  
CHEMISTRY & BIODIVERSITY, vol.17, no.4, 2020 (SCI-Expanded)
44. **A theoretical study on cyclometalated iridium (III) complexes by using a density functional theory**  
ERKAN S., KARAKAŞ D.  
JOURNAL OF THEORETICAL & COMPUTATIONAL CHEMISTRY, vol.19, no.2, 2020 (SCI-Expanded)
45. **Theoretical and Experimental Spectroscopic Properties and Molecular Docking of F8BT p-Type Semiconducting Polymer**  
ERKAN S.  
RUSSIAN JOURNAL OF PHYSICAL CHEMISTRY A, vol.94, no.2, pp.445-452, 2020 (SCI-Expanded)
46. **Computational investigation of structural, nonlinear optical and anti-tumor properties of dinuclear metal carbonyls bridged by pyridyl ligands with alkyne unit**  
Erkan S., Karakaş D.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1199, 2020 (SCI-Expanded)
47. **Structural, spectral characterization and molecular docking analyses of mer-ruthenium (II) complexes containing the bidentate chelating ligands**  
Erkan S., Kaya S., Sayın K., Karakaş D.  
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, vol.224, 2020 (SCI-Expanded)
48. **Evaluation of carbonic anhydrase and paraoxonase inhibition activities and molecular docking studies of highly water-soluble sulfonated phthalocyanines**  
Guzel E., Sonmez F., ERKAN S., Cikrikci K., Ergun A., Gencer N., Arslan O., Koçak M.  
TURKISH JOURNAL OF CHEMISTRY, vol.44, no.6, pp.1565-1577, 2020 (SCI-Expanded)
49. **DFT investigation and molecular docking studies on dinuclear metal carbonyls containing pyridyl ligands with alkyne unit**  
Erkan S., Karakaş D.

- CHEMICAL PAPERS, vol.73, pp.2387-2398, 2019 (SCI-Expanded)
50. **Activity of the rocuronium molecule and its derivatives: A theoretical calculation**  
ERKAN KARİPER S.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1189, pp.257-264, 2019 (SCI-Expanded)
  51. **Computational study of some fluoroquinolones: Structural, spectral and docking investigations**  
SAYIN K., KARAKAŞ D., ERKAN KARİPER S., Sayin T. A.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1156, pp.172-181, 2018 (SCI-Expanded)
  52. **Pamoic acid esters and their xanthene derivatives: Fluorimetric detection of nitroaromatic compounds and non-linear optical properties**  
Gungor S. A., Sahin I., Gungor O., ERKAN KARİPER S., TÜMER F., KÖSE M.  
SENSORS AND ACTUATORS B-CHEMICAL, vol.255, pp.3344-3354, 2018 (SCI-Expanded)
  53. **Theoretical study on the antitumor properties of Ru(II) complexes containing 2-pyridyl, 2-pyridine-4-carboxylic acid ligands**  
ERKAN KARİPER S., SAYIN K., KARAKAŞ D.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1149, pp.473-486, 2017 (SCI-Expanded)
  54. **Multi-properties of a new azo-Schiff base and its binuclear copper(II) chelate: Preparation, spectral characterization, electrochemical, potentiometric and modeling studies**  
Sarigul M., ERKAN KARİPER S., DEVECİ P., Atabay H., KARAKAŞ D., KURTOĞLU M.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1149, pp.520-529, 2017 (SCI-Expanded)
  55. **The new O, O and N, O type ligands and their Cu(II) and Ni(II) complexes: Crystal structure, absorption-emission properties and superoxide dismutase mimetic studies**  
Kose R., Gungor S. A., ERKAN KARİPER S., KÖSE M., KURTOĞLU M.  
INORGANICA CHIMICA ACTA, vol.462, pp.130-141, 2017 (SCI-Expanded)
  56. **Spectroscopic investigation, FMOs and NLO analyses of Zn(II) and Ni(II) phenanthroline complexes: A DFT approach**  
SAYIN K., Karaka D., KARAKUŞ N., Sayin T. A., Zaim Z., ERKAN KARİPER S.  
POLYHEDRON, vol.90, pp.139-146, 2015 (SCI-Expanded)
  57. **Theoretical spectroscopic study of seven zinc(II) complex with macrocyclic Schiff-base ligand**  
SAYIN K., ERKAN KARİPER S., Sayin T. A., KARAKAŞ D.  
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, vol.133, pp.348-356, 2014 (SCI-Expanded)
  58. **Theoretical investigation on the vibrational and electronic spectra of three isomeric forms of dicobalt octacarbonyl**  
KARAKAŞ D., ERKAN KARİPER S.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1062, pp.77-81, 2014 (SCI-Expanded)

