

CURRICULUM VITAE

Education:

1992 PhD in Pharmaceutical Sciences.

1986 Degree in Pharmacy (110/110 *cum laude*) April 3th. Faculty of Pharmacy, University of Catania.

Professional Experience

Department of Drug Sciences University of Catania: **1986-present**.

2017-: Associate Professor (CHIM08).

2017: external reviewer Ph.D School (“Dottorato di Ricerca”) Drug Research and Innovative Treatments (XXX Cycle), Neurosciences, Psychology, Drug Research and Child Health (NEUROFARBA) Department, University of Florence .

2014: National Scientific Qualifications as Associate Professor in the sector 03/D1 (CHIM08) Medicinal, Toxicological and Nutritional Chemistry and Applied Technologies.

2012-: Reviewer REPRISE (Register of Expert Peer-Reviewers for Italian Scientific Evaluation).

2007-: Tutor Professor Scuola Superiore of Catania an University institution for higher education on a residential basis .

2007: Teaching “Drug Modelling” (Molecular Imaging, Drug modelling e Drug Delivery) in the Master *Pharmaceutical and Molecular Diagnostic*.

2007: Member of the European PhD Commitment. Universidad de Navarra (Spagna) C.I.F.A.

2007-2013: Responsible for SOCRATES-ERASMUS project Faculty of Pharmacy and Faculty of Natural, Physical and Mathematical Sciences, University of Catania.

2007-2013: Responsible ERASMUS *Student Placement Life Long Learning* Faculty of Pharmacy and Faculty of Natural, Physical and Mathematical Sciences, University of Catania.

2003: *Invited Scientist* University of Trømsø (Norway), INSTITUTE OF MEDICAL BIOLOGY, Department of Pharmacology.

2002- Aggregate Professor for the Faculty of Pharmacy and of the Degree Course in Biomolecular Chemistry at the Faculty of Natural, Physical and Mathematical Sciences, University of Catania. He was also in the Commitment to establish the latter degree course.

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

2000: Tutor for the students mobility LEONARDO DA VINCI project .

1997-: Senior Researcher.

1996: University of Innsbruck (Prof. T. Langer).

1994: Researcher Department of Pharmaceutical Sciences University of Catania.

1988: Course on Modern Chromatographic Techniques ;

1984: Preliminary School of Photochemistry .

Teaching:

2014- Tutor *Scuola Superiore di Catania* (Higher Education Centre of the University of Catania).

2016-: Phytochemistry. First cycle degree in Applied Pharmaceutical Sciences *curriculum* “Herbal Sciences and Nutraceutical Products”.

2001-: “Molecular Modelling” (Single Cycle Degree in Pharmacy, Pharmaceutical Chemistry and Technology (CTF), second cycle degree Biomolecular 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.

POSITIONS OF RESPONSIBILITY AND ACTIVITIES:

2013-: COST ACTION CM1207 " **GLISTEN: GPCR-Ligand Interactions, Structures, and Transmembrane Signalling: a European Research Network**".

2012-: referee MIUR (Italian Ministry of University and Research).

2011-: referee ISCRA (Italian SuperComputing Resource Allocation).

2010-2013: Member of the International PhD School in Neuropharmacology.

2010-2013: scientific Director spinoff ETNALEAD.

2010: Teaching in the Master "**Discipline Regolatorie del Farmaco**" (**Drug Regulatory Disciplines**) .

2009-2013: COST ACTION BM0806 : Advances in Histamine H₄R Research.

2009-2010: Project co-Ordinator "**PROJECTS IN THE FRAMEWORK OF THE JOINT BILATERAL AGREEMENT CNR-ASRT (Egitto)**" .

2009: formative project "Laboratorio Pubblico-Privato" DM20919(CNR-WYETH).

2008: Organizer Workshop *An Insight into Science Publishing* (28- 29 Aprile), Auditorum "Casa della Cultura" Villa Citelli, Catania.

2008-2013: Book *Series Editor* RSC (**Royal Society of Chemistry**) "**Medicinal Chemistry Series Books**" and "invited" **FRSC (Fellow Royal Society of Chemistry)** .

2008-: COPE member (Committee On Publication Ethics) .

2007: International Scientific Advisory Board e conferenza plenaria “Current Trends in Drug Discovery Research”(CTDDR-2007). 17-20 Febbraio, 2007 (Central Drug Research Institute, Lucknow, India).

2007: International Scientific Advisory Board e conferenza plenaria 11th International Conference (**ISCBC – 2007, February 24-26, 2007**) on “Advances in Drug Discovery Research Hotel Rama International-Aurangabad.

2007-: Scientific Director of the spinoff ETNALEAD awarded by the prize “startup” for scientific innovation.

2006: Organizer Workshop “*A Workshop based in FLO and AlleGrow*” (March 5-8), Catania (Città Universitaria).

2006: International Scientific Advisory Board :

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

2006: Scientific Commitment 3rd School on Advanced BioMedicine and BioInformatics. "Proteoms and Proteins"Lipari Island (Italy), July 9 -July 22 .

2005:*Invited Scientist* F. Hoffmann-La ROCHE, Basilea, Svizzera.

2005- Responsible for (3) PRA research projects (“Progetti Ricerca Ateneo”).

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

2005 Speaker Workshop *Introduction to molecular modelling* (Dicembre 12,13), Università di Tromsø, Norvegia.

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

2004-: *Consulting* BioChemics Consulting SAS (Orleans, France).

2001-2006: *Executive Guest Editor* di Current Pharmaceutical Design (***Special issue: "Pharmacophore Elucidation & their use in Drugs & Design: Experimental Structures, Conformational Analysis and 3D QSAR"***).

2002: Speaker formative event “Ciclo di Vita del Medicinale ad Uso Umano: dalla Sintesi alla Postmarketing Surveillance” (Life cycle of the drug: from sythesis to Postmarketing Surveillance).

Catania (Hotel Baia Verde) 7,8 Settembre (Commissione Nazionale per la Formazione Continua “National Commitment for Continued Learning”).

1999-2016: Editor European Journal of Medicinal Chemistry.

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

Reviewer : 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, European Journal of Medicinal Chemistry, Bioorganic and Medicinal Chemistry, Bioorganic and Medicinal Chemistry Letters, Frontiers in Biosciences, *Chemical Research in Toxicology*, Bioinorganic Chemistry and Applications, Food & Function.

Research

a)Rational Design (Molecular Modelling) and synthesis of new enzyme and receptor ligands; b) *in silico* and experimental ADME(T) studies; c)new softwares for drug design and *life sciences*; d)computational approaches to chemistry and biochemistry; e)Bioinformatic mostly focusing on GPCRs (**G-Protein Coupled Receptors**) .

PUBLICATIONS

1. F. Russo, **S. Guccione**, N.A. Santagati, A. Santagati, A. Caruso, M.G. Leone, A. Felice, G. Attaguile, M. Amico Roxas.

New heterocyclic ring systems-V Synthesis and pharmacological activity of 6H-1,3,4-thiadiazolo [3',2': 1,2]-5-oxopyrimido[5,4-b]indole derivatives and of 1-phenyl-6H-1,2,4-Triazolo [1',5': 1,2]-5-oxopyrimido [5,4-b]Indole.

IL Farmaco Ed. Sc.,**43**,409-420 (1988).

2. F. Russo, G. Romeo, **S. Guccione**, E. Bousquet, A. Caruso, M.G. Leone, G. Attaguile, M. Amico Roxas.

Synthesis and pharmacological activity of 6H-thiazolo[3',2':1,2]-5-oxopyrimido[5,4-b] Indole derivatives, a new heterocyclic ring system.

Pharmazie, **45**, 242-244 (1990).

3. F. Russo, G. Romeo, **S. Guccione**, A. De Blasi.

Pyrimido[5,4-b] Indole derivatives. 1. A new class of potent and selective α_1 adrenoceptor ligands.

J. Med. Chem., **34**, 1850-1854(1991).

4. F. Russo, **S. Guccione**, G. Romeo, L. Monsù Scolaro, A. Caruso, V. Cutuli.

Synthesis and pharmacological evaluation of pyrazolopyrimidobenzoxazole and pyrazolopyrimidobenzothiazole derivatives.

Boll. Chim. Farm., **130**, 89-93, (1991).

5. F. Russo, **S. Guccione**, G. Romeo, L. Monsù Scolaro, S. Pucci, A. Caruso, V. Cutuli, M. Amico Roxas.

Synthesis and pharmacological properties of pyrazolotriazolopyrimidine derivatives.

Eur. J. Med. Chem., **27**, 73-80 (1992).

6. F. Russo, **S. Guccione**, G. Romeo, G. Uccello Barretta, S. Pucci, A. Caruso, M. Amico-Roxas, V. Cutuli.

Pyrazolothiazolopyrimidine derivatives as novel class of anti-inflammatory or antinociceptive agents: synthesis, structural characterization and pharmacological evaluation. Eur. J. Med. Chem., **28**, 363-376 (1993).

7. C. B. Vicentini, A. C. Veronese, **S. Guccione**, M. Guarneri, M. Manfrini and P. Giori.

An efficient procedure for the synthesis of Pyrazolo[3,4-d] [1,3] Thiazin-4-ones.
Heterocycles, **36**, 10, 2291-2301, 1993.

8. G. Romeo, G. Ambrosini , **S. Guccione**, A. De Blasi , F. Russo.

Pyrimido [5,4-b] benzofuran and pyrimido [5,4-b] benzothiophene derivatives.
Ligands for α_1 - and 5HT_{1A}- receptors.

Eur. J. Med. Chem. , **28** , 499-504 (1993).

9. C. B. Vicentini, A. C. Veronese, **S. Guccione**, M. Guarneri, M. Manfrini and P. Giori.

A new procedure for the synthesis of 4H-pyrazolo[1,5-c][1,3,5]thiadiazine-4-thiones.

J. Heterocyclic Chem ., **31**, 1477-1480, 1994.

10. G. Romeo, F. Russo & **S. Guccione**, R. Chabin, D. Kuo & W. B Knight.

Synthesis of new thiazinoindole derivatives and their evaluation as inhibitors of human leukocyte elastase and other related serine proteases.

Bioorg. Med. Chem. Lett ., **20** , 2399-2404, (1994).

11. **S. Guccione**, A. Raffaelli, G. Uccello Barretta , L. Monsù Scolaro, S. Pucci and F. Russo.

Unforeseen alkylating effect of triethylorthoformate in the synthesis of pyrazolotriazolopyrimidine derivatives.

Eur. J. Med. Chem., **30**, 333-337 (1995).

12. **S. Guccione**, A. Raffaelli, G. Uccello-Barretta, L. Monsù Scolaro, S. Pucci and F. Russo.

Potential of alkyl orthoformates as alkylating agents of non-electron rich nitrogen heterocycles.

J. Heterocyclic Chem. **32**, 1149-1158 (1995).

13. **S. Guccione**, M. Modica, J. Longmore, D. Shaw, G. Uccello Barretta, A. Santagati, M. Santagati, F. Russo.

Synthesis and NK-2 antagonist effect of 1,6-diphenyl-pyrazolo [3, 4-d]-thiazolo[3,2-a]4H-pyrimidin-4-one.

Bioorg. & Med. Chem. Lett. **6**, 59-64 (1996).

14. **S. Guccione**, T. Langer, F. Russo.

