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# Siteplanning

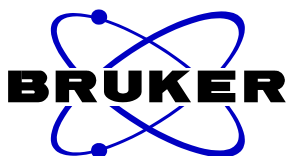
LC-(SPE)-NMR(/MS) equipment

Version 060519

for

Basis instructions for installation of equipment including LC  
coupled to SPE, NMR and MS// Requirements for space,  
powersupply, gas etc.

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# 1. Chapter

## Site planning

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This handbook was written by Dr. Ulrich Braumann. If you have any comments about this handbook or if you need further assistance please contact me.

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## **1.2 Introduction - Important**

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LC-NMR equipment is available in a various range of configurations. The manual describes the default configuration.

Identify the type of setup in the descriptions below and check try to use the default configuration.

***If this is not possible contact us to check if the planned modifications are possible. Orientation of in/outlets tubing and certain requirements for minimal distances do not allow free positioning of the instruments***

### ***1.4 LC-NMR, no cabinet, no MS***

- LC-NMR Interface *without cabinet*  
BSFU, BSFU-O, BMSO standalone, BPSU-12, BPSU-36 standalone, SPE
- Chromatography system consisting of pump, manual injector or autosampler, detector
- LC-NMR probe

### ***1.5 LC-NMR, no cabinet, with esquire MS***

- LC-NMR Interface without cabinet  
BSFU, BSFU-O, BMSO standalone, BPSU-12, BPSU-36 standalone, SPE
- Chromatography system consisting of pump, manual injector or autosampler, detector
- LC-NMR probe
- MS spectrometer and LC-NMR/MS interface

### ***1.6 LC-NMR, with microbay cabinet, withOUT MS***

- LC-NMR Interface mounted in cabinet  
BMSO+BPSU-36/2, BSFU-O+BPSU-36, BPSU-12  
optionally also containing a Bruker DAD detector
- Chromatography system consisting of pump, manual injector or autosampler, detector
- LC-NMR probe

### ***1.7 LC-NMR, compact LC-NMR/MS cabinet ( incl. MS )***

- LC-NMR Interface mounted in cabinet  
BMSO+BPSU-36/2, BSFU-O+BPSU-36, BPSU-12  
optionally also containing a Bruker DAD detector
- Chromatography system consisting of pump, manual injector or autosampler, detector
- MS spectrometer
- LC-NMR probe

## 1.3 Timing

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The Installation of an LC-NMR MS system consists of 2-3 steps

### *Standard NMR Installation*

First the standard NMR installation should take place.

- During the installation a flow probe can be already installed i.e. shimmed and tested for specifications like humptest, pulswidths, sensitivity etc.
- Specific knowledge about LC-NMR is **not** required to install an LC-NMR probe. The service engineer responsible for the NMR installation can perform this task.

### *MS Installation - optional*

An MS spectrometer must be installed **before** the LC-NMR/MS installation starts.

- It is required that the MS spectrometer is working before the LC-NMR/MS installation takes place.
- Before the MS Installation starts, the MS personnel must be advised about the proper positioning of the instrument relatively to the NMR instrument. As the MS has to be positioned relatively to the NMR, even might be positions on top of the NMR console it is best to have the MS installation in between the standard NMR and LC-NMR installation.
- It is not required that the MS fulfils all specifications in terms of sensitivity etc.
- It is helpful if the MS installer is present while the LC-NMR/MS is installed but not necessary.
- A typical esquire or microtof installation will take approx 2-3 days plus some customer training.

### *LC-(SPE)-NMR/(MS)*

The LC-NMR installation is done last. For final tests the attached spectroscopic instruments must work properly.

- The NMR instrument must **work** before the LC-(SPE)-NMR/(MS) can be installed. It is **not required** to have complete acceptance of the NMR instrument. Only the LC NMR probe must fulfil specifications.
- The MS instrument must **work** before the LC-(SPE)-NMR/(MS) can be installed. The MS must give reasonable spectra, it is not required that the MS fulfils specifications about resolution of sensitivity.
- A typical LC-NMR installation will take 2-4 days.
  - 1 day to setup the instruments
  - 1-2 day to calibrate the system parameters and to perform tests of all functions
  - ½ - 1 day basic training.

