

**THOMAS MAVROMOUSTAKOS**  
**Capodistrian University of Athens**  
**Associate Professor of Chemistry Department**

**Date of birth: 18/6/1960**

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**Family status: Married with four children**

## **EDUCATION**

**B.Sc.** 1985 Chemistry, University of Athens, Greece.

**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.

**M.Sc.** 2012 Social Theology School, University of Athens, Greece

**Doctoral Dissertation:** Study of the cannabinoid and anesthetic steroids with artificial and biological membranes. The dissertation can be found in the web site:  
**<http://phdtheses.ekt.gr/eadd/handle/10442/12696>**

## **EMPLOYMENT**

**1985-1987.** Teaching Assistant in School of Pharmacy for introductory and advanced level courses.

**1988-October 1990.** Research Assistant in School of Pharmacy.

**October 1990-June 1991.** Postdoctoral Fellow in School of Pharmacy.

**June 1991-September 2004.** Researcher director at Laboratory of Molecular Analysis (LMA) at the Institute of Organic and Pharmaceutical Chemistry (IOPC) of National Hellenic Research Foundation (NHRF). Use Molecular Modeling to study the conformational analysis of antihypertensive drugs, cannabinoids, steroids, and other bioactive molecules. Perform NMR experiments both in solution and in solid state to study the conformation analysis of biologically active molecules and drug:membranes interactions. Use DSC as a complementary tool to study the thermal changes in membrane bilayers after the incorporation of drugs. Use the modern high technology infrastructure of the institute to collaborate and solve some of the research

problems facing professors at Greek Universities. Such problems include structure determination of zeolithes, inorganic complexes and soil materials.

**September 2004-beginning of January 2005.** Visiting associate professor at the University of Cyprus (Chemistry Department). Teaching of Organic Chemistry laboratory and Medicinal Chemistry.

**January 2005-2007** Director of Laboratory of Molecular Analysis (LMA) at IOPC.

**2007-** Elected since 2007 a President of the new established Center of Applied Research and Technology of Nicosia, Cyprus.

**January of 2007-May of 2007.** Visiting associate professor at the University of Cyprus (Chemistry Department). Teaching of Organic Chemistry laboratory and Medicinal Chemistry.

**September 2007-2012.** Associate Professor at the Chemistry Department of Athens

**June 2012-** Full Professor at the Chemistry Department of Athens

## **AWARDS**

1. Fellowship sponsored by Royal Society for two monthly stayment in Great Britain. During my residence at the University of York I was trained in Molecular Graphics at Prof. Rod Hubbard's laboratory.

2. Award for the 3<sup>rd</sup> best presented poster in the Third International Conference on Applications of Magnetic Resonance in Food Science, Nantes, September 16-18, 1996.

3. Award by the Academy of Athens (29 December 1998) for the best research activity in 1998 related to hypertension.

4. Award of a Fulbright Scholarship for the Summer of 1999.

5. Award for the 3<sup>rd</sup> best presented poster in the Conference of Patras entitled Medicinal Chemistry Design and Development of Drugs in Medicinal Chemistry (1-3, 2001).

6. Award for the 3<sup>rd</sup> best presented poster in the Conference of Patras entitled Medicinal Chemistry Design and Development of Drugs in Medicinal Chemistry (7-9, 2002).

7. In October of 2000, a committee consisting of Prof. E.C. Constable, Prof. G.W. Gray, Prof. M.W. Gray, Prof. P.A. Schubiger and Dr. N. Ragousi, characterized the research activity of Medicinal Chemistry as an excellent ("the work done in this group is excellent") and also the research referred to the adulteration of olive oil ("the

work of the group on virgin olive oil adulteration is worthy of note”). LMA is involved in both activities.

8. Reference of my research activity on peptidomimetism by the company Synergix Ltd in the software of «Molecular Conceptor». A chapter is written on the synthesis of Bioactive Molecules with G. Cohen of the same company and the product is now commercially available.

9. Scholarship by Royal society and COST D22 to perform binding experiments of antihypertensive molecules in AT<sub>1</sub> and AT<sub>2</sub> receptors as well as cell cultures.

10. Selected to teach at the University of Cyprus courses of Organic and Medicinal Chemistry.

11. The article “Conformation and Bioactivity, Design and Development of Novel Antihypertensive Molecules is published in the Journal of “Current and Medicinal Chemistry (IF 4.483) and was selected one of the best articles. This article after being modified was published in the “Frontiers in Medicinal Chemistry (volume 2).

12. Invitation by Prof. A.M. Dopico to write a chapter in the book “Methods in Membrane Lipids” by Humana Press. The book has been circulated in 2007 and the chapter I have written appears with no 39 entitled “The Use of Differential Scanning Calorimetry to Study Drug-Membrane Interactions”.

13. Honored as a second degree Universal Title in Theology (3.2.2008).

14. Selected as evaluator from the Scientific Committee of National Programs of Slovenia during the phases A and B (2007 until now).

15. In Wikipedia there is a web site referred to AMG-3 cannabinoid in which the following publications are mentioned: Mavromoustakos T, Theodoropoulou E, Zervou M, Kourouli T, Papahatjis D. Structure elucidation and conformational properties of synthetic cannabinoids (-)-2-(6a,7,10,10a-tetrahydro-6,6,9-trimethyl-1-hydroxy-6H-dibenzo[b,d]pyranyl)-2-hexyl-1,3-dithiolane and its methylated analog. *Journal of Pharmaceutical and Biomedical Analysis*. 1999 Jan;18(6):947-56. PMID 9925329 and Durdagi S, Papadopoulos MG, Papahatjis DP, Mavromoustakos T. Combined 3D QSAR and molecular docking studies to reveal novel cannabinoid ligands with optimum binding activity. *Bioorganic and Medicinal Chemistry Letters*. 2007 Dec 15;17(24):6754-63. PMID 17980589

17. In <http://www.newsrx.com/article> (NewsRX. Medical News article on Medicinal Chemistry), 16.7.2007 is mentioned the article S. Durdagi *et al* J. Med. Chem. 50, 2875-2885 (2007).

18. In Chemistry, 19.1.2009 is mentioned the article S. Durdagi *et al* J. Chem. Inf. Model. 49,1139-1143 (2009).

19 The article by S. Durdagi *et al* J. Chem. Inf. Model. 49,1139-1143 (2009) is mentioned in the <http://www.rice.edu/nationalmedia/news2009-05-19-hiv.shtml>

20. In Science Daily in the Science news it is published the article entitled “Buckyball Computer Simulations Help Team Find Molecular Key to Combating

