Gabriele Costantino

-Curriculum Vitae -

Personal Data

Date of Birth:

Place of Birth :

Citizen: **Italian**

Marital Status:

Home:

Office: **Dipartimento di Farmacia, Viale Area delle Scienze 27/A – Campus Universitario- 43100 Parma**

Tel. +39 0521 905055 ; E-mail: gabriele.costantino@unipr.it

Education:

1991- October-December: Stage on molecular modeling techniques in drug design. Drug Design Group, Searle R&D (Skokie, IL, USA). Supervisor: Dr. James P. Snyder

1992 April: Laurea Diploma in Chemistry *cum Laude*. Department of Chemistry, University of Perugia.

1992-1993: Research Fellowships at Laboratory of Chemometrics and at Institute of Medicinal Chemistry (under the supervision of Prof. Roberto Pellicciari)

1996 October-December: Fellowship at Organic Chemistry Department, University of Barcelona, Spain (under the supervision of Prof. E. Giralt)

Professionals

November 1994 –November 1998: Research Associate at Istituto di Chimica e Tecnologia del Farmaco, Faculty of Pharmacy, University of Perugia

November 1998 – December 2006: Associate Professor of Medicinal Chemistry at Dipartimento di Chimica e Tecnologia del Farmaco, Faculty of Pharmacy, University of Perugia

December 2006-present: Professor of Medicinal Chemistry at Dipartimento Farmaceutico, Faculty of Pharmacy, University of Parma and Coordinator and chairman of the Doctorate program in 'Design and synthesis of biologically active compounds' – University of Parma

Awards.

Recipient of the 'Italian Chemical Society-Farmindustria' Prize for the best young researcher in Medicinal Chemistry, 2003

Recipient of the 16th Merz Professorship at the Institute for Organic Chemistry – Goethe University, Frankfurt am Main. Oct-2003 Jan-2004

Fundings

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
FIL 2007-2012 (University of Parma)- Principal Investigator
EUROPIN (Erasmus-Mundi Program) Local Coordinator
Principal Investigator in grants supported by Chiesi Farmaceutici, AXXAM, Dompé, IEO**.**

Participation to Scientific Committees and Advisory Board

- President and Treasurer of the Scientific Committee of the Division of Medicinal Chemistry of the Italian Chemical Society
- Member of the Executive Committee of the European Federarion for Medicinal Chemistry
- Editor of *MedChemWatch*, the official newsletter of EFMC
- Member of the Advisory Editorial Board of *Current Medicinal Chemistry*
- 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

Research Interests

Computer-assisted design and synthesis of biologically active compounds. In particular:

- ✓ Design and synthesis of centrally acting compounds: metabotropic glutamate receptor ligands, PARP inhibitors, kynurenine pathway inhibitors
- ✓ Design and synthesis of modulators of transcription factors
- ✓ Molecular dynamics simulations of nuclear receptors and GPCRs

Languages

Italian (mother tongue), English, Spanish (scholar level)

1. **Oral Communications Lectures / Presentations at International and National Symposia**

- 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
- CER Person EUROQSAR (Verona, Italy) September 2016
- Asis Congress (Tirrenia di Pisa, Italy) May 2017
- XII EWDD (Siena, Italy) May 2017
- Carbon Anhydrases Congress (Montecatini, Italy) May 2017
- JMMC (Dubrovnik, Croatia) June 2017
- ESMEC (Urbino, Italy) July 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
- Statale University of Milan October 2016
- University of Florence November 2016
- University of Piemonte Orientale (Novara) January 2017
- Riga meeting Integrate (Lettonia) February 2017
- Simposium University of Florence March 2017
- University of Milan May 2017
- University Gabriele D'Annunzio (Chieti, Italy) 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.

62. Molecular modeling of the mgluR1 metabotropic glutamate receptor transmembrane domain and construction of the model of of its dimer. Pp. 341-345 in *Doklady biochemistry and biophysics*- ISSN: 1607- 6729 vol. 393, **2003**. Belenkin MS; Costantino G.; Palyulin VA; Pellicciari R.; Zefirov NS.