## Articles Published in Other Journals

1. **Investigation of Anticancer Properties of 2-benzylidene-1-indanone and Its Derivatives by DFT and Molecular Docking**  
Yildiz C. A., ERKAN S.  
Turkish Computational and Theoretical Chemistry, vol.8, no.2, pp.101-109, 2024 (Scopus)
2. **Investigation of Antiviral Activities of Nickel and Copper Complexes with Macrocyclic Ligands against Crimean-Congo Hemorrhagic Fever by In Silico Calculations**  
ERKAN S., BULUT N., KARAKAŞ D.  
CUMHURİYET SCIENCE JOURNAL, vol.44, 2023 (Peer-Reviewed Journal)
3. **Investigation of the Effect of Main Components of Wild Thyme on Covid-19 by Computational Methods**  
KAYA S., ERKAN S., KARAKAŞ D.  
CUMHURİYET SCIENCE JOURNAL, vol.44, 2023 (Peer-Reviewed Journal)

4. **Computational Structure Characterization of 1,2,3-Selendiazole Isomers, Investigation of Some Molecular Properties and Biological Activities**  
ERKAN S., dıkyol d. c.  
CUMHURİYET SCIENCE JOURNAL, vol.43, no.2, pp.246-256, 2022 (Peer-Reviewed Journal)
5. **LIGHT-EMITTING PROPERTIES OF PYRIMIDINE-5-CARBONITRILE DERIVATIVES AND DIFFERENTLY SUBSTITUTED CARBAZOLES: A THEORETICAL CALCULATION**  
KARAKOYUN N., ERKAN S.  
International Journal of Innovative Engineering Applications, vol.6, no.1, pp.55-58, 2022 (Peer-Reviewed Journal)
6. **Investigations of structural, spectral (IR and NMR) and in silico analyses of boron compounds as SERM inhibitor**  
KAYA S., SAYIN K., ERKAN S., KARAKAŞ D.  
Chemical Data Collections, vol.37, 2022 (Peer-Reviewed Journal)
7. **The Effect of Electron Donor and Withdrawing Groups Attached to 1,2,3- Selendiazole Based Compounds on Anti-Cancer Properties**  
Erkan S., Usman Sani U. S.  
Journal of Physical Chemistry and Functional Materials, vol.4, no.1, pp.17-23, 2021 (Peer-Reviewed Journal)
8. **Structural, Spectroscopic and Anti-cancer Properties of Hydroxy- and Sulfonamide-Azobenzene Platinum (II) Complexes: DFT and Molecular Docking Studies**  
ERKAN KARİPER S.  
Cumhuriyet Science Journal, vol.39, no.4, pp.1036-1051, 2018 (Peer-Reviewed Journal)
9. **Structural, spectroscopic and activity calculations on methanesulfonylhydrazone derivative chromium pentacarbonyl complexes**  
ERKAN S., SAYIN K., KARAKAŞ D.  
Journal of the Turkish Chemical Society, Section A: Chemistry, vol.5, no.3, pp.1193-1204, 2018 (Scopus)
10. **Spectroscopic and Quantum Chemical Studies on Some  $\beta$ -Lactam Inhibitors**  
ERKAN KARİPER S.  
Turkish Computational and Theoretical Chemistry, vol.1, no.2, pp.13-26, 2017 (Scopus)
11. **Theoretical Studies on Eight Oxovanadium IV Complexes with Salicylaldehyde and Aniline Ligands**  
ERKAN KARİPER S., SAYIN K., KARAKAŞ D.  
Hacettepe Journal of Biology and Chemistry, vol.42, no.3, pp.337-342, 2014 (Peer-Reviewed Journal)
12. **EFFECT OF SOME ELECTRON DONOR AND ELECTRON ACCEPTOR GROUPS ON STABILITY OF COMPLEXES ACCORDING TO THE PRINCIPLE OF HSAB**  
KAYA S., ERKAN KARİPER S., ÜNGÖRDÜ A.  
journal of new results in science, vol.4, pp.82-89, 2014 (Peer-Reviewed Journal)

## Books & Book Chapters

1. **Bor Bileşiklerinde Hesaplamalı Kimya Metodlarıyla Enerji Verimliliği**  
alkaya c., ERKAN S.  
in: MULTİDİSİPLİNER BAKIŞ AÇISIYLA "TÜRKİYE'DE ENERJİ", Hilmi Ataseven, Derya Betül Ünsal, Editor, sivas cumhuriyet üniversitesi, pp.13, 2022
2. **Ionic Liquids as Corrosion Inhibitors**  
Kaya S., Erkan S., Şimşek S., Kumar A.  
in: Sustainable Corrosion Inhibitors II: Synthesis, Design, and Practical Applications, Chaudhery Mustansar Hussain Chandrabhan Verma, Editor, American Chemical Society see ACS Publications, Montana, pp.103-119, 2021
3. **Ionic Liquids as Corrosion Inhibitors**  
KAYA S., ERKAN S., ŞİMŞEK S.  
in: Sustainable Corrosion Inhibitors II: Synthesis, Design, and Practical Applications, Hussain, Chaudhery Mustansar; Verma, Chandrabhan, Editor, ACS, pp.4, 2021
4. **Synthesis Methods in Solid-State Chemistry**

