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International Researcher IDs

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ScopusID: 57201620841

Yoksis Researcher ID: 44772



Biography

It is a great honor that my name has been listed in the World Ranking of Top 2% Scientists in the October 2023 updated database, made at the Stanford University. Stanford University has recently published an update of the list of the top 2% most widely cited scientists in various disciplines, which is considered to be the most prestigious ranking in the world. The selection is based on the top 100,000 scientists by c-score (with and without self-citations) or a percentile rank of 2% or above in the sub-field. This version (6) is based on the October 1, 2023 snapshot from Scopus, updated to end of citation year 2022. This work uses Scopus data provided by Elsevier through ICSR Lab (<https://www.elsevier.com/icsr/icsrlab>). Calculations were performed using all Scopus author profiles as of October 1, 2023. <https://doi.org/10.17632/btchxktzyw.6>

Education Information

1991 - 1994	Doctorate, Ondokuz Mayıs University, Fen Bilimleri Enstitüsü, Fizik (Dr), Turkey
1986 - 1990	Postgraduate, Gazi University, Fen Bilimleri Enstitüsü, Fizik (YI) (Tezli), Turkey
1982 - 1986	Undergraduate, Ondokuz Mayıs University, Eğitim Fakültesi, Matematik ve Fen Bilimleri Eğitimi Bölümü, Turkey

Foreign Languages

English, B1 Intermediate

Dissertations

1994	Anizotropik ortam içindeki elipsoidal parçacığın elastik zorlanma enerjisi, Ondokuz Mayıs University, Fen Bilimleri Enstitüsü, Fizik (Dr), Doctorate
1989	Elastik zorlanma enerjisinin fourier dönüşümü yöntemi ile hesaplanması, Gazi University, Fen Bilimleri Enstitüsü, Fizik (YI) (Tezli), Postgraduate

Research Areas

Health Sciences, Agricultural Sciences, Natural Sciences, Engineering and Technology

Academic Titles / Tasks

2018 - Continues	Associate Professor, Ondokuz Mayıs University, Fen Fakültesi, Fizik Bölümü
1998 - 2017	Assistant Professor, Ondokuz Mayıs University, Fen Fakültesi, Fizik Bölümü
1996 - 1998	Assistant Professor, Ondokuz Mayıs University, Eğitim Fakültesi, Matematik Ve Fen Bilimleri Eğitimi Bölümü
1986 - 1996	Research Assistant, Ondokuz Mayıs University, Eğitim Fakültesi, Matematik Ve Fen Bilimleri Eğitimi Bölümü

Academic and Administrative Experience

2015 - Continues	Deputy Head of Department, Ondokuz Mayıs University, Fen Fakültesi, Fizik Bölümü
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Courses

2021 - 2022	Modern Fizik, Undergraduate
2021 - 2022, 2019 - 2020	Kristalografide Paket Programlar, Postgraduate
2021 - 2022	Elektronik Laboratuvarı, Undergraduate
2021 - 2022	Optik, Undergraduate
2021 - 2022	Kristalografi I, Doctorate
2021 - 2022	Kristalografi, Undergraduate
2021 - 2022	Elektronik, Undergraduate
2019 - 2020	FİZİK VE GEOMETRİK OPTİK I, Associate Degree
2019 - 2020, 2015 - 2016	FİZİK II, Undergraduate
2019 - 2020, 2015 - 2016	MODERN FİZİK (FEN FAK-FİZİK BÖL.), Undergraduate
2016 - 2017	FİZİK VE GEOMETRİK OPTİK II, Undergraduate
2016 - 2017	Fizik Ve Geometrik Optik I, Undergraduate
2015 - 2016	FİZİK I, Undergraduate

Jury Memberships

January 2024	Academic Staff Examination, Academic Staff Examination, Ondokuz Mayıs Üniversitesi
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Published journal articles indexed by SCI, SSCI, and AHCI

- I. **Synthesis, Structural Characterization, DFT Calculations, and Molecular Docking of a Novel Quinoline Derivative**
Jamal A., Faizi M. S. H., Dege N.
JOURNAL OF MOLECULAR STRUCTURE, vol.1300, 2024 (SCI-Expanded)
- II. **Deciphering non-covalent interactions in unprecedented binuclear copper complex: Spectroscopic,**

Hirshfeld surface and DFT investigation

Yilmaz S. K., Alaman Ağar A., Poyraz E. B., Dege N., Vidya V. G., Kumar V. G. V.

