

CURRICULUM VITAE

Minos-Timotheos Matsoukas, MSc, PhD

October 2022

PERSONAL DETAILS

Name: **Minos-Timotheos**
 Surname: **Matsoukas**
 Address: **Giasemion 58, Chalandri, 15233, Greece**
 E-mail: **mmatsoukas@uniwa.gr**
 Date of birth: **13th March, 1981**
 Nationality: **Greek**
 Marital status: **Married**

EDUCATION

Sep 2006 – Mar 2012 **PhD in Medicinal Chemistry** “*Structure Activity Relationship Study of Antihypertensive Agents through Molecular Modelling and NMR*”
 Faculty of Organic Chemistry, Biochemistry and Natural Products,
 Department of Chemistry, University of Patras, Greece
 Oct 2004 – Feb 2006 **Master’s degree in Medicinal Chemistry**
 Departments of Chemistry and Pharmacy, University of Patras, Greece
 Oct 1999 – Sep 2004 **BSc (Hons) in Chemistry**
 Department of Chemistry, University of Patras, Greece

LANGUAGES

1. **Greek** - Native
2. **English** - Exceptional
3. **Spanish** - Basic

POSITIONS

March 2022 – current **Assistant Professor of Computational Chemistry** (coddia@uniwa.gr)
 Department of Biomedical Engineering, University of West Attica, Athens, Greece
 May 2016 - current **Co-founder**
 CloudPharm P.C.
 Cloud-Based Drug Design and Pharmaceutical Research
 Athens, Greece
 Jan 2021 – Feb 2022 **Post-Doctoral Researcher**
 Faculty of Computational Medicine, Medicine Department, Autonomous University of Barcelona, Spain
 Jan 2015 – Sept 2021 **Post-Doctoral Researcher**
 Department of Pharmacy, University of Patras, Greece
 Apr 2012 – Oct 2014 **Post-Doctoral Researcher**
 Faculty of Computational Medicine, Medicine Department, Autonomous University of Barcelona, Spain
 Jul 2006 – Jul 2013 **Administrative Research Associate**

ELDRUG S.A., Drug Research and Development, Patras Science Park,
Greece

PERSONAL FUNDING

- **IKY-SIEMENS, personal grant** for post-doctoral research, **2019-2021**, “*Allosteric targeting, molecular basis of activation and structural studies of the type 1 receptor for corticotropin releasing factor (CRF1R)*”
- **HPC-Europa Short-Term Fellowship** (3 months), for the proposal “*Investigation of GLP-1R dynamics to identify and target hidden allosteric sites for receptor modulation*” Autonomous University of Barcelona, **2019**.
- **EMBO Short-Term Fellowship** (2 months), for the proposal “*Structure Determination of the GHRHR Extracellular Binding Domain in complex with novel non-peptide ligands*” to work at National Cancer Institute, Amsterdam, with Dr. A. Perrakis, **2017**.
- **IKY-SIEMENS, personal grant** for post-doctoral research, **2016-2017**, “*In silico targeting and structural studies of the glucagon like peptide 1 receptor (GLP-1R) towards active compounds against diabetes*”
- **IKY-SIEMENS, personal grant** for post-doctoral research, **2015-2016**, “*Structural elucidation of the extracellular domain of the growth hormone releasing hormone receptor (GHRHR) through molecular modeling and NMR and drug design*”
- **SANTANDER BANK - AUTONOMOUS UNIVERSITY BARCELONA**. 24-month **fellowship** for post-doctoral research, **2013-2014**, *New approaches for G-protein coupled receptor (GPCR) modulation*

