

Curriculum Vitae et Studiorum
Salvatore Guccione

INFORMAZIONI PERSONALI

Nome: Salvatore Guccione

Data di Nascita: 20 Marzo 1962 (Catania).

Stato civile: coniugato con Maria Caruso. Tre figlie: Camilla 25 anni /Beatrice 11 anni/Dafne Maria 7 anni; un figlio : Alessandro 19 anni.

Sede di lavoro: Dipartimento di Scienze del Farmaco , Università degli Studi di Catania, viale Andrea Doria 6, Ed. 2 Città Universitaria, I-95125 Catania .

Telefono Ufficio: +39 (0)95 738-4020

Email: guccione@unict.it

LINGUE Buona conoscenza lingua inglese (scritta e parlata)

Titoli di studio

1980 Maturità Classica (56/60)

1986 Laurea in Farmacia (110/110 e lode) in data 3 Aprile. Facoltà di Farmacia, Università degli Studi di Catania.

Titolo della tesi: *Sintesi e la Valutazione dell' Azione Analgesica ed Antinfiammatoria di Eterocicli Policondensati contenenti 10 Anello Pirimidonico.*

1986: Abilitazione alla Professione di Farmacista (**prima sessione**).

1992 Dottore di Ricerca in Scienze Farmaceutiche.

Titolo della tesi: *Sintesi di Eterocicli Condensati Contenenti il Nucleo Pirazolico. Un nuovo approccio di studio nel campo degli Agenti Antiinfiammatori ed Analgesici.*

Legenda: - = ad oggi.

Afferenza: Dipartimento di Scienze del Farmaco 1986-

1984: Scuola Preliminare di Fotochimica (Università di Perugia).

1986-1988: Volontario o contrattista presso l' Istituto di Chimica Farmaceutica e Tossicologica (oggi Dipartimento di Scienze del Farmaco)Università degli Studi di Catania.

1988-1991: Studente del Dottorato di Ricerca in Scienze Farmaceutiche (IV ciclo).

1987-1991: Partecipazione al Corso Avanzato in Chimica Farmaceutica e Seminario Nazionale per Dottorandi in Scienze Farmaceutiche tenutisi a Bressanone (1987-1990) ed Urbino (1991).

1988: Corso su Moderne Tecniche Cromatografiche (Dipartimento Farmaco- Chimico, Università di Messina);

1992: Conseguimento del titolo di Dottore di ricerca in Scienze Farmaceutiche con una tesi "Sintesi di Eterocicli Policondensati contenenti il Nucleo Pirazolico: un nuovo approccio nel settore degli agenti analgesici-antinfiammatori".

1992-1993: Volontario o contrattista presso l' Istituto di Chimica Farmaceutica e Tossicologica (oggi Dipartimento di Scienze del Farmaco)Università degli Studi di Catania.

1993: Vincitore del concorso per Ricercatore di Chimica Farmaceutica (gruppo disciplinare C07X oggi C08X; settore concorsuale 03/D1).

6 Giugno 1994 (nomina 6 Maggio 1994): presa di servizio con afferenza all' Istituto di Chimica Farmaceutica e Tossicologica (oggi Dipartimento di Scienze del Farmaco), Università degli Studi di Catania.

1996 (febbraio-agosto): Università di Innsbruck (Prof. T. Langer; Institut für Pharmazeutische Chemie).

1997-: Ricercatore confermato con qualifica dal **2007** di Professore Aggregato (Facoltà di Farmacia ; Facoltà di Scienze Matematiche, Fisiche e Naturali (corso di Laurea Magistrale in Chimica Biomolecolare).

2014: A.S.N. (Abilitazione Scientifica Nazionale) Professore associato 03/D1 – Settore Chimica Farmaceutica, Tossicologica, Nutrizionale e Tecnologie Applicate.

Data abilitazione 29/01/2014.

1 Novembre 2017-: Prof. Associato CHIM08

Attività didattica:

A.A. 1994-1995: Attività seminariale per l' insegnamento di Chimica Farmaceutica II (corsi di Laurea in Farmacia e Chimica e Tecnologia Farmaceutiche). Partecipazione a commissioni di esame per discipline del SSD CHIM08. Collaborazione nella preparazione di tesi sperimentali e compilative di laurea.

