

## Res. Asst. PhD İSMAİL ÇELİK

### Personal Information

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### Education Information

Doctorate, Ankara University, Institute Of Health Sciences, Farmasötik Kimya, Turkey 2014 - 2020

Undergraduate, Erciyes Üniversitesi, Eczacılık Fakültesi, Eczacılık, Turkey 2009 - 2014

### Foreign Languages

English, B2 Upper Intermediate

### Research Areas

Pharmacology and Therapeutics, Pharmaceutical Chemistry

### Academic Titles / Tasks

Research Assistant, Erciyes Üniversitesi, Eczacılık Fakültesi, Eczacılık Meslek Bilimleri , 2015 - Continues

### Articles Published in Journals That Entered SCI, SSCI and AHCI Indexes

- I. **Quantum Mechanical, Virtual Screening, Molecular Docking, Molecular Dynamics, ADME and Antimicrobial Activity Studies of Some New Indole-Hydrazone Derivatives as Potent Agents Against *E. faecalis***  
Erol M., Çelik İ., İnce U., Fatullayev H., Uzunhisarcıklı E., Püsküllü M. O.  
Journal Of Biomolecular Structure & Dynamics, vol.40, pp.1-15, 2022 (Journal Indexed in SCI)
- II. **Synthesis, quantum mechanical calculations, antimicrobial activities and molecular docking studies of five novel 2,5-disubstituted benzoxazole derivatives**  
Temiz-Arpaci O., Zeyrek C. T. , Arisoy M., EROL M., Celik I., Kaynak-Onurdag F.  
Journal of Molecular Structure, vol.1245, 2021 (Journal Indexed in SCI Expanded)
- III. **Antidiabetic bioactive compounds from *Tetrastigma angustifolia* (Roxb.) Deb and *Oxalis debilis* Kunth.: Validation of ethnomedicinal claim by in vitro and in silico studies**  
Junejo J. A. , Zaman K., Rudrapal M., ÇELİK İ., Attah E. I.  
South African Journal of Botany, vol.143, pp.164-175, 2021 (Journal Indexed in SCI Expanded)
- IV. **Synthesis, NMR, X-ray crystallography and DFT studies of some regioisomers possessing imidazole heterocycles**  
PÜSKÜLLÜ M. O. , Doganc F., Ozden S., ŞAHİN E., ÇELİK İ., Goker H.  
Journal of Molecular Structure, vol.1243, 2021 (Journal Indexed in SCI)
- V. **Interactions of the receptor binding domain of sars-cov-2 variants with hACE2: Insights from molecular docking analysis and molecular dynamic simulation**

ÇELİK İ., Yadav R., Duzgun Z., Albogami S., El-Shehawi A. M. , Fatimawali F., Idroes R., Tallei T. E. , Emran T. B. *Biology*, vol.10, no.9, 2021 (Journal Indexed in SCI Expanded)

