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Eğitim Bilgileri

Doktora, Erciyes Üniversitesi, Fen Bilimleri Enstitüsü, Fizik (Dr), Türkiye 2009 - 2012
Yüksek Lisans, Süleyman Demirel Üniversitesi, Fen Bilimleri Enstitüsü, Fizik (Yl) (Tezli), Türkiye 2005 - 2008
Lisans, Süleyman Demirel Üniversitesi, Fen-Edebiyat Fakültesi, Fizik Bölümü, Türkiye 2001 - 2005

Yabancı Diller

İngilizce, C1 İleri

Yaptığı Tezler

Doktora, 8b58Ni reaksiyonunun 2- ve 3-cisim yaklaşımları kullanılarak incelenmesi, Erciyes Üniversitesi, Fen Bilimleri Enstitüsü, Fizik (Dr), 2012
Yüksek Lisans, Hatree-fock (HF) ve yoğunluk fonksiyon teori (DFT) metotlarıyla 2-, 3- ve 4- triflorometilbenzaldehit moleküllerinin titreşimsel analizleri ve moleküler yapıları, Süleyman Demirel Üniversitesi, Fen Bilimleri Enstitüsü, Fizik (Yl) (Tezli), 2008

Araştırma Alanları

Fizik, Kimya

Akademik Unvanlar / Görevler

Doç. Dr., Yozgat Bozok Üniversitesi, Sorgun Meslek Yüksekokulu, Motorlu Araçlar ve Ulaştırma Teknolojileri, 2013 - Devam Ediyor
Araştırma Görevlisi, Yozgat Bozok Üniversitesi, Fen-Edebiyat Fakültesi, Fizik, 2007 - 2013

Akademik İdari Deneyim

Yozgat Bozok Üniversitesi, 2014 - 2016
Yozgat Bozok Üniversitesi, 2013 - 2014

Verdiği Dersler

FİZİK, Ön Lisans, 2023 - 2024
MÜHENDİSLİK BİLİMİ, Ön Lisans, 2023 - 2024
MUKAVEMET, Ön Lisans, 2023 - 2024
OTOMOTİV ELEKTRİĞİ, Ön Lisans, 2023 - 2024
OTO103 MESLEKİ MATEMATİK I, Ön Lisans, 2017 - 2018
OTO104 MESLEKİ MATEMATİK II, Ön Lisans, 2017 - 2018
OTO101 FİZİK, Ön Lisans, 2017 - 2018
OTOs102 MESLEKİ İNGİLİZCE I, Ön Lisans, 2017 - 2018
İNT107 FİZİK, Ön Lisans, 2015 - 2016
FİZ568 NÜKLEER SPEKTROSKOPİ, Yüksek Lisans, 2015 - 2016, 2014 - 2015, 2013 - 2014
FİZ540 NÜKLEER FİZİK II, Yüksek Lisans, 2015 - 2016, 2014 - 2015, 2013 - 2014
FİZ8XX UZMANLIK ALAN DERSİ, Yüksek Lisans, 2015 - 2016, 2014 - 2015, 2013 - 2014
FİZ569 NÜKLEER REAKSİYON DİNAMİĞİ, Yüksek Lisans, 2015 - 2016, 2014 - 2015, 2013 - 2014
FİZ539 NÜKLEER FİZİK I, Yüksek Lisans, 2015 - 2016, 2014 - 2015, 2013 - 2014

Yönetilen Tezler

SERT Y., Zayıf bağlı çekirdeklerin elastik saçılmasının optik model yaklaşımıyla incelenmesi, Yüksek Lisans, R.YEGİN(Öğrenci), 2016

SCI, SSCI ve AHCI İndekslerine Giren Dergilerde Yayınlanan Makaleler

I. **Synthesis of novel carbazole hydrazine-carbothioamide scaffold as potent antioxidant, anticancer and antimicrobial agents**
ÇAPAN İ., Hawash M., Qaoud M. T., Gülüm L., Tunoglu E. N. Y., Çifci K., ÇEVRİMLİ B. S., SERT Y., Servi S., KOCA İ., et al.
BMC Chemistry, cilt.18, sa.1, 2024 (SCI-Expanded)

II. **Designing a new bio-active copper(II)-triazole ester type complex based on copper(II)-catalyzed reaction**
Jaafar M. I., Ahmed R. K., Al-Karawi A. J. M., OmarAli A. B., Kansız S., SERT Y., Dege N.
Polyhedron, cilt.256, 2024 (SCI-Expanded)

III. **Deciphering the Biophysical Properties of Ion Channel Gating Pores by Coumarin–Benzodiazepine Hybrid Derivatives: Selective AMPA Receptor Antagonists**
Qneibi M., Hawash M., Gümüş M., Çapan İ., Sert Y., Bdir S., Koca İ., Bdair M.
Molecular Neurobiology, cilt.61, sa.7, ss.4565-4576, 2024 (SCI-Expanded)

IV. **Synthesis and biological studies of pyrimidine derivatives targeting metabolic enzymes**
Korkusuz E., Sert Y., Arslan S., Aydın H., Yıldırım İ., Demir Y., Gülçin İ., Koca İ.
ARCHIV DER PHARMAZIE, cilt.2300634, ss.1-17, 2024 (SCI-Expanded)

V. **Synthesis, X-Ray Diffraction, Spectroscopic Characterization, Hirshfeld Surface Analysis, Molecular Docking Studies, and DFT Calculation of New Pyrazolone Derivatives**
Ait Elmachkouri Y., SERT Y., Irrou E., Anouar E. H., Ouachtak H., Mague J. T., Sebbar N. K., Essassi E. M., Labd Taha M.
Polycyclic Aromatic Compounds, cilt.44, sa.4, ss.2598-2619, 2024 (SCI-Expanded)

VI. **Designing of two new cadmium(II) complexes as bio-active materials: Synthesis, X-ray crystal structures, spectroscopic, DFT, and molecular docking studies**
OmarAli A. B., Ahmed R. K., Al-Karawi A. J. M., Marah S., Kansız S., SERT Y., Jaafar M. I., DEGE N., POYRAZ E. B., Ahmed A. M., et al.
Journal of Molecular Structure, cilt.1290, 2023 (SCI-Expanded)

VII. **Synthesis of novel pyrazole-4-carboxylates by rearrangement reaction: Experimental and theoretical characterization**
Korkusuz E., SERT Y., ŞAHİN E., Yıldırım İ., KOCA İ.
Journal of Physics and Chemistry of Solids, cilt.181, 2023 (SCI-Expanded)

VIII. **Heterojunction solar cell based on donor–acceptor pi-conjugated naphthalene bisbenzimidazole, perylene bisbenzimidazole, and naphthalene imidazole: A spectroscopic, microscopic and DFT assessment**
ÜNSALAN O., SERT Y., ALTUNAYAR ÜNSALAN Ç., Erten-Ela S.
Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, cilt.294, 2023 (SCI-Expanded)

