|  |  |
| --- | --- |
| **Title** | **Nanoparticle-assisted NMR spectroscopy** |
| **PI** | RASTRELLI Federico |
| **Research Group** | Supramolecular Chemistry and Systems Chemistry – DiSC  |
| **Curriculum** | Scienze Chimiche |
| **Location** | Dipartimento di Scienze Chimiche (DiSC) |
| **Contact** | **web:** | www.chimica.unipd.it/federico.rastrelli |
|  | **email:** | federico.rastrelli@unipd.it |

**Project description:**

High-throughput, comprehensive, and accurate multi-profiling assays for metabolites are becoming increasingly popular in modern precision medicine, because they enable personalized diagnosis, uncover metabolic signatures of diseases, facilitate biomarkers discovery, and allow for therapeutic monitoring. In this context, nanoparticle-assisted NMR methods may play a key role due to their ability to output a full NMR spectrum of the analyte as readout signal, which allows an unambiguous detection and quantification of selected classes of molecules.

By exploiting different kinds of non-covalent interactions (namely hydrophobic, ion pairing, and metal−ligand coordination) gold nanoparticles (NPs) can in fact provide tailored binding sites for virtually any class of substrates. Remarkably, the variety of monolayers that can be potentially assembled endow a fine-tuning of these interactions not only in terms of selectivity, but also in terms of their strength.

The reduced translational and rotational diffusion rates resulting from the bulkiness of NPs offer a route to manipulate the magnetization of the receptor spins within the monolayer. We have shown how relaxation- and diffusion-based NMR techniques can be exploited to label and detect interacting analytes either by magnetization transfer or by perturbation of their apparent diffusion coefficient. In particular, when the interaction is weak, the spins located on the NPs monolayer can be used as a source of magnetization that is transferred selectively to the interacting analytes via NOE.

While the intrinsic sensitivity of the first reported protocols was modest, we have recently found that water spins in long-lived association at the nanoparticle monolayer constitute an alternative source of magnetization that can deliver a remarkable boost of sensitivity, especially when combined with saturation transfer experiments. The approach is general and can be applied to analyte-nanoreceptor systems of different compositions, eventually endowing selective analyte detection down to the micromolar range on standard instrumentation.

**Publications**:

F. De Biasi, D. Rosa-Gastaldo, X. Sun, F. Mancin, F. Rastrelli, *J. Am. Chem Soc.* 2019, **141**(12), 4870–4877.

B. Perrone, S. Springhetti, F. Ramadori, F. Rastrelli, and F. Mancin, *J. Am. Chem Soc*. 2013, **135**, 11768−11771.

**Hosting group(s) for the period abroad (**tentative list, may change):

1. Patrick Giraudeau, University of Nantes
2. Óscar Millet, Precision Medicine and Metabolism Lab, CIC bioGUNE