Prof. SAFİYE ERDEM

Personal Information

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Education Information

Postgraduate, Villanova University, College Of Liberal Arts And Sciences, Kimya Bölümü, United States Of America 1986 - 1988
Undergraduate, Bogazici University, Faculty Of Arts And Scıences, Department Of Chemıstry, Turkey 1980 - 1985

Foreign Languages

English, C1 Advanced

Dissertations

Postgraduate, Dimerization of water soluble metalloporphyrins, Villanova University, 1988

Research Areas

Natural Sciences

Academic Titles / Tasks

Professor, Marmara University, Faculty of Arts and Sciences, Chemistry, 2008 - Continues
Associate Professor, Marmara University, Faculty of Arts and Sciences, Chemistry, 2002 - 2008
Assistant Professor, Marmara University, Faculty of Arts and Sciences, Chemistry, 1999 - 2002
Lecturer, Bogazici University, Faculty Of Arts And Scıences, Department Of Chemıstry, 1997 - 1999
Research Assistant, Bogazici University, Faculty Of Arts And Scıences, Department Of Chemıstry, 1992 - 1997
Research Assistant, Villanova University, College Of Liberal Arts And Sciences, Kimya, 1986 - 1988

Academic and Administrative Experience

Marmara University, Faculty of Arts and Sciences, Chemistry, 2013 - Continues
Marmara University, Faculty of Arts and Sciences, 2013 - Continues

Marmara University, Faculty of Arts and Sciences, 2010 - Continues
Marmara University, Faculty of Arts and Sciences, Chemistry, 2005 - 2015
Marmara University, Faculty of Arts and Sciences, Chemistry, 2010 - 2013
Marmara University, Faculty of Arts and Sciences, Chemistry, 2009 - 2010
Marmara University, Institute for Graduate Studies in Pure and Applied Sciences, 2008 - 2010
Marmara University, Faculty of Arts and Sciences, Chemistry, 2008 - 2009
Marmara University, Faculty of Arts and Sciences, Chemistry, 1999 - 2001

Advising Theses

Erdem S., Danış Ö., Arilkumarin türevlerinin beta-laktamaz ve karbapenemaz aktivitesi üzerine etkilerinin incelenmesi, Postgraduate, B.Hamur(Student), 2019
ERDEM S., Flavoenzimlerdeki flavin oksidasyonu mekanizmasının hesapsal modellenmesi, Postgraduate, İ.Demir(Student), 2017
ERDEM S., Flavin redoks tepkimesine sübstitüent etkisinin modellenmesi, Postgraduate, A.Topal(Student), 2017
ERDEM S., Computational and mechanistic studies on the formation of cyclic systems, Doctorate, Ö.SARI(Student), 2017
ERDEM S., Monoamin oksidaz (mao) enzimlerinin hidrür transferi mekanizması tek basamaklı mı çok basamaklı mıdır?, Postgraduate, K.Çakır(Student), 2016
ERDEM S., Asimetrik aldol tepkimeleri için yeni bir katalizör: Homoboroprolin'in asimetrik katalizör etkisinin modellenmesi, Postgraduate, H.DÜLGER(Student), 2016
ERDEM S., Computational modelling of axial chirality of 2-arylimino-3- arylthiazolidine isomers, Postgraduate, G.Sabuncu(Student), 2014
ERDEM S., Erdem S., Monoamin oksidaz (MAO)inhibitör etkili yeni pirazolin türevleri ile moleküler doking, Postgraduate, S.Türkkan(Student), 2013
ERDEM S., Mao inhibitörleri ile akılcı ilaç tasarımına yönelik qsar analizi, Doctorate, M.Köktürk(Student), 2013
ERDEM S., Hidrazon türevi mao inhibitörleri ile akılcı ilaç tasarımına yönelik qsar analizi, Postgraduate, O.Aydın(Student), 2011
ERDEM S., Polihalojenlenmiş nitrobütadienlerin aromatik aminlerle verdiği reaksiyon mekanizmalarının hesapsal olarak modellenmesi, Postgraduate, Ö.Sarı(Student), 2011
ERDEM S., erdem S., Experimental and computational studies of interactions between small molecules and DNA, Postgraduate, M.Biçen(Student), 2011
ERDEM S., MAO A enziminin aktif bölgesinin ONIOM yöntemi ile modellenmesi, Doctorate, V.Enisoğlu(Student), 2010
ERDEM S., Monoamin oksidaz enzimi için önerilen biradikal mekanizma ile ilgili yapı-aktiflik incelemeleri, Postgraduate, B.Büyükmenekşe(Student), 2009
ERDEM S., Klioksalinon-n-oksitlerin senteziyle ilgili reaksiyon mekanizmalarının hesapsal modellenmesi, Doctorate, G.Altınbaş(Student), 2008
ERDEM S., Fulven türevlerinin aromatikliğinin nics yöntemi ile araştırılması, Postgraduate, R.Keleş(Student), 2007
ERDEM S., Para-sübstitüe benzilaminlerin monoamin oksidaz ile tepkimelerinde yapı-aktiflik ilişkisinin incelenmesi, Postgraduate, O.Can(Student), 2007
ERDEM S., Monoamin oksidaz substratlarının enzimin aktif bölgesi içinde QM/MM yöntemi ile modellenmesi, Postgraduate, M.Ali(Student), 2007
ERDEM S., Mao enziminin oksazolidinon ve benzeri heterosiklik bileşikler ile inhibisyonunun kimyasal modellenmesi, Postgraduate, Ü.Boz(Student), 2006
ERDEM S., 2-Asetoksi-2,6,6-trimetilbisiklo [3.1.0] hekzan'ın termal proliz mekanizmasının modellenmesi, Postgraduate, F.Uyar(Student), 2005
ERDEM S., Monoamin oksidaz inhibisyonu ile ilişkili model amin bileşiklerinin koformasyonel analizi, Postgraduate, A.Kırsakal(Student), 2005
ERDEM S., Application of the characteristic root index model to the estimation of physico-chemical and biological properties of selected endocrine disrupting chemicals, Postgraduate, M.ÖZKUL(Student), 2005
ERDEM S., C=N bağını içeren bazı bileşiklerin singlet oksijen reaksiyonları ile önerilen mekanizmaların hesapsal