A.A. 1995-1996: Attività seminariale per l' insegnamento di Chimica Farmaceutica II (corsi di Laurea in Farmacia e Chimica e Tecnologia Farmaceutiche). Partecipazione a commissioni di esame per discipline del SSD CHIM08. Collaborazione nella preparazione di tesi sperimentali e compilative di laurea.

A.A. 1996-1999: Attività seminariale e di assistenza in laboratorio per Analisi dei Medicinali II (3° anno Corso di Laurea in Farmacia) ed Analisi dei Farmaci (3° Anno Corso di Laurea in CTF). Partecipazione a commissioni di esame per discipline del SSD CHIM08. Collaborazione nella preparazione di tesi sperimentali e compilative di laurea.

1999-2010: membro del Collegio Docenti del Dottorato di Ricerca in Scienze Biochimiche e Biomolecolari. **Tutor Tesi dottorato : 3**

A.A. 1999-2005: Attività seminariale per l' insegnamento di Chimica Farmaceutica II (corsi di Laurea in Farmacia e Chimica e Tecnologia Farmaceutiche).

2000: Tutor per il progetto di mobilità studenti LEONARDO DA VINCI .

2000 Docente Garante (“Docente di riferimento”)per le discipline del Settore Scientifico Disciplinare (SSD) CHIM08 per la costituzione del nuovo corso di Laurea specialistica in Chimica Biomolecolare (Facoltà di Scienze Matematiche, Fisiche e Naturali; Dipartimento di Scienze Chimiche).

A.A. 2001-: incarico di insegnamento “Esercitazioni di Chimica Farmaceutica e Tossicologica II” per il corso di Laurea Specialistica in Farmacia.

A.A. 2001- Insegnamenti di a) Chimica Farmaceutica e b) Modelling e Progettazione di Molecole Bioattive (Nuovo Ordinamento.: Progettazione e Sviluppo del Farmaco) per il Corso di Laurea Specialistica (Magistrale) in Chimica Biomolecolare (Dipartimento di Scienze Chimiche).

A.A. 2001- Relatore di tesi di Laurea compilative e sperimentali per i corsi di Laurea in Farmacia, Chimica e Tecnologia Farmaceutiche e Chimica (Dipartimento di Scienze Chimiche).

2007-: Docente Tutor presso la Scuola Superiore di Catania.

2007: Incarico d' insegnamento "Drug Modelling" (Modulo Molecular Imaging, Drug modelling e Drug Delivery presso il Master "Diagnostica Farmaceutica e Molecolare", Facoltà di Farmacia, Università degli Studi di Catania.

2007 : Membro commissione per esame finale Dottorato di Ricerca Internazionale (European PhD). Universidad de Navarra (Spagna) C.I.F.A. (19 Dicembre 2007).

2007-2013: Responsabile progetto SOCRATES-ERASMUS per la Facoltà di Farmacia e la Facoltà di Scienze Matematiche, Fisiche e Naturali.

2007-2013: Responsabile progetto ERASMUS *Student Placement Life Long Learning* per la Facoltà di Farmacia e la Facoltà di Scienze Matematiche, Fisiche e Naturali.

2014- Tutor Scuola Superiore di Catania.

2016-: Insegnamento di Fitochimica (6 CFU). Corso di Laurea in Scienze Farmaceutiche Applicate *curriculum* Scienze Erboristiche dei Prodotti Nutraceutici.

Legenda: - (ad oggi)**Altre attività:**

1999, 2000: *Visiting Scientist* Dipartimento di Chimica Farmaceutica (Institut für Pharmazeutische Chemie), Università di Innsbruck.

1999-2016: Associate Editor European Journal of Medicinal Chemistry.

2000 *Visiting Scientist* , ORGANON, Oss, Olanda.

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"***).

2001- Membro INBB (Istituto Nazionale Biomolecole e Biostrutture).

