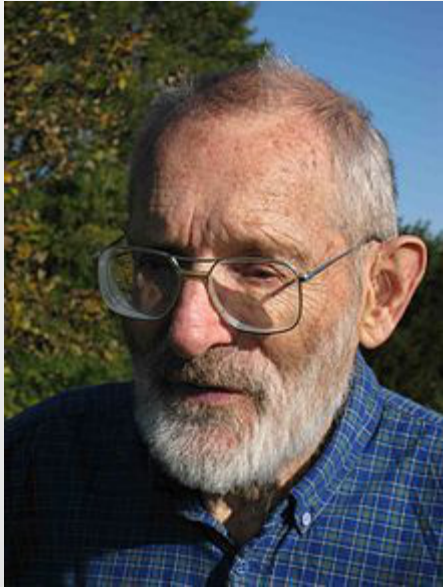


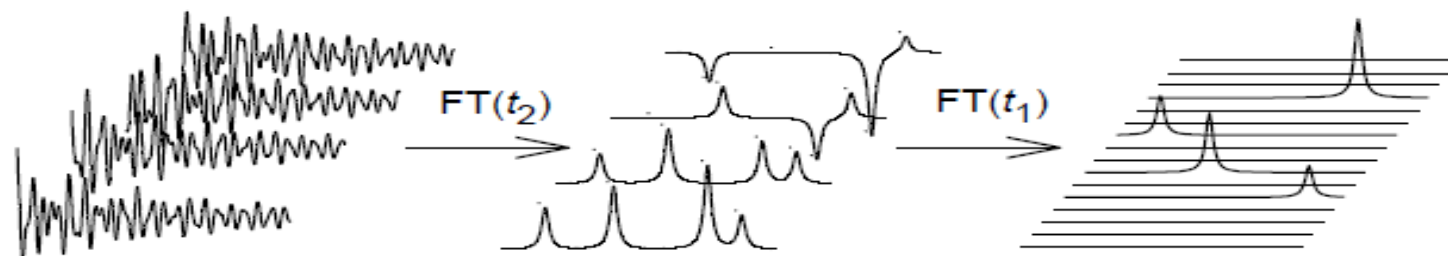
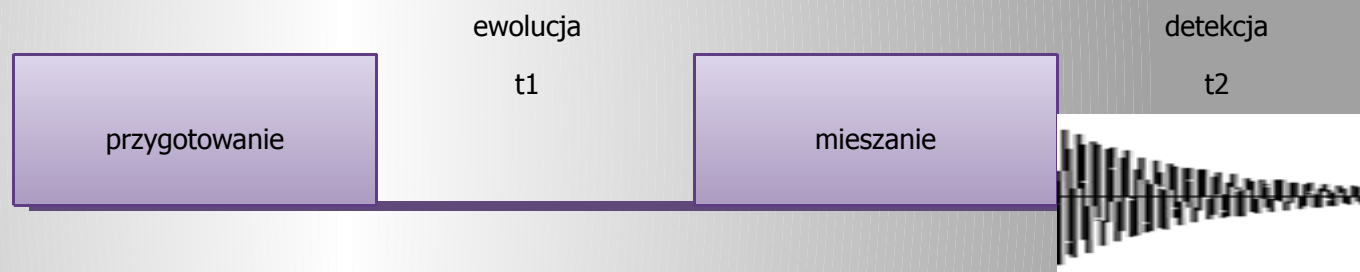
2D NMR



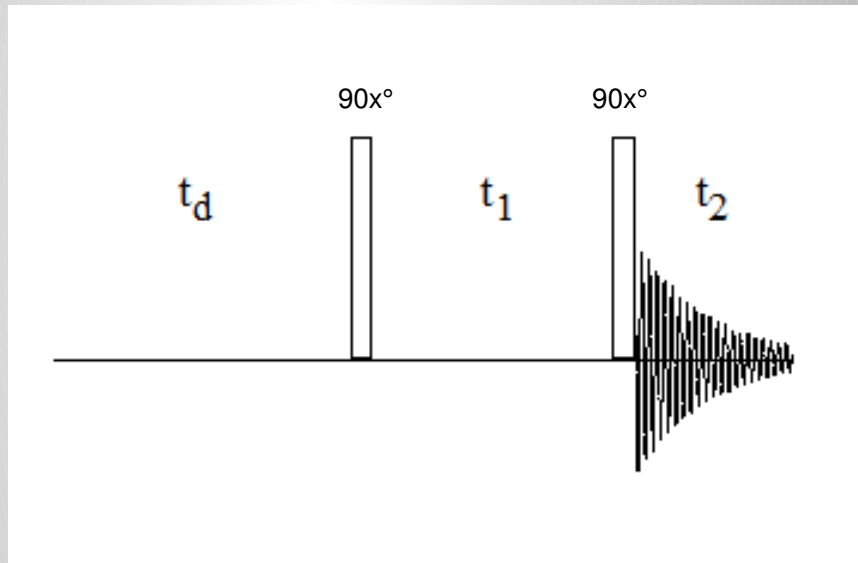
Jean Jeener

Na konferencji AMPERE Summer School , w Jugosławii w1971 r. zaproponował nową technikę pomiarową, dziś znaną jako Correlation Spectroscopy (COSY)

Sekwencja pomiarowa - 2D NMR



COSY Correlation spectroscopy

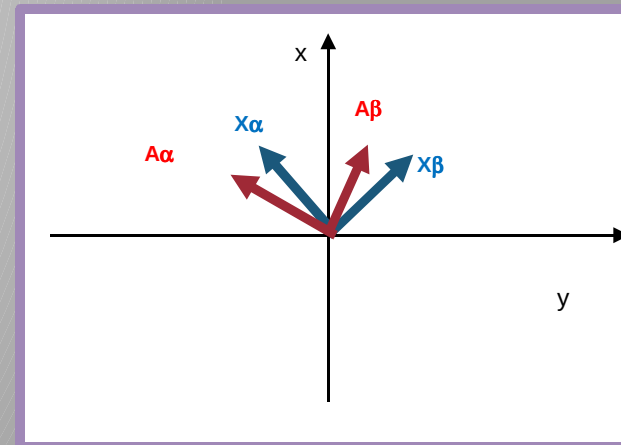
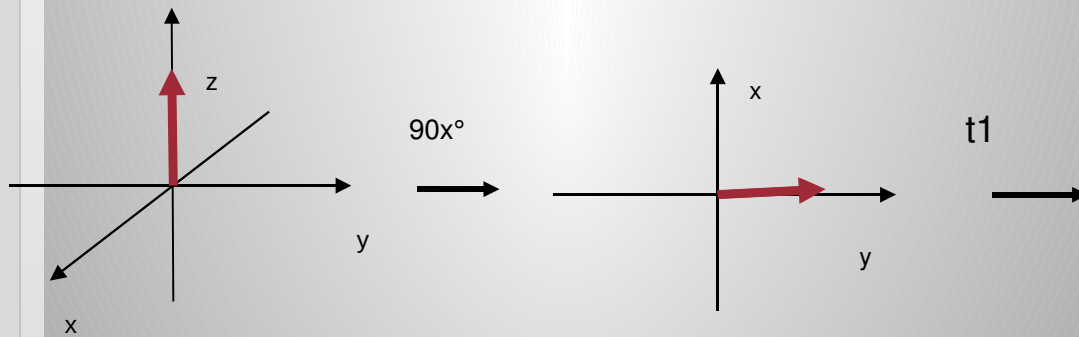


