

THOMAS MAVROMOUSTAKOS
Capodistrian University of Athens
Professor of Chemistry Department

Date of birth: 6.18.1960

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EDUCATION

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

M.Sc. 1988 Medicinal Chemistry, University of Connecticut, USA

Ph.D. 1990, Medicinal Chemistry, University of Connecticut, USA

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

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

Ph.D. 2014- 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 conformational 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

September 2016-June 2017 Sabbatical to work on teaching and doing research in New York College

AWARDS-SCHOLARSHIPS-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 3rd 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 3rd 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 3rd 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 και 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"). As a director of LMA I was 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 AT₁ and AT₂ 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.
16. 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).
17. 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>
18. 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>.
19. In the Genetic Engineering & Biotechnology News is mentioned the published 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>
20. 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>
21. The article Combined 3D QSAR and molecular docking studies to reveal novel cannabinoid ligands with optimum binding activity published in 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>

22. The article Development of Accurate Binding Affinity Predictions of Novel Renin Inhibitors through Molecular Docking Studies. J. Mol. Gr. Mod. 29 425-435 (2010) by 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 (neurodegenerative diseases, diabetes, cancer, hypertension, inflammation and psychotropic)

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 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 deuterated 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 and ELETTRA facilities in Trieste of Italy.
- 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 drugs acting on receptors, DNA and bilayer environment.

- 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}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 (^1H -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, 2016).
6. Visits of National Institute of Chemistry, Ljubljana, Slovenia (Summers of 2010, 2012, 2013, 2014, 2015, 2016)
7. Visit of BMRZ in Frankfurt of Germany, (2011, 2013, 2014, 2015, 2016) running solid state NMR experiments using Bruker 600 and 850 MHz spectrometers.
8. Visit the Technological School in Graz (2016).
9. Visit York University and use 500 MHz Varian spectrometer (2017).

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, Germany 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.
4. Participation as a co-ordinator or participant in **28** funded research projects by the General Secretary of Greece and European Community (EPAN, PAVET, ENTER, bilateral, HERAKLEITOS, etc).

5.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).

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

7.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.

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

9. September 17th 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.

10. 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.

11. Member of the organizing committee of the 32nd European Conference of Peptide Chemistry (September Athens 2-7, 2012).

12. Participation as a co-ordinator and participant in 3 funded research projects by Institute of Promotion of Research in Cyprus with University of Cyprus or Institute of Technology.

13. Participation in the Marie Curie Actions EURODAISY. MEST/CT2005/020575. In that action I guided with Dr. M. Papadopoulos S. Durdagi who is now Professor in the Behcesehir University in Istanbul.

14.Participation in COST, EAST-NMR, BIO-NMR and CERIC programs (2010-2022). These European programs fund the travel expenses and residence for scientists that prove the necessary use of European facilities in order to progress in their research projects.

15. Chairman with Prof. A. Tsotinis for organizing the international 29th Cyprus-Camerino-Noordwijkerhout Trends in Drug Research” conference at Limassol-Cyprus between 18-22 May 2014.

16. Fund from IKY (State Foundation in Athens for giving Fellowships and fund bilateral agreements) of collaborative program with BMRZ located in Frankfurt of Germany (2015-2016)

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**).
3. S. Hadjikakou, C. Banti, A. Rossos, M. Kapetana, A. Meretoudi, P. Raptis, C. Papachristodoulou, T. Mavromoustakos, P. Zoumpoulakis, N. Kourkoumelis. “New Hydrogels for the development of sterile conduct (No 1010095).

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.
2. 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.
- 3.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.
- 4.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.
- 5.T. Mavromoustakos. Use of the NMR in the study of pharmaceutical substances, zeolithes, polymers and archaeological findings. January 2001.
- 6.T. Mavromoustakos, J. Matsoukas. NMR spectroscopy . Application in Medicine, Pharmaceutical Chemistry, Biochemistry and Food and Beverage Chemistry (2006).
7. T. Mavromoustakos and P. Zoumpoulakis.. Molecular Modeling. Applications in Organic and Pharmaceutical Chemistry (2008).
8. T. Mavromoustakos, T. Tselios and C. Papakonstantinou. Fundamental Principles of Organic Chemistry, Ed., Athens 2014.
- 9.T. Mavromoustakos, A. Tzakos, G. Spyroulias, E. Mikros, A. Kolocouris, K. Papakonstantinou, I. Gerothanasis, I. Matsoukas. Nuclear Magnetic Resonance (2018).

SOFTWARE-TRANSLATIONS

- Participate in creating the «Molecular Conceptor» now a commercial product by Synergix Ltd.
- Participate in the translation of Klein's Organic Chemistry Book in Greek Language.
- Participate and in the translation and Editing of Ludon and Parish Organic Chemistry Book in Greek Language.
- Participation in the translation and Editing of Laboratory Techniques and Experiments of Organic Chemistry by D.L. Pavia, G.M. Lampman, G.S. Kriz, R.G. Engel.

Editor

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.

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

6. Editors: T. Mavromoustakos and T. Kellici Editors. Rational Drug Design Methods and Protocols Methods in Molecular Biology 1824, Springer Protocols, 2018.

7. Editors: T. Mavromoustakos, A. Tzakos, S. Durdagi. Τίτλος: Supramolecules in Drug Discovery and Drug Delivery. Methods in Molecular Biology 1824, Springer Protocols, 2020.

Graduate Students acquired Ph.D or Msc 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) 36. J. Andreadelis (Msc) (2012-2014) 37. E. Koulouridi (Msc) (2012-2014) 38. C. Tzoupis (Ph.D.) 39. C. Koukoulitsa (Ph.D.) (2010-2013) 40. M. Vounioti (Msc) (2013-2015) 41. M. Matiatou (Msc) (2014-2015) 42. A. Konstantinidi (Msc) (2015-2016) 43. A. Douros (Msc) (2015-2016) 44. M. Smpili (2015-2016) 45. P. Karapetros (2015-2016) 46. A. Liosi (2015-2016) 47. I. Petropoulou (2015-2016) 48. E. Vrontaki (2012-2015) 49. X. Theodosiou (2016-2017) 50. A. Tikas (2016-2017) 51.K. Moschovou (2017-2018) 52. E. Chontzopoulou (2017-2018). 51. A. Andreadelis (2015-2019). 52. N. Zoupanou (2020) 53. A. Syriopoulou (2020). 54. M. Mavridi (2020). 55. K. Mpatsidis (2020) 56. N. Zoupanou (2020) 57. A. Syriopoulou (20220) 58. D. Sgouropoulou (2021) 59. A. Matzara 60. X. Kotzatstrati (2021) 61. N. Georgiou (2022)

Supervision of Undergraduate Students to complete their diploma work: 1. Gili, A. 2. V. Vasiliki 3. G.Argyriou 4. Gianni, M. 5. Stougiannou, E. 6. Vasiliou, V. 7. Vatougia, G. 8. Kritsi, E. 9. Xenos, C. 10. Stavroula X. 11. Maniati A. 12. Brontaki, E. 13. Stamelaki, V. 14. N. Moustakas 15. L. Kokkinakis 16. C. Papaioannou, 17. S. Mathioudaki 18. M Vanioti 19. L. Katsillis 20. M. Panopoulou 21. G. Skoufas 22. J. Tselios 23. H. Dimitropoulos 24. D. Petropoulou 25. M. Papazachariou 26. E. Vasilopoulos 27. A. Tzekas 28. I. Galdadas 29. D. Karabatsi 30. E. Routsis 31. Y. Elkhonou 32. H. Maggina 33. X. Kotzatrati 34.A. Koutela 35. A. Papasavva 36. M. Aikaterini Daskalopoulou 37. D.D. Neofytos 38. X. Deskouri 39. A. Basdeki 40. D. Mpolka 41. A. Kontou 42. X. Papadimitropoulou 43. A. Gkionis 44. E. Vidali 45. X. Minopoulos, 46. T. Aivaliotis, 47. E. Gronthos 48. A. Anastasia, 49. A. Tsante 50. A. Kontou, 51. G. Apostolopoulos 52. E. Siskou 53. X. Spyropoulou, 54. A. Petroula

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 for Biologists (Biology Department) (Undergraduate Course)
- NMR spectroscopy and Molecular Modeling (Undergraduate Course)
- Organic Chemistry for Physicists (Physics Department) (Undergraduate Course)
- Bioorganic Chemistry (Undergraduate Course)
- Rational Drug Design (Graduate Course)

Teaching at the University of Athens-Chemistry Education

- Organic Chemistry-Life and Education
- Molecular Models in Education

I supervised three graduated students who acquired their Msc in the Graduate Program of Chemistry Education. The first was related to an interdisciplinary approach of teaching about “water” (chemical, physical, poetry, history, geography, religious etc aspects). The second was an approach of teaching about the Greek product “olive oil”. The third was the teaching of acid base concept using examples of drugs.

Teaching at York College

- Essentials of Organic Chemistry (234)
- General Laboratory (109)
- Advanced Topics (450)

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, one as an external evaluator from Australia and fifty six (56) students of Greek Universities. I also participated as one of the major advisors of the graduate student S. Durdagi who received his Ph.D diploma from Frei University, Germany.

• RESEARCH ARTICLES IN PEER JOURNALS

1. C.J. Van der Schyf, **T. Mavromoustakos**, A. Makriyannis: The conformation of (-)-8 α - and (-)-8 α -hydroxy- Δ^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. Herbette, 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 b₅ 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 Δ^8 -THC and its O-methyl analog using differential scanning calorimetry, X-ray diffraction and solid state ²H-NMR. **BBA M BIO** 1103, 25-36 (1992).
6. D.P. Yang, **T. Mavromoustakos**, A. Makriyannis: Small Angle X-Ray Diffraction Studies of Δ^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 NH₂-terminal Domain of ANG II and [Sar¹] ANG II on Conformation and Activity: NMR Evidence for Aromatic Ring Clustering and Peptide Backbone Folding Compared to [Des^{1,2,3}] ANG II **J. Biol. Chem.** 269, 5303-5312 (1994).

9. **T. Mavromoustakos**, De-Ping Yang, A. Makriyannis. Topography of Alphaxalone and Δ^{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-(-)- Δ^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 Δ^{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. Tsotinis, A. Makriyannis. Synthesis of ^2H -Labelled Alkoxyethyl Phosphodiester AZT Derivatives for Solid-State ^2H -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 ³¹P-NMR spectroscopy **LIPS** 3(4), 175-180 (1996).
21. E. Theodoropoulou, **T. Mavromoustakos**, D. Panagiotopoulos, J. Matsoukas, J. Smith. Superimposition of potent non-peptide AT₁ 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 Ser₄₂-Phe-Leu-Leu-Arg₄₆ 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 β-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-NH₂ 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).
26. J.M. Matsoukas, M. Keramida, D. Panagiotopoulos, **T. Mavromoustakos**, H.L.S. Maia, G. Bigam, D. Pati, H. Hoang, H.H. Habibi, G.J. Moore. Structure elucidation and conformational analysis of gonadotropin releasing hormone and its novel synthetic analogue [Tyr(OMe)⁵, D-Lys⁶, Aze⁹NH₂]GnRH: The importance of aromatic clustering in the receptor binding activity. **Eur. J. Med. Chem.** 32(12), 927-940 (1997).

27. **T. Mavromoustakos**, M. Zervou, E. Theodoropoulou, D. Panagiotopoulos, G. Bonas, M. Day, A. Helmis. ^{13}C NMR Analysis of the Triacylglycerol Composition of Greek Virgin Olive Oils **Magn. Reson. Chem.** 35, S3-S7 (1997).
28. **T. Mavromoustakos**, I.K. Stamos, Ch. Kamoutsis, E. Theodoropoulou, M. Zervou, E. Humpfer. Nuclear Magnetic Resonance Spectral Analysis and Conformational Properties of 11-Benzoyl-9,9a,10,11-tetrahydro-4H-indolo[4,4-ab] carbazole **J. Pharmaceut. Biomed.** 16(5) 723-732 (1998).
29. **T. Mavromoustakos**, M. Zervou, D. Panagiotopoulos, E. Theodoropoulou, J. Matsoukas, D. Karussis. Structure Elucidation and Conformational Properties of the Immunomodulator Linomide **J. Pharmaceut. Biomed.** 16(5) 741-751 (1998).
30. **T. Mavromoustakos**, A. Papadopoulos, E. Theodoropoulou, C. Dimitriou, E.A. Byza. Thermal Properties of Adamantanol Derivatives and Their β -Cyclodextrin Complexes in Phosphatidylcholine Bilayers. **Life Sci.** 62(20), 1901-1910 (1998).
31. Alexopoulos, J. Matsoukas, T. Tselios, P. Roumelioti, **T. Mavromoustakos**, K. Holada. A comparative SAR study of Thrombin receptor derived non peptide mimetics. Importance of phenyl/guanidino Proximity for activity **Amino Acids** 15, 211-220 (1998).
32. **T. Mavromoustakos**, E. Theodoropoulou. A combined use of ^{13}C -cross polarization/magic angle spinning, ^{13}C - magic angle spinning and ^{31}P -nuclear magnetic spectroscopy with Differential Scanning Calorimetry to study cannabinoid-membrane interactions. **Chem. Phys. Lipids** 92(1), 37-52 (1998).
33. **T. Mavromoustakos**, E. Theodoropoulou, M. Zervou, T. Kourouli, D. Papahatjis. 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. **J. Pharmaceut. Biomed.** 18(6), 947-956, (1999).
34. K. Alexopoulos, P. Fatseas, E. Melissari, D. Vlahakos, J. Smith, **T. Mavromoustakos**, M. Saifeddine, G. Moore, M. Hollenberg, J. Matsoukas. Design and Synthesis of Thrombin Receptor-derived Nonpeptide Mimetics Utilizing a Piperazine Scaffold. **Bioorg. & Med. Chemistry** 7(6), 1033-1041 (1999).
35. **T. Mavromoustakos**, A. Kolocouris, M. Zervou, P. Roumelioti, J. Matsoukas, R. Weisemann. An effort to understand the molecular basis of hypertension through the study of conformational analysis of losartan and sarlesin using a combination of

Nuclear Magnetic Resonance spectroscopy and theoretical calculations **J. Med. Chem.** 42(10) 1714-1722 (1999).

36.T. Tselios, L. Probert, I. Daliani, E. Matsoukas, A. Troganis, I.P. Gerothanasis, **T. Mavromoustakos**, G.J. Moore, J.M. Matsoukas. Design and Synthesis of a Potent Cyclic Analogue of the Myelin Basic Protein Epitope MBP₇₂₋₈₅: Importance of the Ala⁸¹ Carboxyl Group and of a Cyclic Conformation for Induction of Experimental Allergic Encephalomyelitis **J. Med. Chem.** 42,7, 1170-1177 (1999).

37.**T. Mavromoustakos**, I. Daliani. Effects of Cannabinoids in membrane bilayers containing cholesterol. **BBA M BIO.** 1420, 252-265 (1999).

38.A. Kolocouris, D. Tataridis, G. Fytas, **T. Mavromoustakos**, G.B. Foscolos, N. Kolocouris, E.D. Clercq. Synthesis of 2-(2-adamantyl)piperidines and structure anti-influenza virus A activity relationship study using a combination of NMR spectroscopy and molecular modeling. **Bioorg. & Med. Chem. Lett.**, 9(24), 3465-3470 (1999).

39.J.M. Matsoukas, L. Polevaya, J. Ancas, **T. Mavromoustakos**, A. Kolocouris, P. Roumelioti, D.V. Vlahakos, R. Yamdagni, Q. Wu, G.J. Moore. The Design and Synthesis of a Potent Angiotensin II Cyclic Analogue Confirms the Ring Cluster Receptor Conformation of the Hormone Angiotensin II **Bioorg. & Med. Chem. Lett.**, 8(1), 1-10 (2000).

40.A.Troganis, I.P. Gerothanasis, Z. Athanassiou, **T. Mavromoustakos**, G.E. Hawkes, C. Sakarellos. Thermodynamic Origin of Cis/Trans Isomers of a Proline-Containing β -turn Model Dipeptide in Aqueous Solution: A Combined Variable Temperature ¹H-NMR, Two Dimensional ¹H, ¹H Gradient Enhanced Nuclear Overhauser Effect Spectroscopy (NOESY), One Dimensional Steady-State Intermolecular ¹³C, ¹H-NOE and Molecular Dynamics Study. **Biopolymers** 53, 72-83 (2000).

41.P.Roumelioti, T. Tselios, K. Alexopoulos, **T. Mavromoustakos**, A. Kolocouris, G.J. Moore, J.M. Matsoukas. Structural comparison between type I and type II antagonists: possible implications in the drug design of AT-1 antagonists **Bioorg. & Med. Chem. Lett.**, 10(8), (2000) 755-758.

42.**T. Mavromoustakos**, M. Zervou, G. Bonas, A. Kolocouris, P.Petrakis. A Novel Analytical Method to Detect Adulteration of Virgin Olive Oil by Other Oils. **J Am Oil Chem Soc** 77(4) 405-411 (2000).

43.T. Tselios, I. Daliani, S. Deraos, S. Thymianou, E. Matsoukas, I. Gerothanasis, A. Troganis, A. Mouzaki, **T. Mavromoustakos**, L. Probert, J. Matsoukas. Treatment of Experimental Allergic Encephalomyelitis (EAE) by a Rationally Designed Cyclic

Analogue of Myelin Basic Protein (MBP) Epitope 72-85 **Bioorg. & Med. Chem. Lett.**, 10(24), 2713-2717 (2000).

44.K. Dimas, C. Demetzos, D. Angelopoulou, A. Kolokouris, **T. Mavromoustakos**. Biological Activity of Myricetin and Derivatives Against Human Leukemic Cell Lines *in vitro*. **Pharmacol. Res.**, 42(5) 475-478 (2000).

45.Antonios Kolocouris, **T. Mavromoustakos**, Costas Demetzos, Aris Terzis, Simona Golic Grdadolnik Structure Elucidation and Conformational Properties of a Novel Bioactive Clerodane Diterpene Using a Combination of High Field NMR Spectroscopy, Computational Analysis and X-Ray Diffraction in **Bioorg. Med. Chem. Lett.** 11(6), 837-840 (2001).

46.K. Alexopoulos, D. Panagiotopoulos, **T. Mavromoustakos**, P. Fatseas, M.C. Paredes-Carbajal, D. Mascher, S. Mihailescu, J. Matsoukas. Design, Synthesis and Modeling of Novel Cyclic Thrombin Receptor Derived Peptide Analogues of the Ser₄₂-Phe-Leu-Leu-Arg₄₆ Motif Sequence with Fixed Conformations of Pharmacophoric Groups: Importance of a Phe/Arg/NH₂ Cluster for Receptor Activation and Implications in the Design of Non-Peptide Thrombin Receptor Mimetics. **J. Med. Chem.** 44, 328-339 (2001).

47.M. Matzapetakis, M. Kourgiantakis, M. Dakanali, C. P. Raptopoulou, A. Terzis, A. Lakatos, I. Banyai, T. Kiss, L. Iordanidis, **T. Mavromoustakos**, A. Salifoglou. Synthesis, pH-dependent Structural Characterization and Solution Behavior of Aqueous Aluminum and Gallium Citrate Complexes **Inorg. Chem.** 40, 1734-1744 (2001).

48.**T. Mavromoustakos**, D. Papahatjis, P. Laggner Differential Membrane Fluidization by Active and Inactive Cannabinoid analogs. **BBA M BIO** 1512(2) 183-190 (2001).

49.L. Polevaya, **T. Mavromoustakos**, P. Zoumboulakis, S. G. Grdadolnik, P. Roumelioti, N. Giatas, Ilze Mutule, T. Keivish, D. Vlahakos, E. Iliodromitis, D. Kremastinos, J. Synthesis and Study of Cyclic Angiotensin II Antagonist Analogue reveals the role of π^* - π^* interactions in the C-Terminal Aromatic Residue for agonist activity and its structure resemblance with AT₁ non-peptide antagonists. Matsoukas **Bioorg. Med. Chem.** 9, 1639-1647 (2001).

50.**T. Mavromoustakos**, T. Kalogeropoulou, M. Koufaki, A. Kolocouris, I. Daliani, C. Demetzos, Z. Meng, A. Makriyannis, J. Balzarini, E. De Clercq, Ether Phospholipid-AZT Conjugates Possessing Anti-HIV and Antitumor Cell Activity. Synthesis, Conformational Analysis, and Study of Their Thermal Effects on Membrane Bilayers. **J. Med. Chem.** 44, 1702-1709 (2001).

- 51.D.Angelopoulou, C. Demetzos, A. Kolocouris, I. Daliani, **T. Mavromoustakos** Structure Elucidation, Conformational Analysis and Thermal Effects of Antimicrobial Myricetin Derivatives on Membrane Bilayers **J. Heter. Chem.** 38, 703-710 (2001).
- 52.C.Pappas, P.A. Tarantilis, I. Daliani, **T. Mavromoustakos**, M. Polysiou. Comparison of classical and ultrasound assisted isolation procedures of cellulose from Kenaf and Eucalyptus **Ultrasonics** 9(1), 19-23 (2002).
- 53.T. Tselios, V. Apostolopoulos, I. Daliani, S. Deraos, S. Grdadolnik, **T. Mavromoustakos**, M. Melachrinou, S. Thymianou, A. Mouzaki and J. Matsoukas. Antagonistic Effects of Human Cyclic MBP₈₇₋₉₉ Altered Peptide Ligands in Experimental Allergic Encephalomyelitis and Human T-cell Proliferation. **J. Med. Chem.** 45, 275-283 (2002).
- 54.P. Zoumpoulakis, S.G. Grdadolnik, J. Matsoukas. **T. Mavromoustakos**. Structure elucidation and conformational properties of eprosartan a non peptide Angiotensin II AT₁ antagonist. **J. Pharmaceut. Biomed. Anal.** 28, 125-135 (2002).
- 55.H. Maswadeh, C. Demetzos, K. Dimas, Y. L. Loukas, A. Georgopoulos, **T. Mavromoustakos**, C. Th. Papaioannou. *In vitro* cytotoxic/cytostatic activity of anionic liposomes containing vinblastine against leukemic human cells. **J. Pharm. Pharmacol.** 54, 189-196 (2002).
- 56.S. Prispas, E.S. Kioulafa, N. Hadjichristidis, **T. Mavromoustakos**. Block copolymers with crystalline-amorphous, crystalline-polyelectrolyte and amorphous-polyelectrolyte blocks **Macromol. Chem. Phys.** 203(10-11), 1317-1327, (2002).
- 57.P. Roumelioti, L. Plevaya, P. Zoumpoulakis, N. Giatas, T. Keivish, A. Haritonova, A. Zoga, D. Vlahakos, E. Iliodromitis, D. Kremastinos, S.G. Grdadolnik, **T. Mavromoustakos**, J. Matsoukas. Design, Synthesis and Biological Evaluation of Cyclic Angiotensin II Analogues with 3,5 Side Chain Bridges: Role of C-Terminal Aromatic Residue and Ring Cluster for Activity and Implications in the Drug Design of AT₁ non Peptide Antagonists. **Bioorg. Med. Chem. Letters** 12, 2627-2633 (2002).
- 58.H. Maswadeh, C. Demetzos, I. Daliani, I.Kyrikou, **T. Mavromoustakos**. A. Tsortos, G. Nounesis. A molecular basis explanation of the dynamic and thermal effects of vinblastine sulfate upon dipalmitoylphosphatidylcholine bilayer membranes. **BBA M BIO** 1567 49-55 (2002).
- 59.N. Avlonitis, E. Lekka, A. Detsi, M. Koufaki, T. Calogeropoulou, E. Scoulica, E. Siapi, I. Kyrikou, **T. Mavromoustakos**, A. Tsotinis, S. Golic Grdadolnik, A. Makriyannis. Antileishmanial Ring-Substituted Ether Phospholipids. **J. Med. Chem.** 46, 755-767 (2003).

- 60.P. Zoumpoulakis, A. Zoga, P. Roumelioti, N. Giatas, S.G. Grdadolnik, E. Iliodromitis, D. Vlahakos, D. Kremastinos, J. Matsoukas, **T. Mavromoustakos**. Conformational and biological studies for a pair of novel synthetic AT₁ antagonists. Stereoelectronic requirements for antihypertensive efficacy **J. Pharm. Biomed. Anal.** 31 833-844 (2003).
- 61.I. Kyrikou, S.G. Grdadolnik, M. Tatari, C. Poulos, **T. Mavromoustakos** Structure Elucidation and Conformational Properties of Toxin Paralysin β -Ala-Tyr **J. Pharm. Biomed. Anal.** 31, 713-721 (2003).
- 62.P. Moutevelis-Minakakis, M. Gianni, H.Stougiannou, P. Zoumpoulakis, A. Zoga, A. D. Vlahakos, E. Iliodromitis, **T. Mavromoustakos** Design and Synthesis of Novel Antihypertensive Drugs **Bioorg. Med. Chem. Letters** 13(10), 1737-1740 (2003).
- 63.M. Dakanali, E.T. Kefalas, C. P. Raptopoulou, A. Terzis, **T. Mavromoustakos**, A. Salifoglou. Synthesis, Spectroscopic, and Structural Studies of a New Cadmium (II)-Citrate Aqueous Complex. Potential links to Cadmium toxicity. **Inorg. Chem.** 42, 2531-2537, (2003).
- 64.M. Dakanali, E.T. Kefalas, C.P. Raptopoulou, A. Terzis, G. Voyiatzis, I. Kyrikou, **T. Mavromoustakos**, A. Salifoglou. A New Dinuclear Ti(IV)-Peroxo-Citrate Complex from Aqueous Solutions. Synthetic, Structural, and Spectroscopic Studies in Relevance to Aqueous Titanium(IV)-Peroxo-Citrate Speciation. **Inorg. Chem.** 42, 4632-4639 (2003).
- 65.P. Zoumpoulakis, I. Daliani, M. Zervou, I. Kyrikou, E. Siapi, G. Lamprinidis E. Mikros, **T. Mavromoustakos**. Losartan's molecular basis of interaction with membranes and AT₁ receptor. **Chem. Phys. Lipids** 125, 13-25 (2003).
- 66.R. Kokkinofa, P. Petrakis, **T. Mavromoustakos**, C.R. Theocharis. Authenticity of the traditional Cypriot spirit "Zivania" on the basis of metal content using a combination of coupled plasma spectroscopy and statistical analysis, **J. Agr. Food Chem.** 51(21), 6233-6239 (2003).
- 67.A.N. Batsoulis, M.K. Nacos, C.S. Pappas, P.A. Tarantilis, **T. Mavromoustakos**, M.G. Polissiou. Determination of uronic acids in isolated hemicelluloses from kenaf using diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) and curve-fitting deconvolution method. **Applied Spectroscopy** 58(2) 199-202 (2004).
- 68.I. Kyrikou, I. Daliani, **T. Mavromoustakos**, H. Maswadeh, C., Demetzos, S Xatziantoniou, S. Giatrellis, G. Nounesis. The modulation of thermal and dynamic properties of vinblastine by cholesterol in membrane bilayers **BBA M BIO.** 1661, 1-8 (2004).

- 69.K. Alexopoulos, P. Fatseas, E. Melissari, D. Vlahakos, P. Roumelioti, **T. Mavromoustakos**, S. Mihailescu, M. Christina, P. Carbajal, D. Mascher, J. Matsoukas. Design and Synthesis of Novel Biologically Active Thrombin Receptor Non Peptide Mimetics Based on the Pharmacophoric Cluster Phe/Arg/NH₂ of the Ser₄₂-Phe-Leu-Arg₄₆ Motif Sequence: Platelet Aggregation and Relaxant Activities **J. Med. Chem.** 47(13), 3338-3352 (2004).
- 70.K.S. Triantafyllidis, L. Nalbandian, P.N. Trikalitis, A.K. Ladanos, **T. Mavromoustakos**, C.P. Nicolaides. Structural, compositional and acidic characteristics of nanosized amorphous or partially crystalline ZSM-5 zeolite-based materials. **Microporous and Mesoporous Materials** 75, 89-100 (2004).
- 71.D. Kovala-Demertzi, C. Vidjeluc, M.A. Demertzis, E. Siapi, **T. Mavromoustakos**. The thermal effects of platinum (II) and palladium(II) complexes with 2-acetyl pyridine and pyridine-2-carbaldehyde N(4)-ethyl-thiosemicarbazones in membrane bilayers. **Thermochimica Acta**, 42(1-2), 53-58 (2004)
- 72.I. Kyrikou, S. Xadjikakou, D. Kovala-Demertzi, K.Viras, **T. Mavromoustakos**, Effects of non steroid anti-inflammatory drugs in membrane bilayers containing cholesterol. **Chem. Phys. Lipids** 132, 157-169 (2004).
- 73.I.Kyrikou, **T. Mavromoustakos**, S. Xatziantoniou, A. Georgopoulos, C. Demetzos. A comparative study of the effects of cholesterol and sclareol, a bioactive labdane diterpene, on phospholipids bilayers **Chem. Phys. Lipids** 133, 125-134 (2005).
- 74.E. Siapi, **T. Mavromoustakos**, V.Trandafir, B. Albu and P. Budrugaec. The Use of Differential Scanning Calorimetry to Study the Effects of Gentamycin on Fibrous Collageneous Membranes. **Thermochimica Acta** 425, 165-171 (2005).
- 75.J. Matsoukas, V. Apostolopoulos, H. Kallbacher, A.M. Papini, T. Tselios, K. Chatzantoni, T. Biagioli, F. Lolli, S. Deraos, P. Papathanassopoulos, **T. Mavromoustakos**, A. Mouzaki. Design and synthesis of a novel potent myelin basic epitope 87-99 cyclic analogue: Enhanced stability and biological properties of mimics render them a potentially new class of immunomodulators. **J. Med. Chem.** 48,1470-1480 (2005).
- 76.A. Kapou, **T. Mavromoustakos**, S. Nikolaropoulos, Effects of Steroidal Carriers of Alkylating Agents On DPPC Membrane Bilayers. **Thermochimica Acta** 429, 53-56 (2005).
- 77.E.T. Kefalas, P. Panagiotidis, C.P. Raptopoulou, A. Terzis, **T. Mavromoustakos**, A. Salifoglou. Mononuclear Titanium(IV)-Citrate Complexes from Aqueous Solutions:pH-Specific Synthesis and Structural and Spectroscopic Studies in

Relevance to Aqueous Titanium(IV)-Citrate Speciation. **Inorg. Chem.** 44, 2596-2605 (2005).