63. Molecular modeling of the ligand-binding domains of the NR3A and NR3B subunits of the NMDA receptor. Pp. 83-89 in *Doklady Biochemistry and Biophisics* – ISSN:1607-6729 vol. 389, **2003**. Belenikin MS; Costantino G.; Palyulin VA; Pellicciari R.; Zefirov NS.

64. Molecular dynamic simulation of the ligand-receptor complexes of the aminoterminal domain of the metabotropic glutamate receptor mGluR1. Pp. 98-102 in *Doklady Biochemistry and Biophisics* – ISSN: 1607-6729 vol. 389, **2003**. Belenikin MS; Costantino G.; Palyulin VA; Pellicciari R.; Zefirov NS.

65. Bile acid derivative sas ligands of the farnesoid X receptor. Synthesis, evaluation and structure activity relationship of a series of body and side chain modified analogues of chenodeoxycholic acid. Pp. 4559-4569 in *Journal of Medical Chemistry* – ISSN: 0022-2623 vol. 47, **2004** Pellicciari R.; Costantino G.; Camaioni E.; Sadeghpour BM; Entrena A.; Willson TM; Fiorucci S.; Clerici C.

66. Costantino G, Marinozzi M, Camaioni E, Natalini B, Sarichelou I, Micheli F, Cavanni P, Faedo S, Noe C, Moroni F, Pellicciari R. Stereoselective synthesis and preliminary evaluation of (+)- and (-)-3-methyl-5-carboxy-thien-2-yl-glycine (3-MATIDA): identification of (+)-3-MATIDA as a novel mGluR1 competitive antagonist. *Farmaco*. **2004** 59(2):93-9.

67. A. Macchiarulo, L. De Luca, G. Costantino, M. Barreca, R. Gitto, R. Pellicciari, A. Chimirri. QSAR Study of Anticonvulsant Negative Allosteric Modulators of the AMPA Receptor. *J.Med. Chem*, **2004,** 47:1860-3.

68. Pellicciari R, Camaioni E, Costantino G. Life or Death Decision. The case of Poly(ADP-Ribose)Polymerase (PARP) as therapeutic target for brain ischemia *Prog Med Chem*. **2004**;42:125-69

69. Pellicciari, R; G. Costantino, E. Camaioni, B. Sadeghpour, A. Gioiello, A. Entrena, R. Willson, S. Fiorucci. Bile Acid Derivatives as Agonists of the FXR Receptor. 2. Synthesis, Evaluation, and Structure Activity Relationship of a Series of Body- and Side Chain-Modified Analogs of Chenodeoxycholic acid (CDCA). *J.Med. Chem*, **2004**, 47:4559-69

70. Macchiarulo A, Costantino G, Meniconi M, Pleban K, Ecker G, Bellocchi D, Pellicciari R. Insights into phenylalanine derivatives recognition of VLA-4 integrin: from a pharmacophoric study to 3D-QSAR and molecular docking analyses. *J Chem Inf Comput Sc*i. **2004**;44:1829-39.

71. Pleban K, Macchiarulo A, Costantino G, Pellicciari R, Chiba P, Ecker GF. Homology model of the multidrug transporter LmrA from Lactococcus lactis. *Bioorg Med Chem Lett*. **2004**, 14:5823-6.

72. Bellocchi D., Macchiarulo A, Costantino G, Pellicciari R. Docking studies on PARP-1 inhibitors: insights into the role of a binding pocket water molecule. *Biorg. Med. Chem*. **2005,** 15;13, 1151-7.

73. Costantino G, Entrena A, Macchiarulo A, Gioiello A, Pellicciari R. Molecular Dynamics Simulation of the Ligand Binding Domain of Farnesoid X Receptor (FXR). Insights into Helix-12 Stability and Coactivator Peptide Stabilization in Response to Agonist Binding. *J Med Chem*. **2005**; 48(9):3251-9.

