

Curriculum Vitae

Tiziano Tuccinardi

PERSONAL DETAILS

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

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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

- Apr 2015–present Associate Professor at the Department of Pharmacy, University of Pisa.
- 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

- 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

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 committee advisory board member of the X EWDD European workshop in Drug Design (Siena, May, 17-22 2015).

2015–present Editorial Advisory Board Member of the Journal of Enzyme Inhibition & Medicinal Chemistry published by Inform Healthcare.

2014–present Member of the NutraFood center of the University of Pisa

2014 National scientific qualification for becoming Associate Professor (3/D1 sector)

2013–present Member of the Health Technology Assessment center of the University of Pisa

2013 Scientific committee advisory board member of the IX EWDD European workshop in Drug Design (Siena, May, 19-25 2013)

2011–present Editorial Advisory Board Member of Open Journal of Medicinal Chemistry published by Scientific Research Publishing.

2010–present Editorial Advisory Board Member of Drug Development and Therapeutics published by Organization of Pharmaceutical Unity with BioAllied Sciences (OPUBS).

2010–2012 Editorial Advisory Board Member of Current Chemical Research published by Mehta Press.

2010–2014 Editorial Advisory Board Member of International Journal of Drug Design & Discovery published by Pharma Book Syndicate.

2009 Guest Editor for Current Topics in Medicinal Chemistry

HOBBIES

Running and cycling.

PUBLICATIONS

2016

- 1 Petrou A, Geronikaki A, Terzi E, Ozensoy Guler O, Tuccinardi T, Supuran CT. “Inhibition of carbonic anhydrase isoforms I, II, IX and XII with secondary sulfonamides incorporating benzothiazole scaffolds” J Enzyme Inhib Med Chem. 2016 ASAP.
- 2 Poli G, Gelain A, Porta F, Asai A, Martinelli A, Tuccinardi T. “Identification of a new STAT3 dimerization inhibitor through a pharmacophore-based virtual screening approach” J Enzyme Inhib Med Chem. 2016 ASAP.
- 3 Tabrizi MA, Baraldi PG, Ruggiero E, Saponaro G, Baraldi S, Poli G, Tuccinardi T, Ravani A, Vincenzi F, Borea PA, Varani K. “Synthesis and Structure Activity Relationship Investigation of Triazolo[1,5-a]pyrimidines as CB2 Cannabinoid Receptor Inverse Agonists” Eur J Med Chem. 2016 113:11-27.

