



UNIVERSITY OF PADOVA
DEPARTMENT OF PHARMACEUTICAL AND
PHARMACOLOGICAL SCIENCES

CURRICULUM VITAE ET STUDIORUM

Stefano Moro

Padova, 2018

CURRICULUM VITAE

Stefano Moro is the principal investigator of the Molecular Modeling Section (MMS) at the Department of Pharmaceutical and Pharmacological Sciences. In 2010 he was appointed as Full Professor in Medicinal Chemistry of the University of Padova, Italy. The Molecular Modeling Section (MMS) constitutes the interface among biological/pharmacological and chemical laboratories in our Department, adding its computational expertise as needed in organic synthesis, phytochemistry, biochemistry, molecular biology and pharmacology. In the spirit of the motto "interdisciplinarity is dialog" the aim of the MMS is to face medicinal chemistry and medical problems in collaboration with experts of the field... not mixing our expertises, but summing them up.

BIOGRAPHICAL DATA

Family Name **MORO**
First Name **STEFANO**
Title: **Professor of Medicinal Chemistry**
Place of Birth Treviso (Italy)
Date of Birth February, 05 1965
Citizenship Italian
Family Status Married, two children (Emma and Greta: June 10 1999)



Private Address Via Pullè 55/8
 35100 Padova, ITALY
 phone: +39-049714706

Business Address Molecular Modeling Section (MMS)
 Department of Pharmaceutical and Pharmacological Sciences
 University of Padova
 phone: +39-049-8275704
 fax: +39-049-8275366
 e-mail: stefano.moro@unipd.it
 Webpage URL <http://mms.dsfarm.unipd.it>



QR code:

EDUCATION

November '11 – Today:

Professor of Medicinal Chemistry at the Dept. of Pharmaceutical Sciences, University of Padova (Italy).
Chief of the Molecular Modeling Section (MMS).
Subject: computational medicinal chemistry.

March '06 – October '11:

Associate Professor of Medicinal Chemistry at the Dept. of Pharmaceutical Sciences, University of Padova (Italy).
Chief of the Molecular Modeling Section (MMS).
Subject: computational medicinal chemistry.

January '99 – February '06:

Assistant Professor of Medicinal Chemistry at the Dept. of Pharmaceutical Sciences, University of Padova (Italy).
Principal Investigator of the Molecular Modeling Section (MMS).
Subject: computational medicinal chemistry.

June '02 – November '02: Visiting Professor of Medicinal Chemistry at the Department of Applied BioSciences Institute of Pharmaceutical Chemistry, ETH Zurich (Switzerland).

January '97 – December '98: Post-doctoral research fellow at the Molecular Recognition Section (Laboratory of Bioorganic Chemistry), National Institutes of Diabetes, Digestive and Kidney Diseases (NIDDK), National Institutes of Health (NIH) in Bethesda (USA).
Supervisor: Dr. Kenneth A. Jacobson.
Subject: computational medicinal chemistry.
3D-structure of adenosine and ATP receptors and design of new agonists and antagonists using computer-aided modeling methodologies.

- October '95 - January '97:* "Centro Nazionale delle Ricerche C.N.R." Fellow.
University of Padova (Italy).
Supervisors: Prof. Giorgio Modena
Subject: A mechanistic investigation of bromoperoxidases mimicking system. Evidence of a hypobromite-like vanadium intermediate from experimental data and ab-initio calculations.
- October '92 - October '95:* Ph.D. in Physical Organic Chemistry.
Dept. of Organic Chemistry, University of Padova (Italy).
Supervisor: Prof. Fulvio Di Furia.
Experimental Thesis title: "The chemistry of peroxovanadium complexes: structural aspects, oxidative reactivity and biological implications".
Thesis research: A. Biomimetic vanadium catalyzed oxidations with hydrogen peroxide. Influence of coordination sphere; B. Peroxo vanadium complexes in aqueous solutions. Structure-reactivity relationships by using ⁵¹V-NMR; C. Structure-reactivity relationships of peroxovanadium complexes: ab initio calculations.
- October '91-September '92:* Military service in the Italian Army.
- March-September 1991:* Research fellow in Physical Organic Chemistry at the Dept. of Organic Chemistry, University of Padova (Italy).
Supervisor: Prof. Fulvio Di Furia
During this time the original thesis research project was expanded and completed.
- March 1991* Degree *cum Laude* in Chemistry and Pharmaceutical Technology at the University of Padova (Italy).
Supervisor: Prof. Fulvio Di Furia.
Experimental Thesis title: "Hydroxylation of aromatic substrate by peroxovanadium complexes".
Subject: physical organic chemistry and reaction mechanisms.
- July 1984:* High school certificate *with honors* in Chemistry at the Istituto Tecnico Industriale "G. Natta", Padova (Italy)

TEACHING ACTIVITY

2000 –2007: Lecturer of "Bioinformatics" for undergraduate students In Medical Biotechnology at the School of Medicine - University of Padova.

2000 –2009: Lecturer of "Chemoinformatics" for undergraduate students at the School of Pharmacy of the University of Padova.

1998 - present: Lecturer of "Advance Methodology in Medicinal Chemistry" for undergraduate students at the School of Pharmacy of the University of Padova.

1999 - present: Lecturer of "Advance Course in Molecular Modeling", PhD School at the Pharmaceutical Sciences and Chemistry Departments - University of Padova.

2009 –present: Lecturer of "Pharmaceutical Chemistry – Part 2" for undergraduate students at the School of Pharmacy of the University of Padova.

RESEARCH FIELDS AND EXPERIENCE:

1. Molecular Modeling and Quantitative Structure-Activity Relationships;
2. Integrated Structure-Based Drug Design (SBDD) and Ligand-Based Drug Design (LBDD) approaches;
3. Chemoinformatics;
4. Computational Toxicology;
5. Quantum enzymology;
6. Organic Synthesis;
7. Bioinorganic Chemistry;
8. NMR Spectroscopy;

9. Instrumental Analytic;
10. Enzymology.

HONORS AND AWARDS:

1. *September 2002: Farmindustria Italian National Award for Research Excellence in Medicinal Chemistry.*
2. *May 2000: Federchimica Italian National Award for Research Excellence in Chemistry.*
3. *March 2000: University of Padova Award for Research Excellence in Chemistry.*
4. *January 1998: N.I.H. Fellow Award for Research Excellence, National Institutes of Health (NIH), National Institutes of Diabetes, Digestive and Kidney Diseases (NIDDK), Bethesda (USA).*
5. *October 1993: "IBM Italian Foundation" National Award in "Computational Technology in Chemistry" (Italy).*
6. *March 1991: Federchimica National Award, for the thesis work "Hydroxylation of aromatic substrate by peroxovanadium complexes", University of Padova (Italy).*

COVER STORIES:

1. Journal Medicinal Chemistry, June 1999;
2. Chemical and Engineering News February, 2001;
3. Chemical Communications, December 2003;
4. Medicinal Research Reviews, January 2006;
5. New Journal of Chemistry, March 2006;

6. Current Medicinal Chemistry, May 2006;
7. Current Pharmaceutical Design, June 2007;
8. Medicinal Research Reviews, October 2009;
9. Current Pharmaceutical Design, December 2009;
10. Medicinal Research Reviews, October 2010;
11. ChemMedChem, September 2011;
12. ChemMedChem, December 2011.
13. Structure, April 2017.
14. ChemMedChem, April 2018
15. Molecular Informatics, August 2018

BIBLIOMETRIC INDEXES:

n. publications: 254
total citations: 8136
h-index: 51

source Scopus (26/07/2018):

<https://www.scopus.com/authid/detail.uri?authorId=7004482135>

LIST OF PUBLICATIONS

254. Deganutti G, Salmaso V, **Moro S.** "Could Adenosine Recognize its Receptors with a Stoichiometry Other than 1 : 1?" Mol Inf (2018) in press
253. Salmaso V, Sturlese M, Cuzzolin A, **Moro S.** "Combining self- and cross-docking as benchmark tools: the performance of DockBench in the D3R Grand Challenge 2" J Comput Aided Mol Des. J Comput Aided Mol Des. 32, 251-264 (2018)
252. Cuzzolin A, Deganutti G, Salmaso V, Sturlese M, **Moro S.** "AquaMMapS: an alternative tool to monitor the role of water molecules during protein-ligand association." ChemMedChem ChemMedChem. 1, 1-13 (2018)

251. Bortolozzi R, Mattiuzzo E, Dal Pra M, Sturlese M, **Moro S**, Hamel E, Carta D, Viola G, Ferlin MG. "Targeting tubulin polymerization by novel 7-aryl-pyrroloquinolinones: Synthesis, biological activity and SARs." *Eur J Med Chem.* 1, 244-258 (2018)
250. Bertini S, Ghilardi E, Asso V, Minutolo F, Rapposelli S, Digiacomo M, Saccomanni G, Salmaso V, Sturlese M, **Moro S**, Macchia M, Manera C. "Sulfonamido-derivatives of unsubstituted carbazoles as BACE1 inhibitors." *Bioorg Med Chem Lett.* 27, 4812-4816 (2017)
249. Malvacio I, Cuzzolin A, Sturlese M, Vera DMA, Moyano EL, **Moro S**. "Synthesis and preliminary structure-activity relationship study of 2-aryl-2H-pyrazolo[4,3-c]quinolin-3-ones as potential checkpoint kinase 1 (Chk1) inhibitors." *J Enzyme Inhib Med Chem.* 33, 171-183 (2017)
248. Deganutti G, Welihinda A, Moro S. "Comparison of the Human A_{2A} Adenosine Receptor Recognition by Adenosine and Inosine: New Insight from Supervised Molecular Dynamics Simulations." *ChemMedChem.*12, 1319-1326 (2017)
247. Deganutti G, **Moro S**. "Supporting the Identification of Novel Fragment-Based Positive Allosteric Modulators Using a Supervised Molecular Dynamics Approach: A Retrospective Analysis Considering the Human A_{2A} Adenosine Receptor as a Key Example." *Molecules* 22, 818 (2017)
246. Sissi C, Dovigo L, Greco ML, Ciancetta A, **Moro S**, Trzciński JW, Mancin F, Rossi P, Spalluto G, Tecilla P "Conjugates between minor groove binders and Zn(II)-tach complexes: Synthesis, characterization, and interaction with plasmid DNA" *Tetrahedron.* 73, 3014-3024 (2017).
245. Deganutti G, **Moro S**. "Estimation of kinetic and thermodynamic ligand-binding parameters using computational strategies." *Future Med Chem.* 9, 507-523 (2017)
244. Salmaso V, Sturlese M, Cuzzolin A, **Moro S**. "Exploring Protein-Peptide Recognition Pathways Using a Supervised Molecular Dynamics Approach." *Structure* 25, 655-662 (2017)
243. Zusso M, Mercanti G, Belluti F, Di Martino RM, Pagetta A, Marinelli C, Brun P, Ragazzi E, Lo R, Stifani S, Giusti P, **Moro S**. "Phenolic 1,3-diketones attenuate lipopolysaccharide-induced inflammatory response by an alternative magnesium-mediated mechanism." *Br J Pharmacol.* 174, 1090-1103 (2017)

