

GONCAGÜL SERDAROĞLU

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Öğrenim Bilgisi

Doktora 2004 - 2008	Sivas Cumhuriyet Üniversitesi, Fen Fakültesi, Kimya Bölümü, Türkiye
Yüksek Lisans 1999 - 2003	Sivas Cumhuriyet Üniversitesi, Fen Fakültesi, Kimya Bölümü, Türkiye
Lisans 1994 - 1998	Sivas Cumhuriyet Üniversitesi, Fen Fakültesi, Kimya Bölümü, Türkiye

Yabancı Diller

İngilizce, B2 Orta Üstü

Yaptığı Tezler

Doktora, Sinir sinyal iletimini sağlayan bazı moleküllerin yapısal özelliklerinin ve etkinliklerinin moleküler orbital yöntemleriyle incelenmesi, Sivas Cumhuriyet Üniversitesi, Fen Fakültesi, Kimya Bölümü, 2008

Yüksek Lisans, Spektroskopik verilerden yararlanarak termodinamik büyüklüklerin hesaplanması, Sivas Cumhuriyet Üniversitesi, Fen Fakültesi, Kimya Bölümü, 2003

Akademik Unvanlar / Görevler

Doç. Dr. 2019 - Devam Ediyor	Sivas Cumhuriyet Üniversitesi, Eğitim Fakültesi, Matematik ve Fen Bilimleri Eğitimi Bölümü
Dr. Öğr. Üyesi 2010 - Devam Ediyor	Sivas Cumhuriyet Üniversitesi, Eğitim Fakültesi, Matematik ve Fen Bilimleri Eğitimi Bölümü
Araştırma Görevlisi 2001 - 2010	Sivas Cumhuriyet Üniversitesi, Eğitim Fakültesi, Matematik ve Fen Bilimleri Eğitimi Bölümü

Desteklenen Projeler

1. Şahin Bölükbaşı S., Serdaroğlu G., Şahin N., Yükseköğretim Kurumları Destekli Proje, Ag-NHC komplekslerinin sentezi, spektroskopik karakterizasyonu ve antitümör davranışlarının deneysel ve kuantum kimyasal hesaplama yöntemleri ile incelenmesi, 2019 - 2021
2. Serdaroğlu G., Yükseköğretim Kurumları Destekli Proje, Dasikarpidon türevi bileşiklerin yapısal, elektronik, spektroskopik ve optik özelliklerinin moleküler orbital yöntemlerle incelenmesi, 2019 - 2020
3. SERDAROĞLU G., Yükseköğretim Kurumları Destekli Proje, 1,5-Metanoazosino[4,3-b] indollerin sentezinde kullanılan bileşiklerin elektronik ve optik özelliklerinin kuantum kimyasal yöntemlerle incelenmesi, 2018 - 2018
4. SERDAROĞLU G., Yükseköğretim Kurumları Destekli Proje, 1, 3- disübstitüte- 9H-pyrido[3,4-b] indollerin kimyasal aktiviteleri üzerine sübstitüent etkisinin Hesaplamalı Kimya ile incelenmesi, 2017 - 2018
5. SERDAROĞLU G., ELİK M., Yükseköğretim Kurumları Destekli Proje, Beta Karbonil Bileşiklerinin Antitümör Özellikleri Üzerine Hesaplamalı Kimya Çalışması, 2016 - 2017
6. SERDAROĞLU G., Yükseköğretim Kurumları Destekli Proje, Antiepileptik ilaç moleküllerinin etkinliklerinin açıklanmasında Elektron Propegator Teorinin EPT kullanılması üzerine hesaplamalı Calisma, 2013 - 2014
7. SERDAROĞLU G., Yükseköğretim Kurumları Destekli Proje, Sinir Sinyal İletimini Sağlayan Bazı Moleküllerin Yapısal Özelliklerinin Ve Etkinliklerinin Moleküler Orbital Yöntemleriyle İncelenmesi, 2006 - 2008