- HIV of the article by S. Durdagi *et al* J. Chem. Inf. Model. 49,1139-1143(2009)  
<http://www.sciencedaily.com/releases/2009/05/090519134839.htm>.
21. In the Genetic Engineering&Biotechnology News is mentioned the article by S. Durdagi *et al* J. Chem. Inf. Model. 49,1139-1143(2009)  
<http://www.genengnews.com/news/bnitem.aspx?name=54814928&taxid=3>
  22. It is mentioned in the Blog der Gesundheit. Eine gute Gesundheit ist das wichtigste für den Körper und vor allem für ihren Geist. Achten sie auf diesen! the article of S. Durdagi *et al* J. Chem. Inf. Model. 49,1139-1143(2009)  
<http://gesundheit-blog.weiterlesen.net/new-found-molekule-mai-block-hiv-spread.html>
  23. The article Combined 3D QSAR and molecular docking studies to reveal novel cannabinoid ligands with optimum binding activity Bioorganic & Medicinal Chemistry Letters, Volume 17, Issue 24, December 2007, Pages 6754-6763 by Durdagi, S.; Papadopoulos, M.G.; Papahatjis, D.P.; Mavromoustakos, T. was selected on the top 25 between October-December of 2007  
<http://top25.sciencedirect.com/subject/chemistry/6/journal/bioorganic-medicinal-chemistry-letters/0960894X/archive/14&print=true>
  24. The article Development of Accurate Binding Affinity Predictions of Novel Renin Inhibitors through Molecular Docking Studies. J. Mol. Gr. Mod. 29 425-435 (2010) από τους συγγραφείς A.P. Politi, S. Durdagi, P.M. Minakakis, T. Mavromoustakos, G. Kokotos was elected by the journal as one of the 25 best articles between October-December 2010.  
<http://top25.sciencedirect.com/subject/pharmacology-toxicology-and-pharmaceutical-science/20/journal/journal-of-molecular-graphics-and-modelling/10933263/archive/30>

### **Brief Description of My Research Activities**

- Design of novel drugs against various diseases (i.e hypertension and inflammation)

To achieve this aim I use the following physical chemical methodologies:

- a. Solid State Nuclear Magnetic Resonance in order to study the dynamic changes it causes the antihypertensive drug in the lipid bilayers. In addition, the orientation of drugs in lipid bilayers is sought using deuterium NMR in collaboration with synthetic chemists who deuterate specific sites of drugs.
- b. High Resolution Nuclear Magnetic Resonance in duterated solvents or environments that simulate the active site of action.
- c. Conformational Analysis Using NMR ROE data in combination with computational analysis and molecular modeling to complement the experimental results.
- d. Differential Scanning Calorimetry to study the thermal changes that causes the presence of pharmaceutical compounds with model membranes.
- e. X-ray diffraction where the topography of drugs is sought in lipid bilayers. The X-ray diffraction experiments are run in Graz of Austria under the guidance of Prof. P. Laggner.

- f. Raman Spectroscopy to study the interactions of bioactive compounds with lipid bilayers. In particular, the *trans:gauche* ratio is estimated at the different mesomorphic states of lipid bilayers.
- g. 3D-QSAR studies. CoMFA and CoMSIA softwares are applied to reveal the stereoelectronic requirements for a drug to exert biological activity. 3D-QSAR studies is a valuable tool in the rational design.
- h. Simulation of NMR spectra in liquid and solid state with the collaboration of theoretical physical chemists.
- k. Docking studies of antihypertensive drugs with AT1 receptor.
- l. Searching for pharmacophore models in bioactive drug molecules.

- Authenticity aspects of beverages and foods

- a. Study of geographical origin and adulteration of virgin olive oil by other cheaper oils using high resolution  $^{13}\text{C}$ -NMR of olefinic region. In addition it is studied the adulteration of refined oil by refined hazelnut oil.
- b. Study of authenticity of Cypriot beverage zivania with the combination of different physical chemical methods in collaboration with the University of Cyprus ( $^1\text{H}$ -NMR and Raman Spectroscopies, ICP, Gas Chromatography, Refractometry, Statistical Analysis to facilitate the analysis of the output data etc).

## **VISITS AND SPECIALISATION AFTER PH.D STUDIES**

1. Specialisation in the Computational Analysis and Molecular Modeling at Prof. Rod Hubbard's laboratory (York University, Summer of 1992).
2. Invited visit to Prof. Peter's Laggner laboratory in order to perform small and wide angle x-ray diffraction experiments. The results from this visit are published in the *Biochim. Biophys. Acta* (Summer of 1996).
3. Modern Experimental techniques using NMR spectrometer of AMX 500 MHz and use of modern software to process the experimental data (University of Connecticut, Summer of 1999).
4. Biological experiments related to the binding of novel AT1 antagonists at AT1 and AT2 receptors as well as cell cultures (University of Leeds, Summer of 2004).
5. Visits in the Synchrotron facilities of Trieste, Italy to perform x-ray experiments (Summers 2007, 2009).
6. Visits of National Institute of Chemistry, Ljubluana, Slovenia (Summers of 2010 and 2012)
7. Visit of BMRZ in Frankfurt of Germany, October 2011 and scheduled for September 2013 for running solid state NMR experiments using Bruker 600 and 850 MHz spectrometers.

## **FUNDING-WORKSHOPS**

1. Coordinator of a funded research project by the European Community entitled "Molecular Characterization of Virgin Olive Oil" (148.000 ECU).

2. Participation in the funded research project by the European Community entitled Development and Assessment of Methods for the Detection of Adulteration of Olive Oil with Hazelnut Oil GROWTH (MEDEO 2001).

3. Co-organization of a workshop with Maria Zervou held in Athens on November 22, 1996 about the “Use of Isotope Analyses Applications in Food and Beverage Authentication. Detection of Adulteration.” In this workshop six speakers from France, German and England informed the audience about the new techniques in the analyses and detection of adulteration of foods and beverages. The audience consisted of seventy scientists from Greece and Cyprus working in Food and Beverage Industry, Governmental Organizations related to Food and Beverage Control and Greek Universities.

3. Participation as a co-ordinator or participant in 25 funded research projects by the General Secretary of Greece and European Community.

4. Organization of a partners participating in the MEDEO program which is referred to Development of Novel Methods to Detect Adulteration of Olive Oil by Hazelnut Oil (November 2001).

5. Participation in COST D22 and COST D26 programs. Acquire SMT mission.

6. Participation as a co-ordinator in a research project funded by the Institute of Promotion of Research in Cyprus entitled “New Approaches to face Psoriasis” and bilateral collaborations between Cyprus with Slovenia and Romania.

7. Co-organisation with S. Mavromoustakos in Cyprus a scientific conference to honour D. Poulter (3.11.2008).

10. September 17<sup>th</sup> 2010. Co-organisation with Schrodinger a workshop entitled “From Structural Biology to Drug Discovery”. In this workshop 85 researchers and professors from all over Greece participated actively.

11. Chairman with Prof. A. Tsotinis for organizing the international 29th Cyprus-Camerino-Noordwijkerhout Trends in Drug Research ”. conference at Limassol-Cyprus between 2-7 September 2012.

12. Member of the organizing committee of the 32<sup>nd</sup> European Conference of Peptide Chemistry ( September Athens 2-7, 2012).

## **GREEK PATENTS**

1. T. Mavromoustakos, G. Bonas, M. Zervou, E. Theodoropoulou. A new method to detect Adulteration of Virgin Olive Oil (No **1002879**).

