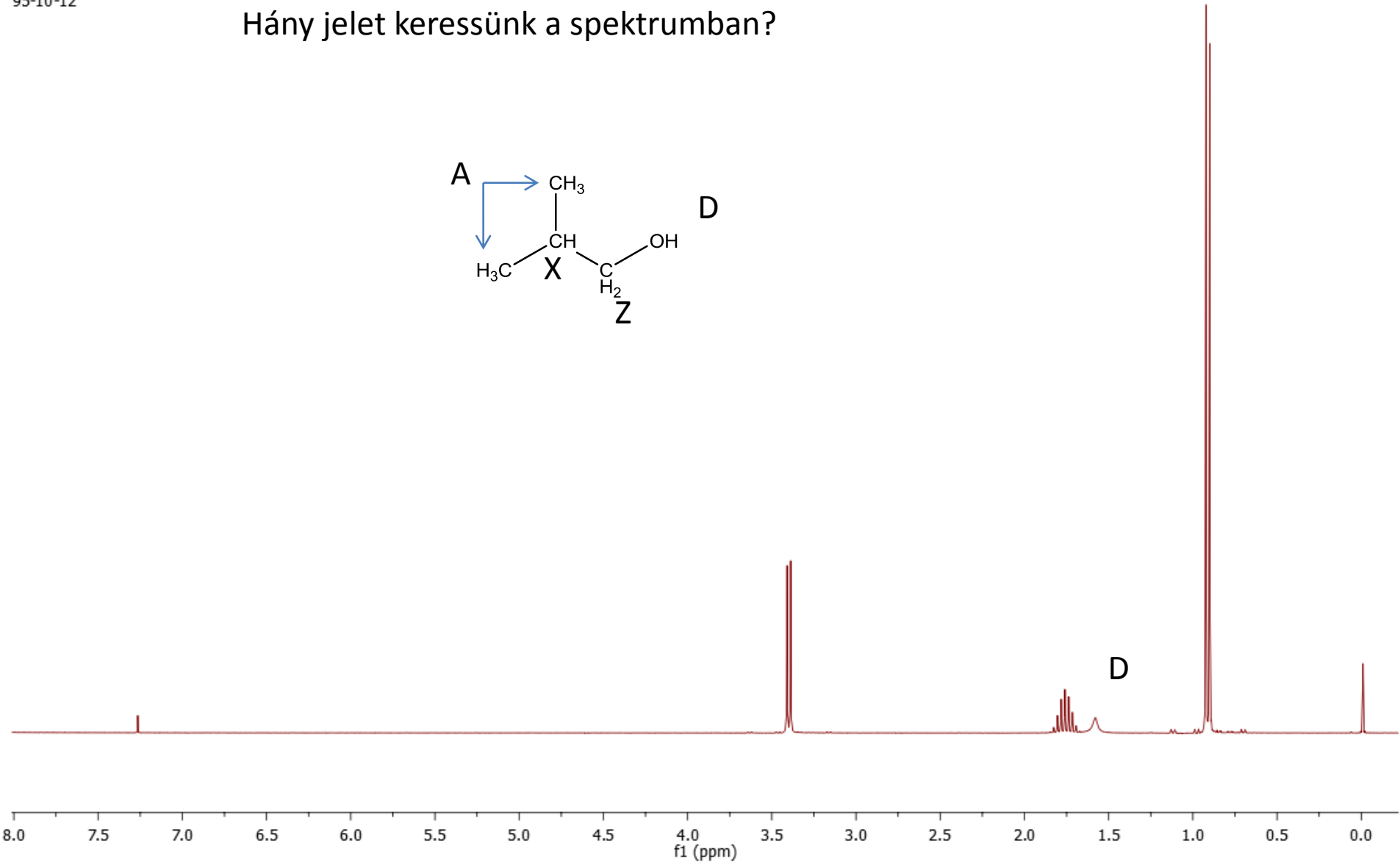
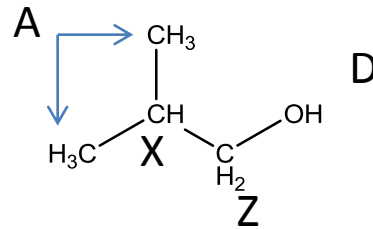


Kémiai eltolódás

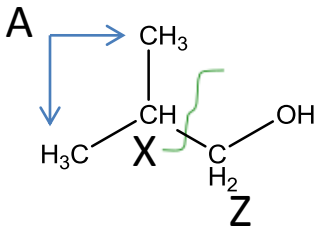
2-METIL-1-PROPANOL_H1 (400 MHz, CDCl₃)
2-metil-1-propanol
[CH₃]₂-CH-CH₂-OH
95-10-12

Hány jelet keressünk a spektrumban?



