

Elenco delle Pubblicazioni

Pubblicazioni *in extenso* su riviste internazionali

1. Bianucci, A.M.; Biagi, G.; **Coï, A.**; Giorgi, I.; Livi, O.; Pacchini, F.; Scartoni, V.; Lucacchini, A.; Costa, B. Bioisosterism, Enantioselectivity, and Molecular Modeling of New Effective N⁶ and/or N(9)-Substituted 2-Phenyl Adenines and 8-Aza Analogs: Different Binding Modes to A₁ Adenosine Receptors. *Drug Development Research*, 2001, 54(2), 52-65. (Codice ISSN 1098-2299)
2. Ganadu, M.L.; Aru, M.; Mura, G.M.; **Coï, A.**; Mlynarz, P.; Kozłowski, H. Effects of divalent metal ions on the α B-crystallin chaperone-like activity: spectroscopic evidence for a complex between copper(II) and protein. *Journal of Inorganic Biochemistry*, 2004, 98(6), 1103-1109. (Codice ISSN 0162-0134)
3. Biagi, G.; Bianucci, A.M.; **Coï, A.**; Costa, B.; Fabbrini, L.; Giorgi, I.; Livi, O.; Micco, I.; Pacchini, F.; Santini, E.; Nofal, F.; LeRoy Salerni, O.; Scartoni, V. 2,9-Disubstituted-N6-(arylcarbamoyl)-8-azaadenines as new Selective A₃ Adenosine Receptor Antagonists: Synthesis, Biochemical and Molecular Modeling Studies. *Bioorganic & Medicinal Chemistry*, 2005, 13(15), 4679-4693. (Codice ISSN 0968-0896)
4. **Coï, A.**; Bianucci, A.M.; Ganadu, M.L.; Mura, G.M. A modeling study of α B-crystallin complexed with zinc for the seek of correlations between *chaperone-like* activity and exposure of hydrophobic surfaces., *International Journal of Biological Macromolecules*, 2005, 36(4), 208-214. (Codice ISSN 0141-8130)
5. **Coï, A.**; Massarelli, I.; Murgia, L.; Saraceno, M.; Calderone, V.; Bianucci, A.M. Prediction of hERG Potassium Channel Affinity by the CODESSA approach. *Bioorganic & Medicinal Chemistry*, 2006, 14(9), 3153-3159. (Codice ISSN 0968-0896)
6. **Coï, A.**; Tonelli, M.; Ganadu, M.L.; Bianucci, A.M. Binding free energy calculations of Adenosine Deaminase inhibitors. *Bioorganic & Medicinal Chemistry*, 2006, 14(8), 2636-2641. (Codice ISSN 0968-0896)
7. Spinozzi, F.; Mariani, P.; Rustichelli, F.; Amenitsh, H.; Bennardini, F.; Mura, G.M.; **Coï, A.**; Ganadu, M.L. Temperature-dependence of chaperone-like activity and oligomeric state of α B-crystallin. *Biochimica et Biophysica Acta*, 2006, 1764(4), 677-687. (Codice ISSN 1570-9639)
8. Calderone, V.; **Coï, A.**; Fiamingo, F.L.; Giorgi, I.; Leonardi, M.; Livi, O.; Martelli, A.; Martinotti, E. Structural modifications of benzanilide derivatives, effective potassium channel openers. *X. European Journal of Medicinal Chemistry*, 2006, 41(12), 1421-1429. (Codice ISSN 0223-5234)