2. T. Mavromoustakos, G. Kokotos, P. Minakaki. Novel Antihypertensive Drugs (**No 1004905**).

### **PUBLISHED BOOKS (Greek language)**

1. T. Mavromoustakos, J.M. Matsoukas. Nuclear Magnetic Resonance.
  - Design of Pharmaceutical Molecules.
  - Applications in Medicine, Food and Beverage Chemistry January 1999.
3. 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 in all high schools of Greece.
4. 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.
5. 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.
6. T. Mavromoustakos. Use of the NMR in the study of pharmaceutical substances, zeolithes, polymers and archaeological findings. January 2001.
7. T. Mavromoustakos, J. Matsoukas. NMR spectroscopy . Application in Medicine, Pharmaceutical Chemistry, Biochemistry and Food and Beverage Chemistry (2006).
8. T. Mavromoustakos and P. Zoumpoulakis.. Molecular Modeling. Applications in Organic and Pharmaceutical Chemistry (pages 307) ISBN 978-960-89486-5- (2008).

### **Editor**

1. Bioactive Peptides in Drug Discovery and Design: Medical Aspects. This book was published by IOS press in January of 1999 as the 22<sup>nd</sup> 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 55<sup>th</sup> 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.

5. Guest Editor in Current Medicinal Chemistry volume 18(17), 2011. Methodologies and Applied Strategiew in the Rationa Drug Design.

***Graduate Students acquired Ph.D or Msc that performed the experimental work under my supervision***

1.E. Theodoropoulou, Ph.D. (1994-1997) 2. E. Matsouka, Ph.D. (2000-2001) 3. I. Daliani, Ph.D. (1998-2002) 4. M. Zervou Ph.D. (1998-2002) 5. I. Kyrikou, Msc (1999-2001) 6. I. Kyrikou, Ph.D. (2001-2004) 6. A. Zoga, Ph.D (2000-2004) 7. P. Zoumpoulakis, Ph.D. (2000-2005) 8. E. Mantzourani, Ph.D (2002-2007) 9. A. Kapou, Msc. (1999-2001) 10. A. Kapou, Ph.D. (2002-2007) 12. K. Pelekoukias, Msc. (2001-2002) 13.M. Smyrniotakis, Msc. (2002-2003) 14. G. Mouselimi, Msc (2003-2004) 15. I. Touris, Msc (2003-2004) 16. S. Gega, Msc. (2003-2005) 17. E. Chalkefs Msc. (2004-2006) 18. V. Mouchlis, Msc. (2005-2007) 19. C. Fotakis Msc. (2005-2007) 20. A. Politi, Msc. (2006-2007) 21. S. Durdagi (2006-2009). 22. A. Politi (Ph.D) (2007-2009) 23. C. Potamitis Ph.D. (2006-2009) 24. N. Neophytou Msc. (2008-2010) 25. V. Michopoulou Msc. (2008-2010) 26. V. Mouchlis Ph.D. (2007-2010) 27. X. Ntaltagianni (Msc.) (2010-2011) 28. N. Stavrinoudakis (Msc.) (2009-2011) 29. N. Varvarigou Msc. (2009-2011, 30. E. Kritsi Msc. (2010-2012) 31. E. Vrontaki, Msc. (2010-2012) 32. T. Kellici Msc. (2011-2013) 33. P. Kolocotroni Msc. (2011-2013) 34. D. Ntountaniotis (2007-2012) 35. P. Chatzigeorgiou Ph.D. (207-2012)

***Undergraduate Students that finished their diploma work under my supervision :***

Gili, A., Vasiliki, V., Argyriou, G., Gianni, M., Stougiannou, E., Vasiliou, V., Vatougia, G., Kritsi, E., Thanopoulos C., Xenos, I., Stavroula X., Maniati A., Brontaki, E. Stamelaki, V., N. Moustakas, L. Kokkinakis, C. Papaioannou, S. Mathioudaki, M Vanioti, L. Katsillis.

**Activity in Education**

1. Participation in different educational programs for teaching graduate students various aspects of Medicinal Chemistry and NMR spectroscopy (EPEAEK programs).
  - a. University of Patras, 1999 (Co-ordinator Prof. J. Matsoukas. Medicinal Chemistry, Drug Discovery and Design.)
  - b. University of Athens (Co-ordinator Prof. N. Xatdjichristidis, Polymer Science).
  - c. University of Ioannina, 2002-2003 (Co-ordinator Prof. N. Xatjihiliadis. Bioinorganic Chemistry).
  - d. University of Athens 2003-2005 (Co-ordinator Prof. G. Kokotos, Organic Synthesis and Application in the Industry).



## Teaching at the University of Cyprus at Chemistry Department of undergraduate courses.

- Laboratory of Organic Chemistry (553).
- Introduction in the Medicinal Chemistry (472)

## Teaching at the University of Athens

- Organic Chemistry (Undergraduate Course)
- NMR spectroscopy and Molecular Modeling (Graduate Course)
- Organic Chemistry for Physicists
- Bioorganic Chemistry (Organic Spectroscopy and Principles of Molecular Modeling)

## Seminars to high school teachers

- Seminars on the Modern Organic Chemistry and applications (May 1998).
- Guidelines on the philosophy of the written chemistry books for the high school students.
- Learning Chemdraw and Power Point (November 2008)

## Seminar for the scientists working in the Cyprus industry for food and beverages.

- Applications of Nuclear Magnetic Resonance as an aid to solve existing problems in industry.

## Participation

- Member of Research Committee for two Ph.D. students of Cyprus University and several students of Greek Universities. I am also participating as one of the majors advisors of the student S. Durdagi who will get Ph.D diploma from Frei University.

## LIST OF PUBLICATIONS

### • PUBLICATION IN JOURNALS

1. C.J. Van der Schyf, **T. Mavromoustakos**, A. Makriyannis: The conformation of (-)-8 $\alpha$ - and (-)-8 $\alpha$ -hydroxy- $\Delta^9$ -tetrahydrocannabinols and their interactions with model membranes. **Life Sci.** 42: 2231-2239 (1988).
2. **T. Mavromoustakos**, D.P Yang, A. Charalambous, L.G. Herbette, A. Makriyannis: Study of the topography of cannabinoids using x-ray diffraction. **BBA M BIO** 1024:336-344 (1990).

