

ANDREA MOZZARELLI

Education/Training

1974 Degree in Chemistry, University of Parma.

1984-1985 Fogarty Fellowship at the Laboratory of Chemical Physics, National Institutes of Health, Bethesda, MD, USA, Dr. William. A. Eaton (member of the National Academy of Sciences, USA)

Positions

1975-1980 Research Assistant in Biochemistry, University of Parma

1980-1988 Senior Researcher in Biochemistry, University of Parma

1988-2000 Associate Professor in Biochemistry, University of Parma

2000-present Full Professor in Biochemistry, Department of Pharmacy, University of Parma, Parma, Italy.

1995-2010 Member of the Interdepartmental Measurement Center board, University of Parma

1998-2003 Member of the committee for the PhD Program in Biochemical Sciences, University of Turin and Parma.

2004-present Member of the committee of the Ph.D program in Biochemistry and Molecular Biology, University of Parma

2011-present Coordinator of the Ph.D program in Biochemistry and Molecular Biology, University of Parma

2011- present Member of the Interdipartimental Center Biopharmanet-tec and SITEIA.PARMA, University of Parma, co-funded by Emilia-Romagna

1999-present Founder and Chair with Proff. Donald Abraham and Glen E Kellogg, Institute for Structural Biology and Drug Discovery, VCU, Richmond, USA, of the course on “From structural biology/genomics to drug discovery”, held every other year.

2008 Chairman of the Symposium on “New Challenges in Protein Science: a Symposium in honor of Dr. William A. Eaton”, with the participation of 13 members of the National Academy of Sciences, USA, and Sir Alan Fersht, Parma.

2009 President of the XII International Symposium on Blood Substitutes, Parma.

2010 Member of the Scientific and Organizing Committee of the Symposium Proteine 2010, Parma.

2012 President of XVII Conference on “Oxygen Binding and Sensing Proteins”, Parma.

2013 Chair of the “Alexander Braunstein Memorial Symposium: Enzymes, cofactors, mechanisms”, 38th FEBS Congress, St. Petersburg, Russia.

2014 President of the IV International Cofactors and Coenzymes Meeting, Parma.

2001 - present Member of the Cofactors and Coenzymes Conference Board.

2007- present Member of the International Blood Substitutes Conference Board.

2007 - present Member of the Editorial Board of Current Medicinal Chemistry.

2008 - present Member of the Editorial Board of Biochimica et Biophysica Acta: Protein and Proteomics.

2008 Guest Editor for a Special issue of Biochimica et Biophysica Acta: Protein and Proteomics. on “Hemoglobin-based oxygen carriers as blood substitutes”

2010 Guest Editor for a Special issue of Biochimica et Biophysica Acta: Protein and Proteomics. on “Protein structure and function in the crystalline state: from x-ray crystallography to spectroscopy”.

2012 Guest Editor for a Special issue of Biochimica et Biophysica Acta: Protein and Proteomics. on “Oxygen binding and sensing proteins”

2003 and 2007 Member of the editorial board for Burger's Medicinal Chemistry VI and VII Edition.

Referee of international high impact factor journals for Biochemistry, Biophysics and Medicinal Chemistry.

Member of the Italian Society of Biochemistry and Molecular Biology, and member of the Protein Society (USA).

Member of National Institute of Biostructures and Biosystems

Member of the COST 2010-2014 "Farm animal proteomics" carrying out activities on meat muscle proteomics.

Member of the COST 2011-2015 "Saffronomics" carrying out activities on saffron proteomics.

Research support

1999-2004 Sub-contractor NIH grant on "Hemoglobin as prototype of allosteric proteins", with Prof. Arthur Arnone and Robert Noble.

2006 – 2010 Italian Ministry of University and Research, International Collaborative grants with Prof. Glen Kellogg, Virginia Commonwealth University, Richmond, Virginia, USA, and Prof. Paul F. Cook, University of Oklahoma, Norman, Oklahoma, USA, for the development of inhibitors of selected pyridoxal 5'-phosphate enzymes, that are drug targets, via complementary computational and experimental methods.

1999 – 2010 Italian Ministry of University and Research, PRIN for the determination of the structure, dynamics and catalytic mechanism of pyridoxal 5'-phosphate enzymes.