IX. **Synthesis, Crystal Structure, Hirshfeld Surface Analysis, Molecular Docking, IR Spectroscopy and DFT Calculations of a Novel 2D Layered Hybrid Compound (C6H10N3O)(2)Cu2Cl6**
Gharbi C., SERT Y., Cinar E. B., Boehme U., DEGE N., Ben Nasr C., Khedhiri L.
JOURNAL OF CLUSTER SCIENCE, cilt.34, sa.3, ss.1423-1435, 2023 (SCI-Expanded)

X. **Metal-Free Synthesis via Intramolecular Cyclization, Enzyme Inhibition Properties and Molecular Docking of Novel Isoindolinones**
ATMACA U., Saglamtas R., SERT Y., ÇELİK M., GÜLÇİN İ.
ChemistrySelect, cilt.8, sa.9, 2023 (SCI-Expanded)

XI. **Using tea bag filter as a sufficient cellulosic membrane for removal of Safranin-O dye from water: adsorption and density functional theory studies**
Al-Kinani E. M., Hadi S. A., Hamud W. M., Al-Karawi A. J. M., Ahmed R. K., Kansiz S., SERT Y.
Desalination and Water Treatment, cilt.287, ss.233-244, 2023 (SCI-Expanded)

XII. **Design, synthesis, characterization, antioxidant, antiproliferative activity and molecular docking studies of new transition metal complexes of 1,2,4-triazole as combretastatin A-4 analogues**
Jawad W. A., Balakit A. A., Al-Jibouri M. N. A., SERT Y., Obies M.
Journal of Molecular Structure, cilt.1274, 2023 (SCI-Expanded)

XIII. **New Heterocyclic Compound as Carbon Steel Corrosion Inhibitor in 1 M H2SO4, High Efficiency at Low Concentration: Experimental and Theoretical Studies**
Allah M. A. A. H., Balakit A. A., Salman H. I., Abdulridha A. A., SERT Y.
JOURNAL OF ADHESION SCIENCE AND TECHNOLOGY, cilt.37, sa.3, ss.525-547, 2023 (SCI-Expanded)

XIV. **Triad pyrazole–thiazole–coumarin heterocyclic core effectively inhibit HSP and drive cancer cells to apoptosis**
Gümüş M., Koca İ., Sert Y., Dişli A., Yenilmez Tunoğlu E. N., Tutar L., Tutar Y.
Journal of Biomolecular Structure and Dynamics, cilt.41, sa.23, ss.14382-14397, 2023 (SCI-Expanded)

XV. **Structure Elucidation, Hirshfeld Surface Analysis, Molecular Docking and Computational Studies of a Jahn-Teller Distorted Octahedral Cobalt (II) Complex with Saccharin Ligand**
Mohammed H. A., SERT Y., Albayati M. R., DEGE N., ŞEN F.
POLYCYCLIC AROMATIC COMPOUNDS, cilt.43, sa.5, ss.4396-4406, 2023 (SCI-Expanded)

XVI. **Synthesis, alpha-Glucosidase Inhibition, Anticancer, DFT and Molecular Docking Investigations of Pyrazole Hydrazone Derivatives**
Karrouchi K., SERT Y., Ansar M., Radi S., El Bali B., Imad R., Alam A., Irshad R., Wajid S., Altaf M.
POLYCYCLIC AROMATIC COMPOUNDS, cilt.43, sa.6, ss.5021-5040, 2023 (SCI-Expanded)

XVII. **Synthesis, molecular docking, molecular dynamics and evaluation of Drug-Likeness properties of the fused N-Formyl pyrazoline substituted new dehydroepiandrosterone derivatives**
ÇAPAN İ., Shehu A., SERT Y., ÇELİK İ., EROL M., KOCA İ., Servi S.
JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS, cilt.41, sa.6, ss.2492-2503, 2023 (SCI-Expanded)

XVIII. **Computational Study of a Novel Compound with Thioether-Bridge**

Şen F., Cukurovalı A., Sert Y.
Polycyclic Aromatic Compounds, cilt.43, sa.10, ss.8632-8652, 2023 (SCI-Expanded)

XIX. **Synthesis, crystal structure, DFT, Hirshfeld surface analysis, energy framework, docking and molecular dynamic simulations of (E)-4-(4-methylbenzyl)-6-styrylpyridazin-3(2H)-one as anticancer agent**
El Kalai F., Çınar E. B., SERT Y., Alhaji Isa M., Lai C., Buba F., Dege N., Benchat N., Karrouchi K.
Journal of Biomolecular Structure and Dynamics, cilt.41, sa.21, ss.11578-11597, 2023 (SCI-Expanded)

XX. **Experimental and computational studies of 1,5-diphenyl-pyrazole-3-carboxamide compounds as potential Cannabinoid receptor type 1**
KOCA İ., YAKAN M., ÇAPAN İ., ŞAHİN E., SERT Y.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1264, 2022 (SCI-Expanded)

XXI. **Utilization of pyrazole-perimidine hybrids bearing different substituents as corrosion inhibitors for 304 stainless steel in acidic media**
Ugus O., GÜMÜŞ M., SERT Y., KOCA İ., KOCA A.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1262, 2022 (SCI-Expanded)

XXII. **Tautomeric, spectroscopic, electronic and NLO analyses of purpald (4-amino-3-hydrazino-5-mercapto-1,2,4-triazole)**
GÖKCE H., Ceylan S., ÖZTÜRK N., SERT Y.
MATERIALS TODAY COMMUNICATIONS, cilt.32, 2022 (SCI-Expanded)

XXIII. **One-step synthesis of novel N1-substituted benzimidazole derivatives: Experimental and theoretical investigations**
Al Garadi W., SERT Y., El Hafi M., El Ibrahimi B., Ramli Y., Mague J. T., El Ghayati L., Sebbar N. K., Essassi E. M.
JOURNAL OF HETEROCYCLIC CHEMISTRY, cilt.59, sa.7, ss.1213-1229, 2022 (SCI-Expanded)

XXIV. **Synthesis, DFT study, molecular docking and drug-likeness analysis of the heteroaryl substituted new pregnenolone derivatives**
ÇAPAN İ., SERT Y., Shehu A., KOCA İ., SERVİ S.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1260, 2022 (SCI-Expanded)

XXV. **Pyrazolyl-Benzoxazinone Derivatives as Dual Hsp Inhibitors in Human Breast Cancer**
KOCA İ., Kamaci V., ÖZSOY C., SERT Y., Kani I., Tutar L., Tutar Y.
CHEMISTRYSELECT, cilt.7, sa.19, 2022 (SCI-Expanded)

XXVI. **Acesulfame based Co(II) complex: Synthesis, structural investigations, solvatochromism, Hirshfeld surface analysis and molecular docking studies**
Kansiz S., Tolan A., Azam M., Dege N., Alam M., SERT Y., Al-Resayes S., Icbudak H.
POLYHEDRON, cilt.218, 2022 (SCI-Expanded)