3. **T. Mavromoustakos**, D.P. Yang, W. Broderick, D. Fournier, L.G. Herbet, A. Makriyannis: Small Angle X-Ray Diffraction Studies on the Topography of cannabinoids in Synaptic Plasma Membranes. **Pharmacol. Biochem. Be.** 40, 547-552 (1991).
4. D.W. Chester, V. Skita, H.S. Young, **T. Mavromoustakos**, P. Shrittmatter: Bilayer structure and physical dynamics of the cytochrome b<sub>5</sub> dimyristoylphosphatidylcholine interaction. **Biophys. J.** 61, 1224-1243 (1992).
5. D.P. Yang, **T. Mavromoustakos**, K. Beshah, A. Makriyannis: Amphipathic interactions of cannabinoids with membranes. A comparison of cannabinoids with membranes. A comparison between  $\Delta^8$ -THC and its O-methyl analog using differential scanning calorimetry, X-ray diffraction and solid state <sup>2</sup>H-NMR. **BBA M BIO** 1103, 25-36 (1992).
6. D.P. Yang, **T. Mavromoustakos**, A. Makriyannis: Small Angle X-Ray Diffraction Studies of  $\Delta^8$ -tetrahydrocannabinol and its O-Methyl Analog in Membranes. **Life Sci** 53, 117-122 (1993).
7. P. Martel, A. Makriyannis, **T. Mavromoustakos**, K. Kelly and K.R. Jeffrey: Topography of tetrahydrocannabinol in model membranes using neutron diffraction. **BBA M BIO** 1151, 51-58 (1993).
8. J. Matsoukas, J. Hondrelis, M. Keramida, **T. Mavromoustakos**, A. Makriyannis R. Yamdagni, Q. Wu, G. Moore: Role of the NH<sub>2</sub>-terminal Domain of ANG II and [Sar<sup>1</sup>] ANG II on Conformation and Activity: NMR Evidence for Aromatic Ring Clustering and Peptide Backbone Folding Compared to [Des<sup>1,2,3</sup>] ANG II **J. Biol. Chem.** 269, 5303-5312 (1994).
9. **T. Mavromoustakos**, De-Ping Yang, A. Makriyannis. Topography of Alphaxalone and  $\Delta^{16}$ -alphaxalone in Membrane Bilayers containing cholesterol **BBA M BIO** 1194(1), 69-74 (1994).
10. **T. Mavromoustakos**, De-Ping Yang, E. Theodoropoulou, A. Makriyannis. Studies of the Conformational Properties of the Cannabinmimetic Aminoalkylindole Pravadoline Using NMR and Molecular Modeling. **Eur. J. Med. Chem** 30(3), 227-234 (1995).
11. **T. Mavromoustakos**, D.P. Yang, A. Makriyannis: Small angle x-ray diffraction and differential scanning calorimetric studies on O-methyl(-)- $\Delta^8$ -Tetrahydrocannabinol and its 5' iodinated derivative in membrane bilayers **BBA M BIO** 1237, 183-188 (1995).

12. **T. Mavromoustakos**, D.P. Yang, A. Makriyannis: Effects of the anesthetic steroids alphaxalone and its inactive analog  $\Delta^{16}$ -analog on the thermotropic properties of membrane bilayers. A model for membrane perturbation. **BBA M BIO** 1239(2), 257-264 (1995).
13. J. M. Matsoukas, G. Agelis, A. Wahhab, J. Hondrelis, D. Panagiotopoulos, R. Yamdagni, Q. Wu, **T. Mavromoustakos**, H.L.S. Maia, R. Ganter, G.J. Moore. Differences in backbone structure between angiotensin II agonists and type I antagonists. **J. Med. Chem.** 38(23), 4660-4669 (1995).
14. **T. Mavromoustakos**, E. Theodoropoulou, D. Papahatjis, T. Kourouli, De-Ping Yang, M. Trumbore, A. Makriyannis: Studies on the thermotropic effects of cannabinoids on phosphatidylcholine bilayers using differential scanning calorimetry and small angle X-ray diffraction. **BBA M BIO** 1281(2), 235-244 (1996).
15. A. Ioannou, A. Dimirkou, **T. Mavromoustakos**. Isotherms of phosphate sorption by hematite and bentonite-hematite (b-h) system **Commun. Soil Sci. Plant Anal.** 27(5-8), 1901-1924 (1996).
16. M. Koufaki, T. Calogeropoulou, **T. Mavromoustakos**, E. Theodoropoulou, A. Tsoinisi, A. Makriyannis. Synthesis of  $^2\text{H}$ -Labelled Alkoxyethyl Phosphodiester AZT Derivatives for Solid-State  $^2\text{H}$ -NMR Studies. **J. Heterocyclic Chem.** 33, 619-622 (1996).
17. J.M. Matsoukas, D. Panagiotopoulos, M. Keramida, **T. Mavromoustakos**, R. Yamdagni, Q. Wu, G.J. Moore, M. Saifeddine, M. D. Hollenberg: Synthesis and Contractile Activities of Cyclic Thrombin Receptor Derived Peptide Analogues with a Phe-Leu-Leu-Arg Motif: Importance of the Phe /Arg Relative Conformation and the Primary Amino Group for Activity. **J. Med. Chem.** 39, 18, 3585-3591 (1996).
18. **T. Mavromoustakos**, E. Theodoropoulou, De-Ping Yang, Sonyyan Lin, M. Koufaki, A. Makriyannis. The conformational properties of the Antineoplastic Ether Lipid 1-thiohexadecyl-2-O-methyl-*rac*-glycero-3-phosphocholine **Chem. Phys. Lipids** 84, 1, 21-34 (1996).
19. **T. Mavromoustakos**, D.P. Yang, A. Makriyannis. Topography and thermotropic properties of cannabinoids in brain sphingomyelin bilayer **Life Sci.** 59, 23, 1969-1979 (1996).
20. **T. Mavromoustakos**, E. Theodoropoulou, C. Dimitriou, J. Matsoukas, D. Panagiotopoulos, A. Makriyannis. Interactions of Angiotensin II with Membranes using a combination of Differential Scanning Calorimetry and  $^{31}\text{P}$ -NMR spectroscopy **LIPS** 3(4), 175-180 (1996).

21. E. Theodoropoulou, **T. Mavromoustakos**, D. Panagiotopoulos, J. Matsoukas, J. Smith. Superimposition of potent non-peptide AT<sub>1</sub> receptor antagonists with angiotensin II. **LIPS** 3, 209-216 (1996).
22. D. Panagiotopoulos, J. Matsoukas, K. Alexopoulos, A. Zebeki, **T. Mavromoustakos**, M. Saifeddine, M. Hollenberg. Synthesis and activities of cyclic thrombin-receptor-derived peptide analogues of the Ser<sub>42</sub>-Phe-Leu-Leu-Arg<sub>46</sub> motif sequence containing D-Phe and/or D-Arg. **LIPS** 3, 233-240 (1996).
23. A. Vyza, E. Tsitsa, E. Theodoropoulou, **T. Mavromoustakos**. Complexation of new active antibacterial adamantan derivatives with  $\beta$ -CD:Preparation and characterization of complexes. Study of the thermotropic properties of pure and complex form with dipalmitoyl phosphatidylcholine bilayers. **JOU INC PHE MOL**, 25 337-340 (1996).
24. J. Matsoukas, M.D. Hollenberg, **T. Mavromoustakos**, D. Panagiotopoulos, K. Alexopoulos, R. Yamdagni, Q. Wu, G.J. Moore. Conformational Analysis of the Thrombin Receptor Agonist Peptides SFLLR and SFLLR-NH<sub>2</sub> by NMR: Evidence for a Cyclic Bioactive Conformation. **J. Protein Chem.** 16, 2, 113-131 (1997).
25. **T. Mavromoustakos**, E. Theodoropoulou, De-Ping Yang. The use of high-resolution solid-state NMR spectroscopy and differential scanning calorimetry to study interactions of anaesthetic steroids with membrane. **BBA M BIO** 1328(1), 65-73 (1997).
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#### **PRESENTATIONS –ABSTRACTS (Partial)**

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172. C. Petrou, S. Mavromoustakos, E. Kokkalou, V. Roussis, E. Christofi, G. Efthimiou, C. Potamitis, S. Durdagi, **T. Mavromoustakos**. Isolation of psoralens from the Ficus sycomorus juice. A novel approach against psoriasis. The Cyprus Conference CNC on New Methods in Drug Research May 11-16, 2008, Limassol, Cyprus (page 28).
173. V. Mouchlis, **T. Mavromoustakos**, G. Kokotos. Application of Docking to study the binding affinity between human nonpancreatic phospholipase A2 (IIA) and bioactive analogues of its inhibitor FPL67047XX. The Cyprus Conference CNC on New Methods in Drug Research May 11-16, 2008, Limassol, Cyprus (page 29).
174. A. Politi, S. Durdagi, E. Papavasiliopoulou, P. Moutevelis-Minakakis, G. Kokotos, **T. Mavromoustakos**. 3D QSAR CoMFA/CoMSIA studies on renin inhibitors. The Cyprus Conference CNC on New Methods in Drug Research May 11-16, 2008, Limassol, Cyprus (page 30).

