

# Curriculum Vitae

## Tiziano Tuccinardi

### PERSONAL DETAILS

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

Nationality: Italian

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### EDUCATION

- 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).  
Supervisor: Prof. Adriano Martinelli
- Nov 2002                      State Examination for Professional Qualification
- July 2002                      MD in Medicinal Chemistry (Marks: 110/110 cum laude)  
Thesis title: "Computational methods for the study of the docking of Adenosine receptors agonists and antagonists"  
Supervisor: Professor Adriano Martinelli, Department of Pharmaceutical Sciences, University of Pisa (Italy).

### WORK EXPERIENCE

- 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

- 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 Farindustria 2010 Award for the best young Italian medicinal chemist (from Farindustria and Pharmaceutical Chemistry Division of the Italian Chemical society).

## RECOGNITIONS

- 2018-present Director of the "Pharmaceutical Chemistry and Technology" MD (long cycle) programme, University of Pisa ([click here](#)).
- 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-VIII 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.
- 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<sup>th</sup> 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 3rd International Bau Drug Design Congress (Istanbul, Turkey, October 1-3 2015).

## **EDITORIAL DUTIES**

- 2023-present Editorial Board Member of Plos One published by PLOS.
- 2019-present Editorial Board Member of Bioorganic Chemistry published by Elsevier.
- 2019-present Editorial Board Member of Letters in Drug Design & Discovery published by Bentham.
- 2018-present Section Editor for Current Bioactive Compounds published by Bentham.
- 2018-present Section Editor (Computer-aided Drug Design) for Medicinal Chemistry published by Bentham
- 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.
- 2018-2022 Section Editor (Computer-aided Drug Design) for Mini-Reviews in Medicinal Chemistry published by Bentham.
- 2019 Co-Guest Editor for Molecules (Special Issue: Breakthroughs in Drug Discovery and Delivery in Oncology) published by MDPI.
- 2018 Guest Editor for Frontiers in Pharmacology (Special Issue: Peptidyl-prolyl Isomerases in Human Pathologies) published by Frontiers.
- 2018 Guest Editor for Molecules (Special Issue: Trends in the Development of Enzyme Inhibitors) published by MDPI.
- 2016–2018 Editorial Board Member of Current Bioactive Compounds published by Bentham.
- 2010–2014 Editorial Board Member of International Journal of Drug Design & Discovery published by Pharma Book Syndicate.
- 2010–2012 Editorial Board Member of Current Chemical Research published by Mehta Press.
- 2009 Guest Editor for Current Topics in Medicinal Chemistry

## **BIBLIOMETRIC PARAMETERS**

Total IF = 1243.6; Average IF = 5.9; Scopus H-Index = 41; Scopus Total Citations = 5308; Scopus Average citation per item = 25.3; First, Last or Corr Author: 74.

## PUBLICATIONS

### 2023

- 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, Ammazalorso 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, Digiacoimo 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  $\gamma$ -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 Nitrofurans 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.  $\alpha/\beta$ -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, Digiacomio 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.