$$A\alpha: \nu_A + (1/2)J(A,X)$$

$$A\beta: \nu_A - (1/2)J(A,X)$$

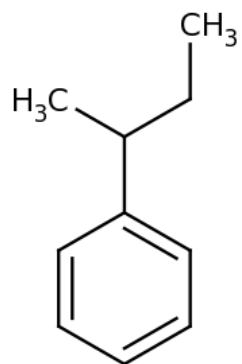
$$X\alpha: \nu_X + (1/2)J(A,X)$$

$$X\beta: \nu_X - (1/2)J(A,X)$$



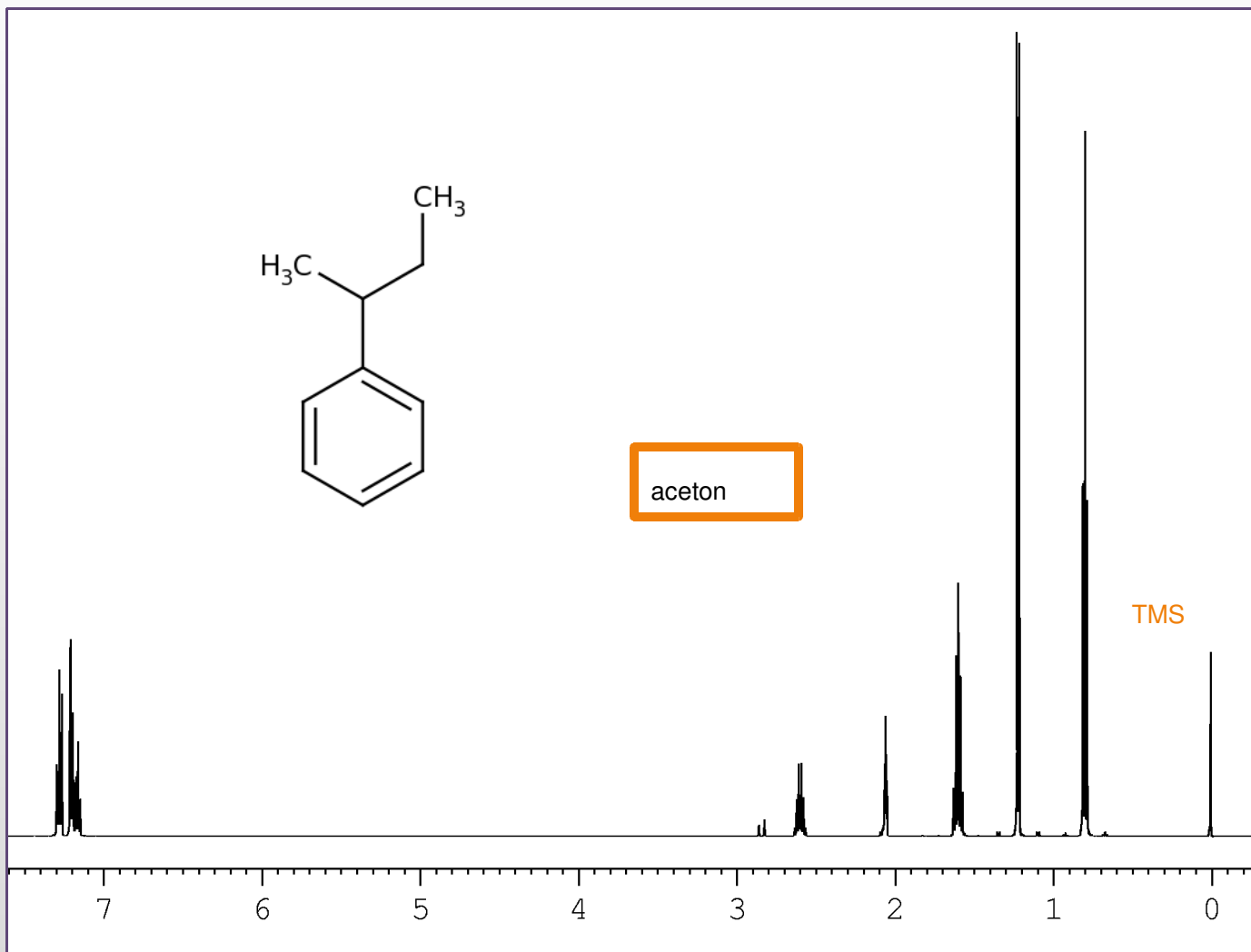
sec-butylobenzen w acetonie

500MHz



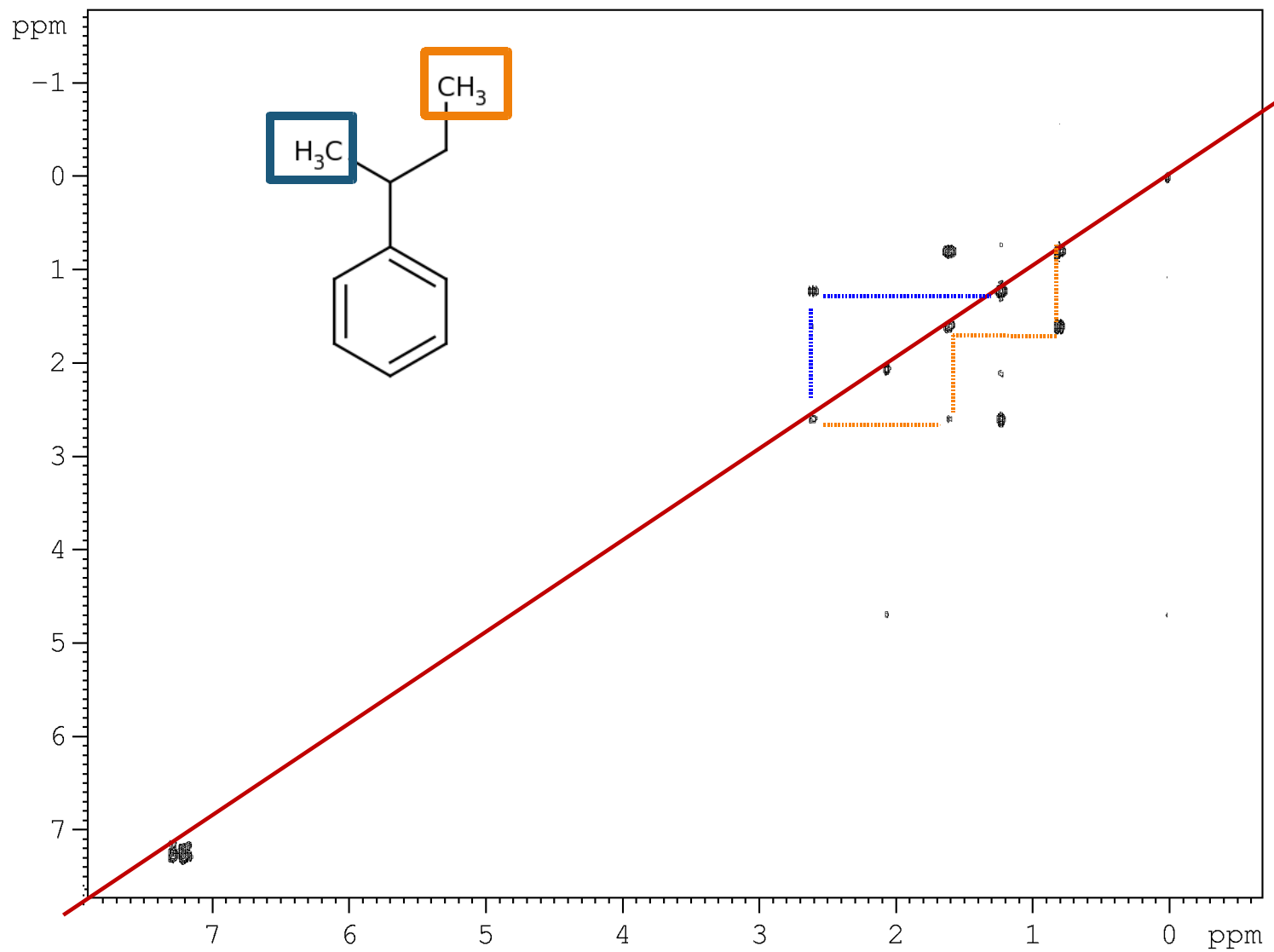
aceton

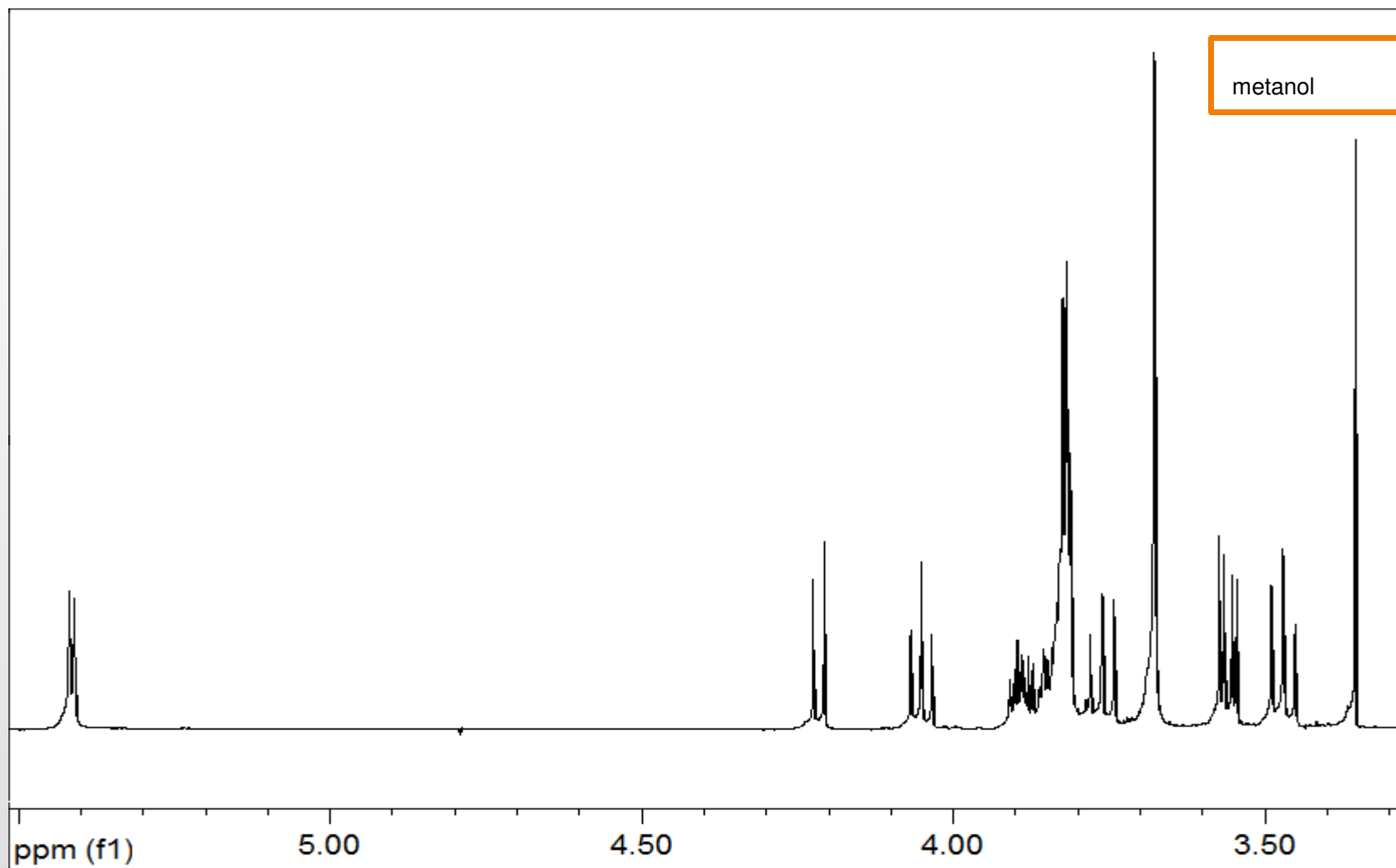
TMS



δ /ppm	Int.
7.294	13.046
7.279	32.091
7.264	24.145
7.208	36.423
7.194	25.150
7.175	10.388
7.160	15.501
7.146	6.192
2.628	1.384
2.615	6.520
2.601	12.807
2.587	12.813
2.572	6.779
2.558	1.342
1.624	7.949
1.609	27.863
1.595	40.381
1.579	27.009
1.566	7.313
1.223	103.799
1.208	102.204
0.807	50.196
0.793	95.290
0.778	46.184

WIDMO 1H-1H COSY

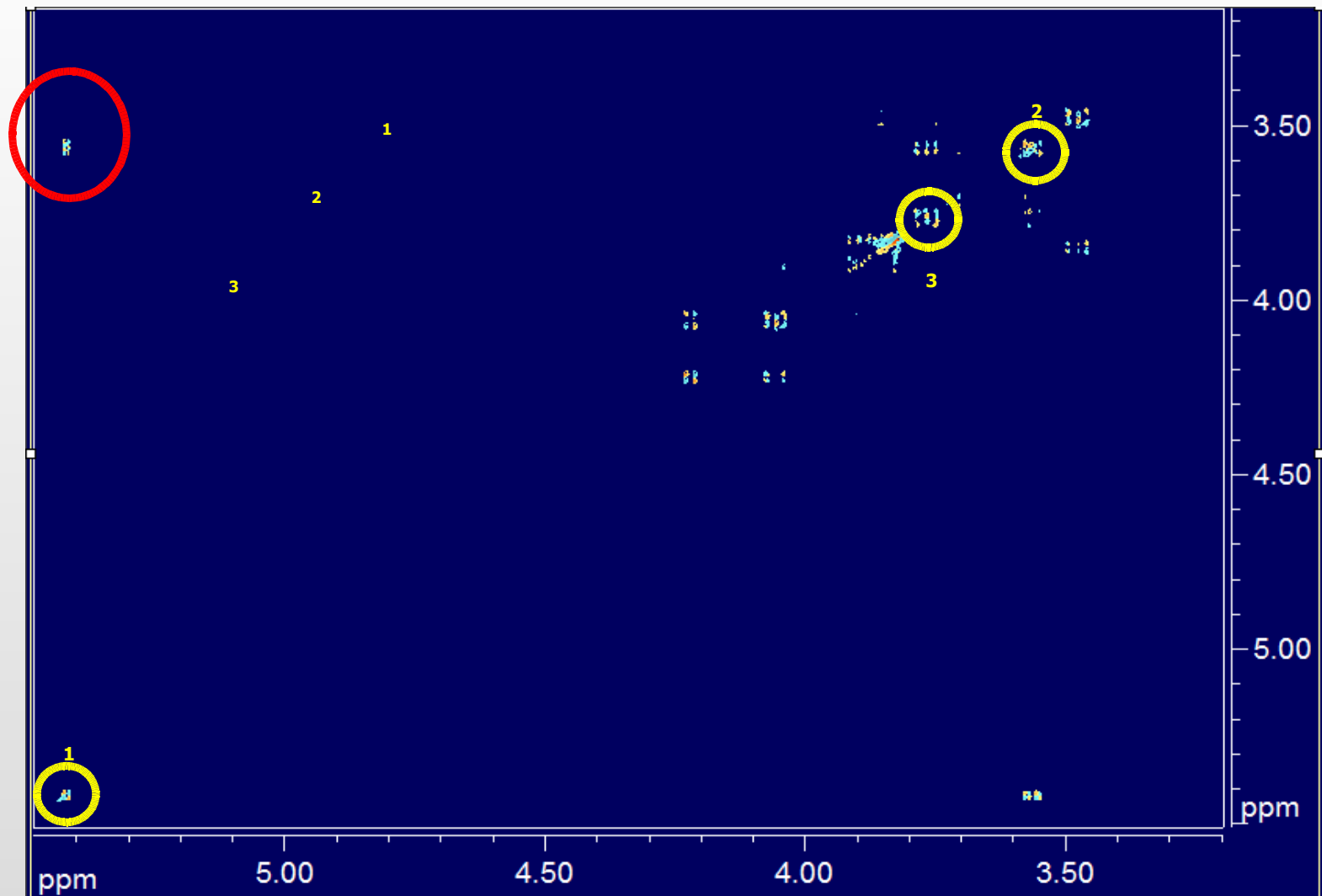




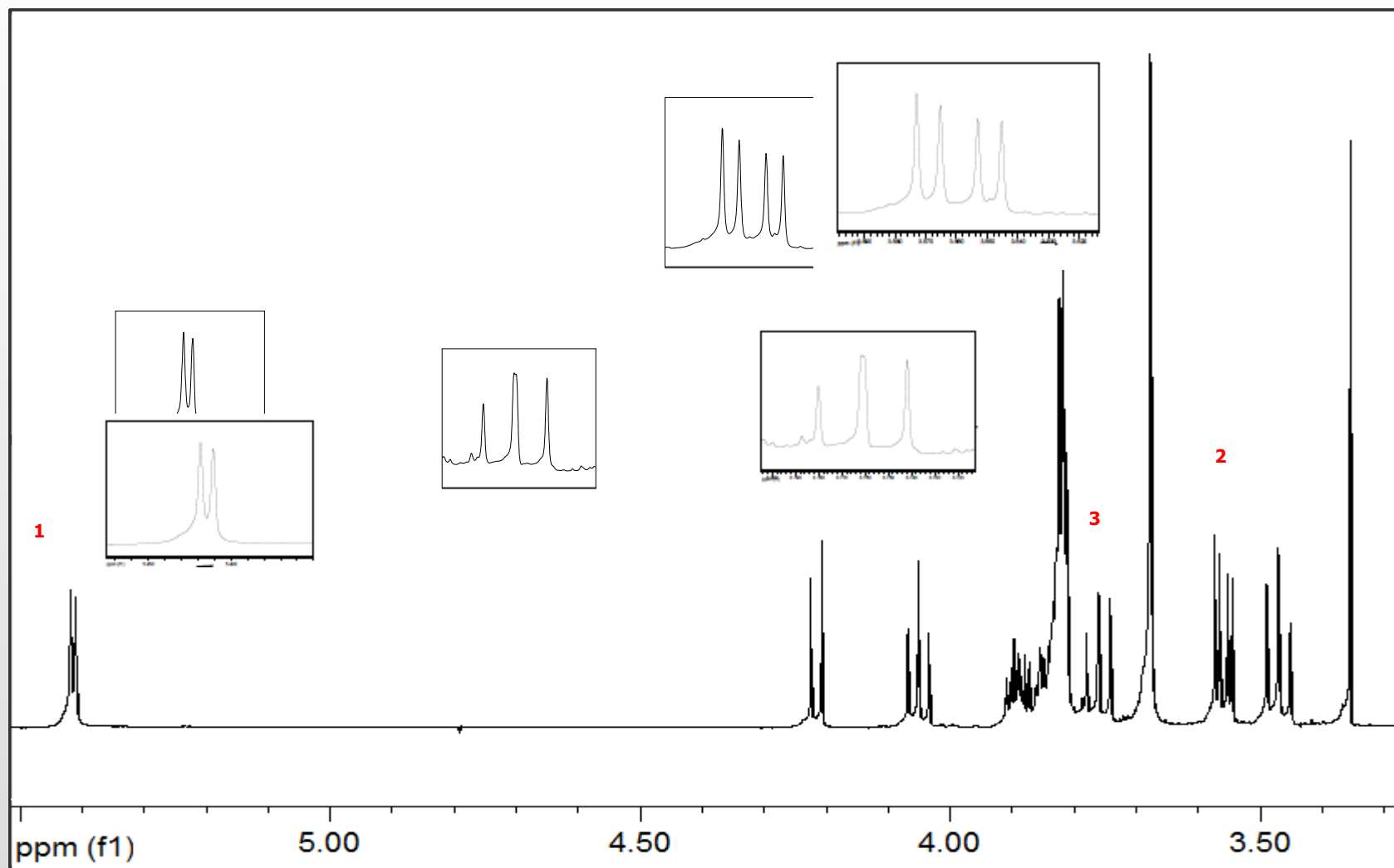
Widmo 1D ¹H NMR roztworu sacharozy w D₂O z dodatkiem metanolu