175. A. Politi, M. Zervou, P. Zoumpoulakis, A. Zoga, P. Moutevelis-Minakakis, G. Kokotos, E.K. Iliodromitis, D.Th. Kremastinos, **T. Mavromoustakos**. Hypertension study in anaesthetized rabbits: A new protocol for AT<sub>1</sub> antagonists screening. The Cyprus Conference CNC on New Methods in Drug Research May 11-16, 2008, Limassol, Cyprus (page 31).
176. C. Potamitis, C. Photakis, S. Gega, E. Siapi, K. Viras, P. Moutevelis-Minakakis, C.G. Kokotos, M. Rappolt, **T. Mavromoustakos**. Comparison study of membrane perturbing ability between AT<sub>1</sub> antagonist valsartan and a novel synthetic pyrrolidinone analog MMK3 as depicted by a combination of Differential Scanning Calorimetry and Raman Spectroscopy. The Cyprus Conference CNC on New Methods in Drug Research May 11-16, 2008, Limassol, Cyprus (page 32).
177. **T. Mavromoustakos**, P.M.Minakakis, G. Kokotos, E. Papavassilopoulou, C. Potamitis, C. Photakis, K. Viras, C. Koukoulitsa, E. Kalatzis, S. Durdagi. Peptide Mimetics and Their Interdigitation with Lipid Bilayers. Page 31. 6<sup>o</sup> Hellenic Forum on Bioactive Peptides, 18-20 May 2008, Conference and Cultural Center of the University page 31.
178. E. Papavassilopoulou, J. Vranas, P.M. Minakakis, G. Michas, M. Papakonstantinou, A. Politi, **T. Mavromoustakos**, G. Kokotos. Synthesis of new 2-pyrrolidinones. 6<sup>o</sup> Hellenic Forum on Bioactive Peptides, 18-20 May 2008, Conference and Cultural Center of the University page 46.
179. E. Papavassilopoulou, P. M. Minakakis, **T. Mavromoustakos**, A. Politi, G. Kokotos. Design and Synthesis of a Novel Potential Renin Inhibitor. 6<sup>o</sup> Hellenic Forum on Bioactive Peptides, 18-20 May 2008, Conference and Cultural Center of the University page 50.
180. C. Potamitis, C. Photakis, S. Gega, E. Siapi, K. Viras, P.M. Minakakis, C.G. Kokotos, M. Rappolt, **T. Mavromoustakos**. Comparison study of the membrane perturbing ability between AT<sub>1</sub> antagonist Valsartan and a novel synthetic pyrrolidinone analog MMK3 as depicted by a combination of Differential Scanning Calorimetry and Raman Spectroscopy. 6<sup>o</sup> Hellenic Forum on Bioactive Peptides, 18-20 May 2008, Conference and Cultural Center of the University page 59.
181. **T. Mavromoustakos**. 2 one hour talks given on a Workshop on Structure Based Drug Discovery June 4 (Athens, 2-6 June 2008, Institute of Organic and Pharmaceutical Chemistry, National Hellenic Research Foundation). Titles of the talks: a. A concerted approach using NMR spectroscopy and Theoretical Calculations to study the Conformational Properties of a Potent Cannabinoid Analogue AMG-3. b. The Contribution of NMR Spectroscopy and other Biophysical Methodologies to study the Molecular Basis of Interdigitation. Natural Products, International Conference, Atheneum Intercontinental 3-8 August 2008, Athens, Greece.
182. **Mavromoustakos, T.**, Petrou, C., Kokkalou, E., Roussis, V., Christofi, V., Efthimiou, G., Potamitis, C., Durdagi, S., Mavromoustakos, S. Ficus sycomorous sap: a psoralene source with potential for the treatment of psoriasis. 202. Koukoulitsa C., Tsantili-Kakoulidou A., T. Mavromoustakos, Chinou I. Natural coumarins and PLS



analysis for antibacterial activity using VolSurf descriptors. Natural Products, International Conference, Atheneum Intercontinental 3-8 August 2008, Athens, Greece.

183. **Mavromoustakos T.**, Durdagi, S., Papahadjis, D., Papadopoulos, M.G. X-ray diffraction studies combined with molecular dynamics calculations to study the effects of cannabinoids in lipid bilayers and CB receptor active site. Hellenic Crystallographic Association 4<sup>th</sup> conference dedicated to the memory of Dr. N. Oikonomakos. 26-27 September 2008, Athens, Greece. Abstract book page 23.

184. (invited speaker) **Mavromoustakos T.**, Durdagi, S., Reis, H., Koukoulitsa, C., Papadopoulos, M. A Concerted Approach Using Physical Chemical Methodologies, Computational Chemistry and 3D QSAR Studies Aiming to Develop Novel Analgesic Cannabinoid Analogs. P-124. Ehrlich II, 2<sup>nd</sup> World Conference on Magic Bullets. Celebrating the 100<sup>th</sup> Anniversary of the Nobel Prize Awarded to Paul Ehrlich. Nurnberg, Germany October 3-5, 2008.

185. **T. Mavromoustakos.** Rational Drug Design. 3.11.2008, (honoured to Prof.) Dale Poulter.

186. **T. Mavromoustakos.** Novel Strategies in the Drug Design. Workshope 5-6 December 2008 held in NHRF, Athens.

187. C. Koukoulitsa, A.Tsantili-Koukoulidou, **T. Mavromoustakos.** Quantitative Structure Retention Relationships for IAM Chromatographic Indices using VolSurf Approach. Comparison with Octanol-Water Distribution Coefficients. logP<sub>2009</sub>. PhysChem and ADMET Profiling in Drug Research. The 4<sup>th</sup> LogP Symposium. February 8-11, 2009, ETH Zurich, Switzerland.

188. C. Koukoulitsa, **T. Mavromoustakos**, S. Durdagi, V. Mouchlis, A. Politi, P. Minakaki, M.G. Papadopoulos, G. Kokotos. Rational Design Applications in the Drug Discovery. 10<sup>th</sup> Conference with International Participation in Medicinal Chemistry, Drug Discovery and Design, March 18-20, Patras, Greece, 2009 (abstract proceedings page 73).

189.C. Potamitis, M. Zervou, T. Tselios, J. Matsoukas, K. Viras, **T. Mavromoustakos.** Study of Myelin Basic Protein Peptide analogues interactions with lipid bilayers using DSC, Raman and Solid State <sup>13</sup>C and <sup>31</sup>P NMR Spectroscopy. 10<sup>th</sup> Conference with International Participation in Medicinal Chemistry, Drug Discovery and Design, March 18-20, Patras, Greece, 2009 (abstract proceedings page 90).