242. Squarcialupi L, Betti M, Catarzi D, Varano F, Falsini M, Ravani A, Pasquini S, Vincenzi F, Salmaso V, Sturlese M, Varani K, **Moro S**, Colotta V. "The role of 5-arylalkylamino- and 5-piperazino- moieties on the 7-aminopyrazolo[4,3-d]pyrimidine core in affecting adenosine A₁ and A_{2A} receptor affinity and selectivity profiles." *J Enzyme Inhib Med Chem.* 32, 248-263 (2017).
241. Vila N, Besada P, Viña D, Sturlese M, **Moro S**, Terán C. "Synthesis, biological evaluation and molecular modeling studies of phthalazin-1(2*H*)-one derivatives as novel cholinesterase inhibitors." *6*, 46170-46185 (2016)
240. Carta D, Bortolozzi R, Sturlese M, Salmaso V, Hamel E, Basso G, Calderan L, Quintieri L, **Moro S**, Viola G, Ferlin MG. "Synthesis, structure-activity relationships and biological evaluation of 7-phenyl-pyrroloquinolinone 3-amide derivatives as potent antimetabolic agents.." *Eur J Med Chem.* 127, 643-660 (2017)
239. Salmaso V, Sturlese M, Cuzzolin A, **Moro S**. "DockBench as docking selector tool: the lesson learned from D3R Grand Challenge 2015." *J Comput Aided Mol Des.* 30, 773-789 (2016)
238. Ciancetta A, Cuzzolin A, Deganutti G, Sturlese M, Salmaso V, Cristiani A, Sabbadin D, **Moro S**. "New Trends in Inspecting GPCR-ligand Recognition Process: the Contribution of the Molecular Modeling Section (MMS) at the University of Padova." *Mol Inform.* 35, 440-448 (2016).
237. **Moro S**, Sturlese M, Ciancetta A, Floris M. "In Silico 3D Modeling of Binding Activities." *Methods Mol Biol.* 1425, 23-35 (2016).
236. Redenti S, Ciancetta A, Pastorin G, Cacciari B, **Moro S**, Spalluto G, Federico S. "Pyrazolo[4,3-*e*][1,2,4]triazolo[1,5-*c*]pyrimidines and Structurally Simplified Analogs. Chemistry and SAR Profile as Adenosine Receptor Antagonists." *Curr Top Med Chem.* (2016)
235. Cuzzolin A, Sturlese M, Deganutti G, Salmaso V, Sabbadin D, Ciancetta A, **Moro S**. "Deciphering the Complexity of Ligand-protein Recognition Pathways using Supervised Molecular Dynamics (SuMD) Simulations." *J Chem Inf Model* 56, 687-705 (2016)
234. Federico S, Ciancetta A, Porta N, Redenti S, Pastorin G, Cacciari B, Klotz KN, **Moro S**, Spalluto G. "5,7-Disubstituted-[1,2,4]triazolo[1,5-*a*][1,3,5]triazines as pharmacological tools to explore the antagonist selectivity profiles toward adenosine receptors." *Eur J Med Chem.* 108:529-41 (2016).
233. Squarcialupi L, Catarzi D, Varano F, Betti M, Falsini M, Vincenzi F, Ravani A, Ciancetta A, Varani K, **Moro S**, Colotta V. "Structural refinement of pyrazolo[4,3-

d]pyrimidine derivatives to obtain highly potent and selective antagonists for the human A₃ adenosine receptor." *Eur J Med Chem.* 108, 117-133 (2016)

232. Federico S, Ciancetta A, Porta N, Redenti S, Pastorin G, Cacciari B, Klotz KN, **Moro S**, Spalluto G. "5,7-Disubstituted-[1,2,4]triazolo[1,5-a][1,3,5]triazines as pharmacological tools to explore the antagonist selectivity profiles toward adenosine receptors." *Eur J Med Chem.* 108, 529-541 (2015).

231. Squarcialupi L, Catarzi D, Varano F, Betti M, Falsini M, Vincenzi F, Ravani A, Ciancetta A, Varani K, **Moro S**, Colotta V. "Structural refinement of pyrazolo[4,3-d]pyrimidine derivatives to obtain highly potent and selective antagonists for the human A₃ adenosine receptor." *Eur J Med Chem.* 108, 117-133 (2015)

230. Ciancetta A, Sabbadin D, Federico S, Spalluto G, **Moro S**. "Advances in Computational Techniques to Study GPCR-Ligand Recognition." *Trends Pharmacol Sci.*(2015) doi: 10.1016/j.tips.2015.08.006.

229. Federico S, Redenti S, Sturlese M, Ciancetta A, Kachler S, Klotz KN, Cacciari B, **Moro S**, Spalluto G. "The Influence of the 1-(3-Trifluoromethyl-Benzyl)-1H-Pyrazole-4-yl Moiety on the Adenosine Receptors Affinity Profile of Pyrazolo[4,3-e][1,2,4]Triazolo[1,5-c]Pyrimidine Derivatives." *PLoS One* 10(12):e0143504 (2015)

228. Carta D, Bortolozzi R, Hamel E, Basso G, Moro S, Viola G, Ferlin MG. "Novel 3-substituted 7-Phenylpyrrolo[3,2-f]quinolin-9(6H)-ones as Single Entities with Multitarget Antiproliferative Activity." *J Med Chem* 58, 7991-8010 (2015)

227. Paoletta S, Sabbadin D, von Kügelgen I, Hinz S, Katritch V, Hoffmann K, Abdelrahman A, Straßburger J, Baqi Y, Zhao Q, Stevens RC, Moro S, Müller CE, Jacobson KA. "Modeling ligand recognition at the P2Y₁₂ receptor in light of X-ray structural information." *J Comput Aided Mol Des.* 29, 737-756 (2015)

226. Sturlese M, Bellanda M. **Moro S**. "NMR-Assisted Molecular Docking Methodologies" *Mol Inf.* 34, 513–525 (2015)

225. Cuzzolin A, Sturlese M, Malvacio I, Ciancetta A, **Moro S**. "DockBench: an integrate informatics platform bridging the gap between the robust validation of docking protocols and virtual screening simulations." *Molecules* 20, 9977-9993 (2015).

224. Sabbadin D, Ciancetta A, Deganutti G, Cuzzolin A, Moro S. "Exploring the recognition pathway at the human A_{2A} adenosine receptor of the endogenous

agonist adenosine using supervised molecular dynamics simulations." *MedChemComm* 6, 1081-1085 (2015)

223. Lovisa F, Cozza G, Cristiani A, Cuzzolin A, Albiero A, Mussolin L, Pillon M, **Moro S**, Basso G, Rosolen A, Bonvini P. "ALK Kinase Domain Mutations in Primary Anaplastic Large Cell Lymphoma: Consequences on NPM-ALK Activity and Sensitivity to Tyrosine Kinase Inhibitors." *PLoS One* 10, e0121378 (2015)

222. Deganutti G, Cuzzolin A, Ciancetta A, **Moro S**. "Understanding allosteric interactions in G protein-coupled receptors using Supervised Molecular Dynamics: a prototype study analysing the human A3 adenosine receptor positive allosteric modulator LUF6000". *Biorg Med Chem.* 23, 4065-4071 (2015)

221. Sissi C, **Moro S**, M Crothers D. "Novel Insights on the Dna Interaction of Calicheamicin gamma1. *Biopolymers* 103, 449-459 (2015).

220. Moschetti I, Faoro F, **Moro S**, Sabbadin D, Sella L, Favaron F, D'ovidio R. "The Xylanase Inhibitor Taxi-Iii Counteracts The Necrotic Activity of A *Fusarium Graminearum* Xylanase in Vitro and in Durum Wheat Transgenic Plants." *Mol Plant Pathol.* 16, 583-592 (2014).

219. Sabbadin D, Ciancetta A, **Moro S**. "Perturbation of fluid dynamics properties of water molecules during GPCR-ligand recognition: the human A2A adenosine receptor as a key study." *J Chem Inf Model*. 54, 2846-2855 (2014)
218. Kufareva I, Katritch V; Participants of GPCR Dock 2013, Stevens RC, Abagyan R. "Advances in GPCR Modeling Evaluated by the GPCR Dock 2013 Assessment: Meeting New Challenges." *Structure*. 22, 1120-1139 (2014)
217. Squarcialupi L, Colotta V, Catarzi D, Varano F, Betti M, Varani K, Vincenzi F, Borea PA, Porta N, Ciancetta A, **Moro S**. "7-Amino-2-phenylpyrazolo[4,3-d]pyrimidine derivatives: Structural investigations at the 5-position to target human A1 and A2A adenosine receptors. Molecular modeling and pharmacological studies." *Eur J Med Chem*. (2014) in press
216. Ciancetta A, Cuzzolin A, **Moro S**. "Alternative Quality Assessment Strategy to Compare Performances of GPCR-Ligand Docking Protocols: The Human Adenosine A2A Receptor as a Case Study." *J Chem Inf Model*. 54, 2243-2254 (2014)
215. Masiero A, Aufiero S, Minervini G, **Moro S**, Costa R, Tosatto SC. "Evaluation of the steric impact of flavin adenine dinucleotide in *Drosophila melanogaster* cryptochrome function." *Biochem Biophys Res Commun*. 450, 1606-1611 (2014)
214. Federico S, Ciancetta A, Porta N, Redenti S, Pastorin G, Cacciari B, Klotz KN, **Moro S**, Spalluto G. "Scaffold Decoration at Positions 5 and 8 of 1,2,4-Triazolo[1,5-c]Pyrimidines to Explore the Antagonist Profiling on Adenosine Receptors: A Preliminary SAR Study." *J Med Chem*. 57, 6210-6215 (2014)
213. Cristiani A, Maset F, De Toni L, Guidolin D, Sabbadin D, Strapazon G, **Moro S**, De Filippis V, Foresta C. "Carboxylation-dependent conformational changes of human osteocalcin." *Front Biosci (Landmark Ed)*. 19, 1105-16 (2014)
212. Cristiani A, Vettore S, Sambado L, Bulfone A, **Moro S**, Girolami A. "Conformational Changes of Congenital FVII Variants with Defective Binding to Tissue Factor ARG304GLN (FVII Padua), ARG 304TRP (FVII Nagoya) and ARG79GLN (FVII Shinjo or Tondabayashi)." *Int J Biomed Sci*. 9(4):185-93, (2014)
211. Frezzato F, Trimarco V, Martini V, Gattazzo C, Ave E, Visentin A, Cabrelle A, Olivieri V, Zambello R, Facco M, Zonta F, Cristiani A, Brunati AM, **Moro S**, Semenzato G, Trentin L. "Leukaemic cells from chronic lymphocytic leukaemia patients undergo apoptosis following microtubule depolymerization and Lyn inhibition by nocodazole." *Br J Haematol*. 165(5):659-72, (2014).