incelenmesi, Postgraduate, A.GENÇÇAKIR(Student), 2004
ERDEM S., Erdem S., Monoamin oksidaz (MAO) enziminin aminleri oksitleme mekanizmasının hesapsal yöntemlerle incelenmesi, Postgraduate, Ö.Karahan(Student), 2004
ERDEM S., Mono Amin Oksidaz (MAO) enziminin ekleme eliminasyon mekanizmasının hesapsal yöntemlerle incelenmesi, Postgraduate, İ.Yıldız(Student), 2003
ERDEM S., 2-Sübstitüe-Metiltiyoetilamin türevlerinin konformasyonel analizi, Postgraduate, M.Durmuş(Student), 2003
ERDEM S., Fulven türevlerinin kararlılığı ve sübstitüent etkisi, Postgraduate, S.Atalay(Student), 2002

Published journal articles indexed by SCI, SSCI, and AHCI

I. **Novel methoxyphenylthio-substituted phthalocyanines: synthesis, characterization, proton-transfer, and acid-sensing properties**
Ağcaabat R., Seslikaya C., FINDIK V., ERDEM S., ODABAŞ Z.
New Journal of Chemistry, vol.48, no.4, pp.1623-1633, 2024 (SCI-Expanded)

II. **In vitro and in silico investigation of inhibitory activities of 3-arylcoumarins and 3-phenylazo-4-hydroxycoumarin on MAO isoenzymes**
Yuce-Dursun B., Danış Ö., Ozalp L., Sahin E., Demir S., Erdem S., Ogan A.
STRUCTURAL CHEMISTRY, vol.34, no.5, pp.1715-1729, 2023 (SCI-Expanded)

III. **New Horizon in Phospha-Michael Reaction: Ultrafast Double Addition of P-H Bond-Bearing Nucleophiles to Electron-Deficient Triple Bonds and Its Use for Functional Monomer Synthesis and Polymer Modification**
Sagdic G., Daglar O., ÇAKMAKÇI E., FINDIK V., ERDEM S., Tunca Ü., Günay U. S., Durmaz H.
Macromolecules, vol.56, no.17, pp.7006-7022, 2023 (SCI-Expanded)

IV. **Cheminformatics and Machine Learning Approaches to Assess Aquatic Toxicity Profiles of Fullerene Derivatives**
Fjodorova N., Novič M., Venko K., Rasulev B., Türker Saçan M., Tugcu G., Sağ Erdem S., Toropova A. P., Toropov A. A.
International Journal of Molecular Sciences, vol.24, no.18, 2023 (SCI-Expanded)

