

Thomas Mavromoustakos

Associate Professor in Organic Chemistry



Education

B.Sc. in Chemistry, University of Athens (1985),
M.Sc. 1988 Medicinal Chemistry, University of Connecticut
Ph.D. 1990, Medicinal Chemistry, University of Connecticut.

B.Sc. 2007 Theology School, University of Athens, Greece

Research Field of Interest

1. Conformational Analysis of bioactive compounds through a combination of NMR spectroscopy and Molecular Modeling.
2. Drug:Membrane interactions using physical chemical methodologies
3. Rational design of novel bioactive molecules through docking and 3D QSAR studies

Teaching

Undergraduate:

Organic Chemistry laboratory for Chemists

Organic Chemistry for Biologists

Organic Chemistry for Physicists

Graduate:

Topics in NMR Spectroscopy and Molecular Modeling

Book Authorship

1. T. Mavromoustakos and P. Zoumpoulakis.. Molecular Modeling. Applications in Organic and Pharmaceutical Chemistry ,2008, (pages 307) ISBN 978-960-89486-5.

2 T. Mavromoustakos, J.M. Matsoukas. Nuclear Magnetic Resonance., 2006 (pages 615)

ISBN 960-88751-5-3

3. T. Mavromoustakos. Use of the NMR in the study of pharmaceutical substances, zeolites, polymers and archaeological findings. January 2001 (pages 198), ISBN 96086193-1-9.

4. T. Mavromoustakos, A. Kolocouris, C. Papakonstantinou, P. Sinigalias, C. Lappas. Two textbooks in Chemistry for the third class of high school . They are published in August of 1998 and are distributed to all high schools of Greece.

5. T. Mavromoustakos, A. Kolocouris, C. Papakonstantinou, P. Sinigalias, C. Lappas. A Chemistry laboratory guide for the third class of high school . They are published in August of 1998 and are distributed in all high schools of Greece.

6. T. Mavromoustakos, A. Kolocouris, C. Papakonstantinou, P. Sinigalias, C. Lappas. Two books containing solutions of the exercises in the textbooks. They are published in August of 1998 and are distributed in all high schools of Greece.

Editing

1. Bioactive Peptides in Drug Discovery and Design: Medical Aspects. This book was published by IOS press in January of 1999 as the 22nd volume of a series of books entitled «Biomedical and Health Research». Eds. J. Matsoukas, T. Mavromoustakos.

2. Review of Clinical Pharmacology and Pharmacokinetics vol. 11, 1997. An issue dedicated in Peptides and Biomedical Research. Eds. J. Matsoukas, T. Mavromoustakos.

3 Bioactive Peptides in Drug Discovery and Design: Medical Aspects. This book is in press 2002 in as the 55th volume of a series of books entitled «Biomedical and Health Research». Eds. J. Matsoukas, T. Mavromoustakos.

4. Guest Editor in Current Reviews in Medicinal Chemistry and more particularly in the issue dedicated to hypertension («Modern Aspects in the Design and Discovery of Novel Antihypertensive Drugs, 2004»). The contributors of this issue included well known scientists of Greece, Europe and USA.

Selected Papers (2008-2009)

1. I. Kyrikou, C. Poulos, N. Benetis, K. Viras, M. Zervou, T. Mavromoustakos. Interactions of the dipeptide paralyisin β -Ala-tyr and the amino acid Glu with phospholipids bilayers. *Biochim. Biophys. Acta* 1778, 113-124 (2008).

2. Mantzourani, E.D., Blokar, K., Tselios, T.V., Matsoukas, J.M., Platts, J.A., Mavromoustakos, T.M., Grdadolnik S.G. A combined NMR and molecular dynamics simulation study to determine the conformational properties of agonists and antagonists against experimental autoimmune encephalomyelitis. *Bioorg. Med. Chem.* 16, 2171–2182, (2008).

3. P. Panagiotidis, E.T. Kefalas, C.P. Raptopoulou, A. Terzis, T. Mavromoustakos, A. Salifoglou. Delving into the complex picture of Ti(IV)-citrate speciation in aqueous media: Synthetic, structural, and electrochemical considerations in mononuclear Ti(IV) complexes containing variably deprotonated citrate ligands. *Inorg. Chem. Acta* 361, 2210-2224 (2008).