78.Nikolas-P. Benetis, Ioanna Kyrikou, **T. Mavromoustakos**, Maria Zervou. Static ^{31}P CP NMR Multilamellar Bilayer Broadlines in the Absence and presence of the Bioactive Dipeptide beta-Ala-Tyr or Glu" **Chemical Physics** 314(1-3) 57-72 (2005).

79.A. Kapou, M.A. Fousteris, S.S. Nikolaropoulos, M. Zervou, S.G. Gardadolnik, P. Zoumpoulakis, I. Kyrikou, **T. Mavromoustakos**. 2D NMR and conformational analysis of a prototype anti-tumor steroidal ester. **J. Pharmaceut. Biomed. Anal.** 38, 428-434 (2005).

80.P. Petrakis, I. Touris, M. Liouni, M. Zervou, C.R. Kokkinofa, R. Theocharis, **T. Mavromoustakos**. Authenticity of the traditional Cyprus spirit "Zivania" on the basis of ^1H NMR Spectroscopy Diagnostic Parameters and Statistical Analysis. P. Petrakis, I. Touris, M. Liouni, M. Zervou, C.R. Kokkinofa, R. Theocharis, T. Mavromoustakos **J. Agric. Food Chem.** 53(13), 5293-5303 (2005).

81.E.T. Kefalas, M. Dakanali, P. Panagiotidis, C.P. Raptopoulou, A. Terzis, **T. Mavromoustakos**, I. Kyrikou, N. Karligiano, A. Bino, A. Salifoglou. pH-Specific Aqueous Synthetic Chemistry in the Binary Cadmium(II)-Citrate System. Gaining Insight into Cadmium(II)-Citrate Speciation with Relevance to Cadmium Toxicity. **Inorg. Chem.** 44(13) 4818-4828 (2005).

82.C. Souli, N. Avlonitis, T. Calogeropoulou, G. Maksay, T. Biro, A. Tsotinis, G. Maksay, T. Biro, A. Politi, **T. Mavromoustakos**, A. Makriyannis, H. Reis, M. Papadopoulos. Novel 17β -substituted conformationally constrained neurosteroids that modulate GABA_A receptors. **J. Med. Chem.** 48(16) 5203-5214 (2005).

83.M.A.C. Preto, A.M. Hermani, L.S. Maia, **T. Mavromoustakos**, M. J. Ramos. Molecular Dynamics Simulations of Angiotensin II in Aqueous and Dimethylsulfoxide Environments. **J. Physical Chem. B** 109, 17743-17751 (2005).

84.P. Zoumpoulakis, A. Politi, S.G. Grdadolnik, J. Matsoukas, **T. Mavromoustakos**. Structure elucidation and conformational study of V8. A novel synthetic non peptide AT₁ antagonist. **J. Pharmaceut. Biomed. Anal.** 40(5) 1097-1104 (2006).

85.Maria K. Keramida, Theodore Tselios, Efthimia Mantzourani, Kostas Papazisis, **T. Mavromoustakos**, Christian Klaussen, George Agelis, Spyros Deraos, Hamid Habibi and John Matsoukas. Design, Synthesis and Molecular Modelling of a Novel Amide Linked Cyclic GnRH Analogue Cyclo(4-9)[Lys⁴,D-Trp⁶,Glu⁹]GnRH: Stimulation of Gonadotropin Gene Expression. **J. Med. Chem.** 49(1) 105-110 (2006).

86.V. Saroglou, S. Xatziantoniou, M. Smyrniotakis, I. Kyrikou, **T. Mavromoustakos**, A. Zompra, V. Magafa, P. Cordopatis, C. Demetzos. Synthesis, liposomal formulation and thermal effects on phospholipids bilayers of leuprolide **J. Pept. Sci** 12, 43-50 (2006)

87.E.D. Mantzourani, T.V. Tselios, S. Golic Grdadolnik, J.M. Matsoukas, A. Brancale, J.A. Platts, T.M. Mavromoustakos. A putative bioactive conformation for the altered

peptide ligand of myelin basic protein and inhibitor of experimental autoimmune encephalomyelitis [Arg⁹¹, Ala⁹⁶] MBP₈₇₋₉₉. **J. Mol. Graph. and Mod.** 25(1),17-29, (2006).

88.**T. Mavromoustakos**, P. Moutevelis-Minakakis, C.G. Kokotos, P. Kontogianni, A. Politi, P. Zoumpoulakis, J. Findlay, A. Cox, A. Balmforth, A. Zoga, E. Iliodromitis. Synthesis, binding studies, and in vivo biological evaluation of novel non-peptide antihypertensive analogs. **Bioorganic and Medicinal Chemistry** 14, 4353-4360 (2006).

89.C. Koukoulitsa, I. Kyrikou, C. Demetzos, **T. Mavromoustakos**. The Role of the Anticancer Drug Vinorelbine in Lipid Bilayers Using Differential Scanning Calorimetry and Molecular Modeling. **Chem. Phys. Lipids** 144, 85-95 (2006).

90.E. Matzourani, T. Tselios, S. Dearos, J. Matsoukas, **T. Mavromoustakos**. Comparison of proposed bioactive conformations of altered peptide ligands of Myelin Basic Protein (Ala⁹¹,96) MBP₈₇₋₉₉ and (Arg⁹¹, Ala⁹⁶) MBP₈₇₋₉₉ by Spectroscopic and Modelling studies. **J. Med. Chem.** 49, 6683-6691 (2006).

91.Agnes Kapou, Nikos Avlonitis, Anastasia Detsi, Maria Koufaki, Theodora Calogeropoulou, Nikolas P. Benetis, Sotirios Nikolaropoulos and **Thomas Mavromoustakos**, CoMFA and CoMSIA 3D-Quantitative Structure-Activity Relationships of New Flexible Antileishmanial Ether Phospholipids **Bioorg. Med. Chem.** 15, 1252-1265 (2007).

92.S. Durdagi, A. Kapou, T. Kourouli, T. Andreou, S.P. Nikas, V.R. Nahmias, D. P. Papahadjis, M.G. Papadopoulos, **T. Mavromoustakos**. The Application of 3D-QSAR Studies for Novel Cannabinoid Ligands Substituted at the C1' Position of the Alkyl Side Chain on the Structural Requirements for Binding to Cannabinoid Receptors CB1 and CB2. **J. Med. Chem** 50(12), 2875-2885 (2007).

93.S. Durdagi, M. Papadopoulos, D. Papahadjis, **T. Mavromoustakos**. Combined 3D QSAR and Molecular Docking Studies to Reveal Novel Cannabinoid Ligands with Optimum Binding Activity. **Bioorg. Med. Chem. Lett.**, 17, 6754-6763 (2007).

94.Mantzourani E.D., Platts J.A., Brancale A., Mavromoustakos T.M., Tselios T.V. Molecular dynamics at the receptor level of immunodominant myelin basic protein epitope 87-99 implicated in multiple sclerosis and its antagonists altered peptide ligands: Triggering of immune response. **J. Mol. Graph. Mod.**, 26 (2), 471-481 (2007).

95.S. Zinovia, D. Georgios, S. Georgios, E. Mantzourani, **T. Mavromoustakos**, I. Friligou, T. Theodore. Putative Bioactive Conformations of Amide Linked Cyclic Myelin Basic Protein Peptide Analogues Associated with Experimental Autoimmune Encephalomyelitis 50, 6039-6047 **J. Med. Chem.** (2007).

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

- 97.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).
- 98.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. Chim. Acta** 361, 2210-2224 (2008).
- 99.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).
- 100.C. Koukoulitsa, M. Zervou, C. Demetzos, **T. Mavromoustakos**. Comparative docking studies of labdane-type diterpenes with forskolin. **Bioorg. Med. Chem.** 16, 8237-8243 (2008).
- 101.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).
- 102.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).
- 103.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).
- 104.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).
- 105.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).
- 106.C. Koukoulitsa, A.T. Kakoulidou, **T. Mavromoustakos**, I. Chinou. PLS Analysis for Antibacterial Activity of Natural Coumarins Using VolSurf Descriptors. **QSAR Comb. Sci.** 28,785-789 (2009).

- 107.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).
- 108.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).
- 109.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).
- 110.L.Mannina, M.D. Imperio, D. Capitani, S. Rezzi, C. Guillou, **T. Mavromoustakos**, M.D. Vilchez, A.H. Fernandez. ^1H NMR-Based Protocol for the Detection of Adulterations of Refined Olive Oil with Refined Hazelnut Oil. **J. Agr. Food Chem.** 57(24) 11550-11556 (2009).
- 111.C. Fotakis, S. Gega, E. Siapi, C. Potamitis, K. Viras, P. Moutevelis-Minakakis, G. Kokotos, S. Durdagi, S. Grdadolnik, B. Sartori, M. Rappolt, **T. Mavromoustakos**. Drug interactions at the bilayer interface and receptor site induced by the novel synthetic pyrrolidinone analog MMK3. **Biochim. Biophys. Acta** 1798(3) 422-432 (2010).
- 112.V.D. Mouchlis, **T.M. Mavromoustakos**, G. Kokotos. Design of new secreted phospholipase A_2 inhibitors based on docking calculations by modifying the pharmacophore segments of the FPL67047XX inhibitor. **J. Comput. Aided. Mol. Des.** 24(2) 107-115 (2010).
- 113.S. Durdagi, M. Papadopoulos, P. Zoumpoulakis, C. Koukoulitsa; **T. Mavromoustakos**. A Computational Study on Cannabinoid receptors and Potent Bioactive Cannabinoid Ligands: Homology Modeling, Docking De novo Drug Design and Molecular Dynamics Analysis. **Molecular Diversity** 14(2) 257-276 (2010).
- 114.A. P. Politi, M. V. Zervou, H. Triantafyllidi, P. G. Zoumpoulakis, T. M. Mavromoustakos, A. A. Zoga, P. Moutevelis-Minakakis, G. Kokotos, E. K. Iliodromitis, D. Th. Kremastinos, Hypertension study in anesthetized rabbits: Protocol proposal for AT1 antagonist screening” **Journal of the Renin-Angiotensin-Aldosterone System**, 11(2) 103-110 (2010).
- 115.P. Roumelioti, A. Resvani, S. Durdagi, M.Eleni, K. Kelaidonis, T. Mavromoustakos, G. Aggelis, J. Matsoukas. An efficient synthesis of a rationally design 1,5 disubstituted imidazole AT1 Angiotensin Receptor Antagonist. Reorientation of imidazole pharmacophore groups in losartan reserves high receptor affinity and confirms docking studies. **J. Comput. Aided. Mol. Des.** 24 749-758 (2010).

- 116.V. Mouchlis, T. Mavromoustakos, G. Kokotos. Molecular Docking and 3D-QSAR CoMFA Studies on Indole Inhibitors of GIIA Secreted Phospholipase A2. **J. Chem. Inf. Mod.** 50, 1589-1601 (2010).
- 117.A.P. Politi, S. Durdagi, P.M. Minakakis, **T. Mavromoustakos**, G. Kokotos. Development of Accurate Binding Affinity Predictions of Novel Renin Inhibitors through Molecular Docking Studies. **J. Mol. Gr. Mod.** 29 425-435 (2010).
- 118.V.Mouchlis, V. Magrioti, E.Barbayianni, N. Cermak, R. C. Oslund, **T. Mavromoustakos**, M. H. Gelb, G. Kokotos. Inhibition of secreted phospholipases A2 by 2-oxoamides based on α -amino acids: Synthesis, in vitro evaluation and molecular docking calculations. **Bioorg. Med. Chem.** 19, 735-743 (2011).
- 119.**T. Mavromoustakos**, P. Chatzigeorgiou, C. Koukoulitsa, S. Durdagi. Partial Interdigitation of Lipid Bilayers. **International Journal of Quantum Chemistry** 6, 1172-1183 (2011).
- 120.C. Potamitis, P. Chatzigeorgiou, E. Siapi, **T. Mavromoustakos**, A. Hodzic, F. Cacho-Nerin, P. Laggner, M. Rappolt. Interactions of the AT₁ antagonist valsartan with dipalmitoyl-phosphatidylcholine bilayers **Biochim. Biophys. Acta** 1808, 1753-1763 (2011).
- 121.Panagiota Moutevelis-Minakakis, Eleni Papavassilopoulou, George Michas, Kalliopi Georgikopoulou, Maria-Eleni Ragoussi, Panagiotis Zoumpoulakis, **Thomas Mavromoustakos**, Dimitra Hadjipavlou-Litina. Synthesis, in silico docking experiments of new 2-pyrrolidinone derivatives and study of their anti-inflammatory activity **Bioorg. Med. Chem.** 19, 2888-2902 (2011).
- 122.N. Neophytou, G. Leonis, N. Stavrinouidakis, M. Simcic, S.G. Grdadolnik, G. Michas, P. Minakaki, E. Papavassiliou, M. Papadopoulos, M. Zheng, S. Grdadolnik, M, Simcic, **T. Mavromoustakos**. Docking and Molecular Dynamics calculations of pyrrolidinone analog MMK16 bound to COX and LOX enzymes **Mol. Inf.** 30, 473-486 (2011).
- 123.Charalambos Fotakis, Dionyssios Christodouleas, P. Zoumpoulakis, Argyro Gili, E. Kritsi, Nikolas-Ploutarch Benetis, Maria Zervou, Heribert Reis, Manthos Papadopoulos, **Thomas Mavromoustakos**. Comparative Biophysical studies of sartan class drug molecules losartan and candesartan (CV-11974) with membrane bilayers **J. Chem. Phys. B** 115, 6180-6192 (2011).
- 124.Koukoulitsa C., Durdagi S., Siapi E., Villalonga-Barber C., Xanthippi A., Barry R. S., Micha-Screttas M., Michael N. Alexis, Anna Kakoulidou, **Mavromoustakos T.** Comparison of thermal effects of stilbenoid analogs in lipid bilayers using differential scanning calorimetry and molecular dynamics: correlation of thermal effects and topographical position with antioxidant activity. **Eur. Biophys. J.** 40, 865-875 (2011).
- 125.M. Poyraza, C. Bantia, N. Kourkoumelis, V. Dokoroud, M.J. Manose, M. Simčič, S. Golič Grdadolnik, T. Mavromoustakos, I.I. Verginadis, K. Charalabopoulos, S.K.

Hadjikakou. Synthesis, structural characterization and biological studies of novel mixed ligand Ag(I) complexes with tri-phenylphosphine and aspirin or salicylic acid **Inorg. Chim. Acta** 375, 114-121 (2011).

126.C. Potamitis, M. Matsoukas, T. Tselios, T. Mavromoustakos, S. Golic Grdadolnik. Conformational Analysis of [Phe⁹¹]MBP₈₃₋₉₉ and [Tyr⁹¹]MBP₈₃₋₉₉ peptide analogues and study of their interactions with HLA-DR2 receptor and human TCR receptors using Molecular Dynamics 25, 837-853 **J. Comput. Aided Mol. Des** (2011).

127.Dimitrios Ntountaniotis, Gregor Mali, Simona Golic Grdadolnik, Halabalaki Maria, Alexios-Leandros Skaltsounis, Constantinos Potamitis, Eleni Siapi, Petros Chatzigeorgiou, Michael Rappolt, **Thomas Mavromoustakos**. Thermal, dynamic and structural properties of drug AT₁ antagonist olmesartan in lipid bilayers **Biochim. Biophys. Acta** 1808, 2995-3006 (2011).

128.X. Tzoupis, G. Leonis, S. Durdagi, V. D. Mouchlis, **T. Mavromoustakos**, M. G. Papadopoulos. Design of a series of novel HIV-1 PR fullerene-based inhibitors **J. Comp. Aided Mol. Des** . 25, 959-976 (2011).

129.A. Politi, G. Leonis, H. Tzoupis, D. Ntountaniotis, H. Reis, M. G. Papadopoulos, S. G. Grdadolnik, **T. Mavromoustakos**. Conformational Properties and Energetic Analysis of Aliskiren in Solution and Receptor Site. **Chem. Informatics** 30, 973-985 (2011).

130.S. Durdagi, M. Papadopoulos, **T. Mavromoustakos**. An effort to discover the preferred conformation of the potent AMG3 cannabinoid analog when reaching the active sites of the cannabinoid receptors. **Eur. J. Med. Chem.** 47(1) 44-51 (2012).

131.G.K. Batsala, V. Dokorou , N. Kourkoumelis, M.J. Manos, A.J. Tasiopoulos, **T. Mavromoustakos**, M. Simcic, S. Golic Grdadolnik, S.K. Hadjikakou Copper(I)/(II) or silver(I) ions towards 2-mercaptopyrimidine: An exploration of a chemical variability with possible biological implication. **Inorg. Chim. Acta** 382 146-157 (2012).

132.V. Mouchlis, V. Michopoulou, V.C.-Kokotou, **T. Mavromoustakos**, E.A. Dennis, G. Kokotos Binding Conformation of 2-Oxoamide Inhibitors to Group IVACytosolic Phospholipase A2 Determined by Molecular Docking Combined with Molecular Dynamics. **Ch. Inf. Mod.** 52(1) 243-254 (2012).

133.A. Hodzic, P. Zoumpoulakis, G. Pabst., **T. Mavromoustakos**, M. Rappolt. Losartan's affinity to fluid bilayers couples to lipid/cholesterol interactions. **Phys. Chem. Chem. Phys.** 14, 4780-4788 (2012).

134.V. Mouchlis, G. Melagraki, **T. Mavromoustakos**, G. Kollias, A. Afantitis. Molecular modeling on pyrimidine-urea inhibitors of TNF- α production: an integrated approach using a combination of molecular docking, classification techniques and 3D-QSAR CoMSIA **J. Ch. Inf. Mod.** 52, 711-723 (2012).

- 135.H. Tzoupis, G. Leonis, G. Megariotis, C.T. Supuran, **T. Mavromoustakos**, M.G. Papadopoulos. Dual Inhibitors for Aspartic Proteases HIV-1 PR and Renin: Advancements in AIDS-Hypertension-Diabetes Linkage via Molecular Dynamics, Inhibition Assays, and Binding Free Energy Calculations. **J. Med. Chem.** 55, 5784-5796 (2012).
- 136.C. Fotakis, G. Megariotis, D. Christodouleas, E. Kritsi, M. Zervou, P. Zoumpoulakis, D. Ntountaniotis, C. Potamitis, A. Hodzic, G. Pabst, M. Rappolt, G. Mali, J. Baldus, C. Glaubitz, M. G. Papadopoulos, A. Afantitis, G. Melagraki, **T. Mavromoustakos**. Comparative study of the AT1 receptor prodrug antagonist candesartan cilexetil with other sartans on the interactions with membrane bilayers. **Biochim. Biophys. Acta** 1818, 3107-3120 (2012).
- 137.N. Varvarigou, G. Megariotis, G. Leonis, E. Vrontaki, A.-M. Maniati, M.Vlachou, A. E.R. Kompogennitaki, M. G. Papadopoulos, S. G. Grdadolnik, D. Komiotis, **Thomas Mavromoustakos**, Andrew Tsotinis. Conformational analysis of two novel cytotoxic C2-substituted pyrrolo[2,3-f]quinolines in aqueous media, organic solvents, membrane bilayers and at the putative active site **Bioorganic & Medicinal Chemistry** 20, 6276-6284 (2012).
- 138.E. Vrontaki, G. Leonis, M. G. Papadopoulos, M. Simcic, S. Golic Grdadolnik, A. Afantitis, G. Melagraki, S. K. Hadjikakou, and **T. Mavromoustakos**. Comparative Binding Effects of Aspirin and Anti-Inflammatory Cu Complex in the Active Site of LOX-1 52(12) **J. Chem. Inf. Mod.** 3293-3301 (2012).
- 139.G. Agelis, A. Resvani, S. Durdagi, K. Spyridaki, T.Tumová, J. Slaninová, P. Giannopoulos, D. Vlahakos, G. Liapakis, **T. Mavromoustakos**, J. Matsoukas. The discovery of new potent non-peptide Angiotensin II AT1 receptor blockers: A concise synthesis, molecular docking studies and biological evaluation of N-substituted 5-butyrimidazole derivatives. **Eur. J. Med. Chem.** 55 358-374 (2012).
- 140.P.M. Minakakis, E. Papavassilopoulou, **T. Mavromoustakos**. Synthesis of new optically active 2-pyrrolidinones. **Molecules** 18, 50-73 (2013).
- 141.E. Kritsi, C. Potamitis, S. Durdagi, P. Zoumpoulakis, S.G. Grdadolnik, **T. Mavromoustakos**. Molecular insights into the AT₁ antagonism based on biophysical and in silico studies of telmisartan. **Med. Chem. Res.** 22(10), 4842-4857 (2013).
- 142.G. Agelis, A. Resvani, C. Koukoulitsa, T. Tumonva, J. Slaninova, D. Kalavrizioti, K. Spyridaki, A. Afantitis, G. Melagraki, A. Siafaka, E. Gkini, G. Megariotis, S.G. Grdadolnik, M. Papadopoulos, D. Vlahakos, M. Maragoudakis, G. Liapakis, **T. Mavromoustakos**, J. Matsoukas. Rational design, efficient syntheses and biological evaluation of N,N'-symmetrically bis-substituted butylimidazole analogs as a new class of potent Angiotensin II receptor blockers. **Eur. J. Med. Chem.** 62, 352-370 (2013).
- 143.H.Tzoupis, G. Leonis, **T. Mavromoustakos**, M. G. Papadopoulos. A Comparative Molecular Dynamics, MM-PBSA and Thermodynamic Integration Study of Saquinavir Complexes with Wild-Type HIV-1 PR and L10I, G48V, L63P,

A71V, G73S, V82A and I84V Single Mutants. **J. Chem. Theory Comput.** 9, 1754-1764 (2013).

144. G. Aggelis, A. Resvani, D. Ntountaniotis, P. Chatzigeorgiou, C. Koukoulitsa, J. Matsoukas, T. Čendak, U. Codec, G. Mali, **T. Mavromoustakos**. Interactions of the potent synthetic AT1 antagonist analog BV6 with membrane bilayers and mesoporous silicate matrices. **Biochim. Biophys. Acta** 1828, 1846-1855 (2013).

145. G. Agelis, K. Kelaidonis, A. Resvani, D. Kalavrizioti, M.E. Androutsou, P. Plotas, D. Vlahakos, C. Koukoulitsa, **T. Mavromoustakos**, J. Matsoukas. Facile and efficient syntheses of a series of N-benzyl and N-biphenylmethyl substituted imidazole derivatives based on (E)-urocanic acid, as Angiotensin II AT1 receptor blockers. **Molecules** 18, 7510-7532 (2013).

146. M. Zervou, Z. Cournia, C. Potamitis, G. Patargias, S. Durdagi, S.G. Grdadolnik, **T. Mavromoustakos**. Insights into the molecular basis of action of the AT1 antagonist losartan using a combined NMR spectroscopy and computational approach. In press. **Biochim. Biophys. Acta**, 1838(3), 1031-1046 (2014).

147. P. Ioannis, **T. Mavromoustakos**. Monounsaturated fatty acid ether oligomers formed during heating of virgin olive oil shows agglutination activity against human red blood cells. **Journal of Agricultural and Food Chemistry**, 62, 867-874 (2014).

148. D. Ntountaniotis, T. Kellici, A. Tzakos, P. Kolokotroni, T. Tselios, J. Becker-Baldus, C. Glaubitz, Sonyan-Lin, A. Makriyannis, **T. Mavromoustakos**. The application of solid state NMR spectroscopy to study Candesartan Cilexetil (TCV-116) membrane interactions. Comparative study with the AT1 antagonist drug olmesartan **Biochim. Biophys. Acta** 1838, 2439-2450 (2014).

149. K. Spyridakis, M.T. Matsoukas, A. Cordomi, K. Gkountelias, M. Papadokostaki, T. Mavromoustakos, D.E. Logothetis, A. N. Margioris, G. Liapakis, L. Pardo, G. Liapakis. Structural-Functional of the Analysis of the Third Transmembrane Domain of the Corticotropin-releasing Factor Type 1. **J. Biol. Chem.** 289,18966-18977 (2014).

150. D. Ntountaniotis, G. Agelis, A. Resvani, M. Halabalaki, G. Liapakis, K. Spyridaki, S. Golic Grdadolnik, F. Merzel, S. Kostidis, C. Potamitis, T. Tselios, J. Matsoukas, A. L. Skaltsounis, **T. Mavromoustakos**. An efficient synthetic method and theoretical calculations of olmesartan methyl ether: Study of biological function of AT1 antagonism in press **Combinatorial Chemistry & High Throughput Screening**;17(8),652-662 (2014).

151. Tzoupis, H., Leonis, G., Avramopoulos, A., Mavromoustakos, T., Papadopoulos, M.G. Systematic molecular dynamics, MM-PBSA, and ab initio approaches to the saquinavir resistance mechanism in HIV-1 PR Due to 11 double and multiple mutations **Journal of Physical Chemistry B** 118(32), 9538-9552 (2014).

152. M. Roulia, **T. Mavromoustakos**, A. Vassiliadis, G. Mali. Distinctive Spectral and Microscopic Features for Characterizing the Three-Dimensional Local

Aluminosilicate Structure of Perlites. **The Journal of Physical Chemistry Part C** 118, 26649-26658 (2014).

153. G.G. Kordopati, T.V. Tselios, T. Kellici, F. Merzel, **T. Mavromoustakos**, S.G. Grdadolnik, G.M. Tsivgoulis. A novel synthetic luteinizing hormone-releasing hormone (LHRH) analogue coupled with modified β -cyclodextrin: Insight into its intramolecular interactions. **Biochimica et Biophysica Acta** 1850, 159–168 (2015).

154. T.F. Kellici, D. Ntountaniotis, G. Leonis, M. Chatziathanasiadou, A.V. Chatzikonstantinou, J. Becker-Baldus, C. Glaubitz, A.G. Tzacos, K. Viras, P. Chatzigeorgiou, S. Tzimas, E. Kefala, G. Valsami, H. Archontaki, M.G. Papadopoulos, **T. Mavromoustakos**. Investigation of the interactions of silibinin with 2-hydroxypropyl- β -cyclodextrin through biophysical techniques and computational methods. **Molecular Pharmaceutics** 12(3), 954-965 (2015)

155. N. Kollatos, S. Manta, A. Dimopoulou, V. Parmenopoulou, V.T. Triantakoustanti, T. Kellici, **T. Mavromoustakos**, D. Schols, D. Komiotis. Branched-chain sugar nucleosides: Stereocontrolled synthesis and bioevaluation of novel 3'-C-trifluoromethyl and 3'-C-methyl pyranonucleosides. **Carbohydrate Research**, 407, 170-178 (2015).

156. E. Vrontaki, G. Leonis, A. Avramopoulos, M.G. Papadopoulos, M. Simcic, S.G. Grdadolnik, A. Afantitis, G. Melagraki, S.K. Hadjikakou, **T. Mavromoustakos**. Stability and binding effects of silver(I) complexes at lipoxygenase-1. **Journal of Enzyme Inhibition and Medicinal Chemistry** 30(4) 539-549 (2015).

157. E. Vrontaki, G. Melagraki, **T. Mavromoustakos**, A. Afantitis. Exploiting ChEMBL database to identify indole analogues as HCV replication inhibitors. **Methods**, 71, 4-13 (2015).

158. A. Sadeghpour, M. Rappolt, D. Ntountaniotis, P. Chatzigeorgiou, K. Viras, G. Megariotis, M. Papadopoulos, E. Siapi, G. Mali, **T. Mavromoustakos**. Comparative Study of Interactions of Aliskiren and AT1 Receptor Antagonists with Lipid Bilayers. **Biochim. Biophys. Acta** 1848(4), 984-994 (2015).

159. E. Vrontaki, G. Melagraki, **T. Mavromoustakos**, A. Afantitis. Searching for anthranilic acid-based thumb pocket 2 HCV NS5B polymerase inhibitors through a combination of molecular docking, 3D-QSAR and virtual screening. **Journal of Enzyme Inhibition and Medicinal Chemistry** 31(1) 38-52 (2016)

160. C. Koukoulitsa, C.V. Barber, R. Csonka, X. Alexi, G. Leonis, D. Dellis, E. Hamelink, O. Belda, B.R. Steele, M.M. Screttas, M. N. Alexis, M. G. Papadopoulos, **T. Mavromoustakos**. Biological and computational evaluation of resveratrol inhibitors against Alzheimer's disease, **Journal of Enzyme Inhibition and Medicinal Chemistry**, 31(1) 66-77 (2016).

161. S. Vasilakaki, E. Barbayianni, G. Leonis, M.G. Papadopoulos, **T. Mavromoustakos**, M.H. Gelp, G. Kokotos. Development of a potent 2-oxoamide inhibitor of secreted phospholipase A2 guided by molecular docking calculations and

molecular dynamics simulations **Bioorganic and Medicinal Chemistry** 24(8) 1683-1695 (2016).

162. A.S. Foskolos, I. Papanastasiou, G.B. Foskolos, A. Tsotinis, T.F. Kellici, **T. Mavromoustakos**, M.C. Taylor, J.M. Kelly. New Hydrazones of 5-nitro-2-furaldehyde with adamantanealkanolhydrazides:synthesis and *in vitro* trypanocidal activity. *Med. Chem. Commun.* 7 1229-1236 (2016).

163. V.G. Kontogianni, M.E. Tsoumani, T.F. Kellici, **T. Mavromoustakos**, I.P. Gerothanasis, A.D. Tselepis, A.G. Tzakos. Deconvoluting the dual antiplatelet activity of a plant extract. **Journal of Agricultural and Food Chemistry** 64(2) 4511-4521 (2016).

164. T.F. Kellici, M. V. Chatziathanasiadou, D. Diamantis, A. V. Chatzikonstantinou, I. Andreadelis, E. Christodoulou, G. Valsami, **T. Mavromoustakos**, A. G. Tzakos, Mapping the interactions and bioactivity of quercetin—(2-hydroxypropyl)- β -cyclodextrin complex. **International Journal of Pharmaceutics** 511 (2016) 303–311.

165. Kritsi, E., Matsoukas, M. Potamitis, C., Karageorgos, V., Detsi, A., Magafa, V., Liapakis, G., **Mavromoustakos, T.**, Zoumpoulakis, P. Exploring new scaffolds for angiotensin II receptor antagonism. **Bioorganic and Medicinal Chemistry** 24(18) 4444-4451 (2016).