210. Sabbadin D, **Moro S.** "Supervised Molecular Dynamics (SuMD) as a helpful tool to depict GPCR-ligand recognition pathway in a nanosecond time scale." *J Chem Inf Model* 54, 372-376 (2014)
209. Sabbadin D, Ciancetta A, **Moro S.** "Bridging molecular docking to membrane molecular dynamics to investigate GPCR-ligand recognition: the human A2A adenosine receptor as a key study." *J Chem Inf Model* 54, 169-183 (2014)
208. Barollo S, Pezzani R, Cristiani A, Redaelli M, Zambonin L, Rubin B, Bertazza L, Zane M, Mucignat-Caretta C, Bulfone A, Pennelli G, Casal Ide E, Pelizzo MR, Mantero F, **Moro S,** Mian C. "The prevalence, the tumorigenic role and the biochemical implications of rare BRAF alterations." *Thyroid* 24(5):809-19, (2014)
207. Floris M, Sabbadin D, Ciancetta A, Medda R, Cuzzolin A, **Moro S.** "Implementing the "Best Template Searching" tool into Adenosiland platform." *In Silico Pharmacology* 1, 1-25 (2013)
206. Ferlin MG, Carta D, Bortolozzi R, Ghodsi R, Chimento A, Pezzi V, **Moro S,** Hanke N, Hartmann RW, Basso G, Viola G."Design, synthesis and SARs of azolymethyl-pyrroloquinolines as non steroidal aromatase inhibitors." *J Med Chem.* 56, 7536-7551 (2013)
205. Barollo S, Pezzani R, Cristiani A, Bertazza L, Rubin B, Bulfone A, Pelizzo MR, Torresan F, Mantero F, Pennelli G, **Moro S,** Mian C."Functional Significance of the Novel H-RAS Gene Mutation M72I in a Patient with Medullary Thyroid Cancer." *Exp Clin Endocrinol Diabetes.* 121, 546-550 (2013)
204. Raffaello A, De Stefani D, Sabbadin D, Teardo E, Merli G, Picard A, Checchetto V, **Moro S,** Szabò I, Rizzuto R. "The mitochondrial calcium uniporter is a multimer that can include a dominant-negative pore-forming subunit." *EMBO J.* 32, 2362-2376 (2013)
203. Fanton M, Floris M, Cristiani A, Olla S, Medda R, Sabbadin D, Bilfone A, **Moro S.** "MMsDusty: an Alternative InChI-Based Tool to Minimize Chemical Redundancy" *Mol Inf.* 8, 681-684 (2013)
202. Minervini G, Masiero A, **Moro S,** Tosatto SC."In silico investigation of PHD-3 specific HIF1- α proline 567 hydroxylation: A new player in the VHL/HIF-1 α interaction pathway?" *FEBS Lett.* 587, 2996-3001 (2013)
201. Bacilieri M, Ciancetta A, Paoletta S, Federico S, Cosconati S, Cacciari B, Taliani

S, Da Settimo F, Novellino E, Klotz KN, Spalluto G, **Moro S**. "Revisiting a Receptor-Based Pharmacophore Hypothesis for Human A2A Adenosine Receptor Antagonists." *J Chem Inf Model*. 53, 1620-1637 (2013)

200. Inamdar GS, Pandya AN, Thakar HM, Sudarsanam V, Kachler S, Sabbadin D, **Moro S**, Klotz KN, Vasu KK. "New insight into adenosine receptors selectivity derived from a novel series of [5-substituted-4-phenyl-1,3-thiazol-2-yl] benzamides and furamides." *Eur J Med Chem*. 63, 924-934 (2013).

199. Pozzi N, Acquasaliente L, Frasson R, Cristiani A, **Moro S**, Banzato A, Pengo V, Scaglione GL, Arcovito A, De Cristofaro R, De Filippis V. " β 2 -Glycoprotein I binds to thrombin and selectively inhibits the enzyme procoagulant functions." *J Thromb Haemost*. 11, 1093-1102 (2013).

198. Squarcialupi L, Colotta V, Catarzi D, Varano F, Filacchioni G, Varani K, Corciulo C, Vincenzi F, Borea PA, Ghelardini C, Di Cesare Mannelli L, Ciancetta A, **Moro S**. "2-Arylpyrazolo[4,3-d]pyrimidin-7-amino Derivatives As New Potent and Selective Human A3 Adenosine Receptor Antagonists. Molecular Modeling Studies and Pharmacological Evaluation." *J Med Chem*. 56, 2256-2269 (2013).

197. Cozza G, Pinna LA, **Moro S**. "Kinase CK2 inhibition: an update." *Curr Med Chem*. 20, 671-693 (2013).

196. Kozma E, Jayasekara PS, Squarcialupi L, Paoletta S, **Moro S**, Federico S, Spalluto G, Jacobson KA. "Fluorescent ligands for adenosine receptors." *Bioorg Med Chem Lett*. 23, 26-36 (2013).

195. Bortolato A, Fanton M, Mason JS, **Moro S**. "Molecular docking methodologies." *Methods Mol Biol*. 924, 339-360 (2013).

194. Floris M, Sabbadin D, Medda R, Bulfone A, **Moro S**. "Adenosiland: walking through adenosine receptors landscape." *Eur J Med Chem*. 58, 248-257 (2012).

193. Federico S, Ciancetta A, Sabbadin D, Paoletta S, Pastorin G, Cacciari B, Klotz KN, **Moro S**, Spalluto G. "Exploring the directionality of 5-substitutions in a new series of 5-alkylaminopyrazolo[4,3-e]1,2,4-triazolo[1,5-c]pyrimidine as a strategy to design novel human α (3) adenosine receptor antagonists." *J Med Chem*. 55, 9654-9668 (2012)

192. Furlanetto V, Zagotto G, Pasquale R, **Moro S**, Gatto B. "Ellagic Acid and Polyhydroxylated Urolithins Are Potent Catalytic Inhibitors of Human Topoisomerase II: An in Vitro Study." *J Agric Food Chem*. 60, 9162-9170 (2012).

191. Cozza G, Pinna LA, **Moro S**. "Protein kinase CK2 inhibitors: a patent review." *Expert Opin Ther Pat*. 22, 1081-1097
190. Colotta V, Lenzi O, Catarzi D, Varano F, Squarzialupi L, Costagli C, Galli A, Ghelardini C, Pugliese AM, Maraula G, Coppi E, Pellegrini-Giampietro DE, Pedata F, Sabbadin D, **Moro S**. "3-Hydroxy-1H-quinazoline-2,4-dione derivatives as new antagonists at ionotropic glutamate receptors: molecular modeling and pharmacological studies." *Eur J Med Chem*. 54, 470-482 (2012)
189. Gaspar A, Reis J, Kachler S, Paoletta S, Uriarte E, Klotz KN, **Moro S**, Borges F. "Discovery of novel A(3) adenosine receptor ligands based on chromone scaffold." *Biochem Pharmacol*. 84, 21-29 (2012)
188. Kozma E, Kumar TS, Federico S, Phan K, Balasubramanian R, Gao ZG, Paoletta S, **Moro S**, Spalluto G, Jacobson KA. "Novel fluorescent antagonist as a molecular probe in A(3) adenosine receptor binding assays using flow cytometry." *Biochem Pharmacol*. 83, 1552-1561 (2012)
187. Viola G, Bortolozzi R, Hamel E, **Moro S**, Brun P, Castagliuolo I, Ferlin MG, Basso G. "MG-2477, a new tubulin inhibitor, induces autophagy through inhibition of the Akt/mTOR pathway and delayed apoptosis in A549 cells." *Biochem Pharmacol*. 83, 16-26 (2012)
186. Cheong SL, Federico S, Venkatesan G, Mandel AL, Shao YM, Spalluto G, **Moro S**, Pastorin G. "The A(3) adenosine receptor as multifaceted therapeutic target: pharmacology, medicinal chemistry, and in silico approaches." *Med Res Rev*. (2011) doi: 10.1002/med.20254.
185. Girolami A, Scarparo P, Bonamigo E, Santarossa L, Cristiani A, **Moro S**, Lombardi AM. "A cluster of factor XI-deficient patients due to a new mutation (Ile 436 Lys) in northeastern Italy" *Eur J Haematol*. (2011) doi: 10.1111/j.1600-0609.2011.01723.x.
184. Bertini S, Asso V, Ghilardi E, Granchi C, Manera C, Minutolo F, Saccomanni G, Bortolato A, Mason J, **Moro S**, Macchia M. "Carbazole-containing arylcarboxamides as BACE1 inhibitors." *Bioorg Med Chem Lett*. 21, 6657-6661 (2011).
183. Cozza G, Gianoncelli A, Bonvini P, Zorzi E, Pasquale R, Rosolen A, Pinna LA, Meggio F, Zagotto G, **Moro S**. "Urolithin as a Converging Scaffold Linking Ellagic acid and Coumarin Analogues: Design of Potent Protein Kinase CK2 Inhibitors." *ChemMedChem* 6, 2273-2286 (2011)

182. Inui M, Manfrin A, Mamidi A, Martello G, Morsut L, Soligo S, Enzo E, **Moro S**, Polo S, Dupont S, Cordenonsi M, Piccolo S. "USP15 is a deubiquitylating enzyme for receptor-activated SMADs." *Nat Cell Biol.* 13, 1368-1375 (2011)
181. Pendin D, Toso J, Moss TJ, Andrezza C, **Moro S**, McNew JA, Daga A. "GTP-dependent packing of a three-helix bundle is required for atlastin-mediated fusion." *Proc Natl Acad Sci U S A.* 108, 16283-16288 (2011)
180. Cheong SL, Dolzhenko AV, Paoletta S, Lee EP, Kachler S, Federico S, Klotz KN, Dolzhenko AV, Spalluto G, **Moro S**, Pastorin G. "Does the combination of optimal substitutions at the C², N(5)- and N(8)-positions of the pyrazolo-triazolo-pyrimidine scaffold guarantee selective modulation of the human A3 adenosine receptors?" *Bioorg Med Chem.* 19, 6120-6134 (2011)
179. Quintieri L, Palatini P, **Moro S**, Floreani M. "Inhibition of cytochrome P450 2C8-mediated drug metabolism by the flavonoid diosmetin." *Drug Metab Pharmacokinet.* 26, 559-568 (2011)
178. Cozza G, Meggio F, **Moro S**. "The Dark Side of Protein Kinase CK2 Inhibition." *Curr Med Chem.* 18, 2867-2884 (2011)
177. Cristiani A, Brisotto N, Cedrati FC, Floris M, Scapozza L, **Moro S**. "ClickMD: an intuitive web-oriented molecular dynamics platform." *Future Med Chem.* 3, 923-931 (2011).
176. Cozza G, Meggio F, **Moro S**. "The Dark Side of Protein Kinase CK2 Inhibition." *Curr Med Chem.* 18, 2867-2884 (2011)
175. Floris M, Masciocchi J, Fanton M, **Moro S**. "Swimming into peptidomimetic chemical space using pepMMsMIMIC." *Nucl. Acids Res.* 39, 1-9 (2011)
174. Cristiani A, Costa G, Cozza G, Meggio F, Scapozza L, **Moro S**. "The Role of the N-Terminal Domain in the Regulation of the "Constitutively Active" Conformation of Protein Kinase CK2: Insight from a Molecular Dynamics Investigation." *ChemMedChem* 7, 1207-1216 (2011)
173. Bacilieri M, Naggi A, Ceol M, Schleicher E, Toso E, Comoli M, Torri G, **Moro S**, Palumbo M, Gambaro G. "Inhibitory effects of glycosaminoglycans on basal and stimulated transforming growth factor-beta1 expression in mesangial cells: biochemical and structural considerations." *Glycobiology* 21, 1029-1037 (2011)