- VI. **An Analysis Based on Molecular Docking and Molecular Dynamics Simulation Study of Bromelain as Anti-SARS-CoV-2 Variants**  
Tallei T. E. , Fatimawali F., Yelnetty A., Idroes R., Kusumawaty D., Emran T. B. , Yesiloglu T. Z. , Sippl W., Mahmud S., Alqahtani T., et al.  
*Frontiers in Pharmacology*, vol.12, 2021 (Journal Indexed in SCI Expanded)
- VII. **Stability and reactivity study of bio-molecules brucine and colchicine towards electrophile and nucleophile attacks: Insight from DFT and MD simulations**  
Mary Y. S. , Mary Y. S. , Armaković S., Armaković S. J. , Yadav R., ÇELİK İ., Mane P., Chakraborty B.  
*Journal of Molecular Liquids*, vol.335, 2021 (Journal Indexed in SCI)
- VIII. **Molecular modeling, density functional theory, ADME prediction and antimicrobial activity studies of 2-(substituted)oxazolo[4,5- B] pyridine derivatives**  
ÇELİK İ., EROL M., Kuyucuklu G.  
*New Journal of Chemistry*, vol.45, no.25, pp.11108-11118, 2021 (Journal Indexed in SCI)
- IX. **Investigation of reactive properties, adsorption on fullerene, DFT, molecular dynamics simulation of an anthracene derivative targeting dihydrofolate reductase and human dUTPase**  
Mary Y. S. , Mary Y. S. , Armakovic S., Armakovic S. J. , Yadav R., ÇELİK İ., Razavi R.  
*JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS*, 2021 (Journal Indexed in SCI)
- X. **Synthesis, Molecular Docking, Molecular Dynamics, DFT and Antimicrobial Activity Studies of 5-substituted-2-(p-methylphenyl)benzoxazole Derivatives**  
EROL M., ÇELİK İ., Kuyucuklu G.  
*Journal of Molecular Structure*, vol.1234, 2021 (Journal Indexed in SCI)
- XI. **Modeling the structural and reactivity properties of hydrazono methyl-4H-chromen-4-one derivatives-wavefunction-dependent properties, molecular docking, and dynamics simulation studies.**  
Mary Y. S. , Mary Y. S. , Resmi K. S. , Sarala S., Yadav R., Celik İ.  
*Journal of molecular modeling*, vol.27, pp.186, 2021 (Journal Indexed in SCI Expanded)
- XII. **Synthesis, in vitro antiprotozoal activity, molecular docking and molecular dynamics studies of some new monocationic guanidinobenzimidazoles.**  
Doganc F., Celik İ., Eren G., Kaiser M., Brun R., Goker H.  
*European journal of medicinal chemistry*, vol.221, pp.113545, 2021 (Journal Indexed in SCI)
- XIII. **Theoretical investigation on the reactive and interaction properties of sorafenib – DFT, AIM, spectroscopic and Hirshfeld analysis, docking and dynamics simulation**  
Mary Y. S. , Mary Y. S. , Rad A. S. , Yadav R., ÇELİK İ., Sarala S.  
*Journal of Molecular Liquids*, vol.330, 2021 (Journal Indexed in SCI)
- XIV. **Investigation of reactive properties of an antiviral azatricyclo derivative–KDFT, MD and docking simulations**  
Mary Y. S. , Mary Y. S. , Armaković S., Armaković S. J. , Pakosinska-Parys M., Yadav R., ÇELİK İ.  
*Journal of Molecular Structure*, vol.1230, 2021 (Journal Indexed in SCI)
- XV. **DFT, docking, MD simulation, and vibrational spectra with SERS analysis of a benzoxazole derivative: an anti-cancerous drug**  
Sheena Mary Y., Shyma Mary Y., Temiz-Arpaci O., Yadav R., ÇELİK İ.  
*CHEMICAL PAPERS*, 2021 (Journal Indexed in SCI)
- XVI. **Molecular docking, DFT analysis, and dynamics simulation of natural bioactive compounds targeting ACE2 and TMPRSS2 dual binding sites of spike protein of SARS CoV-2**  
Yadav R., Hasan S., Mahato S., ÇELİK İ., Mary Y., Kumar A., Dhamija P., Sharma A., Choudhary N., Chaudhary P. K. , et al.  
*Journal of Molecular Liquids*, 2021 (Journal Indexed in SCI Expanded)
- XVII. **Design, synthesis, molecular docking, density functional theory and antimicrobial studies of some novel benzoxazole derivatives as structural bioisosteres of nucleotides**

