

## Assoc. Prof. Sefa ÇELİK

### Personal Information

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### International Researcher IDs

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Publons / Web Of Science ResearcherID: C-8065-2019

ScopusID: 55421873200

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### Education Information

Doctorate, Istanbul University, Faculty Of Science, Fizik / Atom Ve Molekül Fiziği, Turkey 2007 - 2011

Postgraduate, Istanbul University, Faculty Of Science, Fizik / Atom Ve Molekül Fiziği, Turkey 2004 - 2007

Undergraduate, Istanbul University, Faculty Of Science, Fizik, Turkey 2000 - 2004

### Research Areas

Physics, Atomic and Molecular Physics, Theory of Atoms and Molecules, Atomic and Molecular Interactions, Natural Sciences

### Academic Titles / Tasks

Associate Professor, Istanbul University, Faculty of Science, Department of Physics, 2019 - Continues

Associate Professor, İstanbul University-Cerrahpaşa, Faculty Of Engineering, Department Of Electrical And Electronics Engineering, 2018 - 2019

Lecturer PhD, Istanbul University, Elektrik-Elektronik Mühendisliği, 2011 - 2018

Lecturer, Istanbul University, Mühendislik Fakültesi, Elektrik-Elektronik Mühendisliği, 2007 - 2011

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

- I. **Vibrational Spectroscopic and Molecular Docking Studies of Amrinone, a Cardiotonic Inotropic Drug**  
Çelik S., Akyüz S., Özel A., Akalın E.  
OPTICS AND SPECTROSCOPY, vol.130, no.2, pp.215-227, 2022 (SCI-Expanded)
- II. **Structural and vibrational investigations and molecular docking studies of a vinca alkaloid, vinorelbine**  
Çelik S., Akyüz S., Özel A.  
JOURNAL OF BIOMOLECULAR STRUCTURE AND DYNAMICS, vol.1, pp.1-20, 2022 (SCI-Expanded)
- III. **Molecular modeling, DFT quantum chemical analysis, and molecular docking on edotecarin, an indolocarbazole anticancer agent**  
Çelik S., Akyüz S., Özel A.

MOLECULAR CRYSTALS AND LIQUID CRYSTALS, vol.1, pp.1-23, 2022 (SCI-Expanded)

- IV. **Lupeol inhibits pesticides induced hepatotoxicity via reducing oxidative stress and inflammatory markers in rats**  
Çöremen M., Türkyılmaz İ. B., Us H., Sezen Us A., Çelik S., Özel A., Bulan N. Ö., Yanardağ R.  
FOOD AND CHEMICAL TOXICOLOGY, 2022 (SCI-Expanded)
- V. **Synthesis, vibrational spectroscopic investigation, molecular docking, antibacterial and antimicrobial studies of a new anthraquinone derivative compound**  
Çelik S., Vagifli F., Akyuz S., Ozkok F., Özel A., Döşler S., Onul N.  
SPECTROSCOPY LETTERS, vol.55, no.4, pp.259-277, 2022 (SCI-Expanded)
- VI. **Molecular docking of the pentapeptide derived from rice bran protein as anticancer agent inhibiting both receptor and non-receptor tyrosine kinases**  
Gasymov O. K., Kecel-Gunduz S., ÇELİK S., Akyuz S., ÖZEL A., Agaeva G., Suleymanova L. M., Agaeva U., Bakhishova M., Aliyev J. A.  
JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS, 2022 (SCI-Expanded)
- VII. **Vibrational spectroscopic characterization and structural investigations of Cepharranthine, a natural alkaloid**  
Çelik S., Akyüz S., Özel A.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1, pp.1-15, 2022 (SCI-Expanded)
- VIII. **Raman spectroscopic investigation of the wear effect on the titanium carbonitride/aluminum oxide/titanium nitride coated cutting tool**  
Çelik S., Beköz Ülgen N., Akyüz S., Özel A.  
Spectroscopy Letters, vol.1, pp.1-12, 2022 (SCI-Expanded)
- IX. **Structural and spectral analysis of anticancer active cyclo(Ala-His) dipeptide**  
ÇELİK S., Yılmaz G., ÖZEL A., Akyuz S.  
JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS, vol.40, no.2, pp.660-672, 2022 (SCI-Expanded)
- X. **Evaluation of anti-cancer and anti-covid-19 properties of cationic pentapeptide Glu-Gln-Arg-Pro-Arg, from rice bran protein and its d-isomer analogs through molecular docking simulations**  
K.Gasymov O., Çelik S., Agaeva G., Akyüz S., Kecel Gündüz S., M. Qocayev N., Özel A., Agaeva U., Bakhishova M., A. Aliyev J.  
Journal Of Molecular Graphics & Modelling, vol.108, pp.1-15, 2021 (SCI-Expanded)
- XI. **Synthesis, molecular modelling, FT-IR, Raman and NMR characterization, molecular docking and ADMET study of new nickel(II) complex with an N-4-tetradentate thiosemicarbazone**  
Eğlence-Bakır S., Celik S., Şahin M., Ozel A., Akyuz S., Ülküseven B.  
JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS, vol.39, no.12, pp.4212-4224, 2021 (SCI-Expanded)
- XII. **Synthesis, FT-IR and NMR Characterization, Antibacterial and Antioxidant Activities, and DNA Docking Analysis of a New Vanillin-Derived imine Compound**  
Celik S., Özkök F., Ozel A. E., Cakir E., Akyüz S.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1236, 2021 (SCI-Expanded)
- XIII. **Molecular Structure, Molecular Docking and Absorption, Distribution, Metabolism, Excretion and Toxicity study of cellulose II**  
Çelik S., Demirağ A. D., Özel A., Akyüz S.  
Journal Of The Chinese Chemical Society, vol.1, pp.1-13, 2021 (SCI-Expanded)
- XIV. **Synthesis, antimicrobial activity, molecular docking and ADMET study of a caprolactam-glycine cluster**  
ÇELİK S., Albayrak A. T., Akyuz S., ÖZEL A., Sigirci B. D.  
JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS, vol.39, no.7, pp.2376-2386, 2021 (SCI-Expanded)
- XV. **Interactions mechanism of commonly used drugs for the treatment of Covid-19**  
Çelik S., Demirag A. D., Özel A., Akyüz S.  
Bulletin Of The Chemical Society Of Ethiopia, vol.34, no.3, pp.613-623, 2020 (SCI-Expanded)
- XVI. **Vibrational spectroscopic characterization, quantum chemical and molecular docking studies of Valyl-Methionine dipeptide**