- Kaya S., Smida Y. B., Marzouki R., Erkan S., Zid M., Hamzaoui A.  
in: Synthesis Methods and Crystallization, Riadh Marzouki, Editor, intechopen, London, pp.1-16, 2020
5. **Synthesis Methods in Solid-State Chemistry**  
Erkan S., Kaya S.  
in: Synthesis Methods and Crystallization, Riadh Marzouki, Editor, IASP Press see International Association for the Study of Pain (IASP), Budapest, pp.1-26, 2020
6. **Proton Pompa İnhibitörlerinin Kimyası**  
ERKAN S., SAYIN K.  
in: Her Yönüyle Proton Pompaları ve Proton Pompa İnhibitörleri, Hilmi Ataseven, Merve Ergül, Editor, Cumhuriyet Üniversitesi Yayınları, Sivas, pp.63-80, 2020
7. **Proton Pompa İnhibitörlerinin Kimyası**  
ERKAN S., SAYIN K.  
in: Her Yönüyle Proton Pompaları ve Proton Pompa İnhibitörleri, Prof. Dr. Hilmi ATASEVEN, Dr. Öğr. Üyesi Merve ERGÜL, Editor, Sivas Cumhuriyet Üniversitesi Matbaası, Sivas, pp.61-78, 2020
8. **Proton Pompaların Fizikokimyasal Özellikleri**  
SAYIN K., ERKAN S.  
in: Her Yönüyle Proton Pompaları ve Proton Pompa İnhibitörleri, Hilmi Ataseven, Merve Ergül, Editor, Cumhuriyet Üniversitesi Yayınları, Sivas, pp.11-16, 2020
9. **Proton Pompaların Fizikokimyasal Özellikleri**  
SAYIN K., ERKAN S.  
in: Her Yönüyle Proton Pompaları ve Proton Pompa İnhibitörleri, Prof. Dr. Hilmi ATASEVEN, Dr. Öğr. Üyesi Merve ERGÜL, Editor, Sivas Cumhuriyet Üniversitesi Matbaası, Sivas, pp.11-16, 2020

#### Refereed Congress / Symposium Publications in Proceedings

1. **Spectroscopic Analysis of Mifepristone Ru-486 Molecule and Its Derivatives**  
KEBİROĞLU M. H., ERKAN S., BULUT N.  
21st General Assembly of the Federation of Asian Chemical Societies, İstanbul, Turkey, 8 - 14 July 2023
2. **SYNTHESIS, SPECTROSCOPIC ANALYSIS, DFT STUDIES AND MOLECULAR INSERTION APPLICATIONS OF ISATIN HYDRAZONE DERIVATIVE**  
alkaya yıldız c., ERKAN S.  
6 th International Conference on Physical Chemistry & Functional Materials, Elazığ, Turkey, 13 June 2023
3. **Investigation of analysis of mifepristone Ru-486 molecule using Quantum chemical method**  
kebiroğlu h., ERKAN S., BULUT N.  
Global Summit on Advanced Materials & Sustainable Energy, Van, Turkey, 03 October 2022
4. **INVESTIGATION OF CINNAMATE MOLECULE AND ITS DERIVATIVES BY QUANTUM CHEMICAL METHODS**  
kebiroğlu h., alkaya c., ERKAN S., BULUT N.  
III. INTERNATIONAL CANCER DAYS, Sivas, Turkey, 15 September 2022
5. **Investigation of Substituent Effect on Rhenium Complexes by DFT Methods: Structural Analysis, IR Spectrum, Quantum Chemical Parameter, NLO and OLED Properties, Molecular Docking**  
alkaya c., GÜNEY E., nasif v., ERKAN S., KARAKAŞ D.  
5 th International Conference on Physical Chemistry & Functional Materials, Sivas, Turkey, 23 June 2022
6. **A DFT and Molecular Docking studies on Chalcone Base Compounds and Their Anti-Cancer Activities**  
sani u., ERKAN S.  
5 th International Conference on Physical Chemistry & Functional Materials, sivas, Turkey, 23 June 2022
7. **Regorafenib and Its Derivatives on Anticancer Properties; A DFT and Molecular Docking Study**  
alkaya c., ERKAN S.  
5 th International Conference on Physical Chemistry & Functional Materials, Sivas, Turkey, 23 June 2022
8. **INVESTIGATION OF MIFEPRISTON (RU-486) AND ITS DERIVATIVES, MOLECULAR DOKING AND DOS**



**(DESTINY OF STATES) QUANTUM CHEMICAL METHOD**

KEBİROĞLU H., ERKAN S., BULUT N.

