

NMR FACILITY MANUAL

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V1.0/2021

Preamble

Starting on February 2022, the CQE NMR facility will implement a new online booking system using the *Bookkit* platform by *Clustermarket*.

This system will improve time usage and facilitate the communication between NMR Staff and users. This will also make accounting much easier and more transparent as the system allows each user to track his/her own time consumption.

As this is a remotely operated system, presential bookings will end after an adaptation period. Current users will be added to the system during January 2022 and new users will be added after completion of the appropriate training by the NMR staff.

Due to software limitations, some adjustments of the previously used time slots have been made. Also, due to the variable maintenance and consumable prices, it is not possible to define an hour-based price for each machine. Therefore, all time consumption is measured as units per hour. The real cost of utilization will be defined at the end of the year based on the final balance.

This manual describes in detail all the new time slot adjustments and the use of the new booking system.

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Laboratory	Location	Ext.
Low-field NMR lab	Técnico Alameda Complexo Interdisciplinar 4 th floor Room 421	3228
High-Field NMR lab	Técnico Alameda Complexo Interdisciplinar 1 st floor Room 123	3839
SS-NMR lab	Técnico Alameda Complexo Interdisciplinar 1 st floor Room 121	3043

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NMR Facility



NMR Facility description and operation

1. Available equipment

1.1. Bruker 300 MHz Avance II NMR spectrometer, 5 mm BBO probe

The 300 MHz NMR spectrometer is installed in room 421, on the 4th floor of Complexo I. This equipment is permanently outfitted with a 5 mm two-channel (¹H and X) Broad Band probe.

1.1.1. Available nuclei and experiments

Besides the standard ¹H and ¹³C 1D experiments, this equipment allows for the observation of the following nuclei at the respective frequencies.

Nuclei	Tuning frequency (MHz)	Relative abundance (%)
¹ H	300.000	99.99
⁷ Li	116.586	92.58
¹¹ B	96.2520	80.42
¹³ C	75.4350	1.110
¹⁹ F	282.021	100.0
²³ Na	79.3560	100.0
²⁷ Al	78.1710	100.0
³¹ P	121.443	100.0
⁵¹ V	78.8640	99.76
⁹⁵ Mo	19.5450	15.72
¹¹⁹ Sn	111.816	8.850
¹⁹⁵ Pt	64.4940	33.80

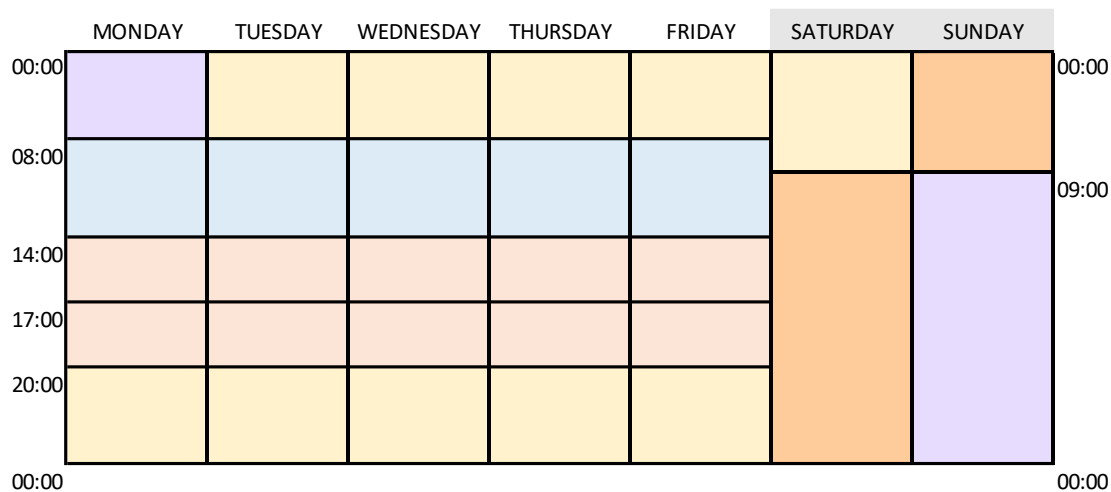
2D experiments are also available in this equipment, as well as temperature variation experiments (VT up and VT down). VT experiments are limited to the temperature range of -80 to +120 °C.



1.1.2. Time slot division and pricing

Time slots in the 300 MHz spectrometer are divided according to the following scheme.

Pricing is fixed at 1 unit/hour of use, being the real cost of each hour of use adjusted based on the year balance. VT experiments have added costs depending on the type and duration of the experiment.