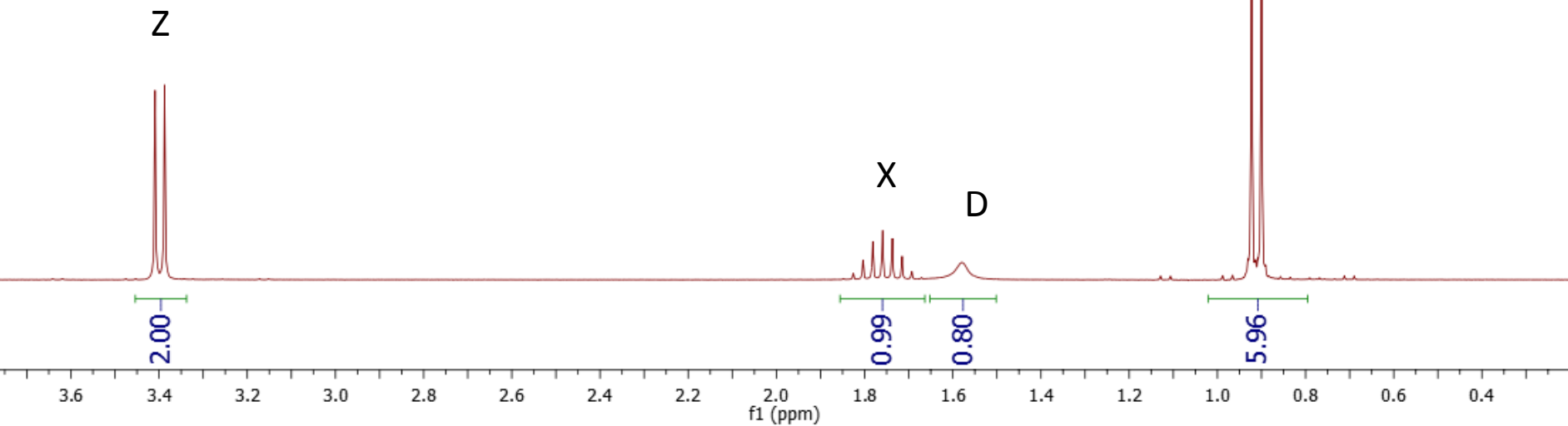
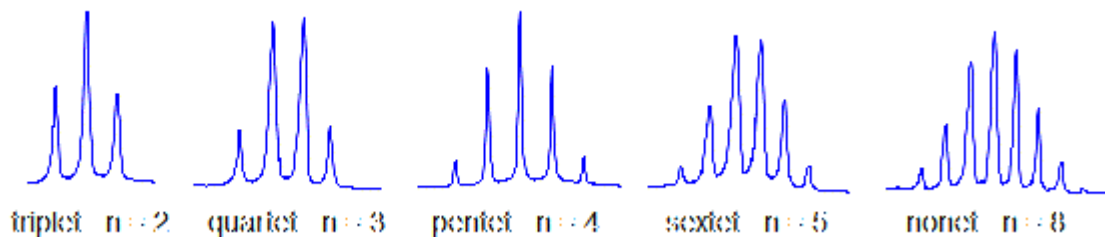
A jelintegrálók információtartalma

2-METIL-1-PROPANOL_H1 (400 MHz, CDCl₃)
 2-metil-1-propanol
 [CH₃]₂-CH-CH₂-OH
 95-10-12



