

GONCAGÜL SERDAROĞLU

ASSOC. PROF.

Email : serdaroglu@cumhuriyet.edu.tr

International Researcher IDs

ORCID: 0000-0001-7649-9168

Yoksis Researcher ID: 101847

Learning Knowledge

Doctorate 2004 - 2008	Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, Turkey
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Postgraduate 1999 - 2003	Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, Turkey
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Undergraduate 1994 - 1998	Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, Turkey
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Foreign Languages

English, B2 Upper Intermediate

Dissertations

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

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

Academic Titles / Tasks

Associate Professor 2019 - Continues	Sivas Cumhuriyet University, Eğitim Fakültesi, Matematik Ve Fen Bilimleri Eğitimi Bölümü
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Assistant Professor 2010 - Continues	Sivas Cumhuriyet University, Eğitim Fakültesi, Matematik Ve Fen Bilimleri Eğitimi Bölümü
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Research Assistant 2001 - 2010	Sivas Cumhuriyet University, Eğitim Fakültesi, Matematik Ve Fen Bilimleri Eğitimi Bölümü
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Supported Projects

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

Awards

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

Published journal articles indexed by SCI, SSCI, and AHCI

1. **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, vol.168, 2024 (SCI-Expanded)
2. **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, vol.112, 2024 (SCI-Expanded)
3. **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, vol.94, no.9, pp.2321-2330, 2024 (SCI-Expanded)
4. **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, vol.94, no.8, pp.2023-2037, 2024 (SCI-Expanded)
5. **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, vol.128, no.27, pp.11392-11400, 2024 (SCI-Expanded)
6. **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, vol.95, 2024 (SCI-Expanded)

7. **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)
8. **Green Synthesis of Pyrrole Derivatives Catalyzed by Molecular Sieves: DFT, ADMT, and Molecular Docking Investigations**
SERDAROĞLU G., Uludağ N., Üstün E.
ChemistrySelect, vol.9, no.9, 2024 (SCI-Expanded)
9. **Advancing Pyrrole Synthesis through DDQ Catalysis: A Comprehensive Research Incorporating DFT, ADMT, and Molecular Docking Analysis**
SERDAROĞLU G., Uludağ N., Üstün E.
ChemistrySelect, vol.9, no.2, 2024 (SCI-Expanded)
10. **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)
11. **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, vol.106, 2023 (SCI-Expanded)
12. **Molecular modeling study on the water-electrode surface interaction in hydrovoltaic energy**
SERDAROĞLU G., KARİPER İ. A., Kariper S. E. B.
Scientific reports, vol.13, no.1, pp.12803, 2023 (SCI-Expanded)
13. **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, vol.47, no.25, pp.11945-11963, 2023 (SCI-Expanded)
14. **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, vol.104, 2023 (SCI-Expanded)
15. **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, vol.1277, 2023 (SCI-Expanded)
16. **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, vol.375, 2023 (SCI-Expanded)
17. **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, vol.102, 2023 (SCI-Expanded)
18. **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, vol.1271, 2023 (SCI-Expanded)
19. **Strychnos alkaloids: total synthesis, characterization, DFT investigations, and molecular docking with AChE, BuChE, and HSA**
Uludag N., Üstün E., SERDAROĞLU G.

Heliyon, vol.8, no.12, 2022 (SCI-Expanded)

20. **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, vol.76, no.6, pp.3413-3423, 2022 (SCI-Expanded)
21. **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, vol.1257, 2022 (SCI-Expanded)
22. **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, vol.1253, 2022 (SCI-Expanded)
23. **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, vol.1253, 2022 (SCI-Expanded)
24. **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, vol.348, 2022 (SCI-Expanded)
25. **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, vol.57, no.3, pp.339-353, 2022 (SCI-Expanded)
26. **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., Rolicek J., Hassen R., SERDAROĞLU G., KAYA S.
JOURNAL OF MOLECULAR STRUCTURE, vol.1248, 2022 (SCI-Expanded)
27. **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, vol.40, no.19, pp.8630-8643, 2022 (SCI-Expanded)
28. **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, vol.1247, 2022 (SCI-Expanded)
29. **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, vol.77, no.1-2, pp.21-36, 2022 (SCI-Expanded)
30. **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, vol.57, no.12, pp.1884-1899, 2022 (SCI-Expanded)
31. **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, vol.346, 2022 (SCI-Expanded)