Ödüller

1. Serdaroğlu G., Kaya S., EN İYİ SÖZLÜ SUNUM ÖDÜLÜ, Abdelmalek Essaadi University, Aralık 2020
2. Serdaroğlu G., EN İYİ POSTER ÖDÜLÜ, International Conference On Physical Chemistry And Functional Materials, Royal Society Of Chemistry, Temmuz 2018
3. Serdaroğlu G., POSTER ÖDÜLÜ, 9Th Global Chemistry Congress, Haziran 2018

SCI, SSCI ve AHCI İndekslerine Giren Dergilerde Yayınlanan Makaleler

1. **Functionalized p-cymene and pyrazine derivatives: Physicochemical, ADMT, drug-likeness, and DFT studies**
SERDAROĞLU G.
Computational Biology and Chemistry, cilt.117, 2025 (SCI-Expanded)
2. **An improved approach to the synthesis of tetrahydroindeno[1,2-d] imidazoles: DFT (FT-IR, NMR, NBO, FMO), ADMET, and drug-likeness studies**
SERDAROĞLU G., Uludag N., SERİN S.
Journal of Molecular Liquids, cilt.423, 2025 (SCI-Expanded)
3. **Bubble energy nanogenerators**
Bolsu Kariper S. E., KARİPER İ. A., SERDAROĞLU G.
Heat and Mass Transfer/Waerme- und Stoffuebertragung, cilt.61, sa.4, 2025 (SCI-Expanded)
4. **Synthesis, Biological Activities, DFT Calculations, and Molecular Docking Studies of O-Methyl-Inositols**
Aksu K., Ayvaz M. Ç., Çelik Ö. F., SERDAROĞLU G., Üstün E., Kelebekli L.
Chemistry and Biodiversity, 2025 (SCI-Expanded)
5. **In silico ADMET and DFT analysis of methoxy substituted curcumin derivatives**
Afrdi M. B., Sardar H., SERDAROĞLU G., Wadood Ali Shah S., Alsharif K. F., Khan H.
Inorganic Chemistry Communications, cilt.168, 2024 (SCI-Expanded)
6. **SwissADME studies and Density Functional Theory (DFT) approaches of methyl substituted curcumin derivatives**
Afridi M. B., Sardar H., SERDAROĞLU G., Shah S. W. A., Alsharif K. F., Khan H.
Computational Biology and Chemistry, cilt.112, 2024 (SCI-Expanded)
7. **CuO-Catalyzed Synthesis, Characterization, and Computational Studies of Ethyl 2-Cyano-3-(1H-indol-3-yl)-3-phenylpropanoate Derivatives**

Mishra A., Das R., SERDAROĞLU G., Pandit J., Mishra P., Bahe A., Shukla N.

Russian Journal of General Chemistry, cilt.94, sa.9, ss.2321-2330, 2024 (SCI-Expanded)

