

CURRICULUM VITAE

PERSONAL

Name: Salvatore Guccione

Date of birth: March 20th 1962 (Catania)

Marital Status: Married with Maria Grazia, nee Caruso . Two daughters:
Camilla 15 years old /Beatrice 15 months years old; one son,
nine years old: Alessandro.

Home Address: via M. Renato Imbriani 183, I-95128 Catania (Italy).

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viale Andrea Doria 6, Ed. 12 Città Universitaria, I-95125
Catania (Italy).

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EDUCATION

1992 Ph.D. in Pharmaceutical Sciences. University of Catania. Advisor: Prof.
Filippo Russo.

1986 Degree in Pharmacy (*curriculum*: Medicinal Chemistry) taken "*summa cum laude*". Faculty of Pharmacy, University of Catania. Supervisor : Prof.
Filippo Russo.

Professional Experience

Dipartimento di Scienze Farmaceutiche 1986-present:

1996: stage in Computational Chemistry (Prof. T. Langer). University of
Innsbruck , Institut für Pharmazeutische Chemie .

1993-1996: Researcher

1992-1993: Grant by the University of Catania

1988-1991: Ph.D. Student

Thesis: *Synthesis of polycondensed heterocycles containing the pyrazole nucleus: a new approach in the area of anti-inflammatory and analgesic agents.*

(1987-1991): Advanced Course in Medicinal Chemistry and National Seminar for Ph.D. Students.

1986-1988: Grant by the University of Catania.

Additional Professional experience:

1988: Course on Modern Chromatographic Techniques ; **1984:** Preliminary School of Photochemistry .

Teaching Experience:

2001- Medicinal Chemistry and Computational Drug Design (Faculty of Pharmacy and graduation course in Biomolecular Chemistry Faculty of Mathematic, Physical and Natural Sciences .

2001-: *Member of the Board Committee* of the new **Magistral Degree** Course in **Biomolecular Chemistry**, Faculty of Mathematic, Physical and Natural Sciences (course in Chemistry).

2000: Tutor of the LEONARDO DA VINCI mobility program for Students.

1999-present: Member of the Dottorato di Ricerca School (Italian Ph.D.) of Biochemical and Biomolecular Sciences (Faculty of Mathematic, Physical and Natural Sciences). Chair: Prof. A Raudino; Founder and *past*-Chair Prof. E. Rizzarelli.

1999-present: Advisor of Student Thesis and Dissertation Committees in the Faculty of Pharmacy and the Faculty of Mathematic, Physical and Natural Sciences (course of Chemistry).

1999-2000: Medicinal Chemistry

1998-1999: Analytical Pharmaceutical Chemistry (Quantitative Chemistry) and Medicinal Chemistry.

1997-1998: Analytical Pharmaceutical Chemistry (Quantitative Chemistry) and Medicinal Chemistry .

1996-1997: Analytical Pharmaceutical Chemistry (Quantitative Chemistry) and Medicinal Chemistry; Lecturer of Computational Medicinal Chemistry in the Ph.D. School in Pharmaceutical Sciences.

1995-1996: Medicinal Chemistry.

1994: Medicinal Chemistry.

1993: Analytical Pharmaceutical Chemistry (Quantitative Chemistry) and Medicinal Chemistry.

Current Professional Affiliations:

Italian Chemical Society

American Chemical Society (Division of Medicinal Chemistry, Organic Chemistry, Chemical Education)

The QSAR & Modelling Society

Molecular Graphic and Modelling Society

Peer Reviews (Journals):

J. Med. Chem., Current Medicinal Chemistry, Eur. J. Pharm. Sci., Letters in Medicinal Chemistry, Journal of Molecular Graphics and Modelling, Internet Electronic Journal of Molecular Design, J. Agricultural and food Chemistry; Biorganic and Medicinal Chemistry; International Journal of Pharmaceutical Medicine(IJPM), J. Computer-Aided Mol. Des. , Biochemical Journal , Journal Biochemical Pharmacology, Journal of Pharmacy and Pharmacology, J. Phys. Org. Chem., J. Heterocyclic Chem

Service and Awards

2008: Book Editor for the Royal Society of Chemistry.