32. **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, vol.42, no.8, pp.5160-5170, 2022 (SCI-Expanded)
33. **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., Serdaroğlu G.
JOURNAL OF MOLECULAR STRUCTURE, vol.1245, 2021 (SCI-Expanded)
34. **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, vol.783, 2021 (SCI-Expanded)
35. **Synthesis, spectroscopic characterization, DFT calculations, and molecular docking studies of new unsymmetric bishydrazone derivatives**
Kaya Y., Erçağ A., Serdaroğlu G., Kaya S., Grillo I. B., Rocha G. B.
JOURNAL OF MOLECULAR STRUCTURE, vol.1244, 2021 (SCI-Expanded)
36. **Synthesis, identification, density functional and Hirshfeld surface studies of 2,2'-disulfanediybis(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, vol.42, no.26, pp.1873-1884, 2021 (SCI-Expanded)
37. **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, vol.12, no.1, 2021 (SCI-Expanded)
38. **Structural, electronic, and spectroscopic study on 1,5-methanoazocino[4,3-b]indole synthesized by TFB-based route**
SERDAROĞLU G., ULUDAĞ N.
CHEMICAL PAPERS, vol.75, no.9, pp.4549-4564, 2021 (SCI-Expanded)
39. **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, vol.6, no.35, pp.9369-9381, 2021 (SCI-Expanded)
40. **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, vol.1237, 2021 (SCI-Expanded)
41. **PEPSI 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, vol.204, 2021 (SCI-Expanded)
42. **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, vol.9, 2021 (SCI-Expanded)
43. **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, vol.202, 2021 (SCI-Expanded)
44. **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, vol.181, pp.322-338, 2021 (SCI-Expanded)

45. **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, vol.331, 2021 (SCI-Expanded)
46. **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, vol.330, 2021 (SCI-Expanded)
47. **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, vol.45, no.5-6, pp.596-607, 2021 (SCI-Expanded)
48. **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, vol.330, 2021 (SCI-Expanded)
49. **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, vol.32, no.2, pp.859-867, 2021 (SCI-Expanded)
50. **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, vol.27, no.4, 2021 (SCI-Expanded)
51. **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)
52. **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, vol.166, pp.707-721, 2021 (SCI-Expanded)
53. **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, vol.1221, 2020 (SCI-Expanded)
54. **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, vol.319, 2020 (SCI-Expanded)
55. **The electronic and spectroscopic investigation of (+/-)- Dasycarpidone**
SERDAROĞLU G., Uludag N.
VIBRATIONAL SPECTROSCOPY, vol.111, 2020 (SCI-Expanded)
56. **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, vol.97, no.10, pp.2026-2030, 2020 (SCI-Expanded)
57. **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, vol.189, 2020 (SCI-Expanded)