NMR Facility



	30 min blocks	weekdays	08 - 14h
	3-hour blocks	weekdays	14 - 17h and 17 - 20h
	Weeknights	weekdays	20 - 08h (09h Friday)
	Weekend (Sat)	Saturday	09 - 09h
	Weekend (Sun)	Sunday	09 - 08h

Slot	Scheduling	Maximum per user
30 min blocks	Monday - Friday 08:00 – 14:00	2 blocks/day
3-hour blocks	Monday – Friday 14:00 – 17:00 – 20:00	6 hours/week or 3h+night/week
Weeknights	Monday - Thursday 20:00 – 08:00 Friday 20:00 – 09:00	1 night/week
Weekends (full day)	Saturday 09:00 – 09:00 Sunday 09:00-08:00	--

Booking of each time slot is restricted to specific time intervals. While *weeknights*, *weekends* and *3-hour blocks* may be booked one week in advance, the *30 min blocks* can only be booked 30 hours before.

1.1.3. User access rules

Only properly trained users have access to this spectrometer. VT experiments can only be performed by qualified personnel and after authorization by the management staff.

VT experiments can only be performed during the 3-hour blocks. VT down experiments cannot be performed at night.

NMR Facility



1.2. Bruker 400 MHz Avance II NMR spectrometer, 5 mm BBO probe

The 400 MHz NMR spectrometer is installed in room 421, on the 4th floor of Complexo I. This equipment is permanently outfitted with a 5 mm two-channel (¹H and X) Broad Band probe.

1.2.1. Available nuclei and experiments

Besides the standard ¹H and ¹³C 1D experiments, this equipment allows for the observation of the following nuclei at the respective frequencies.

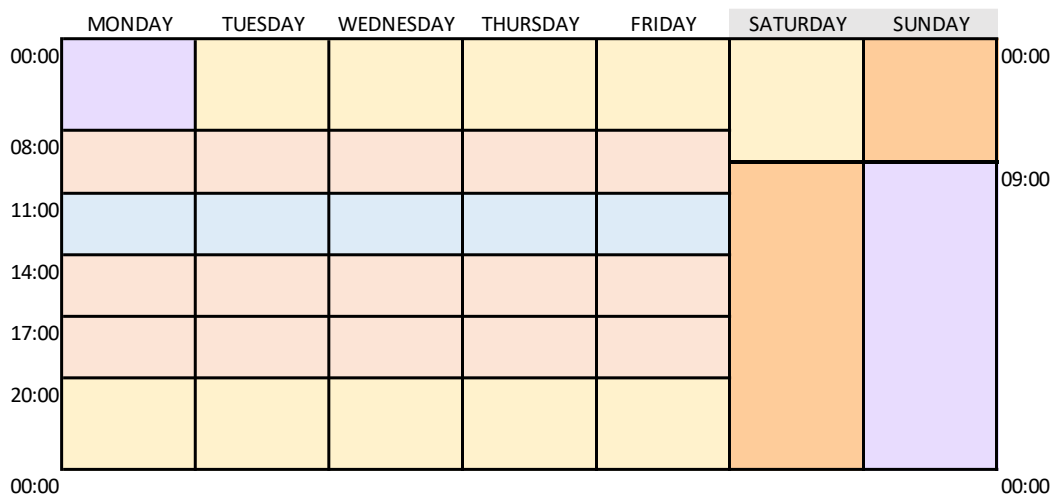
Nuclei	Tuning frequency (MHz)	Relative abundance (%)
¹ H	400.000	99.99
⁷ Li	155.448	92.58
¹¹ B	128.336	80.42
¹³ C	100.58	1.110
¹⁵ N	40.532	0.3700
¹⁹ F	376.028	100.0
²³ Na	105.808	100.0
²⁷ Al	104.228	100.0
²⁹ Si	79.46	4.700
³¹ P	161.924	100.0
⁵¹ V	105.152	99.76
⁹⁵ Mo	26.06	15.72
¹¹⁹ Sn	149.088	8.850
¹⁹⁵ Pt	85.992	33.80

1.2.2. Time slot division and pricing

Time slots in the 400 MHz spectrometer are divided according to the following scheme.

Pricing is fixed at 1 unit/hour of use, being the real cost of each hour of use adjusted based on the year balance. VT experiments have added costs depending on the type and duration of the experiment.

