Remote NMR

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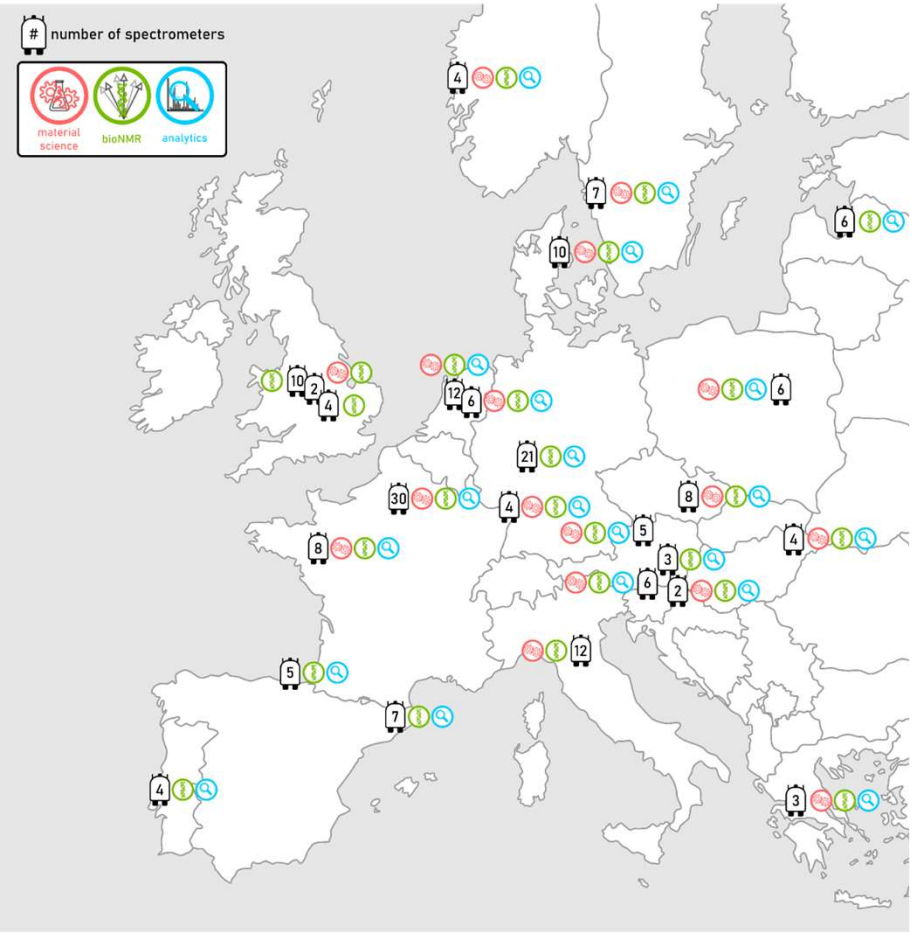
project manager

Remote NMR (R-NMR) moving NMR Infrastrutures to Remote Access Capabilities



Introduce remote measurement at all major NMR Research Infrastructures throughout Europe

Main R-NMR Project Objectives

- Standardized remote access procedures
- Common practices to ship samples
- Training programs on remote access
- FAIR data sharing and archiving
- Monitor carbon footprint of NMR facilities

Review: Remote NMR Landscape

Define: Procedures

Implement: Standardized Remote NMR Procedures

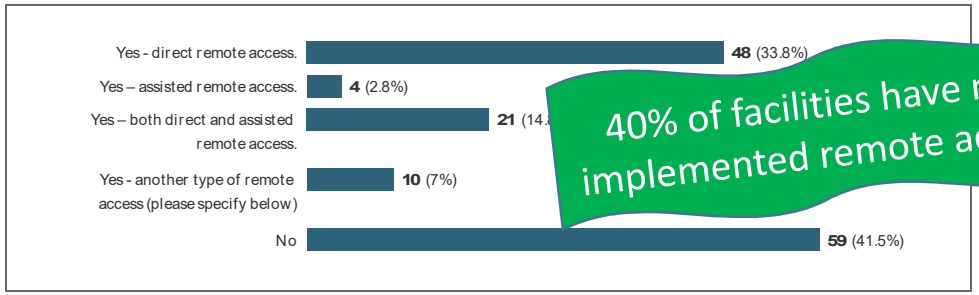
This project has received funding from the European Union's Horizon Europe research and innovation programme under Grant Agreement N. 101058595