58. **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, vol.46, no.1, pp.961-982, 2020 (SCI-Expanded)
59. **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, vol.72, pp.3258-3284, 2019 (SCI-Expanded)
60. **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, vol.43, pp.531-541, 2019 (SCI-Expanded)
61. **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, vol.96, no.9, pp.1221-1226, 2019 (SCI-Expanded)
62. **Spectroscopic (FT-IR, NMR) and Computational Investigation of 2-(2-Aminoethyl)-1,2,3,4,9-Tetrahydrocarbazole: NBO, NLO, FMO, MEP Analysis**
SERDAROĞLU G., Uludag N.
JOURNAL OF STRUCTURAL CHEMISTRY, vol.60, no.8, pp.1267-1284, 2019 (SCI-Expanded)
63. **A DFT Investigation on the Structure, Spectroscopy (FT-IR and NMR), Donor-Acceptor Interactions and Non-Linear Optic Properties of (+/-)-1,2-Dehydroaspidospermidine**
Uludag N., SERDAROĞLU G.
CHEMISTRYSELECT, vol.4, no.23, pp.6870-6878, 2019 (SCI-Expanded)
64. **The synthesis and characterization of 1-(Allyl)-3-(2-methylbenzyl) benzimidazolium chloride: FT-IR, NMR, and DFT computational investigation**
SERDAROĞLU G., ŞAHİN N.
JOURNAL OF MOLECULAR STRUCTURE, vol.1178, pp.212-221, 2019 (SCI-Expanded)
65. **Concise total synthesis of (+/-)-aspidospermidine and computational study: FT-IR, NMR, NBO, NLO, FMO, MEP diagrams**
SERDAROĞLU G., ULUDAĞ N.
JOURNAL OF MOLECULAR STRUCTURE, vol.1166, pp.286-303, 2018 (SCI-Expanded)
66. **A novel synthesis of octahydropyrido[3,2-c]carbazole framework of aspodospermidine alkaloids and a combined computational, FT-IR, NMR, NBO, NLO, FMO, MEP study of the cis-4a-Ethyl-1(2hydroxyethyl)-2,3,4,4a,5,6,7,11c-octahydro-1H-pyrido[3,2-c] carbazole**
ULUDAĞ N., SERDAROĞLU G., YİNANÇ A.
JOURNAL OF MOLECULAR STRUCTURE, vol.1161, pp.152-168, 2018 (SCI-Expanded)
67. **An improved synthesis, spectroscopic (FT-IR, NMR) study and DFT computational analysis (IR, NMR, UV-Vis, MEP diagrams, NBO, NLO, FMO) of the 1,5-methanoazocino[4,3-b]indole core structure**
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1. **Towards Understanding the Corrosion Inhibition Mechanism of Green Imidazolium-Based Ionic Liquids for Mild Steel Protection in Acidic Environments**
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2. **Terpene Derivatives: A Comprehensive Computational Insights in Drug-likeness and ADMT Properties, and DFT Study**
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3. **Geranial benzeri -dienlerin İlaç Benzerliği ve ADMT Özelliklerine İlişkin Hesaplamalı Analizler**
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6. **Conformational analysis and DFT investigations of two triazole derivatives and its halogenated substitution by using spectroscopy, AIM and Molecular docking**
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13. **A Computational Study of 1-Substituted Methyl 9-Methyl-9H-Pyrido[3,4-b]indole-3-Carboxylate: Quantum Chemical Descriptors, FMO and NBO**
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14. **DFT Based Quantum Chemical Descriptors of 1-Substituted THβC, DHβC, βC Derivatives**
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2. **Organic and Inorganic Corrosion Inhibitors A Comparison**
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2. **Drug likeness, in silico ADMET, and antioxidant study of oxindole derivatives**
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3. **A THEORETICAL AND COMPUTATIONAL INSIGHT ON THE TOXICITY OF THE ORGANIC CHEMICALS**
SERDAROĞLU G., KAYA S.
The Third Edition of The International Congress On Water And Environment Studies, Morocco, Morocco, 10 December 2020
4. **The substituent effect on chemical reactivity of (9H-pyrido[3,4-b]indol-3-yl)methanol: Spectroscopic and electronic investigation**
SERDAROĞLU G., KAYA S.
International Virtual Conference on Materials and Environmental Science, Morocco, 18 November 2020
5. **Electrochemical and theoretical study of the behaviour of a Carbon steel in HCl medium by some triazole type compounds**
Merimi İ., B H., Merimi C., SZUMIATA T., SERDAROĞLU G., KAYA S.
4th Edition of the International Virtual Conference on Materials & Environmental Science, Morocco, Morocco, 18 November 2020
6. **The Computational Study on methyl (1R,4S,5R)-4-hydroxy-6-oxo-1,3,4,5,6,7-hexahydro-2H-1,5-methanoazocino[4,3-b]indole-2-carboxylate: FT-IR, NMR, NBO, and FMO Analyses**
SERDAROĞLU G., ULUDAĞ N.
4th Edition of the International Virtual Conference on Materials & Environmental Science, Morocco, Morocco, 18 - 27 November 2020
7. **The metal chelation effect on the chemical reactivity of the (E)-2-(2-(pyridin-2-ylmethylene)hydrazineyl) phenol: Theoretical and computational investigation**
Kaya S., Serdaroglu G., Merimi İ.
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8. **The substituent effect on chemical reactivity of (9H-pyrido[3,4-b]indole-3-yl)methanol: Spectroscopic and electronic investigation**
