

Installation Guide PurityChrom®

1. PurityChrom operates under Microsoft Windows XP, Windows Vista, Windows 7, Windows 8 and Windows 10.

The supported languages are: German and English

2. Automatic switching to energy-saving mode or hibernating has to be disabled i.e. settings for "Turn Off Hardware", "Turn off Computer" or "System Standby" must be set to "Never" in the control panels energy options. Microsoft Security Essentials is installed, please exclude PurityChrom. Therefore, open Microsoft Security Essentials and go to Setup. In "Excluded files and locations" you have to search for C:\PurityChrom and add this folder to excluded files. In "Excluded processes" you have to search for C:\PurityChrom\PurityChrom.exe and add this process to the excluded processes. Furthermore, the Windows Defender has to be deactivated. Therefore, got to "Extras" and/or "Settings". Choose "Administrator" and uncheck "Turn on this program" or Turn on this app".
3. The user account settings have to be set to "Never notify" before installation. After the installation, the settings can be reset. (Start → Control Panel → User Accounts → User Accounts → Change User Account Control Settings → Never notify)
4. Activate the option "Beta: Unicode UTF-8" under the region settings of the computer (Windows settings → Time & Language → Region → additional date, time and regional settings → Region → Administrative → change system localization → select "Beta: Use Unicode UTF-8 for worldwide language support).
5. Set PC to fixed IP Address if it is not connected to a router or a router is connected via a second network card.
6. Insert the CD which includes PurityChrom.
7. Start the installation as an administrator. The installer will ask you to choose the language of the software, your integrated UV-detector and the destination location for the files that will be installed. Do not change the given destination. If not otherwise specified use **English** as the software language.
8. Restart your computer.
9. Installation under Windows versions older than 8 or 10: Go to C:\PurityChrom and right-click the PurityChrom.exe to open the properties. Go to compatibility and check "Run this program in compatibility mode for" and choose "Windows Vista (Service Pack 2). After this, check "Run this program as an administrator". Click "Apply" and "Ok", then close the window.
10. **Installation under Windows 8 or 10:** Run Installation-Setup as administrator, then open the PurityChrom program folder „C:\PurityChrom\“, use a right-click on „PurityChrom.exe“ and select once „Run as administrator“,

Open the „Communication Log“-Window  and the "System Visualisation"  once. Then close the software.

Note:

If the error message "**PrepCon5.dll not found**" appears, run the "Microsoft Visual C++ 2015 Redistributable" setup. You will find the setup in the PurityChrom program folder:
"C:\PurityChrom\DriverDll\vc_redist.x86.exe"

11. Connect your devices. All devices that should be connected by LAN should be set to LAN and need fixed IP addresses.

AZURA L/ VU 4.1	Mobile Control/Service Tool/Firmware Wizard (in folder "Tools" on PurityChrom CD)
UVD 2.1S	Firmware Wizard (in folder "Tools" on PurityChrom CD)
AZURA S/ IFU 2.1	Service Note 0106 (via Lantronix Device Installer)
Conductivity Monitor CM 2.1S/ V 2.1S	FW Wizard via Mac Address
Foxy R1/R2	Device Display
Autosampler AS 6.1L	Service Note 0153 - Point 3
LABOCOL Vario 4000	Internet browser (type in IP 192.168.0.112), more information in the device manual
CT 2.1	FW Wizard via Mac Address
Memmert Oven	Device Display
Eluent Heater	Device Display
Windows Tablet (for Mobile Control)	In adapter settings of tablet
Ethernet Eventbox (SCPA)	Internet browser (type in http://EVENTBOX or the IP 192.168.0.108), more information in the device manual

12. The KNAUER Interface Box IFU 2.1 **USB** requires a separate driver for the built-in USB-to-serial controller. If no VSCOM USBtoCOM box is installed, you can install the driver from the PurityChrom CD, folder:

Drivers\COM Extensions\VSCOM USBtoCOM\Version_2.08.28_Win7, XP, 2003, x86_x64.
The file must be executed with administrator access.

For Windows 8.1 please use the IFU 2.1 driver from the following folder:

Drivers\COM Extensions\VSCOM USBtoCOM\Version_2.08.30_81_Win8.1

The KNAUER Interface box IFU2.1 **LAN** does not require a separate driver

13. The KNAUER RID 2.1L, KNAUER CT 2.1, external 1/4" pressure sensor, SCPA eluent heater, Mikron81 and Shimadzu fluorescence detector require a separate driver. Copy the driver from *C:\PurityChrom\DriverDll\Data Acquisition* or *C:\PurityChrom\DriverDll\Device Control* and rename the file:

RID21L.dll	→ PrepConLF.dll
CT21A.dll	→ ThermoControl.dll *
RF20A.dll	→ PrepConAddCh.dll
PressureSensor.dll	→ PrepConAddCh2.dll
ThermoPrep.dll	→ PrepConTemp.dll
SedexLC.dll	→ PrepConAddCh.dll
Mikron81LF.dll	→ PrepConLF.dll

and paste them to C:\Windows\SysWOW64 (64-bit system) or C:\Windows\System32 (32-bit system).

* the driver *thermocontrol.dll* needs to be additionally pasted to C:/PurityChrom.

14. In the next step, you have to change the "PurityChrom.ini"-file according to the connected devices. This file is located in C:\Windows\

Mobile Control

- If MobileControl is running **on a tablet** using a fixed IP address and PurityChrom is opened, all devices will be logged off from MobileControl and accessed by PurityChrom. To activate this behavior the ini entry under [MainWindow] has to state:
MCMonitorMode=1

WinsockPorts

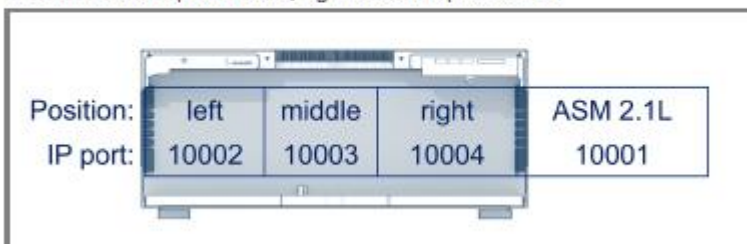
- In [WinsockPorts] the IP addresses and Ports of LAN-connected devices are entered if they do not have a separate entry.

