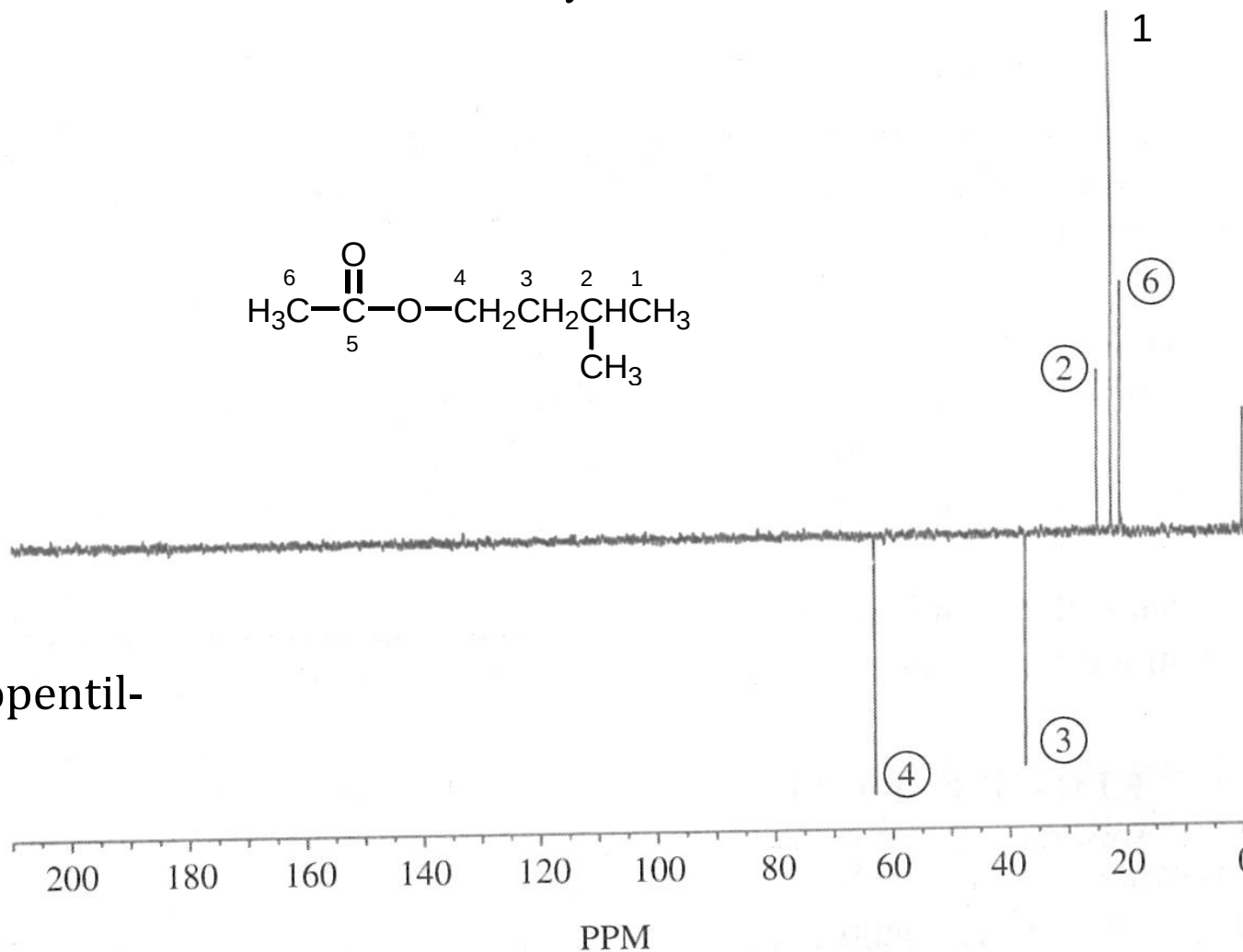
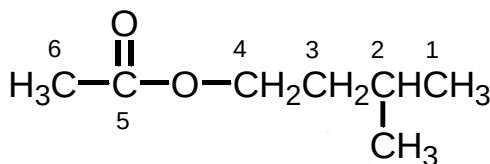


^1H i ^{13}C NMR

Napredne NMR tehnike: APT/DEPT eksperiment, dvodimenzijske spektroskopske metode, COSY, LR COSY, HETCOR, HMBC, NOESY

■ DEPT eksperiment (**D**istortionless **E**nhancement by **P**olarization **T**ransfer)

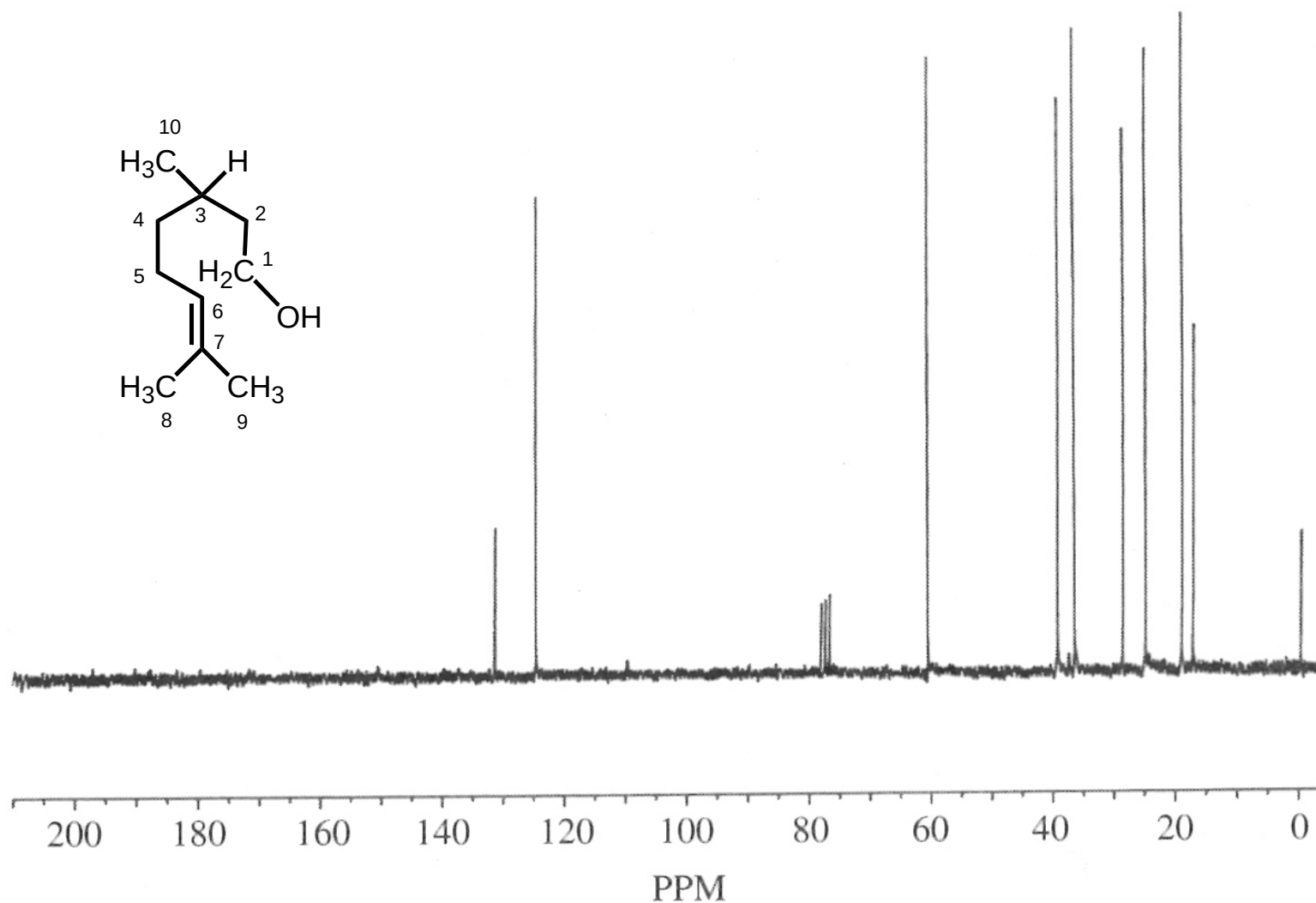


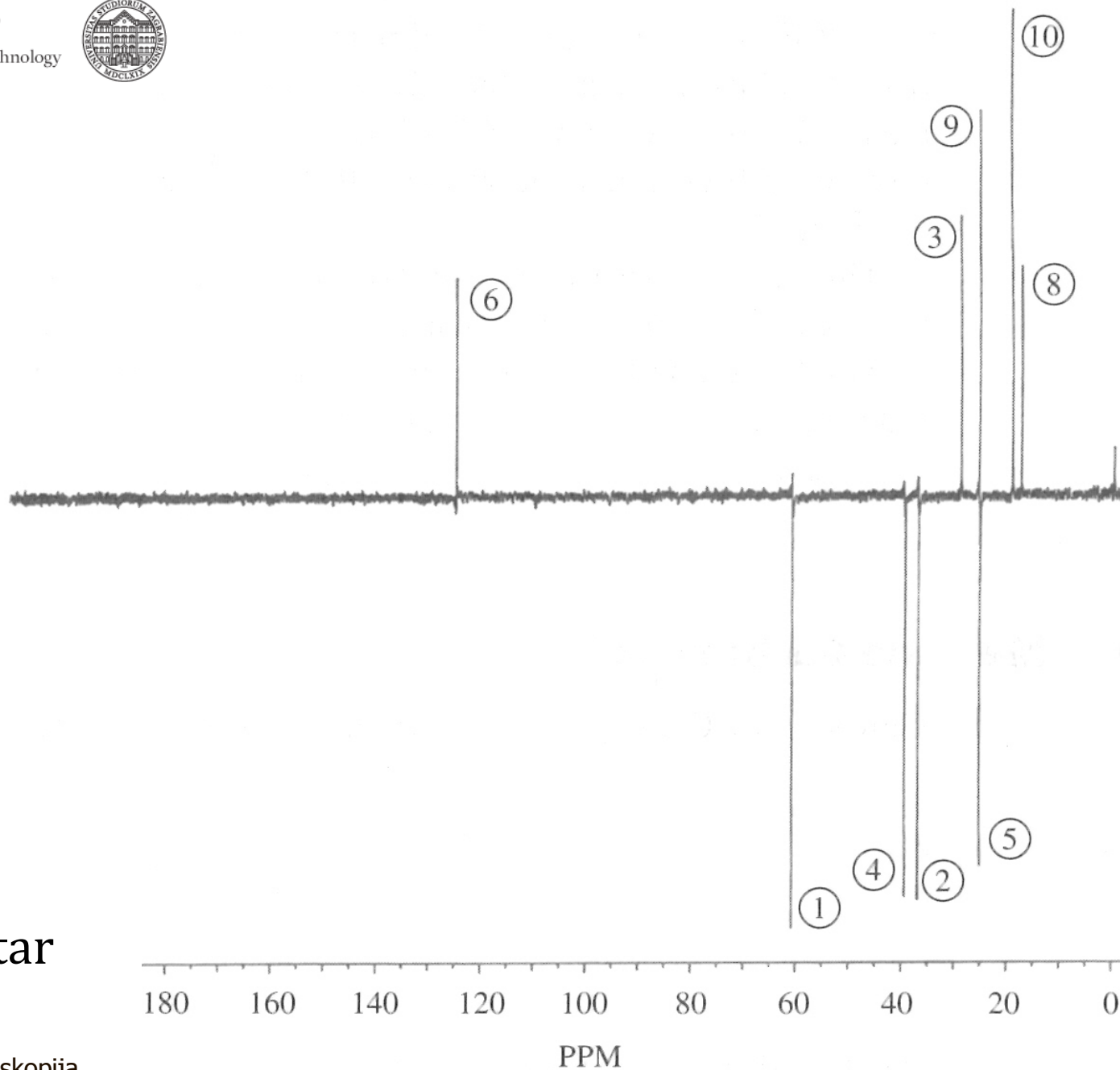
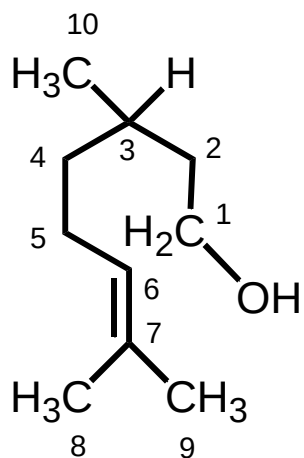
- DEPT spektar izopentil-acetata (u CDCl_3)

■ ^{13}C NMR spektar citronelola



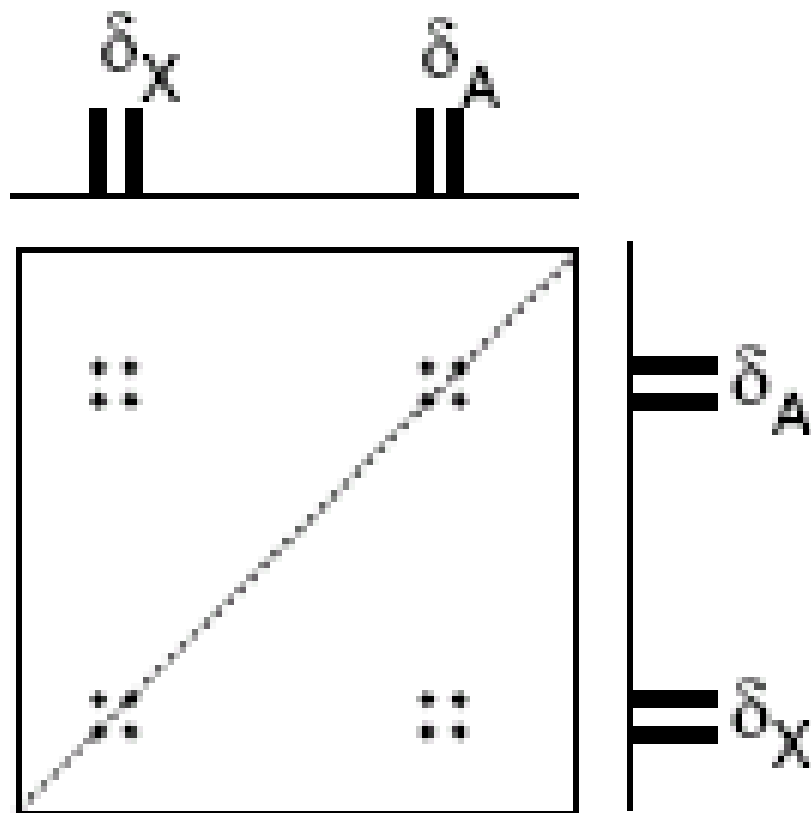
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■ DEPT spektar citronelola

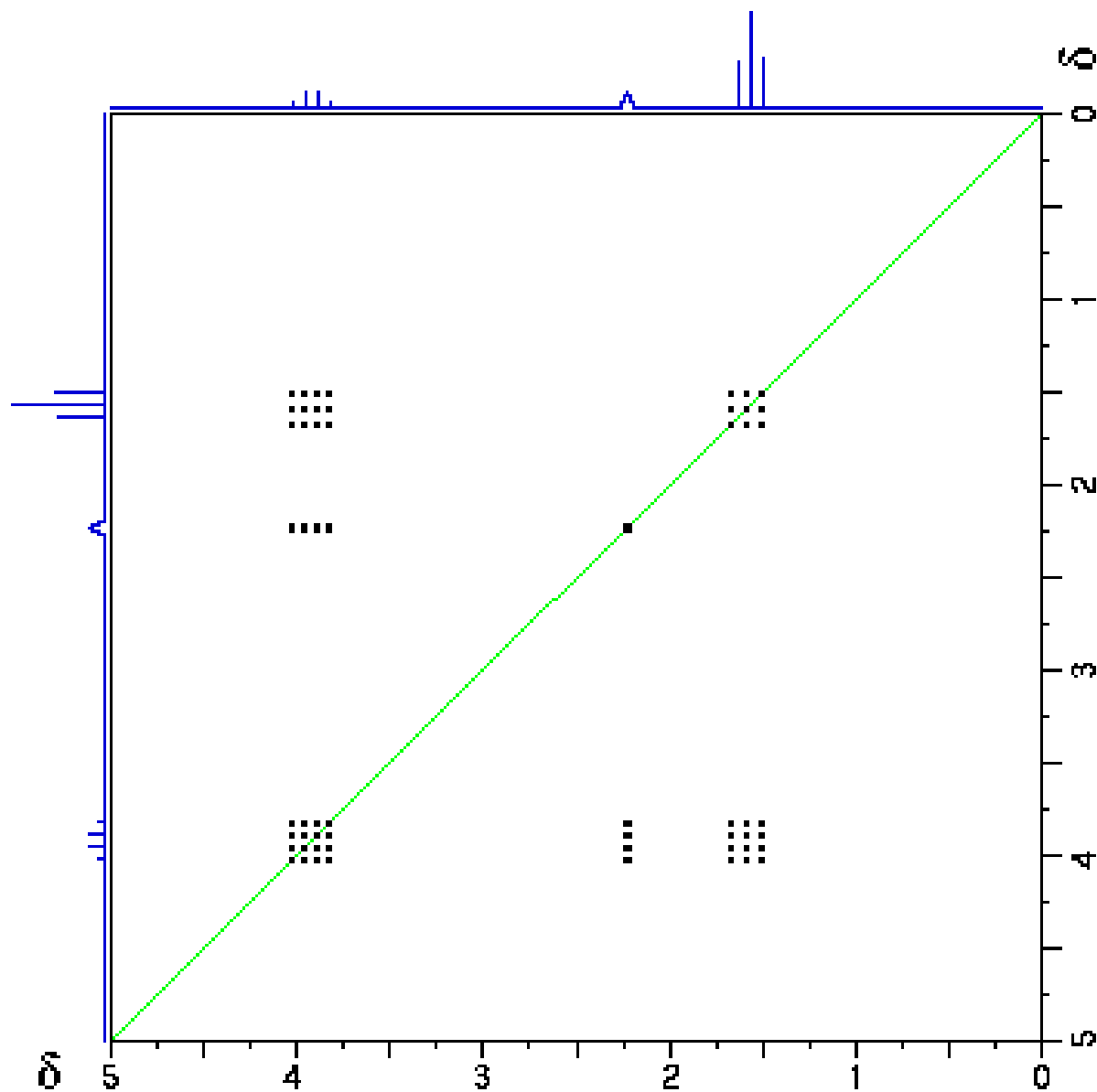
- KORELACIJSKA NMR SPEKTROSKOPIJA; 2D NMR**
 ^1H - ^1H COSY (COrrrelation SpectroscopY)