74. Pellicciari R, Costantino G, Fiorucci S. Farnesoid X receptor: from structure to potential clinical applications. *J Med Chem*. **2005**;48(17):5383-403

75. Meyer U, Costantino G, Macchiarulo A., Pellicciari R. Is Antagonism of *E*/*Z*-Guggulsterone at the Farnesoid X Receptor Mediated by a Noncanonical Binding Site? A Molecular Modeling Study. *J. Med Chem*, **2005**, 48:6948-55

76. Schiaffella F, Macchiarulo A, Milanese L, Vecchierelli A, Costantino G, Pietrella D, Fringuelli R. Design, Synthesis, and Microbiological Evaluation of New CA-CYP51 Inhibitors. *J. Med. Chem*, **2005**, 48:7658-66.

77. Macchiarulo A, Costantino G, Rizzo G, Fiorucci S, Pellicciari R. Unveiling hidden features of orphan nuclear receptors: The case of the small heterodimer partner (SHP). *J Mol Graph Model*. **2006**, 24, 362-72

78. Amori L, Serpi M, Marinozzi M, Costantino G, Diaz MG, Hermit MB, Thomsen C, Pellicciari R. Synthesis and preliminary biological evaluation of (2S,1'R,2'S)- and (2S,1'S,2'R)-2-(2'-phosphonocyclopropyl)glycines, two novel conformationally constrained l-AP4 analogues. *Bioorg Med Chem Lett*. **2006**;16(1):196-9

79. Costantino G. In silico approaches towards the understanding of the structure-function relationships in family C GPRCs. *Curr. Pharm. Des*. **2006**, 12(17):2159-73

80. Pellicciari R., Bellocchi D, Costantino G, Re N, Marrone A, Coletti C. Poly(ADP-ribose)polymerase (PARP)-Catalyzed Hydrolysis of NAD+: QM/MM Simulation of the Enzyme Reaction *ChemMedChem*, **2006,** 1(5):533-9.

81. Pellicciari R, Rizzo RC, Marinozzi M, Costantino G, Amori L, Guidetti P, Wu H-Q, Schwarcz R. Modulators of the Kynurenine Pathway of Tryptophan Metabolism. Synthesis and Preliminary Biological Evaluation of (S)-4-(Ethylsulfonyl)Benzoylalanine, the First Potent and Selective Kynurenine Aminotransferase II (KAT II) Inhibitor *ChemMedChem*, **2006,** 1(5):528-31

82. Filosa R, Marinozzi M, Costantino G, Hermit MB, Thomsen C, Pellicciari R. Synthesis and Biological Evaluation of (2S)- and (2R)-2-(3'-Phosphonobicyclo[1.1.1]pentyl)glycines as Novel Group III Selective Metabotropic Glutamate Receptor Ligands. *Bioorg. Med. Chem*. **2006**, 14(11):3811-7.

83. Pellicciari R, Gioiello A, Costantino G. Potential Therapeutic Applications of Farnesoid X Receptor (FXR) Modulators. *Exp. Opin. Therap. Patents*. **2006**, 16, 333-341

84. Pellicciari R, Gioiello A, Costantino G, Sadeghpour BM, Rizzo G, Meyer U, Parks DJ, Entrena-Guadix A, Fiorucci S. Back door modulation of the farnesoid X receptor: design, synthesis, and biological evaluation of a series of side chain modified chenodeoxycholic acid derivatives *J. Med Chem.* **2006**; 49(14):4208-15

85. Ferrari C, Macchiarulo A, Costantino G, Pellicciari R. Pharmacophore model for bile acids recognition by the FPR receptor. *J Comput Aided Mol Des*. **2006**, 20(5):295-303.

