Gabriele Costantino
-Curriculum Vitae -

Educazione:
1986- Maturità Classica – Liceo A. Mariotti, Perugia.
1991- Parte della tesi di laurea sperimentale (5 mesi) presso Neuroscience/Drug Design Group, Searle R&D (Chicago, IL, USA). Supervisor: Dr. James P. Snyder
1992: Laurea in Chimica *cum Laude*. Dipartimento di Chimica, Università di Perugia.
1992-1994: Research Fellowships presso: Laboratorio di Chemometria (Dipartimento di Chimica, Università di Perugia) e Istituto di Chimica e Tecnologia Farmaceutica (Università di Perugia)
1996: Short-Term Fellowship (CNR) presso Organic Chemistry Department, University of Barcelona, Spain (supervisor: Prof. E. Giralt)

Carriera Professionale
- Novembre 1994 –Novembre 1998: Ricercatore Chimica Farmaceutica (CHIM/08) presso Istituto di Chimica e Tecnologia Farmaceutica, Facoltà di Farmacia, Università di Perugia.
- Novembre 1998 – Dicembre 2006: Professore Associato di Chimica Farmaceutica (CHIM/08) presso Dipartimento di Chimica e Tecnologia del Farmaco, Facoltà di Farmacia, Università di Perugia
- Dicembre 2006-oggi: Professore Ordinario di Chimica Farmaceutica, Dipartimento Farmaceutico, Facoltà di Farmacia, Università di Parma
- Gennaio 2017- oggi: Direttore del Dipartimento di Scienze degli Alimenti e del Farmaco,Università di Parma
- Settembre 2003-Febbraio 2004: Visiting Professor, Istituto di Chimica Organica. Goethe University, Francoforte.

Premi e riconoscimenti scientifici.
- Premio 'Società Chimica Italiana-Farmindustria' per il miglior giovane ricercatore in Chimica Farmaceutica 2003
- Recipient of the 16th Friederich Merz Prize and Professorship at the Institute for Organic Chemistry – Goethe University, Frankfurt am Main.

Principali finanziamenti competitivi:

- INTEGRATE 2015-2018 – Marie Curie ETN project. Coordinator.
- PRIN 2008 (Italian Ministry of University) – National Coordinator and Prinicipal Investigator
- PRIN 2011 (Italian Ministry of University) – Local Coordinator and Principal Investigator
- Vari fondi FIL 2007-2016 (University of Parma)- Principal Investigator
- POR-FESR2011-2014
- POR-FESR2014-2020
- EUROPIN (Erasmus-Mundi Program) Local Coordinator (University of Perugia)

Partecipazione a Società Scientifiche e Organismi di valutazione
- Presidente della Divisione di Chimica Farmaceutica della Società Chimica Italiana
- Membro del Executive Committee of the European Federation for Medicinal Chemistry (EFMC)
- Editor di *MedChemWatch*, the official newsletter of EFMC
- Member of the Information and Communication Committee of the European Federation for Medicinal Chemistry (EFMC)

- Evaluator Expert for the European Commission
- Evaluator Expert for INTAS
- Evaluator Expert for Scientific Agencies in Russia, Romania, Portugal, Spain

Incarichi accademici ed organizzativi

- Presidente del Consiglio di Corso di Studio in CTF (2013-2015)
- Direttore del Centro Interdipartimentale Misure 'G. Casnati'
- Direttore del Dipartimento di Scienze degli Alimenti e del Farmaco

Interessi di Ricerca

Progettazione e sintesi di composti biologicamente attivi. In particolare:

- ✓ Ligandi per i recettori metabotropici del glutammato. Modulatori della via metabolica delle chinurenine del triptofano
- ✓ Progettazione e sintesi di modulatori di recettori nucleari. In particolare, membro del team di ricerca che ha progettato e sintetizzato l'acido 6-etil-chenodesossicolico, oggi in uso clinico con il nome di acido obeticolico per la cirrosi biliare primitiva.
- ✓ Nuovi agenti antibatterici