XXVII. **Quantum computational, spectroscopic investigations on N-(2-((2-chloro-4,5-dicyanophenyl)amino)ethyl)-4-methylbenzenesulfonamide by DFT/TD-DFT with different solvents, molecular docking and drug-likeness researches**
DEGE N., GÖKCE H., Dogan O. E., ALPASLAN G., Agar T., Muthu S., SERT Y.
COLLOIDS AND SURFACES A-PHYSICOCHEMICAL AND ENGINEERING ASPECTS, cilt.638, 2022 (SCI-Expanded)

XXVIII. **Quantum Computational Investigation of (E)-1-(4-methoxyphenyl)-5-methyl-N '-(3-phenoxybenzylidene)-1H-1,2,3-triazole-4-carbohydrazide**
Gökce H., Şen F., Sert Y., Abdel-Wahab B. F., Kariuki B. M., El-Hiti G. A.
MOLECULES, cilt.27, sa.7, 2022 (SCI-Expanded)

XXIX. **Synthesis and inhibition profiles of N-benzyl- and N-allyl aniline derivatives against carbonic anhydrase and acetylcholinesterase - A molecular docking study**
Mahmudov I., Demir Y., SERT Y., Abdullayev Y., Sujayev A., Alwasel S. H., GÜLÇİN İ.
ARABIAN JOURNAL OF CHEMISTRY, cilt.15, sa.3, 2022 (SCI-Expanded)

XXX. **Synthesis, crystal structure, Hirshfeld surface analysis, spectral characterizations and quantum computational assessments of 1-hydroxy-3-methyl-11H-pyrido[2,1-b] quinazolin-11-one**
Lahmidi S., SERT Y., ŞEN F., El Hafi M., Ettahiri W., Gokce H., Essassi E. M., Mague J. T., UCUN F.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1249, 2022 (SCI-Expanded)

XXXI. **Synthesis, antiproliferative activity, molecular docking studies of hydrazone functionalised thioparabanic acid and rhodanine analogues**
KIBRIZ İ. E., AKKOÇ S., SERT Y., Cay U., ÜNGÖREN Ş. H.
PHOSPHORUS SULFUR AND SILICON AND THE RELATED ELEMENTS, cilt.197, sa.9, ss.918-926, 2022 (SCI-Expanded)

XXXII. **Discovery of sulfadrug-pyrrole conjugates as carbonic anhydrase and acetylcholinesterase inhibitors**
Gümüş M., Babacan S. N., Demir Y., Sert Y., Koca İ., Gülçin İ.
ARCHIV DER PHARMAZIE, cilt.355, sa.1, 2022 (SCI-Expanded)

XXXIII. **New tetrazoles compounds incorporating galactose moiety: Synthesis, crystal structure, spectroscopic characterization, Hirshfeld surface analysis, molecular docking studies, DFT calculations and anti-corrosion property anticipation**
Sghyar R., SERT Y., El Ibrahimi B., Moussaoui O., Hadrami E. M. E. L., Ben-Tama A., Mague J. T., Talbaoui A., Kheira Sebbar N., Essassi E. M.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1247, 2022 (SCI-Expanded)

XXXIV. **Synthesis, spectroscopic characterization, DFT, molecular docking and in vitro antibacterial potential of novel quinoline derivatives**
Bouzian Y., SERT Y., Khalid K., Van Meervelt L., Chkirate K., Mahi L., Ahabchane N. H., Talbaoui A., Essassi E. M.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1246, 2021 (SCI-Expanded)

XXXV. **DFT, Molecular Docking and Drug-likeness Analysis: Acrylate molecule bearing perfluorinated pendant unit**
Soykan U., Sert Y., Yildirim G.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1244, 2021 (SCI-Expanded)

XXXVI. **A research on structural vibrational, surface characterization of 2-methyl-3-{5-methyl-[1,2,4]triazolo[1,5-a]pyrimidin-7-yl}-4H-pyrido[1,2-a]pyrimidin-4-one hydrate: SCXRD, FT-IR, MEP, Hirshfeld and molecular docking studies**
Lahmidi S., Şen F., Sert Y., Ucun F., Essassi E. M., Magued J. T.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1235, 2021 (SCI-Expanded)

XXXVII. **Structural, spectral, electronic, and molecular docking investigations on N,N-dimethyl-2-[(1E)-({[(methylsulfanyl)methanethioyl]amino}imino)methyl]aniline**
Bingol Alpaslan Y., SERT Y., Sohtun W. P., Velusamy M., GÖKCE H.
JOURNAL OF THE CHINESE CHEMICAL SOCIETY, cilt.68, sa.6, ss.971-988, 2021 (SCI-Expanded)

XXXVIII. **5-((1H-imidazol-1-yl)methyl)quinolin-8-ol as potential antiviral SARS-CoV-2 candidate: Synthesis, crystal structure, Hirshfeld surface analysis, DFT and molecular docking studies**
Douche D., SERT Y., Brandan S. A., Kawther A. A., Bilmez B., DEGE N., Louzi A. E., Bougrin K., Karrouchi K., Himmi B.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1232, 2021 (SCI-Expanded)

XXXIX. **New alkyl (cyclohexyl) 2-oxo-1-(prop-2-yn-1-yl)-1, 2-dihydroquinoline-4-carboxylates: Synthesis, crystal structure, spectroscopic characterization, hirshfeld surface analysis, molecular docking studies and DFT calculations**
Hayani S., SERT Y., Filali Y., Benhiba F., Chahdi F. O., Laraqui F., Mague J. T., El Ibrahimi B., Sebbar N. K., Rodi Y. K., et al.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1227, 2021 (SCI-Expanded)

XL. **Synthesis, structural, molecular docking and spectroscopic studies of (E)-N'-(4-methoxybenzylidene)-5-methyl-1H-pyrazole-3-carbohydrazide**
Karrouchi K., Brandan S. A., SERT Y., El Karbane M., Radi S., Ferbinteanu M., Garcia Y., Ansar M.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1225, 2021 (SCI-Expanded)

XLI. **Syntheses of novel 1,5-benzodiazepine derivatives: Crystal structures, spectroscopic characterizations, Hirshfeld surface analyses, molecular docking studies, DFT calculations, corrosion inhibition anticipation, and antibacterial activities**
El Ghayati L., SERT Y., Sebbar N. K., Ramli Y., Ahabchane N. H., Talbaoui A., Mague J. T., El Ibrahimi B., Taha M. L., Essassi E. M., et al.

