DOSY

Diffusion Ordered SpectroscopY (DOSY)

An Introduction

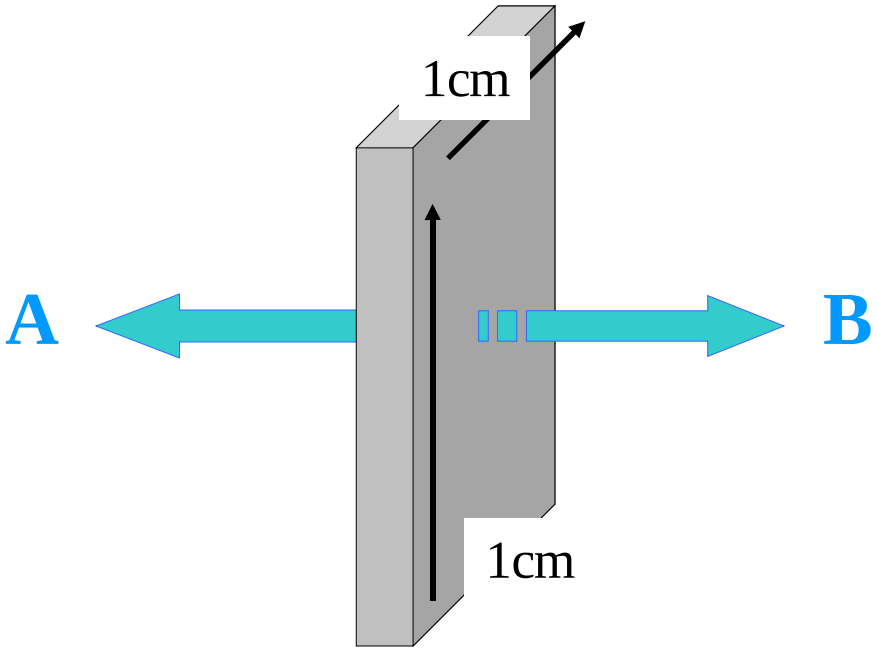
Translational Diffusion

J= dn/dt/A

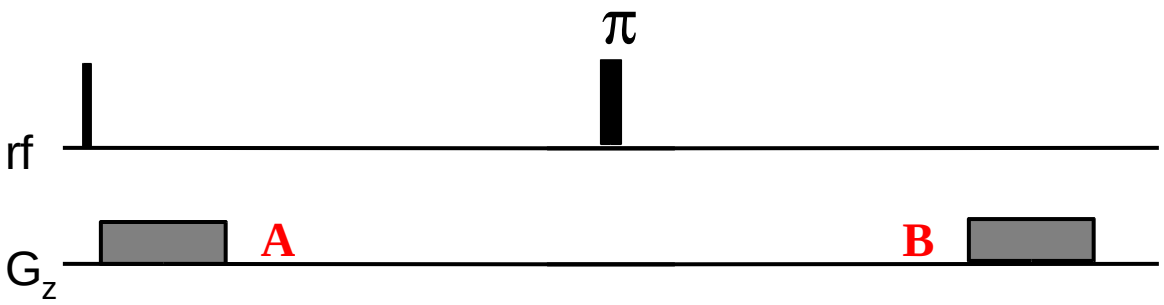
J= flux

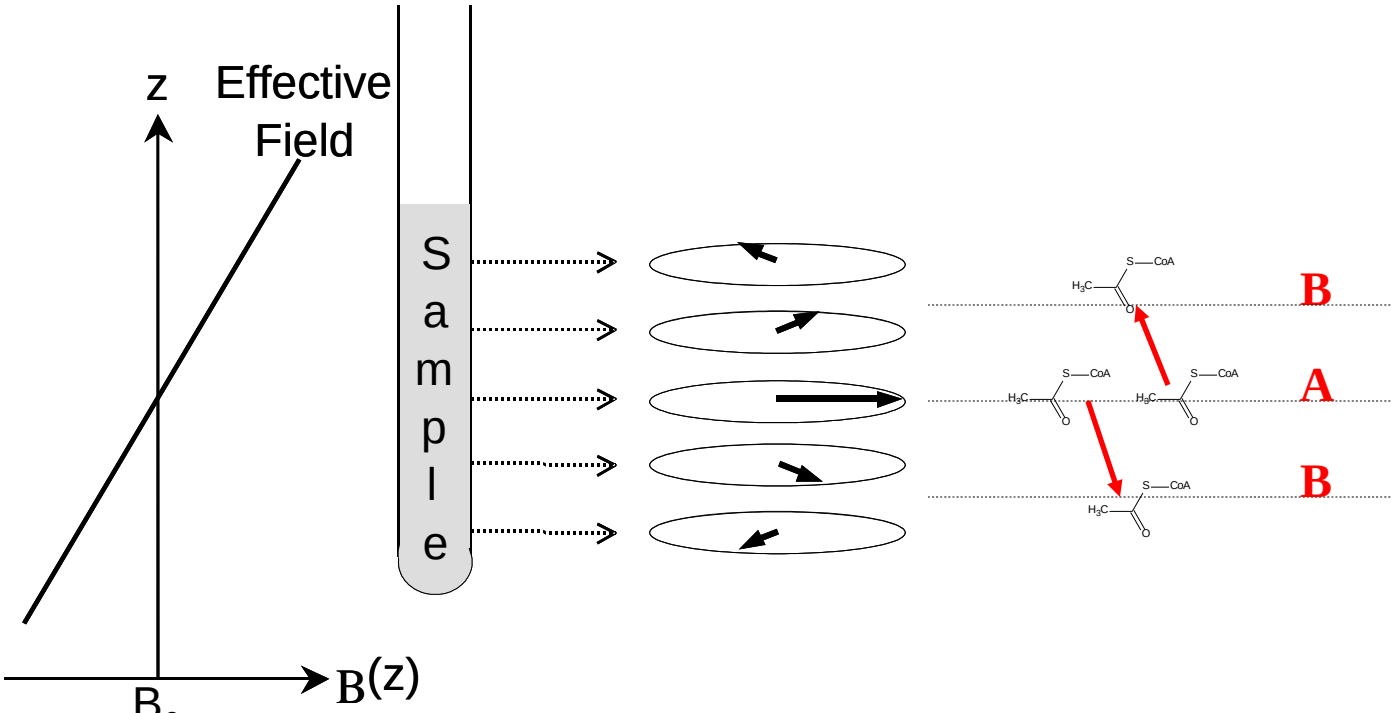
dn/dt= number molecules transported/sec

A= sampling area of the reference plane

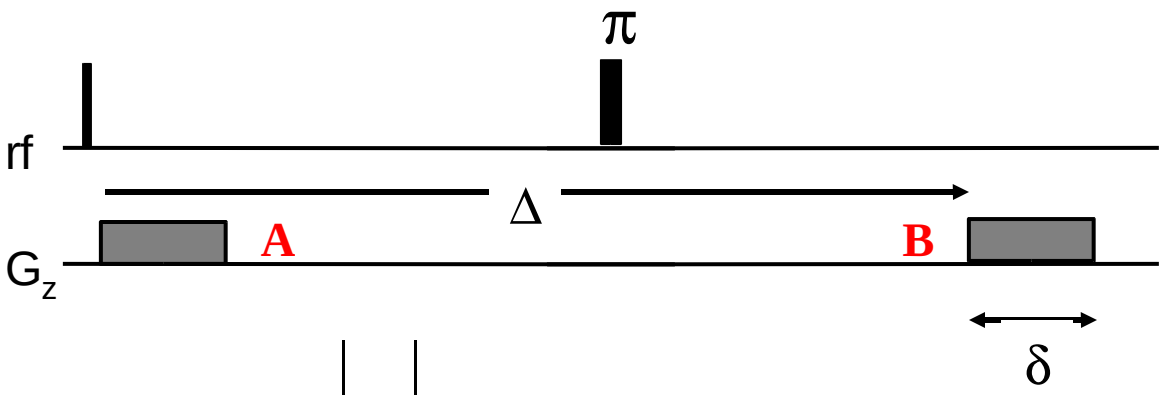


