

One postdoc position (initially: 1+1 year) is available at the Department of Chemistry of the University of Padova and Istituto Italiano di Tecnologia (IIT), ideally starting from March 1, 2021. The position is funded by the AIRC Investigator Grant “Nanoparticle-Based Receptors for Catecholamine Profiling in Diagnosis and Prognosis of Neuroblastoma”. This call is for a postdoc position in Dr. De Vivo’s group at IIT in Genoa (Italy).

**Research area:** computational chemistry, molecular dynamics, high-throughput screening

**Keywords:** monolayer-protected nanoparticles, sensing, molecular recognition, self-assembly.

**Detailed description:**

High-throughput, comprehensive, and accurate multi-profiling assays of catecholamine metabolites are needed to diagnose and profile neuroblastomas. This research project is inspired by the hypothesis that nanoparticle-based receptors can be used to address this need. Prof. Mancin’s group at University of Padova have shown that purposely designed nanoparticles protected by a monolayer of organic molecules (MPNs) can selectively bind small molecule targets. (*J. Am. Chem. Soc.*, **2015**, *137*, 886; *J. Am. Chem. Soc.*, **2015**, *137*, 11399; *Chem Sci*, **2018** *9*, 4777). Thanks to several different NMR methods (“MPN-based NMR chemosensing”), it is possible to selectively and unambiguously detect and quantify multiple markers in solutions as well as metabolites in biological samples (*J. Am. Chem. Soc.*, **2013**, *135*, 1176; *Chem Eur. J.*, **2016**, *22*, 16955; *J. Am. Chem. Soc.*, **2019**, *141*, 4870). We recently demonstrated that computer-aided design can guide the affinity and selectivity of MPNs (*Chem*, **2017**, *3*, 92; *Angew. Chem.Int. Edit.*, **2019**, *58*, 7702). We now plan to develop and apply a computational approach for the fast and efficient in silico screening of MPN receptors for catecholamines. This approach will combine atomistic molecular dynamics simulations, enhanced sampling methods, AI, and high-throughput techniques. The computational effort will benefit from parallel experiments to synthesize and test the best MPN candidates, also on samples from patients, in collaboration with the Gaslini Hospital, in Genova.

**Working environment & conditions:**

We offer a challenging and multidisciplinary environment. The postdoc will work closely with other postdocs and graduate students involved in this and related projects. The ideal candidate will have a PhD in Chemistry, Physics, Physical Chemistry, or a related subject (or suitable postgraduate research experience) and a strong motivation to undertake a highly innovative research project. Other requisites are a good background in computational chemistry, experience in molecular dynamics simulations, and programming skills. Previous experiences with simulations of nanoparticles or computational high-throughput screening of protein-drug interaction are a plus.

**Contact**

The official call will be published in a couple of weeks on the website of University of Padova and its Department of Chemistry. Candidates interested in a pre-assessment should submit a curriculum vitae and the name and addresses of at least two reference scientists by e-mail to [marco.devivo@iit.it](mailto:marco.devivo@iit.it) and [fabrizio.mancin@unipd.it](mailto:fabrizio.mancin@unipd.it)