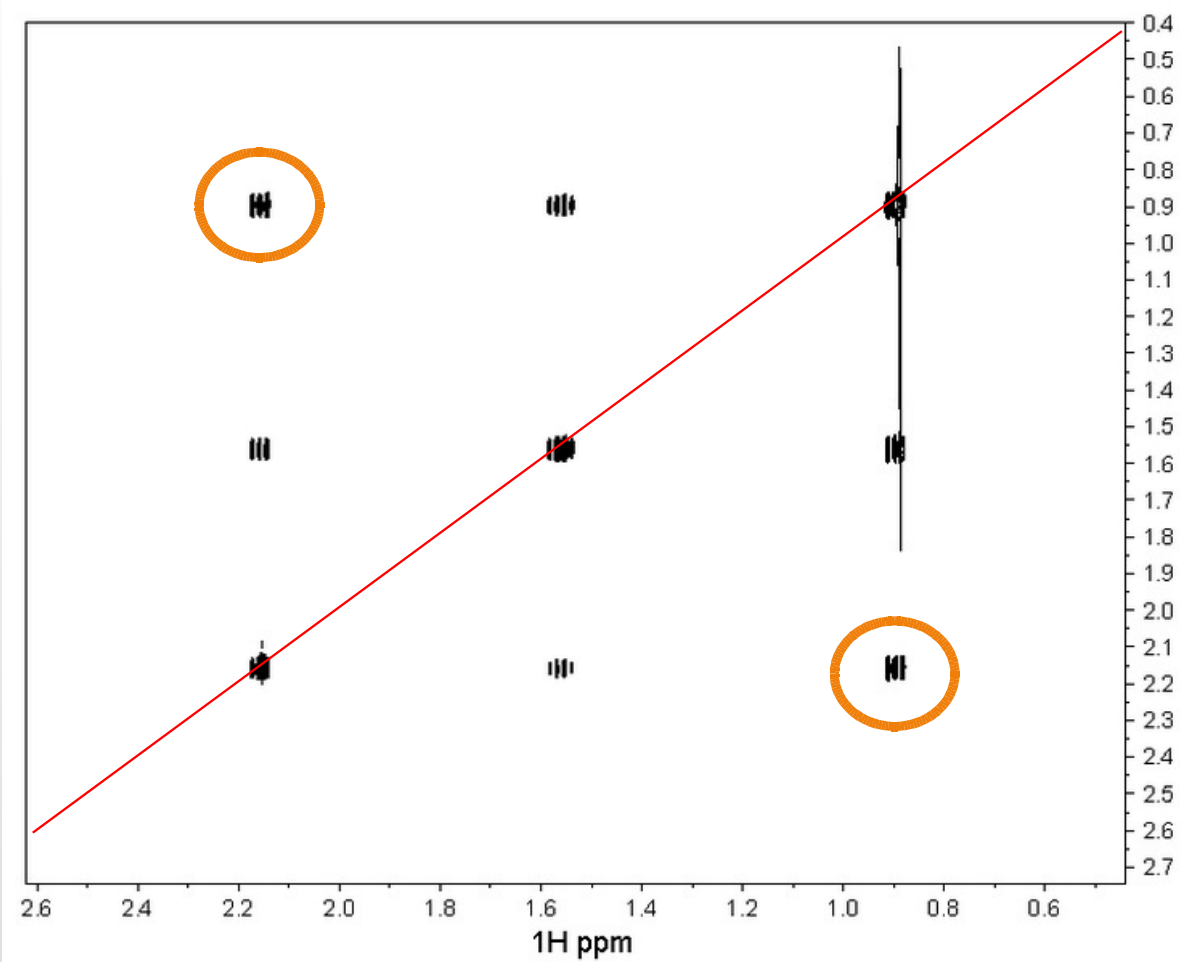
DQF-COSY (dqfCOSY; dq-COSY)

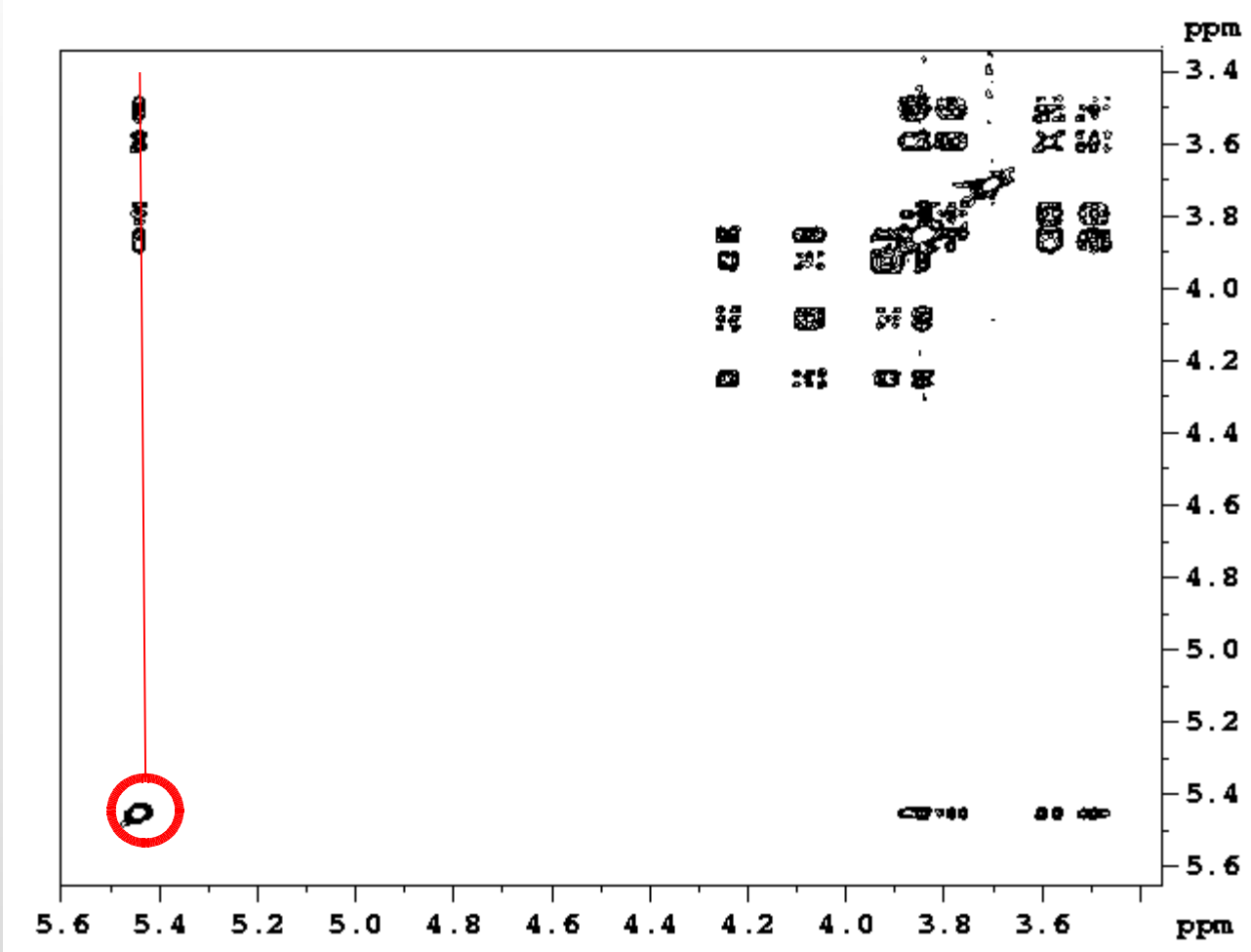
Double Quantum Filtered COSY



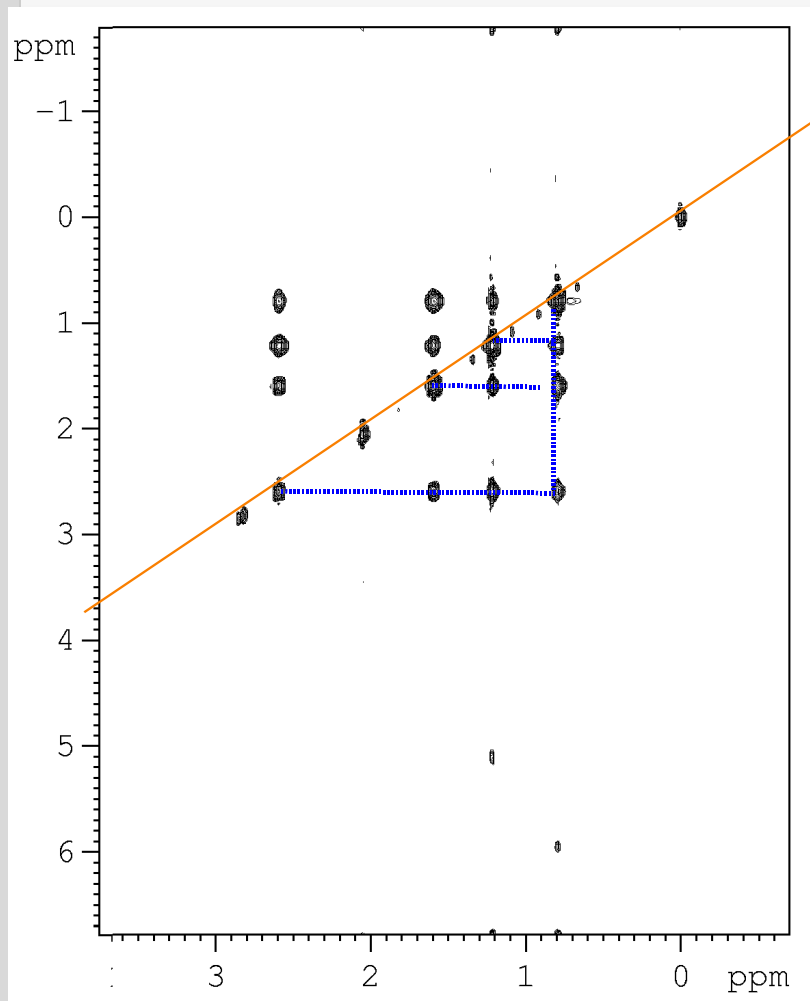
Widmo 2D 1H-1H DQF-COSY roztworu sacharozy w D2O z dodatkiem metanolu