166. D. Ntountaniotis, M. Vanioti, G. G. Kordopati, T. F. Kellici , K. D. Marousis, **T. Mavromoustakos**, G. A. Spyroulias, S. G. Grdadolnik, T. V. Tselios. A combined NMR and molecular dynamics simulation study to determine the conformational properties of rat/mouse 35-55 myelin oligodendrocyte glycoprotein epitope implicated in the induction of experimental autoimmune encephalomyelitis. **Journal of Biomolecular Structure and Dynamics**, 35, 1559–1567 (2017).

167. Kellici, T.F., Ntountaniotis, D., Vanioti, M., Grdadolnik, G.S., Simcic, M., Michas, G., Moutevelis-Minakakis, **Mavromoustakos, T.** The use of J-coupling as a sole criterion to assign the total absolute stereochemistry of new pyrrolidinone class synthetic analogs, derived from S-pyroglutamic acid. **Journal of Molecular Structure**, 1129, 195-199 (2017).

168. Tahsin F. Kellici, **T. Mavromoustakos**, D. Jendrosseck, and A. C. Papageorgiou, Crystal structure analysis, covalent docking, and molecular dynamics calculations reveal a conformational switch in PhaZ7 PHB depolymerase. **Proteins** 85,1351–1361 (2017).

169. A. S. Liossi , D. Ntountaniotis, T.F. Kellici, M.V. Chatziathanasiadou, G. Megariotis, M. Mania, J. Becker-Baldus, M. Kriechbaum, A. Krajnc, E. Christodoulou, C. Glaubitz , M. Rappolt, H. Amenitsch, Gregor Mali, D.N. Theodorou, G. Valsami, M. Pitsikalis, H. Iatrou, A. Tzakos, **T. Mavromoustakos**. Exploring the interactions of irbesartan and irbesartan–2-hydroxypropyl- β -cyclodextrin complex with model membranes. **Biochimica et Biophysica Acta** 1859, 1089–1098 (2017).

170. T. F. Kellici, **T. Mavromoustakos**, P. Stathopoulos, V. Tsikaris, V. Magafa, A. G. Tzakos & A. D. Tselepis, Molecular requirements involving the human platelet

protease-activated receptor-4 mechanism of activation by peptide analogues of its tethered ligand, I. C. Moschonas, **Platelets**, 28(8), 812-821 (2017).

171. G. Raptopoulos, K. Kyriakou, G. Mali, A. Scarpellini, G. C. Anyfantis, **T. Mavromoustakos**, M. Pitsikalis, P. Paraskevopoulou, Copolymerization of Norbornene and Norbornadiene Using a cis-Selective Bimetallic W-Based Catalytic System. **Polymers**, 9, 141, 2017; doi:10.3390/polym9040141.

172. M. Vlachou, A. Siamidi, D. Spaneas, D. Lentzos¹, P. Ladia, K. Anastasiou, I. Papanastasiou, A.S. Foscolos, M.O. Georgiadis, V. Karalis, T. Kellici, **T. Mavromoustakos**. In vitro Controlled Release of two new Tuberculocidal Adamantane Aminoethers from Solid Pharmaceutical Formulations (II). **Drug Res** 67: 1–8 (2017).

173. G. Melagraki, E. Ntougkos, V. Rinotas, C. Papaneophytou, G. Leonis, **T. Mavromoustakos**, G. Kantopidis, E. Douni, A. Afantitis, G. Kol. Cheminformatics-aided discovery of small-molecule protein-protein interaction (PPI) dual inhibitors of Tumor Necrosis Factor (TNF) and receptor activator of NF- κ B ligand (RANKL). **PLOS Computational Biology** 13(4), e1005372 | (2017).

174. P. Chatzigeorgiou, A. Mourelatou, E. Pallatos, **T. Mavromoustakos**, C.E. Semidalas. Comparison of the thermal behavior and conformational changes in partially and fully hydrated dipalmitoylphosphatidylcholine systems. **J. Thermal Anal. Cal.** 1-12 (2017).

175. M. Vlachou, A. Siamidi, E. Diamantidi, A. Iliopoulou, I. Papanastasiou, V. Ioannidou, V. Kourbeli, A.S. Foscolos, A. Vocat, S.T. Cole, V.T. Karalis, T. Kellici, **T. Mavromoustakos**, **Drug Research** 67(8), 447-450 (2017).

176. E.I. Vrettos, N. Sayyad, E.M. Mavrogiannaki, E. Stylos, K.D. Androniki, S. Papas, **T. Mavromoustakos**, V. Theodorou, A.G. Tzakos, Unveiling and tackling guanidinium peptide coupling reagent side reactions towards the development of peptide-drug conjugates. **RSC Advances** 7(80), 50519-50526 (2017).

177. T.F. Kellici, M.V. Chatziathanasiadou, M.Sung Lee, N. Sayyad, E. G. Geromichalou, E.I. Vrettos, A. D. Tsailanis, S.W. Chi, G.D. Geromichalos, **T. Mavromoustakos**, A.G. Tzakos, Rational design and structure–activity relationship studies of quercetin–amino acid hybrids targeting the anti-apoptotic protein Bcl-xL **Organic & Biomolecular Chemistry** 15(37), 7956-7976 (2017).

178. S.B. Mirza R.C. Hua Lee, J.J. Hann Chu., R.E. Salmas, **T. Mavromoustakos**, S. Durdagi, Discovery of selective dengue virus inhibitors using combination of molecular fingerprint-based virtual screening protocols, structure-based pharmacophore model development, molecular dynamics simulations and in vitro studies, **Journal of Molecular Graphics and Modelling** 79, 88-102 (2018).

179. S. Vasilakaki, O. Pastukhov, **T. Mavromoustakos**, A. Huwiler and G. Kokotos, Small Peptides Able to Suppress Prostaglandin E2 Generation in Renal Mesangial Cells, **Molecules**, 23(1), 158 (2018).

180. P. Lagarias, G. Lambrinidis, D. Stamatis, M. Conventino, G. Ortore, T. Mavromoustakos, K. Norbert Klotz, A. Kolocouris, Discovery of Novel Adenosine Receptor Antagonists through a Combined Structure- and Ligand-Based Approach Followed by Molecular Dynamics Investigation of Ligand Binding Mode **J. Chem. Inf. Model.**, 58 (4), 794–815 (2018).
181. E. Kyriakou, A.D. Kostagianni, T.F. Kellici, E. Giannopoulou, K.E. Siatis, N. Sayyad, H.P. Kolofonos, **T. Mavromoustakos**, H. Stamatis, A.G.Tzakos. Three Regioselectively Acylated Flavonoid Derivatives in Equimolar Yield at One Blow. **Chem. Select.** 3(18), 5207-5211 (2018).
182. Chatzigeorgiou, P., Mourelatou, A., Pollatos, E., Margari, D., Zogzas, N., **Mavromoustakos, T.**, Semidalas, C.E. Comparison of the thermal behavior and conformational changes in partially and fully hydrated dipalmitoylphosphatidylcholine systems **Journal of Thermal Analysis and Calorimetry** 131(2), 887-898 (2018).
183. T.F. Kellici, D. Ntountaniotis, G. Liapakis, A.G. Tzakos, **T. Mavromoustakos**, The dynamic properties of angiotensin II type 1 receptor inverse agonists in solution and in the receptor site, **Arabian Journal of Chemistry** 12, 5062-5078 (2019).
184. D. A. Diamantis, S. Ramesova, C. M. Chatzigiannis, I.Degano, P. S. Gerogianni, C. Karadimaf, S. Perikleous, D. Rekkas, I.P. Gerothanassis, D. Galaris, **T. Mavromoustakos**, G.Valsami, R. Sokolova, A. G. Tzakos, Exploring the oxidation and iron binding profile of a cyclodextrin encapsulated quercetin complex unveiled a controlled complex dissociation through a chemical Stimulus **Biochim. Biophys. Acta**, General subjects, 1862, 1913-1924 (2018).
185. Athina Konstantinidi, Nikolaos Naziris, Maria Chountoulesi, Sophia Kiriakidi, Barbara Sartori, Dimitris Kolokouris, Heinz Amentisch, Gregor Mali, Dimitrios Ntountaniotis, Costas Demetzos, **Thomas Mavromoustakos**, and Antonios Kolocouris. Comparative Perturbation Effects Exerted by the Influenza A M2 WT Protein Inhibitors Amantadine and the Spiro[pyrrolidine-2,2'-adamantane] Variant AK13 to Membrane Bilayers Studied Using Biophysical Experiments and Molecular Dynamics Simulations **Journal of Physical Chemistry B** 122(43), 9877-9895 (2019).
186. D. Ntountaniotis, I. Andreadelis, T.F. Kellici, V. Karageorgos, G. Leonis, E. Christodoulou, S. Kiriakidi, J. Becker-Baldus, E.K. Stylos, M.V. Chatziathanasiadou, C.M. Chatzigiannis, D.E. Damalas, B. Aksoydan, U. Javornik, G. Valsami, C. Glaubitz, S. Durdagi, N.S. Thomaidis, A. Kolocouris, J. Plavec, A.G. Tzakos, G. Liapakis, **T. Mavromoustakos**. Host-Guest Interactions between Candesartan and Its Prodrug Candesartan Cilexetil in Complex with 2-Hydroxypropyl- β -cyclodextrin: On the Biological Potency for Angiotensin II Antagonism. **Molecular Pharmaceutics** 16(3),1255-1271 (2019).
187. Mustafa Yilmaz, Apostolos A. Karanastasis, Maria V. Chatziathanasiadou, Mehmet Oguz, Anastasia Kougioumtzi, Nausicaa Clemente, Tahsin F. Kellici, Nikolaos E. Zafeiropoulos, Apostolos Avgeropoulos, **Thomas Mavromoustakos**, Umberto Dianzani, Serdar Karakurt, Andreas G. Tzakos. Inclusion of Quercetin in Gold Nanoparticles Decorated with Supramolecular Hosts Amplifies

Its Tumor Targeting Properties. **ACS Applied Biomaterials** 2(7), 2715-2725 (2019) .

188. A. Papageorgiou, A.S. Foscolos, P Papanastasiou, M. Vlachou, A.Siamidi, A. Vocat, S.T. Cole, T. F. Kellici,T.Mavromoustakos, A. Tsotinis. Synthesis, biology, computational studies and in vitro controlled release of new isoniazid-based adamantane derivatives. **Future Chemistry**, 11(21), 2779–2802 (2019).

189. V.A. Karetsi, C.N. Banti 1, N. Kourkouvelis, C. Papachristodoulou, C.D. Stalikas, C.P. Raptopoulou, V. Psycharis, P. Zoumpoulakis, **T. Mavromoustakos**, I. Sainis, S.K. Hadjikakou An Efficient Disinfectant, Composite Material {SLS@[Zn₃(CitH)₂]} as Ingredient for Development of Sterilized and Non Infectious Contact Lens. **Antibiotics** 8, 213; doi:10.3390/antibiotics8040213, (2019).

190. **T. Mavromoustakos**, D. Ntountaniotis, G. Leonis, E. Christodoulou. Exploring the interactions of irbesartan-2-hydroxypropyl-β-cyclodextrin complex in micelles. Materials, Methods & Technologies ISSN 1314-7269, Volume 13, 2019 **Journal of International Scientific Publications** www.scientific-publications.net pp. 270-278 (2019).

191. S. Kiriakidi, C. Chatzigiannis, C. Papaemmanouil, A.G. Tzakos, **T. Mavromoustakos**. Exploring the role of the membrane bilayer in the recognition of candesartan by its GPCR AT1 receptor. **Biochimica et Biophysica Acta** 1862, 183142 (2020).

192. A. Konstantinidi, M. Chountoulesi, N. Naziris, B. Sartori, Heinz Amenitsch, G. Mali, T. Čendak, M. Plakantonaki, I. Triantafyllakou, Theodore Tselios, C.Demetzos, D. D. Busath, T. Mavromoustakos, A. Kolocouris. The boundary lipid around DMPC-spanning influenza A M2 transmembrane domain channels: Its structure and potential for drug accommodation **Biochimica et Biophysica Acta** 183156 (2020).

193. A.K. Rossos, C.N. Bantia, A. Kalampounias, C. Papachristodoulou, K. Kordatos, P. Zoumpoulakis, **T. Mavromoustakos**, N. Kourkouvelis, S.K. Hadjikakou. pHEMA@AGMNA-1: A novel material for the development of antibacterial contact lens **Materials Science & Engineering C** 111, 110770 (2020).

194.G. Leonis, E. Christodoulou, D. Ntountaniotis1, M. V. Chatziathanasiadou, **T. Mavromoustakos**, N. Naziris, M. Chountoulesi, C. Demetzos, G. Valsami, D. E. Damalas, A. G. Tzakos, N. S. Thomaidis, V. Karageorgos, G. Liapakis. Antihypertensive Activity and Molecular Interactions of Irbesartan in Complex with 2-Hydroxypropyl-β-Cyclodextrin.**Chemical Biology&Drug Design** 96,668–683 (2020).

195. C. Papaemmanouil, M. V. Chatziathanasiadou, C. Chatzigiannis, E. Chontzopoulou, **T. Mavromoustakos**, S. G. Grdadolnik & A. G. Tzakos. Unveiling the interaction profile of rosmarinic acid and its bioactive substructures with serum albumin **Journal of Enzyme Inhibition and Medicinal Chemistry** 35(1),786–804 (2020).

196. A. D. Tsailanis, A. Renziehausen, S. Kiriakidi, E. I. Vrettos, G. S. Markopoulos, N. Sayyad, B. a Hirmizf, M. I. Aguilar, M. P. Del Borgo, E. Kolettas, R. E. Widdop, **T. Mavromoustakos**, T. Crook, N. Syed, A. G. Tzakos. Enhancement of glioblastoma multiforme therapy through a novel Quercetin-Losartan hybrid. **Free Radical Biology and Medicine** 160(20), 391-402 (2020).
197. R. Chayron, N. A. Parisi, M. V. Chatziathanasiadou, E. Vrontaki, K. Moschovou, G. Melagraki, D. Sbirikova, B. Schivachev, M. Schmidtke, Y. Mitrev, M. Sticha, **T. Mavromoustakos**, A. G. Tzakos. Synthetic Analogues of Amino adamantane as Influenza Viral Inhibitors—*In Vitro*, *in Silico* and QSAR Studies. **Molecules** 25(17), 3989 (2020).
198. C. Gkoliniopoulou, F. Soukou, I. Dafnis, T. F. Kellici, D. Sanoudou, **T. Mavromoustakos**, E. Stratikos, A. Chroni. Structure–function analysis of naturally occurring apolipoprotein A-I L144R, A164S and L178P mutants provides insight on their role on HDL levels and cardiovascular risk. **Cellular and Molecular Life Sciences** 160, 391-402 (2020).
199. I. Andreadelis, M. V. Chatziathanasiadou, D. Ntountaniotis, G. Valsami, C. Papaemmanouil, E. Christodoulou, G. Mitropoulou, Y. Kourkoutas, A. G. Tzakos, **T. Mavromoustakos**. Charting the structural and thermodynamic determinants in phenolic acid natural product–cyclodextrin encapsulations. **Molecular Pharmaceutics**, 16(3), 1255-1271 (2020).
200. G. Liapakis, V. Karageorgos, I. Andreadelis, G. G. Holz, E. Dermitzaki, G. G. Kordopati, E. K. Stylos, K. Spyridaki, S. Poulaki, D. Ntountaniotis, S. Sakellaris, M. Vanioti, A. Kostagianni, K. D. Marousis, G. Leonis, G. Kokotos, M. Venihaki, G. A. Spyroulias, T. Tselios, A. M. A. G. Tzakos, **T. Mavromoustakos**. Discovery of a stable tripeptide targeting the N-domain of CRF1 receptor **Amino Acids** 52:1337–1351 (2020).
201. A. Chroni, **T. Mavromoustakos**, S. Pispas. Biocompatible PEO-b-PCL Nanosized Micelles Drug Carriers: Structure and Drug-Polymer Interactions. **Nanomaterials**, 10, 1872 (2020).
202. K. Manta, P. Papakyriakopoulou, M. Chountoules, D. A. Diamantis, D. Spaneas, V. Vakali, N. Naziris, M. V. Chatziathanasiadou, I. Andreadelis, K. Moschovou, I. Athanasiadou, P. Dallas, D. M. Rekkas, C. Demetrios, G. Colombo, S. Banella, U. Javornik, J. Plavec, **T. Mavromoustakos**, A. G. Tzakos, G. Valsami, Preparation and Biophysical Characterization of Quercetin Inclusion Complexes with β -Cyclodextrin Derivatives to be Formulated as Possible Nose-to-Brain Quercetin Delivery Systems, **Molecular Pharmaceutics**, 17(11), 4241-4255 (2020).
203. M. E. K. Stathopoulou, N. Zoupanou, C. V. Banti, A. P. Douvalis, C. Papachristodoulou, K. D. Marousis, G. A. Spyroulias, **T. Mavromoustakos**, S. K. Hadjikakou, Organotin derivatives of cholic acid induce apoptosis into breast cancer cells and interfere with mitochondrion; Synthesis, characterization and biological evaluation. **Steroids**, 167, 108798 (2021).
204. A. Meretoudi, C. N. Banti, P. K. Raptis, C. Papachristodoulou, N. Kourkoumelis, A. A. Ikiades, P. Zoumpoulakis, **T. Mavromoustakos**, S. Hadjikakou, Silver

nanoparticles from oregano leaves' extracts as antimicrobial components for non-infected hydrogel contact lenses **International Journal of Molecular Sciences**, 22(7), 3539 (2021).

205. I. Andreadelis, M.V. Chatziathanasiadou, D. Ntountaniotis, A.G. Tzakos, **T. Mavromoustakos**, Charting the structural and thermodynamic determinants in phenolic acid natural product–cyclodextrin encapsulations, **Journal of Biomolecular Structure and Dynamics**, 2021,39(7), 2642–2658 (2021).

206. S. Kiriakidi, C. Chatzigiannis, C. Papaemmanouil, A.G. Tzakos, Z. Cournia, T. Mavromoustakos. Interplay of cholesterol, membrane bilayers and the AT1R: A cholesterol consensus motif on AT1R is revealed. **Computational and Structural Biotechnology Journal**, 19, 110–120 (2021).

207. A. Chroni, **T. Mavromoustakos**, S. Pispas. Nano-assemblies from amphiphilic pnba-b-poega copolymers as drug nanocarriers **Polymers** 13(7), 1164, (2021).

208. K. Kollias, A. Godelitsas, J. Manuel Astilleros, S. Ladas, A. Lagoyannis, **T. Mavromoustakos**. Dissolution and sorption mechanisms at the aluminosilicate and carbonate mineral-AMD (Acid Mine Drainage) interface. **Applied Geochemistry** 131, 105027 (2021).

209.A.D. Tsailanis, E. Vrettos, M. Choleva, S. Kiriakidi, Ab M. Ganai, T. Tabasum Khand, R. Karpoormath, Rajshekhard, **T. Mavromoustakos**, E. Fragopoulou, A.G. Tzakos. Development of a DHA-Losartan hybrid as a potent inhibitor of multiple pathway-induced platelet aggregation. **Journal of Biomolecular Structure and Dynamics** <https://doi.org/10.1080/07391102.2021.1996461> (2021).

210. E. Chontzopoulou, C. Papaemmanouil, M. Chatziathanasiadou, D. Kolokouris, S. Kiriakidi, A. Konstantinidi, I. Gerogianni, T. Tselios, I. Kostakis, Ioannis C. Evangelia D. L. Hadjipavlou D. Tzeli, **T. Mavromoustakos**. Molecular investigation of artificial and natural sweeteners as potential anti-inflammatory agents *Journal of Biomolecular Structure and Dynamics*. <https://doi.org/10.1080/07391102.2021.1973565>.

211. A. Chroni, **T. Mavromoustakos**, S. Pispas. Poly(2-oxazoline)-Based Amphiphilic Gradient Copolymers as Nanocarriers for Losartan: Insights into Drug-Polymer Interactions. *Macromol* 1,177-200 (2021).

212. N.Zoupanou, C.N. Banti, A.P. Douvalis, C. Papachristodoulou, K. D. Marousis, G.A. Spyroulias, **T. Mavromoustakos**, S.K. Hadjikakou. Organotin derivatives of cholic acid induce apoptosis into breast cancer cells and interfere with mitochondrion; Synthesis, characterization and biological evaluation. **Steroids** 167, 108798 (2021).

213. J. Matsoukas, V. Apostolopoulos, A. Zulli, G. Moore, K. Kelaidonis, K. Moschvou, **T. Mavromoustakos**. From Angiotensin II to Cyclic Peptides and Angiotensin Receptor Blockers (ARBs): Perspectives of ARBs in COVID-19 Therapy. **Molecules**, 26(3), 618 (2021).

214. S. Kiriakidi, C. Chatzigiannis, C. Papaemmanouil, A. G. Tzakos, Z. Cournia,

T. Mavromoustakos. Interplay of cholesterol, membrane bilayers and the AT1R: A cholesterol consensus motif on AT1R is revealed. **Computational and Structural Biotechnology Journal** 19, 110–120(2021).

215. A. Meretoudi, C.N. Banti, P. K. Raptis, C. Papachristodoulou, N. Kourkoumelis, A. A. Ikiades, P. Zoumpoulakis, T. Mavromoustakos, Sotiris K. Hadjidakou. Silver Nanoparticles from Oregano Leaves' Extracts as Antimicrobial Components for Non-Infected Hydrogel Contact Lenses. **Int. J. Mol. Sci.** 22, 3539 (2021).

216. A. Chroni, **T. Mavromoustakos**, S. Pispas. Nano-Assemblies from Amphiphilic PnBA-b-POEGA Copolymers as Drug Nanocarriers. **Polymers** 13, 1164 (2021).

217. E.M. Tomou, C. D. Papaemmanouil, D. A. Diamantis, A. D. Kostagianni, P. Chatzopoulou, **T. Mavromoustakos**, A. G. Tzakos, H. Skaltsa. Anti-Ageing Potential of S. euboea Heldr. Phenolics. **Molecules** 26, 3151 (2021).

218. C.N. Banti, M. Kapetana, C. Papachristodoulou, C.P. Raptopoulou, V. Psycharis, P. Zoumpoulakis, **T. Mavromoustakos**, S.K. Hadjidakou. Hydrogels containing water soluble conjugates of silver(i) ions with amino acids, metabolites or natural products for non infectious contact lenses. Dalton Transaction 50(39), 13712–13727 (2021).

219.A.K. Rossos, C.N. Banti, P.K. Raptis, C. Papachristodoulou, I. Sainis, P. Zoumpoulakis, **T. Mavromoustakos**, S. K. Hadjidakou. Silver Nanoparticles Using Eucalyptus or Willow Extracts (AgNPs) as Contact Lens Hydrogel Components to Reduce the Risk of Microbial Infection. **Molecules** 26(16), 5022 (2021).

220. K. Kollias, A. Godelitsas, J. ManulAstilleros, S. Ladas, A. Lagoyannis, **T.Mavromoustakos**. Dissolution and sorption mechanisms at the aluminosilicate and carbonate mineral-AMD (Acid Mine Drainage) interface **Applied Geochemistry**, 131, 105027 (2021).

221. M. Vlachou, A-S. Foscolos, A. Siamidi, A. Syriopoulou, N. Georgiou, A. Dedeloudi, A. D. Tsailanis, A.G. Tzakos, **T. Mavromoustakos**, I.P. Papanastasiou Biophysical Evaluation and In Vitro Controlled Release of Two Isomeric Adamantane Phenylalkylamines with Antiproliferative/Anticancer and Analgesic Activity. **Molecules** 27(1) 7 (2022).

222. Altunayar-Unsalan, C., Unsalan, O., **T. Mavromoustakos**, Insights into molecular mechanism of action of citrus flavonoids hesperidin and naringin on lipid bilayers using spectroscopic, calorimetric, microscopic and theoretical studies **Journal of Molecular Liquids**, 347, 118411 (2022).

223. V. Palli 1, G. Leonis, N. Zoupanou, N. Georgiou, M. Chountoulesi, N. Naziris, D. Tzeli, C. Demetzos, G. Valsami, K. D. Marousis, G. A. Spyroulias, T.Mavromoustakos. **Molecules** 27, 2421, 1-17 (2022).

224. H. Ridway, G.J. Moore, **T. Mavromoustakos**, S. Tsiodras, I. Ligielli, K. Kelaidonis, C.T. Chasapis, L.K. Gadanec, V.G. Gorgoulis, J.M. Matsoukas. Discovery of a new generation of angiotensin receptor blocking drugs: Receptor

mechanisms and in silico binding to enzymes relevant to covid-19. **Computational and Structural Biotechnology Journal** 20, 2091-2111 (2022).

225. H. Ridgway, C. T. Chasapis,, K. Kelaidonis, I. Ligielli, G. J. Moore, L. K. Gadanec, A. Zulli, V. Apostolopoulos, **T. Mavromoustakos**, J. M. Matsoukas. Understanding the Driving Forces That Trigger Mutations in SARS-CoV-2: Mutational Energetics and the Role of Arginine Blockers in COVID-19 Therapy. **Viruses**,14,1029 (2022).

226. C. Altunayar-Unsalan, O. Unsalan, **T. Mavromoustakos**. Molecular interactions of hesperidin with DMPC/cholesterol bilayers. **Chemico-biological interactions** 366, 110131 (2022).

227. J. M. Matsoukas, L.K. Gadanec, A. Zulli, V.Apostolopoulos, K.Kelaidonis, I. Ligielli, K. Moschovou, N. Georgiou, P. Plotas, C. T. Chasapis, G. Moore, H. Ridgway and T. Mavromoustakos. Diminazene Aceturate Reduces Angiotensin II Constriction and Interacts with the Spike Protein of Severe Acute Respiratory Syndrome Coronavirus 2 **Biomedicines** 10, 1731, (2022).

228. N. Georgiou, Antigoni Cheilari, Danai Karta, Eleni Chontzopoulou, Janez Plavec, Demeter Tzeli, Stamatia Vassiliou, and **Thomas Mavromoustakos**, Conformational Properties and Putative Bioactive Targets for Novel Thiosemicarbazone Derivatives. **Molecules** 27, 4548 (2022).

229. N. Georgiou, A. Katsogiannou, D. Skourtis, H. Iatrou, D. Tzeli, S. Vassiliou, Uroš Javornik, J. Plavec and **Thomas Mavromoustakos** Conformational Properties of New Thiosemicarbazone and Thiocarbohydrazone Derivatives and Their Possible Targets. **Molecules** 27, 2537 (2022).

230. G. J. Moore, H. Ridgway, K. Kelaidonis, C. T. Chasapis, I. Ligielli, **T. Mavromoustakos**, J. Bojarska, J. M. Matsoukas. Actions of Novel Angiotensin Receptor Blocking Drugs, Bisartans, Relevant for COVID-19 Therapy: Biased Agonism at Angiotensin Receptors and the Beneficial Effects of Nephilysin in the Renin Angiotensin System. **Molecules** 27, 4854 (2022).

231. H. Ridgway, C. Ntallis 3 , C. T. Chasapis, K. Kelaidonis, M.Timotheos Matsoukas, P. Plotas, V. Apostolopoulos, G. Moore, S.Tsiodras, D. Paraskevis, **T. Mavromoustakos**, J. M. Matsoukas Molecular Epidemiology of SARS-CoV-2: The Dominant Role of Arginine in Mutations and Infectivity. **Viruses** 2023, 15, 309. <https://doi.org/10.3390/v15020309>.

232. G. Leonis, V. Vakali, N. Zoupanou, N. Georgiou, D. A. Diamantis, A.G. Tzakos, **T. Mavromoustakos**, D. Tzeli. Computational and spectroscopic analysis of the Quercetin encapsulation in (2HP- β -CD)₂ and (2,6Me- β -CD)₂ complexes. **Journal of Molecular Structure** 1294, 136430-136443 (2023).

233. D. P. Kiouri, C. Ntallis, K. Kelaidonis, M. Peana, S. Tsiodras, **T. Mavromoustakos**, A. Giuliani, H. Ridgway, G. J. Moore, J. M. Matsoukas, C. T. Chasapi. Network-Based Prediction of Side Effects of Repurposed Antihypertensive

Sartans against COVID-19 via Proteome and Drug-Target Interactomes. **Proteomes** 11,23-54 (2023).

234. K. Kelaïdonis, I. Ligielli, S. Letsios, P. Vidali, **T. Mavromoustakos**, N. Vassilaki, G. J. Moore, W. Hoffmann, K.W. Egrzyn, H. Ridgway, C. T. Chasapis 10, J. M. Matsoukas. Computational and Enzymatic Studies of Sartans in SARS-CoV-2 Spike RBD-ACE2 Binding: The Role of Tetrazole and Perspectives as Antihypertensive and COVID-19 Therapeutics. **Int. J. Mol. Sci.** 24, 8454-8478 (2023).

235. N. Georgiou, E. Chontzopoulou, A. Cheilari, A. Katsogiannou, D. Karta, K. Vavougyiou, D. Hadjiipavlou-Litina, U. avornik, J. Plavec, D. Tzeli, S. Vassiliou, **T. Mavromoustakos** Thiocarbohydrazones and Chalcone Derived Dihydropyrimidinethiones as Lipid Peroxidation and Soybean Lipoxygenase Inhibitors **ACS Omega** 8, 13, 11966-11977 (2023).

236. A. Chroni, **T. Mavromoustakos**, S. Pispas. Curcumin-Loaded PnBA-b-POEGA Nanoformulations: A Study of Drug-Polymer Interactions and Release Behavior. **Int. J. Mol. Sci.**, 24(5), 4621-4642 (2023).

237. M. Vlachou, A. Siamidi, D. Anagnostopoulou, C. Protopapa, R. Kompogennitaki, A. Sakellaropoulou, N. Efstathiou, I. Papanastasiou, M. Billia, **T. Mavromoustakos**. Potent Lipophilic Melatonergic x-fluoro-y-methoxy Substituted Phenylalkylamides: Molecular Dynamics Calculations and in vitro Modified Release in Aqueous Media from Tablet Formulations. **Current Pharmaceutical Design** 29, 17, 1370 – 1378 (2023).

