UNIVERSITA' DEGLI STUDI DI PADOVA

DIPARTIMENTO DI SCIENZE DEL FARMACO

CURRICULUM DELLA ATTIVITÀ SCIENTIFICA E DIDATTICA

Stefano Moro

Padova, 2019

CURRICULUM VITAE ET STUDIORUM

Stefano Moro

Stefano Moro ha conseguito la Maturità' Tecnica in Chimica Industriale presso l'Istituto Tecnico Industriale "G. Natta" di Padova nel 1984 con punti 56/60.

Si è laureato in Chimica e Tecnologia Farmaceutiche il 13 marzo 1991, con punti 110 su 110 e Lode, presso l'Università degli Studi di Padova, discutendo la Tesi dal titolo: " Idrossilazione di derivati aromatici con perossocomplessi di Vanadio", svolta sotto la direzione del Prof. Fulvio Di Furia, presso il Dipartimento di Chimica Organica dell'Università degli Studi di Padova. Tale lavoro era inerente a tematiche di chimica fisica organica e meccanicistica ed in particolare allo studio del meccanismo delle reazioni di idrossilazione di derivati aromatici catalizzate da complessi metallo perossidici e delle loro possibili implicazioni biologiche.

Nel marzo 1991 ha ricevuto il **Premio Nazionale Federchimica**, per il lavoro di Tesi di Laurea dal titolo "Idrossilazione di derivati aromatici con perossocomplessi di Vanadio".

Dal 20 marzo 1991 al 30 settembre 1991 ha continuato a lavorare sotto la direzione del Prof. Fulvio Di Furia, occupandosi ancora di problemi correlati alla chimica fisica organica e meccanicistica ed in particolare alla reattività di complessi metallo-perossidici.

Dal 2 ottobre 1991 al 28 settembre 1992 ha svolto il servizio militare di leva.

Nel novembre 1991 ha conseguito l'ammissione alla frequenza della Scuola di Dottorato in Scienze Chimiche dell'Università di Padova.

Dal 1 novembre 1992 al 31 ottobre 1995 ha frequentato la Scuola di Dottorato in Scienze Chimiche dell'Università di Padova sotto la supervisione del Prof. Fulvio Di Furia, con una tesi di Dottorato di Ricerca dal titolo "Chimica dei perossocomplessi del vanadio in soluzione acquosa: aspetti strutturali, reattività ed implicazioni biologiche".

Nell' ottobre 1993 ha ricevuto il **Premio Nazionale Fondazione IBM Italia** in "Tecnologie Informatiche in Chimica" per l'attività svolta nella chimica computazionale dei perossocomplessi del vanadio applicati a problematiche strutturali, di reattività e loro implicazioni biologiche".

La tesi di dottorato è stata approvata nella sede di Padova il 5 febbraio 1996 mentre il titolo di Dottore di Ricerca gli è stato conferito il 5 novembre 1996. In

questo perido ha svolto uno studio sulla natura chimica e sulla reattività di specie perossidiche di vanadio in soluzione. Particolare attenzione è stata rivolta all'utilizzo tecnica spettroscopica ^{51}V-NMR ed alle diverse metodologie di calcolo quantomeccanico *ab initio*.

Dal 1 febbraio 1996 al 1 aprile 1997 ha collaborato con il Centro di Studio del Farmaco e delle Molecole Biologicamente Attive del C.N.R. di Padova in qualità di consulente in chimica computazionale presso il laboratorio di grafica computerizzata della suddetta struttura sotto la supervisione del Prof. Francesco Dall'Acqua. In questo periodo ha effettuato ricerche nel campo del meccanismo di interazione tra farmaci e DNA, utilizzando metodologie di chimica computazionale.

Dal 1 maggio 1996 al 14 gennaio 1997 ha conseguito una **Borsa di Studio Nazionale** del Centro Nazionale delle Ricerche (C.N.R.) presso il Centro di Studio sui Meccanismi di Reazioni Organiche di Padova, sotto la direzione del Prof. Giorgio Modena (Bando n.201.03.23 del 12/06/1995). In tale periodo ha effettuato ricerche relative al ruolo dei perossocomplessi di vanadio nell'attività delle bromoperossidasi vanadio-dipendenti ottenendo informazioni sulla reattività e sulla natura delle specie reattive da misure cinetiche, misure spettroscopiche ^{51}V-NMR e da calcoli quantomeccanici *ab initio*.

Dal 15 maggio 1997 al 04 dicembre 1998 ha usufruito di una borsa di studio biennale per attività di ricerca post-dottorato riservata all'area disciplinare delle "Scienze del Farmaco" presso il Dipartimento di Scienze Farmaceutiche dell'Università degli Studi di Padova sotto la supervisione del Prof. Francesco Dall'Acqua (Decreto Rettorale n. 6694/D del 18/10/96). In questo periodo ha svolto ricerche nel campo del meccanismo di interazione tra molecole a potenziale interesse bio-farmacologico e DNA, utilizzando metodologie di chimica computazionale.

