



UNIVERSITA' DEGLI STUDI DI PADOVA

DIPARTIMENTO DI SCIENZE DEL FARMACO

***CURRICULUM DELLA ATTIVITÀ SCIENTIFICA
E DIDATTICA***

Stefano Moro

Padova, 2017

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CURRICULUM VITAE ET STUDIORUM
Stefano Moro

Stefano Moro è nato a Treviso il 5 febbraio 1965 ed 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 periodo 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 $^{51}\text{V-NMR}$ 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 $^{51}\text{V-NMR}$ 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 qualità di **Ricercatore Universitario** presso il Dipartimento di Scienze Farmaceutiche, Facoltà di Farmacia, dell'Università degli Studi di Padova (Decreto Rettoriale 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 Farindustria**, 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 240 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", Università 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 Farindustria**, Settembre 2002 per per il lavoro di lavoro di ricerca svolto nell'ambito delle Scienze Farmaceutiche.

PARAMETRI BIBLIOMETRICI

Stefano Moro

n. pubblicazioni: 245
citazioni totali: 7280
h-index: 48

fonte Scopus (05/06/2017): <https://www.scopus.com/authid/detail.uri?authorId=7004482135>

ELENCO COMPLESSIVO DELLE PUBBLICAZIONI

Stefano Moro

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* (2017) in press
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. Squarzialupi 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).
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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)

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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)
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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)
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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)
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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)

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- Gene Mutation M72I in a Patient with Medullary Thyroid Cancer." *Exp Clin Endocrinol Diabetes*. 121, 546-550 (2013)
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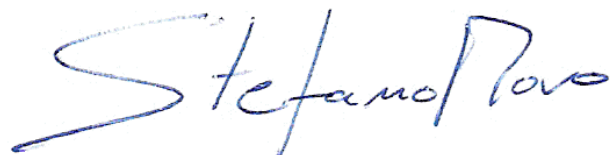
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Padova, 05 Giugno 2017



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