1. **Presentazioni e Conferenze a Congressi Nazionali ed Internazionali**

- VIII International Symposium on Tryptophan Research (Padova, Italy) June 1995
- XV Corso Avanzato di Chimica Farmaceutica (Urbino, Italy) July 1995
- Advanced Course on the Design of Neuroprotective Agents - Universidad de Verano (Baeza, Spain) August 1996
- XIII Congresso Nazionale di Chimica Farmaceutica (Paestum, Italy) September 1996
- II International "Biomed 2" Meeting on Metabotrobic Receptors (Montpellier, France) March 1997
- III° Erasmus meeting (London, UK) October 1997
- III International "Biomed 2" Meeting on Metabotrobic Receptors (Perugia, Italy) June 1998
- XVIII Corso Avanzato di Chimica Farmaceutica (Urbino, Italy) July 1998
- Advanced Course on Drug Design (Salamanca, Spain) July 1998
- IX Meeting Strutture Eterocicliche nella Ricerca Farmaceutica (Palermo, Italy) May 2000
- I° Magna Grecia Medicinal Chemistry Workshop On New Perspectives in Drug Research (Copanello, Italy) June 2001
- XVII International Symposium on Medicinal Chemistry (Barcellona-Spain) September 2002
- IV International Meeting on Metabotropic Glutamate Receptors (Taormina –Italy) September 2002
- XVI Meeting della Divisone di Chimica Farmaceutica (Sorrento, Italy) September 2002
- PARP2003 Meeting (Lisbon, Portugal) April, 2003
- Symposium on" GPCRs as Targets for the Treatment of CNS Disease" (plenary lecture, Frankurt, Germany) January 2004
- Symposium on "Molecular Basis for Signal Transduction Mechanisms" (Warsaw, Poland) August 2005

- XIX International Symposium on Medicinal Chemistry (Istanbul, Turkey) September 2006
- GPCRs in Medicinal Chemistry (RCI-SCI Symposium – Verona, Italy) September 2006
- XXI Meeting Italian Division of Medicinal Chemistry (Verona, Italy) September 2008
- 12° Meeting of the International Society for Tryptophan Research (Firenze, Italy) July, 2009
- 5th Summer School *on* Drug Design (Vienna, Austria) September, 2009
- V New Perspectives in Medicinal Chemistry (Trieste, Italy) May 2011
- 6th Summer School in Drug Design (Vienna, Austria) September 2011
- 7th Summer School in Drug Design (Vienna, Austria) September 2013
- X EWDD, Siena (Italy) May 2015
- XI Joint Meeting of Medicinal Chemistry (Athens, Greece) June 2015
- INNOBALT Drug Discovery Conference (Riga, Latvia) August 2015
- 8th Summer School in Drug Design (Vienna, Austria) September 2015
- 1st International Gazi Pharma Symposium Series (Antalya, Turchia) November 2015
- Chairperson EUROQSAR (Verona) September 2016
- XI EWDD, Siena May 2017
- Satellite Meeting on Carbonic Anhydrase (Montecatini) May 2017
- Gazi Symposium on Pharmaceutical Chemistry (Ankara, Turchi) October 2017

2. **Lectures at Universities and Industries**:
   - Universitat de Barcelona Dept. Quimica (Spain) December 1996
   - GSK (Harlow, UK 2001) October 2001
   - Dompe' S.p.A May 2002
   - University of Frankfurt, Dept. Org. Chem. November 2003
   - Merz Pharma (Frankfurt AM, Germany) December 2003
   - Menarini Ricerche, Roma January 2004
   - Università di Chieti March 2004
   - Institute of Pharmaceutical Chemistry (Uni. Wien, Austria) December 2004
   - Nerviano Medical Sciences, Milano January 2005
   - Department of Chemistry, Moscow State University (Russia) May 2005
   - Università di Parma September 2005
   - Departamento de Quimica Teraputica, Universidad de Granada (Spain) December 2005
   - Novartis Pharma, Vienna (Austria) December 2006
   - Frankfurt Innovation Center / Merz R&D (Germany) January 2008
   - Università di Genova March 2010
   - Aptuit (Verona) Novembre 2010
   - Chiesi Farmaceutici (Parma) December 2011
   - Recordati (Milano) April 2012
   - TES Pharma (Perugia) February 2014
   - La Sapienza University of Rome July 2014
   - Palermo University July 2016
   - Cambridge Workshop Marzo 2016
   - Summer School Helsinki University June 2016
   - University of Zagreb (Croatia) July 2016
   - Statale University of Milan October 2016
   - University of Florence November 2016
   - University of Piemonte Orientale (Novara) January 2017
   - University of Chieti June 2017