## 1.4 LC-NMR, no cabinet, no MS

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### 1.4.1 Configuration

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Configuration for LC-NMR setup which come as *individual* instruments and consist of

- LC-NMR Interface *without cabinet*  
BSFU, BSFU-O, BMSO standalone, BPSU-12, BPSU-36 standalone, SPE
- Chromatography system consisting of  
pump, manual injector or autosampler, detector
- LC-NMR probe

### 1.4.2 Required space

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- Approx. 60x100cm on a table ( not included ) for the installation of the chromatography system and the desktop versions of the LCNMR interfaces ( BSFU, BSFU-O, BMSO standalone, BPSU-12, BPSU-36 standalone, SPE ).
- Approx. 60 x 80cm on a office desk for the computer controlling the chromatography system and the LCNMR interface. The desk of the NMR computer can be used.

### 1.4.3 Positioning of the instruments

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- Distance of the LC-NMR/MS instruments to the NMR Console must be below 10m. The distance is determined by the length of the standard 10m RS232 cable.
  - The data connection can be also established between the chromatography PC and the NMR console.
  - Upon request a prolongation to 20m are possible but may lead to communication problems ( to be tested for each installation )
- Distance of the chromatography system to the chromatography PC must be below 10m. The distance is determined by the length of the standard Ethernet cable.
  - Upon request a 20m cable is available
- The table with the chromatography equipment and the LC-NMR interfaces must be positioned close to the magnet. The distance of the LCNMR interface to the LC-NMR probe must be below 3m the LC-NMR instruments must be outside the 5 gauss line. This distance is determined by standard length of the transfer capillary and the influence of the magnetic field upon electro motors, magnetic valves and the deuterium lamp of the UV detector.
  - Upon request longer capillary can be used but performance of the system will decrease.

- Positioning slightly inside the 5 gauss line is normally possible but has to be tested for each installation..
- The HPLC equipment should be visible from the PC ( It is not necessary that the HPLC PC is near the HPLC equipment ).

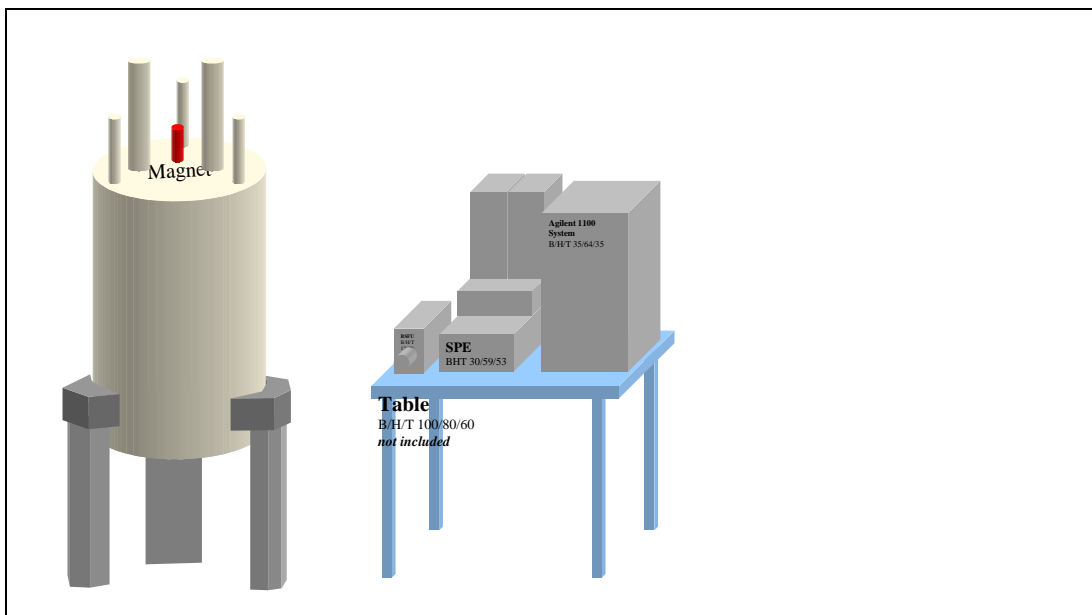


Fig. 1.1: Default configuration with **BSFU**, **SPE** and **Agilent** chromatography.