For example: Port1=192.168.5.1,10001

- Freestanding devices have the IP-Port number 10001,
- IP-Port for Autosampler KNAUER 3950 or AS 6.1L: 2101
- IP-Port for Fraction Collector Foxy R1/R2: 23
- IP-Port for eluent heater (SCPA), Ethernet Eventbox and Labomatic Pump HD-5000 are by default 100 (can be checked in the display of the devices)
- Devices that are connected via serial interface are not filled in.
- Labomatic pumps HD-5000 controlled together via one Labomatic controller unit have all the same IP-Address and need only one Winsock-Port entry. If also a minor pump is managed via the Labomatic controller unit, its IP-Port is calculated by IP-Port of major pumps system + 1 (default 101), for example:
Port1=192.168.1.101,100 → Major Pump system
Port2=192.168.1.101,101 → Minor Pump system
- the left module in an assistant **ASM2.1L** has the port number 10002, the module in the middle the port number 10003 and the right module the port number 10004.

Three modules

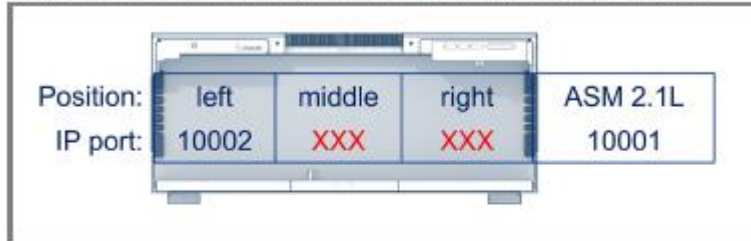
For three modules, the position is as follows: left module: port 10002, middle module: port 10003, right module: port 10004.



- If the assistant **ASM2.1L** contains only one module, it is always connected to the left port (IP port 10002) despite the module position.

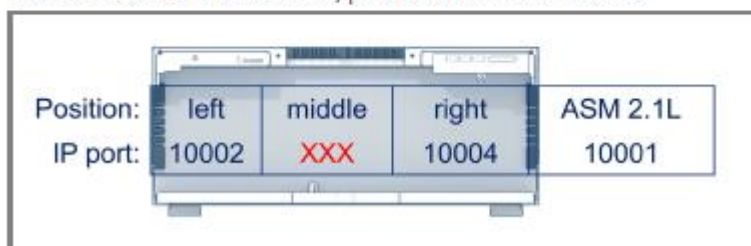
One module

Is one module in the assistant, it is connected to the left (port 10002).

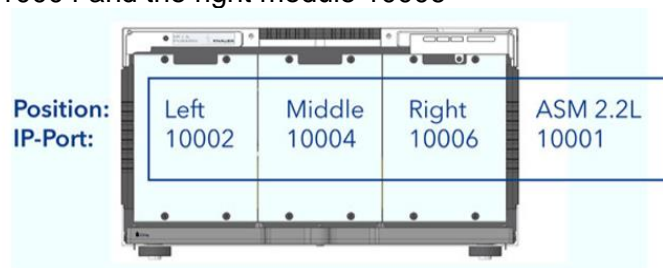


Two modules

For two modules in the assistant, port 10003 is not connected.



- The **ASM2.2L** basic module has the IP port 10001, the left module 10002, the middle module 10004 and the right module 10006



P4.1S/P2.1S (high-pressure gradient system in one assistant) **NOT supported anymore**

- Enter the port of both pumps under one entry under [WinsockPorts]. For example Port1=172.31.5.25,10002,10003
- There is a separate entry for pumps parameter under [Pumps].
→ Set "SoftwareHPG=0" (for isocratic) or "SoftwareHPG=2" (for binary gradient) below "PreciseMixing=0"

High-pressure gradient system (independent pumps, not P6.1L, not Labomatic HD-5000)

- Setting for pumps:
- Enter the IP address and the port of pump A under [WinsockPorts].
- There is a separate entry for pumps parameter under [Pumps].
Set:
SoftwareHPG=1 for isocratic,
SoftwareHPG=2 for binary gradient
SoftwareHPG=3 for ternary gradient or
SoftwareHPG=4 for quaternary gradient

→ additionally, edit lines for pump B, C and D as necessary. For example:

```
SoftwareHPGPort2=127.0.0.2,10001
SoftwareHPGPort3=127.0.0.3,10001
SoftwareHPGPort4=127.0.0.4,10001
```

with the IP-Address and IP-Port of Pump B, C and D.

Low-pressure gradient system (P 2.1L)

- Insert in Puritychrom.ini the following entries:
- Enter the IP address and the port of the pump under [WinsockPorts].
- Additionally, under [Pump] add the appropriate line
LPGType=2 (for binary LPG)
or
LPGType=3 (for ternary LPG)

Gradient system (Labomatic HD-5000)

- Settings according to LPG or HPG have to be done on the screen of the control unit.
- Further settings are not necessary for PurityChrom

Using a Triggersignal

- Change the Puritychrom.ini file as described here:

```
[Pumps]
IOControl=1
```

Pumps do not stop at the command "Stop all"

- You can decide whether pumps should stop or pump further when pressing "Stop all".

```
[Pumps]
PumpStopRequest=1
```

Autosampler

- There is a separate entry for the connected Autosampler in the PurityChrom.ini-file:

[Autosampler]		
TempPrecision=3	[°C]	The precision of set temperature
MaximumSamples=100	[Value]	Maximum sample capacity of the autosampler
VolumeDimension=µl	[µl]	Dimension of the injection volume. Please do not change this entry.
AS3000=0	[0/1]	The autosampler is a Labomatic AS3000.
VarioPrep=0	[0/1]	The autosampler is a SCPA VarioPrep.
Alias=0	[0/1]	The autosampler is a Spark Alias.
Knauer3950=0	[0/1]	The autosampler is a KNAUER 3950 or AS 6.1L.

Wash=0	[0/1]	1: washing cycle begins when starting the software 0: washing cycle after starting the software is turned off
TubingVolume=15	[µl]	Standard tubing volume (volume between needle and valve) (prep mode = 60)
FlushVolume=30	[µl]	Standard flush volume (2x tubing volume) (prep. Mode = 120)
PrepMode	[0/1]	Prep mode OFF = 0, Prep mode ON = 1 Knauer Autosampler with 10 ml Loop and 2,5 ml syringe volume
Transportliquid=	[0/1]	0 = Needle wash 1 = Transport wash
Transportvolume=	[1-9]	Number of syringe loads for washing

- The communication protocol for the KNAUER 3950/AS 6.1L has to be converted from UDP to TCP/IP. If necessary please request for SOP.

