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### Short Presentation/Profile

Associate Professor Theodore Tselios was born in Messolonghi in Greece. He obtained his diploma (Chemistry) in 1994, PhD (Organic Chemistry) in 2001 and MSc (Medicinal Chemistry) in 2003 from the Department of Chemistry, University of Patras in Greece.

He has joined several times, as a visiting scientist, collaborating laboratories abroad such as Austin Research Institute, Melbourne in Australia, School of Chemistry, University of Cardiff in UK, Department of Chemistry and University of Florence in Italy etc.

He is a reviewer in peer review scientific journals (J. Med. Chem., Eur. J. Med. Chem., PLOS ONE, J. Comb. Chem., J. Mol. Graph. Model., Bioin. Chem. and Applic., Molecule, J. Comp. Aid. Mol. Des., J. Drug Del., Prot. Pept. Let.).

He is a member of the editorial board of: i) Journal of Molecular Graphics and Modelling - Elsevier, ii) Mini-Reviews in Medicinal Chemistry - Bentham Science.

He has been honoured by "Leonidas Zervas foundation" of Greece (1998) and he had a scholarship by the State Scholarship's Foundation of Greece, (2002-2003).

He has published seventy (70) research articles, fifty-two (52) the last ten years, in the field of rational drug design, synthesis and evaluation of bioactive molecules. He has twenty-two publications (22) as first or second author and twenty-eight (28) as corresponding author in several journals. Nine (9) research articles were published in "Journal of Medicinal Chemistry", one (1) in "Brain" and four (4) reviews in "Current Medicinal Chemistry". He has published nine (9) book chapters, forty-seven (47) abstracts in international conferences, seventy-three (73) international conference proceedings and ninety-five (95) national (Greek) conference abstracts. Moreover, figures of his research articles have been selected as cover pages in four (4) issues of "Current Medicinal Chemistry". He is a co-inventor of three (3) patents and an applicant in two (2) of them.

Assoc. Prof. T. Tselios' main research activities are in the fields of i) Organic, Peptide and Medicinal Chemistry, ii) Rational Drug Design iii) Structure Activity Relationship (SAR) Studies and iv) Conformational Analysis and Molecular Modelling studies of bioactive molecules.

Since 2004, Assoc. Prof. Theodore Tselios has supervised thirty-six (36) graduate students (PhD and MSc) and forty-two (42) diploma theses.

He has participated in the Organizing Committee of International Conferences (32<sup>nd</sup> European Peptide Symposium, 32<sup>nd</sup> and 29<sup>th</sup> Cyprus-Camerino-Noordwijkerhout: Trends in Drug Research Medicinal Chemistry EFMC Symposium, SEEDRUG project: NMR Applications in Life Sciences - Exploring Peptides & Proteins).

Since 2004, he has joined the faculty of the Chemistry Department of the University of Patras as Lecturer (2004-2009), Assistant Professor (2009-2015) and Associate Professor (2015-today).

## Research Activities

- Organic, Peptide and Medicinal Chemistry: Rational design and synthesis of linear, cyclic peptide analogues and non-peptide mimetics.
- Conformational studies and Molecular Modelling of bioactive and pharmaceutical compounds. Interactions of bioactive molecules (docking studies). Pharmacophore analysis. Homology Modelling.

## Teaching Experience

### ***I) Undergraduate teaching***

*Lectures:*

- a) "Organic Chemistry III" - Department of Chemistry (until 2011)
- b) "Organic Chemistry" - Department of Chemical Engineering (until 2011).
- c) "Organic Chemistry of Functional Groups I" - Department of Chemistry.
- d) "Organic Chemistry of Functional Groups II" - Department of Chemistry.
- e) "Experimental Organic Chemistry I" (Theory) - Department of Chemistry.
- f) "Experimental Organic Chemistry II" (Theory) - Department of Chemistry.

*Laboratories:*

- a) Experimental Organic Chemistry I - Department of Chemistry.
- b) Experimental Organic Chemistry II - Department of Chemistry.