Gabriele Costantino

List of Publications

1. Cruciani, G.; Baroni, M.; Clementi, S.;Costantino, G.; Riganelli, D., Skagerberg, B. Predictive ability of regression models. Part I: Standard Deviation of Prediction Errors (SDEP) *J. Chemometrics*, 6, 335-346, **1992**
2. Baroni, M.; Clementi, S.; Cruciani, G.; Costantino, G.; Riganelli, D.; Oberrauch, E. Predictive ability of regression models. Part II: Selection of the best predictive PLS model. *J. Chemometrics*, 6, 347-356, **1992**
3. Allen, M.S.; LaLoggia, A.J.; Dorn, L. J.; Martin, M.J.; Costantino, G.; Hagen, T. J.; Keohelr, K. K.; Skolnick, P.; Cook, J. M. Predictive binding of β-carboline inverse agonists and antagonists via the CoMFA/GOLPE approach. *J. Med. Chem.*, 35, 4001-4010, **1992**
4. Baroni, M.; Costantino, G.; Cruciani, G, Riganelli, D.; Valigi, R; Clementi S. Generating optimal linear PLS estimation (GOLPE). An advanced chemometric tool for handling 3D-QSAR problems. *Quant. Struct.-Act. Relat*. 12, 9-20 **1993**
5. G. Costantino, B. Natalini, R. Pellicciari, Conformational requirements for interaction of L-Glutamic acid with metabotropic EEA receptors in: "*Trends in QSAR and Molecular Modelling 92*", Escom Science Publishers B.V., Leiden, **1993**, pp. 487-8.
6. Pellicciari, R.; Natalini, B.; Costantino, G.; Garzon, A.; Luneia, R.; Mahmoud, M.R.; Marinozzi, M.; Roberti, M.; Rosato, G. C.; Shiba, S. A. Heterocyclic Modulators of the NMDA Receptor *Il Farmaco*, 48, 151-157 **1993**
7. Clementi, S.; Cruciani, G.; Riganelli, D.; Valigi, R.; Costantino, G.; Baroni, M.; Wold, S: Autocorrelation as a tool for a congruent description of molecules in 3D-QSAR studies. *Pharm. Pharmacol. Lett*. 3, 5-8 **1993**
8. Costantino, G.; Natalini, B.; Pellicciari, R. Moroni, F.; Lombardi, G. Definition of a Pharmacophore for the Metabotropic Glutamate Receptors Negatively Linked to Adenylyl Cyclase *Bioorg. Med. Chem*. 1, 259-264 **1993**
9. Van d. Waterbeemd, H.; Clementi, S.; Costantino, G. Carrupt, P. A.;Testa, B. "Comfa-derived Substituent Descriptors for Structure-Property Correlations" in "*3D-QSAR in Drug Design: Theory, Methods and Applications*" Kubinyi, H. Ed. Escom (Leiden) **1993**
10. Clementi, S.; Cruciani, G.; Baroni, M.; Costantino, G. "Series Design" in "*3D-QSAR in Drug Design: Theory, Methods and Applications*" Kubinyi, H. Ed. Escom (Leiden) **1993**
11. Pellicciari, R.; Natalini, B.; Costantino,G.; Mahmoud, R. M.; Mattoli, L.; Sadeghpour, B.; Moroni, F.; Chiarugi, A.; Carpenedo, F. Modulation of the Kynurenine Pathway in Search for New Neuroprotective Agents. Synthesis and Preliminary Evaluation of (*m*-Nitrobenzoyl)alanine, a Potent Inhibitor of Kynurenine-3-hydroxylase *J. Med. Chem*. 37, 647, **1994**
12. Van d. Waterbeemd, H.; Costantino, G.; Clementi, G.; Cruciani, G.; Valigi, R. "Disjoint Principal Properties of Organic Substituents" in "*Chemometric Methods in Molecular Design*" Mannhold, R.; Krogsgaard-Larsen, P.; Timmerman, H. Eds. VCH (Weinheim) **1994**
13. Marinozzi, M.; Natalini, B.; Thomsen, C.; Ni, M. H.; Costantino, G.; Pellicciari, R. Synthesis and Biological Evaluation of 6-Carboxy-3,4-methanoprolines, New Rigid Glutamate Analogs *Il Farmaco*, 50, 327, **1995**
14. Pellicciari, R.; Luneia, R.; Costantino, G.; Marinozzi, M.; Natalini, B.; Jakobsen, P.; Kanstrup, A.; Lombardi, G.; Moroni, F.; Thomsen, C. 1-Aminoindane-1,5-dicarboxylic Acid: a Novel Antagonist at Phospholipase C Linked Metabotropic Glutamate Receptors *J. Med. Chem*. 38, 3717 **1995**
15. Costantino, G.; Natalini, B.; Mattoli, L.; Pellicciari, R. "The pseudoactive site as a tool for indirect drug design. Application to inhibitors of kynurenine-3-hydroxylase. in *QSAR and Molecular Modeling: Concepts, Computational Tools and Biological Applicarion*. Sanz, F.; Giraldo, J.; Manaut, F, Eds. Prous (Barcelona), pp583-4, **1995**
16. Marinozzi, M.; Natalini, B.; Costantino, G.; Pellicciari, R.; Bruno, V.; Nicoletti, F. Synthesis of 6,6-Dicarboxy-3,4-methano-L-proline, a New Constrained Glutamate Analog Endowed with Neuroprotective Properties *Il Farmaco*. 51, 121-124, **1996**