JOURNAL OF MOLECULAR STRUCTURE, vol.1299, 2024 (SCI-Expanded)

- III. **Comparative assessment of structure-property relationships of new Cu(II) complex in selected density functionals**
AVCI D., Comert H. E., Sonmez F., Dege N., Tamer O., ATALAY Y.
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, vol.305, 2024 (SCI-Expanded)
- IV. **Synthesis, structural determination, in vitro antioxidant and antibacterial efficacy of dispirooxindolopyrrolidine embedded indole heterocycle**
Arumugam N., Almansour A. I., Alkaltham M. F., Soliman S. M., Viswanathan V., Priya R. V., Karuppiah P., Alaqeel S. I., Dege N., Perumal K.
JOURNAL OF MOLECULAR STRUCTURE, vol.1295, 2024 (SCI-Expanded)
- V. **Stereo and regioselective synthesis, structural elucidation and antibacterial activity of novel spiropyrrolidine embedded with two units of oxindoles**
Almansour A. I., Alkaltham M. F., Arumugam N., Soliman S. M., Madhu V., Alaqeel S. I., Dege N., Karuppiah P., Perumal K.
JOURNAL OF MOLECULAR STRUCTURE, vol.1294, 2023 (SCI-Expanded)
- VI. **Synthesis, crystal structure, static and dynamic properties, molecular structure, reactive sites, wavefunction and molecular docking of 1-(3-((4-(diethylamino)-2-hydroxybenzylidene)amino)phenyl)ethan-1-one**
Begaum K. P., Prabhu T., Kaleeswaran S., Kadaikunnan S., Abbas G., Muthu S., Kestek I., Alaman Ağar A., Poyraz E. B., Dege N.
JOURNAL OF MOLECULAR STRUCTURE, vol.1294, 2023 (SCI-Expanded)
- VII. **Environmentally-friendly synthesis, structural determination and antimicrobial activity of new class of spiropyrrolidine embedded with indenoquinoxaline and chromanone heterocyclic units**
Arumugam N., Soliman S. M., Viswanathan V., Almansour A. I., Kumar R. S., Mahalingam S. M., Krishnamoorthy B. S., Dege N., Karuppiah P., Perumal K.
JOURNAL OF MOLECULAR STRUCTURE, vol.1293, 2023 (SCI-Expanded)
- VIII. **Exploring crystal structure, Hirshfeld surface and quantum mechanical attributes of symmetric thiophene Schiff base**
MERAL F. S., Alaman Ağar A., Cinar E. B., Dege N., Kanmazalp S. D., Vidya V. G., Kumar V. G. V.
JOURNAL OF THE IRANIAN CHEMICAL SOCIETY, vol.20, pp.3087-3102, 2023 (SCI-Expanded)
- IX. **Designing of eight-coordinate manganese(II) complexes as bio-active materials: Synthesis, X-ray crystal structures, spectroscopic, DFT, and molecular docking studies**
Ahmed R. K., Omarali A. B., Al-Karawi A. J. M., Marah S., Jaafar M. I., Dege N., Poyraz E. B., Özen T., Loukil M., Alisir S., et al.
POLYHEDRON, vol.244, 2023 (SCI-Expanded)
- X. **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, vol.1290, 2023 (SCI-Expanded)
- XI. **Synthesis, characterization, crystal structure, in silico and computational studies on a novel Schiff base derived from α -chlorocinnamaldehyde and 4-aminoantipyrine**
Adimudo H. C., Agu C. J., Okenyeka O. U., Eddy N. O., Dim E. N., DEGE N., Bonardd S., Vanka K., Ibezim A., Idika D. I., et al.
Journal of Molecular Structure, vol.1289, 2023 (SCI-Expanded)
- XII. **Bifunctional Cu(II)-based 2D coordination polymer and its composite for high-performance photocatalysis and electrochemical energy storage**
Ali A., Khan M. Z., Dege N., Ahmad M., Shahid M.