Dal 15 gennaio 1997 al 04 dicembre 1998 ha svolto attività di ricerca in qualità di "Post-doctoral Fellow" presso il laboratorio di chimica computazionale del Molecular Recognition Section (Bio-organic Chemistry Laboratory), National Institute of Diabetes, Digestive and Kidney Diseases (NIDDK) presso il National Institutes of Health (NIH) di Bethesda (MD) USA, sotto la direzione del Dr. Kenneth Jacobson. Ha collaborato ad un progetto di ricerca sullo "Studio teorico della struttura tridimensionale dei recettori adenosinici e dell'ATP accoppiati alle proteine-G (GPCR) e progettazione tramite metodologie di drug-design di nuovi agonisti ed antagonisti diretti verso questi recettori".

Nell'aprile 1998 è stato premiato con il **N.I.H. Fellow Award for Research Excellence**, conferito dal National Institutes of Health (NIH), Bethesda (USA), come riconoscimento del lavoro svolto nello studio teorico della struttura tridimensionale dei recettori adenosinici e dell'ATP accoppiati alle proteine-G (GPCR).

Dal 04 dicembre 1998 ha preso servizio in qualitità di **Ricercatore Universitario** presso il Dipartimento di Scienze Farmaceutiche, Facoltà di Farmacia, dell' Università degli Studi di Padova (Decreto Rettorale n. 3641 del 18/12/1998).

Attualmente è responsabile della Sezione di Modellistica Molecolare presso il Dipartimento di Scienze Farmaceutiche dell'Università degli Studi di Padova.

Nel febbraio 2000 ha ricevuto **Premio Università di Padova "A. Mion"** per il lavoro scientifico svolto nell'ambito delle scienze chimiche.

Nel maggio 2000 ha ricevuto il **Premio Nazionale Federchimica**, per il lavoro di lavoro di ricerca svolto nell'ambito delle scienze chimiche.

Dal 3 giugno 2002 al 3 dicembre 2002 è stato **Visiting Professor** presso Swiss Federal Institute of Technology (ETH) di Zurigo dove ha condotto attività didattica e di ricerca presso il Department of Applied BioScience (Institut for Pharmaceutical Chemistry) diretto dal Prof. Gerd Folkers.

Nel settembre 2002 ha ricevuto il **Premio Nazionale Farmindustria**, per il lavoro di ricerca svolto nell'ambito delle scienze farmaceutiche.

Dal 27 febbraio 2006 è **Professore Associato** di Chimica Farmaceutica presso la Facoltà di Farmacia dell'Università degli Studi di Padova. E' inoltre responsabile della Sezione di Modellistica Molecolare presso il Dipartimento di Scienze Farmaceutiche dell'Università degli Studi di Padova.

Dal 01 dicembre 2011 è **Professore Straordinario** di Chimica Farmaceutica presso il Dipartimento di Scienze del Farmaco dell'Università degli Studi di Padova. Continua ad essere il responsabile della Sezione di Modellistica Molecolare presso il medesimo dipartimento dell'Università degli Studi di Padova.

Dal 01 dicembre 2015 è **Professore Ordinario** di Chimica Farmaceutica presso il Dipartimento di Scienze del Farmaco dell'Università degli Studi di Padova e responsabile della Sezione di Modellistica Molecolare presso il medesimo dipartimento dell'Università degli Studi di Padova.

Dal 01 gennaio 2014 al 31 dicembre 2016 ha ricoperto il ruolo di **Presidente della Sezione Veneto** della Società Chimica Italiana (SCI.

Il sottoscritto é autore di più di 260 pubblicazioni scientifiche e 2 brevetti internazionali la cui lista é di seguito riportata.

RICONOSCIMENTI DI MERITO

Stefano Moro

a. **Premio Nazionale Federchimica**, Marzo 1991 per la Tesi di Laurea Idrossilazione di derivati aromatici con perossocomplessi di Vanadio", Universita' degli Studi di Padova.

b. **Premio Nazionale Fondazione IBM Italia** in "Tecnologie Informatiche in Chimica", Perugia Ottobre 1993.

c. **N.I.H. Fellow Award for Research Excellence**, Aprile 1998. National Institutes of Health (NIH), National Institutes of Diabetes, Digestive and Kidney Diseases (NIDDK), Bethesda (USA),

d. **Premio Università di Padova "A. Mion"**, Febbraio 2000 per per il lavoro di lavoro di ricerca svolto nell'ambito delle Scienze Chimiche.

e. **Premio Nazionale Federchimica**, Maggio 2000 per per il lavoro di lavoro di ricerca svolto nell'ambito delle Scienze Chimiche.

f. **Premio Nazionale Farmindustria**, Settembre 2002 per per il lavoro di lavoro di ricerca svolto nell'ambito delle Scienze Farmaceutiche.