- Çelik S., Özel A., Durak V., Akyüz S.  
Spectroscopy Letters, vol.1, pp.1-16, 2020 (SCI-Expanded)
- XVII. **Using Raman Spectroscopy to Investigate the Molecular Level Characteristics of Endometriosis**  
Akyuz S., ÇELİK S., USTA A. T., ÖZEL A., Yilmaz G., Yilmaz S.  
OPTICS AND SPECTROSCOPY, vol.128, no.8, pp.1318-1327, 2020 (SCI-Expanded)
- XVIII. **Molecular Structure, Vibrational Spectra, Molecular Docking, and ADMET Study of Cellulose Triacetate II**  
ÇELİK S., Demirag A. D., ÖZEL A., Akyuz S.  
OPTICS AND SPECTROSCOPY, vol.128, no.8, pp.1138-1150, 2020 (SCI-Expanded)
- XIX. **Synthesis, molecular docking and ADMET study of ionic liquid as anticancer inhibitors of DNA and COX-2, TOPII enzymes**  
Celik S., ALBAYRAK A. T., AKYÜZ S., Ozel A.  
Journal of Biomolecular Structure and Dynamics, vol.38, no.5, pp.1354-1364, 2020 (SCI-Expanded)
- XX. **Synthesis, FT-IR and NMR characterization, antimicrobial activity, cytotoxicity and DNA docking analysis of a new anthraquinone derivate compound**  
Celik S., ÖZKÖK F., Ozel A., ŞAHİN Y. M., AKYÜZ S., DİREN SİĞİRCİ B., BAŞARAN KAHRAMAN B., Darici H., Karaoz E.  
Journal of Biomolecular Structure and Dynamics, vol.38, no.3, pp.756-770, 2020 (SCI-Expanded)
- XXI. **Molecular Modeling, Dimer Calculations, Vibrational Spectra, and Molecular Docking Studies of 5-Chlorouracil**  
Akalm E., Çelik S., Akyüz S.  
JOURNAL OF APPLIED SPECTROSCOPY, vol.86, pp.975-985, 2020 (SCI-Expanded)
- XXII. **Investigations of the Neolithic potteries of 6th millennium BC from Göytepe-Azerbaijan by vibrational spectroscopy and chemometric techniques**  
AKYÜZ S., Guliyev F., Celik S., Ozel A., Alakbarov V.  
Vibrational Spectroscopy, vol.105, 2019 (SCI-Expanded)
- XXIII. **Molecular modelling and vibrational investigations of ammonium-based ionic liquid (CLTOAB)**  
Celik S., ALBAYRAK A. T., AKYÜZ S., Ozel A.  
Journal of Biomolecular Structure and Dynamics, vol.37, no.10, pp.2515-2526, 2019 (SCI-Expanded)
- XXIV. **Structural analysis, spectroscopic characterization and molecular docking studies of the cyclic heptapeptide**  
Celik S., Kecel-Gunduz S., AKYÜZ S., Ozel A.  
Journal of Biomolecular Structure and Dynamics, vol.36, no.9, pp.2407-2423, 2018 (SCI-Expanded)
- XXV. **Investigations of Archaeological Glass Bracelets and Perfume Bottles Excavated in Ancient Ainos (Enez) by Multiple Analytical Techniques**  
Celik S., Akyuz T., Akyuz S., Ozel A., Kecel-Gunduz S., Basaran S.  
Journal of Applied Spectroscopy, vol.85, no.1, pp.178-183, 2018 (SCI-Expanded)
- XXVI. **Dielectric and Raman spectroscopy of TlSe thin films**  
Ozel A., Deger D., Celik S., Yakut Ş., Karabak B., Akyuz S., Ulutas K.  
PHYSICA B-CONDENSED MATTER, vol.527, pp.72-77, 2017 (SCI-Expanded)
- XXVII. **Molecular Mechanic Studies on the Zwitterionic and Neutral Conformation Stability of Biological Active Peptide**  
KECEL GÜNDÜZ S., ÇELİK S.  
Süleyman Demirel Üniversitesi Fen Bilimleri Enstitüsü Dergisi, vol.1, pp.1-7, 2017 (SCI-Expanded)
- XXVIII. **Vibrational spectroscopic and structural investigations of bioactive molecule Glycyl-Tyrosine (Gly-Tyr)**  
Celik S., AKYÜZ S., Ozel A.  
Vibrational Spectroscopy, vol.92, pp.287-297, 2017 (SCI-Expanded)
- XXIX. **Structural and spectroscopic investigation on antioxidant dipeptide, L-Methionyl-L-Serine: A combined experimental and DFT study**  
Kecel-Gunduz S., Bicak B., Celik S., Akyuz S., Ozel A.  
Journal of Molecular Structure, vol.1137, pp.756-770, 2017 (SCI-Expanded)