DALTON TRANSACTIONS, vol.52, no.42, pp.15562-15575, 2023 (SCI-Expanded)

- XIII. **Synthesis, crystallographic and spectroscopic investigation, chemical reactivity, hyperpolarizabilities and in silico molecular docking study of (Z)-2N-(tert-butylimino)-3N'-(4-methoxyphenyl)thiazolidin-4-one**
Boudjenane F. Z., Triki-Baara F., Boukabcha N., Belkafouf N. E. H., DEGE N., Saidj M., Khelloul N., Djafri A., Chouaih A.
JOURNAL OF MOLECULAR STRUCTURE, vol.1287, 2023 (SCI-Expanded)
- XIV. **Experimental and Theoretical Biological Probing of Schiff Bases as Esterase Inhibitors: Structural, Spectral and Molecular Insights**
Raza M. A., Mumtaz M. W., Öztürk S., Latif M., Aisha A., Ashraf A., DEGE N., Doğan O. E., Ağar E., Rehman S. U., et al.
Molecules, vol.28, no.15, 2023 (SCI-Expanded)
- XV. **Design, synthesis, structural characterization and computational studies of new class of dispirooxindolopyrrolidine embedded chromanone hybrid heterocycles**
Arumugam N., Alkaltham M. F., Viswanathan V., Almansour A. I., Kumar R. S., Alaqeel S. I., Kumar S. Y., Padmanaban R., Mahalingam S. M., DEGE N.
JOURNAL OF MOLECULAR STRUCTURE, vol.1286, 2023 (SCI-Expanded)
- XVI. **Supramolecular Co(II) complexes based on dithiolate and dicarboxylate ligands: Crystal structures, theoretical studies, magnetic properties, and catalytic activity studies in photocatalytic hydrogen evolution**
Adhikari S., Sheikh A. H., Kansiz S., DEGE N., Baildya N., Mahmoudi G., Choudhury N. A., Butcher R. J., Kaminsky W., Talledo S., et al.
JOURNAL OF MOLECULAR STRUCTURE, vol.1285, 2023 (SCI-Expanded)
- XVII. **Syntheses, characterizations, and Hirshfeld analysis of Ag(I) and Cu(II) complexes: A novel potent Ag(I)-based oxadiazole anticancer agent**
Ayoub M. S., ElShafey M. M., Abdel-Hamid H., Abu-Serie M. M., Teleb M., DEGE N., Soliman S. M.
APPLIED ORGANOMETALLIC CHEMISTRY, vol.37, no.8, 2023 (SCI-Expanded)
- XVIII. **Synthesis, crystal structure, Hirshfeld surface analysis, DFT and antihyperglycemic activity of 9-allyl-2,3,9,10a-tetrahydrobenzo[b]cyclopenta[e][1,4]diazepin-10(1H)-one**
Saddik R., Brandán S. A., Mortada S., Baydere C., Roby O., DEGE N., Tighadouini S., Tahiri M., Faouzi M. A., Karrouchi K.
Journal of Molecular Structure, vol.1283, 2023 (SCI-Expanded)
- XIX. **Synthesis, Structural, Spectroscopic, Hirshfeld Surface Analysis and Computational Study of Copper Complex Containing Salicylaldehyde Ligands**
Alaman E., Agar A. A., Tahir M. N., Ashfaq M., Poyraz E. B., Dege N.
JOURNAL OF STRUCTURAL CHEMISTRY, vol.64, no.7, pp.1314-1328, 2023 (SCI-Expanded)
- XX. **Structural Investigation and Hirshfeld Surface Analysis of N-(3-Chloro-4-Methylphenyl)-2-(3-Nitrobenzamido)Benzamide**
Ayoob M. M., Hawaiz F. E., Dege N., Kansiz S.
JOURNAL OF STRUCTURAL CHEMISTRY, vol.64, no.6, pp.1049-1058, 2023 (SCI-Expanded)
- XXI. **Structural, Spectroscopic and Molecular Characterization of an Asymmetric Schiff Base Compound**
Doğan O. E., Poyraz E. B., Saracoglu H., Agar T., Yasa B., Dege N.
JOURNAL OF STRUCTURAL CHEMISTRY, vol.64, no.6, pp.1147-1163, 2023 (SCI-Expanded)
- XXII. **Computational modeling of imines based anti-oxidant and anti-esterases compounds: Synthesis, single crystal and In-vitro assessment**
Raza M. A., Farwa U., Danish M., Öztürk S., Aagar A. A., DEGE N., Rehman S. U., Al-Sehemi A. G.
COMPUTATIONAL BIOLOGY AND CHEMISTRY, vol.104, 2023 (SCI-Expanded)
- XXIII. **Synthesis, Hirshfeld Surface, FTIR Analysis and Single Crystal X-Ray Structure of 2-Amino-3-Hydroxypyridinium Saccharinate**
Kammazalp S., Sagher M., Dege N., İçbudak H.
Journal of Structural Chemistry, vol.64, no.6, pp.1137-1146, 2023 (SCI-Expanded)
- XXIV. **Synthesis, Crystal Structure and Hirshfeld Surface Analysis of (<i>E</i>)-2-(4-Methylbenzylidene)-N-Phenylhydrazine-1-Carbothioamide**