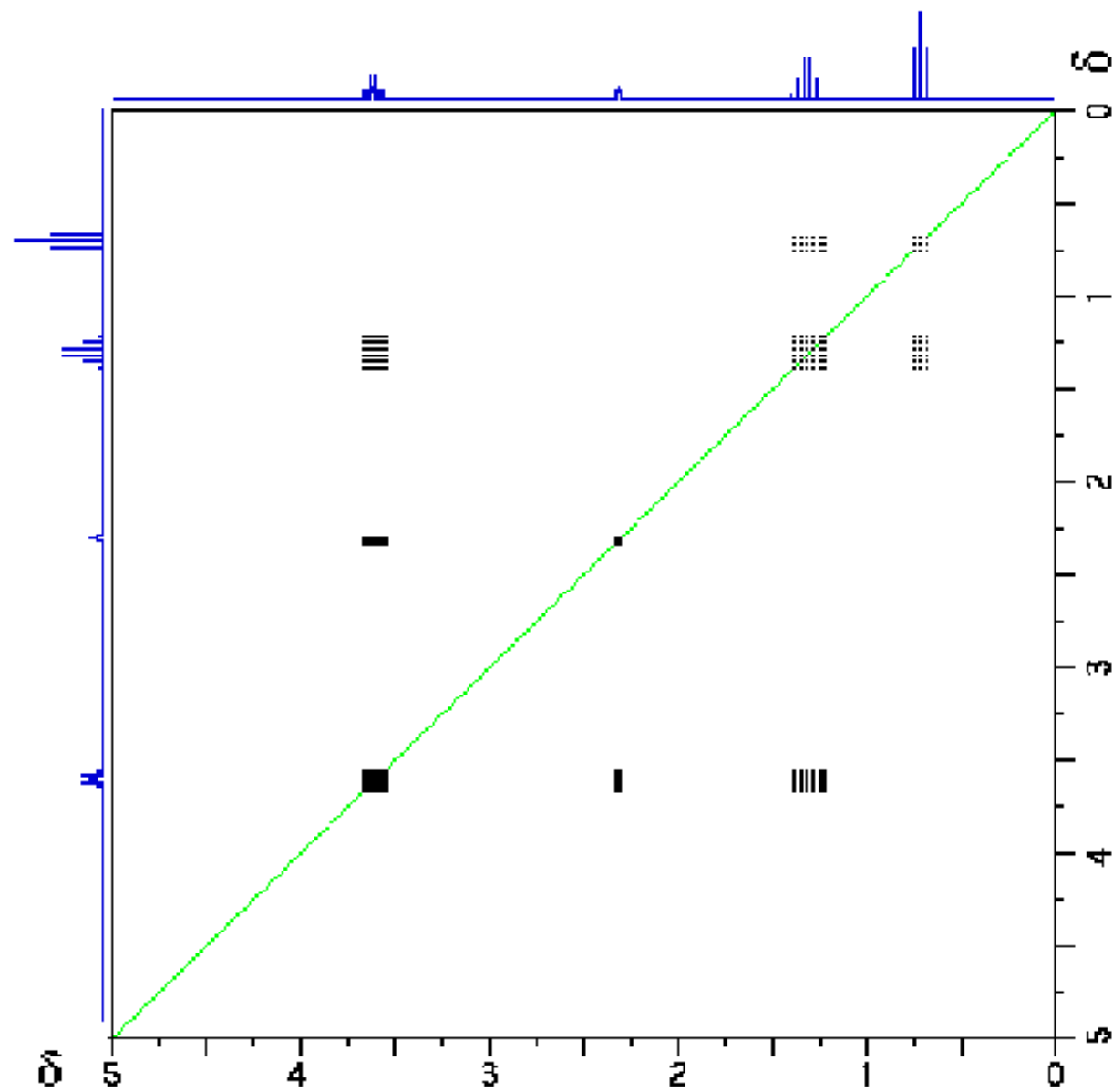
Shematski prikaz COSY spektra za dva spinska sprezanja, A i X

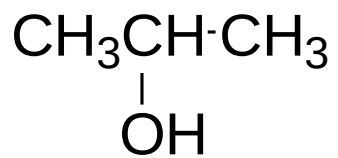
CH₃CH₂-OH

COSY

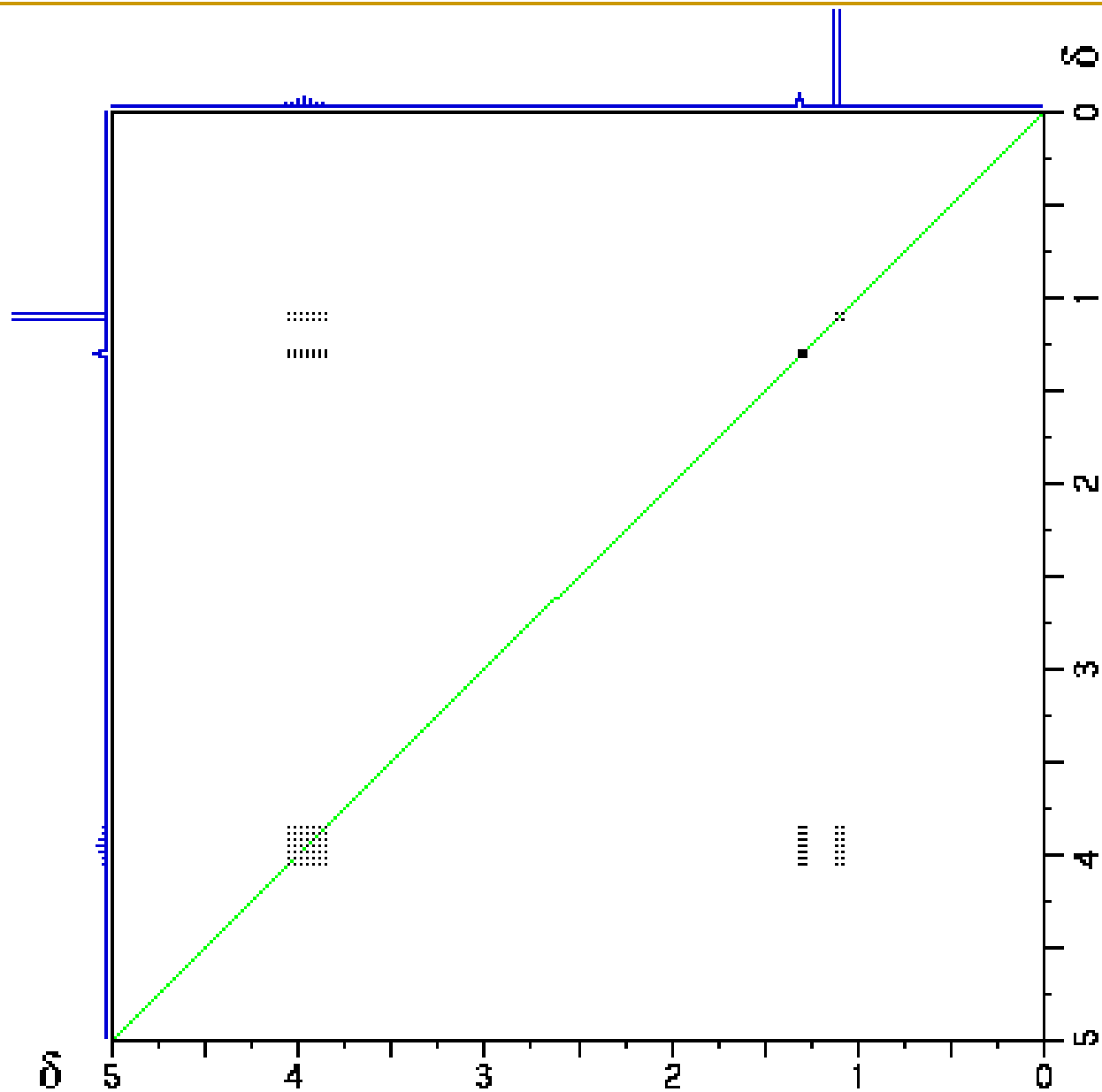


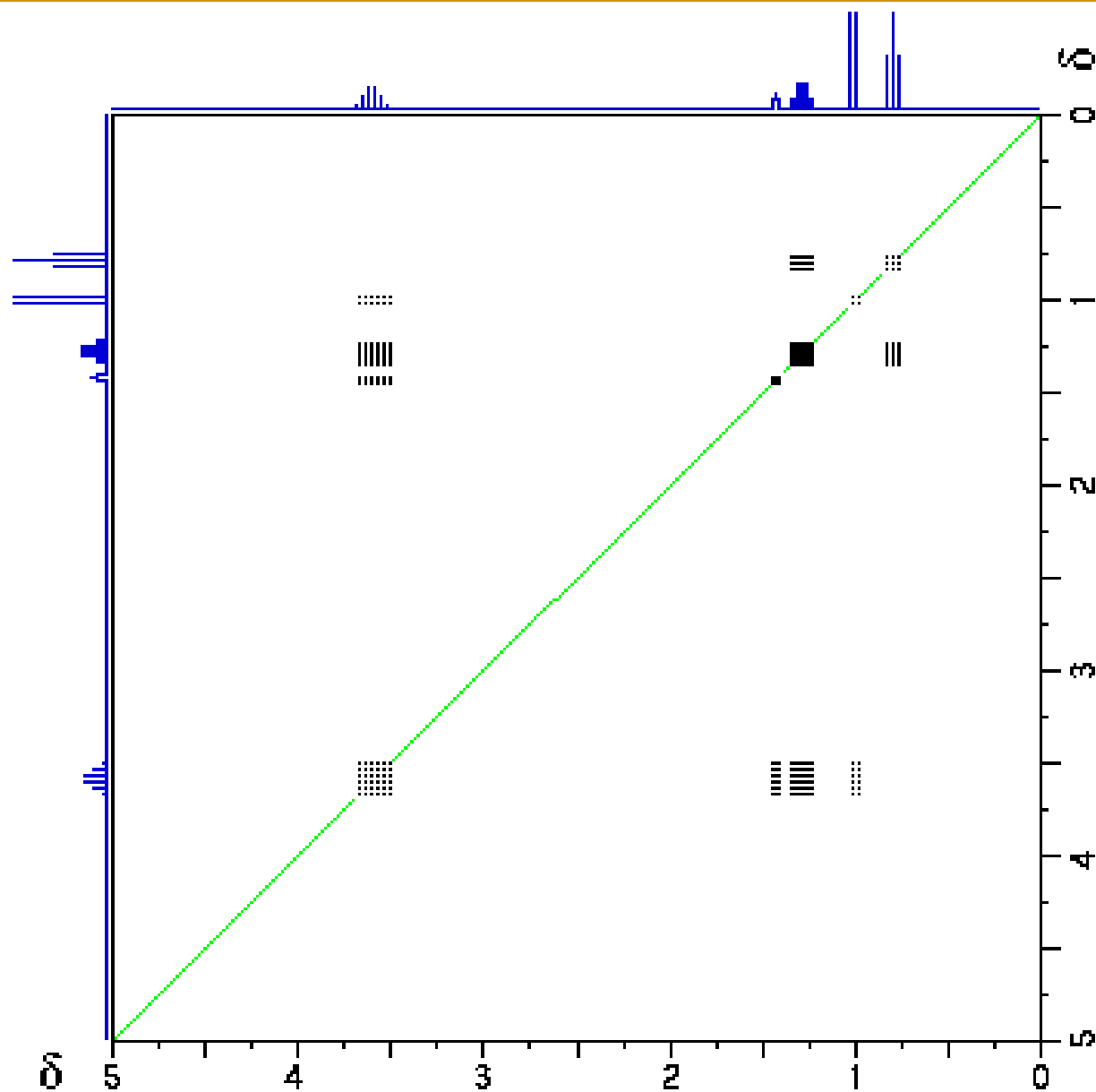
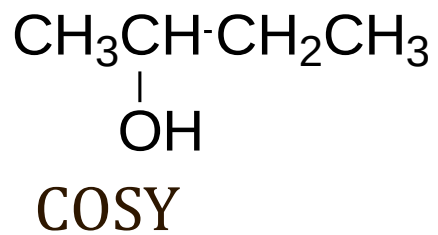
CH₃-CH₂-CH₂-OH
COSY

