GONCAGÜL SERDAROĞLU
ASSOC. PROF.

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International Researcher IDs
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Learning Knowledge

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

Foreign Languages

English, B2 Upper Intermediate

Dissertations

Doctorate, Sinir 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
Assistant Professor 2010 - Continues	Sivas Cumhuriyet University, Eğitim Fakültesi, Matematik Ve Fen Bilimleri Eğitimi Bölümü
Research Assistant 2001 - 2010	Sivas Cumhuriyet University, Eğitim Fakültesi, Matematik Ve Fen Bilimleri Eğitimi Bölümü

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- disübstitüte- 9H-pyrido[3,4-b] indollerin kimyasal aktiviteleri üzerine sübstitüent etkisinin Hesaplamalı Kimya ile incelenmesi, 2017 - 2018
5. ELİK M., SERDAROĞLU G., 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 aciklanmasinda Elektron Propegator Teorinin EPT kullanilmasi üzerine hesaplamali 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. **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)
2. **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)
3. **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)
4. **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)
5. **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)
6. **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)

7. **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)
8. **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)
9. **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)
10. **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)
11. **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)
12. **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, 2023 (SCI-Expanded)
13. **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)
14. **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)
15. **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)
16. **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)
17. **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)
18. **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)
19. **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)

20. **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)
21. **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)
22. **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 FUR NATURFORSCHUNG SECTION C-A JOURNAL OF BIOSCIENCES, vol.77, no.1-2, pp.21-36, 2022 (SCI-Expanded)
23. **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)
24. **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., Serdaroğlu G.
JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS, vol.40, no.19, pp.8630-8643, 2022 (SCI-Expanded)
25. **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)
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. **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)
28. **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)
29. **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)
30. **Synthesis, identification, density functional and Hirshfeld surface studies of 2,2 '-disulfanediylbis(tetrahydro-4H-cyclopenta[d][1,3,2]dioxaphosphole-2-sulfide)**
Mkadmh A. M., Safi Z. S., Elkhaldy A. A., Staples R. J., KAYA S., SERDAROĞLU G.
JOURNAL OF COMPUTATIONAL CHEMISTRY, vol.42, no.26, pp.1873-1884, 2021 (SCI-Expanded)
31. **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)

32. **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)

33. **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)

34. **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)

35. **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, vol.204, 2021 (SCI-Expanded)

36. **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)

37. **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)

38. **The composite microbeads of alginate, carrageenan, gelatin, and poly(lactic-co-glycolic acid): Synthesis, characterization and Density Functional Theory calculations**
Baybaş D., Serdaroğlu G., Semerci B.
International Journal of Biological Macromolecules, vol.181, pp.322-338, 2021 (SCI-Expanded)

39. **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)

40. **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)

41. **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)

42. **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-Celepci D., Sevinçek R., ŞAHİN N., GÜRBÜZ N., ÖZDEMİR İ.
JOURNAL OF CHEMICAL RESEARCH, vol.45, no.5-6, pp.596-607, 2021 (SCI-Expanded)

43. **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)

44. **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)

45. **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)

46. **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)

47. **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)

48. **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)

49. **The electronic and spectroscopic investigation of (+/-)- Dasycarpidone**
SERDAROĞLU G., Uludag N.
VIBRATIONAL SPECTROSCOPY, vol.111, 2020 (SCI-Expanded)

50. **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)

51. **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**
Serdaroğlu G., Uludağ N.
Journal Of The Indian Chemical Society, vol.97, no.10, pp.2026-2030, 2020 (SCI-Expanded)

52. **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)

53. **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)

54. **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)

55. **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)

56. **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)