INTERNATIONAL CONFERENCE ON RESEARCH IN APPLIED SCIENCES, Spain, 09 July 2022, pp.20-24

9. **SPECTROSCOPIC ANALYSIS OF MIFEPRISTONE (RU-486) MOLECULE BY QUANTUM PROGRAMING**  
kebiroğlu h., ERKAN S., BULUT N.  
V-INTERNATIONAL EUROPEAN CONFERENCE ON INTERDISCIPLINARY SCIENTIFIC RESEARCH, Valencia, Spain, 28 January 2022, vol.1, pp.81
10. **LIGHT-EMITTING PROPERTIES OF PYRIMIDINE-5-CARBONITRILE DERIVATIVES AND DIFFERENTLY SUBSTITUTED CARBAZOLES: A THEORETICAL CALCULATION**  
KARAKOYUN N., ERKAN S.  
PCFM2021, 08 April 2021
11. **An approach to DFT on the 1,2,3-Selendiazole Based Compounds on Molecular Properties and Anti-Cancer Properties**  
MUHAMMAD U. S., ERKAN S.  
PCFM2021, Turkey, 08 April 2021
12. **Quantum Chemical Calculations on Manganese Complexes with Penta-Amine Macrocyclic Schiff Base Ligand: Computational and Molecular Docking**  
ERKAN S., SAYIN K., KARAKAŞ D.  
2nd International Conference on Physical Chemistry and Functional Materials, 25 - 27 June 2019
13. **Chemist'xxs Perspective in Cancer**  
ERKAN S.  
I. INTERNATIONAL CANCER DAYS, 19 - 21 September 2019
14. **Computational research on the molecular properties and anti-tumor activity ofPt (II) complexes with a chiral halogenated Schiff base ligand**  
KAYA S., ERKAN S., KARAKAŞ D.  
I. INTERNATIONAL CANCER DAYS, 19 - 21 September 2019
15. **SPECTROSCOPIC AND MOLECULAR DOCKING STUDY ON  $\alpha$ -AMINOPHOSPHONATES CONTAINING THIADIAZOLE MOIETY WITH ANTI-CANCER PROPERTIES**  
KEBİROĞLU H., ERKAN S., BULUT N.  
I. INTERNATIONAL CANCER DAYS, 19 - 21 September 2019
16. **A Theoretical Study on Spectroscopic and Anticancer Activities of PlatinumComplexes**  
MA KHALID H. H., ERKAN S., BULUT N.  
I. INTERNATIONAL CANCER DAYS, 19 - 21 September 2019
17. **Computational research on the molecular properties and anti-tumor activity of Pt (II) complexes with a chiral halogenated Schiff base ligand**  
Kaya S., ERKAN S., KARAKAŞ D.  
I. International Cancer Days, 19 - 21 September 2019, pp.455
18. **Computational Analysis of Structural, Spectroscopic and NLO Propertieson Molybdenum Carbonyl Complexes with 4,4'xx-Dipyridylacetylene BridgeLigand and Triphenyl Phosphine and Triphenoxy Phosphine TerminalLigand**  
ERKAN KARİPER S., KARAKAŞ D.  
2nd International Conference on Physical Chemistry Functional Materials, 25 - 27 June 2019
19. **NLO Properties and Molecular Docking Study Molybdenum CarbonylComplexes with Pyridyl Ligands with Alkyne Unit**  
ERKAN KARİPER S., KARAKAŞ D.  
2nd International Conference on Physical Chemistry Functional Materials, 25 - 27 June 2019
20. **Determination of Biological Reactivity against Lung Cancer Cell andInvestigations of NLO Properties of Ciprofloxacin-Boron Complexes**  
SAYIN K., ERKAN KARİPER S.  
2nd International Conference on Physical Chemistry Functional Materials, 25 - 27 June 2019
21. **Chemical Property of Platinum Complexes**

MA KHALID H. H., ERKAN KARİPER S., BULUT N.