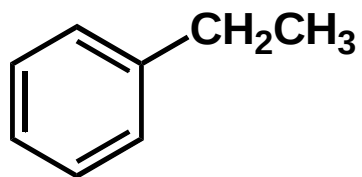




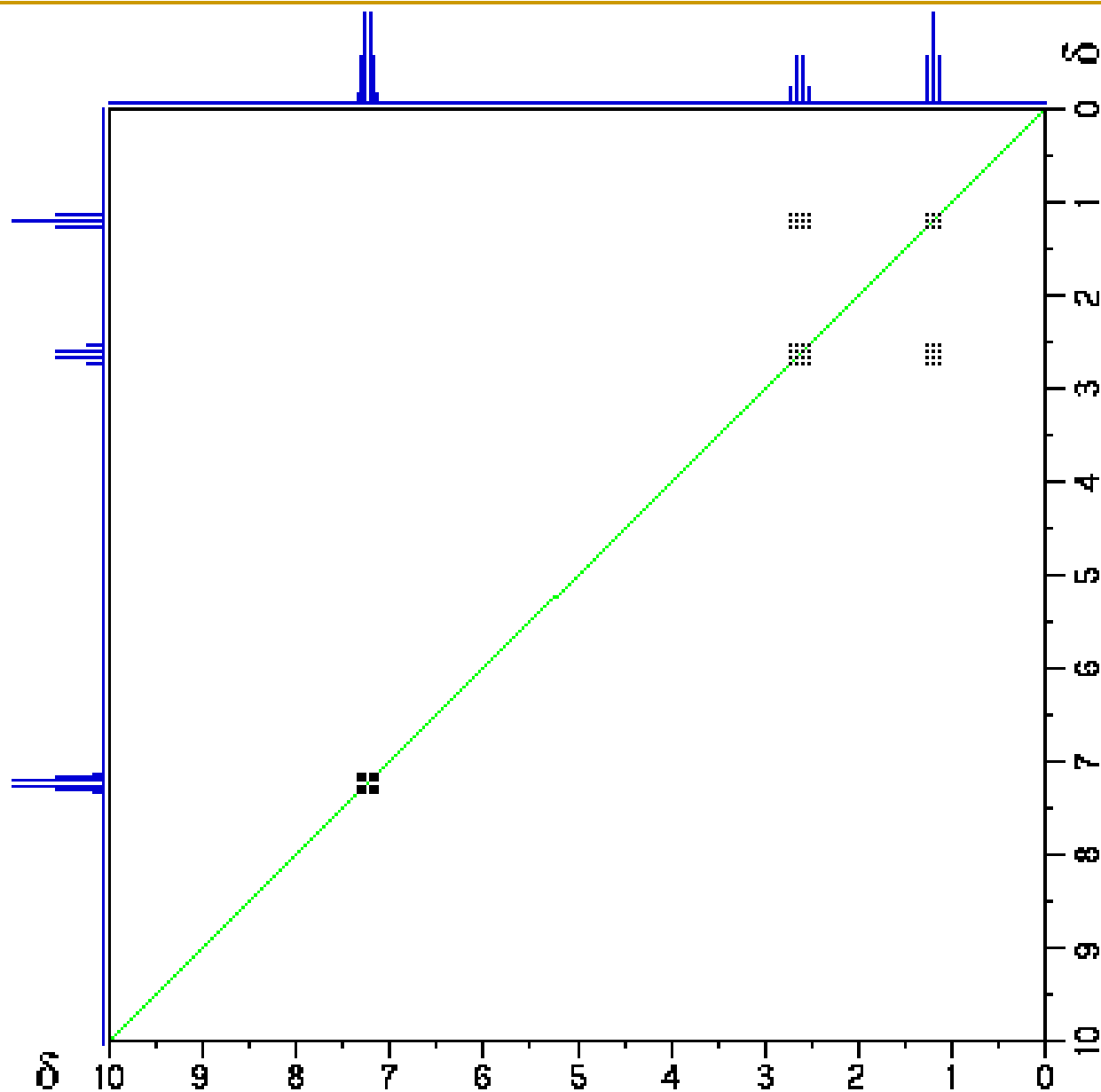
COSY

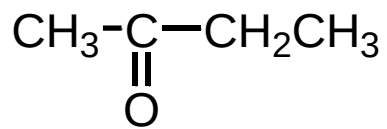




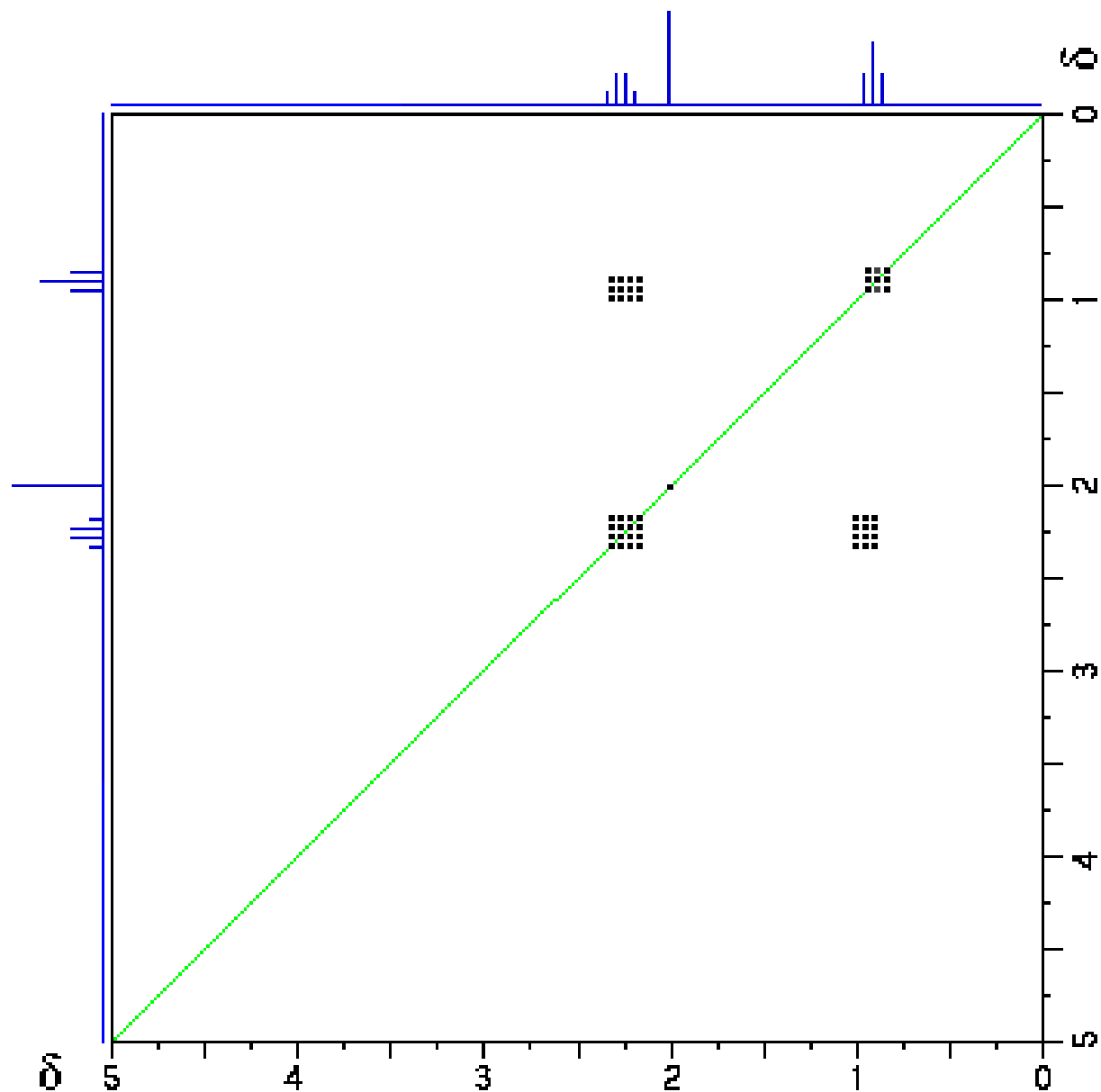


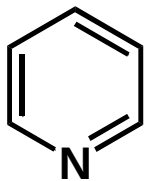
COSY



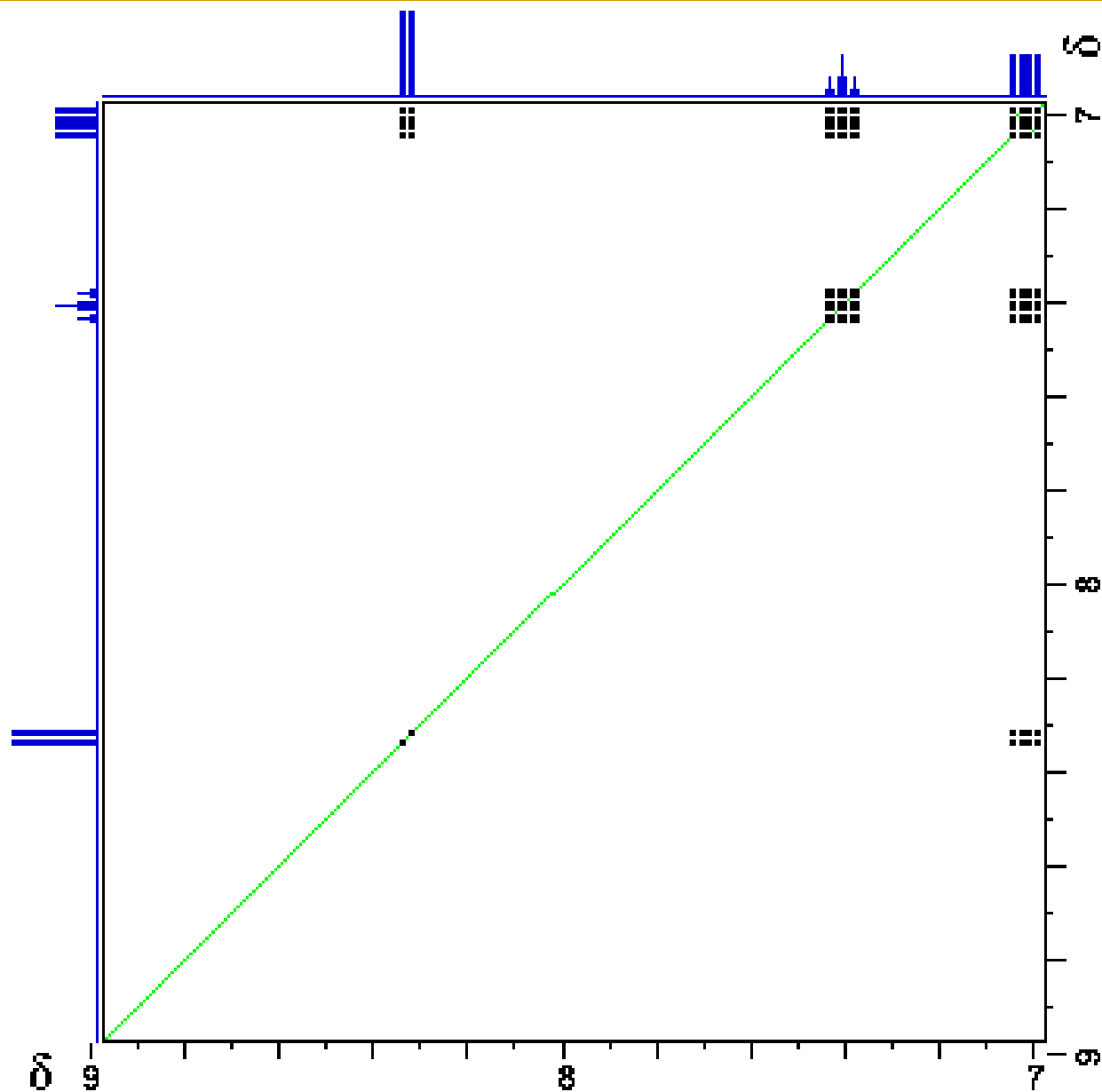


COSY

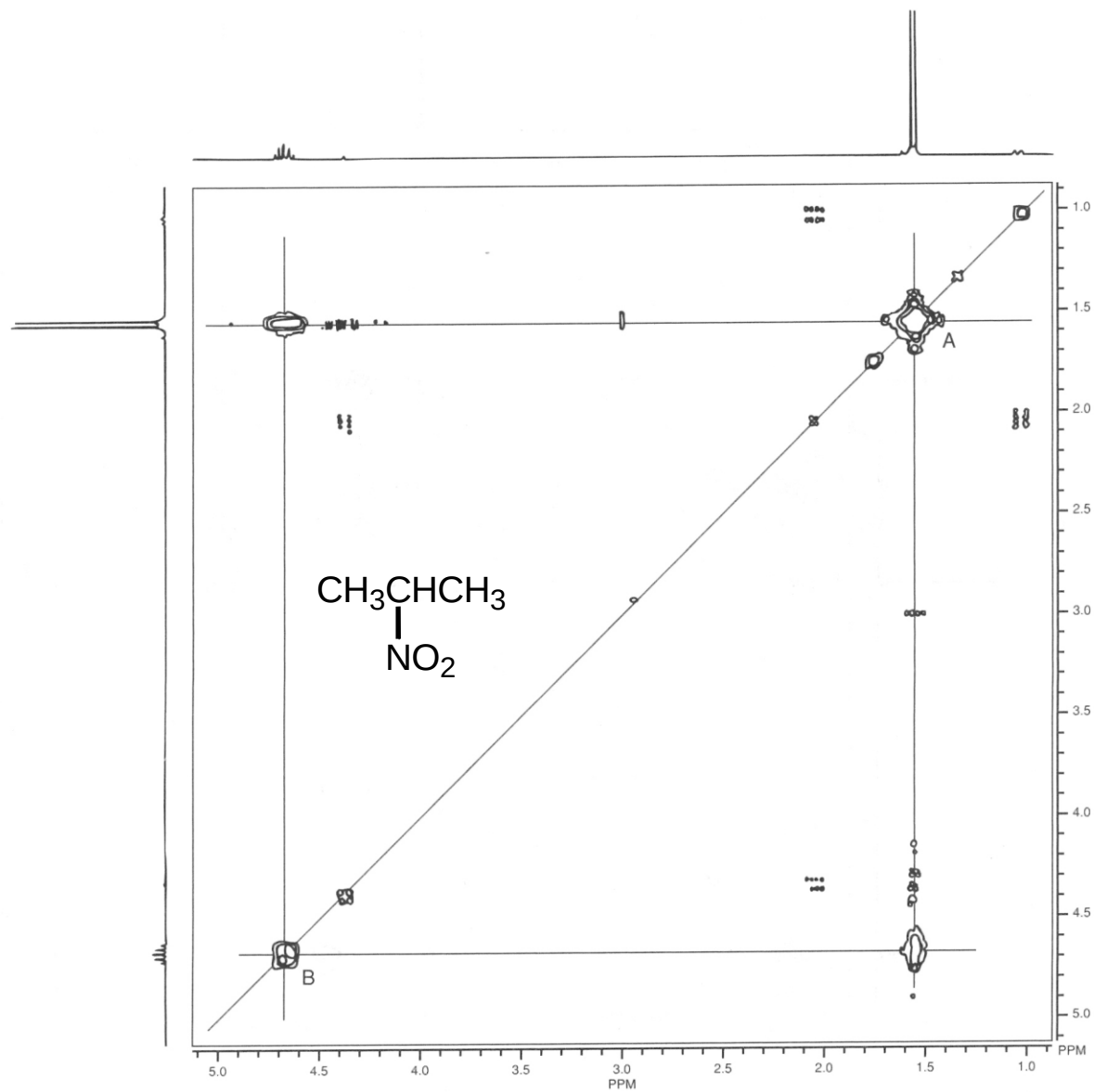




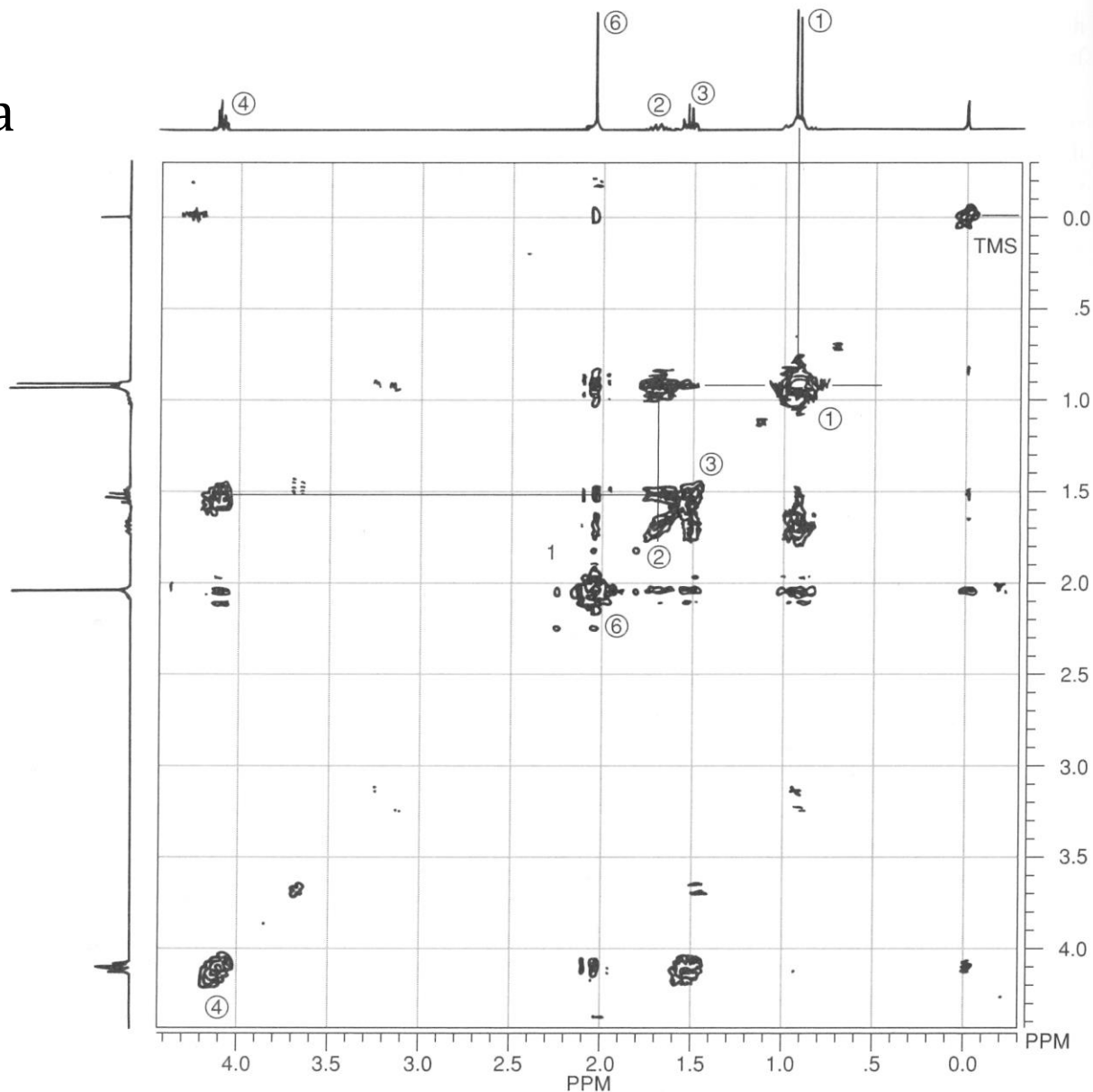
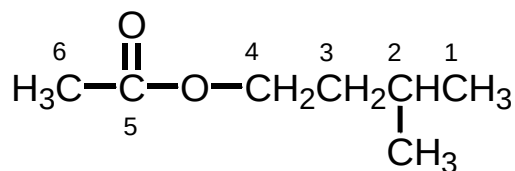
COSY