172. Poli D, Catarzi D, Colotta V, Varano F, Filacchioni G, Daniele S, Trincavelli L, Martini C, Paoletta S, **Moro S**. "The Identification of the 2-Phenylphthalazin-1(2H)-one Scaffold as a New Decorable Core Skeleton for the Design of Potent and Selective Human A(3) Adenosine Receptor Antagonists." *J Med Chem.* 54, 2102-2013 (2011)
171. Federico S, Paoletta S, Cheong SL, Pastorin G, Cacciari B, Stragliotto S, Klotz KN, Siegel J, Gao ZG, Jacobson KA, **Moro S**, Spalluto G. "Synthesis and Biological Evaluation of a New Series of 1,2,4-Triazolo[1,5-a]-1,3,5-triazines as Human A(2A) Adenosine Receptor Antagonists with Improved Water Solubility." *J Med Chem.* 54, 877-889 (2011)
170. Marino SM, Fogal S, Bisaglia M, **Moro S**, Scartabelli G, Gioia LD, Spada A, Monzani E, Casella L, Mammi S, Bubacco L. "Investigation of *S. antibioticus* Tyrosinase reactivity toward Chlorophenols." *Arch Biochem Biophys.* 505, 67-74 (2011)
169. Cozza G, Bortolato A, **Moro S**. "How druggable is protein kinase CK2?" *Med Res Rev* 30, 419-462 (2010)
168. Samorì C, Beretta GL, Varchi G, Guerrini A, Di Micco S, Basili S, Bifulco G, Riccio R, **Moro S**, Bombardelli E, Zunino F, Fontana G. "Structure-activity relationship study of 16 α -thiocamptothecins: an integrated in vitro and in silico approach." *ChemMedChem.* 5, 2006-2015 (2010)
167. Paoletta S, Federico S, Spalluto G, **Moro S**. "Receptor-driven identification of novel human A(3) adenosine receptor antagonists as potential therapeutic agents." *Methods Enzymol.* 485, 225-244 (2010)
166. Bertini S, Ghilardi E, Asso V, Granchi C, Minutolo F, Pineschi M, Di Bussolo V, Bortolato A, Saba A, **Moro S**, Macchia M. "BACE1 inhibitory activities of enantiomerically pure, variously substituted N-(3-(4-benzhydrylpiperazin-1-yl)-2-hydroxypropyl) arylsulfonamides." *Bioorg Med Chem.* 18, 7991-7996 (2010)
165. Quintieri L, Bortolozzo S, Stragliotto S, **Moro S**, Pavanetto M, Nassi A, Palatini P, Floreani M. "Flavonoids diosmetin and hesperetin are potent inhibitors of cytochrome P450 2C9-mediated drug metabolism in vitro." *Drug Metab Pharmacokinet.* 25, 466-476 (2010)
164. Michielan L, **Moro S**. "Pharmaceutical perspectives of nonlinear QSAR strategies." *J Chem Inf Model.* 50, 961-978 (2010).

163. Gianoncelli A, Basili S, Scalabrin M, Sosic A, **Moro S**, Zagotto G, Palumbo M, Gresh N, Gatto B. "Rational design, synthesis, and DNA binding properties of novel sequence-selective peptidyl congeners of ametantrone." *ChemMedChem*. 5, 1080-1091 (2010).
162. Cheong SL, Dolzhenko A, Kachler S, Paoletta S, Federico S, Cacciari B, Dolzhenko A, Klotz KN, **Moro S**, Spalluto G, Pastorin G. "The significance of 2-furyl ring substitution with a 2-(para-substituted) aryl group in a new series of pyrazolo-triazolo-pyrimidines as potent and highly selective hA(3) adenosine receptors antagonists: new insights into structure-affinity relationship and receptor-antagonist recognition." *J Med Chem*. 53, 3361-3375 (2010).
161. Pastorin G, Federico S, Paoletta S, Corradino M, Cateni F, Cacciari B, Klotz KN, Gao ZG, Jacobson KA, Spalluto G, **Moro S**. "Synthesis and pharmacological characterization of a new series of 5,7-disubstituted-[1,2,4]triazolo[1,5-a][1,3,5]triazine derivatives as adenosine receptor antagonists: A preliminary inspection of ligand-receptor recognition process." *Bioorg Med Chem*. 18, 2524-2536 (2010)
160. Michielan L, Pireddu L, Floris M, **Moro S**. "Support Vector Machine (SVM) as Alternative Tool to Assign Acute Aquatic Toxicity Warning Labels to Chemicals." *Mol Info*. 1-2, 51-64 (2010)
159. Morizzo E, Federico S, Spalluto G, **Moro S**. "Human A3 Adenosine Receptor as Versatile G Protein-Coupled Receptor Example to Validate the Receptor Homology Modeling Technology." *Curr Pharm Des*. 15, 4069-4084 (2009)
158. Michielan L, Federico S, Terfloth L, Hristozov D, Cacciari B, Klotz KN, Spalluto G, Gasteiger J, **Moro S**. "Exploring Potency and Selectivity Receptor Antagonist Profiles Using a Multilabel Classification Approach: The Human Adenosine Receptors as a Key Study." *J Chem Inf Model*. 49, 2820-2836 (2009)
157. Michielan L, Terfloth L, Gasteiger J, **Moro S**. "Comparison of Multilabel and Single-Label Classification Applied to the Prediction of the Isoform Specificity of Cytochrome P450 Substrates." *J Chem Inf Model*. 49, 2588-2605 (2009)
156. Lenzi O, Colotta V, Catarzi D, Varano F, Poli D, Filacchioni G, Varani K, Vincenzi F, Borea PA, Paoletta S, Morizzo E, **Moro S**. "2-Phenylpyrazolo[4,3-d]pyrimidin-7-one as a New Scaffold To Obtain Potent and Selective Human A(3) Adenosine Receptor Antagonists: New Insights into the Receptor-Antagonist Recognition." *J Med Chem*. 52, 7640-7652 (2009)

155. Cozza G, Bortolato A, Menta E, Cavalletti E, Spinelli S, **Moro S**. "ATP Non-Competitive Ser/Thr Kinase Inhibitors as Potential Anticancer Agents." *Anti-Cancer Agents in Med Chem* 9, 778-786 (2009)
154. Zonta N, Cozza G, Gianoncelli A, Korb O, Exner TE, Meggio M, Zagotto G, **Moro S**. "Scouting Novel Protein Kinase A (PKA) Inhibitors by Using a Consensus Docking-Based Virtual Screening Approach." *Lett Drug Design Discov* 6, 327-336 (2009)
153. Michielan L, Bolcato C, Federico S, Cacciari B, Bacilieri M, Klotz KN, Kachler S, Pastorin G, Cardin R, Sperduti A, Spalluto G, Moro S. "Combining selectivity and affinity predictions using an integrated Support Vector Machine (SVM) approach: An alternative tool to discriminate between the human adenosine A(2A) and A(3) receptor pyrazolo-triazolo-pyrimidine antagonists binding sites." *Bioorg Med Chem* 17, 5259-5267 (2009)
152. Lebska M, Szczegielniak J, Dobrowolska G, Cozza G, **Moro S**, Muszyn'ska G. "A novel splicing variant encoding putative catalytic alpha subunit, of maize protein kinase CK2." *Physiol Plant.* 136, 251-263 (2009)
151. Cozza G, Mazzorana M, Papinutto E, Bain J, Elliott M, Di Maira G, Gianoncelli A, Pagano MA, Sarno S, Ruzzene M, Battistutta R, Meggio F, **Moro S**, Zagotto G, Pinna LA. "Quinalizarin as a potent, selective and cell permeable inhibitor of protein kinase CK2." *Biochem J.* 421, 387-395 (2009)
150. Colotta V, Catarzi D, Varano F, Lenzi O, Filacchioni G, Martini C, Trincavelli L, Ciampi O, Traini C, Pugliese AM, Pedata F, Morizzo E, **Moro S**. "The Pyrido[2,3-e]-1,2,4-triazolo[4,3-a]pyrazin-1-one as a New Scaffold to Develop Potent and Selective Human A3 Adenosine Receptor Antagonists. Synthesis, Pharmacological Evaluation and Ligand-Receptor Modeling Studies." *J Med Chem* 23, 2407-2419 (2009)
149. Varchi G, Samorì C, Battaglia A, Beretta GL, **Moro S**. "Semi-synthesis, biological activity and molecular modeling studies of C-ring modified camptothecins." *J Med Chem* 52, 1029-1039 (2009)
148. Basili S, **Moro S**. "Novel Camptothecin Derivatives as Topoisomerase I Inhibitors." *Ex Op Ther Patent* 19, 555-574 (2009)
147. Dupont S, Mamidi A, Cordenonsi M, Montagner M, Zacchigna L, Adorno M, Martello G, Stinchfield MJ, Soligo S, Morsut L, Inui M, **Moro S**, Modena N, Argenton F, Newfeld SJ, Piccolo S. "FAM/USP9x, a deubiquitinating enzyme

essential for TGFbeta signaling, controls Smad4 monoubiquitination." *Cell* 136, 123-135 (2009)

146. Richter SN, Menegazzo I, Nadai M, **Moro S**, Palumbo M "Reactivity of clerocidin towards adenine: implications for base-modulated DNA damage." *Org Biomol Chem* 7, 976-985 (2009).

145. Masciocchi J, Frau G, Fanton M, Floris M, Sturlese M, Palla P, Cedrati F, Rodriguez-Tomé P, **Moro S**. "MMsINC: a large-scale chemoinformatics database." *Nucleic Acids Res.* 37, 284-290 (2009)

144. Vilar S, Cozza G, **Moro S**. "Medicinal chemistry and the molecular operating environment (MOE): application of QSAR and molecular docking to drug discovery." *Curr Top Med Chem.* 8, 1555-1572 (2008)

143. Vettore S, Scandellari R, **Moro S**, Lombardi AM, Scapin M, Randi ML, Fabris F. "Novel point mutation in a leucine-rich repeat of the GPIb{alpha} chain of the platelet von Willebrand factor receptor, GPIb/IX/V, resulting in an inherited dominant form of Bernard-Soulier syndrome affecting two unrelated families: the N41H variant." *Haematologica* 93, 1743-1747 (2008)

142. Cozza G, Gianoncelli A, Montopoli M, Caparrotta L, Venerando A, Meggio F, Pinna LA, Zagotto G, **Moro S**. "Identification of novel protein kinase CK1 delta (CK1delta) inhibitors through structure-based virtual screening." *Bioorg Med Chem Lett.* 18, 5672-5675 (2008)

141. Asso V, Ghilardi E, Bertini S, Digiacocono M, Granchi C, Minutolo F, Rapposelli S, Bortolato A, **Moro S**, Macchia M. "alpha-Naphthylaminopropan-2-ol Derivatives as BACE1 Inhibitors." *ChemMedChem.* 3, 1530-1534 (2008)

140. Basili S, Basso G, Faccio A, Granzhan A, Ihmels H, **Moro S**, Viola G. "Diazoniapolycyclic Ions Inhibit the Activity of Topoisomerase I and the Growth of Certain Tumor Cell Lines." *ChemMedChem.* 3, 1671-1376 (2008)

139. Fanton M, Floris M, Frau G, Masciocchi J, Sturlese M, Palla P, Cedrati F, Rodriguez-Tomé P, **Moro S**. "MMsINC: a new web-based large-scale chemoinformatics platform." in *BIOTECHNO 2008 Proceedings*, IEEE Computer Society Press, 64-69(2008)

138. Bazzicalupi C, Bencini A, Bonaccini C, Giorgi C, Gratteri P, **Moro S**, Palumbo M, Simionato A, Sgrignani J, Sissi C, Valtancoli B. "Tuning the Activity of Zn(II)

Complexes in DNA Cleavage: Clues for Design of New Efficient Metallo-Hydrolases." *Inorg Chem.* 47, 5474-5484 (2008)

137. Colotta V, Catarzi D, Varano F, Lenzi O, Filacchioni G, Martini C, Trincavelli L, Ciampi O, Traini C, Pugliese AM, Pedata F, Morizzo E, **Moro S.** "Synthesis, ligand-receptor modeling studies and pharmacological evaluation of novel 4-modified-2-aryl-1,2,4-triazolo[4,3-a]quinoxalin-1-one derivatives as potent and selective human A(3) adenosine receptor antagonists." *Bioorg Med Chem.* 16, 6086-6102 (2008)

