

Arianna Gelain

PERSONAL INFORMATION

Dipartimento di Scienze Farmaceutiche, Università degli Studi di Milano
Via Luigi Mangiagalli 25 - 20133 Milano, Italy
Tel. +39 02 503 19369
Fax. +39 02 503 19359
e-mail: arianna.gelain@unimi.it
<http://www.disfarm.unimi.it>

PERSONAL STATEMENT

Permanent researcher, Assistant Professor

WORK EXPERIENCE

- 2004-today **Assistant Professor**
Faculty of Pharmaceutical Science, Pharmacy, Pharmaceutical Chemistry and Technology degree courses.
- 2004-today **Permanent researcher (scientific-disciplinary sector CHIM/08)**
Department of Pharmaceutical Science (DISFARM), University of Milan
The scientific activity concerns the design and synthesis of novel small molecules with potential pharmacological activity and the related structure-activity relationships studies. The research is mainly focused on the identification of compounds endowed with antiproliferative (in particular STAT3 inhibitors) and antimicrobial (antitubercular, antibiofilm and antimalarial) activities.
- 2000-2003 **Research fellow**
Grant from the University of Milan. Research topic: synthesis of pyridazine derivatives as potentially useful biological tools
- 1998-1999 **Research fellow**
Grant from Abbott Labs. in Milan. Research topic: synthesis of pyridazine derivatives structurally related to epibatidine
- 1996-1997 **Research fellow**
Postdoctoral grant from the University of Modena. Research topic: synthesis of naftalenic derivatives as thymidilate synthase inhibitors.
- 1995 **Research fellow**
Grant from National Research Council (CNR). Research topic: Synthesis of monomers and polymers for CZE analysis.

EDUCATION

- 1995 **PhD in Medicinal Chemistry**
VII cycle, University of Milan
- 1992 **Authorization to practice the Pharmacist profession**
University of Milan
State examination for obtaining the qualification to practice the profession of the Pharmacist
- 1991 **Degree in Pharmaceutical Chemistry and Technology**
University of Milan

PERSONAL SKILLS

Mother tongue Italian

Other languages	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken interaction	Spoken production	
English	Independent user	Independent user	Independent user	Independent user	Independent user

Job-related skills Medicinal Chemistry competences concerning the design and synthesis of organic small molecules as ligands for receptors (protein, enzymes etc.) by conventional synthetic organic chemistry as well as microwave assisted organic chemistry methodologies.
 Ability to use: microwave synthesizer, Flash Chromatography, NMR, ATR-FTIR, analytical HPLC.
 Good knowledge:

- Office suite
- Molecular editor (ChemDraw)
- Data banks (SciFinder, Reaxys, PubMed)

Digital skills

SELF-ASSESSMENT				
Information processing	Communication	Content creation	Safety	Problem solving
Independent user	Independent user	Independent user	Independent user	Basic user

Good skills of Office suite tools (word processor, presentation software) and ChemDraw.