190. M. Smyrniotakis, P. Zoumpoulakis, **T. Mavromoustakos.** Conformational Studies of AT<sub>1</sub> Antagonists in Micelle and Liposomal Environment. 10<sup>th</sup> Conference with International Participation in Medicinal Chemistry, Drug Discovery and Design, March 18-20, Patras, Greece, 2009 (abstract proceedings page 93).

191. C. Fotakis, D. Christodouleas, M. Zervou, N.P. Benetis, K. Viras, **T. Mavromoustakos.** Development of a CP-31 NMR broadline simulation methodology for studying the interactions of antihypertensive AT<sub>1</sub> antagonist losartan with

phospholipid bilayers. 10<sup>th</sup> Conference with International Participation in Medicinal Chemistry, Drug Discovery and Design, March 18-20, Patras, Greece, 2009 (abstract proceedings page 101).

192. (invited speaker). **T. Mavromoustakos**. Interdigitation effects of drugs incorporated in lipid bilayers: Possible consequences in rational drug design. Theobio09. 4<sup>th</sup> International Symposium of Theoretical Biophysics. Roscoff June 29-July 3.

193. (speaker) **T. Mavromoustakos**. 3th Hellenic Symposium on Organic Synthesis.From Chemistry to Biology, Medicine and Materials Science. 15-17 October 2009. University of Athens. The biodiversity in nature provides solutions to synthetic organic chemists.

194. (poster) E. Papavassilopoulou, P. Moutevelis-Minakakis, D. Delivoria, **T. Mavromoustakos**, G. Kokotos. Synthesis of new 2-pyrrolidinones as potential rennin inhibitors. Hellenic Symposium on Organic Synthesis.From Chemistry to Biology, Medicine and Materials Science. 15-17 October 2009. University of Athens.

195. (poster) C. Potamitis, M. Matsoukas, T. Tselios, S.G. Grdadolnik, **T. Mavromoustakos**. Conformational Analysis of Myelin Basic Protein. Peptide Analogues with the use of NMR spectroscopy and molecular dynamic simulations. Hellenic Hellenic Symposium on Organic Synthesis.From Chemistry to Biology, Medicine and Materials Science. 15-17 October 2009. University of Athens.

196. (poster) N. Neophytou, C. Koukoulitsa, V. Mouchlis, E. Papavassilopoulou, K. Georgikopoulou, G. Michas, **T. Mavromoustakos**, P. Moutevelis-Minakakis, G. Kokotos, D. Hadjipavlou. Doking studies of pyrrolidinone derivatives to soybean lipoxygenase-3. Hellenic Symposium on Organic Synthesis.From Chemistry to Biology, Medicine and Materials Science. 15-17 October 2009. University of Athens.

197. (poster) V. Mouchlis, V. Magrioti, N. Cermak, A. Bilger, R. Oslund, **T. Mavromoustakos**, M. Gelb, G. Kokotos. Molecular Modeling studies of secreted phospholipase A<sub>2</sub> inhibition by 2-oxoamides based on  $\alpha$ -amino acids. Hellenic Symposium on Organic Synthesis.From Chemistry to Biology, Medicine and Materials Science. 15-17 October 2009. University of Athens.

198. (poster) V. Mouchlis, M. Kokotou, F. Sympoura, **T. Mavromoustakos**, V. Constantinou-Kokotou. Molecular Modeling studies of secreted phospholipase A<sub>2</sub> inhibition by natural products. Hellenic Symposium on Organic Synthesis.From Chemistry to Biology, Medicine and Materials Science. 15-17 October 2009. University of Athens.

199. C. Potamitis, T. Tselios, J. Matsoukas, M. Matsoukas, **T. Mavromoustakos**. Interdigitation of peptide analogs in lipid bilayers. Dr C Potamitis was one of the 10 Ph.D. students selected to present the oral communication during the XXIX Advanced Course of European School of Medicinal Chemistry and "E. Duvanti", National Seminar for PhD students, Urbino September 13-18, 2009.

200. P. Zoumpoulakis, S. Durdagi, C. Potamitis, E. Kritsi, S.G. Grdadolnik, **T. Mavromoustakos**. Comparative conformational analysis and docking studies between telmisartan and valsartan. Insights on the molecular basis of action of their pharmacophores associated with AT<sub>1</sub> antagonism. 14<sup>th</sup> Hellenic Symposium on Medicinal Chemistry. 23-25 April, 2010. Thessaloniki, Greece.
201. V. Mouchlis, V. Michopoulou, **T. Mavromoustakos**, G. Kokotos. Molecular Docking and Molecular Dynamics simulations on 2-oxoamide cytosolic phospholipase A<sub>2</sub> inhibitors. 14<sup>th</sup> Hellenic Symposium on Medicinal Chemistry. 23-25 April, 2010. Thessaloniki, Greece.
202. (poster) N. Neophytou, E. Papavassilopoulou, G. Michas, V. Mouchlis, C. Koukoulitsa, M. Zheng, D. Hadjipavlou-Litina, G. Kokotos, P. Moutevelis-Minakakis, **T. Mavromoustakos**. An attempt to rationally design inhibitors through docking experiments at the active site of lipoxygenase-3. 11<sup>th</sup> 14<sup>th</sup> Hellenic Symposium on Medicinal Chemistry. 23-25 April, 2010. Thessaloniki, Greece.
203. (poster) V. Michopoulou, V. Mouchlis, **T. Mavromoustakos**, G. Kokotos. Studies on the interactions of the active site of cytosolic phospholipase A<sub>2</sub> with inhibitors containing activated carbonyl functionalities. 14<sup>th</sup> Hellenic Symposium on Medicinal Chemistry. 23-25 April, 2010. Thessaloniki, Greece.
204. (poster) M. Kokotou, V. Mouchlis, **T. Mavromoustakos**, V. Constantinou-Kokotou. Molecular Modeling studies of secreted phospholipase A<sub>2</sub> inhibition by oleuropein. 14<sup>th</sup> Hellenic Symposium on Medicinal Chemistry. 23-25 April, 2010. Thessaloniki, Greece.
205. (invited speaker) **T. Mavromoustakos**. The molecules of the brain. A speech dedicated to composer and chemist M. Plessas. 11<sup>th</sup> Conference with International Participation on Medicinal Chemistry: Drug Discovery and Design. April 25-28, 2010, Patras, Greece.
206. (poster) E. Kritsi, S. Chatziaggeloglou, P. Zoumpoulakis, C. Potamitis, N. Papakonstantopoulos, **T. Mavromoustakos**. Comparative Conformational Analysis Study of Candesartan with Eprosartan and Losartan. 11<sup>th</sup> Conference with International Participation on Medicinal Chemistry: Drug Discovery and Design. April 25-28, 2010, Patras, Greece.
207. (poster) C. Koukoulitsa, M. Chrysanthakopoulos, D. Vrakas, C. Giaginis, **T. Mavromoustakos**, A. T. Kakoulidou. The use of volsurf approach to explore IAM and HAS chromatographic indices. 18<sup>th</sup> EuroQSAR 19-24 September 2010. Rhodes-Greece.
208. (poster) V. Michopoulou, V. Mouchlis, **T. Mavromoustakos**, G. Kokotos. Molecular Docking studies of inhibitors containing activated carbonyl functionalities in the active site of cytosolic phospholipase A<sub>2</sub>. 18<sup>th</sup> EuroQSAR 19-24 September 2010. Rhodes-Greece.