2003-2005 National Research Council, grant with Prof. Martino Bolognesi and other units for "Functional genomics: structural bases of the evolution and the protecting activity against host defense mechanisms of truncated hemoglobins expressed in unicellular organisms", acting as project coordinator in 2004-2005.

2004-2007 FP6 STREP on "Eurobloodsubstitutes" for the development of a hemoglobin-based oxygen carrier, acting as PI of a participating unit.

2006-2011 Cariparma Foundation grant for biotechnological approaches towards the development of hemoglobin-based oxygen carriers.

2010 University of Parma grant for the development of bioreactors and biosensors exploiting protein encapsulation in silica gels.

2012-2014 Cariplo Foundation grant with Prof. Maria Luisa Gelmi aimed at the development of an innovative user-friendly colorimetric biosensor based on aptamer functionalized nanomaterials for the detection of *Staphylococcus aureus* from different biological sources on the development of novel bacteria biosensors.

2010-2011 Research contract with BioChemfor within a EuroTransBio Project on the identification of novel enzyme substrates for fragrance development.

2009-present Research contracts with CHIESI Pharmaceuticals for expression, purification and biochemical characterization of surfactant proteins and their formulation.

2012 Research contract with the Massachusetts General Hospital, Harvard Medical School, Boston, for the identification of novel hemoglobin ligands.

Scientific activities

- Elucidation of structure-dynamics-function relationships of hemoglobins exploiting biochemical and biophysical methods, including single crystal polarized absorption microspectrophotometry and fast kinetic techniques, in solution, in silica gels and in the crystalline state. Main collaborations: Dr. William A. Eaton, NIH, Bethesda, USA; Prof. Cristiano Viappiani, University of Parma; Dr.

William Royer, University of Massachusetts, Worcester, USA; Prof. Paola Dominici, University of Verona.

- Characterization of the stability, catalytic mechanism and specificity of pyridoxal phosphate-dependent enzymes, including tryptophan synthase, *O*-acetylserine sulfhydrylase, tryptophanase, kynurenine aminotransferase and serine racemase. Main collaborations: Prof. Paul Cook, University of Oklahoma, Norman, USA; Prof. Robert Phillips, University of Georgia, Athens, USA; Dr. Edith Miles, NIH, Bethesda, USA; Dr. Tatyana Demidkina, Russian Academy of Sciences, Moscow, Russia; Prof. Menico Rizzi, University of Piemonte Orientale.
- Reactivity of glyceraldehyde-3-phosphate dehydrogenase with substrate in solution and in the crystalline state, and identification of inhibitors of the enzyme from *Plasmodium falciparum*. Main collaborations: Dr. Maria Vas, Hungarian Academy of Sciences, Budapest, Hungary; Prof. Carlo de Micheli, University of Milan.
- Investigation of the stability of green fluorescent proteins via single molecule experiments. Collaboration: Prof. Giuseppe Chirico, University of Milan.
- Development of therapeutic agents for hypo-oxygenation pathologies based on modified hemoglobins. Collaborations: Dr Warren Zapol, Massachusetts General Hospital, Harvard, USA; Dr. Chris Cooper, University of Essex, Colchester, UK; Prof. Andras Eke, Semmelweis University, Budapest, Hungary.
- *In silico* and *in vitro* screening of compounds aimed at regulating the activities of enzyme associated to neuropathologies and bacterial infection. Collaborations: Dr Pietro Cozzini, University of Parma; Prof. Gabriele Costantino, University of Parma.
- Exploitation of protein immobilization in silica gel to select distinct protein conformations, analyzed by spectroscopic methods, and for the development of bioreactors and biosensors.
- Application of computational methods for the evaluation of the interaction between protein and water molecules, ligands, proteins and DNA, and for the design of protein ligands. Collaborators: Drs. Donald Abraham and Glen Kellogg, Virginia Commonwealth University, Richmond, USA; Dr. Pietro Cozzini, University of Parma.
- Proteomic approaches for the analysis of food products and biological fluids. Collaborations: Prof. André de Almeida, University of Lisboa, Lisboa, Portugal; Prof. Jane Thomas-Oates, University of York, UK; Dr. Roberta Virgili, SSCIA, Parma; Drs. Silvia Catinella and Barbara Pioselli, Chiesi Pharmaceuticals.