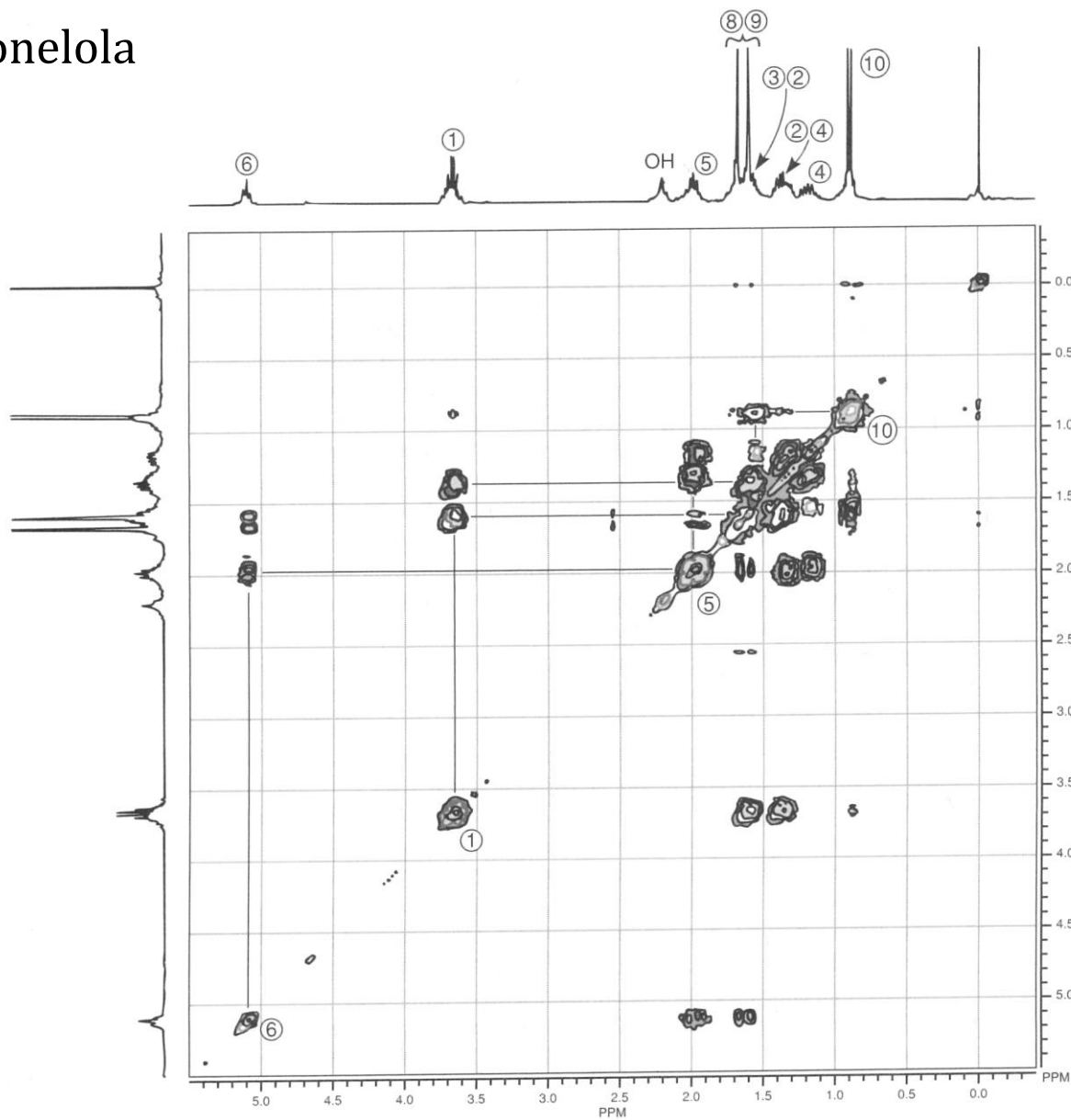
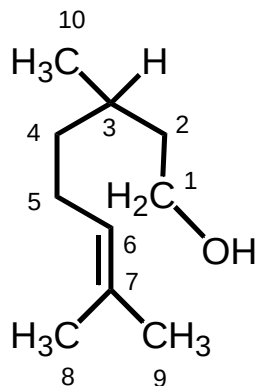
■ COSY spektar
2-nitropropana



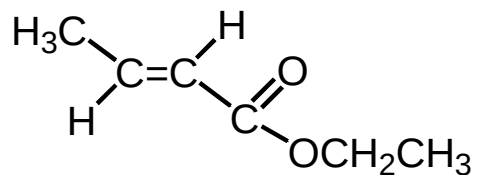
■ COSY spektar izopentil-acetata



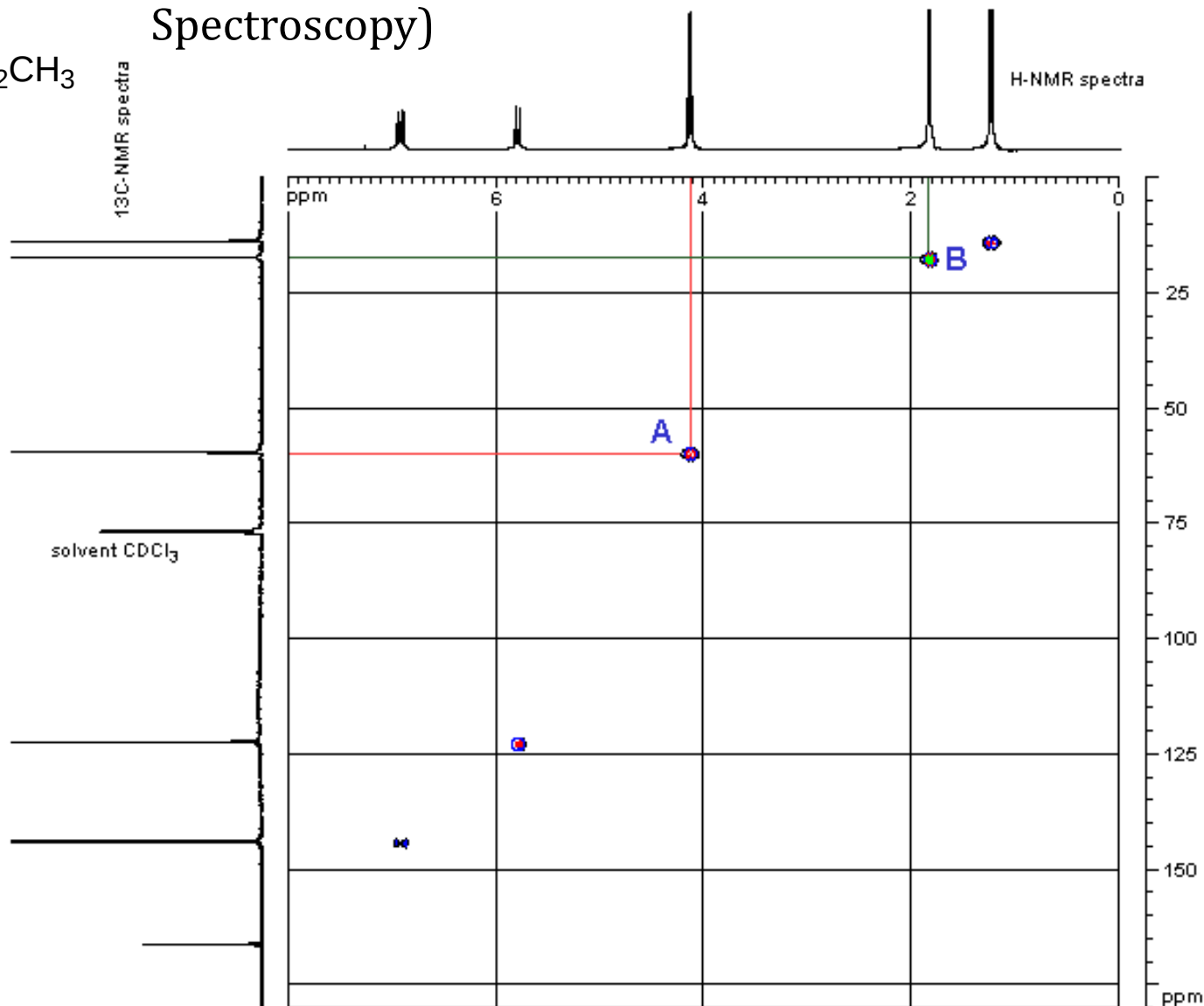
■ COSY spektar citranelola



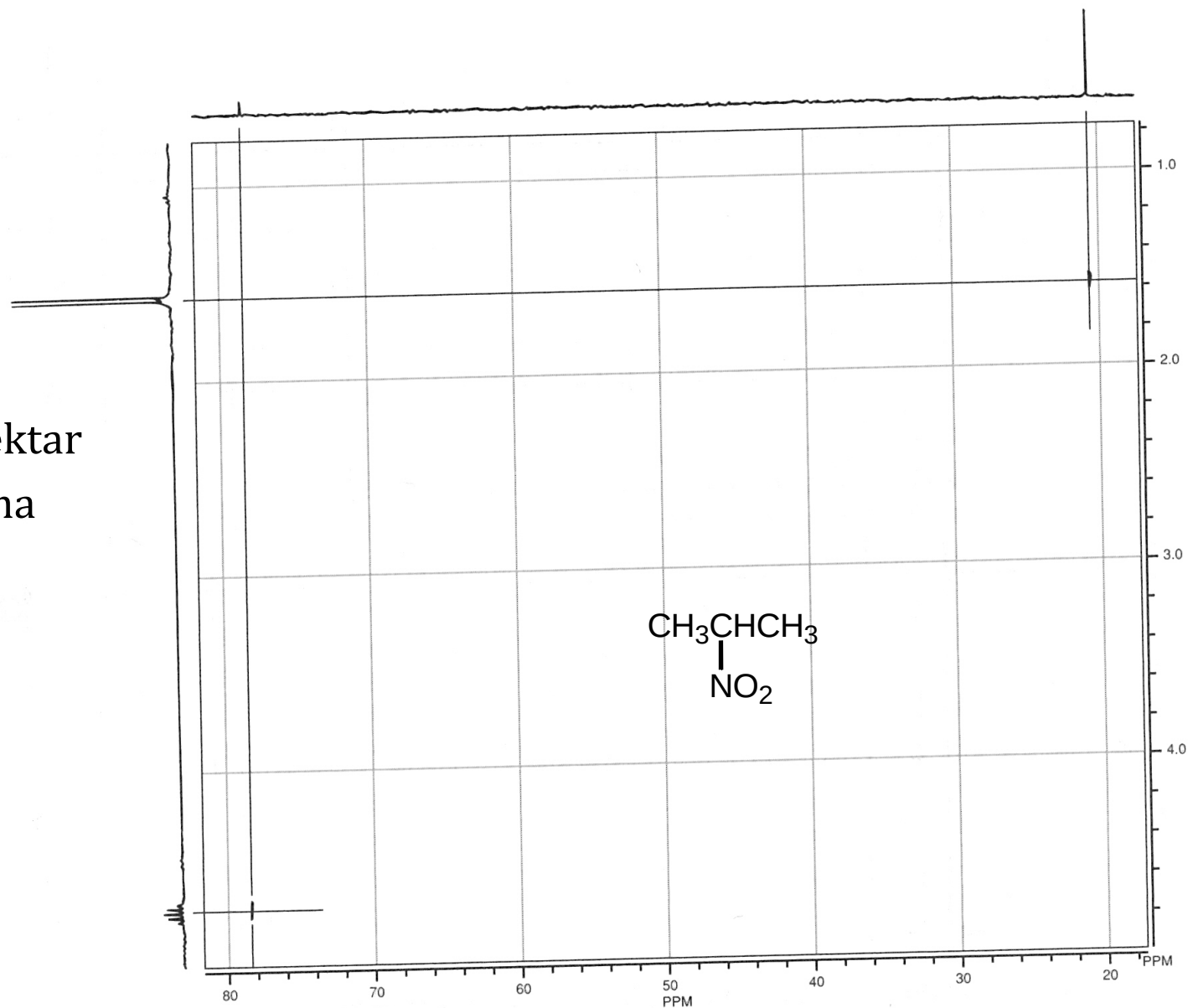




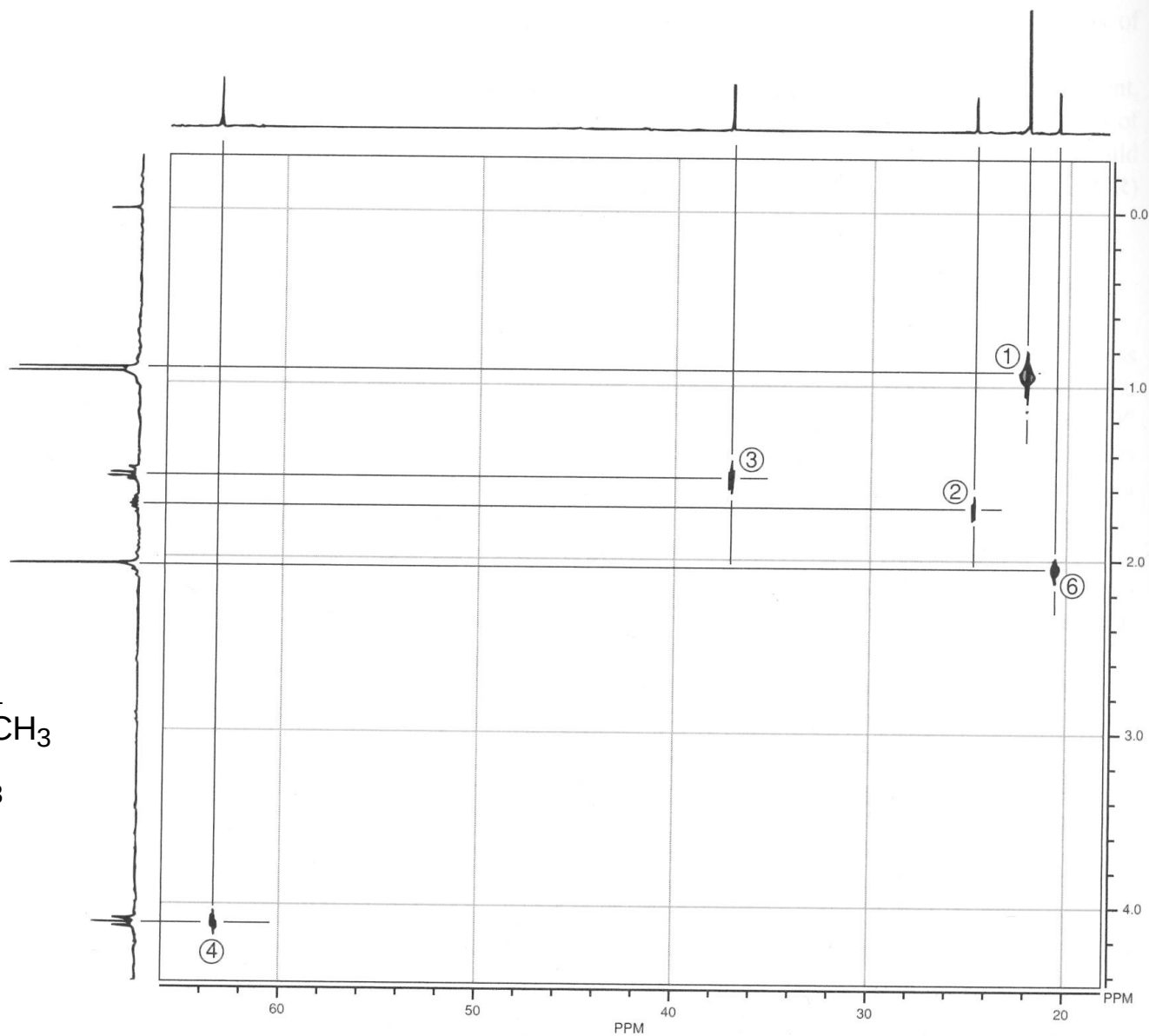
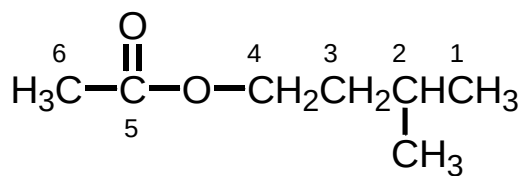
¹³C- ¹H COSY : HETCOR (**H**ETeronuclear **C**ORrelation Spectroscopy)