17. Pellicciari, R.; Marinozzi, M.; Natalini, B.; Costantino, G.; Luneia, R.; Giorgi, G.; Moroni, F.; Thomsen, C. Synthesis and Pharmcological Characterization of All Sixteen Stereoisomers of 2-(2'-Carboxy-3'-phenylcyclopropyl)glycine. Focus on (2*S*,1'*S*,2'*S*,3'*R*)-2-(2'Carboxy-3'-phenylcyclopropyl)glycine, a Novel and Selective Group II Metabotropic Glutamate Receptors Antagonist *J. Med. Chem.*, 39, 2874-2876, **1996**
18. R. Pellicciari, M. Raimondo, M. Marinozzi, B. Natalini, G. Costantino, C. Thomsen, "*S*-(+)-2-(3'-Carboxy-bicyclo[1.1.1]pentyl)glycine, a Structurally New Group I Metabotropic Glutamate Receptor Antagonist", *J. Med. Chem.*, *39*, 2874, **(1996**).
19. Costantino, G. Pellicciari, R. Homology Modeling of Metabotropic Glutamate Receptors (mGluRs). Structural Motifs Affecting Binding Modes and Pharmacological Profile of mGluR1 Agonists and Competitive Antagonists *J.Med. Chem*., 39, 3998-4004, **1996**
20. M. Marinozzi, B. Natalini, G. Costantino, P. Tijskens, C. Thomsen, R. Pellicciari, Asymmetric Synthesis of Enantiomerically Pure (2S,1'S,2'S,3'R)-phenylcarboxycyclopropylglycine (PCCG-4): A Potent and Selective Ligand at Group II Metabotropic Glutamate Receptors, *Bioorg. Med. Chem. Lett.*, 6, 2243,**1996**.
21. Costantino, G.; Mattoli, L.; Natalini, B.; Moroni, F. Pellicciari, R. "Kynurenine-3-hydroxylase and its Selective Inhibitors: Molecular Modelling Studies" in "*Recent Advances in Tryptophan Research*" Allegri-Filippini, G.; Costa, C. V. L.; Bertazzo, A.Eds. Plenum Press, New York, pp 493.497, **1996**
22. C. Clerici, G. Gentili, A. Errico, F. Camilleri, F. Brasacchio, R. Pellicciari, G. Costantino, L. Mattoli, D. Annibali, A. Morelli, "Regulation of Biliary Bicarbonate Secretion by Bile Salts", in "*Vanishing Bile Duct Syndrome - Pathophysiology and Treatment*", Eds. D.Alvaro, A.Benedetti, M.Strazzabosco, Kluwer Academic Publishers, 82 (**1997**)
23. R. Pellicciari, D. Annibali, G. Costantino, M. Marinozzi, B. Natalini, "Dirhodium(II)-tetraacetate-Mediated Decomposition of Ethyldiazo- acetate and Ethyldiazomalonate in the Presence of Fullerene. A New Procedure for the Selective Synthesis of [6-6]-Closed Methanofullerenes", *Synlett,* 1196, **1997**.