Fluorescence Detector

- There is a separate entry for the connected fluorescence detector RF20A in the PurityChrom.ini-file:

[ShimadzuRF20A]		
Enabled=	[0/1]	OFF = 0, ON = 1
Port=	[Port]	Port number
Channels=1	[Value]	Number of channels
Gain=1	[1/2/3]	1=x1, 2=x4, 3=x16
Sensitivity=0	[1/2/3]	0=High, 1=Medium, 2=Low
DataRate=2	[Value]	Data rate of the detector
AnswerTimeOut=1	[Value]	Do no change
ConnectionTimeOut=1	[Value]	Do not change
Output=2	[Value]	0: Excitation energy, 1: Light source correction, 2: Emission not corrected

Do not use USB-to-COM adapter to connect the Shimadzu fluorescence detector.
Settings for Shimadzu RF20A:
Baudrate: 9600, Data Bits 8, Parity 0, Stop Bit 1

UV-Detector

- There is a separate entry for the connected detector in the PurityChrom.ini-file:

[KnauerUVD]		
Enabled=0	[0/1]	OFF = 0, ON = 1 (using a detector connected via serial interface or LAN the value has to be set to 1; using a detector connected via an A/D converter the value has to be set to 0)
IP=	[IP]	IP-address

Port=	[Port]	port number
IP2=	[IP]	IP-address for detector 2*
Port2=	[Port]	port number for detector 2*
IP3=	[IP]	IP-address for detector 3*
Port3=	[Port]	port number for detector 3*
IP4=	[IP]	IP-address for detector 4*
Port4=	[Port]	port number for detector 4*
NDetectors=	[Value]	number of detectors
BaudRate=9600	[Value]	baud rate
Wavelength1=254	[Value]	preset wavelength
DataRate=2	[Value]	Datarate of the detector (don't change the data rate as the detector will send the maximum data rate); Default =50
Channels=1	[Value]	Number of channels; UVD = 1; MWD = up to 4
MaxD2Time=0	[0 – 2000]	0=off, 1-2000 = Hours; When the maximum value is exceeded, an error message occurs. However, work may be continued after confirming the message
Type=UVD2.1S	[Type]	Your detector type (UVD2.1S, UVD2.1L, 50D, MWD2.1L)
NoRefCorr=1	[0/1]	If enabled a reference correction is used on Channel 2.
OptimiseIT=1	[0/1]	Enable/Disable integration time optimization upon software start.

- If the UV-detector is connected via serial interface hide the IP address by using an inverted comma ('IP=) and enter the number of the COMPort under Port.

* only add if more than one UVD2.1/UVD2.1L are used in a system and only possible if all detectors are the same type

RI Detector

- There is a separate entry for the connected RID 2.1L in the PurityChrom.ini-file:

[KnauerRID21L]		
Enabled=	[0/1]	OFF = 0, ON = 1
IP=	[IP]	IP-address
Port=	[Port]	Port number (KNAUER: 10001)
DataRate=	[Value]	Datarate of the detector
Channels=1	[Value]	Number of channels
TimeConst=2000	[Value]	Time constant
SignalMode=0	[Value]	Signal mode, 0=direct, 1=inverted
AnswerTimeOut=1	[Value]	Do no change
ConnectionTimeOut=1	[Value]	Do not change
Temperature=0 / 30-55	[Value]	0 = off, 30-55 = Temperature is set after start
TempZone=1	[1-8]	1= [Temperature] FunctionName1=... 2= [Temperature] FunctionName2=... ...

DAD 2.1L and 6.1L

- There are two separate entries for connecting a DAD in the PurityChrom.ini-file:

[KnauerDAD61L]

Enabled	[0/1]	OFF = 0, ON = 1
IP=	[IP]	IP-address
Port=	[Port]	port number (KNAUER: 10001)
Integration=	[Value]	Preset value for DAD integration time
OptimiseIT=	[0/1]	Enable/Disable integration time optimization upon software start

[DAD]

Enabled=0	[0/1]	OFF = 0, ON = 1
Diodes=1024	[Value]	Number of diodes in the diode array. 1024 = DAD 6.1L / 256 = DAD 2.1L
ScanStart=200	[Value]	Spectrum start of ECOM-DAD.
ScanEnd=600	[Value]	Spectrum end of ECOM-DAD.
SliceWidth=500	[Value]	Preset value for DAD slicewidth.
IntegrationTime=100	[Value]	Preset value for DAD integration time.
IntegrationBandwidth=1	[Value]	Preset value for DAD integration bandwidth.
AutomaticReference=1	[0/1]	Automatic reference spectrum after starting a time control file.
LambertBeer=1	[Value]	This value is required. Do not change!

IFU

- There is a separate entry for the connected IFU in the PurityChrom.ini-file:
- Please make sure that the IFU Baudrate is set to 19200 in the lantronix module

[KnauerIFU21]

Enabled=	[0/1]	OFF = 0, ON = 1
IP=	[IP]	IP-address
Port=	[Port]	port number (COMport or in case of LAN connection port number of the device: default 10001)
DataRate=1	[Value]	datarate of the monitor
Channels=4	[Value]	number of channels

- If the IFU2.1 is connected via USB: the USB connection will be interpreted as COMport. Check your Windows Device Manager to identify the used COM port. To open the Device Manager (using Windows XP / 7) go to the "Control Panel" and open the "Device Manager". Please hide the IP address by using an inverted comma ('IP=)
- If you have an IFU 2.1LAN: please enter an IP address and the IP port
- Data rate: 1 - 10 Hz (4 channels), up to 50 Hz (channel 1 exclusively)
- For data acquisition using the IFU2.1 you have to choose a minimum Slide Width of 500 ms in PurityChrom (Time Table Editor, Function: Start Chromatogram)

Conductivity Monitor (CM 2.1S or Mikron81)

- There is a separate entry for the connected KNAUER conductivity monitor CM2.1S in the PurityChrom.ini-file:

[KnauerCM21S]		
Enabled=0	[0/1]	OFF = 0, ON = 1 (using a detector connected via serial interface or LAN the value has to be set to 1; using a detector connected via an A/D converter the value has to be set to 0)
IP=	[IP]	IP-address
Port=	[Port]	Port number (KNAUER: 10001)
DataRate=1	[Value]	Data rate of the monitor
Channels=1/2/3	[Value]	Number of channels (1 = conductivity, 2 = conductivity and pH 3 = conductivity, pH and Cell-Temperature)

- If the conductivity monitor is connected via serial interface hide the IP address by using an inverted comma ('IP=) and enter the number of the COMPort under Port.
- If the Mikron81 Conductivity Monitor is used please fill in the PurityChrom.ini entry accordingly:

[MicronLF]		
Enabled=0	[0/1]	OFF = 0, ON = 1
Port=	[Port]	Com Port for USB Connection
DataRate=2	[Value]	Data rate of the monitor
Channels=1	[Value]	Number of channels (1 = conductivity, 2 = conductivity and temperature 3 = conductivity and temperature and conductivity raw data (no temp correction))
TimeConstant=1000	[Value]	Time Constant
TempCoeff=17	[Value]	Temperature Coefficient (1.7%)
TempRef=25	[Value]	Reference Temperature (25°C)
AnswerTimeOut=1	[Value]	Do not change
ConnectionTimeOut=1	[Value]	Do not change

Heating devices

- For setting of Temperature Channel Names go to .ini entry [Temperature] and define Function Name1=...; Function Name2=... etc.. If there are different heating devices used in the system, the names should follow the order:
 1. eluent heater channels (Function Names: Eluent Temperature, Column Temperature)
 2. SEDEX LC (Function Name: LSD Temperature)
 3. RID (Function Name: RID Temperature)
 4. Column Oven ATC00 (Function Name: Column Oven Temperature)

Eluent heater

- There is a separate entry for the eluent heater in the PurityChrom.ini-file:

[ThermoControl]		
Enabled=	[0/1]	OFF = 0, ON = 1
IP=	[IP]	IP-address
Port=	[Port]	IP Port
Channels=1	[Value]	number of channels
Zones=1	[Value]	number of adjustable temperatures (1 for one-channel ELH, 2 for two-channel ELH)
Precision=1	[Value]	precision of temperature adjustment
TMax=100	[Value]	maximum temperature

- As "Port" use the port number shown in the display of the eluent heater

CT2.1A / ATC00

- add IP-address of column oven under [Winsock-Port] in the PurityChrom.ini file
- in the setup menu, choose "heater control", the winsock port and as driver "MultComDll"

SEDEX LC

- There is a separate entry for the SEDEX LC in the PurityChrom.ini-file:

[SedexLC]		
Enabled=	[0/1]	OFF = 0, ON = 1
Port=	[Port]	Com Port
Channels=	[Value]	number of channels (1 – Signal, 2 – temperature, 3 – Pressure)
Gain=	[Value]	Dynamic or 1-7
Offset=0	[Value]	-999 till 999
Filter=2	[Value]	0.5,1,2,...,10s
Temperature=20	[Value]	Set point of the temperature
PMax=5.0	[Value]	The software gives warning messages when pressure is outside of the given range
PMin=1.0	[Value]	
TempZone=1	[Value]	Temperature zone in PurityChrom (depends on the number of other heating devices)
LampAutoOn=1	[0/1]	Switches automatically the LED on
LampAutoOff=1	[0/1]	Switches automatically the LED off
AnswerTimeOut=1	[0/1]	Do not change
ConnectionTimeOut=1	[0/1]	Do not change

Leaksensors/Errormessages

- There are separate entries for the **ASM** and its Leaksensor/Errormessages in the PurityChrom.ini-file: Use Option(I) or (II) (it is not allowed to use both entries!)
(I) **ASM with UVD module:**

```
[KnauerASM21L]
Enabled=          [ 0/1 ]      OFF = 0, ON = 1
IP=               [ IP ]       IP-address
Port=             [ Port ]     IP Port
Type=             [1/2]       1=ASM2.1L, 2=ASM2.2L
```

Additionally, under [Detector] CheckLampStatus=1 must be set.

(II) **ASM without UVD module:**

```
[LeakageKnauerASM]
Enabled=          [ 0/1 ]      OFF = 0, ON = 1
IP=               [ IP ]       IP-address
Port=             [ Port ]     IP Port
Message=          "Leakage detected"
```

- Only one ASM can be checked for leakage/Error, please fill in the IP address of the lowest ASM in the tower and connect Error Out of the ones not checked by the software with the one that is, if necessary.
- For the Leaksensor/Error messages of an **AZURA L-Detector** (MWD or DAD) enable this in the entry:
[Detector]
CheckLampStatus=1
You can leave CheckforLeak=0. This would only give you the Leak message in addition to the Error message about the leak.
- For the Leaksensor of the **pumps** define [LeakageInput] with the recommended setting: LeakageCountdown=0

```
[LeakageInput]
LeakageInput1=3 (for major Pump)
LeakageInput2=7 (for Minor Pump (not P2.1S/P4.1S))
LeakageInput3=0
LeakageInput4=0
LeakageCountdown=0
Soundfile=SysAlert.wav
WindowsShutdown=0
Message1=Leakage detected Major Pump
Message2= Leakage detected Minor Pump
Message3=
Message4=
```

Valve Timeout

- To activate, that the Method goes to hold if communication with a **valve** is lost set
[ValveTimeout]
Hold=1

Memmert Oven

- There is a separate entry for the Memmert Oven in the PurityChrom.ini-file:

```
[Memmert]
Enabled=          [ 0/1 ]    OFF = 0, ON = 1
IP=              [ IP ]     IP-address
Tmax=            [ Value ]   Max. Temperature
```

Direct Control

- To use the direct control function during the run to change the flowrate and the gradient composition change the PurityChrom.ini file as described here:

```
[Pumps]
Parameterchange=1
```

Tailing Factor instead of Asymmetry

- If the tailing factor should be calculated instead of the asymmetry, please change the PurityChrom.ini-file as described here:

```
[IntegrationPresets]
TailingFactor=1
```

Deactivate automatic Integration

- Please change the PurityChrom.ini-file as described here to deactivate the integration.

```
[IntegrationPresets]
IntegrateInhibit=1,2,3.... (your data channels)
```

Using an external pressure signal

- Please change the PurityChrom.ini-file as described here to use an external pressure channel:

```
[Pumps]
PressureChannel=0 or 1-8  (0: no external pressure channel
                          1-8: number of your external pressure channel)
```

Demo chromatogram

- Starting PurityChrom in the demo version, there is a possibility to run a demo method Choose the result file here:

```
[DemoMode]
Chromatogram=C: \PurityChrom\Data\ResultFileExample_0001.rfp
```

Tandem switching of two valves

- If you want to link the switching of two valves please change the PurityChrom.ini-file as described here:

```
[Tandem valve]
Index=... (number of tandem valve in the setup of PurityChrom)
SecondPort=...(Com-Port-Number of second valve) OR
SecondWinsockPort =...(Winsock of second valve)
```

You must not configure the second valve in the setup of PurityChrom.