8. **Green Synthesis of Ethyl 2-[(1H-Indol-3-yl)(phenyl)methyl]-3-oxobutanoate Derivatives Using NiO Nanocatalysts**
Pratibha P., Das R., SERDAROĞLU G., Pandit J., Bahe A., Mishra A.
Russian Journal of General Chemistry, cilt.94, sa.8, ss.2023-2037, 2024 (SCI-Expanded)
9. **Mixed Organic Cation in Chiral Two-Dimensional Organic-Inorganic Hybrid Metal Halides—An Ab Initio Study of Nonlinear Optical (NLO) Properties**
Cheng X., Muthukrishnan S., Mi H., Deng S., SERDAROĞLU G., Vidya R., Stroppa A.
Journal of Physical Chemistry C, cilt.128, sa.27, ss.11392-11400, 2024 (SCI-Expanded)
10. **Green synthesis, characterization, anti-cancer and antimicrobial activity of AuNPs extracted from Euphorbia antiquorum stem and flower: Experimental and theoretical calculations**
Venkatesh G., SERDAROĞLU G., Üstün E., Haripriya D., Vennila P., Siva V., Haseena S., Sowmiya V., Pradhiksha A.
Journal of Drug Delivery Science and Technology, cilt.95, 2024 (SCI-Expanded)
11. **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, cilt.28, sa.2, ss.509-530, 2024 (SCI-Expanded)
12. **Green Synthesis of Pyrrole Derivatives Catalyzed by Molecular Sieves: DFT, ADMT, and Molecular Docking Investigations**
SERDAROĞLU G., Uludağ N., Üstün E.
ChemistrySelect, cilt.9, sa.9, 2024 (SCI-Expanded)
13. **Advancing Pyrrole Synthesis through DDQ Catalysis: A Comprehensive Research Incorporating DFT, ADMT, and Molecular Docking Analysis**
SERDAROĞLU G., Uludağ N., Üstün E.
ChemistrySelect, cilt.9, sa.2, 2024 (SCI-Expanded)
14. **Computational Study of Coumarin Compounds as Potential Inhibitors of Casein Kinase 2: DFT, 2D-QSAR, ADMET and Molecular Docking Investigations**
Chennai H. Y., Belaidi S., Ouassaf M., Sinha L., Prasad O., SERDAROĞLU G., Chtita S.
Polycyclic Aromatic Compounds, 2024 (SCI-Expanded)
15. **An efficient new method of ytterbium(III) triflate catalysis approach to the synthesis of substituted pyrroles: DFT, ADMET, and molecular docking investigations**
SERDAROĞLU G., Uludag N., Üstün E.
Computational Biology and Chemistry, cilt.106, 2023 (SCI-Expanded)
16. **Molecular modeling study on the water-electrode surface interaction in hydrovoltaic energy**
SERDAROĞLU G., KARİPER İ. A., Kariper S. E. B.
Scientific reports, cilt.13, sa.1, ss.12803, 2023 (SCI-Expanded)
17. **A novel series of tetrahydrothieno[2,3-c]pyridin-2-yl derivatives: fluorescence spectroscopy and BSA binding, ADMET properties, molecular docking, and DFT studies**
SERDAROĞLU G., Uludag N., Üstün E., Colak N.
New Journal of Chemistry, cilt.47, sa.25, ss.11945-11963, 2023 (SCI-Expanded)
18. **Physicochemical properties, drug likeness, ADMET, DFT studies, and in vitro antioxidant activity of oxindole derivatives**
Ahmad I., Khan H., SERDAROĞLU G.
Computational Biology and Chemistry, cilt.104, 2023 (SCI-Expanded)
19. **Copper(II) chelates derived from an N,N,O-tridentate 2-pyridinecarboxaldehyde-N4-phenylsemicarbazone: Synthesis, spectral aspects, crystal structure, FMO and NBO analysis**
Sithambaresan M., Kurup M. R. P., SERDAROĞLU G., KAYA S.
Journal of Molecular Structure, cilt.1277, 2023 (SCI-Expanded)
20. **Efficient synthesis of chromeno[2,3-b]pyridine derivatives using Zn(OTf)₂ as a catalyst: DFT computations, molecular docking and ADME studies**

SERDAROĞLU G., Uludag N., Üstün E.

Journal of Molecular Liquids, cilt.375, 2023 (SCI-Expanded)