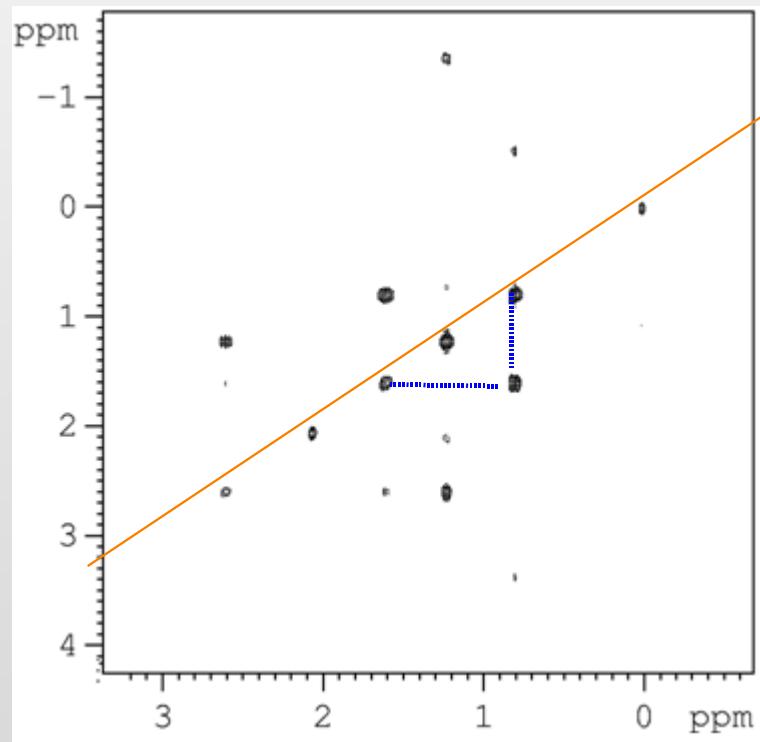




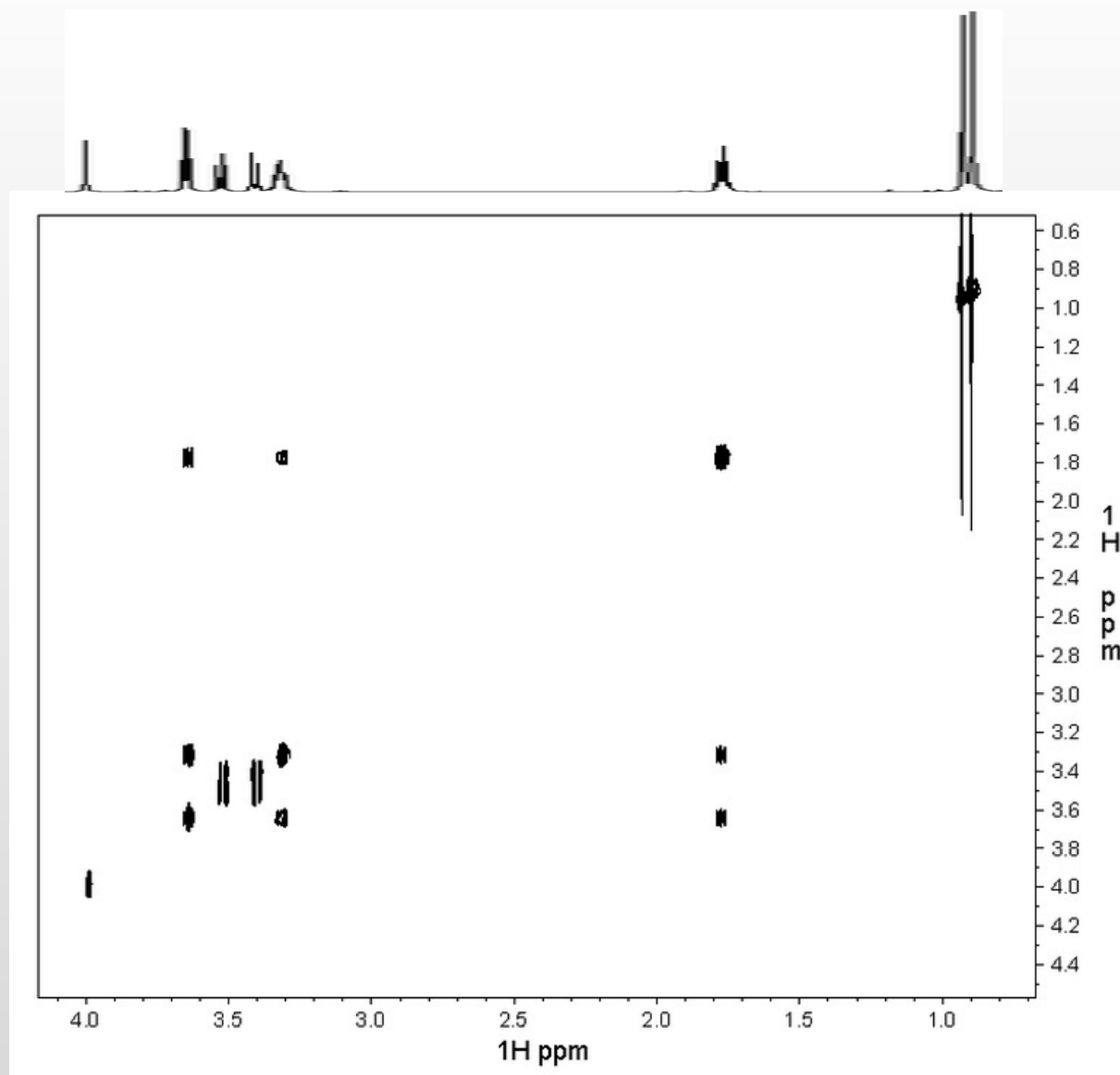
TOCSY

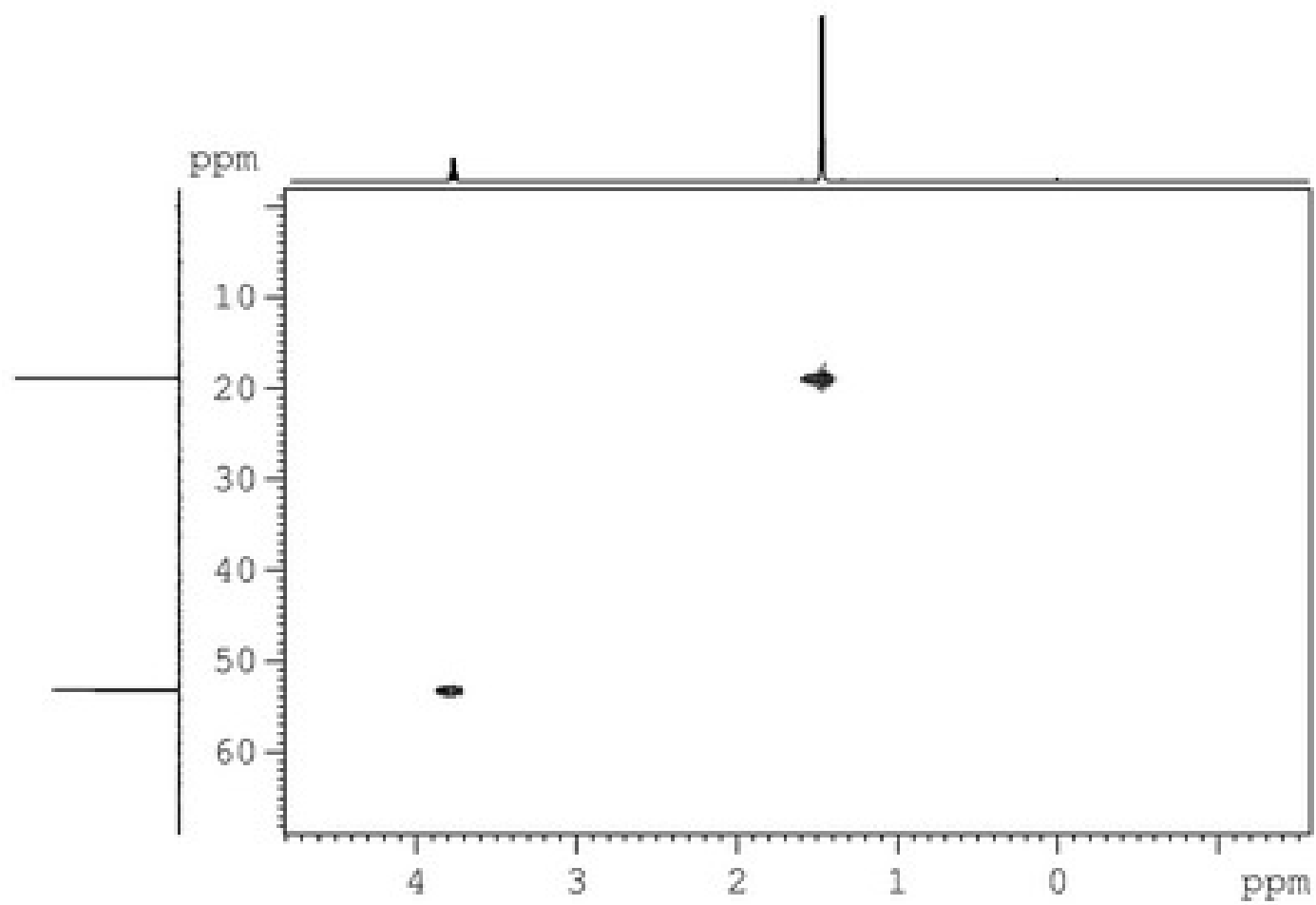


COSY

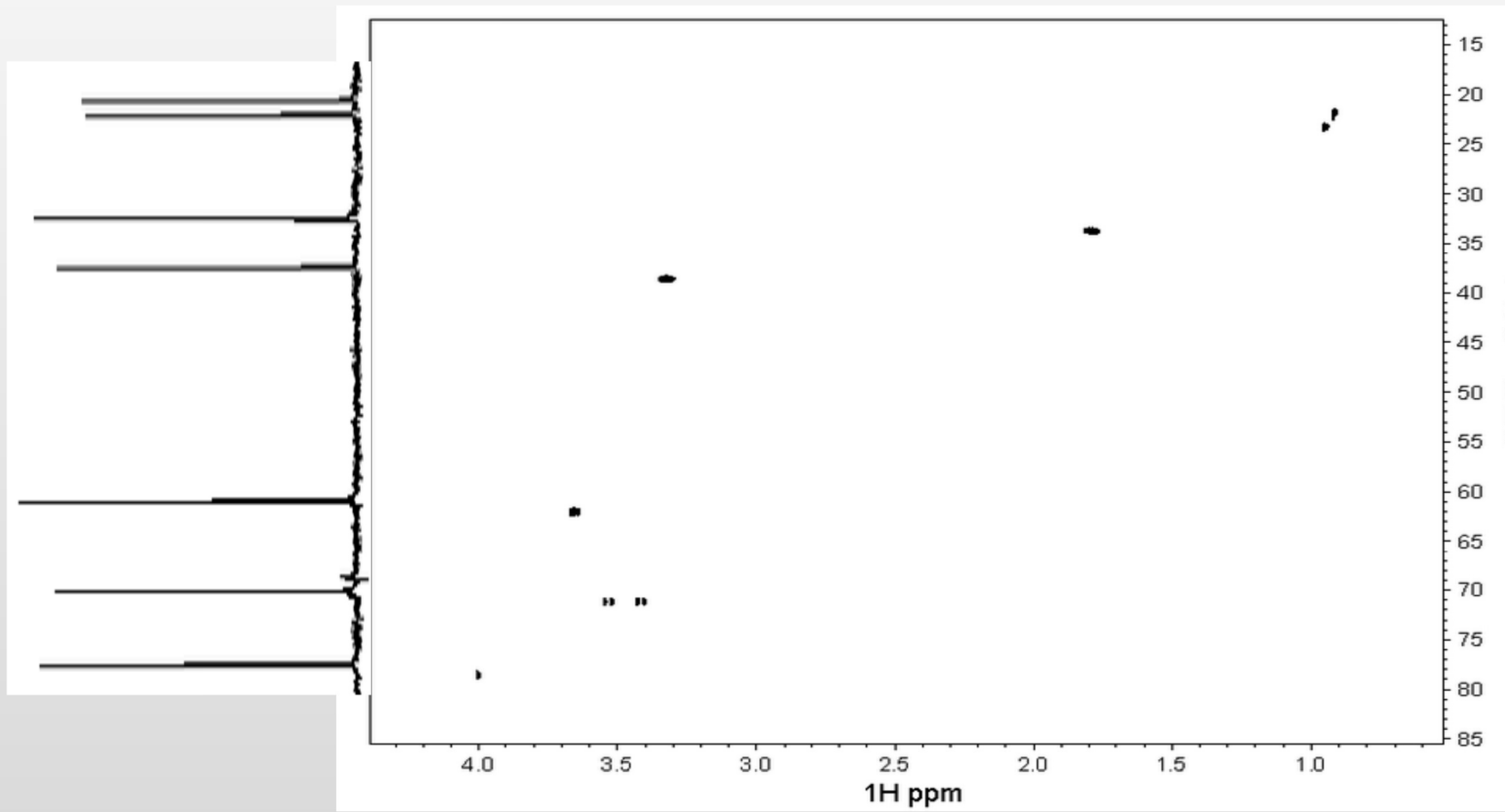


TOCSY

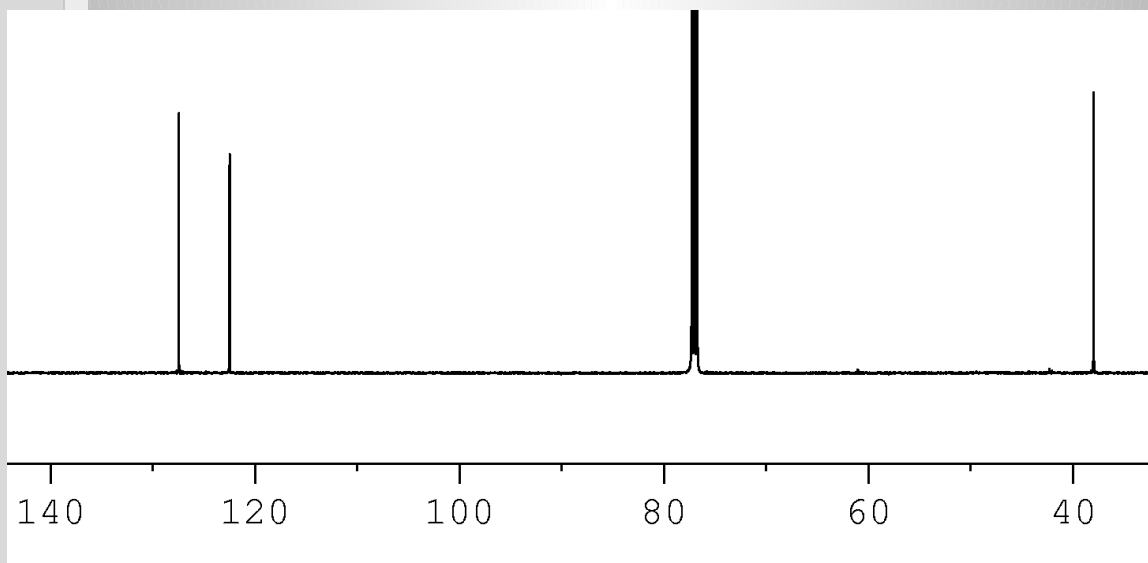
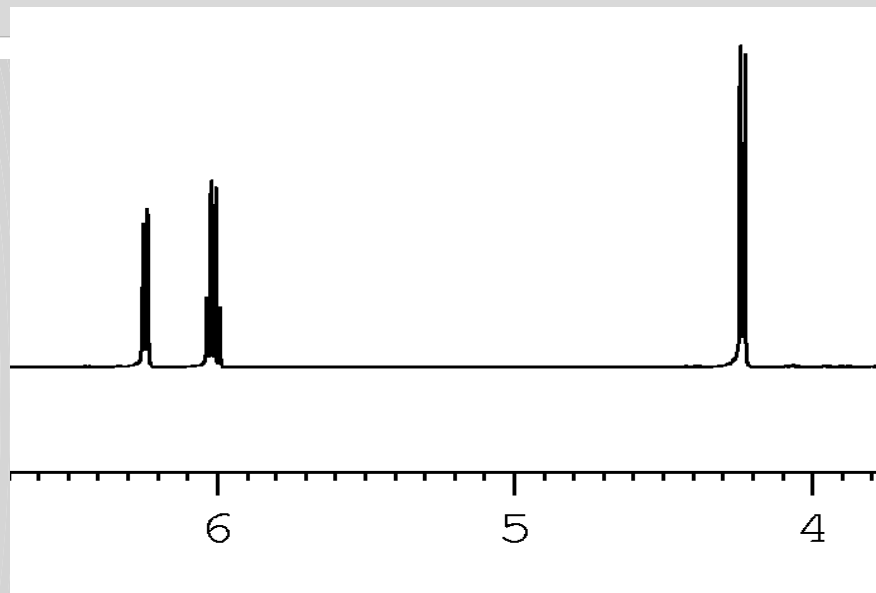




1H-13C HSQC