Acar E., Kansiz S., Dege N.

JOURNAL OF STRUCTURAL CHEMISTRY, vol.64, no.6, pp.974-983, 2023 (SCI-Expanded)

- XXV. **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, vol.34, pp.1423-1435, 2023 (SCI-Expanded)
- XXVI. **Synthesis, DFT calculations, alpha-glucosidase inhibitor activity, and docking studies on Schiff base metal complexes containing isothiocyanate**
Ozge O., AVCI D., Sonmez F., Tamer O., DEGE N., BAŞOĞLU A., ATALAY Y., ZENGİN KURT B.
APPLIED ORGANOMETALLIC CHEMISTRY, vol.37, no.5, 2023 (SCI-Expanded)
- XXVII. **Synthesis, crystal structures, and DFT calculations: novel Mn(II), Co(II) and Ni(II) complexes of N-(pyridin-2-ylmethylene)methanamine with isothiocyanate as promising optical materials**
AVCI D., Ozge O., BAŞOĞLU A., Sonmez F., Tamer O., DEGE N., ATALAY Y.
OPTICAL AND QUANTUM ELECTRONICS, vol.55, no.5, 2023 (SCI-Expanded)
- XXVIII. **A combined experimental, Hirshfeld surface analysis, and theoretical study on fac-[tri(azido)(tris(2-pyridyl)amine)iron(III)]**
Setifi Z., Cubillan N., Glidewell C., Gil D. M., Torabi E., Morales-Toyo M., DEGE N., Setifi F., Mirzaei M.
POLYHEDRON, vol.233, 2023 (SCI-Expanded)
- XXIX. **Synthesis, crystals structures and theoretical studies of novel alkali copper indium orthophosphates ACuIn(PO₄)₂ (A = Na, K and Rb)**
Badri A., Slimi S., Mokni I., DEGE N., Maria Solé R., Aguiló M., Díaz F., Mateos X., Ben Amara M.
Journal of Solid State Chemistry, vol.318, 2023 (SCI-Expanded)
- XXX. **Synthesis, Structural Characterization and Theoretical NLO Activity of N-(4-Acetyl-5-(4-(Nitro) Phenyl)-4,5-Dihydro-1,3,4-Thiadiazol-2-yl)-N-Phenyl Acetamide**
Tabti C., Benmohammed A., Boukabcha N., DEGE N., Djafri A., Boudjenane F. Z., Chouaih A., Djafri A.
POLYCYCLIC AROMATIC COMPOUNDS, vol.43, no.10, pp.9153-9174, 2023 (SCI-Expanded)
- XXXI. **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., cinar E. B., SERT Y., Alhaji Isa M., Lai C., Buba F., DEGE N., Benchat N., Karrouchi K.
JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS, vol.41, no.21, pp.11578-11597, 2023 (SCI-Expanded)
- XXXII. **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, vol.43, no.5, pp.4396-4406, 2023 (SCI-Expanded)
- XXXIII. **Syntheses, X-ray structure and biological studies of binuclear mu-oxo diiron complexes with s-triazine pincer ligand**
Refaat H. M., Alotaibi A. A. M., DEGE N., El-Faham A., Soliman S. M.
INORGANICA CHIMICA ACTA, vol.543, 2022 (SCI-Expanded)
- XXXIV. **Investigation on crystal structure, spectral FT-IR analysis, DFT and molecular docking studies of a novel complex with the N'-(pyridin-2-ylmethylene)nicotinohydrazide**
Mahmoudi G., Sahli S., Tamer O., cinar E. B., Boehme U., DEGE N., Ben Nasr C., Kaabi K.
JOURNAL OF MOLECULAR STRUCTURE, vol.1269, 2022 (SCI-Expanded)
- XXXV. **Above room temperature dielectric switchable organic co-crystal [C₄H₄O₄]. [C₃H₉N] with Hirshfeld surface analyses**
Li X., Wu J., Qian K., Yang J., Cao W., DEGE N., Yan T., Wang F.
INORGANIC CHEMISTRY COMMUNICATIONS, vol.145, 2022 (SCI-Expanded)
- XXXVI. **Synthesis, structural studies, Hirshfeld surface analysis, and molecular docking studies of a thiophene-based Schiff base compound**
Kansiz S., Azam M., Basılı T., Meral S., Aktas F. A., Yesilbag S., Min K., Alaman Ağar A., Dege N.
JOURNAL OF MOLECULAR STRUCTURE, vol.1265, 2022 (SCI-Expanded)