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21. **A DFT AND AB INITIO INVESTIGATION ON THE STRUCTURAL, ELECTRONIC AND SPECTROSCOPIC (FT-IR, UV-VIS) PROPERTIES OF THE TRYPTOLINES**
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9th Global Chemistry Congress, Lizbon, Portugal, 23 - 24 July 2018, vol.6, pp.51
23. **A Computational Approach on the structural, electronic, and spectroscopic properties of the aromatic substituted indole alkaloids**
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9th Global Chemistry Congress, Lisbon, Portugal, 23 - 24 July 2018, vol.6, pp.29
24. **The structural, electronic and specktroskopik properties on the intermediate reagent used in synthesizing of the alkaloids: Computational and Experimental Study**
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36. **A Computational Study on Clobazam**
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XI. Chemical Physics Congress, İstanbul, Turkey, 17 - 18 October 2014, vol.2, pp.42-44
37. **Computational Study on some anti-epileptic drug molecules**
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39. **Solvent effect on active sites of the zwitterionic GABA and its agonists A Theoretical Study**
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40. **A Computational study based on conformational properties of phenethylamine of biochemical and medicinal interest**
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III. Fiziksel Kimya Günleri, Turkey, 12 - 15 July 2012, pp.175
41. **DFT study on conformational dependence of atomic charges Chemical Reactivity Relationship Amphetamine**
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42. **DFT ab initio study on conformational dependence of atomic charges of neutral and cationic epinephrine molecule**
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25. Ulusal Kimya Kongresi, Turkey, 27 June - 02 July 2011, pp.125
43. **A Molecular Orbital Study of the Conformational Properties of Cationic Ephedrine**
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25. Ulusal Kimya Kongresi, Turkey, 27 June - 02 July 2011, pp.124
44. **The conformational dependence of atomic charges of tyramine in gas phase and aqueous phase A DFT ab initio Study**
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Chemical Physics Congress-IX, 14 - 16 October 2010, pp.16
45. **Parabanik Asit İmidazolin 2 4 5 trion Molekülündeki Tautomer Dengesi Üzerine Çözücü Etkisinin DFT Yöntemiyle İncelenmesi**
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24. Ulusal Kimya Kongresi, Zonguldak Karaelmas Üniversitesi, Turkey, 29 June - 02 July 2010
46. **Histamin Molekülünün Konformasyonel Yapılarının Teorik Olarak İncelenmesi**
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24. Ulusal Kimya Kongresi, Turkey, 29 June - 02 July 2010
47. **Serotonin ve kloro fenil alanin Moleküllerinin Reaktif Merkezleri Üzerine DFT Ab initio Çalışması**
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24. Ulusal Kimya Kongresi, Turkey, 29 June - 02 July 2010
48. **Asetilkolin karbakol metakolin ve betanekol moleküllerinin reaktif merkezlerinin DFT ile aydınlatılması**
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49. **GABA ve agonistleri olan DABA TACA CACA ve muskimol moleküllerinin yapı aktivite ilişkileri üzerine çözücü etkisinin DFT ile incelenmesi**
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50. **Histaminin Tautomerik Yapılarının Üzerine Betahistin Etkisi**
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- XXII. Ulusal Kimya Kongresi, Turkey, 6 - 10 October 2008, pp.77
52. **GABA ve Muskimol Moleküllerinin Biyolojik Aktivitelerinin DFT Yöntemiyle İncelenmesi**
ELİK M., SERDAROĞLU G.
XXII. Ulusal Kimya Kongresi, Turkey, 6 - 10 October 2008, pp.138
53. **Sinir Sinyal İletiminde Rol Oynayan Glutamat ve Glisin ile Agonistleri olan Alanin ve Aspartik asit Moleküllerinin Fiziksel Özellikleri ve Etkinliklerinin DFT ile Aydınlatılması**
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XXII. Ulusal Kimya Kongresi, Turkey, 6 - 10 October 2008, pp.78
54. **Ab Initio Study on Biological Activity of Acetylcholine and Carbachol**
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VIII. Kimyasal Fizik Kongresi, 24 - 25 April 2008, pp.27
55. **Tautomerism of The Histamine Molecule A theoretical Study**
SERDAROĞLU G., Durmaz S.
VIII. Kimyasal Fizik Kongresi, 24 - 25 April 2008, pp.28
56. **Dopamin ve Norepinefrin Moleküllerinin Atomik Yükleri**
SERDAROĞLU G.
21. Ulusal Kimya Kongresi, Turkey, 23 - 27 August 2007
57. **Spektroskopik Verilerin Kullanılması ile Termodinamik Büyüklüklerin Hesaplanması**
SERDAROĞLU G.
XVIII. Ulusal Kimya Kongresi, Turkey, 5 - 09 July 2004, vol.23, pp.614

