# Curriculum Vitae

## Tiziano Tuccinardi

**PERSONAL DETAILS**


Birth date and place: November 04, 1977; Pisa (PI), Italy

Nationality: Italian

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**EDUCATION**

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| Jun 2006 | Ph.D. in *Computational Chemistry* (PhD Program: "Medicinal Chemistry and Bioactive Molecules") with the thesis "Computational tools for the study of the structure-property relationship and design of new biologically active compounds", Department of Pharmaceutical Sciences, University of Pisa (Italy).<br>Supervisor: Prof. Adriano Martinelli |
| Nov 2002 | State Examination for Professional Qualification |
| July 2002 | MD in Medicinal Chemistry (Marks: 110/110 cum laude)<br>Thesis title: "Computational methods for the study of the docking of Adenosine receptors agonists and antagonists"<br>Supervisor: Professor Adriano Martinelli, Department of Pharmaceutical Sciences, University of Pisa (Italy). |

**WORK EXPERIENCE**

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| May 2022–present | Full Professor at the Department of Pharmacy, University of Pisa. |
| Apr 2015–April 2022 | Associate Professor at the Department of Pharmacy, University of Pisa. |
| Jul 2016–present | Adjunct Associate Professor at the Department of Biology, College of Science and Technology, Temple University. Philadelphia, PA, USA. |
| Nov 2009–Jul 2014 | Adjunct Assistant Professor at the Sbarro Institute for Cancer Research and Molecular Medicine, Center for Biotechnology, Temple University. Philadelphia, PA, USA. |
| Aug 2009–Dec 2009 | Visiting Researcher (with Prof. Anne Baranger), Department of Chemistry, University of Illinois at Urbana-Champaign. Urbana, IL, USA. |
| Dec 2007–Mar 2015 | Assistant Professor at the Department of Pharmacy, University of Pisa. |
| Jun 2006–Dec 2007 | Post-doctorate in the Molecular Modeling & Virtual Screening Laboratory at the University of Pisa with Professor Adriano Martinelli. |

## AWARDS

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| October 2024 | Second ranked at the Tuscany Start Cup for the MolBook Pro software. The Start Cup initiative aims to stimulate the growth of new start-up businesses by offering them concrete support. |
| October 2024 | Member of the 1% top scientists for the Medicinal & Biomolecular Chemistry field (ranked 172 out of 105998 scientists); as reported by: Ioannidis, John P.A. "August 2024 data-update for "Updated science-wide author databases of standardized citation indicators"" 2024, Mendeley Data, V5, doi: 10.17632/btchxktzyw.7 |
| October 2023 | Member of the 1% top scientists for the Medicinal & Biomolecular Chemistry field (ranked 552 out of 99369 scientists); as reported by: Ioannidis, John P.A. "October 2023 data-update for "Updated science-wide author databases of standardized citation indicators."" 2023, Elsevier Data Repository, V6, doi: 10.17632/btchxktzyw.6 |
| October 2022 | Member of the 1% top scientists for the Medicinal & Biomolecular Chemistry field (ranked 642 out of 94672 scientists); as reported by: Ioannidis, John P.A. "September 2022 data-update for "Updated science-wide author databases of standardized citation indicators."" 2022, Mendeley Data, V5, doi: 10.17632/btchxktzyw.5 |
| June 2021 | ESMEC Alumni Award (First edition). European award given to an outstanding European researcher in the field of Medicinal Chemistry who has participated in one of the forty editions of the European School of Medicinal Chemistry (ESMEC) either as an oral or poster presenter. |
| December 2020 | Member of the 2% top scientists for the Medicinal & Biomolecular Chemistry field (ranked 871 out of 80622 scientists); as reported by: Ioannidis JPA, Boyack KW, Baas J. "Updated science-wide author databases of standardized citation indicators." PLoS Biol. 2020 18(10):e3000918. doi: 10.1371/journal.pbio.3000918. |
| September 2019 | Global Peer Review Awards, for placing in the top 1% of reviewers in Cross-Field and in Chemistry on Publons global reviewer database (from Publons, Clarivate Analytics). |
| June 2019 | Artificial Intelligence Molecular Screen (AIMS) Award 2019 for the Project ID: A19-181, "Identification of new reversible MAGL inhibitors" (from Atomwise Inc., San Francisco, CA 94103. |
| December 2017 | Individual annual funding for academic research activities, top 25% in the associate professor national ranking (from Italian Government). |
| April 2013 | Young Scientist Award for the high publication rating in the 2008-2012 period (from University of Pisa). |
| November 2011 | Young Scientist Award for the high publication rating in the 2006-2010 period (from University of Pisa). |
| July 2010 | Farmindustria 2010 Award for the best young Italian medicinal chemist (from Farmindustria and Pharmaceutical Chemistry Division of the Italian Chemical society). |

