Master position available in
"Protein–ligand structure elucidation using sparse NMR data"
Julien Orts' group "BioNMR and Drug Discovery by Advanced NMR Methods"
University of Vienna

We seek an enthusiastic student to join our dynamic and innovative team in the "BioNMR and Drug Discovery by Adva nced NMR Methods" group at the Department of Pharmaceutical Sciences! You will work on an exciting project to explore new approaches in protein–ligand structure determination methods. This is a unique opportunity to make a significant contribution to the field of drug discovery.

We recently proposed *N*MR^2 as a powerful method to quickly elucidate protein–ligand complex structures not amenable to crystallography without having to perform the tedious step of protein resonance assignment.

As an intern, your task will be to further develop and explore the capabilities of this method. We will teach you how to analyze sparse NMR data and how to use them in molecular dynamic simulations to solve the structure of therapeutically relevant protein/ligand complexes. You should have a deep interest in advanced biophysical and spectroscopic technics applied to biological problems as well as knowledge in biophysical chemistry and/or computational sciences. This project is planned to be completed in a 6-month period. We offer extensive training in structural biology and advance NMR methods, a highly collaborative research environment and the possibility to conduct cutting edge research.

If you are interested in this position, please send your CV and motivation letter:
Nicolas Coudevylle
Department of Pharmaceutical Chemistry
Email: nicolas.coudevylle@univie.ac.at

References:

NMR Molecular Replacement Provides New Insights into Binding Modes to Bromodomains of BRD4 and TRIM24. Torres F *et al*. J Med Chem. **2022** Apr 14;65(7):5565-5574.

Protein-ligand structure determination with the NMR molecular replacement tool, NMR^2.
Orts J, Riek R. J Biomol NMR. **2020** Nov;74(10-11):633-642

Website of the group:
https://bionmr.univie.ac.at