V. **Identification of some novel amide conjugates as potent and gastric sparing anti-inflammatory agents: In vitro, in vivo, in silico studies and drug safety evaluation**
KULABAŞ N., Set İ., Aktay G., GÜRSOY Ş., DANIŞ Ö., OGAN A., Sağ Erdem S., Erzincan P., Helvacıoğlu S., Hamitoğlu M., et al.
Journal of Molecular Structure, vol.1285, 2023 (SCI-Expanded)

VI. **Stable hemiaminals from axially chiral pyridine compounds**
Tuncel S. T., Demir I., ERDEM S., Dogan I.
Chirality, vol.35, no.6, pp.365-375, 2023 (SCI-Expanded)

VII. **A QSAR study to predict the survival motor neuron promoter activity of candidate diaminoquinazoline derivatives for the potential treatment of spinal muscular atrophy**
Sabuncu Gürses G., ERDEM S., Saçan M.
SAR and QSAR in environmental research, vol.34, no.3, pp.247-266, 2023 (SCI-Expanded)

VIII. **Mechanistic Investigation of Lysine-Targeted Covalent Inhibition of PI3K delta via ONIOM QM:QM Computations**
FINDIK V., Gercik B. T. V., Sinek O., ERDEM S., Ruiz-Lopez M. F.
JOURNAL OF CHEMICAL INFORMATION AND MODELING, vol.62, no.24, pp.6775-6787, 2022 (SCI-Expanded)

IX. **Newly synthesized piperazine derivatives as tyrosinase inhibitors: in vitro and in silico studies**
DOKUZPARMAK Ç., ÖZ TUNCAY F., Ozdemir S. B., Kurnaz B., Demir I., ÇOLAK A., ERDEM S., YILDIRIM N.
JOURNAL OF THE IRANIAN CHEMICAL SOCIETY, vol.19, no.7, pp.2739-2748, 2022 (SCI-Expanded)

X. **How fullerene derivatives (FDs) act on therapeutically important targets associated with diabetic diseases**
Fjodorova N., Novic M., Venko K., Drgan V., Rasulev B., SAÇAN M., ERDEM S., Tugcu G., Toropova A. P., Toropov A. A.
COMPUTATIONAL AND STRUCTURAL BIOTECHNOLOGY JOURNAL, vol.20, pp.913-924, 2022 (SCI-Expanded)

XI. **A Bifunctional B,N-Based Asymmetric Catalytic Nitrostyrene-Michael Addition Acting through a 10-Membered Ring Cyclic Transition State**
Du Y., Sari O., ERDEM S., Whiting A.
HELVETICA CHIMICA ACTA, vol.104, no.12, 2021 (SCI-Expanded)

XII. **Mechanistic insights into lysine-targeting covalent inhibition through a theoretical study of ester aminolysis**
FINDIK V., Ruiz-Lopez M. F., ERDEM S.
ORGANIC & BIOMOLECULAR CHEMISTRY, vol.19, no.45, pp.9996-10004, 2021 (SCI-Expanded)

XIII. **Synthesis of hydrazine containing piperazine or benzimidazole derivatives and their potential as a-amylase inhibitors by molecular docking, inhibition kinetics and in vitro cytotoxicity activity studies**
Cakmak U., ÖZ TUNCAY F., Basoglu-Ozdemir S., AYAZOĞLU DEMİR E., Demir I., ÇOLAK A., ÇELİK UZUNER S., ERDEM S., YILDIRIM N.
MEDICINAL CHEMISTRY RESEARCH, vol.30, no.10, pp.1886-1904, 2021 (SCI-Expanded)

XIV. **Insight into the Thiol-yne Kinetics via a Computational Approach**
FINDIK V., Varinca B. T., DEĞİRMENCİ İ., ERDEM S.
JOURNAL OF PHYSICAL CHEMISTRY A, vol.125, no.17, pp.3556-3568, 2021 (SCI-Expanded)

XV. **Synthesis of Benzoxazole-2-carboxylate Derivatives: Electronic- and Position-effect of Functional Groups and Computational Modeling of the Selectivity for Oxazole Ring**
Kuzu B., SARI Ö., ERDEM S., ALGÜL Ö., Mengeş N.
CHEMISTRYSELECT, vol.6, no.10, pp.2529-2538, 2021 (SCI-Expanded)