24. R. Pellicciari, M. Marinozzi, B. Natalini, G. Costantino, D.C. Lankin, J.P. Snyder, J.B. Monahan, "Synthesis, Preliminary Evaluation and Molecular Modeling Studies of New, Conformationally Constrained Analogues of the Competitive NMDA Receptor Antagonist 4-(Phosphonomethyl)-2-piperidinecarboxylic Acid (CGS 19755)", *Il Farmaco,* **52**, (6-7), 477, **1997**
25. R. Pellicciari, G. Costantino, M. Marinozzi, L. Mattoli, B. Natalini, "α-Diazocarbonyl Chemistry - Target Driven Applications", in "*Trends in Drug Research* II", Proceedings of the 11th Noordwijkerhout-Camerino Symposium, 11-15 May 1997, Noordwijkerhout, The Netherlands, Ed.Henk Van der Goot, Elsivier, **1998**.
26. R.Pellicciari, G.Costantino, M.Marinozzi, B.Natalini, C.Thomsen, F.Moroni, "Metabotropic glutamate receptors: new ligads and molecular modelling studies", in "*Metabotropic Glutamate Receptors and Brain Function*", Eds. F.Moroni, F. Nicoletti, D.E. Pellegrini-Giampietro, Portland Press Limited, London, 293-303, **1998**.
27. R. Pellicciari, G. Costantino, E. Giovagnoni, L. Mattoli, I. Brabet, J.-P. Pin. Synthesis and Prelimary evaluation of (S)-2-(4'-carboxycucbly)glycine, a new selective mGluR1 antagonist. *Biorg. Med. Chem. Lett*. 8, 1569, **1998**
28. R. Pellicciari, G. Costantino, M. Marinozzi, B. Natalini. Modulation of glutamate receptor pathways in search for new neuroprotective agents. *Il Farmaco*. 53, 255-261, **1998**
29. R. Pellicciari, M. Marinozzi, G. Costantino, B. Natalini, F. Moroni, D.E. Pellegrini-Giampietro. 2R,1'S,2'R,3'S)-2-(2'-Carboxy-3'-phenylcyclopropyl)glycine (PCCG-13), the first potent and selective competitive antagonist of phospholipase D-coupled metabotropic glutamate receptors: asymmetric synthesis and preliminary biological properties. *J.Med. Chem*. 42, 2716-2720, **1999**
30. B. Natalini, V. Capodiferro, L. Mattoli, M. Marinozzi, G. Costantino, R. Pellicciari. Chromatographic separation and evaluation of the lipophilicity by reversed phase high performane liquid chromatography of fullerene-C60 derivatives. *J. Chromatograph. A*. 847, 339-343, **1999**
31. G. Costantino, A. Macchiarulo, R. Pellicciari. Pharmacophore models of group I and group II metabotropic glutamate receptor agonists. Analysis of conformational, steric, and topological parameters affecting potency and selectivity. *J. Med. Chem*, 42, 2816-2827, **1999**