- 4 Camodeca C, Nuti E, Tepshi L, Boero S, Tuccinardi T, Stura EA, Poggi A, Zocchi MR, Rossello A. "Discovery of a new selective inhibitor of A Disintegrin And Metalloprotease 10 (ADAM-10) able to reduce the shedding of NKG2D ligands in Hodgkin's lymphoma cell models" *Eur J Med Chem*. 2016 111:193-201.
- 5 Granchi C, Rizzolio F, Bordoni V, Caligiuri I, Manera C, Macchia M, Minutolo F, Martinelli A, Giordano A, Tuccinardi T. "4-Aryliden-2-methyloxazol-5(4H)-one as a new scaffold for selective reversible MAGL inhibitors" *J Enzyme Inhib Med Chem*. 2016 31(1):137-146.
- 2015**
- 6 Granchi C, Qian Y, Yeon Lee H, Paterni I, Pasero C, Iegre J, Carlson KE, Tuccinardi T, Chen X, Katzenellenbogen JA, Hergenrother PJ, Minutolo FM. "Salicylketoximes That Target Glucose Transporter 1 Restrict Energy Supply to Lung Cancer Cells" *ChemMedChem*. 2015 10(11):1892-1900.
- 7 Nuti E, Cantelmo AR, Gallo C, Bruno A, Bassani B, Camodeca C, Tuccinardi T, Vera L, Orlandini E, Nencetti S, Stura EA, Martinelli A, Dive V, Albini A, Rossello A. "N-O-Isopropyl Sulfonamido-Based Hydroxamates as Matrix Metalloproteinase Inhibitors: Hit Selection and in vivo Antiangiogenic Activity" *J Med Chem*. 2015 58(18):7224-7240.
- 8 Tuccinardi T, Poli G, dell'Agnello M, Granchi C, Minutolo F, Martinelli A. "Receptor-based virtual screening evaluation for the identification of estrogen receptor β ligands" *J Enzyme Inhib Med Chem*. 2015 30(4):662-670.
- 9 Krasavin M, Korsakov M, Dorogov M, Tuccinardi T, Dedeoglu N, Supuran CT. "Probing the 'bipolar' nature of the carbonic anhydrase active site: aromatic sulfonamides containing 1,3-oxazol-5-yl moiety as picomolar inhibitors of cytosolic CA I and CA II isoforms" *Eur J Med Chem*. 2015 101:334-347.
- 10 Nassini R, Fusi C, Materazzi S, Coppi E, Tuccinardi T, Marone IM, De Logu F, Preti D, Tonello R, Chiarugi A, Patacchini R, Geppetti P, Benemei S. "The TRPA1 channel mediates the analgesic action of dipyrone and pyrazolone derivatives" *Br J Pharmacol*. 2015 172(13):3397-3411.
- 11 Tintori C, La Sala G, Vignaroli G, Botta L, Fallacara AL, Falchi F, Radi M, Zamperini C, Dreassi E, Dello Iacono L, Orioli D, Biamonti G, Garbelli M, Lossani A, Gasparrini F, Tuccinardi T, Laurenzana I, Angelucci A, Maga G, Schenone S, Brullo C, Musumeci F, Desogus A, Crespan E, Botta M. "Studies on the ATP binding site of Fyn kinase for the identification of new inhibitors and their evaluation as potential agents against tauopathies and tumors." *J Med Chem*. 2015 58(11):4590-4609.
- 12 Bader A, Tuccinardi T, Granchi C, Martinelli A, Macchia M, Minutolo F, De Tommasi N, Braca A. "Phenylpropanoids and Flavonoids from *Phlomis kurdica* as Inhibitors of Human Lactate Dehydrogenase" *Phytochem*. 2015 116:262-268.
- 13 Tabrizi MA, Baraldi PG, Ruggiero E, Saponaro G, Baraldi S, Romagnoli R, Martinelli A, Tuccinardi T. "Pyrazole phenylcyclohexylcarbamates as inhibitors of human fatty acid amide hydrolases (FAAH)" *Eur J Med Chem*. 2015 97:289-305.
- 14 Granchi C, Capecchi A, Del Frate G, Martinelli A, Macchia M, Minutolo F, Tuccinardi T. "Development and Validation of a Docking-Based Virtual Screening Platform for the Identification of New Lactate Dehydrogenase Inhibitors" *Molecules*. 2015, 20(5):8772-8790.
- 15 Poli G, Giuntini N, Martinelli A, Tuccinardi T. "Application of a FLAP-Consensus Docking Mixed Strategy for the Identification of New FAAH Inhibitors" *J Chem Inf Model*. 2015 55(3):667-675.
- 16 Di Bussolo V, Calvaresi EC, Granchi C, Del Bino L, Frau I, Dasso Lang MC, Tuccinardi T, Macchia M, Martinelli A, Hergenrother PJ, Minutolo F. "Synthesis and biological evaluation of non-glucose glycoconjugated *N*-hydroxyindole class LDH inhibitors as anticancer agents". *RSC Adv*. 2015, 5(26):19944-19954.
- 17 Paterni I, Bertini S, Granchi C, Tuccinardi T, Macchia M, Martinelli A, Caligiuri I, Toffoli G, Rizzolio F, Carlson KE, Katzenellenbogen BS, Katzenellenbogen JA, Minutolo F. "Highly selective salicylketoxime-based estrogen receptor beta agonists display antiproliferative activities in a glioma model." *J Med Chem*. 2015, 58(3):1184-1194.

- 18 Enyedy EA, Dömötör O, Bali K, Hetényi A, Tuccinardi T, Keppler BK. "Interaction of the anticancer gallium(III) complexes of 8-hydroxyquinoline and maltol with human serum proteins." *J Biol Inorg Chem.* 2015, 20(1):77-88.

2014

- 19 Fusi C, Materazzi S, Benemei S, Coppi E, Trevisan G, Marone I, Minocci D, De Logu F, Tuccinardi T, Di Tommaso M, Susini T, Moneti G, Pieraccini G, Geppetti P, Nassini R. "Steroidal and non-steroidal third-generation aromatase inhibitors induce pain-like symptoms via TRPA1." *Nature Communications* 2014, 5:5736.
- 20 Tuccinardi T, Poli G, Romboli V, Giordano A, Martinelli A. "Extensive consensus docking evaluation for ligand pose prediction and virtual screening studies" *J Chem Inf Model.* 2014, 54(10):2980-2986.
- 21 Poli G, Martinelli A, Tuccinardi T. "Computational Approaches for the Identification and Optimization of Src Family Kinases Inhibitors." *Curr Med Chem.* 2014, 21(28):3281-3293.
- 22 Tuccinardi T, Granchi C, Rizzolio F, Caligiuri I, Battistello V, Toffoli G, Minutolo F, Macchia M, Martinelli A. "Identification and characterization of a new reversible MAGL inhibitor" *Bioorg Med Chem.* 2014, 22(13):3285-3291.
- 23 Wong CH, Nguyen L, Peh J, Luu LM, Sanchez JS, Richardson SL, Tuccinardi T, Tsoi H, Chan WY, Chan HY, Baranger AM, Hergenrother PJ, Zimmerman SC. "Targeting Toxic RNAs that Cause Myotonic Dystrophy Type 1 (DM1) with a Bisamidinium Inhibitor." *J Am Chem Soc.* 2014, 136(17):6355-6361.
- 24 Digilio G, Tuccinardi T, Casalini F, Cassino C, Dias DM, Geraldine CFGC, Catanzaro V, Maiocchi A, Rossello A. "Study of the binding interaction between fluorinated Matrix Metalloproteinase inhibitors and Human Serum Albumin." *Eur J Med Chem.* 2014, 79:13-23.
- 25 Dömötör O, Tuccinardi T, Karcz D, Walsh M, Creaven BS, Enyedy E. "Interaction of anticancer reduced Schiff base coumarin derivatives with human serum albumin investigated by fluorescence quenching and molecular modeling" *Bioorg Chem.* 2014, 52:16-23.