Alkylation of non-electron rich nitrogen heterocycles by alkyl orthoformates: quantum chemistry calculations.

J. Heterocyclic Chem., **33**, 1413-1415 (1996).

15. **S. Guccione**, L. Monsù Scolaro, F. Russo.

Synthesis of 3-methyl substituted pyrazolotriazolopyrimidin-4-one and pyrazolothiazolopyrimidin-4-one derivatives.

J. Heterocyclic Chem. **33**, 459-463 (1996).

16. A. Raffaelli, S. Pucci, G. Uccello Barretta, F. Russo, **S. Guccione**,

Identification of an impurity in the synthesis of pharmacologically active pyrazolotriazolopyrimidines by a combined spectrometric approach.

Rapid Commun.Mass Spectrom., **10**, 1939-1945 (1996).

17. A.Santagati, J. Longmore, **S. Guccione**, T. Langer, E. Tonnel, M. Modica, M. Santagati, L. Monsù Scolaro, F. Russo.

Building a model of interaction at the NK-2 receptors: Polycondensed heterocycles containing the pyrimidoindole skeleton.

Eur. J. Med. Chem., **32**, 973-985 (1997).

18. Cambria, A. Raudino, A. Geronikaki, G. Buemi, G. Raciti, P. Mazzone, **S. Guccione** and S. Ragusa.

Thiazole derivatives as inhibitors of purified bovine liver mitochondrial monoamine oxidase-B: structure-activity relationships and theoretical study.

J. Enzyme Inhib., **14**, 307-321 (1999).

19. T. Langer, **S. Guccione**, F. Russo.

CoMFA study of new acetyl-coa: cholesterol o-acyl transferase (ACAT) inhibitors.

Sci. Pharm., **68**, 65-73 (2000). Invited paper.

20. **S. Guccione**, A. Doweyko, H. M. Chen, G. Uccello Barretta, F. Balzano.

3D-QSAR Using "Multiconformer" Alignment: The Use of HASL in the Analysis of 5-HT_{1A} Thienopyrimidinone Ligands.

J. Comput-Aided Mol. Des, **14**, 647-657 (2000).

21. C.B. Vicentini, M. Guarneri, V. Andrisano, **S. Guccione**, T. Langer, R.

Marschhofer, R. Chabin, A. Edison, X. Huang, W. B. Knight, P. Giori.

Potential of Pyrazolooxadiazinone Derivatives as Serine Protease Inhibitors.

J. Enzyme Inhib., **16**, 15 – 34 (2001).

22. M. Modica, M. Santagati, **S. Guccione**, A. Santagati, F. Russo, A. Cagnotto, M.

Goegan, T. Mennini.

Design, synthesis and binding properties of novel and selective 5-HT₃ and 5-HT₄ receptor ligands.

Eur. J. Med. Chem., **36**, 2001, 287-301

23. S. Gritsch, **S. Guccione**, R. Hoffmann, A. Cambria, G. Raciti and T. Langer.

A 3D QSAR study of Monoamino Oxidase B inhibitors, using the chemical function based pharmacophore generation approach.

J. Enzyme Inhibition, **16**, 199-215, 2001.

24. R. Pignatello, M. Ferro, G. De Guidi, G. Salemi, M. A. Vandelli, **S. Guccione**,

M. Geppi, C. Forte, G. Puglisi.

Preparation, characterisation and photosensitivity studies of solid dispersions of diflunisal and Eudragit RS100[®] and RL100[®].

Int J. Pharm. **218**, 2001, 27-42.

25. Wouters, J., Norberg, B., and Guccione, S. .

4-Methyl-2-[N-(3,4-methylenedioxy-benzylidene)hydrazino]thiazole and its reduction product, 4-methyl-2-[N-(3,4-methylenedioxybenzylidene)-hydrazono]-4,5-dihydrothiazole.

Acta Cryst. Section C, Crystal Struct. Comm., **C57**, 69-71, 2001.

26. Wouters J. , Luque F.J., Uccello Barretta G., Balzano F., Pignatello R. and Guccione S.,

Crystallographic, NMR and ab initio calculation studies of tautomerism among substituted dihydrothiazol-2-ylhydrazones.

J. Chem. Soc. Perkin-Trans 2, **5** (2002), 1012 - 1016.

27. 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 modeling of new 1-aryl-3-[4-arylpiperazin-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.

28. 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**, 3871-3889, 2002.

29. Potemkin V.A., Arslambekov R.M., Bartashevich E.V., Grishina M.A., Belik A.V., Perspicace S., **Guccione S.**

Multi-conformational method for analyzing the biological activity of molecular structures.

Zhurnal Strukturnoi Khimii./ Journal of Structural Chemistry, 43, **6**, 1045 – 1049, 2002.

30. 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 bromobenzensulfonamide into β -cyclodextrin.

Bioorg. Med. Chem., **12**, 2004 , 447-458.

31. 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,

Bioorg. Med. Chem. **12** (2004) 2951–2964.

32. 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.

33. Jordi Muñoz-Muriedas, Samantha Perspicace, Nuria Bech, **Salvatore Guccione**, Modesto Orozco, and F. Javier Luque.

Hydrophobic molecular similarity from MST fractional contributions to the octanol/water partition coefficient.

J. Computer-Aided Mol. Des., **19**, 401-419 (2005).

34. 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.

35. Rosario Pignatello, Antonina Puleo , **Salvatore Guccione** , Giuseppina Raciti , Rosaria Acquaviva , Agatina Campisi , Cinzia A. Ventura , Giovanni Puglisi .

Enhancement of drug affinity for cell membranes by conjugation with lipoamino acids. I. Synthesis and biological evaluation of lipophilic conjugates of tranylcypromine.

Eur. J. Med. Chem., **40**, 1074-1079, 2005.

36. Marco Geppi, **Salvatore Guccione**, Giulia Mollica, Rosario Pignatello, and Carlo A. Veracini.

Molecular Properties of Ibuprofen and Its Solid Dispersions with Eudragit RL100 Studied by Solid-State Nuclear Magnetic Resonance.

Pharm. Res., **22**, 1544-1555, (2005)

37. Rosario Pignatello, **Salvatore Guccione**, Francesco Castelli, Maria G. Sarpietro, Laura Giurato, Massimo Lombardo, Giovanni Puglisi and Istvan Toth.

Enhancement of drug affinity for cell membranes by conjugation with lipoamino acids: II. Experimental and computational evidence using biomembrane models.

Int. J. Pharmaceutics **310** (2006) 53–63.

38. 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**, 258-270, 2006.

39. D. Mares, C. Romagnoli, E. Andreotti, G. Forlani, **S. Guccione**, C.B. Vicentini.

Emerging antifungal azoles and effects on Magnaporthe grisea.

Mycological Research **110**, 2006, 686-696.

40. 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.

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

Theoretical Calculations of the Catalytic Triad in Short Chain Alcohol Dehydrogenases/ Reductases.

Biophys J., **94** , 2008, 1412–1427.

42. Gloria Uccello-Barretta, Federica Balzano, Silvia Bardoni, Letizia Vanni, Laura Giurato, **Salvatore Guccione**.

Chiral discrimination processes by C9 carbamate derivatives of dihydroquinine: interaction mechanisms of diastereoisomeric 9-O-[(S)- or (R)-1-(1-naphthyl)ethylcarbamate]dihydroquinine and the two enantiomers of N-(3,5-dinitrobenzoyl)alanine methyl ester.

Tetrahedron: Asymmetry **19** (2008) 1084–1093.

43. Nadège Piclin, Marco Pintore, Carmela Maria Lanza, Antonio Scacco, Salvatore Guccione, Laura Giurato, Jacques R. Chrétien.

Sensory Analysis on Red Wines: Discrimination by Adaptive Fuzzy Partition (AFP).

J. Sensory Studies , 23, **4**, 2008 , 558-569.

44. Copani, **S. Guccione**, L. Giurato, F. Caraci, M. Calafiore, M.A. Sortino, F. Nicoletti.

The cell cycle molecules behind neurodegeneration in Alzheimer's disease: perspectives for drug development,

Current Medicinal Chemistry, **15**, 2008, 2420-2432.

45. Giovanni Li Volti, Fabio Galvano, Alessandro Frigiola, Salvatore Guccione, Claudia Di Giacomo, Stefano Forte, Giovanni Tringali, Massimo Caruso, Olayiwola Adedotun Adekoya , Diego Gazzolo.

POTENTIAL IMMUNOREGULATORY ROLE OF HEME OXYGENASE 1 IN HUMAN MILK: A COMBINED BIOCHEMICAL AND MOLECULAR MODELLING APPROACH.

The Journal of Nutritional Biochemistry, **21**, 2010, 865-871.

46. KELLY E. DESINO, ROSARIO PIGNATELLO, **GUCCIONE S.**, LIVIA BASILE, SABAH ANSAR, MARY LOU MICHAELIS, RONA R. RAMSAY AND KENNETH L. AUDUS .

TCP-FA4: A DERIVATIVE OF TRANYLCPROMINE SHOWING IMPROVED BLOOD-BRAIN PERMEABILITY. BIOCHEMICAL PHARMACOLOGY, **78**, 2009, 1412–1417.

47. Luis Berrade, Bárbara Aisa, María J. Ramirez, Silvia Galiano, Salvatore Guccione, Lise Román Moltzau, Finn Olav Levy, Ferdinando Nicoletti, Giuseppe Battaglia, Gemma Molinaro, Ignacio Aldana, Antonio Monge, and Silvia Perez-Silanes.

Novel Benzo[b]thiophene Derivatives as New Potential Antidepressants with Rapid Onset of Action.

J. Med. Chem., **54**, **2011**, 3086–3090.

48. Maria Angela Castriciano, Andrea Romeo, Nicola Angelini, Norberto Micali, Salvatore Guccione, Luigi Monsù Scolaro.

Spectroscopic Investigation and Molecular Modeling on Porphyrin/PAMAM Supramolecular Adduct.

Photochemistry and Photobiology. **87**, **2**, 292–301, 2011.

49. B. Maggio, D. Raffa, M.V. Raimondi, F. Plescia, M.L. Trincavelli, C. Martini, F. Meneghetti, L. Basile, Guccione S, G. Daidone (2012). *Synthesis, benzodiazepine receptor binding and molecular modelling of isochromeno[4,3-c]pyrazol-5(1H)-one derivatives.*

EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY, vol. 54, p. 709-720, ISSN: 0223-5234.

50. Livia Basile, Susana Álvarez, Almudena Blanco, Andrea Santagati, Giuseppe Granada, Patrizia Di Pietro, Guccione S, M^a Ángeles Muñoz-Fernández (2012).

Sulfonilamidothiopyrimidone and Thiopyrimidone derivatives as selective COX-2 inhibitors: synthesis, biological evaluation, and docking studies. EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY, vol. 57, p. 149-161, ISSN: 0223-5234, doi: 10.1016/j.ejmech.2012.09.005

51. Valeria Sorrenti, Guccione S, Claudia Di Giacomo, Maria N. Modica, Valeria Pittalà, Rosaria Acquaviva, Livia Basile, Morena Pappalardo, Loredana Salerno (2012).