238. N. Georgiou, N. Gouleni, E. Chontzopoulou, G.S. Skoufas, A. Gkionis, D. Tzeli, S. Vassiliou, **T. Mavromoustakos**. Structure assignment, conformational properties and discovery of potential targets of the Ugi cinnamic adduct NGI25. **Journal of Biomolecular Structure and Dynamics**, 41,4, 1253-1266 (2023).

239. P. Mavroeidi, L. P. Zorba, N. V. Tzouras, S. P. Neofotistos, N. Georgiou, K. Sahin, M. Şentürk, S. Durdagi, G.C. Vougioukalakis and **T. Mavromoustakos**, Are Terminal Alkynes Necessary for MAO-A/MAO-B Inhibition? A New Scaffold Is Revealed. **Molecules** (2024), 29, 2486. <https://doi.org/10.3390/molecules29112486>,

240. N. Georgiou, D. Karta, A. Cheilari, F. Merzel, D. Tzeli, S. Vassiliou and **T. Mavromoustakos**. Synthesis of Thiazolidin-4-Ones Derivatives, Evaluation of Conformation in Solution, Theoretical Isomerization Reaction Paths and Discovery of Potential Biological Targets. **Molecules** 29(11), 2458 (2024).

241. V. Apostolopoulos, N. Georgiou, D. Tzeli, **T. Mavromoustakos**, G.J. Moore, Konstantinos Kelaïdonis, M.T. Matsoukas, S. Tsiodras, J. Swiderski. Density functional theory and enzyme studies support interactions between angiotensin receptor blockers and angiotensin converting enzyme-2: Relevance to coronavirus 2019. **Bioorganic Chemistry** 150 (2024) 107602.

242. P. Ntavaroukas 1. Konstantinos Michail, R. Tsiakalidou, E. Stampouloglou, K. Tsiggene, D. Komiotis, N. Georgiou, **T. Mavromoustakos**, S. Manta, D. Aje, P.

Michael, B. J. Campbell, S.Papoutsopoulou. A Novel Quinoline Inhibitor of the Canonical NF- κ B **Transcription Factor Pathway Biology** 2024, 13, 910. <https://doi.org/10.3390/biology13110910>

243. N.Georgiou, T. **Mavromoustakos**, D. Tzeli, Docking, MD Simulations, and DFT Calculations: Assessing W254's Function and Sartan Binding in Furin. **Curr. Issues Mol. Biol.** 46(8), 8226-8238 (2024).

244. H. Ridgway, G.J. Moore, L.K. Gadanec, A. Zulli, V. Apostolopoulos, W. Hofmann, K. Wegrzyn, N. Vassilaki, G. Mpekoulis, M. Zouridakis, P. Giastas, V.P. Vidali, K. Kelaionis, M.T. Matsoukas, M. Dimitriou, T. **Mavromoustakos**, S. Tiodras, V.G. Georgoulis, I. Karakasiliotis, C. Chasapis, J.M. Matsoukas. Novel benzimidazole angiotensin receptor blockers with anti-SARS-CoV-2 activity equipotent to that of nirmatrelvir: computational and enzymatic studies *Expert Opinion on Therapeutic Targets* 28, 5, 437 – 459 (2024).

245. N. Georgiou, N., A. Tzani, ., K. Vavougyiou,. C. Papadopoulos, N. Eleftheriadis, P. Sket, D. Tzelis, Tiemi-Aro, T. **Mavromoustakos** Synthesis of Anti-Inflammatory Drugs' Chalcone Derivatives and a Study of Their Conformational Properties Through a Combination of Nuclear Magnetic Resonance Spectroscopy and Molecular Modeling **Pharmaceuticals**, 2025, 18(1), 88.

REVIEW ARTICLES IN INTERNATIONAL JOURNALS WITH PEER REVIEWERS -BOOK CHAPTERS

246. N. Georgiou, M. G. Kakava, E. A. Routsis, E. Petsas, N. Stavridis, C. Freris, N. Zoupanou, K. Moschovou, S. Kiriakidi. T. **Mavromoustakos**. Quercetin: A Potential Polydynamic Drug. **Molecules**, 2023, 28, 8141.

247.T. **Mavromoustakos**, V. Apostolopoulos, J. Matsoukas. Antihypertensive drugs that act on Renin-Angiotensin System with emphasis in AT₁ antagonists **Mini Rev. Med. Chem.** 1, 207-217 (2001).

248. J. Matsoukas, T. **Mavromoustakos**, V. Apostolopoulos, Designing peptide mimetics for the treatment of multiple sclerosis, **Mini Rev. Med. Chem.** 1, 273-282 (2001).

249. V. Apostolopoulos, J. Matsoukas, M. Plebanski, T. **Mavromoustakos**, Applications of Peptide Mimetics in Cancer. **Curr. Med. Chem.** 9, 411-420 (2002).

250. T. **Mavromoustakos**, P. Zoumpoulakis, I. Kyrikou, A. Zoga, E. Siapi, M. Zervou, I. Daliani, D. Dimitriou, A. Pitsas, C. Kamoutsis, P. Laggner.Efforts to Understand the Molecular Basis of Hypertension Trough Drug:Membrane Interactions. **Current Topics in Medicinal Chemistry**, 4, 445-459 (2004).

251. T. **Mavromoustakos**, M. Zervou, P. Zoumpoulakis, I. Kyrikou, N.P. Benetis, L. Polevaya, P. Roumelioti, N. Giatas, A. Zoga, P. Moutevelis Minakakis, A. Kolocouris, D. Vlahakos, S. Golic Grdadolnik, J. Matsoukas. Conformation and

Bioactivity. Design and Discovery of Novel Antihypertensive Drugs. **Current Topics in Medicinal Chemistry**, 4, 385-401, (2004).

252. K.P. Marathias, B. Agroyannis, **T. Mavromoustakos**, J. Matsoukas, D.V. Vlahakos. Hematocrit-lowering Effect Following Inactivation of Renin-Angiotensin System with Angiotensin Converting Enzyme Inhibitors and Angiotensin Receptor Blockers. **Current Topics in Medicinal Chemistry**, 4, 483-486 (2004).

253. **T. Mavromoustakos**, A. Kapou, N.P. Benetis, M. Zervou. Conformational Analysis Using 2D NMR Spectroscopy Coupled with Computational Analysis as an Aid in the Alignment Procedure of 3D-QSAR studies. **Drug Design Reviews-Online** 1(3) 235-245 (2004).

254. E.D. Manzourani, **T.M. Mavromoustakos**, J.A. Platts, J.M. Matsoukas, T.V. Tselios. Structural Requirements for Binding of Myelin Basic Protein (MBP) Peptides to MHC II: Effects on Immune Regulation. **Current Medicinal Chemistry**, 12, 1521-1535 (2005).

255. P. Zoumpoulakis and **T. Mavromoustakos**. Seeking the Active Site of the AT₁ Receptor for Computational Docking. **Drug Design Reviews-Online**. 2, 537-544, (2005).

256. **T. Mavromoustakos**, S. Durdagi, C. Koukoulitsa, M. Simcic, M.G. Papadopoulos, M. Hodoscek, S. Golic Grdadolnik. Strategies in the Rational Drug Design. **Current Medicinal Chemistry**, 18, 2517-2530 (2011).

257. V.D. Mouchlis, E. Barbayianni, **T.M. Mavromoustakos** and G. Kokotos. The Application of Rational Design on Phospholipase A2 Inhibitors. **Current Medicinal Chemistry**, 18, 2566-2582 (2011).

258. **T. Mavromoustakos**, G. Aggelis, S. Durdagi, AT₁ antagonists: a patent review (2008-2012). **Expert Opin. Ther. Patents** 23(11), 1-12 (2013).

259. T. Kellici, D. Ntountaniotis, E. Vrontaki, G. Liapakis, P. Moutevelis-Minakakis, G. Kokotos, S. Hadjikakou, A.G. Tzakos, A. Afantitis, G. Melagraki, S. Bryant, T. Langer, V. Di Marzo, **T. Mavromoustakos**. Rational Drug Design Paradigms: The Odyssey for designing better Drugs. In press **Combinatorial Chemistry & High Throughput Screening** 18(3) 238-256 (2015).

260. T.F. Kellici, A.G. Tzakos, **T. Mavromoustakos**. Rational Design and Synthesis of Molecules Targeting the Angiotensin II Type 1 and Type 2 Receptors. **Molecules**, 20, 3868-3897 (2015).

261. T.F. Kellici, G. Liapakis, A.G. Tzakos, **T. Mavromoustakos**. Pharmaceutical compositions for antihypertensive treatments: a patent review. **Expert Opin. Ther. Patents** 25(11), 1-12 (2015).

262. S. Karakurt, T.F. Kellici, **T. Mavromoustakos**, A.G. Tzakos, M. Yilmaz. Calixarenes in Lipase Biocatalysis and Cancer Therapy. **Curr. Org. Chem.** 20, 1043-1057 (2016).
263. T.F. Kellici, D. Ntountaniotis, E. Kritsi, P. Zoumpoulakis, C. Potamitis, S. Durdagi, R.E. G. Salmas, E. Ergum, E. Gokdemir, M. Halabalaki, I.P. Gerothanasis, G. Liapakis, A.G. Tzakos, **T. Mavromoustakos**. Leveraging NMR and X-ray data of the free ligands to build better drugs targeting angiotensin II Type 1 G-Protein coupled receptor. **Curr. Med. Chem.** 23(1), 36-59, (2016).
264. Goulas, V., Stylos, F., Chatziathanasiadou, M.V., **Mavromoustakos, T.**, Tzakos, A.G. Functional components of carob fruit: Linking the chemical and biological space. **International Journal of Molecular Sciences** 17(11), 1875-1895 (2016).
265. D.P. Kiouri, C. Chasapis, **T. Mavromoustakos**, T., Spiliopoulou, C.A., Stefanidou, M.E. Zinc and its binding proteins: essential roles and therapeutic potential **Archives of Toxicology**, 2025, 99(1), pp. 23–41, e201204005

• ΠΡΩΤΟΤΥΠΑ ΑΡΘΡΑ ΚΑΙ ΑΡΘΡΑ ΑΝΑΣΚΟΠΗΣΗΣ ΣΕ ΒΙΒΛΙΑ

258. A. Makriyannis, **T. Mavromoustakos**, H. Jarrel, H. Banijamali: Role of the phenolic hydroxyl group in psychoactive cannabinoids. Studies on the interaction of Δ^8 -tetrahydrocannabinol and its O-methyl ether with model membranes, **Marihuana '87**. G. Chester, P. Consroe, R. Musty, eds Australian Govt Publishing Service, Canberra 1988 pp. 321-326.
259. A. Makriyannis, D.P. Yang, **T. Mavromoustakos**: The molecular features of membrane perturbation by anaesthetic steroids: a study using differential scanning calorimetry, small angle x-ray diffraction and solid state ^2H "Steroids and Neuronal Activity" Ciba Foundation Symp. No. 153. J. Wiley London 172-189 (1990).
260. A. Makriyannis, D.P. Yang, **T. Mavromoustakos**: Combined Use of Solid State Nuclear Magnetic Resonance, Small Angle X-ray Diffraction and Differential Scanning Calorimetry in Studies of Cannabinoid:Membrane Interactions. **Emerging Technologies and New Directions in Drug Abuse Research** 106-128 (1991).
261. A. L. Petrou, M. Kollia, A.I. Scourti, M. Chrycikopoulou, **T. Mavromoustakos**, E. Theodoropoulou, M.H. Karatza, J.M. Tsangaris. Complexes of Aluminium(III) with biologically important ligands. **NATO series: Advanced Study Institute on Cytotoxic, Mutogenic and Carcinogenic Potential of Heavy Metals Related to Human Environment** 253-263 (1997), Kluwer Academic Publishers. N. Hadjiiliadis ed.
262. A. Kolocouris, M. Zervou, **T. Mavromoustakos**, P. Roumelioti, T. Tselios, J. Matsoukas, E. Humpher, Conformational analysis of peptidic and peptidomimetic AII antagonists using a combination of NMR spectroscopy and theoretical calculations **Bioactive Peptides in Drug Discovery and Design: Medical Aspects** vol. 22, 3-12 (1999). IOS Press. Ed. J. Matsoukas, T. Mavromoustakos.

263. **T. Mavromoustakos**, I. Daliani, J. Matsoukas. The application of biophysical methods to study Drug:Membrane Interactions **Bioactive Peptides in Drug Discovery and Design: Medical Aspects** vol. 22, 13-24 (1999). IOS Press. Ed. J. Matsoukas, T. Mavromoustakos.
264. N. Giatas, P. Roumelioti, **T. Mavromoustakos**, J. Matsoukas. Peptide Conformation and the Design of Mimetics: From Angiotensin to non-Peptide Receptor Antagonist. **2nd Hellenic Forum on Bioactive Peptides**, 335-342 (2001). Ed. P. Cordopatis.
265. I. Daliani, M. Zervou, P. Zoumboulakis, A. Kolocouris, S.G. Grdadolnik, **T. Mavromoustakos**. Interactions of AT₁ Antagonist Losartan with Phospholipid Bilayers Using MAS ¹³C NMR Spectroscopy. **2nd Hellenic Forum on Bioactive Peptides**, 455-460 (2001). Ed. P. Cordopatis.
266. **T. Mavromoustakos**, M. Zervou, A. Kolocouris, P. Zoumboulakis, S.G. Grdadolnik, P. Roumelioti, J. Matsoukas. Can Nuclear Magnetic Resonance Be of Aid to Treat Hypertension? **2nd Hellenic Forum on Bioactive Peptides**, 461-466 (2001). Ed. P. Cordopatis.
267. L. Polevaya, P. Roumelioti, **T. Mavromoustakos**, P. Zoumpoulakis, N. Giatas, I. Mutule, T. Keivish, A. Zoga, D. Vlahakos, E. Iliodromitis, D. Kremastinos, J. Matsoukas. Design, Synthesis and Biological Evaluation of Cyclic Angiotensin II Analogues with 3,5 Side-Chain Bridges: Role of C-Terminal Aromatic Residue and Positions. **Bioactive Peptides in Drug Discovery and Design: Medical Aspects** 3-12 (2002). vol. 55, IOS Press. Ed. J. Matsoukas, T. Mavromoustakos.
268. S. Deraeos, T. Tselios, P. Zoumpoulakis, L. Probert, A. Troganis, **T. Mavromoustakos**, J. Matsoukas. Design, Synthesis and Conformational Properties of Linear Analogues of Human Myelin Basic Protein Epitope MBP₁₋₁₁. **Bioactive Peptides in Drug Discovery and Design: Medical Aspects** 116-124 (2002). vol. 55, IOS Press. Ed. J. Matsoukas, T. Mavromoustakos.
269. H. Wasmadeh, C. Demetzos, I. Daliani, T. Mavromoustakos, G. Nounesis, A. Tsortos. The Effects of Vinblastine Sulfate on Dipalmitoylphosphatidylcholine Single and Multiple Bilayer Membranes. **Bioactive Peptides in Drug Discovery and Design: Medical Aspects** 125-130 (2002). vol. 55, IOS Press. Ed. J. Matsoukas, T. Mavromoustakos.
270. I. Kyrikou, T. Mavromoustakos, C. Poulos. Structural Elucidation, Conformational Properties and Effects in Membrane Bilayers of the Toxin Paralysis, β-Ala-Tyr from Larvae of the Gray Flesh Fly. **Bioactive Peptides in Drug Discovery and Design: Medical Aspects** 142-149 (2002). vol. 55, IOS Press. Ed. J. Matsoukas, T. Mavromoustakos.
271. T. Mavromoustakos, I. Kyrikou, A. Kapou, D. Kovala. Effects of NSAIDs in Membrane Bilayers. **Bioactive Peptides in Drug Discovery and Design: Medical Aspects** 150-160 (2002). vol. 55, IOS Press. Ed. J. Matsoukas, T. Mavromoustakos.

272. A. Kapou, T. Mavromoustakos, S.G. Grdadolnik, S. Nikolaropoulos. Synthesis and Conformational Analysis of Steroidal Carriers of Alkylating Agents with the Use of Two-Dimensional Nuclear Magnetic Resonance. **Bioactive Peptides in Drug Discovery and Design: Medical Aspects** 167-173 (2002). vol. 55, IOS Press. Ed. J. Matsoukas, T. Mavromoustakos.
273. P. Zoumpoulakis, M. Zervou, T. Mavromoustakos, S.G. Grdadolnik. Structure Elucidation and Conformational Properties of Irbesartan. **Bioactive Peptides in Drug Discovery and Design: Medical Aspects** 174-179 (2002). vol. 55, IOS Press. Ed. J. Matsoukas, T. Mavromoustakos.
274. I. Kyrikou, M. Zervou, P. Petrakis, T. Mavromoustakos. An Effort to Develop an Analytical Method to Detect Adulteration of Olive Oil by Hazelnut Oil. **Magnetic Resonance in Food Science**. 223-230 Editors: P.S. Belton, A.M. Gil, G.A. Webb, D. Rutledge. Atjemaum Press Ltd, Gateshead, Tyne and Wear, UK, 2003.
275. **T. Mavromoustakos**, P. Zoumpoulakis, M. Zervou, I. Kyrikou, A. Kapou, N. Benetis. The Use of Computational Analysis to Design Novel Drugs. Proceedings of the ICCMSE 2003 by World Scientific, 413-417 editor: T.E. Simos .
276. T. Tselios, S. Deraos, I. Daliani, G. Deraos, **T. Mavromoustakos**, L. Rrobert, J. Matsoukas. Design and Synthesis of Potent Human Cyclic MBP87-99 Altered Peptide Ligands: Inhibition of Experimental Allergic Encephalomyelitis (EAE). **3rd Hellenic Forum on Bioactive Peptides** 227-234 (2003) Ed. P. Cordopatis, E. Manessi, Z.G. Pairas.
277. N. Giatas, P. Roumelioti, A. Zoga, M.E. Androutsou, L. Polevaya, I. Mutule, T. Keivish, **T. Mavromoustakos**, P. Zoumpoulakis, D. Vlahakos, J. Matsoukas. Structural Resemblance of Angiotensin II Ring Cluster Conformation with AT₁ Non-Peptide Antagonists **3rd Hellenic Forum on Bioactive Peptides** 361-366 (2003) Ed. P. Cordopatis, E. Manessi, Z.G. Pairas.
278. P. Zoumpoulakis, M. Zervou, I. Kyrikou, S.G. Grdadolnik, P. Roumelioti, A. Zoga, N. Giatas, J. Matsoukas, **T. Mavromoustakos**. Comparative Conformational Analysis Between Losartan Derivatives. **3rd Hellenic Forum on Bioactive Peptides** 367-370 (2003) Ed. P. Cordopatis, E. Manessi, Z.G. Pairas.
279. I. Kyrikou, S.G. Grdadolnik, C. Poulos, **T. Mavromoustakos**. Structural Elucidation, Conformational Properties in Hydrophilic and Amphoteric Environments and Interactions With Phospholipid Bilayers of the Toxin Paralysin β -Ala-Tyr From Larvae of the Gray Flesh Fly. **3rd Hellenic Forum on Bioactive Peptides** 371-375(2003) Ed. P. Cordopatis, E. Manessi, Z.G. Pairas.
280. P. Zoumpoulakis, M. Zervou, I. Kyrikou, E. Siapi, S.G. Grdadolnik, P. Laggner, A. Hickel, **T. Mavromoustakos**. Relationship Between Conformation and Bioactivity in the Hypertension Disease. **3rd Hellenic Forum on Bioactive Peptides** 355-360 (2003) Ed. P. Cordopatis, E. Manessi, Z.G. Pairas.
281. S. Deraos, T. Tselios, I. Daliani, P. Zoumpoulakis, L. Probert, A. Troganis, **T. Mavromoustakos**, J. Matsoukas. Human Myelin Basic Protein Epitope MBP₁₋₁₁:

Synthesis and Conformational Analysis of Altered Peptide Ligands. **3rd Hellenic Forum on Bioactive Peptides** 601-605 (2003) Ed. P. Cordopatis, E. Manessi, Z.G. Pairas.

282. **T. Mavromoustakos**, M. Zervou, P. Zoumpoulakis. Design and Discovery of Novel Antihypertensive Drugs through Conformation and Bioactivity Studies. Bentham Science Publishers Ltd. Co-Editors: Atta-ur-Rahman, Allen B. Reitz. Associate Editors: M. Iqbal Choudhary, Cheryl P. Kordik. Ur **Frontiers in Medicinal Chemistry**, 3, 87-113 (2006).

283. **T. Mavromoustakos**. The Use of Differential Scanning Calorimetry to Study Drug-Membrane Interactions. **Methods in Molecular Biology**, vol 400. Methods in Membrane Lipids. Edited by A.M. Dopico, Humana Press Inc., Tutuowas, NJ. pages 587-600 (chapter 39) (2008).

284. **T. Mavromoustakos**, S. Golic Grdadolnik, M. Zervou, P. Zoumpoulakis, C. Potamitis, A. Politi, E. Mantzourani, J. A. Platts, C. Koukoulitsa, P. Minakakis, G. Kokotos, T. Tselios, J. Matsoukas, S. Durdagi, M. G. Papadopoulos, D. P. Papahadjis, Z. S. Spyridi, G. A. Dalkas and G. A. Spyroulias. Putative Bioactive Conformers of Small Molecules: A Concerted Approach Using NMR Spectroscopy and Computational Chemistry. **Medicinal Chemistry Research Progress**, Chapter 7, page 175-207. Editors, Giulia P. Colombo and Sofia Ricci, Nova publishers Inc., New York, (2009).

266. **T. Mavromoustakos**. Peptide Mimetics Drugs and their Interdigitation Effects on Lipid Bilayers. **6th Hellenic Forum on Bioactive Peptides**. Pp 571-575. Eds. P. Cordopatis, E. Manesi, Z.G. Pairas, 2011.

267. **T. Mavromoustakos**, P. Moutevelis-Minakakis, G. Kokotos, E. Papavassilopoulou, C. Potamitis, C. Fotakis, P. Chatzigeorgiou, K. Vyras, C. Koukoulitsa, E. Kalatzis and S. Durdagi **Essays on Contemporary Peptide Science** "Chapter 6: Peptide mimetics drugs and their interdigitation with lipid bilayers" pp 95-113, Cordopatis, P. (Ed.) Research SignPost 2011 ISBN: 978-81-308-0428-6.

268. H. Tzoupis, A. Avramopoulos, H. Reis, G. Leonis, S. Durdagi, **T. Mavromoustakos**, G. Megariotis, M. Papadopoulos. **Theoretical Studies of Interactions in Nanomaterials and Biological Systems** RSC Nanoscience & Nanotechnology No. 25 Chapter 8m pp. 148-184. Towards Efficient Designing of Safe Nanomaterials: Innovative Merge of Computational Approaches and Experimental Techniques Edited by Jerzy Leszczynski and Tomasz Puzyn. Published by the Royal Society of Chemistry, 2012 www.rsc.org.

269. S. Vasilakaki, E. Barbayianni, **T.M. Mavromoustakos**, M.H. Gelb, G. Kokotos. Hydrophobic α -Amino Acids Favour the Inhibition of Human GIIA Phospholipase A₂ by 2-Oxoamides, **32nd European Peptide Symposium**, 2-7 September 2012, Athens, Greece. Proceedings pp. 274-276.

270. 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. Abstracts **32nd European Peptide Symposium**, 2-7 September 2012, Athens, Greece. Proceedings pp. 318-320.

271. 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-butylimidazole analogues as potent angiotensin II receptor blockers, S116. Abstracts **32nd European Peptide Symposium**, 2-7 September 2012, Athens, Greece. Proceedings pp. 342-344.

272. 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 Angiotensin II Receptor Blockers, **32nd European Peptide Symposium**, 2-7 September 2012, Athens, Greece. Journal of Peptide Science. Proceedings pp. 358-360.

273. G. Agelis, A. Resvani, C. Koukoulitsa, A. Afantitis, G. Melegraki, A. Siafaka, 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, **32nd European Peptide Symposium**, 2-7 September 2012, Athens, Greece Proceedings pp. 376-378.

274. E. Vrontaki, G. Melagraki, T. Mavromoustakos. Chapter 14: Quantitative Nanostructure-Activity Relationship models for the Risk Assessment of NanoMaterials for the forthcoming book "**Quantitative Structure-Activity Relationships in Drug Design, Predictive Toxicology, and Risk Assessment**" Publisher: IGI Global Editor: Kunal Roy (2015).

275. E. Vrontaki, G. Melagraki, E. Kaffe, **T. Mavromoustakos**, G. Kokotos, V. Aidinis, A. Afantitis. Computer Aided Drug Design Approaches for Identification of Novel Autotaxin (ATX) Inhibitors. **Curr. Med. Chem.**, 23, 1708-1724, (2016).

276. Vrontaki, E., Melagraki, G., Afantitis, A., **Mavromoustakos**, T., Kollias, G. Searching for Novel Janus Kinase-2 Inhibitors Using a Combination of Pharmacophore Modeling, 3D QSAR Studies and Virtual Screening **Mini Reviews in Medicinal Chemistry** 17(3) 268-294 (2017).

277. Vrontaki, E., Melagraki, G., Voskou, S., Phylactides, M.S., **Mavromoustakos**, T., Kleanthous, M., Afantitis, A. Development of a predictive pharmacophore model and a 3D-QSAR study for an in silico screening of new potent BCR-ABL kinase inhibitor **Mini Reviews in Medicinal Chemistry** 17(3) 188-204 (2017).

278. G. Liapakis, M.T. Matsoukas, V. Karageorgosi, M. Venihaki, **T. Mavromoustakos**. Family B G Protein-coupled Receptors and their Ligands: From Structure to Function **Current Medicinal Chemistry**, 3323-3355(31), 24 (2017).

279. E. Vrontaki, **T. Mavromoustakos**, G. Melagraki, A. Afantitis, Quantitative nanonstructure-activity relationship models for the risk assessment of nanomaterials,

Materials Science and Engineering: Concepts, Methodologies, Tools and Applications, 1-3, 20-44 (2017).

280. G. Melagraki, G. Leonis, E. Ntougkos, V. Rinotas, C. Papaneophytou, **T. Mavromoustakos**, G. Kontopidis, E. Douni, G. Kollias, A. Afantitis, Current Status and Future Prospects of Small-Molecule Protein-Protein Interaction (PPI) Inhibitors of Tumor Necrosis Factor (TNF) and Receptor Activator of NF- κ B Ligand (RANKL). **Current Topics in Medicinal Chemistry** 18(8), pp. 661-673 (2018).

281. P. Lagarias, Y. Elkhoul, J. Vedad, A. Konstantinidi, A. A. Profit, T. F. Kellici, A. Kolocouris, Ruel Desamero, and **Thomas Mavromoustakos** Molecular Dynamics Simulations on the Bioactive Molecule of hIAPP22–29 (NFGAILSS) and Rational Drug Design. Thomas Mavromoustakos and Tahsin F. Kellici (eds.), **Rational Drug Design: Methods and Protocols, Methods in Molecular Biology**, vol. 1824, https://doi.org/10.1007/978-1-4939-8630-9_22, © Springer Science+Business Media, LLC, part of Springer Nature 2018.

282. A. Tsailanis, M. Tsoumani, E. K. Stylos, M. V. Chatziathanasiadou, T. F. Kellici, **T. Mavromoustakos**, A. D. Tselepis, and A. G. Tzakos Designing Natural Product Hybrids Bearing Triple Antiplatelet Profile and Evaluating Their Human Plasma Stability. Thomas Mavromoustakos and Tahsin F. Kellici (eds.), **Rational Drug Design: Methods and Protocols, Methods in Molecular Biology**, vol. 1824, https://doi.org/10.1007/978-1-4939-8630-9_22, © Springer Science+Business Media, LLC, part of Springer Nature 2018.

283. D. Ntountaniotis, T. F. Kellici, P. Gkeka, Z. Cournia, I. Galdadas, G. Mali, J. B. Baldus, C. Glaubitz, M. Kriechbaum, M. Rappolt, G. Liapakis, **T. Mavromoustakos**. Drug-Membrane Interactions in the Renin Angiotensin System Thermodynamics and **Biophysics of Biomedical Nanosystems: Applications and Practical Considerations** C. Demetzos and N. Pippa (eds.), **Thermodynamics and Biophysics of Biomedical Nanosystems, Series in BioEngineering, Springer** 339-364 (2019).

284. G. Leonis, E. C. Semidalas, P. Chatzigeorgiou, E. Pollatos, C. E. Semidalas, M. Rappolt, K. Viras, **T. Mavromoustakos**. Vinblastine: cholesterol interactions in lipid bilayers. **Advances in Biomembranes and Self-Assembly**. 29, 127-159 (2019). Edited by Ales Iglic, Michael Rappolt and Ana J. Garcia Saez. Elsevier, Academic Press.

285. S. Kiriakidi, A. Kolocouris, G. Liapakis, S. Ikram, S. Durdagi, **T. Mavromoustakos**. Effects of Cholesterol on GPCR Function: Insights from Computational and Experimental Studies 89-103 (2019). Springer Nature Switzerland AG 2019 89. A. Rosenhouse-Dantsker, A. N. Bukiya (eds.), **Direct Mechanisms in Cholesterol Modulation of Protein Function, Advances in Experimental Medicine and Biology** 1135.

286. Kalliopi Moschovou, Georgia Melagraki, **Thomas Mavromoustakos**, Lefteris C. Zacharia & Antreas Afantitis. Cheminformatics and virtual screening studies of

COMT inhibitors as potential Parkinson's disease therapeutics **Expert Opinion on Drug Discovery**, 15(1), 2020.

287. Catherine Koukoulitsa, Eleni Chontzopoulou, Sofia Kiriakidi, Andreas G. Tzakos and Thomas Mavromoustakos A Journey to the Conformational Analysis of T-Cell Epitope Peptides Involved in Multiple Sclerosis **Brain** 2020, 10, 356; doi:10.3390/brainsci10060356.

288. E. Christodoulou, D. Ntountaniotis, G. Leonis, **T. Mavromoustakos**, G. Valsami. Application of Neutralization and Freeze-Drying Technique for the Preparation of the Beneficial in Drug Delivery 2-Hydroxypropyl- β -Cyclodextrin Complexes with Bioactive Molecules. **Rational Drug Design: Methods and Protocols, Methods in Molecular Biology**, vol. 1825, pp. 77-80 https://doi.org/10.1007/978-1-4939-8630-9_22, © Springer Science+Business Media, LLC, part of Springer Nature 2021.