XVI. **One-pot synthesis of oxazolidinones and five-membered cyclic carbonates from epoxides and chlorosulfonyl isocyanate: theoretical evidence for an asynchronous concerted pathway**
Demir E., SARI Ö., ÇETİNKAYA Y., ATMACA U., ERDEM S., ÇELİK M.
BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY, vol.16, pp.1805-1819, 2020 (SCI-Expanded)

Refereed Congress / Symposium Publications in Proceedings

I. **ANTIOXIDANT AND ANTI-COLLAGENASE ACTIVITY OF ST. JOHN'S WORT (HYPERICUM PERFORATUM L.)**
YILDIZ İ., Özalp L., ERDEM S., MOUTSİNGA E. G. B. K., DANIŞ Ö., OGAN A.
3. INTERNATIONAL MARMARA SCIENTIFIC RESEARCH AND INNOVATION CONGRESS 19-20 NOVEMBER 2022 İSTANBUL/ TURKE, İstanbul, Turkey, 19 November 2022, vol.1

II. **Etakrinik Asit Oxidazol Türevlerinin Glutatiyon S-transferazİnhibisyonu Üzerine Moleküler Doking Çalışması**
FINDIK V., ERDEM S.
30. ULUSAL KİMYA KONGRESİ, Turkey, 5 - 08 November 2018

III. **Tiyol-en Tepkimelerinin Bölgeseçici HalkalaşmaReaksiyonuna Hesapsal Bir Yaklaşım**
SİNEK Ö., FINDIK V., ERDEM S.
30. ULUSAL KİMYA KONGRESİ, Turkey, 5 - 08 November 2018

IV. **Tiyol-in Reaksiyon Mekanizmalarının Teorik Olarakİncelenmesi**
VARINCA B. T., FINDIK V., ERDEM S.
30. ULUSAL KİMYA KONGRESİ, Turkey, 5 - 08 November 2018

V. **Tiyil Radikali ve Alkenler Arasında Gerçekleşen BölgeseçiciHalkalaşma Reaksiyonuna Hesapsal Yaklaşım**
SERT E. M., FINDIK V., ERDEM S.
30. ULUSAL KİMYA KONGRESİ, Turkey, 5 - 08 November 2018

VI. **Monoamin Oksidaz Kataliz Mekanizmasının KuvantumÖbeği ve ONIOM Yöntemleri İle Bütünleşik Modellenmes**
ERDEM S., ÇAKIR K., ENGİN H.
30. ULUSAL KİMYA KONGRESİ, Turkey, 5 - 08 November 2018

VII. **In vitro and In silico Investigation of Tyrosinase Inhibition By Some Novel Triazole Derivative Compounds Containing Fluoroquinolone Skeleton**
KURNAZ B., ÇOLAK A., ÖZDEMİR S. B., DEMİRBAŞ N., DEMİR İ., ERDEM S.
1.Euroasia Biochemical Approaches Technologies Congress, 27 - 30 October 2018

VIII. **Molecular Dynamics and Docking Simulations on the Formate Dehydrogenase Enzymes**
FINDIK V., ÇAKAR M. M., ERDEM S., BİNAY B.
1.Euroasia Biochemical Approaches Technologies Congress, 27 - 30 October 2018

IX. **In Silico Investigation on Anti-Depression Effects of Hypericum Perforatum Flavanoids: Molecular Docking with Monoamin Oxidases**
YILDIZ İ., ERDEM S., OGAN A.
1.Euroasia Biochemical Approaches Technologies Congress, 27 - 30 October 2018

X. **Molecular Docking of New Hybrid Triazole Derivatives into Tyrosinase Enzyme**
DEMİR İ., ERDEM S., ÇOLAK A., DEMİRBAŞ N.
1.Euroasia Biochemical Approaches Technologies Congress, 27 - 30 October 2018

XI. **The effect of substituents on Phthalocyanine-DNA binding: molecular dynamics and docking studies**
ÖZALP L., ERDEM S., ÖZBİL M.
International conference on applied mathematics, modeling and Life Sciences, 3 - 05 October 2018

XII. **In slico modelling on fish toxicity of Pharmaceuticals**
EMİNOĞLU E. M., SAÇAN M., ERDEM S.
International conference on applied mathematics, modeling and Life Sciences, 3 - 05 October 2018

XIII. **Modelling the catalytic and inhibition mechanisms of monoamine oxidase: A combined ONIOM and quantum cluster approach**
ERDEM S.
International conference on applied mathematics, modeling and life Sciences, 3 - 05 October 2018

