



**CURRICULUM VITAE**

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Doctorate	KİMYA (DR)	Hacettepe University	2011
Master's Degree	KİMYA (YL) (TEZLİ)	Hacettepe University	2005
Bachelor's Degree	KİMYA BÖLÜMÜ	Hacettepe University	2002

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Research Assistant	Hacettepe University	2002-2011

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1. Springer Nature Editorial Contribution Award (2025)
2. Springer Nature Author Service Award (2025)
3. Visiting Professorship and Fellowship (2018)
4. Visiting Professorship and Fellowship (2017)

**PUBLICATIONS**

**A. Articles published in international peer-reviewed journals:**

- A1.** Hoti D., Nixha A. R., Duran H. E., Arslan M., Yıldıztekin G., Ece A., Türkeş C., "Phthalimide–benzoic acid hybrids as potent aldose reductase inhibitors: Synthesis, enzymatic kinetics, and in silico characterization", *Bioorganic and Medicinal Chemistry*, vol. 131, 2025.
- A2.** Shendrikov V. P., Kot E. F., Makrinsky K. I., Ece A., Boldyrev I. A., "Phospholipid conjugates: formation of the intramolecular  $\pi$ -cation complex", *BMC Chemistry*, vol. 19, no. 1, 2025.
- A3.** Güleç Ö., Duran H. E., Arslan M., Yıldıztekin G., Ece A., Türkeş C., "Chalcone-inspired indole, carbazole, and phenothiazine hybrids as potent aldose reductase inhibitors with selective anticancer potential: Rational design, synthesis, and multi-level characterization", *Bioorganic Chemistry*, 2025.
- A4.** Zognjani B., Nixha A. R., Duran H. E., Arslan M., Yıldıztekin G., Ece A., Türkeş C., "N-substituted phthalimide–carboxylic acid hybrids as dual-targeted aldose reductase inhibitors: Synthesis, mechanistic insights, and cancer-relevant profiling", *Bioorganic Chemistry*, vol. 163, 2025.
- A5.** Zhang T., Chan K., Ece A., Daly R., Cannon A., Scalabrino G. A., Frankish N., O'sullivan J., Fallon P., Sheridan H., "Bioactive Indanes: Design, synthesis and bioactivity investigation of 2,2-substituted Indane derivatives, a new bioactive Indane scaffold", *Bioorganic Chemistry*, vol. 159, 2025.