NMR Facility



	30 min blocks	weekdays	11 - 14h
	3-hour blocks	weekdays	08 - 11h, 14 - 17h and 17 - 20h
	Weeknights	weekdays	20 - 08h (09h Friday)
	Weekend (Sat)	Saturday	09 - 09h
	Weekend (Sun)	Sunday	09 - 08h

Slot	Scheduling	Maximum per user
30 min blocks	Monday - Friday 11:00 – 14:00	2 blocks/day
3-hour blocks	Monday – Friday 08:00 – 11:00 14:00 – 17:00 – 20:00	6 hours/week or 3h+night/week
Weeknights	Monday - Thursday 20:00 – 08:00 Friday 20:00 – 09:00	1 night/week
Weekends (full day)	Saturday 09:00 – 09:00 Sunday 09:00-08:00	--

Booking of each time slot is restricted to specific time intervals. While *weeknights*, *weekends* and *3-hour blocks* may be booked one week in advance, the *30 min blocks* can only be booked 30 hours before.

1.2.3. User access rules

Only properly trained users have access to this spectrometer. VT experiments can only be performed by qualified personnel and after authorization by the management staff.

VT experiments can only be performed during the 3-hour blocks. VT down experiments cannot be performed at night.

NMR Facility



1.3. Bruker 500 MHz Avance II+ NMR spectrometer

The 500 MHz NMR spectrometer is installed in room 123, on the 1st floor of Complexo I.

This equipment is only available for used that have completed the advanced training program and whose work justifies the recurrent use of this machine. Punctual uses of the 500 MHz spectrometer are possible under the supervision of one of the staff members and upon authorization.

Major operations in the hardware (ex. cable and filter connections, probe exchange) can only be performed by the staff.

1.3.1. Available probes and experiments

A wide variety of probes is available:

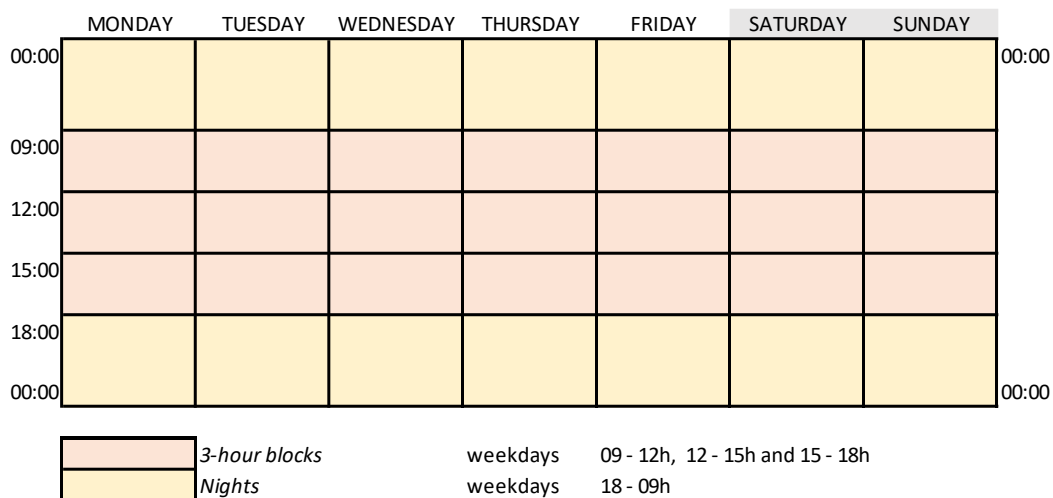
Probe	Sample holder	Nuclei
BBO 3 mm	3 mm tube	^1H , ^{31}P - ^{15}N
BBO 5 mm	5 mm tube	^1H , ^{31}P - ^{15}N
BBO 10 mm	10 mm tube	^1H , ^{31}P - ^{15}N
TXI 5 mm	5 mm tube	^1H , ^{13}C , ^{15}N
HR-MAS	4 mm rotor	^1H , ^{13}C , ^{31}P
Low Band	10 mm tube	^1H , $<^{15}\text{N}$
Diffusion	5 mm tube	^1H , ^{31}P - ^{15}N
SS-NMR	4 mm rotors	^1H , ^{19}F , ^{31}P - ^{15}N (CP-MAS)

1.3.2. Time slot division and pricing

Time slots in the 500 MHz spectrometer are divided according to the following scheme.

Pricing is fixed at 10 unit/hour of use, being the real cost of each hour of use adjusted based on the year balance. VT experiments have added costs depending on the type and duration of the experiment.