Driving licence B

ADDITIONAL INFORMATION

Teaching activity	<p>2012-today, Drug Analysis (qualitative, 7 CFU), Pharmacy degree course, University of Milan.</p> <p>2010-2011, Drug Analysis (quantitative, 9 CFU), Pharmaceutical Chemistry and Technology degree course, University of Milan.</p> <p>2009-2010, Drug Analysis (quantitative, 11 CFU), Pharmaceutical Chemistry and Technology degree course, University of Milan.</p> <p>2007-2009, Drug Analysis (qualitative, 7 CFU), Pharmacy degree course, University of Milan.</p> <p>2004-2006, Drug Analysis (quantitative, module I, 5 CFU) Chemical Safety and Toxicological Environmental Sciences degree course, University of Milan.</p> <p>2006-2016, member of examination commission of Medicinal Chemistry I of Pharmaceutical Chemistry and Technology degree course, University of Milan.</p>
Tutorial activity	<p>Supervisor for preparation of degree thesis (more than 40) in Pharmaceutical Chemistry and Technology (7 Erasmus Programme) and Pharmacy (University of Milan).</p> <p>2009-2011, PhD tutor (Doctorate School in Chemical Sciences and Technologies, Curriculum Pharmaceutical Sciences, XXIV cycle) University of Milan</p>
Institutional activities	<p>Participation at the collegial governance: member of Department Council and Interdepartmental didactic board of Pharmacy degree course.</p> <p>Scientific responsible of Erasmus programme for Granada (Spain) and Semmelweis (Budapest, Hungary) Universities.</p> <p>Member of the supervisory committee for the practical tests of dosing and recognition of drugs within the state exams for the qualification to practice as pharmacist.</p> <p>Member of the supervisory committee for the admission test.</p>
Projects	<p>Participant in peer-reviewed research projects:</p> <p>Linea 2 "Dotazione annuale per attività istituzionali" (2015-2018)</p> <p>PRIN 2010-2011 (20105YY2HL_007), Natural and Synthetic Systems with antitumor activity, (2013-2015)</p> <p>Fondazione Cariplo grant n. 2011-0277 ANFOMAT-Novel materials for medical devices based on bifunctionalized surfaces with antifouling properties (2012-2014).</p>
Memberships	<p>Division of Pharmaceutical Chemistry and Organic Chemistry of the Italian Chemical Society.</p> <p>Member of CRC LaMPo</p>
Conferences	<p>Recently attended at:</p> <p><i>XXXVIII Convegno Nazionale della Divisione di Chimica Organica della Società Chimica Italiana CDCO 2018, 9-13 Settembre 2018, Milano</i></p> <p>Poster: A click chemistry approach to explore a new scaffold for potential antitubercular agents, A. Gelain, M. Mori, S. Villa, L.R. Chiarelli, F. Meneghetti, P61, pag. 197</p> <p><i>4th International Workshop on Pericyclic Reactions and Synthesis of Hetero- and Carbocyclic Systems, 28-30 June, 2017, Milan</i></p> <p>Poster: A click chemistry approach to synthesize novel potential antimalarial agents targeting Atg8-Atg3 protein-protein interaction, A. Gelain, S. Villa, L. Legnani, D. Colombo, J. Bosch, G. Grazioso, P7, pag. 58</p> <p><i>6th World Congress on Medicinal Chemistry and Drug Design, June 7-8, 2017, Milan</i></p> <p>Posters:</p> <p>New 1,2,5-oxadiazole Pt(II) complex endowed with STAT3 inhibitory properties as promising anticancer agents, A. Gelain, S. Villa, F. Meneghetti, G. Facchetti, N. Ferri, A. Asai, V. Gandin, C. Marzano, I. Rimoldi, MCPP009</p> <p>Synthesis of novel furan-based antituberculars potentially targeting the methionine aminopeptidases (<i>MtMetAP1a</i>), A. Gelain, S. Villa, M. Mori, L. R. Chiarelli, L. Costantino, T. Tuccinardi, F. Meneghetti, MCPP010</p> <p><i>XXIV National Meeting in Medicinal Chemistry, September 11-14, 2016, Perugia</i></p> <p>Poster: New inhibitors of Salicylate Synthase (MbtI) from <i>M. Tuberculosis</i>. A promising strategy to antitubercular drugs, S. Villa, A. Gelain, D. Barlocco, E. Pini, G. Beretta, M. Mori, L. Costantino, L.R. Chiarelli, M.R. Pasca, D. Bonanni, T. Tuccinardi, F. Meneghetti, PC-161</p> <p>Poster: Oxadiazole Pt(II) complex as STAT3 inhibitor in anticancer therapy, F. Porta, G. Facchetti, S. Villa, A. Gelain, M. Porcino, F. Meneghetti, D. Barlocco, N. Ferri, A. Asai, I. Rimoldi, FC-1</p>

XXV Congresso Nazionale della Società Chimica Italiana, 7-12 Settembre 2014, Rende (CS)
 Oral communication: Sviluppo di MD77: nuovi derivati eterociclici inibenti STAT3, **A. Gelain**, Far-O-13

XXII National meeting on Medicinal Chemistry, September 10-13, 2013, Rome

Poster: Identification of a novel STAT3 inhibitor structurally related to the oxadiazole derivative MD77, D. Masciocchi S. Villa, F. Porta, D. Barlocco, F. Meneghetti, B.-M. Kwon, A. Asai, **A. Gelain**, P.OE.15

Publications

Author and co-author of 46 scientific publications in peer reviewed and SCOPUS indexed international journals, one chapter book and more than 50 contributions (oral and poster communications) presented at national and international congresses.