57. **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)
58. **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)
59. **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)
60. **A novel synthesis of octahydropyrido[3,2-c]carbazole framework of aspidospermidine 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)
61. **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**
ULUDAĞ N., SERDAROĞLU G.
JOURNAL OF MOLECULAR STRUCTURE, vol.1155, pp.548-560, 2018 (SCI-Expanded)
62. **A computational study on relationship between quantum chemical parameters and reactivity of the zwitterionic GABA and its agonists: Solvent effect**
SERDAROĞLU G.
INDIAN JOURNAL OF CHEMISTRY SECTION A-INORGANIC BIO-INORGANIC PHYSICAL THEORETICAL & ANALYTICAL CHEMISTRY, vol.56, no.11, pp.1143-1153, 2017 (SCI-Expanded)
63. **Ab Initio Calculations on some Antiepileptic Drugs such as Phenytoin, Phenbarbital, Ethosuximide and Carbamazepine**
Serdaroglu G., Ortiz J. V.
STRUCTURAL CHEMISTRY, vol.28, no.4, pp.957-964, 2017 (SCI-Expanded)
64. **DFT and Ab Initio Computational Study on the Reactivity Sites of the GABA and its Agonists, Such as CACA, TACA, DABA, and Muscimol: In the Gas Phase and Dielectric Media**
Serdaroglu G.
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, vol.111, no.14, pp.3938-3948, 2011 (SCI-Expanded)
65. **A DFT Study of Determination of the Reactive Sites of the Acetylcholine and Its Agonists: In the Gas Phase and Dielectric Medium**
Serdaroglu G.
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, vol.111, no.10, pp.2464-2475, 2011 (SCI-Expanded)
66. **DFT and statistical mechanics entropy calculations of diatomic and polyatomic molecules**
Serdaroglu G., Durmaz S.
INDIAN JOURNAL OF CHEMISTRY SECTION A-INORGANIC BIO-INORGANIC PHYSICAL THEORETICAL & ANALYTICAL CHEMISTRY, vol.49, no.7, pp.861-866, 2010 (SCI-Expanded)

Articles Published in Other Journals

1. **Pyrimidine and cumene derivatives functionalized by hydroxy and methoxy: Computational insights in drug-likeness, ADM, and toxicity studies**
SERDAROĞLU G., Soyutek E., Koçarslan Ş., Uludağ C.

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3. **Experimental and Theoretical Spectroscopic Studies of the Electronic Structure of 2-Ethyl-2-phenylmalonamide**
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4. **Conformational analysis and DFT investigations of two triazole derivatives and its halogenated substitution by using spectroscopy, AIM and Molecular docking**
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8. **Effect of substitution on corrosion inhibition properties of three Imidazole derivatives on mild steel in 1M HCl**
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9. **A Computational study predicting the chemical reactivity behavior of 1-substituted 9-ethyl-βCCM derivatives: DFT- Based Quantum Chemical Descriptors**
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10. **An entry to the synthesis of uleine-type alkaloids by Fischer indole synthesis reactions: FT-IR, NMR spectroscopy and computational study of the substituted carbazole compound**
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11. **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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12. **DFT Based Quantum Chemical Descriptors of 1-Substituted THβC, DHβC, βC Derivatives**
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13. **Investigation with Molecular Orbital Method of Electron Charge Distribution and Electrostatic Properties of Dopamine and Amphetamine Molecules**
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14. **Mirisetin ve Kuersetin Bileşiklerinin Antioksidan Etkinliklerinin DFT Yöntemleriyle İncelenmesi**
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15. **Dopamin ve Amfetamin Moleküllerinin Elektron Yük Dağılımları ve Elektrostatik Özelliklerinin Moleküler Orbital Yöntem ile İncelenmesi**
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2. **Organic and Inorganic Corrosion Inhibitors A Comparison**
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Refereed Congress / Symposium Publications in Proceedings

1. **RECENT TRENDS IN QUANTUM CHEMICAL CALCULATION**
SERDAROĞLU G.
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2. **Drug likeness, in silico ADMET, and antioxidant study of oxindole derivatives**
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4th Commonwealth Chemistry, England, 4 - 05 October 2023
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 substituent effect on chemical reactivity of (9H-pyrido[3,4-b]indole-3-yl)methanol: Spectroscopic and electronic investigation**
SERDAROĞLU G., KAYA S.
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., Serdaroğlu G., Merimi İ.
4th Edition of the International Virtual Conference on Materials & Environmental Science, 18 - 27 November 2020, pp.15-21
8. **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**
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16. **INTRAMOLECULAR INTERACTIONS OF (S)-2-(1-(ANTHRACEN-9-YL)-9-ETHYL-9H-PYRIDO[3,4-B]INDOL-3-YL)PROPANE-2-OL**
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21. **A COMPUTATIONAL STUDY ON THE N-HETEROCYCLIC CARBENE COMPOUND: THE ELECTRONIC (FMO, NBO, MEP) AND SPECTROSCOPIC (FT-IR, NMR) INVESTIGATION**
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23. **A Computational Approach on the structural, electronic, and spectroscopic properties of the aromatic substituted indole alkaloids**
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24. **A DFT study: the structural and electronic properties of substituted 3-hydoxymethyl-β-carboline**
SERDAROĞLU G.
International Conference on Physical Chemistry and Functional Materials, Elazığ, Turkey, 19 - 21 June 2018, vol.1, pp.285