Evaluation of Imidazole-based Compounds as Heme Oxygenase-1 inhibitors. CHEMICAL BIOLOGY & DRUG DESIGN, vol. 80, p. 876-886, ISSN: 1747-0285, doi: 10.1111/cbdd.12015

52. Deboprosad Mondal, Song YeLi, Luca Bellucci, Teodoro Laino, Andrea Tafi, Guccione S, and Salvatore D. Lepore (2013). *Stereoretentive Chlorination of Cyclic Alcohols Catalyzed by Titanium (IV) Tetrachloride: Evidence for a Front Side Attack Mechanism.*

JOURNAL OF ORGANIC CHEMISTRY, vol. 78, p. 2118-2127, ISSN: 0022-3263.

53. Luca Vanella, Giovanni Li Volti, Guccione S, Giancarlo Rappazzo, Eliana Salvo, Morena Pappalardo, Michal L Schwartzman, Nader G Abraham . *Heme Oxygenase-2/adiponectin Protein-Protein Interaction in Metabolic syndrome.*

Biochemical and Biophysical research Communications, ISSN: 0006-291X 432 (2013) 606-611.

54. Livia Basile , Matteo Pappalardo, Salvatore Guccione , Danilo Milardi, and Rona R. Ramsay.

Computational Comparison of Imidazoline Association with the I2 Binding Site in Human Monoamine Oxidases.

J. Chem. Inf. Model., **2014**, 54 (4), pp 1200–1207

Matteo Pappalardo, Nir Shachaf, Livia Basile, Danilo Milardi, Mouhammed Zeidan, Jamal Raiyn, Salvatore Guccione, Anwar Rayan

Sequential application of ligand and structure based modeling approaches to index chemicals for their hH4R antagonism Research Article | published 16 Oct 2014 | PLOS ONE 10.1371/journal.pone.0109340

56. Agata Antonina Rita Impellizzeri, Matteo Pappalardo, Livia Basile, Ornella Manfra, Kjetil Wessel Andressen, Kurt Allen Krobert, Angela Messina, Finn Olav Levy and Salvatore Guccione

Identification of essential residues for binding and activation in the human 5-HT_{7(a)} serotonin receptor by molecular modeling and site-directed mutagenesis Front. Behav. Neurosci., 08 May 2015 |

57. Andrea Carletta, Anaelle Tilborg, Laurence Moineaux, Jerome de Ruyck, Livia Basile, Loredana Salerno, Giuseppe Romeo, Johan Wouters and Salvatore Guccione.

How does Binding of Imidazole-based inhibitors to Heme Oxygenase-1 influence their Conformation? Insights combining Crystal Structures and Molecular Modelling.

Acta Cryst. (2015). B71, 447–454

58. Belma Zengin Kurt, Isil Gazioglu, Livia Basile, Fatih Sonmez, Tiziana Ginex, Mustafa Kucukislamoglu and Salvatore Guccione

Potential of Aryl-urea-Benzofuranylthiazoles hybrids as multitasking agents in Alzheimer's disease

European Journal of Medicinal Chemistry 102 (2015) 80-92

59. Gisella E. Alfonsino, Andrea Santagati, Livia Basile, Ettore Novellino, Corey Gaul, Carley Squires, Michael Braden, John M. Gerdes, Silvia Pérez Silanes, Salvatore Guccione, and Keith K. Parker

5HT_{1a} Receptor Binding Affinities of a Series of Serotonin Transporter (SERT) Inhibitors and Related Thermodynamic Insights

Journal of Advances in Medical and Pharmaceutical Sciences 4(1): 1-12, 2015

60. Filippo Caraci, Giuseppe Pappalardo, Livia Basile, Alessandro Giuffrida, Agata Copani, Rita Tosto, Alessandro Sinopoli, Maria Laura Giuffrida, Emanuele Pirrone, Filippo Drago, Rosario Pignatello, Salvatore Guccione
Neuroprotective effects of the monoamine oxidase inhibitor tranylcypromine and its amide derivatives against A β (1-42)-induced toxicity
European Journal of Pharmacology 764 (2015) 256- 263
61. Sara Merlo, Livia Basile, Maria Laura Giuffrida, Maria Angela Sortino, Salvatore Guccione, Agata Copani
Identification of 5-Methoxyflavone as a Novel DNA Polymerase-beta Inhibitor and Neuroprotective Agent against Beta-amyloid Toxicity
Journal of Natural Products *J. Nat. Prod.*, 2015, 78 (11), pp 2704-2711
62. Giuseppe Amico, Livia Basile, Giuseppe Romeo, Loredana Salerno, Maria N. Modica, Maria A. Siracusa, Agostino Marrazzo, Valeria Pittalà and Salvatore Guccione
Rescuing abandoned molecules as Nav1.7 and PCSK9 Inhibitors
Journal of Advances in Medical and Pharmaceutical Sciences 5(2): 1-10, 2016.
63. Nir Shahaf, Matteo Pappalardo, Livia Basile, **Salvatore Guccione**, and Anwar Rayan.
How to choose the suitable template for homology modelling of GPCRs: 5-HT7 receptor as a test case.
MOLECULAR INFORMATICS, 2016, 35, 414-423. **I.F.: 1.955**
64. Fatih Sonmez, Belma Zengin Kurt, Isil Gazioglu, Livia Basile, Aydan Dag, Valentina Cappello, Tiziana Ginex, Mustafa Kucukislamoglu and Salvatore Guccione
Design, synthesis and docking study of novel coumarin ligands as potential selective acetylcholinesterase inhibitors
JOURNAL OF ENZYME INHIBITION AND MEDICINAL CHEMISTRY, 2017 32, 285–297. DOI: 10.1080/14756366.2016.1250753. **I.F.: 4.293**

65. Matteo Pappalardo; Mahmoud Rayan; Saleh Abu-Lafi; Martha E. Leonardi; Danilo Milardi; Guccione S; and Anwar Rayan
Homology-based modeling of rhodopsin-like family members in the inactive state: structural analysis and deduction of tips for modeling and optimization
MOLECULAR INFORMATICS 2017, 36, 1700014
DOI:10.1002/minf.201700014. I.F.: 1.955
66. Lucia Crascì, Livia Basile, Annamaria Panico, Carmelo Puglia, Francesco P. Bonina, Pierluigi Maria Basile, Luisa Rizza and Salvatore Guccione
Correlating in Vitro Target-Oriented Screening and Docking: Inhibition of Matrix Metalloproteinases Activities by Flavonoids
PLANTA MEDICA, 2017, 83, 901-911. **DOI: 10.1002/minf.201700014. I.F.: 2.342**
67. Federica Porta, Arianna Gelain, Daniela Barlocco, Nicola Ferri, Silvia Marchianò, Valentina Cappello, Livia Basile, Salvatore Guccione, Fiorella Meneghetti, and Stefania Villa
A field-based disparity analysis of new 1,2,5-oxadiazole derivatives endowed with antiproliferative activity.
Chemical Biology & Drug Design, 2017, 90, 820-839.
DOI: 10.1111/cbdd.13003. I.F.: 2.396
68. Salvatore Ferla, Natalie E. Netzler, Sebastiano Ferla, Sofia Veronese, Daniel Enosi Tuipulotu, Salvatore Guccione, Andrea Brancale, Peter A. White, Marcella Bassetto
In silico screening for human norovirus antivirals reveals a novel non-nucleoside inhibitor of the viral polymerase
Scientific Reports (NATURE), (2018) 8:4129. **DOI:10.1038/s41598-018-22303-y. I.F.: 4.259**

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 and R. Ganellin Eds. Ed. IUPAC 2006.
- II. Laura Giurato and **Salvatore Guccione**, *Comparing Log_P 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 and R. Ganellin Eds. IUPAC 2006.

INVITED LECTURES

- a. **S. Guccione.** *Therapeutic Potential of Condensed Heterocycles* ; Russian Academy of Medical Science: Cancer Research Centre, Moscow (Russia), September 1994.
- b. **S. Guccione.** *Condensed Heterocycles as biological active agents: : summing up. Current status of the Research.* Russian Academy of Medical Science: Cancer Research Centre, Moscow (Russia), September 1994.
- c. **S. Guccione.** *Protein-tyrosin kinase inhibitors hybrid heterocycles as pp 60c-src protein tyrosine kinase inhibitors .* Wroclaw University of Medicine (Poland): Department of Organic Chemistry, Wroclaw (Poland), May 1995.
- d. **S. Guccione.** *Bioisosterism and Molecular Hybridization in the Design of New enzyme Inhibitors.*
Collegium Medicum of the Jagiellonian University : Department of Chemical Technology of Drugs, Kraków (Poland) May 1995.
- e. **S. Guccione.** *Building a hypothesis on Human Leukocyte Elastase Inhibition by Difunctional Heterocycles .* Warsaw University of Medicine (Warsaw Academy of Medicine). Faculty of Pharmacy, Warsaw (Poland), May 1995.
- f. **S. Guccione.** *Synthesis of Heterocycles of Pharmaceutical interest.* University of Pisa: Centro CNR di Studio delle Macromolecole Stereordinate ed Ottica- mente Attive, Pisa (Italy), June 1995.
- g. **S. Guccione:** *3D-QSAR (HASL) in DRUG DESIGN .* Aristotelian University of Thessaloniki (Greece). Department of Pharmaceutical Chemistry , Thessaloniki (Greece), September 28th 1997 .
- h. **S. Guccione:** *Use of different 3D-QSAR techniques in mapping unknown (not X-ray determined) biological targets.*
Pharmaceutical Research Institute Warsaw (Poland), May 19th 1999.
Organized in collaboration with the Medical University in Lublin,

Department of Medicines Synthesis and Technology, Faculty of Pharmacy, Lublin (Poland).

- i. **S. Guccione**: *Combining different 3D-QSAR methodologies in a multiconformer context: a new approach to map not X-ray determined targets of pharmaceutical interest overcoming alignment problems.*

Proceedings of the conference "Crystallography and Drug Design '99" (CDD 99), Lodz (Poland), May 20th-22nd 1999, **85**.

- j. **S. Guccione**: *Molecular Modelling for Pharmaceutical Development.*
NV Organon, Oss (The Netherlands), September 4th 2000

- k. **S. Guccione**: *3D-QSAR in Medicinal Chemistry: Problems, Solutions and Novel Applications.*

Faculté des Sciences -Facultés Universitaires Notre-Dame de la Paix-
Département de Chimie, Namur (BELGIUM), January 15th 2001.

- l. **S. Guccione**: *Computational approaches and their use in Drug Design : an overview.*

Institut Jacques Monod, Paris (France), January 16th 2001.

- m. **S. Guccione**: *Rational Drug Design: Computer Approaches in Structure-Property Relationships.*

Faculty of Pharmacy, University of Barcelona (Spain), June 12th 2001.

- n. **S. Guccione**: *Conformation and Alignment in 3D-QSAR Analyses.*

Faculty of Pharmacy, University of Barcelona (Spain), June 12th 2001.

- 15) S. Guccione**: *Combining Different Computational and Experimental Methodologies to Rationalize the Drug Design and Delivery Process .*

CHEMOVATION, Ltd., Horsham U.K., February 11th 2002.

- 16) S. Guccione**: *A New Potential Approach in the Anti-obesity Therapy: Molecular Modelling Studies of NPY-5 Receptor Antagonists.*

University of Milan, Institut of Pharmaceutical Chemistry and Toxicology, Ph. D School, May 16th 2002.