NMR Facility



Slot	Scheduling	Maximum per user
<i>3-hour blocks</i>	09:00 – 12:00 – 15:00 – 18:00	--
<i>Nights</i>	18:00 – 09:00	--

1.3.3. User access rules

Access to the 500 MHz spectrometer is restricted to specialized users. Access may be granted upon request and after specific training.

Users failing to comply with the established rules will lose access to this facility.

Booking system



NMR booking system

2. *Bookkit* management system

In 2022 the automated booking and accounting system *Bookkit* by *Clustermarket* will be implemented. This system is designed to increase flexibility and improve time usage of the available NMR spectrometers.

2.1. User types and permissions

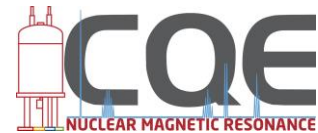
The booking system has been configured to allow the existence of two types of user: **Administrator** and **Researcher**. Each user type has different permission levels.

Administrator-type users can override all the operations performed by other users. These can also add and remove users, add permissions to each user and allocate each user to a specific accounting group. Administrators can also make the facility unavailable for maintenance purposes, delete booking slots and book special time slots for a specific user if requested.

All NMR users are added to the system as **Researcher**. This allows each user to browse the booking system for each spectrometer, schedule time slots and manage his own booked slots.

Important note: Time slots can be booked in advance according to the established rules for each machine and scheduling. Each user may cancel his own booking up to 1 hour before starting time. Once the booked time as started, it is not possible to cancel it.

Booking system



2.2. Registration and access

Each registered user will receive an e-mail with a link to the registration page. Upon clicking the link, the Sign Up page of *Bookkit* will show up asking you to register on the system.

Please fill in the fields as requested. In the *Email* box use your institutional e-mail address (ex. john.smith@tecnico.ulisboa.pt). Gmail, Hotmail, etc. are not allowed.

In the *Phone* field, please indicate your research group using the numbers 1 to 9 for CQE groups and the number 999 for external users.

In the *Sector* field, please select “Academia”.

After checking the “I agree” box and clicking “Sign Up”, you will receive an e-mail with instruction to confirm your registration. Please check your spam box if you have not received the e-mail.

Follow the instructions given in the e-mail.

Sign Up

Already have an account? [Log in here.](#)

First Name

Last Name

Email

Phone

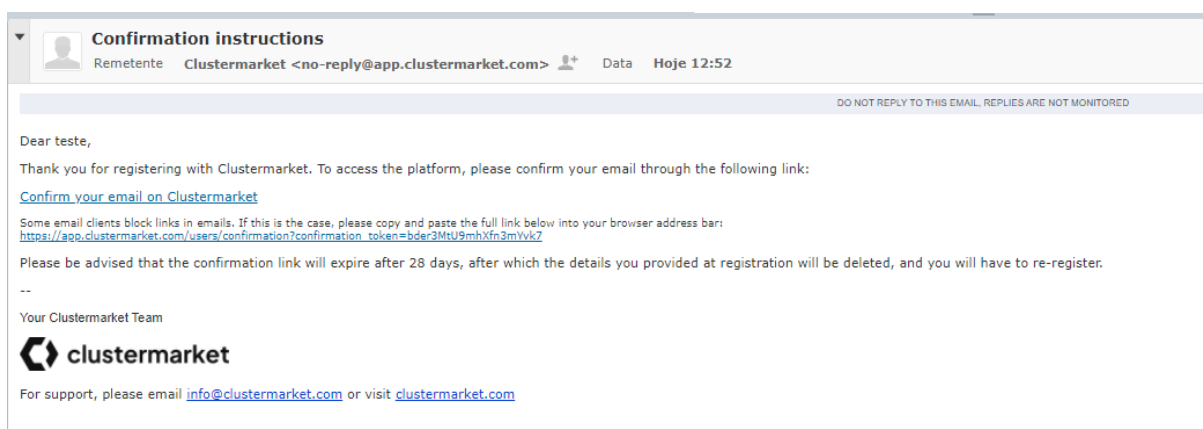
Password

Sector

How did you hear about us?