2001-: Responsabile progetti SOCRATES-ERASMUS.

2002: **Organizzatore del Workshop** International Course “Multivariate QSAR Modelling”, June 11-14, Capomulini, Acireale, (CT) sponsorizzato da UMETRICS, Umea (Svezia).

2002: *Invited Scientist* CHEMOVATION , Horsham, U.K..

2002: *Visiting Scientist* F. Hoffmann- La ROCHE, Basilea .

2002: Relatore evento formativo Ciclo di Vita del Medicinale ad Uso Umano: dalla Sintesi alla Postmarketing Surveillance. Catania (Hotel Baia Verde) 7,8 Settembre sotto il patrocinio Commissione Nazionale per la Formazione Continua.

2003: *Invited Scientist* Università di Trømso, INSTITUTE OF MEDICAL BIOLOGY, Department of Pharmacology.

*Nominato Supervisore *esterno* “graduation theses” Università di Tromso.

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

2004-2013: Attività di *Consulting* BioChemics Consulting SAS (Orleans, France).

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

2005, 2007: Responsabile PRA (Progetti Ricerca Ateneo).

2005 Membro dell' 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.

2006: Membro dell' International Scientific Advisory Board :

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

2006 Membro del Comitato Scientifico 3rd School on Advanced BioMedicine and BioInformatics. "Proteoms and Proteins" Lipari Island (Italy), July 9 (Sunday)-July 22 (Saturday).

2006: Organizzatore del Workshop *A Workshop based in FLO and AlleGrow* (5-8 marzo), Catania (Città Universitaria) in collaborazione con Thistlesoft, Colebrook, CT, USA.

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

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

2007-2015: Responsabile progetto SOCRATES-ERASMUS ed ERASMUS *Student Placement Life Long Learning* .

2010-2013: Direzione Scientifica dello spinoff universitario ETNALEAD . Premio "STARTCUP CATANIA" per l' Innovazione Scientifica e Partecipante al PNI (Premio Nazionale Innovazione) di Napoli (4 Dicembre 2007).

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

2008-2016: membro COPE (Committee On Publication Ethics) .

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

2009: docente progetto di formazione Laboratorio Pubblico-Privato DM20919(CNR-WYETH).

2010-2013: Membro del Collegio del **Dottorato Internazionale in Neurofarmacologia.**

2010-: Docente Master Discipline Regolatorie del Farmaco .

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

2011-: Institutional Co-Ordinator Lilly Open Innovation Drug Discovery (OIDD) Program.

2012-: revisore (referee) MIUR (REPRISE).

2017: revisore esterno Dottorato in Area del Farmaco e Trattamenti Innovativi XXX Ciclo Dipartimento di NEUROFARBA Sezione di Farmaceutica e Nutraceutica Universita' degli Studi di Firenze.

Principali Tematiche di Ricerca

1. Progettazione razionale (Modellistica Molecolare) e sintesi di nuovi ligandi enzimatici e recettoriali con particolare riferimento a GPCRs (**G-Protein Coupled Receptors**) ;
2. Bioinformatica con particolare riferimento a GPCRs (**G-Protein Coupled Receptors**) ;
3. Predizione *in silico* e validazione sperimentale proprietà ADME(T);
4. Sviluppo di nuovi softwares per 3D-QSAR;
5. Applicazione di tecniche computazionali a problemi chimici e biologici.

Collaborazioni Scientifiche Nazionali ed Internazionali

1. Istituto di Ricerche Farmacologiche “Mario Negri”, Consorzio Mario Negri Sud, via Nazionale, 66030,S. Maria Imbaro (CH). Italy.
2. Centro CNR di Studio per le Macromolecole Stereordinate ed Otticamente Attive, Università di Pisa, via Risorgimento 35,I-56126 Pisa, Italy.
3. Dipartimento di Scienze Farmaceutiche, Università di Ferrara, Italy.