A jel $2n+1$ db vonalra bomlik fel

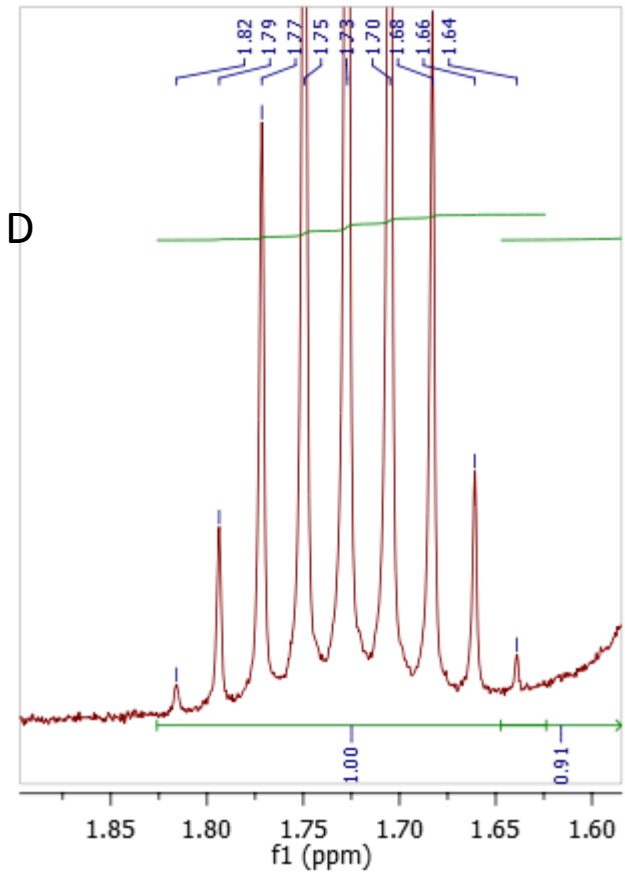
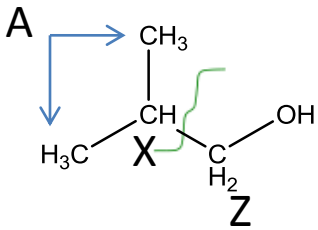
n=0	1
n=1	1 1
n=2	1 2 1
n=3	1 3 3 1
n=4	1 4 6 4 1
n=5	1 5 10 10 5 1
n=6	1 6 15 20 15 6 1



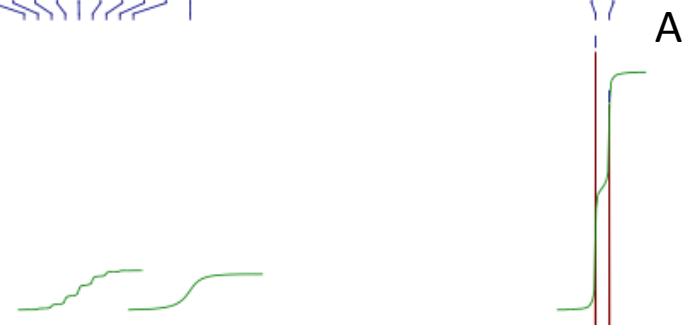
A finomfelhasadások, Elsőrendű spinrendszer

A_6XZ_2 spinrendszer

2-METIL-1-PROPANOL-H1
2-metil-1-propanol
[CH₃]₂-CH-CH₂-OH
95-10-12



1.82
1.79
1.77
1.75
1.73
1.70
1.68
1.66
1.64
1.55

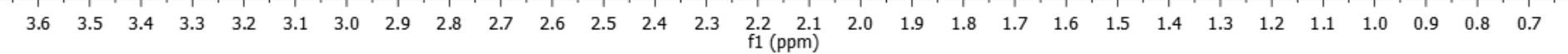
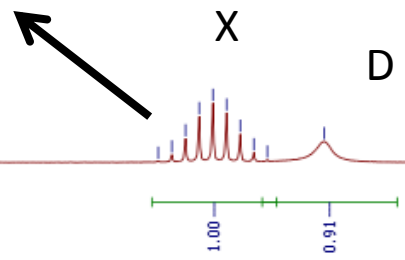
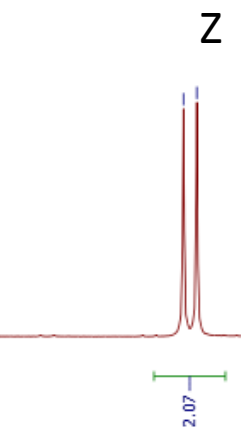