- XXX. **Conformational Analysis of Cyclo(Tyr-Cys) and Cyclo(Phe-Cys) Dipeptides**  
ÇELİK S., KECEL GÜNDÜZ S.  
Süleyman Demirel Üniversitesi Fen Bilimleri Enstitüsü Dergisi, vol.1, pp.1-5, 2017 (SCI-Expanded)
- XXXI. **Conduction mechanisms, molecular modelling and micro-Raman studies of TlInSe<sub>2</sub> chalcogenide crystal**  
Kalkan N., Celik S., Bas H., Ozel A.  
Journal of Optoelectronics and Advanced Materials, vol.19, pp.234-245, 2017 (SCI-Expanded)
- XXXII. **The conformational and vibrational behavior of the inhibitory neuropeptide derived from beta-endorphin**  
Kecel-Gunduz S., Celik S., Ozel A., AKYÜZ S.  
Journal of Biomolecular Structure and Dynamics, vol.35, no.3, pp.585-602, 2017 (SCI-Expanded)
- XXXIII. **Comparative study of antitumor active cyclo(Gly-Leu) dipeptide: A computational and molecular modeling study**  
ÇELİK S., ÖZEL A., Akyuz S.  
Vibrational Spectroscopy, vol.83, pp.57-69, 2016 (SCI-Expanded)
- XXXIV. **Structural and vibrational study of primidone based on monomer and dimer calculations**  
Celik S., Kecel-Gunduz S., Ozel A., Akyuz S.  
Journal of Biomolecular Structure and Dynamics, vol.33, no.4, pp.911-923, 2015 (SCI-Expanded)
- XXXV. **Structural and vibrational spectroscopic elucidation of sulphiride in solid state**  
Kecel-Gunduz S., Celik S., Ozel A. E., Akyuz S.  
JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS, vol.33, no.2, pp.322-343, 2015 (SCI-Expanded)
- XXXVI. **Counterpoise Correction on the Geometries and Vibrational Frequencies of Acetazolamide Dimers**  
Ozel A., Gunduz S., Celik S., Akyuz S.  
ASIAN JOURNAL OF CHEMISTRY, vol.25, no.14, pp.8151-8156, 2013 (SCI-Expanded)
- XXXVII. **Structural and Vibrational Study on Monomer and Dimer Forms and Water Clusters of Acetazolamide**  
Ozel A., Gunduz S., Celik S., Akyuz S.  
JOURNAL OF SPECTROSCOPY, 2013 (SCI-Expanded)
- XXXVIII. **Structural and IR and Raman spectral analysis of cyclo(His-Phe) dipeptide**  
Celik S., Ozel A., Kecel S., Akyuz S.  
VIBRATIONAL SPECTROSCOPY, vol.61, pp.54-65, 2012 (SCI-Expanded)
- XXXIX. **Conformational preferences, experimental and theoretical vibrational spectra of cyclo(Gly-Val) dipeptide**  
Celik S., Ozel A., Akyuz S., Kecel S., Agaeva G.  
JOURNAL OF MOLECULAR STRUCTURE, vol.993, pp.341-348, 2011 (SCI-Expanded)
- XL. **Conformational analysis and vibrational spectroscopic investigation of L-proline-tyrosine (L-Pro-Tyr) dipeptide**  
Kecel S., Ozel A., Akyuz S., Celik S., Agaeva G.  
JOURNAL OF MOLECULAR STRUCTURE, vol.993, pp.349-356, 2011 (SCI-Expanded)
- XLI. **Conformational analysis and vibrational spectroscopic investigation of L-alanyl-L-glutamine dipeptide**  
Kecel S., Ozel A., Akyuz S., Celik S.  
Spectroscopy, vol.24, pp.219-232, 2010 (SCI-Expanded)
- XLII. **Infrared and Raman spectroscopic and quantum chemical investigations of zinc halide complexes of 3-aminoquinoline**  
Ozel A., Celik S., Akyuz S., Kecel S.  
VIBRATIONAL SPECTROSCOPY, vol.53, no.1, pp.151-157, 2010 (SCI-Expanded)
- XLIII. **Vibrational spectroscopic investigation of free and coordinated 5-aminoquinoline: The IR, Raman and DFT studies**  
Ozel A., Celik S., Akyuz S.  
JOURNAL OF MOLECULAR STRUCTURE, vol.924, pp.523-530, 2009 (SCI-Expanded)