XIV. **Nontarget binding of canabinoids in central nervous system: molecular docking with monoamine oxidases**
DERVİŞOĞLU C., ERDEM S.
International conference on applied mathematics, modeling and life Sciences, 3 - 05 October 2018

XV. **Revisiting Fish Toxicity of Active Pharmaceutical Ingredients:Mechanistic Insights from Integrated Ligand-/Structure-basedAssessments on Acetylcholinesterase**
SAÇAN M., Minovski N., Eminoğlu E. M., ERDEM S., Novic M.
18th International Conference on QSAR in Environmental and Health Sciences, 11 - 15 June 2018

XVI. **Molecular dynamics and docking studies on theinteractions of DNA with quaternary metallo phthalocyanines**
ÖZALP L., ERDEM S., ÖZBİL M.
International Symposium on Chemistry Via Computation Applications on Molecular Nanoscience, 30 October 2017

XVII. **Synthesis of stable tetrahedral intermediates(hemiaminals) and kinetics of their conversion to thiazol-2-imines**
GÜNAL Ş. E., GÜRSES G. S., ERDEM S., DOĞAN H. İ.
International Symposium on Chemistry Via Computation Applications on Molecular Nanoscience, 30 October 2017

XVIII. **Mechanistic dft study on the function of homoboroprolineas asymmetric catalyst in enantioselective aldol reactions**
ERDEM S., DÜLGER H., DEMİREL N.
International Symposium on Chemistry Via Computation Applications on Molecular Nanoscience, 30 October 2017

XIX. **Mechanistic DFT study on one-pot synthesis of heterocyclic compounds**
atbakar m., ERDEM S., ÖCAL SUNGUROĞLU Z. N., erden i.
International Symposium on Chemistry V A Computation Applications on Molecular Nanoscience, 30 October 2017

XX. **Molecular docking of arylcoumarins to carbapenemaseenzyme**
ERDEM S., HAMUR B., DANIŞ Ö.
International Symposium on Chemistry Via Computation Applications on Molecular Nanoscience, 30 October 2017

XXI. **A combined experimental and theoretical study for the formation of indolizine,**

pyrrolo[1,2,a]pyrazine, pyrrolo[1,2-a]pyrazinone
SARI Ö., MENGEŞ N., ERDEM S., BALCI M.
Chemistry ViA Computation – International Symposium on Chemistry ViA Computation Applications on Molecular Nanoscience, 30 - 31 October 2017

XXII. **Synthesis of stable tetrahedral intermediates (hemiaminals) andkinetics of their conversion to thiazol-2-imines**
EROL GÜNAL Ş., sabuncu gürses g., ERDEM S., DOĞAN H. İ.
International Symposium on Chemistry via Computation applications on Molecular Nanoscience, 30 October 2017

XXIII. **Novel Chiral Monoamine Oxidase Inhibitors: Molecular Docking Studies on N-aryloxazolidinedionees**
YÜCE DURSUN B., ERDEM S., GÖKHAN KELEKÇİ N., DOĞAN H. İ., EROL Ş.
5th International BAU Drug Design Congress, 19 October 2017 - 21 January 2018

XXIV. **Novel Chiral Monoamine Oxidase Inhibitors: Molecular Docking Studies on N-Aryloxazolidinediones**
YÜCE DURSUN B., ERDEM S., GÖKHAN KELEKÇİ N., DOĞAN H. İ., Erol Günal Ş.
5th International BAU Drug Design Congress, 19 - 21 October 2017

XXV. **Potansiyel Karbapenemaz İnhibitörü Arilkumarin Türevleri ile Moleküler Doking Hesapları**
HAMUR B., ERDEM S.
3. Hesaplamalı Kimya Kongresi, Turkey, 12 - 14 October 2017

XXVI. **Flavinin re-Yüzünden Oksidasyon Mekanizmasının Hesapsal Modellenmesi**
DEMİR İ., ERDEM S.
3. Hesaplamalı Kimya Kongresi, 12 - 14 October 2017

XXVII. **DFT computations on the mechanism of flavinoxidative half-reaction**
ERDEM S., DEMİR İ.
11the European Conference on Theoretical and Computational Chemistry, 4 - 07 September 2017