I agree to the [Terms of Use](#) and [Privacy Policy](#)

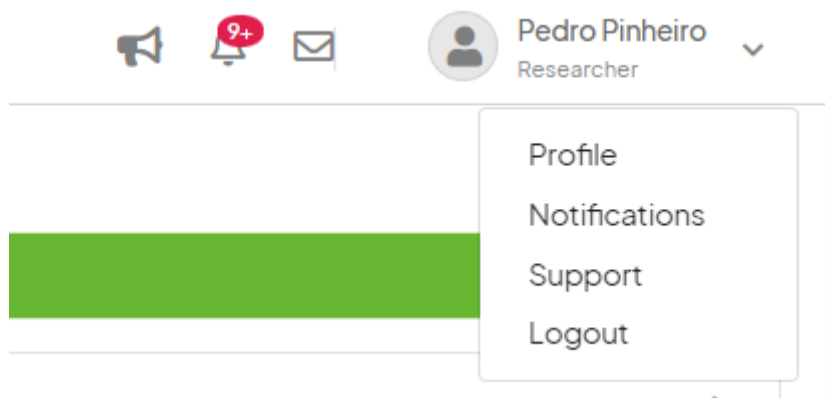
[Log in with your organisation](#)



2.3. Account setup

The *Bookkit* system allows each user to select the level of information sent by e-mail. By default, each user will receive an e-mail for each action performed by any user on the system. This is undesirable. You can control this in the “Notifications” tab of the personal area. Click the arrow right to your username (upper right corner of the screen).

Booking system



Select “Notifications” and select the appropriate level of notifications you wish to receive. It is advisable to deselect all the notifications in the “Equipment Sharing” tab:

	As Provider	As Customer	On behalf of labs
All	No <input type="radio"/> Yes <input type="radio"/>	No <input type="radio"/> Yes <input type="radio"/>	No <input type="radio"/> Yes <input type="radio"/>
About external equipment bookings.	No <input type="radio"/> Yes <input type="radio"/>	No <input type="radio"/> Yes <input type="radio"/>	No <input type="radio"/> Yes <input type="radio"/>
About external equipment preapprovals.	No <input type="radio"/> Yes <input type="radio"/>	No <input type="radio"/> Yes <input type="radio"/>	No <input type="radio"/> Yes <input type="radio"/>
About external equipment requests.	No <input type="radio"/> Yes <input type="radio"/>	No <input type="radio"/> Yes <input type="radio"/>	No <input type="radio"/> Yes <input type="radio"/>
About changes to equipment bookings.	No <input type="radio"/> Yes <input type="radio"/>	No <input type="radio"/> Yes <input type="radio"/>	
About internal equipment bookings.	No <input type="radio"/> Yes <input type="radio"/>	No <input type="radio"/> Yes <input type="radio"/>	
About internal equipment requests.	No <input type="radio"/> Yes <input type="radio"/>	No <input type="radio"/> Yes <input type="radio"/>	
When a lab member uploads a new equipment.	No <input type="radio"/> Yes <input type="radio"/>		No <input type="radio"/> Yes <input type="radio"/>

Please note that, by doing this, you will not receive any e-mail notifications regarding your own bookings. However, you will be informed of any Administrator-performed operations.

2.4. Login

We recommend that you save the link (<https://app.clustermarket.com>) as a bookmark in your internet browser. You may also choose to access the system via the link in the Lab webpage or on CQE’s NMR webpage.

The login credentials are the same used when registering the *Bookkit* system. Please note that your login credentials should not be shared with other users. If you suspect that your account has been compromised, please notify the staff immediately.

2.5. Browsing time slots and booking

On the main page of the *Bookkit* system you will find on the left side the navigation pane where you can visualize all your booked slots (clicking on My Dashboard), check your bookings (My Bookings), visualize all the available equipment (Equipment), and where you can also find a summary of all the equipment and booked slots (Lab Dashboard). There is also a dropdown list where you can select the lab you want to consult if your account is linked to other labs.

Booking system



Slot booking is performed easily in two steps.

STEP 1 – CHOOSE THE EQUIPMENT

Except for the 500 MHz spectrometer, due to the fact that each machine has different time slots, each one has been divided into three “pieces of equipment”.

Spectrometer	Piece of equipment	Time slots available
300 MHz	NMR300 30 min blocks (08h-14h)	30 min slots, Mon-Fry, 08-14h
	NMR300 3 h blocks (14h-20h+night)	3h slots, Mon-Fry, 14-20h+night
	NMR300 weekends (09h-09h)	Weekend full day
400 MHz	NMR400 30 min blocks (11h-14h)	30 min slots, Mon-Fry, 11-14h
	NMR400 3h blocks (8h-11h; 14h-20h+night)	3h slots, Mon-Fry, 8h-11h and 14-20h+night
	NMR400 weekends (09h-09h)	Weekend full day
500 MHz	NMR 500	3h slots

These different pieces of equipment appear in your Dashboard and Lab Dashboard as follows:

Booking system



Equipment	
123	NMR 500
421	NMR300 30 min blocks (08h-14h)
	NMR300 3 h blocks (14h-20h+night)
	NMR300 weekends (09h-09h)
	NMR400 30 min blocks (11h-14h)
	NMR400 3h blocks (8h-11h;14h-20h+night)
	NMR400 weekends (09h-09h)

To book a time slot in one of these equipment, just click on it.

