

# Curriculum Vitae

## Tiziano Tuccinardi

### 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

- Apr 2015–present 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

- 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

2021	Director of the "Computer-Aided Drug Design" International Summer School (VI CADDISS, Pisa, Italy, July 12-17 2021).
2020	Director of the webinar series entitled "I molteplici profili professionali per il laureato in Chimica e Tecnologia Farmaceutiche" (Pisa, November 30-December 4 2020)
2020	Director of the "Computer-Aided Drug Design" International Summer School (V CADDISS, Pisa, Italy, July 20-25 2020).
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	Director of the "Computer-Aided Drug Design" International Summer School (IV CADDISS, Pisa, Italy, July 8-13 2019).
2019	Chairman of the XII EWDD European workshop in Drug Design (Siena, May, 19-24 2019).
2019	Scientific Advisory Board Member of the XII EWDD European workshop in Drug Design (Siena, May, 19-24 2019).
2018-present	Director of the "Pharmaceutical Chemistry and Technology" MD (long cycle) programme, University of Pisa ( <a href="#">click here</a> ).
2018-present	Member of the Marine pharmacology center of the University of Pisa
2018	Director of the "Computer-Aided Drug Design" International Summer School (III CADDISS, Pisa, Italy, July 9-14 2018).
2017	Scientific Advisory Board Member of the XI EWDD European workshop in Drug Design (Siena, May, 21-26 2017).
2017	National Scientific Qualification as Full Professor for the 03/D1 (CHIM08) area
2017	Director of the "Computer-Aided Drug Design" International Summer School (II CADDISS, Pisa, Italy, July 10-15 2017).
2016-present	Scientific Advisory Board Member of the Bio Future Medicine (BFM) startup.

2016	Director of the “Computer-Aided Drug Design” International Summer School (I CADDISS, Pisa, Italy, July 11-16 2016).
2015	Co-chairman of the “Molecular modelling studies” session of the 3rd International Bau Drug Design Congress (Istanbul, Turkey, October 1-3 2015).
2015	Scientific Advisory Board Member of the X EWDD European workshop in Drug Design (Siena, May, 17-22 2015).
2014–present	Member of the NutraFood research center of the University of Pisa
2014-2016	Member of University Scientific Committee (chemistry sector), University of Pisa.
2013–present	Member of the Health Technology Assessment center of the University of Pisa
2013	Scientific Advisory Board Member of the IX EWDD European workshop in Drug Design (Siena, May, 19-25 2013)

### **EDITORIAL DUTIES**

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.
2018-present	Section Editor (Computer-aided Drug Design) for Mini-Reviews in Medicinal Chemistry published by Bentham.
2015–present	Editorial Board Member of the Journal of Enzyme Inhibition & Medicinal Chemistry published by Taylor & Francis.
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 = 1003.8; Average IF = 5.4; Scopus H-Index = 35; Scopus Total Citations = 3903 Scopus Average citation per item = 21.1; First, Last or Corr Author: 68.

## PUBLICATIONS

2021

- 186 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*. 2021 Accepted
- 185 Tuccinardi T. What is the current value of MM/PBSA and MM/GBSA methods in drug discovery? *Exp. Opin. on Drug Disc*. 2021 ASAP 10.1080/17460441.2021.1942836
- 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, Pellicchia 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, Digiacomo 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.
- 151 Azam F, Suliman Abodabos H, Taban IM, Rfieda AR, Mahmood D, Anwar MdJ, Khan S, Sizochenko N, Poli G, Tuccinardi T, Ali HI. Rutin as promising drug for the treatment of Parkinson's disease: an assessment of MAO-B inhibitory potential by docking, molecular dynamics and DFT studies. *Mol. Sim*. 2019 45(18):1563-1571
- 150 D'Andrea F, Vagelli G, Granchi C, Guazzelli L, Tuccinardi T, Poli G, Iacopini D, Minutolo F, Di Bussolo V. Synthesis and Biological Evaluation of New Glycoconjugated LDH Inhibitors as Anticancer Agents. *Molecules*. 2019;24(19). pii: E3520.
- 149 Tuccinardi T, Rizzolio F. Peptidyl-Prolyl Isomerases in Human Pathologies. *Front Pharmacol*. 2019, 10:794.
- 148 Maggini V, De Leo M, Granchi C, Tuccinardi T, Mengoni A, Gallo ER, Biffi S, Fani R, Pistelli L, Firenzuoli F, Bogani P. The influence of *Echinacea purpurea* leaf microbiota on chicoric acid level. *Sci Rep*. 2019, 9(1):10897.
- 147 Mancini S, Fratini F, Turchi B, Mattioli S, Dal Bosco A, Tuccinardi T, Nozic S, Paci G. Former Foodstuff Products in *Tenebrio Molitor* Rearing: Effects on Growth, Chemical Composition, Microbiological Load, and Antioxidant Status. *Animals (Basel)*. 2019, 9(8):E484.