209. (poster) V. Mouchlis, **T. Mavromoustakos**, G. Kokotos. Molecular Docking and 3D-QSAR COMFA studies on indole inhibitors of GIIA secreted phospholipase A<sub>2</sub>. 18<sup>th</sup> EuroQSAR 19-24 September 2010. Rhodes-Greece.
210. (poster) N. Neophytou, G. Michaw, D. Hadjipavlou-Litina, M. Zheng, G. Kokotos, P. Moutevelis-Minakakis, **T. Mavromoustakos**. Comparative docking studies at the active site of lipoxygenase-3, lipoxygenase-5 and cyclooxygenase-2. 18<sup>th</sup> EuroQSAR 19-24 September 2010. Rhodes-Greece.
211. (invited speaker). **T. Mavromoustakos**. The Use of High Resolution Liquid and Solid State NMR Spectroscopy in the Rational Drug Design. EAST-NMR meeting. Satellite of 18<sup>th</sup> EuroQSAR 24-26 September 2010. Rhodes-Greece.
212. **T. Mavromoustakos**. Cerebrosides, myelin, hormone LHRH, brain. Review of Clinical Pharmacology and Pharmacokinetics. 25, 21, 2011.
213. E. Kritsi, S. Chatziaggeloglou, P. Zoumpoulakis, C. Potamitis, N. Papakonstantopoulos, **T. Mavromoustakos**. Review of Clinical Pharmacology and Pharmacokinetics. 25, 31, 2011.
214. (invited speaker) **T. Mavromoustakos**, S. Durdagi, C. Koukoulitsa, M.G. Papadopoulos, C. Tzoupis. Strategies in the Rational Drug Design. 25<sup>th</sup> National Chemistry Congress with International Participation. Erzurum Turkey, 27 June-2 July 2011.
215. S. Durdagi, H.J. Duff, S.Y. Noskov, **T. Mavromoustakos**, M.G. Papadopoulos, C.T. Supuran, M. Senturk, D. Ekinici. Applications of Computational Chemistry Approaches to Biological Systems: Recent Advances and Future Directions in Computer-Aided Drug Design Studies. 25<sup>th</sup> National Chemistry Congress with International Participation. Erzurum Turkey, 27 June-2 July 2011.
216. (invited speaker) **T. Mavromoustakos**. Strategies used to design new medicine. Austin, Texas, USA, August 4, 2011.
217. V. Mouchlis, V. Magrioti, E. Barbayianni, **T. Mavromoustakos**, M.H. Gelb, G. Kokotos. 29<sup>th</sup> Trends in Drug Research. Cyprus-Noordwijkerhout-Camerino Symposium. Limassol, Cyprus, October 2-7, 2011.
218. K. Gkountelias, K. Spyridaki, P. Giannopoylos, A. Akritides, M. Papadokostaki, **T. Mavromoustakos**, G. Liapakis. Determination of Residues in the Third Membrane Spanning Segment of CRF1, which are accessible in the ligand binding-site crevice of receptor. Cyprus-Noordwijkerhout-Camerino Symposium. Limassol, Cyprus, October 2-7, 2011.
219. E. Vrontaki, S.K. Hadjidakou, S. Golic Grdadolnik, **T. Mavromoustakos**. NMR spectroscopy and docking study of complex Ag(tpp)<sub>3</sub>(asp) to soybean lipoxygenase-1. Cyprus-Noordwijkerhout-Camerino Symposium. Limassol, Cyprus, October 2-7, 2011.

220. C. Koukoulitsa, G. Agelis, A. Resvani, J. Matsoukas, **T. Mavromoustakos**. Structural elucidation conformational properties and molecular docking study at Bace-1 of bioactive molecule BV6. Cyprus-Noordwijkerhout-Camerino Symposium. Limassol, Cyprus, October 2-7, 2011.
221. V. Nikoletta, M. Gregory, A. Tsotinis, M. Papadopoulos, **T. Mavromoustakos**. Docking, molecular dynamics and NMR spectroscopy study of two new cytotoxic c2-substituted pyrrolo [2,3-f] quinolines. Cyprus-Noordwijkerhout-Camerino Symposium. Limassol, Cyprus, October 2-7, 2011.
222. D. Ntountaniotis, G. Mali, S.G. Grdadolnik, M. Halabalaki, A.L. Skaltsounis, C. Potamitis, E. Siapi, P. Hatzigeorgiou, M. Rappolt, T. Mavromoustakos. Thermal and dynamic properties of drug AT<sub>1</sub> antagonist olmesartan in lipid bilayers using various physical-chemical methodologies. Cyprus-Noordwijkerhout-Camerino Symposium. Limassol, Cyprus, October 2-7, 2011.
223. (invited) T. Mavromoustakos. Rational Drug Design. Structure-&Computer-aided Design Workshop:Bioactive Molecules&Materials. 7-11 November, 2011. Athens, Greece.
224. H. Tzoupis, G. Leonis, S. Durdagi, V. Mouchlis, **T. Mavromoustakos**, M.G. Papadopoulos. Binding of Novel Fullerene Inhibitors to HIV-1 Protease:Insight through Molecular Dynamics and Molecular Mechanics Poisson-Boltzmann Surface Area Calculations.Structure-&Computer-aided Design Workshop:Bioactive Molecules&Materials. 7-11 November, 2011. Athens, Greece.
225. (invited speaker) **T. Mavromoustakos**, C. Koukoulitsa, X. Tzoupis, M. Papadopoulos, G. Leonis, D. Ntountaniotis, G. Aggelis, T. Tselios, J. Matsoukas, G. Liapakis, E. Vrontaki, S.K. Hadjidakou, S. Golic Grdadolnik, M. Simcic, G. Mali, C. Glaubitz, J. Baldus, S. Durdagi. Applications of NMR Spectroscopy in the Organic and Medicinal Chemistry, EuAsC<sub>2</sub>S-12 April 16-21 2012, Corfu, Greece.
226. (poster) E. Vrontaki, A. Maniati, N. Varvarigou, G. Megariotis, G. Leonis, M. Vlachou, A. Eikosipentaki, R. Kompogennitaki, M. Papadopoulos, S.G. Grdadolnik, **T. Mavromoustakos**, A. Tsotinis. Conformational Analysis of two novel cytotoxic C2-substituted pyrrolo[2,3-f]quinolines in organic and aqueous media, membrane bilayers and at the putative active site. 30<sup>th</sup> Noordwijkerhout-Camerino-Cyprus-Symposium. May 13<sup>th</sup>- 17<sup>th</sup>, 2012, Royal Tropical Institute Amsterdam.
227. C. Koukoulitsa, C. Villalonga-Barber, B.R. Steele, O. Belda, M. Micha-Screttas, **T. Mavromoustakos**. Rational Design and Biological Evaluation of Novel Resveratrol and Glyoxylato-arylhyazone analogs against Alzheimer disease. 15<sup>th</sup> Hellenic Symposium on Medicinal Chemistry Athens, May 25-27, 2012.
228. T. Charalambos, G. Leonis, S. Durdagi, V. Mouchlis, **T. Mavromoustakos**, M. Papadopoulos. Binding of novel fullerene inhibitors to HIV-1 protease: Insight through molecular dynamics and molecular mechanics poisson-boltzmann surface area calculations. 15<sup>th</sup> Hellenic Symposium on Medicinal Chemistry Athens, May 25-27, 2012.