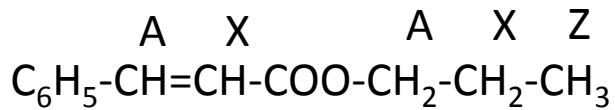
A (d)
3.37

B (m)
1.73

C (s)
1.55

D (d)
0.88



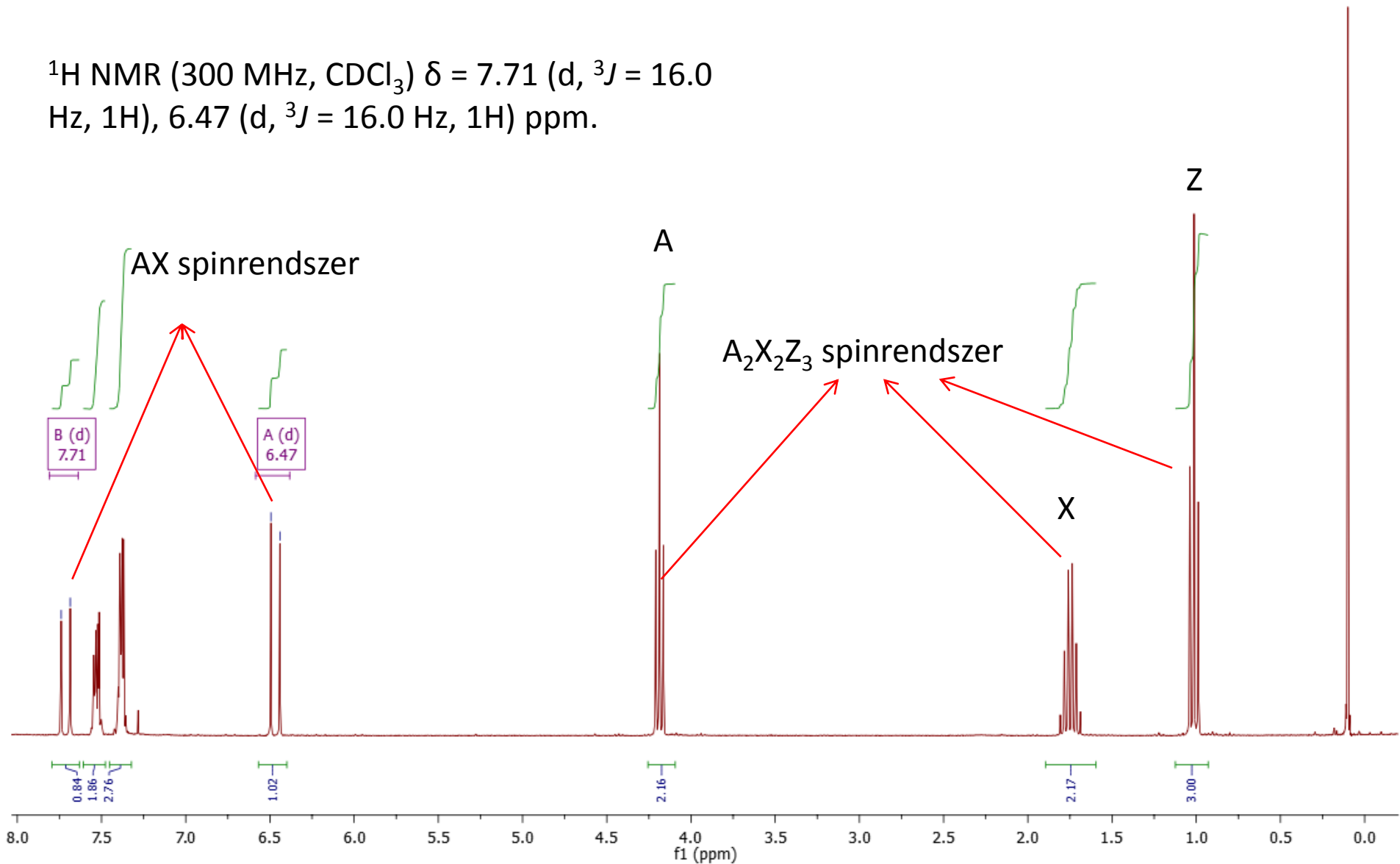


7.74
7.69

6.49
6.44

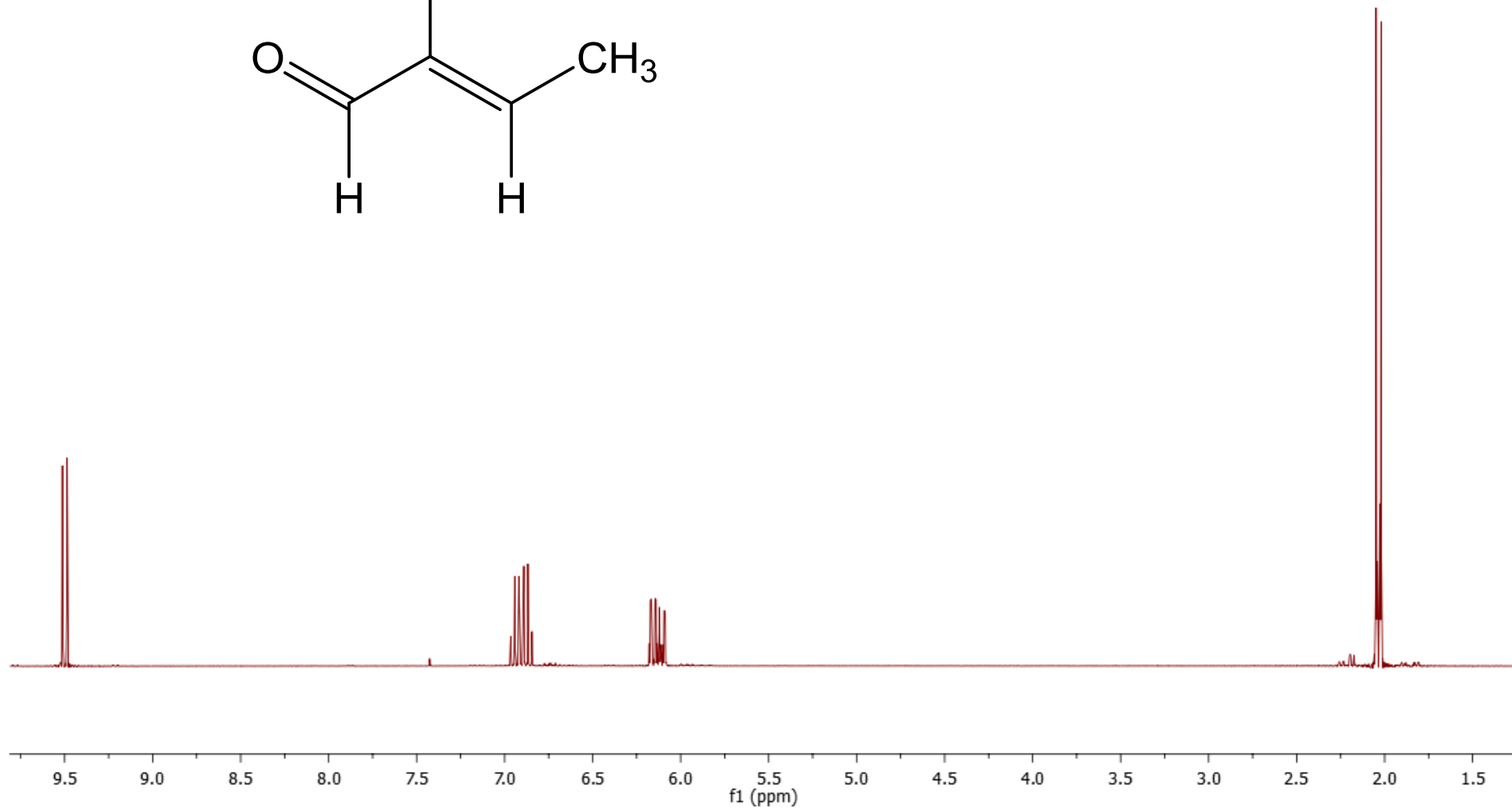
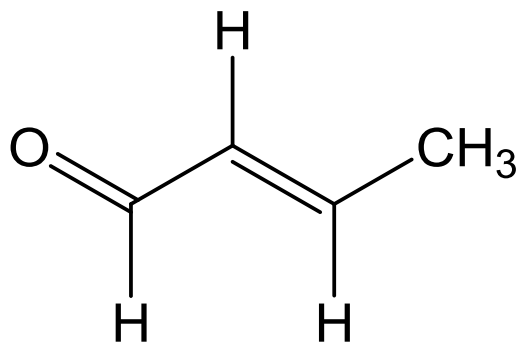
Cisz vagy transz?

^1H NMR (300 MHz, CDCl_3) $\delta = 7.71$ (d, $^3J = 16.0$ Hz, 1H), 6.47 (d, $^3J = 16.0$ Hz, 1H) ppm.



Elsőrendű spinrendszer többféle csatolással