www.r-nmr.eu

Review: Remote NMR landscape

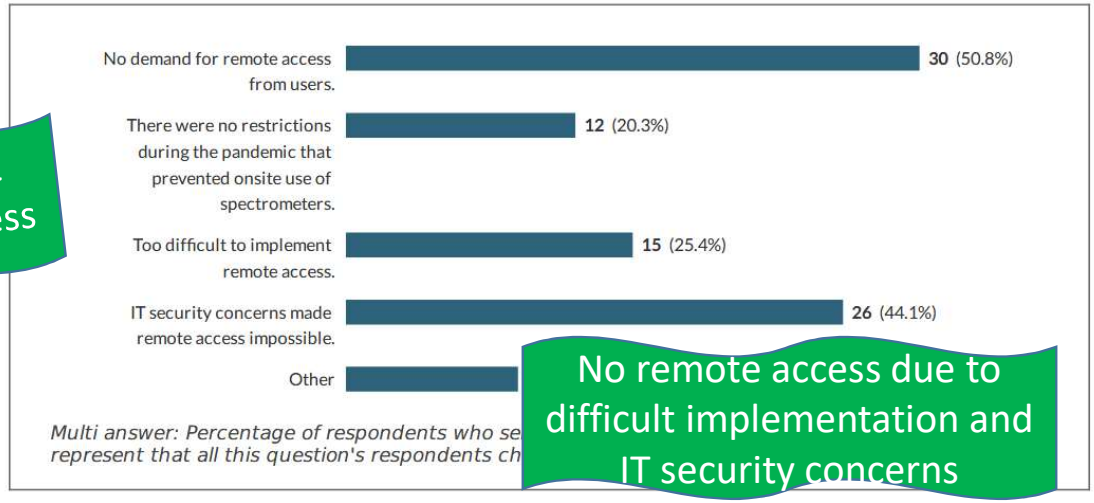
- **NMR facility manager (142) survey and NMR user (401) survey**
- **Research field, software, sample handling, data security, interactions with users, sample shipment, remote access**

23 Prior to, during and since the Covid19 pandemic, did you provide remote access to one or more of the NMR spectrometers in your facility? By remote access, we mean that either: 1) users could directly operate the NMR spectrometer by remote login to the NMR spectrometer computer (direct remote access), or 2) users could communicate via a computer linkup (Zoom/Teams etc) or telephone with a local operator who controlled the NMR spectrometer based on the information provided by the remote user (assisted remote access), or 3) some other type of remote access.



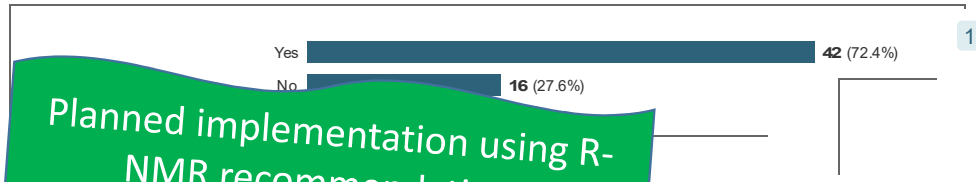
40% of facilities have not implemented remote access

23.b Why has remote access to spectrometers not been implemented in your facility? (select any that apply)



No remote access due to difficult implementation and IT security concerns

23.c The aim of the Remote-NMR project is to develop a common framework for remote spectrometer access taking into account best practice across the EU/UK. Standardized training for remote access will also be put in place. Once this has been completed, would your NMR facility be interested in implementing remote spectrometer access?



Planned implementation using R-NMR recommendations

11.d Do you consider sample shipment/delivery to an NMR facility to be a barrier to remote spectrometer access?

Sample shipment is a barrier

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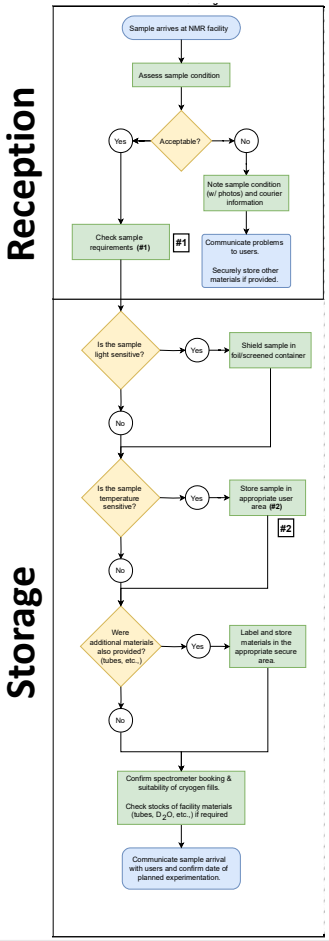
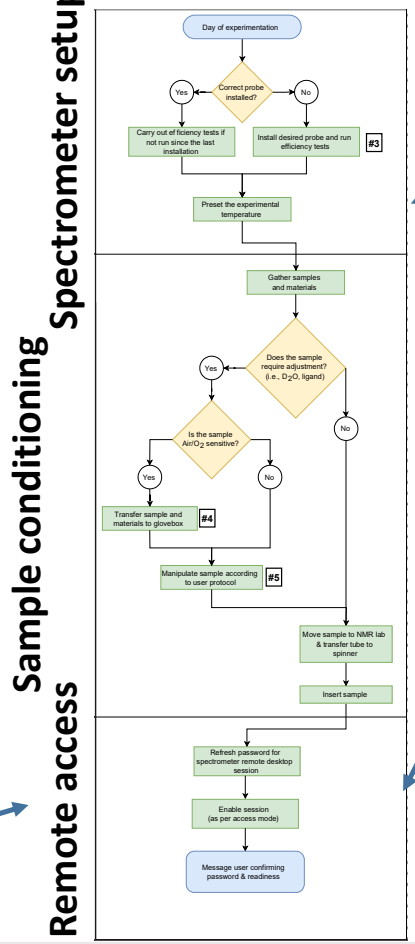
Procedures for remote NMR



