

## Assoc. Prof. GONCAGÜL SERDAROĞLU

### Personal Information

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### Education Information

Doctorate, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, Turkey 2004 - 2008

Postgraduate, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, Turkey 1999 - 2003

Undergraduate, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, Turkey 1994 - 1998

### Foreign Languages

English, B2 Upper Intermediate

### Dissertations

Doctorate, Sınır sinyali 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

### Research Areas

Chemistry, Computational Chemistry, Statistical Mechanics, Quantum Mechanics

### Academic Titles / Tasks

Associate Professor, Sivas Cumhuriyet University, Eğitim Fakültesi, Matematik Ve Fen Bilimleri Eğitimi Bölümü, 2019 - Continues

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

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

### 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

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

- 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, vol.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, vol.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, vol.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, vol.8, no.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, vol.76, no.6, pp.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, vol.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, vol.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, vol.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, vol.57, no.3, pp.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, vol.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, vol.40, no.19, pp.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, vol.42, no.8, pp.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, vol.77, no.1-2, pp.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, vol.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, vol.57, no.12, pp.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, vol.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, vol.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, vol.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, vol.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, vol.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)**  
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)
- 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, vol.12, no.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, vol.75, no.9, pp.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, vol.6, no.35, pp.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, vol.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, vol.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, vol.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, vol.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, vol.181, pp.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, vol.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, vol.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, vol.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, vol.45, no.5-6, pp.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, vol.32, no.2, pp.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, vol.27, no.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, vol.166, pp.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, vol.66, pp.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, vol.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, vol.319, 2020 (SCI-Expanded)
- XL. **The electronic and spectroscopic investigation of ( +/- )- Dasycarpidone**  
SERDAROĞLU G., Uludag N.  
VIBRATIONAL SPECTROSCOPY, vol.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, vol.97, no.10, pp.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, vol.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, vol.46, no.1, pp.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, vol.43, pp.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, vol.72, pp.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, vol.96, no.9, pp.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, vol.60, no.8, pp.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, vol.4, no.23, pp.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, vol.1178, pp.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, vol.1166, pp.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, vol.1161, pp.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, vol.1155, pp.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, vol.56, no.11, pp.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, vol.28, no.4, pp.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, vol.111, no.14, pp.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, vol.111, no.10, pp.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, vol.49, no.7, pp.861-866, 2010 (SCI-Expanded)

## Articles Published in Other Journals

- 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, vol.10, no.3, pp.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, vol.31, pp.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, vol.6, no.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, vol.29, pp.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.  
HELIYON, vol.6, no.6, 2020 (ESCI)
- VI. **Effect of substitution on corrosion inhibition properties of three Imidazole derivatives on mild steel in 1M HCl**  
Bouklah M., Elmsellem H., Krim O., SERDAROĞLU G., B H., Elidrissi A., KAYA S., I Warad I. W.  
Arabian Journal of Chemical and Environmental Researches, vol.7, no.2, pp.126-143, 2020 (Peer-Reviewed Journal)
- VII. **A Computational study predicting the chemical reactivity behavior of 1-substituted 9-ethyl-βCCM derivatives: DFT- Based Quantum Chemical Descriptors**  
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- VIII. **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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- IX. **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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- X. **DFT Based Quantum Chemical Descriptors of 1-Substituted TH $\beta$ C, DH $\beta$ C,  $\beta$ C Derivatives**  
Serdaroğlu G., Elik M.  
Cumhuriyet Science Journal, vol.38, no.4, pp.647-660, 2017 (Peer-Reviewed Journal)
- XI. **Investigation with Molecular Orbital Method of Electron Charge Distribution and Electrostatic Properties of Dopamine and Amphetamine Molecules**  
Serdaroğlu G., Elik M.  
C.Ü. Fen Edebiyat Fakültesi Fen Bilimleri Dergisi, vol.28, no.2, pp.39-52, 2007 (Peer-Reviewed Journal)
- XII. **Mirisetin ve Kuersetin Bileşiklerinin Antioksidan Etkinliklerinin DFT Yöntemleriyle İncelenmesi**  
ELİK M., SERDAROĞLU G., Özkan R.  
C.Ü. Fen Edebiyat Fakültesi Fen Bilimleri Dergisi, vol.28, no.2, pp.53-65, 2007 (Peer-Reviewed Journal)
- XIII. **Dopamin ve Amfetamin Moleküllerinin Elektron Yük Dağılımları ve Elektrostatik Özelliklerinin Moleküler Orbital Yöntem ile İncelenmesi**  
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## Books & Book Chapters