- 168 Mori M, Stelitano G, Gelain A, Pini E, Chiarelli LR, Sammartino JC, Poli G, Tuccinardi T, Beretta G, Porta A, Bellinzoni M, Villa S, Meneghetti F. Shedding X-ray light on the role of magnesium in the activity of *M. tuberculosis* salicylate synthase (MbtI) for drug design. *J Med Chem.* 2020, 63(13):7066-7080.
- 167 Balestri F, Poli G, Pineschi C, Moschini R, Cappiello M, Mura U, Tuccinardi T, Del Corso A. Aldose Reductase Differential Inhibitors in Green Tea. *Biomolecules.* 2020, 10(7):E1003.
- 166 Gütschow M, Eynde JJV, Jampilek J, Kang C, Mangoni AA, Fossa P, Karaman R, Trabocchi A, Scott PJH, Reynisson J, Rapposelli S, Galdiero S, Winum JY, Brullo C, Prokai-Tatrai K, Sharma AK, Schapira M, Azuma YT, Cerchia L, Spetea M, Torri G, Collina S, Geronikaki A, García-Sosa AT, Vasconcelos MH, Sousa ME, Kosalec I, Tuccinardi T, Duarte IF, Salvador JAR, Bertinaria M, Pellecchia M, Amato J, Rastelli G, Gomes PAC, Guedes RC, Sabatier JM, Estévez-Braun A, Pagano B, Mangani S, Ragno R, Kokotos G, Brindisi M, González FV, Borges F, Miloso M, Rautio J, Muñoz-Torrero D. Breakthroughs in Medicinal Chemistry: New Targets and Mechanisms, New Drugs, New Hopes-7. *Molecules.* 2020, 25(13):E2968.
- 165 Poli G, Bozdog M, Berrino E, Angeli A, Tuccinardi T, Carta F, Supuran CT. N-aryl-N'-ureido-O-sulfamates as potent and selective inhibitors of hCA VB over hCA VA: Deciphering the binding mode of new potential agents in mitochondrial dysfunctions. *Bioorg Chem.* 2020, 4;100:103896.
- 164 Poli G, Tuccinardi T. Consensus Docking in Drug Discovery. *Curr Bioact Comp.* 2020, 16(3):182-190.
- 163 Poli G, Granchi C, Rizzolio F, Tuccinardi T. Application of MM-PBSA Methods in Virtual Screening. *Molecules.* 2020, 25(8):E1971.
- 162 Bisio A, Schito AM, Pedrelli F, Danton O, Reinhardt JK, Poli G, Tuccinardi T, Bürgi T, De Riccardis F, Giacomini M, Calzia D, Panfoli I, Schito GC, Hamburger M, De Tommasi N. Antibacterial and ATP Synthesis Modulating Compounds from *Salvia tingitana*. *J Nat Prod.* 2020, 83(4):1027-1042.
- 161 El Hassouni B, Granchi C, Vallés-Martí A, Supadmanaba IGP, Bononi G, Tuccinardi T, Funel N, Jimenez CR, Peters GJ, Giovannetti E, Minutolo F. The Dichotomous Role of the Glycolytic Metabolism Pathway in Cancer Metastasis: Interplay with the Complex Tumor Microenvironment and Novel Therapeutic Strategies. *Semin Cancer Biol.* 2020, 60:238–248.
- 160 D'Ascenzio M, Secci D, Carradori S, Zara S, Guglielmi P, Cirilli R, Pierini M, Poli G, Tuccinardi T, Angeli A, Supuran CT. 1,3-Dipolar cycloaddition, HPLC enantioseparation and docking studies of saccharin/isoxazole and saccharin/isoxazoline derivatives as selective carbonic anhydrase IX and XII inhibitors. *J Med Chem.* 2020, 63(5):2470-2488.
- 159 Vanden Eynde JJ, Mangoni AA, Rautio J, Leprince J, Azuma YT, García-Sosa AT, Hulme C, Jampilek J, Karaman R, Li W, Gomes PAC, Hadjipavlou-Litina D, Capasso R, Geronikaki A, Cerchia L, Sabatier JM, Ragno R, Tuccinardi T, Trabocchi A, Winum JY, Luque FJ, Prokai-Tatrai K, Spetea M, Gütschow M, Kosalec I, Guillou C, Vasconcelos MH, Kokotos G, Rastelli G, de Sousa ME, Manera C, Gemma S, Mangani S, Siciliano C, Galdiero S, Liu H, Scott PJH, de Los Ríos C, Agrofoglio LA, Collina S, Guedes RC, Muñoz-Torrero D. Breakthroughs in Medicinal Chemistry: New Targets and Mechanisms, New Drugs, New Hopes-6. *Molecules.* 2020, 25(1):E119.
- 158 Bayda S, Adeel M, Tuccinardi T, Cordani M, Rizzolio F. The History of Nanoscience and Nanotechnology: From Chemical-Physical Applications to Nanomedicine. *Molecules.* 2020, 25(1):E112.
- 157 Gado F, Arena C, Fauci C, Reynoso-Moreno I, Bertini S, Digiacocono M, Meini S, Poli G, Macchia M, Tuccinardi T, Gertsch J, Chicca A, Manera C. Modification on the 1,2-dihydro-2-oxo-pyridine-3-carboxamide core to obtain multi-target modulators of endocannabinoid system. *Bioorg Chem.* 2020; 94:103353.
- 156 Mancini S, Fratini F, Tuccinardi T, Degl'Innocenti C, Paci G. *Tenebrio molitor* reared on different substrates: is it gluten free? *Food Control* 2020, 110:107014.

155 Poli G, Galati S, Martinelli A, Supuran CT, Tuccinardi T. Development of a cheminformatics platform for selectivity analyses of carbonic anhydrase inhibitors. *J Enzyme Inhib Med Chem*. 2020, 35(1):365-371.

## 2019

154 Carpi S, Scoditti E, Massaro M, Polini B, Manera C, Digiacomo M, Esposito Salsano J, Poli G, Tuccinardi T, Doccini S, Santorelli FM, Carluccio MA, Macchia M, Wabitsch M, De Caterina R, Nieri P. The Extra-Virgin Olive Oil Polyphenols Oleocanthal and Oleacein Counteract Inflammation-Related Gene and miRNA Expression in Adipocytes by Attenuating NF- $\kappa$ B Activation. *Nutrients*. 2019, 11(12):E2855.