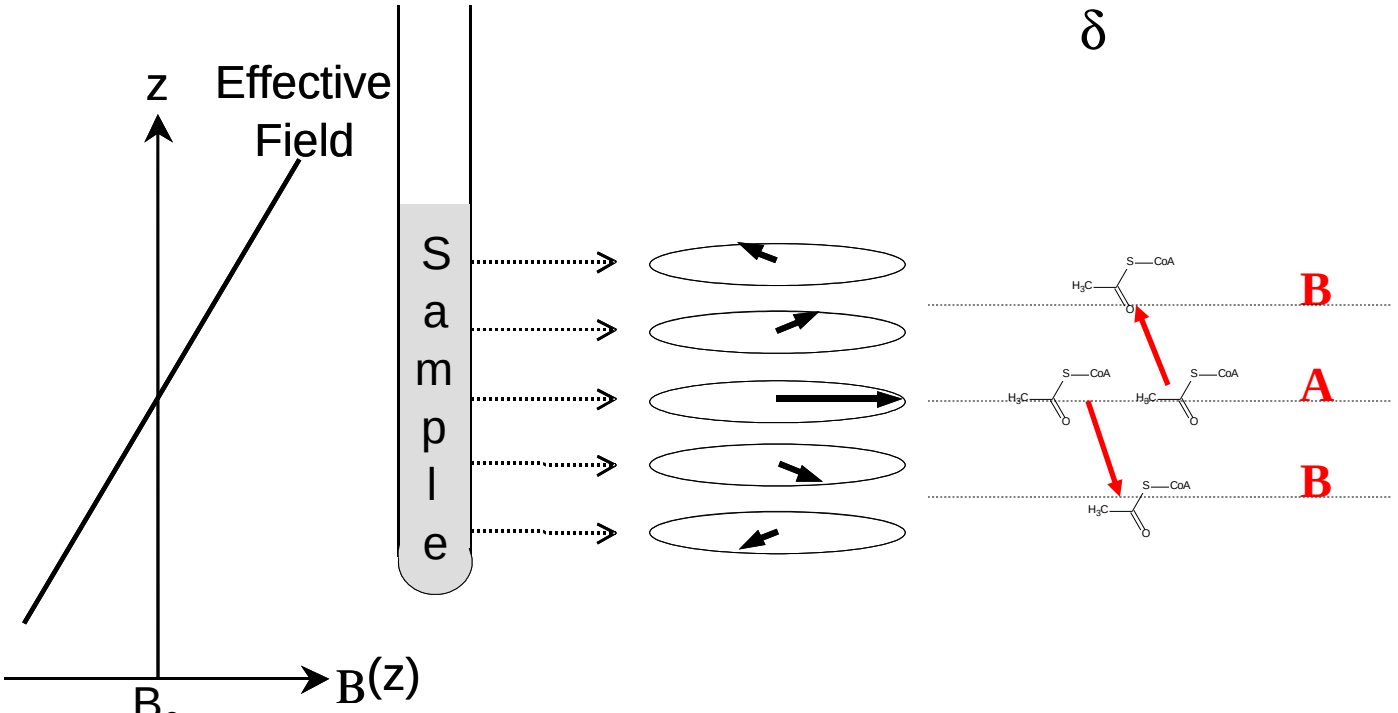
Translational Diffusion





Translational Diffusion





Translational Diffusion

$$I(q) = I_o \, e^{-Dq^2\Delta'}$$

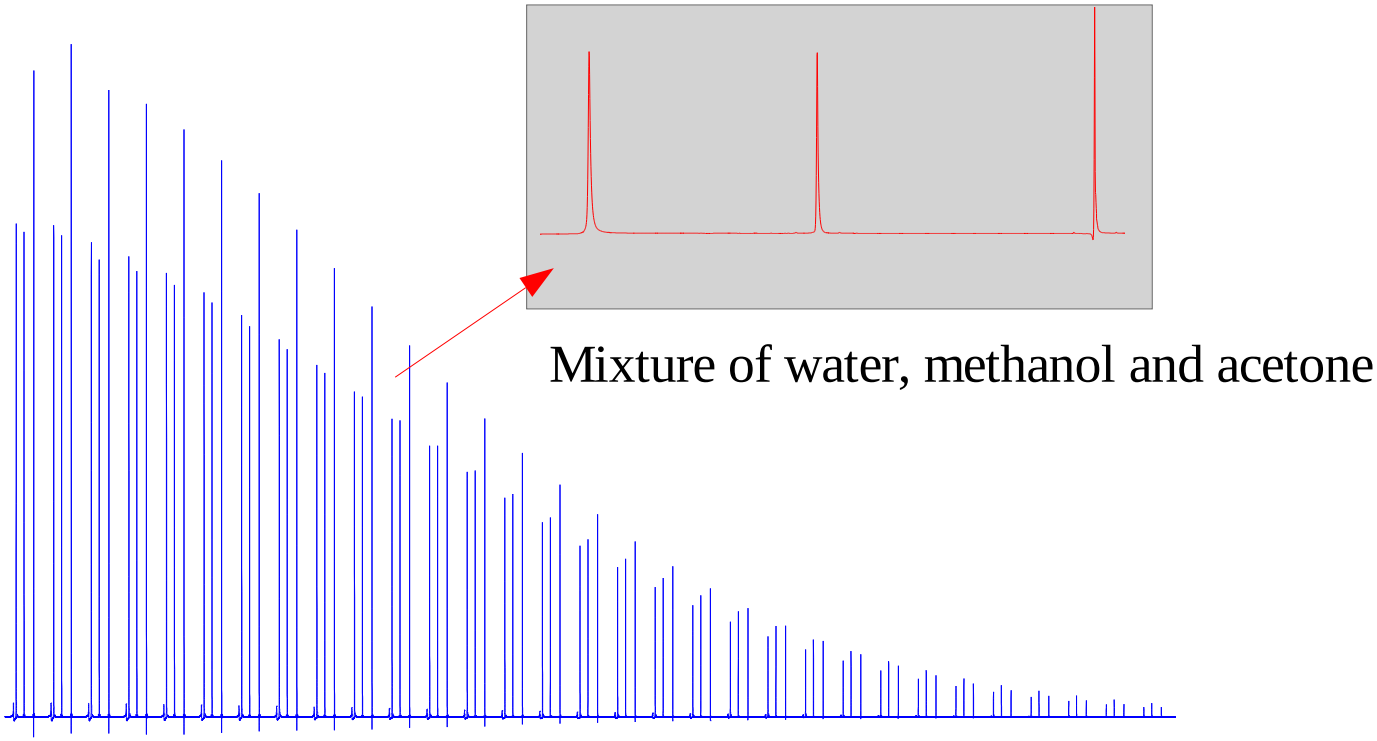
D : diffusion coefficient
Δ' $= \Delta - \delta/3$
Δ : diffusion time and δ is a correction factor for finite gradients
