

# Prof. RAHİME ŞİMŞEK

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## Education Information

Post Doctorate, Virginia Commonwealth University, School Of Pharmacy, Medicinal Chemistry, United States Of America  
2001 - 2003

Doctorate, Hacettepe University, Sağlık Bilimleri Ens., Farmasötik Kimya, Turkey 1996 - 2000

Postgraduate, Hacettepe University, Sağlık Bilimleri Ens., Farmasötik Kimya, Turkey 1993 - 1996

Undergraduate, Hacettepe University, Eczacılık Fak., Turkey 1988 - 1993

## Dissertations

Doctorate, Kalsiyum modölatör etkili hegzahidrokinolin türevleri üzerinde çalışmalar, Hacettepe Üniversitesi, Eczacılık Fakültesi, Eczacılık Meslek Bilimleri Bölümü, 2000

Postgraduate, 1-açıl-3,5-diaril-2-pirazolin türevleri üzerinde çalışmalar, Hacettepe Üniversitesi, Eczacılık Fakültesi, Eczacılık Meslek Bilimleri Bölümü, 1996

## Research Areas

Health Sciences, Pharmacology and Therapeutics, Professional Sciences, Pharmaceutical Chemistry

## Advising Theses

ŞİMŞEK R., Synthesis of condensed 1,4-dihydropyridine derivatives and evaluation of their calcium channel modulating and antioxidant activities, Doctorate, A.SAMİR(Student), 2014

ŞİMŞEK R., Kondanse 1,4-dihidropiridin türevleri ve kalsiyum kanalları üzerine etileri, Postgraduate, B.BÜLBÜL(Student), 2008

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

- Implication of Toll-Like Receptors in growth and management of health and diseases: Special focus as a promising druggable target to Prostate Cancer**  
Khan S., ŞİMŞEK R., Fuentes J. D. B., Vohra I., Vohra S.  
BIOCHIMICA ET BIOPHYSICA ACTA-REVIEWS ON CANCER, vol.1880, no.1, 2025 (SCI-Expanded)
- Synthesis, crystal structure, spectroscopy and quantum chemical investigations of hexahydroquinoline molecule**

Bülbül H., ÇETİN G., Köysal Y., ŞİMŞEK R., YILDIRIM S., Tanak H., Butcher R. J.

Molecular Physics, 2024 (SCI-Expanded)

III. **Exploring novel fluorine-rich fuberidazole derivatives as hypoxic cancer inhibitors: Design, synthesis, pharmacokinetics, molecular docking, and DFT evaluations**

Taj M. B., Raheel A., Ayub R., Alnajeebi A. M., Abualnaja M., Habib A. H., Alelwani W., Noor S., Ullah S., Al-Sehemi A. G., et al.

PLoS ONE, vol.18, no.2 February, 2023 (SCI-Expanded)

IV. **Neurological Effects of SARS-CoV-2 and Neurotoxicity of Antiviral Drugs Against COVID-19**

Ünlü B., Simsek R., Köse S. B. E., Yirün A., Erkekoglu P.

MINI-REVIEWS IN MEDICINAL CHEMISTRY, vol.22, no.2, pp.213-231, 2022 (SCI-Expanded)

## Articles Published in Other Journals

- I. **Toxicity of serotonin-norepinephrine reuptake inhibitors (SNRIs) during pregnancy and lactation**  
Canitez G., ŞİMŞEK R., ÇAKIR D. A., Yalcin H., BAYDAR T., ERKEKOĞLU Ü. P.  
ISTANBUL JOURNAL OF PHARMACY, no.2, pp.255-267, 2024 (ESCI)
- II. **Migraine and Its Treatment from the Medicinal Chemistry Perspective**  
Pehlivanlar E., Carradori S., ŞİMŞEK R.  
ACS Pharmacology and Translational Science, vol.7, no.4, pp.951-966, 2024 (ESCI)
- III. **Syntheses, characterizations, crystal structures and Hirshfeld surface analyses of methyl 4-[4-(difluoro-methoxy)phenyl]-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate, isopropyl 4-[4-(difluoromethoxy)phenyl]-2,6,6-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate and tert-butyl 4-[4-(difluoromethoxy)phenyl]-2,6,6-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate**  
Yıldırım S. Ö., AKKURT M., Pehlivanlar E., ÇETİN G., ŞİMŞEK R., Butcher R. J., Bhattarai A.  
Acta Crystallographica Section E: Crystallographic Communications, vol.80, pp.281-288, 2024 (ESCI)
- IV. **Synthesis, characterization, crystal structure and Hirshfeld surface analysis of isobutyl 4-[4-(difluoromethoxy)phenyl]-2,6,6-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate**  
Yıldırım S. Ö., AKKURT M., ÇETİN G., ŞİMŞEK R., Butcher R. J., Bhattarai A.  
Acta Crystallographica Section E: Crystallographic Communications, vol.79, no.Pt 12, pp.1132-1136, 2023 (ESCI)
- V. **Synthesis, crystal structure and Hirshfeld surface analysis of tert-butyl 4-[4-(difluoromethoxy)phenyl]-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate**  
Pehlivanlar E., Yıldırım S. Ö., ŞİMŞEK R., AKKURT M., Butcher R. J., Bhattarai A.  
Acta Crystallographica Section E: Crystallographic Communications, vol.79, pp.664-668, 2023 (ESCI)
- VI. **Crystal structure and Hirshfeld surface analysis of isopropyl 4-[2-fluoro-5-(trifluoromethyl)phenyl]-2,6,6-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate**  
Yıldırım S. Ö., AKKURT M., ÇETİN G., ŞİMŞEK R., Butcher R. J., Bhattarai A.  
Acta Crystallographica Section E: Crystallographic Communications, vol.79, no.Pt 3, pp.187-191, 2023 (Scopus)
- VII. **Synthesis, characterization, crystal structure and Hirshfeld surface analysis of a hexahydroquinoline derivative: tert-butyl 4-([1,1'-biphenyl]-4-yl)-2,6,6-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate**  
Yıldırım S. Ö., AKKURT M., ÇETİN G., ŞİMŞEK R., Butcher R. J., Bhattarai A.  
ACTA CRYSTALLOGRAPHICA SECTION E-CRYSTALLOGRAPHIC COMMUNICATIONS, vol.78, pp.798-821, 2022 (ESCI)