### ***II) Graduate teaching***

*Lectures:*

- a) "NMR Spectroscopy and Molecular Design" - Interdepartmental Master Degree Program "Medicinal Chemistry: Drug Discovery and Design", Departments of Chemistry, Pharmacy & Medicine (until 2018).
- b) "Synthetic Inorganic, Organic & Organometallic Chemistry" (Heterocyclic Chemistry) - Master Degree Program "Synthetic Chemistry & Advanced Polymeric & Nanostructured Materials", Department of Chemistry (until 2018).
- c) "Structural and Computational Medicinal Chemistry" - Interdepartmental Master Degree Program "Medicinal Chemistry and Chemical Biology", Departments of Chemistry & Medicine.

*Laboratory:*

"Laboratory of Medicinal Chemistry" (Synthetic Chemistry & Molecular Design) - Interdepartmental Master Degree Program "Medicinal Chemistry: Drug Discovery and Design", Departments of Chemistry, Pharmacy & Medicine (until 2018).

## Funded Programs

**2007-2010:** 24.000,00 €. K. Karatheodoris Program, University of Patras. Scientific Supervisor: Assist. Prof. T. Tselios. Project title: "Design, Synthesis and Molecular Modeling of Cyclic GnRH analogues for the Treatment of Cancer".

**2011-2015:** 3.000.000,00 €. Greek General Secretariat of Research and Technology. Cooperation Program. Scientific Supervisor: Prof. J. Matsoukas; Collaborator, Scientific Supervisor the last three months and responsible for the last evaluation of the program: Assoc. Prof. T. Tselios. Project title: “Pre-clinical and Toxicology Evaluation of Immunodominant Myelin Peptides/Mimetics Conjugated with Mannan towards Clinical Phase I-II Studies: A Potential Therapeutic Vaccine Drug in the Treatment of Multiple Sclerosis (MS)”.

**2011-2015:** 3.200.000,00 €. Seventh Framework Programme. Research Potential. Call Identifier FP7-REGPOT-2011-1. Scientific Supervisor: Assoc. Prof. G. Spyroulias; Collaborator: Assist. Prof. T. Tselios. Project title: “Establishment of a centre of excellence for structure-based drug target characterization: Strengthening the research capacity of south-eastern Europe”

**2012-2014:** 150.000,00 € 4New B2012, Greek General Secretariat of Research and Technology, EYΔE – ETAK. Coordinator: Eldrug SA, Subcontractor: Department of Chemistry, University of Patras (22.500,00 €); Scientific Supervisor of subcontracting: Assist. Prof. T. Tselios. Project Title: “Synthesis and pre-clinical evaluation of bioactive BV6 compound”.

**2014-2015:** 480.500,00 €. Greece-Israel cooperation program, Greek General Secretariat of Research and Technology. Scientific Supervisor: Assoc. Prof. T. Tselios. Project Title: “A novel combined approach for the Immunotherapy of Multiple Sclerosis”.

**2018-2021:** 834.800,71 € (total); 150.000,00 € (Department of Chemistry, University of Patras) Greek General Secretariat of Research and Technology. Scientific Supervisor for Department of Chemistry, University of Patras: Assoc. Prof. T. Tselios. Project Title: “Development of an advanced humanized mouse model for multiple sclerosis: application for pre-clinical studies and drug testing”.

## Awards

- Award from the Leonidas Zervas foundation, Athens, Greece, 1998.
- Scholarship by the State Scholarship's Foundation of Greece, 2002-2003