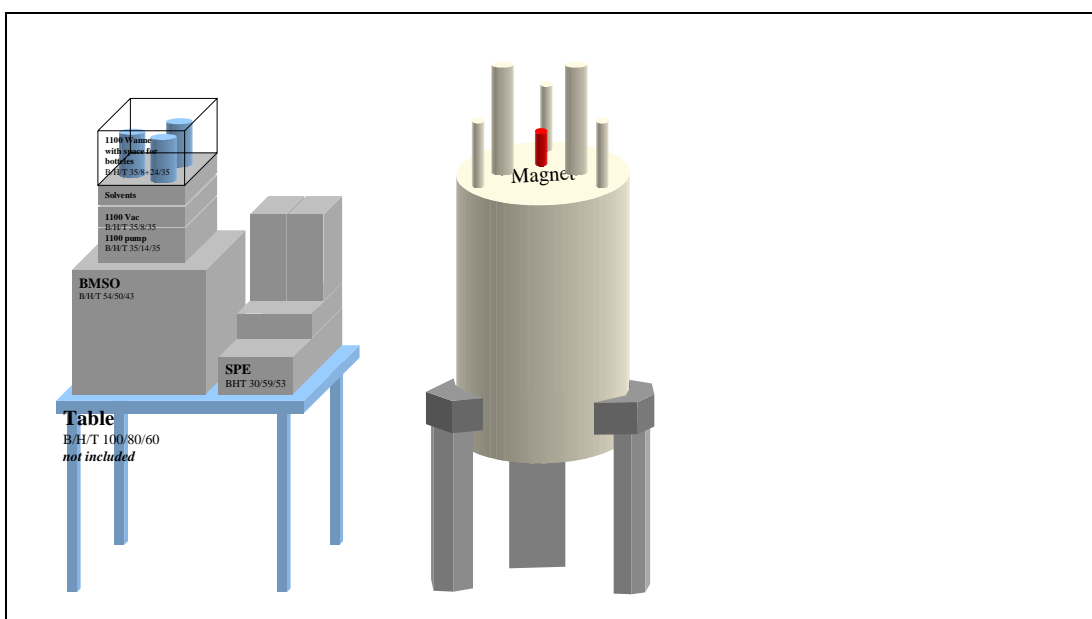


Fig. 1.2: Default configuration with **BMSO**, **SPE** and **Agilent** chromatography.



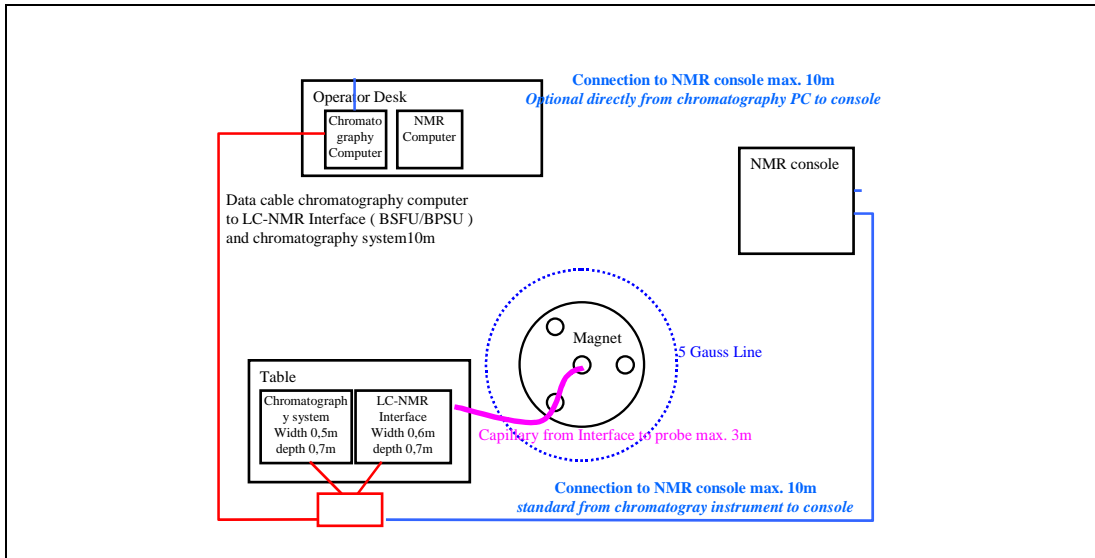


Fig. 1.3: Default configuration for the setup of a LC-NMR system.