- A6.** Efeoglu C., Serttas R., Demir B., Sahin E., Yabalak E., Seferoglu N., Erdogan S., Ece A., Nural Y., "1,4-Naphthoquinone thiazoles: Synthesis, crystal structure, anti-proliferative activity, and inverse molecular docking study", *Journal of Molecular Structure*, vol. 1322, 2025.
- A7.** Reymova F., Sever B., Topalan E., Sevimli-gur C., Can M., Tuyun A. F., Başoğlu F., Ece A., Otsuka M., Fujita M. vd., "Design, Synthesis, and Mechanistic Anticancer Evaluation of New Pyrimidine-Tethered Compounds", *Pharmaceuticals*, vol. 18, no. 2, 2025.
- A8.** Dincel E. D., Kuran E. D., Ece A., Başoğlu Ünal F., Renzi G., Badii G., Carta F., Supuran C. T., Güzeldemirci N., "Preliminary Investigations on Acyl Hydrazones Bearing Sulfonamides as Inhibitors of the Human Carbonic Anhydrase Isoforms I, II, IX, and XII", *Anti-Cancer Agents in Medicinal Chemistry*, vol. 25, 2025.
- A9.** Tok F., Abas B. İ., Başoğlu F., Çevik Ö., Karakuş S., Ece A., "Synthesis, Biological Evaluation and in Silico Studies of Novel Urea/Thiourea Derivatives of Lenalidomide", *Journal of Biochemical and Molecular Toxicology*, vol. 38, no. 12, 2024.
- A10.** Ece A., Mirzaei M., Ghnim Z., Al-hussainy A., Wabdan A., Saadh M., Mohany M., Mascarenhas-melo F., "Assessing the structural and electronic features of C24, B12C12 and Al12C12 fullerenes for the adsorption of methimazole to develop potential drug delivery systems", *Computational and Theoretical Chemistry*, vol. 1241, 2024.
- A11.** Güleç Ö., Türkeş C., Arslan M., Demir Y., Dincer B., Ece A., Küfrevioğlu Ö. İ., Beydemir Ş., "Bioactivity, cytotoxicity, and molecular modeling studies of novel sulfonamides as dual inhibitors of carbonic anhydrases and acetylcholinesterase", *Journal of Molecular Liquids*, vol. 410, 2024.
- A12.** Kolancılar H., Özcan H., Yılmaz A. Ş., Salan A. S., Ece A., "2,3-Dichloronaphthoquinone derivatives: Synthesis, antimicrobial activity, molecular modelling and ADMET studies", *Bioorganic Chemistry*, vol. 146, 2024.
- A13.** Güleç Ö., Türkeş C., Arslan M., Demir Y., Dincer B., Ece A., İrfan Küfrevioğlu Ö., Beydemir Ş., "Novel spiroindoline derivatives targeting aldose reductase against diabetic complications: Bioactivity, cytotoxicity, and molecular modeling studies", *Bioorganic Chemistry*, vol. 145, 2024.
- A14.** Caglayan C., Temel Y., Türkeş C., Ayna A., Ece A., Beydemir Ş., "The effects of morin and methotrexate on pentose phosphate pathway enzymes and GR/GST/TrxR enzyme activities: An in vivo and in silico study", *Archiv der Pharmazie*, vol. 357, no. 2, 2024.
- A15.** Güleç Ö., Türkeş C., Arslan M., Demir Y., Dincer B., Ece A., Beydemir Ş., "Novel beta-lactam substituted benzenesulfonamides: in vitro enzyme inhibition, cytotoxic activity and in silico interactions", *Journal of Biomolecular Structure and Dynamics*, vol. 42, no. 12, pp. 6359-6377, 2024.
- A16.** Maryam A., Siddiqi A. R., Chaitanya Vedithi S., Ece A., Khalid R. R., "Identification of selective inhibitors for phosphodiesterase 5A using e-pharmacophore modelling and large-scale virtual screening-based structure guided drug discovery approaches", *Journal of Biomolecular Structure and Dynamics*, vol. 42, no. 15, pp. 7812-7827, 2024.
