

Spektroskop Nukleární Magnetické Resonance

Ústav: 402 - Ústav analytické chemie

Odpovědná osoba: doc. Ing. Bohumil Dolenský, Ph.D.





OP Výzkum a vývoj
pro inovace

Kvalalab****



VYSOKÁ ŠKOLA
CHEMICKO-TECHNOLOGICKÁ
V PRAZE



EVROPSKÁ UNIE
EVROPSKÝ FOND PRO REGIONÁLNÍ ROZVOJ
INVESTICE DO VAŠÍ BUDOUCNOSTI

NMR ECZ 500R / S3 JEOL

Katalogová cena

17 810 928 Kč

Zakoupeno za

9 411 203 Kč

Sleva

8 399 725 Kč

NMR ECZ 500R JEOL

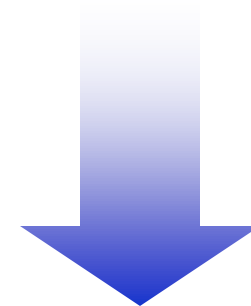
Supravodičový magnet
(4,2 K)

11,74736 Tesla

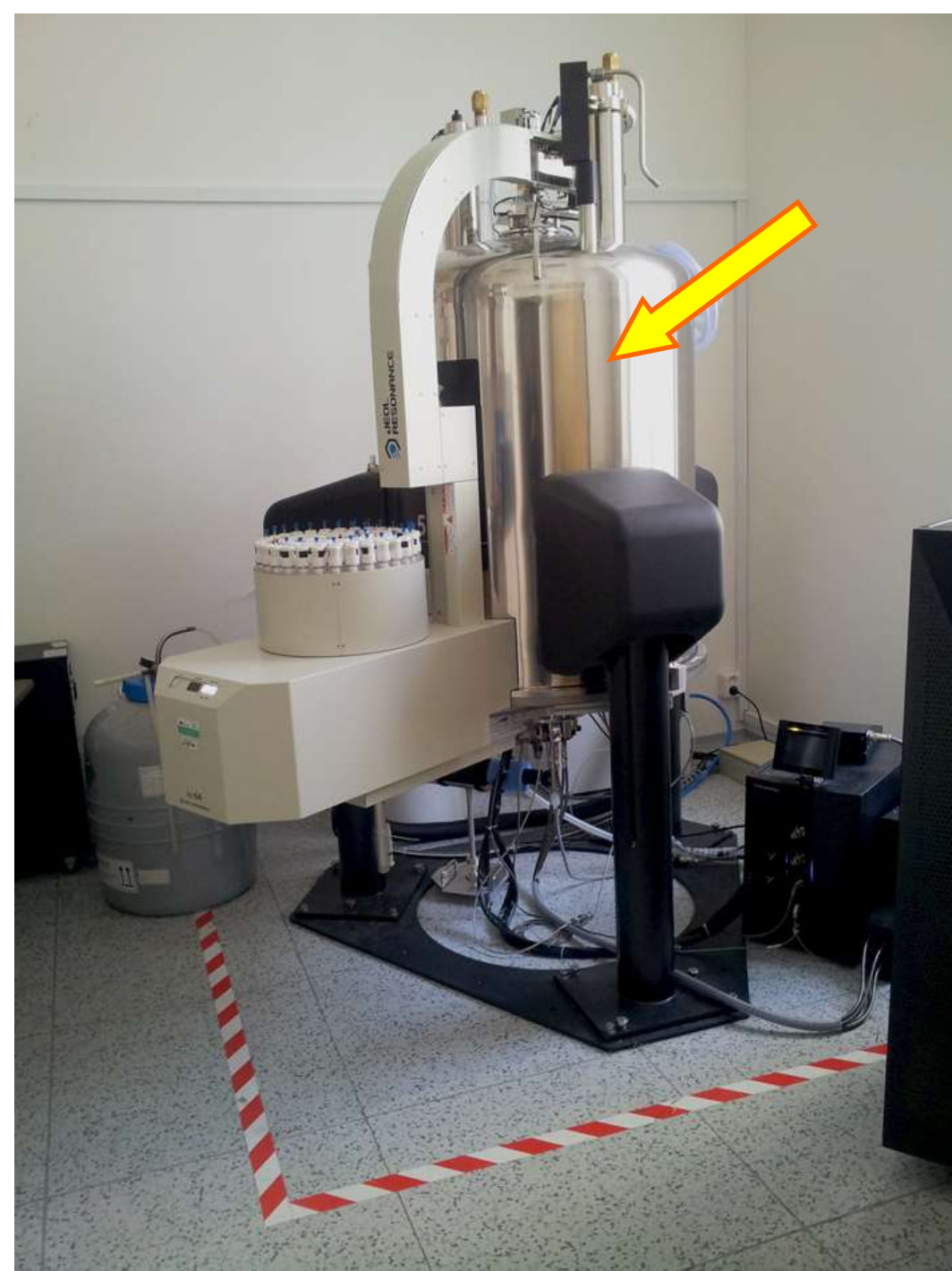
261052-krát pole Země

^1H 500,1599 MHz

^{13}C 125,7653 MHz



vysoce rozlišená spektra



NMR ECZ 500R JEOL

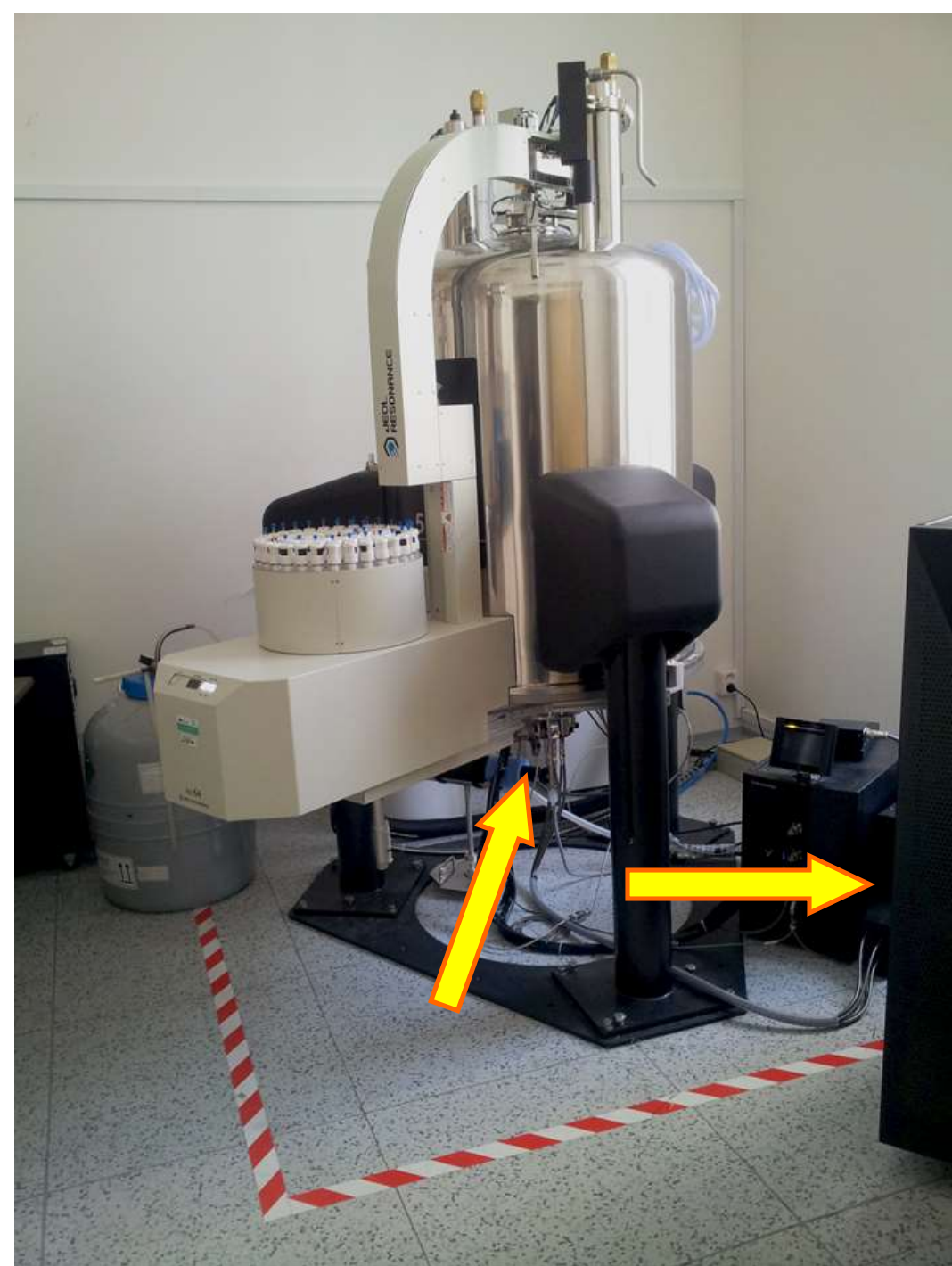
500 MHz 5 mm FG/RO
Digital Auto Tune Probe S
+
Auto-Tuning Unit 2