q : $\gamma g \delta$
γ : gyromagnetic ratio
g : is the amplitude of the applied gradient
δ : duration of the applied gradient

I(q) is a function of:

size, shape, aggregation etc. of molecule
temperature
viscosity

Translational Diffusion

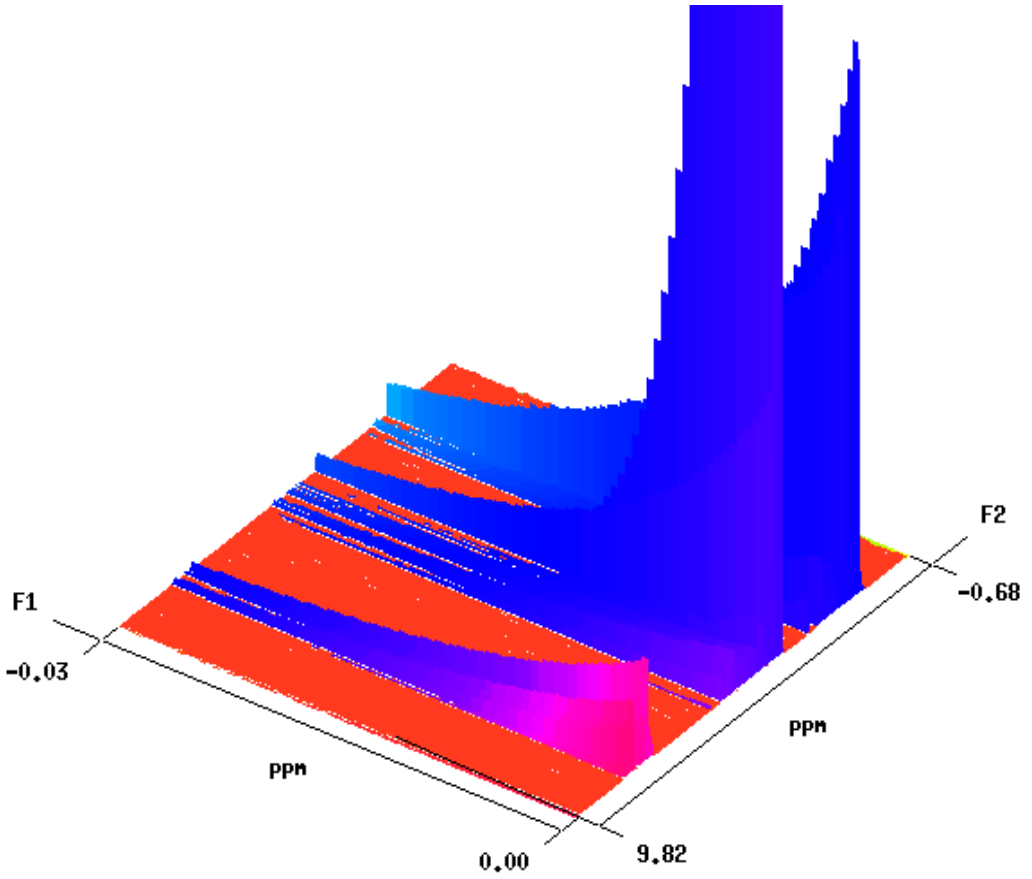
Decay of magnetization as function of gradient intensity