- A17.** Karakuş F., Ece A., Kuzu B., "New targets and biomarkers for doxorubicin-induced cardiotoxicity in humans: implications drawn from toxicogenomic data and molecular modelling", *Journal of Biomolecular Structure and Dynamics*, 2024.
- A18.** Ece A., "Computer-aided drug design", *BMC Chemistry*, vol. 17, no. 1, 2023.
- A19.** Efeoglu C., Taskin S., Selcuk O., Celik B., Tumkaya E., Ece A., Sari H., Seferoglu Z., Ayaz F., Nural Y., "Synthesis, anti-inflammatory activity, inverse molecular docking, and acid dissociation constants of new naphthoquinone-thiazole hybrids", *Bioorganic and Medicinal Chemistry*, vol. 95, 2023.
- A20.** Guven O., Sever B., Başoğlu-ünal F., Ece A., Tateishi H., Koga R., Radwan M. O., Demir N., Can M., Dilsiz Aytemir M. vd., "Structural Characterization of TRAF6 N-Terminal for Therapeutic Uses and Computational Studies on New Derivatives", *Pharmaceuticals*, vol. 16, no. 11, 2023.
- A21.** Çelik Onar H., Özden E. M., Taslak H. D., Gülçin İ., Ece A., Erçağ E., "Novel coumarin-chalcone derivatives: Synthesis, characterization, antioxidant, cyclic voltammetry, molecular modelling and biological evaluation studies as acetylcholinesterase,  $\alpha$ -glycosidase, and carbonic anhydrase inhibitors", *Chemico-Biological Interactions*, vol. 383, 2023.
- A22.** Erdönmez B., Altıntop M. D., Akalın Çiftçi G., Özdemir A., Ece A., "Design, Synthesis, and Evaluation of a New Series of Hydrazones as Small-Molecule Akt Inhibitors for NSCLC Therapy", *ACS Omega*, vol. 8, no. 22, pp. 20056-20065, 2023.
- A23.** Bulut Z., Abul N., Poslu A. H., Gülçin İ., Ece A., Erçağ E., Koz Ö., Koz G., "Structural characterization and biological evaluation of uracil-appended benzylic amines as acetylcholinesterase and carbonic anhydrase I and II inhibitors", *Journal of Molecular Structure*, vol. 1280, 2023.
- A24.** Orujova T., Ece A., Akalın Çiftçi G., Özdemir A., Altıntop M. D., "A new series of thiazole-hydrazone hybrids for Akt-targeted therapy of non-small cell lung cancer", *Drug Development Research*, vol. 84, no. 2, pp. 185-199, 2023.
- A25.** Shendrikov V. P., Alekseeva A. S., Kot E. F., Mineev K. S., Tretiakova D. S., Ece A., Boldyrev I. A., "Indane Based Molecular Motors: UV-Switching Increases Number of Isomers", *Molecules*, vol. 27, no. 19, 2022.
- A26.** Efeoglu C., Yetkin D., Nural Y., Ece A., Seferoğlu Z., Ayaz F., "Novel urea-thiourea hybrids bearing 1,4-naphthoquinone moiety: Anti-inflammatory activity on mammalian macrophages by regulating intracellular PI3K pathway, and molecular docking study", *Journal of Molecular Structure*, vol. 1263, no. 1, 2022.
- A27.** Yamali C., Gul H. I., Tugrak Sakarya M., Nurpelin Saglik B., Ece A., Demirel G., Nenni M., Levent S., Cihat Oner A., "Quinazolinone-based benzenesulfonamides with low toxicity and high affinity as monoamine oxidase-A inhibitors: Synthesis, biological evaluation and induced-fit docking studies", *Bioorganic Chemistry*, vol. 124, 2022.
- A28.** Şenol Z. M., Çetinkaya S., Yenidünya A. F., Başoğlu-ünal F., Ece A., "Epichlorohydrin and tripolyphosphate-crosslinked chitosan-kaolin composite for Auramine O dye removal from aqueous solutions: Experimental study and DFT calculations", *International Journal of Biological Macromolecules*, vol. 199, pp. 318-330, 2022.