PARAMETRI BIBLIOMETRICI

Stefano Moro

n. pubblicazioni: 261
citazioni totali: 8594
h-index: 52

fonte Scopus (05/03/2019): https://www.scopus.com/authid/detail.uri?authorId=7004482135

ELENCO COMPLESSIVO DELLE PUBBLICAZIONI

Stefano Moro

261. Redenti S, Marcovih I, De Vita T, Perez C, De Zorzi R, Demitri N, Perez DI, Bottegoni G, Bisignano P, Bissaro M, **Moro S**, Martinez A, Storici P, Spalluto G, Cavalli A, Federico S. "A Triazolotriazine-based Dual GSK-3β/CK-1δ Ligand as a Potential Neuroprotective Agent Presenting Two Different Mechanisms of Enzymatic Inhibition." ChemMedChem. 14, 310-314 (2019).

260. Margiotta E, Deganutti G, **Moro S.** "Could the presence of sodium ion influence the accuracy and precision of the ligand-posing in the human A_{2A} adenosine receptor orthosteric binding site using a molecular docking approach? Insights from Dockbench." J Comput Aided Mol Des. 32, 1337-1346 (2018).

259. Bissaro M, Federico S, Salmaso V, Sturlese M, Spalluto G, **Moro S.** "Targeting protein kinase CK1δ with Riluzole: could it be one of the possible missing bricks to interpret its effect in the treatment of ALS from a molecular point of view?" ChemMedChem. 13, 2601-2605 (2018).

258. Salmaso V, **Moro S.** "Bridging Molecular Docking to Molecular Dynamics in Exploring Ligand-Protein Recognition Process: An Overview." Front Pharmacol. 22, 9, 923 (2018).

257. Federico S, Margiotta E, Salmaso V, Pastorin G, Kachler S, Klotz KN, **Moro S**, Spalluto G. "[1,2,4]Triazolo[1,5-c]pyrimidines as adenosine receptor antagonists: Modifications at the 8 position to reach selectivity towards A_3 adenosine receptor subtype." Eur J Med Chem. 5, 157, 837-851 (2018).

256. Pandya AN, Baraiya AB, Jalani HB, Pandya D, Kaila JC, Kachler S, Salmaso V, **Moro S**, Klotz KN, Vasu KK. "Discovery of 2-aminoimidazole and 2-amino imidazolyl-thiazoles as non-xanthine human adenosine A_3 receptor antagonists: SAR and molecular modeling studies." Medchemcomm. 13; 9, 676-684 (2018)

255. Sabbadin D, Salmaso V, Sturlese M, **Moro S.** "Supervised Molecular Dynamics (SuMD) Approaches in Drug Design." Methods Mol Biol. 1824, 287-298 (2018)

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 A2A 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 A_1 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 antimitotic 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 A_3 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 A_3 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 A2A 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. Moscetti 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, Strapazzon 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 azolylmethyl-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-a proline 567 hydroxylation: A new player in the VHL/HIF-1a 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. "β2 -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 a(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, Squarcialupi 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, Tosetto J, Moss TJ, Andreazza 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 C^2, 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, Tosetto 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 a-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, Digiacomo 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 Descov. 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 Triazoloquinoxaline 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 Descov. 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 Dibenzoquinolizinium 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-(Substituted)-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-Substituted 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 A_3 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 A_3 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 A_1 and A_3 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 A_1 and A_3 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.Orsolinib, M. Veronese "Anchimeric assistance e.ect on regioselective hydrolysis of branched PEGS: a mechanistic investigatigation". *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. Orsoline, A. Guitto, F.M. Veronese "PEG-ARAC conjugates for controllaled release. *Eur. J. Med. Chem.* **39**, 123-133 (2004)

78. C. Sissi, E. Leo, **S. Moro**, G. Capranico, 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. Chemm. 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 ▪-/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 A_3 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 A_3 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 Acedemic/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 A_3 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 studing 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 Flavinoids in Cell Function. Buslig B, and Manthey J eds., 2001, Kluwer Acedemic/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 $P2Y_1$ 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.-l. 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 A_3 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 entracellular 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 regioisomeres 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. Nandanan, S.Y. Jang, D.P. Guo, X.D. Ji, I. Kugelgen, **S. Moro** "Molecular recognition in P_2 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 analysys, and receptor docking of 3,5-diacyl-2,4-dislkylpyridine derivatives as selective A_3 adenosine receptor." *J. Med. Chem.* **42**, 706-721 (1999)

33. K.A. Jacobson, **S. Moro**, Y.C. Kim, A.H. Li "A_3 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 A_3 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 A_3 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 $P2Y_1$ 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 Bisantrene-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 Pubblication 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 ^{51}V-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, Phofochemical 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 Transfert 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 Potentail." *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 ^{51}V-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 Theorethical 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". 14^{th} Confernce 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 d^o 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)

Brevetti Internazionali

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 A_3 Adenosine Receptor Binding Assays Using Flow Cytometry." U.S. Patent N. HHS E-073-2012/0-US-01 (2012)

Capitoli di Libri

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.

In fede.

Padova, 05 Marzo 2019

Il sottoscritto, ai sensi della Legge 675/96 D.lgs 196/03 sulla riservatezza dei dati personali, dichiara di essere stato compiutamente informato delle finalità e modalità del trattamento dei dati consapevolmente forniti nel presente curriculum e di autorizzarne l'utilizzo e l'archiviazione in banca dati.