## RECOGNITIONS

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| 2024-present | President of University Scientific Committee (chemistry sector), University of Pisa. |
| 2023-present | Coordinator of the PhD program "Science of Drug and Bioactive Substances", Department of Pharmacy, University of Pisa. |
| 2023-present | Member of the PhD program "Genomic and experimental medicine (GEM)", Scuola Superiore Meridionale (SSM). |
| 2023-2024 | Member of University Scientific Committee (chemistry sector), University of Pisa. |

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| 2018-present | Member of the Marine pharmacology center of the University of Pisa. |
| 2016-present | Scientific Advisory Board Member of the Bio Future Medicine (BFM) startup. |
| 2016-present | Director of the "Computer-Aided Drug Design" International Summer School (I-IX CADDISS edition), Pisa, Italy. |
| 2014-present | Member of the NutraFood research center of the University of Pisa |
| 2013-present | Member of the Health Technology Assessment center of the University of Pisa |
| 2009-present | Member of the PhD program "Science of Drug and Bioactive Substances", Department of Pharmacy, University of Pisa. |
| 2018-2024 | Director of the "Pharmaceutical Chemistry and Technology" MD (long cycle) programme, University of Pisa. |
| 2013-2019 | Scientific Advisory Board Member of the EWDD European workshop in Drug Design (IX-XII edition) Siena, Italy. |
| 2019 | Opinion leader guest at the international master "Design a Contamination Control Strategy for Aseptic/Sterile Products and Processes" November 26-28, 2019, Rome (Italy). |
| 2019 | Chairman of the 4$^{th}$ Satellite Meeting on Carbonic Anhydrases (Parma, Italy, November, 14-17 2019). |
| 2019 | Chairman of the XII EWDD European workshop in Drug Design (Siena, May, 19-24 2019). |
| 2014-2016 | Member of University Scientific Committee (chemistry sector), University of Pisa. |
| 2015 | Co-chairman of the "Molecular modelling studies" session of the 3nd International Bau Drug Design Congress (Istanbul, Turkey, October 1-3 2015). |

**MAIN EDITORIAL DUTIES**

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| 2023-present | Editor in Chief of Mini-Reviews in Medicinal Chemistry published by Bentham. |
| 2023-present | Editorial Board Member of Plos One published by PLOS. |
| 2019-present | Editorial Board Member of Bioorganic Chemistry published by Elsevier. |
| 2018-present | Editorial Board Member of Molecules (Medicinal Chemistry section) published by MDPI. |
| 2015-present | Editorial Board Member of the Journal of Enzyme Inhibition & Medicinal Chemistry published by Taylor & Francis. |

**BIBLIOMETRIC PARAMETERS**

Total IF = 1243.2; Average IF = 5.5; Scopus H-Index = 46; Scopus Total Citations = 7453; Scopus Average citation per item = 32.7; First, Last or Corr Author: 80.

**PUBLICATIONS**

**2024**

228 Bononi G, Di Bussolo V, Tuccinardi T, Minutolo F, Granchi C. A patent review of lactate dehydrogenase inhibitors (2014-present). Expert Opin Ther Pat. 2024 34(11):1121-1135.

227 Di Stefano M, Galati S, Lonzi C, Granchi C, Poli G, Tuccinardi T, Macchia M. WaSPred: A reliable AI-based water solubility predictor for small molecules. Int J Pharm. 2024, 666:124817.

226 Palazzolo S, Saorin G, Corona G, Granchi C, Tuccinardi T, Kamensek U, Brezar SK, Cemazar M, Canzonieri V, Rizzolio F. A carrier free delivery system of a MAGL inhibitor is effective on ovarian cancer. Eur J Pharm Biopharm. 2024, 203:114397.

225 Cuffaro D, Burkhard T, Bernardoni BL, Di Leo R, Zhang X, Galati S, Tuccinardi T, Macchia M, Rossello A, Santamaria S, de Groot R, Nuti E. Design, synthesis and biological evaluation of arylsulfonamides as ADAMTS7 inhibitors. RSC Med Chem. 2024, 15(8):2806-2825.

224 de Freitas Silva M, Juliet Cristancho Ortiz C, Ferreira Coelho L, Pruccoli L, Pagliarani B, Pisani L, Catto M, Poli G, Tuccinardi T, Cardoso Vilela F, Giusti-Paiva A, Amaral Alves M, Ribeiro de Souza HM, Tarozzi A, Silva Gontijo V, Viegas C Jr. Synthesis and pharmacological evaluation of novel N-aryl-cinnamoyl-hydrazone hybrids designed as neuroprotective agents for the treatment of Parkinson's disease. Bioorg Chem. 2024, 150:107587.

223 Alberti M, Poli G, Broggini L, Sainas S, Rizzi M, Boschi D, Ferraris DM, Martino E, Ricagno S, Tuccinardi T, Lolli ML, Miggiano R. An alternative conformation of the N-terminal loop of human dihydroorotate dehydrogenase drives binding to a potent antiproliferative agent. Acta Crystallogr D Struct Biol. 2024, 80(Pt 6):386-396.

222 Di Stefano M, Galati S, Piazza L, Gado F, Granchi C, Macchia M, Giordano A, Tuccinardi T, Poli G. Watermelon: setup and validation of an in silico fragment-based approach. J Enzyme Inhib Med Chem. 2024, 39(1):2356179.

