

(NECMETTIN PIRINCCIOGLU)



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Research Interest

The main research area involves the application of computational tools in drug development and in understanding of biochemical processes in livings as well as organic reaction mechanisms, including asymmetric reactions catalyzed by organocatalysts. The molecular modelling approaches also apply to supramolecular complexes between artificial organic receptors and small ligands to explain the main driving forces in the selective recognition and high activity occurring in living cells. The research also covers designing molecules for biologically relevant applications.

Current Position

- 2006- Working as a full-time professor of organic chemistry at Department of Chemistry, University of Dicle.

Work Experiences

- 2000-2005 Worked as an associate professor of organic chemistry at Department of Chemistry, University of Dicle.
- 2003 (for 4 months) Worked as visiting fellow at Department of Chemistry, University of Bath.
- 2004 (for 3 months) Worked as visiting fellow at Department of Chemistry, University of Bath.
- 1997-2000 Worked as an assistant professor at Department of Chemistry, University of Dicle.
- 1998 (for 3 months) Worked as visiting fellow at Department of Chemistry, University of Uppsala.
- 1999 (for 3 months) Worked as visiting fellow at Department of Chemistry, University of Uppsala.
- 1996-1997 Worked as a postdoctoral fellow at Department of Chemistry, University of Uppsala.

Education

- 1990-1996 Completed a PhD thesis under supervision of Professor Andrew Williams titled "Modification of Reactivity by Supramolecular Complex Formation" at Department of Chemistry, University of Kent.
- 1984-1986 Received a BSc degree in chemistry from Department of Chemistry, University of Ege.

Supervised MSc Theses

-) Özhan, ., “Studying mechanism of addition of bromine to aqueous solution of disodium salts of citraconic and mesaconic acids”, 2002-2004, Graduate School of Science, University of Dicle.
-) Varhan, E., “A theoretical study of mechanism of acid-catalyzed dehydration of arene hydrates and oxides”, 2002-2004, Graduate School of Science, University of Dicle.
-) Yüksel U., “A theoretical study of the extraction abilities of 1,3-diols designed for the liquid-liquid extraction of boron”, 2002-2004, Graduate School of Science, University of Dicle.
-) Atar, M., “An investigation of the molecular recognition of sugars by chiral host compounds derived from cyclodextrin and calix(4) arenes by NMR and molecular model calculations”, 2002-2004, Graduate School of Science, University of Ege.
-) Arslan, N., “Design of a new chiral micelle as esterase model” 2004-2006, Graduate School of Science, University of Dicle.
-) Akdeniz M., “A theoretical study of binding mode of vancomycin” 2004-2006, Graduate School of Science, University of Dicle.

Supervised PhD Theses

-) Kocakaya Ö., “Experimental and Computational Study of Various Chemical Processes” 2004-2009, Graduate School of Science, University of Dicle.
-) Ercan, S., “Computer-aided anti-HIV drug design” 2005-2012, Graduate School of Science, University of Dicle.
-) Arslan, N., “Design of piroline-based chiral organocatalysts and their application in asymmetric Aldol reactions: an experimental and theoretical approach” 2006-2014, Graduate School of Science, University of Dicle.

Administration Positions

-) Vice-chair of Department of Chemistry, Dicle University 1997-2000
-) Vice-chair of Graduate School of Science, Dicle University 2002-2003
-) Vice-chair of Department of Chemistry, Dicle University 2003-2005
-) Chair of Research Project Council, Dicle University 2002-2008
-) Chair of Graduate School of Science, Dicle University 2005-2008

Courses Lectured

Autumn	Spring
Undergraduate	
Organic Chemistry I	Organic Chemistry II
Postgraduate	
Computational Chemistry and Molecular Modelling I	Computational Chemistry and Molecular Modelling II
Computer-Aided Drug Design I	Computer-Aided Drug Design II