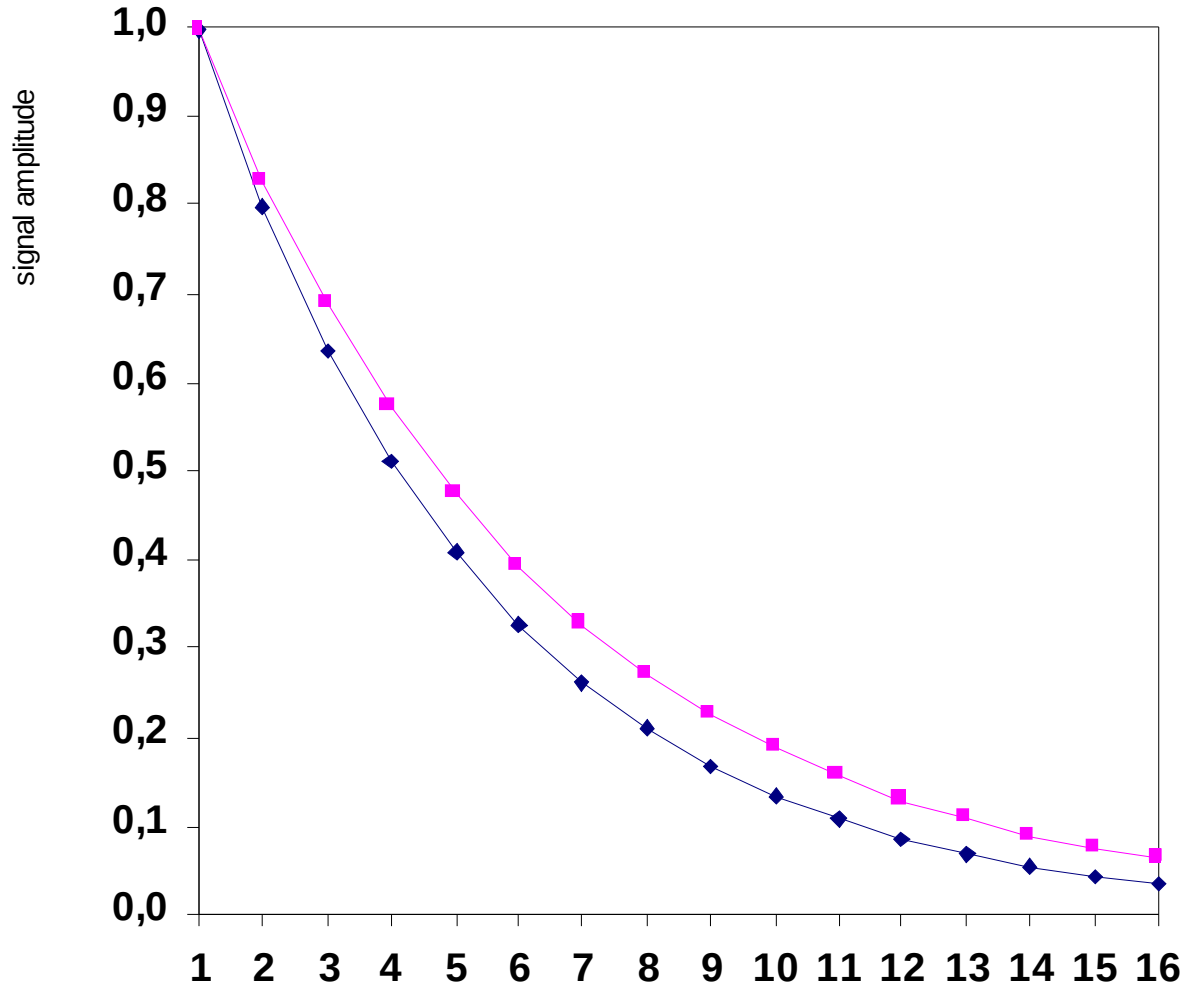
Mixture of water, methanol and acetone

Diffusion und DOSY

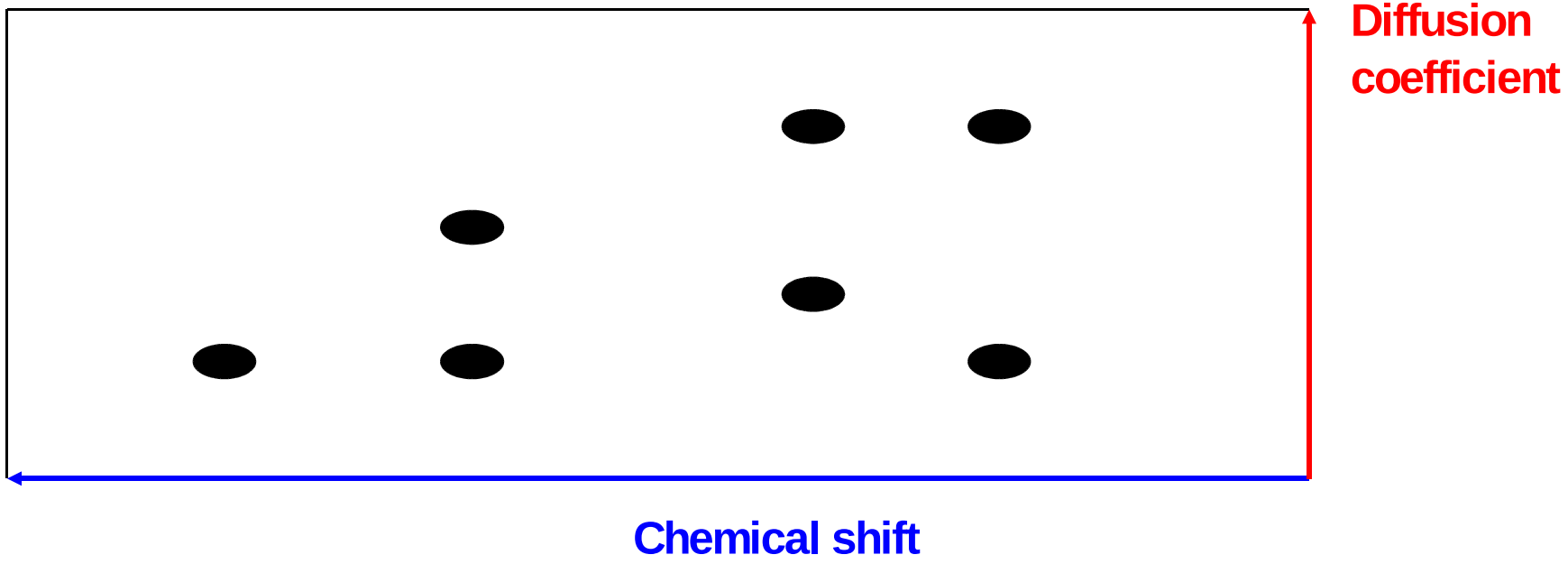
Stacked plot of a diffusion spectrum after F2 transformation. On the F2 axis some of the strong signals of the peptide mixture are visible. The F1 axis shows the decay of the signals with increased gradient strength due to the diffusion of the molecules in solution.



