**To start working you need**: the Elmathron<sup>®</sup> measuring device; capillary and accesories included in the standard version; vacuum pump capable to generate vacuum of 0.1-0.3 Pa; computational server; any computer or mobile telephone with internet access and browser support.





You must turn on Elmathron, connect a vacuum, start up the device, connect a capillary to the inlet and place the inlet capillary in the liquid to be measured.

You can access the continuous measurement settings in the Continuous Measurements screen.



To optimize the feeding of samples to the Elmathron<sup> $\mathbb{R}$ </sup> measuring device, including sample viscosity and the chosen analysis method, a built-in software calculator can be used to precheck all the inlet parameters.

There are several precautions regarding the viscosity of the fluid being measured, please check the documentation. For example, it is necessary to use an inlet filter if some particles can enter the measured area through a capillary.



Start Page Elegant NMR® Software v1.08 ©Elegant Mathematics LLC

Continuous	📳 🔇 🕢 🕃 🔐 🧿
Device Name:	Elmathron_SN_1
Experiment Name:	Mixture_Aug_3_2021
Fluid Viscosity:	≤2.0 mPa•s (propanol/25°C)
Delay (Velocity) Range: ?	8.4 m (483 nL/m) 13.5 h (5 nL/m)
Total Inlet Volume:	4.04 μL
Extra-Detector Volume: ?	Done
Total Inlet L/K <sub>d</sub> /S:	2.2e+8 mm <sup>-3</sup>
Inlet Parameters: Capillary ? L <sub>ce</sub> Add More Calculate	a: 400 mm D <sub>ca</sub> : 0.1 mm X

	AR® Software v1.08 ©Elegant Mathematics LLC	- Advanced Parameters	- Device Inspection     Verify Inlet Parameters:     Perform Cleaning:     Check Baseline:     C
Device Name:	Elmathron_SN_1	Suppress V (mol/L) < (mol/L) ? < (%) ? < (%) ? < (%) X	Speed/Accuracy Balance: ? Fast v
Experiment Name:	Mixture_Aug_3_2021	? ["er":"C4H1002","eq":"0","td":"1","wr3":"0","op1":[25,2]}	Cleaning Substances: ?
Fluid Viscosity:	<a>2.0 mPa•s (propanol/25°C)</a>	Suppress > (mol/L) < (mol/L) ? < (%) ? < (%) ? < (%)	S1:
Delay (Velocity) Range:	<b>?</b> [8.4 m (483 nL/m) [13.5 h (5 nL/m)	Check	S2:
Total Inlet Volume:	<b>?</b> 4.04 μL Open	Add More	Cleaning Stages: ?
Extra-Detector Volume:	2   0.05 μL   Calculator	To optimize an analysis, ad-	1. Place the inlet in clean air Run not active
+ Device Inspection		ditional Advanced Parameters	2. Place the inlet in the S1 fluid Run not active
Maximum Volume:	? 50 µL v	are supported in which you can	3. Place the inlet in the S2 fluid Run not active
Maximum Time: Mixture Lifetime:	? 2 hours v ? (seconds v	specify the classes of analyzed	4. Place the inlet in the S1 fluid Run not active
+ Advanced Parameters		substances.	5. Place the inlet in the S2 fluid Run not active
	Run Measurements		6. Place the inlet in the S1 fluid Run not active
			7. Place the inlet in clean air Run not active
	art continious mea- with default param-		Estimated Parameters: ?
	field is filled), or re-		Export to Calculator
•	surement time, vol-		Baseline: ?
ume, etc.			Suggested Cleaning Substances: ?
			The appropriateness of the in-