289. S. Kiriakidi, **T. Mavromoustakos**, Study of Candesartan Cilexetil: 2-Hydroxypropyl- β -Cyclodextrin Interactions: A Computational Approach Using Steered Molecular Dynamics Simulation. **Supramolecules in Drug Discovery and Drug Delivery: Methods and Protocols, Methods in Molecular Biology**, vol. 1825, pp. 88-90 https://doi.org/10.1007/978-1-4939-8630-9_22, © Springer Science+Business Media, LLC, part of Springer Nature 2021.

290. E. Soumelidou, S.G. Grdadolnik, **T. Mavromoustakos**. Drug Incorporation in the Drug Delivery System of Micelles. **Supramolecules in Drug Discovery and Drug Delivery: Methods and Protocols, Methods in Molecular Biology**, vol. 1825, pp. 99-101 https://doi.org/10.1007/978-1-4939-8630-9_22, © Springer Science+Business Media, LLC, part of Springer Nature 2021.

291. G. Leonis, D. Ntountaniotis, E. Christodoulou, T. Mavromoustakos. **Molecular Dynamics Protocols for the Study of Cyclodextrin Drug Delivery Systems. Supramolecules in Drug Discovery and Drug Delivery:: Methods and Protocols, Methods in Molecular Biology**, vol. 1825, pp. 102-105-101 https://doi.org/10.1007/978-1-4939-8630-9_22, © Springer Science+Business Media, LLC, part of Springer Nature 2021.

292. A.F. Metaxa, E. Vrontaki, E.K. Efthimiadou, **T. Mavromoustakos**. Drug Delivery Systems Based on Modified Polysaccharides: Synthesis and Characterization. **Molecular Dynamics Protocols for the Study of Cyclodextrin Drug Delivery Systems. Supramolecules in Drug Discovery and Drug Delivery:: Methods and Protocols, Methods in Molecular Biology**, vol. 1825, pp. 151-153 https://doi.org/10.1007/978-1-4939-8630-9_22, © Springer Science+Business Media, LLC, part of Springer Nature 2021.

293. N. Naziris, M. Chountoules, D. Ntountaniotis, T. Mavromoustakos, C. Demetzos. Differential Scanning Calorimetry (DSC) on Sartan/Cyclodextrin Delivery Formulations. **Molecular Dynamics Protocols for the Study of Cyclodextrin Drug Delivery Systems. Supramolecules in Drug Discovery and Drug Delivery:: Methods and Protocols, Methods in Molecular Biology**, vol. 1825, pp. 163-

165https://doi.org/10.1007/978-1-4939-8630-9_22, © Springer Science+Business Media, LLC, part of Springer Nature 2021.

294. M. V. Chatziathanasiadou, T. Mavromoustakos, A. Tzakos. Unveiling the Thermodynamic Aspects of Drug-Cyclodextrin Interactions Through Isothermal Titration Calorimetry. **Molecular Dynamics Protocols for the Study of Cyclodextrin Drug Delivery Systems. Supramolecules in Drug Discovery and Drug Delivery:: Methods and Protocols, Methods in Molecular Biology**, vol. 1825, pp. 187-190 https://doi.org/10.1007/978-1-4939-8630-9_22, © Springer Science+Business Media, LLC, part of Springer Nature 2021.

295. N. Naziris, A. Skandalis, T. Mavromoustakos, S. Pispas, C. Demetzos. Association of the Thermodynamics with the Functionality of Thermoresponsive Chimeric Nanosystems. **Molecular Dynamics Protocols for the Study of Cyclodextrin Drug Delivery Systems. Supramolecules in Drug Discovery and Drug Delivery:: Methods and Protocols, Methods in Molecular Biology**, vol. 1825, pp. 221-224 https://doi.org/10.1007/978-1-4939-8630-9_22, © Springer Science+Business Media, LLC, part of Springer Nature 2021.

296. C.M. Chatzigiannis, S. Kiriakidi, A.G. Tzakos, T. Mavromoustakos. 2D DOSY NMR: A Valuable Tool to Confirm the Complexation in Drug Delivery Systems. **Molecular Dynamics Protocols for the Study of Cyclodextrin Drug Delivery Systems. Supramolecules in Drug Discovery and Drug Delivery: Methods and Protocols, Methods in Molecular Biology**, vol. 1825, pp. 221-224 https://doi.org/10.1007/978-1-4939-8630-9_22, © Springer Science+Business Media, LLC, part of Springer Nature 2021.

297. Chountoulesi, N. Naziris, T. Mavromoustakos, C. Demetzos. A Differential Scanning Calorimetry (DSC) Experimental Protocol for Evaluating the Modified Thermotropic Behavior of Liposomes with Incorporated Guest Molecules. **Molecular Dynamics Protocols for the Study of Cyclodextrin Drug Delivery Systems. Supramolecules in Drug Discovery and Drug Delivery: Methods and Protocols, Methods in Molecular Biology**, vol. 1825, pp. 299-303 https://doi.org/10.1007/978-1-4939-8630-9_22, © Springer Science+Business Media, LLC, part of Springer Nature 2021.

298. D. Ntountaniotis, G. Leonis, E. Christodoulou, T. Mavromoustakos. Applications of NMR in Drug:Cyclodextrin Complexes. **Molecular Dynamics Protocols for the Study of Cyclodextrin Drug Delivery Systems. Supramolecules in Drug Discovery and Drug Delivery: Methods and Protocols, Methods in Molecular Biology**, vol. 1825, pp. 213-317 https://doi.org/10.1007/978-1-4939-8630-9_22, © Springer Science+Business Media, LLC, part of Springer Nature 2021.

299. J. Matsoukas, V. Apostolopoulos, A. Zulli, G. Moore, K. Kelaidonis, K. Moschovou, T. Mavromoustakos. From Angiotensin II to Cyclic Peptides and Angiotensin Receptor Blockers (ARBs): Perspectives of ARBs in COVID-19 Therapy **Molecules** 26(3), 618 (2021).

300. A.D. Tsailanis, A.D. Tzakos, A.G. **T. Mavromoustakos**. Advancing the therapeutic efficacy of bioactive molecules by delivery vehicle platforms. **Current Medicinal Chemistry**, 2021, 28(14), pp. 2697–2706
301. E. Chontzopoulou, A.G. Tzakos, **T. Mavromoustakos**. On the rational drug design for hypertension through NMR spectroscopy. **Molecules** 26(1), 12 (2021).
302. N. Georgiou, V. K. Gkalpinos, S. D. Katsakos, S. Vassiliou, A. G. Tzakos, **T. Mavromoustakos**. Rational Design and Synthesis of AT1R Antagonists. **Molecules** 26, 2927 (2021).
303. J.M. Matsoukas, I. C.T. V. Apostolopoulos, K.Kelaidonis, T. Mavromoustakos. Novel Approaches in the Immunotherapy of Multiple Sclerosis: Cyclization of Myelin Epitope Peptides and Conjugation with Mannan. **Brain Sciences**, 11(12), 1583 (2021).
304. A. Syriopoulou, I. Markopoulos, A. Tzakos, **T. Mavromoustakos**. Methods in Molecular Biology. AutoDock in Drug Design, Chapter 5, Ligand–Receptor, Ligand–DNA Interactions, and Drug Design, 2021. DOI:10.1007/978-1-0716-1209-5_5.
305. S.Kiriakidi, Z. Cournia, T. Mavromoustakos Effects of cholesterol on the GPCR AT1 receptor and its interplay with AT1 antagonists. **Cholesterol from Chemistry and Biophysics to the Clinic**. Edited by A.N. Bakiya and A.M. Dopico. Academic Press, 2022.
- 306.N. Zoupanou, N. Georgiou, K. Moschovou, C.T.Chasapis, K. Kelaidonis, V. P. Chavda, **T. Mavromoustakos**, J. M. Matsoukas,V. Apostolopoulos. Peptide-based vaccines and altered peptide ligands: Multiple sclerosis paving. Advanced Vaccination Technologies for Infectious and Chronic Diseases A guide to Vaccinology the way. Editors: V.P. Chavda, A. Gujarat, L.K. Vora. Academic Press, 2024, 63-72 (Chapter 5).
307. N. Georgiou, E. Chontzopoulou, E.A. Routsi, **T. Mavromoustakos**, S.Kiriakidi, Exploring Hypertension: The Role of AT1 Receptors, Sartans, and Lipid Bilayers **ACS Omega**, 2024, 9(45), pp. 44876–44890.
308. J.M. Matsoukas, I. C.T. V. Apostolopoulos, K.Kelaidonis, **T. Mavromoustakos**. Novel Approaches in the Immunotherapy of Multiple Sclerosis: Cyclization of Myelin Epitope Peptides and Conjugation with Mannan. **Brain Sciences**, 11(12), 1583 (2021).
309. S.Kiriakidi, Z. Cournia, **T. Mavromoustakos** Effects of cholesterol on the GPCR AT1 receptor and its interplay with AT1 antagonists. **Cholesterol from Chemistry and Biophysics to the Clinic**. Edited by A.N. Bakiya and A.M. Dopico. Academic Press, 2022.

ARTICLES FOR CONFERENCES

1. T. Mavromoustakos. The European Peptide Society Newsletter 47, 4-7 (2013).

2. T. Mavromoustakos, A. Tsotinis, 32nd Cyprus-Noordwijkerhout-Camerino Symposium: Trends in Drug Research 2014, Chem. Med. Chem. DOI: 10.1002/cmdc.201402227

➤ **ARTICLES WRITTEN IN ENGLISH LANGUAGE AND PUBLISHED IN GREEK JOURNALS**

1.A. Makriyannis, **T. Mavromoustakos**: Studies on drug:membrane interactions using solid-state NMR, small angle x-ray diffraction and differential scanning calorimetry. **Rev. Clin. Pharmacol.** 3(2):95-114 (1989).

2.T. Mavromoustakos, De-Ping Yang, E. Theodoropoulou, A. Makriyannis. **BIOMED** Aminoacids, Peptides, Proteins, Use of Molecular Graphics as an aid in the Study of Conformational Properties of the Aminoalkylindole Pravadoline and the Analgesic Cannabinoid CP-55,940, Drug Discovery and Design, Patras 1993, pp. 78-83 Ed. J. Matsoukas.

3.**T. Mavromoustakos**, E. Theodoropoulou, J. Matsoukas, G. Moore, J. Smith, Superimposition of Angiotensin II with potent Non-Peptide AT-1 Receptor Antagonists. **BIOMED** Aminoacids, Peptides, Proteins, Drug Discovery and Design, Patras 1994, pp. 74-80 Ed. J. Matsoukas.

4.**T. Mavromoustakos**, E. Theodoropoulou, J. Matsoukas, D. Panagiotopoulos, G. Moore, A. Makriyannis. Interactions of ANG II with membranes using a combination of Differential Scanning Calorimetry and ³¹P-NMR. **BIOMED**, Aminoacids, Peptides, Proteins, Drug Discovery and Design, Patra 1994, Ed. J. Matsoukas p. 88-94.

5.D. Panagiotopoulos, J. Matsoukas, M. Keramida, T. Mavromoustakos, H.L.S. Maia, R. Yamdagni, Q. Wu, G.J. Moore, M. Saifeddine, M.D. Hollenberg. Cyclic Thrombin Receptor Derived Peptide Analogues of the S²FLLR⁴⁶ motif: Novel Synthesis and Biological Activities. **BIOMED**, Aminoacids, Peptides, Proteins, Drug Discovery and Design, Patra s1994, Ed. J. Matsoukas p. 108-111.

6.**T. Mavromoustakos**, E. Theodoropoulou, J. Matsoukas, G. Moore, J. Smith. Use of Molecular Modeling to Study Superimposition of Angiotensin II with its Non-Peptide Receptor Antagonists **Rev. Clin. Pharmacol** 8, 137-142 (1994).

7.**T. Mavromoustakos**, De-Ping Yang, E. Theodoropoulou, A. Makriyannis. Use of Molecular Graphics as an aid in the Study of Conformational Properties of Aminoalkylindole Pravadoline and the Analgesic Cannabinoid CP-55,940. **Rev. Clin. Pharmacol** 9, 113-116 (1995).

8.**T. Mavromoustakos**, M. Bensaia, E. Theodoropoulou, M. Zervou, D. Karussis, J. Matsoukas. The conformational Properties of the Immunomodulator Linomide. **Biomed** 1995, **Aminoacids, Peptides, Proteins-Drug Discovery and Design**, J. Matsoukas ed. 23-30, Patras, Greece 1996.

9. **T. Mavromoustakos**, E. Theodoropoulou, K. Alexopoulos, J. Matsoukas, M. Hollenberg. Use of Molecular Modeling to Study Superimposition of the Thrombin receptor motif S₄₂FLLR₄₆ with its Peptidomimetic Analogs. **Biomed 1995, Aminoacids, Peptides, Proteins-Drug Discovery and Design**, J. Matsoukas ed. 102-107, Patras, Greece 1996.
10. D. Panagiotopoulos, K. Alexopoulos, J.M. Matsoukas, T. Mavromoustakos, E. Theodoropoulou, H.L.S. Maia, M. Saifeddine, M.D. Hollenberg. Synthesis and Activities of Cyclic Thrombin Receptor-Derived Peptide Analogues of the Ser₄₂-Phe-Leu-Leu-Arg₄₆. Motif Sequence, containing 2,3 Diaminopropionic acid. **Biomed 1995, Aminoacids, Peptides, Proteins-Drug Discovery and Design**, J. Matsoukas ed. 108-113, Patras, Greece 1996.
11. J. M. Matsoukas, K. Alexopoulos, T. Tselios, R. Yamdagni, Q. Wu, **T. Mavromoustakos**, G.J. Moore. Differences in Backbone Structure between the Super Agonis [Sar^I] and its Type I Antagonist Sarilesin. **Biomed 1995, Aminoacids, Peptides, Proteins-Drug Discovery and Design**, J. Matsoukas ed. 114-119, Patras, Greece 1996.
12. A. Dimirkou, A. Ioannou, **T. Mavromoustakos**. Kinetics of Phosphate Adsorption by Calcium-Bentonite **Chimica Chronika, New Series** 25, 195-214 (1996).
13. **T. Mavromoustakos**, E. Theodoropoulou, K. Alexopoulos, D. Karussis, J. Matsoukas. Conformational Properties of the Immunomodulator Linomide **Rev. Clin. Pharmacology** 11:70-74 (1997)
14. **T. Mavromoustakos**, E. Theodoropoulou, K. Alexopoulos, J. Matsoukas. M. Hollenberg, G.J. Moore. Use of Molecular Modeling to Study Superimposition of the thrombin receptor motif S₄₂FLLR₄₆ with its Peptidomimetic Analogs **Rev. Clin. Pharmacology** 11:125-127 (1997).
15. D. Panagiotopoulos, K. Alexopoulos, J. M. Matsoukas, **T. Mavromoustakos**, E. Theodoropoulou, E. Kalatzis, P. Fatseas, M. Saifeddine, M.D. Hollenberg. Synthesis and activities of Cyclic Thrombin Receptor-Derived Peptide Analogues of the Ser₄₂-Phe-Leu-Leu-Arg₄₆ Motif Sequence containing 2,3 Diaminopropanic Acid **Rev. Clin. Pharmacology** 11:128-131 (1997).
16. J. M. Matsoukas, K. Alexopoulos, T. Tselios, P. Roumelioti, R. Yamdagni, Q. Wu, **T. Mavromoustakos**, E. Kalatzis, E. Siapi, G. J. Moore. Differences in Backbone Structure between the Super Agonist [Sar^I] Angiotensin II and its Type I Antagonist Sarilesin **Rev. Clin. Pharmacology** 11:132-136 (1997).
17. **T. Mavromoustakos**. Drug:Membrane Interactions. An example with the pair of Anesthetic Steroids Alphaxalone and Δ^{16} -alphaxalone **Rev. Clin. Pharmacology** 12:15-22 (1998).
18. **T. Mavromoustakos**, M. Zervou, G. Bonas, A. Kolocouris, P. Petrakis. A novel Analytical Method to detect adulteration of virgin olive oil by other oils. International

Conference. Instrumental Methods of Analysis, Modern Trends and Applications. 19-22 September 1999, Chalkidiki, Greece. IMA '99 490-495.

Published Articles presented in Books:

1. Cell Membranes 37, 21, 1996

Mavromoustakos T, Yang DP, Makriyannis A// Natl Hellen Res Fnd, Inst Organ @ Pharmaceut Chem, 48 Vas Constantinou Ave, GR-11635 Athens, Greece BIOCHIM BIOPHYS ACTA-BIOMEMB 1994, 1194 (1) 69

Topography of alphaxalone and delta (16)-alphaxalone in membrane bilayers containing cholesterol.

2. Cell Membranes 39, 16, 1996.

Mavromoustakos T, Theodoropoulou E, Papahatjis D, Kourouli T, Yang DP, Trumbore M, Makriyannis A//Natl Hellen Re Fdn, Inst Organ @ Pharmaceut Chem, GR-11635 Athens, Greece BBA-BIOMEMB 1996, 1281 (2) 235

Studies on the thermotropic effects of cannabinoids on phosphatidylcholine bilayers using differential scanning calorimetry and small angle X-ray diffraction.

3. Progress in Anesthetic Mechanism

Mavromoustakos T, Yang DP, Makriyannis A// Natl Hellen Res Fnd, Inst Organ @ Pharmaceut Chem, 48 Vas Constantinou Ave, GR-11635 Athens, Greece BIOCHIM BIOPHYS ACTA-BIOMEMB 1994, 1194 (1) 69 Topography of alphaxalone and delta (16)-alphaxalone in membrane bilayers containing cholesterol.

Proceedings-Abstracts

1.T. **Mavromoustakos**, E. Theodoropoulou, A. Makriyannis. Comparison of the conformational properties of the aminoalkylindole pravadoline and non classical cannabinoid. **Pharmaceutical Proceedings of the 6th Pharmaceutical Conference in Athens (1992)** Edit. A. Adamos p. 111-118.

2.T. **Mavromoustakos**, E. Theodoropoulou, M. Koufaki, D.P. Yang, A. Makriyannis. Conformational Analysis of 1-thiohexadecyl-2-O-methyl-rac-glycero-3-phosphocholine. **Pharmaceutical Proceedings of the 7th Hellenic Pharmaceutical Conference in Athens (1994).**

3.E. Theodoropoulou, T. **Mavromoustakos**, A. Byza. Thermotropic changes of biologically active molecules in presence of cyclodextrins. **Pharmaceutical Proceedings of the 7th Hellenic Pharmaceutical Conference in Athens (1994).**

4.T. **Mavromoustakos**, E. Theodoropoulou, B. Polychroniou, A. Dimitriou. Drug:Membrane interactions using ^{31}P -NMR spectroscopy. **Chemistry Proceedings of the 16th National Hellenic Conference in Athens (1995)**, Vol. A p 157-160.

5.T. **Mavromoustakos**, E. Theodoropoulou. Study of Drug:Cannabinoid Interactions using various Biophysical Methods. **Proceedings of the 16th National Hellenic Conference in Athens (1995)**, Vol. B 1087-1090.

6.A. Petrou, T. **Mavromoustakos**, A. Skourti, M. Kollia, M. Chrysikopoulou, M. Karatza, I. Tsagaris. Complexes of Al(III) with molecules of biological importance.

Proceedings of 5th Chemistry Conference between Cyprus and Greece. Nicosia, September 4-7, 1996.

7.T. Mavromoustakos, M. Bensaia, M. Zervou, E. Theodoropoulou. Conformational analysis of linomide. **Proceedings of the 17th National Hellenic Conference in Patras (1996), 553-556.**

8.M. Zervou, T. Mavromoustakos, G. Bonas, E. Theodoropoulou, M. Bensaia, A. Xelmis. Use of ^{13}C to detect virgin olive oil adulteration. **Proceedings of the 17th National Hellenic Conference in Patras (1996), December 1-5 479-482.**

9.D. Panagiotopoulos, K. Alexopoulos, T. Tselios, J. Matsoukas, E. Theodoropoulou, T. Mavromoustakos, M. Hollenberg. Synthesis and Biological Activity of epitope of thrombin using Ser⁴²-Phe-Leu-Leu-Arg⁴⁶. The approach of the key aminoacids Phe-Arg in the biological activity. **Proceedings of the 17th National Hellenic Conference in Patras (1996), December 1-5 219-222.**

10.T. Mavromoustakos, G. Bonas, M. Zervou, E. Theodoropoulou, D. Panagiotopoulos, A. Helmis. Quantitative determination of the most abundant fatty acids in Greek virgin olive oils using ^{13}C NMR spectroscopy. **Proceedings of the Conference held in Kalamata (1996), November, 8-10.**

11. A. Kolocouris, T. Mavromoustakos, M. Efstathiou, S. Photopoulou. A chromatic analogue used to teach the Hybridization of Carbon. **1st Hellenic Meeting on the Teaching of Chemistry in High Schools. University of Athens, December 4-6, 166-168, 1998.**

12.T. Mavromoustakos, M. Efstathiou. Spontaneous processes. **1st Hellenic Meeting on the Teaching of Chemistry in High Schools. University of Athens, December 4-6, 169-173, 1998.**

13.T. Mavromoustakos, M. Efstathiou, A. Kolocouris. The magnificent of Retro-Synthesis in Organic Chemistry. **1st Hellenic Meeting on the Teaching of Chemistry in High Schools. University of Athens, December 4-6, 173-178, 1998.**

14.A. Kolocouris, T. Mavromoustakos, T. Kalogeropoulou, M. Koufaki, I. Daliani, A. Makriyannis, K. Demetzos, E. Declercq. Conformation studies of a novel synthetic glycerol derivative of AZT with anticancer and anti-HIV biological action. **Pharmaceutical Proceedings of the 9th Hellenic Pharmaceutical Conference in Athens (2000).**

15.T. Tselios, I. Daliani, S. Deraos, P. Roumelioti, E. Matsouka, I. Probert, T. Mavromoustakos. Design and Synthesis of Cyclic Peptides of the Basic Protein Myelin. Induction of the Experimental Allergic Encephalomyelitis (E.A.E.). **Pharmaceutical Proceedings of the 9th Hellenic Pharmaceutical Conference in Athens (2000).**

16.M. Zervou, A. Kolocouris, T. Mavromoustakos, I. Matsoukas. Conformational analysis of the peptide mimetics and peptide antagonists of angiotensin II with the aid of combined Nuclear Magnetic Resonance and Computational Chemistry.

Perspectives for the design and synthesis of Novel Antihypertensive Molecules. **Pharmaceutical Proceedings of the 9th Hellenic Pharmaceutical Conference in Athens (2000).**

17.H. Maswadeh, K. Demetzos, M. Rallis, **T. Mavromoustakos**, I. Daliani, A. Kolocouris, P. Dallas, G. Papaioannou. Inclusion of Vinblastine in liposomes with different lipid synthesis. Study of the thermotropic metabolites in artificial membranes using a combination of DSC and Solid State NMR spectroscopy. **Pharmaceutical Proceedings of the 9th Hellenic Pharmaceutical Conference in Athens (2000).**

18.**T. Mavromoustakos**, M. Zervou, G. Bonas, A. Kolocouris, P. Petrakis. A novel Analytical Method to detect adulteration of virgin olive oil by other oils. **International Conference. Instrumental Methods of Analysis, Modern Trends and Applications.** 19-22 September 1999, Chalkidiki, Greece. IMA '99 410-415.

19.N. Giatas, P. Roumelioti, **T. Mavromoustakos**, J. Matsoukas. Peptide Conformation and the Design of Mimetics: From Angiotensin to non-Peptide Receptor Antagonist. **2nd Hellenic Forum on Bioactive Peptides**, 335-342 (2001). Ed. P. Cordopatis.

20.I. Daliani, M. Zervou, P. Zoumboulakis, A. Kolocouris, S.G. Grdadolnik, **T. Mavromoustakos**. Interactions of AT₁ Antagonist Losartan with Phospholipid Bilayers Using MAS ¹³C NMR Spectroscopy. **2nd Hellenic Forum on Bioactive Peptides**, 455-460 (2001). Ed. P. Cordopatis.

21.**T. Mavromoustakos**, M. Zervou, A. Kolocouris, P. Zoumboulakis, S.G. Grdadolnik, P. Roumelioti, J. Matsoukas. Can Nuclear Magnetic Resonance Be of Aid to Treat Hypertension? **2nd Hellenic Forum on Bioactive Peptides**, 461-466 (2001). Ed. P. Cordopatis.

22.Differential Scanning Calorimetry. An invaluable tool in Medicinal Chemistry (invited speaker). **T. Mavromoustakos**, I. Kyrikou, E. Siapi, P. Zoumpoulakis. 1st National Conference in Thermal Analysis, Kerkini, September 27-29, 2002. Proceedings 19-23.

23.Study the adulteration of olive oil with hazelnut oil using ¹³C NMR spectroscopy. I. Kyrikou, M. Zervou, P. Petrakis, **T. Mavromoustakos**. 19^o Greek Conference of Chemistry, Iraklion, Crete, 6-10 November 2002, 438-441.

24.Biophysical studies of gentamycin in collagen membranes. I. Kyrikou, E. Siapi, P. Zoumpoulakis, M. Zervou, D. Dimitriou, A. Pitsas, Ch. Camoutsis, Eng. V. Trandafir, A. Buzor, G. Popescu, **T. Mavromoustakos**, 19^o Greek Conference of Chemistry, Iraklion, Crete, 6-10 November 2002, 542-546.

25.P. Zoumpoulakis, A. Zoga, I. Kyrikou, M. Zervou, E. Siapi, **T. Mavromoustakos**. Interaction and diffusion of AT₁ antagonists in membrane bilayers. 19^o Greek Conference of Chemistry, Iraklion, Crete, 6-10 November 2002, 546-549.

➤ **65 ARTICLES WRITTEN IN GREEK LANGUAGE AND PUBLISHED IN GREEK JOURNALS (not included)**

PRESENTATIONS–ABSTRACTS (not included the national with Greek language as the official of the conference)

1.T. Mavromoustakos, A. Banijamali, A. Charalambous, A. Makriyannis: Deuterium labeling of Δ^9 -tetrahydrocannabinol. A tool for the study of drug alignment in model membrane. 2nd national meeting and exposition of American Association of Pharmaceutical Scientists. Boston, MA June, 1987.

2.T. Mavromoustakos, A. Charalambous, C.J. Van der Schyf, A. Makriyannis: Interactions of (-)- Δ^8 -tetrahydrocannabinols with membranes. Proceeding: 3rd Annual Meeting of the American Association of Pharmaceutical Scientists. Orlando, Florida, 1988.

3.T. Mavromoustakos, A. Makriyannis: Study of the topography and thermotropic properties of cannabinoids in model membranes using small angle x-ray diffraction and differential scanning calorimetry. XIV NERMCA Meeting, April 1989.

4.T. Mavromoustakos, D.P. Yang, A. Charalambous, L. Herbet, A. Makriyannis: Effects of Δ^8 -THC Me- Δ^8 -THC on model membranes as studied by DSC, x-ray diffraction and solid state ^2H -NMR. 3rd Cyprus Conference on New Methods in Drug Research, Paphos, Cyprus, May, 1989.

5.T. Mavromoustakos, D.P. Yang, X. Xie, A. Makriyannis: Interactions of Anesthetic Steroids with model membranes. 3rd Cyprus Conference on New Methods in Drug Research, Paphos, Cyprus, May, 1989.

6.T. Mavromoustakos, D.P. Yang, A. Charalambous, L.G. Herbet, A. Makriyannis: Topography of (-)- Δ^8 -tetrahydrocannabinol in synthetic lipid and bovine extract bilayers as studied by small angle x-ray diffraction. XV NERMCA Meeting, April 1990.

7.T. Mavromoustakos, D.P. Yang, A. Makriyannis: The effects of Cannabinoids and Anesthetic Steroids on Model Membranes: 5th Cyprus Conference, April 1992.

8.T. Mavromoustakos, A. Makriyannis: Conformational Properties of Pravastatin. 6th Hellenic Conference of Medicinal Chemistry, Athens, Greece, May, 1993.

9.T. Mavromoustakos: The use of Molecular Graphics as an aid in the study of Conformational Properties of Pharmaceutical Molecules. BIOMED EUROWORKSHOP, Aminoacids, Peptides, Proteins, University of Patras, Greece 1993.

10.T. Mavromoustakos, E. Theodoropoulou, A. Makriyannis. The conformational analysis of the Antineoplastic Ether Lipid 1-thiohexadecyl-2-O-methyl-*rac*-glycero-3-phosphocholine. 6th Hellenic Conference on Pharmaceutics, Athens, June 1994.

- 11.**T. Mavromoustakos**, E. Theodoropoulou, J. Matsoukas, G. Moore, J. Smith. Use of Molecular Modeling to Study Superimposition of ANG II with its Non-Peptide Receptor Antagonist. BIOMED EUROWORKSHOP, Aminoacids, Peptides, Proteins, Patra, November 1994.
- 12.**T. Mavromoustakos**, A. Ioannou, A. Dimirkou. Isotherms of phosphate sorption by hematite and hematite-bentonite (h-b) system. International Symposium on Soil and Plant Analysis August 5-10, 1995, Wageningen, the Netherlands.
- 13.**T. Mavromoustakos**, E. Theodoropoulou, J. Matsoukas, G. Moore, A. Makriyannis. Interactions of ANG II with membranes using a combination of Differential Scanning Calorimetry and ^{31}P -NMR. BIOMED, Aminoacids, Peptides, Proteins, Drug Discovery and Design, Patra 1994, Ed. J. Matsoukas p. 88-94.
- 14.**T. Mavromoustakos**, E. Theodoropoulou, V. Polychroniou, A. Dimitriou Effects of biologically active molecules in membranes using ^{31}P NMR spectroscopy 16th Hellenic Conference in Chemistry, Athens (1995).
- 15.**T. Mavromoustakos**, E. Theodoropoulou. Study of the effects of a pair of cannabinoid molecules in phospholipid bilayers. Pharmaceutical Proceedings of the 8th Hellenic Pharmaceutical Conference in Athens (1995).
- 16.**T. Mavromoustakos**, E. Theodoropoulou, A. Makriyannis. Thirteenth European Experimental N.M.R. Conference, EENC 1996, Paris. Study of Drug Membrane Interactions Using Solid State Nuclear Magnetic Resonance Spectroscopy.
- 17.**T. Mavromoustakos**. International Food & Drinks Exhibition Feb 8-12, 1996. Use of Nuclear Magnetic Resonance in the Food Industry. European Exhibition and Promotion Centre, Athens, Greece.
- 18.**T. Mavromoustakos**. Applications of Thermal Analysis. A day for the Thermal Analysis April 5, 1996, Polytechnic School in Athens, Greece.
- 19.**T. Mavromoustakos**, G. Bonas, M.P. Day, M. Zervou, E. Theodoropoulou, M. Bensaia. A ^{13}C NMR spectroscopy approach to the Authentication of Olive Oil. The Third International Conference on Applications of Magnetic Resonance in Food Science, Nantes, September 15-18, 1996 p. 212-213.
- 20.**T. Mavromoustakos**, M. Bensaia, M. Zervou, E. Theodoropoulou. Conformational analysis of linomide. Proceedings of the 17th National Hellenic Conference in Patras (1996).
- 22.**T. Mavromoustakos**, P. Laggner, E. Theodoropoulou, D. Papahadjis, T. Kourouli. Study of the thermotropic and dynamic properties of cannabinoid molecules using x-ray diffraction and Differential Scanning Calorimetry. 80 Hellenic Symposium of Medicinal Chemistry 28-29 of November, 1997, Athens, Greece.
- 23.M. Zervou, A. Kolocouris, **T. Mavromoustakos**, C. Screttas, J. Matsoukas. Conformational Analysis of the active metabolite EXP-3174 of the antihypertensive

drug Losartan. 8o Hellenic Symposium of Medicinal Chemistry 28-29 of November, 1997, Athens, Greece.