Invited speakers to national and international conferences, and referee of national and international funding agencies.

Publication record

163

ISI/SCOPUS H_{index} 30

Sum of the times cited 3059

Average citation per publication 18.77

Publications (2007-2013)

Spyrakis F, Cozzini P, Bertoli C, Marabotti A, Abraham DJ, Kellogg GE, Mozzarelli A.
Energetics of the protein-DNA-water interaction
BMC Structural Biology, 2007, on-line

Baldini G, Cannone F, Chirico G, Collini M, Campanini B, Bettati S, Mozzarelli A.
Evidence of discrete substates and unfolding pathways in green fluorescent protein
Biophys. J., 2007, 92 1724-1731

Bruno S, Ronda L, Bettati S, Mozzarelli A.

Trapping hemoglobin in rigid matrices: fine tuning of oxygen binding properties by modulation of encapsulation protocols

Artificial Cells, Blood Substitutes & Biotechnology, 2007, 35, 69-79

Bruno S, Faggiano S, Spyrakis F, Mozzarelli A, Abbruzzetti S, Grandi E, Viappiani C, Feis A, Mackowiak S, Smulevich G, Cacciatori E, Dominici P

The Reactivity with CO of AHb1 and AHb2 from *Arabidopsis thaliana* is Controlled by the Distal HisE7 and Internal Hydrophobic Cavities.

J Am Chem Soc 2007, 129, 2880-2889

Amadasi A, Bertoldi M, Contestabile R, Bettati S, Cellini B, di Salvo ML, Borri Voltattorni C, Bossa F, Mozzarelli A.

Pyridoxal 5'-Phosphate Enzymes as Targets for Therapeutic Agents

Curr. Med Chem. 2007, 14, 1291-1324

Spyrakis F, Amadasi A, Fornabaio M, Abraham DJ, Mozzarelli A, Kellogg GE, Cozzini P.

Simple, Intuitive Calculations of Free Energy of Binding for Protein-Ligand Complexes. 4. Scoring Docked Ligand Conformations using Free Energy Correlations.

Eur. J. Med. Chem., 2007, 42, 921-933

Chattopadhyay A, Meier M; Ivaninskii S; Burkhard P; Speroni F; Campanini B; Bettati S, Mozzarelli A; Rabeh W, Li L. Cook PF

Structure, Mechanism and Conformational Dynamics of O-Acetylserine Sulphydrylase from *Salmonella typhimurium*: Comparison of A and B Isozymes

Biochemistry 2007, 46, 8315-8330

Iaboli L, Zerbini A, Bruno S, Bettati S, Rossi U, Mozzarelli A

Il sangue artificiale: la ricerca del Sacro Graal?

Novità in Urgenza, Bollettino Scientifico della Società Italiana di Medicina d'Emergenza-Urgenza, CG Edizioni Medico Scientifiche, 2007, 67, 12-22.

Ronda L, Faggiano S, Bettati S, Hellmann N, Decker H, Weidenbach T, Mozzarelli A.

Hemocyanin from *E. californicum* encapsulated in silica gels: oxygen binding and conformational states

Gene, 2007, 398, 202-207

Bruno S, Faggiano S, Spyrakis F, Mozzarelli A, Cacciatori E, Dominici P, Grandi E, Abbruzzetti S, Viappiani C.

Different roles of protein dynamics and ligand migration in non-symbiotic hemoglobins AHb1 and AHb2 from *Arabidopsis thaliana*

Gene, 2007, 398, 224-233

Eaton WA, Henry ER, Hofrichter J, Bettati S, Viappiani C, Mozzarelli A.

Evolution of Allosteric Models for Hemoglobin.

IUMB Life. 2007, 59, 586-599

Cannone F, Collini M, Chirico G, Baldini G, Bettati S, Campanini B, Mozzarelli A.

Environmental effects on the oscillatory unfolding kinetics of GFP

Eur. Biophys. J. 2007, 36, 795-803

Ronda L, Pioselli B, Bruno S, Micaella C, Bettati S, Mozzarelli A.