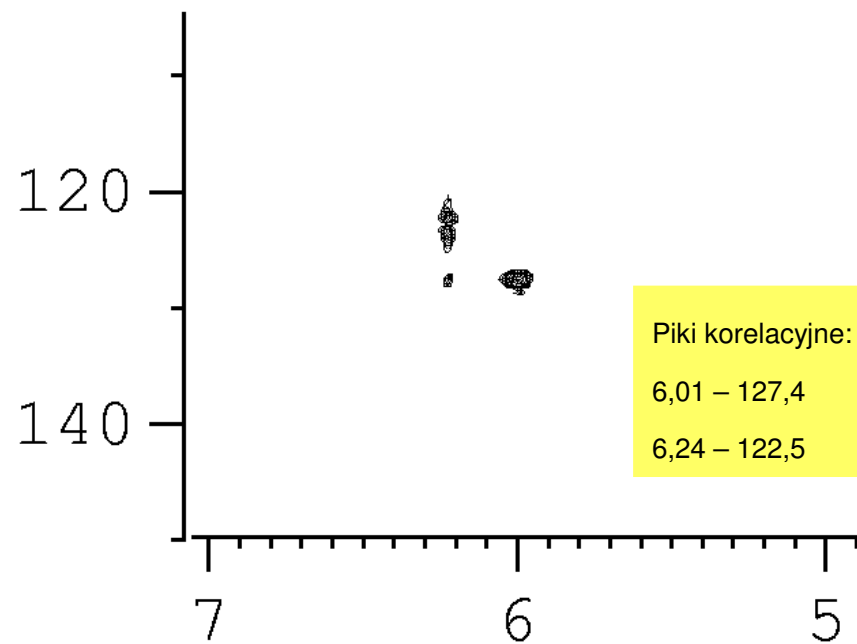


proton	δ/ppm
1	6,240
2	6,013
3	4,232
	J/Hz
	7,5 Hz
	7,5 Hz



proton	δ/ppm
1	6,240
2	6,013
3	4,232
	J/Hz
	7,5 Hz
	7,5 Hz

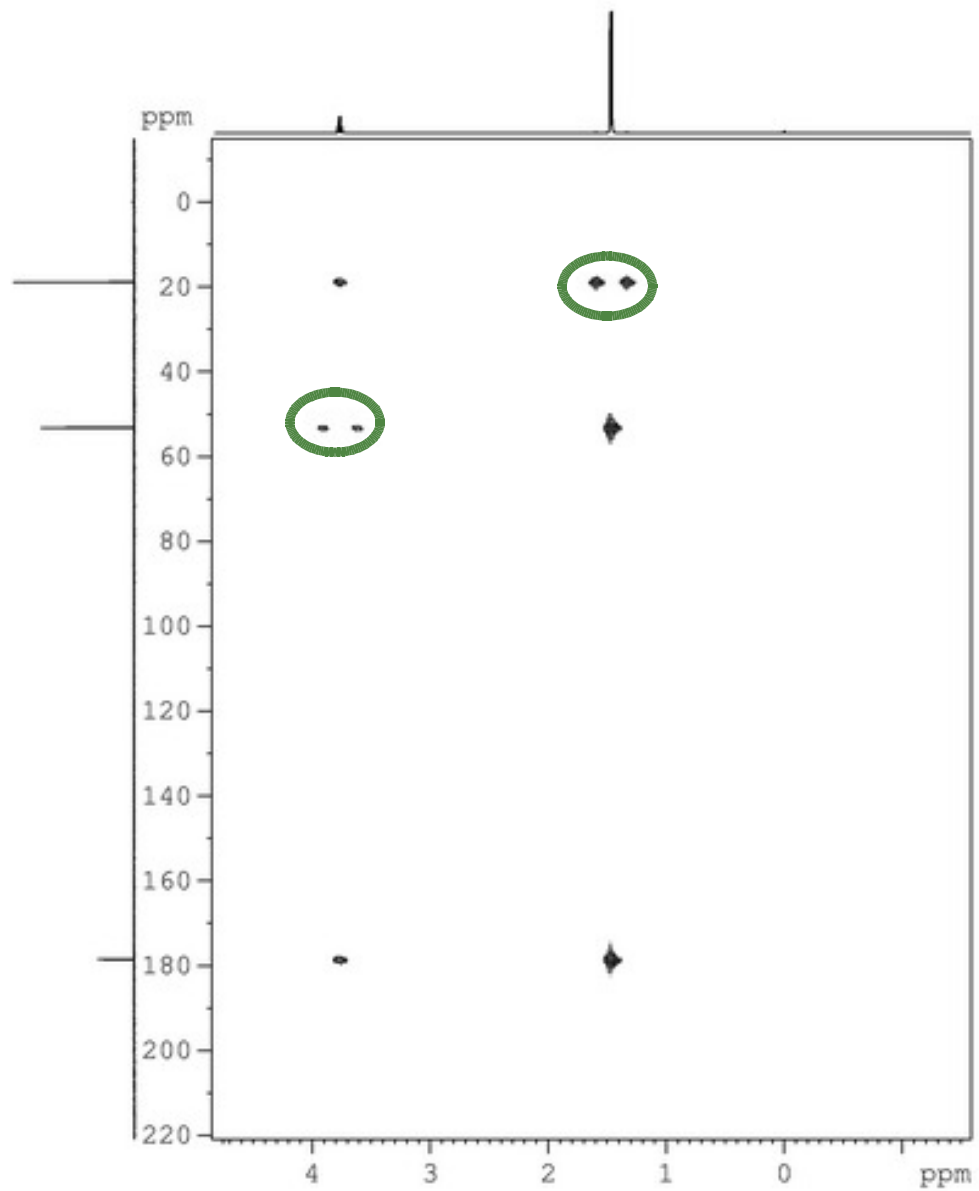
pik	δ/ppm
2	127.434
1	122.509
3	37.981



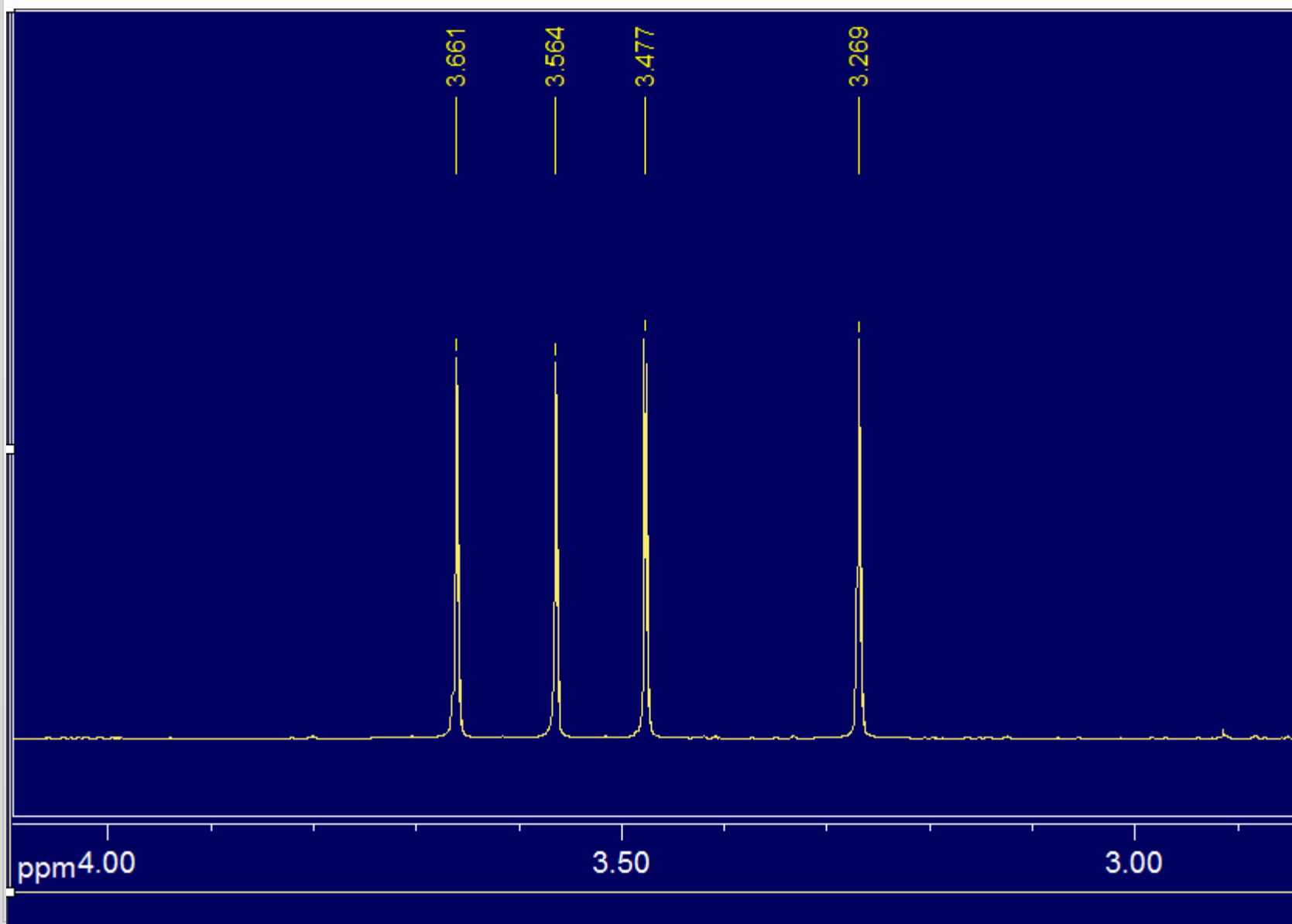
Piki korelacione:

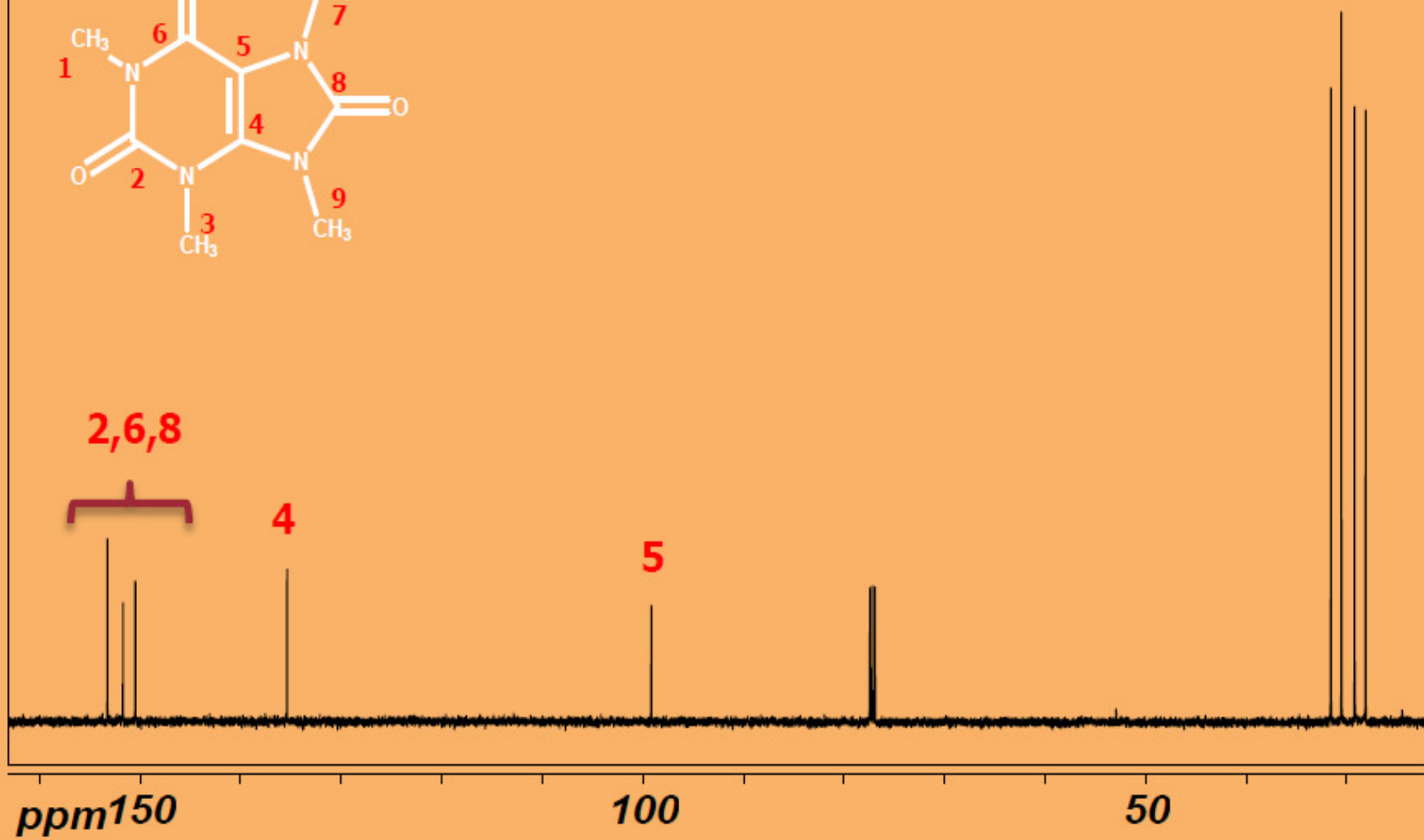
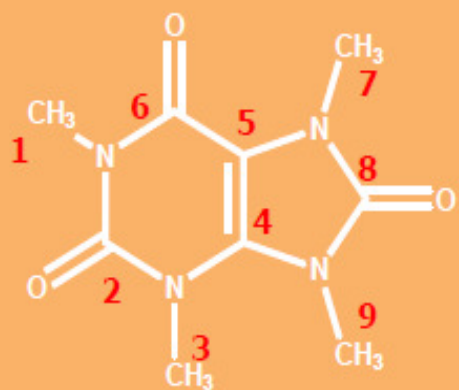
6,01 – 127,4

6,24 – 122,5

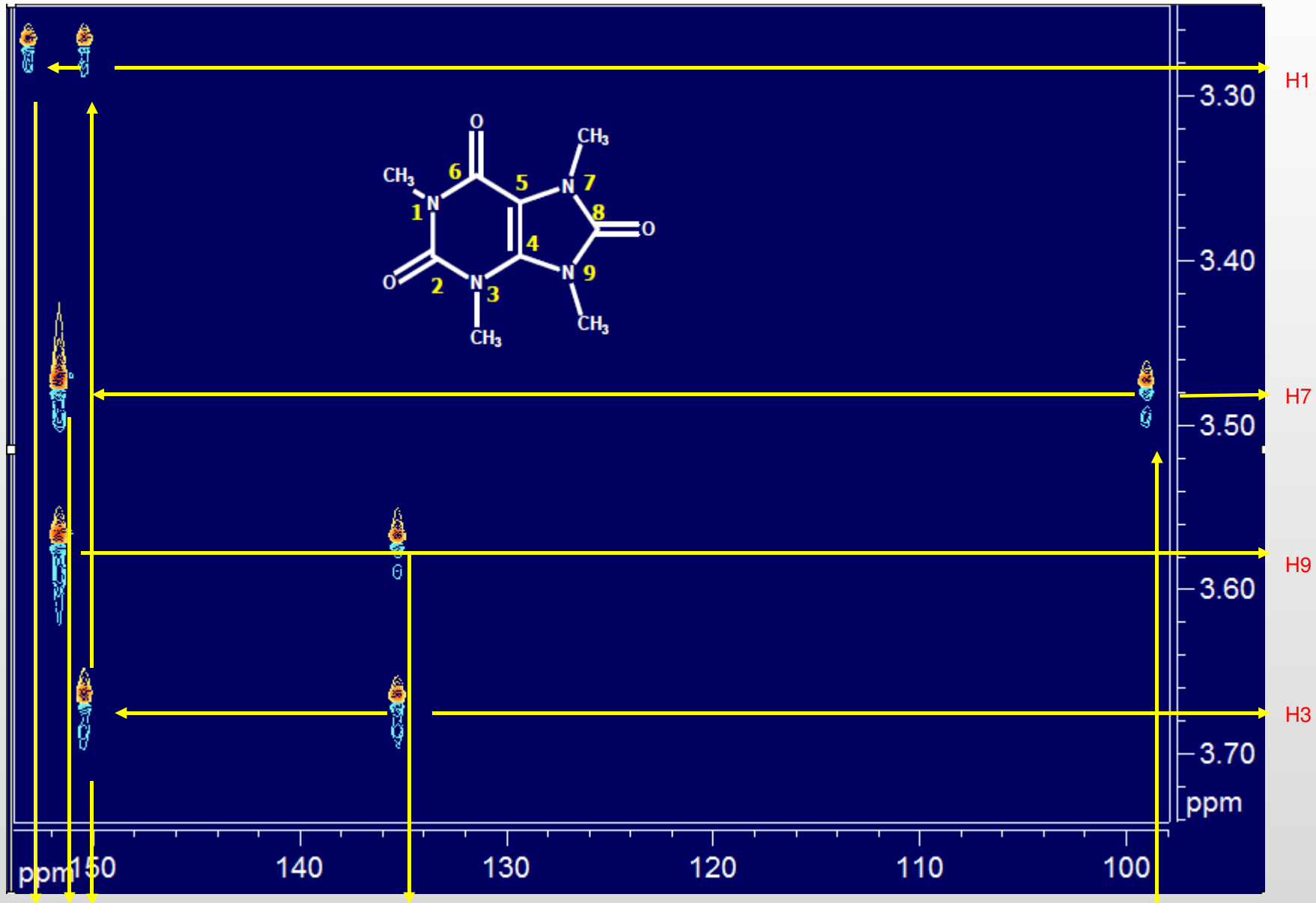


Widmo ¹H NMR teakryny w CDCl₃





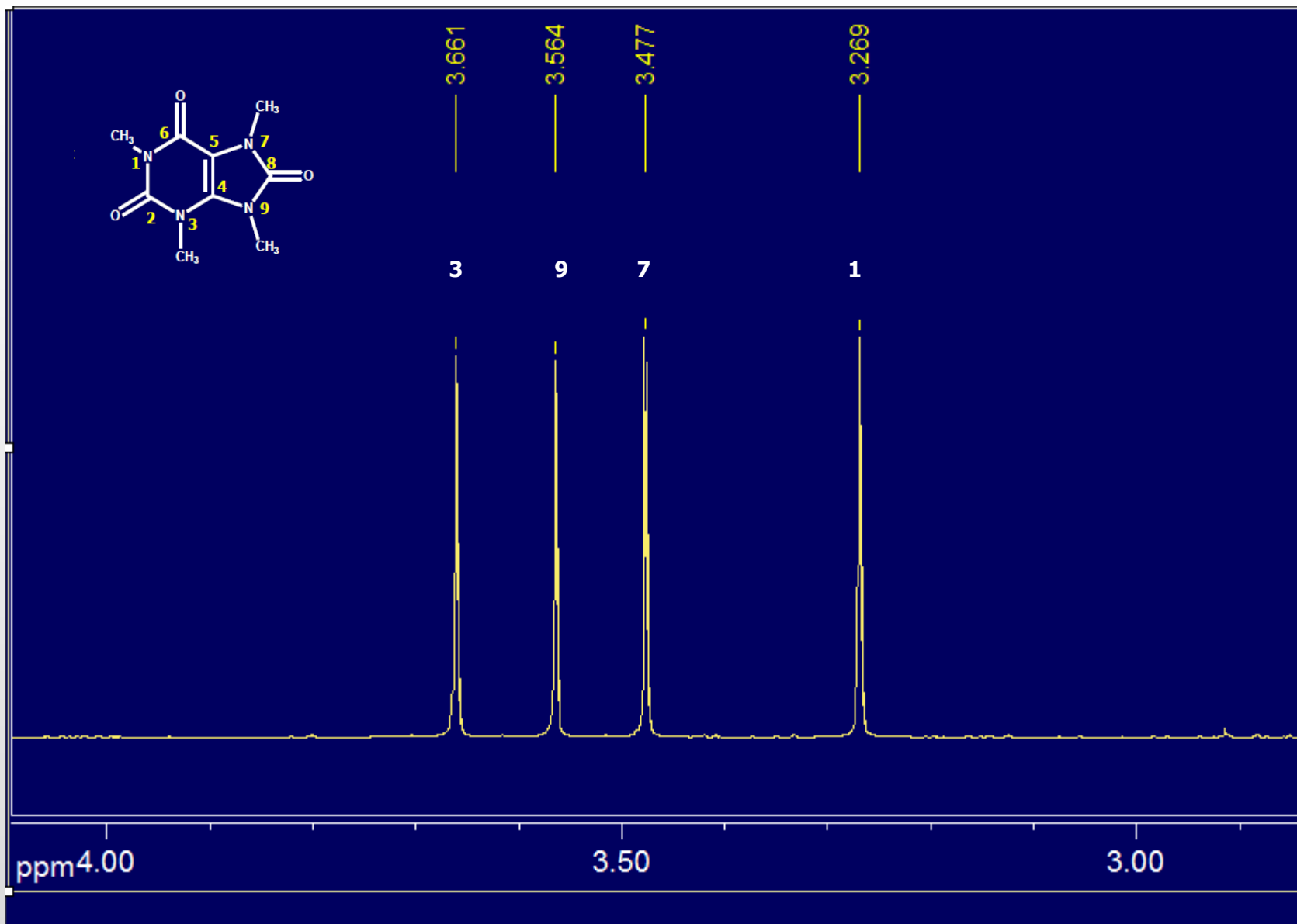
Detekcja odwrotna. Widmo 2D¹H-¹³C HMBCTeakryny.