136. Bortolato A, Cozza G, **Moro S.** "Protein kinase CK2 inhibitors: emerging anticancer therapeutic agents? " *Anti-Cancer Agents in Medicinal Chemistry* 8, 798-806 (2008)

135. Michielan L, Bacilieri M, Kaseda C, **Moro S** "Prediction of the aqueous solvation free energy of organic compounds by using autocorrelation of molecular electrostatic potential surface properties combined with response surface analysis." *Bioorg Med Chem.* 16, 5733-5742 (2008)

134. Leone S, Mutti C, Kazantsev A, Sturlese M, **Moro S**, Cattaneo E, Rigamonti D, Contini A "SAR and QSAR study on 2-aminothiazole derivatives, modulators of transcriptional repression in Huntington's disease." *Bioorg Med Chem.* 16, 5695-5703 (2008)

133. Bortolato A, Moro S. "Designing a ligand for pharmaceutical purposes." *Expert Opin. Drug Discov.* 3, 579-590 (2008)

132. Chilin A, Battistutta R, Bortolato A, Cozza G, Zanatta S, Poletto G, Mazzorana M, Zagotto G, Uriarte E, Guiotto A, Pinna LA, Meggio F, **Moro S** "Coumarin as Attractive Casein Kinase 2 (CK2) Inhibitor Scaffold: An Integrate Approach To Elucidate the Putative Binding Motif and Explain Structure-Activity Relationships." *J Med Chem* 51, 752-759 (2008)

131. Michielan L, Bacilieri M, Schiesaro A, Bolcato C, Pastorin G, Spalluto G, Cacciari B, Klotz KN, Kaseda C, **Moro S** "Linear and Nonlinear 3D-QSAR Approaches in Tandem with Ligand-Based Homology Modeling as a Computational Strategy To Depict the Pyrazolo-Triazolo-Pyrimidine Antagonists Binding Site of the Human Adenosine A(2A) Receptor." *J. Chem. Inf. Model.* 48, 350-363 (2008)

130. Zagotto G, Sissi C, **Moro S**, Dal Ben D, Parkinson GN, Fox KR, Neidle S, Palumbo M "Amide bond direction modulates G-quadruplex recognition and

telomerase inhibition by 2,6 and 2,7 bis-substituted anthracenedione derivatives." *Bioorg. Med. Chem.* 16, 354-361 (2008)

129. Bolcato C, Cusan C, Pastorin G, Spalluto P, Cacciari B, Klotz HN, Morizzo E, **Moro S** "Pyrazolo-Triazolo-Pyrimidines as adenosine receptor antagonists: Effect of the N-5 bond type on the affinity and selectivity at the four adenosine receptor subtypes." *Purinergic Signalling* 4, 39-46 (2008)

128. Spinelli S, **Moro S** "2-Heteroarylbenzamide derivatives as MEK kinase inhibitors with antitumor activity." *European Patent N.* 07003478.0-2101 (2007)

127. Morizzo E, Capelli F, Lenzi O, Catarzi D, Varano F, Filacchioni G, Vincenzi F, Varani K, Andrea Borea P, Colotta V, **Moro S** "Scouting Human A3 Adenosine Receptor Antagonist Binding Mode Using a Molecular Simplification Approach: From Triazoloquinoline to a Pyrimidine Skeleton as a Key Study." *J. Med. Chem.* 50, 6596-6606 (2007)

126. Basili S, Dall'Acqua F, Faccio A, Granzhan A, **Moro S**, Viola G, Ihmels H "Relationship between the Structure and the DNA-Binding Properties of Diazoniapolycyclic Duplex- and Triplex-DNA Binders: Efficiency, Selectivity and Binding Model." *Biochemistry* 46, 12721-12736 (2007)

125. Cozza G, **Moro S**, Gotte G "Elucidation of the ribonuclease A aggregation process mediated by 3D domain swapping: A computational approach reveals possible new multimeric structures." *Biopolymers* 89, 26-39 (2007)

124. Bacilieri M, Varano F, Deflorian F, Marini M, Catarzi D, Colotta V, Filacchioni G, Galli A, Costagli Chiara, Kaseda C, **Moro S** "Tandem 3D-QSARs approach as valuable tool to predict binding affinity data: design of new Gly/NMDA receptor antagonists as a key study" *J. Chem. Inf. Model.* 47, 1913-1922 (2007)

123. Battistutta R, Mazzorana M, Cedron L, Bortolato A, Sarno S, Kazimierczuk Z, Zanotti G, **Moro S**, Pinna LA "The ATP-binding site of protein kinase CK2 holds a positive electrostatic area and conserved water molecules." *ChemBioChem* 8, 1804-1809 (2007)

122. Colotta V, Catarzi D, Varano F, Capelli F, Lenzi O, Filacchioni G, Martini C, Trincavelli L, Ciampi O, Pugliese AM, Pedata F, Schiesaro A, Morizzo E, **Moro S** "New 2-Arylpyrazolo[3,4-c]quinoline Derivatives as Potent and Selective Human A3 Adenosine Receptor Antagonists. Synthesis, Pharmacological Evaluation and Ligand-Receptor Modeling" *J. Med. Chem.* 50, 4161-4074 (2007)

121. Dal Ben D, Capranico G, Zagotto G, Palumbo M, **Moro S** "DNA topoisomerase II structures and anthracycline activity: insights into ternary complex formation." *Curr. Pharm. Des.* 13, 2766-2780 (2007)
120. Bacilieri M, **Moro S**. "Ligand-based drug design methodologies in drug discovery process: an overview." *Curr Drug Discov Technol.* 3, 155-165 (2006).
119. Bortolato A, **Moro S** "In Silico Binding Free Energy Predictability by Using Linear Interaction Energy (LIE) Method: "Bromo-Benzimidazole CK2 Inhibitors as Case Study." *J. Chem. Inf. Model.* 47, 572-582 (2007)
118. Cacciari B, Bolcato C, Spalluto G, Klotz KN, Bacilieri M, Deflorian F, **Moro S** "Pyrazolo-Triazolo-Pyrimidines as adenosine receptor antagonists: a complete structure-activity profile." *Purinergic Signalling* 3, 183-193 (2007)
117. Pagano MA, Poletto G, Di Maira G, Cozza G, Ruzzene M, Sarno S, Bain J, Elliott M, **Moro S**, Zagotto G, Meggio F, Pinna LA. "Tetrabromocinnamic Acid (TBCA) and Related Compounds Represent a New Class of Specific Protein Kinase CK2 Inhibitors." *ChemBioChem.* 8, 129-139 (2007)
116. **Moro S**, Bacilieri M, Deflorian F "Combining ligand-based and structure-based design in the virtual screening arena" *Expert Opin. Drug Discov.* 2, 37-49 (2007)
115. Cristalli G, Cacciari B, Dal Ben D, Lambertucci C, **Moro S**, Spalluto G, Volpini R. " Highlights on the Development of A(2A) Adenosine Receptor Agonists and Antagonists." *ChemMedChem* 2, 260-281 (2007)
114. Bacilieri M, **Moro S** "Ligand-based drug design methodologies in drug discovery process: an overview." *Curr Drug Discov Technol.* 3, 155-165 (2006).
113. H. Ihmels, D. Otto, A. Faccio, F. Dall'Acqua, G. Viola, **S. Moro** "Comparative Studies on the DNA-binding Properties of Linear and Angular Dibenzoquinolinium Ions." *J. Org. Chem.* 71, 8401-8411 (2006)
112. **S. Moro**, M. Bacilieri, B. Cacciari, C. Bolcato, C. Cusan, G. Pastorin, K. N. Klotz, G. Spalluto "The application of a 3D-QSAR (autoMEP/PLS) approach as an efficient pharmacodynamic-driven filtering method for small-sized virtual library: application to a lead optimization of a human A3 adenosine receptor antagonist." *Biorg. Med. Chem.* 14, 4923-4932 (2006)
111. G. Cozza, P. Bonvini, E. Zorzi, G. Poletto, M.A. Pagano, S. Sarno, A. Donella-Deana, G. Zagotto, A. Rosolen, L.A. Pinna, F. Meggio, **S. Moro** "Identification of

ellagic acid as potent inhibitor of protein kinase CK2: a successful example of a virtual screening application." *J. Med. Chem.* 49, 2363-2366 (2006)

110 O. Lenzi, V. Colotta, D. Catarzi, F. Varano, G. Filacchioni, C. Martini, L. Trincavelli, O. Ciampi, K. Varani, F. Marighetti, E. Morizzo, **S. Moro** "4-amido-2-aryl-1,2,4-triazolo[4,3-a]quinoxalin-1-ones as new potent and selective human A3 adenosine receptor antagonists. synthesis, pharmacological evaluation, and ligand-receptor modeling studies. *J. Med. Chem.* 49, 3916-3925 (2006)

109. **S. Moro**, F. Varano, G. Cozza, M. A. Pagano, G. Zagotto, A. Chilin, A. Guiotto, D. Catarzi, V. Calotta, L. A. Pinna, F. Meggio "Pyrazoloquinazoline tricyclic system as novel scaffold to design new kinase CK2 inhibitors". *Letter in Drug Design & Discov.* 3, 281-284 (2006)

108. **S. Moro**, F. Deflorian, M. Bacilieri, G. Spalluto "Ligand-based homology modeling as attractive tool to inspect GPCR structural plasticity." *Curr. Pharm. Des.* 12, 2175-2185 (2006)

107. **S. Moro**, F. Deflorian, M. Bacilieri, G. Spalluto "G protein-coupled receptors as challenging druggable targets: insights from in silico studies." *New J. Chem.* 30, 301-308 (2006)

106 **S. Moro**, F. Deflorian, M. Bacilieri, G. Spalluto "Novel strategies for the design of new potent and selective human A3 receptor antagonists: an update." *Curr. Med. Chem.* 13, 763-771 (2006)

105. **S. Moro**, G. Spalluto, Z.-G. Gao, K. A. Jacobson "Progress in the pursuit of therapeutic adenosine receptor antagonists." *Med. Res. Rev.* 26, 131-159 (2006)

104. B. Cacciari, G. Pastorin, C. Bolcato, G. Spalluto, M. Bacilieri, **S. Moro** "A2B adenosine receptor antagonists: recent developments." *Mini Rev. Med. Chem.* 5, 1053-1060 (2005)

103. D. Catarzi, V. Colotta, F. Varano, O. Lenzi, G. Filacchioni, L. Trincavelli, C. Martini, C. Montopoli, **S. Moro** "1,2,4-Triazolo[1,5-a]quinoxaline as a versatile tool for the design of selective human A3 adenosine receptor antagonists: synthesis, biological evaluation, and molecular modeling studies of 2-(hetero)aryl- and 2-carboxy-substituted derivatives." *J. Med. Chem.* 48, 7932-7945 (2005)

102. **S. Moro**, M. Bacilieri, B. Cacciari, G. Spalluto "Autocorrelation of Molecular Electrostatic Potential Surface Properties Combined with Partial Least Squares

Analysis as New Strategy for the Prediction of the Activity of Human A3 Adenosine Receptor Antagonists." *J. Med. Chem.* **48**, 5698-5704 (2005)