Biocatalysis in a confined environment: lessons from enzymes immobilized in wet, nanoporous silica gels

Chemistry-Today, 2007, 25, 10-15

Abbruzzetti S, Grandi E, Bruno S, Faggiano S, Spyrakis F, Mozzarelli A, Cacciatori E, Dominici P, Viappiani C.

Ligand migration in non-symbiotic hemoglobin AHb1 from *Arabidopsis thaliana*

J.Phys. Chem. B 2007, 111, 12582-12590

Raboni S, Mozzarelli A, Cook PF.

Control of ionizable residues in the catalytic mechanism of tryptophan synthase from *Salmonella typhimurium*

Biochemistry, 2007, 46, 13223-13234

Tripathi A, Fornabaio M, Spyrakis F, Mozzarelli A, Cozzini P, Kellogg GE

Complexity in Modeling and Understanding Protonation States: Computational Titration of HIV-1 Protease Inhibitor Complexes.

Chemistry and Biodiversity, 2007, 4, 2564-2577

Amadasi A, Surface JA, Spyrakis F, Cozzini P, Mozzarelli A, Kellogg GE

Robust classification of “relevant” water molecules in putative protein binding sites

J. Med. Chem. 2008, 51, 1063-1067

Ronda L, Bruno S, Faggiano S, Bettati S, Mozzarelli A.

Oxygen binding to haem proteins in solution, encapsulated in silica gels and in the crystalline state

Methods Enzymol. 2008, 437B, 309-326

Abbruzzetti S, Bruno S, Faggiano S, Ronda L, Grandi E, Mozzarelli A, Viappiani C

Characterization of ligand migration mechanisms inside haemoglobins from the analysis of geminate rebinding kinetics

Methods Enzymol. 2008, 437B, 327-342

Portoro I, Kocsis L, Herman P, Caccia D, Perrella M, Ronda L, Bruno S, Bettati S, Micalella C, Mozzarelli A, Varga A, Vas M, Lowe KC, Eke A.

Towards a novel haemoglobin-based oxygen carrier: Euro-PEG-Hb, physico-chemical properties, vasoactivity and renal filtration

Biochim. Biophys. Acta. 2008, 1784, 1402–1409

Mozzarelli A. Hemoglobin-based oxygen carriers as blood substitutes, Biochim. Biophys. Acta. 2008, 1784, 1363-1364

Marabotti A, Spyrakis F, Facchiano A, Cozzini P, Alberti S, Kellogg GE, Mozzarelli A.

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J. Compt. Chem. 2008, 29, 1955-1969

Moniot S, Bruno S, Vornrhein C, Didierjean C, Boschi-Muller S, Vas M, Bricogne G, Branlant G, Mozzarelli A, Corbier C.

Trapping of the thioacyl-glyceraldehyde-3-phosphate dehydrogenase intermediate from *Bacillus stearothermophilus*: direct evidence for a flip-flop mechanism.

J. Biol. Chem. 2008, 283, 21693-21702.

Ronda L, Abbruzzetti S, Bruno S, Bettati S, Mozzarelli A, Viappiani C.
Ligand-induced tertiary relaxations during the T-to-R quaternary transition in hemoglobin
J. Phys. Chem. B 2008, 112, 12790-12794

Amadasi A, Mozzarelli A, Meda C, Maggi A, Cozzini P.
Identification of xenoestrogens in food additives by an integrated *in silico* and *in vitro* approach.
Chemical Research in Toxicology, 2009, 22, 52-63

Raboni S, Bettati S, Mozzarelli A.
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Cellular and Molecular Life Science, 2009, 66, 2391- 2403

Caccia D, Ronda L, Frassi R, Perrella M, Del Favero E, Bruno S, Pioselli B, Abbruzzetti S,
Viappiani C, Mozzarelli A.
PEGylation promotes hemoglobin tetramer dissociation
Bioconjug. Chem. 2009, 20, 1356-66.

Bettati S, Viappiani C, Mozzarelli A.
Hemoglobin: an “evergreen” red protein
Biochim. Biophys. Acta, 2009, 1794, 1317–1324.