21. **Substituted naphthoxy-phthalonitrile derivatives: Synthesis, substituent effects, DFT, TD-DFT Calculations, antimicrobial properties and DNA interaction studies**
Erdoğan M., Başkan C., SERDAROĞLU G.
Computational Biology and Chemistry, cilt.102, 2023 (SCI-Expanded)
22. **Nitrobenzamido substitution on thiophene-3-carboxylate: Electrochemical investigation, antioxidant activity, molecular docking, DFT calculations**
SERDAROĞLU G., Uludag N., Colak N., Rajkumar P.
Journal of Molecular Structure, cilt.1271, 2023 (SCI-Expanded)
23. **Strychnos alkaloids: total synthesis, characterization, DFT investigations, and molecular docking with AChE, BuChE, and HSA**
Uludag N., Üstün E., SERDAROĞLU G.
Heliyon, cilt.8, sa.12, 2022 (SCI-Expanded)
24. **Mathematical modeling studies for the adsorptive removal of ciprofloxacin drug from water samples using functionalized silica resin**
Junejo R., Jalbani N. S., KAYA S., SERDAROĞLU G., ELİK M.
CHEMICAL PAPERS, cilt.76, sa.6, ss.3413-3423, 2022 (SCI-Expanded)
25. **Synthesis of thiophene derivatives: Substituent effect, antioxidant activity, cyclic voltammetry, molecular docking, DFT, and TD-DFT calculations**
ULUDAĞ N., SERDAROĞLU G., Sugumar P., Rajkumar P., ÇOLAK N., Ercag E.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1257, 2022 (SCI-Expanded)
26. **Cyanomethylation of 2,3,4,9-tetrahydro-1H-carbazol-1-one based on using two different reagents: Antioxidant activity and DFT studies**
SERDAROĞLU G., ULUDAĞ N., Ercag E.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1253, 2022 (SCI-Expanded)
27. **Spectral, thermal and DFT studies of novel nickel(II) complexes of 2-benzoylpyridine-N-4-methyl-3-thiosemicarbazone: Crystal structure of a square planar azido-nickel(II) complex**
Jayakumar K., Seena E. B., Kurup M. R. P., Kayac S., SERDAROĞLU G., Suresh E., Marzouki R.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1253, 2022 (SCI-Expanded)
28. **Corrosion inhibition of steel using different families of organic compounds: Past and present progress**
Aslam R., SERDAROĞLU G., Zehra S., Verma D. K., Aslam J., Guo L., Verma C., Ebenso E. E., Quraishi M. A.
JOURNAL OF MOLECULAR LIQUIDS, cilt.348, 2022 (SCI-Expanded)
29. **Experimental and DFT Modeling Studies for the Adsorptive Removal of Reactive Dyes from Wastewater**
Junejo R., Shams Jalbani N., KAYA S., SERDAROĞLU G., ŞİMŞEK S., Memon S.
SEPARATION SCIENCE AND TECHNOLOGY, cilt.57, sa.3, ss.339-353, 2022 (SCI-Expanded)
30. **Synthesis, crystal structure, Hirshfeld surface analysis and DFT calculations of 2, 2, 2-tribromo-1-(3,5-dibromo-2-hydroxyphenyl)ethanone**
Brahmia A., Bejaoui L., Roliczek J., Hassen R., SERDAROĞLU G., KAYA S.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1248, 2022 (SCI-Expanded)
31. **Equilibrium, thermodynamic, and kinetic modeling studies for the adsorptive removal of oxyanions from water**
Junejo R., Shams Jalbani N., KAYA S., SERDAROĞLU G., ELİK M., Memon S.
SEPARATION SCIENCE AND TECHNOLOGY, cilt.57, sa.12, ss.1884-1899, 2022 (SCI-Expanded)
32. **Novel Ag(I)-NHC complex: synthesis, in vitro cytotoxic activity, molecular docking, and quantum chemical studies**
SERDAROĞLU G., ŞAHİN N., ŞAHİN BÖLÜKBAŞI S., ÜSTÜN E.
ZEITSCHRIFT FÜR NATURFORSCHUNG SECTION C-A JOURNAL OF BIOSCIENCES, cilt.77, sa.1-2, ss.21-36, 2022 (SCI-Expanded)