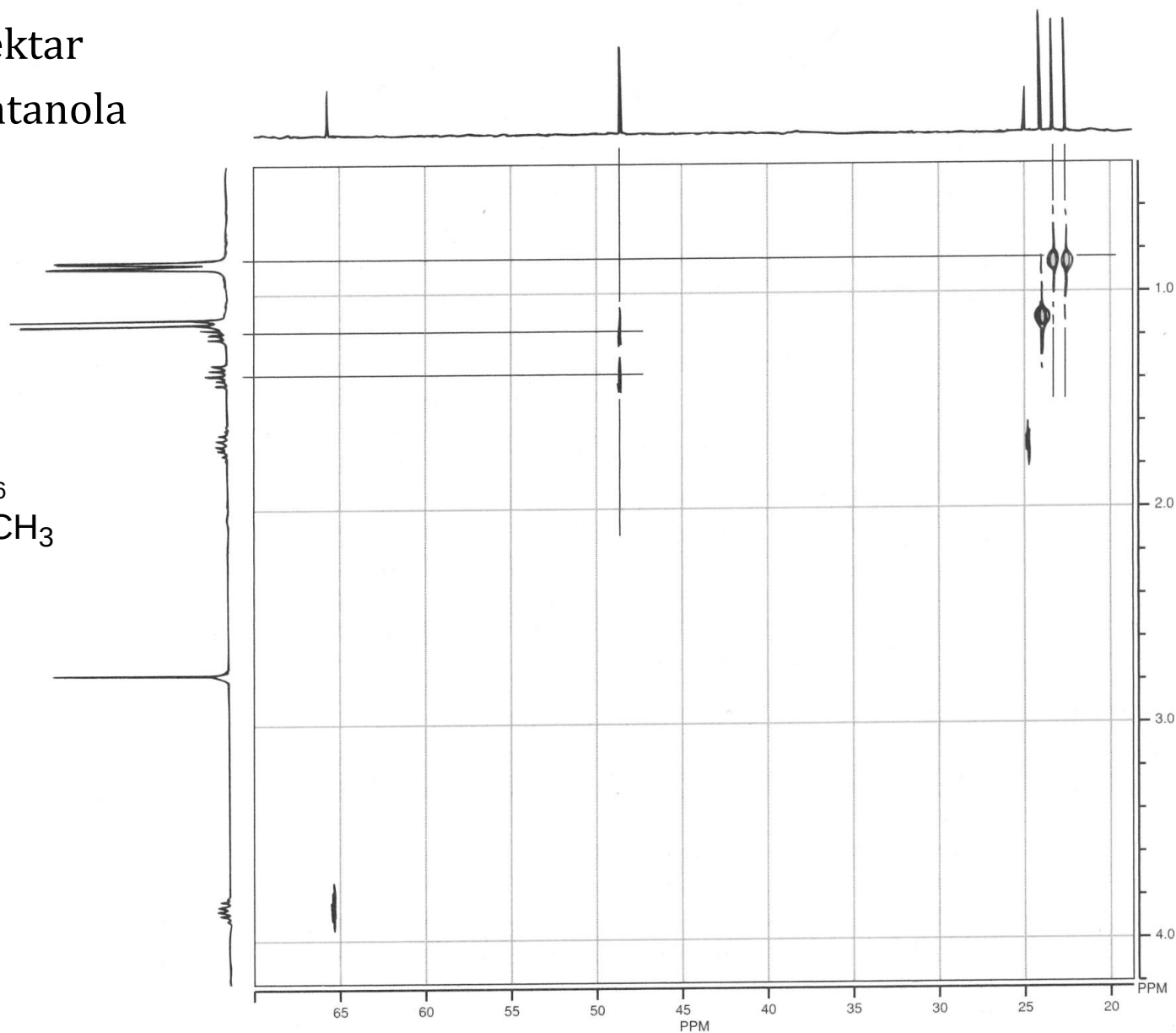
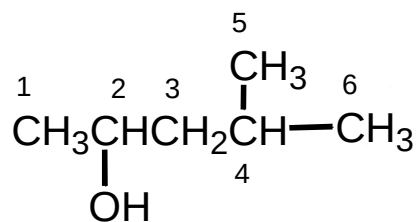
■ HETCOR spektar
2-nitropropana



■ HETCOR spektar
izopentil-acetata

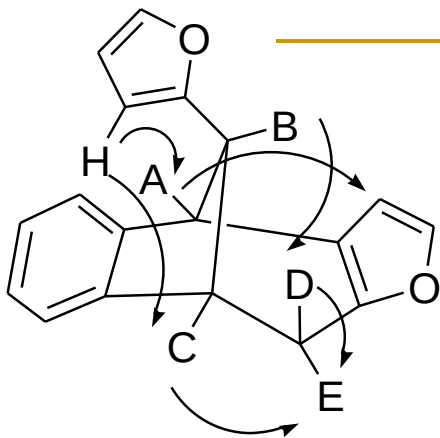


- HETCOR spektar
4-metil-2-pentanola

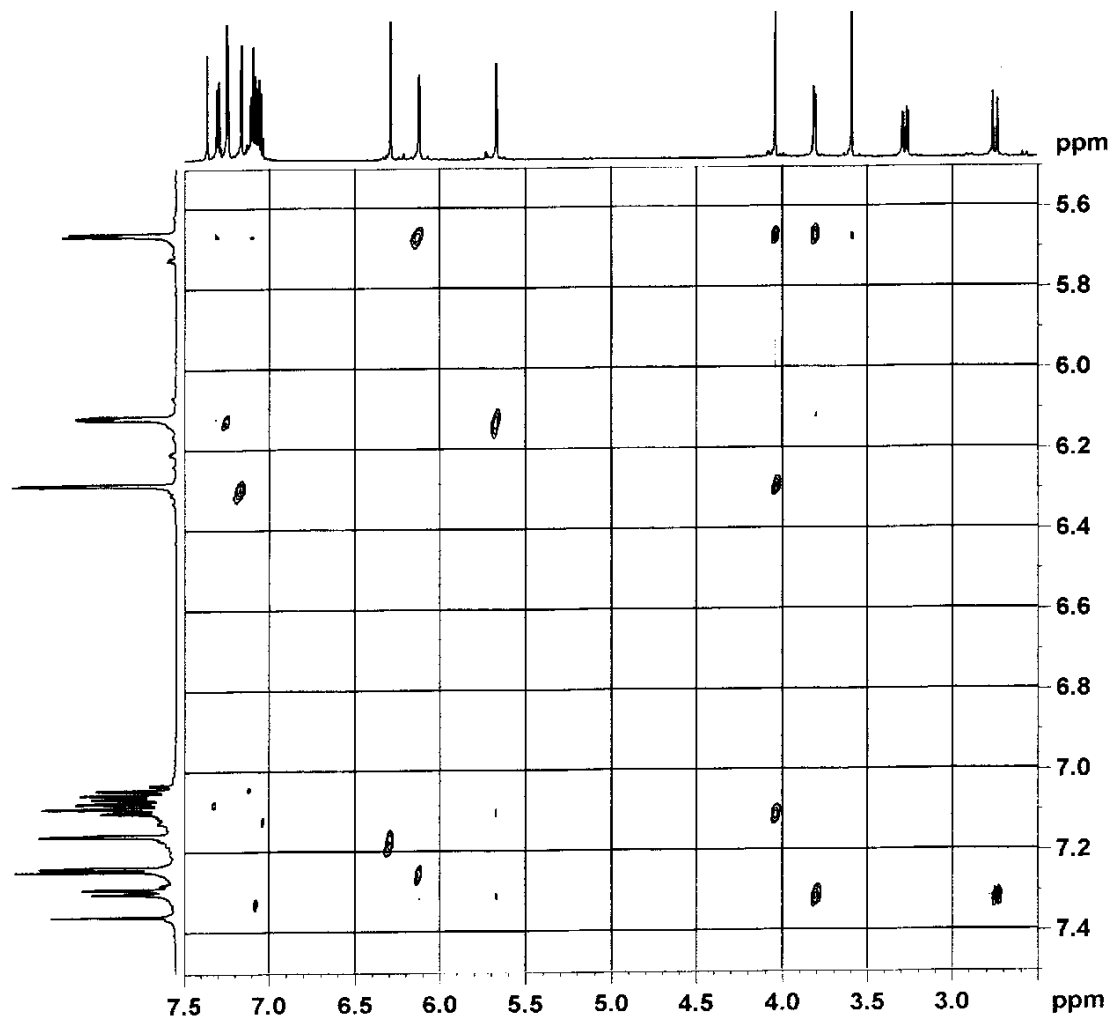
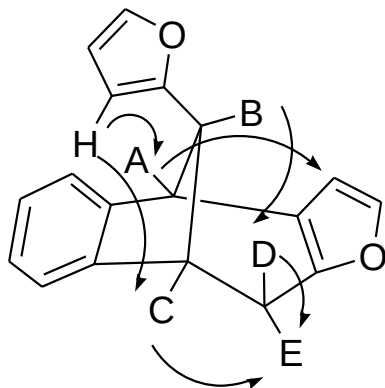


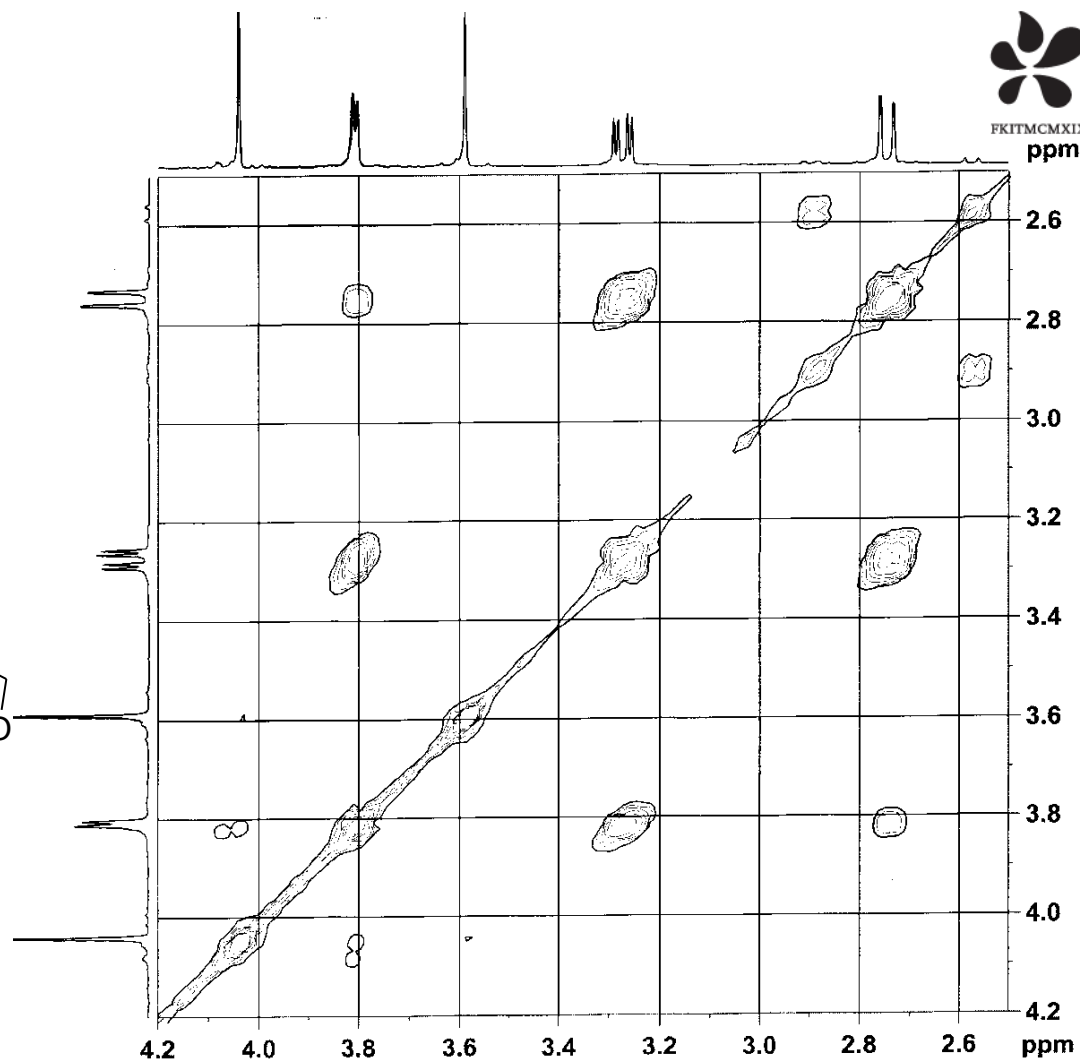
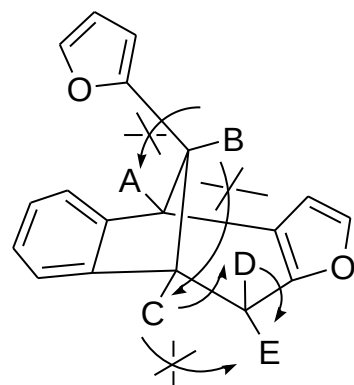
NOESY

(Nuclear Overhauser Effect Spectroscopy)



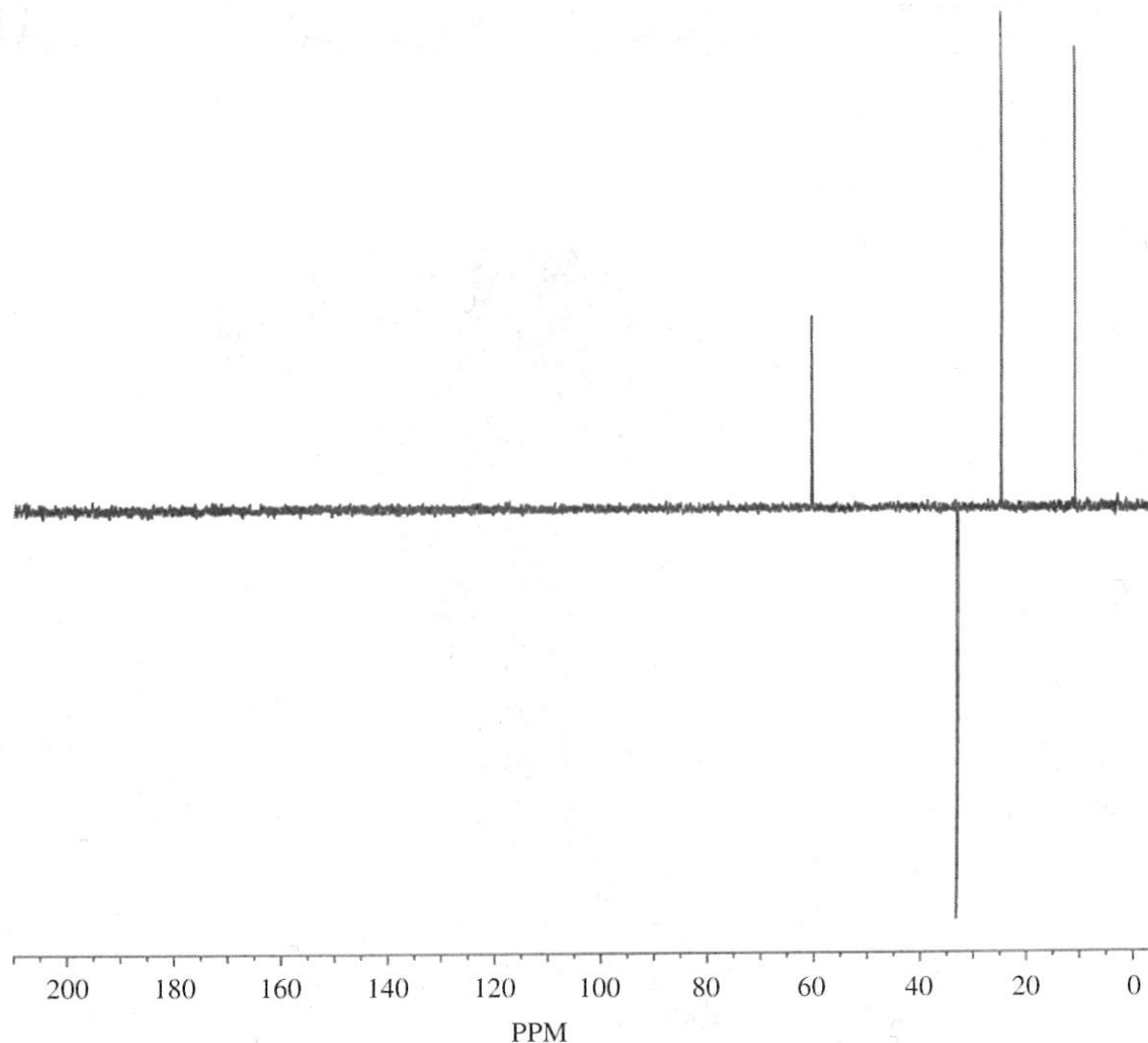
- NOE interakcije (lijevo) i **NOESY** spektar (desno) *exo*-biciklo[3.2.1]oktadienske strukture dobivene fotokemijskom [2+2]-cikloadicijom.