Singh R, Mozzarelli A
Cofactor Chemogenomics in “Chemogenomics Methods and Applications” Jacoby E. (Ed.)
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Jacoby E, Mozzarelli A.
Chemogenomic Strategies to Expand the Bioactive Chemical Space.
Curr. Med. Chem. 2009, 16, 4374-4381

Abbruzzetti S, Faggiano S, Bruno S, Spyrakis F, Mozzarelli A, Dewilde S, Moens L, Viappiani C.
Ligand migration through the internal hydrophobic cavities in human neuroglobin
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Faggiano S, Abbruzzetti S, Spyrakis F, Grandi E, Viappiani C, Bruno S, Mozzarelli A, Cozzini P,
Astegno A, Dominici P, Brogioni S, Feis A, Smulevich G, Carrillo O, Schmidtke P, Bidon CA,
Luque FJ.
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Non-Symbiotic Hemoglobin AHb1 from *Arabidopsis thaliana*.
J. Phys. Chem. B. 2009, 113, 16028–16038

Salsi E, Bayden A, Spyrakis F, Amadasi A, Campanini B, Bettati S, Cozzini P, Kellogg GE,
Cook PF, Dodatko T, Roderick SL, Mozzarelli A.
Design of *O*-acetylserine sulfhydrylase inhibitors by mimicking Nature
J. Med Chem. 2010, 53, 345-356

Raboni S, Contestabile R, Spyrakis F, Campanini B, Amadasi A, Bettati S, Peracchi A, Mozzarelli
A.
Pyridoxal 5'-Phosphate-Dependent Enzymes: Catalysis, Conformation and Genomics
Comprehensive Natural Products II Chemistry and Biology; Mander, L., Lui, H.-W, Eds., Elsevier:
Oxford, 2010; Vol. 7, pp 253-350.

Salsi E, Campanini B, Bettati S, Raboni S, Roderick S, Cook PF, Mozzarelli A.
A two-step process controls the formation of the bienzyme cysteine synthase complex
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Mozzarelli A, Ronda L, Faggiano S, Bettati S, Bruno S.
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Faggiano S, Bruno S, Ronda L, Jankevics H, Mozzarelli A.
Polymerized and PEG-conjugated hemoglobins: a globin-based calibration curve for dynamic light scattering analysis
Anal. Biochem., 2010, 401, 266–270

Tian H, Guan R, Salsi E, Campanini B, Bettati S, Kumar VP, Karsten WE, Mozzarelli A, Cook PF.
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Bruno S, Ronda L, Faggiano S, Bettati S, Mozzarelli A
Oxygen delivery via allosteric effectors of haemoglobin and blood substitutes
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Ronda L, Pioselli B, Bruno S, Faggiano S, Mozzarelli A.
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Anal. Biochem. 2011, 408, 118-123.

Faggiano S, Bruno S, Ronda L, Pizzonia P, Pioselli B, Mozzarelli A (2011). Modulation of expression and polymerization of hemoglobin Polytaur, a potential blood substitute.
Arch. Biochem. Biophys. 2011, 505, 42-47.

Salsi E., Campanini B, Bettati S, Guan R, Cook PF, Mozzarelli A.
Exploring *O*-acetylserine sulfhydrylase-B isoenzyme from *Salmonella typhimurium* by fluorescence spectroscopy
Arch. Biochem. Biophys. 2011, 505, 178-185

Spyrakakis F, Faggiano S, Abbruzzetti S, Dominici P, Cacciatori E, Astegno A, Droghetti E, Feis A, Smulevich G, Bruno S, Mozzarelli A, Cozzini P, Viappiani C, Bidon CA, Luque FJ.
Histidine E7 Dynamics Modulates Ligand Exchange between Distal Pocket and Solvent in AHb1 from *Arabidopsis thaliana*
J. Phys. Chem. B 2011, 115, 4138-4146

Pearson A, Mozzarelli A.
X-ray crystallography marries spectroscopy to unveil structure and function of biological macromolecules
Biochim. Biophys. Acta 2011, 1814, 731-733

Ronda L, Bruno S, Bettati S, Mozzarelli A.
Protein crystal microspectrophotometry

Biochim. Biophys. Acta 2011, 1814, 734-741

Ronda L, Bazhulina NP, Morozova EA, Revtovich SV, Chekhov VO, Nikulin AD, Demidkina TV, Mozzarelli A.