9. Giorgi, I.; Bianucci, A.M.; Biagi, G.; Livi, O.; Scartoni, V.; Leonardi, M.; Pietra, D.; **Coï, A.**; Massarelli, I.; Nofal, F.A.; Fiamingo, F.L.; Anastasi, P.; Giannini, G. Synthesis, biological activity and molecular modelling of new trisubstituted 8-azaadenines with high affinity for A₁ Adenosine Receptors. *European Journal of Medicinal Chemistry*, 2007, 42(1), 1-9. (Codice ISSN 0223-5234)
10. Massarelli, I.; Ahmad Nofal, F.; **Coï, A.**; Pietra, D.; Biagi, G.; Giorgi, I.; Bianucci, A.M. QSAR study on a novel series of 8-azaadenine analogues proposed as A₁ adenosine receptor antagonists. *European Journal of Medicinal Chemistry*, 2007, 43(1), 114-121. (Codice ISSN 0223-5234)
11. **Coï, A.**; Bianucci, A.M.; Bonomi, F.; Rasmussen, P.; Mura, G.M.; Ganadu, M.L. Structural Perturbation of α B-Crystallin by Zinc and Temperature related to its *chaperone-like* activity. *International Journal of Biological Macromolecules*, 2008, 42(3), 229-34. (Codice ISSN 0141-8130)
12. Saraceno, M.; **Coï, A.**; Bianucci, A.M.; Molecular Modelling of human CYP2D6 and molecular docking of a series of *ajmalicine*- and *quinidine-like* inhibitors. *International Journal of Biological Macromolecules*, 2008, 42(4), 362-71. (Codice ISSN 0141-8130)
13. **Coï, A.**; Massarelli, I.; Testai, L.; Calderone, V.; Bianucci, A.M. Identification of "toxicophoric" features for predicting drug-induced QT interval prolongation, *European Journal of Medicinal Chemistry*, 2008, 43(11), 2479-2488. (Codice ISSN 0223-5234)
14. **Coï, A.**; Fiamingo, F.L.; Livi, O.; Calderone, V.; Martelli, A.; Bianucci, A.M. QSAR studies on BK channel activators. *Bioorganic & Medicinal Chemistry*, 2009, 17(1), 319-325. (Codice ISSN 0968-0896)
15. Massarelli, I.; Imbriani, M.; **Coï, A.**; Saraceno, M.; Carli, N.; Bianucci, A.M. Development of QSAR models for predicting hepatocarcinogenic toxicity of chemicals. *European Journal of Medicinal Chemistry*, 2009, 44(9), 3658-3664. (Codice ISSN 0223-5234)
16. **Coï, A.**; Bianucci, A.M.; Calderone, V.; Testai, L.; Digiaco, M.; Rapposelli, S.; Balsamo, A. Predictive models, based on classification algorithms, for compounds potentially active as mitochondrial ATP-sensitive potassium channel openers, *Bioorganic & Medicinal Chemistry*, 2009, 17(15), 5565-5571. (Codice ISSN 0968-0896)
17. **Coï, A.**; Massarelli, I.; Saraceno, M.; Carli, N.; Testai, L.; Calderone, V.; Bianucci, A.M. QSAR models for predicting biological properties, developed by combining structure- and ligand-based approaches: an application to the hERG potassium channel inhibition, *Chemical Biology & Drug Design*, 2009, 74(4), 416-433. (Codice ISSN 1747-0285)
18. **Coï, A.**; Bianucci, A.M.; Rapposelli, S.; Balsamo, A. Classification models for the identification of P-gp inhibitors. *Drugs of the Future*, (2010), 35(suppl. A). (Codice ISSN 0377-8282)