2nd International Conference on Physical Chemistry Functional Materials, 25 - 27 June 2019

22. **Quantum Chemical Calculations on Ag and Pb Complexes with Penta-Amine Macrocylic Schiff Base Ligand: Computational and Molecular Docking Analyses**  
SAYIN K., ERKAN KARİPER S., KARAKAŞ D.  
2nd International Conference on Physical Chemistry Functional Materials, 25 - 27 June 2019
23. **Quantum Chemical Calculations on Manganese Complexes with PentaAmine Macrocylic Schiff Base Ligand: Computational and Molecular Docking**  
ERKAN KARİPER S., SAYIN K., KARAKAŞ D.  
2nd International Conference on Physical Chemistry Functional Materials, 25 - 27 June 2019
24. **Computational study on molybdenum-based metal carbonyl complexes**  
ERKAN KARİPER S., KARAKAŞ D.  
2nd International Conference on Physical Chemistry Functional Materials, 25 - 27 June 2019
25. **Computational study on molybdenum-based metal carbonyl complexes**  
ERKAN S., KARAKAŞ D.  
2nd International Conference on Physical Chemistry and Functional Materials(PCFM'19), 25 - 27 June 2019, pp.1
26. **Computational Analysis of Structural, Spectroscopic and NLO Properties on Molybdenum Carbonyl Complexes with 4,4'-xx-Dipyridylacetylene Bridge Ligand and Triphenyl Phosphine and Triphenoxy Phosphine Terminal Ligand**  
ERKAN S., KARAKAŞ D.  
2nd International Conference on Physical Chemistry and Functional Materials(PCFM'19), Nevşehir, Turkey, 25 - 27 June 2019, pp.8
27. **NLO Properties and Molecular Docking Study Molybdenum Carbonyl Complexes with Pyridyl Ligands with Alkyne Unit**  
ERKAN S., KARAKAŞ D.  
2nd International Conference on Physical Chemistry and Functional Materials(PCFM'19), Nevşehir, Turkey, 25 - 27 June 2019, pp.15
28. **Quantum Chemical Calculations on Ag and Pb Complexes with Penta-Amine Macrocylic Schiff Base Ligand: Computational and Molecular Docking Analyses**  
SAYIN K., ERKAN S., KARAKAŞ D.  
2nd International Conference on Physical Chemistry and Functional Materials, 25 - 27 June 2019
29. **Quantum Chemical Calculations on Ag and Pb Complexes with Penta-Amine Macrocylic Schiff Base Ligand: Computational and Molecular Docking Analyses**  
SAYIN K., ERKAN S., KARAKAŞ D.  
2nd International Conference on Physical Chemistry and Functional Materials (PCFM'xx19), 25 - 27 June 2019, pp.82
30. **Quantum Chemical Calculations on Manganese Complexes with Penta-Amine Macrocylic Schiff Base Ligand: Computational and Molecular Docking Analyses**  
ERKAN S., SAYIN K., KARAKAŞ D.  
2nd International Conference on Physical Chemistry and Functional Materials(PCFM'19), Nevşehir, Turkey, 25 - 27 June 2019, pp.21
31. **Determination of Biological Reactivity against Lung Cancer Cell and Investigations of NLO Properties of Ciprofloxacin-Boron Complexes**  
SAYIN K., ERKAN S.  
2nd International Conference on Physical Chemistry and Functional Materials, 25 - 27 June 2019
32. **The computational analysis on NLO properties and molecular docking studies for some cyclophosphazenes compounds**  
ERKAN KARİPER S., TÜZÜN B.  
2rd International Symposium on Innovative Approaches in Scientific Studies, 30 November - 02 December 2018
33. **Computational studies on the vanadocene dithiocarbamate complexes**  
ERKAN KARİPER S.

- 2nd International Symposium on Innovative Approaches in Scientific Studies, 30 November - 02 December 2018
34. **Investigation of Spectroscopic, Theoretical and Molecular Docking of vanilin thiosemicarbazone derivatives**  
TÜZÜN B., ERKAN S.
- 2nd international symposium on innovative approaches in scientific studies, 30 November - 02 December 2018
35. **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
36. **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
37. **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
38. **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
39. **Investigation of Some Antibiotics with Computational Chemistry Methods**  
ERKAN KARİPER S.
- International Eurasian Congress on Natural Nutrition and Healthy Life'xx 2018, 12 - 15 July 2018
40. **Investigation of  $\beta$ -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
41. **Spectroscopic Analysis of Complexes with N-alkyl-N-phenyl Dithiocarbamate Ligand Containing Trace Mine Zinc Metals with Computational Chemistry Methods**  
ERKAN KARİPER S.
- International Trace Analysis Congress, 20 May - 23 June 2018
42. **Computational Studies on Schrock Type  $\text{Mo}(\text{CO})_5(\text{Cme}_2)$  and  $\text{Mo}(\text{CO})_5(\text{Cmeet})$  Alkyliden Complexes Based on Density Functional Theory**  
özçiftci h., ERKAN S., SAYIN K., KARAKAŞ D.
- International Trace Analysis Congress (iTAC 2018), 20 - 23 June 2018
43. **Examination of Vaniline Thiosemicarbazone Ligand and Trace Metal Copper Spectroscopic Properties by Computational Chemistry Methods**  
ERKAN KARİPER S., TÜZÜN B.
- International Trace Analysis Congress (iTAC 2018), Sivas, Turkey, 20 - 23 June 2018
44. **Investigation of 1-Allyl-3-Butylbenzimidazolium-Derived Silver (I) Complexes in Terms of Structure and Biological Activity by Computational Chemistry Methods**  
SAYIN K., ERKAN KARİPER S., KARAKAŞ D.
- International Conference on Physical Chemistry and Functional Materials, 19 - 21 June 2018
45. **Bazı  $\beta$ -Lactam İnhibitörleri Üzerine Kuantum Kimyasal Çalışmalar**  
ERKAN KARİPER S., SAYIN K., KARAKAŞ D.
- v. ulusal anorganik kimya kongresi, Turkey, 22 April 2015 - 25 April 2018
46. **Yoğunluk Fonksiyon Teori Metoduyla  $[\text{MgO}_2\text{Ti}_2(\text{OPri})_6]$ ,  $[\text{MgO}_2\text{Ti}_2(\text{OPri})_2(\text{Acac})_4]$  ve  $[\text{MgO}_2\text{Ti}_2(\text{OPri})_2(\text{bzac})_4]$  Kompleksleri Üzerine Hesapsal Çalışmalar**  
SAYIN K., KARAKAŞ D., ERKAN KARİPER S.
- v. ulusal anorganik kimya kongresi, Turkey, 22 - 25 April 2018
47. **Investigation of Structural, Spectroscopic and Optical Properties of Some Dinuclear Metal Carbonyls Containing Pyridyl Ligands with Alkyne Unit by Using Quantum Chemical Calculations and Quantum Chemical Approaches on the Catalytic Activities of Complexes**