2013

- 26 Malfitano AM, Laezza C, Saccomanni G, Tuccinardi T, Manera C, Martinelli A, Ciaglia E, Pisanti S, Vitale M, Gazzero P, Bifulco M. "Immune-Modulation and Properties of Absorption and Blood Brain Barrier Permeability of 1,8-Naphthyridine Derivatives." *J Neuroimmune Pharmacol.* 2013, 8(5):1077-1086.
- 27 Tuccinardi T, Granchi C, Iegre J, Paterni I, Bertini S, Macchia M, Martinelli A, Qian Y, Chen X, Minutolo F. "Oxime-based inhibitors of glucose transporter 1 displaying antiproliferative effects in cancer cells." *Bioorg Med Chem. Lett.* 2013, 23(24):6923-6927.
- 28 Calvaresi EC, Granchi C, Tuccinardi T, Di Bussolo V, Huigens III RW, Lee HY, Palchaudhuri R, Macchia M, Martinelli A, Minutolo F, Hergenrother PJ. "Dual Targeting of the Warburg Effect with a Glucose-Conjugated Lactate Dehydrogenase Inhibitor" *Chembiochem.* 2013, 14(17):2263-2267.
- 29 Poli G, Tuccinardi T, Rizzolio F, Caligiuri I, Botta L, Granchi C, Ortore G, Minutolo F, Schenone S, Martinelli A. "Identification of new FYN kinase inhibitors using a FLAP-based approach." *J Chem Inf Model.* 2013, 53(10):2538-2547.
- 30 Granchi C, Calvaresi EC, Tuccinardi T, Paterni I, Macchia M, Martinelli A, Hergenrother PJ, Minutolo F. "Assessing the differential action on cancer cells of LDH-A inhibitors based on the N-hydroxyindole-2-carboxylate (NHI) and malonic (Mal) scaffolds." *Org Biomol Chem.* 2013, 11(38):6588-6596.
- 31 Aghazadeh Tabrizi M, Baraldi PG, Saponaro G, Moorman A, Romagnoli R, Preti D, Baraldi S, Ruggiero E, Tintori C, Tuccinardi T, Vincenzi F, Borea PA, Varani K. "Discovery of 7-Oxo-pyrazolo[1,5-a]pyrimidine-6-carboxamides as Potent and Selective CB2 Cannabinoid Receptor Inverse Agonists." *J Med Chem.* 2013, 56(11):4482-4496.

32 Malfitano AM, Laezza C, D'Alessandro A, Procaccini C, Saccomanni G, Tuccinardi T, Manera C, Macchia M, Matarese G, Gazzero P, Bifulco M. "Effects on Immune Cells of a New 1,8-Naphthyridin-2-One Derivative and Its Analogues as Selective CB2 Agonists: Implications in Multiple Sclerosis" *PLoS One*. 2013 May 1;8(5):e62511.

33 Tuccinardi T, Bertini S, Granchi C, Ortore G, Macchia M, Minutolo F, Martinelli A, Supuran CT. "Salicylaldehyde derivatives as new leads for the development of Carbonic Anhydrase inhibitors" *Bioorg Med Chem*. 2013, 21(6):1511-1515.

2012

34 Wong CH, Richardson SL, Ho YJ, Lucas AM, Tuccinardi T, Baranger AM, Zimmerman SC. "Investigating the Binding Mode of an Inhibitor of the MBNL1·RNA Complex in Myotonic Dystrophy Type 1 (DM1) Leads to the Unexpected Discovery of a DNA-Selective Binder." *Chembiochem*. 2012, 13(17):2505-2509.

35 Manera C, Saccomanni G, Malfitano AM, Bertini S, Castelli F, Laezza C, Ligresti A, Lucchesi V, Tuccinardi T, Rizzolio F, Bifulco M, Di Marzo V, Giordano A, Macchia M, Martinelli A. "Rational design, synthesis and anti-proliferative properties of new CB2 selective cannabinoid receptor ligands: An investigation of the 1,8-naphthyridin-2(1H)-one scaffold." *Eur J Med Chem*. 2012, 52:284-294.

36 Ortore G, Tuccinardi T, Martinelli A. "Computational Studies on Translocator Protein (tspo) and its Ligands." *Curr Top Med Chem*. 2012, 12(4):352-359.

2011

37 Marques SM, Tuccinardi T, Nuti E, Santamaria S, André V, Rossello A, Martinelli A, Santos MA. "Novel 1-hydroxypiperazine-2,6-diones as new leads in the inhibition of metalloproteinases." *J Med Chem*. 2011, 54(24):8289-8298.