JOURNAL OF HETEROCYCLIC CHEMISTRY, cilt.58, sa.1, ss.270-289, 2021 (SCI-Expanded)

XLII. **Synthesis, X-ray structure, vibrational spectroscopy, DFT, biological evaluation and molecular docking studies of (E)-N'-(4-(dimethylamino)benzylidene)-5-methyl-1H-pyrazole-3-carbohydrazide**
Karrouchi K., Brandan S. A., SERT Y., El-marzouqi H., Radi S., Ferbinteanu M., Faouzi M. E. A., Garcia Y., Ansar M.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1219, 2020 (SCI-Expanded)

XLIII. **Synthesis, spectrophotometric and DFT studies of new Triazole Schiff bases as selective naked-eye sensors for acetate anion**
Balakit A. A., Makki S. Q., SERT Y., UCUN F., Alshammari M. B., Thordarson P., El-Hiti G. A.
SUPRAMOLECULAR CHEMISTRY, cilt.32, sa.10, ss.519-526, 2020 (SCI-Expanded)

XLIV. **Corrosion inhibition of carbon steel in 1 M H2SO4 using new Azo Schiff compound: Electrochemical, gravimetric, adsorption, surface and DFT studies**
Abdulridha A. A., Allah M. A. A. H., Makki S. Q., SERT Y., Salman H. E., Balakit A. A.
JOURNAL OF MOLECULAR LIQUIDS, cilt.315, 2020 (SCI-Expanded)

XLV. **Synthesis, crystal structure, Hirshfeld surface analysis, spectral characterization, and quantum computational evaluation of (E)-2-(((4-bromophenyl)imino)methyl)-6-methylphenol**
SERT Y., Dogan O. E., GÖKCE H., Agar T., UCUN F., DEGE N.
JOURNAL OF PHYSICS AND CHEMISTRY OF SOLIDS, cilt.144, 2020 (SCI-Expanded)

XLVI. **DFT, molecular docking and experimental FT-IR, laser-Raman, NMR and UV investigations on a potential anticancer agent containing triazole ring system**
SERT Y., El-Hiti G. A., GÖKCE H., UCUN F., Abdel-Wahab B. F., Kariuki B. M.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1211, 2020 (SCI-Expanded)

XLVII. **Synthesis, spectroscopic characterization, crystal structure, DFT, molecular docking and in vitro antibacterial potential of novel quinoline derivatives**
Bouzian Y., Karrouchi K., SERT Y., Lai C., Mahi L., Hamou Ahabchane N., Talbaoui A., Mague J. T., Essassi E. M.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1209, 2020 (SCI-Expanded)

XLVIII. **Spectral, DFT/B3LYP and molecular docking analyses on ethyl 2-(5-methyl-1,2,4-triazolo[1,5-a]pyrimidin-7-yl)pent-4-enoate**
SERT Y., Lahmidi S., El Hafi M., GÖKCE H., Essassi E. M., Ejjoumamany A., Mague J. T.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1206, 2020 (SCI-Expanded)

XLIX. **A new series of sulfa drugs containing pyrazolyl acylthiourea moiety: Synthesis, experimental and theoretical spectral characterization and molecular docking studies**
KOCA İ., Yigitcan S., GÜMÜŞ M., GÖKCE H., SERT Y.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1204, 2020 (SCI-Expanded)

L. **Hirshfeld Surface analysis, spectroscopic, biological studies and molecular docking of (4E)-4-((naphthalen-2-yl)methyleneamino)-1,2-dihydro-2,3-dimethyl-1-phenylpyrazol-5-one**
Eltayeb N. E., ŞEN F., Lasri J., Hussien M. A., Elsilk S. E., Babgi B. A., GÖKCE H., SERT Y.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1202, 2020 (SCI-Expanded)

LI. **Syntheses of N-substituted benzimidazolone derivatives: DFT calculations, Hirshfeld surface analysis, molecular docking studies and antibacterial activities**
Saber A., Sebbar N. K., SERT Y., Alzaqri N., HÖKELEK T., El Ghayati L., Talbaoui A., Mague J. T., Baba Y. F., Urrutigoity M., et al.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1200, 2020 (SCI-Expanded)

LII. **Theoretical and experimental spectroscopic studies, XPS analysis, dimer interaction energies and molecular docking study of 5-(adamantan-1-yl)-N-methyl-1,3,4-thiadiazol-2-amine**
Al-Wahaibi L. H., SERT Y., UCUN F., Al-Shaalan N. H., Alsfouk A., El-Emam A. A., KARAKAYA M.
JOURNAL OF PHYSICS AND CHEMISTRY OF SOLIDS, cilt.135, 2019 (SCI-Expanded)

LIII. **Molecular docking, Hirshfeld surface analysis and spectroscopic investigations of 1-(adamantan-1-yl)-3-(4-fluorophenyl)thiourea: A potential bioactive agent**
SERT Y., Al-Wahaibi L. H., GÖKCE H., Hassan H. M., Alsfouk A., El-Emam A. A.
CHEMICAL PHYSICS LETTERS, cilt.735, 2019 (SCI-Expanded)

LIV. **Hirshfeld Surface, Molecular Docking Study, Spectroscopic Characterization and NLO Profile of 2-**

Methoxy-4,6-Diphenylnicotinonitrile
GÖKCE H., SERT Y., ALPASLAN G., El-Azab A. S., Alanazi M. M., Al-Agamy M. H. M., Abdel-Aziz A. A. -.
CHEMISTRYSELECT, cilt.4, sa.33, ss.9857-9870, 2019 (SCI-Expanded)

LV. **Synthesis, crystal structure, spectroscopic characterization, Hirshfeld surface analysis, molecular docking studies and DFT calculations, and antioxidant activity of 2-oxo-1,2-dihydroquinoline-4-carboxylate derivatives**
Filali Baba Y., SERT Y., Kandri Rodi Y., Hayani S., Mague J. T., Prim D., Marrot J., Ouazzani Chandi F., Kheira Sebbar N., Essassi E. M.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1188, ss.255-268, 2019 (SCI-Expanded)

LVI. **Combined experimental and theoretical investigations on a half-sandwich organometallic Os(II) complex**
SERT Y., Clayton H. S., GÖKCE H., Tapala K. C.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1188, ss.86-98, 2019 (SCI-Expanded)

LVII. **Molecular docking and vibrational spectroscopy studies of (E)-N '-hydroxy-1,3-diphenyl-4,5-dihydro-1H-pyrazole-5-carboximidamide**
SERT Y., GÖKCE H., Chandra C., Mahendra M., Srikantamurthy N., ÇIRAK Ç.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1184, ss.79-91, 2019 (SCI-Expanded)

LVIII. **Molecular Structure, DFT, Vibrational Spectra with Fluorescence Effect, Hirshfeld Surface, Docking Simulation and Antioxidant Activity of Thiazole Derivative**
Khamees H. A., Mohammed Y. H. E., Swamynayaka A., Al-Ostoot F. H., SERT Y., Alghamdi S., Khanum S. A., Madegowda M.
CHEMISTRYSELECT, cilt.4, sa.15, ss.4544-4558, 2019 (SCI-Expanded)

LIX. **Synthesis, Experimental and Theoretical Characterization of Novel Pyrimidine-5-Carboxamides**
GÜMÜŞ M., SERT Y., Yalkin A., GÖKCE H., KOCA İ.
CHEMISTRYSELECT, cilt.4, sa.16, ss.4695-4708, 2019 (SCI-Expanded)