17) **S. Guccione**: *Windows to the world of Ligands-Macromolecular Receptor Interactions.*

International Symposium on Drug Discovery and Process Research (DDPR-2003), Kolhapur (INDIA) January 23-25 , 2003. **I-13**

18) **S. Guccione** *Application of Computational Methods to Drug Design and Drug Delivery Studies.*

Department of Pharmacology, University of Tromsø, September 5th, 2003.

19) **S. Guccione** *Molecular Alignment Based on Hydrophobic Similarity as a tool in Drug Design*

Computational Methods in Toxicology and Pharmacology Integrating Internet Resources (CMTPI-2003). September 17-19, 2003. Hotel Kinissi Palace Thessaloniki, Greece. **SV3**

20) **S. Guccione** *Computational Techniques to Speed up the Drug Discovery Process.*

Centre for Biomolecular Sciences, - University of St. Andrews - September 22nd 2004.

21) **S. Guccione** *Introduction to molecular modelling.*

Faculty of Medicine University of Tromsø. Arranged by the Functional Genomics (FUGE) Bioinformatics Laboratory Project, University of Tromsø. December 10-18 2005.

22) **S. Guccione** *Dual UAL 5-HT_{1A} or 5-HT₇ Receptor Ligands –SERT Blockers. Implications for Ligand-Selective Receptor Conformations : Phenotype-Based Selectivity.*

Current Trends in Drug Discovery research (CTDDR-2007) Central Drug Research Institute Lucknow (India) .Medicinal Chemistry Research 15, 1/6, 2007 (Special issue). **67**

23) **S. Guccione** *NEW APPROACHES TO CANCER THERAPY*

11th International Conference (ISCBC – 2007, February 24-26, 2007) on “Advances in Drug Discovery Research”. Hotel Rama International- Aurangabad **PL12**.

24) **S. Guccione** *Identification of novel scaffolds leading to small molecule beta polymerase inhibitors with potential in neurodegenerative and oncology disorders*.

Modelling and Design of Molecular Materials 2008, Piechowice, Poland June 23-28 2008. **L33**.

25) **S. Guccione** *“Computational fishing in protein interactions and neurodegeneration hypotheses”*.

Workshop on Molecular Modelling: Approaches to Computational Biophysics” Marie Curie ToK programme “DRUGDESI”. Dedicated to the memory of Coordinator, Dr. Nikos G. Oikonomakos”. Athens, 5 – 6 December 2008.

26) **S. Guccione** *“Targeting the Neuronal Cell Cycle: “Field Screen” guided design of DNA Polymerase- β Inhibitors as potential neuro-protectant agents”*.

ZING Medicinal Chemistry Conference 2009 “Lead optimisation and lead discovery”. Ocean Maya Hotel Playa del Carmen (Mayan Rivera, México). February 1-4 2009.

27) **S. Guccione** *“Potential of the Nature’ s Biochemistry for Drug Design”*. 9th International Symposium on Pharmaceutical Sciences (ISOPS-9) . Ankara University, Faculty of Pharmacy, Tandokan, Ankara(Turkey). June 23-26, 2009.

28) **S. Guccione** *“In silico approaches as a tool in drug discovery”*.

Department of Pharmacology, University of Oslo and Oslo University Hospital, N-0316 Oslo, Norway. September 26th 2011.

29) **S. Guccione** *“Heme oxygenase-1 and -2 interactions as new targets for drug design: interactive links between virtual and experimental approaches”*.

WORKSHOP "Advances in Heme oxygenases and oxidative stress". Villa San Saverio, Catania, Italy, April 12th- 13th, 2012.

30)**S. Guccione** "Principles and operational strategies of Rational Drug Design". Institute for Microbiology and Genetics. Dept. of Molecular Structural Biology University of Goettingen (Germany). September 23 2013.

31)**S. Guccione**

Better understanding of the MAO B-associated I2 binding site combining molecular modelling and enzymology.

Fourth International Meeting on Pharmacy & Pharmaceutical Sciences (IMPPS-4). Istanbul Marmara University-Faculty of Pharmacy. September 18-21, 2014, TURKEY.

32)**S. Guccione**

Interfacing In Silico and Experimental Approaches to Advance Drug Discovery in Central Nervous System (CNS) Disorders

10th AFMC International Medical Chemistry Symposium (AIMECS2015) Jeju, Korea, October 18 - 21, 2015 .

PROCEEDINGS

1. G. Romeo, F. Russo, **S. Guccione**, D. Barbarulo, A. De Blasi.

Heterocyclic systems containing the pyrimido-2,4-dione ring as selective ligands for the α_1 -adrenoceptors.

Il Farmaco, **50**, 471, (1995) (Proceedings of VI Meeting: Strutture Eterocicliche nella Ricerca Farmaceutica).

2. **S. Guccione**: *Combining different 3D-QSAR methodologies in a multiconformer context: a new approach to map not X-ray determined targets of pharmaceutical interest overcoming alignment problems.*

Proceedings of the conference "Crystallography and Drug Design '99" (CDD 99), Lodz (Poland), May 20th-22nd 1999, **85-93**.

3. M. Santagati, A. Doweyko, A. Santagati, M. Modica, **S. Guccione**, H.M. Chen, G. Uccello Barretta, F. Balzano.

5-HT_{1A} receptors mapping by conformational analysis (2D NOESY/MM) and "three way modelling" (HASL, CoMFA, PARM).

Molecular Modelling and Prediction of Bioactivity, K. Gundertofte & F.S. Jorgensen Eds. Proceedings of the 12th European Symposium on Quantitative Structure-Activity Relationships, Copenhagen, Denmark, August 23-28, 1998.

2000 Kluwer Academic/Plenum Publishers, New York, **183**.

4. M. Sarpietro, M. Marino, A. Cambria, G. Uccello Barretta, F. Balzano, **S. Guccione**.

Determination of the cholecalciferol-lipid complex using a combination of comparative modelling and nmr spectroscopy.

Molecular Modelling and Prediction of Bioactivity, K. Gundertofte & F.S. Jorgensen Eds. Proceedings of the 12th European Symposium on Quantitative Structure-Activity Relationships, Copenhagen, Denmark, August 23-28, 1998. 2000 Kluwer Academic/Plenum Publishers, New York, **325**.

5. T. Langer, M. A. König, G. Schischkow, **S. Guccione**.

De Novo Design of Inhibitors of Protein Tyrosine Kinase pp60^{c-src}

Molecular Modelling and Prediction of Bioactivity, K. Gundertofte & F.S. Jorgensen Eds. Proceedings of the 12th European Symposium on Quantitative Structure-Activity Relationships, Copenhagen, Denmark, August 23-28, 1998. 2000 Kluwer Academic/Plenum Publishers, New York, **361**.

6. M. Santagati, H. Chen, A. Santagati, M. Modica, **S. Guccione**, G. Uccello

Barretta, F. Balzano.

Application of PARM to constructing and comparing 5-HT_{1A} and α_1 receptor models,

Molecular Modelling and Prediction of Bioactivity, K. Gundertofte & F.S. Jorgensen Eds. Proceedings of the 12th European Symposium on Quantitative Structure-Activity Relationships, Copenhagen, Denmark, August 23-28, 1998. 2000 Kluwer Academic/Plenum Publishers, New York, **433**.

7. V. A. Potemkin, E. V. Bartashevich, M. A. Grishina and **Salvatore Guccione**.

An Alternative Method for 3D-QSAR and the Alignment of Molecular Structures: BiS (Biological Substrate Search),

13th European Symposium on Quantitative Structure-Activity Relationships, Rational Approaches to Drug Design.

QSAR 2000 Düsseldorf, Heinrich-Heine-Universität, Düsseldorf, Germany, 27 August-1 September, 2000. Prous Science Publishers, **349**.

8. R. Bursi, P. Verwer, A. Gazit, A. R. Beccari, G. Uccello Barretta, F. Balzano and **S. Guccione**.

From Molecular Spectra to Biological Activities: a Comparative Spectra Analysis (CoSA) study on Epidermal Growth Factor Receptor Protein Tyrosine Kinase Inhibitors.

13th European Symposium on Quantitative Structure-Activity Relationships, Rational Approaches to Drug Design.

QSAR 2000 Düsseldorf, Heinrich-Heine-Universität, Düsseldorf, Germany, 27 August-1 September, 2000. 2001 Prous Science Publishers, **211-213**.

9. R.R. Ramsay, R. James E. Bradley, L.Giurato, **S. Guccione**.

The shape of the flavin in monoamine oxidase.

The 16th International Symposium on Flavins and Flavoproteins Palacio de Congresos, Jaca, Spain, 8-13 Giugno 2008, Prensas de la Universidad de Zaragoza.

Editors: S. Frago, C. Gomez-Moreno, M. Medina. **183-186** .

COMUNICAZIONI

- (1) F. Russo, **S. Guccione**, N.A. Santagati, A. Santagati.
Synthesis and pharmacological activity of new 5H-thiadiazolo [3'2':1,2] pyrimido[5,4-b]indol-5-one.
French-Italian joint meeting on Medicinal Chemistry. Pisa, September 22-26th 1987, **P 126.**
- (2) F. Russo, G. Romeo, **S. Guccione**, E. Bousquet.
Synthesis and pharmacological activity of 6H-thiazolo [3'2':1,2]5-oxopyrimido[5,4-b]indolo. New heterocyclic ring system.
BONONIACHEM 88, XVIth National Meeting of Chemistry, Bologna, October 9-14th 1988, **F 110.**
- (3) F. Russo, G. Romeo, **S. Guccione**,
Synthesis of pyrimido[5,4-b]indoles-3-substituted as potential anti-hypertensive agents.
1er Congreso Conjunto Hispano-Italiano de Quimica Terapeutica, Granada (Spain), September 19-22 1989, **P.A. 098.**
- (4) F. Russo, **S. Guccione**, G. Romeo e L. Monsù Scolaro.
New polycondensed heterocycles containing the pyrazolo[3,4-d]pyrimidine system as potential drugs.
Regional meeting (Sicily) of the Italian Chemical Society, Catania, November 13-14 1989, **P 28.**
- (5) F. Russo, **S. Guccione**, G. Romeo, L. Monsù Scolaro, S. Pucci, A. Caruso, M. V. Cutuli, M. Amico Roxas.
Synthesis and pharmacological activity of new 1H-pirazolo[3,4-d] [1,2,4]8H-triazolo[2,3-a]4H-pirimidin-4-one.
CISCI 90, National Meeting of the Italian Chemical Society, San Benedetto del Tronto, September 30 - October 5th 1990, **FP 74.**

(6) F. Russo, W. B. Knight, **S. Guccione**, G. Romeo.

Synthesis of new pyrazolo-thiazin-4-one and pyrazolo-oxazin-4-one as potential inhibitors of Human Leukocyte Elastase.

CISCI 90, National Meeting of the Italian Chemical Society, San Benedetto del Tronto, September 30 -October 5th 1990, **FP 89**.

(7) **S. Guccione**,

Nuovi potenziali agenti analgesici ed antinfiammatori

VIII National Seminary for Ph. D. Students -XI Advanced Course of Medicinal Chemistry. Urbino, July 8-13th 1991, **181**.

(8) F. Russo, **S. Guccione**, G. Romeo, G. Uccello Barretta, S. Pucci, A. Caruso, V. Cutuli,

Synthesis, structural characterization and biological activity of new 1H-pyrazolo [3,4-d]thiazolo [3,2-a] – 4H -pyrimidin - 4 – one,

X National Meeting of the Medicinal Chemistry Division of the Italian Chemical Society, Siena, September 16-20th 1991, **P10**.