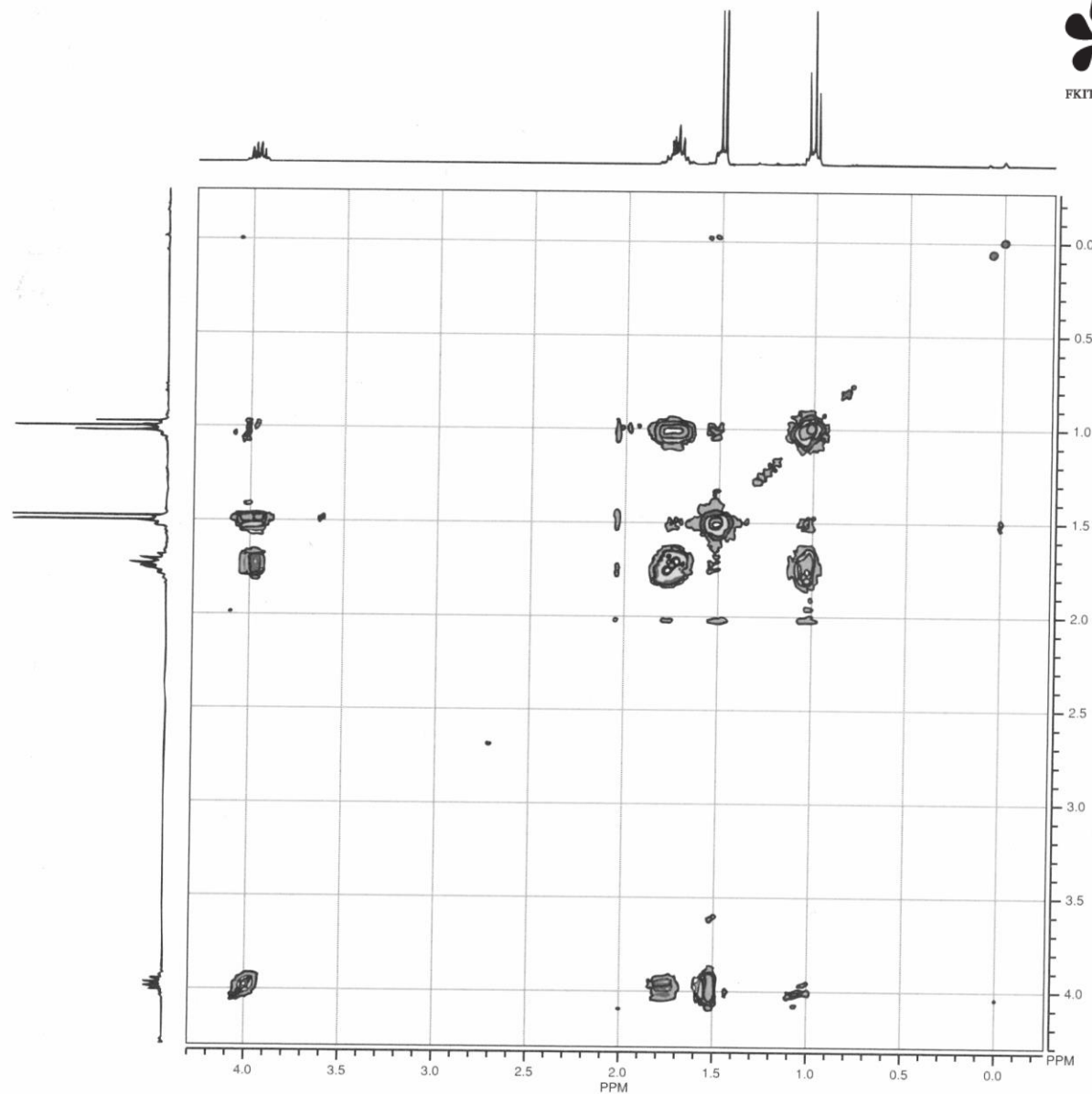


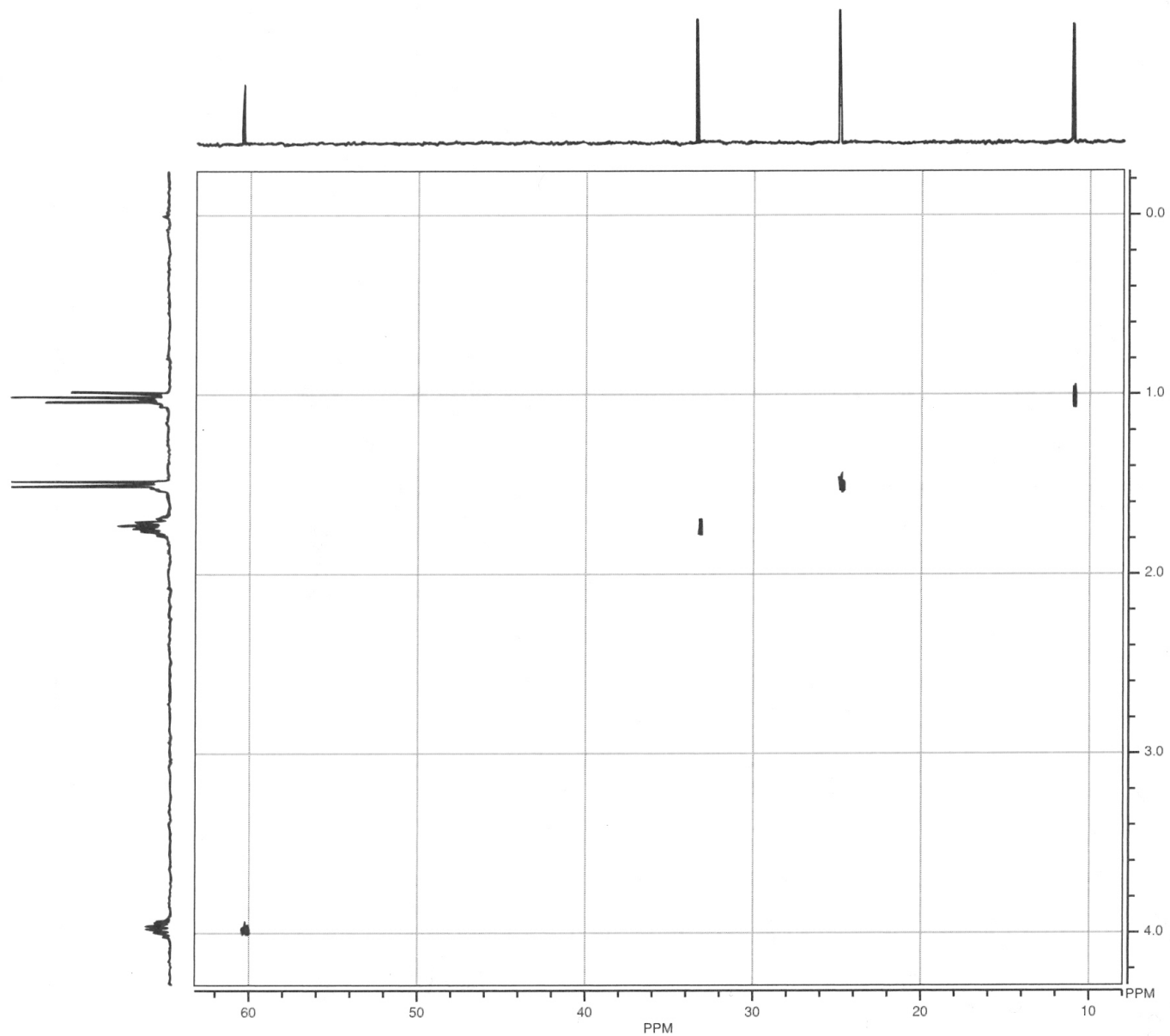


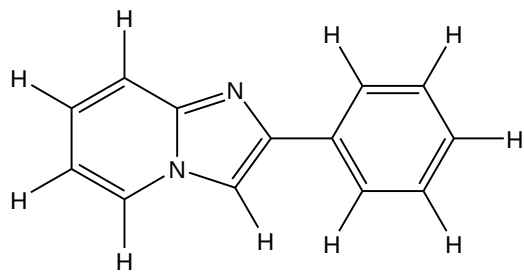
- Ključne interakcije (lijevo) i ***COSY*** spektar (desno) *exo*-biciklo[3.2.1]oktadienske strukture.

- **Zadatak.** Na osnovu DEPT-tehnike, COSY i HETCOR spektra u potpunosti asignirajte protone i ugljike za spoj bruto formule C_4H_9Cl i predložite strukturu spoja.

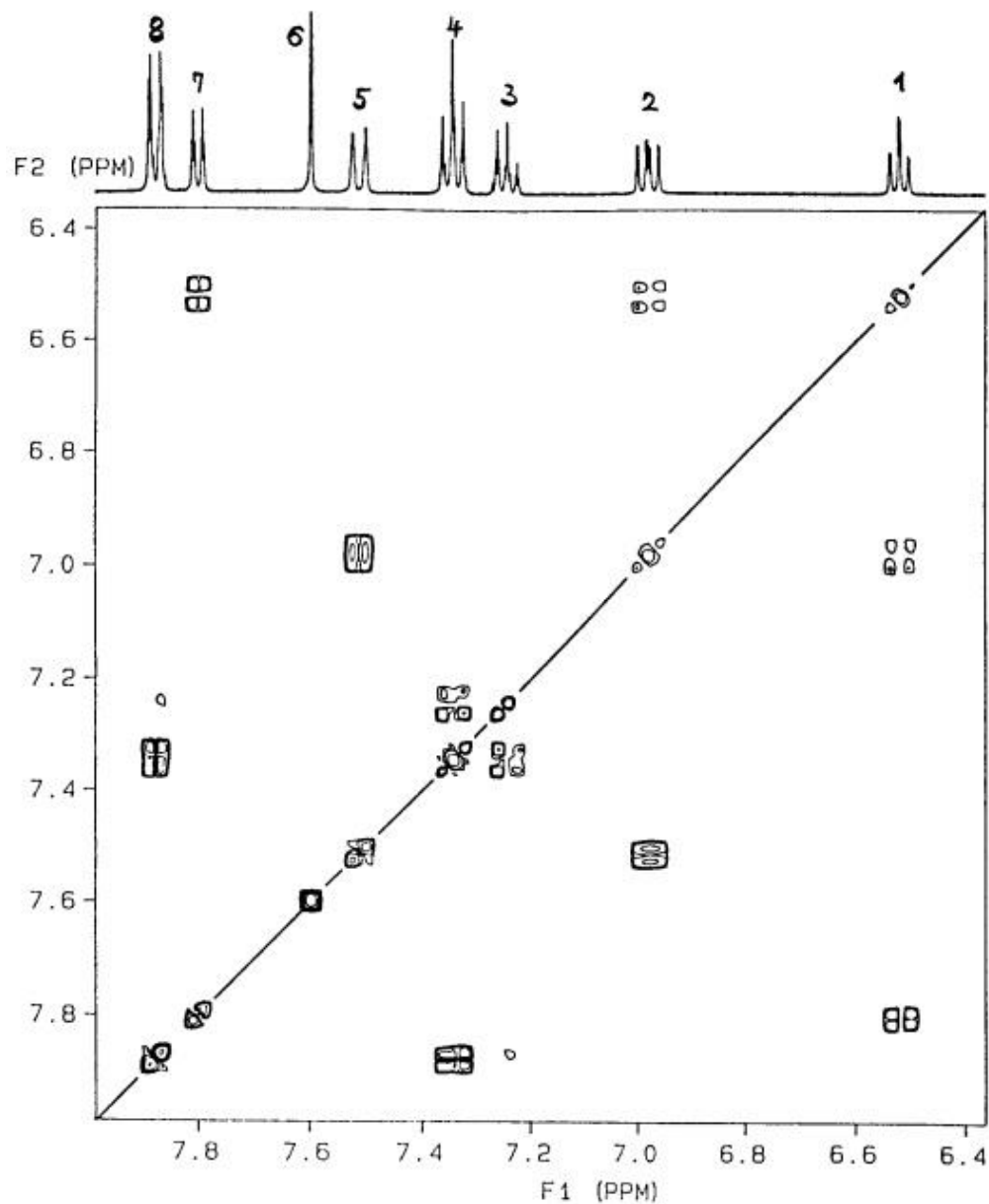


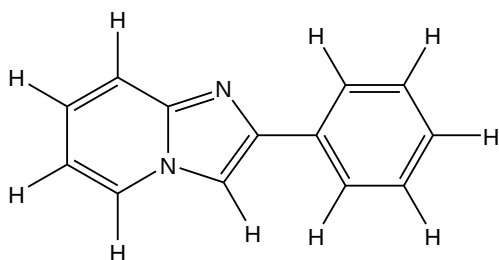




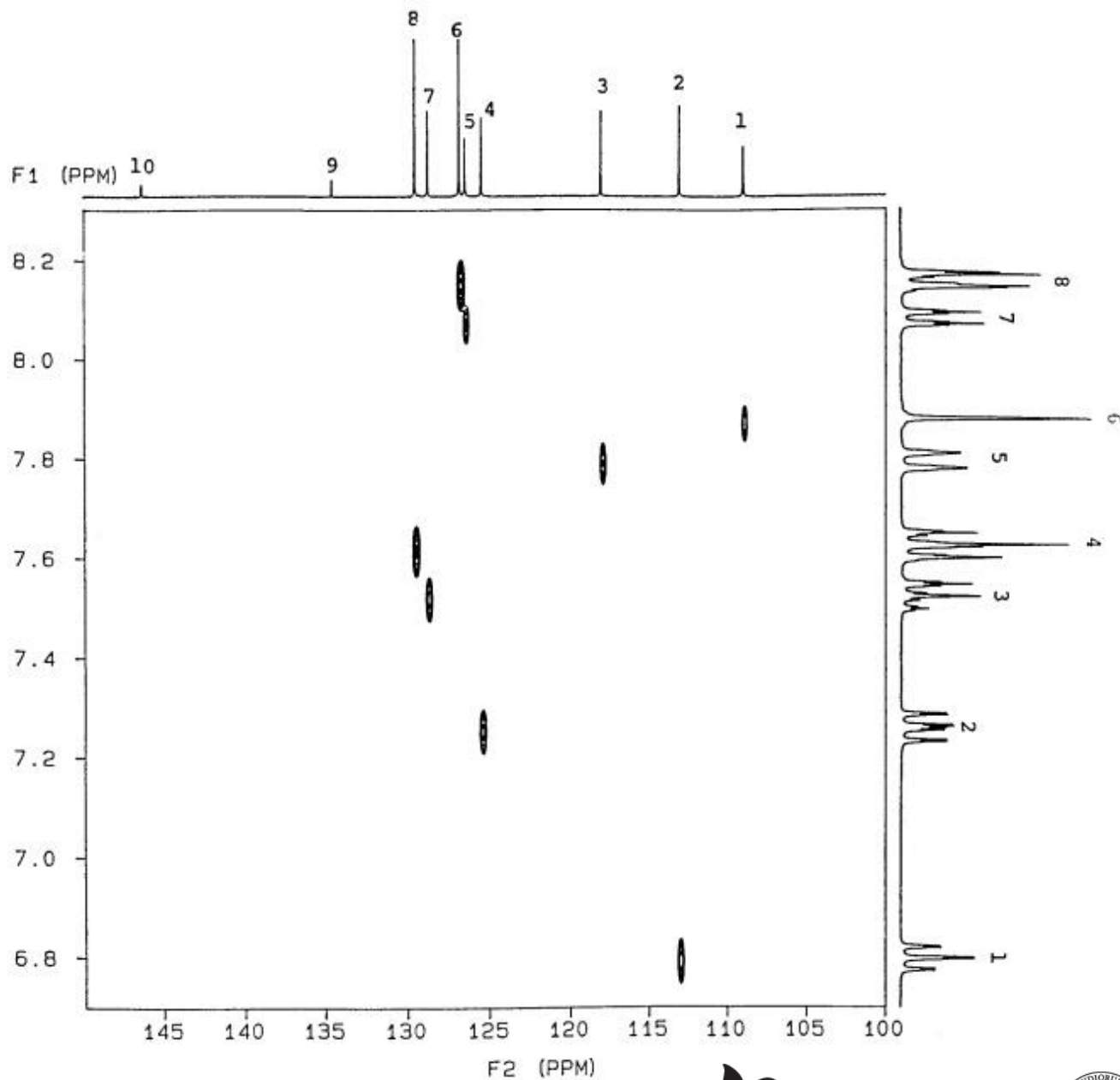


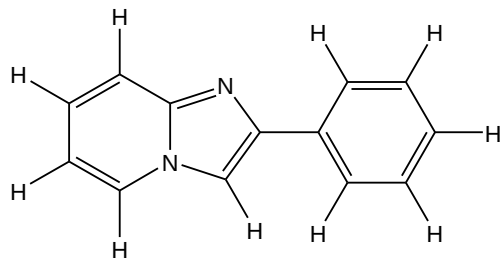
$^1\text{H} - ^1\text{H}$ COSY spektar



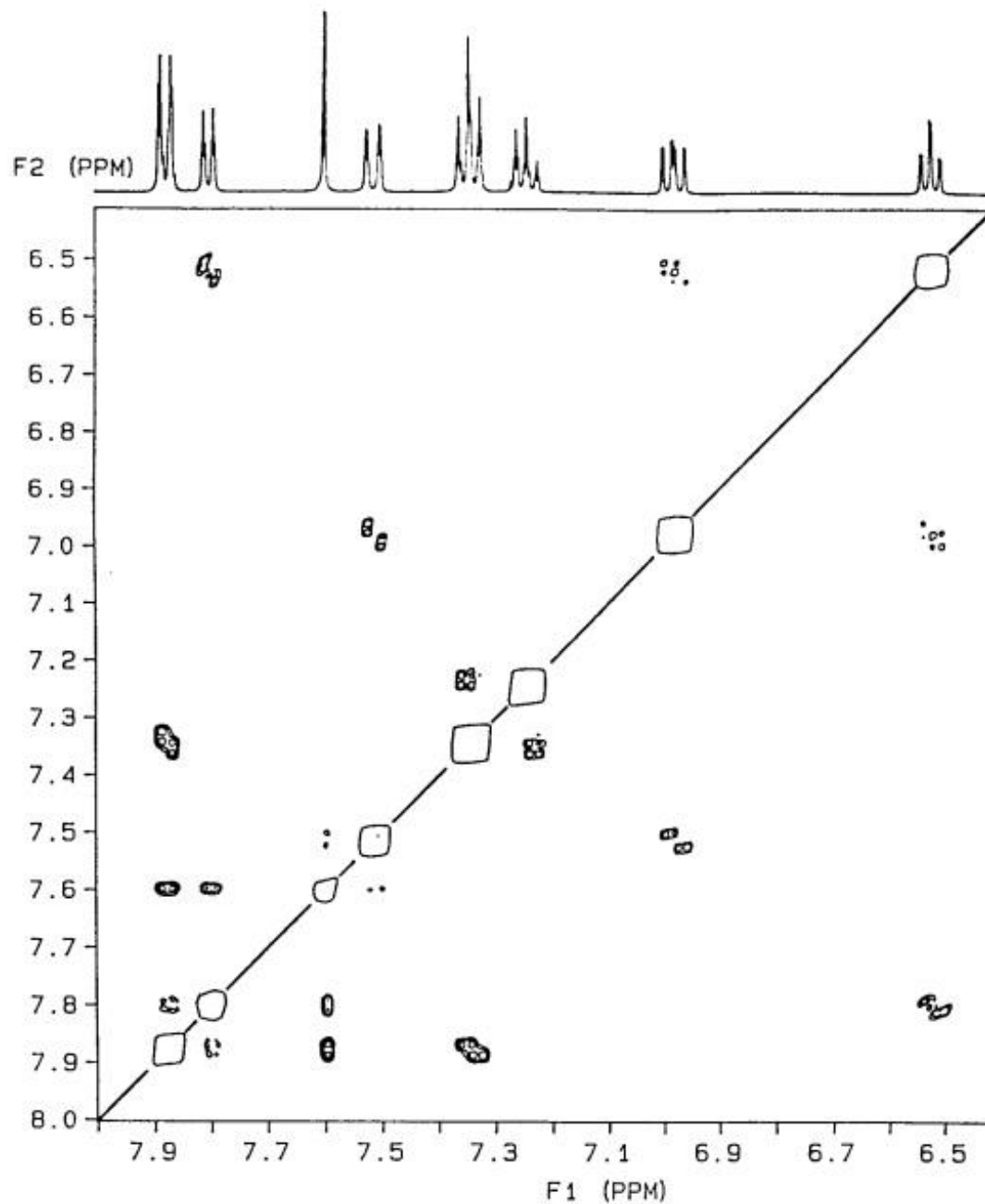


$^1\text{H} - ^{13}\text{C}$ COSY spektar
(HETCOR)