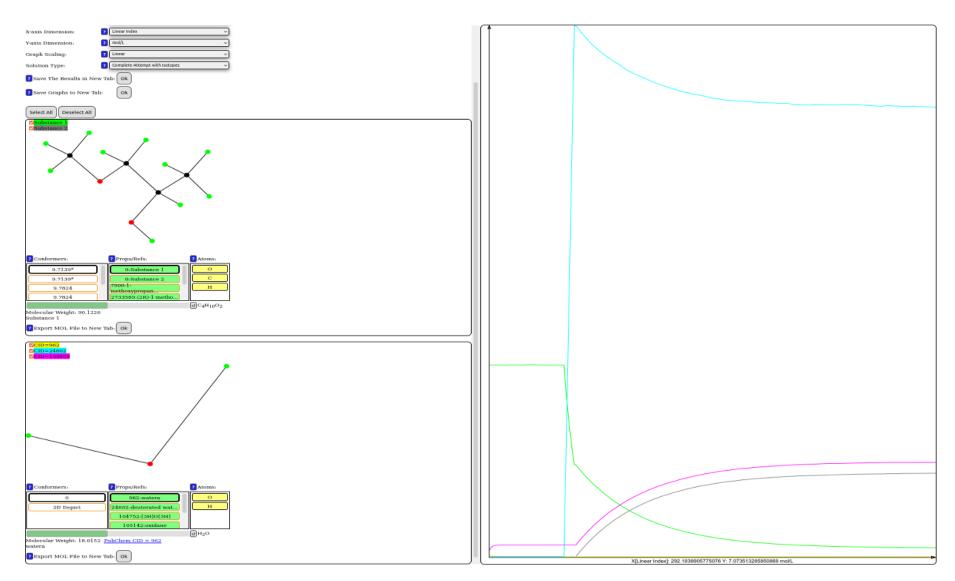
The appropriateness of the inlet settings can be checked through the Device Inspection section.

Measurements are carried out fully automatically, and the results are transmitted to the computing unit.

Start Page Elegant NMR® Software v1.08 ©Elegant Mathematics LLC	Start Page Elegant NMR® Software v1.08 © Elegant Mathematics LLC
Search Records	Start Computations
Devices: ?	
Elmathron_SN_1	Multiple Solutions: ?
Demo_Dev_2	
Demo_Dev_3 Demo_Dev_4	Experiment Correlations: ? No v
Dello Dev 4	Advanced Computation Methods: ? Only Al
List of Search Criteria: ?	Advanced Computation Methods:
Experiment Nr Range V	Purpose of Calculations:  Molecules and Concentrations
Add More	+ Advanced Parameters
Search Records	List of Datasets for Computation and Display: ?
List of Search Records: ?	Elmathron_SN_1 V
Select All Deselect All Demonstrate Results Permanently Delete	Add More Check in Database
Append to Starting Computations Continuous Measurements with Autosampler	Start Computations Start Batch Computations

You can explore and search for measurements, and perform calculations, including many correlation methods, based on measured datasets.

## Elegant NMR®



The results are presented in the form of a list of detected substances with their conformers and the corresponding concentration graphs for each of them. You can explore it and apply various correlation methods based on the measured datasets.

## FAQ

**Q:** What is the magnetic strength in Tesla?

A: We use very weak magnets, only 1 T, because DNP in liquids only works well with magnetic fields less than 1 T. In turn, DNP improves the signal-to-noise ratio for one-dimensional spectra by about 400 times, and almost 100,000 times for multidimensional spectra. Therefore, the sensitivity of 1D is approximately as if we were capturing spectra at 100 MHz, and the sensitivity of 2D+ is approximately as if we were capturing spectra at 400 MHz.

**Q:** Can I get 1D spectra from Elegant NMR system?

**A:** The ability of the Elegant NMR measuring system to automatically interpret heteronuclear DNP NMR spectra on an adaptive grid completely disrupts the status quo in which 7- and 8-dimensional DNP NMR spectra, having sparsity values less than 0.1%, are very difficult not only to interpret, but even to visualize.

In the Elegant NMR system, such spectra are identified with reference to a huge database containing about 1.7 billion spatial molecular structures.

7-8-dimensional spectra can be projected onto one-dimensional slices and then visualized. We will implement this approach in the expert mode of the Elegant NMR software for reference purposes.

## FAQ

Q: Do we need to use external MW source for DNP?

**A:** No, Elegant NMR System is equipped with internal DNP source according to recently patented technology US 10773092 B2.

Q: Do you have HPLC/GCMS inside, or how you separate unknown mixtures?

**A**: We do not separate molecules, we separate signals. In classical HPLC, for separation to occur, we need the substances to be separated to form complexes with a stationary phase and the energy of formation of such complexes is significantly different. It is often possible to find a stationary phase that would orientate the substances to be separated well, but would not separate these mixtures well enough, for instance, because of the insufficient number of theoretical plates. In our apparatus we do not separate substances, namely, we orient them differently. This orientation affects the two-dimensional NMR spectra and it is possible, without separation, to obtain slightly different HSQC or NOE spectra, and on the basis of their correlations, to get relative concentration and pure spectra of the substances themselves.

The patent pending technology US 16/695,200 is fully implemented inside Elegant NMR system.