AWARDS - DISTINCTIONS

- **Best poster award**, GLISTEN GPCR SYMPOSIUM, **2017, Porto, Portugal**. *The Size Matters: Computational Design and Analysis of GPCR Bivalent Ligands*. Pérez-Benito L, Henry A, **Matsoukas M-T**, Cordoní A, Tresadern G, Pardo L.
- **1st scored scholarship nationwide** (94/100) amongst 100 granted fellowships for post-doctoral research from Greek State Scholarships Foundation, year **2017**, for the proposal “*In silico targeting and structural studies of the glucagon like peptide 1 receptor (GLP-1R) towards active compounds against diabetes*”
- European Commission **Seal of Excellence** for the **Marie Skłodowska-Curie Actions 2016** proposal “*Structural Determination of the GHRH Extracellular Binding Domain and Dual Targeting for Novel Anti-cancer Compounds*”.
- **Best oral presentation award**, Hellenic Bioinformatics Symposium, Bioinformatics as a growth engine for Greece, **2016, Thessaloniki, Greece**. *A multi-pharmacophore virtual screening methodology and the discovery of novel compounds targeting pharmacological targets*.
- Greek State Scholarships Foundation: Distinction and money prize for 1st entree position in the

Chemistry Department, **1998**, Department of Chemistry, University of Patras, Greece.

GRANT COORDINATION

- EPAnEK 2014-2020, Competitiveness, Entrepreneurship & Innovation. “CloudScreen, A one stop shop integrated platform for drug repositioning”, **Jan 2020 –**, Cloudpharm PC, **Coordinator**. (budget 0.5M)
- European Regional Development Fund (NSRF), GREECE-EU co-funded grant “Synthesis and Preclinical evaluation of an active substance, BV6, towards approval of clinical trials”, **Jan 2012 – Dec 2013**, Eldrug SA, **Scientific Coordinator**. (budget 0.3M)

GRANT PARTICIPATION

- ΕΠΑΝΕΚ 2014-2020. Competitiveness, Entrepreneurship & Innovation “CloudScreen: A one-stop-shop computational platform for drug repurposing”, **Researcher**, **1/10/2020 - 28/2/2022**.
- ΕΠΑΝΕΚ 2014-2020. Competitiveness, Entrepreneurship & Innovation “NextGFS”, **Researcher**, **1/6/2020 - 31/9/2020**.
- INSPIRED - The National Research Infrastructures on Integrated Structural Biology, Drug Screening Efforts and Drug Target Functional Characterization MIS 5002550, **Researcher**, **1/8/2019 - 31/12/2019**.
- Partnership Agreement (PA) 2014-2020, “Novel functional activators of soluble guanylate cyclase (sGC)”, **May 2018 – July 2019**, University of Patras, **Researcher**.
- EU FP7, RD-CONNECT, “An integrated platform connecting registries, biobanks and clinical bioinformatics for rare disease research”, **Sep 2016 – Feb 2017**, University of Patras, **Researcher**.
- European Regional Development Fund (NSRF), GREECE-EU co-funded grant “Pre-clinical and toxicologic evaluation of peptide mimetics, analogues of myelin conjugated immunodominant epitopes towards clinical trials”, **Jan 2011 – Dec 2013**, Eldrug SA, **Legal representative** and **Scientific associate**.
- Operational Programme Competitiveness (OPCE II), GREECE-EU co-funded grant “Research and Development of sartans towards pre-clinical studies on hypertension and cardiovascular diseases”, **Mar 2007 – Oct 2008**, Eldrug SA, **Legal representative** and **Scientific associate**.
- General Secretariat for Research and Technology (GSRT), “Design, synthesis and biological evaluation of Myelin Basic protein analogues against Multiple Sclerosis”, **Jan 2006 – Dec 2008**, University of Patras, **Researcher**.
- General Secretariat for Research and Technology (GSRT), “Design of dual action antagonists against hypertension”, **Jan 2005 – Dec 2005**, University of Patras, **Researcher**.