LX. **Structural, Spectroscopic, Electronic and Molecular Docking Studies on (11R,12 S)-16-Aminotetracyclo[6.6.2.0(2,7).0(9,14)]hexadeca-2(7),3,5,9(14),10,12-hexaen-15-ol**
KAYA S., GÖKCE H., El-Azab A. S., SERT Y., Alanazi M. M., ÖZTÜRK N., Al-Agamy M. H. M., Abdel-Aziz A. A.
CHEMISTRYSELECT, cilt.4, sa.3, ss.825-837, 2019 (SCI-Expanded)

LXI. **Experimental and theoretical investigations on structural, spectroscopic, electronic and thermodynamic properties of (adamantan-1-yl)(phenylsulfanyl)methanone**
GÖKCE H., SERT Y., ÖZTÜRK N., Abdel-Aziz A. A., El-Azab A. S., Al-Obaid A. M.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1173, ss.596-607, 2018 (SCI-Expanded)

LXII. **Molecular structure, Hirshfeld surface analysis, spectroscopic (FT-IR, Laser-Raman, UV-vis. and NMR), HOMO-LUMO and NBO investigations on N-(12-amino-9,10-dihydro-9,10-ethanoanthracen-11-yl)-4-methylbenzenesulfonamide**
ALAŞALVAR C., Orturk N., Abdel-Aziz A. A. -., GÖKCE H., El-Azab A. S., El-Gendy M. A., SERT Y.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1171, ss.696-705, 2018 (SCI-Expanded)

LXIII. **Molecular docking, Hirshfeld surface, structural, spectroscopic, electronic, NLO and thermodynamic analyses on novel hybrid compounds containing pyrazole and coumarin cores**
SERT Y., GÜMÜŞ M., GÖKCE H., KANİ İ., KOCA İ.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1171, ss.850-866, 2018 (SCI-Expanded)

LXIV. **Spectroscopic (FT-IR, Laser-Raman and NMR) and conformational analysis on novel pyrazole beta-keto ester compound**
GÜMÜŞ M., SERT Y., Ozdemir S., GÖKCE H., KANİ İ., KOCA İ.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1167, ss.280-293, 2018 (SCI-Expanded)

LXV. **4-[(1,3-Dioxoisoindolin-2-yl)methyl]benzenesulfonamide: Full Structural and Spectroscopic Characterization and Molecular Docking with Carbonic Anhydrase II**
GÖKCE H., ÖZTÜRK N., SERT Y., El-Azab A. S., Alsae N. A., Abdel-Aziz A. A.
CHEMISTRYSELECT, cilt.3, sa.35, 2018 (SCI-Expanded)

LXVI. **Experimental (FT-IR, Laser-Raman and NMR) and theoretical comparative study on 2-**

benzylsulfanyl-4-pentyl-6-(phenylsulfanyl)pyrimidine-5-carbonitrile, a potential bioactive agent
Al-Wahaibi L. H., ÖZTÜRK N., Hassan H. M., SERT Y., El-Emam A. A., Al-Tamimi A. S., GÖKCE H.
JOURNAL OF THEORETICAL & COMPUTATIONAL CHEMISTRY, cilt.17, sa.5, 2018 (SCI-Expanded)

LXVII. **Computational Studies on the Ground State Tautomer, Hydrogen Conformations and Vibrational Spectroscopic Analysis of Antitumor Agents: 3-Deazauracil and 6-Azauracil**
ÇIRAK Ç., KÖRÖZLÜ N., SERT Y., UCUN F.
SPECTROSCOPY AND SPECTRAL ANALYSIS, cilt.38, sa.4, ss.1276-1282, 2018 (SCI-Expanded)

LXVIII. **Synthesis, Vibrational Spectra, and DFT Simulations of 3-bromo-2-methyl-5-(4-nitrophenyl)thiophene**
Balakit A. A., Sert Y., ÇIRAK Ç., Smith K., Kariuki B. M., El-Hiti G. A.
JOURNAL OF APPLIED SPECTROSCOPY, cilt.84, sa.5, ss.888-899, 2017 (SCI-Expanded)

LXIX. **Experimental and Quantum Chemical Calculations of 2-Amino-4,5,6,7-Tetrahydrobenzo[b]Thiophene-3-Carbonitrile**
Oturak H., Kinayturk N. K., Topuz M. A., Kutlu N., Kaynaker E., Talip P., Sert Y.
ACTA PHYSICA POLONICA A, cilt.132, sa.3, ss.1192-1199, 2017 (SCI-Expanded)

LXX. **Spectroscopic investigation of 2-(4-benzoyl-1,5-diphenyl-1H- pyrazol-3-yl)-4H-naphto[2,3-d][1,3] oxazin-4-one molecule**
SERT Y., GÜMÜŞ M., Kamaci V., GÖKCE H., KANİ İ., KOCA İ.
JOURNAL OF THEORETICAL & COMPUTATIONAL CHEMISTRY, cilt.16, sa.5, 2017 (SCI-Expanded)

LXXI. **; Experimental (FT-IR, Laser-Raman and NMR) and theoretical spectroscopic analysis of 3-[(N-methylanilino) methyl]-5-(thiophen-2-yl)-1,3,4-oxadiazole-2(3H)-thione**
SERT Y., ÖZTÜRK N., Al-Omary F. A. M., ALAŞALVAR C., Al-Shehri M. M., El-Emam A. A., GÖKCE H.
JOURNAL OF THEORETICAL & COMPUTATIONAL CHEMISTRY, cilt.16, sa.3, 2017 (SCI-Expanded)

LXXII. **Radial sensitivity of the optical model potentials for He-4+Sn-120 and He-6+Sn-120**
Sert Y., Boztosun I.
INTERNATIONAL JOURNAL OF MODERN PHYSICS E, cilt.25, sa.9, 2016 (SCI-Expanded)

LXXIII. **Spectroscopic Investigations and DFT Calculations on 3-(Diacetylamino)-2-ethyl-3H-quinazolin-4-one**
SERT Y., UCUN F., El-Hiti G. A., Smith K., Hegazy A. S.
JOURNAL OF SPECTROSCOPY, cilt.2016, 2016 (SCI-Expanded)

LXXIV. **A theoretical investigation of Be-9+Al-27 reaction: phenomenological and microscopic model approximation**
Sert Y., Yegin R., Dogan H.
INDIAN JOURNAL OF PHYSICS, cilt.89, sa.10, ss.1093-1100, 2015 (SCI-Expanded)

LXXV. **Theoretical and experimental investigations on vibrational and structural properties of tolazamide**
KARAKAYA M., SERT Y., Kurekci M., Eskiyurt B., ÇIRAK Ç.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1095, ss.87-95, 2015 (SCI-Expanded)

LXXVI. **Structural optimization and vibrational analysis of an antidiabetic drug: tolbutamide**
SERT Y., KARAKAYA M., ÇIRAK Ç., Eskiyurt B., Kurekci M.
JOURNAL OF SULFUR CHEMISTRY, cilt.36, sa.4, ss.450-461, 2015 (SCI-Expanded)

LXXVII. **Monomer spectroscopic analysis and dimer interaction energies on N-(4-methoxybenzoyl)-2-methylbenzenesulfonamide by experimental and theoretical approaches**
KARAKAYA M., SERT Y., Sreenivasa S., Suchetan P. A., ÇIRAK Ç.
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, cilt.142, ss.169-177, 2015 (SCI-Expanded)

LXXVIII. **Phenomenological and microscopic analysis of elastic scattering reactions: Be-9+Al-27 new results**
SERT Y., Yegin R.
JOURNAL OF THE KOREAN PHYSICAL SOCIETY, cilt.66, sa.5, ss.748-753, 2015 (SCI-Expanded)

LXXIX. **FT-IR, Laser-Raman spectra and computational analysis of 5-Methyl-3-phenylisoxazole-4-carboxylic acid**
SERT Y., Mahendra M., Keskinoglu S., Chandra C., Srikantamurthy N., Umesha K. B., ÇIRAK Ç.

SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, cilt.139, ss.145-155, 2015 (SCI-Expanded)

LXXX. **FT-IR and Raman vibrational analysis, B3LYP and M06-2X simulations of 4-bromomethyl-6-tert-butyl-2H-chromen-2-one**
SERT Y., Puttaraju K. B., Keskinoglu S., Shivashankar K., UCUN F.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1079, ss.194-202, 2015 (SCI-Expanded)

LXXXI. **Experimental and computational study on molecular structure and vibrational analysis of an antihyperglycemic biomolecule: Gliclazide**
KARAKAYA M., Kurekci M., Eskiyurt B., SERT Y., ÇIRAK Ç.
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, cilt.135, ss.137-146, 2015 (SCI-Expanded)

LXXXII. **Structural and spectroscopic analysis of 3-[(4-phenylpiperazin-1-yl)methyl]-5-(thiophen-2-yl)-2,3-dihydro-1,3,4-oxadiazole-2-thione with experimental (FT-IR, Laser-Raman) techniques and ab initio calculations**
Al-Omary F. A. M., KARAKAYA M., SERT Y., Haress N. G., El-Emam A. A., ÇIRAK Ç.
JOURNAL OF MOLECULAR STRUCTURE, cilt.1076, ss.664-672, 2014 (SCI-Expanded)

LXXXIII. **Experimental (FT-IR, NMR and UV) and theoretical (M06-2X and DFT) investigation, and frequency estimation analyses on (E)-3-(4-bromo-5-methylthiophen-2-yl)acrylonitrile**
SERT Y., Balakit A. A., Ozturk N., UCUN F., El-Hiti G. A.
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, cilt.131, ss.502-511, 2014 (SCI-Expanded)

LXXXIV. **Vibrational frequency analysis, FT-IR and Laser-Raman spectra, DFT studies on ethyl (2E)-2-cyano-3-(4-methoxyphenyl)-acrylate**
SERT Y., Sreenivasa S., Dogan H., Mohan N. R., Suchetan P. A., UCUN F.
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, cilt.130, ss.96-104, 2014 (SCI-Expanded)

LXXXV. **Vibrational spectroscopy investigation using M06-2X and B3LYP methods analysis on the structure of 2-Trifluoromethyl-10H-benzo[4,5]-imidazo[1,2-a]pyrimidin-4-one**
SERT Y., Mahendra M., Chandra C., Shivashankar K., Puttaraju K. B., Dogan H., ÇIRAK Ç., UCUN F.
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, cilt.128, ss.109-118, 2014 (SCI-Expanded)

LXXXVI. **Vibrational spectroscopy (FT-IR and Laser-Raman) investigation, and computational (M06-2X and B3LYP) analysis on the structure of 4-(3-fluorophenyl)-1-(propan-2-ylidene)-thiosemicarbazone**
SERT Y., Miroslaw B., ÇIRAK Ç., Dogan H., Szulczyk D., Struga M.
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, cilt.128, ss.91-99, 2014 (SCI-Expanded)

LXXXVII. **Experimental FT-IR, Laser-Raman and DFT spectroscopic analysis of 2,3,4,5,6-Pentafluoro-trans-cinnamic acid**
SERT Y., Dogan H., Navarrete A., Somanathan R., Aguirre G., ÇIRAK Ç.
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, cilt.128, ss.119-126, 2014 (SCI-Expanded)

LXXXVIII. **Vibrational frequency analysis, FT-IR, DFT and M06-2X studies on tert-Butyl N-(thiophen-2yl)carbamate**
SERT Y., Singer L. M., Findlater M., Dogan H., ÇIRAK Ç.
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, cilt.128, ss.46-53, 2014 (SCI-Expanded)

LXXXIX. **Effect of intermolecular hydrogen bonding, vibrational analysis and molecular structure of a biomolecule: 5-Hydroxymethyluracil**
ÇIRAK Ç., SERT Y., UCUN F.
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, cilt.127, ss.41-46, 2014 (SCI-Expanded)

XC. **FT-IR, Laser-Raman spectra and quantum chemical calculations of methyl 4-(trifluoromethyl)-1H-pyrrole-3-carboxylate-A DFT approach**
Sett Y., Sreenivasa S., Dogan H., Manojkumar K. E., Suchetan P. A., UCUN F.
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, cilt.127, ss.122-130, 2014 (SCI-Expanded)

XCI. **Use of vibrational spectroscopy to study 4-benzyl-3-(thiophen-2-yl)-4,5-dihydro-1H-1,2,4-triazole-5-thione: A combined theoretical and experimental approach**
SERT Y., El-Emam A. A., Al-Abdullah E. S., Al-Tamimi A. S., ÇIRAK Ç., UCUN F.
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, cilt.126, ss.280-290, 2014 (SCI-Expanded)

XCII. **The biomolecule, 2-[(2-methoxyl)sulfanyl]-4-(2-methylpropyl)-6-oxo-1,6-dihydropyrimidine-5-carbonitrile: FT-IR, Laser-Raman spectra and DFT**
SERT Y., El-Emam A. A., Al-Deeb O. A., Al-Turkistani A. A., UCUN F., ÇIRAK Ç.
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, cilt.126, ss.86-97, 2014 (SCI-Expanded)

XCIII. **Micro-Raman, Mid-IR, Far-IR and DFT studies on 2-[4-(4-Fluorobenzamido)phenyl]benzothiazole**
ÜNSALAN O., Sert Y., Ari H., Simao A., Yilmaz A., BÖYÜKATA M., Bolukbasi O., Bolelli K., Yalcin I.
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, cilt.125, ss.414-421, 2014 (SCI-Expanded)

XCIV. **Experimental FT-IR, Laser-Raman and DFT spectroscopic analysis of a potential chemotherapeutic agent 6-(2-methylpropyl)-4-oxo-2-sulfanylidene-1,2,3,4-tetrahydropyrimidine-5-carbonitrile**
SERT Y., Al-Turkistani A. A., Al-Deeb O. A., El-Emam A. A., UCUN F., ÇIRAK Ç.
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, cilt.120, ss.97-105, 2014 (SCI-Expanded)