HF kanál 455 - 535 MHz

^1H , ^{19}F

LF kanál 10 - 210 MHz

^{31}P , ^{15}N , ^{109}Ag , ^{39}K



500 MHz 5 mm FG/RO Digital Auto Tune Probe S

^1H line shape of chloroform (spinning)

Peak width at half height: $\leq 0.5 \text{ Hz}$

Peak width at 0.55% height: $\leq 6 \text{ Hz}$

Peak width at 0.11% height: $\leq 12 \text{ Hz}$

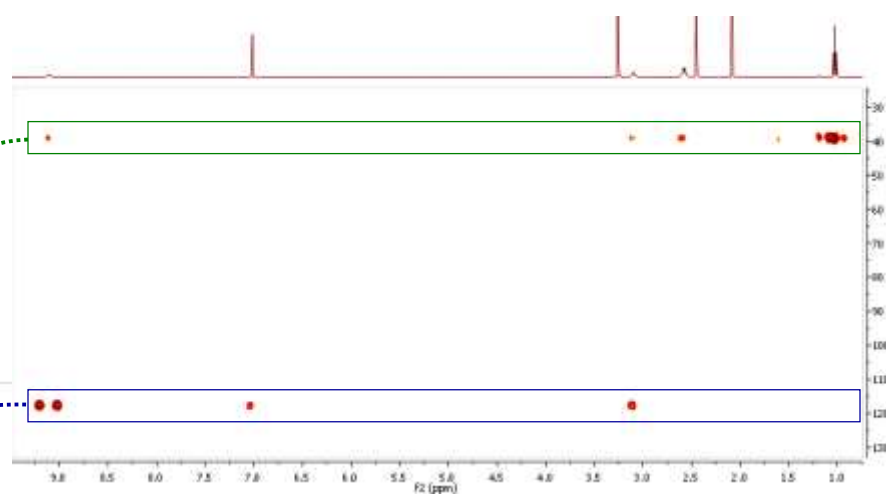
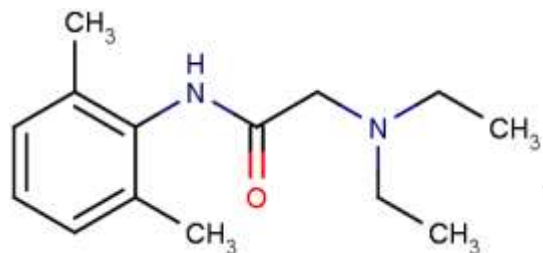
Spinning side band: $\leq 1\%$ for ^1H

Sensitivity: ≥ 630 for ^1H (0.1% ethylbenzene, one scan)
 ≥ 750 for ^{19}F (0.05% TFT, one scan)
 ≥ 270 for ^{13}C (10% ethylbenzene, one scan)
 ≥ 135 for ^{31}P (0.0485M TPP, one scan)
 ≥ 35 for ^{15}N (90% formamide, one scan)

90° pulse width: $\leq 8 \mu\text{s}$ for ^1H at 30W
 $\leq 10 \mu\text{s}$ for ^{19}F at 30W
 $\leq 12 \mu\text{s}$ for ^{13}C at 100W
 $\leq 15 \mu\text{s}$ for ^{31}P at 125W
 $\leq 24 \mu\text{s}$ for ^{15}N at 150W

Variable temperature range: -100 to $+150 \text{ }^\circ\text{C}$

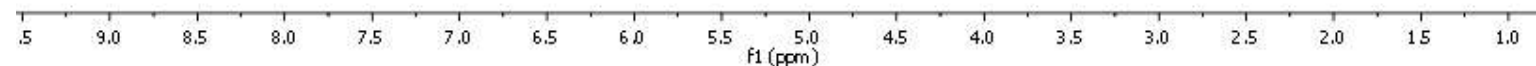
$^1\text{H}\{^{15}\text{N}\}$ gHMBC 2D NMR