101. E. Del Grosso, D. Boschi, L. Lazzarato, C. Cena, A. Di Stilo, R. Fruttero, **S. Moro**, A. Gasco "The Furoxan System as a Flexible Tool to Designing Selective NO-donor COX-2 Inhibitors Endowed with Antiaggregatory and Vasodilating Activities." *Chem. Biodiv.* **2**, 886-900 (2005)

100. M.G. Ferlin, C. Marzano, L.D. Via, A. Chilin, G. Zagotto, A. Guiotto, **S. Moro** "New water soluble pyrroloquinoline derivatives as new potential anticancer agents." *Bioorg. Med. Chem.* **13**, 4733-4739 (2005)

99. E. Del Grosso, D. Boschi, L. Lazzarato, C. Cena, A. Di Stilo, R. Fruttero, **S. Moro**, A. Gasco "The Furoxan System as a Flexible Tool to Designing Selective NO-donor COX-2 Inhibitors Endowed with Antiaggregatory and Vasodilating Activities." *Chem. Biodiv.* **2**, 886-900 (2005)

98. M.G. Ferlin, C. Marzano, L.D. Via, A. Chilin, G. Zagotto, A. Guiotto, **S. Moro** "New water soluble pyrroloquinoline derivatives as new potential anticancer agents." *Bioorg. Med. Chem.* **13**, 4733-4739 (2005)

97. G. Pastorin, C. Bolcato, B. Cacciari, K.A. Jacobson, K.-N. Klotz, **S. Moro**, G. Spalluto "Synthesis and Biological studies of 1,3-Di-n-Propyl-2,4-Dioxo-6-Methyl-8-(Substitued) 1,2,3,4-Tetrahydro [1,2,4]-Triazolo [3,4-f]-Purines as Adenosine Receptor Antagonists: A Molecular Modeling Investigation." *Il Farmaco* **60**, 643-651 (2005)

96. G. Pastorin, C. Bolcato, B. Cacciari, K.A. Jacobson, K.-N. Klotz, C. Montopoli, **S. Moro**, G. Spalluto "Synthesis, Biological studies and Molecular Modeling Investigation of 1,3-Dimethyl-2,4-Dioxo-6-Methyl-8-(Substitued)-1,2,3,4-Tetrahydro [1,2,4]-Triazolo [3,4-f]-Purines as Adenosine Receptor Antagonists." *Il Farmaco* **60**, 299-306 (2005)

95. A. Brigo, G. I. Mustata, J.M. Briggs, **S. Moro** "Discovery of HIV-1 Integrase Inhibitors through a Novel Combination of Ligand and Structure-based Drug Design." *Med. Chem.* **1**, 263-275, (2005)

94. F. Varano, D. Catarzi, V. Colotta, F.R. Calabri, O. Lenzi, G. Filacchioni, A. Galli, C. Costagli, V. Carlà, F. Deflorian, **S. Moro** "1-Substitued Pyrazolo[1,5-c]quinazolines as Novel Gly/NMDA Receptor Antagonists: Synthesis, Biological Evaluation and Molecular Modeling Study." *Bioorg. Med. Chem.* **13**, 5536-5549 (2005)

93. S. N. Richter, D. Fabris, **S. Moro**, M. Palumbo "Dissecting reactivity of clerocidin toward common buffer systems by means of selected drug analogues." *Chem. Res. Toxicol.* **18**, 35-40 (2005)
92. **S. Moro**, G. Spalluto, K. A. Jacobson "Recent development on computer aided engineering of GPCR ligands: the human A₃ adenosine receptors as an example." *Trends Pharmacol. Sci.* **26**, 44-51 (2005)
91. **S. Moro**, P. Braiuca, F. Deflorian, G. Pastorin, C. Ferrari, B. Cacciari, P. G. Baraldi, K. Varani, P. A. Borea, G. Spalluto "Combined Target-based and Ligand-based Drug Design Approach as Tool to Define a Novel 3D-Pharmacophore Model of Human A₃ Adenosine Receptor Antagonists: Pyrazolo[4,3-*e*]1,2,4-Triazolo[1,5-*c*]Pyrimidine Derivatives as a Key Study." *J Med. Chem.* **48**, 152-162 (2005)
90. D. Catarzi, V. Colotta, F. Varano, F.R. Calabri, O. Lenzi, G. Filacchioni, L. Trincavelli, C. Martini, A. Tralli, C. Monopoli, **S. Moro** "2-Aryl-8-chloro-1,2,4-triazolo[1,5-*a*]quinoxalin-4-amines as Highly Potent A₁ and A₃ Adenosine Receptor Antagonists." *Bioorg. Med. Chem.* **13**, 705-715 (2005)
89. M. Yarim, **S. Moro**, B. Hagenbuch, R. Huber, P. Meier-Abt, C. Kaseda, T. Kashima, G. Folkers "Application of QSAR Analysis to Organic Anion Transporting Polypeptide 1a5 (Oatp1a5) Substrates". *Bioorg. Med. Chem.* **13**, 463-471 (2005)
88. D. Catarzi, V. Colotta, F. Varano, F.R. Calabri, O. Lenzi, G. Filacchioni, L. Trincavelli, C. Martini, A. Tralli, C. Monopoli, **S. Moro** "2-Aryl-8-chloro-1,2,4-triazolo[1,5-*a*]quinoxalin-4-amines as Highly Potent A₁ and A₃ Adenosine Receptor Antagonists." *Bioorg. Med. Chem.* **13**, 705-715 (2005)
87. **S. Moro**, M. Bacilieri, C. Ferrari, G. Spalluto "Autocorrelation of Molecular Electrostatic Potential Surface Properties combined with Partial Least Squares Analysis as alternative attractive tool to generate ligand-based 3D-QSARs. *Curr. Drug Disc. Tech.* **2**, 13-21 (2005)
86. B. Cacciari, G. Pastorin, **S. Moro**, G. Spalluto "Potent and Selective A_{2A} Adenosine Receptor Antagonists: Recent improvements". *Frontiers in Medicinal Chemistry*, vol. 2, pp. 49-62, Bentham Science Publishers Ltd. (2005)
85. T. De Ros, **S. Moro**, S. Bosi, L. Feruglio, B. Gregoretti, M. Terdoslavich, S. Passamonti, G. Decorti, G. Spalluto, M. Prato "Hemolytic effects of water-soluble fullerene derivatives." *J Med. Chem.* **47**, 6711-6715 (2004)

84. F. Meggio, M. A. Pagano, **S. Moro**, G. Zagotto, M. Ruzzene, S. Sarno, G. Cozza, J. Bain, M. Elliott, A. Donella Deana, A. M. Brunati, L. A. Pinna "Inhibition of protein kinase CK2 by condensed polyphenolic derivatives. An in vitro and in vivo study." *Biochemistry* **43**, 12931-12936 (2004)
83. A. Guiotto, M. Canevari, M. Pozzobon, **S. Moro**, P. Orsolini, M. Veronese "Anchimeric assistance effect on regioselective hydrolysis of branched PEGs: a mechanistic investigation". *Bioorg. Med. Chem.* **19**, 5031-5037 (2004)
82. Colotta V, Catarzi D, Varano F, Calabri FR, Lenzi O, Filacchioni G, Martini C, Trincavelli L, Deflorian F, **Moro S.** "1,2,4-triazolo[4,3-a]quinoxalin-1-one moiety as an attractive scaffold to develop new potent and selective human A3 adenosine receptor antagonists: synthesis, pharmacological, and ligand-receptor modeling studies." *J Med. Chem.* **47**, 3580-3590 (2004)
81. **S. Moro**, G.L. Beretta, D. Dal Ben, J. Nitiss, M. Palumbo, G. Caprinico "Interaction model for anthracycline activity against DNA topoisomerase II." *Biochemistry* **43**, 7503-7513 (2004)
80. E. Boseggia, **S. Moro**, M. Gatos, L. Lucatello, F. Mancin, M. Palumbo, C. Sissi, P. Tecilla, U. Tonellato, G. Zagotto "Toward efficient Zn(II)-based artificial nucleases." *J. Am. Chem. Soc.* **126**, 4543-4549 (2004)
79. O. Schiavon, G. Pasut, **S. Moro**, P. Orsolini, A. Guiotto, F.M. Veronese "PEG-ARAC conjugates for controlled release." *Eur. J. Med. Chem.* **39**, 123-133 (2004)
78. C. Sissi, E. Leo, **S. Moro**, G. Caprinico, A. Mancia, E. Menta, A.P. Krapcho, M. Palumbo "Antitumor Aza-anthrapyrazoles: biophysical and biochemical studies on 8- and 9-aza regioisomers." *Biochem. Pharmacol.* **67**, 631-42 (2004)
77. D. Vedaldi, A. Dolmella, **S. Moro**, G. Miolo, G. Viola, S. Caffieri, F. Dall'Acqua "1-Thioangelicin: crystal structure, computer-aided studies and photobiological activity." *Farmaco* **59**, 125-132 (2004)
76. **S. Moro**, F. Deflorian, K.A. Jacobson, G. Spalluto, G. Pastorin, B. Cacciari "Demystifying the Three Dimensional Structure of G Protein-Coupled Receptors with the Aid of Molecular Modeling." *J. Chem. Soc. Chem. Comm.* **24**, 2949-2956 (2003)
75. P. Pengo, L. Pasquato, **S. Moro**, A. Brigo, F. Fogolari, Q.B. Broxterman, B. Kaptein, P. Scrimin "Quantitative Correlation of Solvent Polarity with the ν_{310} -

Helix Equilibrium: A Heptapeptide Behaves as a Solvent-Driven Molecular Spring." *Angew. Chem. Int. Ed.* **42**, 3388–3392 (2003)

74. G. Pastorin, T. Da Ros, G. Spalluto, B. Cacciari, **S. Moro**, F. Deflorian, K. Varani, S. Gessi, P.A. Borea "Pyrazolo[4,3-e]1,2,4-triazolo[1,5-c]pyrimidine derivatives as adenosine receptor antagonists: influence of the N5 substituent on the affinity at the human A₃ and A_{2B} adenosine receptor subtypes." *J Med. Chem.* **46**, 4287-4296 (2003)

73. M. Bonchio, O. Bortolini, G. Licini, **S. Moro**, W. A. Nugent "On The Mechanism of the Oxygen Transfer to Sulfoxides by Ti(IV)/Trialkanolamine/Peroxo Complexes. Evidence for a Metal Template Process." *Eur. J. Org. Chem.* ,507-511(2003)

72. E. De Moliner, **S. Moro**, S. Sarno, G. Zagotto, G. Zanotti, L.A. Pinna, R. Battistutta "Inhibition of protein kinase CK2 by anthraquinone related compounds: A structural insight." *J. Biol. Chem.* **278**, 1831-1836 (2003)

71. O. Bortolini, M. Carraro, V. Conte, **S. Moro**, "Vanadium-Bromoperoxidase-Mimicking Systems: Direct Evidence of a Hypobromite-like Vanadium Intermediate." *Eur. J. Inorg. Chem.* **12**, (2002)

70. M. Palumbo, B. Gatto, **S. Moro**, C. Sissi, G. Zagotto "Sequenze-specific interactions of drugs interfering with the topoisomerase-DNA cleavage complex." *Biochim. Biophys. Acta* **1587**, 145-154 (2002)

69. **S. Moro**, K. A. Jacobson "Molecular modeling as tool to investigate molecular recognition in P2Y receptors." *Curr. Pharm. Des.* **8**, 99-110 (2002)