32. R. Pellicciari, G. Costantino. Metabotropic G-protein-coupled glutamate receptors as therapeutic targets. *Curr. Opin. Chem. Biol*. 3, 433-440, **1999**
33. G. Costantino, A. Macchiarulo, R. Pellicciari. Modeling of Amino terminal domains of group I metabotropic glutamate receptors: structural motifs affecting ligand selectivity. *J. Med. Chem*. 42, 5390-5401, **1999**
34. R. Pellicciari, G. Costantino, A. Macchiarulo. Metabotropic Glutamate receptors: a structural view point. *Pharmaceutica Acta Helv*. 74, 231-237, **2000**
35. L. Amori, G. Costantino, M.Marinozzi, R. Pellicciari, F. Gasparini, P.J. Flor, R. Kuhn, I. Vranesic. Synthesis, molecular modeling and preliminary biological evaluation of 1-amino-3-phosphono-3-cyclopentene-1-carboxylic acid and 1-amino-3-phosphono-2-cyclopentene-1-carboxylic acid, two novel agonists of metabotropic glutamate receptors of group III. *Bioorg. Med. Chem. Lett*. 10, 1447-1450, **2000**
36. I.I. Baskin, M.S. Belenikin, E.V. Ekimova, G.Costantino, V.A.Palyulin, R.Pellicciari, N.S. Zefirov, "Molecular Modeling of the Amino-terminal Domain of Metabotropic Glutamate Receptor mGluR1", *Doklady Chemistry*, 374, 191-194, **2000**
37. G. Costantino, C. Wolf, B. Natalini, R. Pellicciari. Evaluation of hydrophobic / hydrophilic balance of bile acids by comparative molecular field analysis (CoMFA). *Steroids*, 65, 483-489, **2000**
38. G. Costantino, K. Maltoni, M. Marinozzi, E. Camaioni, L. Preazau, J.P. Pin, R. Pellicciari. Synthesis and Biological Evaluation of 2-(3'-(1H-tetrazol-5-yl)bicyclo[1.1.1]pent-1-yl)glycine (S-TBPG), a Novel mGlu1 Receptor Antagonist. *Bioorg. Med. Chem*. 9, 221-227 **2001**,
39. R. Pellicciari, G. Costantino, M. Marinozzi, A. Macchiarulo, E. Camaioni, B. Natalini. Metabotropic Glutamate Receptors: Structure and New Subtype Selective Ligands *Il Farmaco*. 56, 91-94, **2001**
40. G. Costantino, A. Macchiarulo, R. Pellicciari. Homology Model of the Closed, Functionally Active, Form of the Amino Terminal Domain of mGluR1. *Bioorg. Med. Chem*. **2001**, 9, 847-852
41. M. C. Teràn Moldes, G. Costantino, M. Marinozzi, R. Pellicciari. Synthesis and preliminary biological evaluation at the $glycine_B$ site of (+)- and (-)-Oxetanylglycine, a Novel Non-Proteinogenic Amino Acid. *Il Farmaco*. **2001**, *56*, 609-613
42. G. Costantino, A. Macchiarulo, A. Entrena Guadix, R. Pellicciari. QSAR and Molecular Modeling Studies of Baclofen Analogs as $GABA_B$ Agonists. Insights into the Role of the Aromatic Moiety in $GABA_B$ Binding and Activation. *J. Med. Chem*. **2001**, 44, 1827-1832
43. G. Costantino, A. Macchiarulo, E. Camaioni, R. Pellicciari. Modeling of Poly(ADP-Ribose)polymerase (PARP) inhibitors. Docking of Ligands and QSAR Analysis. *J. Med. Chem*. **2001**, *44*, 3786-3794
44. R. Pellicciari, G. Costantino, M. Marinozzi, A. Macchiarulo, L. Amori, P.J. Flor, F. Gasparini, R. Kuhn, S. Urwyler. Design, Synthesis and Preliminary Evaluation of Novel 3'-Substituted Carboxycyclopropylglycines as Antagonists at Group 2 Metabotropic Glutamate Receptors. *Bioorg. Med. Chem. Lett*. **2001**, *11*, 3170-3182
45. A. Macchiarulo, A. Entrena-Guadix, G. Costantino. Conformational Analysis of Carboxyphenylglycine (CPG) Derivatives: Insight into Bio-active and Bio-selective Conformations of Group-I mGluRs Antagonists. *Il Farmaco*, **2001**, 56, 891-898
46. G. Costantino, A.Macchiarulo, R. Pellicciari Metabotropic Glutamate Receptors: Targets for Cerebral Ischemia. *Expert Opinions In Therapeutic Agents*. **2001**, 5, 669-683.
47. G. Costantino, A. Macchiarulo, R. Rovito. R. Pellicciari. Structure of Metal-Carbenoid Intermediates Derived from the Dirhodium(II)-Tetracarboxylate Mediated Decomposition of α-Diazocarbonyl Compounds. An *ab initio* and DFT Study. *J. Mol. Struct.(TEOCHEM)*. **2002**, 581, 111-115
48. Pellicciari R, Marinozzi M, Camaioni E, del Carmen Nunez M, Costantino G, Gasparini F, Giorgi G, Macchiarulo A, Subramanian N. Spiro[2.2]pentane as a dissymmetric scaffold for conformationally constrained analogues of glutamic acid: focus on racemic 1-aminospiro[2.2]pentyl-1,4-dicarboxylic acids. *J Org Chem*. **2002**;67:5497-507
49. Pellicciari R, Fiorucci S, Camaioni E, Clerici C, Costantino G, Maloney PR, Morelli A, Parks DJ, Willson TM. 6alpha-ethyl-chenodeoxycholic acid (6-ECDCA), a potent and selective FXR agonist endowed with anticholestatic activity.*J Med Chem*. **2002** ;45: 3569-72