- A29.** Nural Y., Ozdemir S., Yalcin M. S., Demir B., Atabey H., Seferoglu Z., Ece A., "New bis- and tetrakis-1,2,3-triazole derivatives: Synthesis, DNA cleavage, molecular docking, antimicrobial, antioxidant activity and acid dissociation constants", *Bioorganic and Medicinal Chemistry Letters*, vol. 55, 2022.
- A30.** Askin S., Tahtaci H., Türkes C., Demir Y., Ece A., Akalın Çiftçi G., Beydemir Ş., "Design, synthesis, characterization, in vitro and in silico evaluation of novel imidazo[2,1-b][1,3,4]thiadiazoles as highly potent acetylcholinesterase and non-classical carbonic anhydrase inhibitors", *Bioorganic Chemistry*, vol. 113, 2021.
- A31.** Başoğlu F., Ulusoy-güzeldemirci N., Akalın-çiftçi G., Çetinkaya S., Ece A., "Novel imidazo[2,1-b]thiazole-based anticancer agents as potential focal adhesion kinase inhibitors: Synthesis, in silico and in vitro evaluation", *Chemical Biology and Drug Design*, vol. 98, no. 2, pp. 270-282, 2021.
- A32.** Nural Y., Ozdemir S., Yalcin M. S., Demir B., Atabey H., Ece A., Seferoglu Z., "Synthesis, Biological Evaluation, Molecular Docking, and Acid Dissociation Constant of New Bis-1,2,3-triazole Compounds", *ChemistrySelect*, vol. 6, no. 28, pp. 6994-7001, 2021.
- A33.** Yamali C., Sakagami H., Uesawa Y., Kurosaki K., Satoh K., Masuda Y., Yokose S., Ece A., Bua S., Angeli A. vd., "Comprehensive study on potent and selective carbonic anhydrase inhibitors: Synthesis, bioactivities and molecular modelling studies of 4-(3-(2-arylidenehydrazine-1-carbonyl)-5-(thiophen-2-yl)-1H-pyrazole-1-yl) benzenesulfonamides", *European Journal of Medicinal Chemistry*, vol. 217, 2021.
- A34.** Maryam A., Khalid R. R., Siddiqi A. R., Ece A., "E-pharmacophore based virtual screening for identification of dual specific PDE5A and PDE3A inhibitors as potential leads against cardiovascular diseases", *Journal of Biomolecular Structure and Dynamics*, vol. 39, no. 7, pp. 2302-2317, 2021.
- A35.** Chan K., Frankish N., Zhang T., Ece A., Cannon A., O'sullivan J., Sheridan H., "Bioactive indanes: insight into the bioactivity of indane dimers related to the lead anti-inflammatory molecule PH46A", *Journal of Pharmacy and Pharmacology*, vol. 72, no. 7, pp. 927-937, 2020.
- A36.** Ece A., "Towards more effective acetylcholinesterase inhibitors: a comprehensive modelling study based on human acetylcholinesterase protein-drug complex", *Journal of Biomolecular Structure and Dynamics*, vol. 38, no. 2, pp. 565-572, 2020.
- A37.** Dizdaroglu Y., Albay C., Arslan T., Ece A., Turkoglu E. A., Efe A., Senturk M., Supuran C. T., Ekinci D., "Design, synthesis and molecular modelling studies of some pyrazole derivatives as carbonic anhydrase inhibitors", *Journal of Enzyme Inhibition and Medicinal Chemistry*, vol. 35, no. 1, pp. 289-297, 2020.
- A38.** Maryam A., Khalid R. R., Vedithi S. C., Ece A., Çınaroğlu S. S., Siddiqi A. R., Blundell T. L., "Exploring the structural basis of conformational heterogeneity and autoinhibition of human cGMP-specific protein kinase Ia through computational modelling and molecular dynamics simulations", *Computational and Structural Biotechnology Journal*, vol. 18, pp. 1625-1638, 2020.
- A39.** Yamali C., Gul H. I., Ece A., Bua S., Angeli A., Sakagami H., Sahin E., Supuran C. T., "Synthesis, biological evaluation and in silico modelling studies of 1,3,5-trisubstituted pyrazoles carrying benzenesulfonamide as potential anticancer agents and selective cancer-associated hCA IX isoenzyme inhibitors", *Bioorganic Chemistry*, vol. 92, 2019.
- A40.** Türk S., Karaku Ş S., Ece A., Ulusoy S., Boşgelmez-tnaz G., "Synthesis, structure elucidation and biological activities of some novel 4(3h)-quinazolinones as anti-biofilm agents", *Letters in Drug Design and Discovery*, vol. 16, no. 3, pp. 313-321, 2019.
- A41.** Er M., Abounakhl A. M., Tahtaci H., Bawah A. H., Çınaroğlu S. S., Onaran A., Ece A., "An integrated approach towards the development of novel antifungal agents containing thiadiazole: Synthesis and a combined similarity search, homology modelling, molecular dynamics and molecular docking study", *Chemistry Central Journal*, vol. 12, 2018.
- A42.** Yamali C., Gul H. I., Ece A., Taslimi P., Gulcin I., "Synthesis, molecular modeling, and biological evaluation of 4-[5-aryl-3-(thiophen-2-yl)-4,5-dihydro-1H-pyrazol-1-yl] benzenesulfonamides toward acetylcholinesterase, carbonic anhydrase I and II enzymes", *Chemical Biology and Drug Design*, vol. 91, no. 4, pp. 854-866, 2018.
- A43.** Tahtaci H., Karacık H., Ece A., Er M., Şeker M. G., "Design, Synthesis, SAR and Molecular Modeling Studies of Novel Imidazo[2,1-b][1,3,4]Thiadiazole Derivatives as Highly Potent Antimicrobial Agents", *Molecular Informatics*, vol. 37, no. 3, 2018.
- A44.** Karakurt T., Cukurovali A., Subasi N. T., Onaran A., Ece A., Eker S., Kani I., "Experimental and theoretical studies on tautomeric structures of a newly synthesized 2,2''(hydrazine-1,2-diylidenebis(propan-1-yl-1-ylidene))diphenol", *Chemical Physics Letters*, vol. 693, pp. 132-145, 2018.
- A45.** Altuntas T. G., Yılmaz N., Ece A., Altanlar N., Ölgün S., "In vitro antibacterial and antifungal activity and computational evaluation of novel indole derivatives containing 4-substituted piperazine moieties", *Letters in Drug Design and Discovery*, vol. 15, no. 10, pp. 1079-1086, 2018.
- A46.** Karakus G., Ece A., Yaglioglu A. S., Zengin H. B., Karahan M., "Synthesis, structural characterization, and antiproliferative/cytotoxic effects of a novel modified poly(maleic anhydride-co-vinyl acetate)/doxorubicin conjugate", *Polymer Bulletin*, vol. 74, no. 6, pp. 2159-2184, 2017.
- A47.** Er M., Ergüven B., Tahtaci H., Onaran A., Karakurt T., Ece A., "Synthesis, characterization, preliminary SAR and molecular docking study of some novel substituted imidazo[2,1-b][1,3,4]thiadiazole derivatives as antifungal agents", *Medicinal Chemistry Research*, vol. 26, no. 3, pp. 615-630, 2017.
- A48.** Ece A., Pejin B., "A computational insight into acetylcholinesterase inhibitory activity of a new lichen depsidone", *Journal of Enzyme Inhibition and Medicinal Chemistry*, vol. 30, no. 4, pp. 528-532, 2015.
- A49.** Ece A., Sevin F., "The discovery of potential cyclin A/CDK2 inhibitors: A combination of 3D QSAR pharmacophore modeling, virtual screening, and molecular docking studies", *Medicinal Chemistry Research*, vol. 22, no. 12, pp. 5832-5843, 2013.