24.**T. Mavromoustakos**, M. Zervou, G. Bonas, E. Theodoropoulou, M. Bensaia, A. Xelmis. Use of ^{13}C to detect virgin olive oil adulteration. Proceedings of the 17th National Hellenic Conference in Patras (1996), 479-482.

25.**T. Mavromoustakos**, A. Kolocouris, M. Zervou, I. Matsoukas. The molecular basis of hypertension. EENC 98, Bled. 14th European Experimental Conference, May 10-15, 1998 Bled, Slovenia.

26.A. Kolocouris, **T. Mavromoustakos**, M. Zervou, I. Matsoukas, E. Humphreys. An effort to understand the molecular Basis of Hypertension through the conformational analysis of Losartan and Sarmsin using a combination of NMR spectroscopy and theoretical calculations. XVth EFMC International Symposium of Medicinal Chemistry, Edinburgh, Scotland, 6-10 September 1998.

27.A. Kolocouris, **T. Mavromoustakos**, J. Matsoukas. The molecular basis of the antihypertensive activity of Losartan 9o Hellenic Conference in Medicinal Chemistry Athens, 7-9 November 1998. Proceedings, Pharmakeftiki 11, (3), 122-123 (1998).

28.**T. Mavromoustakos**, A. Kolocouris, M. Zervou, I. Daliani, The Combination of NMR Spectroscopy and Molecular Modeling in Drug Design: Implications in the Synthesis of Non-Peptide Mimetics of ANG II, TRAP, MBP and GnRH. Workshop. "Peptides and Peptide Mimetics, Drug Discovery and Design". December 7, 1998

29.J. M. Matsoukas, **T. Mavromoustakos**, C.J. Moore. The Molecular Basis of Hypertension. Workshop. "Peptides and Peptide Mimetics, Drug Discovery and Design". December 7, 1998.

30.K. Alexopoulos, D. Panagiotopoulos, P. Roumelioti, **T. Mavromoustakos**, M. Paredes-Carbajal, D. Mascher, S. Mihailescu and J. Matsoukas. Design and Biological Activities of Novel Cyclic Thrombin Receptor-Derived Peptide Analogues of the Ser₄₂-Phe-Lue-Leu-Arg₄₆ Motif Sequence, Containing 2,3 Diaminopropionic acid, Lys and L- or D-Phe with Fixed Conformations: Importance of a Phe/Arg/NH₂ Cluster for Receptor Activation. Workshop. "Peptides and Peptide Mimetics, Drug Discovery and Design". December 7, 1998.

32.**T. Mavromoustakos**, I. Daliani, A. Kolocouris, A. Makriyannis. The Interactions of Cannabinoids with Membranes as Studied by DSC and Solid State NMR. The 8th Cyprus Conference on New Methods in Drug Research Limassol, Cyprus April 25-30, 1999.

33.**T. Mavromoustakos**, A. Kolocouris, J.M. Matsoukas, M. Zervou. Study of the Molecular Basis of Hypertension Using NMR spectroscopy and Computational Analysis Studies. The 8th Cyprus Conference on New Methods in Drug Research Limassol, Cyprus April 25-30, 1999.

34.**T. Mavromoustakos**, M. Zervou, G. Bonas, A. Kolocouris, P. Petrakis. A novel Analytical Method to detect adulteration of virgin olive oil by other oils. International

Conference. Instrumental Methods of Analysis, Modern Trends and Applications. 19-22 September 1999, Chalkidiki, Greece. IMA '99.

35.A. Kolocouris, **T. Mavromoustakos**, T. Kalogeropoulou, M. Koufaki, I. Daliani, A. Makriyannis, K. Demetzos, E. Declercq. Conformation studies of a novel synthetic glycerol derivative of AZT with anticancer and anti-HIV biological action. Pharmaceutical Conference of the 9th Hellenic Pharmaceutical Conference in Athens 14-15 January 2000.

36.T. Tselios, I. Daliani, S. Deraos, P. Roumelioti, E. Matsouka, I. Probert, **T. Mavromoustakos**. Design and Synthesis of Cyclic Peptides of the Basic Protein Myelin. Induction of the Experimental Allergic Encephalomyelitis (E.A.E.). Pharmaceutical Conference of the 9th Hellenic Pharmaceutical Conference in Athens 14-15 January 2000.

37.M. Zervou, A. Kolocouris, **T. Mavromoustakos**, I. Matsoukas. Conformational analysis of the peptide mimetics and peptide antagonists of angiotensin II with the aid of combined Nuclear Magnetic Resonance and Computational Chemistry. Perspectives for the design and synthesis of Novel Antihypertensive Molecules. Pharmaceutical Conference of the 9th Hellenic Pharmaceutical Conference in Athens 14-15 January 2000.

38.H. Maswadeh, K. Demetzos, M. Rallis, **T. Mavromoustakos**, I. Daliani, A. Kolocouris, P. Dallas, G. Papaioannou. Inclusion of Vinblastine in liposomes with different lipid synthesis. Study of the thermotropic metabolism in artificial membranes using a combination of DSC and Solid State NMR spectroscopy. Pharmaceutical Conference of the 9th Hellenic Pharmaceutical Conference in Athens 14-15 January 2000.

39. C. Dagas, V. Barbarousi, M. Zervou, **T. Mavromoustakos**, D. Liakos, A. Petrou. Potentiometric and ^{27}Al -NMR Spectroscopic Study of the Al(III)-D-Ribose System. 34th International Conference on Coordination Chemistry. The University of Edinburgh, Scotland.. 9-14 July 2000.

40.**T. Mavromoustakos** Study of Drug:Active Site Interactions using NMR spectroscopy. Frontiers of Biomolecular NMR. Five Years of Slovenian NMR centre. Ljubljana, Slovenia, 16-17.2.2001.

41.P. Zoumboulakis, S.G. Gardadolnik, L. Polevaya, D. Vlahakos, J. Matsoukas, **T. Mavromoustakos** Synthesis and Study of Cyclic Angiotensin II Antagonist Analogue reveals the role of C-Terminal Aromatic Residue for agonist activity and its structure resemblance with AT₁ non-peptide antagonists. Frontiers of Biomolecular NMR. Five Years of Slovenian NMR centre. Ljubljana, Slovenia, 16-17.2.2001.

42.**T. Mavromoustakos** NMR spectroscopy. A Powerful Tool in the Rational Drug Design. 2nd Conference Medicinal Chemistry: Drug Design and Development. 2nd Conference Medicinal Chemistry: Drug Design and Development 1-3 March 2001.

- 43.N. Giatas, P. Roumelioti, A. Zoga, P. Zoumpoulakis, D. Vlahakos, **T. Mavromoustakos**, J. Matsoukas. Design and Biological Activity of Novel non-Peptide Imidazole Based Angiotensin II Receptor Antagonists. 2nd Conference Medicinal Chemistry: Drug Design and Development 1-3 March 2001.
- 44.P. Roumelioti, N. Giatas, A. Zoga, L. Polevaya, **T. Mavromoustakos**, P. Zoumboulakis, D. Vlahakos, E. Iliodromitis, J. Matsoukas. Design and Synthesis of Amide-linked Angiotensin II Analogues with 3,5 side Chain Bridges: Structural Resemblance of Ring Cluster Conformation with AT₁ non-Peptide Antagonists. 2nd Conference Medicinal Chemistry: Drug Design and Development 1-3 March 2001.
- 45.I. Daliani, T. Tselios, L. Probert, S. Deraos, **T. Mavromoustakos**, J. Matsoukas. Rational Design and Synthesis of a Potent Amide-Linked Cyclic Analogue of MBP₈₇₋₉₉ based on 2D-NMR studies and Molecular Dynamics. 2nd Conference Medicinal Chemistry: Drug Design and Development 1-3 March 2001.
- 46.**T. Mavromoustakos**, D. Papahatjis and P. Laggner. Differential Membrane Fluidization by Active and Inactive Cannabinoid Analogs. The 9th Cyprus Conference of New Methods in Drug Research. Limassol, Cyprus. 17-22 May, 2001.
- 47.**T. Mavromoustakos**, T. Calogeropoulou, M. Koufaki, A. Kolocouris, I. Daliani, C. Demetzos, Z. Meng, A. Makriyannis, J. Balzarini and E. De Clercq. Ether Phospholipid-AZT Conjugates possessing Anti-HIV and Anti-Tumor Cell Activity. Synthesis, Conformational Analysis and Study of their Thermal Effects on Membrane Bilayers. The 9th Cyprus Conference of New Methods in Drug Research. Limassol, Cyprus. 17-22 May, 2001.
- 48.**T. Mavromoustakos**. Nuclear Magnetic Resonance: A valuable tool in the detection of adulteration in Food and Beverages. Invited Speak in the University of Cyprus (28.5.2001).
- 49.K. Agni, **T. Mavromoustakos**, G. Spyroulias, S. Nikolaropoulos. Conformational Analysis of a steroidal derivative of Chlorombucil, using NMR studies and Computational Chemistry. 7th Conference in Advanced Medicinal Chemistry. 18-20 May 2001.
- 50.**T. Mavromoustakos**. The role of Differential Scanning Calorimetry in the Interactions of Drug Molecules with Membranes. Speech in the Polytechnic School of Athens. 29.9.2001. Proceedings pages 9-16.
- 51.I. Daliani, T. Tselios, L. Probert, S. Deraos, **T. Mavromoustakos**, J. Matsoukas. Rational Design and Synthesis of a Potent Amide-Linked Cyclic Analogue of MBP₈₇₋₉₉ Based on 2D-NMR Studies and Molecular Dynamics. Peptides: The Wave of the Future Michal Lebl and Richard A. Houghten (Editors) American Peptide Society, 2001.
- 52.P. Roumelioti, L. Polevaya, N. Giatas, A. Zoga, I. Mutule, T. Keivish, **T. Mavromoustakos**, P. Zoumpoulakis, D. Vlahakos, J. Matsoukas. Design and Synthesis of an Amide-Linked Angiotensin II Analogue with 3,5 Side Chain Bridge: Structural Resemblance of Ring Cluster Conformation with AT₁ Non-Peptide

Antagonists. Peptides: The Wave of the Future Michal Lebl and Richard A. Houghten (Editors) American Peptide Society, 2001.

53.**T. Mavromoustakos**, P. Zoumpoulakis, M. Zervou, N. Zoga, N. Giatas, P. Roumelioti, J. Matsoukas. Conformation and Bioactivity. 3rd Conference of Medicinal Chemistry: Drug Design and Development. Patra, March 7-9,2002. (invited speaker). A corresponding poster forr this work was prized.

54.S. Deraos, T. Tselios, I. Daliani, P. Zoumpoulakis, L. Probert, A. Troganis, **T. Mavromoustakos**, J. Matsoukas. Design, Synthesis and Conformational Properties of Linear Analogues of Human Myelin Basic Protein Epitope MBP₁₋₁₁. 3rd Conference of Medicinal Chemistry: Patra, Drug Design and Development. March 7-9,2002.

55.N. Giatas, M.E. Androutsou, A. Zoga, P. Roumelioti, P. Zoumpoulakis, **T. Mavromoustakos**, D. Vlahakos, E. Iliodromitis, J. Matsoukas. Synthesis of Imidazole-based Non-peptide Angiotensin II Receptor Antagonists as Potent Antihypertensives. 3rd Conference of Medicinal Chemistry: Drug Design and Development. March 7-9,2002.

56.I. Kyrikou, C. Poulos, **T. Mavromoustakos**. Structure Elucidation, Conformational Properties and Interactions of the Toxin Paralysin, β -Ala-Tyr from Larvae of the Gray Flesh Fly with Phospholipid Bilayers Using MAS ¹³C-NMR Spectroscopy. 3rd Conference of Medicinal Chemistry: Drug Design and Development. Patra, March 7-9,2002.

57.A. Zoga, N. Giatas, P. Roumelioti, M.E. Androutsou, P. Zoumpoulakis, **T. Mavromoustakos**, D. Vlahakos, E. Iliodromitis, J. Matsoukas. Biological Essays on non-Peptide Angiotensin II AT₁-Receptor Antagonists. Drug Design and Development. Patra, March 7-9,2002.

58.P. Zoumpoulakis, A. Zoga, E. Zervou, N. Giatas, P. Roumelioti, J. Matsoukas, **T. Mavromoustakos**.Conformational and Biophysical Studies of AT₁ Non-Peptide Antagonists. Drug Design and Development. Patra, March 7-9,2002.

59.T. Tselios, I. Daliani, S. Deraos, **T. Mavromoustakos**, L. Probert, J. Matsoukas. Design and Synthesis of Potent Human Cyclic MBP₈₇₋₉₉ Altered Peptide Ligands: Inhibition of Experimental Allergic Encephalomyelitis (EAE) 3rd Hellenic Forum on Bioactive Peptides. April 11-14, 2002. Coference and Cultural Center of the University of Patras.

60.P. Zoumpoulakis, M. Zervou, I. Kyrikou, E. Siapi, S.G. Grdadolnik, **T. Mavromoustakos**. Relationship between Conformation and Bioactivity in the Hypertension Disease. April 11-14, 2002. Conference and Cultural Center of the University of Patras.

61.N. Giatas, P. Roumelioti, A. Zoga, M.E. Androutsou, L. Polevaya, I. Mutule, T. Keivish, **T. Mavromoustakos**, P. Zoumpoulakis, D. Vlahakos, J. Matsoukas.Structural Resemblance of Angiotensin II Ring Cluster Conformation with an AT₁ Non-Peptide Antagonist. April 11-14, 2002. Conference and Cultural Center of the University of Patras.

- 62.P. Zoumpoulakis, M. Zervou, I. Kyrikou, S.G. Grdadolnik, A. Zoga, N. Giatas, P. Roumelioti, J. Matsoukas, **T. Mavromoustakos**. Comparative Conformational Analysis Studies Between Losartan Derivatives. April 11-14, 2002. Conference and Cultural Center of the University of Patras.
- 63.I. Kyrikou, S.G. Grdadolnik, C. Poulos, **T. Mavromoustakos**. Structural Elucidation, Conformational Properties in Hydrophilic and Amphoteric Environments and Interactions with Phospholipid Bilayers of the Toxin Paralysis β -Ala-Tyr from Larvae of the Gray Flesh Fly. April 11-14, 2002. Conference and Cultural Center of the University of Patras.
- 64.T. Calogeropoulou, M. Koufaki, N. Avlonitis, E. Lekka, A. Detsi, E. Scoulica, P. Papazafiri, E. Siapi, I. Kyrikou, **T. Mavromoustakos**, A. Makriyannis. Design and synthesis of novel ether phospholipids embodying cyclic moieties. Comparative study of their anticancer and antileishmanial activity. *Drugs Fut* 2002, 27(Suppl. A):XVIIth Int. Symp. on MEDICINAL CHEMISTRY.
- 65.**T. Mavromoustakos**, I. Kyrikou, P. Petrakis. The adulteration of olive oil by other oils. 6th International Conference on Applications of Magnetic Resonance in Food Science, Paris 4-6 September, 2002.
- 66.**T. Mavromoustakos**, E. Siapi. The Use of Differential Scanning Calorimetry to study the thermal effects of gentamycin on Synthetic Polymeric Collageneous Membranes. The VIIth Symposium of Colloid and Surface Chemistry. 143-149. Bucarest 20-21 September 2002.
- 67.**T. Mavromoustakos** (invited speaker). I. Kyrikou, E. Siapi, T. Calogeropoulou, M. Koufaki, D. Papahadjis. Differential Scanning Calorimetry. An invaluable tool in Medicinal Chemistry 1st National Conference in Thermal Analysis, Kerkini, September 27-29, 2002.
- 68.A. Kapou, **T. Mavromoustakos**, S. Nikolaropoulos. Thermal changes caused by Synthetic Steroids in Membrane Bilayers. 1st Greek Conference of Thermal Analysis, Kerkini, September 27-29, 2002.
- 69.I. Kyrikou, M. Zervou, P. Petrakis, **T. Mavromoustakos**. Study the adulteration of olive oil with hazelnut oil using ¹³C NMR spectroscopy. 19^o Greek Conference of Chemistry, Iraklion, Crete, 6-10 November 2002.
- 70.I. Kyrikou, E. Siapi, P. Zoumpoulakis, M. Zervou, D. Dimitriou, A. Pitsas, Ch. Camoutsis, Eng. V. Trandafir, A. Buzor, G. Popescu, **T. Mavromoustakos**. Biophysical studies of gentamycin in collagen membranes. 19^o Greek Conference of Chemistry, Iraklion, Crete, 6-10 November 2002.
- 71.P. Zoumpoulakis, A. Zoga, I. Kyrikou, M. Zervou, E. Siapi, **T. Mavromoustakos**. Interaction and diffusion of AT1 antagonists in membrane bilayers. 19^o Greek Conference of Chemistry, Iraklion, Crete, 6-10 November 2002.

- 72.S. Deraos, T. Tselios, I. Daliani, P. Zoumpoulakis, L. Probert, A. Troganis, **T. Mavromoustakos**, J. Matsoukas. Design, Synthesis and Conformational Properties of Linear Analogues of Human Myelin Basic Protein Epitope MBP₁₋₁₁. 17(2) 98 2003. Review of Clinical Pharmacology and Pharmacokinetics.
- 73.N. Giatas, M-E. Androutsou, A. Zoga, P. Roumelioti, P. Zoumpoulakis, **T. Mavromoustakos**, D. Vlahakos, E. Iliodromitis, J. Matsoukas. Synthesis of Imidazole-based Non-peptide Angiotensin II Receptor Antagonists As Potent Antihypertensives 17(2) 98 2003. Review of Clinical Pharmacology and Pharmacokinetics.
- 74.P. Zoumpoulakis, A. Zoga, E. Zervou, N. Giatas, P. Roumelioti, J. Matsoukas, **T. Mavromoustakos**. Conformational and Biophysical Studies of AT₁ Non-Peptide Antagonists. 17(2) 103 2003. Review of Clinical Pharmacology and Pharmacokinetics.
- 75.I. Kyrikou, C. Poulos, **T. Mavromoustakos**. Structural Elucidation, Conformational Properties and Interactions of the Toxin Paralysin, β -Ala-Tyr from Larvae of the Gray Flesh Fly with Phospholipid Bilayers Using MAS ¹³C-NMR Spectroscopy. 17(2) 104 2003. Review of Clinical Pharmacology and Pharmacokinetics.
- 76.A Zoga, N. Giatas, P. Roumelioti, M-E. Androutsou, P. Zoumpoulakis, **T. Mavromoustakos**, D. Vlahakos, E. Iliodromitis, J. Matsoukas. Biological Essays of non-Peptide Angiotensin II AT₁-Receptor Antagonists. 17(2) 110 2003. Review of Clinical Pharmacology and Pharmacokinetics.
- 77.M.K.Keramida, T. Tselios, H. Habibi, G. Agelis, **T. Mavromoustakos**, K. Papazisis, J. Matsoukas. Design and Synthesis of Two Novel Cyclic GnRH Analogues: Biological and Conformational Studies. March 13-14, 2003, Patras, Greece.
- 78.K. Agnes, **Mavromoustakos, T.**, Golic, S., Nikolaropoulos, S. 2-D NMR and Molecular Modeling in the Conformational Analysis of an Anticancer Steroidal Ester. 11th Panhellenic Pharmaceutical Congress, Athens, Greece, March 29-31, 2003.
- 79.K. Ioanna, D. Ioanna, **T. Mavromoustakos**, H. Maswadeh, C. Demetzos, S. Xatziantoniou, T. Achilleas, G. Nounesis. The modulation of thermal and dynamic properties of vinblastine by cholesterol in membrane bilayers. 11th Panhellenic Pharmaceutical Congress, Athens, Greece, March 29-31, 2003.
- 80.E. Siapi, **T. Mavromoustakos**, I. Kyrikou, V. Trandafir, B. Albu, G. Popescu, A. Pitsas, D. Demetriou. Thermal Effects of Collageneous Membranes Containing the Antibiotic Gentamycin. Progrese in stiinta compusilor or organici si macromoleculari, 25-27 September, 2003, Iasi, Romania.
- 81.**T. Mavromoustakos**, P. Minakakis, G. Kokotos, M. Zervou, I. Kyrikou, A. Kapu, A. Zoga, P. Zoumpoulakis, S. Gega, I. Chailkefs, C. Potamitis, E. Siapi, A. Pitsas, D. Demetriou, E. Iliodromitis. The Use of NMR and Molecular Modeling to study the molecular basis of hypertension. Progrese in stiinta compusilor or organici si macromoleculari, 25-27 September, 2003, Iasi, Romania.

82. **T. Mavromoustakos**, P. Zoumpoulakis, M. Zervou, I. Kyrikou, A. Kapou, N. Benetis. The Use of Computational Analysis to Design Novel Drugs. Proceedings of the ICCMSE 2003 by World Scientific, editor: T.E. Simos.
83. **Mavromoustakos, T.**, Zoumpoulakis P., Roumelioti, P., Giatas, N., Vlahakos, D., Iliodromytis, E., Matsoukas, Design, conformation and bioactivity of novel angiotensin II receptor antagonists. J. Biopolymers 71(3), 266 (2003).
84. Macpherson A, Neti S, Mannisi J, **Mavromoustakos T**, Macpherson P Quantitative predictions from echocardiograms JOURNAL OF HYPERTENSION 21: S326-S327 Suppl. 4 JUN 2003.
85. E. Siapi, **T. Mavromoustakos**, D. Kovala-Demertzi, C. Vidjeluc, M.A. Demertzis. The thermal effects of platinum (II) and palladium (II) complexes with 2-acetyl pyridine and pyridine-2-carbaldehyde N(4)-ethyl-thiosemicarbazones in membrane bilayers. Inorganic Reaction Mechanisms, 8-10 2004, Athens, Greece.
86. **T. Mavromoustakos**, K. Ioanna, D. Ioanna, M. Hamzah, D. Costas, S. Xatziantoniou, S. Giatrellis, G. Nounesis. The Modulation of Thermal Properties of Vinblastine by Cholesterol in Membrane Bilayers. Medicinal Chemistry: Drug Design and Development, March 11-13, 2004, Patras, Greece.
87. A. Kapou, S. Nikolaropoulos, **T. Mavromoustakos**. DSC-Evaluated Thermal Effects of Steroidal Carriers of Alkylating Agents on Membrane Bilayers. Medicinal Chemistry: Drug Design and Development, March 11-13, 2004, Patras, Greece.
88. I. Kyrikou, C. Poulos, N. Benetis, **T. Mavromoustakos**. A ^{31}P NMR study of interactions of β -Ala-Tyr and Aminoacid Glu with Phospholipid Bilayers. Medicinal Chemistry: Drug Design and Development, March 11-13, 2004, Patras, Greece.
89. E. Mantzourani, T. Tselios, J. Matsoukas, **T. Mavromoustakos**. Structural Elucidation and Conformational Properties of $[\text{Arg}^{91}, \text{Ala}^{96}]$ an Antagonist Suppressing the Induction of Experimental Autoimmune Encephalomyelitis (EAE). Medicinal Chemistry: Drug Design and Development, March 11-13, 2004, Patras, Greece.
90. V. Saroglou, S. Hatziantoniou, M. Smyrniotakis, **T. Mavromoustakos**, A. Zompra, V. Magafa, P. Cordopatis, C. Demetzos. Design of New Liposome Formulation and Encapsulation of the Synthetic Anticancer Drug Leuprolide Acetate and Study of its Thermal Effects on Membrane Bilayers. J. Peptide Sci. 2004 (10 Sup)H41. 4th Hellenic Forum on Bioactive Peptides. April 22-24 2004, Patras-Hellas.
91. M. Smyrniotakis, I. Kyrikou, K. Demetzos, K. Viras, **T. Mavromoustakos**. Efforts to Esterify Captopril with Polyethylenoglycol. J. Peptide Sci. 2004 (10 Sup)H52. 4th Hellenic Forum on Bioactive Peptides. April 22-24, 2004 Patras-Hellas.
92. N. P. Benetis, I. Kyrikou, **T. Mavromoustakos**. Spectral Simulations of Static ^{31}P CP NMR Multilamella Bilayer Spectra in the Absence and Presence of Bioactive

Dipeptide β -Ala-Tyr or Glu. J. Peptide Sci. 2004 (10 Sup)H53. 4th Hellenic Forum on Bioactive Peptides. April 22-24, 2004 Patras-Hellas.

93.A. Zoga, I. Kyrikou, S. Gega, E. Chalkefs, P.M. Minakakis, **T. Mavromoustakos**. Biophysical Studies on a Novel Antihypertensive AT₁ Antagonism MM1. J. Peptide Sci. 2004 (10 Sup)H54. 4th Hellenic Forum on Bioactive Peptides. April 22-24, 2004 Patras-Hellas.

94.A. Kapou, M. Zervou, S.G. Grdadolnik, **T. Mavromoustakos**. 3D-QSAR Antihypertensive Models Based on 2D-NMR and Computational Analysis Driven Low Energy Conformers of Losartan. J. Peptide Sci. 2004 (10 Sup)H54. 4th Hellenic Forum on Bioactive Peptides. April 22-24, 2004 Patras-Hellas.

95.K. Potamitis, M. Zervou, I. Kyrikou, E. Siapi, P. Zoumpoulakis, C. Fotakis, D. Christodouleas, K. Viras, A. Kolocouris, S.G. Grdadolnik, **T. Mavromoustakos**. Conformational Analysis Using 2D NMR Spectroscopy Coupled with Computational Analysis of Valsartan and its Drug:Membrane Interactions. J. Peptide Sci. 2004 (10 Sup)H55. 4th Hellenic Forum on Bioactive Peptides. April 22-24, 2004 Patras-Hellas.

96.G. Mousselimi, I. Kyrikou, E. Siapi, C. Fotakis, D. Christodouleas, K. Viras, **T. Mavromoustakos**. Comparative Thermal and Dynamic Effects of Captopril and Enalapril in Lipid Bilayers Using DSC, Solid State NMR and Raman Spectroscopy. J. Peptide Sci. 2004 (10 Sup) H55. 4th Hellenic Forum on Bioactive Peptides. April 22-24, 2004 Patras-Hellas.

97.E. Mantzourani, T. Tselios, J. Matsoukas, **T. Mavromoustakos**. Structural Elucidation and Conformational Analysis of a Potent Altered Peptide Ligand, [Arg⁹¹, Ala⁹⁶]MBP₈₇₋₉₉ Employing Experimental ROE Constraints Combined with Theoretical Calculations and Molecular Modelling. J. Peptide Sci. 2004 (10 Sup)H56. 4th Hellenic Forum on Bioactive Peptides. April 22-24, 2004 Patras-Hellas.

98.I. Kyrikou, C. Poulos, N. Benetis, K. Viras, **T. Mavromoustakos**. Conformational Properties and Interactions of the Toxin Paralysis β -Ala-Tyr and Glu with Phospholipid Bilayers. J. Peptide Sci. 2004 (10 Sup) H58. 4th Hellenic Forum on Bioactive Peptides. April 22-24, 2004 Patras-Hellas.

99.**T. Mavromoustakos**, P. Zoumpoulakis, A. Politi, P. Minakaki, G. Kokotos. The Contribution of Docking in the Rational Drug-Design. 6th Conference Medicinal Chemistry:Drug Discovery and Design. March 10-12, 2005, Patras-Hellas.

100.P. Moutevelis-Minakakis, K. Georgikopoulou, C.G. Kokotos, P. Kontogiannis, **T. Mavromoustakos**. Design and synthesis of novel (S)-pyroglutamic based antihypertensive agents. J. Peptide Science vol. 10, 2004, 3rd International and 28th European Peptide Symposium. September 5-10, 2004. Prague, Czech Republic.

101. P. Moutevelis-Minakakis, C.G. Kokotos, P. Kontogianni, **T. Mavromoustakos**. Design and synthesis of novel (S)-pyroglutamic acid based antihypertensive agents. Acids and Proteins. Rome, Italy. September 5-9, 2003 and Aminoacids 25(2), 2003.