(9) F. Russo, **S. Guccione**, G. Romeo, V. Andrisano, M. Guarneri, P. Giori, C. Vicentini, R. Chabin, W.B. Knight.

Human Leukocyte Elastase inhibitors : a new approach to the disorders with connective destruction,

X National Meeting of the Medicinal Chemistry Division of the Italian Chemical Society, Siena, September 16-20th 1991, **C18**.

(10) F. Russo, G. Romeo, **S. Guccione**, A. De Blasi, M. Foti.

Pyrimido[5,4-b]indoles as highly active and selective $\alpha 1$ antagonists.

X National Meeting of the Medicinal Chemistry Division of the Italian Chemical Society, Siena, September 16-20th 1991, **C8**.

(11) S. Pucci, A. Raffaelli, F. Russo, **S. Guccione**, G. Romeo.

Mass spectrometry study of some pyrazolotriazolopyrimidine derivatives.

JANUACHEM 92, National Meeting of the Italian Chemical Society, Genova, October 25-30th 1991, **MS7C5**.

- (12) **S. Guccione**, F. Russo, G. Romeo, R. Chabin, D. Kuo and W.B Knight.
Preliminary research on indolothiazines -4-one as HLE inhibitors.
XII International Symposium on Medicinal Chemistry, Basel(Switzerland), September 13-17th 1992, **P-163 A**.
- (13) **S. Guccione**, F. Russo, G. Romeo, C.B. Vicentini, M. Guarneri, P. Giori, R. Chabin, D. Kuo, W.B Knight.
HLE inhibition from oxadiazinone derivatives.
XII International Symposium on Medicinal Chemistry, Basel (Switzerland), September 13-17th 1992, **164 B**.
- (14) **S. Guccione**, F. Russo, G. Romeo, V. Andrisano, M. Recanatini, R. Chabin, D. Kuo and W.B Knight.
Design and synthesis of pyrazolothiazines - 4 - thione as novel class of Human Leukocyte Elastase inhibitors (HLE).
XII International Symposium on Medicinal Chemistry, Basel (Switzerland) September 13-17th 1992, **165 C**. Abstracted in Drug Data Report, **15**,4, 1993.
- (15) S. Pucci, A. Raffaelli, G. Uccello Barretta, P. Salvadori, F. Russo, **S. Guccione**, G. Romeo.
Structural characterization of impurities present in samples of pyrazolotriazolopyrimidine derivatives by EI, FAB and IS mass spectrometry and NMR.
11th Informal Meeting on Mass Spectrometry, Budapest (Hungary), April 26-28th 1993, **19**.
- (16) S. Pucci, A. Raffaelli, P. Salvadori, F. Russo, **S. Guccione**, G. Romeo.
Studio di alcuni derivati pirazolotriazolopirimidinici mediante spettrometria di massa.
I° MS-PHARMADAY, Siena, June 2-4th 1993, **P9**.
- (17) C.B. Vicentini, M. Guarneri, V. Andrisano, **S. Guccione**, R. Chabin, A. Edison, X. Huang, W.B. Knight and P. Giori.
Pyrazolo [4,3-c][1,2,5]oxadiazin-3(5H)-ones as potential mechanistic inhibitors of Serine Proteases.

6th Cyprus Conference on New Methods in Drug Research, Limassol (Cyprus), May 7-14 1994, **35**.

- (18) **S. Guccione**, V. Andrisano, M. Recanatini, C.B. Vicentini, P. Giori, M. Guarneri, A. Rescifina, A. Edison, X. Huang, R. Chabin, F. Russo and W.B. Knight.

Bioisosterism and molecular hybridization as criterion in the design of bifunctional heterocycles as new serine protease inhibitors: synthesis, biological activity and enzymology mechanistic studies.

XIII International Symposium on Medicinal Chemistry, Paris (France), September 19-23th 1994, **P200**.

- (19) **S. Guccione**, M. Modica, D. Shaw, G. Uccello Barretta, A. Santagati and M. Santagati.

Study on the tachykinins antagonist effect of combinatorial functionalized heterocycle replacements in tricyclic pyrimidine derivatives.

XIII International Symposium on Medicinal Chemistry, Paris (France), September 19-23th 1994, **P285**.

- (20) F. Russo, V. Ligresti, **S. Guccione**, A. Edison, X. Huang and W.B. Knight.

Molecular hybrids as Human Leukocyte Elastase inhibitors.

Regional Meeting (Sicily) of the Italian Chemical Society, Palermo, October 20-22th 1994, **C23**.

- (21) F. Russo, **S. Guccione**, C.B. Vicentini, P. Giori, M. Guarneri, V. Andrisano, M. Recanatini, T. Langer, R. Marschhofer, A. Edison, X. Huang, R. Chabin and W. B. Knight.

Building a hypothesis for Human Leukocyte Elastase inhibition by bifunctional condensed heterocycles.

National Meeting su Orientamenti e Metodologie in Chimica Farmaceutica, Organica e Bioorganica, Numana (AN), June 2-6 1995, **O41**.

- (22) S. Vomero, F. Russo, M. Anzini, A. Cappelli, **S. Guccione**, T. Langer, A. Edison, X. Huang, W.B. Knight.

1,4-Benzodiazepine derivatives as Potential Inhibitors of Human Leukocyte Elastase(HLE).

II Italian-Spanish Joint Meeting on Medicinal Chemistry, Ferrara, August 30th-September 2nd 1995, **P131**.

(23) M. Artico, S. Massa, F. Russo, A. Mai, **S. Guccione**, A. Edison, X. Huang, W. B. Knight.

Pyrrlobenzodiazepine moiety as original support to design novel Human Leukocyte Elastase inhibitors.

II Italian-Spanish Joint Meeting on Medicinal Chemistry, Ferrara, August 30th-September 2nd 1995, **P133**.

(24) C.B. Vicentini, M. Guarneri, V. Andrisano, **S. Guccione**, T. Langer, R. Marschhofer, R. Chabin, A. Edison, X. Huang, W.B. knight, P. Giori.

Human Leukocyte Elastase inhibitor design: CoMFA contributions to pyrazolooxadiazinones design.

II Italian-Spanish Joint Meeting on Medicinal Chemistry, Ferrara, August 30th-September 2nd 1995, **P135**.

(25) F. Russo, Z. Machon', A. Regiec, R. Jaszold-Howorko, **S. Guccione**, L. Monsù Scolaro, A. Edison, X. Huang, W. B. Knight.

Human Leukocyte Elastase inhibitors: isothiazolooxazinones and 6-acylamino or 6-aminocarboxylate substituted pyrazolothiazinones and pyrazolooxazinones.

II Italian-Spanish Joint Meeting on Medicinal Chemistry, Ferrara, August 30th-September 2nd 1995, **P148**.

(26) **S. Guccione**, M. Santagati, A. Santagati, M. Modica, G. Uccello Barretta, T. Langer, E. Tonnel, F. Russo.

CoMFA contributions to a binding mode for NK-2 receptor antagonists.

10th Camerino Noordwijkerhout Symposium **Perspectives in Receptor Research**
Camerino, September 10-14 1995, **P77**.

(27) M. Modica, A. Santagati, M. Santagati, L. Monsù Scolaro, **S. Guccione**, F. Russo,

Potential of Indole Skeleton Containing Heterocycles as Antagonists at the Neurokinin (NK) receptor System .

Regional Meeting (Sicily) of the Italian Chemical Society, Taormina Mare (Italy), December 18-20 1995, **12**.

(28) R. Marschhofer, T. Langer, **S. Guccione**,

Human-Leukozyten-Elastase. zur untersuchung neuartiger inhibitoren mittels molecular modelling.

Wissenschaftliche Tagung der Österreich Pharmazeutischen Gesellschaft, Innsbruck (Austria), October 26th-28th ,1995.

Sci. Pharm.*, **63**, 331, 1995.

*Official journal of the Austrian Pharmaceutical Society.

(29) T. Langer, R. Hoffmann, **S. Guccione**.

Inhibitors of Human Leukocyte Elastase. modelling and 3D search,

11th European Symposium on Quantitative Structure-Activity Relationships: Computer Assisted Lead Finding and optimization, Lausanne (Switzerland), September 1-6, 1996, **P4b**.

(30) **S. Guccione**, T. Langer , F. Russo, N. A. Santagati, M. Guarneri, C.B. Vicentini, W.B. Knight, A. Edison.

Modelling Study on potential Mechanism Based Inhibitors of Human Leukocyte Elastase.

11th European Symposium on Quantitative Structure-Activity Relationships: Computer Assisted Lead Finding and optimization, Lausanne (Switzerland), September 1-6, 1996, **P20d**.

(31) T. Langer , **S. Guccione**, F. Russo, M. Artico, S. Massa, A. Mai, W.B. Knight, A. Edison.

Comparative Modelling Study on Serine Protease Inhibitors,

11th European Symposium on Quantitative Structure-Activity Relationships: Computer Assisted Lead Finding and optimization, Lausanne (Switzerland), September 1-6, 1996, **P21d**.

(32) **S. Guccione**, T. Langer, F. Russo, V. Andrisano, M. Recanatini, W. B. Knight, A.M. Edison.

Modelling study on hydrophobic subsites (S'1-S'3) binding of pyrazolothiaziniones to HLE.

XIVth International Symposium on Medicinal Chemistry, September 8-12, 1996, Maastricht (Olanda) , **P5.25**.

(33) **S. Guccione** , F. Russo, K. Kiec'-Kononowicz, T. Langer, W. B. Knight, A.M. Edison.

Potential Serine Protease inhibitors: fused hydantoins and imidazoquinazolidindiones.

XIVth International Symposium on Medicinal Chemistry, September 8-12 1996, Maastricht (Olanda), **P5.26**.

(34) F. Russo, **S. Guccione** , A.M. Edison, T. Langer, and W. B. Knight.

Protein Tyrosine Kinase inhibitors: an approach for anticancer drug development.

XIII National Meeting of the Medicinal Chemistry Division of the Italian Chemical Society, Paestum, September 23-27 1996, **C-F6**.

(35) F. Russo , A.Santagati, J. Longmore, **S. Guccione** , T. Langer , E. Tonnel , M. Modica, M. Santagati, L. Monsù Scolaro.

Building a model of interaction at the NK-2 receptors: polycondensed heterocycles containing the pyrimidoindole skeleton.

XIII National Meeting of the Medicinal Chemistry Division of the Italian Chemical Society Paestum, September 23-27 1996, **P44**.

(36) F. Russo, M. Modica, J. Longmore, **S. Guccione** , M. Santagati, A.Santagati, F. Balzano, G. Uccello Barretta, S. Pucci, T. Langer.

NK-2 Receptor Antagonists: Pyrazolopyrimidothiazole and Pyrazolopyrimidoxazole derivatives.

XIII National Meeting of the Medicinal Chemistry Division of the Italian Chemical Society, Paestum, September 23-27 1996, **P123**.

(37) M. König, T. Langer und **S. Guccione**.

Neue inhibatoren der protein-tyrosin-kinase pp60^{c-src}: untersuchung des bindungsverhaltens mittels molecular modelling.

Wissenschaftliche Tagung der OEPHG'(13th Meeting of the Austrian Pharmaceutical Society), April 2-4 1997, Wien (Austria).