## **1.5 LC-NMR, no cabinet, *with* esquire MS**

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### **1.5.1 Configuration**

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Configuration for LC-NMR setup which come as individual instruments and consist of

- LC-NMR Interface without cabinet  
BSFU, BSFU-O, BMSO standalone, BPSU-12, BPSU-36 standalone, SPE
- Chromatography system consisting of  
pump, manual injector or autosampler, detector
- LC-NMR probe
- MS spectrometer and LC-NMR/MS interface

### **1.5.2 Required space**

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- Approx. 60x180cm on a table ( not included ) for the installation of the chromatography system and the desktop versions of the LCNMR interfaces BSFU, BSFU-O, BMSO standalone, BPSU-12, BPSU-36 standalone, SPE ) and the MS spectrometer. The LC-NMR/MS interface is typically placed on top of the MS spectrometer.
- Approx. 30x70cm for the rough pump, preferably below the MS.
- Approx. 60 x 80cm on a office desk for the computer controlling the chromatography system and the LCNMR interface. The desk of the NMR computer can be used.
- Additionally approx. 60 x 80cm on a office desk if a dedicated MS PC ( optional ) is delivered.

### **1.5.3 Positioning of the instruments**

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- Distance of the LC-NMR/MS instruments to the NMR Console must be below 10m. The distance is determined by the length of the standard 10m RS232 cable.
  - The data connection can be also established between the chromatography PC and the NMR console.
  - Upon request a prolongation to 20m are possible but may lead to communication problems ( to be tested for each installation )
- Distance of the chromatography system to the chromatography and the dedicated MS PC ( optional ) must be below 10m. The distance is determined by the length of the standard Ethernet cable.
  - Upon request a 20m cable is available.
- The table with the chromatography equipment and the LC-NMR interfaces must be positioned close to the magnet. Distance of the LCNMR interface to LC-NMR probe must be below 3m and the LC-NMR/MS instruments must be outside the 5 gauss line. This distance is determined by standard length of

the transfer capillary and the influence of the magnetic field upon electro motors, magnetic valves and the deuterium lamp of the UV detector.

- Upon request longer capillary can be used but performance of the system will decrease.
- Positioning slightly inside the 5 gauss line is normally possible but has to be tested for each installation.
- Distance of the LC-NMR/MS interface ( BNMI ) to the ion source of the MS spectrometer must be as short as possible ( below 20cm ).
  - Position the chromatography system between MS and LC-NMR interface.
  - Position the MS spectrometer so that the ion source points towards the chromatography system.
  - Position the BNMI on top of the MS with the front over the Ion source.
- The HPLC equipment should be visible from the PC ( It is not necessary that the HPLC PC is near the HPLC equipment ).