## Patents

- J. Matsoukas, **T. Tselios**, V. Apostolopoulos. “Peptide analogues of Myelin Basic Protein epitopes in the treatment of Experimental Autoimmune Encephalomyelitis (EAE) and Multiple Sclerosis (MS)”. GPO AGIK 38/17, CO7K 14/47, 09/05/2002/USA.
- J. Matsoukas, **T. Tselios** et al. “Peptide Analogues and Conjugates Thereof”: PCT/IB2008/003493, WO 2009/066175, (28.05.2009), European No. 08851987.1 / 1402/2227486 (Granted). Short Description: “MBP analogues conjugated with mannan using KLH bridge”.
- **T. Tselios** et al. “Immunotherapy of Multiple Sclerosis Using Mannosylated Peptides as Therapeutic Vaccines”: PCT/IB2009/000382, WO 2009/093143 (30.07.2009). Greece (OBI) No. 1006998/30.09.2010 (Granted). European No. 09703874.9 / 1412/2240200 (Granted); Short Description: “MBP analogues conjugated with mannan via KGn bridge”. Divisional No. 14156495.5 (Granted); Short Description: “MOG analogues conjugated with mannan via KGn bridge”. Australia No. 2009207345 (Granted); Short Description: “MOG analogues conjugated with mannan via KGn bridge”. Divisional No. 2014200921 (Granted);

Short Description: "MBP analogues conjugated with mannan via KGn bridge". USA No. 12/864,019 (Granted); Short Title: "Conjugates comprising mannan and myelin oligodendrocyte glycoprotein (MOG)"; Short Description: "MOG analogues conjugated with mannan via KGn bridge". Divisional: No. 14/877,679 (Granted); Short Title: "Conjugates comprising mannan and myelin basic protein (MBP)"; Short Description: "MBP analogues conjugated with mannan via KGn bridge".

### **Publications in Peer Reviewed Journals (70) [Impact Factor 2016]**

- 1. T. Tselios**, L. Probert, G. Kollias, E. Matsoukas, P. Roumelioti, K. Alexopoulos, G. Moore, J. Matsoukas\*. Design and synthesis of small semi-mimetic peptides with Immunomodulatory activity based on Myelin Basic Protein (MBP). *Amino Acids*, **1998**, 14: 333-341. [IF: 3.173]
- 2.** K. 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*, **1998**, 15: 211-220. [IF: 3.173]
- 3.** J. Pires, **T. Tselios**, J. Matsoukas, G. Moore\*. Role of Myelin Basic Protein Epitope MBP<sub>74-85</sub> in Experimental Autoimmune Encephalomyelitis: Elaboration of Agonist and Antagonist Motifs. *Drug Development Research*, **1999**, 48: 1-5. [IF: 1.909]
- 4. T. Tselios**, L. Probert, I. Daliani, E. Matsoukas, A. Troganis, I. Gerothanasis, T. Mavromoustakos, G. Moore, J. Matsoukas\*. Design and Synthesis of a Potent Cyclic Analogue of the Myelin Basic Protein Epitope MBP<sub>72-85</sub>: Importance of the Ala<sup>81</sup> Carboxyl Group and of a Cyclic Conformation for Induction of Experimental Allergic Encephalomyelitis (E.A.E.). *J. Med. Chem.*, **1999**, 42, 7:1170-1177. [IF: 6.259]
- 5.** P. Roumelioti, **T. Tselios**, K. Alexopoulos, T. Mavromoustakos, A. Kolocouris, G. Moore, J. Matsoukas\*. Structural Comparison Between Type I and type II Antagonists: Possible Implications in the Drug Design of AT1 Antagonists. *Bioorg. Med. Chem. Lett.*, **2000**, 10: 1-4. [IF: 2.454]
- 6. T. Tselios**, I. Daliani, L. Probert, S. Deraos, E. Matsoukas, S. Roy, J. Pires, G. Moore, J. Matsoukas\*. Treatment of Experimental Allergic Encephalomyelitis (EAE) Induced by Guinea Pig Myelin Basic Protein Epitope 72-85 with a Human MBP<sub>87-99</sub> Analogue and Effects of Cyclic Peptides. *Bioorg. Med. Chem.*, **2000**, 8: 1903-1909. [IF: 2.93]
- 7. T. Tselios**, I. Daliani, S. Deraos, S. Thymianou, E. Matsoukas, A. Troganis, I. Gerothanassis, 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.*, **2000**, 10: 2713-2717. [IF: 2.454]
- 8. T. Tselios**, V. Apostolopoulos, I. Daliani, S. Deraos, S. Grdadolnik, T. Mavromoustakos, M. Melachrinou, S. Thymianou, L. Probert, A. Mouzaki, J. Matsoukas\*. Antagonistic Effects of Human Cyclic MBP<sub>87-99</sub> Altered Peptide Ligands in Experimental Allergic Encephalomyelitis and Human T-Cell Proliferation. *J. Med. Chem.*, **2002**, 45, 275-283. [IF: 6.259]
- 9.** A.G. Tzakos, P. Fuchs, N.A. van Nuland, A. Troganis, **T. Tselios**, S. Deraos, J. Matsoukas, I.P. Gerothanassis\*, A.M. Bonvin. NMR and molecular dynamics studies of an autoimmune myelin basic protein peptide and its antagonist: structural implications for the MHC II (I-Au)-peptide complex from docking calculations. *Eur. J. Biochem. (FEBS)*, **2004**, 271(16): 3399-3413. [IF: 3.902]
- 10.** A. Mouzaki\*, **T. Tselios**, P. Papathanassopoulos, I. Matsoukas, K. Chatzantoni.