- I. **Materials Development and Processing for Biomedical Applications**  
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## Refereed Congress / Symposium Publications in Proceedings

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

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- V. **The metal chelation effect on the chemical reactivity of the (E)-2-(2-(pyridin-2-ylmethylene)hydrazineyl) phenol: Theoretical and computational investigation**  
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- VII. **A NEW EQUATION TO CALCULATE THE CHEMICAL HARDNESS OF THE MOLECULES**  
KAYA S., SERDAROĞLU G., Katin K. P.  
5nd International Conference on Material Science and Technology, Kapadokya, Turkey, 16 October 2020, vol.5, pp.282
- VIII. **New Developments on the Application Maximum Entropy Principle: A Theoretical Study**  
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- IX. **DFT investigation of Chloro[1-(2-Methyl-2-propenyl)-3-(4-chlorobenzyl)benzimidazole-2-ylidene]silver(I)**  
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- X. **A Computational Study Of 2,3-Dihydrospiro[Carbazole-1,2'-[1,3]Dithiolan]-4(9H)-One Compound: Structure, FT-IR, NMR, NLO, and NBO Analyses**  
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- XI. **A DFT Investigation on 2-((3R)-3-ethyl-2,3,4,9-tetrahydrospiro[carbazole-1,2'xx-[1,3]dithiolan]-2-yl)-1-(methyl-azaneyl)ethan-1-one**  
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- XII. **The electronic and spectroscopic investigation of uleine: A Computational Study**  
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4. International Conference on Material Science and Technology, Ankara, Turkey, 18 - 20 October 2019, vol.4, pp.775-779
- XIII. **THE STRUCTURAL, ELECTRONIC AND PHYSICAL PROPERTIES OF CATIONIC NHC-AG(II) COMPLEX: A DFT STUDY**  
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4. International Conference on Material Science and Technology, Ankara, Turkey, 18 - 20 October 2019, vol.4, pp.765-769
- XIV. **A QUANTUM CHEMICAL INVESTIGATION ON CATIONIC 2-BROMO-1-(4-(TERT-BUTYL)BENZYL)-3-(2-METHYLALLYL)-2,3-DIHYDRO-1H-BENZO[D]IMIDAZOLE**  
SERDAROĞLU G.  
I. International Cancer Days, Sivas, Turkey, 19 - 21 September 2019, vol.1, pp.561-567
- XV. **INTRAMOLECULAR INTERACTIONS OF (S)-2-(1-(ANTHRACEN-9-YL)-9-ETHYL-9H-PYRIDO[3,4-B]INDOL-3-YL)PROPANE-2-OL**

SERDAROĞLU G.