Diffusion and DOSY



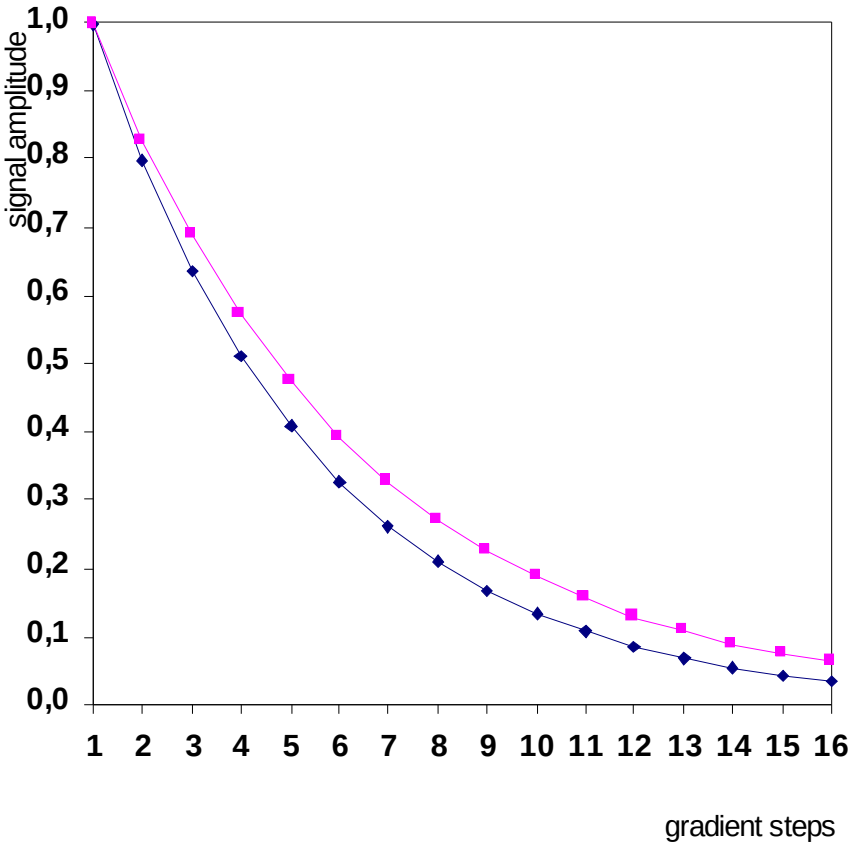
DOSY: the principle



Diffusion and DOSY

overlapping signals

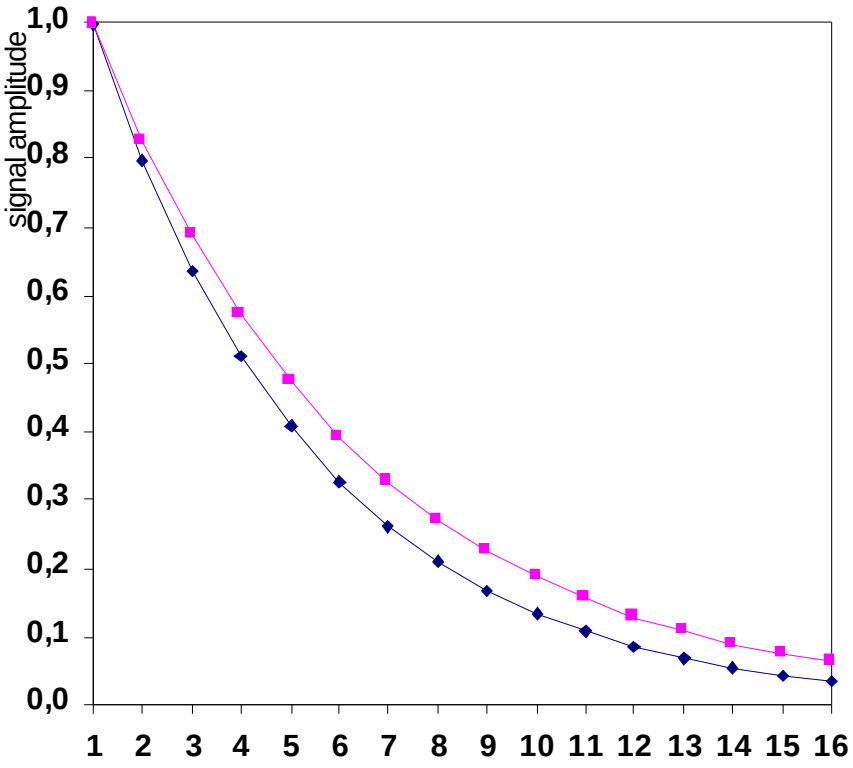
Signal decay: low noise



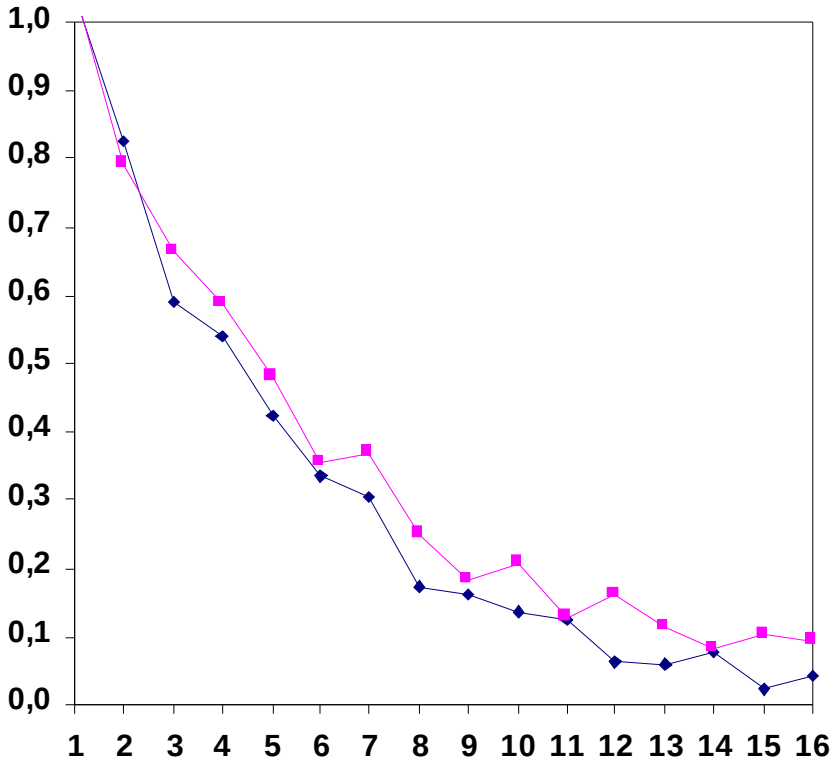
Diffusion and DOSY

overlapping signals and S/N

Signal decay: high S/N