XCV. **Synthesis, spectroscopic and theoretical studies of ethyl (2E)-3-amino-2-({[(4-benzoyl-1,5-diphenyl-1H-pyrazol-3-yl)carbonyl]amino}carbonothioyl)but-2-enoate butanol solvate**
KOCA İ., SERT Y., GÜMÜŞ M., KANİ İ., ÇIRAK Ç.
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, cilt.118, ss.816-827, 2014 (SCI-Expanded)

XCVI. **Synthesis, characterization and vibrational spectra analysis of ethyl (2Z)-2-(2-amino-4-oxo-1,3-oxazol-5(4H)-ylidene)-3-oxo-3-phenylpropanoate**
KIBRIZ İ. E., SERT Y., SAÇMACI M., ŞAHİN E., YILDIRIM İ., UCUN F.
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, cilt.114, ss.491-501, 2013 (SCI-Expanded)

XCVII. **Effect of intermolecular hydrogen bonding, vibrational analysis and molecular structure of 4-chlorobenzothioamide**
ÇIRAK Ç., SERT Y., UCUN F.
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, cilt.113, ss.130-136, 2013 (SCI-Expanded)

XCVIII. **Vibrational spectroscopic investigation of p-, m- and o-nitrobenzonitrile by using Hartree-Fock and density functional theory**
Sert Y., Ucun F.
INDIAN JOURNAL OF PHYSICS, cilt.87, sa.8, ss.809-818, 2013 (SCI-Expanded)

XCIX. **Vibrational analysis of 4-chloro-3-nitrobenzonitrile by quantum chemical calculations**
SERT Y., ÇIRAK Ç., UCUN F.
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, cilt.107, ss.248-255, 2013 (SCI-Expanded)

C. **Vibrational spectroscopic studies of 3-hydroxyphenylboronic acid: molecular structure**
Sert Y., Ucun F., BÖYÜKATA M.
INDIAN JOURNAL OF PHYSICS, cilt.87, sa.2, ss.113-119, 2013 (SCI-Expanded)

CI. **Molecular structures and vibrational spectra of 2-, 3-and 4-ethylpyridines and 2-, 3-and 4-**

vinylpyridines by density functional theory and ab initio Hartree-Fock calculations
Sert Y., Ucun F., BÖYÜKATA M.
INDIAN JOURNAL OF PHYSICS, cilt.86, sa.10, ss.859-869, 2012 (SCI-Expanded)

CII. **Role of the cluster deformations in explaining the exotic decay half-lives**
Soylu A., Sert Y., Bayrak O., Boztosun I.
EUROPEAN PHYSICAL JOURNAL A, cilt.48, sa.9, 2012 (SCI-Expanded)

CIII. **RADIAL SENSITIVITY OF THE ELASTIC SCATTERING AROUND THE COULOMB BARRIER ENERGIES FOR WEAKLY-BOUND AND HALO NUCLEI**
Sert Y., Caner T., Bayrak O., Boztosun I.
MODERN PHYSICS LETTERS A, cilt.27, sa.21, 2012 (SCI-Expanded)

CIV. **Experimental and computational study on molecular structure and vibrational analysis of a modified biomolecule: 5-Bromo-2 '-deoxyuridine**
ÇIRAK Ç., SERT Y., UCUN F.
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, cilt.92, ss.406-414, 2012 (SCI-Expanded)

CV. **Adsorption of Cr(VI) from Aqueous Solutions Onto Raw and Acid-Activated Resadiye and Hancili Clays**
GÖDE F., Ozturk N., Sert Y., Bahceli S.
SPECTROSCOPY LETTERS, cilt.43, sa.1, ss.68-78, 2010 (SCI-Expanded)

CVI. **Ab Initio Hartree-Fock and Density Functional Theory Study on Molecular Structures, Energies, and Vibrational Frequencies of 2-Amino-3-, 4-, and 5-Nitropyridine**
SERT Y., UCUN F., BÖYÜKATA M.
ZEITSCHRIFT FUR NATURFORSCHUNG SECTION A-A JOURNAL OF PHYSICAL SCIENCES, cilt.65, ss.107-112, 2010 (SCI-Expanded)

CVII. **Conformational and vibrational analysis of 2-, 3- and 4-trifluoromethylbenzaldehyde by ab initio Hartree-Fock, density functional theory and Moller-Plesset pertubasyon theory calculations**
SERT Y., UCUN F., BÖYÜKATA M.
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, cilt.861, ss.122-130, 2008 (SCI-Expanded)

Diğer Dergilerde Yayınlanan Makaleler

I. **Synthesis of new N-alkylated 6-bromoindoline-2.3-dione derivatives: Crystal structures, spectroscopic characterizations, Hirschfeld surface analyses, molecular docking studies, DFT calculations, and antibacterial activity**
Rharmili N., SERT Y., Kandri Rodi Y., Ouazzani Chahdi F., Haoudi A., Mague J. T., Mazzah A., El Hachlafi N., Benkhaira N., Fikri-Benbrahim K., et al.
Results in Chemistry, cilt.7, 2024 (ESCI)

II. **Design, synthesis, molecular docking and biological evaluation of new carbazole derivatives as anticancer, and antioxidant agents**
Çapan İ., Hawash M., Jaradat N., Sert Y., Servi R., Koca İ.
BMC Chemistry, cilt.17, sa.1, 2023 (Scopus)

III. **Molecular docking and antioxidant activity studies of imidodithiocarbonate derivatives containing pyrimidine**
Korkusuz E., SERT Y., Selvi E. K., Aydın H., KOCA İ., Yıldırım İ.
Organic Communications, cilt.16, sa.1, ss.1-10, 2023 (ESCI)

IV. **A quinoline-benzotriazole derivative: Synthesis, crystal structure and characterization by using spectroscopic, DFT and molecular docking methods**
Himmi B., Brandán S. A., SERT Y., Ahmed Kawther A., Dege N., Berrin Cinar E., El Louzi A., Bougrin K., Karrouchi K.
Results in Chemistry, cilt.5, 2023 (Scopus)

V. **Çift Katlama Modeli İle Elastik Saçılma: 8B+27Al**

Sert Y.
Erzincan University Journal of Science and Technology, cilt.14, sa.1, ss.241-248, 2021 (Hakemli Dergi)

VI. **Synthesis, characterization and theoretical studies of novel sulfonamide-aldehydes derivatives having tautomeric forms**
GÜMÜŞ M., SERT Y., KOCA İ.
ORGANIC COMMUNICATIONS, cilt.12, sa.4, ss.176-187, 2019 (ESCI)

VII. **Vibrational, Geometrical and HOMO/LUMO/MEP Analyses by Using DFT/B3LYP and DFT/M06-2X Methods: 3-Amino-1,2,4-triazole**
SERT Y.
Pamukkale University Journal of Engineering Sciences, cilt.24, sa.7, ss.1272-1277, 2018 (ESCI)