Bronkhorst Flowmeter

- There is a separate entry for the Flowmeter in the PurityChrom.ini-file:

```
[BronkFlow]
Enabled=          [ 0/1 ]    OFF = 0, ON = 1
Port=             [ Port ]   Com Port
Port2=            [ Value ]  Com Port
Port3=            [ Value ]  Com Port
Port4=            [ Value ]  Com Port
SearchNodes=0     [ 0/1 ]    OFF = 0, ON = 1
SearchRange=1,8   [ Value ]  Range of nodes in which the software
                           should search for active flowmeters
Node1=            [ Value ]  If the functions "SearchNode" and
Node2=            [ Value ]  "SearchRange" are not used, add here
Node3=            [ Value ]  the node addresses of each flowmeter
Node4=            [ Value ]
Channels=         [ Value ]  numbers of channels in total
Message=          [ 0/1 ]    OFF = 0, ON = 1
                           If activated, a message box with
                           information about found flowmeters and
                           their respective capacities will appear
                           after software start
Logfile=          [ 0/1 ]    OFF = 0, ON = 1
                           If activated, the communication between
                           software and flowmeters will be logged in
                           a separated file saved in the program
                           folder C:/PurityChrom-MCC-Plus/
UseBus=           [ 0/1 ]    OFF = 0, ON = 1
                           for using the BUS system for
                           communication of flowmeters with the
                           software choose 1, for using individual
                           RS-232 cables for each flowmeter
                           choose 0
```


External 1/4" Pressure Sensors

- There is a separate entry for the Sensors in the PurityChrom.ini-file:

```
[PressureSensor]
Enabled=          [ 0/1 ]    OFF = 0, ON = 1
IP=              [ IP ]     IP-address for first sensor
Port=            [ Port ]   IP Port for first sensor (SCPA
                           Default:100)
IP2=             [ IP ]     IP-address for second sensor
Port2=           [ Port ]   IP Port for second sensor (SCPA
                           Default:100)
Channels=        [Value]    Number of sensors
```

15. Start the software. If the connection has been successful green ticks will appear behind the port number and if the connection was not successful a red cross will appear behind the port number.

16. Configuration of PurityChrom

- The menu option SETUP  in the main window will open the program settings window:

[Communication]

Please choose the correct Ports, baud rates and drivers for your devices according to the PurityChrom manual.

Note: Do not change the number of addresses in the Addr. Row!

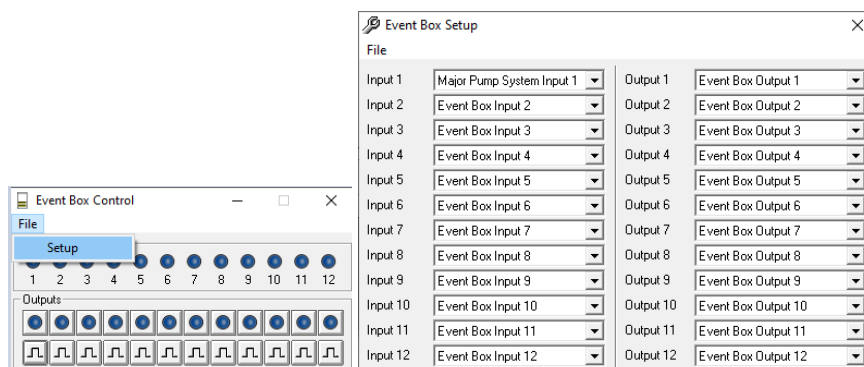
For fraction collector LABOCOL Vario 4000, choose driver "Multcom Interface" and for the pump Labomatic HD-5000, choose the driver "Multcom Interface (Serial Control)". For the Ethernet Eventbox (SCPA), activate the option "Serial Event Box" and choose the driver "Multcom Interface (Serial Control)".

Using trigger signal from the air sensor or a manual injection valve you can choose under "Control Inputs" to stop all, to start a run (Time Control Start) or to pause a run (Time Control Hold/Continue) depending on the signal. Using a manual injection valve connected to the pump via a trigger cable you have to choose the respective Event Box Input that is configured in the event box setup as "Major Pump System Input 1". Using an air sensor connected via gameport adapter you have to choose "Gameport Input 1, 2, 3 or 4". Using an air sensor connected via Ethernet Eventbox (SCPA), choose the respective eventbox input.



Control Inputs	
Stop all	Event Box Input 1
Time Control Start	Gameport Input 1
Time Control Hold/Continue :	Disabled

If eventbox signals are used, configure the respective signals in the event box setup:

Event Box Setup			
File			
Input 1	Major Pump System Input 1	Output 1	Event Box Output 1
Input 2	Event Box Input 2	Output 2	Event Box Output 2
Input 3	Event Box Input 3	Output 3	Event Box Output 3
Input 4	Event Box Input 4	Output 4	Event Box Output 4
Input 5	Event Box Input 5	Output 5	Event Box Output 5
Input 6	Event Box Input 6	Output 6	Event Box Output 6
Input 7	Event Box Input 7	Output 7	Event Box Output 7
Input 8	Event Box Input 8	Output 8	Event Box Output 8
Input 9	Event Box Input 9	Output 9	Event Box Output 9
Input 10	Event Box Input 10	Output 10	Event Box Output 10
Input 11	Event Box Input 11	Output 11	Event Box Output 11
Input 12	Event Box Input 12	Output 12	Event Box Output 12

Valves:

The valves must be configured additionally

Device	Address	Positions	Port	Type
Foxy R1/R2	1	2	Driver 5	Standard Valve
LABOCOL Vario 4000	1	2	WinsockPort	Standard Valve
RID 2.1L	1	2	Driver 3	Standard Valve
P 6.1L HPG – SSV A	1	2	Driver 1	Standard Valve
P 6.1L HPG – SSV B	2	2	Driver 1	Standard Valve
Injection valve	1	2	WinsockPort	Knauer injection valve
Multiposition valve	1	XX	WinsockPort	Knauer multiposition valve
Knauer VU4.1 (for example column selection valve)	1	11	WinsockPort	Knauer VU4.1 Valve
Column selection valve (Vici-Valve drive)	1	11	Com Port	Vici Valve*
Multi-Injection Valve	1	4	WinsockPort	Knauer multiposition valve
Valves of Labomatic Pump HD-5000	1-12 (device screen)	2	WinsockPort of the pump system	Standard valve
Gas valve of SEDEX LC	1	2	Com Port des SEDEX LC	Standard valve
Valves of Liquid handler LH 2.1: → Fraction valve → Dispenser valve → Injection valve (VU4.1)	1 1 2	2 4 2	WinsockPorts of Collector, Autosampler, Autosampler	Standard valve

*For a VICI valve drive please consider that the ID needs to be set to 1. This can be done either by the remote display or via a terminal tool (e.g. Hyper terminal).