$^1\text{H} - ^1\text{H}$ NOESY spektar



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$^1\text{H} - ^1\text{H}$ COSY spektar:

H 1 --- 2, 7
 2 --- 1, 5
 3 --- 4, 8 (slabo)
 4 --- 3, 8
 5 --- 2
 6 --- -
 7 --- 1
 8 --- 4, 3 (slabo)

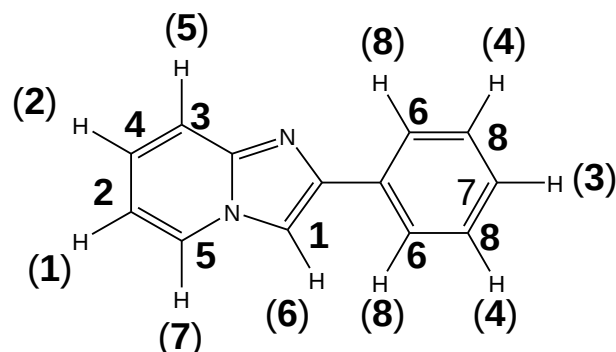
$^1\text{H} - ^{13}\text{C}$ COSY spektar
 (HETCOR):

H	C
1	2
2	4
3	7
4	8
5	3
6	1
7	5
8	6

$^1\text{H} - ^1\text{H}$ NOESY spektar:

H 1 --- 2, 7
 2 --- 1, 5
 3 --- 4
 4 --- 3, 8
 5 --- 2, 6 (slabo)
 6 --- 5, 7, 8
 7 --- 1, 6, 8
 8 --- 4, 6, 7

Asignacija strukture:



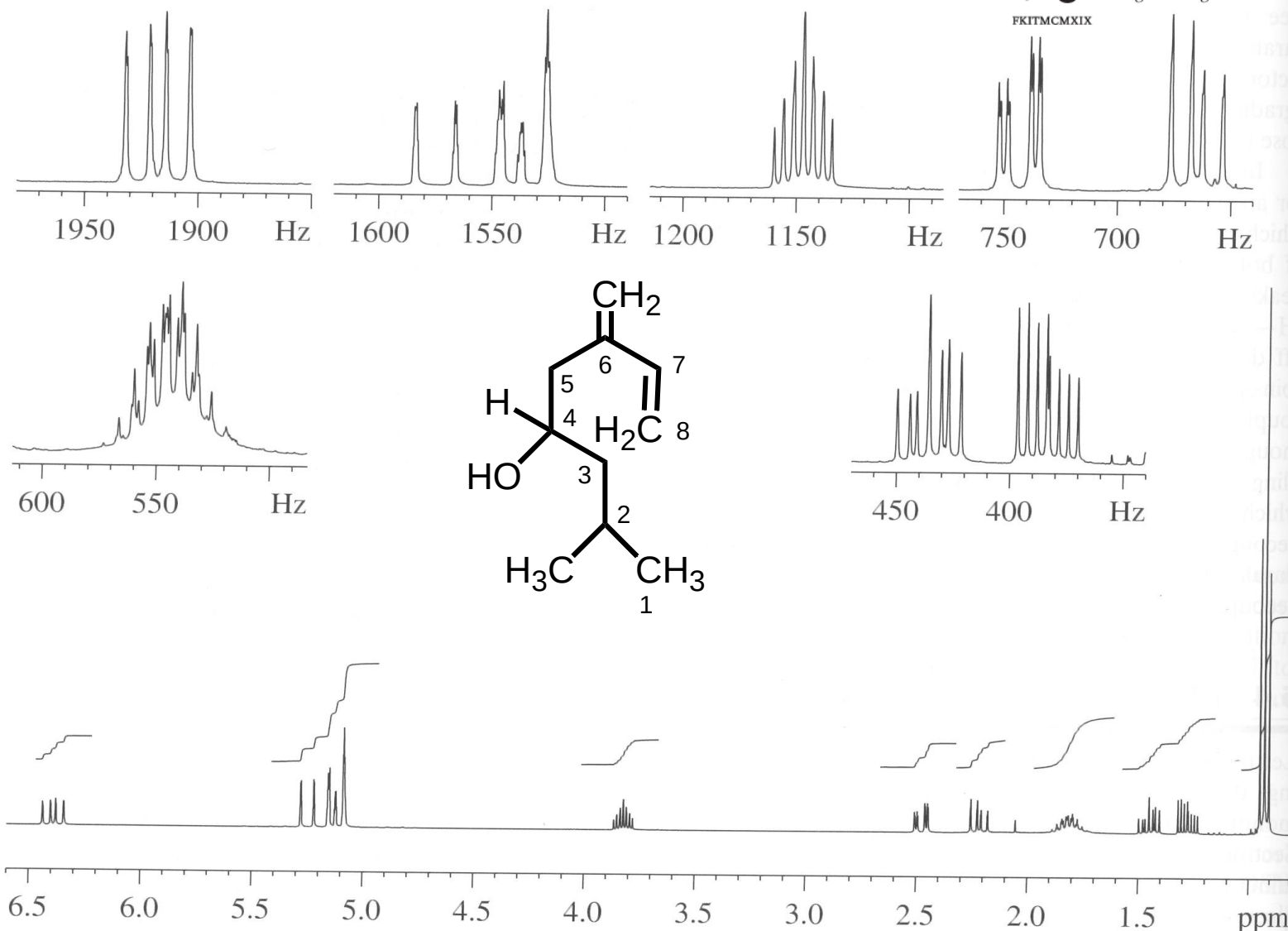
^1H NMR 300 MHz



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■ ^1H NMR spektar **ipsenola**

■ ^{13}C NMR (a) i DEPT (b) spektar ipsenola



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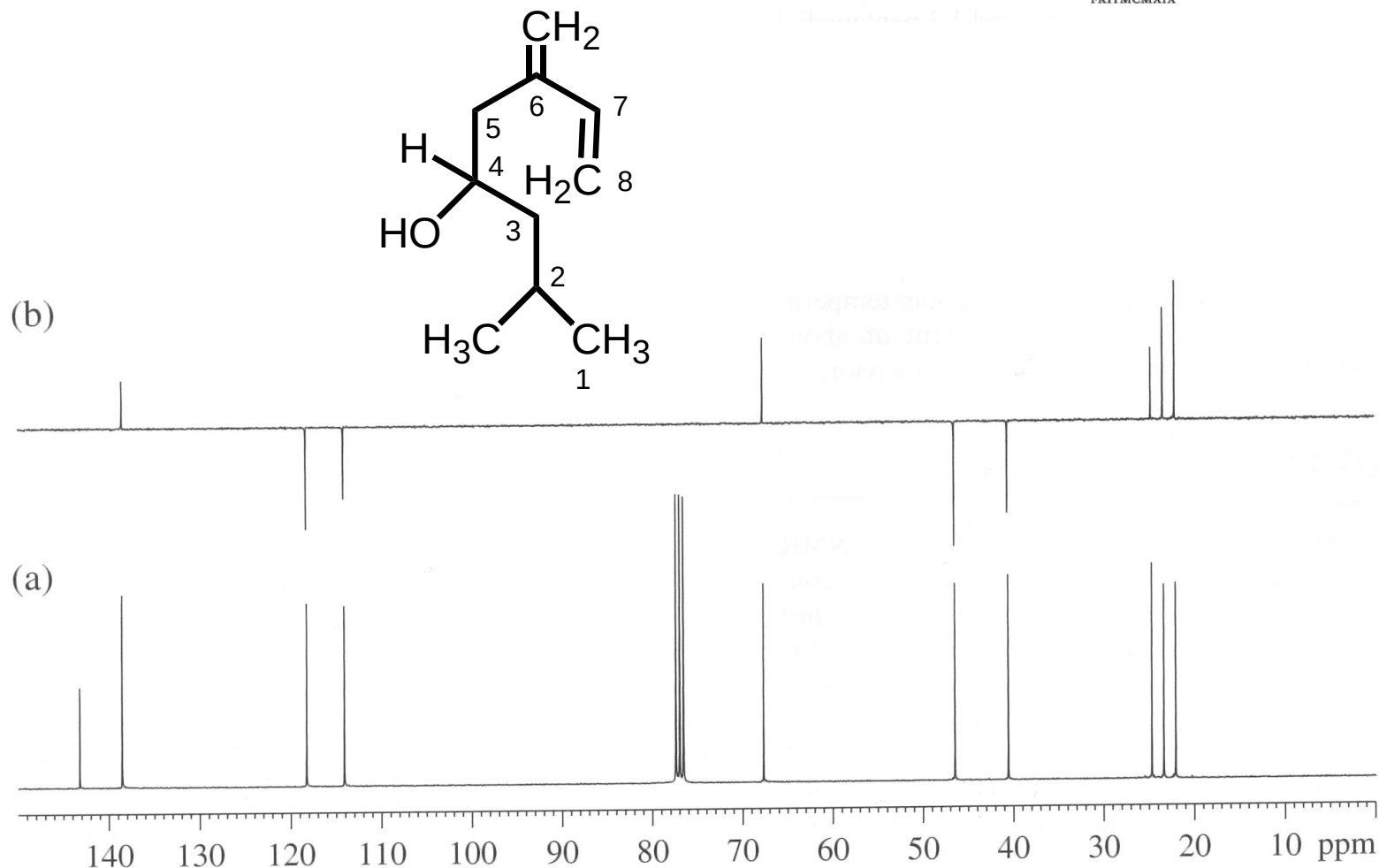
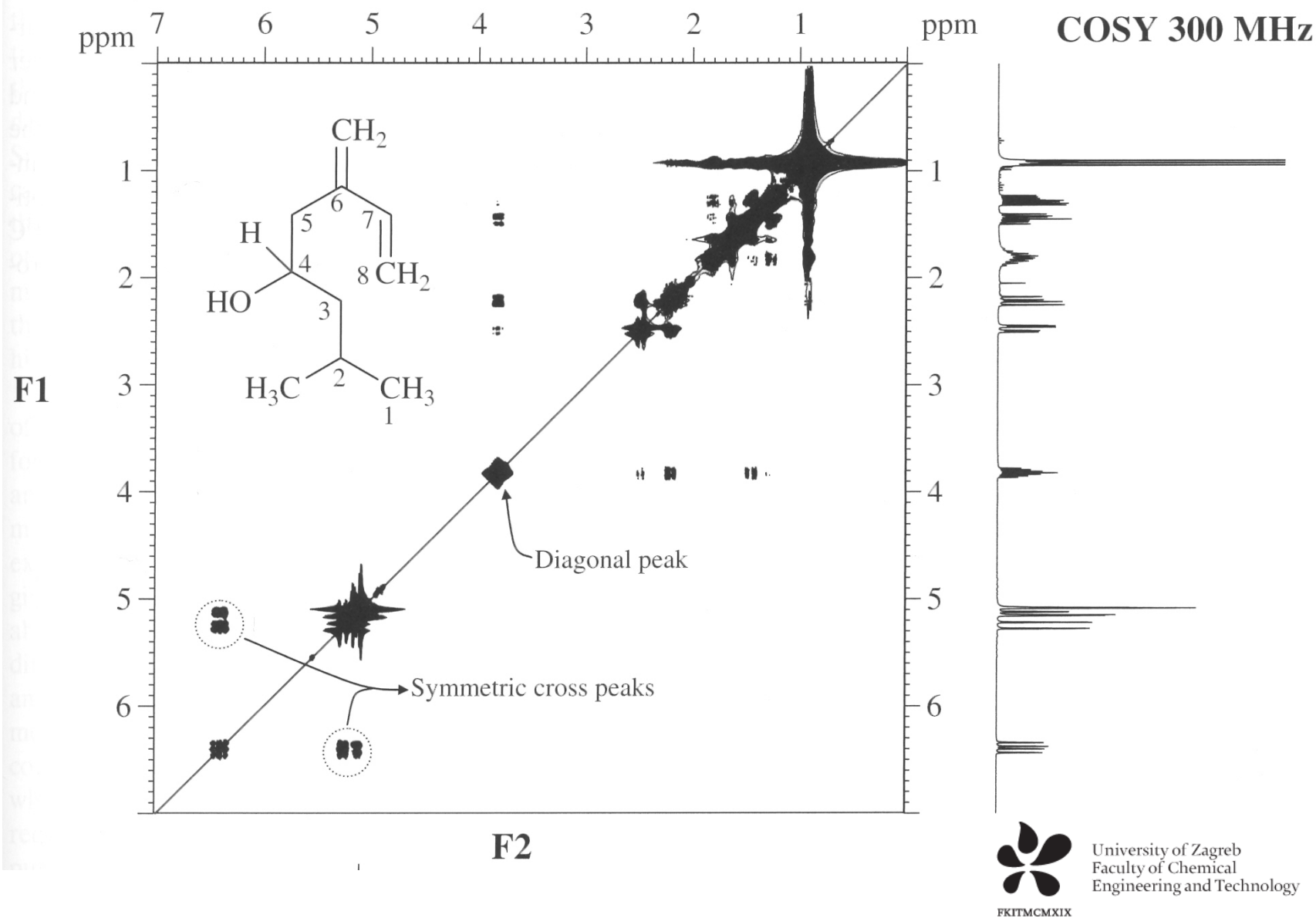


FIGURE 4.12 (a) Standard ^{13}C decoupled spectrum of ipsenol in CDCl_3 at 75.5 MHz. (b) DEPT subspectra: DEPT 135° CH and CH_3 up, CH_2 down.