221 Bononi G, Lonzi C, Tuccinardi T, Minutolo F, Granchi C. The Benzoylpiperidine Fragment as a Privileged Structure in Medicinal Chemistry: A Comprehensive Review. Molecules. 2024, 29(9):1930.

220 Åbacka H, Masoni S, Poli G, Huang P, Gusso F, Granchi C, Minutolo F, Tuccinardi T, Hagström-Andersson AK, Lindkvist-Petersson K. SMS121, a new inhibitor of CD36, impairs fatty acid uptake and viability of acute myeloid leukemia. Sci Rep. 2024, 14(1):9104.

219 Di Stefano M, Galati S, Piazza L, Granchi C, Mancini S, Fratini F, Macchia M, Poli G, Tuccinardi T. VenomPred 2.0: A Novel In Silico Platform for an Extended and Human Interpretable Toxicological Profiling of Small Molecules. J Chem Inf Model. 2024, 64(7):2275-2289.

218 Sharma M, Pandey V, Poli G, Tuccinardi T, Lolli ML, Vyas VK. A comprehensive review of synthetic strategies and SAR studies for the discovery of PfDHODH inhibitors as antimalarial agents. Part 1: triazolopyrimidine, isoxazolopyrimidine and pyrrole-based (DSM) compounds. Bioorg Chem. 2024, 146:107249.

217 Di Stefano M, Masoni S, Bononi G, Poli G, Galati S, Gado F, Manzi S, Vagaggini C, Brai A, Caligiuri I, Asif K, Rizzolio F, Macchia M, Chicca A, Sodi A, Di Bussolo V, Minutolo F, Meier P, Gertsch J, Granchi C, Dreassi E, Tuccinardi T. Design, synthesis, ADME and biological evaluation of benzylpiperidine and benzylpiperazine derivatives as novel reversible monoacylglycerol lipase (MAGL) inhibitors. Eur J Med Chem. 2024, 263:115916.

216 Mattioli S, Fratini F, Cacchiarelli C, Martinis V, Tuccinardi T, Paci G, Dal Bosco A, Mancini S. Chemical composition, fatty acid profile, antioxidant content, and microbiological loads of lesser mealworm, mealworm, and superworm larvae. Ital J An Sc. 2024, 23(1):125-137.

**2023**

215 Bononi G, Citi V, Martelli A, Poli G, Tuccinardi T, Granchi C, Testai L, Calderone V, Minutolo F. Sirtuin 1-activating derivatives belonging to the anilinopyridine class displaying in vivo cardioprotective activities. RSC Medicinal Chemistry 2023, 15(1):267-282.

214 Galati S, Di Stefano M, Bertini S, Granchi C, Giordano A, Gado F, Macchia M, Tuccinardi T, Poli G. Identification of New GSK3β Inhibitors through a Consensus Machine Learning-Based Virtual Screening. Int J Mol Sci. 2023, 24(24):17233.

213 Berrino E, Carradori S, Carta F, Melfi F, Gallorini M, Poli G, Tuccinardi T, Fernández-Bolaños JG, López Ó, Petzer JP, Petzer A, Guglielmi P, Secci D, Supuran CT. A Multitarget Approach against Neuroinflammation: Alkyl Substituted Coumarins as Inhibitors of Enzymes Involved in Neurodegeneration. Antioxidants (Basel). 2023, 12(12):2044.

212 Saorin G, Mauceri M, Cavarzerani E, Caligiuri I, Bononi G, Granchi C, Bartoletti M, Perin T, Tuccinardi T, Canzonieri V, Adeel M, Rizzolio F. Enhanced Activity of a Pluronic F127 Formulated Pin1 Inhibitor for Ovarian Cancer Therapy. J. Drug Deliv. Sci. Technol. 2023, 87, 104718.

211 Galati S, Di Stefano M, Macchia M, Poli G, Tuccinardi T. MolBook UNIPI - create, manage, analyze and share your chemical data for free. J Chem Inf. 2023, 63(13):3977-3982.

210 Poli G, Demontis GC, Sodi A, Saba A, Rizzo S, Macchia M, Tuccinardi T. An in silico toolbox for the prediction of the potential pathogenic effects of missense mutations in the dimeric region of hRPE65. J Enzyme Inhib Med Chem. 2023, 38(1):2162047.

209 De Logu F, Maglie R, Titiz M, Poli G, Landini L, Marini M, Souza Monteiro de Araujo D, De Siena G, Montini M, Cabrini DA, Otuki MF, Pawloski PL, Antiga E, Tuccinardi T, Calixto JB, Geppetti P, Nassini R, André E. miRNA-203b-3p Induces Acute and Chronic Pruritus through 5-HTR2B and TRPV4. J Invest Dermatol. 2023, 143(1):142-153.e10.