2007: International Scientific Advisory Board and invited Speaker “Current Trends in Drug Discovery Research”(CTDDR-2007). February 17-20, 2007. Central Drug Research Institute, Lucknow (India).

2007: International Scientific Advisory Board & Invited Speaker 11th International Conference (ISCBC – 2007, February 24-26, 2007) on “Advances in Drug Discovery Research Hotel Rama International-Aurangabad

2007: Guest and Chairman at the 6th EWDD (6th European Workshop in Drug Design) , Certosa di Pontignano, Siena, June 3-10.

2007 : European PhD Board of Examiners Universidad de Navarra C.I.F.A. of Pamplona.

2007: Scientific Director of the Spinoff EtnaLead.

2006: International Scientific Advisory Board &Invited Speaker

2nd INTERNATIONAL SYMPOSIUM ON DRUG DISCOVERY AND PROCESS RESEARCH, CDDPR 2006. February 10-12, 2006. Belgaum, Karnataka, (India).

2006 Organizing&Scientific Committee 3rd School on Advanced BioMedicine and BioInformatics. "Proteoms and Proteins"Lipari Island (Italy), July 9 (Sunday)-July 22 (Saturday),

2005-Invited Scientist ROCHE, Basilea, Svizzera. PhD grants allowed by the Company.

2005 International Scientific Advisory Board, Bioactive Heterocycles and Drug Discovery Paradigm, January 8-10, 2005, Rajkot(India).

2004 *Consulting- Invited Scientist* Drug Discovery Ltd, Glasgow (Scozia).

2004-Center for β -testing of the software CATALYST (ACCELRYN INC).

2004-: *outsourcing* Center of BioChemics Consulting SAS (Orleans, France).PhD grants allowed by the Company.

2003 *Invited Scientist* Università di Trømso, INSTITUTE OF MEDICAL BIOLOGY, Department of Pharmacology and appointed as Supervisor of Graduation Thesis University of Tromso.

2002 Group Leader European Commission Human Potential Programme Access To Research Infrastructure

2002: Organization and Chairman of the International Course “Multivariate QSAR Modelling”, June 11-14, Capomulini, Acireale, (CT).

2002:Visiting and consulting Scientist to CHEMOVATION , Horsham, U.K.; Visiting Scientist to ROCHE, Basle. PhD grants allowed by the Company.

2002-. Editorial board Member of several journal of the Bentham Publisher. Invited speaker course for continuing learning in medicine (for Pharmacists), organized by the Health Ministry of the Italian Republic.

2001- INBB member (Institute National of Biosystems and Biostructures)- Academic National Consortium.

2001: Coordinator of the SOCRATES-ERASMUS project

2000 Visiting Scientist to ORGANON, Oss, The Netherlands.

2000-2005: Executive Guest Editor of Current Pharmaceutical Design.

1999-present: Associate Editor of the European Journal of Medicinal Chemistry.

1999-2000: Invited Speaker, "Crystallography and Drug Design '99" (CDD 99) Conference, Lodz (Poland), May 20th-22nd .

1999, 2000: Invited Computational Scientist at the University of Innsbruck, Pharmaceutical Chemistry Department (formerly Institut für Pharmazeutische Chemie).

1998-2000: Italian Co-ordinator of the European Science Exchange Program granted by the Royal Society.

Research : Salvatore Guccione is involved in both experimental and theoretical research. He has expertise in computational chemistry, molecular modelling, Ligand- and Structure-Based Drug Design (pharmacophore generation, 3D-QSAR, virtual libraries generation), and synthesis of bioactive heterocycles.

RECENT SELECTED PUBLICATIONS (10)

1. Orús L. , Pérez-Silanes S. , Oficialdegui A-M., Martínez-Esparza J., Del Castillo J-C., Mourelle M. , Langer T. , Guccione S. , Donzella G .^{d§}, Krovat E.M., Poptodorov K., Lasheras B. , Ballaz S. , Hervías I. , Tordera R., Del Río J., Monge A .