- EROL M., ÇELİK İ., Temiz-Arpaci O., Kaynak-Onurdag F., Okten S.  
Journal of Biomolecular Structure and Dynamics, vol.39, no.9, pp.3080-3091, 2021 (Journal Indexed in SCI)
- XVIII. **In silico evaluation of potential inhibitory activity of remdesivir, favipiravir, ribavirin and galidesivir active forms on SARS-CoV-2 RNA polymerase**  
ÇELİK İ., EROL M., Duzgun Z.  
Molecular Diversity, 2021 (Journal Indexed in SCI)
- XIX. **1 H -Benzimidazole-5-carboxamide derivatives: Design, synthesis, molecular docking, DFT and antimicrobial studies**  
EROL M., ÇELİK İ., Temiz-Arpaci O., Goker H., Kaynak-Onurdag F., Okten S.  
New Journal of Chemistry, vol.44, no.48, pp.21309-21317, 2020 (Journal Indexed in SCI)
- XX. **Synthesis, molecular docking and ADME prediction of some new benzimidazole carboxamides derivatives as antimicrobial agents**  
EROL M., ÇELİK İ., Temiz-Arpaci O., Goker H., Kaynak-Onurdag F., Okten S.  
Medicinal Chemistry Research, vol.29, no.11, pp.2028-2038, 2020 (Journal Indexed in SCI)
- XXI. **Antimicrobial and antiproliferative activity studies of some new quinoline-3-carbaldehyde hydrazone derivatives**  
PÜSKÜLLÜ M. O. , ÇELİK İ., EROL M., FATULLAYEV H., UZUNHİSARCIKLI E., Kuyucuklu G.  
Bioorganic Chemistry, vol.101, 2020 (Journal Indexed in SCI)
- XXII. **Approach to the mechanism of action of hydroxychloroquine on SARS-CoV-2: a molecular docking study**  
Celik K., Onay-Besikci A., Ayhan-Kilcigil G.  
JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS, 2020 (Journal Indexed in SCI)
- XXIII. **Synthesis, Molecular Docking, and DFT Studies of Some New 2,5-Disubstituted Benzoxazoles as Potential Antimicrobial and Cytotoxic Agents**  
EROL M., ÇELİK İ., UZUNHİSARCIKLI E., Kuyucuklu G.  
Polycyclic Aromatic Compounds, 2020 (Journal Indexed in SCI)
- XXIV. **Evaluation of Activity of Some 2,5-Disubstituted Benzoxazole Derivatives against Acetylcholinesterase, Butyrylcholinesterase and Tyrosinase: ADME Prediction, DFT and Comparative Molecular Docking Studies**  
ÇELİK İ., EROL M., Temiz Arpacı O., ŞENOL DENİZ F. S. , ERDOĞAN ORHAN İ.  
Polycyclic Aromatic Compounds, 2020 (Journal Indexed in SCI Expanded)
- XXV. **In Vitro and In Silico Studies of Quinoline-2-Carbaldehyde Hydrazone Derivatives as Potent Antimicrobial Agents**  
ÇELİK İ., EROL M., PÜSKÜLLÜ M. O. , UZUNHİSARCIKLI E., İNCE U., Kuyucuklu G., Suzen S.  
Polycyclic Aromatic Compounds, 2020 (Journal Indexed in SCI)
- XXVI. **Design, synthesis and docking studies of benzimidazole derivatives as potential EGFR inhibitors**  
Celik İ., Ayhan-Kilcigil G., Guven B., Kara Z., Gurkan-Alp A. S. , Karayel A., Onay-Besikci A.  
European Journal of Medicinal Chemistry, vol.173, pp.240-249, 2019 (Journal Indexed in SCI)

## Articles Published in Other Journals

- I. **Molecular Docking and Dynamics Simulations Study of Selected Phytoconstituents of "Pangi" (Pangium edule Reinw) Leaf as Anti-SARS-CoV-2**  
Sailah I., Tumilaar S. G. , Lombogia L. T. , Çelik İ., Tallei T. E.  
Philippine Journal of Science, vol.150, no.5, pp.925-937, 2021 (Refereed Journals of Other Institutions)
- II. **2-(p-Florofenil)-5-(2-(4-asetilpiperazin-1-il)asetamido)benzoksazol'ün Sentezi, Moleküler Doking, DFT ve Antimikrobiyal Aktivite Çalışmaları**  
Erol M., Çelik İ., Kuyucuklu G.  
İğdır Üniversitesi Fen Bilimleri Enstitüsü Dergisi, vol.11, no.3, pp.2122-2132, 2021 (National Refreed University Journal)