**2022**

208 Carradori S, Fantacuzzi M, Ammazzalorso A, Angeli A, De Filippis B, Galati S, Petzer A, Petzer JP, Poli G, Tuccinardi T, Agamennone M, Supuran CT. Resveratrol Analogues as Dual Inhibitors of Monoamine Oxidase B and Carbonic Anhydrase VII: A New Multi-Target Combination for Neurodegenerative Diseases? Molecules. 2022, 27(22):7816.

207 Bononi G, Masoni S, Di Bussolo V, Tuccinardi T, Granchi C, Minutolo F. Historical perspective of tumor glycolysis: A century with Otto Warburg. Semin Cancer Biol. 2022, 86(Pt 2):325-333.

206 Bononi G, Citi V, Lapillo M, Martelli A, Poli G, Tuccinardi T, Granchi C, Testai L, Calderone V, Minutolo F. Sirtuin 1-Activating Compounds: Discovery of a Class of Thiazole-Based Derivatives. Molecules. 2022, 27(19):6535.

205 Sainas S, Giorgis M, Circosta P, Poli G, Alberti M, Passoni A, Gaidano V, Pippione AC, Vitale N, Bonanni D, Rolando B, Cignetti A, Ramondetti C, Lanno A, Ferraris DM, Canepa B, Buccinnà B, Piccinini M, Rizzi M, Saglio G, Al-Karadaghi S, Boschi D, Miggiano R, Tuccinardi T, Lolli ML. Targeting Acute Myelogenous Leukemia Using Potent Human Dihydroorotate Dehydrogenase Inhibitors Based on the 2-Hydroxypyrazolo[1,5-a]pyridine Scaffold: SAR of the Aryloxyaryl Moiety. J Med Chem. 2022, 65(19):12701-12724.

204 Di Stefano M, Galati S, Ortore G, Caligiuri I, Rizzolio F, Ceni C, Bertini S, Bononi G, Granchi C, Macchia M, Poli G, Tuccinardi T. Machine Learning-Based Virtual Screening for the Identification of Cdk5 Inhibitors. Int J Mol Sci. 2022, 23(18):10653.

203 Balestri F, Poli G, Piazza L, Cappiello M, Moschini R, Signore G, Tuccinardi T, Mura U, Del Corso A. Dissecting the Activity of Catechins as Incomplete Aldose Reductase Differential Inhibitors through Kinetic and Computational Approaches. Biology. 2022, 11(9):1324.

202 Ceni C, Benko MJ, Mohamed KA, Poli G, Di Stefano M, Tuccinardi T, Digiacomo M, Valoti M, Laprairie RB, Macchia M, Bertini S. Novel Potent and Selective Agonists of the GPR55 Receptor Based on the 3-Benzylquinolin-2(1H)-One Scaffold. Pharmaceuticals. 2022, 15(7):768.

201 Mancini S, Fratini F, Provera I, Dovicchi J, Tuccinardi T, Minieri S, Papini RA, Forzan M, Paci G. Growth performances, chemical composition, and microbiological loads of mealworm reared with brewery spent grains and bread leftovers. Ital J An Sc. 2022, 21(1):1419-1429.

200 Galati S, Sainas S, Giorgis M, Boschi D, Lolli ML, Ortore G, Poli G, Tuccinardi T. Identification of Human Dihydroorotate Dehydrogenase Inhibitor by a Pharmacophore-Based Virtual Screening Study. Molecules. 2022, 27(12):3660.

199 Poli G, Barravecchia I, Demontis GC, Sodi A, Saba A, Rizzo S, Macchia M, Tuccinardi T. Predicting potentially pathogenic effects of hRPE65 missense mutations: a computational strategy based on molecular dynamics simulations. J Enzyme Inhib Med Chem. 2022, 37(1):1765-1772.

198 Bononi G, Di Stefano M, Poli G, Ortore G, Meier P, Masetto F, Caligiuri I, Rizzolio F, Macchia M, Chicca A, Avan A, Giovannetti E, Vagaggini C, Brai A, Dreassi E, Valoti M, Minutolo F, Granchi C, Gertsch J, Tuccinardi T. Reversible Monoacylglycerol Lipase Inhibitors: Discovery of a New Class of Benzylpiperidine Derivatives. J Med Chem. 2022, 65(10):7118-7140.

197 Bononi G, Flori L, Citi V, Acciai C, Nocilla V, Martelli A, Poli G, Tuccinardi T, Granchi C, Testai L, Calderone V, Minutolo F. New Synthetic Analogues of Natural Polyphenols as Sirtuin 1-Activating Compounds. Pharmaceuticals (Basel). 2022, 15(3):339.

196 Cazzaniga G, Mori M, Meneghetti F, Chiarelli LR, Stelitano G, Caligiuri I, Rizzolio F, Ciceri S, Poli G, Staver D, Ortore G, Tuccinardi T, Villa S. Virtual screening and crystallographic studies reveal an unexpected γ-lactone derivative active against MptpB as a potential antitubercular agent. Eur J Med Chem. 2022, 234:114235.