Published Articles

1. Mehmet Çolak, Deniz Baris Cebe, Necmettin Pirinccioglu, Halil Ho gören. Novel bis(aminoalcohol)oxalamide organogelators and their diglycolylamide analogs: evaluation of gelation efficiency in various organic fluids. *Turk J Chem*, 2017, 41, 658-671.
2. Gül en Öztürk, Salih Subari, Sevil eker, Mahmut To rul, Safak Özhan Kocakaya, Selami Ercan, Necmettin Pirinçcio lu. A facile synthesis of amide-based receptors under microwave conditions: investigation of their anion recognition properties by experimental and computational tools. *J. Mol. Mod.* 2017, 23(9). 249. DOI: 10.1007/s00894-017-3390-0.
3. Süleyman Özakin, Robert W. Davis, Thomas P. Umile, Necmettin Pirinccioglu, Murat Kizil, Gurbet Celik, Alaattin Sen, Kevin P. C. Minbiole, Ebru nce. The isolation of tetrangomycin from terrestrial *Streptomyces* sp. CAH29: evaluation of antioxidant, anticancer, and anti-MRSA activity. *Med Chem Res* 2016. DOI 10.1007/s00044-016-1708-6.
4. Michal ezanka, Ivan Stibor, Murat Azizoglu, Yilmaz Turgut, Necmettin Pirinccioglu. Enantiomeric recognition of amino acid ester salts by -cyclodextrin derivatives: an experimental and computational study. *ARKIVOC* 2016 (v) 249-267.
5. Murat Azizoglu, Asli Erdogan, Nevin Arslan, Yilmaz Turgut, Halil Hosgoren and Necmettin Pirinccioglu. A series of novel beta-hydroxyamide based catalysts for borane-mediated enantioselective reductions of prochiral ketones. *Tetrahedron-Asymmetry* 2016, 27(14-15), 614-622. DOI: 10.1016/j.tetasy.2016.06.003.
6. Safak O. Kocakaya, Yilmaz Turgut and Necmettin Pirinccioglu. Enantiomeric discrimination of chiral organic salts by chiral aza-15-crown-5 ether with C-1 symmetry: experimental and theoretical approaches. *J. Mol. Model.* 2015, 21(3):55. DOI: 10.1007/s00894-015-2604-6
7. Fulwah Alqahtani, Jafar Mahdavi, Lee M Wheldon, Matthew Vassey, Necmettin Pirinccioglu, Pierre-Joseph Royer, Suzan M Qarani, Shaun Morroll, Jeroen Stoof, Nicholas D Holliday, Teo Y Siew, Neil J Oldfield, Karl G Wooldridge, Dlawer A A Ala'Aldeen. Deciphering the complex three-way interaction between the non-integrin laminin receptor, galectin-3 and *Neisseria meningitidis*. *Open Biology*, 2014, 4(10):UNSP 140053. DOI: 10.1098/rsob.140053.
8. Sevil Seker, Deniz Baris, Nevin Arslan, Yilmaz Turgut, Necmettin Pirinccioglu and Mahmut Togrul. Synthesis of rigid and C-2-symmetric pyridino-15-crown-5 type macrocycles bearing diamide-diester functions: enantiomeric recognition for chiral primary organoammonium perchlorate salts. *Tetrahedron-Asymmetry* 2014, 25(5):411-417. DOI: 10.1016/j.tetasy.2014.01.009.
9. Selami Ercan, Nevin Arslan, Safak Ozhan Kocakaya, Andrew Williams, Necmettin Pirinccioglu. Experimental and Theoretical Study of Mechanism of Hydrolysis of Substituted Phenyl Hexanoates Catalysed by Globin in the Presence of Surfactant. *J Mol Model* 2014, 20(3):2096. DOI: 10.1007/s00894-014-2096-9.
10. Jafar Mahdavi, Necmettin Pirinccioglu, Neil J. Oldfield, Elisabet Carlsohn, Jeroen Stoof, Akhmed Aslam, Tim Self, Shaun Cawthraw, Liljana Petrovska, Natalie Colborne, Carina Sihlbom, Thomas Boren, Karl G. Wooldridge, Dlawer A.A. Ala'Aldeen. A novel O-linked glycan modulates *Campylobacter jejuni* major outer membrane protein-mediated adhesion to human histo-blood group antigens and chicken colonization. *Open Biology*, 2013, 4(1): 130202. DOI: 10.1098/rsob.130202.
11. Selami Ercan and Necmettin Pirinccioglu Computational design of a full-length model of HIV-1 integrase: modeling of new inhibitors and comparison of their calculated

binding energies with those previously studied J Mol Model 2013 19(10): 4349-4368. DOI: 10.1007/s00894-013-1943-4