→Remote Display:

Connect the remote display to valve drive.

Press the HOME/SETUP button for 5 seconds to enter the Setup menu.

Use the arrow button to select “Interface Setup” and press HOME/SETUP button.

Use the arrow button to select “RS-232” and press HOME/SETUP button.

Use the arrow button to select “Set ID” and press HOME/SETUP button.

Use the arrow button to set the ID to 1 (default is asterisk [*]) and confirm with HOME/SETUP button.

→Terminal program:

Chose correct COM-port for the valve drive and use the following communication settings to connect:

Baudrate: 9600

Data: 8
Stop: 1
Parity: none
Then, type “*ID1” and press ENTER to set the ID from default (asterisk [*]) to 1.

[Presets]
Choose the right maximum pressure for the major and minor pump system.
Choose the right maximum flow rate for the major and minor pump system.

[Limiter]
The fraction limiter is a feature that calculates the volume after which the collector will step to the next position dependent on the flow rate. In the limiter setup, the fraction limiter can be configured.

[Annotation]
The automatic annotations in the chromatograms are configured in the annotation setup

[Dead Time / Volume]
A considerable dead volume can occur in the tubing and valves between the detector cell and the waste/fraction switching valve, which results in a time delay when fractionating, especially at low flow rates. In the Dead Time / Dead Volume setup, you can define the dead volume or dead time of your system

[Description]
You can define names to the event box inputs and outputs, valves and the auxiliary output of the pump interface in the description's setup. This makes it easier to program time control files. It also makes the visualizations clearer, since the inputs, outputs and valves can be listed by function.

Valves:		
Injection Valve:	Position 1:	Load
	Position 2:	Inject
Valve of the Fraction Collector:	Position 1:	Waste
	Position 2:	Fraction
Multiposition Valve for Fractionation:	Position 1:	Waste
	Position 2:	Fraction 1...
Solvent Selection Valve A/B (HPG)	Position 1:	A1/B1
	Position 2:	A2/B2
Column Selection Valve	Position1-11:	Bypass Column 1-5 Rev Column 1-5
Multi-Injection Valve	Position 1:	Manual load
	Position 2:	Inject

Gas Valve of SEDEX LC

Interface Box des
Liquid Handler

Input 1
Input 2
Input 3
Input 4
Input 6
Output 1

Position 3: Direct Inject

Position 4: Pump Load

Position 1: Open

Position 2: Close

Fraction collector BUSY

Injection valve position (LOAD/INJECT)

Hold status activated

Front door opened

Device/Communication error

Start Washing

Configuration of fraction valves OR Valves of the fraction collector

[Limiter]

a) Limiter activation

Activate **Controlled Valve**, select the fraction valve or the valve of the fraction collector and choose **"Not waste"**

The fractionation should start if the fraction valve or the valve of your fraction collector changes the position from "Waste" to "Not waste" and the pumps are running. Therefore, choose your fraction collector valve in "Controlled Valve".

b) Limiter Output

Choose **Controlled Collector (Next Vial)** for a fraction collector.

Choose **Controlled Valve (Next Position)** for a fractionation valve.

[Annotation]

c) Waste Annotation Device

Choose the fraction valve or the valve of the fraction collector and **Waste**.

d) Fraction Annotation Device

Choose the fraction valve or the valve of the fraction collector and **Not Waste**.

e) Step Annotation Device

Choose **Controlled Collector Step** for fraction collector.

Choose **Controlled Valve Position Change** for fractionation valve.

[Dead Time / Volume]

f) Controlled Collector AND Controlled Valves

Here, enter the delay volume (volume from detector cell to fraction collector)

Note: if no fraction valve or fraction collector is used, please deactivate Controlled Valve in the Limiter activation section

Configuration of P 6.1L HPG

Main Window configuration using P6.1L (high-pressure gradient version)

- Using the P6.1L HPG remove the buttons for C and D from the toolbar.
Therefore, double-click on an empty area on the toolbar. The "Customize Toolbar" will open, where you can remove these buttons. To hide a button, deselect the checkbox under it. The settings will be saved when you exit the program.
- Configuration of the solvent selection valve of P6.1L (high-pressure gradient version) in the Setup:

[Communication]

a) Choose two standard valves:

The first valve can switch between A1 (position 1) and A2 position 2. Here you have to program the following:

Addr.: 1, Pos.: 2, Port: Driver 1, Type: Standard Valve

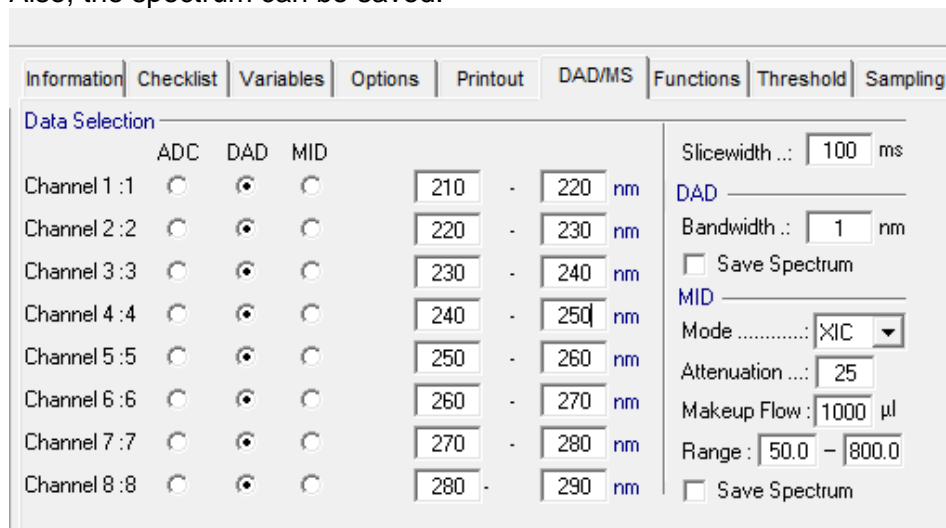
The second valve can switch between B1 (position 1) and B2 position 2. Here you have to program the following:

Addr.: 2, Pos.: 2, Port: Driver 1, Type: Standard Valve

Configuration DAD 2.1L/DAD 6,1L

Channels are configured in Time Control File Editor in section DAD and are saved to the method.

The wavelength function and cannot be used to set the wavelength of DAD channels. Also, the spectrum can be saved.