- XXXVII. **A zinc(II) metal-organic complex based on 2-(2-aminophenyl)-1H- benzimidazole ligand: Exhibiting high adsorption capacity for aromatic hazardous dyes and catecholase mimicking activity**
Muslim M., Ali A., Ahmad M., Alarifi A., Afzal M., Sepay N., DEGE N.
JOURNAL OF MOLECULAR LIQUIDS, vol.363, 2022 (SCI-Expanded)
- XXXVIII. **Synthesis, structural determination, molecular docking and biological activity of 1-(4-fluorobenzyl)-5-bromolindolin-2,3-dione**
Belhachemi M. H. M., Benmohammed A., Saiah H., Boukabcha N., Saidj M., DEGE N., Djafri A., Chouaih A.
JOURNAL OF MOLECULAR STRUCTURE, vol.1265, 2022 (SCI-Expanded)
- XXXIX. **Stabilization of supramolecular network of fluconazole drug polyiodide: Synthesis, computational and spectroscopic studies**
Ferjani H., Bechaieb R., DEGE N., Abd El-Fattah W., Elamin N. Y., Frigui W.
JOURNAL OF MOLECULAR STRUCTURE, vol.1263, 2022 (SCI-Expanded)
- XL. **Synthesis, structural, photo-physical properties and DFT studies of some diarylheptanoids**
Al-Balushi R. A., Al-Busaidi I. J., Al-Sharji H., Haque A., Faizi M. S. H., DEGE N., Khan M. S., Mohamed T. A.
JOURNAL OF MOLECULAR STRUCTURE, vol.1264, 2022 (SCI-Expanded)
- XLI. **Photophysical Properties and Single-Molecule Magnet Behavior in Heterobimetallic 3d4 f Schiff Base Complexes**
Fellah F. Z. C., Pointillart F., Guizouarn T., Roisnel T., DEGE N., Fellah A. C., Hassaine R.
EUROPEAN JOURNAL OF INORGANIC CHEMISTRY, vol.2022, no.27, 2022 (SCI-Expanded)
- XLII. **Synthesis of 3-Methoxy-6- [(2, 4, 6-trimethyl-phenylamino)-methyl]-phenol Schiff base characterized by spectral, in-silco and in-vitro studies**
Murugan S., Nehru J., Arputharaj D. S., Catherine Paul A., Gunasekaran P., DEGE N., POYRAZ E. B., Balasubramani K., Savaridasson J. K., Al-Sehemi A. G., et al.
Heliyon, vol.8, no.8, 2022 (SCI-Expanded)
- XLIII. **New Organic-Inorganic Salt Based on Fluconazole Drug: TD-DFT Benchmark and Computational Insights into Halogen Substitution**
Ferjani H., Bechaieb R., Alshammari M., Lemine O. M., DEGE N.
INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES, vol.23, no.15, 2022 (SCI-Expanded)
- XLIV. **Solvothermal synthesis, crystal structure, thermal, magnetic properties and DFT computations of a Ytterbium(III) complex derived from pyridine-2,6-dicarboxylic acid**
Sharif S., Saeed M., DEGE N., Bano R., Ahmad S., Gilani M. A., ŞAHİN O., Ahmad S., Ch A. R.
JOURNAL OF MOLECULAR STRUCTURE, vol.1260, 2022 (SCI-Expanded)
- XLV. **Supramolecular assembly in designing co-crystals of fumaric acid and pyrimidine/picolinate derivatives**
Kansiz S., Azam M., DEGE N., Ermis N., Al-Resayes S., Alam M.
GREEN CHEMISTRY LETTERS AND REVIEWS, vol.15, no.3, pp.825-836, 2022 (SCI-Expanded)
- XLVI. **Experimental and theoretical approaches on structural, spectroscopic (FT-IR and UV-Vis), nonlinear optical, and molecular docking analyses for Zn (II) and Cu (II) complexes of 6-chloropyridine-2-carboxylic acid**
DEGE N., Tamer O., Simsek M., AVCI D., Yaman M., BAŞOĞLU A., ATALAY Y.
APPLIED ORGANOMETALLIC CHEMISTRY, vol.36, no.6, 2022 (SCI-Expanded)
- XLVII. **X-ray Structure Analyses and Biological Evaluations of a New Cd(II) Complex with S-Triazine Based Ligand**
Dahlous K. A., Alotaibi A. A. M., DEGE N., El-Faham A., Soliman S. M., Refaat H. M.
CRYSTALS, vol.12, no.6, 2022 (SCI-Expanded)
- XLVIII. **Synthesis, Structure and Biological Evaluations of Zn(II) Pincer Complexes Based on S-Triazine Type Chelator**
Refaat H. M., Alotaibi A. A. M., DEGE N., El-Faham A., Soliman S. M.
MOLECULES, vol.27, no.11, 2022 (SCI-Expanded)
- XLIX. **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., İçbudak H.
POLYHEDRON, vol.218, 2022 (SCI-Expanded)