I. International Cancer Days, Sivas, Turkey, 19 - 21 September 2019, vol.1, pp.555-560

- XVI. **CONFORMATIONAL DEPENDENCE OF THE INTRA MOLECULAR INTERACTIONS IN N-HETEROCYCLIC CARBENE COMPLEX**  
ŞAHİN N., SERDAROĞLU G.  
III. Uluslararası Battalgazi Bilimsel Çalışmalar Kongresi, Malatya, Turkey, 21 - 23 September 2019, vol.1, pp.766-770
- XVII. **SOLVENT EFFECT ON THE ELECTRONIC STRUCTURE, PHYSICOCHEMICAL PROPERTIES AND QUANTUM CHEMICAL PARAMETERS OF THE SUBSTITUTED INDOLE COMPOUND**  
SERDAROĞLU G., ŞAHİN N.  
III. Battalgazi Bilimsel Araştırmalar Kongresi, Malatya, Turkey, 21 - 23 September 2019, vol.1, pp.771-777
- XVIII. **A DFT AND AB INITIO INVESTIGATION ON THE STRUCTURAL, ELECTRONIC AND SPECTROSCOPIC (FT-IR, UV-VIS) PROPERTIES OF THE TRYPTOLINES**  
SERDAROĞLU G.  
2ND INTERNATIONAL CONFERENCE ON PHYSICAL CHEMISTRY FUNCTIONAL MATERIALS, Nevşehir, Turkey, 25 - 27 June 2019, vol.1, pp.189-195
- XIX. **A COMPUTATIONAL STUDY ON THE N-HETEROCYCLIC CARBENE COMPOUND: THE ELECTRONIC (FMO, NBO, MEP) AND SPECTROSCOPIC (FT-IR, NMR) INVESTIGATION**  
SERDAROĞLU G., ŞAHİN N.  
2ND INTERNATIONAL CONFERENCE ON PHYSICAL CHEMISTRY FUNCTIONAL MATERIALS, Nevşehir, Turkey, 25 - 27 June 2019, vol.1, pp.61
- XX. **A Computational Approach on the structural, electronic, and spectroscopic properties of the aromatic substituted indole alkaloids**  
SERDAROĞLU G.  
9th Global Chemistry Congress, Lisbon, Portugal, 23 - 24 July 2018, vol.6, pp.29
- XXI. **The structural, electronic, and spectroscopic properties of the potential neuroactive alkaloids: A Computational Study**  
SERDAROĞLU G.  
9th Global Chemistry Congress, Lisbon, Portugal, 23 - 24 July 2018, vol.6, pp.51
- XXII. **The structural, electronic and spectroscopic properties on the intermediate reagent used in synthesizing of the alkaloids: Computational and Experimental Study**  
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International Conference on Physical Chemistry and Functional Materials, Elazığ, Turkey, 19 - 21 June 2018, vol.1, pp.170
- XXIII. **A DFT study: the structural and electronic properties of substituted 3-hydroxymethyl- $\beta$ -carboline**  
SERDAROĞLU G.  
International Conference on Physical Chemistry and Functional Materials, Elazığ, Turkey, 19 - 21 June 2018, vol.1, pp.285
- XXIV. **A Computational study on the structural, electronic and spectroscopic properties of the (3-oxocyclohexyl)acetonitrile**  
SERDAROĞLU G., ULUDAĞ N.  
International Conference on Physical Chemistry and Functional Materials, Elazığ, Turkey, 19 - 21 June 2018, vol.1, pp.246
- XXV. **The FT-IR, NMR spectroscopy and computational study of the substituted carbazole used in synthesizing of the Strychnos alkaloids**  
SERDAROĞLU G., ULUDAĞ N.  
4th International Conference on New Trends in Chemistry, St Petersburg, Russia, 11 - 13 May 2018, pp.49
- XXVI. **A Computational Approaches on the structural, electronic and spectroscopic properties of the phenylhydrazine**  
SERDAROĞLU G., ULUDAĞ N.  
4th International Conference on New Trends in Chemistry, St Petersburg, Russia, 11 - 13 May 2018, pp.102