86. Pellicciari R, Sato H, Gioiello A, Costantino G, Macchiarulo A, Sadeghpour BM, Giorgi G, Schoonjans K, Auwerx J. Nongenomic actions of bile acids. Synthesis and preliminary characterization of 23- and 6,23-alkyl-substituted bile acid derivatives as selective modulators for the G-protein coupled receptor TGR5. *J Med Chem*. **2007** Sep 6;50(18):4265-8

87. Marinozzi M, Serpi M, Amori L, Gavilan Diaz M, Costantino G, Meyer U, Flor PJ, Gasparini F, Heckendorn R, Kuhn R, Giorgi G, Hermit MB, Thomsen C, Pellicciari R. Synthesis and preliminary pharmacological evaluation of the four stereoisomers of (2S)-2-(2'-phosphono-3'-phenylcyclopropyl)glycine, the first class of 3'-substituted trans C1'-2'-2-(2'-phosphonocyclopropyl)glycines. *Bioorg Med Chem*. **2007**;15(9):3161-70

88. Pellicciari R., Camaioni E, Costantino G, Formentoni L, Sabbatici P, Venturosi F, Eren G, Bellocci D, Chiarugi A, Moroni F.On the Way to Selective PARP-2 Inhibitors. Design, Synthesis, and Preliminary Evaluation of a Series of Isoquinolinone Derivatives. *ChemMedChem*, **2008,** Published Online**:** 11 Apr 2008

89. Cozzini P, Kellogg GE, Spyrakis F, Abraham DJ, Costantino G, Emerson A, Fanelli F, Gohlke H, Kuhn LA, Morris GM, Orozco M, Pertinhez TA, Rizzi M, Sotriffer CA. Target flexibility: an emerging consideration in drug discovery and design. *J Med Chem*. **2008** Oct 23;51(20):6237-55

90. Synthesis and biological evaluation of 4,5-diphenyloxazolone derivatives on route towards selective COX-2 inhibitors. Dündar Y, Unlü S, Banoğlu E, Entrena A, Costantino G, Nunez MT, Ledo F, Sahin MF, Noyanalpan N. *Eur J Med Chem*. **2009** May;44(5):1830-7

91. New promises for manipulation of kynurenine pathway in cancer and neurological diseases. Costantino G. *Expert Opin Ther Targets*. **2009** Feb;13(2):247-58

92. Molecular Dynamics Simulation of the Heterodimeric mGluR2/5HT(2A) Complex. An Atomistic Resolution Study of a Potential New Target in Psychiatric Conditions. Bruno A, Guadix AE, Costantino G. *J Chem Inf Model*. **2009**, 49(6), 1602-1616

93. Bulky 1,4-benzoxazine derivatives with antifungal activity. Fringuelli R, Giacchè N, Milanese L, Cenci E, Macchiarulo A, Vecchiarelli A, Costantino G, Schiaffella F. *Bioorg Med Chem*. **2009**, **17**(11), 3838-3846

94. Sodium channel blockers for neuropathic pain. Zuliani V, Rivara M, Fantini M, Costantino G. *Expert Opin Ther Pat*. **2010** Jun;20(6):755-79

95. Synthesis, biological evaluation, and docking studies of novel heterocyclic diaryl compounds as selective COX-2 inhibitors.Eren G, Unlü S, Nuñez MT, Labeaga L, Ledo F, Entrena A, Banoğlu E, Costantino G, Sahin MF. *Bioorg Med Chem*. **2010**;18(17):6367-76

96. Derivates of Nicotinic Acid N-Oxide, their preparation and their use as inhibitors of enzyme 3-hydroxyanthranilate-3,4-dioxygenase. G. Costantino; L. Amori; R. Schwarcz

97. Bruno A., Amori L., and Costantino, G. Addressing the Conformational Flexibility of Serine Racemase by Combining Targeted Molecular Dynamics, Conformational Sampling and Docking Studies. *Mol. Informatics*, **2011**, 30, 317-328

98. Gioiello A, Macchiarulo A, Carotti A, Filipponi P, Costantino G**,** Rizzo G, Adorini L, Pellicciari R. Extending SAR of bile acids as FXR ligands: discovery of 23-N-(carbocinnamyloxy)-3α,7α-dihydroxy-6α-ethyl-24-nor-5β-cholan-23-amine. *Bioorg Med Chem*. **2011** Apr 15;19(8):2650-8