XXVIII. **Substituent effect on the reduction tendency andconformation of flavin ring: a DFT study**
ERDEM S., TOPAL A.
11the European Conference on Theoretical and Computational Chemistry, 4 - 07 September 2017

XXIX. **Enzim Kataliz Mekanizmaları ile Rasyonel İlaç Tasarımı: Monoamin Oksidaz Enziminin Kovalent Geri-dönüşümlü İnhibisyonu**
ERDEM S.
5. İlaç Kimyası: İlaç Etkin Maddesi Tasarımı, Sentezi,Üretimi ve Standardizasyonu Kongresi, 30 March - 02 April 2017

XXX. **Flavinin si-Yüzünden Oksidasyon Mekanizmasının Hesapsal Modellenmesi**
DEMİR İ., ERDEM S.
5. İlaç Kimyası: İlaç Etkin Maddesi Tasarımı, Sentezi,Üretimi ve Standardizasyonu Kongresi, 30 March - 02 April 2017

XXXI. **In Silico Modelling of DNA Quaternized Metallophthalocyanine Binding M Zn Ni Cu**
Özalp L., ERDEM S., YÜCE DURSUN B.
4. BAU DRUG DESIGN Congress, İstanbul, Turkey, 13 - 15 October 2016

XXXII. **A Hybrid Proton and Hydride Transfer Mechanism for the Serotonin Oxidation of Monoamine Oxidase A**
Çakır K., ERDEM S., ENİSOĞLU ATALAY V., Dülger H.
4. BAU DRUG DESIGN Congress, 13 - 15 October 2016

XXXIII. **Synthesis anti inflammatory activity and molecular modeling studies on cox 1 and cox 2 inhibition of novel amide conjugates of some NSAIDs**
kulabaş n., Gürsoy Ş., Erzincan P., YÜCE DURSUN B., AKTAY G., ERDEM S., OGAN A., Küçükgüzel İ.
17th Tetrahedron Symposium, 28 Haziran-1 Temmuz 2016, Barselona, Spain, 28 June - 01 July 2016

XXXIV. **Synthesis anti inflammatory activity and molecular modeling studies on cox 1 and cox 2 inhibition of novel amide conjugates of some NSAIDs**
KULABAŞ N., GÜRSOY Ş., ERZİNCAN P., YÜCE DURSUN B., AKTAY G., ERDEM S., OGAN A., KÜÇÜKGÜZEL İ.
17th TETRAHEDRON SYMPOSIUM : Challenges in Biological, Bioorganic & Medicinal Chemistry, Sitges, Spain, 28 June - 01 July 2016

XXXV. **QSAR for Butyrylcholine Esterase BuChE Inhibition by Substituted Pyridylene hydrazone Derivatives**
ERDEM S., SAÇAN M., Çomak H.
17th International Conference on QSAR in Environmental and Health Sciences (QSAR 2016), Miami, United States Of America, 13 - 17 June 2016

XXXVI. **In Silico Approach to Monoamine Oxidase A Inhibitory Potential of New Coumarine Derivatives**
Erzincan P., Erdem S., Saçan M., Yüce Dursun B., Danış Ö., Demir S., Ogan A.
. 17th International Conference on QSAR in Environmental and Health Sciences (QSAR 2016), Florida, United States Of America, 13 - 17 June 2016

XXXVII. **QSAR Approach to Acetylcholine Esterase AChE Inhibitory Potential of Rasagiline and Selegiline Related Carbamate Derivatives**
ERDEM S., SAÇAN M.
17th International Conference on QSAR in Environmental and Health Sciences (QSAR 2016), Miami, United States Of America, 13 - 17 June 2016

XXXVIII. **ZnIIFtalosiyanin Türevinin DNA Bağlanma Özelliklerinin in vitro vein siliko Yöntemlerle İncelenmesi**
YÜCE DURSUN B., ÖZALP L., BAŞAK A. S., ERDEM S.
2. Bilgisayar Destekli İlaç Tasarımı Uygulamalı Kursu, Turkey, 16 - 17 May 2016

XXXIX. **Farmasötik Bileşiklerin Toksisitelerinin Torpedo californica ACHE İnhibisyonu ile İlişkisi**
EMİNOĞLU E. M., ERDEM S., SAÇAN M.
2. Bilgisayar Destekli İlaç Tasarımı Uygulamalı Kursu, Turkey, 16 - 17 May 2016

