

Doç.Dr. GONCAGÜL SERDAROĞLU

Kişisel Bilgiler

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Eğitim Bilgileri

Doktora, Sivas Cumhuriyet Üniversitesi, Fen Fakültesi, Kimya Bölümü, Türkiye 2004 - 2008

Yüksek Lisans, Sivas Cumhuriyet Üniversitesi, Fen Fakültesi, Kimya Bölümü, Türkiye 1999 - 2003

Lisans, Sivas Cumhuriyet Üniversitesi, Fen Fakültesi, Kimya Bölümü, Türkiye 1994 - 1998

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

Araştırma Alanları

Kimya, Hesapsal Kimya, İstatiksel Mekanik, Kuantum Mekanik

Akademik Unvanlar / Görevler

Doç.Dr., Sivas Cumhuriyet Üniversitesi, Eğitim Fakültesi, Matematik Ve Fen Bilimleri Eğitimi Bölümü, 2019 - Devam Ediyor

Dr.Öğr.Üyesi, Sivas Cumhuriyet Üniversitesi, Eğitim Fakültesi, Matematik Ve Fen Bilimleri Eğitimi Bölümü, 2010 - Devam Ediyor

Araştırma Görevlisi, Sivas Cumhuriyet Üniversitesi, Eğitim Fakültesi, Matematik Ve Fen Bilimleri Eğitimi Bölümü, 2001 - 2010

Verdiği Dersler

Öğretmenlik Uygulaması, Lisans, 2018 - 2019

Genel Kimya - I, Lisans, 2019 - 2020

Genel Kimya - I, Lisans, 2019 - 2020

Topluma Hizmet Uygulaması, Lisans, 2018 - 2019

Genel Kimya - II, Lisans, 2018 - 2019
Kimya - I, Lisans, 2019 - 2020
IFO 1012 GENEL KİMYA II, Lisans, 2017 - 2018, 2016 - 2017
Genel Kimya Lab - I, Lisans, 2018 - 2019
İFÖ 4036 Öğretmenlik Uygulaması, Lisans, 2017 - 2018
Genel Kimya - II, Lisans, 2017 - 2018
IFO 1011 GENEL KİMYA I, Lisans, 2017 - 2018, 2016 - 2017
Kimyada Özel Konular, Lisans, 2018 - 2019
ILK 5015 FEN EĞİTİMİNDE İLERİ KİMYA, Yüksek Lisans, 2017 - 2018, 2016 - 2017
IFO 1014 GENEL KİMYA LABORATUVARI II, Lisans, 2016 - 2017
IFO 3020 TOPLUMA HİZMET UYGULAMALARI, Lisans, 2016 - 2017
Genel Kimya Lab - II, Lisans, 2016 - 2017
Öğretmenlik Uygulaması, Lisans, 2016 - 2017
Topluma Hizmet Uygulamaları, Lisans, 2016 - 2017
İSÖ 3024 TOPLUMA HİZMET UYGULAMALARI, Lisans, 2016 - 2017
Fen Eğitiminde İleri Kimya, Yüksek Lisans, 2017 - 2018
IFO 1013 GENEL KİMYA LABORATUVARI I, Lisans, 2016 - 2017
IFO 3017 KİMYADA OZEL KONULAR, Lisans, 2016 - 2017
Genel Kimya Lab - I, Lisans, 2016 - 2017
Kimyada Özel Konular, Lisans, 2016 - 2017
Fen Teknoloji ve Toplum, Lisans, 2015 - 2016
Fen Teknoloji ve Toplum, Lisans, 2015 - 2016
Genel Kimya Lab - II, Lisans, 2015 - 2016
Topluma Hizmet Uygulamaları, Lisans, 2015 - 2016
Genel Kimya, Lisans, 2014 - 2015
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Çevre Kimyası, Lisans, 2014 - 2015
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Topluma Hizmet Uygulaması, Lisans, 2014 - 2015
Genel Kimya, Lisans, 2014 - 2015
Öğretmenlik Uygulaması, Lisans, 2014 - 2015
Genel Kimya, Lisans, 2009 - 2010
Kimya-II, Lisans, 2009 - 2010

SCI, SSCI ve AHCI İndekslerine Giren Dergilerde Yayınlanan Makaleler

- I. **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)
- II. **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)
- III. **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)
- IV. **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)