Courses

- Öğretmenlik Uygulaması, Undergraduate, 2018 - 2019
- Genel Kimya - I, Undergraduate, 2019 - 2020
- Genel Kimya - I, Undergraduate, 2019 - 2020
- Topluma Hizmet Uygulaması, Undergraduate, 2018 - 2019
- Genel Kimya - II, Undergraduate, 2018 - 2019
- Kimya - I, Undergraduate, 2019 - 2020
- IFO 1012 GENEL KİMYA II, Undergraduate, 2017 - 2018, 2016 - 2017
- Genel Kimya Lab - I, Undergraduate, 2018 - 2019
- İFÖ 4036 Öğretmenlik Uygulaması, Undergraduate, 2017 - 2018
- Genel Kimya - II, Undergraduate, 2017 - 2018
- IFO 1011 GENEL KİMYA I, Undergraduate, 2017 - 2018, 2016 - 2017
- Kimyada Özel Konular, Undergraduate, 2018 - 2019
- ILK 5015 FEN EĞİTİMİNDE İLERİ KİMYA, Postgraduate, 2017 - 2018, 2016 - 2017
- IFO 1014 GENEL KİMYA LABORATUVARI II, Undergraduate, 2016 - 2017
- IFO 3020 TOPLUMA HİZMET UYGULAMALARI, Undergraduate, 2016 - 2017
- Genel Kimya Lab - II, Undergraduate, 2016 - 2017
- Öğretmenlik Uygulaması, Undergraduate, 2016 - 2017
- Topluma Hizmet Uygulamaları, Undergraduate, 2016 - 2017
- İSÖ 3024 TOPLUMA HİZMET UYGULAMALARI, Undergraduate, 2016 - 2017
- Fen Eğitiminde İleri Kimya, Postgraduate, 2017 - 2018
- IFO 1013 GENEL KİMYA LABORATUVARI I, Undergraduate, 2016 - 2017
- IFO 3017 KİMYADA OZEL KONULAR, Undergraduate, 2016 - 2017
- Genel Kimya Lab - I, Undergraduate, 2016 - 2017
- Kimyada Özel Konular, Undergraduate, 2016 - 2017
- Fen Teknoloji ve Toplum, Undergraduate, 2015 - 2016
- Fen Teknoloji ve Toplum, Undergraduate, 2015 - 2016
- Genel Kimya Lab - II, Undergraduate, 2015 - 2016

Topluma Hizmet Uygulamaları, Undergraduate, 2015 - 2016
Genel Kimya, Undergraduate, 2014 - 2015
Topluma Hizmet Uygulamaları, Undergraduate, 2014 - 2015
Çevre Kimyası, Undergraduate, 2014 - 2015
Topluma Hizmet Uygulamaları, Undergraduate, 2014 - 2015
Çevre Kimyası, Undergraduate, 2014 - 2015
Topluma Hizmet Uygulaması, Undergraduate, 2014 - 2015
Genel Kimya, Undergraduate, 2014 - 2015
Öğretmenlik Uygulaması, Undergraduate, 2014 - 2015
Genel Kimya, Undergraduate, 2009 - 2010
Kimya-II, Undergraduate, 2009 - 2010

Activities in Scientific Journals

Turkish Computational and Theoretical Chemistry, Editor, 2017 - Continues

Tasks In Event Organizations

Serdaroğlu G., 2nd International Conference on Physical Chemistry and Functional Materials, Scientific Congress, Nevşehir, Turkey, Haziran 2019
Serdaroğlu G., 8th European Chemistry Congress, Scientific Congress, France, Haziran 2018
Serdaroğlu G., II.Ulusal Okul Öncesi Eğitimi Öğrenci Kongresi, Scientific Congress, Sivas, Turkey, Mayıs 2007

Mobility Activity

Post Doc, Post Doc, Auburn University, United States Of America, 2013 - 2014
Erasmus Programme, Lecturing, Aalborg Universitet (Aalborg University), Denmark, 2010 - 2010

Metrics

Publication: 149
Citation (WoS): 497
Citation (Scopus): 712
H-Index (WoS): 14
H-Index (Scopus): 16

Congress and Symposium Activities

Biyomolekül Modelleme Teknikleri ve Uygulamaları, Working Group, İstanbul, Turkey, 2010

Research Areas

Chemistry, Computational Chemistry, Statistical Mechanics, Quantum Mechanics

Non Academic Experience

Laquila University
IQM-CSIC,
Auburn University