99. Bruno A, Beato C, Costantino G. Molecular dynamics simulations and docking studies on 3D models of the heterodimeric and homodimeric 5-HT(2A) receptor subtype. *Future Med Chem.* **2011** Apr;3(6):665-81

100. Discovery and characterizationof novel potent PARP-1 inhibitors andowed with neuroprotective propertiesPellicciari R., Camaioni E., Gilbert A. M., Macchiarulo M., Bikker J.A:, Shah F., Bard J., Costantino G., Gioiello A., Robertson G.M., Sabbatini P., Venturoni F., Liscio P., Carotti A., Bellocchi D., Cozzi A., Wood A, Gonzales C., Zaleska MM., Ellingboe JW; Moroni F. *Med. Chem. Commun.*, **2011**, 2, 559-565

101. Carmi C, Galvani E, Vacondio F, Rivara S, Lodola A, Russo S, Aiello S, Bordi F, Costantino G, Cavazzoni A, Alfieri RR, Ardizzoni A, Petronini PG, Mor M. Irreversible inhibition of epidermal growth factor receptor activity by 3-aminopropanamides. *J Med Chem.* **2012** Mar 8;55(5):2251-64

102. Amori L, Katkevica S, Bruno A, Campanini B, Felici P, Mozzarelli A, Costantino G. Design and synthesis of trans-2-substituted-cyclopropane-1-carboxylic acids as the first non-natural small molecule inhibitors of O-acetylserine sulfhydrylase *Med. Chem. Commun.*, **2012**, 3, 1111-1116

103. Bruno A, Costantino G, De Fabritis G, Pastor M, Selent J.Membrane-Sensitive Conformational States of Helix 8 in the Metabotropic Glu2 Receptor, a Class C GPCR. *PLoS ONE*, **2012** e42023. doi: 10.1371/journal.pone.0042023. Epub 2012 Aug 1.

104. G. Costantino, M. Mor, C. Pecchini, GP Vallerini, E. Della Turca, F. Micheli, A Worby, R. Di Fabio, A. Giacometti, A. Roth, E. Merlo-Pich, M. Biagetti, G. Bonanomi, D. Montanari, L. Tarsi, F. Tonelli, R Longhi, A.M Capelli Further insights in 5-phenyl-2-[2-(1-piperidinylcarbonyl) phenyl]-2,3-dihydro-1H-pyrrolo[1,2-c]imidazol-1-ones, a recently disclosed class of Neuropeptide S antagonists. 2013, *Letters in Drug Design and Discovery, **2013**, 10, 396-401*

99. Artese A, Alcaro S, Moraca F, Reina R, Ventura M, Costantino G, Beccari AR, Ortuso F. State of-the-art and dissemination of computational tools for drug-design purposes: a survey among Italian academics and industrial institutions. *Future Med Chem*. **2013** May;5(8):907-27

100. Beccari AR, Cavazzoni C, Beato C, Costantino G. LiGen: A High Performance Workflow for Chemistry Driven de Novo Design. *J Chem Inf Model*. **2013**, 53(6), 1518-1527

101. Beato C, Beccari AR, Cavazzoni C, Lorenzi S, Costantino G. Use of Experimental Design To Optimize Docking Performance: The Case of LiGenDock, the Docking Module of Ligen, a New De Novo Design Program. *J Chem Inf Model*. **2013**, 53(6), 1503-1517

102. Bruno A., Amori L., Costantino G.. Computational Insights into the mechanism of inhibition of OASS-A by a small molecule inhibitor. *Mol. Informatics*, **2013**, 32(5-6), 447-457

103.Capelli AM, Bruno A, Entrena Guadix A, Costantino G. Unbinding pathways from the glucocorticoid receptor shed light on the reduced sensitivity of glucocorticoid ligands to a naturally occurring, clinically relevant mutant receptor. *J Med Chem*. **2013** 56(17):7003-14

104.Radi, M., Vallerini, G.P., Petrelli, A., Vincetti, P., Costantino, G. A one-pot two-step microwave-assisted synthesis of N1-substituted 5,6-ring-fused 2-pyridones. *Tetrahedron Letters*, **2013**, 54(50), 6905-6908

105.Vallerini GP, Amori L, Beato C, Tararina M, Wang XD, Schwarcz R, Costantino G. 2-Aminonicotinic acid 1-oxides are chemically stable inhibitors of quinolinic acid synthesis in the mammalian brain: a step towards new anti-excitotoxic agents. *J Med Chem*. **2013**,12;56(23):9482-95.