Exploring methionine gamma-lyase structure-function relationship via microspectrophotometry and X-ray crystallography.

Biochim Biophys Acta. 2011, 1814, 834-842

Spyrakakis F, Bruno S, Bidon-Chanal A, Luque FJ, Abbruzzetti S, Viappiani C, Dominici P, Mozzarelli A.

Oxygen binding to *Arabidopsis thaliana* AHb2 nonsymbiotic hemoglobin: evidence for a role in oxygen transport.

IUBMB Life 2011, 63, 355-62

Passera E, Campanini B, Rossi F, Casazza V, Rizzi M, Pellicciari R, Mozzarelli A.

Human kynurenine aminotransferase II: reactivity with substrates and inhibitors

FEBS J. 2011, 278, 1882-1900

Peracchi A, Mozzarelli A

Exploring and exploiting allostery: Models, evolution, and drug targeting

Biochim. Biophys. Acta - Proteins and Proteomics, 2011, 1814, 922-933

Bisht NK, Abbruzzetti S, Uppal S, Bruno S, Spyrakakis F, Mozzarelli A, Viappiani C, Kundu S.

Ligand migration and hexacoordination in type 1 non symbiotic rice hemoglobin

Biochim. Biophys. Acta - Proteins and Proteomics, 2011, 1814, 1042-1053

Pioselli B, Paredi G, Mozzarelli A.

Proteomic analysis of pork meat in the production of cooked ham

Molecular BioSystems, 2011, 7, 2252-2260

Bruno S, Ronda L, Abbruzzetti S, Viappiani C, Bettati S, Maji S, Mozzarelli A.

Protein encapsulation, conformations, and nanobiotools.

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Mozzarelli A., Bettati S. Eds.

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Kim HW, Mozzarelli A, Sakai H, Jahr J.

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"Chemistry and biochemistry of oxygen therapeutics: from transfusion to artificial blood", Mozzarelli A., Bettati S. Eds. John Wiley and Sons Ltd, Chichester, UK, 2011, 413-428

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Bound Water at Protein-Protein Interfaces: Partners, Roles and Hydrophobic Bubbles as a Conserved Motif.

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The multifaceted pyridoxal 5'-phosphate-dependent *O*-acetylserine sulfhydrylase
Biochem. Biophys. Acta - Proteins and Proteomics, 2011, 1814, 1497–1510

Conti P, Tamborini L, Pinto A, Blondel A, Minoprio P, Mozzarelli A, De Micheli C.

Drug Discovery Targeting Amino Acid Racemases

Chem. Rev. 2011, 111, 6919-6946, **IF 33**

Oxygen and nitric oxide rebinding kinetics in nonsymbiotic hemoglobin AHB1 from *Arabidopsis thaliana*.

Abbruzzetti S, Faggiano S, Spyrakis F, Bruno S, Mozzarelli A, Astegno A, Dominici P, Viappiani C.

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Low affinity PEGylated hemoglobin from *Trematomus bernacchii*, a model for hemoglobin-based blood substitutes

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"Muscle to meat" molecular events and technological transformations: the proteomics insight

J. Proteomics, 2012, 75, 4275-4289

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Design and synthesis of *trans*-2-substituted-cyclopropane-1-carboxylic acids as the first non-natural small molecule inhibitors of *O*-acetylserine sulfhydrylase

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Fine tuning of the active site modulates specificity in the interaction of *O*-acetylserine sulfhydrylase isozymes with serine acetyltransferase

BBA - Proteins and Proteomics, 2013, 1834, 169–181

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PlosOne, on line

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J Enzyme Inhib Med Chem. 2011 in press

Patents

Italian patent: TO2009A000082 deposited: 09/02/2009

Catechol 1,2 dioxygenase encapsulated in silica gels, procedure of encapsulation, and exploitation for bioremediation of materials polluted with catechols and derivatives

European patent: n. 12002678.6. data di deposito 17/04/2012

Method for the expression of surfactant peptides

Italian patent: MI2012A001636 deposited 01/10/2012

Method for the determination of alpha-amylase activity in hemolytic samples.