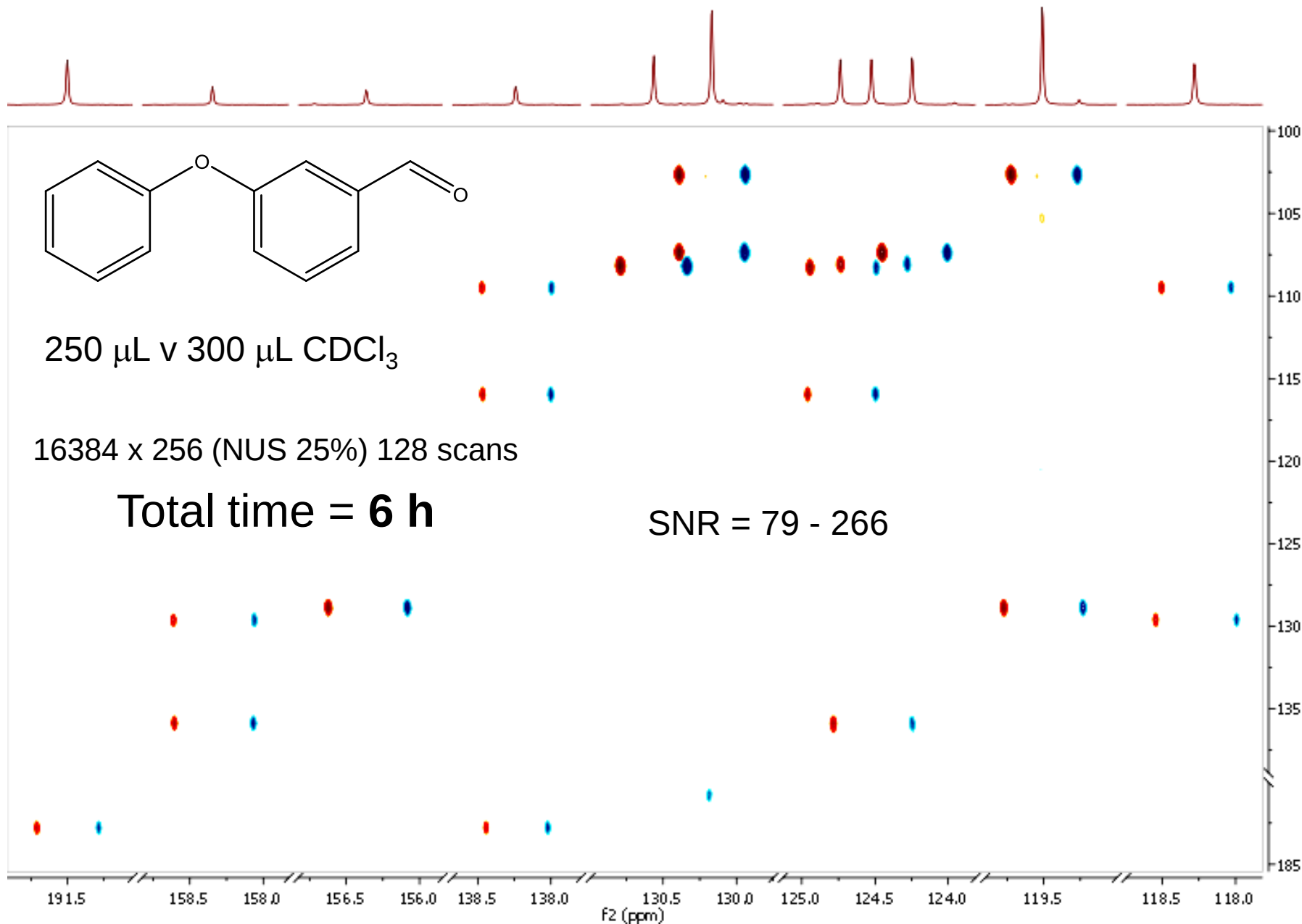
$\delta(^{15}\text{N})$
117,8 ppm

$\delta(^{15}\text{N})$