33. **DFT computational study of trihalogenated aniline derivative's adsorption onto graphene/fullerene/fullerene-like nanocages, X12Y12 (X = Al, B, and Y = N, P)**
Al-Otaibi J. S., Mary Y. S., Mary Y. S., Kaya S., Serdaroglu G.
JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS, cilt.40, sa.19, ss.8630-8643, 2022 (SCI-Expanded)
34. **An efficient studies on C-2 cyanomethylation of the indole synthesis: The electronic and spectroscopic characterization (FT-IR, NMR, UV-Vis), antioxidant activity, and theoretical calculations**
ULUDAĞ N., SERDAROĞLU G.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1247, 2022 (SCI-Expanded)
35. **Synthesis, characterization, biological and DFT studies of charge-transfer complexes of antihyperlipidemic drug atorvastatin calcium with Iodine, Chloranil, and DDQ**
Niranjani S., Nirmala C. B., Rajkumar P., SERDAROĞLU G., Jayaprakash N., Venkatachalam K.
JOURNAL OF MOLECULAR LIQUIDS, cilt.346, 2022 (SCI-Expanded)
36. **Conformational Analysis, Spectroscopic Insights, Chemical Descriptors, ELF, LOL and Molecular Docking Studies of Potential Pyrimidine Derivative with Biological Activities**
Mary Y. S., Mary Y. S., SERDAROĞLU G., KAYA S., Sarojini B. K., Umamahesvari H., Mohan B. J.
POLYCYCLIC AROMATIC COMPOUNDS, cilt.42, sa.8, ss.5160-5170, 2022 (SCI-Expanded)
37. **Spectral studies and quantum chemical ab initio calculations for Copper(II) complexes of two heterocyclic aroylhydrazones**
Sheeja S. R., Mangalam N. A., Sithambaresan M., Kurup M. R. P., Kaya S., Serdaroglu G.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1245, 2021 (SCI-Expanded)
38. **Performance of curing epoxy resin as potential anticorrosive coating for carbon steel in 3.5% NaCl medium: Combining experimental and computational approaches**
Hsissou R., Benhiba F., Echihi S., Benzidia B., Cherrouf S., Haldhar R., Alvi P. A., KAYA S., SERDAROĞLU G., Zarrouk A.
CHEMICAL PHYSICS LETTERS, cilt.783, 2021 (SCI-Expanded)
39. **Synthesis, spectroscopic characterization, DFT calculations, and molecular docking studies of new unsymmetric bishydrazone derivatives**
Kaya Y., Erçağ A., Serdaroglu G., Kaya S., Grillo I. B., Rocha G. B.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1244, 2021 (SCI-Expanded)
40. **Synthesis, identification, density functional and Hirshfeld surface studies of 2,2 '-disulfaneylbis(tetrahydro-4H-cyclopenta[d][1,3,2]dioxaphosphole-2-sulfide)**
Mkadmh A. M., Safi Z. S., Elkhalidy A. A., Staples R. J., KAYA S., SERDAROĞLU G.
JOURNAL OF COMPUTATIONAL CHEMISTRY, cilt.42, sa.26, ss.1873-1884, 2021 (SCI-Expanded)
41. **Electrochemical investigations and theoretical studies of biocompatible niacin-modified carbon paste electrode interface for electrochemical sensing of folic acid**
Ganesh P., Kim S., Choi D., KAYA S., SERDAROĞLU G., Shimoga G., Shin E., Lee S.
JOURNAL OF ANALYTICAL SCIENCE AND TECHNOLOGY, cilt.12, sa.1, 2021 (SCI-Expanded)
42. **Structural, electronic, and spectroscopic study on 1,5-methanoazocino[4,3-b]indole synthesized by TFB-based route**
SERDAROĞLU G., ULUDAĞ N.
CHEMICAL PAPERS, cilt.75, sa.9, ss.4549-4564, 2021 (SCI-Expanded)
43. **New Hybrid (E)-4-((pyren-1-ylmethylene)amino)-N-(thiazol-2-yl)benzenesulfonamide as a Potential Drug Candidate: Spectroscopy, TD-DFT, NBO, FMO, and MEP Studies****
Erdogan M., SERDAROĞLU G.
CHEMISTRYSELECT, cilt.6, sa.35, ss.9369-9381, 2021 (SCI-Expanded)
44. **PEPPSI type complexes: Synthesis, x-ray structures, spectral studies, molecular docking and theoretical investigations**
SERDAROĞLU G., ŞAHİN N., ÜSTÜN E., Tahir M. N., Arici C., GÜRBÜZ N., ÖZDEMİR İ.
POLYHEDRON, cilt.204, 2021 (SCI-Expanded)
45. **Modeling the DFT structural and reactivity studies of a pyrimidine-6-carboxylate derivative with reference to its wavefunction-dependent, MD simulations and evaluation for potential antimicrobial**