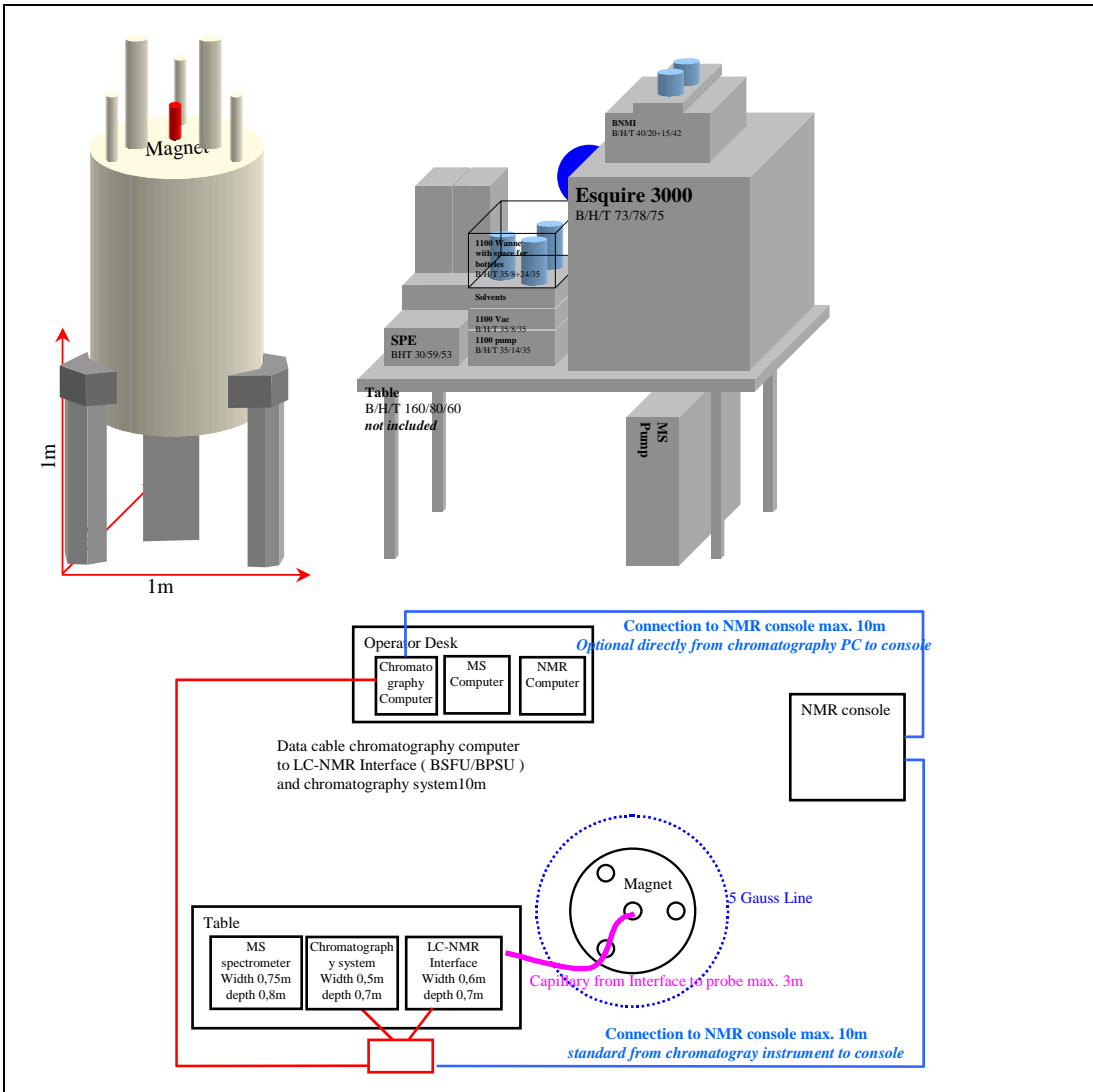


Fig. 1.4: Default configuration for the setup of a LC-NMR/MS system without cabinet including an MS.

## **1.6 LC-NMR, with microbay cabinet, withOUT MS**

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### **1.6.1 Configuration**

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Configuration for LC-NMR setup which includes a cabinet for the installation of the 19" instruments .

- LC-NMR Interface mounted in cabinet  
BMSO+BPSU-36/2, BSFU-O+BPSU-36, BPSU-12  
optionally also containing a Bruker DAD detector
- Chromatography system consisting of  
pump, manual injector or autosampler, detector
- LC-NMR probe

### **1.6.2 Required space**

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- Approx. 65x85cm for the installation of the LC-NMR cabinet ( same size as one microbay NMR console ).
- Interfaces are mounted in the cabinet ( except the SPE Prospekt2 ).
- The chromatography equipment can be positioned on top of the LC-NMR microbay cabinet. A Bruker DAD detector can be mounted in the cabinet.
- If an SPE System is included an additional table is required. ( It can be also positioned on top of the cabinet besides the chromatography equipment but the space is very limited )
- Approx. 60 x 80cm on a office desk for the computer controlling the chromatography system and the LCNMR interface. The desk of the NMR computer can be used.

### **1.6.3 Positioning of the instruments**

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- The Distance of the LC-NMR instruments to the NMR Console must be below 10m. The distance is determined by the length of the standard 10m RS232 cable.
  - The data connection can be also established between the chromatography PC and the NMR console.
  - Upon request a prolongation to 20m are possible but may lead to communication problems ( to be tested for each installation )
- Distance of the chromatography system to the chromatography PC must be below 10m. The distance is determined by the length of the standard Ethernet cable.
  - Upon request a 20m cable is available.
- The LC-NMR cabinet must be positioned close to the magnet. Distance of the LCNMR interface to the LC-NMR probe must be below 3m the LC-NMR instruments must be outside the 5 gauss line. This distance is determined by standard length of the transfer capillary and the influence of

the magnetic field upon electro motors, magnetic valves and the deuterium lamp of the UV detector.

- Upon request longer capillary can be used but performance of the system will decrease.
- Positioning slightly inside the 5 gauss line is normally possible but has to be tested for each installation..
- If the NMR console is also a microbay console it is recommended to put the two consoles next to each other to enlarge the area on top of the console for the chromatography and the LC-NMR interfaces.
- The screen of the control unit should be visible from the NMR computer and vice versa.
- The HPLC equipment should be visible from the PC ( It is not necessary that the HPLC PC is near the HPLC equipment ).