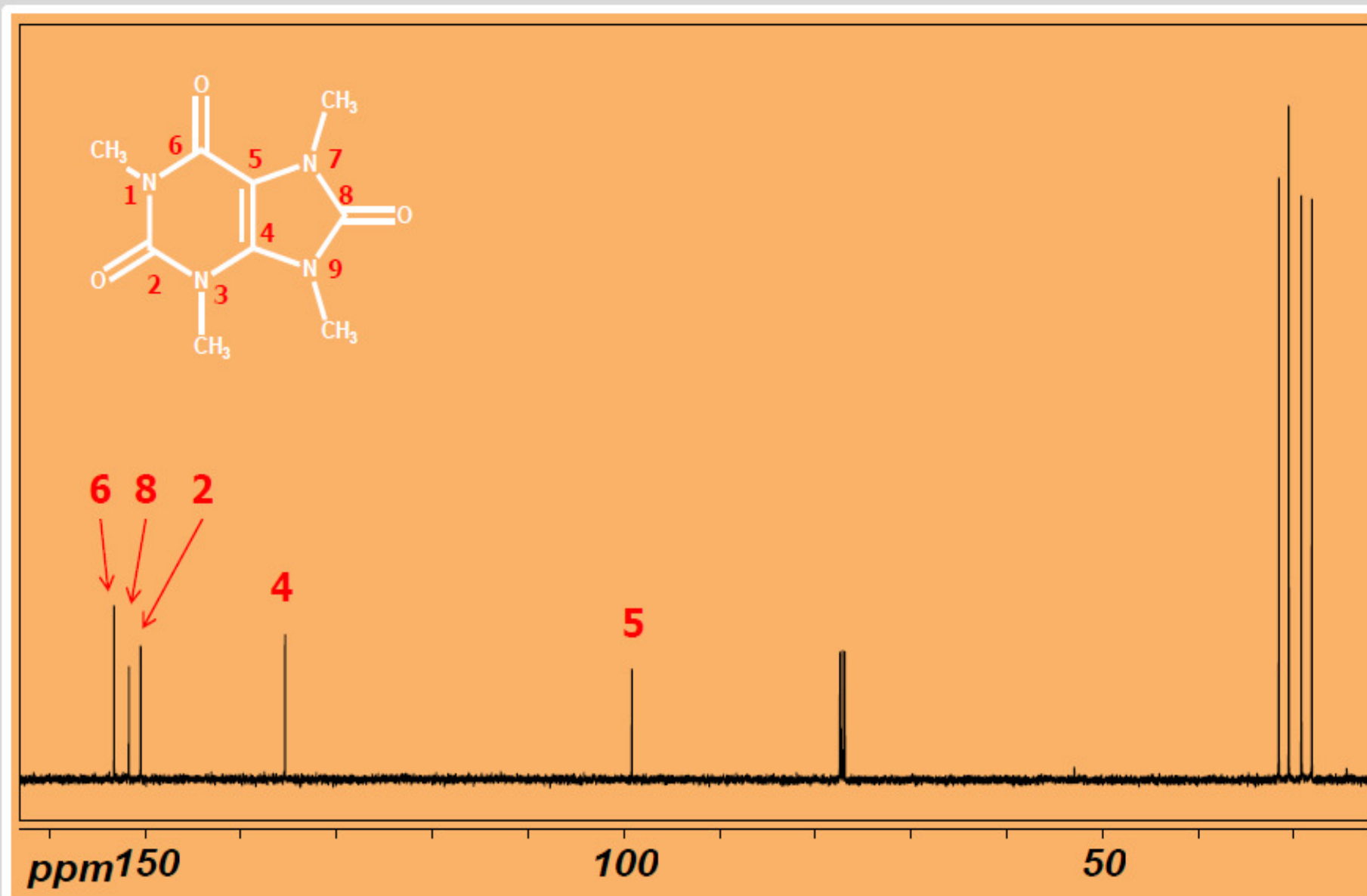
C6 C8 C2

C4

C5

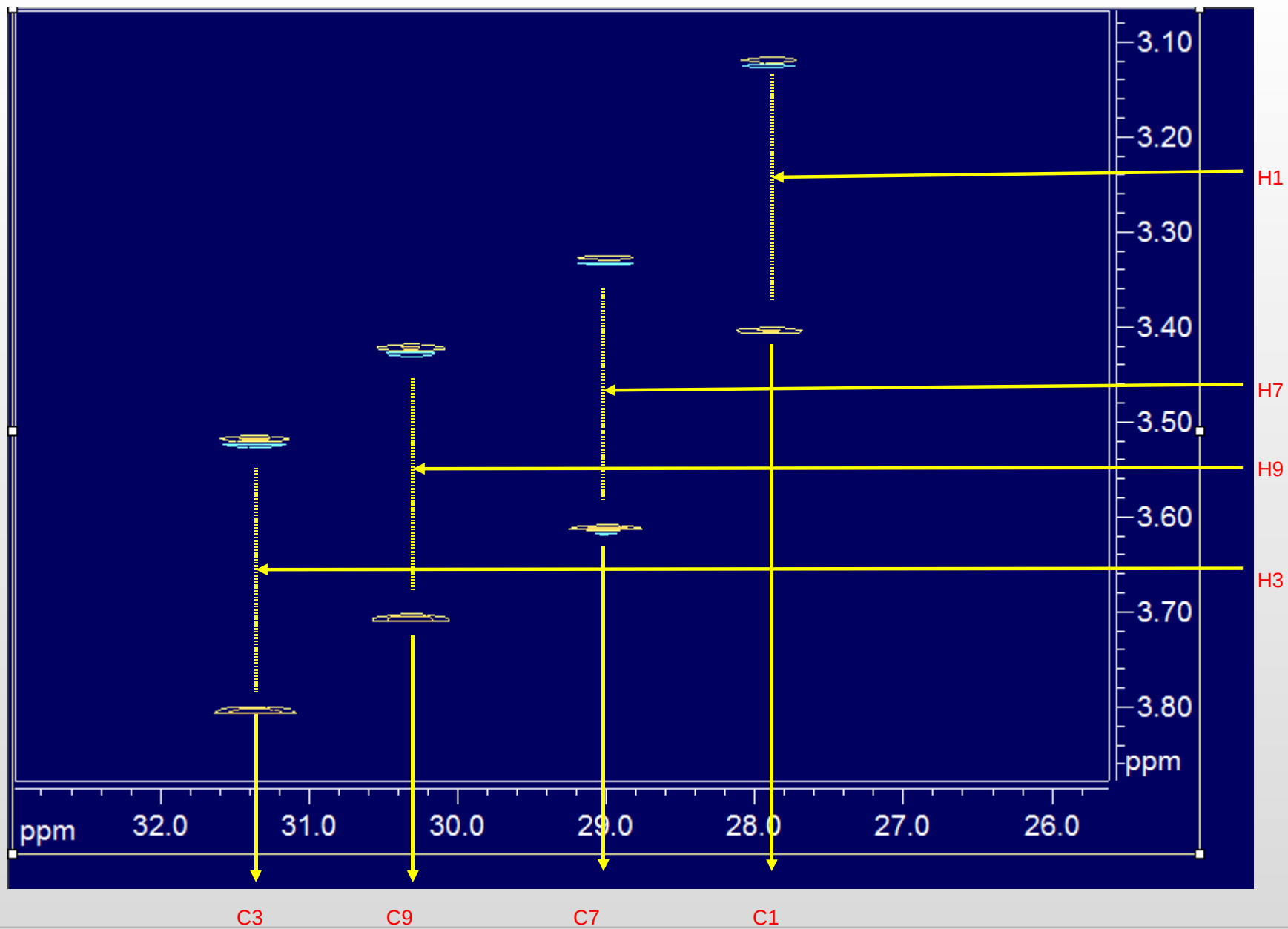


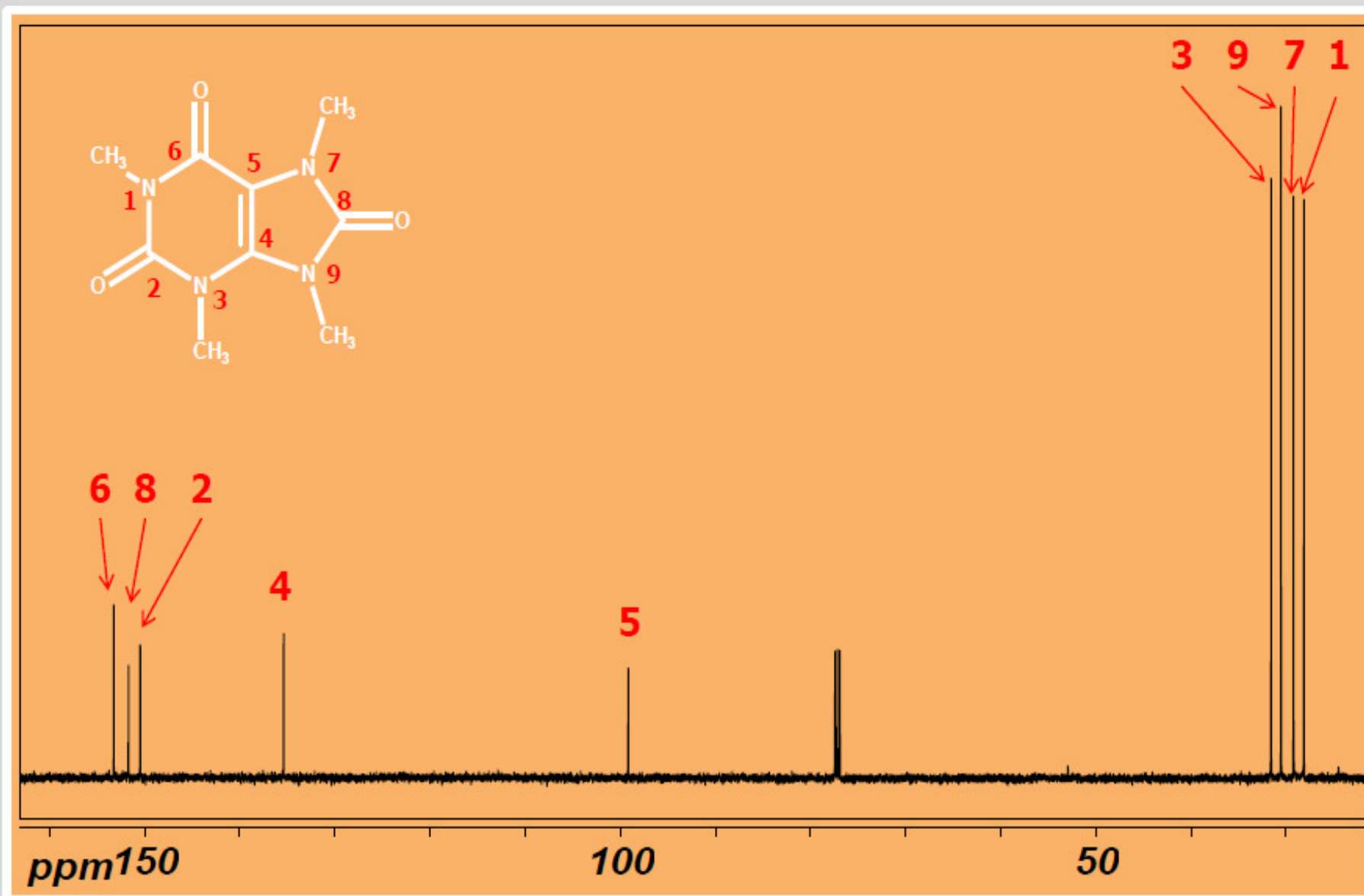
Widmo ¹H NMR teakryny w CDCl₃



Widmo ¹³C NMR teakryny w CDCl₃

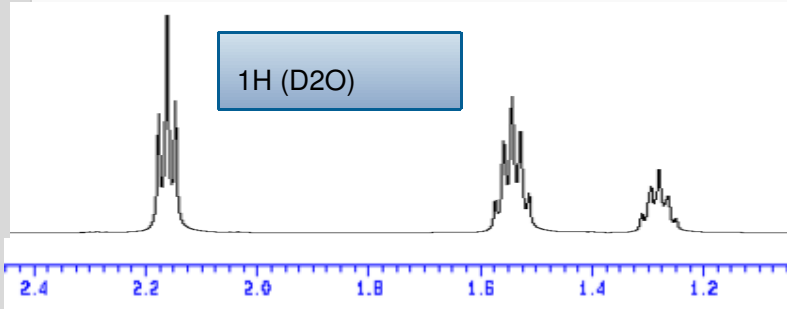
Widmo 1H-13C HSQCteakryny



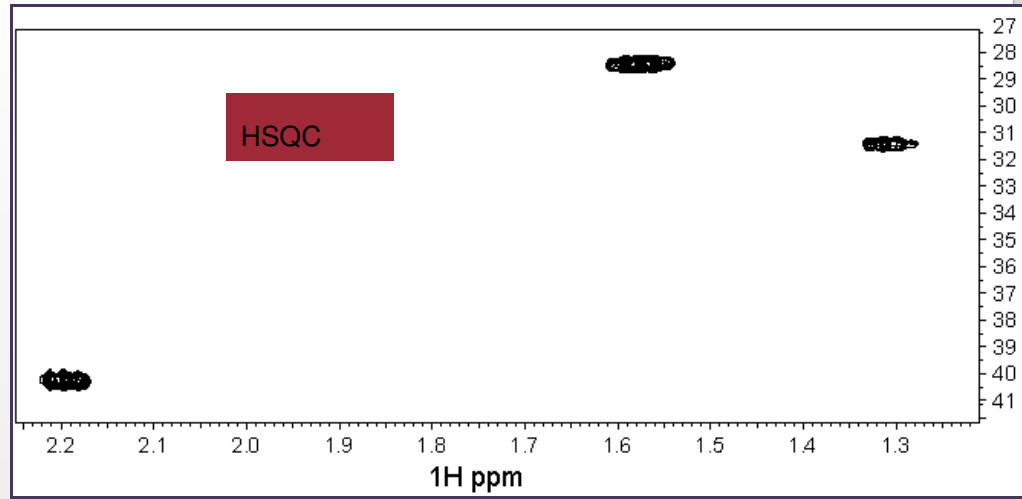


C7 H12 O4

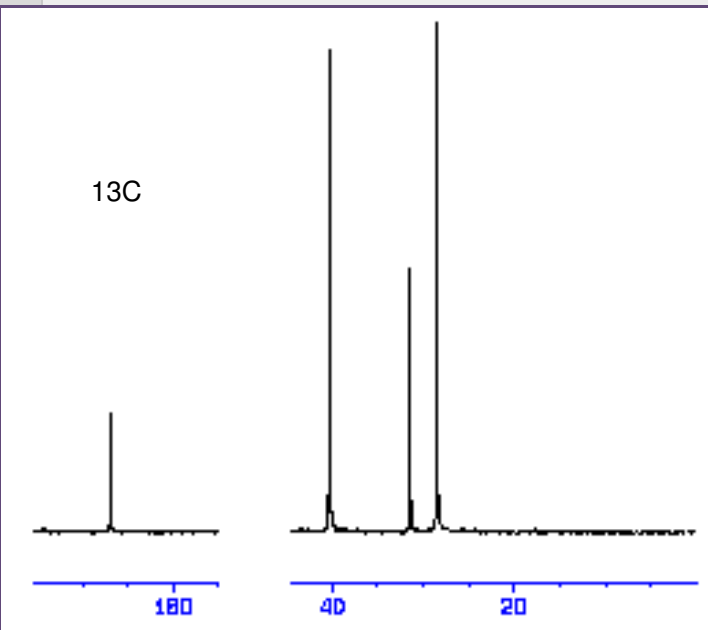
1H (D2O)