TEACHING EXPERIENCE

Post-graduate courses

- **2017-2020:** Master's Degree – Informatics for Life Sciences, University of Patras, Greece, (<https://goo.gl/tUHgtj>) "*Biomolecular Simulations*" (invited lectures)
- **2016-2018:** Master's Degree – Translational Research in Molecular Biology and Genetics, Department of Molecular Biology & Genetics of Democritus University of Thrace, (<https://goo.gl/gd2Nta>) "*Computational methods in the identification of bioactive molecules*" (invited lectures)
- **2012-2014:** Official Master's Degree in Bioinformatics, Autonomous University of Barcelona, Spain, (<https://goo.gl/a6NJBX>), *Computational methods in Drug Discovery* (theory and practice)

Undergraduate Courses

- **2022-2023:** Department of Biomedical Engineering, University of West Attica, *Undergraduate course "Inorganic and Analytical Chemistry"* (theory)
- **2022-2023:** Department of Biomedical Engineering, University of West Attica, *Undergraduate course "Pharmaceutical Mechanics"* (theory)
- **2021-2022:** Department of Biomedical Engineering, University of West Attica, *Undergraduate course "Biochemistry"* (theory)
- **2021-2022:** Department of Biomedical Engineering, University of West Attica, *Undergraduate course "Organic Chemistry"* (theory)
- **2017-2020:** Department of Pharmacy, University of Patras, Greece, *Undergraduate course "Molecular simulation: Bioinorganic Chemistry"* (theory and practice)
- **2005-2006:** Department of Chemistry, University of Patras, Greece, *Undergraduate course "Organic Chemistry II"* (laboratory assistance)

INVITED SEMINARS

1. **iNext** Workshop: Bridging Solution Methods: From NMR to X-ray Scattering and Biophysics, Dept of Pharmacy, University of Patras, **2017, Patras, Greece**. *Structure-Based Drug Design*.
2. Workshop in **Targeted Drug Discovery**, National Hellenic Research Foundation, **2016, Athens, Greece**. *Pharmacophore modeling and virtual Screening in Drug Discovery*.
3. **2016 Golden Helix Summer School, Syros, Greece**. *In silico drug design methods*.

ORAL PRESENTATIONS

1. 4th Annual User Meeting of iNEXT, **2019, Lund, Sweden**. Conformational state sampling and dual targeting of the GHRHR, a class B GPCR. **Invited Speaker**
2. 69th Panhellenic Conference of the Hellenic Society for Biochemistry and Molecular Biology, **2018, Larisa, Greece**. *Conformational sampling and dual targeting of the GHRHR*.

3. 2nd Synthetic & Medicinal Chemistry Symposium, **2018, Patras, Greece**. *A virtual screening methodology for the discovery of novel compounds*. **Invited Speaker**
4. Hellenic Symposium on Medicinal Chemistry, **2017, Thessaloniki, Greece**. *An in silico multi-pharmacophore virtual screening methodology for the discovery of novel compounds against pharmacological targets*. **Invited Speaker**
5. Hellenic Bioinformatics Symposium, Bioinformatics as a growth engine for Greece, **2016, Thessaloniki, Greece**. *A multi-pharmacophore virtual screening methodology and the discovery of novel compounds targeting pharmacological targets*. **Best oral presentation award**
6. The International Conference HeCrA-HSCBB-16, **2016, Athens, Greece**. *Discovery of novel immunosuppressants targeting Calcineurin through computational methods*.
7. 17th International Conference in Medicinal Chemistry, **2016, Spetses, Greece**. *Discovery of novel immunosuppressants targeting Calcineurin through pharmacophore virtual screening*. **Invited Speaker**
8. 22nd Panhellenic Chemistry Conference, **2016, Thessaloniki, Greece**. *Identification of novel immunosuppressant agents targeting the Calcineurin/NFAT pathway through pharmacophore virtual screening*.
9. SEE-DRUG: NMR Applications in Life Sciences – Exploring Peptides & Proteins, **2015, Patras, Greece**. *The discovery of novel immunosuppressant agents targeting the Calcineurin/NFAT pathway*. **Invited Speaker**
10. Congress of The Hellenic Society of Biochemistry and Molecular Biology (FEBS), **2015, Athens, Greece**. *Discovery of novel immunosuppressants targeting the calcineurin-NFAT substrate interaction site through pharmacophore virtual screening*
11. Computational Methods in Toxicology and Pharmacology Integrating Internet Resources, **2015, Chios, Greece**. *Structure based pharmacophore virtual screening for novel immunosuppressants against calcineurin*
12. 9th Conference of the Hellenic Society for Computational Biology and Bioinformatics (HSCBB14), **2014, Athens, Greece**. *Computational approaches towards identification of structural and signaling properties of peptide binding G Protein-coupled receptors*. **Invited Speaker**
13. International Conference in Medicinal Chemistry, **2011, Patras, Greece**. *Conformational Elucidation of Aliskiren, a Potent Renin Inhibitor*. **Invited Speaker**