## Refereed Congress / Symposium Publications in Proceedings

- I. **Experimental and Molecular Modeling Investigation of Isopropyl 4-(Biphenyl-4-Yl)-2,6,6-Trimethyl-5-Oxo-1,4,5,6,7,8-Hexahydroquinoline-3-Carboxylate**  
Yıldırım S. Ö., ÇETİN G., BÜYÜKMUMCU Z., ŞİMŞEK R., Safak C., Butcher R. J., Pakdur O. S.

33rd International Physics Congress of the Turkish-Physical-Society (TPS), Bodrum, Turkey, 6 - 10 September 2017, vol.1935

## II. Antimicrobial Screening of 1 4 Dihydropyridine Derivatives

EKİZOĞLU M., GÜNDÜZ M. G., KART D., ŞİMŞEK R., ŞAFAK O. C.

4th International Meeting on Medicinal and Pharmaceutical Chemistry-6th International Symposium on Pharmaceutical Chemistry Joint Meeting, 30 September - 02 October 2010

## Supported Projects

ŞİMŞEK R., ERKEKOĞLU Ü. P., ÇETİN G., YİRÜN A., ORAL D., BALCI A., Project Supported by Higher Education Institutions, Yeni Hekzahidrokinolin Türevlerinin Sentezi Karakterizasyonu Dönüştürücü Büyüme Faktörü-Beta (TGF-beta) ve İnflamasyon Mediyatörlerine İnhibitör Etkilerinin İn Vitro ve İn Silico Olarak İncelenmesi, 2020 - 2022

KOCAEFE Y. Ç., ÖZDEMİR SAKA C., ŞİMŞEK R., BORA G., DÖKMECİ S., Project Supported by Higher Education Institutions, Mezenkimal dokularda TGFB1 ve IGF1 faktörlerinin bir epigenetik düzenleyici olarak Klf5 kontrolündeki rolünün araştırılması, 2018 - 2021

ŞİMŞEK R., ŞAFAK O. C., GÜNDÜZ M. G., ÇETİN G., Project Supported by Higher Education Institutions, Alkil 2,6,6(2,7,7)-trimetil-4-(bifenil)-5-okso-1,4,5,6,7,8-hekzahidrokinolin 3-karboksilat türevlerinin sentezi ve karakterizasyonu, 2017 - 2018

GÜNDÜZ M. G., ÇETİN G., ŞİMŞEK R., ŞAFAK O. C., Project Supported by Higher Education Institutions, L-Tipi Kalsiyum Kanal Blokörü Kondanse 1,4-Dihidropiridin Türevlerinin Mikrodalga Yardımıyla Sentezi, 2016 - 2017

ŞİMŞEK R., Project Supported by Higher Education Institutions, BOSS XV 15 Belçika Organik Sentez Sempozyumu, 2016 - 2016

ŞAFAK O. C., ŞİMŞEK R., GÜNDÜZ M. G., EKİZOĞLU M., Baydar E., Project Supported by Higher Education Institutions, Kondanse 14Dihidropiridin Türevlerinin Sentezi ile Antimikrobiyal ve Antioksidan Etkileri Üzerinde Çalışmalar, 2016 - 2016

ŞİMŞEK R., KÜRKÜOĞLU B., Project Supported by Higher Education Institutions, Hacettepe Üniversitesi Medya İletişim ve Tanıtım Koordinatörlüğü Altyapı Geliştirme Projesi, 2015 - 2016

ŞİMŞEK R., Project Supported by Higher Education Institutions, Kondanse 1,4-Dihidropiridin Türevlerinin Sentezi, Kalsiyum Nodulatör Etkilerinin ve Antioksidan Özelliklerinin Araştırılması, 2013 - 2016

ŞİMŞEK R., Project Supported by Higher Education Institutions, Sentetik Kimya 2015, Orta Vadede Yükselen Hedefler ve Moleküller, 2015 - 2015

ŞİMŞEK R., Project Supported by Higher Education Institutions, Hacettepe Üniversitesi Ulusal ve Uluslararası Tanıtım Etkinliklerinin Yeniden Düzenlenmesi, 2014 - 2015

ŞİMŞEK R., TUBITAK Project, Kalsiyum Kanal Modulatör Etkili Kondanse 1 4 Dihidropiridin Türevleri, 2013 - 2014

## Metrics

Publication: 69

Citation (WoS): 579

Citation (Scopus): 732

H-Index (WoS): 13

H-Index (Scopus): 14

## Non Academic Experience

Virginia Commonwealth University