STEP 2 – SELECT AVAILABLE SLOT

Example for time slot booking on “NMR300 30 min blocks (08-14h)”

Once the appropriate equipment has been selected, the calendar for the current week will be presented with all the available time slots, booked slots and bookings by the current user. Other users' bookings will be presented in grey, your bookings will appear green, and the unavailable slots will be marked red or dark grey.

Booking system



Book equipment

Booking calendar

Learn more about using the calendar: ?

today < >

20 - 26 Dec 2021

day week month

	Mon 20/12	Tue 21/12	Wed 22/12	Thu 23/12	Fri 24/12	Sat 25/12	Sun 26/12
07							
08	8:00 - 9:00 My own booking						
09							
10			9:30 - 10:00 César Reis 10:00 - 10:30 Carina Fialho 10:30 - 11:00 Vanessa Cacho				
11		10:30 - 11:00 Claudia Figueira 11:00 - 12:00 Vanessa Cacho					
12		12:00 - 13:00 César Reis					
13							

■ Announcements ■ Mybooking ■ Member booking ■ External booking ■ Not available

To book a slot, just click the time you wish to start your booking. This will be presented in blue.

Please remember that booking of some time slots is only available 30 hours in advance. Other slots may be booked up to 7 days in advance. Also, the system does not allow for booking overlap and will also prevent booking outside the predetermined slots. This will be shown as a red message on the top of the screen. Also, if you exceed the daily or weekly booking limit, a message will be shown. Exceptions may be granted to users who request it to the NMR staff.

Booking system



Book equipment

Booking calendar Learn more about using the calendar: ?

today < > 20 - 26 Dec 2021 day week month

	Mon 20/12	Tue 21/12	Wed 22/12	Thu 23/12	Fri 24/12	Sat 25/12	Sun 26/12
07							
08	8:00 - 9:00 My own booking		8:00 - 8:30 Equipment				
09							
10			9:30 - 10:00 César Reis 10:00 - 10:30 Carina Fialho				
11		10:30 - 11:00 Claudia Figueira 11:00 - 12:00 Vanessa Cacho	10:30 - 11:00 Vanessa Cacho				
12		12:00 - 13:00 César Reis					
13							

■ Announcements
 ■ My booking
 ■ Member booking
 ■ External booking
 ■ Not available

Scroll down the window and the booking details will be presented, as well as the “Book” blue button. After confirming your booking details, click “Book”.

Booking details

Dates	Time	Quantity	Unit Price	Cost
22/12/2021	08:00 - 08:30	0.5 hrs	1 per hr	0.5
Subtotal				0.50 EUR
VAT incl. service fee ?				0.00 EUR
Total cost				0.50 EUR

Notes

Write your notes

Book

Booking system



If available, special addons will be shown, as demonstrated here for the “NMR300 3 h blocks (14h-20h+night)” machine.

Booking details

Dates	Time	Quantity	Unit Price	Cost
24/12/2021	17:00 - 20:00	3 hrs	1 per hr	3
Optional Add-ons				
<input type="checkbox"/> Vt up		0 hrs	1 per hour	0 EUR
<input type="checkbox"/> Vt up overnight		0 hrs	4 per hour	0 EUR
<input type="checkbox"/> Vt down		0 hrs	1 per hour	0 EUR
Subtotal				3.00 EUR
VAT incl. service fee ⓘ				0.00 EUR
Total cost				3.00 EUR



Notes

Write your notes

Book

Important note: If you intend to perform a VT experiment, besides selecting the type of experiment, you must also contact the staff directly by e-mail to arrange the necessary materials (LN₂, N₂, dewars, etc.).

After clicking “Book”, you will see a green message on the top of the screen indicating that your booking is confirmed. This will also appear in our “MyLab Activities” separator.

Lab Dashboard

✓ Success The equipment has been booked successfully.

My Lab Activities

✓ in 3 days	Equipment	NMR300 3h blocks (14h-20h...	🔄	24/12/2021 17:00	24/12/2021 20:00	Single	Booked	✕ >
✓ in 5 days	Equipment	NMR400 weekends (09h-09h)	🔄	26/12/2021 09:00	27/12/2021 08:00	Single	Booked	✕ >

10 ▾ First < 1 > Last

Booking system



2.6. Special requests and mandatory information

As already mentioned, special experiments such as VT require the user to contact the staff to arrange the necessary materials. These experiments also present added costs that are computed into the final experiment price. It is absolutely mandatory to register the type of experiment in the booking system and to inform the staff. Otherwise, the booking will be cancelled by the Administrator.