39,0 ppm

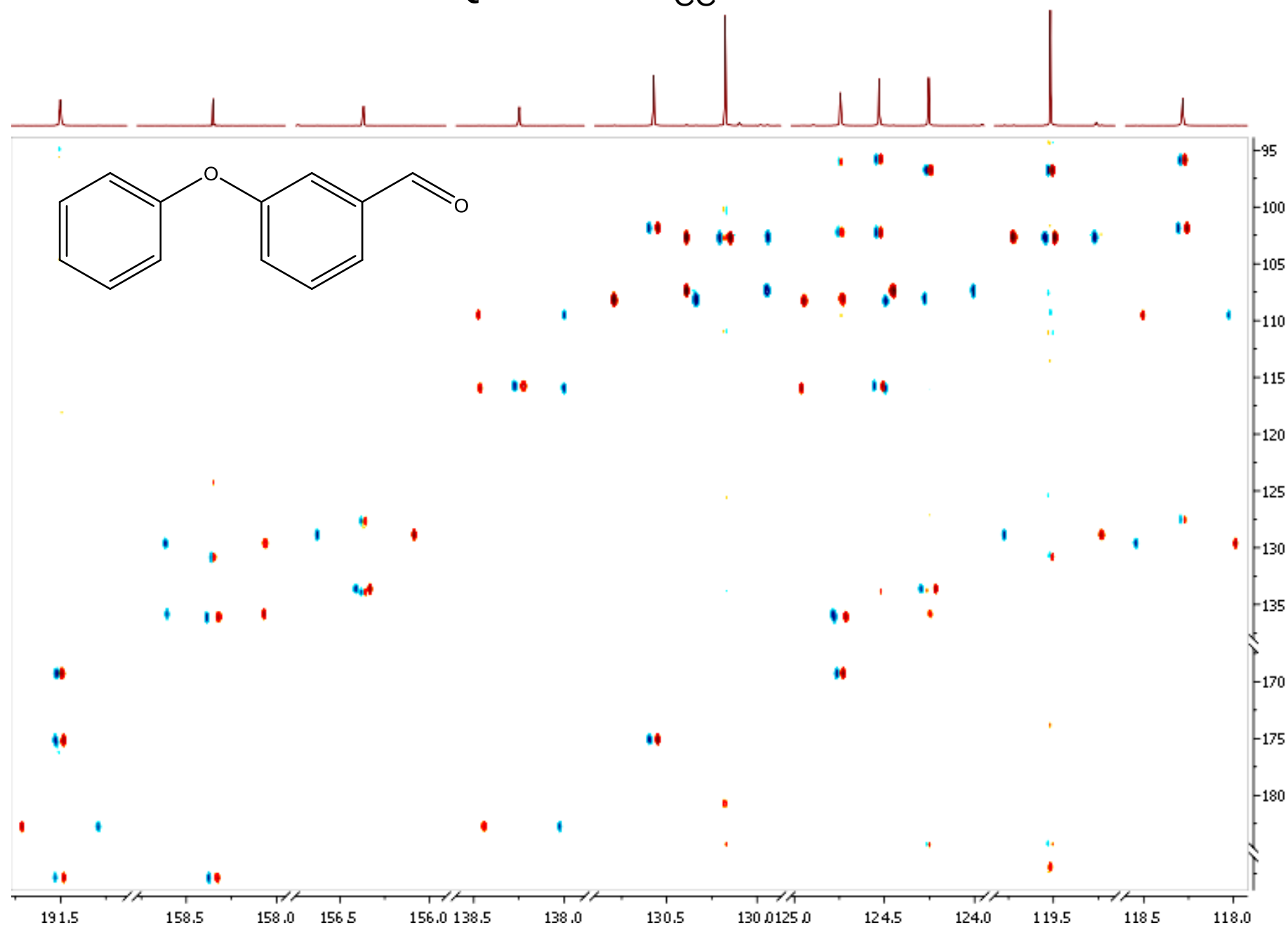
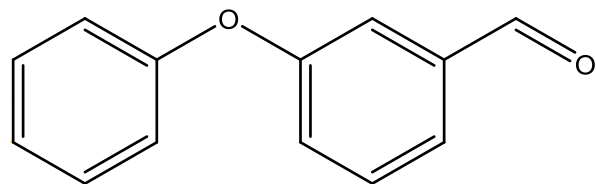
^1H NMR