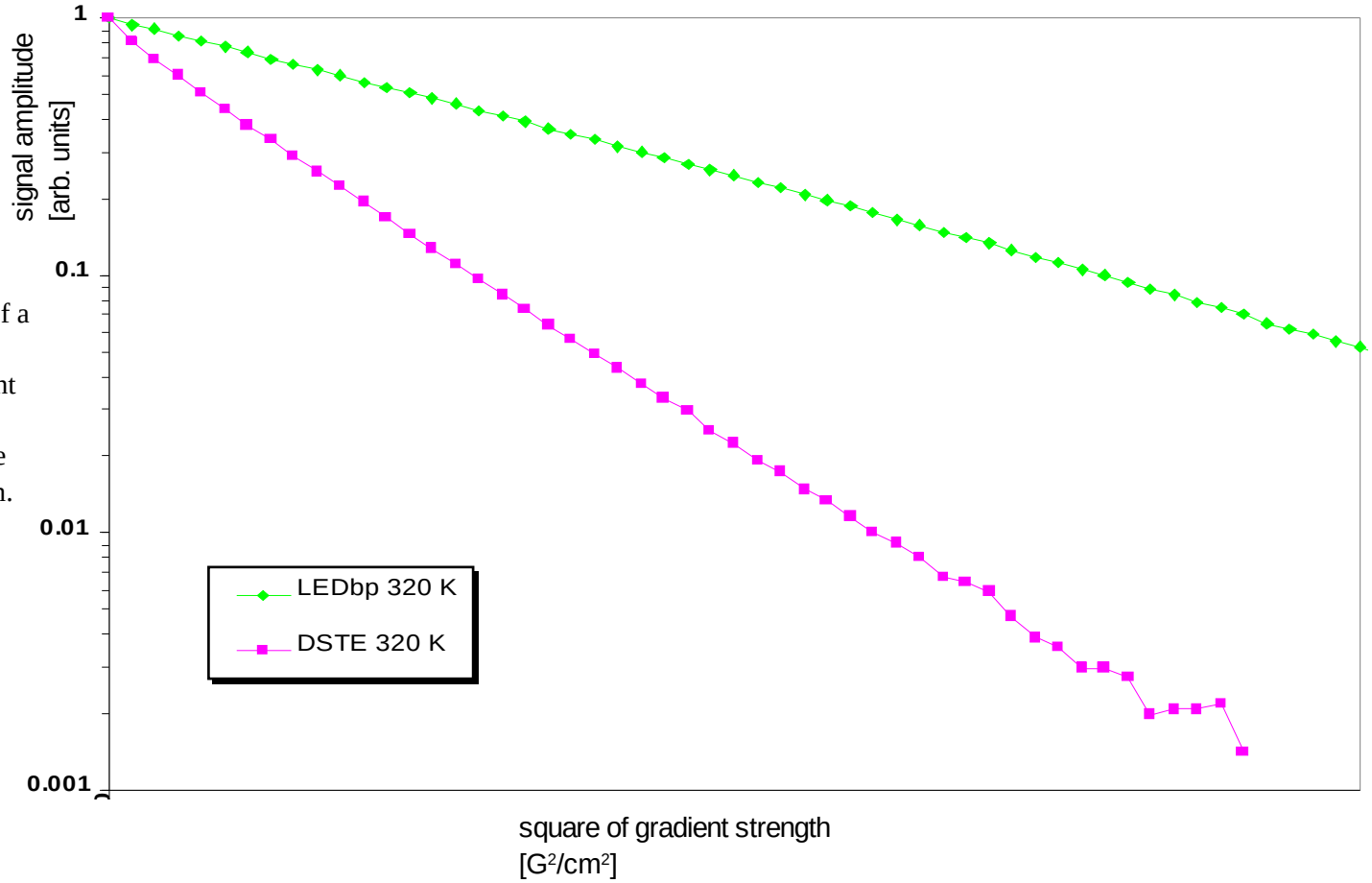
Signal decay: low S/N



Diffusion and DOSY

Convection

self diffusion measurements of a peptide in DMSO at different temperatures and with different pulse sequences. The signal amplitude is plotted versus the square of the gradient strength.