38 Granchi C, Roy S, Mottinelli M, Nardini E, Campinoti F, Tuccinardi T, Lanza M, Betti L, Giannaccini G, Lucacchini A, Martinelli A, Macchia M, Minutolo F. Synthesis of sulfonamide-containing N-hydroxyindole-2-carboxylates as inhibitors of human lactate dehydrogenase-isoform 5. *Bioorg Med Chem Lett*. 2011, 21(24):7331-7336.

39 Granchi C, Roy S, De Simone A, Salvetti I, Tuccinardi T, Martinelli A, Macchia M, Lanza M, Betti L, Giannaccini G, Lucacchini A, Giovannetti E, Sciarrillo R, Peters GJ, Minutolo F. "N-Hydroxyindole-based inhibitors of lactate dehydrogenase against cancer cell proliferation." *Eur J Med Chem*. 2011, 46(11):5398-5407.

40 Granchi C, Roy S, Del Fiandra C, Tuccinardi T, Lanza M, Betti L, Giannaccini G, Lucacchini A, Martinelli A, Macchia M, Minutolo F. "Triazole-substituted N-hydroxyindol-2-carboxylates as inhibitors of isoform 5 of human lactate dehydrogenase (hLDH5)" *MedChemComm*. 2011, 2(7), 638-643.

41 Enyedy EA, Horváth L, Hetényi A, Tuccinardi T, Hartinger CG, Keppler BK, Kiss T. "Interactions of the carrier ligands of antidiabetic metal complexes with human serum albumin: a combined spectroscopic and separation approach with molecular modeling studies" *Bioorg Med Chem*. 2011, 19(14):4202-4210.

42 Tuccinardi T, Martinelli A. Protein Kinase Homology Models: Recent Developments and Results. *Curr Med Chem*. 2011;18(19):2848-2853.

43 Carrasco MP, Enyedy EA, Krupenko NI, Krupenko SA, Nuti E, Tuccinardi T, Santamaria S, Rossello A, Martinelli A, Santos MA. "Novel Folate-Hydroxamate Based Antimetabolites: Synthesis and Biological Evaluation." *Med Chem*. 2011, 7(4):265-274.

44 Tuccinardi T, Zizzari AT, Brullo C, Daniele S, Musumeci F, Schenone S, Trincavelli ML, Martini C, Martinelli A, Giorgi G, Botta M. "Substituted pyrazolo[3,4-b]pyridines as human A(1) adenosine antagonists: Developments in understanding the receptor stereoselectivity." *Org Biomol Chem*. 2011, 9(12):4448-4455 (cover of the Volume).

45 Bertini S, De Cupertinis A, Granchi C, Bargagli B, Tuccinardi T, Martinelli A, Macchia M, Gunther JR, Carlson KE, Katzenellenbogen JA, Minutolo F. "Selective And Potent Agonists For Estrogen Receptor Beta Derived From Molecular Refinements Of Salicylaldehydes" *Eur Med Chem*. 2011, 46(6):2453-2462.

- 46 Granchi C, Roy S, Giacomelli C, Macchia M, Tuccinardi T, Martinelli A, Lanza M, Betti L, Giannaccini G, Lucacchini A, Funel N, León LG, Giovannetti E, Peters GJ, Palchadhuri R, Calvaresi EC, Hergenrother PJ, Minutolo F. "Discovery of N-Hydroxyindole-Based Inhibitors of Human Lactate Dehydrogenase Isoform A (LDH-A) as Starvation Agents against Cancer Cells." *J Med Chem*. 2011, 54(6):1599-1612.
- 47 Bajorath J, Barreca ML, Bender A, Bryce R, Hutter M, Laggner C, Laughton C, Martin Y, Mitchell J, Padova A, Renner S, Selzer PM, Sherman W, Sippl W, Taft C, Tuccinardi T, Vistoli G, Willett P. "Ask the experts: focus on computational chemistry" *Future Med Chem*. 2011, 3(8):909-21.
- 48 Tuccinardi T. "Binding-interaction prediction of RNA-binding ligands" *Future Med Chem*. 2011, 3(6):723-733.

2010

- 49 Ortore G, Tuccinardi T, Orlandini E, Martinelli A. "Different Binding Modes of Structurally Diverse Ligands for Human D3DAR." *J Chem Inf Model*. 2010, 50(12):2162-2175.
- 50 Bertini S, Calderone V, Carboni I, Maffei R, Martelli A, Martinelli A, Minutolo F, Rajabi M, Testai L, Tuccinardi T, Ghidoni R, Macchia M. "Synthesis of heterocycle-based analogs of resveratrol and their antitumor and vasorelaxing properties." *Bioorg Med Chem*. 2010, 18(18):6715-6724.
- 51 Rizzolio F, La Montagna R, Tuccinardi T, Russo G, Caputi M, Giordano A. "Adenosine Receptor Ligands in Clinical Trials." *Curr Top Med Chem*. 2010; 10(10):1036-1045.
- 52 Chaves S, Marques SM, Matos AM, Nunes A, Gano L, Tuccinardi T, Martinelli A, Santos MA. "New Tris(hydroxypyridinones) as Iron and Aluminium Sequestering Agents: Synthesis, Complexation and In Vivo Studies." *Chemistry - A European Journal* 2010, 16(34):10535-10545.
- 53 Tuccinardi T, Botta M, Giordano A, Martinelli A. "Protein Kinases: Docking and Homology Modeling Reliability." *J Chem Inf Model*. 2010, 50(8):1432-1441.
- 54 Rizzolio F, Tuccinardi T, Caligiuri I, Lucchetti C, Giordano A. "CDK inhibitors: from the bench to clinical trials." *Curr. Drug Targets*. 2010;11(3):279-290.