activity

Smitha M., Mary Y. S., Mary Y. S., SERDAROĞLU G., Chowdhury P., Rana M., Umamahesvari H., Sarojini B. K., Mohan B. J., Pavithran R.

JOURNAL OF MOLECULAR STRUCTURE, cilt.1237, 2021 (SCI-Expanded)

46. **Two empirical formulae for estimating standard entropy of inorganic ionic solids and a possible connection between two associated electronic structure principles**
KAYA S., Chattaraj P. K., SERDAROĞLU G.
POLYHEDRON, cilt.202, 2021 (SCI-Expanded)
47. **Zeolite/Cellulose Acetate (ZCA) in Blend Fiber for Adsorption of Erythromycin Residue From Pharmaceutical Wastewater: Experimental and Theoretical Study**
Jodeh S., Erman I., Hamed O., Massad Y., Hanbali G., Samhan S., Dagdag O., KAYA S., SERDAROĞLU G.
FRONTIERS IN CHEMISTRY, cilt.9, 2021 (SCI-Expanded)
48. **The composite microbeads of alginate, carrageenan, gelatin, and poly(lactic-co-glycolic acid): Synthesis, characterization and Density Functional Theory calculations**
Baybaş D., Serdaroglu G., Semerci B.
International Journal of Biological Macromolecules, cilt.181, ss.322-338, 2021 (SCI-Expanded)
49. **Adsorption of Eriochrome Black T on the chitin surface: Experimental study, DFT calculations and molecular dynamics simulation**
Boumya W., Khnifira M., Machrouhi A., Abdennouri M., Sadiq M., Achak M., SERDAROĞLU G., KAYA S., ŞİMŞEK S., Barka N.
Journal of Molecular Liquids, cilt.331, 2021 (SCI-Expanded)
50. **Synthesis, in vitro anticancer activities, and quantum chemical investigations on 1,3-bis-(2-methyl-2-propenyl)benzimidazolium chloride and its Ag(I) complex**
SERDAROĞLU G., ŞAHİN BÖLÜKBAŞI S., Barut-Celepçi D., Sevinçek R., ŞAHİN N., GÜRBÜZ N., ÖZDEMİR İ.
JOURNAL OF CHEMICAL RESEARCH, cilt.45, sa.5-6, ss.596-607, 2021 (SCI-Expanded)
51. **Carbazole derivatives: Synthesis, spectroscopic characterization, antioxidant activity, molecular docking study, and the quantum chemical calculations**
SERDAROĞLU G., ULUDAĞ N., Ercag E., Sugumar P., Rajkumar P.
JOURNAL OF MOLECULAR LIQUIDS, cilt.330, 2021 (SCI-Expanded)
52. **Hydroxy phenyl hydrazides and their role as corrosion impeding agent: A detail experimental and theoretical study**
Singh A. K., Chugh B., Singh M., Thakur S., Pani B., Guo L., KAYA S., SERDAROĞLU G.
JOURNAL OF MOLECULAR LIQUIDS, cilt.330, 2021 (SCI-Expanded)
53. **Conformational analysis and quantum descriptors of two bifonazole derivatives of immense anti-tuber potential by using vibrational spectroscopy and molecular docking studies**
Mary Y. S., Mary Y. S., SERDAROĞLU G., Sarojini B. K.
STRUCTURAL CHEMISTRY, cilt.32, sa.2, ss.859-867, 2021 (SCI-Expanded)
54. **Adsorption of adipic acid in Al/B-N/P nanocages: DFT investigations**
Al-Otaibi J. S., Mary Y. S., Mary Y. S., SERDAROĞLU G.
JOURNAL OF MOLECULAR MODELING, cilt.27, sa.4, 2021 (SCI-Expanded)
55. **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, cilt.66, ss.379-388, 2021 (SCI-Expanded)
56. **A combined molecular dynamic simulation, DFT calculations, and experimental study of the eriochrome black T dye adsorption onto chitosan in aqueous solutions**
Khnifira M., Boumya W., Abdennouri M., Sadiq M., Achak M., SERDAROĞLU G., KAYA S., ŞİMŞEK S., Barka N.
International Journal of Biological Macromolecules, cilt.166, ss.707-721, 2021 (SCI-Expanded)
57. **Synthesis, crystal structure, hirshfeld surface analysis, spectroscopic, biological and first-principles studies of novel aminocoumarins**
Bejaoui L., Brahmia A., Marzouki R., Dusek M., Eigner V., SERDAROĞLU G., KAYA S., Bour M. E., Hassen R. B.