Sample shipment

GDPR factsheet

Software for remote access



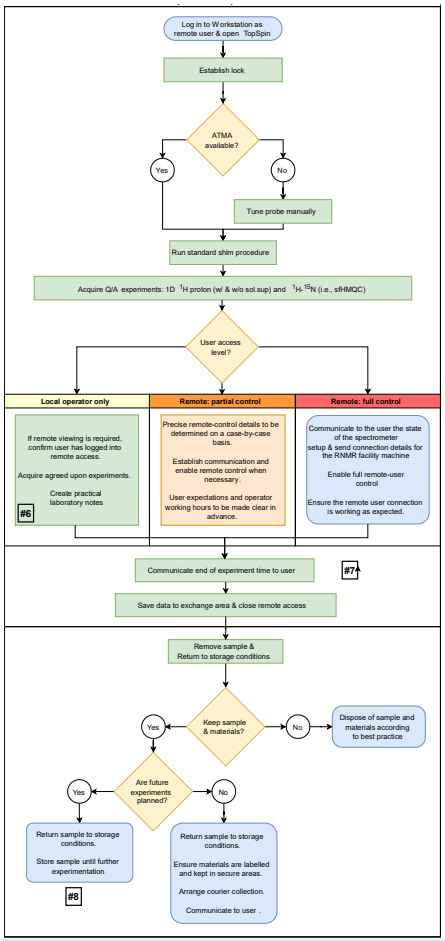
Standardization of experiments

Data & Metadata standards

User access levels

Data storage and access

Sample shipment



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CO_2 footprint

Carbon footprint of NMR instruments

Country: Germany

CO_2 equivalents: 80 g/kWh

Site setup			CO_2 equivalents	Boil off		Power consumption			
Magnet	Console	Helium supply		Helium	Nitrogen	Spectrometer	He liq	N liq	
800 (4K)	Solid state	Remote (USA)	15462 kg/ year	7.9 L/ week	100 L/ week	3.8 kW	0.66 kW	0.30 kW	details
600 (4K)	Liquid state	Remote (Qatar/Algeria)	8479 kg/ year	2.7 L/ week	50 L/ week	2.1 kW	0.23 kW	0.15 kW	details
600 (4K)	Liquid w/cryo	Remote (Qatar/Algeria)	45899 kg/ year	2.7 L/ week	50 L/ week	13.7 kW	0.23 kW	0.15 kW	details
1000 (4K)	Solids & liquids	Local coldhead/pulsed tube	13337 kg/ year	13.4 L/ week	67 L/ week	3 kW	0.93 kW	0.20 kW	details
1200 (2K)	Solids & liquids w/cryo	Local turbine	38072 kg/ year	42.0 L/ week	150 L/ week	9.3 kW	1.56 kW	0.45 kW	details
		Total		3584 L/ year	21758 L/ year				

Add spectrometer

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Add spectrometer

Calculation details

Item	Consumption	Conversion	Energy	CO_2 equiv
He boil off (1200 MHz)	42.0 L/week	6.22 kWh/L 368 gCO_2/kWh (Germany)	13636 kWh/year	5018 kg/year
N boil off (1200 MHz)	150.0 L/week	500 Wh/L 368 gCO_2/kWh (Germany)	3913 kWh/year	1440 kg/year
Console (Solids & liquids w/cryo)	8.8 kW	368 gCO_2/kWh (Germany)	81524 kWh/year	30001 kg/year
Magnet pumping	500 W	368 gCO_2/kWh (Germany)	4383 kWh/year	1613 kg/year
Total			103456 kWh/year	38072 kg/year

Calculation explanations

See explanations and justification of calculations here.

The carbon calculator version 1.1.3 is created by Thomas Vosegaard from the R-NMR report "Monit

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Opportunities and Challenges of remote access

- **Resilience of critical infrastructures**
- **Less traveling necessary/ Access possible for researchers from lower-income countries**
- **Focus on in person access for training**
- **Better reconciliation of family, care and work**

- **Standardized processes save time and increase quality of access**
  - Sample shipment
  - Standard experiments
  - User access levels
  - Standardized data, metadata, data storage and access

- **Data security needs to be improved**
- **IT infrastructure needs to be improved**
- **Remote measurement requires in house assistance**

Financial consequences of remote access is such that IT and assistance is more work and requires more resources at the facilities.

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