- L. **Co (II) Complexes Based on the Bis-Pyrazol-S-Triazine Pincer Ligand: Synthesis, X-ray Structure Studies, and Cytotoxic Evaluation**
Refaat H. M., Alotaibi A. A. M., DEGE N., El-Faham A., Soliman S. M.
CRYSTALS, vol.12, no.5, 2022 (SCI-Expanded)
- LI. **Synthesis, structure and acetylcholinesterase inhibition activity of new diarylpyrazoles**
Zia M., Hameed S., Nadeem H., Kharl A. A., DEGE N., Paracha R. Z., Arshad I., Naseer M. M.
Bioorganic Chemistry, vol.121, 2022 (SCI-Expanded)
- LII. **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., Doğan O. E., ALPASLAN G., Agar T., Muthu S., SERT Y.
COLLOIDS AND SURFACES A-PHYSICOCHEMICAL AND ENGINEERING ASPECTS, vol.638, 2022 (SCI-Expanded)
- LIII. **New Schiffbases with a 2,6-bis(2-aminophenylthio)pyridine moiety acting as glutathione reductase activator and inhibitors: Synthesis and molecular docking studies**
TUNÇ T., Ortaakarsu A. B., Hatipoglu S. M., Kazanci U., Karabocek S., Karabocek N., DEGE N., Karacan N.
JOURNAL OF MOLECULAR STRUCTURE, vol.1254, 2022 (SCI-Expanded)
- LIV. **Stereoselective synthesis, structural determination, computational studies and antimicrobial activity of novel class of spiropyrroloquinoxaline engrafted ferrocenoindole hybrid heterocycle**
Arumugam N., Almansour A. I., Kumar R. S., Soliman S. M., Viswanathan E., DEGE N., Alaqeel S. I., Amaladass P., Perumal K.
Journal of Molecular Structure, vol.1252, 2022 (SCI-Expanded)
- LV. **Growth, crystal structure, Hirshfeld surface analysis, DFT studies, physicochemical characterization, and cytotoxicity assays of novel organic triphosphate**
Oueslati Y., Kansiz S., DEGE N., de la Torre Paredes C., Llopis-Lorente A., Martinez-Manez R., Sta W. S.
JOURNAL OF MOLECULAR MODELING, vol.28, no.3, 2022 (SCI-Expanded)
- LVI. **Therapeutical Potential of Imines; Synthesis, Single Crystal Structure, Computational, Molecular Modeling, and ADMET Evaluation**
Tatildil D., Raza M. A., DEGE N., Alaman Ağa A., Farwa U., Rehman S. U.
ACS OMEGA, vol.7, no.12, pp.10568-10579, 2022 (SCI-Expanded)
- LVII. **Synthesis, spectroscopic analyses, DFT calculations and molecular docking studies of Pd(II) complex of hydrazone ligand derived from ethyl carbazate**
İsler E., Zulfikaroglu A., VURAL H., DEGE N.
MOLECULAR CRYSTALS AND LIQUID CRYSTALS, vol.736, no.1, pp.72-92, 2022 (SCI-Expanded)
- LVIII. **(E)-N-(3-chlorophenyl)-1-(5-nitro-2-(piperidin-1-yl)phenyl)methanimine: X-Ray, DFT, ADMET, Boiled-Egg Model, Druggability, Bioavailability, and Human Cyclophilin D (CypD) Inhibitory Activity**
Şahin S., DEGE N.
JOURNAL OF MOLECULAR STRUCTURE, vol.1250, 2022 (SCI-Expanded)
- LIX. **Polymorphism, spectroscopic, DFT and anticancer activity of a palladium (II) complex with a thiophenyl azoimine-quinoline SNN ' N '' ligand**
Al-Noaimi M., Awwadi F. F., Mansi I. A., Sawwan M., Abu-Irmaileh B., DEGE N.
POLYHEDRON, vol.211, 2022 (SCI-Expanded)
- LX. **Synthesis, characterization, computational analyses, in silico ADMET studies, and inhibitory action against SARS-CoV-2 main protease (Mpro) of a Schiff base**
Şahin S., DEGE N.
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- L. **Crystal structure, Hirshfeld surface analysis and DFT studies of 2-[5-(4-methylbenzyl)-6-oxo-3-phenyl-1,6-dihydropyridazin-1-yl]acetic acid**