- Journal of Molecular Structure, cilt.1221, 2020 (SCI-Expanded)
58. **Eco-friendly sodium gluconate and trisodium citrate inhibitors for low carbon steel in simulated cooling water system: Theoretical study and molecular dynamic simulations**
SERDAROĞLU G., KAYA S., Touir R.
JOURNAL OF MOLECULAR LIQUIDS, cilt.319, 2020 (SCI-Expanded)
59. **The electronic and spectroscopic investigation of (+/-)- Dasycarpidone**
SERDAROĞLU G., Uludag N.
VIBRATIONAL SPECTROSCOPY, cilt.111, 2020 (SCI-Expanded)
60. **Mixed ligand copper(II) chelates derived from an O, N, S- donor tridentate thiosemicarbazone: Synthesis, spectral aspects, FMO, and NBO analysis**
Jacob J. M., Kurup M. R. P., Nisha K., SERDAROĞLU G., KAYA S.
POLYHEDRON, cilt.189, 2020 (SCI-Expanded)
61. **Computational Study of 2,3-dihydrospiro[carbazole-1,2'-xx-[1,3]dithiolan]-4(9H)-one compound: Structure, FT-IR, NMR, NLO, and NBO Analyses**
Serdaroglu G., Uludag N.
Journal Of The Indian Chemical Society, cilt.97, sa.10, ss.2026-2030, 2020 (SCI-Expanded)
62. **Harmine derivatives: a comprehensive quantum chemical investigation of the structural, electronic (FMO, NBO, and MEP), and spectroscopic (FT-IR and UV-Vis) properties**
SERDAROĞLU G.
RESEARCH ON CHEMICAL INTERMEDIATES, cilt.46, sa.1, ss.961-982, 2020 (SCI-Expanded)
63. **Direct arylation of heteroarenes by PEPPSI-type palladium-NHC complexes and representative quantum chemical calculations for the compound which the structure was determined by X-ray crystallography**
ŞAHİN N., SERDAROĞLU G., Dusunceli S. D., Tahir M. N., Arici C., ÖZDEMİR İ.
JOURNAL OF COORDINATION CHEMISTRY, cilt.72, ss.3258-3284, 2019 (SCI-Expanded)
64. **The synthesis and spectroscopic characterization of (+)-demethoxyaspidospermine: Density functional theory calculations of the structural, electronic, and non-linear optic and spectroscopic properties**
Serdaroglu G., Uludag N.
JOURNAL OF CHEMICAL RESEARCH, cilt.43, ss.531-541, 2019 (SCI-Expanded)
65. **An efficient method for the azocino[4,3-b]indole framework of strychnos alkaloids: OFT investigations on the electronic and spectroscopic properties**
Uludag N., SERDAROĞLU G., Colak N.
JOURNAL OF THE INDIAN CHEMICAL SOCIETY, cilt.96, sa.9, ss.1221-1226, 2019 (SCI-Expanded)
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