- A50.** Zorluoğlu S. L., Taşdemir I. H., Ece A., Kiliç E., "A cooperative computational and experimental investigation on electrochemical behavior of metoprolol and its voltammetric determination", *Canadian Journal of Chemistry*, vol. 91, no. 10, pp. 951-959, 2013.
- A51.** Pamuk D., Taşdemir I. H., Ece A., Canel E., Kiliç E., "Redox pathways of aliskiren based on experimental and computational approach and its voltammetric determination", *Journal of the Brazilian Chemical Society*, vol. 24, no. 8, pp. 1276-1286, 2013.
- A52.** Taşdemir I. H., Ece A., Kiliç E., "Experimental and theoretical study on the electrochemical behavior of Zofenopril and its voltammetric determination", *Current Pharmaceutical Analysis*, vol. 8, no. 4, pp. 339-348, 2012.
- A53.** Ece A., Sevin F., "Exploring QSAR on 4-cyclohexylmethoxypyrimidines as antitumor agents for their inhibitory activity of CDK2", *Letters in Drug Design and Discovery*, vol. 7, no. 9, pp. 625-631, 2010.
- A54.** Sökmen I., Ece A., Düz B., Sevin F., "Reaction of atomic carbon with isomeric cresols", *Letters in Organic Chemistry*, vol. 6, no. 8, pp. 650-653, 2009.
- A55.** Düz B., Elbistan C. K., Ece A., Sevin F., "Application of carbon arc-generated Mo and W-based catalyst systems to the ROMP of norbornene", *Applied Organometallic Chemistry*, vol. 23, no. 9, pp. 359-364, 2009.
- A56.** Düz B., Yüksel D., Ece A., Sevin F., "The first example of tungsten-based carbene generation from WCl<sub>6</sub> and atomic carbon and its use in olefin metathesis", *Tetrahedron Letters*, vol. 47, no. 29, pp. 5167-5170, 2006.

#### **D. Articles published in national peer-reviewed journals:**

- D1.** Ece A., "E-pharmacophore mapping combined with virtual screening and molecular docking to identify potent and selective inhibitors of P90 Ribosomal S6 Kinase (RSK) E-Farmakofor Haritalanması, Sanal Tarama ve Moleküler Kenetlenmenin birleştirilmesi ile etkili ve Seçici P90 Ribosomal S6 Kinaz (RSK) İnhibitörlerinin Belirlenmesi", *Turkish Journal of Pharmaceutical Sciences*, vol. 13, no. 2, 2016.