Author ID: 0000-0001-9104-732X ORCID

Reviewer for several journal as Journal of Medicinal Chemistry, ChemMedChem e Journal of Heterocyclic Chemistry.

Recent papers (total list available on <https://air.unimi.it>):

- 1) **A. Gelain**, M. Mori, F. Meneghetti, F. Porta, L. Basile, G. Marverti, A. Asai, M. Hyeraci, A.N. Garcia-Argaez, L. Dalla Via, S. Guccione, S. Villa, "Exploring the biological activity of a library of 1,2,5-oxadiazole derivatives endowed with antiproliferative activity", *Anticancer Research*, 2019, 39, 1, 135-144
- 2) L. R. Chiarelli, M. Mori, D. Barlocco, G. Beretta, **A. Gelain**, E. Pini, M. Porcino, G. Mori, G. Stelitano, L. Costantino, M. Lapillo, D. Bonanni, G. Poli, T. Tuccinardi, S. Villa, F. Meneghetti, "Discovery and Development of Novel Salicylate Synthase (MbtI) Furanic Inhibitors as Antitubercular Agents", *Eur. J. Med. Chem.*, 2018, 155, 754-763.
- 3) S. Villa, L. Legnani, D. Colombo, **A. Gelain**, C. Lammi, D. Bongiorno, D.P. Iboudo, K.E. McGee, J. Bosch, G. Grazioso, "Structure-based drug design, synthesis and biological assays of *P. falciparum* Atg3-Atg8 protein-protein interaction inhibitors", *J. Comput. Aided Mol. Des.*, 2018, 32 (3), 473-486.
- 4) E. Pini, G. Poli, T. Tuccinardi, L. R. Chiarelli, M. Mori, **A. Gelain**, L. Costantino, S. Villa, F. Meneghetti, D. Barlocco, "New chromane-based derivatives as inhibitors of *Mycobacterium tuberculosis* salicylate synthase (MbtI): preliminary biological evaluation and molecular modeling studies", *Molecules*, 2018, 23, 1506-1520.
- 5) S. Dell'orto, C. Cattò, F. Villa, F. Forlani, E. Vassallo, M. Morra, F. Cappitelli, S. Villa, **A. Gelain**, "Low density polyethylene functionalized with antibiofilm compounds inhibits *Escherichia coli* cell adhesion", *Journal of Biomedical Materials Research - Part A* 2017, 105, 3251-3261.
- 6) F. Porta, G. Facchetti, N. Ferri, **A. Gelain**, F. Meneghetti, S. Villa, D. Barlocco, D. Masciocchi, A. Asai, N. Miyoshi, S. Marchianò, B.-M. Kwon, Y. Jin, V. Gandin, C. Marzano, I. Rimoldi, "An in vivo active 1,2,5-oxadiazole Pt(II) complex: a promising anticancer agent endowed with STAT3 inhibitory properties", *Eur. J. Med. Chem.* 2017, 131:196-206.
- 7) F. Porta, **A. Gelain**, D. Barlocco, N. Ferri, S. Marchianò, V. Cappello, L. Basile, S. Guccione, F. Meneghetti, S. Villa, "A field-based disparity analysis of new 1,2,5-oxadiazole derivatives endowed with antiproliferative activity", *Chem. Biol. Drug Des.*, 2017, 90, 820-839.
- 8) C. Cattò, G. Grazioso, S. Dell'Orto, **A. Gelain**, S. Villa, V. Marzano, A. Vitali, F. Villa, F. Cappitelli, F. Forlani, "The response of *Escherichia coli* biofilm to salicylic acid", *Biofouling*, 2017, 33(4), 235-251.
- 9) E. Gabriele, F. Porta, G. Facchetti, C. Galli, **A. Gelain**, F. Meneghetti, I. Rimoldi, S. Romeo, S. Villa, C. Ricci, N. Ferri, A. Asai, D. Barlocco, A. Sparatore, "Synthesis of new dithiolethione and methanethiosulfonate systems endowed with pharmaceutical interest", *Arkivoc*, 2017, (2), 235-250.
- 10) F. Meneghetti, S. Villa, **A. Gelain**, D. Barlocco, L. R. Chiarelli, M. R. Pasca, L. Costantino, "Iron acquisition pathways as targets for antitubercular drugs", *Curr. Med. Chem.*, 2016, 23, 4009-4026.
- 11) G. Poli, **A. Gelain**, F. Porta, A. Asai, A. Martinelli, T. Tuccinardi, "Identification of a new STAT3 dimerization inhibitor through a pharmacophore-based virtual screening approach", *Journal of Enzyme Inhibition and Medicinal chemistry*, 2016, 31, 1011-1017.
- 12) F. Meneghetti, S. Villa, D. Masciocchi, D. Barlocco, L. Toma, D.C. Han, B.-M. Kwon, N. Ogo, A. Asai, L. Legnani, **A. Gelain**, "Ureido-Pyridazinone Derivatives: Insights into the Structural and Conformational Properties for STAT3 Inhibition", *Eur. J. Org. Chem.*, 2015, 22, 4907-4912.
- 13) L. Fanzani, F. Porta, F. Meneghetti, S. Villa, **A. Gelain**, A. P. Lucarelli, E. Parisini,