153 Mancini S, Fratini F, Tuccinardi T, Turchi B, Nuvoloni R, Paci G. Effects of different blanching treatments on microbiological profile and quality of the mealworm (*Tenebrio molitor*). *J. Insects as Food and Feed*. 2020, 5(3):225-234

152 Balestri F, Barracco V, Renzone G, Tuccinardi T, Pomelli CS, Cappiello M, Lessi M, Rotondo R, Bellina F, Scaloni A, Mura U, Del Corso A, Moschini R. Stereoselectivity of Aldose Reductase in the Reduction of Glutathionyl-Hydroxynonanal Adduct. *Antioxidants (Basel)*. 2019, 8(10):E502.

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## BOOK CHAPTERS

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## ORAL COMMUNICATIONS

- 1 T. Tuccinardi. *From ESMEC 23<sup>rd</sup> to ESMEC 40<sup>th</sup>: Diary of a Medicinal Chemist.* (Invited Speaker) "European School of Medicinal Chemistry ESMEC" June 28-July 1, 2021, Urbino (Italy).

- 2 T. Tuccinardi. *The University - Industry network: Present and future of a successful partnership*. Opening lecture at the international master “Design a Contamination Control Strategy for Aseptic/Sterile Products and Processes” November 26-28, 2019, Rome (Italy).
- 3 T. Tuccinardi. *Development of a chemoinformatic platform for selectivity analyses of carbonic anhydrase inhibitors*. “4<sup>th</sup> Satellite Meeting on Carbonic Anhydrases” November 14-17, 2019, Parma (Italy).
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- 5 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).
- 6 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”.
- 7 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)
- 8 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”.
- 9 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”.
- 10 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)
- 11 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”.
- 12 T. Tuccinardi. *Consensus Docking as a Tool for the Identification and Optimization of New Lead Compounds*. (Invited Speaker) “3rd International Bau Drug Design Congress” October 1-3, 2015 Istanbul (Turkey).
- 13 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”.
- 14 T. Tuccinardi. *Computational Methods in Drug Discovery*. (Invited Seminar) Centro Ricerche Oncologiche Mercogliano (CROM), July 24 2012 Mercogliano (AV, Italy).
- 15 T. Tuccinardi. *Computational Studies of the Molecular Modeling and Virtual Screening Laboratory*. “Computationally Driven Drug Discovery” November 21-23, 2011 L’Aquila (Italy).
- 16 T. Tuccinardi. *Small modifications for improving the ligand activity*. (Invited Speaker) “XX National Meeting on Medicinal Chemistry” September 12-16, 2010 Abano Terme (Italy).
- 17 T. Tuccinardi, A. Martinelli. *Protein kinases: docking and homology modeling reliability*. “28<sup>th</sup> Camerino-Cyprus-Noordwijkerhout Symposium, Trekking through Receptor Chemistry” May 16-20, 2010, Camerino (Italy).
- 18 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).
- 19 T. Tuccinardi. *GPCR modeling: methods and validation*. (Invited Seminar) University of Florence, February 15 2007 Firenze (Italy).

- 20 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).
- 21 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 (NRRP), 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) – "Development of modulators of the endocannabinoid system".
- 3 University of Pisa (2023) – "TOTEM – Therapeutic protac targeting MAGL".
- 4 Italian Ministry of Health, Ricerca Finalizzata 2016 – "Development of medical innovative treatments for retinitis pigmentosa" NET-2016-02363765.
- 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 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".
- 2 Multiple Sclerosis Italian Foundation (FISM 2020) – "Targeting the endocannabinoid system to fight MS: monoacylglycerol lipase degradation by PROTACs" 2020/PR-Single/005.
- 3 University Research Projects PRA 2018-2019 "Modulators of the endocannabinoid system in the treatment of glaucoma and related ocular pathologies" PRA\_2018\_18.
- 4 Multiple Sclerosis Italian Foundation (FISM 2017) – "Multi-target modulation of the endocannabinoid system as an innovative therapeutic approach for multiple sclerosis" 2017/R/16.
- 5 University Research Projects PRA 2016-2017 – "Sviluppo di derivati eterociclici azotati quali modulatori dei processi vita/morte della cellula" PRA\_2016\_59.
- 6 US National Institutes Of Health (NIH 2012) – "Design, synthesis, and evaluation of lactate dehydrogenase inhibitors" NIH 1R01GM098453-01A1.
- 7 Italian Ministry of Public Education, PRIN 2011 – "Design and optimization of new anticancer compounds" 20105YY2HL\_008.
- 8 IRCCS European Oncology Institute (2013) – "Application and Optimization of Virtual Screening Techniques".
- 9 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.
- 10 IRCCS European Oncology Institute (2012) – "Evaluation of new LDH inhibitors".
- 11 IRCCS European Oncology Institute (2011) – "Identification of new kinase inhibitors".

- 12 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.
- 13 Italian Ministry of Public Education, PRIN 2008 – “Design and synthesis of endocannabinoid modulators” 20088SPEFN\_004.
- 14 Monte dei Paschi di Siena Foundation (2007) – “Modulation of MMPs involved in brain pathologies”.