2D ^{13}C - ^{13}C INADEQUATE $J_{\text{CC}} = 61 \text{ Hz}$

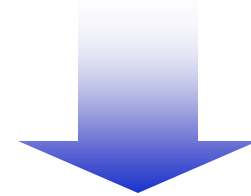


2D ^{13}C - ^{13}C INADEQUATE $J_{\text{CC}} = 8 \text{ Hz}$

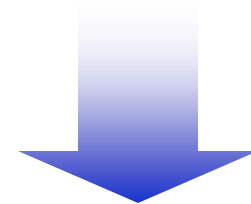


NMR ECZ 500R JEOL

Zesilovač 30 A

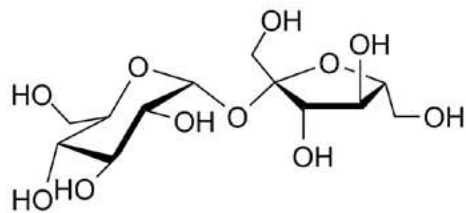


gradientové pulsy až
900 mT / m

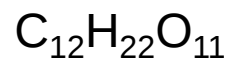


DOSY NMR



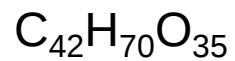


Sacharóza

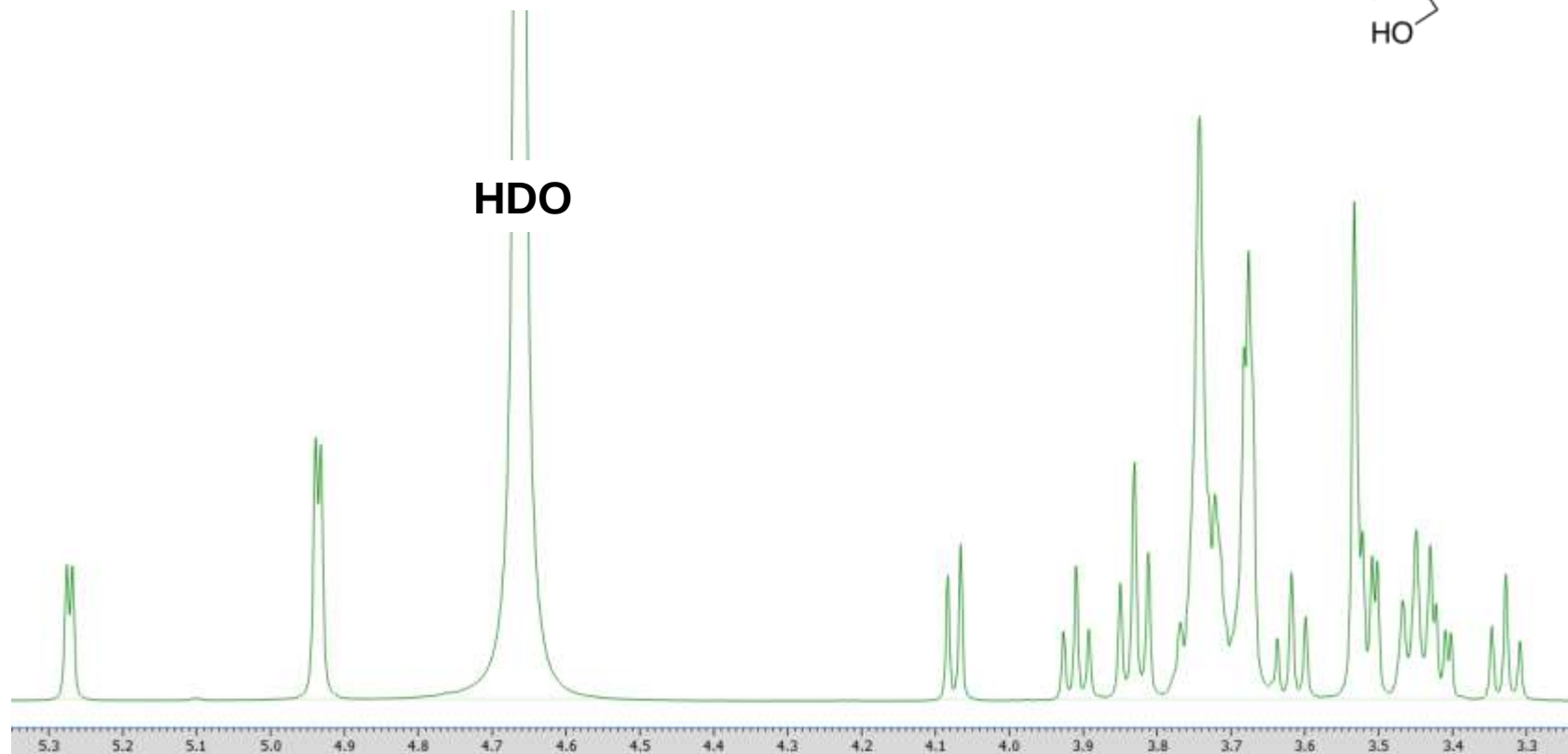
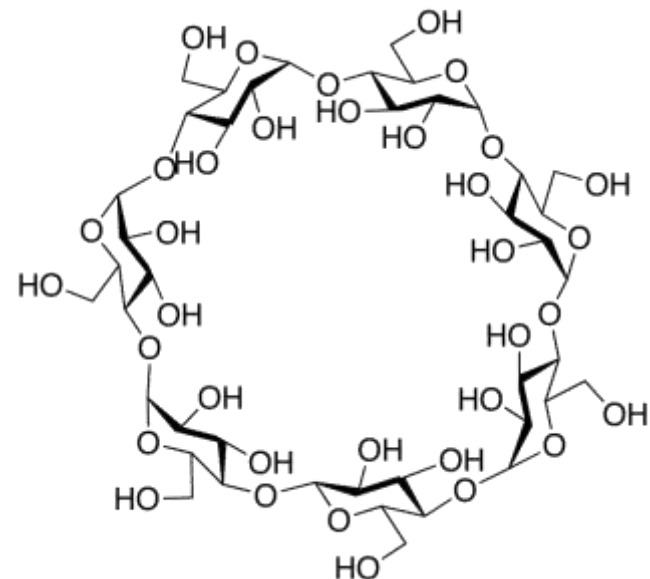