68. G. Viola, F. Dall'Acqua, N. Gabellini, **S. Moro**, D. Vedaldi, H. Ihmels "Indolo [2,3-b]-quinolizinium bromide: An efficient intercalator with DNA-Photodamaging Properties" *ChemBioChem.* **3**, 101-109 (2002)

67. A. Maconi, G. Pastorin, T. Da Ros, G. Spalluto Z.-g. Gao, K.A. Jacobson, P.G. Baraldi, B. Cacciari, K. Varani, **S. Moro**, P.A. Borea "Synthesis, Biological Properties and Molecular Modeling Investigation of the First Potent, Selective and Water Soluble Human A₃ Adenosine Receptor Antagonist" *J Med. Chem.* **45**, (2002)

66. P.G. Baraldi, **S. Moro**, R. Makaeva, M.G. Pavani, M. delC. Nunez, G. Spalluto, G. Falzoni, F. Di Virgilio, R. Romagnoli "Synthesis, biological activity and molecular modeling studies of 1,2,3,4-tetrahydroisoquinoline derivatives as conformationally

constrained analogues of KN62, a potent antagonist of the P2X7-receptor containing a tyrosine moiety." *Arzneimittelforschung* **52**, 273-285 (2002)

65. K.A. Jacobson, **S. Moro**, J.A. Manthey, P. West, X.-d. Ji "Interaction of flavonoids and other phytochemicals with adenosine receptors. In *Flavonoids in Cell Function*." Buslig, B., Manthey, J., eds., 2002, Kluwer Academic/Plenum, New York, pp. 163-171

64. S. Sarno, **S. Moro**, F. Meggio, G. Zagotto, D. Dal Ben, L. A. Pinna "Toward the rational design of protein kinase CK2 inhibitors." *Pharmacol. Ther.* **93**, 1-10 (2002)

63. P.G. Baraldi, B. Cacciari, **S. Moro**, R. Romagnoli, G. Spalluto, G. Pastorin, T. Da Ros, K.N. Klotz, E. Leung, K. Varani, S. Gessi, S. Merighi, P.A. Borea "Synthesis, biological activity, and molecular modeling investigation of new pyrazolo[4,3-e]1,2,4-triazolo[1,5-c]pyrimidine derivatives as human A₃ adenosine receptor antagonists." *J Med. Chem.* **45**, 770-780(2002)

62. T. Da Ros, M. Bergamin, G. Spalluto, B. Baiti, **S. Moro**, M. Prato, A. Boutorine "Synthesis, molecular modeling and biological evaluation of fullerene-trimethoxyindole-oligonucleotide conjugates: a possible probe for studying photochemical reactions in DNA triple helices." *Eur. J. Org. Chem.* **3**, 405-413 (2002)

61. M. Palumbo, **S. Moro**, B. Gatto, C. Sissi, G. Zagotto "Quantitation of camptothecin and related compounds." *J. Chromatogr. B Biomed. Sci. Appl.* **64**, 121-140 (2001)

60. G. Zagotto, **S. Moro**, B. Gatto, C. Sissi, M. Palumbo "Anthracyclines: recent developments in their separation and quantitation." *J. Chromatogr. B Biomed. Sci. Appl.* **64**, 161-171 (2001)

59. S. Richter, L. Panella, **S. Moro**, G. Capranico, M. Palumbo, B. Gatto "Clerocidin alkylates DNA: implications for irreversible topoisomerase II-mediated DNA damage." *Nucleic Acid Res.* **29**, 4224-30 (2001)

58. M. Bonchio, O. Bortolini, V. Conte **S. Moro** "Characterization and Reactivity of Triperoxo Vanadium Complexes In Protic Solvents." *Eur. J. Inorg. Chem.* **11**, 2719-2738 (2001)

57. F. Meggio, **S. Moro**, A. D. Deana, D. Dal Ben, S. Sarno, G. Fagotto, L. A. Pinna "Molecular Features of selective polyphenolic inhibitors of Protein kinase CK2." *Cell. Biol. Mol. Lett.* **6**, 503-506 (2001)
56. K. A. Jacobson, R.G. Ravi, **S. Moro**, E. Nandanan, H. S. Kim, Y. C. Kim, K. Lee, Barak, D., Marquez, V.E., and Ji, X.D. "Ribose modified nucleosides and nucleotides as ligands for purine receptors." *Nucleosides Nucleotides* **20**, 333-341 (2001)
55. K. A. Jacobson, **S. Moro**, P. West, X.-d. Ji "Interaction of flavonoids and other phytochemical with adenosine receptors. in *Flavonoids in Cell Function*. Buslig B, and Manthey J eds., 2001, Kluwer Academic/Plenum, New York.
54. P. G. Baraldi, B. Cacciari, **S. Moro**, R. Romagnoli, X.D. Ji, K. A. Jacobson, G. Spalluto "Fluorosulfonyl- and bis-(-chloroethyl)amino- phenylamino functionalized pyrazolo[4,3e]1,2,4-triazolo[1,5-c]pyrimidine derivatives as irreversible antagonists at the human A3 adenosine receptor. *J Med. Chem.* **44**, 2735-2742 (2001)
53. C. Sissi, **S. Moro**, S. Richter, B. Gatto, E. Menta, S. Spinelli, A.P. Krapcho, F. Zunino, M. Palumbo "DNA-interactive aza-anthrapyrazoles: biophysical and biochemical studies relevant to the mechanism of action". *Mol. Pharmacol.* **59**, 96-103 (2001)
52. K. A. Jacobson, **S. Moro**, C. Hoffmann, Y.-C. Kim, H. S. Kim, R. G. Ravi, T. K. Harden, J. L. Boyer "Structurally related nucleotides as selective agonists and antagonists at P2Y₁ receptors" *Farmaco* **56**, 71-75 (2001)
51. P.G. Baraldi, B. Cacciari, **S. Moro**, R. Romagnoli, G. Spalluto, K.N. Klotz, E. Leung, K. Varani, S. Gessi, S. Merighi, P.A. Borea "Pyrazolo[4,3-e]1,2,4-triazolo[1,5-c]pyrimidine derivatives as highly potent and selective human A(3) adenosine receptor antagonists: influence of the chain at the N(8) pyrazole nitrogen. *J Med. Chem.* **43**, 4768-4780 (2000)
50. E. Nandanan, S.-Y- Jang, **S. Moro**, H. Kim, M. A. Siddiqui, P. Russ, V. E. Marquez, R. Busson, P. Herdewijn, K. Harden, J. L. Boyer, K. J. Jacobson "Synthesis, biological activity, and molecular modeling of ribose-modified deoxyadenosine bisphosphate analogues as P2Y₁ receptor ligands". *J Med. Chem.* **43**, 829-842 (2000)
49. I. Menegazzo, **S. Moro**, G. Sandonà, V. Sheeba, G. Zagotto "A versatile synthesis of the 1,4-dihydroxynaphthoquinone nucleus". *Tetrahedron Lett.* **31**, 6631-6634 (2000)

48. V. Cecchetti, **S. Moro**, C. Parolin, T. Pecere, E. Filipponi, A. Calistri, O. Tabarrini, B. Gatto, M. Palumbo, A. Fravolini, G. Palù "6-amino quinolones as new potential anti-HIV agents." *J. Med. Chem.* **43**, 3799-802. (2000)
47. G. Viola, E. Uriarte, **S. Moro** "Interactions between DNA and benzopsoralen analogues: thermodynamic and molecular modeling studies." *Farmaco* **55**, 276-86 (2000)
46. O. Bortolini, M. Carraro, V. Conte, **S. Moro**, "Models for the active site of vanadium dependent haloperoxidases: insight into the solution structure of peroxo vanadium compounds." *J. Bioinorg. Chem.* **80**, 41-49 (2000)
45. G. Zagotto, **S. Moro**, R. Supino, E. Favini, M. Palumbo "New 1,4-anthracene-9,10-dione derivatives as potential anticancer agents." *Farmaco* **55**, 1-5 (2000)
44. E. Soldaini, **S. Moro**, S. John, J. Bollenbacher, U. Schindler, W.J. Leonard "Dna binding site selection of dimeric and tetrameric Stat5 proteins reveals a large repertoire of divergent tetrameric Stat5a binding sites." *Mol. Cell. Biol.* **20**, 389-401 (2000)
43. G.G. Aloisi, F. Elisei, **S. Moro**, D. Vedaldi, F. Dall'Acqua "Photophysical behavior of thio- and seleno-psoralens." *Photochem. Photobiol.* **71**, 506-513 (2000)
42. O. Bortolini, M. Carraro, V. Conte, **S. Moro** "Histidine containing diperoxovanadium (V) compounds: insight on the solution structure by a 51V-NMR and ESI-MS comparative study." *Eur. J. Inorg. Chem.* **9**, 1489-1495 (1999)
41. **S. Moro**, M. Bonchio, G. Licini, G. Modena, O. Bortolini, W. A. Nugent "Enantioselective Ti(IV) sulfoxidation catalysts bearing C3-symmetric trialkanolamine ligands: solution speciation by 1H NMR and ESI-MS analysis." *J. Am. Chem Soc.* **121**, 6258-6268 (1999)
40. J.-I. Jiang, **S. Moro**, A.H. Li, S.-Y. Jang, L. Chang, N. Melman, X.D. Ji, E.B. Lobkovsky, J.C. Clardy, K.A. Jacobson "Chiral resolution and stereospecificity of 4-phenylethynyl-6-phenyl-1,4-dihydropyridines as selective A₃ adenosine receptor antagonists." *J. Med. Chem.* **42**, 3055-3065 (1999)
39. G. Miolo, **S. Moro**, D. Vedaldi, S. Caffieri, A. Guiotto, F. Dall'Acqua "New benzoquinolizin-5-one derivatives as furocoumarin analogs: DNA-interactions and molecular modeling studies." *Farmaco.* **54**, 551-61 (1999)

38. C. Hoffmann, **S. Moro**, R.A. Nicholas, T.K. Harden, K.A. Jacobson "The role of amino acids in intracellular loops of the human P2Y1 receptor surface expression and activation processes." *J. Biol. Chem.* **274**, 14639-14647 (1999)
37. C. Sissi, **S. Moro**, A.P. Krapcho, E. Menta, M. Palumbo "Binding of 2-aza-antracenedione regioisomers to DNA: effects of the relative position of the side-chain groups." *Anticancer-Drug Des.* **14**, 265-274 (1999)
36. **S. Moro**, C. Hoffmann, K.A. Jacobson "Role of the extracellular loops of G protein-coupled receptors in ligand recognition: a molecular modeling study of the human P2Y1 receptor." *Biochemistry* **38**, 3498-3507 (1999)
35. K.A. Jacobson, C. Hoffmann, Y.C. Kim, E. Camaioni, E. Nandan, S.Y. Jang, D.P. Guo, X.D. Ji, I. Kugelgen, **S. Moro** "Molecular recognition in P₂ receptors: ligand development aided by molecular modeling and mutagenesis." *Prog. Brain Res.* **120**, 119-132 (1999)
34. A.H. Li, **S. Moro**, N. Forsyth, N. Melman, X.D. Ji, K.A. Jacobson "Synthesis, CoMFA analysis, and receptor docking of 3,5-diacyl-2,4-disubstituted pyridine derivatives as selective A₃ adenosine receptor." *J. Med. Chem.* **42**, 706-721 (1999)
33. K.A. Jacobson, **S. Moro**, Y.C. Kim, A.H. Li "A₃ adenosine receptors: protective vs. damaging effects identified using novel agonists and antagonists." *Drug Devel. Res.* **55**, 113-124 (1998)
32. C. Sissi, L. Bolgan, **S. Moro**, G. Zagotto, C. Bailly, E. Menta, G. Capranico, M. Palumbo "DNA-binding preferences of bisantrene analogues: Relevance to sequence specificity of drug-mediated topoisomerase II poisoning." *Mol. Pharmacol.* **54**, 1036-1054 (1998)
31. Y.-C. Kim, **S. Moro**, M. de Zwart, L. Chang, N. Melman, A. P. Ijzerman, K.A. Jacobson "Derivatives of the Triazoloquinazoline Adenosine Antagonist (CGS15943) Having High Potency at the Human A_{2B} Receptor." *J. Med. Chem.* **41**, 2835-2845 (1998)
30. **S. Moro**, A.-H. Li, K.A. Jacobson "Molecular Modeling Studies of Human A₃ Adenosine Antagonists: Structural Homology and Receptor Docking." *J. Chem. Inf. Comput. Sci.* **38**, 1239-1248 (1998)