KROTONALD_H1
Krotonaldehid (400 MHz, CDCl₃)
H1 CDCl₃
1993-12-15



^1H NMR (400 MHz, CDCl_3)

C Elsőrendű spinrendszer többféle csatolással

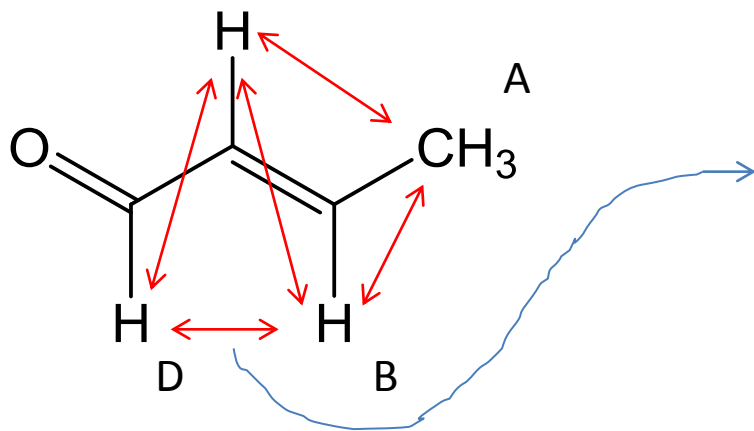
Távolható allilcsatolás:

$$^4J = 0,5-2 \text{ Hz}$$

Csatolások kettős kötésen:

$$^3J_{\text{cisz}} = 5-14 \text{ Hz}$$

$$^3J_{\text{transz}} = 12-19 \text{ Hz}$$



$$^4J = 0-2 \text{ Hz}$$

Miért így mérjük le a csatolást?