2009

- 55 Nuti E, Panelli L, Casalini F, Avramova SI, Orlandini E, Santamaria S, Nencetti S, Tuccinardi T, Martinelli A, Cercignani G, D'Amelio N, Maiocchi A, Uggeri F, Rossello A. "Design, Synthesis, Biological Evaluation, and NMR Studies of a New Series of Arylsulfones As Selective and Potent Matrix Metalloproteinase-12 Inhibitors." *J Med Chem* 2009, 52(20):6347-6361.
- 56 Tuccinardi T, Taliani S, Bellandi M, Da Settimo F, Da Pozzo E, Martini C, Martinelli A. "A virtual screening study of the 18-kDa translocator protein using pharmacophore models combined with 3D-QSAR studies." *ChemMedChem* 2009, 4(10):1686-1694.
- 57 Nuti E, Casalini F, Avramova SI, Santamaria S, Cercignani G, Marinelli L, La Pietra V, Novellino E, Orlandini E, Nencetti S, Tuccinardi T, Martinelli A, Lim NH, Visse R, Nagase H, Rossello A. "N-O-Isopropyl Sulfonamido-Based Hydroxamates: Design, Synthesis and Biological Evaluation of Selective Matrix Metalloproteinase-13 Inhibitors as Potential Therapeutic Agents for Osteoarthritis." *J Med Chem* 2009, 52(15):4757-4773.
- 58 Tuccinardi T, Ortore G, Santos MA, Marques SM, Nuti E, Rossello A, Martinelli A. "Multitemplate Alignment Method for the Development of a Reliable 3D-QSAR Model for the Analysis of MMP3 Inhibitors", *J Chem Inf Model*. 2009, 49(7):1715-1724.
- 59 Manera C, Saccomanni G, Adinolfi B, Benetti V, Ligresti A, Cascio M, Tuccinardi T, Lucchesi V, Martinelli A, Nieri P, Masini E, Di Marzo V, Ferrarini PL. "Rational Design, Synthesis and Pharmacological Properties of New 1,8-Naphthyridin-2(1*H*)-on-3-Carboxamide Derivatives as Highly Selective Cannabinoid-2 Receptor Agonists." *J Med Chem* 2009, 52(12):3644-3651.
- 60 Tuccinardi T. "Docking-Based Virtual Screening: Recent Developments" *Comb. Chem. High Throughput Screen*. 2009, 12(3):303-314.

- 61 Brizzi A, Brizzi V, Cascio MG, Corelli F, Guida F, Ligresti A, Maione S, Martinelli A, Pasquini S, Tuccinardi T, Di Marzo V. "New Resorcinol-Anandamide "Hybrids" as Potent Cannabinoid Receptor Ligands Endowed with Antinociceptive Activity in Vivo", *J Med Chem* 2009, 52(8):2506-2514.
- 62 La Motta C, Sartini S, Tuccinardi T, Nerini E, Da Settimo F, Martinelli A. "Computational Studies of Epidermal Growth Factor Receptor: Docking Reliability, Three-Dimensional Quantitative Structure-Activity Relationship Analysis, and Virtual Screening Studies", *J Med Chem* 2009, 52(4):964-975.
- 63 Minutolo F, Bertini S, Granchi C, Marchitello T, Prota G, Rapposelli S, Tuccinardi T, Martinelli A, Gunther J R, Carlson K E, Katzenellenbogen J A, Macchia M. "Structural Evolutions of Salicylaldoximes as Selective Agonists for Estrogen Receptor Beta", *J Med Chem* 2009, 52(3):858-867.