- 146 Mangoni AA, Eynde JJV, Jampilek J, Hadjipavlou-Litina D, Liu H, Reynisson J, Sousa ME, Gomes PAC, Prokai-Tatrai K, Tuccinardi T, Sabatier JM, Luque FJ, Rautio J, Karaman R, Vasconcelos MH, Gemma S, Galdiero S, Hulme C, Collina S, Gütschow M, Kokotos G, Siciliano C, Capasso R, Agrofoglio LA, Ragno R, Muñoz-Torrero D. Breakthroughs in Medicinal Chemistry: New Targets and Mechanisms, New Drugs, New Hopes-5 Molecules. 2019, 24(13):E2415.
- 145 Bozdog M, Poli G, Angeli A, Lucarini E, Tuccinardi T, Di Cesare Mannelli L, Selleri S, Ghelardini C, Winum JY, Carta F, Supuran CT. N-aryl-N'-ureido-O-sulfamates: Potent and selective inhibitors of the human Carbonic Anhydrase VII isoform with neuropathic pain relieving properties Bioorg Chem. 2019, 89:103033.
- 144 Lapillo M, Salis B, Palazzolo S, Poli G, Granchi C, Minutolo F, Rotondo R, Caligiuri I, Canzonieri V, Tuccinardi T, Rizzolio F. First-of-its-kind STARD3 Inhibitor: In Silico Identification and Biological Evaluation as Anticancer Agent ACS Med Chem Lett. 2019, 10(4):475-480.
- 143 Russo Spina C, De Stefano L, Poli G, Granchi C, El Boustani M, Ecça F, Grassi G, Grassi M, Canzonieri V, Giordano A, Tuccinardi T, Caligiuri I, Rizzolio F. Virtual screening identifies a PIN1 inhibitor with possible anti-ovarian cancer effects J. Cell Phys. 2019, 234(9):15708-15716.
- 142 Schlomann U, Dorzweiler K, Nuti E, Tuccinardi T, Rossello A, Bartsch JW. Metalloprotease inhibitor profiles of human ADAM8 in vitro and in cell-based assays. Biol Chem. 2019, 400(6):801-810.
- 141 Chiarelli LR, Mori M, Beretta G, Gelain A, Pini E, Sammartino JC, Stelitano G, Barlocco D, Costantino L, Lapillo M, Poli G, Caligiuri I, Rizzolio F, Bellinzoni M, Tuccinardi T, Villa S, Meneghetti F. New insight into structure-activity of furan-based salicylate synthase (MbtI) inhibitors as potential antitubercular agents J Enzyme Inhib Med Chem. 2019, 34(1):823-828.
- 140 Buran K, Bua S, Poli G, Önen Bayram FE, Tuccinardi T, Supuran CT. Novel 8-Substituted Coumarins That Selectively Inhibit Human Carbonic Anhydrase IX and XII Int J Mol Sci. 2019, 20(5) pii: E1208.
- 139 Krasavin M, Shetnev A, Baykov S, Kalinin S, Nocentini A, Sharoyko V, Poli G, Tuccinardi T, Korsakov M, Tennikova TB, Supuran CT. Pyridazinone-substituted benzenesulfonamides display potent inhibition of membrane-bound human carbonic anhydrase IX and promising antiproliferative activity against cancer cell lines. Eur J Med Chem. 2019, 168:301-314.
- 138 Lapillo M, Tuccinardi T, Martinelli A, Macchia M, Giordano A, Poli G. Extensive Reliability Evaluation of Docking-Based Target-Fishing Strategies. Int J Mol Sci. 2019, 20(5) pii: E1023.
- 137 Granchi C, Lapillo M, Glasmacher S, Bononi G, Licari C, Poli G, El Boustani M, Caligiuri I, Rizzolio F, Gertsch J, Macchia M, Minutolo F, Tuccinardi T, Chicca A. Optimization of a benzoylpiperidine class identifies a highly potent and selective reversible monoacylglycerol lipase (MAGL) inhibitor. J Med Chem. 2019, 62(4):1932-1958.
- 136 De Logu F, Li Puma S, Landini L, Tuccinardi T, Poli G, Preti D, De Siena G, Patacchini R, Tsagareli MG, Geppetti P, Nassini R. The acyl-glucuronide metabolite of ibuprofen has analgesic and anti-inflammatory effects via the TRPA1 channel. Pharmacol Res. 2019 142:127-139.
- 135 Poli G, Lapillo M, Mouawad N, Caligiuri I, Macchia M, Minutolo F, Rizzolio F, Tuccinardi T, Granchi C. Computationally driven discovery of phenyl(piperazin-1-yl)methanone derivatives as reversible monoacylglycerol lipase (MAGL) inhibitors. J Enzyme Inhib Med Chem. 2019, 34(1):589-596.
- 134 El Boustani M, De Stefano L, Caligiuri I, Mouawad N, Granchi C, Canzonieri V, Tuccinardi T, Giordano A, Rizzolio F. A Guide to PIN1 Function and Mutations Across Cancers Front. Pharmacol. 2019, 9:1477.
- 133 Gado F, Di Cesare Mannelli L, Lucarini E, Bertini S, Cappelli E, Digiaco M, Stevenson LA, Macchia M, Tuccinardi T, Ghelardini C, Pertwee RG, Manera C. Identification of the first synthetic allosteric modulator of the CB2 receptors and evidence of its efficacy for neuropathic pain relief. J Med Chem. 2019 62(1):276-287.