4. S. Durdagi, H. Reis, M.G. Papadopoulos, T. Mavromoustakos. Comparative Molecular Dynamics Simulations of the Potent Synthetic Classical Cannabinoid Ligand AMG3 in Solution and at Binding Site of the CB1 and CB2 Receptors *Bioorg. Med. Chem.* 16, 7377-7387 (2008).

5. C. Koukoulitsa, M. Zervou, C. Demetzos, T. Mavromoustakos. Comparative docking studies of labdane-type diterpenes with forskolin. *Bioorg. Med. Chem.* 16, 8237-8243 (2008).
6. A. Kapou, N.P. Benetis, S. Durdagi, S. Nikolaropoulos, T. Mavromoustakos. Synthesis and 3D QSAR/CoMFA and CoMSIA Studies on Antileukemic Steroidal Esters coupled with Conformationally Flexible Nitrogen Mustards. *Journal of Chemical Information and Modeling*, 48(11) 2254-2264 (2008).
7. S. Durdagi, T. Mavromoustakos, M.G. Papadopoulos. 3D QSAR CoMFA/CoMSIA, molecular docking and molecular dynamics studies of fullarene-based HIV-1 PR inhibitors, *Bioorg. Med. Chem. Lett.* 18, 6283-6289 (2008).
8. S. Durdagi, T. Mavromoustakos, N. Chronakis, MG Papadopoulos. Computational design of novel fullerene analogs as potential HIV 1 PR inhibitors: Analysis of the binding interactions between fullerene Inhibitors and HIV 1 PR residues using 3D QSAR, molecular docking and molecular dynamics simulations. *Bioorg. Med. Chem.*, 16, 9957-9974 (2008).
9. C. Potamitis, M Zervou, V. Katsiaras, P Zoumpoulakis, S. Durdagi, M. Papadopoulos, J. Hayes, S. Grdadolnik, I. Kyrikou, D. Argyropoulos, G.Vatougia, T. Mavromoustakos. Antihypertensive Drug Valsartan in solution and at the AT₁ Receptor: Conformational Analysis, Dynamic NMR Spectroscopy, in silico Docking and Molecular Dynamics Simulations. *J. Chem. Inf. Mod.* 49, 726-739 (2009).
10. C. Fotakis, D. Christodouleas, P. Chatzigeorgiou, M. Zervou, N. P. Benetis, K. Viras, T.M. Mavromoustakos. Application of a novel CP-³¹P NMR methodology to study the possible interdigitation effect of losartan in phospholipids bilayers. Comparison with Raman spectroscopy data *Biophys. J.* 96, 2227-2236 (2009).
11. C. Koukoulitsa, A.T. Kakoulidou, T. Mavromoustakos, I. Chinou. PLS Analysis for Antibacterial Activity of Natural Coumarins Using VolSurf Descriptors. *QSAR Comb. Sci.* 785-789 (2009).
12. Kotzabasakis, V., Kostakis, K., Pitsikalis, M., Hadjichristidis, N., L.D., David, Mavromoustakos, T., Potamitis, C. Polymerization of Higher α -Olefins Using a Cs-Symmetry Hafnium Metallocene Catalyst. Kinetics of the Polymerization and Microstructural Analysis. *J. Polym. Sci. Part A* 47, 4314-4325 (2009).
13. Durdagi S., Supuran, T., Amalda, T.S, Doostdar, N., Kumar, M.K., Barron, A.R., Mavromoustakos, T., Papadopoulos, M.G. *In Silico* Drug Screening Approach for the Design of Magic Bullets: A Successful Example with Anti-HIV Fullerene Derivatized Amino Acids. *J. Chem. Inf. Model.* 49, 1139-1143 (2009).
14. Aggeliki Politi, Serdar Durdagi, Panagiota Moutevelis-Minakakis, George Kokotos, Manthos G. Papadopoulos, Thomas Mavromoustakos. Application of 3D QSAR CoMFA/CoMSIA and in silico docking studies on novel renin inhibitors against cardiovascular diseases. *Eur. J. Med. Chem.* 44(9) 3703-3711 (2009).

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