Booking of equipment that allows the installation of different hardware, such as probes, will be closely monitored by the staff. The installation of different probe heads must be requested in advance and registered in the booking system. This is particularly relevant for the 500 MHz spectrometer. The probe head to be used must be selected when booking the slot. Please note that probe heads will not be exchanged every day to extend the lifetime of the hardware. Therefore, experiments requiring a type of probe will be grouped according to the installed probe. To facilitate this, experiments in this machine may be booked 2 weeks in advance.

Booking details

Dates	Time	Quantity	Unit Price	Cost
22/12/2021	12:00 - 15:00	3 hrs	10 per hr	30
Optional Add-ons				
<input type="checkbox"/> Bbo3		0 hrs	0 per hour	0 EUR
<input type="checkbox"/> Bbo5		0 hrs	0 per hour	0 EUR
<input type="checkbox"/> Bbo10		0 hrs	0 per hour	0 EUR
<input type="checkbox"/> Txi		0 hrs	0 per hour	0 EUR
<input type="checkbox"/> Hr-mas		0 hrs	0 per hour	0 EUR
<input type="checkbox"/> Low band		0 hrs	0 per hour	0 EUR
<input type="checkbox"/> Diff		0 hrs	0 per hour	0 EUR
<input type="checkbox"/> Ss-nmr		0 hrs	0 per hour	0 EUR
Subtotal				30.00 EUR
VAT incl. service fee ⓘ				0.00 EUR
Total cost				30.00 EUR

2.7. Cancelling a booking

Each user can cancel his own bookings up to 1 hour before the starting time. To do so, go to the “MyLab Activities” in the “Lab Dashboard” and click the arrow on the right of the booking you wish to cancel.

Lab Dashboard

My Lab Activities								
✓ in 3 days	Equipment	NMR300 3h blocks (14h-20h...	🔄	24/12/2021 17:00	24/12/2021 20:00	Single	Booked	✕ >
✓ in 5 days	Equipment	NMR400 weekends (09h-09h)	🔄	26/12/2021 09:00	27/12/2021 08:00	Single	Booked	✕ >

You may also click your own booking displayed in the calendar (marked in green).

This will open the booking detail window where you can find the “Cancel” button. By clicking this, your booking will be immediately cancelled and eliminated from the Dashboard.

Booking system



My Booking - Details

NMR300 3 h blocks (14h-20h+night)
Laboratório de RMN IST CQE

Back Book again

Status
Booked

Booking Reference
EQP4195627

Last Updated By
Pedro Pinheiro

Location
Lisboa, PT

Contact
Maria João Ferreira

Dates	Time	Quantity	Unit Price	Cost
24/12/2021	17:00 - 20:00	3.0 hrs	1.0 per hr	3.0 EUR
Subtotal				3.0 EUR
VAT incl. service fee				0 EUR
Total cost				3.0 EUR

Last note
N/A

Edit booking Cancel booking

Notes

Details

Additional Information

Besides deleting you may also choose to edit the booking by clicking the “Edite Booking” button. Use this to change the type of experiment you wish to perform (ex. if you initially booked a VT experiment but decide not to do it).

2.8. Transfer a booking

A common scenario in this facility is the booking of a time slot and then its transfer to another user. In the past this was easily done by changing the name of the user in the registering sheet. However, the *Bookkit* system does not allow for this. One hypothesis is to cancel your booking and have the other user book the now available slot. However, this can only be done up to 60 minutes before the starting time.

The other hypothesis is to communicate the booking reference code to the staff, indicating the person who will use it. Please note that his only makes sense if you are giving your booking to a member of a different group.

My Booking - Details

NMR400 weekends (09h-09h)
Laboratório de RMN IST CQE

Back Book again

Status
Booked

Booking Reference
EQP4192539

Last Updated By
Pedro Pinheiro

Location
Lisboa, PT

Contact
Maria João Ferreira

Booking system



2.9. System availability and announcements

Every week has slots reserved for programmed maintenance operations. These appear in the booking system as unavailable time (marked in light grey).

Emergency maintenance operations that require down time will be locked in the booking system as either “unavailable time” or as a booking performed by one member of the staff, overriding any other bookings. If necessary, the announcements tab will be used, as well as the mailing list.