342,30 g/mol

***β*-Cyklodextrin**



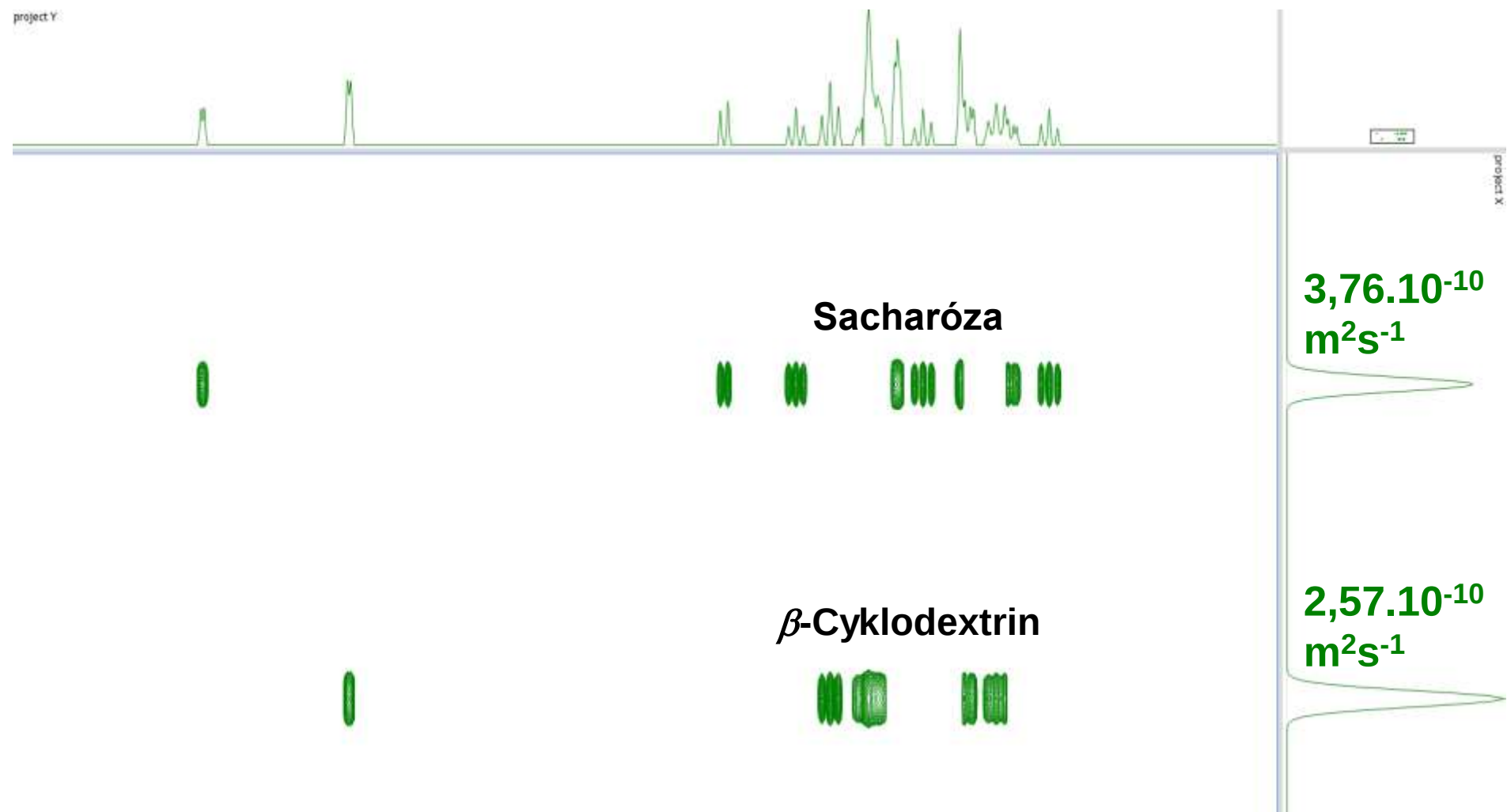
1134,98 g/mol



2D DOSY NMR

„NMR chromatografie“

Diffusion Ordered SpectroscopY

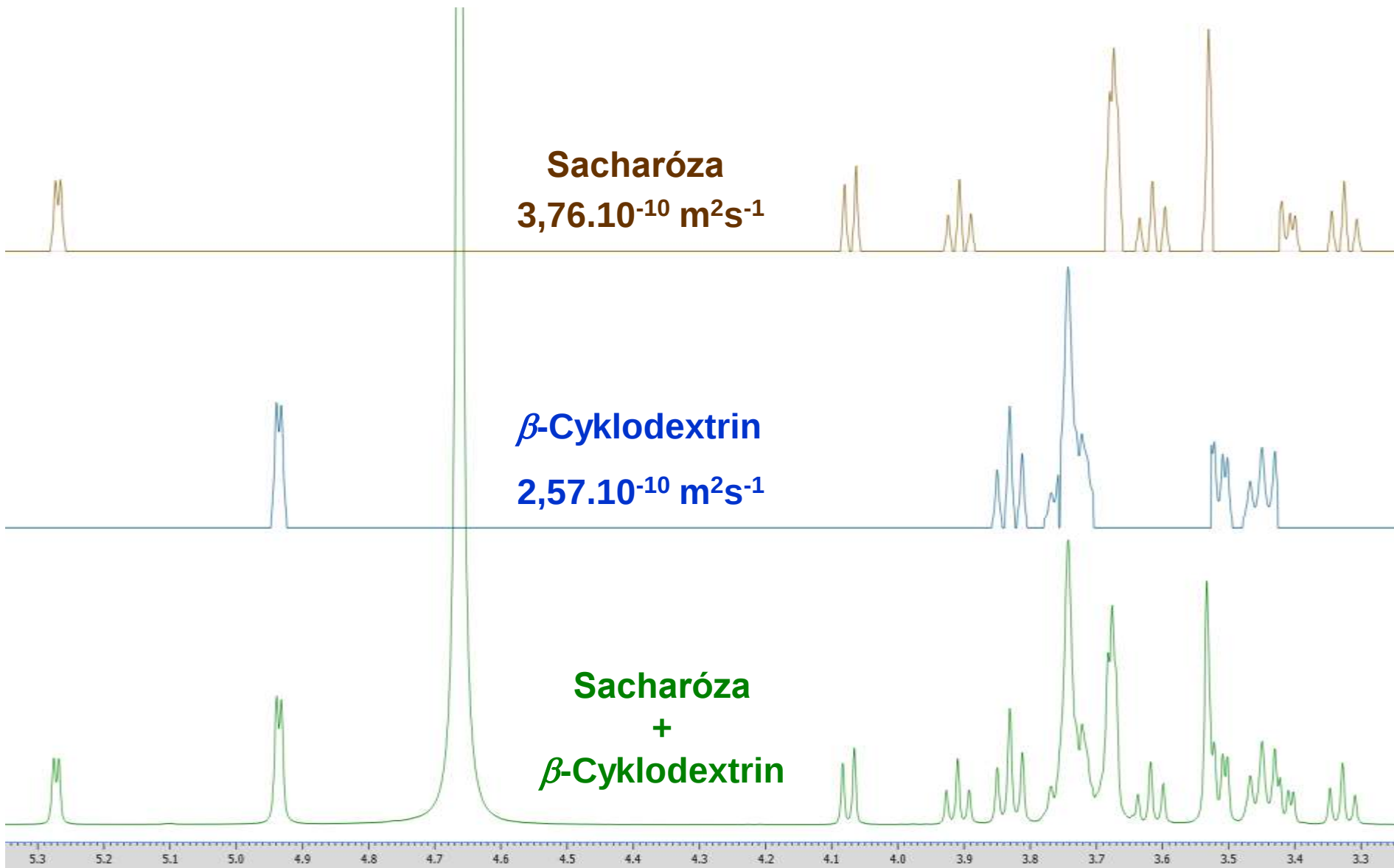


2D DOSY NMR → NMR spektra jednotlivých složek

Sacharóza
 $3,76 \cdot 10^{-10} \text{ m}^2 \text{s}^{-1}$

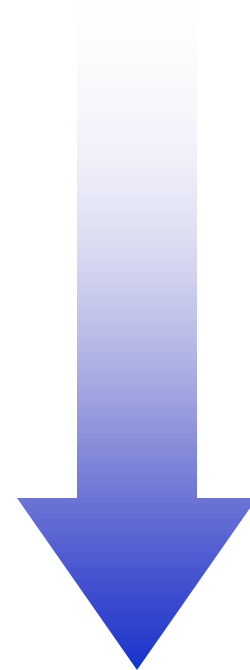
β -Cyklodextrin
 $2,57 \cdot 10^{-10} \text{ m}^2 \text{s}^{-1}$

**Sacharóza
+
 β -Cyklodextrin**



NMR ECZ 500R JEOL

AirJet XR9021



-90 °C

bez chladících médií

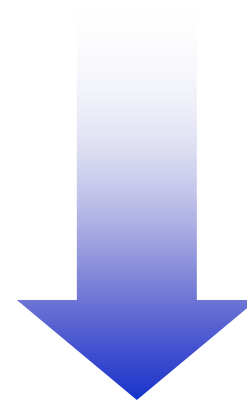


NMR ECZ 500R JEOL

ASC64

automatická výměna

64 vzorků



využití

24 h / den