- V. **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)
- VI. **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)
- VII. **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)
- VIII. **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)
- IX. **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)
- X. **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)
- XI. **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)
- XII. **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)
- XIII. **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)
- XIV. **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)
- XV. **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)
- XVI. **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)
- XVII. **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, cilt.1248, 2022 (SCI-Expanded)
- XVIII. **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, cilt.1245, 2021 (SCI-Expanded)
- XIX. **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, cilt.1244, 2021 (SCI-Expanded)
- XX. **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)
- XXI. **Synthesis, identification, density functional and Hirshfeld surface studies of 2,2 '-disulfanediybis(tetrahydro-4H-cyclopenta[d][1,3,2]dioxaphosphole-2-sulfide)**
 Mkdahm A. M., Safi Z. S., Elkhaldy A. A., Staples R. J., KAYA S., SERDAROĞLU G.
 JOURNAL OF COMPUTATIONAL CHEMISTRY, cilt.42, sa.26, ss.1873-1884, 2021 (SCI-Expanded)
- XXII. **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)
- XXIII. **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)
- XXIV. **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)
- XXV. **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)
- XXVI. **PEPSSI 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)
- XXVII. **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)
- XXVIII. **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)

- XXIX. **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)
- XXX. **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)
- XXXI. **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)
- XXXII. **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)
- XXXIII. **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)
- XXXIV. **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)
- XXXV. **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)
- XXXVI. **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)
- XXXVII. **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)
- XXXVIII. **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)
- XXXIX. **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., Tourir R.
JOURNAL OF MOLECULAR LIQUIDS, cilt.319, 2020 (SCI-Expanded)
- XL. **The electronic and spectroscopic investigation of (+/-)- Dasycarpidone**
SERDAROĞLU G., Uludag N.
VIBRATIONAL SPECTROSCOPY, cilt.111, 2020 (SCI-Expanded)
- XLI. **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)
- XLII. **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)
- XLIII. **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)
- XLIV. **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)
- XLV. **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)
- XLVI. **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)
- XLVII. **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, cilt.60, sa.8, ss.1267-1284, 2019 (SCI-Expanded)
- XLVIII. **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, cilt.4, sa.23, ss.6870-6878, 2019 (SCI-Expanded)
- XLIX. **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, cilt.1178, ss.212-221, 2019 (SCI-Expanded)
- L. **Concise total synthesis of (+/-)-aspidospermidine and computational study: FT-IR, NMR, NBO, NLO, FMO, MEP diagrams**
SERDAROĞLU G., ULUDAĞ N.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1166, ss.286-303, 2018 (SCI-Expanded)
- LI. **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, cilt.1161, ss.152-168, 2018 (SCI-Expanded)
- LII. **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, cilt.1155, ss.548-560, 2018 (SCI-Expanded)
- LIII. **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, cilt.56, sa.11, ss.1143-1153, 2017 (SCI-Expanded)

- LIV. **Ab Initio Calculations on some Antiepileptic Drugs such as Phenytoin, Phenbarbital, Ethosuximide and Carbamazepine**
Serdaroglu G., Ortiz J. V.
STRUCTURAL CHEMISTRY, cilt.28, sa.4, ss.957-964, 2017 (SCI-Expanded)
- LV. **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, cilt.111, sa.14, ss.3938-3948, 2011 (SCI-Expanded)
- LVI. **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, cilt.111, sa.10, ss.2464-2475, 2011 (SCI-Expanded)
- LVII. **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, cilt.49, sa.7, ss.861-866, 2010 (SCI-Expanded)

Diğer Dergilerde Yayınlanan Makaleler

- I. **Experimental and Theoretical Spectroscopic Studies of the Electronic Structure of 2-Ethyl-2-phenylmalonamide**
Selvaraj S., RamKumar A., Ahilan T., Kesavan M., SERDAROĞLU G., P R., Mani M., Gunesakaran S., Kumaresan S.
Physical Chemistry Research, cilt.10, sa.3, ss.333-344, 2022 (ESCI)
- II. **Conformational analysis and DFT investigations of two triazole derivatives and its halogenated substitution by using spectroscopy, AIM and Molecular docking**
KUMAR V. S., Mary Y. S., Mary Y. S., SERDAROĞLU G., Rad A. S., Roxy M. S., Manjula P., Sarojini B.
Chemical Data Collections, cilt.31, ss.100625, 2021 (Scopus)
- III. **Conformational analysis and quantum descriptors of two new imidazole derivatives by experimental, DFT, AIM, molecular docking studies and adsorption activity on graphene**
Kumar V. S., Mary Y. S., Pradhan K., Brahman D., Mary Y. S., SERDAROĞLU G., Rad A. S., Roxy M. S.
HELIYON, cilt.6, sa.10, 2020 (ESCI)
- IV. **Experimental and theoretical investigations on electronic structure of 5-(hydroxymethyl)-2-furaldehyde: An antisickling agent identified from terminalia bellirica**
P R., S S., Suganya R., M Kesavan K., SERDAROĞLU G., Gunasekaran S.
Chemical Data Collections, cilt.29, ss.100498, 2020 (Scopus)
- V. **New route for synthesis of 2-(2,2-dimethoxyethyl)-1,2,3,4,5,6-hexahydro-1,5-methanoazocino[4,3-b]indole and DFT investigation**
ULUDAĞ N., SERDAROĞLU G.
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