2.10. Adding new users

It is strictly forbidden to add any new user by sharing the personal registering e-mail link.

New users can only be added by the staff upon completion of the mandatory training program.

To enrol a new user, the group leader or supervisor should directly contact the NMR staff.

General rules



NMR facility general rules

3. General rules of conduct

3.1. Access to the NMR facility

Access to the NMR facility is divided into four levels:

Level	Type of user	Access
A	Student/trainee	Low-field Lab (for training only)
B	Researcher	Low-field Lab
C	Advanced Researcher	Low-field Lab 500 MHz Lab
D	Staff	Low-field Lab 500 MHz Lab SS-NMR Lab

Each new user must complete a training program, provided by the NMR staff, in order to be able to perform experiments in the Low-field laboratory. Access to the other laboratories is restricted to users that have completed an extended training program and whose work requires the recurrent use of the 500 MHz spectrometer. The use of the SS-NMR laboratory is restricted to the SS-NMR staff.

3.2. Performing experiments

Users can only perform pre-defined experiments available in the experiment lists.

Sample preparation inside the Low-field laboratory is prohibited.

NMR tubes must be wiped and dry before introduction in the holder and in the spectrometer bore.

When removing a tube from the spectrometer, check for its label on the desk of the control station. Properly label the tube and place it in the rack.

When placing a tube in the holder, check that the tube is properly fitted inside the holder and that the solvent level is adequate (using the acrylic gauge). Do not remove the gauge from the bench.

When performing VT experiments, use the appropriate holder (HDPE or Ceramic).

When conducting "exotic nuclei" experiments, make sure that you tune the correct frequency and that you register the nuclei tuned in the logbook by order of use.

J-Young NMR tubes are lowered into the magnet using a string system to allow for their easy recovery. This type of tubes should be introduced and removed from the magnet without

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using the air cushion (“lift”). When using one of these tubes, a sign must be placed on top of the station keyboard stating that there is a *J-Young* tube inside the machine.

3.3. Experiment registration

Each user must register, in the appropriate logbooks, the experiments conducted, indicating the NMR program name (ex. PROTON), the solvent (ex. DMSO-d6), date, user and the status of the machine.

3.4. Data retrieving

Spectra data may be retrieved from each machine via the NMRServer machine. Each user has a folder located in the NMRServer machine to which data must be exported from the NMR computer terminals. NMR data can then be retrieved to the personal computer of each user using a remote FTP app (ex. FileZilla). The transfer of one’s files to the NMRServer machine doubles as a data backup system.

The use of USB pens, external hard drives and other mobile storage devices is strictly forbidden.

3.5. Hardware operations

Only Level D users can perform major hardware changes in the spectrometers. This includes probe head change and cable connections. Some C level users are also habilitated to assemble the VT down systems, upon staff approval.

No operations of any type are allowed in the NMR consoles, gas controls or UPS systems.

3.6. Hardware protection and backup systems

All spectrometers and accessory machines are connected to specialized power sources. The electrical supply is guaranteed by a set of high-power UPS systems that allow the equipment to operate for at least 30 minutes without external power. However, in the event of a prolonged power failure, the NMR spectrometers will be shut down to prevent damage to the coil systems.

Please note that besides electrical power, all spectrometers require a constant supply of compressed air. This is supplied by the compressed air line of the building, in normal conditions, and by a backup compressor if the standard supply fails. However, there is no compressed air supply during power failures. In the event of a power failure, please contact a member of the staff immediately.

Each NMR room is equipped with an A/C system set to keep the room temperature at a constant value of 21 °C. Spring-loaded doors ensure the maintenance of the constant temperature. Windows can only be opened during maintenance operations and in emergency situations.

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3.7. Emergency situations

Situation	Procedure
Tube stuck in NMR bore	Stop air flow by unselecting "lift" in the BSMS control Place sign on top of control station monitor Contact staff
Broken tube in the NMR	Place sign on top of control station monitor Contact staff immediately
Gas leak	Do not perform any operation in the spectrometer Leave the room Contact staff immediately
Power failure	Do not perform any operation in the spectrometer Contact staff immediately
Compressed air failure	Do not perform any operation in the spectrometer Contact staff immediately
Vapours escaping the NMR magnet	Do not perform any operation in the spectrometer Leave the room Contact staff immediately
Failure to connect to the machine	Contact staff
NMR console off	Do not perform any operation in the spectrometer Contact staff
Temperature warning	Do not perform any operation in the spectrometer Contact staff immediately
Room temperature too high	Contact staff
Locked computer terminal	Contact staff