- XXVII. **A DFT Investigation on the Electronic Structure, Chemical Reactivity Behaviour, MEP Diagrams of the Harman Derivatives**  
Serdaroğlu G., Elik M.  
INTERNATIONAL CONGRESS ON CHEMISTRY AND MATERIALS SCIENCE, Ankara, Turkey, 5 - 07 October 2017, vol.1, pp.224
- XXVIII. **A Computational Study on  $\beta$ C alkaloids: Solvent effect, Quantum Chemical Descriptors, FMO Analysis**  
SERDAROĞLU G.  
INTERNATIONAL CONGRESS ON CHEMISTRY AND MATERIALS SCIENCE, Ankara, Turkey, 5 - 07 October 2017, vol.1, pp.57
- XXIX. **MEP Diagrams and Solvation Free Energies of the C1- substituted 9-methyl- $\beta$ C alkaloids**  
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International Conference on Applications in Chemistry and Chemical Engineering (ICACChE), Saray Bosna, Bosnia And Herzegovina, 11 - 15 October 2017, vol.1, pp.7-13
- XXX. **Computational Study on the Nor-Harman derivatives**  
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International Conference on Applications in Chemistry and Chemical Engineering (ICACChE), Sarajevo, Bosnia And Herzegovina, 11 - 15 October 2017, vol.1, pp.14-19
- XXXI. **The DFT Calculations on relationship between Solvation Energies and aromaticity of TH $\beta$ C, DH $\beta$ C,  $\beta$ C**  
SERDAROĞLU G.  
4th European Chemistry Congress, Barcelona, Spain, 11 - 13 May 2017, vol.8
- XXXII. **Substituent effect on reactivity of  $\beta$ CCM: A Computational Study**  
SERDAROĞLU G.  
4th European Chemistry Congress, Spain, 11 - 13 May 2017, vol.8, pp.105
- XXXIII. **A Computational Study on Clobazam**  
SERDAROĞLU G., Ortiz J. V.  
XI. Chemical Physics Congress, İstanbul, Turkey, 17 - 18 October 2014, vol.2, pp.42-44
- XXXIV. **A Computational Study on Relationship between Solubility and Molecular Structure: Lamotrigine**  
SERDAROĞLU G., Ortiz J. V.  
XI. Chemical Physics Congress, İstanbul, Turkey, 17 - 18 October 2014, vol.2, pp.39-41
- XXXV. **Computational Study on some anti-epileptic drug molecules**  
SERDAROĞLU G., Ortiz J. V.  
Meeting of the Southeastern Theoretical Chemistry Association, Atlanta, United States Of America, 15 - 17 May 2014, pp.81
- XXXVI. **The Conformational Dependence on Phenobarbitone Molecule s Reactivity in Gas phase and Dielectric media**  
SERDAROĞLU G., Ortiz J. V.  
Research Week, Auburn, ALABAMA, United States Of America, 14 - 17 April 2014
- XXXVII. **Solvent effect on active sites of the zwitterionic GABA and its agonists A Theoretical Study**  
SERDAROĞLU G.  
Chemical Physics Congress-X, 10 - 12 October 2012, pp.110
- XXXVIII. **DFT study on conformational dependence of atomic charges Chemical Reactivity Relationship Amphetamine**  
SERDAROĞLU G.  
III. Fiziksel Kimya Günleri, Turkey, 12 - 15 July 2012, pp.174
- XXXIX. **A Computational study based on conformational properties of phenethylamine of biochemical and medicinal interest**  
SERDAROĞLU G.  
III. Fiziksel Kimya Günleri, Turkey, 12 - 15 July 2012, pp.175
- XL. **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