- 102.P. Moutevelis-Minakakis, K. Georgikopoulou, V. Magrioti, **T. Mavromoustakos**, G. Kokotos. Synthesis of new 2-pyrrolidinone antihypertensives starting from natural amino acids. 9th International Congress on Amino Acids and Proteins. Vienna 8-12 August 2005.
- 103.**T. Mavromoustakos**, P. Zoumpoulakis, M. Zervou, I. Kyrikou, A. Kapou, N. Benetis. The Use of Computational Analysis to Design Novel Drugs. Proceedings of the ICCMSE 2003 by World Scientific, editor: T.E. Simos.
- 104.**Mavromoustakos, T.**, Zoumpoulakis P., Roumelioti, P., Giatas, N., Vlahakos, D., Iliodromytis, E., Matsoukas, J. Design, conformation and bioactivity of novel angiotensin II receptor antagonists. Biopolymers 71(3), 266 (2003).
105. Macpherson A, Neti S, Mannisi J, **Mavromoustakos T**, Macpherson P. Quantitative predictions from echocardiograms JOURNAL OF HYPERTENSION 21: S326-S327 Suppl. 4 JUN 2003.
- 106.E. Siapi, **T. Mavromoustakos**, D. Kovala-Demertzi, C. Vidjeluc, M.A. Demertzis. The thermal effects of platinum (II) and palladium (II) complexes with 2-acetyl pyridine and pyridine-2-carbaldehyde N(4)-ethyl-thiosemicarbazones in membrane bilayers. Inorganic Reaction Mechanisms, 8-10 2004, Athens, Greece.
- 107.**T. Mavromoustakos**, K. Ioanna, D. Ioanna, M. Hamzah, D. Costas, S. Xatziantoniou, S. Giatrellis, G. Nounesis. The Modulation of Thermal Properties of Vinblastine by Cholesterol in Membrane Bilayers. Medicinal Chemistry: Drug Design and Development, March 11-13, 2004, Patras, Greece.
- 108.A. Kapou, S. Nikolaropoulos, **T. Mavromoustakos**. DSC-Evaluated Thermal Effects of Steroidal Carriers of Alkylating Agents on Membrane Bilayers. Medicinal Chemistry: Drug Design and Development, March 11-13, 2004, Patras, Greece.
- 109.I. Kyrikou, C. Poulos, N. Benetis, **T. Mavromoustakos**. A ³¹P NMR study of interactions of β-Ala-Tyr and Aminoacid Glu with Phospholipid Bilayers. Medicinal Chemistry: Drug Design and Development, March 11-13, 2004, Patras, Greece.
- 110.E. Mantzourani, T. Tselios, J. Matsoukas, **T. Mavromoustakos**. Structural Elucidation and Conformational Properties of [Arg⁹¹,Ala⁹⁶] an Antagonist Suppressing the Induction of Experimental Autoimmune Encephalomyelitis (EAE). Medicinal Chemistry: Drug Design and Development, March 11-13, 2004, Patras, Greece.
- 111.V. Saroglou, S. Hatziantoniou, M. Smyrniotakis, **T. Mavromoustakos**, A. Zompra, V. Magafa, P. Cordopatis, C. Demetzos. Design of New Liposome Formulation and Encapsulation of the Synthetic Anticancer Drug Leuprolide Acetate and Study of its Thermal Effects on Membrane Bilayers. J. Peptide Sci. 2004 (10 Sup)H41. 4th Hellenic Forum on Bioactive Peptides. April 22-24 2004, Patras-Hellas.
- 112.M. Smyrniotakis, I. Kyrikou, K. Demetzos, K. Viras, **T. Mavromoustakos**. Efforts to Esterify Captopril with Polyethyleneglycol. J. Peptide Sci. 2004 (10 Sup)H52. 4th Hellenic Forum on Bioactive Peptides. April 22-24, 2004 Patras-Hellas.

- 113.N. P. Benetis, I. Kyrikou, **T. Mavromoustakos**. Spectral Simulations of Static ^{31}P CP NMR Multilamella Bilayer Spectra in the Absence and Presence of Bioactive Dipeptide β -Ala-Tyr or Glu. J. Peptide Sci. 2004 (10 Sup)H53. 4th Hellenic Forum on Bioactive Peptides. April 22-24, 2004 Patras-Hellas.
- 114.A. Zoga, I. Kyrikou, S. Gega, E. Chalkefs, P.M. Minakakis, **T. Mavromoustakos**. Biophysical Studies on a Novel Antihypertensive AT_1 Antagonism MM1. J. Peptide Sci. 2004 (10 Sup)H54. 4th Hellenic Forum on Bioactive Peptides. April 22-24, 2004 Patras-Hellas.
- 115.A. Kapou, M. Zervou, S.G. Grdadolnik, **T. Mavromoustakos**. 3D-QSAR Antihypertensive Models Based on 2D-NMR and Computational Analysis Driven Low Energy Conformers of Losartan. J. Peptide Sci. 2004 (10 Sup)H54. 4th Hellenic Forum on Bioactive Peptides. April 22-24, 2004 Patras-Hellas.
- 116.K. Potamitis, M. Zervou, I. Kyrikou, E. Siapi, P. Zoumpoulakis, C. Fotakis, D. Christodouleas, K. Viras, A. Kolocouris, S.G. Grdadolnik, **T. Mavromoustakos**. Conformational Analysis Using 2D NMR Spectroscopy Coupled with Computational Analysis of Valsartan and its Drug:Membrane Interactions. J. Peptide Sci. 2004 (10 Sup)H55. 4th Hellenic Forum on Bioactive Peptides. April 22-24, 2004 Patras-Hellas.
- 117.G. Mousselimi, I. Kyrikou, E. Siapi, C. Fotakis, D. Christodouleas, K. Viras, **T. Mavromoustakos**. Comparative Thermal and Dynamic Effects of Captopril and Enalapril in Lipid Bilayers Using DSC, Solid State NMR and Raman Spectroscopy. J. Peptide Sci. 2004 (10 Sup) H55. 4th Hellenic Forum on Bioactive Peptides. April 22-24, 2004 Patras-Hellas.
- 118.E. Mantzourani, T. Tselios, J. Matsoukas, **T. Mavromoustakos**. Structural Elucidation and Conformational Analysis of a Potent Altered Peptide Ligand, $[\text{Arg}^{91}, \text{Ala}^{96}]\text{MBP}_{87-99}$ Employing Experimental ROE Constraints Combined with Theoretical Calculations and Molecular Modelling. J. Peptide Sci. 2004 (10 Sup)H56. 4th Hellenic Forum on Bioactive Peptides. April 22-24, 2004 Patras-Hellas.
- 119.I. Kyrikou, C. Poulos, N. Benetis, K. Viras, **T. Mavromoustakos**. Conformational Properties and Interactions of the Toxin Paralysin β -Ala-Tyr and Glu with Phospholipid Bilayers. J. Peptide Sci. 2004 (10 Sup) H58. 4th Hellenic Forum on Bioactive Peptides. April 22-24, 2004 Patras-Hellas.
- 120.A. Kapou, N. Avlonitis, A. Detsi, M. Koufaki, T. Calogeropoulou, N.P. Benetis, **T. Mavromoustakos**. CoMFA and CoMSIA 3D-Quantitative Structure-Activity Relationships of New Flexible Antileishmanial Ether Phospholipids. Vol. 1. 253,-256, International Conference of Computational Methods in Sciences and Engineering 2004. (ICCMSE 2004) Editors: T. Simos, G. Maroulis.
- 121.**T. Mavromoustakos**, P. Zoumpoulakis, A. Politi, P. Minakaki, G. Kokotos. The Contribution of Docking in the Rational Drug-Design. 6th Conference Medicinal Chemistry:Drug Discovery and Design. March 10-12, 2005, Patras-Hellas.

- 122.P. Moutevelis-Minakakis, K. Georgikopoulou, C.G. Kokotos, P. Kontogiannis, **T. Mavromoustakos**. Design and synthesis of novel (S)-pyroglutamic based antihypertensive agents. J. Peptide Science vol. 10, 2004, 3rd International and 28th European Peptide Symposium. September 5-10, 2004. Prague, Czech Republic.
- 123.P. Moutevelis-Minakakis, C.G. Kokotos, P. Kontogianni, **T. Mavromoustakos**. Design and synthesis of novel (S)-pyroglutamic acid based antihypertensive agents. Acids and Proteins. Rome, Italy. September 5-9, 2003 and Aminoacids 25(2), 2003.
- 124.P. Moutevelis-Minakakis, K. Georgikopoulou, V. Magrioti, **T. Mavromoustakos**, G. Kokotos. Synthesis of new 2-pyrrolidinone antihypertensives starting from natural amino acids. 9th International Congress on Amino Acids and Proteins. Vienna 8-12 August 2005.
- 125.N.P. Benetis, A. Gili, C. Fotakis, D. Christodouleas, K. Viras, I. Kyrikou, M. Zervou, **T. Mavromoustakos**. Quantitative Simulation of Static P-1 NMR Spectra under Cross Polarization condition as an aid in the Rational Design of Novel Antihypertensive Drugs. Designing Molecules Against Diseases of Modern Societies. Telloglio Institute of Arts, 159A, Aghiou Dimitriou Str., Thessaloniki, 20-21 May 2005. p. 87-90.
- 126.**T. Mavromoustakos**, N. Benetis, M. Zervou, P. Zoumpoulakis, I. Kyrikou, A. Politi, G. Kokotos, M. Minakaki. Design, Synthesis and Biological Evaluation of Novel AT₁ Antagonists. Interactions with Membrane Bilayers and AT₁ receptor. Designing Molecules Against Diseases of Modern Societies. Telloglio Institute of Arts, 159A, Aghiou Dimitriou Str., Thessaloniki, 20-21 May 2005. p. 128-130.
- 127.Panagiota Moutevelis-Minakakis, Christoforos G. Kokotos, Panagiota Kontogianni, Kalliopi Georgikopoulou and **Thomas Mavromoustakos**. (S)-Pyroglutamic acid based design and synthesis of new antihypertensive agents. Peptides 2004. Proceedings of the Third International and Twenty-Eight European Peptide Symposium. September 5-10, 2004-Prague, Czech Republic pages 244-245.
- 128.Efthimia Mantzourani, Thoedore Tselios, John Matsoukas and **Thomas Mavromoustakos**. Exploring conformational space and enlightening the structure of a potent altered peptide ligand, [Arg⁹¹, Ala⁹⁶] MBP₈₇₋₉₉, applying a combination of 2D NMR and molecular modeling. Peptides 2004. Proceedings of the Third International and Twenty-Eight European Peptide Symposium. September 5-10, 2004-Prague, Czech Republic pages 1041-1042,
- 129.E.D. Mantzourani, T.V. Tselios, S. Golic-Grdadolnik, J.M. Matsoukas, A. Brancale, J.A. Platts, **T.M. Mavromoustakos**. Exploration of conformational space of linear EAE antagonist [Arg⁹¹, Ala⁹⁶] MBP₈₇₋₉₉ and proposal of a putative bioactive conformation in DMSO-d₆. ICCMSE 2005, Vol. 4A pages 398-401 Advances in Computational Methods in Sciences and Engineering 2005. Editors T. Simos and G. Maroulis, Loutraki 22-26 October 2005.
- 130.**T. Mavromoustakos**, P. Zoumpoulakis, M. Zervou, N. Benetis. Theoretical Calculations constitute a Valuable Tool to Understand the Molecular Basis of

Hypertension. Vol. 4A pages 401-405 Advances in Computational Methods in Sciences and Engineering 2005. Editors T. Simos and G. Maroulis, Loutraki 22-26 October 2005.

131.V. Saroglou, S. Hatziantoniou, M. Smyrniotakis, **T. Mavromoustakos**, A. Zompra, V. Magafa, P. Cordopatis, C. Demetzos. Design of a New Liposomal Formulation and Encapsulation of the Synthetic Anticancer Drug Leuprolide Acetate. Study of its Thermal Effects on Membrane Bilayers. 4th Hellenic Forum on Bioactive Peptides, 225-233 (2005).

132.N. Benetis, I. Kyrikou, **T. Mavromoustakos**. Static ³¹P CP NMR spectral simulations of DPPC bilayers in the absence and presence of bioactive dipeptide β -Ala-Tyr or Glu. 4th Hellenic Forum on Bioactive Peptides, 301-304 (2005).

133.A. Zoga, I. Kyrikou, E. Siapi, S. Gega, E. Chalkefs, P.M-Minakakis, D. Vlahakos, E. Iliodromytis, **T. Mavromoustakos**. Biophysical Studies on MM1; a Novel Antihypertensive AT₁ Antagonist. 4th Hellenic Forum on Bioactive Peptides, 305-308 (2005).

137.A. Kapou, M. Zervou, S.G. Grdadolnik, **T. Mavromoustakos**. 3D-QSAR Antihypertensive models based on 2D-NMR and Computational Analysis Driven low energy conformers of losartan. 4th Hellenic Forum on Bioactive Peptides, 309-312 (2005).

134.G. Mousselimi, I. Kyrikou, E. Siapi, C. Fotakis, S. Gega, D. Christodouleas, K. Viras, **T. Mavromoustakos**. Comparative thermal and dynamic effects of captopril and enalapril in lipid bilayers using DSC, solid state NMR and Raman Spectroscopy. 4th Hellenic Forum on Bioactive Peptides, 317-320 (2005).

135.E. Mantzourani, T. Tselios, S.G. Grdadolnik, J. Matsoukas, **T. Mavromoustakos**. Structural Elucidation and Conformational Analysis of a Potent Altered Peptide Ligand [Arg⁹¹, Ala⁹⁶]MBP₈₇₋₉₉, Employing Experimental NOEs Constraints Combined with Theoretical Calculations and Molecular Modeling. 4th Hellenic Forum on Bioactive Peptides, 321-325 (2005).

136.I. Kyrikou, C. Poulos, N. Benetis, K. Viras, **T. Mavromoustakos**. Conformational Properties and Interaction of the Toxin Paralysin β -Ala-Tyr and Glu with Phospholipid Bilayers. 4th Hellenic Forum on Bioactive Peptides, 337-340 (2005).

137.**T. Mavromoustakos**, M. Zervou, P. Zoumpoulakis. NMR Spectroscopy: A valuable tool in the weaponry of Medicinal Chemistry. 7th Conference "Medicinal Chemistry:Drug Discovery and Design", March 8-11, 2006, Patras, Greece.

138.E.D. Mantzourani, **T.M.Mavromoustakos**, S. Golic-Grdadolnik, J.A. Platts, G.N. Deraos, J.M. Matsoukas, T.V. Tselios. A putative bioactive conformation for the APL of Myelin Basic Protein and inhibitor of Experimental Autoimmune Encephalomyelitis, [Ala⁹⁶]MBP₈₇₋₉₉. 7th Conference "Medicinal Chemistry:Drug Discovery and Design", March 8-11, 2006, Patras, Greece.

- 139.C. Potamitis, H. Reis, M. Zervou, M. Papadopoulos, **T. Mavromoustakos**. Conformational Analysis of AT₁ antagonist Valsartan using 2D NMR spectroscopy and Computational Analysis, Determination of thermodynamic parameters through dynamic NMR spectroscopy and semi-empirical calculations. 7th Conference “Medicinal Chemistry: Drug Discovery and Design”, March 8-11, 2006, Patras, Greece.
- 140.P.M. Minakakis, E. Papavassilopoulou, **T. Mavromoustakos**, P. Zoumpoulakis, G. Kokotos. Design and Synthesis of a new 2-pyrrolidone antihypertensive starting from natural amino acid. 5^o Hellenic Forum on Bioactive Peptides. 14-16 May 2006, Conference and Cultural Center of the University of Patras.
- 141.C. Potamitis, H. Reis, M. Zervou, M. Papadopoulos, **T. Mavromoustakos**. Conformational Analysis of AT₁ antagonist valsartan using 2D NMR spectroscopy and computational analysis. Determination of thermodynamic parameters through dynamic NMR spectroscopy and semi-empirical calculations. 5^o Hellenic Forum on Bioactive Peptides, 14-16 May 2006, Conference and Cultural Center of the University of Patras.
- 142.E. Chalkefs, K. Viras, P. Moutevelis-Minakakis, C. Kokotos, **T. Mavromoustakos**. Conformational Studies of MMK2 and its interaction with model membrane bilayers. 5^o Hellenic Forum on Bioactive Peptides, 14-16 May 2006, Conference and Cultural Center of the University of Patras.
- 143.A. Politis, P. Zoumpoulakis, M. Zervou, K. Georgikopoulou, G. Kokotos, P. Moutevelis-Minakakis, **T. Mavromoustakos**. Rational design of the potential molecule (5S)-1-(3-hydroxybenzyl)-5-(1H-imidazol-1-ylmethyl)-2-pyrrolidinone (MMK8) for the treatment of hypertension. 5^o Hellenic Forum on Bioactive Peptides, 14-16 May 2006, Conference and Cultural Center of the University of Patras.
- 144.E.D. Mantzourani, **T.M. Mavromoustakos**, S.G. Gardadolnik, J.A. Platts, G.N. Deraos, J.M. Matsoukas, T.V. Tselios. Towards the proposal of a structural motif for the bioactive APL of myelin basic protein and inhibitor of experimental autoimmune encephalomyelitis, [Ala⁹⁶]MBP₈₇₋₉₉. 5^o Hellenic Forum on Bioactive Peptides, 14-16 May 2006, Conference and Cultural Center of the University of Patras.
- 145.A. Kapou, N.P. Benetis, N. Avlonitis, T. Calogeropoulou, M. Koufaki, **T. Mavromoustakos**. CoMFA and CoMSIA 3D-QSAR studies of new synthetic antileishmanal ring-substituted ether phospholipids. 3rd Cost B22 Annual Congress, Oral Communications. 1-4 October 2006.
- 146.S. Durdagi, C. Koukoulitsa, T. Kourouli, T. Andreou, S. Nikas, V. Nahmias, D. Papahadjis, M.G. Papadopoulos, **T. Mavromoustakos**. Theoretical Investigation of Pharmacokinetic Profile of Synthetic Cannabinoids. The XVI European Symposium on Quantitative Structure-Activity Relationships and Molecular Modelling. 10-17 September 2006 Mediterranean Sea/Italy.

- 147.E. Mantzourani, T. Tselios, S. Golič Grdadolnik, A. Brancale, J. Matsoukas, J. Platts, **T. Mavromoustakos**. Conformational Analysis and Molecular Dynamics at the Receptor Level of the Immunodominant Myelin Basic Protein Epitope 87-99 Implicated in Multiple Sclerosis, and its Antagonists Linear Altered Peptide Ligands MGMS *Young Modellers' Forum in Conjunction with the RSC MMG*, School of Oriental & African Studies (SOAS), London, UK, September 1, 2006. abstracts p.40.
- 148.P. Moutevelis-Minakakis, **T. Mavromoustakos**, P. Zoumpoulakis, A. Politi, G. Kokotos. Synthesis of 2-pyrrolidinones as potential antihypertensive drugs. 2nd Hellenic Symposium on Organic Synthesis. From Chemistry to Biology, Medicine and Materials Science. 19-21 April 2007. p44 page 110
- 149.A. Politi, E. Papavasiliopoulou, P. Moutevelis-Minakaki, G. Kokotos, **T. Mavromoustakos**. Design and Computational Study of Novel Renin Inhibitors. Hellenic Symposium on Organic Synthesis. From Chemistry to Biology, Medicine and Materials Science. 19-21 April 2007 p55 page 121.
- 150.S. Durdagi, P.G. Zoumpoulakis, M.G. Papadopoulos, C. Koukoulitsa, D.P. Papahatjis, **T. Mavromoustakos**. An algorithm for the conformational analysis of flexible drug molecules: A critical aspect for the 3D-QSAR studies and rational drug design. Hellenic Symposium on Organic Synthesis. From Chemistry to Biology, Medicine and Materials Science. 19-21 April 2007 p56 page 122.
- 151.V. Mouchlis, **T. Mavromoustakos**, G. Kokotos. Computational Study of binding interactions between human nonpancreatic phospholipase A₂ (IIA) and inhibitor FPL 67047XX and analogues. Hellenic Symposium on Organic Synthesis. From Chemistry to Biology, Medicine and Materials Science. 19-21 April 2007 p57 page 123.
- 152.**T. Mavromoustakos** (speech). Swedish-Hellenic Life Science Research Conference. 24-26 May 2007, Orebro Sweden. Presentation of Laboratory of Molecular Analysis and talk about the Relationship between bioactivity and Conformation.
- 153.C. Potamitis, M. Zervou, S. Golic Grdadolnik, I. Kyrikou, V. Katsiara, P. Zoumpoulakis, D. Argyropoulos, G. Vatougia, S. Nikaloropoulos, **T. Mavromoustakos**. Antihypertensive Drug Valsartan: Conformational Analysis and Determination of the Amide Rotational Barrier using dynamic NMR spectroscopy, comparative superimposition and docking studies with the prototype AT₁ antagonist losartan. 8th Conference "Medicinal Chemistry:Drug Discovery and Design", March 15-17, 2007, PatrasGreece. (Abstract cited in the Review of Clinical Pharmacology and Pharmacokinetics page 28).
- 154.S. Durdagi, C. Koukoulitsa, A. Kapou, T. Kourouli, T. Andreou, S.P. Nikas, V.R. Nahmias, D.P. Papahatjis, M.G. Papadopoulos, **T. Mavromoustakos**. The application of 3D-QSAR and pharmacokinetic studies for the novel cannabinoid ligands substituted at the C1' position of the alkyl side chain. Medicinal Chemistry:Drug Discovery and Design", March15-17,2007, PatrasGreece. (Abstract cited in the

155.V. Katsiaras, C. Potamitis, P. Zoumpoulakis, S. Nikolaropoulos, **T. Mavromoustakos**. Docking Studies of the Antihypertensive Drug Valsartan at the Active Site of the AT₁ Receptor. Medicinal Chemistry:Drug Discovery and Design”, March 15-17, 2007, Patras Greece. (Abstract cited in the Review of Clinical Pharmacology and Pharmacokinetics page 54).

156.C. Koukoulitsa, P. Zoumpoulakis, A. Resvani, J. Matsoukas, **T. Mavromoustakos**. *In silico* studies of ADME properties of AT₁ receptor Antagonists. Medicinal Chemistry:Drug Discovery and Design”, March 15-17, 2007, Patras Greece. (Abstract cited in the Review of Clinical Pharmacology and Pharmacokinetics page 59).

157.**T. Mavromoustakos**, M. Zervou, P. Zoumpoulakis, C. Potamitis, V. Katsiaras, A. Politi, E. Mantzourani, S. Durdagi, C. Koukoulitsa. Putative Bioactive Conformers of Small Molecules: A Concerted Approach Using NMR Spectroscopy and Computational Chemistry. Drugs Fut 2007, 32,33 (Suppl. A) 6th AFMC International Medicinal Chemistry Symposium.

158.S. Durdagi, C. Koukoulitsa, A. Kapou, T. Kourouli, T. Andreou, S.P. Nikas, V.R. Nahmias, D.P. Papahatjis, M.G. Papadopoulos, **T. Mavromoustakos**. Drugs Fut 2007, 32 (Suppl. A), 79 6th AFMC International Medicinal Chemistry Symposium.

159.P. Zoumpoulakis, **T. Mavromoustakos**, M. Rappolt, P. Laggner, G. Rabst. The Role of Membrane Hydrocarbon Chain Composition in Interactions with Antihypertensive Drugs. 51th Annual Biophysical Meeting, March 3-7 Baltimore, Maryland, 2007.

160.T. Tselios, E. Mantzourani, I. Friligou, J. Platts, **T. Mavromoustakos**, J. Matsoukas. Rational Design of Potent Myelin Basic Protein (MBP) Cyclic Analogues: Exploring the Molecular Basis of Experimental Autoimmune Encephalomyelitis (EAE) Inhibition. 5o Hellenic Forum on Bioactive Peptides, 14-16 May 2006, Conference and Cultural Center of the University of Patras, 209-215 (2007).

161.C. Potamitis, H. Reis, M. Zervou, M. Papadopoulos, **T. Mavromoustakos**. Conformational Analysis of AT₁ Antagonist Valsartan Using 2D NMR Spectroscopy and Computational Analysis. Determination of Thermodynamic Parameters through Dynamic NMR Spectroscopy and Semi-empirical Calculations. 5o Hellenic Forum on Bioactive Peptides, 14-16 May 2006, Conference and Cultural Center of the University of Patras, 267-272 (2007).

162.E. D. Mantzourani, **T.M. Mavromoustakos**, S.G. Grdadolnik, J.A. Platts, G.N. Deraos, J.M. Matsoukas, T.V. Tselios. Towards the Proposal of a Structural Motif for the Bioactive APL of Myelin Basic Protein and Inhibitor of Experimental Autoimmune Encephalomyelitis, [Arg⁹¹, Ala⁹⁶]MBP₈₇₋₉₉. 5o Hellenic Forum on Bioactive Peptides, 14-16 May 2006, Conference and Cultural Center of the University of Patras, 273-276 (2007).

163.(invited speaker) **T. Mavromoustakos**. Invited by Prof. P. Laggner from Institute of Biophysical Research (IBR) of Graz Austria to give a lecture. The lecture was given in 14.1.2008 and was entitled "The Molecular Basis of Interdigitation".

164.S. Durdagi, P.G. Zoumpoulakis, H. Reis, M.G. Papadopoulos, C. Koukoulitsa, D.P. Papahatjis, **T. Mavromoustakos**. Molecular Docking and Molecular Dynamics Simulations of the potent Δ^8 -THC analogue AMG3. 13th Hellenic Symposium of Medicinal Chemistry. 14-15 March, Athens, 2008, Greece.

165.A. Politi, S. Durdagi, E. Papavasiliopoulou, P. Moutevelis-Minakakis, G. Kokotos, **T. Mavromoustakos**. 3D QSAR CoMFA/CoMSIA studies on renin inhibitors. 3th Hellenic Symposium of Medicinal Chemistry. 14-15 March, Athens, 2008, Greece.

166.C. Potamitis, M. Zervou, J.M. Hayes, P. Zoumpoulakis, D. Argyropoulos, S. Golic Grdadolnik, **T. Mavromoustakos**. Antihypertensive drug valsartan: Conformational analysis, thermodynamic properties and docking studies using NMR spectroscopy and *in silico* methods. 3th Hellenic Symposium of Medicinal Chemistry. 14-15 March, Athens, 2008, Greece.

167.S. Durdagi, H. Reis, M. Papadopoulos, C. Koukoulitsa, **T. Mavromoustakos**. Synergetic Use of 3D QSAR, Molecular Docking and Molecular Dynamics Simulations for the Conformational Analyses of Drugs. 9th International Conference Medicinal Chemistry. Drug Discovery and Design. March 26-28, 2008, Patras, Greece.

168.A. Politi, M. Zervou, P. Zoumpoulakis, A. Zoga, P. Moutevelis-Minakakis, G. Kokotos, **T. Mavromoustakos**, E.K. Iliodromitis, D.Th.Kremastinos. Hypertension Study in Anaesthetized Rabbits: A New Protocol for AT₁ Antagonists Screening. 9th International Conference Medicinal Chemistry. Drug Discovery and Design. March 26-28, 2008, Patras, Greece.

169.C. Potamitis, M. Zervou, T. Tselios, J. Matsoukas, **T. Mavromoustakos**. Interactions of a pair of synthetic peptide analogues of myelin basic protein with lipid bilayers using DSC and High Resolution Solid State ¹³C NMR. Screening. 9th International Conference Medicinal Chemistry. Drug Discovery and Design. March 26-28, 2008, Patras, Greece.

170.(invited speaker) **T. Mavromoustakos**. Membrane Interdigitation and Its Role in Drug Function. The Cyprus Conference CNC on New Methods in Drug Research May 11-16, 2008, Limassol, Cyprus (page 17).

171.S. Durdagi, M. G. Papadopoulos, D. P. Papahatjis, **T. Mavromoustakos**. Molecular Docking and Molecular Dynamics Simulations on the Improvement of 3D QSAR Results of Novel Δ^8 -THC Analogues. The Cyprus Conference CNC on New Methods in Drug Research May 11-16, 2008, Limassol, Cyprus (page 26).

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 AT₁ 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 the membrane perturbing ability between AT₁ 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. Papavasiliopoulou, C. Potamitis, C. Photakis, K. Viras, C. Koukoulitsa, E. Kalatzis, S. Durdagi. Peptide Mimetics and Their Interdigitation with Lipid Bilayers. Page 31. 6^o Hellenic Forum on Bioactive Peptides, 18-20 May 2008, Conference and Cultural Center of the University page 31.

178.E. Papavasiliopoulou, J. Vranas, P.M. Minakakis, G. Michas, M. Papakonstantinou, A. Politi, **T. Mavromoustakos**, G. Kokotos. Synthesis of new 2-pyrrolidinones. 6^o Hellenic Forum on Bioactive Peptides, 18-20 May 2008, Conference and Cultural Center of the University page 46.

179.E. Papavasiliopoulou, P. M. Minakakis, **T. Mavromoustakos**, A. Politi, G. Kokotos. Design and Synthesis of a Novel Potential Renin Inhibitor. 6^o 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 AT₁ antagonist Valsartan and a novel synthetic pyrrolidinone analog MMK3 as depicted by a combination of Differential Scanning Calorimetry and Raman Spectroscopy. 6^o 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 4th 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, 2nd World Conference on Magic Bullets. Celebrating the 100th 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. logP₂₀₀₉. PhysChem and ADMET Profiling in Drug Research. The 4th 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. 10th 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 ^{13}C and ^{31}P NMR Spectroscopy. 10th 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 AT₁ Antagonists in Micelle and Liposomal Environment. 10th 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 AT₁ antagonist losartan with phospholipid bilayers. 10th 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. 4th 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 A₂ inhibition by 2-oxoamides based on α -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 A₂ 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 AT₁ antagonism. 14th 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 A₂ inhibitors. 14th 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. 11th 14th 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 A₂ with inhibitors containing activated carbonyl functionalities. 14th 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 A₂ inhibition by oleuropein. 14th 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. 11th 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. 11th 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. 18th 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 A₂. 18th 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 A₂. 18th 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. 18th 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 18th 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. 25th 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. 25th 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. 29th Trends in Drug Research. Cyprus-Noordwijkerhout-Camerino Symposium. Limassol, Cyprus, October 2-7, 2011.
- 218.K. Gkoutelias, 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. Hadjikakou, S. Golic Grdadolnik, **T. Mavromoustakos**. NMR spectroscopy and docking study of complex $\text{Ag}(\text{tpp})_3(\text{asp})$ 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_1 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. Hadjikakou, S. Golic Grdadolnik, M. Simcic, G. Mali, C. Glaubitz, J. Baldus, S. Durdagi. Applications of NMR Spectroscopy in the Organic and Medicinal Chemistry, EuAsC₂S-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. 30th Noordwijkerhout-Camerino-Cyprus-Symposium. May 13th- 17th, 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-arylhydrazone analogs against Alzheimer disease. 15th 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. 15th Hellenic Symposium on Medicinal Chemistry Athens, May 25-27, 2012.