12. Mehmet Karakaplan, Devran Ak, Mehmet Colak, Safak Ozhan Kocakaya and Necmettin Pirinccioglu, Synthesis of new diaza-18-crown-6 ethers derived from trans-(R,R)-1,2-diaminocyclohexane and investigation of their enantiomeric discrimination ability with amino acid ester salts, Tetrahedron, 2013, 69, 349-358 DOI: 10.1016/j.tet.2012.10.020.
13. Safak Ozhan Kocakaya, Necmettin Pirinccioglu. A theoretical study of the effects of polar substitution on the activation barriers for internal rotation around the C-N bond in p-substituted nitrosobenzenes: comparison of DFT and MP2 calculations. Turk J Chem 2010, 34(3): 399-410. DOI: 10.3906/kim-0909-272.
14. Giorgio Cevasco, Andrea Galatini, Necmettin Pirinccioglu, Sergio Thea, Andrew Williams. A study on a primitive artificial esterase model: reactivity of a calix[4]resorcinarene bearing carboxyl groups. J Phys Org Chem 2008, 21(6): 498-504. DOI: 10.1002/poc.1371.
15. Necmettin Pirinccioglu, James Robinson, Mary Mahon, J. Grant Buchanan, Ian H. Williams. Ian H.) Experimental and computational evidence for alpha-lactone intermediates in the addition of aqueous bromine to disodium dimethyl-maleate and - fumarate. Org Biomol Chem 2007, 5(24): 4001-4009. DOI: 10.1039/b711538e.
16. S. Seyhan, O. Ozbayrak, N. Demirel, M. Merdivan, N. Pirinccioglu. Chiral separation of amino acids by chiral octamide derivatives of calixarenes derived from resorcinol by impregnation on a polymeric support. 2005, 16(22): 3735-3738. DOI: 10.1016/j.tetasy.2005.10.012.
17. N. Demirel, M. Merdivan, N. Pirinccioglu, C. Hamamci. Thorium(IV) and uranium(VI) sorption studies on octacarboxymethyl-C-methylcalix[4]resorcinarene impregnated on a polymeric support. 2003, 485(2): 213-219. DOI: 10.1016/S0003-2670(03)00415-X.
18. Murat Kizil, Ebru Ince Yilmaz, Necmettin Pirinccioglu, M. Cetin Aytekin. DNA cleavage activity of diazonium salts: Chemical nucleases. Turk J Chem 2003, 27(5): 539-544.
19. N. Pirinccioglu, ZS Jia, A Thibblin. Acid-catalysed aromatization of anthranil derivatives. A kinetic and thermodynamic study. J Chem Soc PT2 2001, (12): 2271-2275. DOI: 10.1039/b107121a.
20. Necmettin Pirinccioglu, Flora Zaman, Andrew Williams. Reactions within association complexes: The reaction of imidazole with substituted phenyl acetates in the presence of detergents in aqueous solution. J Org Chem 2000 65(8): 2537-2543. DOI: 10.1021/jo991887o.
21. Necmettin Pirinccioglu, Alf Thibblin. Acid-catalyzed solvolysis of allylic ethers and alcohols. Competing elimination and substitution via a thermodynamically "stable" carbocation. J Am Chem Soc 1998, 120(26): 6512-6517. DOI: 10.1021/ja9807800.
22. Necmettin Pirinccioglu, Andrew Williams. Studies of reactions within molecular complexes: alkaline hydrolysis of substituted phenyl benzoates in the presence of xanthenes. J Chem Soc PT2 1998, (1): 37-40. DOI: 10.1039/a705499h.
23. Necmettin Pirinccioglu, Flora Zaman, Andrew Williams. A calixresorcinarene provides the framework for an artificial esterase. J Chem Soc PT2 (12): 2561-2562. DOI: 10.1039/p29960002561.
24. KB Ray, RH Weatherhead, N Pirinccioglu, A Williams. Enhanced alkaline-hydrolysis of monoesterified 4-tert-butylcalix[4]arenes involving intramolecular electrophilic catalysis by the phenolic hydroxy group. J Chem Soc PT2 1994 (1): 83-88. DOI: 10.1039/p29940000083.

COMPUTATIONAL CHEMISTRY GROUP MEMBERS

Dr. Afak Özhan KOCAKAYA
Murat KURT (PhD Student)
Murat AZ ZO LU (PhD Student)
Barı KURT (Phd Student)
Sema Çakır (MSc Student)
Samet Ay (MSc Student)
Ükran Demir (MSc Student)
Alev Bingöl (MSc Student)

COLLABORATIONS

Professor Ian H Williams (University of Bath, UK)
Dr Jafar Mahdavi (University of Nottingham, UK)

FACILITIES

The group has access to various research facilities including an excellent synthetic organic laboratory supplied with various instruments, 400 MHz NMR, FT-IR, UV/Vis, GC and HPLC, chemical analysis. The group also have the opportunities to use a variety of computational tools to model a range of chemical and biological processes. They include quantum and molecular dynamic calculations using Gaussian 03 and AMBER programmes. We have also access to TR-GRID facilities for computational applications.