ERKAN KARİPER S.

2nd International Conference on Catalysis and Chemical Engineering, 19 - 21 February 2018

48. **ANTI-KANSER ÖZELLİĞİ TAŞIYAN SİKLOMETALAT İRİDYUM(III) KOMPLEKSLERİ ÜZERİNE YAPISAL, SPEKTROSKOPİK VE KUANTUM KİMYASAL HESAPLAMALAR**  
ERKAN KARİPER S., KARAKAŞ D.  
3. Hesaplamalı Kimya Kongresi, Turkey, 12 - 14 October 2017
49. **Mer-[Ru(Cl-Ph-tpy)(N-N)(X)] Tipi Rutenyum (II) Komplekslerinin Yapısal, Elektronik ve Antikanser Özelliklerinin Hesaplamalı Kimya Yöntemleriyle Araştırılması**  
ERKAN KARİPER S., SAYIN K., KARAKAŞ D.  
3. Hesaplamalı Kimya Kongresi, Turkey, 12 - 14 October 2017
50. **SPECTROSCOPIC AND QUANTUM CHEMICAL STUDIES ON SOME  $\beta$ -LACTAM INHIBITORS**  
ERKAN KARİPER S.  
2nd International Gazi Pharma Symposium Series, 11 - 13 October 2017
51. **Structural, Spectroscopic and Quantum Chemical Calculations on Cyclometalated Iridium (III) Complexes with Anticancer Properties**  
ERKAN KARİPER S., KARAKAŞ D.  
2nd International Gazi Pharma Symposium Series, 11 - 13 October 2017
52. **INVESTIGATIONS OF BIOLOGICAL PROPERTIES OF SOME METAL (MN, PD AND AG) COMPLEXES WITH PENTA-AMINEMACROCYCLIC SCHIFF BASE LIGAND: MOLECULAR DOCKING CALCULATIONS**  
SAYIN K., KARAKAŞ D., ERKAN KARİPER S.  
2nd International Gazi Pharma Symposium Series, 11 - 13 October 2017
53. **2-[(E)-(3,4-dimethylphenyl)imino]methyl]-6-methoxy-4-[(E)-phenyldiazenyl]phenol esaslı Cu(II), Zn(II) Komplekslerinin Sentezi ve Bazı Spektral Özellikleri**  
tekerek e., ERKAN KARİPER S., KURTOĞLU M.  
6th National Inorganic Chemistry Congress with International Participation, 18 - 21 May 2017
54. **YENİ AZO-AZOMETİN ESASLI Cu(II), Zn(II) KOMPLEKSLERİNİN SENTEZİ ve SPEKTRAL ÖZELLİKLERİ**  
tekerek e., ERKAN KARİPER S., KURTOĞLU M.  
6th National Inorganic Chemistry Congress with International Participation, 18 - 21 May 2017
55. **Investigation of solvent effect on biological reactivity, UV-VIS and NMR analyses of Zn(II) complexes with pentaaza macrocyclic schiff-base ligand**  
SAYIN K., KARAKAŞ D., KARAKUŞ N., ERKAN KARİPER S.  
TURCMOS 2015, 13 - 18 September 2015
56. **Bazı Çinko(II) Komplekslerinin Biyolojik Aktivite Sıralamasının Hesapsal Yöntemlerle Belirlenmesi**  
SAYIN K., ERKAN KARİPER S., SAYIN ALAGÖZ T., KARAKAŞ D.  
v. ulusal anorganik kimya kongresi, Turkey, 22 - 25 April 2015
57. **Bipridin ve Pridil-Primidin-4-Karboksilik Asit Temelli Ligantları İçeren Ru(II) Komplekslerinin Yapısal ve Antitümör Özellikleri Üzerine Teorik Çalışma**  
KARAKAŞ D., SAYIN K., ERKAN KARİPER S.  
v. ulusal anorganik kimya kongresi, Turkey, 22 - 25 April 2015
58. **Metansülfonilhidrazon Temelli Krompentakarbonil Kompleksleri Üzerine Yapısal, Spektroskopik ve Aktivite Hesaplamaları**  
ERKAN KARİPER S., SAYIN K., KARAKAŞ D.  
v. ulusal anorganik kimya kongresi, Turkey, 22 - 25 April 2015
59. **Azo-azometin Ligandı ve Cu(II) Kompleksinin Sentezi, Kararlılık ve Elektrokimyasal Özellikleri**  
sarıgül m., ERKAN S., ATABEY H., DEVECİ P., KURTOĞLU M.  
V. ULUSAL ANORGANİK KİMYA KONGRESİ, Turkey, 22 - 25 April 2015
60. **Oksimato Köprülü trans-Platin(II) Kompleksi Üzerine Kuantum Kimyasal Çalışmalar**  
SAYIN K., KARAKAŞ D., ERKAN KARİPER S.  
IV. Fiziksel Kimya Kongresi, Turkey, 5 - 08 June 2014
61. **Oksimato köprülü trans platin II kompleksi üzerine kuantum kimyasal çalışmalar**  
SAYIN K., KARAKAŞ D., ERKAN S.