Sci. Pharm.*, **65**, 95.

*Official journal of the Austrian Pharmaceutical Society.

(38) J. Longmore, F. Guerrera, L. Salerno, M. C. Sarv  , M. A.,Siracusa, C. J. Cramer, F. Russo, **S. Guccione**.

Synthesis and pharmacological evaluation of benzothieno- and [1]pyridothieno [2,3- d]triazole derivatives as antagonists at NK-1 receptors.

First Italian-Swiss Meeting on Medicinal Chemistry , Torino Incontra Congress Center, 23-26 Settembre 1997, Torino. **A39**.

(39) F. Russo, J. Longmore, M. Modica, M. Santagati, A. Santagati , **S. Guccione**.

Synthesis of 1-phenyl-6-aryl substituted pyrazolopyrimidothiazole as antagonists at NK-2 receptors.

First Italian-Swiss meeting on Medicinal Chemistry , Torino Incontra Congress Center, 23-26 Settembre 1997- Torino. **A40**

(40) F. Russo, K. Kiec'-Kononowicz, A. Drabczyska, **S. Guccione**, T. Langer, M. A. Koenig.

CoMFA based design of new inhibitors of protein tyrosin kinase pp60c-src,

First Italian-Swiss Meeting on Medicinal Chemistry , Torino Incontra Congress Center, 23-26 Settembre 1997- Torino. **A78**.

(41) C. B. Vicentini, F. Russo, M. Reboud-Ravaux, C. Doucet , M. Manfrini , **S.**

Guccione. *Pyrazolo[4,3-c][1,2,5]oxadiazinones as human leukocyte elastase (HLE) inhibitors.*

First Italian-Swiss Meeting on Medicinal Chemistry , Torino Incontra Congress Center, 23-26 Settembre 1997- Torino. **A90**.

(42) M. Sarpietro, M. Marino, A. Cambria, G. Uccello Barretta, F. Balzano, F. Russo, **S. Guccione**.

Determination of the cholecalciferol-lipid complex using a combination of comparative modelling and NMR spectroscopy,

12th European Symposium on Quantitative Structure-Activity Relationships. Copenhagen, Denmark, August 23-28, 1998. **P.75.**

(43) M. Santagati, A. Doweyko, A. Santagati, M. Modica, **S. Guccione**, H. Chen , F. Russo, G. Uccello Barretta , F. Balzano.

5-HT_{1A} receptors mapping by conformational analysis (2D NOESY/MM) and "three way modelling" (HASL, CoMFA, PARM),

12th European Symposium on Quantitative Structure-Activity Relationships. Copenhagen, Denmark, August 23-28, 1998. Abstract book, **O.17.**

(44) M. Santagati, H. Chen , A. Santagati, M. Modica, **S. Guccione** , F. Russo , G. Uccello Barretta, F. Balzano.

Application of PARM to constructing and comparing 5-HT_{1A} and α_1 receptor models.

12th European Symposium on Quantitative Structure-Activity Relationships. Copenhagen, Denmark, August 23-28, 1998. **P.122.**

(45) M.P.Giovannoni, V. Dal Piaz, B.M. Kwon, M.K. Kim, Y.K. Kim, **S. Guccione**, D. Barlocco.

Inibitori dell'acil-CoA: colesterolo aciltransferasi a struttura 5,6-difenilpiridazinica.

XIV Convegno Nazionale, Division of Medicinal Chemistry of the Italian Chemical Society. Salsomaggiore Terme (Parma), September 21-25, 1998. **133.**

(46) R. Bursi, V. Van Geerestein, A. Gazit, **S. Guccione**.

Comparative Spectra Analysis (CoSA): A Tyrosine Kinase Inhibitors Study.

1999 QSAR Gordon Research Conference, Tilton, New Hampshire, July 25-30, 1999. Quantitative Structure-Activity Relationships. **Session IV (Thursday).**

(47) A.M. Doweyko, **S. Guccione**, H. Chen, M. Modica, M. Santagati, A. Santagati, G. Uccello-Barretta, F. Balzano.

Receptor modeling using multiconformer alignment: Comparison of HASL and CoMFA in the analysis of 5HT_{1A} thienopyrimidione ligands.

1999 QSAR Gordon Research Conference, Tilton, New Hampshire, July 25-30, 1999. Quantitative Structure-Activity Relationships. **Session IV (Thursday).**

(48) R. Marschhofer, **S. Guccione**, and T. Langer.

Strukturbasiertes Alignment fuer 3D-QSAR: Vergleich FlexX-LUDI am Beispiel von HLE-Inhibitoren,

Wissenschaftliche Tagung der OEPHG(14th Meeting of the Austrian Pharmaceutical Society), September 9-October 2 1999 2-4 1997, Innsbruck (Austria).
Sci. Pharm.*, 67, **S84** (1999).

*Official journal of the Austrian Pharmaceutical Society.

(49) V. A. Potemkin, E. V. Bartashevich, A. R. Beccari, M. A. Grishina and **S. Guccione**.

An Alternative Method for 3D-QSAR and the Alignment of Molecular Structures: BiS (Biological Substrate Search),

13th European Symposium on Quantitative Structure-Activity Relationships, Rational Approaches to Drug Design. **P110.**

QSAR 2000 Düsseldorf, Heinrich-Heine-Universität, Düsseldorf, Germany, 27 August-1 September, 2000.

*Selected for the *Proceedings* book.

(50) S. Gritsch, **S. Guccione**, A. Cambria, G. Raciti, R. Hoffmann, and T. Langer.
Chemical features based pharmacophore models of MAO-B inhibitors.

13th European Symposium on Quantitative Structure-Activity Relationships, Rational Approaches to Drug Design.

QSAR 2000 Düsseldorf, Heinrich-Heine-Universität, Düsseldorf, Germany, 27 August-1 September, 2000. **P114.**

(51) **S. Guccione**, M. Fresta, A. R. Beccari, P. M. Furneri and Giovanni Puglisi.

Combining Differential Scanning Calorimetry (DSC) and Computational Approaches: A New "Self-Promoted" Entrance Pathway of Ofloxacin.

13th European Symposium on Quantitative Structure-Activity Relationships, Rational Approaches to Drug Design.

QSAR 2000 Düsseldorf, Heinrich-Heine-Universität, Düsseldorf, Germany, 27 August-1 September, 2000. **P100**

(52) **S. Guccione**, B. S. Capuano and R. Bursi.

3D-QSAR and Receptor Mapping of Steroid Progesterone Receptor Ligands by CoMFA, HASL and PARM.

13th European Symposium on Quantitative Structure-Activity Relationships, Rational Approaches to Drug Design.

QSAR 2000 Düsseldorf, Heinrich-Heine-Universität, Düsseldorf, Germany, 27 August-1 September, 2000. **P40**.

(53) **S. Guccione**, M. Modica, A. M. Doweyko, M. Santagati, A. B. Nordquist, J. R. Torrente, H. Chen, and R. J. Mattson.

PARM Mapping of Rat and Human Serotonin 1A (5-HT_{1A}) Receptor.

13th European Symposium on Quantitative Structure-Activity Relationships, Rational Approaches to Drug Design.

QSAR 2000 Düsseldorf, Heinrich-Heine-Universität, Düsseldorf, Germany, 27 August-1 September, 2000. **P12**.

(54) E. Fioravanzo, **S. Guccione**, H. Chen, M. C. Calogero, and M. Mabilia.

A PARM study of non-peptide angiotensinII receptor antagonists from SEA alignment.

13th European Symposium on Quantitative Structure-Activity Relationships, Rational Approaches to Drug Design.

QSAR 2000 Düsseldorf, Heinrich-Heine-Universität, Düsseldorf, Germany, 27 August-1 September, 2000. **P109**.

(55) R. Bursi, P. Verwer, A. Gazit, A. R. Beccari, G. Uccello Barretta, F. Balzano and **S. Guccione**.

From Molecular Spectra to Biological Activities: a Comparative Spectra Analysis (CoSA) study on Epidermal Growth Factor Receptor Protein Tyrosine Kinase Inhibitors.

13th European Symposium on Quantitative Structure-Activity Relationships, Rational Approaches to Drug Design.

QSAR 2000 Düsseldorf, Heinrich-Heine-Universität, Düsseldorf, Germany, 27 August-1 September, 2000. **P39.**

*Selected for the *Proceedings* book.

(56) A.P. Borosy, A.R. Beccari and **S. Guccione.**

DISCO based 3D QSAR analysis of 5-HT_{1A} receptor ligands by COMFA and HASL.

EUCO-CC3. Third European Conference on Computational Chemistry.

Budapest, Hungary, 4-8 September 2000.

(57) A.P. Borosy, F. Signorelli, M. Santagati, M. Modica, F. Russo, A. Santagati and **S. Guccione.**

Pharmacophore mapping of serotonin 5-HT₄ receptor by new piperazinyl acylaminodimethyl- thiophene ligands: conformational analysis and DISCO .

EUCO-CC3. Third European Conference on Computational Chemistry.

Budapest, Hungary, 4-8 September 2000.

(58) Potemkin V.A., Grishina M.A., Rusinov G.L, Fedorova O.V., Chupakhin O.N. and **Guccione S.**

New 3D-QSAR Algorithm BiS for orientation and alignment of molecules to receptor. Analysis of anti-tubercular action of podands.

The 2-nd Russian Conference "Molecular Modelling", 24-26 April, Moscow, 2001, **p. 95.**

(59) Bartashevich E.V., Belik A.V., Potemkin V.A. and **Guccione S.**

A method for determination of form and sizes of pocket in "receptor-ligand" complexes.

The 2-nd Russian Conference "Molecular Modelling", 24-26 April, Moscow, 2001, **p. 51.**

(60) Potemkin V.A., Arslambekov R.M., Belik A.V., Perspicace S., **Guccione S.**

Multigen: A New Paradigm For “Multiconformational” Alignment of Molecular Structures in 3D-Qsar Studies.

Computer Assistance to Chemical Research -2001, International Symposium. Zelinsky Institute of Organic Chemistry of Russian Academy of Sciences, Moscow, Russia, May 22-23, 2001. **RegNo 440**

(61) Potemkin V.A., Arslambekov R.M., Belik A.V., Perspicace S., Guccione S.
Multigen: A New Paradigm For “Multiconformational” Alignment of Molecular Structures in 3D-Qsar Studies.

Fock School on Computational and Quantum Chemistry, Novgorod the Great, Russia, May 22-23, 2001. **A-32.**

*(60), (61): Cooperative sessions of two conferences.

(62) Grishina M.A., Potemkin V.A., Rusinov G.L., Bertashevitch E.V., **Guccione S.**,
Perspicace S. and Chupakin O.N.

Comparing A Bis (Biological Substrate Search) Alignment Of Anticancer Dna And Dna/Rna Antimetabolites Into Their Active Sites With .Pdb Co-Crystals.

From Genes to Drugs via Crystallography, Maiorana Centre, Erice, Italy, May 23 – June 2, 2002. **P. 23**

(63) Lara Orús, Silvia Pérez-Silanes, Ana-M. Oficialdegui, Javier Martínez-Esparza, Juan-C Del Castillo, Marisa Mourelle, Thierry Langer, **Salvatore Guccione**, Giuseppina Donzella, Eva M. Krovat, Konstantin Poptodorov, Berta Lasheras, Santiago Ballaz, Isabel Hervías, Rosa Tordera, Joaquín Del Río, Antonio Monge.