“Mycobacterium tuberculosis low molecular weight phosphatases (MPtpA and MPtpB): from biological insight to inhibitors”, Curr. Med. Chem., 2015, 22, 3110-3132.

14) S. Dell’Orto, D. Masciocchi, S. Villa, F. Meneghetti, G. Celentano, D. Barlocco, D. Colombo, L. Legnani, L. Toma, Y. J. Jeon, B.-M. Kwon, A. Asai, **A. Gelain**, *“Modeling, synthesis and NMR characterization of novel chimera compounds targeting STAT3”*, MedChemComm., 2014, 5, 1651-1657.

15) **A. Gelain**, L. Rizzi, L. Legnani, A. Pacini, K. Spyridaki, V. Karageorgos, G. Liapakis, S. Villa, *“Novel peptidomimetics related to gonadotropin-releasing hormone (GnRH)”*, MedChemComm., 2015, 6, 1656-1665.

16) C. Cattò, S. Dell’Orto, F. Villa, S. Villa, **A. Gelain**, A. Vitali, V. Marzano, S. Baroni, F. Forlani, F. Cappitelli, *“Unravelling the structural and molecular basis responsible for the anti-biofilm activity of zosteric acid”*, PLoS One, 2015, 10, Article number 0131519

17) F. Villa, S. Villa, **A. Gelain**, F. Cappitelli, *“Sub-lethal Activity of Small Molecules from Natural sources and their synthetic”*, Topics in Medicinal Chemistry, 2013, 13, 3184-3204.

18) F. Meneghetti, D. Masciocchi, **A. Gelain**, S. Villa, *“Crystal structure of 3-(3-oxo-4,4a,5,6-tetrahydro-3H-benzof[h]cinnolin-2-yl-propionic acid”*, Acta Cryst., 2014, 70, o1088-o1089.

19) D. Masciocchi, **A. Gelain**, F. Porta, F. Meneghetti, A. Pedretti, G. Celentano, D. Barlocco, L. Legnani, L. Toma, B-M Kwon, A. Asai, S. Villa, *“Synthesis, structure-activity relationships and stereochemical investigations on new tricyclic pyridazinone derivatives as potential STAT3 inhibitors”*, MedChemComm., 2013, 4, 1181-1188.

Personal information

I authorize the handling of personal information in this curriculum, according to D.Lgs n. 196/03 and following modifications and Regulations EU 679/2016 (General Regulations concerning Data Protection or GRDP) and art. 7 of University Regulations concerning protection of personal information.

I authorize, according to D.lgs 14/03/2013 n. 33 concerning transparency, in case of conferment of the position and of the fellowship, the publication of this curriculum in the web site of Università degli Studi di Milano in the section “Amministrazione trasparente”, “Consulenti e collaboratori”

Milan, 21/02/2019

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