XL. **Yüksek Antioksidan Aktiviteye Sahip Yeni Kumarin Türevleri ile Kantitatif Yapı Aktivite İlişkileri ve Moleküler Doking**
ERDEM S.
4. İlaç Kimyası: İlaç Etkin Maddesi Tasarımı, Sentezi, Üretimi veStandardizasyonu Kongresi, Turkey, 17 - 20 March 2016

XLI. **In Silico Design of Potent Coumarin Derivatives for Treatment of Neurodegenerative Diseases**
ERDEM S.
COST Action CM1103 Final Meeting, 21 - 23 October 2015

XLII. **Molecular Modeling Studies on COX 1 and COX 2 Inhibition of Novel Amide Conjugates of Some NSAIDs with Anti inflammatory Activity**
KULABAŞ N., ERZİNCAN P., DANIŞ Ö., ERDEM S., OGAN A., KÜÇÜKGÜZEL İ.
International Symposium on Drug Research & Development, Turkey, 15 - 17 October 2015

XLIII. **Effect of active site residues and water molecules in amine oxidation mechanism of monoamine oxidase A quantum cluster approach**
ERDEM S., ÇAKIR K., ENGİN H., ENİSOĞLU ATALAY V., DÜLGER H.
10th European Conference on Computational Chemistry, 31 August - 03 September 2015

XLIV. **3 Aril Kumarin Türevlerinin Sentezi Ve İnsan Monoamin Oksidaz A Ve B İnhibitörleri Olarak Etkilerinin İncelenmesi**
YÜCE DURSUN B., Şahin E., DANIŞ Ö., DEMİR S., OGAN A., ERDEM S.
27. Ulusal Kimya Kongresi, Turkey, 23 - 28 August 2015

XLV. **3 Aril kumarin türevlerinin sentezi ve insan monoamin oksidaz B ve B inhibitörleri olarak etkilerinin incelenmesi**
YÜCE DURSUN B., ŞAHİN E., DANIŞ Ö., DEMİR S., OGAN A., ERDEM S.
27. Ulusal Kimya Kongresi, Çanakkale, Turkey, 23 - 28 August 2015

XLVI. **QSAR Models for Antioxidant Activity of New Coumarin Derivatives**
ERZİNCAN P., SAÇAN M., YÜCE DURSUN B., DANIŞ Ö., DEMİR S., ERDEM S., OGAN A.
8th International Symposium on Computational Methods in Toxicology and Pharmacology Integrating Internet Resources (CMTPI-2015), 21 - 25 June 2015

XLVII. **Monoamine Oksidaz Enzimindeki Flavin N5 Araürün Oluşumu Kataliz mi İnhibisyon mu**
ÇAKIR K., DÜLGER H., ENİSOĞLU ATALAY V., ERDEM S.
2. Ulusal Hesaplamalı Kimya Kongresi, Kars, Turkey, 2 - 05 June 2015

XLVIII. **Pirolo Pirazin İndolizin Türevlerinin Sentezi ve Oluşum Mekanizmalarının Hesapsal Olarak**

Modellenmesi
SARI Ö., MENGEŞ N., ERDEM S., BALCI M.
2. Ulusal Hesaplamalı Kimya Kongresi, Kars, Turkey, 2 - 05 June 2015

XLIX. **Monoamin Oksidaz Enzimi Tarafından Katalizlenen Dopamin Oksidasyon Mekanizmasının Modellenmesi**
DÜLGER H., ÇAKIR K., ENİSOĞLU ATALAY V., ERDEM S.
2. Ulusal Hesaplamalı Kimya Kongresi, Kars, Turkey, 2 - 05 June 2015

L. **Monoamine Oksidaz A ve B Enzimlerinin Nörotransmitter Aminleri Serotonin Dopamin Oksitlemesi Aynı Mekanizmayla mı Farklı Mekanizmalarla mı Gerçekleşir**
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LX. **Structure Activity Relationship on Monoamine Oxidase Catalyzed Oxidation of Substituted Benzylamines Competing Proton Hydride Transfer Mechanisms**
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XCV. **The Effect of Active Site Tyrosine Orientation on Binding Of New Pyrazoline Derivatives To MAO B Molecular Docking and Dynamic Simulations**
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CII. **ONIOM Calculations On The Active Site Of Human MAO A And Its Tyrosine 444 Mutant Enzymes**
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CXXXII. **DFT Calculations For the Determination of Aromaticity of 1 3 4 Thiodiazole 2 Thione and Its Oxygen Analogs**
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Metrics

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