7,9 Hz

D

B

6,8 Hz

15,5 Hz

C

7,9 Hz

15,5 Hz

1,6 Hz

1,6 Hz

6,8 Hz

A

9.6 9.5 9.4 9.3
f1 (ppm)

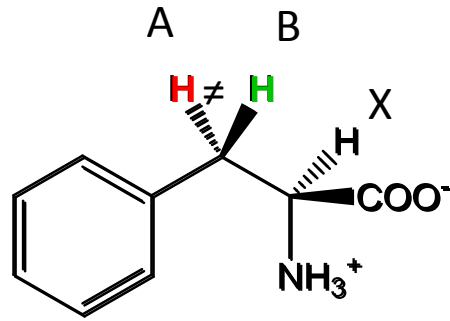
7.00 6.95 6.90 6.85
f1 (ppm)

6.21 6.18 6.15 6.12
f1 (ppm)

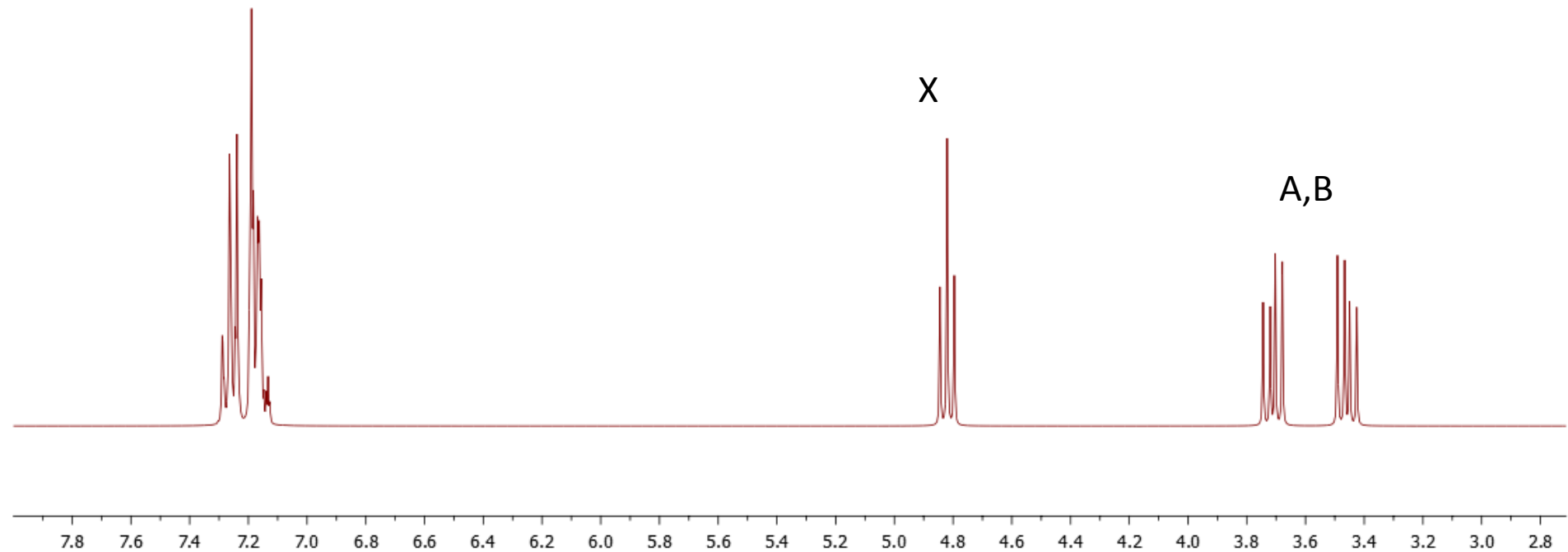
2.06 2.03
f1 (ppm)

Kémiaailag nem ekvivalens diasztereotóp csoportok

^1H NMR (400 MHz, CDCl_3)