## Articles Published in Other Journals

- I. **Computational Investigation of the Interaction Mechanism of Some anti-Alzheimer Drugs with the Acetylcholinesterase Enzyme**  
Çelik S., Demirağ A. D., Coşgun A. O., Özel A., Akyüz S.  
Open Journal of Nano, vol.8, pp.11-21, 2023 (Peer-Reviewed Journal)
- II. **Molecular Docking Study of Midostaurin, an Effective Drug in the Treatment of Myeloid Leukemia**  
Çelik S., Yılmaz G., Özel A., Akyüz S.  
Open Journal of Nano, vol.8, no.1, pp.1-9, 2023 (Peer-Reviewed Journal)
- III. **Molecular Docking Analysis on the Antiviral Effects of Curcumin on SARS-CoV-2**  
Demirağ A. D., Çelik S., Özel A., Akyüz S.  
Bayburt Üniversitesi Fen Bilimleri Dergisi, vol.5, no.2, pp.223-228, 2022 (Peer-Reviewed Journal)
- IV. **Clarification of the Structure of 1,4-Bis(2-Chloro-4-Nitrophenyl)Piperazine Molecule and Its Molecular Docking Analysis with DNA**  
Demirağ A. D., Çelik S., Ilgın B., Özel A., Akyüz S.  
Bayburt Üniversitesi Fen Bilimleri Dergisi, vol.5, pp.19-25, 2022 (Peer-Reviewed Journal)
- V. **Comparative Conformational Analysis of Anticancer Pentapeptide Glu-Gln-Arg-Pro-Arg Isolated From Rice Bran Protein and Its Single- and All D-Amino Acid Isomers Analogs**  
K. Gasymov O., A. Agaeva G., Qocayev N. M., Çelik S., Akyüz S., Kecel Gündüz S., Özel A., Agaeva U. T., Bakhishova M., Aliyev J. A.  
Transactions of Azerbaijan National Academy of Sciences, vol.42, no.2, pp.23-32, 2022 (Peer-Reviewed Journal)
- VI. **Conformational, Toxic, Physicochemical and Molecular Docking Analysis of the Anticancer Acalabrutinib Molecule**  
Çelik S., Demirağ A. D., Arslan S., Özel A., Akyüz S.  
Open Journal of Nano, vol.1, pp.1-9, 2022 (Peer-Reviewed Journal)
- VII. **Alzheimer Hastalığı Tedavisinde Etkili Cyclo(Phe-Phe) Dipeptidinin Konformasyon Analizi**  
Çelik S., Akyüz S., Özel A.  
Yüzüncü Yıl Üniversitesi Fen Bilimleri Enstitüsü Dergisi, vol.26, no.3, pp.135-142, 2021 (Peer-Reviewed Journal)
- VIII. **Molecular Docking Analysis of Used Drugs for the Treatment of Cancer**  
Demirağ A. D., Çelik S., Akyüz S., Özel A.  
Süleyman Demirel Üniversitesi Fen Bilimleri Enstitüsü Dergisi, vol.12, no.3, pp.539-547, 2021 (Peer-Reviewed Journal)
- IX. **Molecular Docking Analysis Of N-[2-(3-Methylthio(1,2,4-Thiadiazol-5-Ylthio))Acetyl] Benzamide Molecule With Integrin And DNA**  
Demirağ A. D., Çelik S., Özen D., Özel A., Akyüz S.  
Open Journal of Nano, vol.6, no.2, pp.19-27, 2021 (Peer-Reviewed Journal)
- X. **Molecular Structure And Docking Analysis Of The Integrin Inhibitor Cyclo (Arg-Gly-Asp-D-Phe-Val) Peptide**  
Çelik S., Demirağ A. D., Civelek H., Özel A., Akyüz S.  
Open Journal of Nano, vol.6, no.2, pp.1-6, 2021 (Peer-Reviewed Journal)
- XI. **3-Dimensional Molecular Structure of Cyclo (Trp-Trp) Dipeptide with Antimicrobial and Anticancer Activity**  
Çelik S., Akyüz S., Özel A.  
Yüzüncü Yıl Üniversitesi Fen Bilimleri Enstitüsü Dergisi, vol.26, no.2, pp.80-87, 2021 (Peer-Reviewed Journal)
- XII. **Cyclo(Tyr-Tyr) Dipeptidinin Teorik IR, Raman ve Moleküler Yapı Analizi**  
Çelik S., Akyüz S., Özel A.  
Süleyman Demirel Üniversitesi Fen Bilimleri Enstitüsü Dergisi, vol.25, no.2, pp.401-409, 2021 (Peer-Reviewed Journal)
- XIII. **Biological evaluation and pharmacokinetic profiling of a coumarin-benzothiazole hybrid as a new scaffold for human gliomas**  
Gabr M. T., Çelik S., Akyüz S., Özel A.