229. N. Stavrinouidakis, N. Neophytou, V. Magrioti, **T. Mavromoustakos**, G. Kokotos. Probing for novel and selective monoglyceride lipase inhibitors. 15<sup>th</sup> Hellenic Symposium on Medicinal Chemistry Athens, May 25-27, 2012.
230. A. Afantitis, G. Melagraki, C. Koukoulitsa, M. Koufaki, **T. Mavromoustakos**. Modelling and predicting oxidative stress-induced neuronal damage by chroman analogues. 15<sup>th</sup> Hellenic Symposium on Medicinal Chemistry Athens, May 25-27, 2012.
231. E. Vrontaki, M. Simcic, S. Golic-Grdadolnik, S.K. Hadjiikakou, T. Mavromoustakos. Study of the conformation of Cu complexes with aspirin. 15<sup>th</sup> Hellenic Symposium on Medicinal Chemistry Athens, May 25-27, 2012.
232. K. Spyridaki, K. Gkoutelias, T. Tselios, V. Magafa, R. Exarchakou, M. Papadokostaki, **T. Mavromoustakos**, G. Liapakis. Structure-function analysis of the second extracellular loop of type 1 receptor of the corticotrophin releasing factor, S90. Abstracts 32<sup>nd</sup> European Peptide Symposium, 2-7 September 2012, Athens, Greece. Journal of Peptide Science 18, S1, 1-224.
233. S. Vasilakaki, E. Barbayianni, **T.M. Mavromoustakos**, M.H. Gelb, G. Kokotos. Hydrophobic  $\alpha$ -Amino Acids Favour the Inhibition of Human GIIA Phospholipase A<sub>2</sub> by 2-Oxoamides, S95-S96. Abstracts 32<sup>nd</sup> European Peptide Symposium, 2-7 September 2012, Athens, Greece. Journal of Peptide Science 18, S1, 1-224.
234. A. Politi, G. Leonis, H. Tzoupis, D. Ntountaniotis, M.G. Papadopoulos, S.G. Gardadolnik, T. Mavromoustakos. Conformational properties and energetic analysis of aliskiren in solution and receptor site, S109. Abstracts 32<sup>nd</sup> European Peptide Symposium, 2-7 September 2012, Athens, Greece. Journal of Peptide Science 18, S1, 1-224.
- 235.G. Aggelis, A. Resvani, S. Durdagi, T. Tumova, J. Slaninov, P. Giannopoulos, K. Spyridaki, G. Liapakis, D. Vlahakos, **T. Mavromoustakos**, J. Matsoukas. A concise synthesis, docking studies and biological evaluation of N-substituted 5-butyylimidazole analogues as potent angiotensin II receptor blockers, S116. Abstracts 32<sup>nd</sup> European Peptide Symposium, 2-7 September 2012, Athens, Greece. Journal of Peptide Science 18, S1, 1-224.
236. A. Resvani, C. Nikolis, G. Liapakis, D. Vlahakos, C. Koukoulitsa, D. Ntountaniotis, **T. Mavromoustakos**, J. Matsoukas, G. Agelis. Facile and Efficient Syntheses of Structurally Modified E-urocanic Acid Analogs as Potent Anagiotensin II Receptor Blockers, S120. Abstracts 32<sup>nd</sup> European Peptide Symposium, 2-7 September 2012, Athens, Greece. Journal of Peptide Science 18, S1, 1-224.
237. G. Agelis, A. Resvani, C. Koukoulitsa, A. Afantitis, G. Melegraki, A. Sifaka, E. Gkini, T. Tumova, K. Spyridaki, D. Kalaviziotti, M-E Androutsou, J. Sianinova, G. Liapakis, D. Vlahakos, **T. Mavromoustakos**, J. Matsoukas. Rational Design, Efficient Synthesis, Biological Evaluation of New N,N '-bis-substituted Butylimidazole Analogs as Potent Angiotensin Receptor Blockers,, S123. Abstracts

32<sup>nd</sup> European Peptide Symposium, 2-7 September 2012, Athens, Greece. Journal of Peptide Science 18, S1, 1-224.

238. H. Tzoupis, G. Leonis, G. Megariotis, C.T. Supuran, **T. Mavromoustakos**, M.G. Papadopoulos. Effective inhibition of aspartic proteases: Advancements in aids-hypertension-diabetes linkage. International Conference on Chemistry for Health. Athens, 9-14 September 2012, Athens, Greece.

239. A. Politi, G. Leonis, H. Tzoupis, D. Ntountaniotis, M.G. Papadopoulos, S.G. Gardadolnik, **T. Mavromoustakos**. Conformational properties and energetic analysis of aliskiren in solution and receptor site. International Conference on Chemistry for Health. Athens, 9-14 September 2012, Athens, Greece.

240. (invited speech and poster) D. Ntountaniotis, P. Kolokotroni, J. Baldus, C. Glaubitz, **T. Mavromoustakos**. Exploring the molecular basis of interactions of candesartan cilexetil (TCV-116) in lipid bilayers using solid state NMR spectroscopy. 3<sup>rd</sup> Annual East-NMR User Meeting. Lasko, Slovenia, November 13-16, 2012.

241. (invited speech) **T. Mavromoustakos**. “Successful and Unsuccessful stories in the Rational Drug Design”. BAU International Drug Design Symposium Istanbul, 21-23 March 2013.

242. (invited workshop) **T. Mavromoustakos**. Theoretical Background for the use of NMR Spectroscopy and Molecular Modeling to Predict of Putative Bioactive Conformation of Drugs”. BAU International Drug Design Symposium Istanbul, 21-23 March 2013.

243. (invited workshop) **T. Mavromoustakos**. A reaction in the NMR tube can be converted to a facile method of preparing methyl ethers. 2<sup>nd</sup> SEE-dRUG Workshop-NMR Basics&Applications in Life Sciences.

244. **T. Mavromoustakos**. A facile and efficient drug:active site interactions and a synthetic method for methyl ethers.NMR in protein dynamics and structural biology 10-13 June, 2013 Budapest.

245. G. Kordopati, T. Tselios, **T. Mavromoustakos**, S.G. Gardadolnik, G. Tsivgoulis. Synthesis and interaction studies of  $\beta$ -cyclodextrin/hrh analogue conjugate by using nmr spectroscopy. NMR in protein dynamics and structural biology 10-13 June, 2013 Budapest.



**A**

#### **ARTICLES OF GENERAL INTEREST**

Author of **60** various articles in Greek language, related to education as well as of general interest (i.e. thermodynamics and entropy, the use of analogs in quantum chemistry, olive oil health and tradition etc).



#### **ARTICLES RELATED TO THEOLOGY AND CIVILISATION** Author

of **21** articles in theology and civilisation published in Greek and Cypriot journals.