106.Pieroni M, Wan, B. Cho S, Franzblau SG, Costantino G. Design, Synthesis and Investigation on the Structure–Activity Relationships of N-Substituted 2-Aminothiazole Derivatives as Antitubercular Agents. *Eur. J. Med. Chem.* **2014** Jan 24;72:26-34

107. Gioiello A, Cerra B, Zhang W, Vallerini GP, Costantino G, Franco FD, Passeri D, Pellicciari R, Setchell KD. Synthesis of atypical bile acids for use as investigative tools for the

genetic defect of 3β-hydroxy-Δ5-C27-steroid oxidoreductase deficiency. *J Steroid Biochem Mol Biol*. **2014** :348-360

108. Costantino G. Inhibitors of quinolinic acid synthesis: new weapons in the study of neuroinflammatory diseases *Future Med Chem*. **2014**:841-3.

109 Costantino, G. Computationally driven drug discovery meeting-3 - Verona (Italy): 4 - 6th of March 2014. *Expert Opin Drug Discov*. **2014** Aug 4:1-3

110. Capelli, A.M.; Costantino, G. Unbinding pathways of VEGFR2 inhibitors revealed by steered molecular dynamics. *J. Chem.Inf. Model*. **2014** 10.1021/ci500527j

111. Moriconi A, Cunha TM, Souza GR, Lopes AH, Cunha FQ, Carneiro VL, Pinto LG, Brandolini L, Aramini A, Bizzarri C, Bianchini G, Beccari AR, Fanton M, Bruno A, Costantino G, Bertini R, Galliera E, Locati M, Ferreira SH, Teixeira MM, Allegretti M. Targeting the minor pocket of C5aR for the rational design of an oral allosteric inhibitor for inflammatory and neuropathic pain relief. *Proc Natl Acad Sci U S A*. **2014**;111(47):16937-42

112. Blocking cysteine biosynthesis in Salmonella typhimurium the the moonlighting enzyme CysK as a potential antibiotic target in metabolism meets virulance 2. Bettati S.; Spyrakis F.; Benoni R.; Pieroni M.; Costantino G.; Pecchini C.; zani F.; Mozzarelli A.

112. Campanini, B.; Pieroni, M.; Raboni, S.; Bettati, S.; Benoni, S.; Pecchini, C.; Costantino, G.; Mozzarelli. A.; Inhibitors of the Sulfur Assimilation Pathway in Bacterial Pathogens as Enhancers of Antibiotic Therapy. *Curr. Med. Chem*. **2015**, 22, 187-213

113. Pieroni M, Annunziato G, Azzali E, Dessanti P, Mercurio C, Meroni G, Trifiró P, Vianello P, Villa M, Beato C, Varasi M, Costantino G. Further insights into the SAR of α-substituted cyclopropylamine derivatives as inhibitors of histone demethylase KDM1A. *Eur J Med Chem*. **2015** Mar 6; 92:377-86.

114. Pieroni M, Machado D, Azzali E, Santos Costa S, Couto I, Costantino G, Viveiros M. Rational Design and Synthesis of Thioridazine Analogues as Enhancers of the Antituberculosis Therapy. *J Med Chem*. **2015** Aug 13;58(15):5842-53.