Medicine in Drug Discovery, vol.1, pp.1-18, 2020 (Scopus)

**XIV. Non-Linear Optical Properties of Primidone**

ÖZEL A., ÇELİK S., AKYÜZ S.

ASIAN JOURNAL OF CHEMISTRY, vol.27, no.5, pp.1932-1934, 2015 (Scopus)

**XV. Three-Dimensional Structure Of The Cyclic Dipeptides**

Çelik S., Agaeva G., Özel A., Akyüz S.

Journal of Qafqaz University, vol.23, pp.97-102, 2008 (Peer-Reviewed Journal)

## Books & Book Chapters

**I. Atom ve Molekül Fiziği**

Akyüz S., Çelik S.

Nobel Yayınevi, Ankara, 2023

**II. OMEGA-3, OMEGA-6 YAĞ ASİTLERİ VE SPEKTROSKOPİ UYGULAMALARI**

Çelik S., Çakır E., Er A.

in: YENİLENEBİLİR KAYNAKLARDAN ELDE EDİLEN MALZEMELER VE UYGULAMALARI-I, Gökhan ÇAYLI, Editor, Artikel Akademi, İstanbul, pp.131-145, 2022

**III. YOSUNLAR VE TİTREŞİM SPEKTROSKOPİSİ UYGULAMALARI**

Er A., Çelik S.

in: YENİLENEBİLİR KAYNAKLARDAN ELDE EDİLEN MALZEMELER VE UYGULAMALARI-I, Gökhan ÇAYLI, Editor, Artikel Akademi, İstanbul, pp.117-130, 2022

**IV. The importance of polymers in medicine and their FTIR and Raman spectroscopic investigations**

Çelik S., Akyüz S., Özel A.

in: Development, Properties, and Industrial Applications of 3D Printed Polymer Composites, R.

Keshavamurthy, Vijay Tambrallimath, J. Paulo Davim, Editor, IGI Global, New York, pp.1-20, 2022

**V. SÜRDÜRÜLEBİLİR GIDA KAYNAĞI OLARAK BİTKİSEL PROTEİNLER VE TİTREŞİM SPEKTROSKOPİSİ UYGULAMALARI**

Çelik S., Çakır E., Er A.

in: Sürdürülebilirlik alanında akademik çalışmalar - V, Gökhan Çaylı, Mustafa Güler, Editor, artikel akademi, İstanbul, pp.57-72, 2022

**VI. Coronaviruses: Molecular Modeling and Docking Studies of Potential Drug Candidates Showing Anti-Covid-19 Activity**

Çelik S., Demirağ A. D., Akyüz S., Özel A.

in: Biologically Active Small Molecules, Debarshi Kar Mahapatra, Sanjay Kumar Bharti, Editor, Apple academic press, Florida, pp.1-27, 2022

**VII. Spectroscopic Applications in Pharmaceuticals and Food**

Çelik S., Kaya Kınaytürk N., Çakır E.

in: Quality Control Applications in the Pharmaceutical and Medical Device Manufacturing Industry, Eugenia

Gabriela Carrillo-Cedillo, Karina Cecilia Arredondo-Soto, Kenia Palomino-Vizcaino, Héctor Alfonso Magaña-Badilla, Editor, IGI Global, New York, pp.122-137, 2022

**VIII. Flavonoids: Their Anticarcinogenic Effects and Molecular Modeling Studies**

Çelik S., Çakır E., Akyüz S., Özel A.

in: Handbook of Research on Natural Products and Their Bioactive Compounds as Cancer Therapeutics, Ashok

Kumar Pandurangan, Suresh Kumar Anandasadagopan, Fahad A. Alhumaydhi, Editor, IGI Global, New York, pp.265-296, 2022

**IX. Characterization and Spectroscopic Applications of Metal Foams From New Lightweight Materials**

Çelik S., Beköz Üllen N., Akyüz S., Karabulut G., Özel A.

in: Handbook of Research on Advancements in the Processing, Characterization, and Application of Lightweight Materials, Kaushik Kumar, B. Sridhar Babu, J. Paulo Davim, Editor, IGI Global, New York, pp.1-25, 2021

**X. Shedding Light on New Drug Designs by Modeling Peptide Structures via Quantum Chemical Methods**

### **in the Health Field**

Çelik S., Kecel Gündüz S., Akyüz S., Özel A.

in: Emerging Trends of Research in Chemical Sciences, Tanmoy Chakraborty, Shalini Chaudhary, Editor, Apple Academic Press, Florida, pp.123-145, 2021