- 132 Mangoni AA, Guillou C, Vanden Eynde JJ, Hulme C, Jampilek J, Li W, Prokai-Tatrai K, Rautio J, Collina S, Tuccinardi T, Sousa ME, Sabatier JM, Galdiero S, Karaman R, Kokotos G, Torri G, Luque FJ, Vasconcelos MH, Hadjipavlou-Litina D, Siciliano C, Gütschow M, Ragno R, Gomes PAC, Agrofoglio LA, Muñoz-Torrero D. Breakthroughs in Medicinal Chemistry: New Targets and Mechanisms, New Drugs, New Hopes-4. *Molecules*. 2019 24(1) pii: E130.
- 131 Krasavin M, Shetnev A, Sharonova T, Baykov S, Kalinin S, Nocentini A, Sharoyko V, Poli G, Tuccinardi T, Presnukhina S, Tennikova TB, Supuran CT. Continued exploration of 1,2,4-oxadiazole periphery for carbonic anhydrase-targeting primary arene sulfonamides: Discovery of subnanomolar inhibitors of membrane-bound hCA IX isoform that selectively kill cancer cells in hypoxic environment. *Eur J Med Chem*. 2019 164:92-105.
- 130 Cuffaro D, Nuti E, Gifford V, Ito N, Camodeca C, Tuccinardi T, Nencetti S, Orlandini E, Itoh Y, Rossello A. Design, synthesis and biological evaluation of bifunctional inhibitors of membrane type 1 matrix metalloproteinase (MT1-MMP). *Bioorg Med Chem*. 2019 27(1):196-207.
- 2018**
- 129 Bononi G, Granchi C, Lapillo M, Giannotti M, Nieri D, Fortunato S, Boustani ME, Caligiuri I, Poli G, Carlson KE, Kim SH, Macchia M, Martinelli A, Rizzolio F, Chicca A, Katzenellenbogen JA, Minutolo F, Tuccinardi T. Discovery of long-chain salicylketoxime derivatives as monoacylglycerol lipase (MAGL) inhibitors. *Eur J Med Chem*. 2018 157:817-836.
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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).
- 4 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".
- 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).
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- 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".
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- 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).

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- 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).
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- 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 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 Italian Ministry of Health, Ricerca Finalizzata 2016 – “Development of medical innovative treatments for retinitis pigmentosa” NET-2016-02363765.
- 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 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 Multiple Sclerosis Italian Foundation (FISM 2017) – “Multi-target modulation of the endocannabinoid system as an innovative therapeutic approach for multiple sclerosis” 2017/R/16.
- 2 University Research Projects PRA 2016-2017 – “Sviluppo di derivati eterociclici azotati quali modulatori dei processi vita/morte della cellula” PRA\_2016\_59.
- 3 US National Institutes Of Health (NIH 2012) – “Design, synthesis, and evaluation of lactate dehydrogenase inhibitors” NIH 1R01GM098453-01A1.

- 4 Italian Ministry of Public Education, PRIN 2011 – “Design and optimization of new anticancer compounds” 20105YY2HL\_008.
- 5 IRCCS European Oncology Institute (2013) – “Application and Optimization of Virtual Screening Techniques”.
- 6 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.
- 7 IRCCS European Oncology Institute (2012) – “Evaluation of new LDH inhibitors”.
- 8 IRCCS European Oncology Institute (2011) – “Identification of new kinase inhibitors”.
- 9 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.
- 10 Italian Ministry of Public Education, PRIN 2008 – “Design and synthesis of endocannabinoid modulators” 20088SPEFN\_004.
- 11 Monte dei Paschi di Siena Foundation (2007) – “Modulation of MMPs involved in brain pathologies”.