Pamukkale Üniversitesi, IV. Fiziksel Kimya Kongresi, Denizli, Turkey, 5 - 08 June 2014

62. **Schiff baz ligantlı oksovanadyum IV komplekslerinin antidiabetik aktivitesi üzerine elektronik yapı etkisinin teorik olarak araştırılması**  
KARAKAŞ D., ERKAN S., SAYIN K.  
Yüzüncü Yıl Üniversitesi, I. Uluslar Arası Katılımlı Ulusal Hesaplamalı Kimya Çalıştayı, Van, Turkey, 29 - 31 May 2014
63. **Platin II oksim kompleksinin  $^{13}\text{C}$  ve  $^1\text{H}$  NMR spektrumlarının hesaplamalı kimya yöntemleriyle incelenmesi**  
KARAKAŞ D., SAYIN K., ERKAN S.  
Yüzüncü Yıl Üniversitesi, I. Uluslar Arası Katılımlı Ulusal Hesaplamalı Kimya Çalıştayı, Van, Turkey, 29 - 31 May 2014
64. **Bazı iki dişli Schiff baz ligandlarının bakır(II) komplekslerinin hesaplamalı yöntemlerle yapısal analizi**  
ERKAN KARİPER S., KAYA S., KARAKAŞ D.  
IV Ulusal Anorganik Kimya Kongresi, Turkey, 30 May - 02 June 2013
65. **Ab initio moleküler orbital yöntemleri ile  $\text{Co}_2(\text{CO})_8$  izomerlerinin moleküler yapı parametrelerinin ve titreşim frekanslarının hesaplanması**  
ERKAN S., KARAKAŞ D.  
GOP Üniversitesi, IV Ulusal Anorganik Kimya Kongresi, Turkey, 30 May - 02 June 2013
66. **AB initio moleküler orbital yöntemleri ile  $\text{Co}_2(\text{CO})_8$  izomerlerinin moleküler yapı parametrelerinin ve titreşim frekanslarının hesaplanması**  
ERKAN KARİPER S., KARAKAŞ D.  
IV Ulusal Anorganik Kimya Kongresi, Turkey, 30 May - 02 June 2013
67. **Bazı iki dişli Schiff baz ligandlarının bakır II komplekslerinin hesaplamalı yöntemlerle yapısal analizi**  
ERKAN S., KAYA S., KARAKAŞ D.  
GOP Üniversitesi, IV Ulusal Anorganik Kimya Kongresi, Turkey, 30 May - 02 June 2013
68. **Quantum chemical studies on the corrosion inhibition of  $\text{CrO}_4^{2-}$ ,  $\text{MoO}_4^{2-}$  and  $\text{NO}_3^-$**   
SAYIN K., KARAKAŞ D., ERKAN KARİPER S.  
10. Kimyasal Fizik Kongresi, 10 October 2012
69. **DFT structural studies on copper(II) complexes with symmetric and unsymmetric tripodal tetramine ligands**  
ERKAN KARİPER S., SAYIN K., KARAKAŞ D.  
10. Kimyasal Fizik Kongresi, 10 - 12 October 2012
70. **Theoretical studies on zinc complexes with schiff base ligand**  
SAYIN K., ERKAN KARİPER S., KARAKAŞ D.  
10. Kimyasal Fizik Kongresi, 10 - 12 October 2012
71. **The investigation of inhibition efficiency some imidazole derivatives against iron with quantum chemical methods**  
ERKAN KARİPER S., SAYIN K., KARAKAŞ D.  
10. Kimyasal Fizik Kongresi, 10 - 12 October 2012
72. **Quantum chemical studies on the corrosion inhibition of  $\text{CrO}_4^{2-}$ ,  $\text{MoO}_4^{2-}$  and  $\text{NO}_3^-$**   
SAYIN K., KARAKAŞ D., ERKAN S.  
TOBB Ekonomi ve Teknoloji Üniversitesi 10. Kimyasal Fizik Kongresi (CPC-X), 10 - 12 October 2012
73. **Theoretical studies on zinc complexes with schiff base ligand**  
SAYIN K., ERKAN S., KARAKAŞ D.  
TOBB Ekonomi ve Teknoloji Üniversitesi 10. Kimyasal Fizik Kongresi (CPC-X), 10 - 12 October 2012
74. **DFT structural studies on copper II complexes with symmetric and unsymmetric tripodal tetramine ligands**  
ERKAN S., SAYIN K., KARAKAŞ D.  
TOBB Ekonomi ve Teknoloji Üniversitesi 10. Kimyasal Fizik Kongresi (CPC-X), 10 - 12 October 2012
75. **The investigation of inhibition efficiency some imidazole derivatives against iron with quantum chemical methods**  
ERKAN S., KARAKAŞ D.