Immunotherapy for Multiple Sclerosis: Basic insights for new clinical strategies. *Current Neurovascular Research*, **2004**, 1(4): 325-340. [IF: 2.298]

**11.** J. Matsoukas\*, V. Apostolopoulos, H. Kalbacher, A.M. Papini, **T. Tselios**, K. Chatzantoni, T. Biagioli, F. Lolli, S. Deraos, P. Papatthanassopoulos, A. Troganis, E. Mantzourani, T. Mavromoustakos, A. Mouzaki\*. Design and synthesis of a novel potent myelin basic protein epitope 87-99 cyclic analogue: enhanced stability and biological properties of mimics render them a potentially new class of immunomodulators. *J. Med. Chem.*, **2005**, 10, 48(5):1470-1480. [IF: 6.259]

**12.** A. Tzakos, P. Kursula, V. Theodorou, **T. Tselios**, C. Svarnas, J. Matsoukas, A. Troganis, V. Apostolopoulos, I. Gerotheranassis\*. Structure and Function of the Myelin Proteins: Current Status and Perspectives in Relation to Multiple Sclerosis. *Cur. Med. Chem.*, **2005**, 12, 13, 1569-1587. [IF: 3.249]

**13.** N. Grigoriadis\*, **T. Tselios**, S. Deraos, A. Orologas, G. Deraos, J. Matsoukas, I. Mavromatis, I. Milonas. Animal models of central nervous system immune-mediated diseases: Therapeutic interventions with Bioactive Peptides and Mimetics. *Cur. Med. Chem.*, **2005**, 12, 13, 1513-1519. [IF: 3.249]

**14.** E.D. Mantzourani, 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 in Immune Regulation. *Cur. Med. Chem.*, **2005**, 12, 13, 1569-1587. [IF: 3.249]

**15.** **T.V. Tselios**, F.N. Lamari, I. Karathanasopoulou, M. Katsara, V. Apostolopoulos, G.A. Pietersz, J.M. Matsoukas, N.K. Karamanos\*. Synthesis and study of the electrophoretic behavior of mannan conjugates with cyclic peptide analogue of myelin basic protein using lysine-glycine linker. *Anal. Biochem.*, **2005**, 1, 347(1):121-128. [IF: 2.334]

**16.** M.K. Keramida\*, **T. Tselios**, E. Mantzourani, K. Papazisis, T. Mavromoustakos, C. Klaussen, G. Agelis, S. Deraos, I. Friligou, H. Habibi, J. Matsoukas\*. Design, synthesis, and molecular modeling of a novel amide-linked cyclic GnRH analogue cyclo(4-9)[Lys4,D-Trp6,Glu9]GnRH: stimulation of gonadotropin gene expression. *J. Med. Chem.*, **2006**, 49(1): 105-110. [IF: 6.259]

**17.** M. Katsara, **T. Tselios**, S. Deraos, G. Deraos, J. Matsoukas, V. Apostolopoulos\*. Round and round we go: cyclic peptides in disease. *Cur. Med. Chem.*, **2006**, 13(19): 2221-2232. [IF: 3.249]