229.N. Stavrinos, N. Neophytou, V. Magrioti, **T. Mavromoustakos**, G. Kokotos. Probing for novel and selective monoglyceride lipase inhibitors. 15th 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. 15th 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. 15th 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 32nd 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 α -Amino Acids Favour the Inhibition of Human GIIA Phospholipase A₂ by 2-Oxoamides, S95-S96. Abstracts 32nd 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 32nd 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-butylimidazole analogues as potent angiotensin II receptor blockers, S116. Abstracts 32nd 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 Angiotensin

II Receptor Blockers, S120. Abstracts 32nd 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. Siafaka, 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 32nd 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. 3rd 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. 2nd 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 β -cyclodextrin/hrh analogue conjugate by using nmr spectroscopy. NMR in protein dynamics and structural biology 10-13 June, 2013 Budapest.

246. Maria Zervou,Zoe Cournia, Constantinos Potamitis,George Patargias, Serdar Durdagi, Simona Golic Grdadolnik,**Thomas Mavromoustakos**. The Molecular Basis

of Action of the AT1 antagonist Losartan. Coupling between protein, water, and lipid dynamics in complex biological systems: Theory and Experiments Conference, September 24-27, 2013, CECAM-HQ-EPFL, Lausanne, Switzerland.

247. E.Koulouridi, V. Magrioti, G. Kokotos, **T. Mavromoustakos**, In Silico screening for new inhibitors of human cytosolic phospholipase cPLA2 and molecular docking experiments Review Clinical Pharmacology and Pharmacokinetics International Edition 27,79 (2013).

248. C. Koukoulitsa, C. Kontogiorgis, D. Hadjipavlou-Litina, **T. Mavromoustakos** In Silico studies of 3-aryl-coumarins as MAO-B receptor inhibitors Review Clinical Pharmacology and Pharmacokinetics International Edition 27,80 (2013).

249. G. Kordopati, T. Tselios, **T. Mavromoustakos**, S. Golic Grdadolnik, G. Tsivgoulis, Synthesis and 2D NMR studies of a α -cyclodextrin/LHRH analogue conjugate. Review Clinical Pharmacology and Pharmacokinetics International Edition 27,81 (2013).

250.P. Kolokotroni, D. Ntountaniotis, J. Baldus, C. Glaubitz, **T. Mavromoustakos**, Exploring the molecular basis of interactions of Candesartan Cilexetil (TCV-116) in lipid bilayers using ^1H and ^{13}C CP/MAS solid state NMR spectroscopy. Review Clinical Pharmacology and Pharmacokinetics International Edition 27,83 (2013).

251.T. Kellici, V. Magrioti, G. Kokotos, **T. Mavromoustakos**, Identification of novel selective MAGL inhibitors using pharmacophore models and molecular docking. Review Clinical Pharmacology and Pharmacokinetics International Edition 27,85 (2013).

252. S. Vasilakaki, C. Koukoulitsa, E. Barbagianni, **T. Mavromoustakos**, G. Kokotos In silico studies of the inhibition properties of GK241 and its analogues against secretory phospholipase sPLA2 GIIA. Review Clinical Pharmacology and Pharmacokinetics International Edition 27,87 (2013).

253. (invited speaker) **T. Mavromoustakos**, Drug:Membrane Interactions, November 14, 2013. Novartis Institutes for Biomedical Research, Horsham, RH12 5AB.

254.(invited speaker) **T. Mavromoustakos**, Drug:Membrane Interactions and Drug Discovery. 2nd International Bau Drug Design Congress. Novel Methods and Emerging Targets in Drug Discovery&Patented Drug Development. Istanbul April 17-19, 2014.

255.**T. Mavromoustakos**, Honorium to Prof. A. Makriyannis. 32nd Cyprus-Noordwijkerhout-Camerino Symposium. Limassol, 18-22 May 2014

256.G. Kordopati, T. Tselios, T. Kellici, F. Merzel, **T. Mavromoustakos**, S.G. Grdadolnik, G. Tsivgoulis. Conformational studies of LHRH analogue conjugated with cyclodextrin using 2D NMR and Molecular Modeling. 32nd Cyprus-Noordwijkerhout-Camerino Symposium. Limassol, 18-22 May 2014

257. G. Kordopati, T. Tselios, T. Kellici, F. Merzel, **T. Mavromoustakos**, S.G. Grdadolnik, G. Tsivgoulis. Conformational studies of LHRH analogue conjugated

with cyclodextrin using 2D NMR and Molecular Modeling. 32nd Cyprus-Noordwijkerhout-Camerino Symposium. Limassol, 18-22 May 2014.

258. T. Kellici, D. Ntountaniotis, G. Leonis, M. Chatziathanasiadou, A. Tzakos, J. Baldus, C. Glaubitz, G. Valsami, E. Archontaki, K. Viras, M.G. Papadopoulos, **T. Mavromoustakos**. Interactions of silybin A with cyclodextrin derivatives using solid and liquid state NMR spectroscopy, differential scanning and isothermal titration calorimetry as well as molecular dynamics simulations. 32nd Cyprus-Noordwijkerhout-Camerino Symposium. Limassol, 18-22 May 2014.

259. E. Vrontaki, G. Melagraki, **T. Mavromoustakos**, A. Afantitis. An *in silico* effort to discover new HCV Replication Inhibitors. 32nd Cyprus-Noordwijkerhout-Camerino Symposium. Limassol, 18-22 May 2014.

260. E. Vrontaki, G. Leonis, A. Avramopoulos, M.G. Papadopoulos, M. Simcic, S.Golic Grdadolnik, A. Afantitis, G. Melagraki, S.K. Hadjikakou, **T. Mavromoustakos**. Stability and Binding Effects of Ag Metal Complexes at LOX-1. 32nd Cyprus-Noordwijkerhout-Camerino Symposium. Limassol, 18-22 May 2014.

261. S. Vasilakaki, G. Leonis, M.G. Papadopoulos, **T. Mavromoustakos**, G. Kokotos, Molecular Dynamics Simulations and MM-PBSA Binding Free Energy Estimation in GK241-sPLA₂ GIIA complex. 32nd Cyprus-Noordwijkerhout-Camerino Symposium. Limassol, 18-22 May 2014.

262. A.S. Foscolos, I. Papanastasiou, G. Foscolos, A. Tsotinis, T. Kellici, **T. Mavromoustakos**. Hydrazones of 5-nitro-2-furanecarboxaldehyde with 1-adamantanealkanoic acid hydrazides with probable trypanocidal activity. 32nd Cyprus-Noordwijkerhout-Camerino Symposium. Limassol, 18-22 May 2014.

263. (poster presentation) S. Vasilakaki, **T. Mavromoustakos**, G. Kokotos. Review Clinical Pharmacology and Pharmacokinetics International Edition p. 28 devoted to the 15th Conference with International Participation held in Patras, April 9-11, 2014.

264. (poster presentation) S. Vasilakaki, **T. Mavromoustakos**, G. Kokotos. Docking studies on coumarin and quinolinone derivatives against sPLA₂GIIA. Clinical Pharmacology and Pharmacokinetics International Edition p. 28 devoted to the 15th Conference with International Participation held in Patras, April 9-11, 2014, p. 44.

265. (poster presentation) T. Kellici, D. Ntountaniotis, G. Leonis, M. Chatziathanasiadou, A. Tzakos, J. Baldus, C. Glaubitz, G. Valsami, E. Archontaki, K. Viras, M.G. Papadopoulos, **T. Mavromoustakos**. Clinical Pharmacology and Pharmacokinetics International Edition p. 28 devoted to the 15th Conference with International Participation held in Patras, April 9-11, 2014, p. 45.

266. E. Vrontaki, G. Melagraki, **T. Mavromoustakos**, A. Afantitis. Exploiting ChEMBL Database to identify indole analogues as HCV replication inhibitors. Clinical Pharmacology and Pharmacokinetics International Edition p. 28 devoted to the 15th Conference with International Participation held in Patras, April 9-11, 2014, p. 31.

267. **T. Mavromoustakos**, Honarium to Prof. A. Makriyannis. 32nd Cyprus-Noordwijkerhout-Camerino Symposium. Limassol, 18-22 May 2014
268. **G. Kordopati**, T. Tselios, T. Kellici, F. Merzel, T. Mavromoustakos, S.G. Grdadolnik, G. Tsivgoulis. Conformational studies of LHRH analogue conjugated with cyclodextrin using 2D NMR and Molecular Modeling. 32nd Cyprus-Noordwijkerhout-Camerino Symposium. Limassol, 18-22 May 2014
269. **G. Kordopati**, T. Tselios, T. Kellici, F. Merzel, T. Mavromoustakos, S.G. Grdadolnik, G. Tsivgoulis. Conformational studies of LHRH analogue conjugated with cyclodextrin using 2D NMR and Molecular Modeling. 32nd Cyprus-Noordwijkerhout-Camerino Symposium. Limassol, 18-22 May 2014.
270. T. Kellici, D. Ntountaniotis, G. Leonis, M. Chatziathanasiadou, A. Tzakos, J. Baldus, C. Glaubitz, G. Valsami, E. Archontaki, K. Viras, M.G. Papadopoulos, **T. Mavromoustakos**. Interactions of silybin A with cyclodextrin derivatives using solid and liquid state NMR spectroscopy, differential scanning and isothermal titration calorimetry as well as molecular dynamics simulations. 32nd Cyprus-Noordwijkerhout-Camerino Symposium. Limassol, 18-22 May 2014.
271. E. Vrontaki, G. Melagraki, **T. Mavromoustakos**, A. Afantitis. An *in silico* effort to discover new HCV Replication Inhibitors. 32nd Cyprus-Noordwijkerhout-Camerino Symposium. Limassol, 18-22 May 2014.
272. E. Vrontaki, G. Leonis, A. Avramopoulos, M.G. Papadopoulos, M. Simcic, S.Golic Grdadolnik, A. Afantitis, G. Melagraki, S.K. Hadjikakou, **T. Mavromoustakos**. Stability and Binding Effects of Ag Metal Complexes at LOX-1. 32nd Cyprus-Noordwijkerhout-Camerino Symposium. Limassol, 18-22 May 2014.
273. S. Vasilakaki, G. Leonis, M.G. Papadopoulos, **T. Mavromoustakos**, G. Kokotos, Molecular Dynamics Simulations and MM-PBSA Binding Free Energy Estimation in GK241-sPLA₂ GIIA complex. 32nd Cyprus-Noordwijkerhout-Camerino Symposium. Limassol, 18-22 May 2014.
274. A.S. Foscolos, I. Papanastasiou, G. Foscolos, A. Tsotinis, T. Kellici, **T. Mavromoustakos**. Hydrazones of 5-nitro-2-furanecarboxaldehyde with 1-adamantanealkanoic acid hydrazides with probable trypanocidal activity. 32nd Cyprus-Noordwijkerhout-Camerino Symposium. Limassol, 18-22 May 2014.
275. E. Vrontaki, G. Melagraki, **T. Mavromoustakos**, A. Afantitis. Development of predictive pharmacophore model and 3D-QSAR CoMSIA study for the *in silico* screening of new potent β -thalassaemia agents. IXth Joint Meeting in Medicinal Chemistry, 7-10 June 2015, Athens, Greece.
276. P. Gkeka, I. Galdadas, **T. Mavromoustakos**, Z. Cournia. Investigation of the molecular basis of action of the AT₁ antagonist losartan and its metabolite EXP3174 using all-atom MD simulations. IXth Joint Meeting in Medicinal Chemistry, 7-10 June 2015, Athens, Greece.

277. S. Vasilakaki, **T. Mavromoustakos**, G. Kokotos. Study of the pyrrophenone-cytosolic phospholipase A₂ binding by molecular dynamics simulations. IXth Joint Meeting in Medicinal Chemistry, 7-10 June 2015, Athens, Greece.
278. T. Kellici, D. Ntountaniotis, G. Leonis, M. Chatziathanasiadou, A. Tzakos, J. Baldus, C. Glaubitz, G. Valsami, E. Archontaki, K. Viras, M. Papadopoulos, **T. Mavromoustakos**. Preparation and investigation of the inclusion complex of silibinin with 2-hydroxypropyl- β -cyclodextrin. IXth Joint Meeting in Medicinal Chemistry, 7-10 June 2015, Athens, Greece.
279. **T. Mavromoustakos** (speaker), P. Patrikios. Oligomers formed during the boiling of virgin olive oil. GREEK LIPID FORUM, NHRF 11-12 June 2015. (Abstract Book p. 24).
280. E. Semidalas, K. Viras, P. Chatzigeorgiou, T. Kellici, G. Leonis, **T. Mavromoustakos** and C. Semidalas. The effects of vinblastine in the lipid bilayers SCINTE 4.11-6.11.2015 NHRF, Athens
281. **T. Mavromoustakos** (invited speaker). Targeted biologically active compounds. 16 Medical Conference 11.11.2015, Patras, Greece.
282. (poster) A. Tsotinis, A.S. Foscolos, I. Papanastasiou, G.B. Foskolos, T. Kellici, **T. Mavromoustakos**, M.C. Taylor, J.M. Kelly. New hydrazones of 5-nitro-furaldehyde with adamantane alkanohydrazides: synthesis, conformational analysis and *in vitro* trypanocidal activity. 33rd Camerino-Cyprus Symposium. Receptor Chemistry: Reality and Vision. Camerino May 15-19, 2016.
283. G. Megariotis, **T. Mavromoustakos**, D.N. Theodorou, A Molecular Dynamics Study of Irbesartan in a Lipid Membrane παρουσιάστηκε στο 13th International Conference on Nanosciences & Nanotechnologies Thessaloniki, 05/07/16 -08/07/16.
284. G. Megariotis, **T. Mavromoustakos**, D.N. Theodorou, A Molecular Dynamics Study of Irbesartan in a Lipid Membrane παρουσιάστηκε στο 13th International Conference on Nanosciences & Nanotechnologies που έλαβε χώρα στη Θεσσαλονίκη κατά το χρονικό διάστημα από 05/07/16 έως 08/07/16.
285. Design and Synthesis of Novel pyrimidinopyrimidines as VEGFR2/EGFR inhibitors. P. Konstantinos, T. Kellici, M. Michailidou, **T. Mavromoustakos**, T. Efferth, H. Loutrari, A.L. Skaltsounis, I. K. Kostakis. Kinase 2016: Next Generation Inhibitors on Monday 16 – Tuesday 17 May 2016 at BioCity, Nottingham, UK.
286. (invited and honoured speaker) T. Mavromoustakos, The contribution of Differential Scanning Calorimetry in Medicinal Chemistry, Ioannina 17-19 May 2016.
287. (poster) A. Tsotinis, A.S. Foscolos, I. Papanastasiou, G.B. Foskolos, T. Kellici, **T. Mavromoustakos**, M.C. Taylor, J.M. Kelly. New hydrazones of 5-nitro-

furaldehyde with adamantane alkanohydrazides: synthesis, conformational analysis and *in vitro* trypanocidal activity. 33rd Camerino-Cyprus Symposium. Receptor Chemistry: Reality and Vision. Camerino May 15-19 2016.

288. G. Megariotis, **T. Mavromoustakos**, D.N. Theodorou, A Molecular Dynamics Study of Irbesartan in a Lipid Membran, 13th International Conference on Nanosciences & Nanotechnologies, Thessaloniki, 5.7.16 until 8.7.2016.

289. Design and Synthesis of Novel pyrimidinopyrimidines as VEGFR2/EGFR inhibitors. P. Konstantinos, T. Kellici, M. Michailidou, **T. Mavromoustakos**, T. Efferth, H. Loutrari, A.L. Skaltsounis, I. K. Kostakis. Kinase 2016: Next Generation Inhibitors on Monday 16 – Tuesday 17 May 2016 at BioCity, Nottingham, UK.

290. A.S. Foscolos, I. Papanastasiou, G. B. Foscolos., A. Tsotinis, T.F. Kellici, **T. Mavromoustakos**, M.C. Taylor and M.J. Kelly New Hydrazones of 5-nitro-2-furaldehyde with adamantane kanohydrazides: Synthesis and *in vitro* trypanocidal activity. 17th Hellenic Symposium on Medicinal Chemistry Thessaloniki, 1-3 June 2017.

291. Kritsi E., Matsoukas M. T., Potamitis C., Karageorgos V., Detsi A., Magafa V., Liapakis G., **Mavromoustakos T.**, Zoumpoulakis P. Exploring new scaffolds for angiotensin receptor antagonism. 17th Hellenic Symposium on Medicinal Chemistry Thessaloniki, 1-3 June 2017.

292. Tahsin F. K., Nisar S., Min-Sung L., Chatziathanasiadou, M.V., Vrettos, E.I., Tsailanis, A.D., Seung-Wook C., **Mavromoustakos, T.**, Tzakos, A.G. Rational Design and Structure-Activity Relationship Studies of Quercetin-Amino Acid hybrids targeting the anti-apoptotic protein BCL-XL. 17th Hellenic Symposium on Medicinal Chemistry Thessaloniki, 1-3 June 2017.

293. A. Konstantinidi, G. Mali, H. Wilfried Amenitsch, **T. Mavromoustakos**, A. Kolocouris. SSNMR, X-rays and Molecular Dynamics Study of the interactions between aminoadamantane ligands and their complexes with the influenza A M2TM in DMPC bilayers. 17th Hellenic Symposium on Medicinal Chemistry Thessaloniki, 1-3 June 2017.

294. A. Konstantinidi, Gregor Mali, Heinz Wilfried Amenitsch, **T. Mavromoustakos**, A. Kolocouris. Solid state NMR and Molecular Dynamics Study of the Interactions between Aminoadamantanes and their Complexes with the Influenza A M2TM in DMPC bilayers. Conference of Medicinal Chemistry, Thessaloniki 1-3 June 2017.

295. **T. Mavromoustakos** (invited speaker). The amelioration of the undesired property of lipophilicity. Drug Delivery. 5th International Bahçeşehir University (BAU) Drug Design Congress, Istanbul 19-21 October 2017.

296. S. Kiriakidi, D. Ntountaniotis, T. Kellici, J. Andreadelis, G. Liapakis, A. Kolocouris, **T. Mavromoustakos**. Candesartan cyclodextrin interactions. 5th International Bahçeşehir University (BAU) Drug Design Congress, Istanbul 19-21 October 2017 (poster and oral presentation by S. Kiriakidi).

297. S. Kiriakidi, E. Chontzopoulou, A. Kolocouris, **T. Mavromoustakos**. A computational approach in the drug binding mechanism of candesartan to AT1R Molecular Dynamics. Poster No4 page 200. EuroQsar 22, Thessaloniki 16-20 September 2018.
298. **T. Mavromoustakos**, D. Ntountaniotis, J. Andreadelis, T. Kellici, G. Valsami, E. Christodoulou, S. Durdagi, E. Stylos, M. Chatziathanasiadou, C. Chatzigiannis, J. Baldus, S. Kiriakidi, A. Kolocouris, A. Tzakos, G. Liapakis. Interactions between candesartan and its prodrug candesartan cilexetil in complex with HP- β -cyclodextrin (OP39) page 146. EuroQsar 22, Thessaloniki 16-20 September 2018.
299. A. Konstantinidi, N. Naziris, M. Chountoulesi, H. W. Amentisch, B. Sartori, G. Mali, D. Kolocouris, C. Demetzos, **T. Mavromoustakos**, A. Kolocouris. Application of a combined methodology including computational chemistry, biophysics and synthetic organic chemistry to optimize the structure of aminoadamantane drugs acting at influenza A/M2 protein Poster 332, EuroQsar 22, Thessaloniki 16-20 September 2018.
300. (invited speaker) **T. Mavromoustakos**, Interactions between candesartan and its prodrug candesartan cilexetil in complex with HP-beta-cyclodextrin. 11th Swedish-Hellenic Life Science Research Conference, 4 - 5 October 2018, Athens, Greece.
301. (invited speech) **T. Mavromoustakos**, Interactions of bioactive molecules with lipid bilayers using X-ray diffraction and complementary biophysical techniques, 5th HECRA, Patras, 5-8 October, 2018.
302. (invited speech) **T. Mavromoustakos**, DSC: A valuable tool to study drug:membrane interactions, Therma 2018, Athens, 12-13 October 2018.
303. D. Stamatis, E. Vrontaki, P. Lagarias, T. Mavromoustakos, A. Kolocouris. Structure-activity relationships of new selective adenosine receptor antagonists using molecular dynamics simulations. ACAC, Athens, Greece 30 October-2 November 2018.
304. E. Chontzopoulou, S. Kiriakidi, **T. Mavromoustakos**. Interactions between candesartan and its prodrug candesartan cilexetil in complex with HP- β -cyclodextrin. ACAC, Athens, Greece 30 October-2 November 2018.
305. S. Kiriakidi, E. Chontzopoulou, A. Kolocouris, **T. Mavromoustakos**. A computational approach in the drug binding mechanism of candesartan to AT1 receptor using Molecular Dynamics. ACAC, Athens, Greece 30 October-2 November 2018.
306. (invited speech) **T. Mavromoustakos**, I. Andreadelis. Nanotechnology and Drug Discovery. 6th International Bau Drug Design Congress, Istanbul, 13-15 December 2018.
307. (invited workshop) **T. Mavromoustakos**, Investigation of Bioactive Therapeutic Molecules Using NMR Spectroscopy. 6th International Bau Drug Design Congress, Istanbul, 13-15 December 2018.

308. M.K. Δασκαλοπούλου, Δ. Ματιάδης, Μ. Σαγνού, Μ. Πελεκάνου, **Θ. Μανρομούστακος**, Α. Παναγιωτοπούλου. Isolation, characterization and Quantitation of Curcuminoids: NMR studies in turmeric market products and pharmaceutical supplements. 12^ο Πανελλήνιο Συνέδριο Χημικής Μηχανικής, Αθήνα 29-31 Μαΐου 2019.
309. A. Papageorgiou, A.S. Foscolos, I. Papanastasiou, M. Vlachou, A. Siamidi, A. Vocat, S.T. Cole, T. Kellici, **T. Mavromoustakos**, A. Tsotinis. Synthesis, biology, computational studies and *in vitro* controlled release of new isoniazid-based adamantane derivatives. Medicinal Chemistry Frontiers June 10-13, Krakow, Poland.
310. **T. Mavromoustakos**, Molecular Interactions of Irbesartan complex with 2-hydroxypropyl- β -Cyclodextrine. CMTPI Ioannina, 23-27 June, 2019.
311. **T. Mavromoustakos**, I. Andreadelis, G. Leonis, D. Ntountaniotis, E. Christodoulou. Nanotechnology and Drug Delivery. 2nd International Conference, Burgas, Bulgaria 1-5th July 2019.
312. **T. Mavromoustakos** (invited speaker-plenary lecture). Drug Delivery Systems for Optimising the Therapeutic Index. 4th International Turkish Congress on Molecular Spectroscopy 05-09 August 2019.
313. **T. Mavromoustakos**, A. Syriopoulou and S. Kiriakidi (workshop). 2nd Summer Chaos School 10-13 September 2019, Friday September 13th.
314. **T. Mavromoustakos**, Basic principles of Computational Chemistry (speech). 2nd Summer Chaos School 10-13 September 2019, Friday September 13th.
315. **T. Mavromoustakos** (invited) Delivery Systems for Drug Optimization Properties. 3rd Global Conference of Cardiovascular Diseases-2019, Athens 15-16 November 2019.
316. **T. Mavromoustakos** (invited) Medicinal Chemist and Rational Drug Design 7th International Bau Drug Design Congress, Istanbul 18-21 December 2019.
317. **T. Mavromoustakos** (invited) Delivery Systems for Drug Optimization Properties. 3rd Global Conference of Cardiovascular Diseases-2019, Athens 15-16 November 2019.
318. **T. Mavromoustakos** (invited) Medicinal Chemist and Rational Drug Design 7th International Bau Drug Design Congress, Istanbul 18-21 December 2019.
319. (poster) N. Zoupanou, S. Chadjikakou, C. Banti, M.E Stathopoulou, S. Kyriakidi, Carlos Silva Lopez, **T. Mavromoustakos**. Poster entitled "Conformational characteristics decisive for their biological action of organotin metalloterapeutics". 1st International Workshop on Emerging and Disruptive next-GEneration Technologies for POC (EDGE-Tech) Lecce and online 26th - 31st October 2020, Italy.

320. A. Syriopoulou, E. Chontzopoulou, D. Diamantis, A.G. Tzakos, **T. Mavromoustakos**. In silico study of protein/ligand interactions aiming to design novel drugs, 1st International Workshop on Emerging and Disruptive next-Generation Technologies for POC (EDGE-Tech), 26th- 31st October 2020, Lecce, Italy.
321. **T. Mavromoustakos** (invited) Efforts to discover novel AT1 antagonists and drug delivery systems. 18th Hellenic Symposium in Medicinal Chemistry. 25-27, Athens, 2021.
322. C. Kotzatrati, M-Eleni Aggistrioti, K. Barbidi, S. G. Detos, **T. Mavromoustakos**. In Silico Molecular Docking on Spookier, A Halloween Enzyme Regulating the Ecdysteroidogenic Pathway in Insects. 18th Hellenic Symposium in Medicinal Chemistry. 25-27, Athens, 2021.
323. P. Mavroeidi, A. Syriopoulou, N. Georgiou, N. Tzouras, S. Neofotistos, G. Vougioukalakis, S. Durdagi, **T. Mavromoustakos**. Searching for targets against neurodegenerative diseases. 18th Hellenic Symposium in Medicinal Chemistry. 25-27, Athens, 2021.
324. (poster) N. Zoupanou, S. Chadjikakou, C. Banti, M.E Stathopoulou, S. Kyriakidi, Carlos Silva Lopez, **T. Mavromoustakos**. Poster entitled “Spectroscopic analysis and Molecular Modeling of organotin metallotherapeutics ”. 18th Hellenic Symposium on Medicinal Chemistry, Athens and online 25st -27th February 2021, Greece.
- 325.(poster presentation) S.Kiriakidi, C. Chatzigiannis, C. Papaemmanouil, A.G. Tzakos, Z. Cournia, **T. Mavromoustakos**, A cholesterol Concensus Motif on AT1R is revealed, 18th Panhellenic Symposium on Medicinal Chemistry, Athens, Greece, February 25-27 2021.
326. (poster) A. Syriopoulou, E. Chontzopoulou, D. Diamantis, A. G. Tzakos, T. Mavromoustakos, In silico study of protein/ligand interactions aiming to design novel drugs.", 18th Hellenic Symposium on Medicinal Chemistry, 25-27 February 2021.
327. E. Tsagkogiannis, A. Syriopoulou, A. Tzakos, T. Mavromoustakos, A.I. Koukou. Directed Evolution of 3,4-Dioxygenase of Protocatechuic Acid: Emergence of Alternative Substrate Specificity. 18th Hellenic Symposium in Medicinal Chemistry. 25-27, Athens, 2021.
328. (flash representation) P. Mavroeidi, A. Syriopoulou, N. Georgiou, N. Tzouras, S. Neofotistos, G. Vougioukalakis, S. Durdagi. T. Mavromoustakos. Searching for novel synthetic MAO inhibitors.
329. (flash representation) E. Tsagkogiannis, A. Syriopoulou, A. Tzakos, **T. Mavromoustakos**, Anna-Irini Koukou. Directed evolution of 3,4-dioxygenase of protocatechuic acid: Emergence of alternative substrate specificity. ACAC 2020, Athens, March 10-14 2021, Greece.

330. (flash representation) K. Manta, P. Papakyriakopoulou, M. Chountoulesi, D. A. Diamantis, D. Spaneas, V. Vakali, Nikolaos Naziris, M.V. Chatziathanasiadou, I. Andreadelis, K. Moschovou, I. Athanasiadou, P. Dallas, D. M. Rekkas, C. Demetzos, G. Colombo, U. Javornik, J. Plavec, **T. Mavromoustakos**, A.G. Tzakos, G. Valsami. Comparative study mparative NMR study of the complexation of Quercetin with two β -CD. ACAC 2020, Athens, March 10-14 2021, Greece.

331. (flash representation) N. Zoupanou, S. Chadjikakou, C. Banti, M.E Stathopoulou, S. Kyriakidi, C.S. Lopez and **T. Mavromoustakos**. Conformational characteristics decisive for their biological action of organotin metallotherapeutics. ACAC 2020, March 10-14 2021, Greece.

332. (flash representation) S. Kiriakidi, C. Chatzigiannis, C. Papaemmanouil, A. G. Tzakos, Z. Cournia and **T. Mavromoustakos**. Interplay of cholesterol, membrane bilayers and the AT1R: A cholesterol consensus motif on AT1R is revealed. ACAC 2020, Athens, March 10-14 2021, Greece.

333. (flash representation) E. Chontzopoulou, S. Kiriakidi, U. Javornik, J. Plavec, A. Tzakos, **T. Mavromoustakos**. Unveiling the molecular mechanism of action of the anti-hypertensive drug irbesartan through 2D NMR Spectroscopy. ACAC 2020, Athens, March 10-14 2021, Greece.

334. (flash representation). A. Gkionis, G. Skoufas, E. Chontzopoulou, N. Georgiou, N. Gouleni, **T. Mavromoustakos**, S. Vasiliou Conformational analysis of cinnamic compound NGI27 using a combination of 2D NMR Spectroscopy and Molecular Dynamics studies. ACAC 2020, Athens, March 10-14 2021, Greece.

335. (invited speech). T. Mavromoustakos. NMR and Rational Design. 17th Euromar 2021, July 5-8, Portoroz, Slovenia.

336. (poster) T. Mavromoustakos, E. Chontzopoulou, C. Papaemmanouil, M.V. Chatziathanasiadou, D. Kolokouris, S. Kyriakidis, A. Konstantinidi, I. Gerogianni, T. Tselios, I.K. Kostakis, E.D. Chrysina, D. Hadjipavlou-Litina, D. Tzeli, A.G. Tzakos, Combined NMR Spectroscopy and Computational Studies Reveal Novel Lox Inhibitor. 17th Euromar 2021, July 5-8, Portoroz, Slovenia.

337. (poster) T. Mavromoustakos, N. Zoupanou, S. Chadjikakou, C. Banti, M.E. Stathopoulou, S. Kyriakidi, C. Silva Lopez, Nuclear Magnetic Resonance and *ab initio* studies of organotin metallotherapeutics. 17th Euromar 2021, July 5-8, Portoroz, Slovenia.

- **CONTRIBUTION IN 20 MASTERS IN TEACHING OF CHEMISTRY AS SUPERVISOR AND MEMBER OF EXAMINATION COMMITTEE.**
- **ARTICLES OF GENERAL INTEREST**

Author of **120** 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) and theology.

Author of a Chemical Theology book on the Resurrections of Lazarus and Jesus Christ according to John Gospel