BiblioSketch

Stefano Moro

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

Bibliographic Sketch:

Stefano Moro received his M.S. degree in Medicinal Chemistry (1991) from University of Padova (Italy) and the Ph.D. degrees in Physical Organic Chemistry (1995) with Prof. Fulvio Di Furia at University of Padova. Following his doctoral studies, he was Fogarty Postdoctoral Associate with Dr. Kenneth Jacobson in the Molecular Recognition Section, National Institute of Diabetes, Digestive, and Kidney Diseases, of the National Institutes of Health in Bethesda (MD, USA), before joining again the University of Padova in 1999 as Assistant Professor. In 2003, Dr. Moro was invited as Visiting Professor at the School of Pharmacy of the ETH of Zurich, Switzerland.

He has authored or co-authored more than 250 original research papers and 2 EU patent. Until today, its H-index is equal to 51 extracted from more than 8000 citations (Scopus, 21/07/2018).

Stefano Moro is also the recipient of several national and international awards: March 1991: **Federchimica National Award for Young Research Excellence in Chemistry**; October 1993: **IBM Foundation National Award for Research Excellence in Chemistry**; January 1998: **N.I.H. Fellow Award for Research Excellence**; May 2000: **Federchimica National Award for Research Excellence in Chemistry**; September 2002: **Farmindustria National Award for Research Excellence in Medicinal Chemistry**. His name was included in the **VIA-Academy Top Italian Scientists**.

Selected publications:

1. 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. 1, 1-13 (2018)

2. 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)

3. Deganutti G, Moro S. "Estimation of kinetic and thermodynamic ligand-binding parameters using computational strategies." Future Med Chem. 9, 507-523 (2017)

4. Salmaso V, Sturlese M, Cuzzolin A, Moro S. "Exploring Protein-Peptide Recognition Pathways Using a Supervised Molecular Dynamics Approach." Structure 25, 655-662 (2017)

5. 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)

6. 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)

7. Ciancetta A, Sabbadin D, Federico S, Spalluto G, Moro S. "Advances in Computational Techniques to Study GPCR-Ligand Recognition." Trends Pharmacol Sci. 36, 878-890 (2015)

8. 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)

9. 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)

10. 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)

11. 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)

12. 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)

13. 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)

14. 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)

15. 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)