19. Rapposelli, S.; **Coï, A.**; Imbriani, M.; Bianucci, A.M. Development of classification models for identifying "true" P-gp inhibitors through inhibition, ATPase activation and monolayer efflux assays. *International Journal of Molecular Sciences*, (2012), 13(6), 6924-6943. (Codice ISSN 14220067)
20. **Coï A.**, Bianucci A.M., Combining structure- and ligand-based approaches for studies of interactions between different conformations of the hERG K⁺ channel pore and known ligands. *Journal of Molecular Graphics and Modelling*, (2013), 46, 93-104. (Codice ISSN 10933263)
21. Bustaffa E., Minichilli F. Andreassi M.G., Carone S, **Coï A.**, Cori L., Fatta F., Fatta F., Grecchi S., Minoia C., Ronchi A., Scovassi I., Sicari R., Stea F., Bianchi F e Gruppo di Lavoro SEpiAs, Sorveglianza epidemiologica in aree interessate da inquinamento ambientale da arsenico di origine naturale o antropica (SEpiAS CCM 2010). *Epidemiologia e Prevenzione*, (2014), 38(3-4) suppl 1, 25-94.

Poster

- P1. F. Spinozzi, G. M. Mura, **A. Coï**, M. L. Ganadu, P. Mariani. Correlation between aggregation behavior and the chaperone-like activity of human α B-crystallin. National Conference on Nanoscience and Nanotechnology: The Molecular Approach, Area del CNR di Bologna, 25-27 Febbraio 2004.
- P2. A. M. Bianucci, **A. Coï**, I. Massarelli, L. Murgia, M. Saraceno. Prediction of hERG Potassium Channel Affinity by Traditional QSAR and Volsurf Approach. XV Noordwijkerout-Camerino Symposium, vol. abstracts, pp. 32, Noordwijkerout (Netherlands) 8-14 Maggio 2005.
- P3. **A. Coï**, A. M. Bianucci, F. Bonomi, M. L. Ganadu, G. M. Mura, P. Rasmussen. Structural Studies and Molecular Modeling of α B-Crystallin. Effects of Zinc and Temperature. XXXIII Congresso Nazionale, Divisione di Chimica Inorganica della Società Chimica Italiana, vol. abstracts, P024, Siena 11-16 Luglio 2005.
- P4. F.L. Fiamingo, **A. Coï**, G. Amato, V. Calderone, I. Giorgi, M. Leonardi, O. Livi, A. Martelli. Sintesi e valutazione farmacologica di potenziali BK-openers. 6° SAYCS (Sigma-Aldrich Young Chemists) Symposium, Riccione 9-11 Ottobre 2006.
- P5. M. Saraceno, **A. Coï**, A.M. Bianucci. Molecular Modeling of CYP2D6 complexes and molecular docking of a series of ajmalicine- and quinidine-like inhibitors. 8th Tetrahedron Symposium, vol. abstracts, P1.73, Berlino 26-29 Giugno 2007.
- P6. I. Giorgi, G. Biagi, M. Leonardi, A.M. Bianucci, **A. Coï**, D. Pietra. Novel 8-azapurine derivatives as ligands of A₃ adenosine receptors. 8th Tetrahedron Symposium, vol. abstracts, P2.44, Berlino 26-29 Giugno 2007.
- P7. **A. Coï**, A.M. Bianucci, S. Rapposelli, V. Calderone, A. Balsamo. Theoretical Models to classify the 4-Spiro-substituted Benzopyran derivatives as new Mitochondrial-K_{ATP} Channel Openers (mito-KCOs) endowed of Cardioprotective activity. XIII Meeting SERF Heterocyclic Structures in Medicinal Chemistry, vol. abstracts, pp. 222, P-21, Palermo 18-21 Maggio 2008.
- P8. **A. Coï**, A.M. Bianucci, V. Calderone, L. Testai, M. Manganaro, S. Rapposelli, A. Balsamo. Theoretical Models for Classification as Cardioprotective Agents of Mitochondrial-K_{ATP} Channel Openers (mito-KCOs) Possessing the 4-Spiro-substituted Benzopyranic Structure. 9th Tetrahedron Symposium, vol. abstracts, pp. 108, P-2, Berkeley, CA, USA 22-25 July 2008.
- P9. **A. Coï**, A.M. Bianucci. Classification Models for the risk of drug-induced Torsades de Pointes. 10th Tetrahedron Symposium, vol. abstracts, A038, Paris, France 23-26 June 2009.
- P10. **A. Coï**, A.M. Bianucci, S. Rapposelli, A. Balsamo. Classification Models for the identification of P-gp inhibitors. 21st International Symposium on Medicinal Chemistry, vol. abstracts, 479, Brussels, Belgium, September 5-9, 2010.
- P11. M. Santoro, **A. Coï**, M. Lipucci, S. Gainotti, E. Mollo, L. Vittozzi, D. Taruscio, F. Bianchi. Classificazione e caratterizzazione dei fabbisogni informativi dei Registri di Malattie Rare attraverso l'utilizzo di analisi esplorative dei dati. XXXVII Congresso dell'Associazione Italiana di Epidemiologia, Roma, 4-6 Novembre 2013.
- P12. **A. Coï**, M. Santoro, M. Lipucci, A.M. Bianucci, S. Gainotti, E. Mollo, L. Vittozzi, D. Taruscio, F. Bianchi. Characterization and classification of Rare Disease Registries by using exploratory data analyses. ECRD 2014 : The European Conference on Rare Diseases & Orphan Products – Berlino, 8-10 Maggio 2014.
- P13. M. Santoro, A. Kole, F. Faurisson, M. Ensini, **A. Coï**, M. Lipucci, L. Vittozzi, D. Taruscio, F. Bianchi. The Patient's Perspective on Rare Disease Registries: evidence of associations with disease characteristics. ECRD 2014 : The European Conference on Rare Diseases & Orphan Products – Berlino, 8-10 Maggio 2014.
- P14. **Coï A.**, Cori L., Minichilli F., Santoro M., Bianchi F. Risk perception in four areas of Italy affected by arsenic pollution derived from natural or anthropic sources. Abstract accettato alla XXVI Conferenza dell'International Society of Environmental Epidemiology (ISEE), che si terrà a Seattle il 24-28 Agosto 2014.
- P15. Bianchi F., **Coï A.**, Cori L., Minichilli F., Bustaffa E., Biomonitoring of urinary organic and inorganic arsenic in four different polluted areas in Italy. Abstract accettato alla XXVI Conferenza dell'International Society of Environmental Epidemiology (ISEE), che si terrà a Seattle il 24-28 Agosto 2014.