EDITOR IN PEER REVIEW JOURNALS

Editorial Board Member

2018 – 2020: Biochemistry and Molecular Biology

FUNDING BODY REVIEWER

- Czech Science Foundation, “Research, experimental development and innovation to support basic research grant projects for Standard Projects”, 2023
- EPAnEK 2014-2020, Competitiveness, Entrepreneurship & Innovation. Scientific evaluator.
- Greek state Scholarship Foundation, “Strengthening human resources through doctoral research”, ESPA 2014-2020.
- “European Digital Innovation Hubs- EDIHs”, Digital Europe, 2021-2027

REVIEWER IN PEER REVIEW JOURNALS

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| • Journal Medicinal Chemistry | • Scientific Reports (Nature) |
| • Current Molecular Pharmacology | • Frontiers in Pharmacology |
| • Current Pharmaceutical Discovery | • Gene Reports |
| • Frontiers in Pediatrics | • Computational and Structural Biotechnology Journal |
| • Journal of Chemical Information and Modeling | • Molecules (MDPI) |
| • Journal of Peptide Science | • Journal of Molecular Graphics and Modelling |
| • SAR and QSAR in Environmental Research | |
| • Antiviral Research | |

MEMBER IN CONSORTIA

- Cancer nanomedicine - from the bench to the bedside (COST action CA17140), **Management Committee**

PARTICIPATION IN EU INFRASTRUCTURES

- Access to ARIS Supercomputing Center, Greek National HPC Infrastructure, Athens, *“Extending 3D Drug Repurposing predictions to the human Variome and extended (AlphaFold) Proteome space”*. 12th call, **2022**
- Access to MARENOSTRUM Barcelona Supercomputing Center, *“New strategies in GPCR drug discovery”*. call IDs: BCV-2014-2-0012, BCV-2014-3-0008, BCV-2014-3-0013, BCV-2014-3-0015, **2014-2015**

EXAMINATION/EVALUATION COMMITTEES

- June 2019: **PhD thesis Examination Board**, Eduardo Mayol Escuer, *“Development of Bioinformatic Tools for the Study of Membrane Proteins”*, Universitat Autònoma de Barcelona, Barcelona, Spain
- June 2019: **PhD thesis External Evaluator**, Mireia Jimenez Roses, *“Structure and function of GPCRs”*, Universitat Autònoma de Barcelona, Barcelona, Spain

- February 2019: **MSc thesis External Evaluator**, Robin du Preez, “*Characterisation of potential novel small molecule therapeutics targeting the growth hormone releasing hormone receptor*”, Department of Physiology, at the Faculty of Health Sciences, University of Pretoria, South Africa.
- September 2017: **PhD thesis External Evaluator**, Santiago Ríos Azuara, “*Sequence and structure-based bioinformatics tools to the characterization, clustering and modeling of G-protein-coupled receptors (GPCRs)*”, Universitat Autònoma de Barcelona, Barcelona, Spain
- November 2016: **PhD thesis Examination Board**, Jose Carlos-Tamayo, “*Development and application of computational techniques to drug discovery and structure-function relationships*”, Universitat Autònoma de Barcelona, Barcelona, Spain

PATENTS

- P12223EP00 (EU)** - M. Pérez-Riba, Á. Aranguren, **M.-T. Matsoukas**, L. Pardo (inventors). Therapeutic Uses of non-Peptide Inhibitors of the Calcineurin - NFAT Signalling Pathway.
- WO2021197574A1 (WIPO)** – A Garcia Pino, CP Govaerts, H Ainelo, H Tamma, V Haurlyuk, L Pardo Carasco, **M-T Matsoukas** (inventors). Rel/rela/spot small molecules modulators and screening methods.