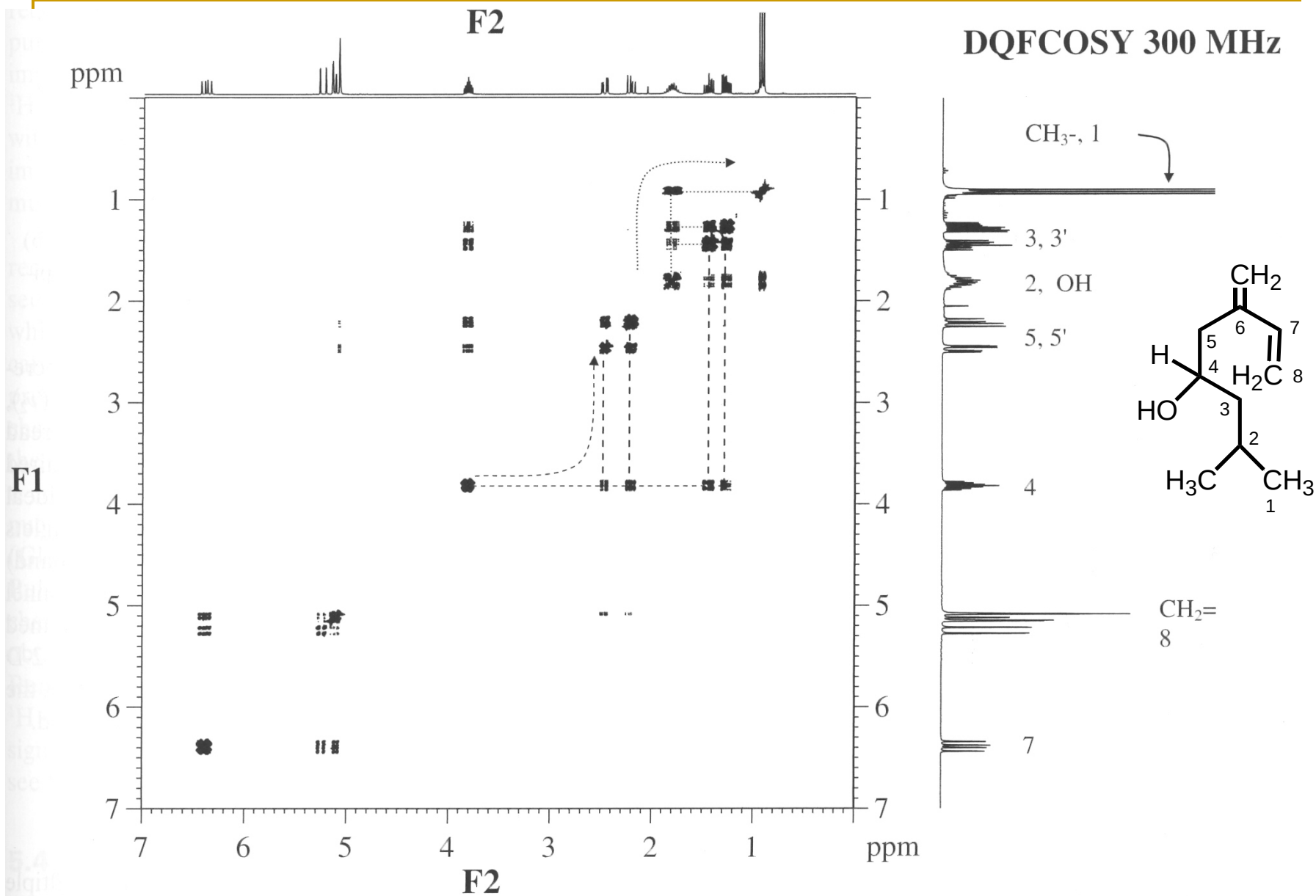


■ COSY spektar ipsenola

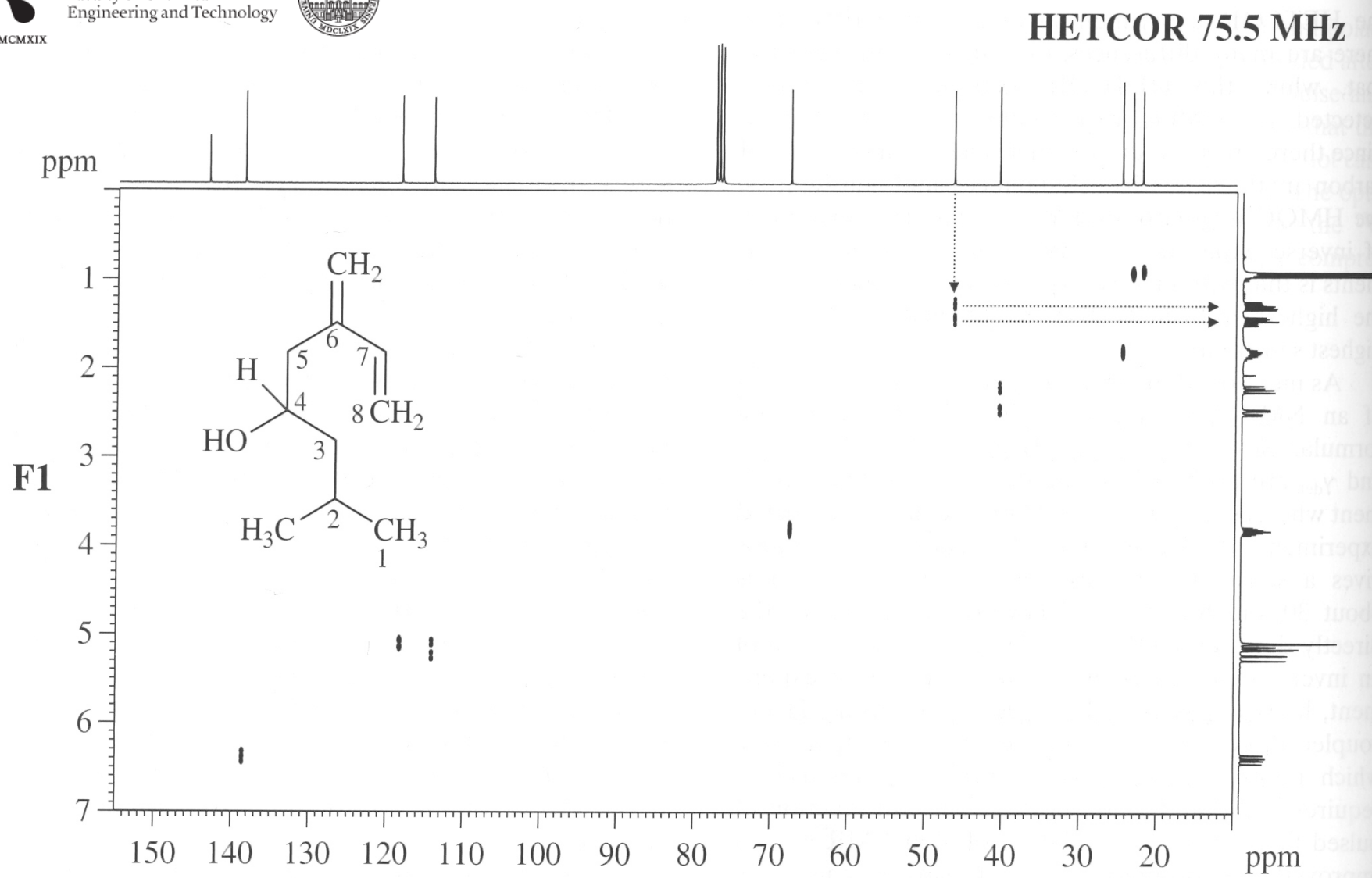


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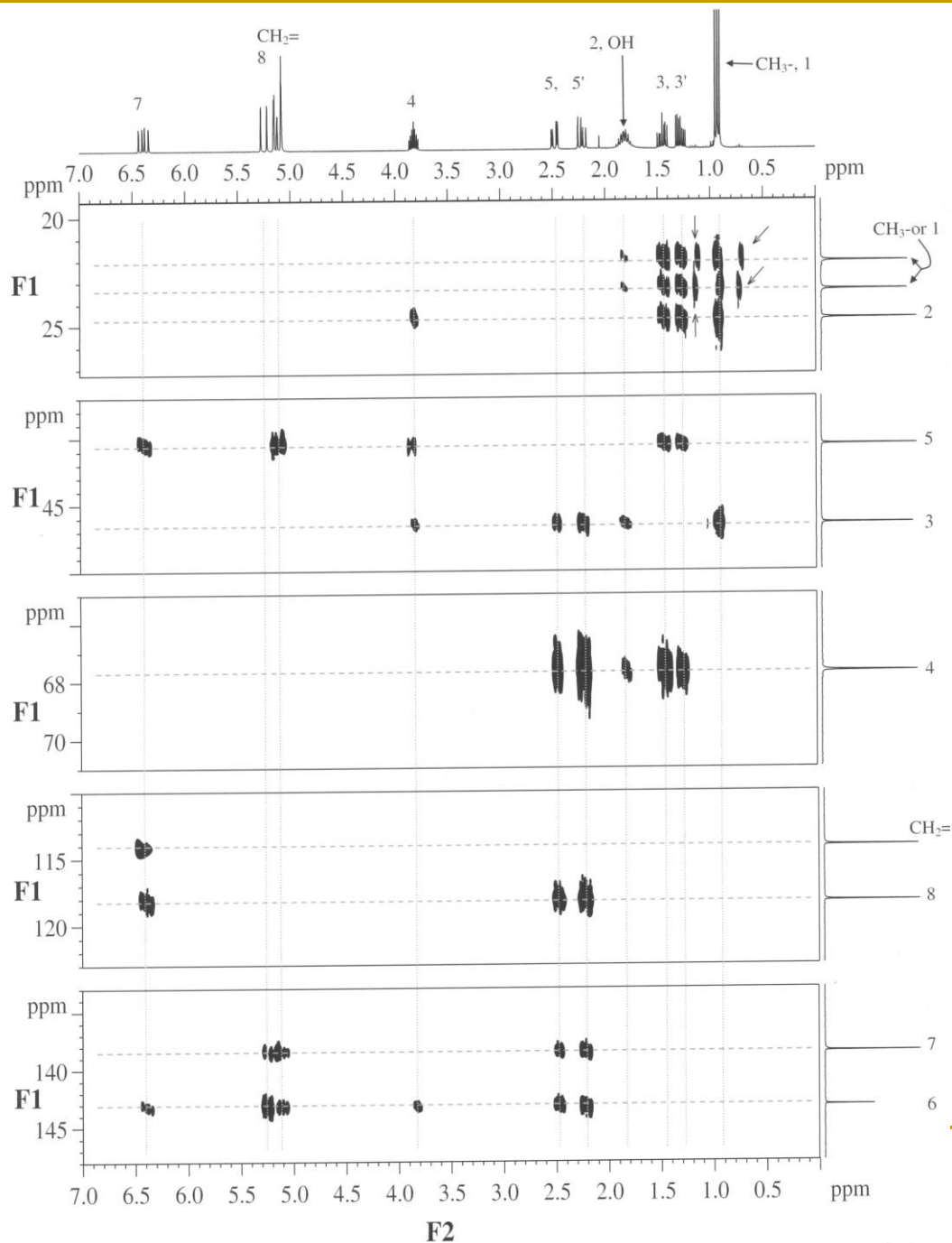


- Double Quantum Filtered (DQF) COSY spektar ipsenola



■ HETCOR spektar ipsenola

■ HMBC spektar ipsenola

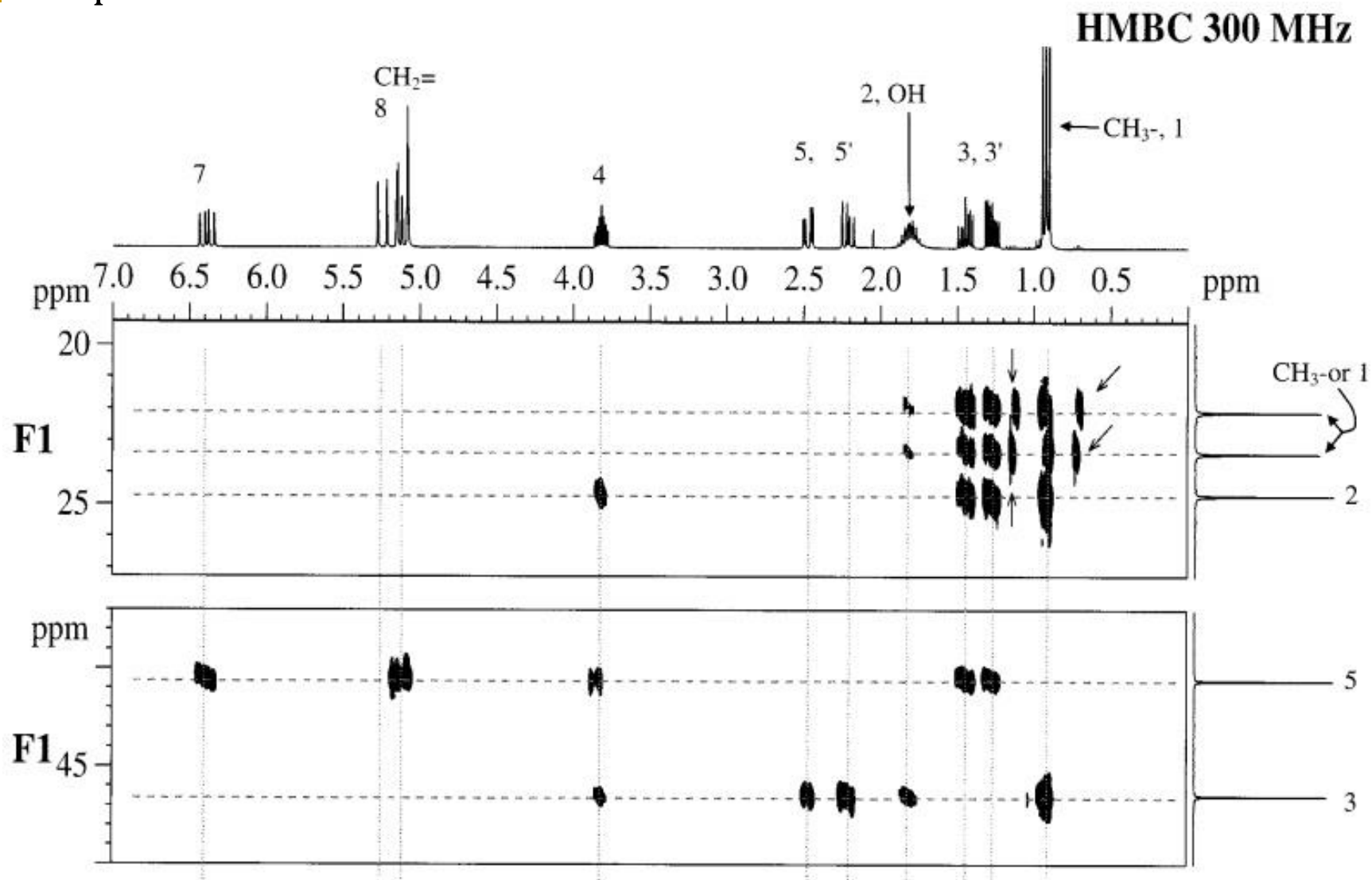


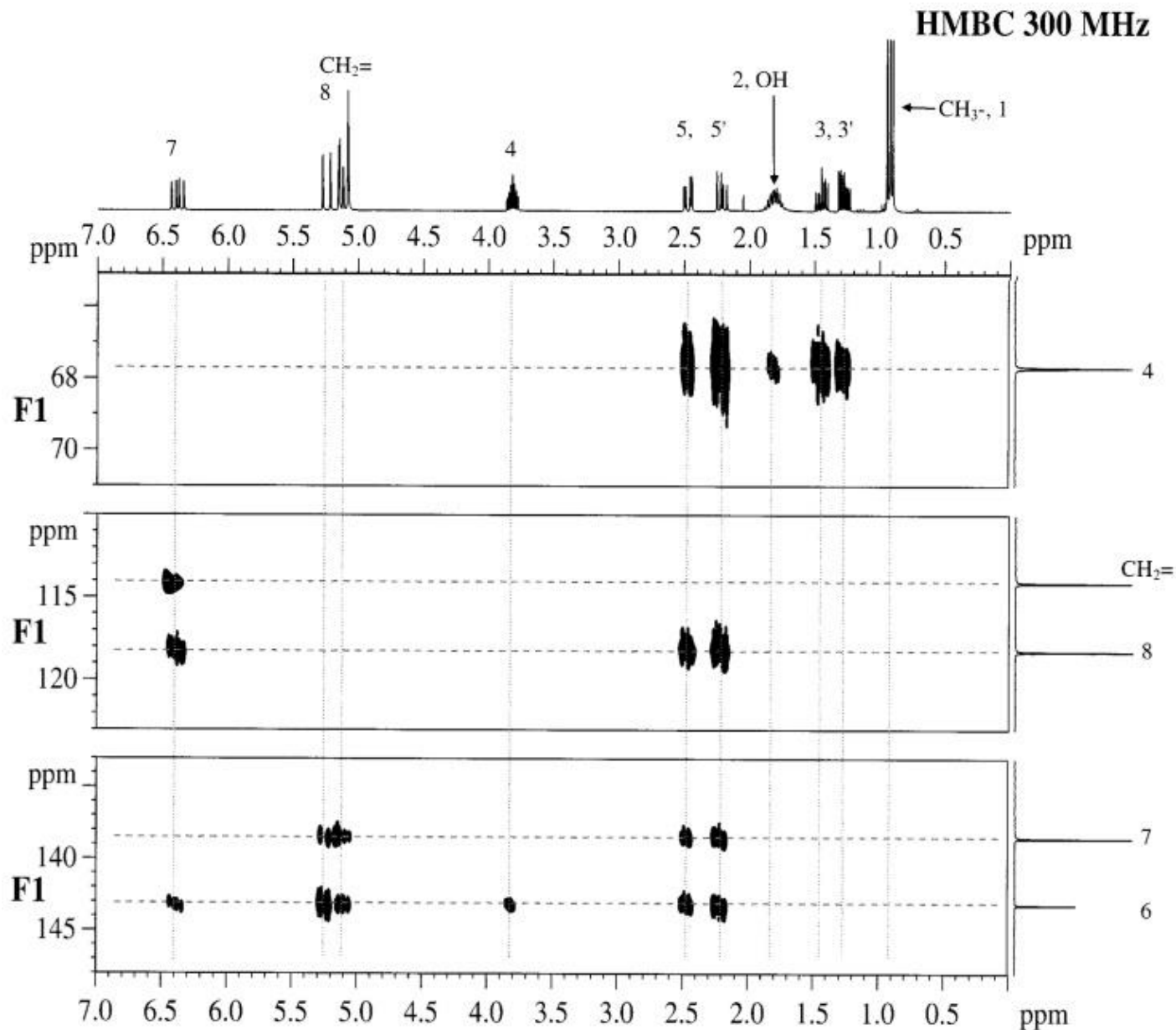
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- HMBC spektar ipsenola





■ **IPSENOL** (nastavak HMBC spektra)