**18.** E. Mantzourani, **T. Tselios**, S. Golič Grdadolnik, A. Brancale, J. Matsoukas, T. Mavromoustakos\*. A putative bioactive conformation for the altered peptide ligand of myelin basic protein and inhibitor of experimental autoimmune encephalomyelitis [Arg<sup>91</sup>, Ala<sup>96</sup>]MBP<sub>87-99</sub>. *J. Mol. Graph. Model.*, **2006**, 25/1, 17-29. [IF: 1.754]

**19.** E.D. Mantzourani, **T.V. Tselios\***, S. Golič Grdadolnik; J.A. Platts, A. Brancale, G. Deraos, J.M. Matsoukas, T.M. Mavromoustakos\*. Comparison of Proposed Putative Active Conformations of Linear Altered Peptide Ligands of Myelin Basic Protein Epitope 87-99 by Spectroscopic and Modelling studies: The Role of Position 91 and 96 in T-cell Receptor Activation. *J. Med. Chem.*, **2006**, 49, 6683-6691. [IF: 6.259]

**20.** E.D. Mantzourani, J.A. Platts, A. Brancale, T.M. Mavromoustakos, **T.V. Tselios\***. 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. Model.*, **2007**, 26(2): 471-481. [IF: 1.754]

21. Z. Spyrinti, G.A. Dalkas, G.A. Spyroulias\*, E.D. Mantzourani, T. Mavromoustakos, I. Friligou, J.M. Matsoukas, **Tselios TV\***. Putative Bioactive Conformations of Amide Linked Cyclic Myelin Basic Protein Peptide Analogues Associated with Experimental Autoimmune Encephalomyelitis. *J. Med. Chem.*, **2007**, 29, 50(24):6039-6047. [IF: 6.259]
22. **T. Tselios\***, K. Kelaidonis, A. Resvani, K. Prousalis, J. Matsoukas, T. Tsegenidis\*. Solid Phase Synthesis of a Glycopeptide analogue using the acid sensitive 4-Methoxybenzhydryl bromide resin. *Protein & Peptide Letters*, **2008**, 15(1):1-5. [IF: 0.964]
23. G. Agelis, N. Tzioumaki, **T. Tselios**, T. Botić, A. Cencic, D. Komiotis\*. Synthesis and molecular modelling of unsaturated exomethylene pyranonucleoside analogues with antitumor and antiviral activities. *Eur. J. Med. Chem.*, **2008**, 43(7): 1366-1375. [IF: 4.519]
24. E.D. Mantzourani, K. Blokar, **T.V. Tselios**, J.M. Matsoukas, J.A. Platts, T.M. Mavromoustakos, S.G. Grdadolnik\*. A combined NMR and molecular dynamics simulation study to determine the conformational properties of agonists and antagonists against experimental autoimmune encephalomyelitis. *Bioorg. Med. Chem.*, **2008**, 1, 16(5): 2171-2182. [IF: 2.93]
25. Z.D. Sofianos, T. Katsila, N. Kostomitsopoulos, V. Balafas, J. Matsoukas, **T. Tselios**, C. Tamvakopoulos\*. In vivo evaluation and in vitro metabolism of leuprolide in mice-mass spectrometry-based biomarker measurement for efficacy and toxicity. *J. Mass. Spectrom.*, **2008**, 43(10): 1381-1392. [IF: 2.422]
26. M. Katsara, E. Yuriev, P.A. Ramsland, G. Deraos, **T. Tselios**, J. Matsoukas, V. Apostolopoulos\*. Mannosylation of mutated MBP83-99 peptides diverts immune responses from Th1 to Th2. *Mol. Immunol.*, **2008**, 45(13): 3661-3670. [IF: 3.236]
27. M. Katsara, G. Deraos, **T. Tselios**, J. Matsoukas, V. Apostolopoulos\*. Design of novel cyclic altered peptide ligands of myelin basic protein MBP83-99 that modulate immune responses in SJL/J mice. *J. Med. Chem.*, **2008**, 10, 51(13): 3971-3978. [IF: 6.259]
28. M. Katsara, E. Yuriev, P.A. Ramsland, G. Deraos, **T. Tselios**, J. Matsoukas, V. Apostolopoulos\*. A double mutation of MBP(83-99) peptide induces IL-4 responses and antagonizes IFN-gamma responses. *J. Neuroimmunol.*, **2008**, 30, 200(1-2): 77-89. [IF: 3.236]
29. E. Mantzourani, D. Laimou, M.T. Matsoukas, **T. Tselios\***. Peptides as therapeutic agents or drug leads for autoimmune, hormone dependent and cardiovascular diseases. *Anti-Inflammatory & Anti-Allergy Agents in Medicinal Chemistry*, **2008**, 7, 294-306.
30. K. Gkountelias, **T. Tselios**, M. Venihaki, G. Deraos, I. Lazaridis, O. Rassouli, A. Gravanis, G. Liapakis\*. Alanine scanning mutagenesis of the second extracellular loop of type 1 corticotropin-releasing factor receptor revealed residues critical for peptide binding. *Mol. Pharmacol.*, **2009**, 75(4): 793-800. [IF: 3.911]
31. M. Katsara, G. Deraos, **T. Tselios**, M.T. Matsoukas, I. Friligou, J. Matsoukas, V. Apostolopoulos\*. Design and synthesis of a cyclic double mutant peptide (cyclo(87-99)[A91,A96]MBP87-99) induces altered responses in mice after conjugation to mannan: implications in the immunotherapy of multiple sclerosis. *J. Med. Chem.*, **2009**, 8, 52(1): 214-218. [IF: 6.259]
32. G. Deraos, K. Chatzantoni, M.T. Matsoukas, **T. Tselios**, S. Deraos, M. Katsara, P. Papathanasopoulos, D. Vynios, V. Apostolopoulos\*, A. Mouzaki\*, J. Matsoukas\*. Citrullination of linear and cyclic altered peptide ligands from myelin basic protein