- XI. **Role of Alloying Elements on Powder Metallurgy Steels and Spectroscopic Applications on Them**  
Çelik S., Beköz Üllen N., Akyüz S., Özel A.  
in: Advanced Surface Coating Techniques for Modern Industrial Applications, Supriyo Roy, Goutam Kumar Bose, Editor, IGI Global, New York, pp.226-246, 2020
- XII. **The Role of Multivariate Analysis on the Interpretation of FTIR and Raman Spectra**  
ÇELİK S., Albayrak A. T., AKYÜZ S., ÖZEL A.  
in: Design of Experiments for Chemical, Pharmaceutical, Food, and Industrial Applications, Gabriela Carrillo-Cedillo E., Rodriguez-Avila J. A., Arredondo-Soto K. C., Manuel Cornejo-Bravo J., Editor, IGI Global Publications, Hershey, pp.104-129, 2019
- XIII. **The Importance of Ionic Liquids and Applications on Their Molecular Modeling**  
ÇELİK S., Albayrak A. T., AKYÜZ S., ÖZEL A.  
in: Computational Models for Biomedical Reasoning and Problem Solving, Chung-Hao C., Sen-Ching Samson C., Editor, IGI Global Publications, Hershey, pp.206-230, 2019
- XIV. **The Importance of Anthraquinone and Its Analogues and Molecular Docking Calculation**  
ÇELİK S., ÖZKÖK F., AKYÜZ S., ÖZEL A.  
in: Computational Models for Biomedical Reasoning and Problem Solving, Chung-Hao C., Sen-Ching Samson C., Editor, IGI Global, Hershey, pp.177-205, 2019
- XV. **Practical aspects**  
KECEL GÜNDÜZ S., ÇELİK S., ÖZEL A.  
in: Nanobiomaterials Science, Development and Evaluation, Mehdi Razavi, Avnesh Thakor, Editor, Woodhead Publishing, Duxford, pp.281-299, 2017

### **Refereed Congress / Symposium Publications in Proceedings**

- I. **THE EFFECT OF PENTAPEPTIDE EQRPR DERIVED FROM RICE BRAN ON THE DPPC MONOLAYER.**  
Bakhishova M., Çelik S., Kecel Gündüz S., Akyüz S., Özel A., Agaeva G., M. Suleymanova L., Agaeva U., Gasymov O. K., Aliyev J.  
International Korkut Ata Scientific Researches Conference, Osmaniye, Turkey, 28 - 30 June 2022, pp.40
- II. **TOXICOLOGICAL AND MOLECULAR DOCKING ANALYSES OF ANTICANCER DRUG CLADRIBINE**  
Çelik S., Gökdelen A. C., Demirağ A. D., Özel A., Akyüz S.  
Turkish Physical Society 37 th International Physics Congress, Muğla, Turkey, 1 - 05 September 2021, pp.69
- III. **MOLECULAR DOCKING STUDY OF MIDOSTAURIN, AN EFFECTIVE DRUG IN THE TREATMENT OF MYELOID LEUKEMIA**  
Yılmaz G., Çelik S., Özel A., Akyüz S.  
Turkish Physical Society 37 th International Physics Congress, Muğla, Turkey, 1 - 05 September 2021, pp.78
- IV. **Molecular structure and docking analysis of the factor Xa inhibitor Edoxaban**  
Çelik S., Avcular E., Demirağ A. D., Özel A., Akyüz S.  
Turkish Physical Society 37 th International Physics Congress, Muğla, Turkey, 1 - 05 September 2021, pp.76
- V. **COVID-19 MAJOR PROTEASE ENZYME AND SARS-COV-2 SPIKE GLYCOPROTEIN MOLECULAR DOCKING ANALYSIS WITH RUXOLITINIB**  
Çelik S., Arslan S., Demirağ A. D., Özel A., Akyüz S.  
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- CIX. Conformational Analysis Of Cyclo(Gly-Leu):Comparison Of Experimental And Dft Vibrational Spectra**

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- CXV. **Vibrational and conformational analysis of Pyroglutamyl-asparagine amide ( Pglu-Asn-NH<sub>2</sub> ) dipeptide**  
KECEL S., ÖZEL A., ÇELİK S., AKYÜZ S.  
14th European Conference on the Spectroscopy of Biological Molecules, Portugal, 1 - 04 August 2011, pp.2
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27 th International Physics Congress, Turkey, 1 - 04 September 2010, pp.463
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27 th International Physics Congress, Turkey, 1 - 04 September 2010, pp.436
- CXVIII. **Conformational preferences, experiment and theoretical vibrational spectra of cyclo(gly-val) dipeptide**  
ÇELİK S., ÖZEL A., AKYÜZ S., KECEL S., Agaeva G.  
30th European Congress on Molecular Spectroscopy (EUCMOS 2010), Italy, 1 - 04 August 2010, pp.131
- CXIX. **Structural and spectroscopic elucidation of L-proline tyrosine (L-pro-tyr) dipeptide**  
KECEL S., ÖZEL A., AKYÜZ S., ÇELİK S., Agaeva G.  
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- CXX. **Conformational Analysis And Vibrational Spectroscopic Investigation of L-Alanyl-L-Glutamine Dipeptide**  
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- CXXI. **Conformational analysis and vibrational spectroscopic investigation of L-Alanyl- L-Glutamine dipeptide**  
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- CXXII. **Conformational Analysis, FT-IR and Raman Spectroscopic Study of Cyclo (His-Phe) Dipeptide**  
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- CXXIII. **FT-IR , Raman Spectroscopic and Quantum Chemical Investigations of Zinc Halide Complexes of 3-aminoquinoline**  
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- CXXIV. **FT-IR , Micro-Raman Spectroscopic And Quantum Chemical Investigation of Zinc Halide Complexes**