VIII. **Global Potential for 11Be64Zn Elastic Scattering**
SERT Y.
Cumhuriyet Science Journal, cilt.38, sa.2, ss.305, 2017 (Hakemli Dergi)

IX. **A DFT study on vibrational spectra and conformational stability of2,4-difluorophenylboronic acid**
SERT Y., ÇIRAK Ç.
Asian Chemistry Letters, cilt.19, ss.53-60, 2015 (Hakemli Dergi)

Hakemli Kongre / Sempozyum Bildiri Kitaplarında Yer Alan Yayınlar

I. **Synthesis, Characterization and Molecular Docking Studies of Novel Sulfadrugs-Pyrrole Conjugates**
GÜMÜŞ M., BABACAN Ş. N., SERT Y., KOCA İ.
4th International Eurasian Conference on Biological and Chemical Sciences (EurasianBioChem 2021), Ankara, Türkiye, 24 - 26 Kasım 2021

II. **Experimental and theoretical characterization and molecular docking studies of novel sulfonamide derivatives**
KOCA İ., SERT Y., GÜMÜŞ M., Gökçe H.
8. International Drug Chemistry Conference, Antalya, Türkiye, 4 - 07 Mart 2020

III. **ETİL 2E 3 AMİNO 2 4 BENZOİL 1 5 DİFENİL 1H PİRAZOL 3 İL KARBONİL AMİNO KARBONOTİYOLİL BÜT 2 ENOAT SENTEZ SPEKTROSKOPİ VE TEORİK ÇALIŞMALAR**
KOCA İ., SERT Y., GÜMÜŞ M., KANİ İ., UCUN F.
13. Ulusal Spektroskopi Kongresi, Burdur, Türkiye, 15 - 18 Mayıs 2013

Desteklenen Projeler

GÜMÜŞ M., SERT Y., Yükseköğretim Kurumları Destekli Proje, Çok hedefli ilaçlar (Multitarget drugs) olarak kumarin tiyazol hibrit sistemlerinin sentezi ve bilgisayar destekli analizleri, 2024 - Devam Ediyor
KOCA İ., SERT Y., ÇAPAN İ., Yükseköğretim Kurumları Destekli Proje, Amino Benzamit Köprülü Yeni Hibrit Moleküllerin Sentezi ve Potansiyel Biyolojik Etkinliğinin Teorik Olarak İncelenmesi, 2024 - Devam Ediyor
Sert Y., Yükseköğretim Kurumları Destekli Proje, Yeni Pirazol Türevi Moleküllerin Sentezi COX İnhibitörü Olarak Değerlendirilmesi, 2024 - 2026
Sert Y., Yükseköğretim Kurumları Destekli Proje, Üre Temelli Yeni Hibrit Moleküllerin Sentezi Karakterizasyonu ve Biyolojik, 2023 - 2025
Sert Y., Yükseköğretim Kurumları Destekli Proje, Hidrazit Grubu İçeren Pirazol Türevi Hibrit Moleküllerin Moleküler Docking ve Antioksidan Aktivite Çalışmaları, 2023 - 2025
Gümüş M., Koca İ., Tutar Y., Sert Y., Açıkalın Coşkun K., TÜBİTAK Projesi, Kinoksalinon-Tiyazol Hibrit Yapılarının Tasarımı, Sentezi ve Antikanser Çalışmaları, 2022 - 2025
Koca İ., Korkusuz E., Çapan İ., Sert Y., TÜBİTAK Projesi, Antipirin Türevi Hibrit Moleküllerin Tasarımı ve Karbonik Anhidraz Aktivitesinin Araştırılması, 2023 - 2024
KOCA İ., SERT Y., Ürünveren M., Yükseköğretim Kurumları Destekli Proje, Potansiyel Yeni Nitroredüktaz İnhibitörler

Üzerine Deneysel ve Teorik Çalışmalar, 2022 - 2024
Koca İ., SERT Y., Yükseköğretim Kurumları Destekli Proje, Pirimidin Halkası İçeren İmidoditiyokarbonat Türevi Moleküllerin Moleküler Docking ve Antioksidan Aktivite Çalışmaları, 2022 - 2023
Koca İ., SERT Y., Yükseköğretim Kurumları Destekli Proje, Pirazolopirimidin Halkalarını İçeren Hibrit Moleküllerin Moleküler Docking ve Antikanser Aktivite Çalışmaları, 2022 - 2023
SERT Y., COŞAR K., KÖKSAL F., ORHAN E., ANADUT H. O., SOYKAN U., Yükseköğretim Kurumları Destekli Proje, Stiren-Divinil Benzen Kopolimer Emdirilmiş Betonların Mekanik Özelliklerin Araştırılması Ve Kuantum Kimyasal Hesaplamalar, 2021 - 2023
SERT Y., ANIL B., GÜMÜŞ M., KOCA A., Yükseköğretim Kurumları Destekli Proje, Azo-Hetero Halkalı Sistemler İçeren Yeni Korozyon İnhibitörleri Üzerine Deneysel ve Teorik İncelemeler, 2021 - 2023
SERT Y., Yükseköğretim Kurumları Destekli Proje, Organik Temelli Bazı Pirrol Türevi Moleküllerin Spektrospik Teorik ve Deneysel İncelenmesi, 2020 - 2021
Gümüş M., Koca İ., Sert Y., Yükseköğretim Kurumları Destekli Proje, Potansiyel Biyoaktif Sülfonamit Türevi Bileşiklerin Karakterizasyonu Üzerine Deneysel ve Teorik Çalışmalar, 2018 - 2019
Gümüş M., Sert Y., Yükseköğretim Kurumları Destekli Proje, FARKLI HETEROSİKLİK ÇEKİRDEKLER İÇEREN YENİ HİBRİT BİLEŞİKLERİN SENTEZ, KARAKTERİZASYON VE TEORİK ÇALIŞMALARI, 2017 - 2018
SERT Y., Yükseköğretim Kurumları Destekli Proje, ADAMANTAN TÜREVLERİNİN DENEYSEL VE TEORİK YAKLAŞIMLAR İLE SPEKTRAL ÖZELLİKLERİ VE DİMER ETKİLEŞİM ENERJİLERİ, 2015 - 2016
SERT Y., Yükseköğretim Kurumları Destekli Proje, 86,88 İzotoplarının Fotonükleer Reaksiyon Ürün Çekirdeklerinin Enerji Seviyelerinin ve Yarı Ömürlerinin Deneysel Olarak Belirlenmesi ve Spekturum Analizleri, 2014 - 2016
SERT Y., Yükseköğretim Kurumları Destekli Proje, 86 88Sr İZOTOPLARININ FOTONÜKLEER REAKSİYON ÜRÜN ÇEKİRDEKLERİNİN ENERJİ SEVİYELERİNİN VE YARI ÖMÜRLERİNİN DENEYSEL OLARAK BELİRLENMESİ VE SPEKTRUM ANALİZLERİ, 2014 - 2016

Metrikler

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