25. **The structural, electronic and specktroskopic properties on the intermediate reagent used in synthesizing of the alkaloids: Computational and Experimental Study**
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27. **A Computational Approaches on the structural, electronic and spectroscopic properties of the phenylhydrazine**
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34. **Substituent effect on reactivity of βCCM: A Computational Study**
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35. **A Computational Study on Clobazam**
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XI. Chemical Physics Congress, İstanbul, Turkey, 17 - 18 October 2014, vol.2, pp.42-44

36. **A Computational Study on Relationship between Solubility and Molecular Structure: Lamotrigine**
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XI. Chemical Physics Congress, İstanbul, Turkey, 17 - 18 October 2014, vol.2, pp.39-41

37. **Computational Study on some anti-epileptic drug molecules**
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Meeting of the Southeastern Theoretical Chemistry Association, Atlanta, United States Of America, 15 - 17 May 2014, pp.81

38. **The Conformational Dependence on Phenobarbitone Molecule s Reactivity in Gas phase and Dielectric media**
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Research Week, Auburn, ALABAMA, United States Of America, 14 - 17 April 2014

39. **Solvent effect on active sites of the zwitterionic GABA and its agonists A Theoretical Study**
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Chemical Physics Congress-X, 10 - 12 October 2012, pp.110

40. **DFT study on conformational dependence of atomic charges Chemical Reactivity Relationship Amphetamine**
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III. Fiziksel Kimya Günleri, Turkey, 12 - 15 July 2012, pp.174

41. **A Computational study based on conformational properties of phenethylamine of biochemical and medicinal interest**
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42. **A Molecular Orbital Study of the Conformational Properties of Cationic Ephedrine**
SERDAROĞLU G.
25. Ulusal Kimya Kongresi, Turkey, 27 June - 02 July 2011, pp.124

43. **DFT ab initio study on conformational dependence of atomic charges of neutral and cationic epinephrine molecule**
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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**
KARAKUŞ N., SERDAROĞLU G.
24. Ulusal Kimya Kongresi, Zonguldak Karaelmas Üniversitesi, Turkey, 29 June - 02 July 2010

46. **Histamin Molekülünün Konformasyonel Yapılarının Teorik Olarak İncelenmesi**
SERDAROĞLU G.
24. Ulusal Kimya Kongresi, Turkey, 29 June - 02 July 2010
47. **Serotonin ve kloro fenil alanin Moleküllerinin Reaktif Merkezleri Üzerine DFT Ab initio Çalışması**
SERDAROĞLU G.
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48. **Asetilkolin karbakol metakolin ve betanekol moleküllerinin reaktif merkezlerinin DFT ile aydınlatılması**
SERDAROĞLU G.
XXIII. Ulusal Kimya Kongresi, Turkey, 16 - 20 June 2009
49. **GABA ve agonistleri olan DABA TACA CACA ve muskimol molekülerinin yapı aktivite ilişkileri üzerine çözücü etkisinin DFT ile incelenmesi**
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XXIII. Ulusal Kimya Kongresi, Turkey, 16 - 20 June 2009
50. **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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51. **Histaminin Tautomerik Yapılarının Üzerine Betahistin Etkisi**
KARAKUŞ N., SERDAROĞLU G.
XXII. Ulusal Kimya Kongresi, Turkey, 6 - 10 October 2008, pp.152
52. **GABA ve Muskimol Moleküllerinin Biyolojik Aktivitelerinin DFT Yöntemiyle İncelenmesi**
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XXII. Ulusal Kimya Kongresi, Turkey, 6 - 10 October 2008, pp.138
53. **Norepinefrin Epinefrin ve Dopamin Molekülleri Üzerine Amfetamin Etkisinin Moleküler Orbital Yöntemle İncelenmesi**
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XXII. Ulusal Kimya Kongresi, Turkey, 6 - 10 October 2008, pp.77
54. **Tautomerism of The Histamine Molecule A theoretical Study**
SERDAROĞLU G., Durmaz S.
VIII. Kimyasal Fizik Kongresi, 24 - 25 April 2008, pp.28
55. **Ab Initio Study on Biological Activity of Acetylcholine and Carbachol**
SERDAROĞLU G., Durmaz S.
VIII. Kimyasal Fizik Kongresi, 24 - 25 April 2008, pp.27
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 EGİTİMİNDE ILERİ KİMYA, Postgraduate, 2017 - 2018, 2016 - 2017
IFO 1014 GENEL KİMYA LABORATUVARİ II, Undergraduate, 2016 - 2017
IFO 3020 TOPLUMA HİZMET UYGULAMALARİ, 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 LABORATUVARİ 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: 141
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