1. Please describe the principles of Nuclear Magnetic Resonance (NMR) in 10 sentences.

Which of the following sentences are correct? explain why:

1. Hydrogen atom nuclei possess magnetic moments

Yes. Hydrogen atom nuclei consist of a single proton. Protons (and electrons) possess magnetic moments.

1. Nuclear Magnetic Resonance uses an external magnetic field

Yes. An external magnetic field is used in NMR measurements – this also includes Magnetic Resonance Imaging. The magnetic moments of hydrogen atom nuclei can take in the external magnetic field two orientations: parallel or anti-parallel to the field. The difference in the number of the populations of these two state is responsible for creating a macroscopic magnetisation of the sample.

1. Relaxation time can be expressed in seconds

Yes. When one changes the magnetic field, the macroscopic magnetisation changes as well. This process is referred to as relaxation. The relaxation time describes how fast the magnetisation is changing – in other words, it gives the time that is needed for the magnetisation to reach the value that corresponds to the new magnetic field. For instance, the time for water in bulk (pure water) is about 2 s.

1. Magnetic Resonance Imaging (MRI) monitors differences in water relaxation times in tissue

Yes. Because of different structure and composition of various kinds of tissue, water molecules in tissue exhibit different dynamics.

1. MRI uses X ray irradiation

NO!!! in MRI one does not use X ray – therefore the method is a breakthrough in medical diagnosis – no side effects.

1. MRI can be performed only for pathological tissues

NO of course. It would be nonsense. Actually the examination is performed to see the shape of the tissue. One would need to be ill for sure to be admitted to NMR scans – not much sense. And, from the physical view point – healthy tissues also contain water molecules than move.

1. Water molecules perform translational and rotational dynamics

Yes. Water molecules (and also other molecules) can rotate around their axes (rotational dynamics) as well as move in the space (translational dynamics).

1. MRI exploits graphical software

Yes. Sure.

1. NMR investigations exploits only for water molecules

No. Other molecules also include hydrogen atoms. Moreover, one can perform NMR investigations also for some other nuclei – such as 19F and 31P.

1. Magnetic moments interact with a magnetic field

Yes. This is the reason why the magnetic moments can take only the two orientations in an external magnetic field.

1. Please describe in 10 sentences the concept of fitting a model to experimental data.

Which of the following sentences are correct? explain why:

1. Fitting a model to experimental data means to find theoretical parameters for which one obtains the best agreement between the experimental data and the model

Yes.

1. Fitting procedures exploit minimisation algorithms

Yes. One takes a difference between the experimental values and the theoretically predicted one (for a given set of parameters) for each data point (Yexp- Ytheor). Then, as two situations are possible: Yexp> Ytheor or Yexp< Ytheor, the difference can be positive (>0) or negative (<0). Therefore one takes (Yexp- Ytheor)2. Then one makes a sum of these squared differences for all data points. Then one looks for which values of the model parameters the sum will reach a minimum.

1. Linear regression means fitting a linear function y(x)=ax+b to the data

Yes. Linear regression is just the name for this specific case. It is worth to know that when a non-linear function is fitted (for instance an exponential function) the fitting is called non-linear regression.

1. To be able to fit data, the data must have an extremum (minimum, maximum)

No. One performs for instance, linear regression, and linear functions do not have extrema.

1. The number of the fitted parameters might not exceed the number of experimental points

Yes. Imagine: you have 2 data points and a linear function: y=ax+b

The coordinates of the points are: (x1, y1) and (x2,y2)

One gets: y1=ax1+b

y2=ax2+b

One can calculate: a=(y2-y1)/(x2-x1). Then one can get b from one of the equations.

Well known statement: one can draw a line through each two points.

If the number of points is equal to the number of the parameters, one can just calculate the parameters (no need to fit anything).

Important remark: It might happen that one gets in this way a set of equations contradicting each other. This means that the assumed model is wrong.

Rule: the number of points must be larger than the number of the parameters.

1. The obtained parameters have some inaccuracies (fitting errors)

Yes. Typically one asks the question: how much must one change one of the model parameters to enlarge the values of the sum of (Yexp- Ytheor)2 by a certain factor, for instance 2. And then the answer is provided by the uncertainty of the parameter: a ± a (3.2 ± 0.2)

1. The model parameters must be positive

No. Of course not. One can for sure fit a curve: y=-2x+7

1. The number of the model parameters cannot exceed 5

No. The number of the model parameters can be large, as long as we have a sufficient number of the data points.

1. The model cannot include products of parameters

No

Let us consider two examples:

Y(x)=(A\*B)x2 +Cx+D - wrong: one cannot independently determine A and B

However

Y(x)=(A\*B)x2 +Bx+D - right: one determines B and then one can determine A from the value of the product A\*B (because one knows B)

1. The number of experimental data must exceed 16

No. nonsense

1. Knowing that the magnetization follows the equation:

calculate the magnetisation for *t*=T. After how long time the magnetisation changes by factor 2.