

Biomolecular Structures

www.chimica.unipd.it/stefano.mammi

+39 049 827 5293 (SM)



Stefano Mammi (stefano.mammi@unipd.it); Roberto Battistutta (roberto.battistutta@unipd.it); Massimo Bellanda (massimo.bellanda@unipd.it); Elisabetta Schievano (elisabetta.schievano@unipd.it); Andrea Calderan (andrea.calderan@unipd.it); Paolo Ruzza (paolo.ruzza@unipd.it)

The research of the Biomolecular Structure Group is addressed to the study of peptides and proteins. We investigate their chemical and structural properties with the goal to elucidate the molecular mechanisms at the basis of their biological activity in natural processes. We then apply this knowledge to try to modify the properties of selected targets (for instance for biotechnological applications) or to correct them when correlated to pathological states. The main experimental techniques we employ are multidimensional NMR and protein crystallography. Another focus of our research is the application of NMR, in combination with multivariate statistical analysis, to the metabolomic study of complex matrices such as food extracts and biological fluids. The applications range from the development of new methods to the traceability of food products to the development of new analytical tools to establish the *in vivo* effects of exogenous substances. Our main research lines are the following:

- Structural, functional and inhibition studies of oncogenic protein kinases CK2 and CDK2;
- Structural and functional characterization of SulP/SLC26 anion transporters;
- Enzyme engineering for industrial applications;
- Structure and interactions of proteins involved in the peculiar redox metabolism of pathogenic organisms;
- Fragment-based drug discovery by NMR and crystallography;
- Metabolomic analysis of food extracts and biological fluids;
- Traceability of foodstuff;
- Synthesis and characterization of peptide and peptidomimetics.
- *Molecular architecture and the structural basis for anion interaction in prestin and SLC26 transporters*, Nat. Comm., **2014**, 5, 3622-35.
- *Objective Definition of Monofloral and Polyfloral honeys Based on NMR Metabolomic Profiling*, J. Agric. Food Chem., **2016**, 64, 3645-3652.
- *Interactions of GFAP with ceftriaxone and phenytoin: SRCD and molecular docking and dynamic simulation*, Biochim. Biophys. Acta-Gen. Subj., **2016**, 1860, 2239-2248.
- *NMR Quantification of Carbohydrates in Complex Mixtures. A Challenge on Honey*, Anal. Chem., **2017**, 89, 13405-13414.
- *Polyamine-Based Thiols in Trypanosomatids: Evolution, Protein Structural Adaptations, and Biological Functions*. Antioxid. Redox Signal., **2018**, 28, 463– 486.