DOSY: Pulse and AU Programs

- AU Programs
  - dosy, setdiffparm
- Pulse Programs (1D-versions not shown)

  Stimulated Echo Sequences:
  - stegp1s, stebpgp1s — bp: bipolar gradients
  - stebpgp1s19 — 19: 3919 WATERGATE
  - stebpgpin1s — in: INEPT, for X-nuclei

  Double Stimulated Echo Sequences:
  - dstegp3s

DOSY: Pulse and AU Programs

Stimulated Echo plus LED Sequences:

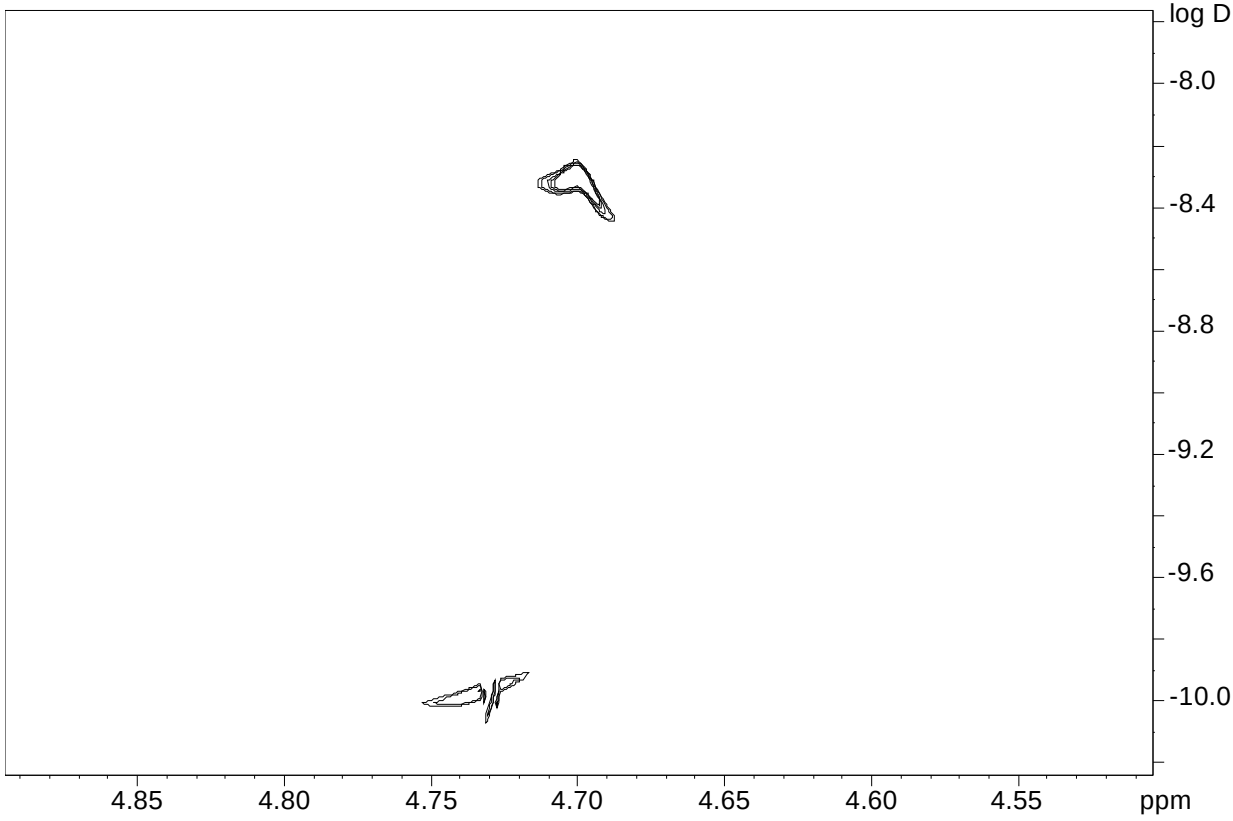
- ledgp2s
- ledbpgp2s — bp: bipolar gradients
- ledbpgpml2s2d — ml: diffusion filtered 2DTOCSY
- ledbpgpml2s192d — 19: additional WATERGATE
- ledbpgpco2s3d — co: 3D DOSY-COSY
- ledbpgpml2s3d — ml: 3D DOSY-TOCSY
- ledbpgpno3s3d — no: 3D DOSY-NOESY

DOSY: Data

- Data are compatible with T_1/T_2 software
- F1 axis shows diffusion constant:
  - logarithmic: log D
  - linear: D * 1e9