195 Galati S, Di Stefano M, Martinelli E, Macchia M, Martinelli A, Poli G, Tuccinardi T. VenomPred: A Machine Learning Based Platform for Molecular Toxicity Predictions. Int J Mol Sci. 2022, 23(4):2105.

194 Ibrahim AIM, Batlle E, Sneha S, Jiménez R, Pequerul R, Parés X, Rüngeler T, Jha V, Tuccinardi T, Sadiq M, Frame F, Maitland NJ, Farrés J, Pors K. Expansion of the 4-(Diethylamino)benzaldehyde Scaffold to Explore the Impact on Aldehyde Dehydrogenase Activity and Antiproliferative Activity in Prostate Cancer. J Med Chem. 2022, 65(5):3833-3848.

193 Ortore G, Poli G, Martinelli A, Tuccinardi T, Rizzolio F, Caligiuri I. From Anti-infective Agents to Cancer Therapy: A Drug Repositioning Study Revealed a New Use for Nitrofuran Derivatives. Med Chem. 2022, 18(2):249-259.

192 Abdalla AN, Di Stefano M, Poli G, Tuccinardi T, Bader A, Vassallo A, Abdallah ME, El-Readi MZ, Refaat B, Algarni AS, Ahmad R, Alkahtani HM, Abdel-Aziz AA-, El-Azab AS, Alqathama A. Co-inhibition of p-gp and hsp90 by an isatin-derived compound contributes to the increase of the chemosensitivity of mcf7/adr-resistant cells to doxorubicin. Molecules 2022, 27(1):90.

191 Adeel M, Saorin G, Boccalon G, Sfriso AA, Parisi S, Moro I, Palazzolo S, Caligiuri I, Granchi C, Corona G, Cemazar M, Canzonieri V, Tuccinardi T, Rizzolio F. A Carrier Free Delivery System of a Monoacylglycerol Lipase Hydrophobic Inhibitor. Int J Pharm. 2022, 613:121374.

190 Poli G, Di Stefano M, Estevez JA, Minutolo F, Granchi C, Giordano A, Parisi S, Mauceri M, Canzonieri V, Macchia M, Caligiuri I, Tuccinardi T, Rizzolio F. New PIN1 inhibitors identified through a pharmacophore-driven, hierarchical consensus docking strategy. J Enzyme Inhib Med Chem. 2022, 37(1):145-150.

**2021**

189 Cuffaro D, Camodeca C, Tuccinardi T, Ciccone L, Bartsch JW, Kellermann T, Cook L, Nuti E, Rossello A. Discovery of Dimeric Arylsulfonamides as Potent ADAM8 Inhibitors. ACS Med Chem Lett. 2021, 12(11):1787-1793.

188 Podolski-Renić A, Dinić J, Stanković T, Tsakovska I, Pajeva I, Tuccinardi T, Botta L, Schenone S, Pešić M. New Therapeutic Strategy for Overcoming Multidrug Resistance in Cancer Cells with Pyrazolo[3,4-d]pyrimidine Tyrosine Kinase Inhibitors. Cancers (Basel). 2021, 13(21):5308.

187 Tuccinardi T. What is the current value of MM/PBSA and MM/GBSA methods in drug discovery? Exp. Opin. on Drug Disc. 2021, 16(11):1233-1237.

186 Santamaria S, Buemi F, Nuti E, Cuffaro D, De Vita E, Tuccinardi T, Rossello A, Howell S, Mehmood S, Snijders AP, de Groot R. Development of a fluorogenic ADAMTS-7 substrate. J Enzyme Inhib Med Chem. 2021, 36(1):2160-2169.

185 Asif K, Memeo L, Palazzolo S, Frión-Herrera Y, Parisi S, Caligiuri I, Canzonieri V, Granchi C, Tuccinardi T, Rizzolio F. STARD3: A Prospective Target for Cancer Therapy. Cancers (Basel). 2021, 13(18):4693.

184 Galati S, Di Stefano M, Martinelli E, Poli G, Tuccinardi T. Recent Advances in In Silico Target Fishing. Molecules. 2021, 26(17):5124.

183 Bononi G, Tuccinardi T, Rizzolio F, Granchi C. α/β-Hydrolase Domain (ABHD) Inhibitors as New Potential Therapeutic Options against Lipid-Related Diseases. J Med Chem. 2021, 64(14):9759-9785.

182 Bononi G, Tonarini G, Poli G, Barravecchia I, Caligiuri I, Macchia M, Rizzolio F, Demontis GC, Minutolo F, Granchi C, Tuccinardi T. Monoacylglycerol lipase (MAGL) inhibitors based on a diphenylsulfide-benzoylpiperidine scaffold. Eur J Med Chem. 2021, 223:113679.

181 Jha V, Galati S, Volpi V, Ciccone L, Minutolo F, Rizzolio F, Granchi C, Poli G, Tuccinardi T. Discovery of a new ATP-citrate lyase (ACLY) inhibitor identified by a pharmacophore-based virtual screening study. J Biomol Struct Dyn. 2021, 39(11):3996-4004.