## Courses

Üniversite Kültürü, Associate Degree, 2019 - 2020  
Genel Kimya - I, Associate Degree, 2019 - 2020  
Çevre Kimyası, Associate Degree, 2018 - 2019  
Organik Kimya, Associate Degree, 2018 - 2019  
Bilim Adamları ve Buluşları, Associate Degree, 2019 - 2020  
Anorganik Kimya, Associate Degree, 2019 - 2020  
Analitik Kimya, Associate Degree, 2019 - 2020  
Genel Kimya Laboratuvarı, Associate Degree, 2018 - 2019  
Organik Kimya, Associate Degree, 2017 - 2018  
Genel Kimya Laboratuvarı, Associate Degree, 2017 - 2018  
Sosyal Bilimlerde Araştırma Yöntemleri, Associate Degree, 2018 - 2019  
Staj, Associate Degree, 2017 - 2018  
Yönlendirilmiş Çalışma, Associate Degree, 2016 - 2017  
Grafik ve Tasarım, Associate Degree, 2017 - 2018  
Kimyasal Hesaplamalar, Associate Degree, 2016 - 2017  
Özel Gıdalar Teknolojisi, Associate Degree, 2016 - 2017

## Activities in Scientific Journals

Turkish Computational and Theoretical Chemistry, Committee Member, 2017 - Continues

## Scientific Refereeing

Project Supported by Higher Education Institutions, BAP Research Project, Kahramanmaraş Sutcu Imam University, Turkey, December 2019  
Turkish Computational and Theoretical Chemistry , Other Indexed Journal, November 2019  
Cumhuriyet Science Journal, National Scientific Refreed Journal, November 2019  
CHEMICAL PAPERS, SCI Journal, June 2019

## Tasks In Event Organizations

Erkan S., 2nd International Conference on Physical Chemistry & Functional Materials, Scientific Congress, Nevşehir, Turkey, Haziran 2019

## Metrics

Publication: 155  
Citation (WoS): 969  
Citation (Scopus): 969  
H-Index (WoS): 18  
H-Index (Scopus): 18

## Congress and Symposium Activities

International Energy Days 2022, Moderator, Sivas, Turkey, 2022

5th International Conference on Physical Chemistry & Functional Materials, Moderator, Sivas, Turkey, 2022

1. ULUSLARARASI KANSER GÜNLERİ, Panelists, Sivas, Turkey, 2019

2nd International Conference on Physical Chemistry & Functional Materials, Moderator, Elazığ, Turkey, 2019

## Invited Talks

Investigation of Structural, Spectroscopic, Optical Properties and Catalytic Activities of Some Dinuclear Metal Carbonyls Containing Pyridyl Ligands with Alkyne Unit by Using Quantum Chemical Calculations, Conference, 2nd International Conference on Catalysis and Chemical Engineering, France, February 2018

## Research Areas

Bioinorganic Chemistry, Organometallic Chemistry