4. Department of Enzymology, Merck, Sharp and Dohme Research Laboratories, Rahway, NJ 07065, USA.
5. School of Pharmacy, Aristotelian University of Thessaloniki, Department of Pharmaceutical Chemistry, 540 06 Thessaloniki, Greece.
6. Macromolecular Structure-CADD, Bristol Meyers Squibb, Pharmaceutical Research Institute, P.O. Box 4000, Princeton, NJ 08543, USA.
7. Laboratory of Computer Chemistry, Institute of Chemical Metallurgy, Chinese Academy of Science, Beijing, 100081, P.R. China.
8. Dipartimento di Scienze Farmaceutiche, Università di Modena e Reggio Emilia, via Campi, 183-I-41100, Modena, Italy.
9. Institut für Pharmazeutische Chemie, University of Innsbruck, A-6020 Innsbruck, Austria.
10. Department of Pharmacology, Centro de Investigación en Farmacobiología Aplicada (CIFA), Universidad de Navarra, C/ Irunlarrea s/n, 31080, Pamplona, Spain .
11. Chelyabinsk State University Chelyabinsk.
12. Institute of Organic Synthesis, Ural Branch Russian Academy of Sciences Ekaterinburg.
13. Departament de Físicoquímica, Facultat de Farmàcia, Universitat de Barcelona, Av. Diagonal 643, 08028, Barcelona, Spain.
14. School of Molecular and Microbial Sciences and School of Pharmacy, University of Queensland, Brisbane, Australia.
15. Abteilung für Molekulare Strukturbiologie, Institut für Mikrobiologie und Genetik & GZMB, Justus-von-Liebig Weg 11, 37077 Goettingen, Germany;
16. Department of Molecular Genetics and Preparative Molecular Biology Institute for Microbiology und Genetics, Grisebachstr. 8, 37077 Goettingen, Germany
17. Department of General Chemistry and Istituto Nazionale di Biostrutture e Biosistemi, University of Parma, 43100 Parma, Italy.

18. Department of Pharmacology, yDepartment of Medical Biochemistry, and Institute of Medical Biology, Faculty of Medicine, University of Tromsø, 9037 Tromsø, Norway.
19. BioChemics Consulting 111 Bld. Duhamel du Monceau 45166 Olivet Cedex, France.
20. Università degli Studi di Pisa, Dipartimento di Chimica e Chimica Industriale, Via Risorgimento 35, I-56126 Pisa, Italy.
21. The University of Kansas, Department of Pharmacology & Toxicology, 1251 Wescoe Hall Drive, Lawrence, KS 66045, USA.
22. Department of Pharmacology, Institute of Medical Biology, University of Tromsø, 9037 Tromsø, Norway.
23. Neonatal Intensive Care Unit, “Cesare Arrigo” Children Hospital, 15100 Alessandria, Italy Department of Pediatrics, G. Gaslini Children's University Hospital, 16167 Genoa, Italy.
24. Dipartimento di Chimica Inorganica, Chimica Analitica e Chimica Fisica, University of Messina, and C.I.R.C.M.S.B., Vill. S. Agata, Messina, Italy.
25. Dipartimento di Scienze e Tecnologie Molecolari e Biomolecolari-Sezione di Chimica e Tecnologie Farmaceutiche, Università degli Studi di Palermo, Via Archirafi 32, 90123 Palermo, Italy;
26. Dipartimento di Psichiatria, Neurobiologia, Farmacologia e Biotecnologie, Università degli Studi di Pisa, Via Bonanno 6, 56126 Pisa, Italy;
27. Dipartimento di Scienze Farmaceutiche “P. Pratesi”, Università degli Studi di Milano, Via L. Mangiagalli 25, 20133 Milano, Italy
28. Lab. Inmuno-Biología Molecular, Hospital General Universitario Gregorio Marañón, 28007 Madrid, Spain.
29. Dipartimento Farmaco Chimico Tecnologico, Università degli Studi di Siena, I-53100 Siena, Italy.
30. Department of Chemistry, Florida Atlantic University, Boca Raton, Florida 33431, United States