ABX spinrendszer

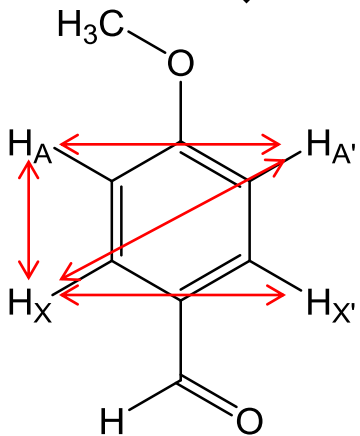


Példa másodrendű spinrendszerre

^1H NMR (400 MHz, CDCl_3)

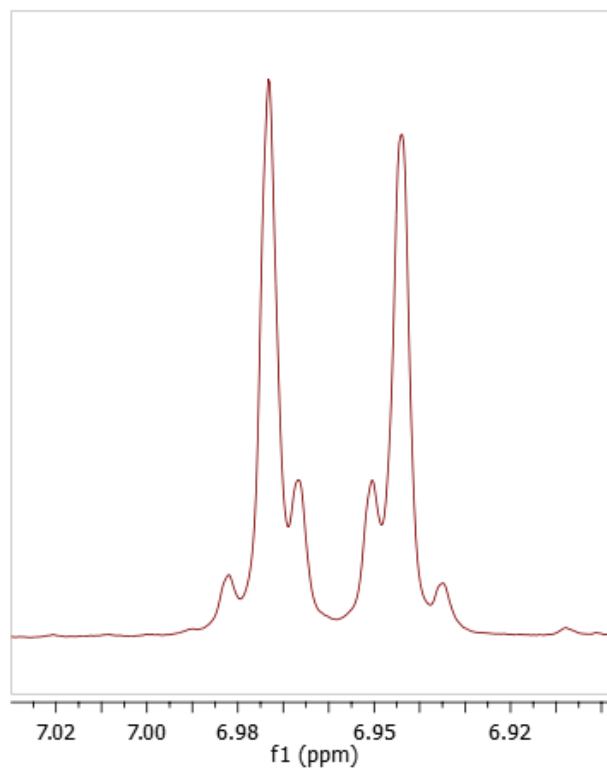
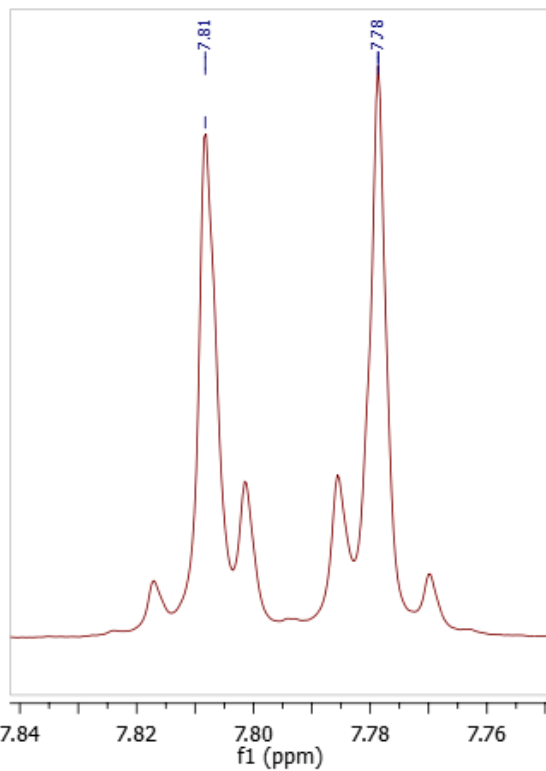
ANIZSALDEHID_H1
Anizsaldehyd
COH-C6H4-O-CH3
H1 CDCl3
95-1016

AA'XX' spinrendszer!