180 Mattioli S, Paci G, Fratini F, Dal Bosco A, Tuccinardi T, Mancini S. Former foodstuff in mealworm farming: Effects on fatty acids profile, lipid metabolism and antioxidant molecules. LWT - Food Science and Technology 2021, 147: 111644.

179 Mancini S, Mattioli S, Paolucci S, Fratini F, Dal Bosco A, Tuccinardi T, Paci G. Effect of Cooking Techniques on the in vitro Protein Digestibility, Fatty Acid Profile, and Oxidative Status of Mealworms (Tenebrio molitor). Front Vet Sci. 2021, 8:675572.

178 Peng S, Guo P, Lin X, An Y, Sze KH, Lau MHY, Chen ZS, Wang Q, Li W, Sun JK, Ma SY, Chan TF, Lau KF, Ngo JCK, Kwan KM, Wong CH, Lam SL, Zimmerman SC, Tuccinardi T, Zuo Z, Au-Yeung HY, Chow HM, Chan HYE. CAG RNAs induce DNA damage and apoptosis by silencing NUDT16 expression in polyglutamine degeneration. Proc Natl Acad Sci U S A. 2021, 118(19):e2022940118.

177 Åbacka H, Hansen JS, Huang P, Venskutonytė R, Hyrenius-Wittsten A, Poli G, Tuccinardi T, Granchi C, Minutolo F, Hagström-Andersson AK, Lindkvist-Petersson K. Targeting GLUT1 in acute myeloid leukemia to overcome cytarabine resistance. Haematologica. 2021, 104(4):1163-1166.

176 Galati S, Yonchev D, Rodríguez-Pérez R, Vogt M, Tuccinardi T, Bajorath J. Predicting Isoform-Selective Carbonic Anhydrase Inhibitors via Machine Learning and Rationalizing Structural Features Important for Selectivity. ACS Omega. 2021, 6(5):4080-4089.

175 Bononi G, Poli G, Rizzolio F, Tuccinardi T, Macchia M, Minutolo F, Granchi C. An updated patent review of monoacylglycerol lipase (MAGL) inhibitors (2018-present). Expert Opin Ther Pat. 2021, 31(2):153-168.

174 Santamaria S, Cuffaro D, Nuti E, Ciccone L, Tuccinardi T, Liva F, D'Andrea F, de Groot R, Rossello A, Ahnström J. Exosite inhibition of ADAMTS-5 by a glycoconjugated arylsulfonamide. Sci Rep. 2021, 11(1):949.

173 Jha V, Biagi M, Spinelli V, Di Stefano M, Macchia M, Minutolo F, Granchi C, Poli G, Tuccinardi T. Discovery of Monoacylglycerol Lipase (MAGL) Inhibitors Based on a Pharmacophore-Guided Virtual Screening Study. Molecules. 2021, 26(1):E78.

172 Granchi C, Bononi G, Ferrisi R, Gori E, Mantini G, Glasmacher S, Poli G, Palazzolo S, Caligiuri I, Rizzolio F, Canzonieri V, Perin T, Gertsch J, Sodi A, Giovannetti E, Macchia M, Minutolo F, Tuccinardi T, Chicca A. Design, synthesis and biological evaluation of second-generation benzoylpiperidine derivatives as reversible monoacylglycerol lipase (MAGL) inhibitors. Eur J Med Chem. 2021, 209:112857.

**2020**

171 Palazzolo S, Memeo L, Hadla M, Duzagac F, Steffan A, Perin T, Canzonieri V, Tuccinardi T, Caligiuri I, Rizzolio F. Cancer Extracellular Vesicles: Next-Generation Diagnostic and Drug Delivery Nanotools. Cancers (Basel). 2020 12(11):E3165.

170 Arena C, Gado F, Di Cesare Mannelli L, Cervetto C, Carpi S, Reynoso-Moreno I, Polini B, Vallini E, Chicca S, Lucarini E, Bertini S, D'Andrea F, Digiacomo M, Poli G, Tuccinardi T, Macchia M, Gertsch J, Marcoli M, Nieri P, Ghelardini C, Chicca A, Manera C. The endocannabinoid system dual-target ligand N-cycloheptyl-1,2-dihydro-5-bromo-1-(4-fluorobenzyl)-6-methyl-2-oxo-pyridine-3-carboxamide improves disease severity in a mouse model of multiple sclerosis. Eur J Med Chem. 2020, 208:112858.

169 Jha V, Macchia M, Tuccinardi T, Poli G. Three-Dimensional Interactions Analysis of the Anticancer Target c-Src Kinase with Its Inhibitors. Cancers (Basel). 2020, 12(8):E2327.

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## PATENTS

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3 Rossello A, Nuti E, Orlandini E, Tuccinardi T. "Arylsulfonamide derivatives, especially dimeric hydroxamic acid-containing amino acids, metalloproteases inhibitors and their preparation, pharmaceutical compositions and use in the treatment of degenerative disorders." PCT Int. Appl. WO2010010080 (2010). Assignee: Bracco Imaging S.p.A, Italy.