PUBLICATIONS

Overview

Publications	Citations	Total IF	<i>h</i> -index
57	1086 Scopus	229 (Web of Science)	17 Scopus
	1002 Web of Science	210 (without abstracts)	16 Web of Science
	1429 Google Scholar	4.42 (mean)	18 Google Scholar

1 st Author (or equal)	2 nd Author	Corresponding Author (*)	Total
10/57 (18%)	11/57 (19%)	8/57 (14%)	52%

- Salgado-Polo F, Borza R, **Matsoukas M-T**, Marsais F, Jagerschmidt C, Waeckel L, Moolenaar WH, Ford P, Heckmann B, Perrakis A. Autotaxin facilitates selective LPA receptor signaling. *Cell Chemical Biology*, **2023**, 30, 69.
- Ridgway H, Ntallis C, Chasapis CT, Kelaidonis K, **Matsoukas M-T**, Plotas P, Apostolopoulos V, Moore G, Tsiodras S, Paraskevis D, Mavromoustakos T, Matsoukas JM. Molecular Epidemiology of SARS-CoV-2: The Dominant Role of Arginine in Mutations and Infectivity. *Viruses*. **2023**, 15, 309.
- Sánchez-Morales A, Biçer A, Panagiotopoulos V, Crecente-Garcia S, Benaiges C, Bayod S, Hernández JL, Busqué F, **Matsoukas M-T***, Pérez-Riba M*, Alibés R*. Design and synthesis