- XLI. DFT ab initio study on conformational dependence of atomic charges of neutral and cationic epinephrine molecule**  
SERDAROĞLU G.  
25. Ulusal Kimya Kongresi, Turkey, 27 June - 02 July 2011, pp.125
- XLII. The conformational dependence of atomic charges of tyramine in gas phase and aqueous phase A DFT ab initio Study**  
SERDAROĞLU G.  
Chemical Physics Congress-IX, 14 - 16 October 2010, pp.16
- XLIII. 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
- XLIV. Serotonin ve kloro fenil alanin Moleküllerinin Reaktif Merkezleri Üzerine DFT Ab initio Çalışması**  
SERDAROĞLU G.  
24. Ulusal Kimya Kongresi, Turkey, 29 June - 02 July 2010
- XLV. Histamin Molekülünün Konformasyonel Yapılarının Teorik Olarak İncelenmesi**  
SERDAROĞLU G.  
24. Ulusal Kimya Kongresi, Turkey, 29 June - 02 July 2010
- XLVI. Asetilkolin karbakol metakolin ve betanekol moleküllerinin reaktif merkezlerinin DFT ile aydınlatılması**  
SERDAROĞLU G.  
XXIII. Ulusal Kimya Kongresi, Turkey, 16 - 20 June 2009
- XLVII. GABA ve agonistleri olan DABA TACA CACA ve muskimol moleküllerinin yapı aktivite ilişkileri üzerine çözücü etkisinin DFT ile incelenmesi**  
SERDAROĞLU G.  
XXIII. Ulusal Kimya Kongresi, Turkey, 16 - 20 June 2009
- XLVIII. Histaminin Tautomerik Yapılarının Üzerine Betahistin Etkisi**  
KARAKUŞ N., SERDAROĞLU G.  
XXII. Ulusal Kimya Kongresi, Turkey, 6 - 10 October 2008, pp.152
- XLIX. GABA ve Muskimol Moleküllerinin Biyolojik Aktivitelerinin DFT Yöntemiyle İncelenmesi**  
ELİK M., SERDAROĞLU G.  
XXII. Ulusal Kimya Kongresi, Turkey, 6 - 10 October 2008, pp.138
- L. Norepinefrin Epinefrin ve Dopamin Molekülleri Üzerine Amfetamin Etkisinin Moleküler Orbital Yöntemle İncelenmesi**  
SERDAROĞLU G., ELİK M.  
XXII. Ulusal Kimya Kongresi, Turkey, 6 - 10 October 2008, pp.77
- LI. Sinir Sinyal İletiminde Rol Oynayan Glutamat ve Glisin ile Agonistleri olan Alanin ve Aspartik asit Moleküllerinin Fiziksel Özellikleri ve Etkinliklerinin DFT ile Aydınlatılması**  
SERDAROĞLU G., ÜSTÜN E.  
XXII. Ulusal Kimya Kongresi, Turkey, 6 - 10 October 2008, pp.78
- LII. Ab Initio Study on Biological Activity of Acetylcholine and Carbachol**  
SERDAROĞLU G., Durmaz S.  
VIII. Kimyasal Fizik Kongresi, 24 - 25 April 2008, pp.27
- LIII. Tautomerism of The Histamine Molecule A theoretical Study**  
SERDAROĞLU G., Durmaz S.  
VIII. Kimyasal Fizik Kongresi, 24 - 25 April 2008, pp.28
- LIV. Dopamin ve Norepinefrin Moleküllerinin Atomik Yükleri**  
SERDAROĞLU G.  
21. Ulusal Kimya Kongresi, Turkey, 23 - 27 August 2007
- LV. Spektroskopik Verilerin Kullanılması ile Termodinamik Büyüklüklerin Hesaplanması**  
SERDAROĞLU G.

## Supported Projects

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

Serdaroğlu G., Project Supported by Higher Education Institutions, Dasikarpidon türevi bileşiklerin yapısal, elektronik, spektroskopik ve optik özelliklerinin moleküler orbital yöntemlerle incelenmesi, 2019 - 2020

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

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

ELİK M., SERDAROĞLU G., Project Supported by Higher Education Institutions, Beta Karbonil Bileşiklerinin Antitümör Özellikleri Üzerine Hesaplamalı Kimya Çalışması, 2016 - 2017

SERDAROĞLU G., Project Supported by Higher Education Institutions, Antiepileptik ilaç moleküllerinin etkinliklerinin açıklanmasında Elektron Propegator Teorinin EPT kullanılması üzerine hesaplamalı Calisma, 2013 - 2014

SERDAROĞLU G., Project Supported by Higher Education Institutions, Sinir Sinyal İletimini Sağlayan Bazı Moleküllerin Yapısal Özelliklerinin Ve Etkinliklerinin Moleküler Orbital Yöntemleriyle İncelenmesi, 2006 - 2008

## 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: 128

Citation (WoS): 500

Citation (Scopus): 562

H-Index (WoS): 14

H-Index (Scopus): 15

## Congress and Symposium Activities

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

## **Awards**

Serdarođlu G., Kaya S., EN İYİ SÖZLÜ SUNUM ÖDÜLÜ, Abdelmalek Essaadi University, December 2020

Serdarođlu G., EN İYİ POSTER ÖDÜLÜ, International Conference On Physical Chemistry And Functional Materials, Royal Society Of Chemistry, July 2018

Serdarođlu G., POSTER ÖDÜLÜ, 9Th Global Chemistry Congress, June 2018