31. New York Medical College, Department of Pharmacology, Valhalla, NY 10595, USA; Marshall University's Joan C. Edwards School of Medicine, Huntington, WV 25701, USA .
32. IBB-CNR, Istituto di Biostrutture e Bioimmagini, UOS di Catania c/o Dipartimento di Scienze Chimiche, Università degli Studi di Catania, Viale A.Doria 6 Ed.3, Città Universitaria, I- 95125 Catania, Italy.
33. Biomedical Sciences Research Complex, University of St. Andrews, North Haugh, St. Andrews KY16 8QP, U.K.
34. Drug Discovery Informatics Lab, QRC-Qasemi Research Center, Al-Qasemi Academic College, Baka El-Garbiah, Israel.
35. Department of Pharmacology, Institute of Clinical Medicine, University of Oslo and Oslo University Hospital, Oslo, Norway, 2 K.G. Jebsen Cardiac Research Centre and Center for Heart Failure Research, Faculty of Medicine, University of Oslo, Oslo, Norway
36. Chemistry Department (member of NAMEDIC), University of Namur, 61 Rue de Bruxelles, Namur B-5000, Belgium.
37. Sakarya University, Pamukova Vocational High School, 54900, Sakarya, Turkey
38. Molecular Modelling Laboratory, Department of Food Science, University of Parma, Parco Area delle Scienze 17/A, Parma 43124, Italy
39. National Research Council, Institute of Biostructures and Bioimaging, Catania, Italy
40. Dipartimento di Scienze Biomediche e Biotecnologiche, Università degli Studi di Catania.
41. BIONAP s.r.l. , Contrada Fureria Belpasso, Italy
42. Dipartimento di Scienze del Farmaco, Università degli Studi di Padova, Padua, Italy.
43. Dipartimento di Scienze Farmacologiche e Biomolecolari, Università degli Studi di Milano, Milan, Italy.

44. School of Pharmacy and Pharmaceutical Sciences, Cardiff University, Cardiff, United Kingdom.
45. PEPTICOM LTD., Malha Technology Park (GATI), Building 8, 3rd floor, Jerusalem, Israel.
46. Elvysys Microfluidic Innovation Center, 83 avenue Philippe Auguste 75011 Paris, FRANCE.
47. Università di Southampton (Biological Sciences: Prof. Nallin Divecha), UK. e
48. Dipartimento di Scienze Farmaceutiche, Sezione di Chimica Generale e Organica "A. Marchesini" DISFARM (Università degli Studi di Milano) .
49. School of Pharmacy and Pharmaceutical Sciences, Cardiff University, Cardiff, United Kingdom.
50. Dipartimento di Farmacia – Scienze del Farmaco, Università di Bari.

Progetti e Networks di Ricerca Internazionali:

1. **1998-2000:** Co-ordinatore del programma European Science Exchange finanziato dalla Royal Society of Chemistry (Dr. Chaman Chander, University of Luton: Nitric oxide levels using a cartilage explant model).
2. **2002** Group Leader European Commission Human Potential Programme Access To Research Infrastructure.
3. **1999-2000:** Co-ordinatore del programma European Science Exchange finanziato dalla Royal Society of Chemistry (Dr. Chaman Chander, University of Luton: Nitric oxide levels using a cartilage explant model).
4. **2009-2010:** Coordinatore Progetto **“PROJECTS IN THE FRAMEWORK OF THE JOINT BILATERAL AGREEMENT CNR-ASRT (Egitto)”** **2009-10:** **“Molecular Modelling Design, Synthesis and Studies on the effects of Gem-Bisphosphonic Acids on bone cancer processes of activated macrophages”**

(Partner : Dr. Wafaa M. Abdou, Department of Pesticide Chemistry, Chemical Industries Research Division, National Research Centre, El-Tahrir St., Dokki, D-12622 Dokki, Cairo, Egypt).

5. **2009-2013:** membro COST ACTION BM0806 : Advances in Histamine H₄R Research.
6. **2013-2017:** membro COST ACTION CM1207 " GLISTEN: GPCR-Ligand Interactions, Structures, and Transmembrane Signalling: a European Research Network".
7. **2018-:** Responsabile Accordo Internazionale di Collaborazione con PEPTICOM LTD.(Israele), Università di Southampton (Biological Sciences), UK. e Dipartimento di Scienze Farmaceutiche, Sezione di Chimica Generale e Organica "A. Marchesini" DISFARM (Università degli Studi di Milano) .