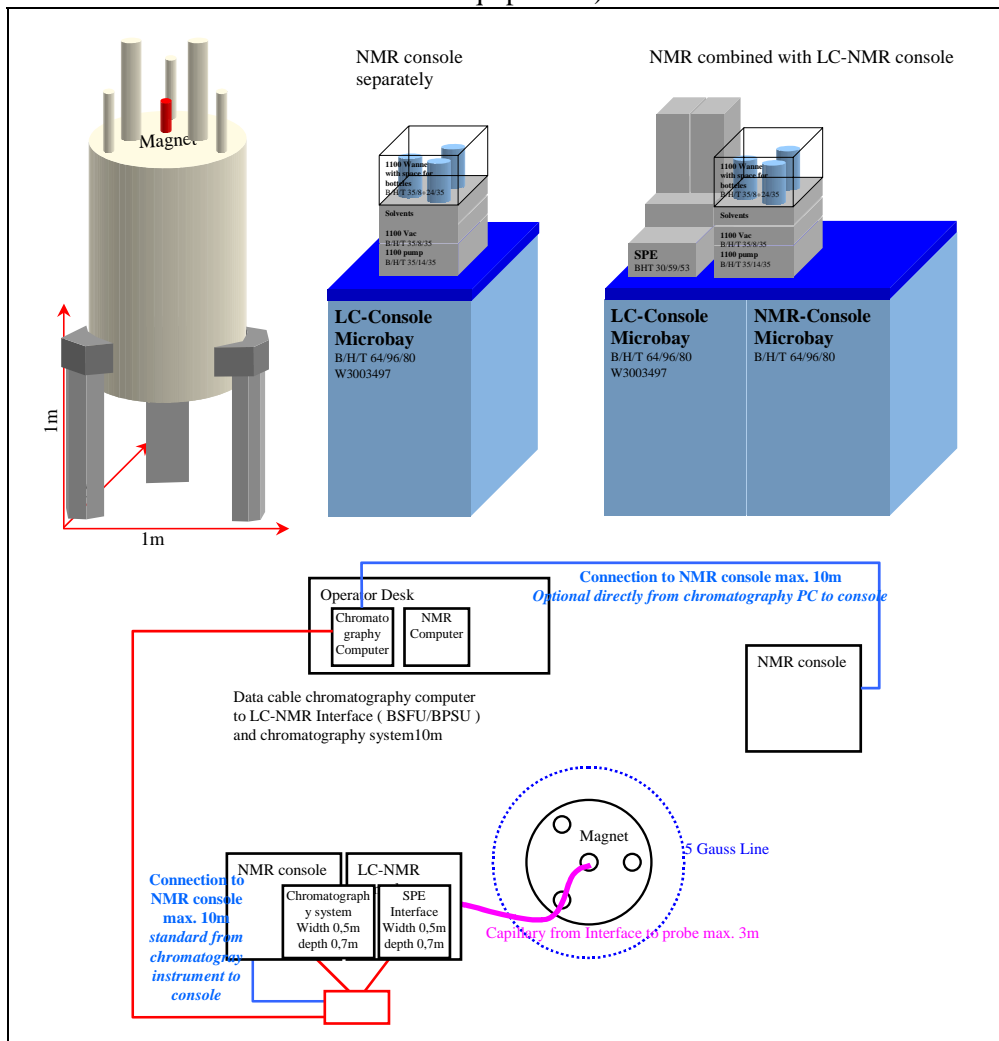


Fig. 1.5: Default configuration for a LC-NMR system with microbay cabinet.

## **1.7 LC-NMR, compact LC-NMR/MS cabinet ( incl. MS )**

### **1.7.1 Configuration**

Configuration for LC-NMR setup which includes a compact LC-NMR/MS cabinet holding the LC-NMR instruments and the NMR console as well as the MS rough pump in an integrated cabinet.