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1 Ferrarini PL, Martinelli A, Manera C, Benetti V, Cascio MG, Di Marzo V, Saccomanni G, Tuccinardi T. "Selective ligands of cannabinoid receptor CB2 and their possible uses." PI2007A000017 (2007). Assignee: Universita' di Pisa, Italy.

**ORAL COMMUNICATIONS**

1 T. Tuccinardi. Artificial intelligence in drug discovery. (Invited Seminar) BIO & Pharmaceutical Materials Science - european master, September 11, 2024 – Pisa (Italy).

2 T. Tuccinardi. In silico pathogenicity prediction of missense mutations. (Invited Seminar) Tigem (Telethon Institute of Genetics and Medicine), June 11, 2024 Pozzuoli (Naples, Italy).

3 T. Tuccinardi. I*n silico studies for evaluating the potential pathogenic impact of hRPE65 missense mutations.* (Invited Keynote Speaker) "SGOF 2023 meeting (Société de la Génétique Ophtalmologique Francophone)" October 13-14, 2023, Venice (Italy).

4 T. Tuccinardi. *Artificial Intelligence: A Modern Approach.* (Invited Speaker) "NEXT ONCOLOGY - Supporting oncology through innovation" October 09-10, 2023, Milan (Italy).

5 T. Tuccinardi. *Compose, manage and analyze chemical-based databases.* (Invited Speaker) "12$^{th}$ International conference on Carbonic Anhydrases" July 05-07, 2023, Naples (Italy).

6 T. Tuccinardi. *From ESMEC 23$^{rd}$ to ESMEC 40$^{th}$: Diary of a Medicinal Chemist.* (Invited Speaker) "European School of Medicinal Chemistry ESMEC" June 28-July 1, 2021, Urbino (Italy).

7 T. Tuccinardi. *The University - Industry network: Present and future of a successful partnership.* Invited opening lecture at the international master "Design a Contamination Control Strategy for Aseptic/Sterile Products and Processes" November 26-28, 2019, Rome (Italy).

8 T. Tuccinardi. *Development of a chemoinformatic platform for selectivity analyses of carbonic anhydrase inhibitors.* "4$^{th}$ Satellite Meeting on Carbonic Anhydrases" November 14-17, 2019, Parma (Italy).

9 T. Tuccinardi. *New trends in Computer-aided Drug Design.* (Invited Seminar) University of Genoa, October 7, 2019 Genova (Italy), PhD School "Scienze e Tecnologie della Chimica e dei Materiali".

10 T. Tuccinardi. *Identification and optimization of new reversible MAGL inhibitors: a computer-aided drug design history.* "VI National Meeting on Computational and Theoretical Chemistry" September 19-20, 2019, Arcavacata (CS, Italy).

11 T. Tuccinardi. *Principles of Computer-aided Drug Design.* (Invited Seminar) University of Genoa, October 22 2018 Genova (Italy), PhD School "Scienze e Tecnologie della Chimica e dei Materiali".

12 T. Tuccinardi. *Development of a fingerprint scoring function for the prediction of the binding mode of Carbonic Anhydrase inhibitors.* "The 11th International Conference on Carbonic Anhydrases" June 27-30, 2018, Bucharest (Romania).

13 T. Tuccinardi. *Recent advances in Computer-aided Drug Design.* (Invited Seminar) University of Genoa, October 16 2017 Genova (Italy), PhD School "Scienze e Tecnologie della Chimica e dei Materiali".

14 T. Tuccinardi. *New trends in Computer-aided Drug Design.* (Invited Seminar) University of Genoa, October 17 2016 Genova (Italy), PhD School "Scienze e Tecnologie della Chimica e dei Materiali".

15 T. Tuccinardi. *Structure-based computational studies for the identification and optimization of reversible MAGL inhibitors*. "IV National Meeting on Computational and Theoretical Chemistry" October 3-5, 2016, Pisa (Italy)

16 T. Tuccinardi. *Principles of Computer-aided Drug Design.* (Invited Seminar) University of Genoa, October 26 2015 Genova (Italy), PhD School "Scienze e Tecnologie della Chimica e dei Materiali".

17 T. Tuccinardi. *Consensus Docking as a Tool for the Identification and Optimization of New Lead Compounds.* (Invited Speaker) "3nd International Bau Drug Design Congress" October 1-3, 2015 Istanbul (Turkey).

18 T. Tuccinardi. *New trends in Computer-aided Drug Design.* (Invited Seminar) University of Genoa, December 9 2014 Genova (Italy), PhD School "Scienze e Tecnologie della Chimica e dei Materiali".

19 T. Tuccinardi. *Computational Methods in Drug Discovery.* (Invited Seminar) Centro Ricerche Oncologiche Mercogliano (CROM), July 24 2012 Mercogliano (AV, Italy).

20 T. Tuccinardi. *Computational Studies of the Molecular Modeling and Virtual Screening Laboratory*. "Computationally Driven Drug Discovery" November 21-23, 2011 L'Aquila (Italy).