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## Supported Projects

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Özel A., Akyüz S., Çelik S., Kecel Gündüz S., Darıcı H., Karaöz E., Ulukaya E., TÜBİTAK International Bilateral Joint Cooperation Program Project, Pirinç Kepeği Türevi Pentapeptidinin Konformasyon Davranışının ve D-Amino Asit Sübstitüsyonlarının Antikanser Aktivitesi Üzerindeki Etkisinin Değerlendirilmesi: Antikanser İlaç Keşfine Yönelik Çıkarımlar, 2020 - 2022

ÖZEL A., KALKAN N., ÇELİK S., Project Supported by Higher Education Institutions, Conduction mechanisms molecular modelling and microRaman studies of TlInSe2 chalcogenide crystal, 2018 - 2019

KECEL GÜNDÜZ S., ÖZEL A., AKYÜZ S., BIÇAK B., ÇELİK S., Project Supported by Higher Education Institutions, Conformational behavior structural and vibrational characterization of the carboxy terminal dipeptide of b-endorphin, 2018 - 2019

KECEL GÜNDÜZ S., AKYÜZ S., BIÇAK B., ÖZEL A., ÇELİK S., Project Supported by Higher Education Institutions, Structural and spectroscopic investigation on antioxidant dipeptide L-Methionyl-L-Serine A combined experimental and DFT study, 2018 - 2019

ÇELİK S., AKYÜZ S., ÖZEL A., KECEL GÜNDÜZ S., AKYÜZ T., BAŞARAN S., Project Supported by Higher Education Institutions, Investigations of Archaeological Glass Bracelets and Perfume Bottles Excavated in Ancient Ainos (Enez) by Multiple Analytical Techniques, 2018 - 2018

ÇELİK S., AKYÜZ S., ÖZEL A., Project Supported by Higher Education Institutions, Vibrational Spectroscopic and Structural Investigations of Bioactive Molecule Glycyl-Tyrosine(Gly-Tyr), 2018 - 2018

KECEL GÜNDÜZ S., ÖZEL A., ÇELİK S., Project Supported by Higher Education Institutions, Nanobiomaterials Science Development and Evaluation, 2017 - 2018

ÖZEL A., ÇELİK S., AKYÜZ S., Project Supported by Higher Education Institutions, BINDING INTERACTIONS OF TYR-ILE-GLY-SER-ARG LIGAND WITH LAMININ RECEPTOR MODELS, 2017 - 2018

ÖZEL A., AKYÜZ S., KECEL GÜNDÜZ S., ÇELİK S., Project Supported by Higher Education Institutions, THEORETICAL VIBRATIONAL SPECTRA AND MOLECULAR DOCKING STUDIES WITH PROTEIN AND DNA ON CYCLOHEPTAPEPTIDE, 2017 - 2018

ÇELİK S., KECEL GÜNDÜZ S., ALBAYRAK A. T., AKYÜZ S., ÖZEL A., Project Supported by Higher Education Institutions, MOLECULAR MODELLING AND VIBRATIONAL INVESTIGATIONS OF AMMONIUM-BASED IONIC LIQUID (CLTOAB), 2017 - 2017

ÇELİK S., ÖZEL A., Project Supported by Higher Education Institutions, TİROZİN İÇEREN HALKA VE AÇIK UÇLU BAZI DİPEPTİTLERİN TEORİK KONFORMASYON ANALİZİ, 2017 - 2017

ÇELİK S., AKYÜZ S., ÖZEL A., Project Supported by Higher Education Institutions, Comparative study of antitumor active cyclo(Gly-Leu) dipeptide : A computational and molecular modeling study, 2017 - 2017

ÖZEL A., ÇELİK S., AKYÜZ S., Project Supported by Higher Education Institutions, CONFORMATIONAL STABILITY AND SPECTROSCOPIC ANALYSIS OF THE CYCLIC HEPTAPEPTIDE, 2016 - 2016

ÇELİK S., AKYÜZ T., AKYÜZ S., ÖZEL A., KECEL GÜNDÜZ S., KURAP G., BAŞARAN S., Project Supported by Higher Education Institutions, Investigations of Archaeological glass bracelets and perfume bottles excavated in Ancient Ainos (Enez) by Multiple Analytical Techniques, 2016 - 2016

ÇELİK S., Project Supported by Higher Education Institutions, Structural and vibrational study of primidone based on monomer and dimer calculations, 2014 - 2016

ÇELİK S., Project Supported by Higher Education Institutions, Spectroscopic Identification of the Ancient Glasses