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- LI. **Crystal structures and Hirshfeld surface analyses of 4-benzyl-6-phenyl-4,5-dihydropyridazin-3(2H)-one and methyl 2-[5-(2,6-dichlorobenzyl)-6-oxo-3-phenyl-1,4,5,6-tetrahydropyridazin-1-yl]acetate**

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- LII. **Crystal structure and Hirshfeld surface analysis of (E)-6-(4-hydroxy-3-methoxystyryl)-4,5-dihydropyridazin-3(2H)-one**

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- LIII. **Crystal structure and Hirshfeld surface analysis of 2,2'-bis[(1E,1'E)-[ethane-1,2-diylbis(azanylyunene)]-bis(methanylylidene)]bis[4-(trifluoromethoxy)-phenol]copper(II) hydroquinone hemisolvate**

Kansiz S., Meral S., DEGE N., Alaman Ağar A., Fritsky I. O.

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- LIV. **Crystal structure and DFT study of a zinc xanthate complex**

Qadir A. M., Kansiz S., DEGE N., Rosair G. M., Fritsky I. O.

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- LV. **Crystal structure and Hirshfeld surface analysis of N-(tert-butyl)-2-(phenylethynyl)imidazo[1,2-a]pyridin-3-amine**

Tber Z., Kansiz S., El Hafi M., Loubidi M., Jouha J., DEGE N., Essassi E. M., Mague J. T.