- LC-NMR Interface mounted in cabinet  
BMSO+BPSU-36/2, BSFU-O+BPSU-36, BPSU-12  
optionally also containing a Bruker DAD detector
- Chromatography system consisting of  
pump, manual injector or autosampler, detector
- MS spectrometer
- LC-NMR probe

### **1.7.2 Required space**

- Approx. 160x85cm for the installation of the LC-NMR/MS cabinet ( two microbay consoles plus rough pump housing ).
- Interfaces are mounted in the cabinet ( except an optional SPE Prospekt2 ).
- The NMR equipment is installed in one of the microbay consoles.
- The MS rough pump is installed in the integrated rough pump housing between the NMR console and the LC-NMR cabinet.
- The chromatography equipment, the MS and an optional SPE system can be positioned on top of the LC-NMR microbay cabinets. A Bruker DAD detector can be mounted in the cabinet.
- Approx. 60 x 80cm on a office desk for the computer controlling the chromatography system and the LCNMR interface. The desk of the NMR computer can be used.

### **1.7.3 Positioning of the instruments**

- Distance of the chromatography system to the chromatography PC must be below 10m. The distance is determined by the length of the standard Ethernet cable.
  - Upon request a 20m cable is available.
- The LC-NMR cabinet must be positioned close to the magnet. Distance of the LCNMR interface to the LC-NMR probe must be below 3m the LC-NMR instruments must be outside the 5 gauss line. This distance is determined by standard length of the transfer capillary and the influence of the magnetic field upon electro motors, magnetic valves and the deuterium lamp of the UV detector.
  - The magnet must be on the left side of the LC-NMR/MS compact console.

- The compact LC-NMR/MS console is an integrated system. NMR and LC-NMR console cannot be separated.
- Upon request longer capillary can be used but performance of the system will decrease.
- Positioning slightly inside the 5 gauss line is normally possible but has to be tested for each installation..
- The screen of the control unit should be visible from the NMR computer and vice versa.
- The HPLC equipment should be visible from the PC ( It is not necessary that the HPLC PC is near the HPLC equipment ).