- of a novel non peptide CN-NFATc signaling inhibitor for tumor suppression in triple negative breast cancer. *European Journal of Medicinal Chemistry*, **2022**, 238, 114514.
4. Swarbrick C, Zogali V, Chan KWK, Kioussis D, Gwee CP, Wang S, Lescar J, Luo D, von Itzstein M, **Matsoukas M-T**, Panagiotakopoulos G, Vasudevan SG, Rassias G. Amidoxime prodrugs convert to potent cell-active multimodal inhibitors of the dengue virus protease. *European Journal of Medicinal Chemistry*, **2021**, 224, 113695.
 5. Bisyris E, Zingkou E, Kordopati GG, **Matsoukas M-T**, Magriotis P, Pampalakis G, Sotiropoulou G. Generation of a quenched phosphonate activity-based probe for labelling the active KLK7 protease. *Organic and Biomolecular Chemistry*, **2021**, 19, 6834.
 6. Bisyris E, Zingkou E, Kordopati GG, **Matsoukas M-T**, Magriotis P, Pampalakis G, Sotiropoulou G. A novel theranostic activity-based probe targeting kallikrein 7 for the diagnosis and treatment of skin diseases. *Chemical Communications*, **2021**, 57, 6507.
 7. Kantsadi A, Cattermole E, **Matsoukas M-T**, Spyroulias GA, Vakonakis I. A COVID moonshot: assessment of ligand binding to the SARS-CoV-2 main protease by saturation transfer difference NMR spectroscopy. *Journal of Biomolecular NMR*. **2021**, 75, 167.
 8. Rodríguez-Espigares I, Torrens-Fontanals M, Tiemann J, Aranda-García D, Ramírez-Anguita JM, Maciej Stepniowski T, Worp N, Varela-Rial A, Morales-Pastor A, Medel-Lacruz B, Pándy-Szekeres G, Mayol E, Giorgino T, Carlsson J, Deupi X, Filipek S, Filizola M, Gómez-Tamayo JC, Gonzalez A, Gutiérrez-de-Terán H, Jiménez-Rosés M, Jespers W, Kapla J, Khelashvili G, Kolb P, Latek D, Marti-Solano M, Matricon P, **Matsoukas M-T**, Misztal P, Olivella M, Perez-Benito L, Provasi D, Ríos S, Torrecillas I, Sallander J, Sztyler A, Vasile S, Weinstein H, Zachariae U, Hildebrand PW, De Fabritiis G, Sanz F, Gloriam DE, Cordomi A, Guixà-González R, Selent J. GPCRmd uncovers the dynamics of the 3D-GPCRome. *Nature Methods*. **2020** (in press).
 9. Busch J, **Matsoukas M-T**, Musgaard M, Spyroulias GA, Biggin P, Vakonakis I. Identification of compounds that bind the centriolar protein SAS-6 and inhibit its oligomerisation. *Journal of Biological Chemistry*. **2020**, 295, 17922.
 10. Zachmann J, Kritsi E, Tapeinou A, Zoumpoulakis P, Tselios T, **Matsoukas M-T***. A Combined Computational and Structural Approach into Understanding the Role of Peptide Binding and Activation of the Melanocortin Receptor 4, *Journal of Chemical Information and Modeling*. **2020**, 60, 1461.
 11. Jenko Bizjan B, Katsila T, Tesovnik T, Šket R, Debeljak M, **Matsoukas M.-T.** Kovač J. Challenges in identifying large germline structural variants for clinical use by long read sequencing. *Computational and Structural Biotechnology Journal*. **2020**, 18, 83.
 12. Roumana A, Argyriou A, Makrynitsa G, Chasapi S, Matsoukas M-T, Topouzis S. Rational design of soluble guanylate cyclase (sGC) activators and modified synthesis of HMR-1766 (Ataciguat). *Review of Clinical Pharmacology And Pharmacokinetics, International Edition*. **2020**, 34.
 13. Rassias G, Zogali V, Swarbrick C, Chan KWK, Chan SA, Gwee CP, Wang S, Kaplanai E, Canko A, Kioussis D, Lescar J, Luo D, **Matsoukas M-T**, Vasudevan DG. Cell-active carbazole derivatives as inhibitors of the Zika virus protease. *European Journal of Medicinal Chemistry*. **2019**, 180, 536.
 14. Kritsi E, **Matsoukas M-T**, Potamitis C, Detsi A, Ivanov M, Sokovic M, Zoumpoulakis P. Novel Hit Compounds as Putative Antifungals: The Case of *Aspergillus fumigatus*. *Molecules*, **2019**, 24, 3853.
 15. Magafa V†, **Matsoukas M-T†**, Karageorgos V, Dermizaki E, Exarchakou R, Stylos EK, Pardalos M, Margioris AN, Varvounis G, Tzakos AG, Spyroulias GA, Liapakis G. Novel stable

analogues of the neurotensin C-terminal hexapeptide containing unnatural amino acids. *Amino Acids*. **2019**, 51, 1009.