Synthesis and Molecular Modeling of new 1-aryl-3-[4-arylpiperazin-1-yl]-1-propane derivatives with high affinity at the serotonin transporter and at 5-HT_{1A} receptors.
XVIIth International Symposium on Medicinal Chemistry, September 1-5, 2002, Barcelona, Spain.. Drugs of the Future, 27A, September 2002, Prouss Science. **P 409.**

(64) Jordi Muñoz, F. Javier Luque, Glen E. Kellogg, Daniela Barlocco, Rosa Poidomani and Salvatore Guccione.

Potential of the Hydrophobic Similarity Index in Drug Design: Mapping the binding of 5,6-Diphenylpyridazinone Acyl-CoA:cholesterol O-acyl transferase (ACAT) INHIBITORS.

V Congresso I.N.B.B., 3-5 Ottobre **2002**, Catania, **P100**.

(65) Glen E. Kellogg , Rosa Poidomani, Samantha Perspicace and **Salvatore Guccione**.

Free Energy Predictions of Carbohydrate-Ligand Complex Binding .

V Congresso I.N.B.B., 3-5 Ottobre **2002**, Catania, **P101**.

(66) Antonina Puleo, Rosario Pignatello, Rosa Poidomani, Samantha Perspicace, Giovanni Puglisi, Salvatore Guccione, and Istvan Toth.

Molecular Modelling of Lipophilic Conjugates of Methotrexate with Lipoamino Acids.

V Congresso I.N.B.B., 3-5 Ottobre **2002**, Catania, **P102**.

(67) Nuria Bech, F. Javier Luque, Samantha Perspicace, Maria Modica and Salvatore Guccione.

Mapping the 5-HT₃ Receptor Agonist Binding by Molecular Hydrophobic Index, Electrostatic and Van der Waals Interaction Energy.

V Congresso I.N.B.B., 3-5 Ottobre **2002**, Catania, **P103**

(68) Rosario Pignatello, Gabriele Cruciani, Rosa Poidomani, Antonina Puleo, Giovanni Puglisi, Samantha Perspicace and Salvatore Guccione.

Molecular Modelling of Non-Steroidal Antiinflammatory Drugs in Eudragit Retard Polymers Solid Dispersions.

V Congresso I.N.B.B., 3-5 Ottobre 2002, Catania, **P104**.

(69) Perspicace S., Kohler J., **Guccione S.**, Huber W.

Binding Studies Using Surface Plasmon Resonance (Spr) Technique.

Regional Meeting of The Italian Chemical Society. Hotel Delle Terme. Acireale (Catania), December 2-3 2002. **C4**.

(70) M. Geppi, **S. Guccione**, G. Mollica, R. Pignatello and C.A. Veracini.

Study of Structural and Dynamic Behaviour of Ibuprofen and its Complexes with Eudragit RL100 by Means of Solid State NMR .

10th Chianti Workshop on Magnetic Resonance. Nuclear and Electron Relaxation.

The Neon Jubilee Edition San Miniato (Pisa), Italy - May 25 - 30, 2003. **p. 128**

(71) V.A. Potemkin, M.A. Grishina, S. Guccione, S. Perspicace.

Determination of orientation of DNA-antimetabolites in the real receptor cavity using 3D QSAR method BiS, 3-D Russian Conference "Molecular Modelling", 15-17 April 2003, Moscow, **P. 100**.

(72) Potemkin V.A., Arslambekov R.M., Belik A.V., **Guccione S.**

Parallel version of MultiGen.

Computer Applications in fundamental and applied Chemistry, Biology, Pharmaceutics and Medicine, Moscow, 2003. **P. 11**.

(73) Glen E. Kellogg , Samantha Perspicace and **Salvatore Guccione.**

Carbohydrate-Ligand Complex Binding: Empirical free Energy Modeling.

3rd International Workshop on New Approaches in Drug Design & Discovery , Marburg, Germany, March, 24-27, 2003. **P5**.

(74) M. Geppi, **S. Guccione**, G. Mollica, R. Pignatello , C.A. Veracini.

Solid state NMR of drugs: A Study of Non-steroidal Anti-inflammatory drugs and Their dispersions with polymeric carriers .

XXXIV National Congress on Magnetic Resonance : Porto Conte Ricerche, September 21-24 2004. **P 29 O**.

(75) Kurt Kristiansen, Ingebrigt Sylte , Rebecca Ciaccio , Stefano Forte, and **Salvatore Guccione.**

A Preliminary Human Endothelin-A(ET_A) Receptor Model.

2nd Workshop on *The state-of-the-art of Computational Chemistry* ,The University of Calabria and Basilicata", Campus Universitario, Germaneto-Catanzaro 5,6 Feb. 2004. **P5**

(76) Pietro Cozzini, Francesca Spyrakis , Micaela Fornabaio· Stefano Forte, **Salvatore Guccione**, Laura Giurato.

The Significance of Ph Effects In Protein-Ligand Interaction Models.

2nd Workshop on *The state-of-the-art of Computational Chemistry* ,The University of Calabria and Basilicata", Campus Universitario, Germaneto-Catanzaro 5,6 Feb. 2004. **P10**

(77) Kurt Kristiansen, Ingebrigt Sylte , Rebecca Ciaccio , Stefano Forte Laura Giurato
Pietro Cozzini, Francesca Spyrakis and **Salvatore Guccione.**

Molecular Modelling of endothelin Et_A and ET_B .

XVIIIth International Symposium on Medicinal Chemistry, August 15-19, 2002, Copenhagen Denmark & Malmö Sweden . p. 202 drugs Future 2004 29 (suppl. A) .

(78) M. Geppi, **S. Guccione**, G. Mollica, R. Pignatello, C. A. Veracini.

Study of structural and dynamic behaviour of ibuprofen and its solid dispersions with eudragit RL100 by means of solid state NMR **PO 188**.

The first EENC/AMPERE joint meeting in Lille France), Lille France from 6th to 11th September 2004. **PO 188**

(79) F. Spyraakis, L. Giurato, P. Cozzini, M. Modica, I. Sylte, **S. Guccione**.

5-HT_{1A} receptor binding analysis of thienopyrimidinones partial agonists: a paradigm breaking study regarding the pharmacophoric leadership of the protonated piperazine ring in GPCR ligands,

VI Congresso I.N.B.B., 4-6 novembre **2004**, Chiesa S.Croce di Lucca, Napoli. **P79**

(80) Uccello-Barretta G., Balzano F., Paolino D. , Ciaccio R. , **Guccione S.**

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

VI Congresso I.N.B.B., 4-6 Novembre **2004**, Chiesa S.Croce di Lucca, Napoli. **P64**

(81) Osman A.B.S.M. Gani, Olaiywola Adekoya, Laura Giurato, **Salvatore Guccione**, Jan Olof Winberg and Ingebrigt Sylte .

The Catalytic Mechanism of Short-Chain Dehydrogenase/Reductases.

The Norwegian biochemical society 41st contact meeting, 13-16 January 2005

RICA Ishavs Hotel Tromsø. **P30**

(82) Tadeusz Z.E. Jones, Laura Giurato, **Salvatore Guccione** and Rona R. Ramsay.

Binding of imidazoline ligands to the active site of purified MAO A .

12th Amine Oxidase and Trace Amines Workshop AO 2006 . From Bench to

Bedside. **P1**

(83) L. Berrade, S. Perez, P. Egea, L. Giurato, **S. Guccione**, I. Aldana, G. Molinaro, F. Nicoletti, A. Monge.

Design and synthesis of multiple ligands: new arylamines and their binding affinity toward 5-HT transporter (SERT) and 5-HT₇ receptors.

XIX International Symposium on Medicinal Chemistry, 29 Agosto-2 Settembre **2006**, Istanbul, Turchia. **P241**.

(84) Andrea Santagati , Giuseppe Granata , Venera Cardile, **Salvatore Guccione**, Laura Giurato.

Molecular Modelling of a novel class of N5-methanesulfonamide dihydrothienopyrimidinones as as potential dual COX-2 inhibitor/nitric oxide anti-releasing agents.

Drug Discovery research (CTDDR-2007) Central Drug Research Institute Lucknow (India). **P. 144**. Medicinal Chemistry Research 15, 1/6, 2007 . (Special issue **p. 372**).

(85) Laura Giurato, Rona R. Ramsay and **Salvatore Guccione**.

Models of imidazoline isomers in the active site of monoamine oxidase B.

Drug Discovery research (CTDDR-2007) Central Drug Research Institute Lucknow (India). **P143**.

Medicinal Chemistry Research 15, 1/6, 2007 (Special issue **p. 370**) .

(86) Maria Angela Castriciano, Andrea Romeo, Luigi Monsù Scolaro, Nicola Angelici, Norberto Micali, **Salvatore Guccione**, Laura Giurato.

Supramolecular Complexation of Tetrakis(4-carboxyphenyl)porphyrin with PAMAM Starburst Dendrimers: Structural Features and Interactions with Nucleic Acids. A Combined Experimental and Molecular Modeling Approach.

8th Tetrahedron Symposium 26-29 June 2007, Berlin, Germany. **P87** (session 3 June 28,29)

(87) M. T. Cambria, M. Falconi, S. Guccione, M. Rizzi, S. Ragusa, A. Cambria.

Docking Simulation of the Complex between 2,5-Xylidine and *Rigidoporous Lignosus* Laccase.

SIB 2007, RICCIONE 26-28 SETTEMBRE 2007.

THE ITALIAN JOURNAL OF BIOCHEMISTRY 56, 3, 2007. **P. 15.14**

(88) R.R. Ramsay, R. James E. Bradley, L.Giurato, **S. Guccione**.

The shape of the flavin in monoamine oxidase.

16th International Symposium on Flavins and Flavoproteins Palacio de Congresos, Jaca, Spain, 8-13 Giugno 2008. **P115**.

(89)L. Giurato, S. Forte, A. Geronikaki, P. Eleftheriou, **S. Guccione**.

Insights into the binding mode of new 3-((furan-2-yl)methyl)-2-phenyl thiazolidin-4-one derivatives as Protein Tyrosine Phosphatase 1B (PTP 1B) inhibitors.

40th Erice Course: From Molecules To Medicine: Integrating Crystallography In Drug Discovery (29 Maggio - 8 Giugno 2008), Erice, Italia. **P39**.

(90)Stefano Forte , Francesca Gullo, **Salvatore Guccione**, Fabio Galvano , Giovanni Li Volti.

Computational Studies on the role of Human Milk heme Oxygenase as Immuno Modulating Factor. 40th Erice Course: From Molecules To Medicine: Integrating Crystallography In Drug Discovery (29 Maggio - 8 Giugno 2008), Erice, Italia. **P44**.

(91)Luis Berrade, Silvia Pérez, Adela Mendoza, Silvia Galiano, Bárbara Aisa, Maria Javier Ramírez, Salvatore Guccione, Lise Roman Moltzau, Finn Olav Levy, Ignacio Aldana, Antonio Monge.

NEW 5-HT₇ RECEPTOR ANTAGONISTS AS PUTATIVE ANTIDEPRESSANTS WITH RAPID ONSET OF ACTION. XXth International Symposium on Medicinal Chemistry. Vienna August 31-September 4 2008. **P204**.

Drugs Fut. 2008, 33(Suppl. A): 41.

