Gabriele Costantino
-Curriculum Vitae -

Dati Personali
Data di nascita: **8 Aprile 1968**
Luogo di Nascita: **Roma**
Cittadinanza **Italiana**
Stato Civile: **Sposato, due figli**
Residenza: **Via Varese, 11 - Parma**
Ufficio: **Dipartimento di Scienze degli Alimenti e del Farmaco, Viale Area delle Scienze 27/A – Campus Universitario- 43125 Parma**
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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

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.
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