(MBP(87-99)) epitope elicits a Th1 polarized response by T cells isolated from multiple sclerosis patients: implications in triggering disease. *J. Med. Chem.*, **2008**, 25, 51(24): 7834-7842. [IF: 6.259]

**33.** Z. Spyralanti, **T. Tselios**, G. Deraos, J. Matsoukas, G.A. Spyroulias\*. NMR structural elucidation of myelin basic protein epitope 83-99 implicated in multiple sclerosis. *Amino Acids*, **2010**, (38)3: 926-936. [IF: 3.173]

**34.** M. Katsara, E. Yuriev, P.A. Ramsland, **T. Tselios**, G. Deraos, A. Lourbopoulos, N. Grigoriadis, J. Matsoukas, V. Apostolopoulos\*. Altered peptide ligands of myelin basic protein (MBP87-99) conjugated to reduced mannan modulate immune responses in mice. *Immunology*, **2009**, 128, 521-533. [IF: 3.701]

**35.** M. Emmanouil, E. Taoufik, V. Tseveleki, S.S. Vamvakas, **T. Tselios**, M. Karin, H. Lassmann, L. Probert\*. Neuronal I $\kappa$ B kinase  $\beta$  protects mice from autoimmune encephalomyelitis by mediating neuroprotective and immunosuppressive effects in the CNS. *Journal of Immunology*, **2009**, 15, 183(12): 7877-7889. [IF: 4.856]

**36.** D.K. Laimou, M. Katsara, M.T. Matsoukas, V. Apostolopoulos, A.N. Troganis, **T.V. Tselios\***. Structural elucidation of Leuprolide and its analogues in solution: insight into their bioactive conformation. *Amino Acids*, **2010**, 39(5): 1147-1160. [IF: 3.173]

**37.** I. Friligou, E. Papadimitriou, D. Gatos, J. Matsoukas, **T. Tselios\***. Microwave-Assisted Solid-Phase Peptide Synthesis of the 60-110 Domain of Human Pleiotrophin (hPTN) on 2-Chlorotriptyl Resin. *Amino Acids*, **2011**, 40(5): 1431-1440. [IF: 3.173]

