

# Guest lectures

<b>Speaker</b>	<b>Dr. Andrea Cesari</b>
<b>Address</b>	<b>Fixed-term Junior Researcher (RTDa), Organic Chemist and NMR Spectroscopist at Università di Pisa</b>
<b>Title</b>	<b>1. From Sample to Spectrum: good practises in liquid-state NMR Spectroscopy</b> <b>2. Exploring the NMR toolkit for molecular recognition studies - from relaxation times to 2D maps</b> <b>3. Applications of liquid-state NMR spectroscopy in pharmaceutical technology</b> <b>4. Nanoparticle-based chemosensors using NMR spectroscopy</b>
<b>Date</b>	<b>13-17 May 2024</b>
<b>Time</b>	<b>See below</b>
<b>Place</b>	<b>Feringa Building &amp; ADL</b>
<b>Host</b>	<b>Prof.dr. P.C.A. van der Wel</b>
<b>Tel</b>	<b>+31 50 36 32 683</b>

## **Monday 13 May 2024 from 3-5 p.m. in room 5616.0125: Lecture 1**

### **1. From Sample to Spectrum: good practises in liquid-state NMR Spectroscopy (2 hours)**

This lecture will provide a practical guide to the proper NMR sample preparation, spectrometer setting-up, acquisition parameters selection, and FIDs processing/manipulation. A good routinary practice become necessary for the obtainment of quantitative and reproducible NMR spectra required for accurate analytical investigations (e.g. for pharmaceutical formulations) or complex mixtures characterization (e.g. metabolomics).

## **Tuesday 14 May 2024 from 1-3 p.m. in room 5615.0118: Lecture 2**

### **2. Exploring the NMR toolkit for molecular recognition studies - from relaxation times to 2D maps (2 hours)**

Nuclear Magnetic Resonance (NMR) spectroscopy is widely recognized as one of the most powerful and versatile analytical techniques. Stereochemical, dynamic, and thermodynamic features of a wide range of molecular entities (from small organic/organometallic species to polymeric materials) can be obtained. More advanced topics in liquid-state NMR spectroscopy will be explored in this lecture, including the measurements of relaxation times ( $T_1$ ,  $T_2$ ) and how 2D maps are constructed and

exploited. These pieces of information are fruitfully applied to the study of nanomaterials (e.g. loaded nanoparticles), sensors (through NOEs), and even hybrid materials (e.g. perovskites).

**Wed. 15 May 2024 from 9 a.m.-11a.m in ADL1\* room 3219.0024C: Lecture 3**

**3. Applications of liquid-state NMR spectroscopy in pharmaceutical technology (2 hours)**

This seminar focuses on applications of liquid-state NMR spectroscopy in pharmaceutical technology including structural and conformational elucidation, mucoadhesivity assessments, encapsulation efficiency quantification, and kinetic/controlled release analysis. Several case-studies will be discussed on drug delivery systems mainly based on oligosaccharides (cyclodextrins as pure, modified, nanosponges, or nanogels) and polysaccharides (modified chitosans).

**Friday 17 May 2024 from 9-11 a.m. in room 5616.0144: Lecture 4**

**4. Nanoparticle-based chemosensors using NMR spectroscopy (2 hours)**

NMR chemosensing take advantage of the use of Saturation Transfer Different (STD) techniques in combination with nanosized receptors. The aim is to extract an NMR spectrum containing only the resonances of the target analyte bound to the sensor, ultimately reducing the complexity of crowded spectra. In this seminar a general description of the NMR chemosensing approach will be given considering the description and characterization of supramolecular assemblies (monolayer-coated gold nanoparticles and cavitand-decorated silica nanoparticles) and the NMR methods used from NOE pumping towards novel high-power water STD.

\*ADL1 = Antonius Deusinglaan 1, 9713 AV Groningen; ADL1 building

All other lectures are on the Zernike campus.