DOSY: two water species

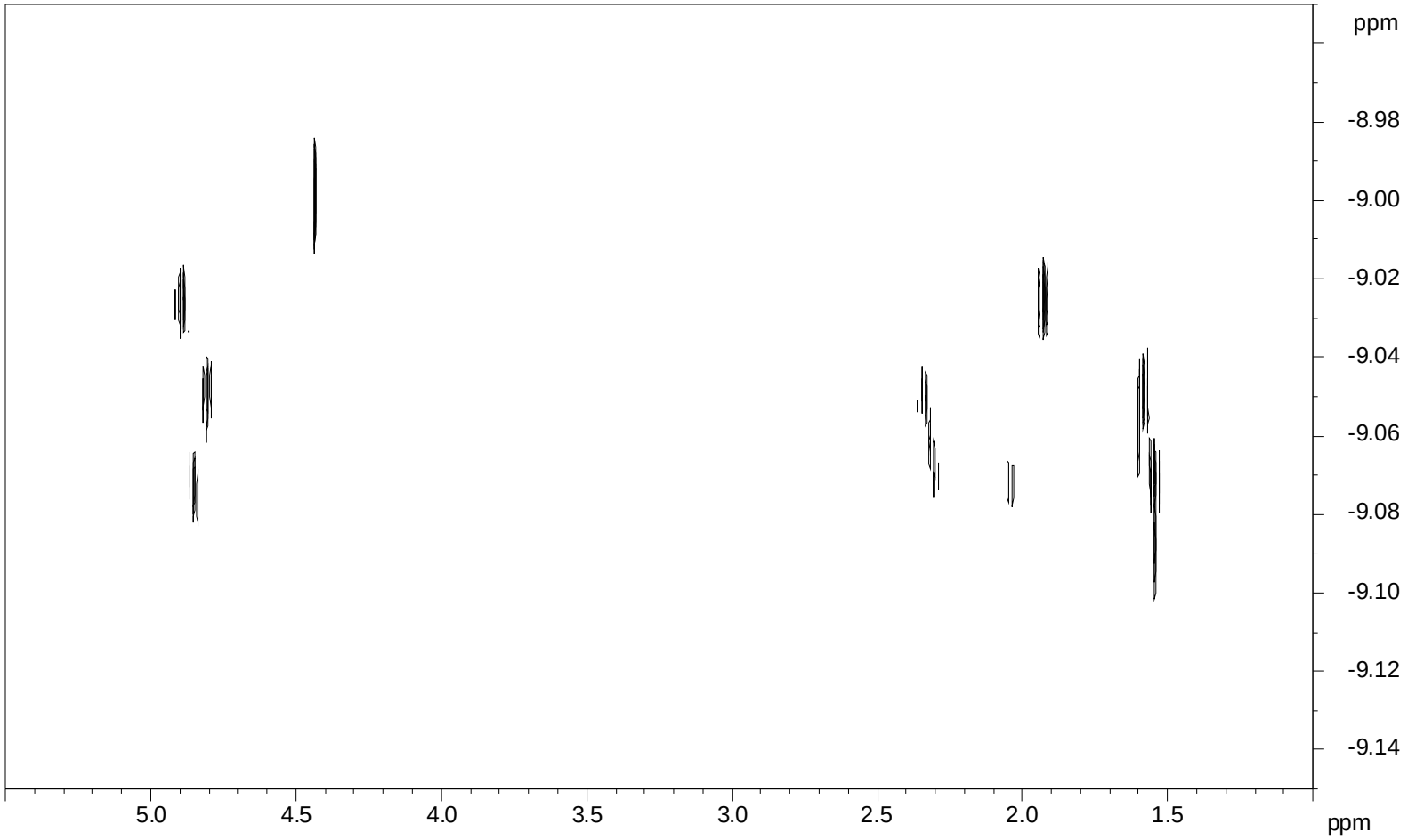
Intra- and inter cellular water

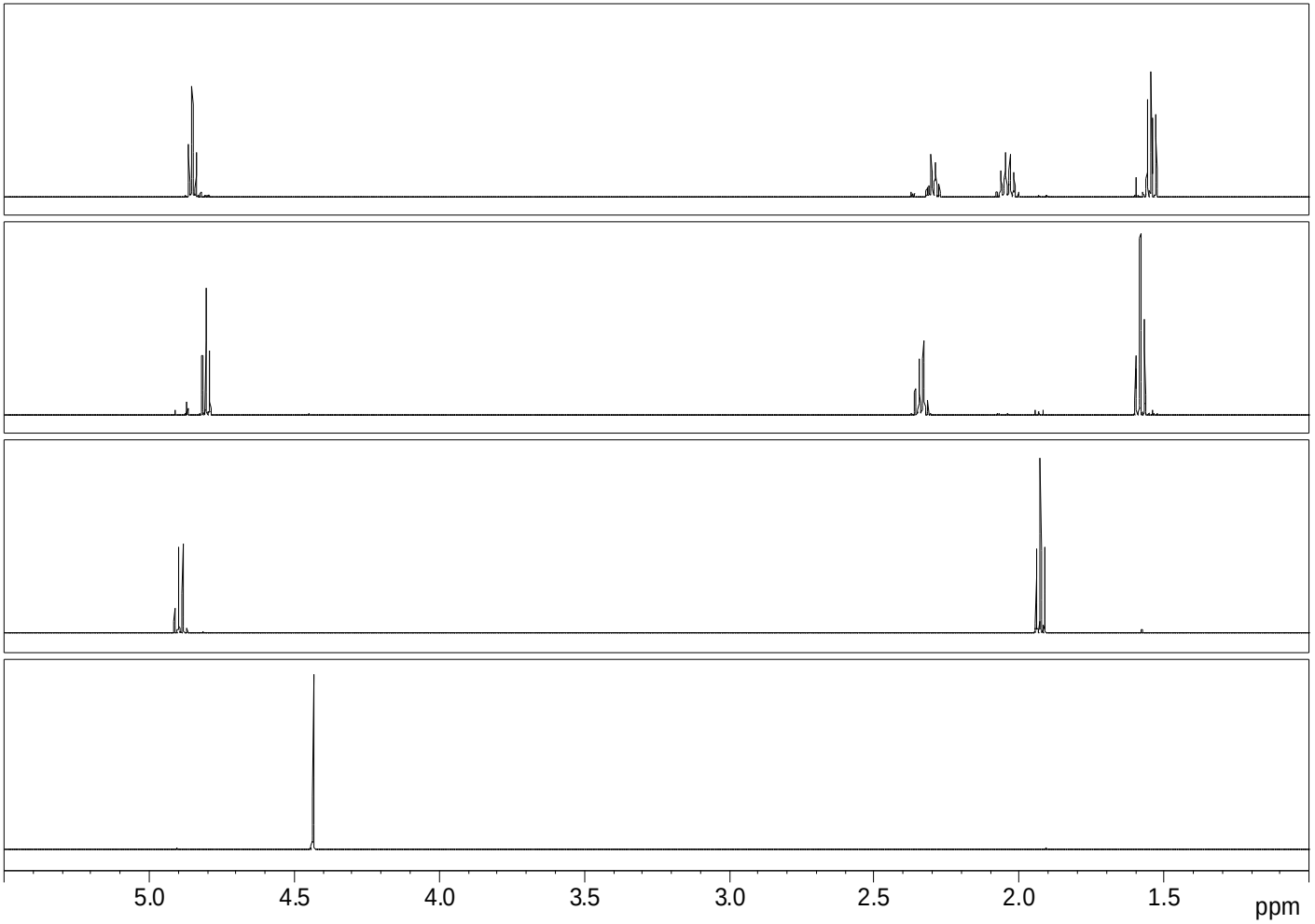


DOSY: mixture of 4 esters

P-Hydroxybenzoic acid ester

R= -Me, -Et, -Prop, -But



DOSY: mixture of 4 esters

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