- III. **MD, DFT Investigations and Inhibition of the Novel SARS- CoV-2 Mainprotease in Three Cocystals of Hydrochloro- thiazide**  
Mary Y. S. , Mary Y. S. , Yadav R., Çelik İ., Rad A. S.  
Analytical Chemistry Letters, vol.11, no.4, pp.450-468, 2021 (Refereed Journals of Other Institutions)
- IV. **Bioactive antidiabetic flavonoids from the stem bark of cordia dichotoma forst.: Identification, docking and ADMET studies**  
Hussain N., Kakoti B. B. , Rudrapal M., Sarwa K. K. , ÇELİK İ., Attah E. I. , Khairnar S. J. , Bhattacharya S., Sahoo R. K. , Walode S. G.  
MolBank, vol.2021, no.2, 2021 (Journal Indexed in ESCI)
- V. **Synthesis, Antimicrobial and Cytotoxic Activity Studies of Some New Benzoxazole Derivatives**  
Erol M., Çelik İ., Kuyucuklu G., Uzunhisarcıklı E.  
Avrupa Bilim ve Teknoloji Dergisi, vol.21, pp.455-462, 2021 (Other Refereed National Journals)
- VI. **Synthesis, antimicrobial and in silico studies of new 2,5-disubstituted benzoxazole derivative**  
Erol M., Çelik İ., Kuyucuklu G.  
Medicine Science, vol.10, no.2, pp.400-408, 2021 (Other Refereed National Journals)

### Books & Book Chapters

- I. **TARGETING EGFR L858R1T790M AND EGFR L858R1T790M/C797S RESISTANCE MUTATIONS IN NON-SMALL CELL LUNG CANCER: CURRENT APPROACHES IN MEDICINAL CHEMISTRY**  
Çelik İ., Kılıçgil G.  
in: Eczacılıkta Yenilikler-3, Gülbin Özçelikay, İlknay Yıldız, Editor, Ankara Üniversitesi, Ankara, pp.249-264, 2020

### Refereed Congress / Symposium Publications in Proceedings

- I. **SYNTHESIS OF SOME CYCLOHEXYL SUBSTITUTED OXADIAZOLE DERIVATIVES LINKED 1H-BENZIMIDAZOLE**  
Çelik İ., Kılıçgil G.  
International Symposium on Pharmaceutical Sciences (ISOPS-12), Ankara, Turkey, 26 June 2018 - 29 May 2019, pp.384-385
- II. **Molecular Docking Studies of Some Novel Benzimidazole Derivatives as EGFR Inhibitors**  
Alp A. S. , Çelik İ., Kılıçgil G.  
International Symposium on Pharmaceutical Sciences (ISOPS-12), Ankara, Turkey, 26 June 2018 - 29 May 2019, pp.400
- III. **SYNTHESIS OF SOME 1H-BENZIMIDAZOLE COMPOUNDS BEARING BIS-THIOSEMICARBAZIDE AND TRIAZOLE DERIVATIVES AS INHIBITORS OF EGFR TYROSINE KINASE**  
Çelik İ., Kılıçgil G., Güven B., Kara Z., Beşikci A.  
International Symposium on Pharmaceutical Sciences (ISOPS-12), Ankara, Turkey, 26 - 29 June 2018, pp.384
- IV. **SYNTHESIS OF SOME 1H-BENZIMIDAZOLES CONTAINING CYCLOHEXYL SUBSTITUTED THIOSEMICARBAZIDES, TRIAZOLES, THIA DIAZOLES AS INHIBITORS OF EGFR TYROSINE KINASE**  
ÇELİK İ., KILCIGİL G., KARA Z., GÜVEN B., BEŞİKÇİ A.  
GPSS2017, 11 - 13 October 2017
- V. **SYNTHESIS OF SOME THIA DIAZOLE/TRIAZOLE LINKED 1H-BENZIMIDAZOLE DERIVATIVES AS INHIBITORS OF EGFR TYROSINE KINASE**  
Çelik İ., Kılıçgil G., Kara Z., Güven B., Beşikci A.  
2nd International Gazi Pharma Symposium Series (GPSS-2017), Ankara, Turkey, 11 - 13 October 2017, pp.249
- VI. **Synthesis of Some 1H-Benzimidazoles as Inhibitors of EGFR Tyrosine Kinase**  
Çelik İ., Kılıçgil G., Beşikci A.  
ICPC 2016 : International Conference on Physical Chemistry, Kobenhavn, Denmark, 27 - 28 June 2016, vol.10, no.6

## VII. The cytotoxic effects of *Chrysophthalmum dichotomum* on A549 and HepG2 cell lines

AYCAN M. B. , DOKUMACI A. H. , AKŞİT A. , ÇELİK İ. , GÜRBÜZ P.