BANDI PRIN

1. Sintesi di Liganti per i recettori serotoninergici (area 03) PRIN 1997.
2. Progettazione e Sintesi di nuovi Ligandi Selettivi per il Recettore alfa1-adrenergico (area 03) PRIN 1999.
3. Sviluppo di Ligandi Selettivi per le sottoclassi alfa1-adrenergiche (area 03) PRIN 2001.
4. Sviluppo di ligandi selettivi per i recettori dell'endotelina (area 03) PRIN 2003.
5. Basi Molecolari nei processi di aggregazione di peptici fibrillogenici (area 03) PRIN 2005.
6. Surface Plasmon Resonance Imaging per la rivelazione parallela di target di RNA e microRNA mediante acidi peptido-nucleici (area 03) PRIN 2007.
7. Riconoscimento selettivo di micro RNA mediante surface plasmon resonance imaging e microfluidica digitale (area 03) PRIN 2009.
8. Meccanismi di patogenesi negli stadi precoci della malattia di Alzheimer: identificazione di target farmacologici e biomarkers (CHIM 03) PRIN 2015.

FINANZIAMENTI DI ATENEO

1. **2005, 2007:** Responsabile PRA (Progetti Ricerca Ateneo).
2. **2014-2016: FIR (Finanziamento Ricerca di Ateneo)** *Sviluppo di nuovi ligandi del recettore Sigma-1 come radiotraccianti per PET imaging dell'adenocarcinoma della prostata (CHIM03/SSD CHIM08).*
3. **2016-2018: FIR (Finanziamento Ricerca di Ateneo)** *In silico design and biological investigations of Diabetic Neuropathy modulators (CHIM03/SSD CHIM08).*

Associazioni:

- Società Chimica Italiana (Divisione di Chimica Farmaceutica).
- INBB (Istituto Nazionale Biosistemi e Biostrutture)-Consorzio Accademico Nazionale.
- Molecular Graphics and Modelling Society.

Attività di “referaggio”:

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, Letters in Drug Design, Reference Module, Current Perspectives in Medicinal Chemistry.

ELENCO DELLE PUBBLICAZIONI

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). **I.F.:** 1.126

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). **I.F.:** 6.259

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). **I.F.:** 4.519

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). **I.F.: 4.519**

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. **I.F.: 0.805**

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). **I.F.: 4.519**

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. **I.F.: 0.893**

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). **I.F.: 2.454**

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). **I.F.: 4.519**

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). **I.F.:** **0.893**

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). **I.F.:** **2.454**

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). **I.F.:** **0.893**

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). **I.F.:** **0.893**

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). **I.F.:** **1.998**

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 (1998). **I.F.:** **4.519**

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). **I.F.:** **4.293**

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). **I.F.: 3.028**

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). **I.F.: 4.293**

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. **I.F.: 4.519**

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. **I.F.: 4.293**

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. **I.F: 3.629**

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., **C58**, 69-71, 2001. **I.F.:** **4.099**

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. **I.F.:** **6.259**

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. **I.F.:** **2.930**

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. **I.F.:** **0.472**

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

bromobenzenesulfonamide into β -cyclodextrin.

Bioorg. Med. Chem., **12**, 2004 , 447-458. **I.F.:** **2.930**

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. **I.F.:** **2.930**

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. **I.F.:** **3.154**

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). **I.F.:** **3.028**

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. **I.F.:** **2.930**

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. **I.F.:** **4.519**

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). **I.F.:** **3.002**

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. **I.F.:** **3.629**

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. **I.F.:** **2.599**

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. **I.F.:** **2.184**

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. **I.F.:** **3.902**

41. Osman A.B.S.M Gani, Olayiwola A. Adekoya, Laura Giurato, Francesca Spyrakis, 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. **I.F.:** **3.656**

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. **I.F.:** **2.126**

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. **I.F.:** **1.540**

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. **I.F.:** **3.249**

45. KELLY E. DESINO, ROSARIO PIGNATELLO, **SALVATORE GUCCIONE**, 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. **I.F.:** **4.581**

46. 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. **I.F.: 4.518**

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. **I.F.: 6.259**

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. **I.F.: 2.121**

49. B. Maggio, D. Raffa, M.V. Raimondi, F. Plescia, M.L. Trincavelli, C. Martini, F. Meneghetti, L. Basile, **S. Guccione**, G. Daidone (2012).