2008

- 64 Marques SM, Nuti E, Rossello A, Supuran CT, Tuccinardi T, Martinelli A, Santos MA. "Dual Inhibitors of Matrix Metalloproteinases and Carbonic Anhydrases: Iminodiacetyl-Based Hydroxamate-Benzenesulfonamide Conjugates." *J Med Chem* 2008, 51(24):7968-7979.
- 65 Cincinelli R, Cassinelli G, Dallavalle S, Lanzi C, Merlini L, Botta M, Tuccinardi T, Martinelli A, Penco S, Zunino F. "Synthesis, modeling and RET protein kinase inhibitory activity of 3- and 4-substituted- β -carbolin-1-ones." *J Med Chem* 2008, 51(24):7777-7787.
- 66 Baraldi PG, Preti D, Tabrizi MA, Romagnoli R, Saponaro G, Baraldi S, Botta M, Bernardini C, Tafi A, Tuccinardi T, Martinelli A, Varani K, Borea PA. "Structure-Activity Relationship Studies of a New Series of Imidazo[2,1-*f*]purinones as Potent and Selective A₃ Adenosine Receptor Antagonists" *Bioorg Med Chem* 2008, 16(24):10281-10294.
- 67 Tuccinardi T, Nuti E, Ortore G, Rossello A, Avramova SI, Martinelli A. "Development of a receptor-based 3D-QSAR study for the analysis of MMP2, MMP3, and MMP9 inhibitors", *Bioorg Med Chem* 2008, 16(16):7749-7758.
- 68 Manera C, Tuccinardi T, Martinelli A. "Indoles and related compounds as cannabinoid ligands" *Mini rev. Med. Chem.* 2008, 8(4):370-387.
- 69 Tuccinardi T, Schenone S, Bondavalli F, Brullo C, Bruno O, Ranise A, Zizzari A, Tintori C, Ciampi O, Trincavelli ML, Martini C, Martinelli A, Botta M. "Substituted Pyrazolo[3,4-*b*]pyridines as potent and selective A₁ adenosine antagonists: synthesis, biological evaluation and development of an A₁ bovine receptor model", *ChemMedChem* 2008, 3(6):898-913.
- 70 Rapposelli S, Cuboni S, Digiacocono M, Lapucci A, Trincavelli ML, Tuccinardi T, Balsamo A. "Synthesis and AT1 affinity evaluation of benzamidophenyl analogs of known AT1 receptor ligands with similar aromatic skeleton", *Arkivoc* 2008, (ii) 268-286.
- 71 Martinelli A, Tuccinardi T. "Molecular modeling of adenosine receptors: new results and trends" *Med. Res. Rev.* 2008 28(2):247-277.
- 72 Cosimelli B, Greco G, Ehlardo M, Novellino E, Da Settimo F, Taliani S, La Motta C, Bellandi M, Tuccinardi T, Martinelli A, Ciampi O, Trincavelli ML, Martini C. "Derivatives of 4-Amino-6-hydroxy-2-mercaptopyrimidine (AHMP) as Novel, Potent, and Selective A₃ Adenosine Receptor Antagonists" *J Med Chem.* 2008, 51(6):1764-1770.
- 73 Minutolo F, Bellini R, Bertini S, Carboni Isabella, Lapucci A, Pistolesi L, Prota G, Rapposelli S, Solati F, Tuccinardi T, Martinelli A, Stossi F, Carlson K, Katzenellenbogen B, Katzenellenbogen J, Macchia M. "Monoaryl-substituted Salicylaldoximes as Ligands for Estrogen Receptor Beta" *J Med Chem.* 2008, 51(5):1344-1351.

2007

- 74 Tuccinardi T, Ortore G, Supuran CT, Rossello A, Martinelli A. "Homology Modelling and Receptor-Based 3D-QSAR study of Carbonic Anhydrase IX", *J Chem Inf Mod.* 2007, 47(6):2253-2262.