$$J_{AX'} = J_{A'X}$$

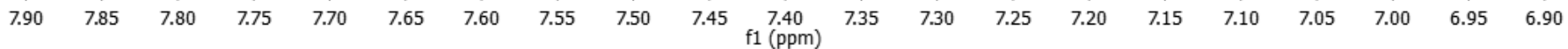
$$J_{AX} = J_{A'X'}$$



$$J_{\text{orto}} = 7-10 \text{ Hz}$$

$$J_{\text{meta}} = 1-3 \text{ Hz}$$

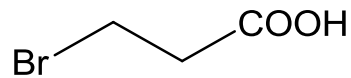
$$J_{\text{para}} = 0-1 \text{ Hz}$$



Ismeretlen minta szerkezetének megállapítása ^1H NMR spektrum alapján

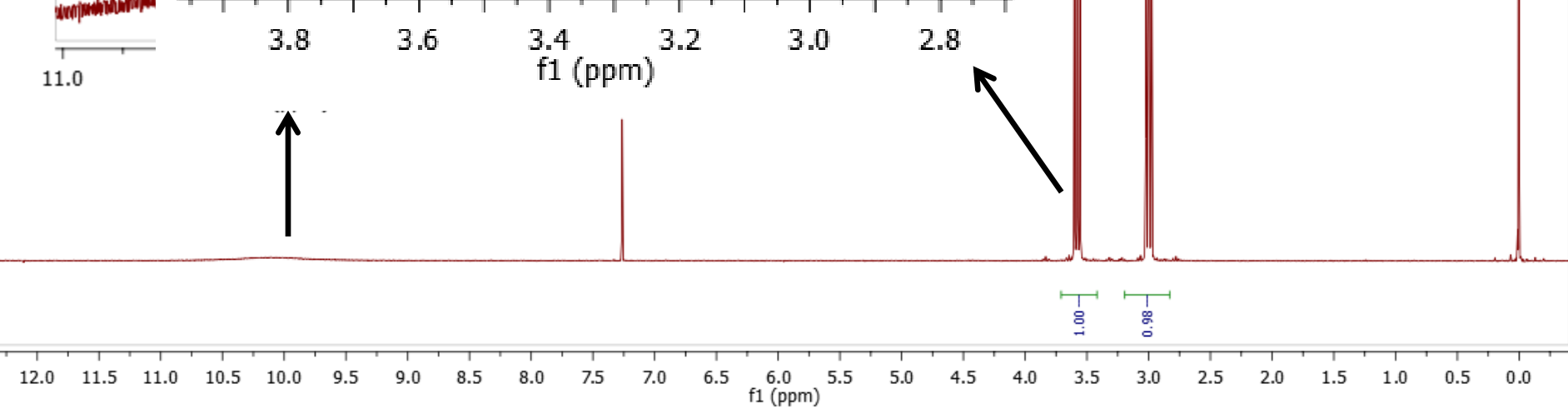
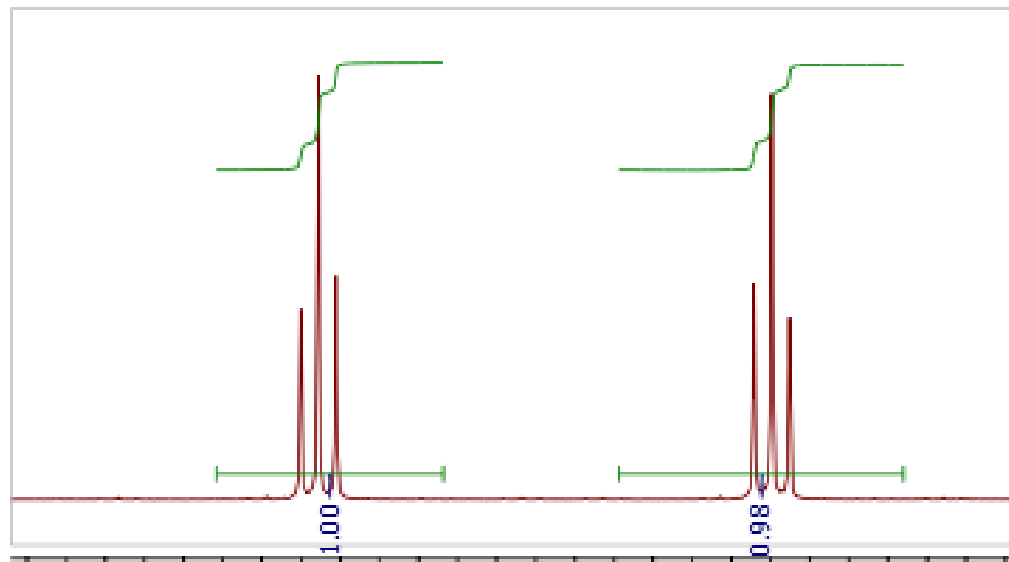
^1H NMR (400 MHz, CDCl_3)

$\text{BrC}_3\text{H}_5\text{O}_2$



A X

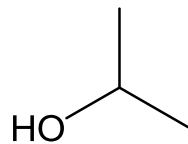
A_2X_2 spinrendszer



Ismeretlen minta szerkezetének megállapítása ^1H NMR spektrum alapján

^1H NMR (400 MHz, CDCl_3)

$\text{C}_3\text{H}_8\text{O}$



AX_6 spinrendszer

X

