

Title	Rational design of nanoreceptors for sensing and molecular bio-trafficking
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## **Project description:**

The potential of macromolecular receptors is demonstrated by Nature. Proteins control almost any biological event using recognition to drive catalysis, signaling processes, ions translocation, etc. In the classic *supramolecular* approach, the receptor is a molecular entity designed following the principles of *complementarity* and *preorganization*. However, the complexity and specificity of natural receptors are still far from being reached. Monolayer Protected Gold Nanoparticles (MPGNs) offer an interesting shortcut to the development of macromolecular receptors by self-organization. Their coating can be considered as a threedimensional array of organic molecules grafted to the particle surface. The functional groups implemented can provide the in-



teractions for substrate recognition and the radial organization of the molecules on the particle surface multiply the number of interactions and provide some degree of preorganization. We have demonstrated that MPGNs can be turned into sensors and catalysts. Such an activity intrinsically implies the cooperative (or collective) recognition of substrate. However, the characterization and prediction of monolayer structure and activity are still challenging.

In this project, we aim at performing a deep investigation on the recognition properties of MPGNs. This will include synthesis of coating molecules and MPGNs, their structural characterization, the assessment of their binding properties, the investigation of their interactions with biological entities. The results obtained will be integrated with atomic molecular dynamic simulations (performed by our collaborators) to obtain a detailed picture. The **final goal will be the realization of nanoparticles with programmed molecular recognition** ability capable to detect **and translocate selected molecules in complex media**, including biological fluids and living organisms.

## Publications:

B. Perrone, F. Rastrelli, F. Mancin et al. *JACS* 2013, *135*, 11768; M.-V. Salvia, F. Rastrelli, F. Mancin, et al. *JACS* 2015, *137*, 886; M.-V. Salvia, G. Salassa, F. Rastrelli, F. Mancin *JACS* 2015, *137*, 11399; L. Riccardi, L. Gabrielli, X. Sun, F. De Biasi, F. Rastrelli, F. Mancin, M. De Vivo *Chem* 2017, *accepted*.

## **Collaborations/Network:**

Marco De Vivo, Istituto Italiano di Tecnologia, **Genova**; Monica Carril, CIG BIOMAguna, S. Sebastian, **Spagna**; Euan Kay, St. Andrew University, **UK**; Tomas Buergi, University of Geneve, **CH**.

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