16. Chepurny OG‡, **Matsoukas M-T‡**, Liapakis G, Leech C, Milliken B, Doyle RP, Holz GG. Non-conventional glucagon and GLP-1 receptor agonist and antagonist interplay at the GLP-1 receptor revealed in high-throughput FRET assays for cAMP. *Journal of Biological Chemistry*, **2019**, 294, 3514.
17. Makrynitsa GI, Ntonti D, Marousis KD, Bikrou M, **Matsoukas M-T**, Asami S, Bentrop D, Papageorgiou N, Canard B, Coutard B, Spyroulias GA. Conformational plasticity of the VEEV macro domain is important for binding of ADP-ribose. *Journal of Structural Biology* **2019**, 206, 119.
18. Sakellaris S‡, **Matsoukas M-T‡**, Karageorgos V, Poulaki S, Kuppast B, Margioris A, Venihaki M, Fahmy H, Liapakis G. Selective antagonism of CRF1 receptor by a substituted pyrimidine. *Hormones*, **2019**, 18, 215.
19. Katsila T, **Matsoukas M-T.*** How far have we come with contextual data integration in drug discovery? *Expert Opinion on Drug Discovery*, **2018**, 13, 791.
20. Salgado-Polo F, Fish A, **Matsoukas M-T**, Heidebrecht T, Keune WJ, Perrakis A. Lysophosphatidic acid produced by Autotaxin acts as an allosteric modulator of its catalytic efficiency. *Journal of Biological Chemistry*, **2018**, 293, 14312.
21. Perez-Benito L, Henry A, **Matsoukas M-T**, Lopez L, Pulido D, Royo M, Cordini A, Tresadern G, Pardo L. The Size Matters? A Computational Tool to Design Bivalent Ligands. *Bioinformatics*, **2018**, bty422.
22. Jiménez-Rosés M, **Matsoukas M-T**, Caltabiano G, Cordini A. Ligand-Triggered Structural Changes in the M2 Muscarinic Acetylcholine Receptor. *Journal of Chemical Information and Modeling*, **2018**, 58, 1074.
23. Karageorgos V, Venihaki M, Sakellaris S, Pardalos M, Kontakis G, **Matsoukas M-T**, Gravanis A, Margioris A, Liapakis G. Current understanding of the structure and function of family B GPCRs to design novel drugs. *Hormones*, **2018**, 17, 45.
24. Deraos G‡, Kritsi E‡, **Matsoukas M-T‡**, Christopoulou K‡, Kalbacher H, Zoumpoulakis P, Apostolopoulos V, Matsoukas J. Design of Linear and Cyclic Mutant Analogues of Dirucotide Peptide (MBP82–98) against Multiple Sclerosis: Conformational and Binding Studies to MHC Class II. *Brain Sciences*, **2018**, 8, 213.
25. Loubopoulos A, **Matsoukas M-T**, Katsara M, Deraos G, Giannakopoulou A, Lagoudaki R, Grigoriadis N, Matsoukas J, Apostolopoulos V. Cyclization of PLP 139-151 peptide reduces its encephalitogenic potential in experimental autoimmune encephalomyelitis. *Bioorganic & Medicinal Chemistry*, **2018**, 29, 2221.
26. Smiljkovic M, **Matsoukas M-T**, Kritsi E, Zelenko U, Grdodolnik SG, Calhelha, R, Ferreira I, Sankovic-Babic S, Glamoclija J, Fotopoulou T, Koufaki M, Zoumpoulakis, Sokovic M. Nitrate esters of heteroaromatic compounds as novel *Candida albicans* CYP51 enzyme inhibitors. *ChemMedChem*. **2018**, 13, 251.
27. **Matsoukas M-T,*** Spyroulias GA. Dynamic properties of the growth hormone releasing hormone receptor (GHRHR) and molecular determinants of GHRH binding. *Molecular BioSystems*, **2017**, 13, 1313.
28. Liapakis G‡, **Matsoukas M-T‡**, Karageorgos V, Venihaki M, Mavromoustakos T. Family B G Protein-coupled Receptors and their Ligands: From Structure to Function. *Current Medicinal Chemistry*, **2017**, 24, 3323.