21 T. Tuccinardi. *Small modifications for improving the ligand activity.* (Invited Speaker) "XX National Meeting on Medicinal Chemistry" September 12-16, 2010 Abano Terme (Italy).

22 T. Tuccinardi, A. Martinelli. *Protein kinases: docking and homology modeling reliability.* "28$^{th}$ Camerino-Cyprus-Noordwijkerhout Symposium, Trekking through Receptor Chemistry" May 16-20, 2010, Camerino (Italy).

23 T. Tuccinardi, S. Taliani, M. Bellandi, E. Da Pozzo, G. Greco, E. Novellino, A. Martinelli, F. Da Settimo, C. Martini. *3D-QSAR and virtual screening studies for the translocator protein(TSPO).* "XIX National Meeting on Medicinal Chemistry" September 14-18, 2008 Verona (Italy).

24 T. Tuccinardi. *GPCR modeling: methods and validation.* (Invited Seminar) University of Florence, February 15 2007 Firenze (Italy).

25 S.L. Baroncini, T. Tuccinardi, A. Martinelli. *MMPs: "Receptor Based" 3D QSAR, "*Riunione Scientifica della Società Chimica Italiana, Sezione Toscana", December 18 2006 Firenze (Italy).

26 A. Martinelli, S. Lazzarotti, T. Tuccinardi. *La selettività CB2/CB1 dei recettori dei cannabinoidi. Uno studio di docking automatico, "*XXIV Convegno Interregionale – Toscana Umbria Marche Abruzzo", September 30 – October 1 2005 Firenze (Italy).

**ONGOING RESEARCH SUPPORT**

1 National Recovery and Resilience Plan (PNRR), Mission 4 Component 2 Investment 1.4 "National Centre for HPC, Big Data and Quantum Computing" - Spoke 7 "Materials & Molecular Sciences" (European Union – NextGenerationEU).

2 Synendos Therapeutics AG (2022-2024) – "Development of modulators of the endocannabinoid system".

3 Novartis Farma S.p.A. (2023) – “Development of an extended in silico toolbox for the prediction of the potential pathogenic effects of hRPE65 missense mutations”.

4 Industria Farmaceutica Galenica Senese Srl (2023-2025) – “Delivery-optimized therapeutic nanomaterials for human health”.

5 Associazione Italiana per la Ricerca sul Cancro (AIRC 2015) – "Inhibition of Pin1 to improve carboplatin and taxol cytotoxicity in high-grade serous ovariancancer" (AIRC MFAG 15639).

**COMPLETED RESEARCH SUPPORT**

1 University of Pisa (2023) – “TOTEM – Therapeutic protac targeting MAGL”.

2 Italian Ministry of Health, Ricerca Finalizzata 2016 – “Development of medical innovative treatments for retinitis pigmentosa” NET-2016-02363765.

Novartis Farma S.p.A. (2021) – “Development of an innovative in silico and in vitro protocol for evaluation of pathogenicity of RPE65 VUS to assess eligibility to gene therapy”.

3 Multiple Sclerosis Italian Foundation (FISM 2020) – “Targeting the endocannabinoid system to fight MS: monoacylglycerol lipase degradation by PROTACs” 2020/PR-Single/005.

4 University Research Projects PRA 2018-2019 “Modulators of the endocannabinoid system in the treatment of glaucoma and related ocular pathologies” PRA_2018_18.

5 Multiple Sclerosis Italian Foundation (FISM 2017) – “Multi-target modulation of the endocannabinoid system as an innovative therapeutic approach for multiple sclerosis” 2017/R/16.

6 University Research Projects PRA 2016-2017 – “Sviluppo di derivati eterociclici azotati quali modulatori dei processi vita/morte della cellula” PRA_2016_59.

7 US National Institutes Of Health (NIH 2012) – “Design, synthesis, and evaluation of lactate dehydrogenase inhibitors” NIH 1R01GM098453-01A1.

8 Italian Ministry of Public Education, PRIN 2011 – “Design and optimization of new anticancer compounds” 20105YY2HL_008.

9 IRCCS European Oncology Institute (2013) – “Application and Optimization of Virtual Screening Techniques”.

10 Amyotrophic Lateral Sclerosis Research Agency (ARISLA 2011) – “Positron Emission Tomography and Amyotrophic Lateral Sclerosis: Study of Cannabinoid subtype 2 receptor expression in ALS experimental model” PETALS II.

11 IRCCS European Oncology Institute (2012) – “Evaluation of new LDH inhibitors”.

12 IRCCS European Oncology Institute (2011) – “Identification of new kinase inhibitors”.

13 Multiple Sclerosis Italian Foundation (FISM 2009) – “Design, synthesis and study of the therapeutic efficacy of novel modulators of the endocannabinoid system in multiple sclerosis” 2009/R/3/C1.

14 Italian Ministry of Public Education, PRIN 2008 – “Design and synthesis of endocannabinoid modulators” 20088SPEFN_004.

15 Monte dei Paschi di Siena Foundation (2007) – “Modulation of MMPs involved in brain pathologies”.