Synthesis, benzodiazepine receptor binding and molecular modelling of isochromeno[4,3-c]pyrazol-5(1H)-one derivatives.

Eur. J. Med. Chem, 54, 709-720. **I.F.: 4. 519**

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

Sulfonilamidothiopyrimidone and Thiopyrimidone derivatives as selective COX-2 inhibitors: synthesis, biological evaluation, and docking studies.

Eur. J. Med. Chem., 57, 149-161. **I.F.: 4.519.**

51. Valeria Sorrenti, **Salvatore Guccione**, 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, 80, 876-886, 2012. **I.F.: 2.396**

52. Deboprosad Mondal, Song YeLi, Luca Bellucci, Teodoro Laino, Andrea Tafi, **Salvatore Guccione**, and Salvatore D. Lepore.

Stereoretentive Chlorination of Cyclic Alcohols Catalyzed by Titanium (IV) Tetrachloride: Evidence for a Front Side Attack Mechanism.

JOURNAL OF ORGANIC CHEMISTRY, 78, 2118-2127, 2013. **I.F.: 4.849**

53. Luca Vanella, Giovanni Li Volti, **Salvatore Guccione**, 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. **I.F.: 2.466**

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. **I.F.: 3.760**

55. 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. **I.F.: 2.806**

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 . **I.F.:** **3.104**

57. Andrea Carletta, Anaëlle Tilborg, Laurence Moineaux, Jérôme 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. **I.F.:** **4.099**

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. **I.F.:** **4.519**

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. **I.F.: 2.896**

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

J. Nat. Prod., **2015**, 78 (11), pp 2704–2711. **I.F.: 3.281**

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. 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**

66. 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
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**

Capitoli in Libri:

- 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 LogP 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

- 1) **S. Guccione.** *Therapeutic Potential of Condensed Heterocycles* ; Russian Academy of Medical Science: Cancer Research Centre, Moscow (Russia), September 1994.
- 2) **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.
- 3) **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.
- 4) **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.
- 5) **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.

- 6) **S. Guccione**. *Synthesis of Heterocycles of Pharmaceutical interest*. University of Pisa: Centro CNR di Studio delle Macromolecole Stereordinate ed Otticamente Attive, Pisa (Italy), June 1995.
- 7) **S. Guccione**: *3D-QSAR (HASL) in DRUG DESIGN* . Aristotelian University of Thessaloniki (Greece). Department of Pharmaceutical Chemistry , Thessaloniki (Greece), September 28th 1997 .
- 8) **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).
- 9) **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**.
- 10) **S. Guccione**: *Molecular Modelling for Pharmaceutical Development*.
NV Organon, Oss (The Netherlands), September 4th 2000
- 11) **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.
- 12) **S. Guccione**: *Computational approaches and their use in Drug Design : an overview*.
Institut Jacques Monod, Paris (France), January 16th 2001.

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

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

- 14) **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 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 (India) **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, South 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. Dowejko, 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. Konig, 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 Conjuncto 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.

Pyrralobenzodiazepine 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, 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 Tyrosyne 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. Doweiko, **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 Spyraakis , 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 Spyraakis 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-H_{T1A} 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 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 Rauschholzhausen, 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 5HT1A 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. **P 48**
- (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** ; *Inflamm. Res.* (2016) 65 (Suppl 1):S1–S53 DOI 10.1007/s00011-016-0958-6 **S44**

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

KEY TIPS FOR MODELLING 3D STRUCTURE OF GPCR.

GLISTEN in Prague 2016 **P4-17**, Prague September 25-27 2016.

(119) 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.