- 75 Da Settimo F, Primofiore G, Taliani S, Marini AM, La Motta C, Simorini F, Salerno S, Sergianni V, Tuccinardi T, Martinelli A, Cosimelli B, Greco G, Novellino E, Trincavelli ML, Martini C. "5-Amino-2-phenyl[1,2,3]triazolo[1,2-a][1,2,4]benzotriazin-1-one: A Versatile Scaffold to Obtain Potent and Selective A₃ Adenosine Receptor Antagonists", *J Med Chem.* 2007, 50(23):5676-5684.
- 76 Tuccinardi T, Martinelli A. "Computational Approaches on Angiotensin Receptors and their Ligands: Recent Developments and Results" *Curr. Med. Chem.* 2007, 14(29):3105-3121.
- 77 Manera C, Cascio MG, Benetti V, Allarà M, Tuccinardi T, Martinelli A, Saccomanni G, Vivoli E, Ghelardini C, Di Marzo V, Ferrarini PL. "New 1,8-naphthyridine and quinoline derivatives as CB₂ selective agonists" *Bioorg Med Chem Lett.* 2007, 17(23):6505-6510.
- 78 Brizzi A, Brizzi V, Martinelli A, Tuccinardi T, Cascio MG, Bisogno T, Di Marzo V. "Design, Synthesis and binding studies of new potent ligands of cannabinoid receptor (II)", *Bioorg Med Chem.* 2007, 15(16):5406-5416.
- 79 Tuccinardi T, Manetti F, Schenone S, Martinelli A, Botta M. "Construction and Validation of a RET TK Catalytic Domain by Homology Modeling", *J Chem Inf Mod.* 2007 47(2):644-655.
- 80 Nuti E, Tuccinardi T, Rossello A. "Matrix Metalloproteinase Inhibitors: New Challenges in the Era of Post Broad-Spectrum Inhibitors" *Curr. Pharm. Design.* 2007, 13(20):2087-2100.
- 81 Tuccinardi T, Nuti E, Ortore G, Supuran CT, Rossello A, Martinelli A. "Analysis of human Carbonic Anhydrase II: Docking Reliability and Receptor-Based 3D-QSAR study", *J Chem Inf Mod.* 2007 47(2):515-525.
- 82 Tuccinardi T, Cascio MG, Di Marzo V, Manera C, Ortore G, Saccomanni G, Martinelli A. "Structure-Based Virtual screening: Identification of novel CB₂ receptor ligands", *LDDD.* 2007, 4(1):15-19.
- 2006**
- 83 Santos AM, Marques SM, Tuccinardi T, Carelli P, Panelli L, Rossello A. "Design, Synthesis And Molecular Modeling Study Of Iminodiacetyl Monohydroxamic Acid Derivatives As Mmp Inhibitors", *Bioorg Med Chem.* 2006, 14(22):7539-7550.
- 84 Manera C, Benetti V, Castelli MP, Cavallini T, Lazzarotti S, Pibiri F, Saccomanni G, Tuccinardi T, Vannacci A, Martinelli A, Ferrarini PL. "Design, synthesis and biological evaluation of new 1,8-naphthyridin-4(1H)-on-3-carboxamide and quinolin-4(1H)-on-3-carboxamide derivatives as CB₂ selective agonists", *J Med Chem.* 2006, 49(16):5947-5957.
- 85 Tuccinardi T, Bertini S, Martinelli A, Minutolo F, Ortore G, Placanica G, Prota G, Rapposelli S, Carlson KE, Katzenellenbogen JA, Macchia M. "Synthesis of Anthranilyldoxime Derivatives as Estrogen Receptor Ligands and Computational Prediction of Binding Modes", *J Med Chem.* 2006, 49(16):5001-5012.
- 86 Tafi A, Bernardini C, Botta M, Corelli F, Andreini M, Martinelli A, Ortore G, Baraldi PG, Fruttarolo F, Borea PA, Tuccinardi T. "Pharmacophore based receptor modeling: a novel approach to protein model optimization. The case of Adenosine A₃ receptor antagonists", *J Med Chem.* 2006, 49(14):4085-4097.
- 87 Martinelli A, Tuccinardi T. "GPCR modeling: methods and validation. An overview of recent developments" *Exp. Opin. on Drug Disc.* 2006, 1(5):459-476.
- 88 Tuccinardi T, Calderone V, Rapposelli S, Martinelli A. "Proposal of a new binding orientation for non-peptide AT₁ antagonists: homology model, docking and 3D-QSAR analysis", *J Med Chem.* 2006, 49(14):4305-4316.
- 89 Minutolo F, Bertini S, Martinelli A, Ortore G, Placanica G, Prota G, Rapposelli S, Tuccinardi T, Sheng S, Carlson KE, Katzenellenbogen BS, Katzenellenbogen JA, Macchia M. "Salicylaldoximes and anthranilyldoximes as alternatives phenol-based estrogen receptor ligands", *Arkivoc* 2006, (viii) 83-94.

- 90 Tuccinardi T, Martinelli A, Nuti E, Carelli P, Balzano F, Uccello-Barretta G, Murphy G, Rossello A. "Amber force field implementation, molecular modelling study, synthesis and MMP-1/MMP-2 inhibition profile of (*R*)- and (*S*)-*N*-hydroxy-2-(*N*-isopropoxybiphenyl-4-ylsulfonamido)-3-methylbutanamides", *Bioorg Med Chem*. 2006, 14(12):4260-4276 (cover of the Volume).
- 91 Tuccinardi T, Manera C, Ortore G, Saccomanni G, Martinelli A. "Adenosine receptor modelling. A₁/A_{2a} selectivity", *Eur J Med Chem*. 2006, 41(3):321-329.
- 92 Ortore G, Tuccinardi T, Bertini S, Martinelli A. "A theoretical study to investigate D2DAR/D4DAR selectivity: receptor modeling and molecular docking of dopaminergic ligands", *J Med Chem*. 2006, 49(4):1397-1407.
- 93 Tuccinardi T, Ferrarini PL, Manera C, Ortore G, Saccomanni G, Martinelli A. "Cannabinoid CB2/CB1 selectivity. Receptor modelling and automated docking analysis", *J Med Chem*. 2006, 49(3):984-994.
- 94 Minutolo F, Bertini S, Betti L, Danesi R, Gervasi G, Giannaccini G, Martinelli A, Papini A, Peroni E, Placanica G, Rapposelli S, Tuccinardi T, Macchia M. "Synthesis of stable analogues of geranylgeranyl diphosphate possessing a (z,e,e)-geranylgeranyl side-chain, docking analysis and biological assays for their prenyl protein transferase inhibitory activity", *Chem Med Chem*. 2006, 1(2):218-224.
- 2005**
- 95 Manera C, Betti L, Cavallini T, Giannaccini G, Martinelli A, Ortore G, Saccomanni G, Trincavelli L, Tuccinardi T, Ferrarini PL. "1,8-Naphthyridin-4-one derivatives as new ligands of A_{2A} adenosine receptors", *Bioorg Med Chem Lett*. 2005, 15(20):4604-4610.
- 96 Rossello A, Nuti E, Catalani MP, Carelli P, Orlandini E, Rapposelli S, Tuccinardi T, Atkinson SJ, Murphy G, Balsamo A. "A new development of matrix metalloproteinase inhibitors: twin hydroxamic acids as potent inhibitors of MMPs", *Bioorg Med Chem Lett*. 2005, 15(9):2311-2314.
- 2004**
- 97 Ferrarini PL, Betti L, Cavallini T, Giannaccini G, Lucacchini A, Manera C, Martinelli A, Ortore G, Saccomanni G, Tuccinardi T. "Study on affinity profile toward native human and bovine adenosine receptors of a series of 1,8-naphthyridine derivatives", *J Med Chem*. 2004, 47(12):3019-3031.