29. Wilsher NE, Arroo RR, **Matsoukas M-T**, Tsatsakis AM, Spandidos DA, Androutsopoulos VP. Cytochrome P450 CYP1 metabolism of hydroxylated flavones and flavonols: Selective bioactivation of luteolin in breast cancer cells. *Food and Chemical Toxicology*, **2017**, 110, 383.
30. Qaradakh T, **Matsoukas M-T**, Hayes A, Rybalka E, Caprnda M, Rimarova K, Sepsi M, Büsselberg D, Kruzliak P, Matsoukas J. Alamandine reverses hyperhomocysteinemia-induced vascular dysfunction via PKA-dependent mechanisms. *Cardiovascular Therapeutics*, **2017**, 35, e12306.
31. Loubopoulos A, Deraos G, **Matsoukas M-T**, Touloumi O, Giannakopoulou A, Kalbacher H, Grigoriadis N, Apostolopoulos V, Matsoukas J. Cyclic MOG 35-55 ameliorates clinical and neuropathological features of experimental autoimmune encephalomyelitis. *Bioorganic & Medicinal Chemistry*, **2017**, 25, 4163.
32. Katsila T, **Matsoukas M-T**, Patrinos GP, Kardamakis D. Pharmacometabolomics Informs Quantitative Radiomics for Glioblastoma Diagnostic Innovation. *OMICS: A Journal of Integrative Biology*, **2017**, 21, 429.
33. Cordomi A, Liapakis G, **Matsoukas M-T**.* Understanding Corticotropin Releasing Factor Receptor (CRFR) Activation Using Structural Models. *Current Molecular Pharmacology*, **2017**, 10, 1.
34. Apostolopoulos V, Deraos G, **Matsoukas M-T**, Day S, Stojanovska L, Tselios T, Androutsou M-E, Matsoukas J. Cyclic citrullinated MBP 87–99 peptide stimulates T cell responses: Implications in triggering disease. *Bioorganic & Medicinal Chemistry*, **2017**, 25, 528.
35. Semidalas C, Semidalas E, **Matsoukas M-T**, Nixarlidis C, Zoumpoulakis P. In silico studies reveal the mechanisms behind the antioxidant and anti-inflammatory activities of hydroxytyrosol. *Medicinal Chemistry Research*, **2016**, 25, 2498.
36. Kritsi E, **Matsoukas M-T**, Potamitis C, Karageorgos V, Detsi A, Magafa V, Liapakis G, Mavromoustakos T, Zoumpoulakis P. Exploring new scaffolds for angiotensin II receptor antagonism. *Bioorganic & Medicinal Chemistry*, **2016**, 24, 4444.
37. Katsila T, Spyroulias GA, Patrinos GP, **Matsoukas M-T**.* Computational approaches in target identification and drug discovery. *Computational and Structural Biotechnology Journal*, **2016**, 14, 177.
38. Bratakos S, Sinanoglou V, **Matsoukas M-T**, Siapi E, Papahatjis D, Riganakos K, Zoumpoulakis P. Fragmentation Patterns of Aromatic 2, 5-Diketopiperazines using Liquid Chromatography/mass Spectrometry. *Current Analytical Chemistry*, **2016**, 12, 439.
39. Tapeinou A, **Matsoukas M-T**, Simal C, Tselios T. Cyclic peptides on a merry-go-round; towards drug design. *Peptide Science*, **2015**, 104, 453.
40. **Matsoukas M-T**‡, Aranguren-Ibáñez Á‡, Lozano T, Nunes V, Lasarte JJ, Pardo L, Pérez-Riba M. Identification of small-molecule inhibitors of calcineurin-NFATc signaling that mimic the PxlIT motif of calcineurin binding partners. *Science Signaling*, **2015**, 8, 63.
41. Lattanzi R, Congiu C, Onnis V, Deplano A, Salvadori S, Marconi V, Mattei D, Francioso A, Ambrosio C, Casella I, Costa T, Caltabiano G, **Matsoukas M-T**, Balboni G, Negri L. Halogenated Triazinediones Behave as Antagonists of PKR1: in vitro and in vivo Pharmacological Characterization. *International Journal of Pharmaceutical Sciences and Research*, **2015**, 6, 1033.
42. Cordomí A, Ismail S, **Matsoukas M-T**, Escruiet C, Gherardi M-J, Pardo L, Fourmy D. Functional elements of the gastric inhibitory polypeptide receptor: Comparison between secretin- and rhodopsin-like G protein-coupled receptors. *Biochemical Pharmacology*, **2015**, 96, 237.

43. Spyridaki K, **Matsoukas M-T**, Cordomi A, Gkountelias K, Papadokostaki M, Mavromoustakos T, Logothetis DE, Margioris AN, Pardo L, Liapakis G. Structural-Functional Analysis of the Third Transmembrane Domain of the CRF1 Receptor: Role in Activation and Allosteric Antagonism. *Journal of Biological Chemistry*, **2014**, 289, 18966.
44. **Matsoukas M-T**, Potamitis C, Plotas P, Androutsou M-E, Agelis G, Matsoukas J, Zoumpoulakis P. Insights into AT1 Receptor Activation through AngII Binding Studies. *Journal of Chemical Information and Modeling*, **2013**, 53, 2798.
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