**38.** A. Aggelis, A. Resvani, M-T. Matsoukas, **T. Tselios**, K. Kelaidonis, D. Kalavrizioti, D. Vlahakos, J. Matsoukas\*. Towards non-peptide ANG II AT1 receptor antagonists based on urocanic acid: rational design, synthesis and biological evaluation. *Amino Acids*, **2011**, 40(2): 411-420. [IF: 3.173]

**39.** T. Katsila, E. Balafas, G. Liapakis, P. Limonta, M. Montagnani Marelli, K. Gkountelias, **T. Tselios**, N. Kostomitsopoulos, J. Matsoukas, C. Tamvakopoulos\*. Evaluation of a stable gonadotropin-releasing hormone analog in mice for the treatment of endocrine disorders and prostate cancer. *J. Pharmacol. Exp. Ther.*, **2011**, 336(3): 613-623. [IF: 3.867]

**40.** M-T. Matsoukas, P. Zoumpoulakis, **T. Tselios\***. Conformational analysis of aliskiren, a potent renin inhibitor, using high-resolution nuclear magnetic resonance and molecular dynamics simulations. *J. Chem. Inf. Model.*, **2011**, 26, 51(9): 2386-2397. [IF: 3.76]

**41.** C. Potamitis, M.T. Matsoukas, **T. Tselios\***, T. Mavromoustakos\*, S. Golič Grdadolnik\*. Conformational analysis of the MBP(83-99) (Phe (91)) and MBP (83-99) (Tyr (91)) peptide analogues and study of their interactions with the HLA-DR2 and human TCR receptors by using Molecular Dynamics. *J. Comput. Aided Mol. Des.*, **2011**, 25(9): 837-853. [IF: 3.028]

**42.** E. Taoufik, V. Tseveleki, S.Y. Chu, **T. Tselios**, M. Karin, H. Lassmann, D.E. Szymkowski, L. Probert\*. Transmembrane tumour necrosis factor is neuroprotective and regulates experimental autoimmune encephalomyelitis via neuronal nuclear factor-kappaB. *Brain*, **2011**, 134(9): 2722-2735. [IF: 10.292]

**43.** D. Laimou, E. Lazoura, A.N. Troganis, M-T. Matsoukas, S.N. Deraos, M. Katsara, J. Matsoukas, V. Apostolopoulos, **T.V. Tselios\***. Conformational studies of immunodominant myelin basic protein 1-11 analogues using NMR and molecular modelling. *J. Comput. Aided Mol. Des.*, **2011**, 25(11): 1019-1032. [IF: 3.028]

44. D. Laimou, T. Katsila, J. Matsoukas, A. Schally, K. Gkountelias, G. Liapakis, C. Tamvakopoulos, **T. Tselios\***. Rationally designed cyclic analogues of luteinizing hormone-releasing hormone: enhanced enzymatic stability and biological properties. *Eur. J. Med. Chem.*, **2012**, 58: 237-247. [IF: 4.519]
45. M.T. Matsoukas, A. Cordoní, S. Ríos, L. Pardo, **T. Tselios\***. Ligand binding determinants for angiotensin II type 1 receptor from computer simulations. *J. Chem. Inf. Model.*, **2013**, 25, 53(11): 2874-2883. [IF: 3.76]
46. I. Friligou, F. Rizzolo, F. Nuti, **T. Tselios\***, M. Evangelidou, M. Emmanouil, M. Karamita, J. Matsoukas, M. Chelli, P. Rovero, A.M. Papini\*. Divergent and convergent synthesis of polymannosylated dibranched antigenic peptide of the immunodominant epitope MBP(83-99). *Bioorg. Med. Chem.*, **2013**, 1, 21(21): 6718-6725. [IF: 2.93]
47. G. Agelis\*, K. Kelaidonis, A. Resvani, D. Kalavrizioti, M.E. Androutsou, P. Plotas, D. Vlahakos, C. Koukoulitsa, **T. Tselios**, 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*, **2013**, 27, 18(7): 7510-7532. [IF: 2.861]
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