BOOK CHAPTERS

- 98 Martinelli A, Tuccinardi T. "QSAR of carbonic anhydrase inhibitors and their impact on drug design", *Drug Design of Zinc-Enzyme Inhibitors: Functional, Structural, and Disease Applications*. John Wiley & Sons, Inc.
- 99 Tuccinardi T, Martinelli A. "QSAR studies of MMP inhibitors", *Drug Design of Zinc-Enzyme Inhibitors: Functional, Structural, and Disease Applications*. John Wiley & Sons, Inc.
- 100 Marques SM, Chaves S, Rossello A, Tuccinardi T, Santos MA. "Iminodiacetyl-monohydroxamate derivatives as potent and selective MMP inhibitors", *Metal Ions in Biology and Medicine* 2006, 9, 117-121.

PATENTS

- 101 Varasi M, Di Bussolo V, Granchi C, Macchia M, Martinelli A, Minutolo F, Morelli M, Tuccinardi T. "Compounds inhibiting the enzyme lactate dehydrogenase (LDH), pharmaceutical compositions and uses thereof", EP13172098.9 (2013)
- 102 Rossello A, Nuti E, Orlandini E, Tuccinardi T. "Aryl-sulphonamidic dimers as metalloproteases inhibitors." PCT Int. Appl. WO2010010080 (2010).
- 103 Rossello A, Nuti E, Orlandini E, Balsamo A, Tuccinardi T. "Compounds having aryl-sulphonamidic structure useful as metalloproteases inhibitors." PCT Int. Appl. WO2008113756 (2008).

- 104 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).

BIBLIOMETRIC PARAMETERS

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ORAL COMMUNICATIONS

- 1 T. Tuccinardi. Principles of Computer-aided Drug Design. (Invited Seminar) University of Genoa, October 26 2015 Genova (Italy).
- 2 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).
- 3 T. Tuccinardi. New trends in Computer-aided Drug Design. (Invited Seminar) University of Genoa, December 9 2014 Genova (Italy).
- 4 T. Tuccinardi. *Computational Methods in Drug Discovery*. (Invited Seminar) Centro Ricerche Oncologiche Mercogliano (CROM), July 24 2012 Mercogliano (AV, Italy).
- 5 T. Tuccinardi. *Computational Studies of the Molecular Modeling and Virtual Screening Laboratory*. "Computationally Driven Drug Discovery" November 21-23, 2011 L'Aquila (Italy).
- 6 T. Tuccinardi. *Small modifications for improving the ligand activity*. "XX National Meeting on Medicinal Chemistry" September 12-16, 2010 Abano Terme (Italy).
- 7 T. Tuccinardi, A. Martinelli. *Protein kinases: docking and homology modeling reliability*. "28th Camerino-Cyprus-Noordwijkerhout Symposium, Trekking through Receptor Chemistry" May 16-20, 2010, Camerino (Italy).
- 8 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).
- 9 T. Tuccinardi. *GPCR modeling: methods and validation*. (Invited Seminar) University of Florence, February 15 2007 Firenze (Italy).
- 10 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).
- 11 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 Institutes Of Health (2012) – "Design, synthesis, and evaluation of lactate dehydrogenase inhibitors"
- 2 Italian Ministry of Public Education, PRIN 2011 – "Design and optimization of new anticancer compounds".
- 3 Associazione Italiana per la Ricerca sul Cancro (AIRC 2015) – "Inhibition of Pin1 to improve carboplatin and taxol cytotoxicity in high-grade serous ovariancancer".

COMPLETED RESEARCH SUPPORT

- 1 IRCCS European Oncology Institute (2013) – “Application and Optimization of Virtual Screening Techniques”.
- 2 Amyotrophic Lateral Sclerosis Research Agency (ARISLA 2012) – “Positron Emission Tomography and Amyotrophic Lateral Sclerosis: Study of Cannabinoid subtype 2 receptor expression in ALS experimental model”.
- 3 IRCCS European Oncology Institute (2012) – “Evaluation of new LDH inhibitors”.
- 4 IRCCS European Oncology Institute (2011) – “Identification of new kinase inhibitors”.
- 5 Multiple Sclerosis Italian Foundation (FISM 2011) – “Design, synthesis and study of the therapeutic efficacy of novel modulators of the endocannabinoid system in multiple sclerosis”.
- 6 Italian Ministry of Public Education, PRIN 2010 – “Design and synthesis of endocannabinoid modulators”.
- 7 Monte dei Paschi di Siena Foundation (2007) – “Modulation of MMPs involved in brain pathologies”.

REFERENCES

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