2nd Anticancer Agents Congress, Muğla, Turkey, 23 - 25 April 2014

## Supported Projects

EROL M., PÜSKÜLLÜ M. O. , ÇELİK İ., DEMİRPOLAT E., ARPACI Ö., TUBITAK Project, BENZOKSAZOL YAPISI TAŞIYAN BAZI YENİ BİLEŞİKLERİN TASARIMI, MOLEKÜLER DOCKING ÇALIŞMASI, SENTEZİ İLE EGFR ve VEGFR-2 KINAZ AKTİVİTELERİ ÜZERİNE ETKİLERİNİN DEĞERLENDİRİLMESİ, 2020 - Continues

Uzunhisarcıklı E., Çelik İ., Aycan M. B. , Project Supported by Higher Education Institutions, Virtual Screening ve Moleküler Docking Çalışmaları ile Doğal Yapılı Bileşiklerin Tespiti ve in vitro Alzheimer Modelinde Tau Düzeyi Üzerine Etkilerinin Değerlendirilmesi, 2020 - 2021

Erol M., Çelik İ., Uzunhisarcıklı E., Project Supported by Higher Education Institutions, Bazı Yeni 2,5-Disübstitüe Benzoksazol Türevi Bileşiklerin Sentezi Yapılarının Aydınlatılması ve MCF-7 Hücre Hatında İn Vitro Sitotoksik Etkisinin İncelenmesi, 2020 - 2021

Erol M., Arpacı Ö., Püsküllü M. O. , Demirpolat E., Çelik İ., TUBITAK Project, Benzoksazol Yapısı Taşıyan Bazı Yeni Bileşiklerin Tasarımı, Moleküler Docking Çalışması, Sentezi İle EGFR ve VEGFR-2 Kinaz Aktiviteleri Üzerine Etkilerinin Değerlendirilmesi, 2020 - 2021

Püsküllü M. O. , Erol M., Çelik İ., Fatullayev H., Project Supported by Higher Education Institutions, Yeni Bazı Kinolin 3-Karbaldehit Hidrazon Türevlerinin Sentezi Yapılarının Aydınlatılması Antimikrobiyal Etkilerinin Değerlendirilmesi ve Moleküler Docking Çalışmaları, 2019 - 2020

Erol M., Arpacı Ö., Püsküllü M. O. , Çelik İ., Fatullayev H., Hızlısoy H., Project Supported by Higher Education Institutions, Bazı Yeni Benzoksazol Türevi Bileşiklerin Sentezi, Moleküler Docking Çalışmaları ve Antimikrobiyal Etkilerinin Değerlendirilmesi, 2019 - 2020

PÜSKÜLLÜ M. O. , ÇELİK İ., FATULLAYEV H., Project Supported by Higher Education Institutions, Yeni Bazı Kinolin 3-Karbaldehit Hidrazon Türevlerinin Sentezi, 2019 - 2019

EROL M., ÇELİK İ., FATULLAYEV H., Project Supported by Higher Education Institutions, Bazı Yeni 2-Merkapto Pirimidin Türevlerinin Sentezi, 2019 - 2019

## Scientific Refereeing

COMPUTERS IN BIOLOGY AND MEDICINE, SCI Journal, June 2021

JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS, SCI Journal, February 2021

## Edit Congress and Symposium Activities

2nd International Gazi Pharma Symposium Series (GPSS-2017), Attendee, Ankara, Turkey, 2017

XII. Türk Eczacılık Tarihi Toplantısı, Attendee, Eskişehir, Turkey, 2016

## Citations

Total Citations (WOS):43

h-index (WOS):4

## Scholarships

2211-C Yurt İçi Öncelikli Alanlar Doktora Burs Programı, TUBITAK, 2016 - 2018