The screenshot shows the 'DAD/MS' tab in the 'Time Control File Editor'. The 'Data Selection' section is active, showing a table of 8 channels. Each channel has radio buttons for ADC, DAD, and MID. The DAD columns are selected for all channels. The wavelength range is specified in nm for each channel. On the right, there are settings for 'Slicewidth' (100 ms), 'Bandwidth' (1 nm), 'Save Spectrum' (unchecked), 'MID Mode' (XIC), 'Attenuation' (25), 'Makeup Flow' (1000 µl), 'Range' (50.0 - 800.0), and another 'Save Spectrum' checkbox (unchecked).

Channel	ADC	DAD	MID	Wavelength Range (nm)
Channel 1:1	<input type="radio"/>	<input checked="" type="radio"/>	<input type="radio"/>	210 - 220 nm
Channel 2:2	<input type="radio"/>	<input checked="" type="radio"/>	<input type="radio"/>	220 - 230 nm
Channel 3:3	<input type="radio"/>	<input checked="" type="radio"/>	<input type="radio"/>	230 - 240 nm
Channel 4:4	<input type="radio"/>	<input checked="" type="radio"/>	<input type="radio"/>	240 - 250 nm
Channel 5:5	<input type="radio"/>	<input checked="" type="radio"/>	<input type="radio"/>	250 - 260 nm
Channel 6:6	<input type="radio"/>	<input checked="" type="radio"/>	<input type="radio"/>	260 - 270 nm
Channel 7:7	<input type="radio"/>	<input checked="" type="radio"/>	<input type="radio"/>	270 - 280 nm
Channel 8:8	<input type="radio"/>	<input checked="" type="radio"/>	<input type="radio"/>	280 - 290 nm

Configuration of RID 2.1L

The flush valve needs to be configured separately:

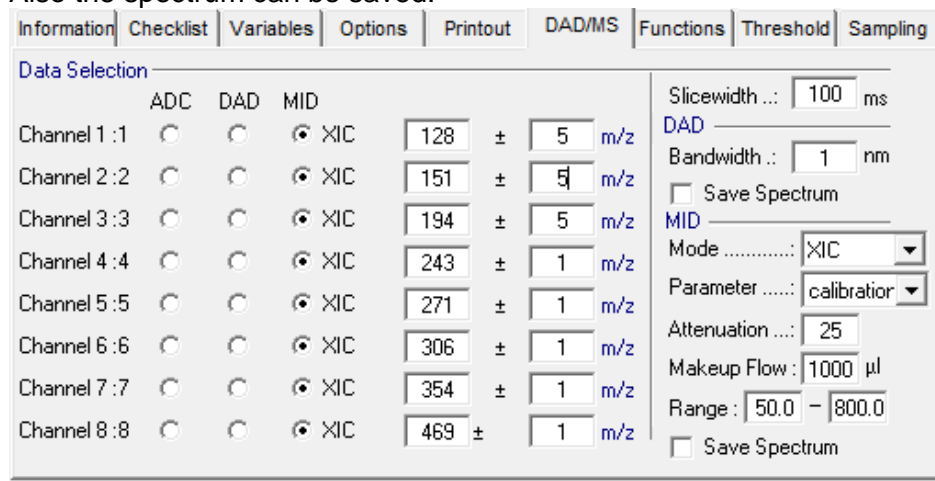
Addr.: 1, Pos.: 2, Port: Driver 3, Type: Standard Valve

Data output is in nRIU. For µRIU please change the factor in the channel setup to 0,001.

Configuration 4000MiD

Channels are configured in Time Control File Editor in section DAD/MS and are saved to the method. Here mode, calibration, Attenuation, Make Up Flow and Mass Range can be specified.

Also the spectrum can be saved.

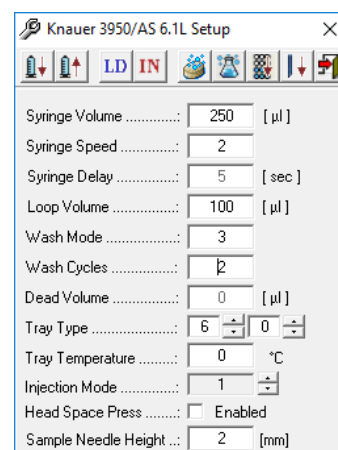


The screenshot shows the 'DAD/MS' tab in the 'Time Control File Editor'. The 'Data Selection' section is active, showing a table of 8 channels. Each channel has radio buttons for ADC, DAD, and MID. The MID columns are selected for all channels. The mass range is specified in m/z for each channel. On the right, there are settings for 'Slicewidth' (100 ms), 'Bandwidth' (1 nm), 'Save Spectrum' (unchecked), 'MID Mode' (XIC), 'Parameter' (calibration), 'Attenuation' (25), 'Makeup Flow' (1000 µl), 'Range' (50.0 - 800.0), and another 'Save Spectrum' checkbox (unchecked).

Channel	ADC	DAD	MID	Mass Range (m/z)
Channel 1:1	<input type="radio"/>	<input type="radio"/>	<input checked="" type="radio"/>	128 ± 5 m/z
Channel 2:2	<input type="radio"/>	<input type="radio"/>	<input checked="" type="radio"/>	151 ± 5 m/z
Channel 3:3	<input type="radio"/>	<input type="radio"/>	<input checked="" type="radio"/>	194 ± 5 m/z
Channel 4:4	<input type="radio"/>	<input type="radio"/>	<input checked="" type="radio"/>	243 ± 1 m/z
Channel 5:5	<input type="radio"/>	<input type="radio"/>	<input checked="" type="radio"/>	271 ± 1 m/z
Channel 6:6	<input type="radio"/>	<input type="radio"/>	<input checked="" type="radio"/>	306 ± 1 m/z
Channel 7:7	<input type="radio"/>	<input type="radio"/>	<input checked="" type="radio"/>	354 ± 1 m/z
Channel 8:8	<input type="radio"/>	<input type="radio"/>	<input checked="" type="radio"/>	469 ± 1 m/z

Configuration of KNAUER 3950/AS 6.1L

In the menu option “File” in the main window of PurityChrom you will find the Autosampler Setup:



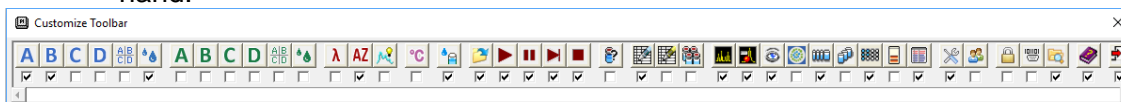
Syringe Volume	The volume of the autosampler syringe. (2500µl for prep mode)
Syringe Speed	1: slow, 2: middle, 3: fast
Syringe Delay	Leave the syringe delay at 5 sec.
Loop Volume	The volume of your sample loop. (10000µl for prep mode)
Wash Mode	0: washing cycle is turned off 2: between vials 3: between injection
Wash Cycles	How many wash cycles (1 – 3 times).
Dead Volume	Not important for KNAUER 3950/AS 6.1L.
Tray Type	0: Well-plate 96 low 1: Well-plate 96 high, 2: Well-plate 384 low 3: 48 vials 4: 12 vials 5: 108 vials (the second tray don't need to be selected) 6: 84+3 vials (the second tray don't need to be selected) 7: 30 vials (the second tray don't need to be selected) If a tray is used twice put the same number twice
Tray Temperature	0°C: off Sample tray cooling for KNAUER 3950/AS 6.1L with cooling option: 4 – 40 °C (make sure that the tray temperature is off when no cooling option is available!)
Injection Mode	0: None 1: Partial Loop Fill – max inject volume: 50 % of the sample loop 2: Flushed Loop – full loop 3: Microliter Pickup – max inject volume: 50 % of the sample loop
Head Space Press	Activate the HEAD SPACE PRESSURE option to support the sample transport to the sample loop by clicking.
Sample Needle Height	Select a distance between 2 and 6 mm

After changing settings in the Autosampler Setup always exit the setup via the door in the upper right corner, otherwise, your changes will not be saved.

Methods with an autosampler injection are started about the autosampler control file or a sequence. Please read the manual for more information.

Configuration of toolbar buttons

If toolbar buttons are missing, double-clicking on an empty area next to the toolbar buttons will open a selection window. Tick all boxes needed for the configuration at hand.



Note: The Toolbar buttons for the Solvent Composition of Major and Minor pump determine the calculation in the time control editor. (In the example picture composition will be calculated only for A and B). For a P6.1L LPG please choose A – D.


Configuration of Function Tab in Time Table Editor


To deactivate unnecessary functions, press shift and untick the functions, which should not be available.

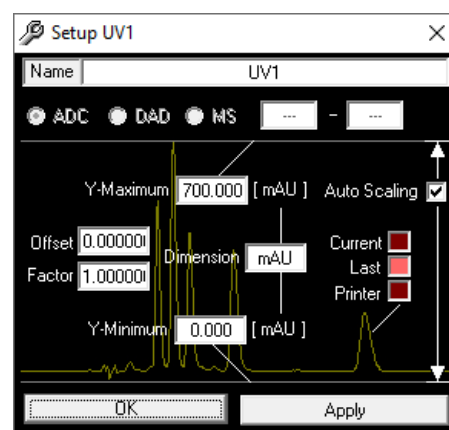
Configuration of used data channels

Order of data channels:

1. UVD/MWD
2. CM (+pH) or RID
3. FLD or IFU channels
4. DAD
5. MS

The menu option „Chromatogram“  in the main window opens the „Analysis window“.

Using the icon „tools“  the selected channel can be configured (for example the name and the dimension). Read the manual for more information.



Device	Channel Name	Modus	Dimension	Factor
UWD/MWD	UV1/ UV2*/ UV3*/ UV4*	ADC	mAU	1
CM	Conductivity Monitor	ADC	mS/cm	1
pH	pH	ADC	-	1
RID	RID	ADC	nRIU	1
External Pressure Sensors (AZG10/AZG10-1)	Pressure before column	ADC	bar	0.05
	Pressure after column	ADC	bar	0.05
External Pressure Sensor (AZG10-2)	Pressure before column	ADC	bar	0.004
	Pressure after column	ADC	bar	0.004
External Pressure Sensor (AZG10-3/AZG10-4/ AZG10-5)	Pressure before column	ADC	bar	1
	Pressure after column	ADC	bar	1
DAD	UV1/ UV2**/ UV3**/ UV4**	DAD	mAU	1
MS	MS1/ MS2**/ MS3**/ MS4**	MS	cts	1
Eluent heater***	Temperature/Column/Column In/Column Out	ADC	°C	1

*depending on Channel number of device (as set in .ini file)

** special for DAD/MS: all leftover channels can be filled with DAD channels (not in .ini)

*** when eluent heater and DAD are combined, then channel 1-4 is used for eluent heater and channel 5-8 for DAD

17. If the installation and configuration is finished, close the software. Copy the license file (PurityChrom.lic) on the CD (in the folder: *License*) to C:\PurityChrom and insert the USB license dongle into a free USB port of the computer. The license will be recognized and can be used. Do not remove the dongle while PurityChrom is running.
18. KNAUER is not responsible for lost dongles. Losing the dongle means losing the license.
19. Restart your computer and the software PurityChrom once a week.

Attachment: IP addresses

- Use following IP addresses (subnet mask: 255.255.255.0, gateway: 192.168.1.1)

Device	IP-Address
Computer	192.168.1.100
Major Pumpe 1 (not in ASM)	192.168.1.101
Major Pumpe 2 (binary HPG, not in ASM)	192.168.1.102
Major Pumpe 3 (ternary HPG, not in ASM)	192.168.1.103
Major Pumpe 4 (quaternary HPG, not in ASM)	192.168.1.104
Assistant 1 (In the tower from bottom to top)	192.168.1.105
Assistant 2 (In the tower from bottom to top)	192.168.1.106
Assistant 3 (In the tower from bottom to top)	192.168.1.107
Assistant 4 (In the tower from bottom to top)	192.168.1.108
Assistant 5 (In the tower from bottom to top)	192.168.1.109
Detector	192.168.1.110
CM2.1S/RID 2.1L/Mikron 81	192.168.1.111
Fraction Collector	192.168.1.112
Autosampler	192.168.1.113
Minor Pump P4.1S/P2.1S (not in ASM)	192.168.1.114
Valve 1 (not in ASM)	192.168.1.115
Valve 2 (not in ASM)	192.168.1.116
Valve 3 (not in ASM)	192.168.1.117
Valve 4 (not in ASM)	192.168.1.118
Valve 5 (not in ASM)	192.168.1.119
IFU	192.168.1.120
CT2.1/Memmert Oven	192.168.1.121
Eluent Heater	192.168.1.122
MiD	192.168.1.123
Windows Tablet (Mobile Control)	192.168.1.125
Ethernet Eventbox (SCPA)	192.168.1.130

Mark devices with stickers: „Fixed IP-Address: 192.168.1.XXX“