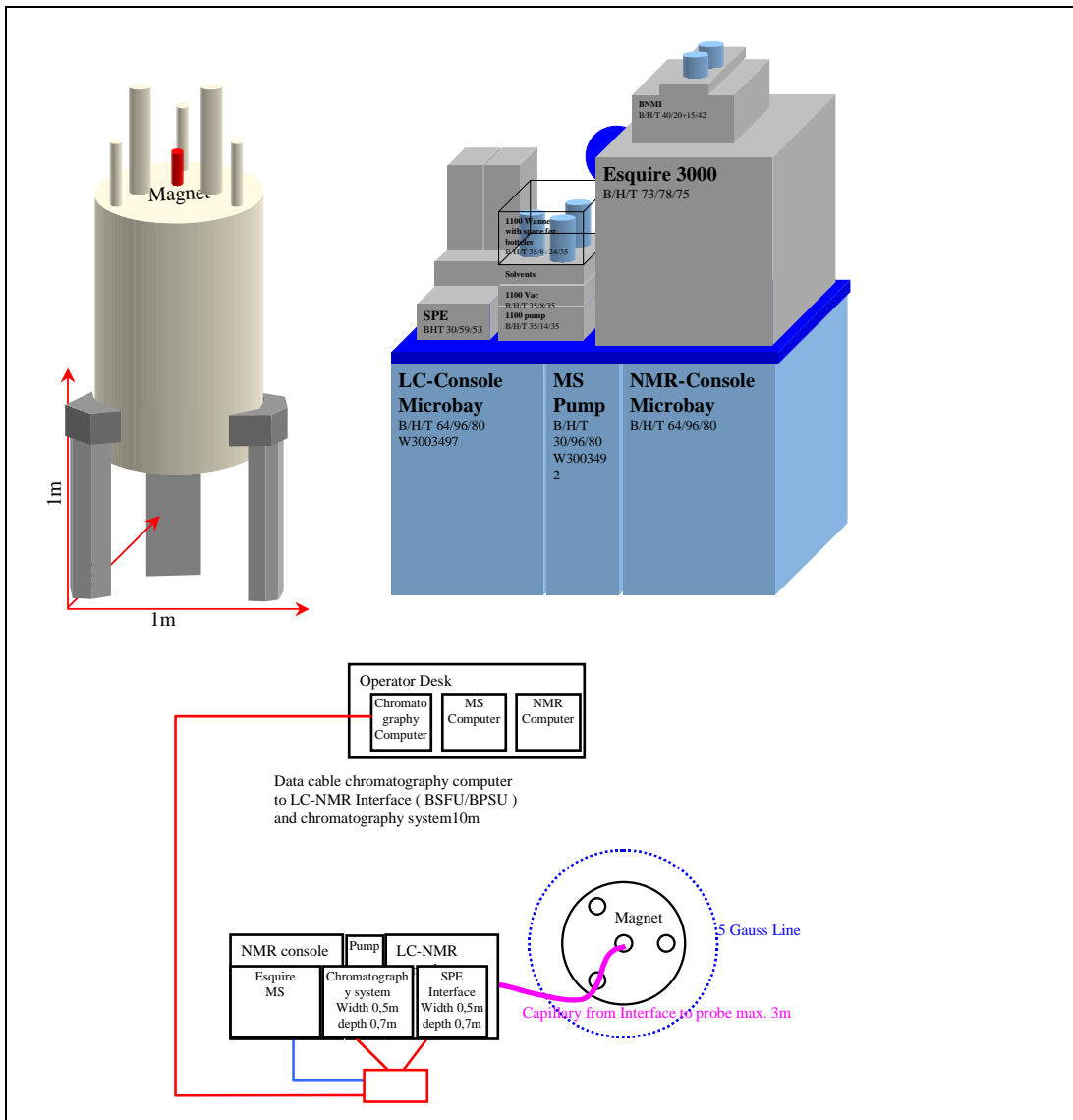


Fig. 1.6: Default configuration for a LC-NMR system in a integrated microbay cabinet.



## 1.8 General Requirements

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### 1.8.1 Material

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The following material must be provided for the installation *by the customer*.

- 500ml of *non* deuterated acetonitrile gradient grade. ( CH<sub>3</sub>CN )
- 2 glass bottles, approx. 500ml as waste containers.

If an LC-NMR interface (BSFU, BPSU-12, BMSO, BPSU-36 ) is included

- 200ml of *deuterated* water ( D<sub>2</sub>O )

If LC-SPE-NMR is included

- 100ml of *deuterated* acetonitrile ( CD<sub>3</sub>CN 99,8% do *not* use special LC-NMR quality with 15% D<sub>2</sub>O )
- 1000ml of *non*-deuterated water H<sub>2</sub>O for chromatography, gradient grade.

### 1.8.2 Venting

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In chromatography system toxic solvents are used. The customer is responsible to provide proper venting of the system.

### 1.8.3 Power and Gas supply

- 110/240 indicates that the instrument can be adjusted to either one of the voltage ranges. 110-240V means that the instruments adjusts automatically.
- The table below is only for a overview of the required power consumption. For details check the manuals of the individual instruments.
- Make sure that enough power outlets are available. An extension lead with 5 outlets is supplied with each LC-NMR setup and additional extension lead with 5 outlets comes with the LC-SPE-NMR system.

Instrument		Powersupply		Gas
Computer + Monitor	2	110/240V	400VA	
<b>Chromatography</b>				
Agilent 1100 pump	2	110-240V	180VA Pump 30VA degasser	
Agilent 1100 Autosampler	1	110-240V	180VA	
Agilent Oven 1100	1	110-240V	320VA	
Gilson Autosampler	1	115/230V	250VA	
Bruker DAD Detector	1	110/240V	300VA	
Agilent 1100 Detector	1	110-240V	300VA	
<b>Interfaces</b>				
BSFU	1	110-240V	75VA	none
BPSU-12	1	110-240V	70VA	none
BMSO+BPSU-36/2	2	110-240V	400VA BMSO 250VA BPSU-36/2	3-8bar N <sub>2</sub> /Air 2-6 l/h
BMSO standalone	2	110-240V	420VA	3-8bar N <sub>2</sub> /Air 2-6 l/h
BNMI	1	115-230V	100VA	
SPE Interface	2	115/230V	200VA ACE 150VA HPD	3-5bar N <sub>2</sub> 6-18l/h <sup>1)</sup>
	2	100-240V	250VA pump 10VA N <sub>2</sub> valve	40l/h <sup>2)</sup>
<b>Other</b>				
MS spectrometer		Check documentation of MS instrument		
ISCO Fraction collector	1	230V <sup>3)</sup>	20VA	
Gilson Sample collector	1	115/230V	250VA	
<b>Sum</b>	–		_____ VA	

<sup>1)</sup> Cartridge and probe head drying. N<sub>2</sub> quality of NMR probe VT sufficient.

<sup>2)</sup> Optional protective flushing of cartridge compartment with constant flow of N<sub>2</sub>

<sup>3)</sup> 230V powersupply with 14V DC output delivered. Instrument requires 14V DC.