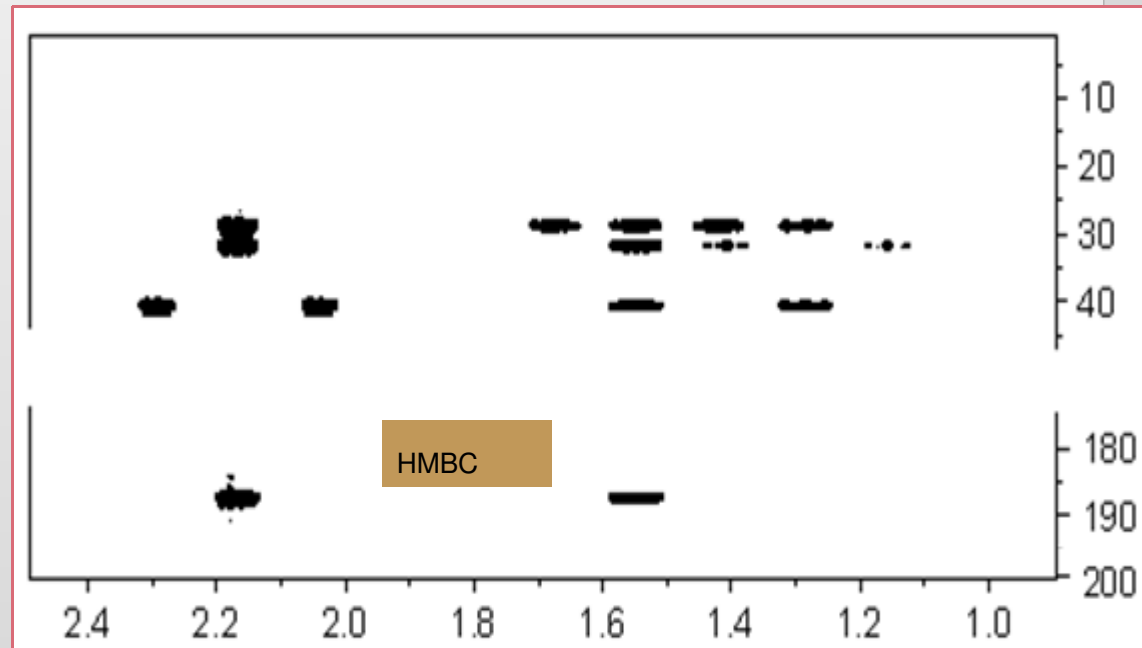
HSQC



13C



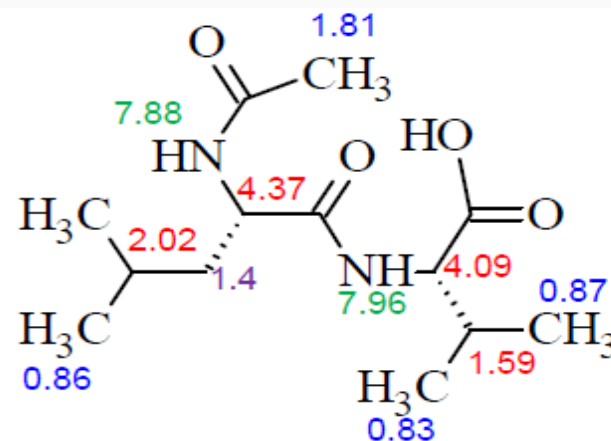
HMBC



NOESY

Nuclear Overhauser effect spectroscopy

N-acetyl-leu-val-OH



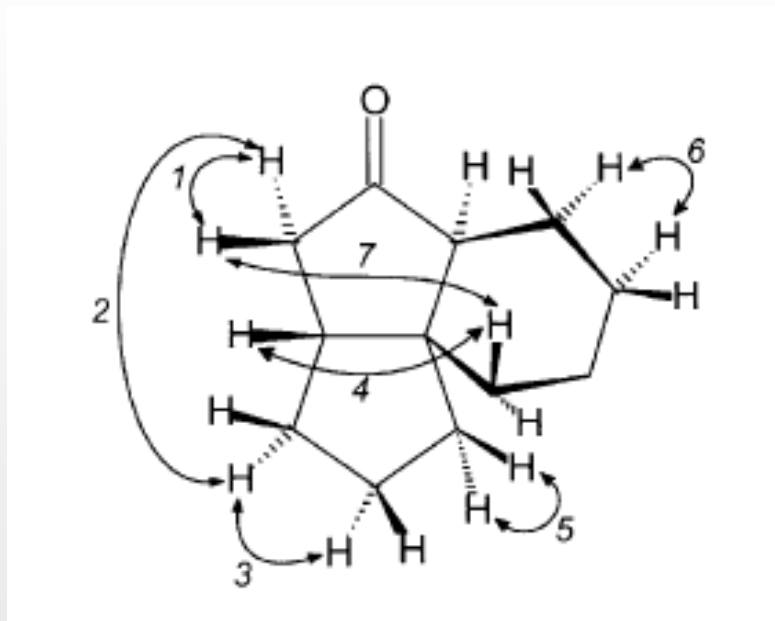
$^1\text{H-NMR}$ (DMSO- d_6) d: 0.83 (3H, d, $J = 6.7$ Hz), 0.86 (6H, d, $J = 6.7$ Hz), 0.87 (3H, d, $J = 6.7$ Hz), 1.38–1.42 (2H), 1.59 (1H, m), 1.81 (3H, s), 2.02 (1H, m), 4.09 (1H, dd, $J = 5.5, 8.5$ Hz), 4.37 (1H, m), 7.88 (1H, d, $J = 8.5$ Hz), 7.96 (1H, d, $J = 8.5$ Hz)

ROESY

Rotating frame nuclear Overhauser effect spectroscopy

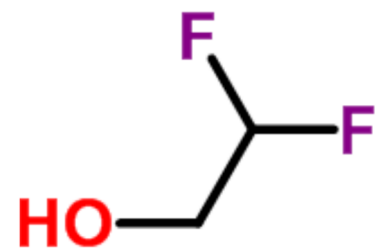
Wyniki eksperymentu NOESY

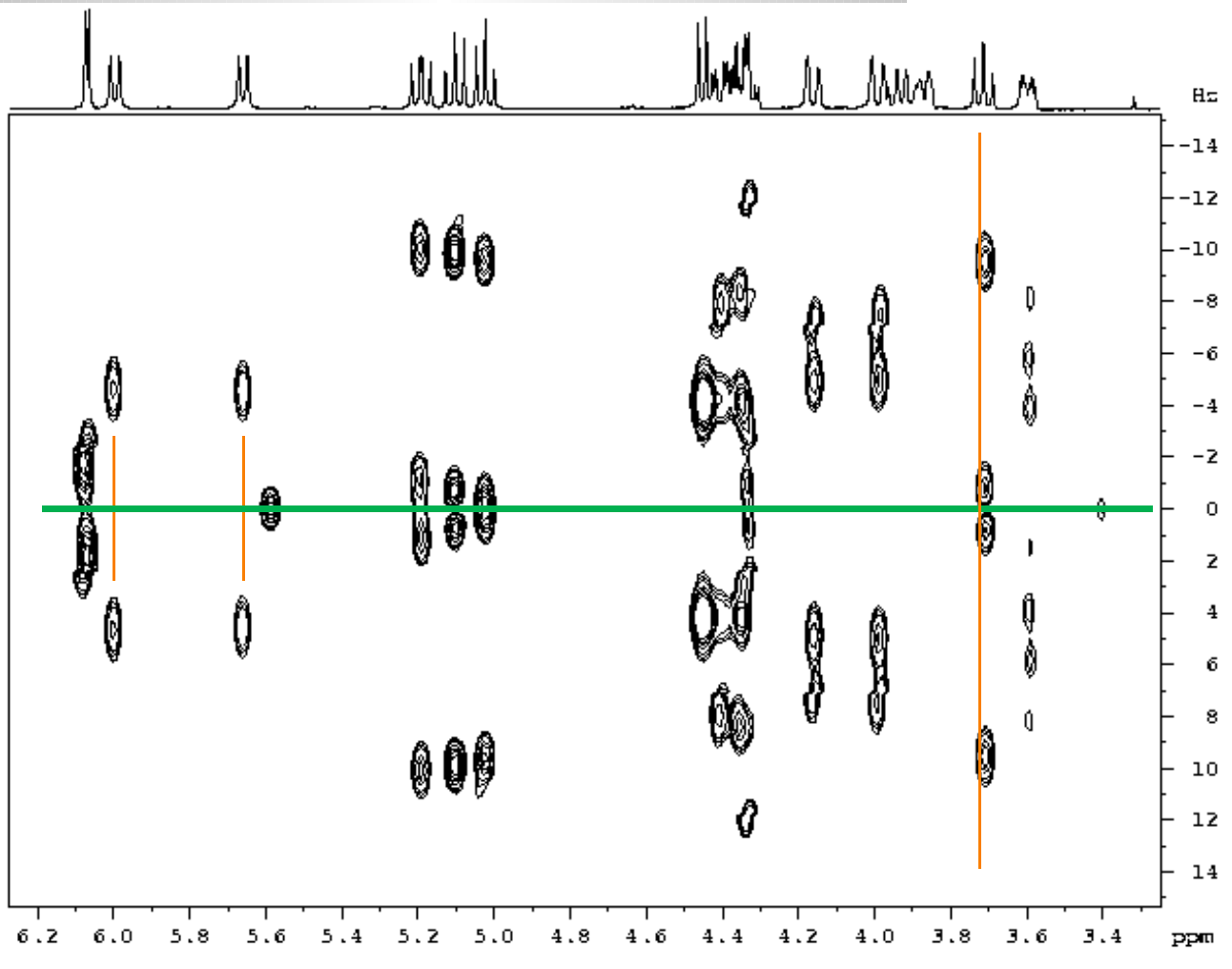
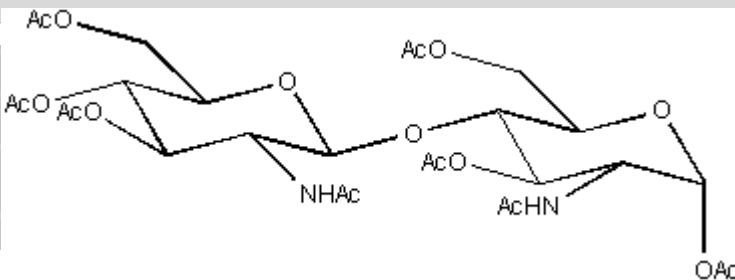
Nr	r(NOESY) / Å
1	1.79
2	2.28
3	2.13
4	2.62
5	1.77
6	2.35
7	2.65



Wzorzec (odnośnik)

2D JRES NMR





Widmo 2D 1H-1H JRES NMR

2D JRES NMR

Homojądrowe
Np. 1H-1H

Heterojądrowe
Np. 1H-13C



$^1J_{C,H}$ [Hz]

Alifatyczne, C-H	125-135
Alifatyczne, CX-H (X=N,O,S)	135-155
Alken, =C-H	155-170
Alkin, \equiv C-H	240-250
Aromatyczne, C-H	155-165

SELJRES (strychnina)

ang. selective J-resolved spectra

C-14