115. Beato C, Pecchini C, Cocconcelli C, Campanini B, Marchetti M, Pieroni M, Mozzarelli A, Costantino G. Cyclopropane derivatives as potential human serine racemase inhibitors: unveiling novel insights into a difficult target. *J Enzyme Inhib Med Chem*. **2015** Jul 2:1-8

116. Pieroni M, Wan B, Zuliani V, Franzblau SG, Costantino G, Rivara M. Discovery of antitubercular 2,4-diphenyl-1H-imidazoles from chemical library repositioning and rational design. *Eur J Med Chem*. **2015** Jul 15;100:44-9

117. Vincetti P, Caporuscio F, Kaptein S, Gioiello A, Mancino V, Suzuki Y, Yamamoto N, Crespan E, Lossani A, Maga G, Rastelli G, Castagnolo D, Neyts J, Leyssen P, Costantino G, Radi M Discovery of Multitarget Antivirals Acting on Both the Dengue Virus NS5-NS3 Interaction and the Host Src/Fyn Kinases. *J Med Chem*. **2015** Jun 25;58(12):4964-75

118. Pieroni M, Machado D, Azzali E, Santos Costa S, Couto I, Costantino G, Viveiros M. Rational Design and Synthesis of Thioridazine Analogues as Enhancers of the Antituberculosis Therapy. *J Med Chem*. **2015**, 58:5842-53

119. Pieroni M, Annunziato G, Beato C, Wouters R, Benoni R, Campanini B, Pertinhez T, Bettati S, Mozzarelli A, Costantino G. Rational Design, Synthesis and Preliminary Structure-Activity Relationships of α-Substituted-2-Phenylcyclopropane Carboxylic Acids as Inhibitors of Salmonella Typhimurium O-Acetylserine Sulfhydrylase. *J Med Chem*. **2016**; 59(6):2567-78

120. Paolo Vincetti, Anna Brianza, Nicolò Scalacci, **Gabriele Costantino,** Daniele Castagnolo, and Marco Radi. A microwave-assisted multicomponent protocol for the synthesis of benzofuran-2-carboxamides. *Tetrahedron Lett.* **2016**

121. Annunziato G, Angeli A, D'Alba F, Bruno A, Pieroni M, Vullo D, De Luca V, Capasso C, Supuran CT, **Costantino G**. Discovery of New Potential Anti-Infective Compounds Based on

Carbonic Anhydrase Inhibitors by Rational Target-Focused Repurposing Approaches. *ChemMedChem*. **2016** Jun 15. doi: 10.1002/cmdc.201600180.

122. Vucicevic J, Srdic-Rajic T, Pieroni M, Laurila JM, Perovic V, Tassini S, Azzali E, **Costantino G**, Glisic S, Agbaba D, Scheinin M, Nikolic K, Radi M, Veljkovic N A combined ligand- and structure-based approach for the identification of rilmenidine-derived compounds which synergize the antitumor effects of doxorubicin. *Bioorg Med Chem*. **2016**; 24(14):3174-83.

123. Bruno A, Aiello F, **Costantino** G, Radi M.
Mol Inform. 2016 Sep;35(8-9):333-9.
Homology Modeling, Validation and Dynamics of the G Protein-coupled Estrogen Receptor 1 (GPER-1).

124. Tassini S, Sun L, Lanko K, Crespan E, Langron E, Falchi F, Kissova M, Armijos-Rivera JI, Delang L, Mirabelli C, Neyts J, Pieroni M, Cavalli A, **Costantino** G, Maga G, Vergani P, Leyssen P, Radi M. Discovery of Multi-Target Agents Active as Broad-Spectrum Antivirals and Correctors of Cystic Fibrosis Transmembrane Conductance Regulator (CFTR) for Associated Pulmonary Diseases. J Med Chem. 2017 Jan 25.

125. Accepting the Invitation to Open Innovation in Malaria Drug Discovery: Synthesis, Biological Evaluation and Investigation on the Structure‐Activity Relationships of Benzo[b]thiophene-2-carboxamides as Antimalarial Agents.
Pieroni M, Azzali E, Basilico N, Parapini S, Zolkiewski M, Beato C, Annunziato G, Bruno A, Vacondio F, Costantino G.
J Med Chem. 2017 Jan 27