(92)IMPELLIZZERI AAR, ANDRESSEN KW, KROBERT KA, MANFRA O, MESSINA A, GUCCIONE S, LEVY FO

Molecular Modelling and Site-Directed Mutagenesis Reveal Essential Residues for 5-HT₇ Receptor Binding.

Winter Meeting of the Norwegian Society of Pharmacology and Toxicology, from January 28-31 at Beito. **BF8**

(93)Stefano Forte, Giancarlo Rappazzo, Giovanni Li Volti, and Salvatore Guccione.

Heme Oxygenase-1 and -2 interactions and their possible implications in drug design.

6th International Workshop on New Approaches in Drug Design & Discovery
Schloss Rauischholzhausen, March 22-25, 2010 . **P5**.

(94) Chiara B.M. Platania, Matteo Pappalardo, Danilo Milardi, Salvatore Guccione and Anwar Rayan.

*New insights into the human Histaminergic type 4 receptor: increasing hit rates of antagonists by multiple focusing Membrane Proteins: **Structure and Function.***

Lady Margaret Hall, Oxford, UK April 6th -. April 6th - April 8th, 2011. **P29**

(95) L. Basile, V. Greco, C.B.M. Platania, C. La Rosa, D. Milardi, S. Sciuto, S. Guccione.

Drug delivery of synthetic antisense “Bioconjugates” for anticancer therapy DNA.

4th BBBB - Bled International Conference on Pharmaceutical Sciences, Bled, Slovenia, 29 Settembre – 1 Ottobre 2011. European Journal of Pharmaceutical Sciences, 44 (suppl. 1), 146,2011 . **P089**.

(96) Basile L., Floris M., Medda R., Guccione S., Doweyko A.

A Python implementation of the Hypothetical Active Site Lattice.

Consorzio Interuniversitario “Istituto Nazionale di Biostrutture e Biosistemi”

X Convegno Nazionale “Scienze della vita”- Roma 22-23 Ottobre 2012.

Abstract book pag. 56.

(97) Pappalardo M., Basile L., Guccione S.

Heme Oxygenase 1 and Heme Oxygenase 2 as druggable targets: docking and two hybrid system to identifying and characterizing protein-protein and protein-ligand interactions.

Consorzio Interuniversitario “Istituto Nazionale di Biostrutture e Biosistemi”

X Convegno Nazionale “Scienze della vita”- Roma 22-23 Ottobre 2012.

Abstract book pag. 64-65.

(98) Livia Basile, Matteo Pappalardo, Danilo Milardi, Salvatore Guccione, Rona R. Ramsay.

Computational comparison of the I₂ binding site in monoamine oxidases A and B (MAO A and MAO B).

Convegno Congiunto delle Sezioni Calabria e Sicilia 2012. Arcavacata di Rende (CS), 6-7 Dicembre 2012. **O-02.**

(99) Matteo Pappalardo, Danilo Milardi, Anwar Rayan, Nir Shachaf, Livia Basile, Salvatore Guccione.

Compounds repositioning to H4 antagonists combining in silico approaches.

Cost Action BM0806. Final conference & MC Meeting. Recent Advances in Histamine H4R research. Cape Sounion, Athens, Greece, 21-23 Marzo 2013. **O11.**

(100) Livia Basile, Matteo Pappalardo, Danilo Milardi, Salvatore Guccione.

Preliminary Results on In vitro and in Silico Comparing of 5-HT₇ Receptor Mutants by Molecular Dynamics and Docking.

COST Action CM1207. GLISTEN MC/WG meeting and workshop. Biological and Chemical Research Centre, University of Warsaw, Varsavia, 7-9 Ottobre 2013. **1.**

(101) L. Basile, M. Pappalardo, D. Milardi, S. Guccione.

Studio in Silico dei residui chiave per l'attività di ligandi al recettore 5HT-7.

Convegno Congiunto delle Sezioni Calabria e Sicilia 2013. Catania, 2-3 Dicembre 2013. **O20.**

(102) S. Guccione, L. Basile, C. Squires, C. Gaul and K.K. Parker

THERMODYNAMIC PROPERTIES OF A 5HT_{1A} RECEPTOR LIGAND

69th Northwest Regional Meeting (NORM 2014) of the American Chemical Society (on behalf of the Montana Local Section of the American Society) June 22-25, 2014 University of Montana campus Missoula, Montana.

(103) Livia Basile, Salvatore Guccione, Gisella Alfonsino, Danilo Milardi, Matteo Pappalardo.

GPCR-interacting proteins and their individual functional roles.

4th International Meeting on Pharmacy & Pharmaceutical Sciences (IMPPS-4),
Faculty of

Pharmacy, Marmara University, Istanbul, Turchia, 18-21 Settembre 2014.

(104) L. Basile, S. guccione, C. Squires, C. Gaul and K.K. Parker

Insights into the Thermodynamic Properties of a 5HT1A Ligand.

COST Action CM1207. GLISTEN Budapest 2014 Conference. Research Centre for
Natural Sciences (RCNS-HAS). Budapest, Ungheria, 2-4 Ottobre 2014. **P410**

(105) Livia Basile, Matteo Pappalardo, Danilo Milardi, Salvatore Guccione,
Rona R. Ramsay.

*Computational comparison of imidazoline association with the I2 binding site
in human monoamine oxidases .*

The 16th International Amine Oxidase Conference and Workshop . 15th - 17th July
2014. Garvan Institute of Medical Research , Sydney, NSW (Australia). Abstract book
(oral comm.): 2 (page 24).

(106) Salvatore Ferla, Marcella Bassetto, Sebastiano Ferla, Salvatore Guccione,
Johan Neyts, Joana Rocha-Pereira, Pieter Leyssen, Andrea Brancale

Computer-aided discovery of small-molecules against norovirus

Twenty-Eighth International Conference on Antiviral Research, Rome Italy May
11-15 2015. **Poster 48 page 62**

(107) L. BASILE, M. SORTINO, F. NICOLETTI, S. GUCCIONE, A. G.
COPANI

*Identification of 5-methoxyflavone as a novel DNA polymerase-beta inhibitor and
neuroprotective agent against beta-amyloid toxicity.*

2014 Neuroscience Meeting Planner. Washington, DC: Society for Neuroscience,
2014. Online. **Poster 042.**

(108) Livia Basile, Gisella Alfonsino , Matteo Pappalardo, Salvatore Guccione,
Saheem A. Zaidi and Glen E. Kellogg

*Insight into the G protein mediated 5-HT7 receptor signal transduction by
Molecular Dynamics simulations*

XXIII National Meeting on Medicinal Chemistry & 9th Young Medicinal Chemists Symposium (NMMC & 9th NPCF) - September 6-9 2015, Salerno (Italy) **OC39**

(109) Livia Basile, Belma Zengin Kurt , Isil Gazioglu , Fatih Sonmez , Mustafa Kucukislamoglu , Tiziana Ginex ,Valentina Cappello , Salvatore Guccione

Novel coumarin derivatives as selective acetylcholinesterase inhibitors

XXIII National Meeting on Medicinal Chemistry & 9th Young Medicinal Chemists Symposium (NMMC & 9th NPCF) - September 6-9 2015, Salerno (Italy) **PC60**

(110) Benedetta Maggio, Demetrio Raffa, Maria Valeria Raimondi, Stella Cascioferro, Fabiana Plescia, Domenico Schillaci, Maria Grazia Cusimano, Ainars Leonchiks, Dmitrijs Zhulenkovs, Livia Basile, Salvatore Guccione, Giuseppe Daidone

Discovery of a New Class of Sortase A Transpeptidase Inhibitors to Tackle Gram-positive Pathogens: 2-Phenylhydrazonoalkanoic Acid Derivatives

XXIII National Meeting on Medicinal Chemistry & 9th Young Medicinal Chemists Symposium (NMMC & 9th NPCF) - September 6-9 2015, Salerno (Italy) **PC154**

(111) Matteo Floris, Ricardo Medda, Roberta Di Martina, Livia Basile, Salvatore Guccione

The Mimesis Toolkit: applications for peptidomimetics drug design and 3D QSAR

XXIII National Meeting on Medicinal Chemistry & 9th Young Medicinal Chemists Symposium (NMMC & 9th NPCF) - September 6-9 2015, Salerno (Italy). **PC160**

(112) Matteo Pappalardo, Martha Leonardi, Danilo Milardi, Livia Basile, Salvatore Guccione and Anwar Ryan

Tips for modeling human G-Protein Coupled Receptors

XXIII National Meeting on Medicinal Chemistry & 9th Young Medicinal Chemists Symposium (NMMC & 9th NPCF) - September 6-9 2015, Salerno (Italy). **PC167**

(113) Matteo Pappalardo, Livia Basile, Martha Leonardi, Salvatore Guccione, Danilo Milardi, Anwar Ryan

A new approach for modelling G-Protein Coupled Receptors

Convegno Nazionale della Divisione di Chimica dei Sistemi Biologici, Siracusa
24-25 Settembre 2015 . **P1**

- (114) Martha Leonardi, Matteo Pappalardo, Livia Basile, Danilo Milardi, Salvatore Guccione, and Anwar Ryan

TOWARDS IMPROVED QUALITY OF GPCR MODELS BY USAGE OF SUITABLE TEMPLATES AND STATISTICALLY DETERMINATED STRUCTURAL CONSERVED COMMON MOTIFS. Società Chimica Italiana. *Convegno congiunto delle Sezioni Calabria e Sicilia (SCICASI)* Catanzaro 3, 4 Dicembre 2015. **O12**

- (115) Valentina Cappello , Livia Basile , Salvatore Guccione , Federica Porta , Stefania Villa , Daniela Barlocco , Fiorella Meneghetti , Nicola Ferri and Arianna Gelain.

OXADIAZOLE DERIVATIVES AS POTENTIAL DUAL STAT 3 - TOPOISOMERASE INHIBITORS: BIOLOGICAL AND IN SILICO STUDIES.

Società Chimica Italiana. *Convegno congiunto delle Sezioni Calabria e Sicilia (SCICASI)* Catanzaro 3, 4 Dicembre 2015. **O24**

- (116) Roberta Di Martina, Matteo Floris, Ricardo Medda, Livia Basile, Salvatore Guccione

THREE WAYS TO REFRAME A PROBLEM AND FIND INNOVATIVE SOLUTIONS TO IMPROVE BOTH PEPTIDE AND NON PEPTIDE DRUGS: THE MIMESIS TOOLKIT. Società Chimica Italiana. *Convegno congiunto delle Sezioni Calabria e Sicilia (SCICASI)* Catanzaro 3, 4 Dicembre 2015. **O25**

- (117) Salvatore Guccione, Matteo Pappalardo, Martha E. Leonardi, and Anwar Rayan

TIPS FOR MODELLING HISTAMINE RECEPTORS.

45° ANNUAL MEETING OF EHRS (European Histamine Research Society)
FLORENCE, MAY 11-14 2016 **O16**

(118) Federica Porta, Stefania Villa, Arianna Gelain, Fiorella Meneghetti, Daniela Barlocco, Nicola Ferri, Livia Basile, Valentina Cappello and Salvatore Guccione.

Design, Synthesis and Field-Based Disparity Analysis of New N-Aryl-benzamides Endowed with Antiproliferative Activity.

IASOC: Ischia Advanced School of Organic Chemistry, Ischia, September 25-26, 2016.