29. A.-H. Li, **S. Moro**, N. Melman, K.A. Jacobson "Structure Activity Relationships of 3,5-Diacyl-2,4-Dialkyl-6-Phenylpyridine Derivatives as Selective A₃ Adenosine Receptor Antagonists." *J. Med. Chem.* **41**, 3186-3201 (1998)
28. **S. Moro**, G. Danping, E. Camaioni, J.L. Boyer, K.T. Harden, K.A. Jacobson "Human P2Y₁ Receptor: Molecular Modeling and Site-Directed Mutagenesis as Tools to Identify Agonist and Antagonist Binding Sites." *J. Med. Chem.* **41**, 1456-1466 (1998)
27. G. Capranico, F. Guano, **S. Moro**, G. Zagotto, C. Sissi, B. Gatto, F. Zunino, E. Menta, M. Palumbo, "Mapping Drug Interactions at the Covalent Topoisomerase II-DNA Ccomplex by Bisantrone-Amsacrine Congeners." *J. Biol. Chem.* **273**, 12732-12739 (1998)
26. O. Bortolini, V. Conte, F. Di Furia, **S. Moro** "Direct Evidence on Solvent-Peroxovanadium Clusters by Electrospray Ionization Mass Spectrometry." *Eur. J. Inorg. Chem.* **8**, 1193-1197 (1998)
25. V. Conte, F. Di Furia, **S. Moro** "From the Speciation of Peroxovanadium Complexes in Aqueous Solution to the Chemistry of Haloperoxidases." in *Chemistry, Biochemistry and Therapeutic Application of Vanadium Compounds*. American Chemical Society Publication Division, 1155 Sixteenth street, N.W. Washington DC, 20036 (1998)
24. V. Conte, F. Di Furia, **S. Moro** "Solvation, Preferential Solvation and Complexation by the Solvent of Peroxovanadium Complexes Studied by ⁵¹V-NMR Spectroscopy. Correlations with the Oxidative Reactivity." *Inorg. Chim. Acta* **272**, 62-67 (1998)
23. **S. Moro**, M. A. van Rhee, L. H. Sanders, K. A. Jacobson "Flavonoid Derivatives as Adenosine Receptor Antagonist: a Comparison of the Hypothetical Binding Sites Based on a Comparative Molecular Field Analysis Model." *J. Med. Chem.* **41**, 46-52 (1998)
22. D. Vedaldi, **S. Moro**, G. G. Piazza, S. Caffieri, G. Miolo, G.G. Aloisi, F. Alisei, F. Dall'Acqua "1-Thiopsoralen, a New Photobiologically Active Heteropsoralen. Photophysical, Photochemical and Computer-Aided Studies." *Farmaco* **52**, 645-652 (1997)
21. M. Bonchio, S. Calloni, F. Di Furia, G. Licini, G. Modena, **S. Moro**, W. A. Nugent "Titanium(IV)-(R,R,R)-tris(2-phenylethoxy)amine Alkylperoxo Complex

Mediated Oxidations: the Biphilic Nature of the Oxygen Transfer to Organic Sulfur Compounds." *J. Am. Chem. Soc.* **119**, 6935-6936 (1997)

20. M. Bonchio, G. Licini, G. Modena, **S. Moro**, O. Bortolini, P. Traldi, W. A. Nugent "Use of Electrospray Ionization Mass Spectrometry to Characterize Reactive Intermediates in a Titanium Alkoxide Mediated Sulfoxidation Reaction." *Chem. Comm.* **7**, 869-870 (1997)

19. Bagno, V. Conte, F. Di Furia, **S. Moro** "The First Evidence of the Structure of Peroxovanadium Complexes in Aqueous Solution As Provided by *Ab Initio* Calculations." *J. Phy. Chem.* **101**, 4637-4640 (1997)

18. G. Zagotto, **S. Moro**, E. Uriarte, E. Ferrazzi, G. Palu', M. Palumbo "Amido Analogues of Mitoxantrone: Physico-Chemical Properties, Molecular Modeling, Cellular Effects and Antineoplastic Potential." *Anticancer-Drug Des.* **12**, 99-112 (1997)

17. R. Fornasier, S. Mammi, F. Marcuzzi, M. Morandin, **S. Moro** "Synthesis and Computational Study of a Capped Multifunctional Supramolecular Receptor: Eptakis-(6^A,6^C-Deoxy-6^B,6^D,6^E,6^F,6^G-Pentamino- β -Cyclodextrin." *Gazz. Chim. Ital.* **127**, 63-67 (1997)

16. V. Conte, F. Di Furia, **S. Moro** "The Chemistry of Peroxovanadium Species in Aqueous Solution. Structure and Reactivity of a Neutral Diperoxovanadium Complex as Provided by ⁵¹V-NMR, *Ab Initio* Calculations and Kinetic Results." *J. Mol. Cat.* **120**, 93-99 (1997)

15. V. Conte, F. Di Furia, **S. Moro** "Peroxovanadium Complexes as Radical Oxidants in Organic Solvents and in Aqueous Solutions." *J. Mol. Cat.* **117**, 139-148 (1997)

14. V. Conte, F. Di Furia, **S. Moro** "Synthesis of Brominated Compounds. A Convenient Molybdenum-Catalyzed Procedure Inspired by the Mode of Action of Haloperoxidases." *Tetrahedron Lett.* **37**, 8609-8612 (1996)

13. V. Conte, F. Di Furia, **S. Moro**, S. Rabbolini "A Mechanistic Investigation of Bromoperoxidases Mimicking System. Evidence of a Hypobromite-like Vanadium Intermediate from Experimental Data and *ab initio* Calculations." *J. Mol. Cat.* **113**, 175-184 (1996)

12. V. Conte, F. Di Furia, **S. Moro** "The Versatile Chemistry of Peroxometal Complexes as Oxidants of Organic Compounds." *J. Phys. Org. Chem.* **9**, 329-336 (1996)
11. M. Bonchio, S. Campestrini, V. Conte, F. Di Furia, **S. Moro** "A Theoretical and Experimental Investigation of the Electrophilic Oxidation of Thioethers and Sulfoxides by Peroxide." *Tetrahedron* **51**, 12363-12372 (1995)
10. V. Conte, F. Di Furia, **S. Moro** "A Possible Role of Vanadium in Biological Oxidations. The Oxidation of Uracil." *Gazz. Chim. Ital.* **125**, 563-568 (1995)
9. V. Conte, F. Di Furia, **S. Moro** "Studies Directed Toward the Prediction of the Oxidative Reactivity of Vanadium Peroxocomplexes in Aqueous Solution. Correlation between the Nature of the Ligands and ^{51}V -NMR Chemical Shifts." *J. Mol. Cat.* **104**, 159-169 (1995)
8. M. Anderson, V. Conte, F. Di Furia, **S. Moro** "Vanadium Bromoperoxidases Mimicking System: Bromohydrins Formation as Evidence of the Occurrence of a Hypobromite-like Vanadium Complex." *Tetrahedron Lett.* **36**, 2675-2678 (1995)
7. V. Conte, F. Di Furia, **S. Moro** " ^{51}V -NMR investigation on the formation of peroxo vanadium complexes in aqueous solution: some novel observations." *J. Mol. Cat.* **94**, 323-333 (1994)
6. Conte, F. Di Furia, **S. Moro** "Mimicking the Vanadium Bromoperoxidases Reactions: Mild and Selective Bromination of arenes and Alkenes in a Two-Phase System." *Tetrahedron Lett.* **35**, 7429-7432 (1994)
5. M. Bonchio, V. Conte, F. Di Furia, G. Modena, **S. Moro** "Mechanism of arenes hydroxylation by vanadium picolinato peroxocomplexes." *Org. Chem.* **59**, 6262-6267 (1994)
4. M. Bonchio, V. Conte, F. Di Furia, G. Modena, **S. Moro**, J. O. Edwards "Nature of the radical intermediates in the decomposition of peroxovanadium species in protic and aprotic media." *Inorg. Chem.* **33**, 1631-1637 (1994)
3. M. Bonchio, V. Conte, F. Di Furia, G. Modena, **S. Moro**; Reactivity of d^0 transition metal peroxocomplexes. in "Contribution to development of Coordination Chemistry". 14th Conference on Coordination Chemistry. Slovak Technical University press, 311-314 (1993)

2. M. Bonchio, T. Carofiglio, V. Conte, F. Di Furia, F. Magno, G. Modena, **S. Moro**, P. Pastore "Toward the prediction of d⁰ transition metal peroxo complexes oxidative behavior. The correlation between one electron reduction and oxygen-oxygen bond strength." *Inorg. Chem.* **32**, 5797-5799 (1993)
1. M. Bianchi, M. Bonchio, V. Conte, F. Coppa, F. Di Furia, G. Modena, **S. Moro**, S. Standen "Hydroxylation of aromatics with hydrogen peroxide catalyzed by vanadium(V) peroxocomplexes." *J. Mol. Cat.* **83**, 107-116 (1993)

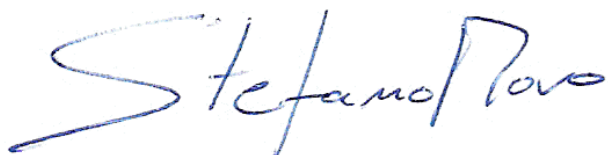
LIST OF PATENTS (2):

1. Spinelli S, **Moro S.** "2-Heteroarylbenzamide derivatives as MEK kinase inhibitors with antitumor activity." European Patent N. 07003478.0-2101 (2007)
2. Jacobson KA, Thatikonda, Kozma E, Spalluto G, **Moro S.** "Novel Fluorescent Antagonist as a Molecular Probe in A₃ Adenosine Receptor Binding Assays Using Flow Cytometry." U.S. Patent N. HHS E-073-2012/0-US-01 (2012)

LIST OF BOOK CHAPTERS (2):

1. Moro S, Morizzo E, Jacobson KA. "Molecular modeling and re-engineering of A₃ adenosine receptors" in *A₃ Adenosine Receptors from Cell Biology to Pharmacology and Therapeutics*. Springer (2009) - ISBN: 978-90-481-3143-3.
2. Bortolato A, Perruccio F, **Moro S.** "Successful Applications of In Silico Approaches for Lead/Drug Discovery" in *In silico Lead Discovery*. Benthan (2011) - ISBN: 978-1-60805-142-7.

Padova, 26 July 2018

A handwritten signature in blue ink that reads "Stefano Moro". The signature is written in a cursive, flowing style.