50. Macchiarulo A, Costantino G, Fringuelli D, Vecchiarelli A, Schiaffella F, Fringuelli R.1,4-Benzothiazine and 1,4-benzoxazine imidazole derivatives with antifungal activity: a docking study. *Bioorg Med Chem*. **2002,** 10: 3415-23
51. Belenikin MS, Baskin II, Costantino G, Palyulin VA, Pellicciari R, Zefirov NS. Molecular modeling of the closed forms of the kainate-binding domains of kainate receptors and qualitative analysis of the structure-activity relationships for some agonists. *Dokl Biochem Biophys*. **2002**;386:239-44.
52. Belenikin MS, Baskin II, Costantino G, Palyulin VA, Pellicciari R, Zefirov NS. Comparative analysis of the ligand-binding sites of the metabotropic glutamate receptors mGluR1-mGluR8. *Dokl Biochem Biophys*. **2002**;386:251-6.
53. Macchiarulo A, Costantino G, Sbaglia R, Aiello S, Meniconi M, Pellicciari R. The role of electrostatic interaction in the molecular recognition of selective agonists to metabotropic glutamate receptor *Proteins*. **2003**;50:609-19.
54. De Luca L, Macchiarulo A, Costantino G, Barreca ML, Gitto R, Chimirri A, Pellicciari R. Binding modes of noncompetitive AMPA antagonists: a computational approach. *Farmaco*. **2003** 58:107-13.
55. Chiarugi A, Meli E, Calvani M, Picca R, Baronti R, Camaioni E, Costantino G,Marinozzi M, Pellegrini-Giampiero DE, Pellicciari R, Moroni F. Novel isoquinolinone-derived inhibitors of poly(ADP-ribose) polymerase-1:pharmacological characterization and neuroprotective effects in an in vitromodel of cerebral ischemia. *J Pharmacol Exp Ther*. **2003**, 305, 943-949
56. Costantino G, Macchiarulo A, Belenikin M, Pellicciari R. Molecular Dynamic Simulation of the ligand binding domain of mGluR1 in response to agonist and antagonist binding. *J. Comp. Aided. Mol. Des*., **2002** 16(11): 779-84.
57. 6alpha-ethyl-chenodeoxycholic acid (6- ECDCA), a potent and selective FXR agonist endowed with anticholestatic activity. Pp. 3569-3572 in *Journal of Medical Chemistry* – ISSN: 0022-2623 vol. 45, **2002.** Pellicciari R.; Fiorucci S.; Camaioni E.; Clerici C.; Malonev PR; Morelli A.; Parks DJ; Costantino G.
58. Pellicciari R, Camaioni E, Costantino, G, Marinozzi M, Macchiarulo A, Moroni F, Natalini B. Towards New Neuroprotective Agents: Design and Synthesis of 4*H*-Thieno[2,3-*c*] isoquinolin-5-one Derivatives as Potent PARP-1 Inhibitors. *Il Farmaco*, **2003**, 58(9): 851-8.
59. Costantino G, Macchiarulo A, Entrena-Guadix A, Camaioni E, Pellicciari, R. Binding Mode of 6ECDCA, Potent Bile Acid Agonist of the Farnesoid X Receptor (FXR). *Bioorg. Med. Chem. Lett*. **2003,** 13):1865-8
60. Traversa U, Bombi G, Camaioni E, Macchiarulo A, Costantino G, Palmieri C, Caciagli F, Pellicciari R. Rat brain guanosine binding site. Biological studies and pseudo-receptor construction. *Bioorg Med Chem*. **2003** 11(24): 5417-25.
61. Pellicciari R, Amori L, Costantino G, Giordani A, Macchiarulo A, Mattoli L, Pevarello P, Speciale C, Varasi M. Modulation of the kynurine pathway of tryptophan metabolism in search for neuroprotective agents. Focus on kynurenine-3-hydroxylase. *Adv Exp Med Biol.* **2003**;527:621-8.
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