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ÇELİK S., Project Supported by Higher Education Institutions, CONFORMATIONAL PREFERENCES AND STRUCTURAL ELUCIDATION OF BIOLOGICALLY ACTIVE PENTAPEPTIDE, 2014 - 2014

ÇELİK S., Project Supported by Higher Education Institutions, QUANTUM CHEMICAL AND CONFORMATIONAL INVESTIGATION ON HYDROGEN BONDING INTERACTION OF H-GLY-TYR-OH DIMER AT VARIOUS MUTUAL ORIENTATION, 2013 - 2013

ÇELİK S., Project Supported by Higher Education Institutions, Conformational preferences, experimental and theoretical vibrational spectra of cyclo(Gly?Val) dipeptide, 2012 - 2012

ÇELİK S., Project Supported by Higher Education Institutions, CONFORMATIONAL PREFERENCES AND VIBRATIONAL SPECTRA OF GLYCYL-TYROSINE DIPEPTIDE, 2012 - 2012

ÇELİK S., Project Supported by Higher Education Institutions, Conformational Analysis of Cyclo (GLY-LEU): Comparison of Experimental and DFT Vibrational Spectra, 2011 - 2011

## Congress and Symposium Activities

International Conferences on Science and Technology (ICONST- NST-2019), Attendee, Prizren, Kosova, 2019

İstanbul Üniversitesi Fen Fakültesi Fizik Kulübü - 9. Fizik Çalıştayı, Attendee, İstanbul, Turkey, 2019

Protein-Ligand Docking and Molecular Dynamics (MD) Simulations-6th International BAU Drug Design Congress (Workshop), Attendee, İstanbul, Turkey, 2018

2nd International Conference on Innovations in Natural Science and Engineering (ICINSE 2018), Attendee, Kyiv, Ukraine, 2018

2nd International Congress on Advances in Bioscience and Biotechnology (ICABB 2018), Attendee, Podgorica, Serbia And Montenegro, 2018

ADIM Fizik Günleri VII, Attendee, Aydın, Turkey, 2018

İstanbul Üniversitesi Fen Fakültesi Fizik Kulübü - 8. Fizik Çalıştayı, Attendee, İstanbul, Turkey, 2018

Turkish Physical Society 33 th International Physics Congress, Attendee, Muğla, Turkey, 2017

The 25 th Colloquium on High-Resolution Molecular Spectroscopy HRMS 2017, Attendee, Helsinki, Finland, 2017

Adım Fizik Günleri VI, Attendee, Balıkesir, Turkey, 2017

İstanbul Üniversitesi Fen Fakültesi Fizik Kulübü - 7. Fizik Çalıştayı, Attendee, İstanbul, Turkey, 2017

TÜBİTAK 1000 Projeleri AR-GE Strateji Çalıştayı, Attendee, İstanbul, Turkey, 2016

33th European Congress on Molecular Spectroscopy (EUCMOS 2016), Attendee, Szeged, Hungary, 2016

XVI. International Symposium on "Disordered Systems: Theory and Its Applications", Attendee, İstanbul, Turkey, 2016

Adım Fizik Günleri V, Attendee, Eskişehir, Turkey, 2016

İstanbul Üniversitesi Fen Fakültesi Fizik Kulübü - 6. Fizik Çalıştayı, Attendee, İstanbul, Turkey, 2016

Ab initio Modeling in Solid State Chemistry-MSSC2015 (International Summer School), Attendee, İngiltere-Londra, United Kingdom, 2015

9th International Physics Conference of the Balkan Physical Union, Attendee, İstanbul, Turkey, 2015

4th World Conference on Design and Arts - WCDA-2015, Attendee, St. Petersburg, Russia, 2015

2nd International Conference on Global Trends in Pure and Applied Chemical Sciences, Attendee, Hong Kong, Turkey, 2014

Turkish Physical Society 31 th International Physics Congress, Attendee, Muğla, Turkey, 2014

Turkish Physical Society 30 th International Physics Congress, Attendee, İstanbul, Turkey, 2013

15th European Conference on the Spectroscopy of Biological Molecules, Attendee, Oxford, United Kingdom, 2013

Turkish Physical Society 29 th International Physics Congress, Attendee, Muğla, Turkey, 2012

31th European Congress on Molecular Spectroscopy, Attendee, Cluj-Napoca, Romania, 2012

Turkish Physical Society 28 th International Physics Congress, Attendee, Muğla, Turkey, 2011

14th European Conference on the Spectroscopy of Biological Molecules, Attendee, Coimbra, Portugal, 2011

Turkish Physical Society 27 th International Physics Congress, Attendee, İstanbul, Turkey, 2010

30th European Congress on Molecular Spectroscopy, Attendee, Florensa, Italy, 2010

XIII European Conference on the Spectroscopy of Biological Molecules, Attendee, Palermo, Italy, 2009

The International Congress on Spectroscopic Methods for Conservation of Cultural Heritage, Attendee, İstanbul , Turkey, 2007

XXVIII European Congress on Molecular Spectroscopy, Attendee, İstanbul, Turkey, 2006

Workshop on Neutron spin-echo (NSE2005), Attendee, Grenoble, France, 2005