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- LVI. **Crystal structure and Hirshfeld surface analysis of 4-(4-methylbenzyl)-6-phenylpyridazin-3(2H)-one**

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- LVIII. **Crystal structure, DFT and MEP study of (E)-2-[(2-hydroxy-5-methoxybenzylidene)amino]benzonitrile**
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- LIX. **Crystal structure and the DFT and MEP study of 4-benzyl-2-[2-(4-fluorophenyl)-2-oxoethyl]-6-phenylpyridazin-3(2H)-one**
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- LX. **Crystal structure and Hirshfeld surface analysis of ethyl 2-[5-(3-chlorobenzyl)-6-oxo-3-phenyl-1,6-di-hydropyridazin- 1-yl]acetate**
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- LXI. **Crystal structure and Hirshfeld surface analysis of (Z)-6-[(2-hydroxy-4-methylanilino)methylidene]-4-methylcyclohexa-2,4-dien-1-one**
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- LXII. **Crystal structure and Hirshfeld surface analysis of 4-[4-(1H-benzo[d]imidazol-2-yl)phenoxy]phthalonitrile dimethyl sulfoxide monosolvate**
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- LXIII. **Crystal structure and Hirshfeld surface analysis of (Z)-6-[(2-hydroxy-5-nitroanilino)methylidene]-4-methylcyclohexa-2,4-dien-1-one**
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- LXVI. **Crystal structure and DFT study of (E)-2-chloro-4-[[2-(2,4-dinitrophenyl)hydrazin-1-ylidene]methyl]phenol acetonitrile hemisolvate**
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- LXVII. **Dichlorido{ $\text{Ni}(\text{H}_2\text{O})_2$, $\text{Ni}(\text{H}_2\text{O})_2$, $\text{Ni}(\text{H}_2\text{O})_2$ -trimethyl- $\text{Ni}(\text{H}_2\text{O})_2$ -(1 H_2O -pyrazol-1-yl- κ^2 $\text{Ni}(\text{H}_2\text{O})_2$ sup²/sup²)methyl]ethane-1,2-diamine- κ^2 sup²/sup² $\text{Ni}(\text{H}_2\text{O})_2$, $\text{Ni}(\text{H}_2\text{O})_2$ }copper(II) methanol monosolvate**
Singh R., Ali A., Faizi M. S., Singh R., Iskenderov T. S., DEGE N.
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- LXVIII. **Crystal structure and Hirshfeld surface analysis of 3-(4-methoxyphenyl)-1-methyl-4-phenyl-1H-pyrazolo[3,4-d]pyrimidine**
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- LXIX. **Crystal structure and Hirshfeld surface analysis of 4-(2,6-dichlorobenzyl)-6-phenylpyridazin-3(2H)-one**
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- LXX. **Crystal structure and Hirshfeld surface analysis of two 5,11-methanobenzo[g][1,2,4]triazolo[1,5 c][1,3,5]oxadiazocine derivatives**
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- LXXI. **(Z)-3-([3-Methoxy-5-(trifluoromethyl)phenyl]imino)methylbenzene-1,2-diol**
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- LXXII. **Synthesis, crystal structure, spectroscopic features and Hirshfeld surfaces of 2-methyl-3-[(2-methylphenyl)carbamoyl]phenyl acetate**
Yaman M., ÇAKMAK Ş., DEGE N., ODABAŞOĞLU M., Pavlenko V. A., Kütük H.
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- LXXIII. **Crystal structure and Hirshfeld surface analysis of a Schitt base: (Z)-6-[(5-chloro-2-methoxyanilino)-methylidene]-2-hydroxycyclohexa-2,4-dien-1-one**
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- LXXV. **Crystal structure and Hirshfeld surface analysis of N-{2-[(E)-(4-methylbenzylidene)amino]phenyl}-2-(5-methyl-1-H-pyrazol-3-yl)acetamide hemihydrate**
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- LXXX. **Crystal structure and Hirshfeld surface analysis of 5-[(5-nitro-1H-indazol-1-yl)methyl]-3-phenyl-4,5-dihydroisoxazole**
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