Synthesis and molecular modelling of new 1-(aryl)-3-[4-(aryl)piperazin-1-yl]-1-propane derivatives with high affinity at the serotonin transporter and at 5-HT_{1A} receptors

J. Med. Chem., 45, 19, 4128-4139, 2002.

2. Massimo Fresta, Salvatore Guccione, Andrea R. Beccari, Pio M. Furneri, and Giovanni Puglisi

Combining Molecular Modeling with Experimental Methodologies: Mechanism of Membrane Permeation and Accumulation of Ofloxacin

Bioorg. Med. Chem., 10,12,3871-3889, 2002.

3. Uccello-Barretta, G. , Balzano, F. ,Sicoli, G. , Friglola, C. , Aldana, I. , Monge, A. , Paolino, D. , Guccione, S..

Combining NMR and molecular modelling in a drug delivery context: investigation of the multi-mode inclusion of a new NPY-5 antagonist bromobenzenesulfonamide into β -cyclodextrin.

Bioorganic and Medicinal Chemistry, 12, 2004 , 447-458

4. Rosario Pignatello, Salvatore Guccione, Stefano Forte, Claudia Di Giacomo, Valeria Sorrenti, Luisa Vicari, Gloria Uccello Barretta, Federica Balzano, and Giovanni Puglisi,

Lipophilic conjugates of methotrexate with short-chain alkylamino acids as DHFR inhibitors.

Synthesis, biological evaluation, and molecular modeling.

Bioorganic & Medicinal Chemistry 12 (2004) 2951–2964.

5. Chiara B. Vicentini, Salvatore Guccione, Laura Giurato, Rebecca Ciaccio, Donatella Mares, and Giuseppe Forlani.

Pyrazole Derivatives as Photosynthetic Electron Transport Inhibitors: New Leads and Structure-Activity Relationship.

J. Agric. Food Chem. **2005**, 53, 3848-3855

6. Muñoz-Muriedas J. , Perspicace S. , Bech N., Guccione S. , Orozco M., and Luque F. J.

Hydrophobic Molecular Similarity from MST Fractional Contributions to the Octanol/Water Partition Coefficient

J. Comput-Aided Mol. Des., (2005) 19: 401–419.

7. Gloria Uccello-Barretta, Federica Balzano, Donatella Paolino, Rebecca Ciaccio, and Salvatore Guccione.

Combined NMR-crystallographic and modelling investigation of the inclusion of molsidomine into α -, β - and γ -cyclodextrins.

Bioorg. Med.Chem., 13 (2005) 6502–6512.

8. C. Hildmann, D. Wegener, D. Riester, R. Hempel, A. Schober, J. Merana, L. Giurato, S. Guccione, T.K. Nielsen, R. Ficner, A. Schwienhorst

Substrate and inhibitor specificity of class 1 and class 2 histone deacetylases .

J. Biotechnol., 124, **1**, 258-270, 2006.

9. Tadeusz Z.E. Jones, Laura Giurato, Salvatore Guccione, and Rona R. Ramsay .

Interactions of imidazoline ligands with the active site of purified monoamine oxidase A.

FEBS Journal 274 (2007) 1567–1575.

10. Osman A.B.S.M Gani, Olayiwola A. Adekoya, Laura Giurato, Francesca Spyraakis, Pietro Cozzini, Salvatore Guccione, Jan-Olof Winberg, and Ingebrigt Sylte

Physicochemical features of the catalytic triad of short chain alcoholde hydrogenases/reductases. Biophys. J., 94 February 2008, 1412–1427.

More than **100** presentations (invited lectures, poster and oral communications at National and International Conferences, Meetings and Symposia).

Book Chapters:

- I. Francesca Spyrakis, Laura Giurato, Salvatore Guccione , Pietro Cozzini, ***Structural data: the basis for molecular modelling.*** In: Practical Studies in Medicinal Chemistry, A. Monge Ed. IUPAC 2006.
- II. Laura Giurato and Salvatore Guccione, ***Comparing Log_SP calculations by the Ghose-Crippen and the Villar methods. Scientific Computation is not an end itself. It must be implemented in the context of problems to be solved .*** In: Practical Studies in Medicinal Chemistry, A. Monge Ed. IUPAC 2006.