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ULisboa

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Centro
de Química
e Bioquímica

U LISBOA

UNIVERSIDADE
DE LISBOA

Mestrado em Química, Métodos Avançados de Análise 2017/2018

Bloco de Ressonância Magnética Nuclear

Exercícios TP, Novembro 2017

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Gab 8.5.49, Lab 8.5.55

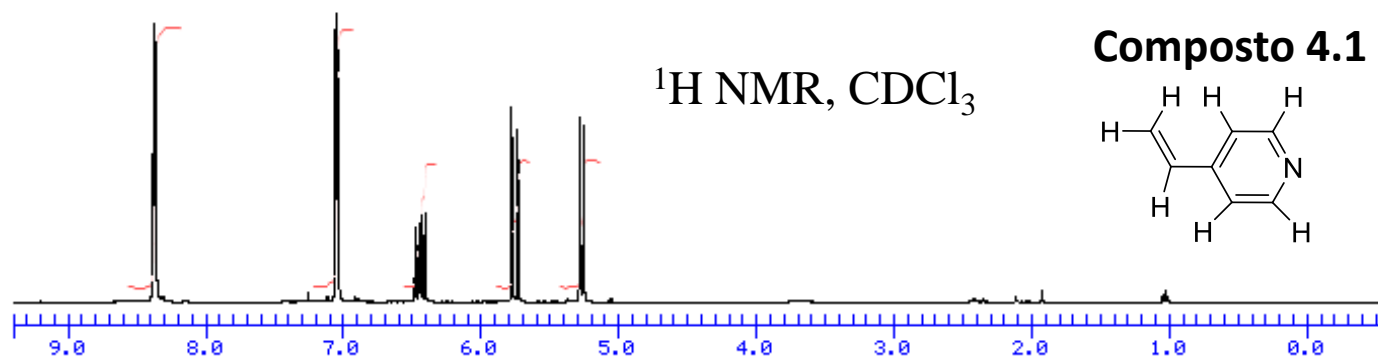
1- Quais dos seguintes núcleos são activos em RMN? Justifique

Nucleus	Yes/No
$^{17}\text{O}_8$	
$^{19}\text{F}_9$	
$^{16}\text{O}_8$	
$^{14}\text{N}_7$	

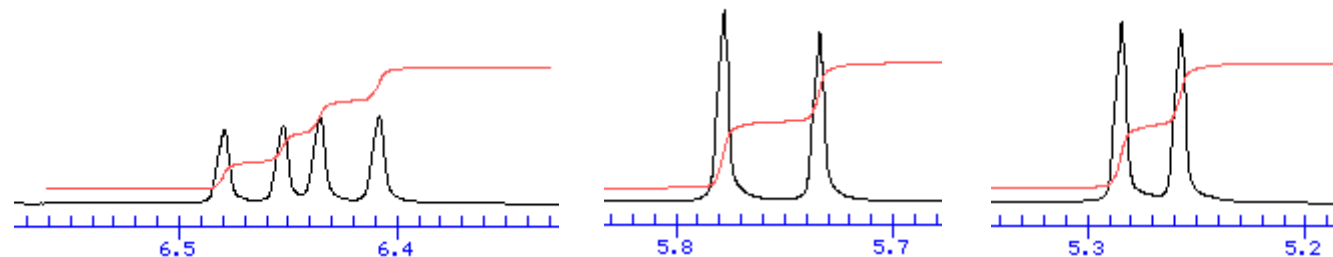
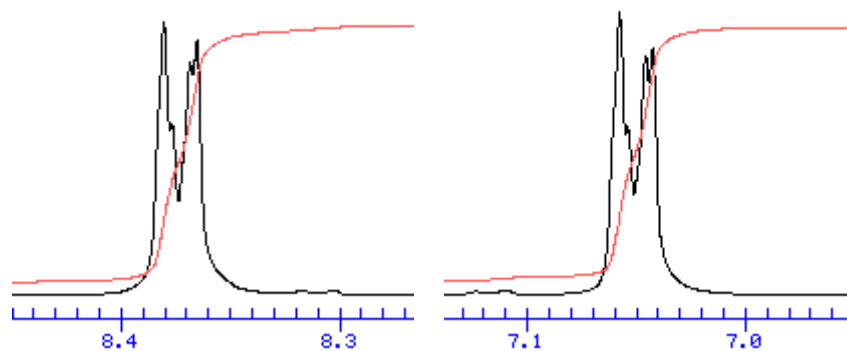
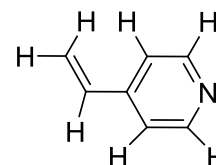
2- Preencha a seguinte tabela (360 MHz for ^1H):

Proton	ν [Hz]	δ [ppm]
R-CH ₂ -R	468	
C ₆ H ₅ -H	2620	
R-CH ₂ -Cl		3.7
R-CHO		9.5

4- Atribuir os sinais dos H dos seguintes compostos:
 (apresente os sinais na forma δ 2.95, 1H, d, J=2Hz)

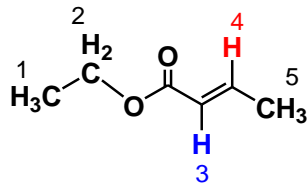


Composto 4.1

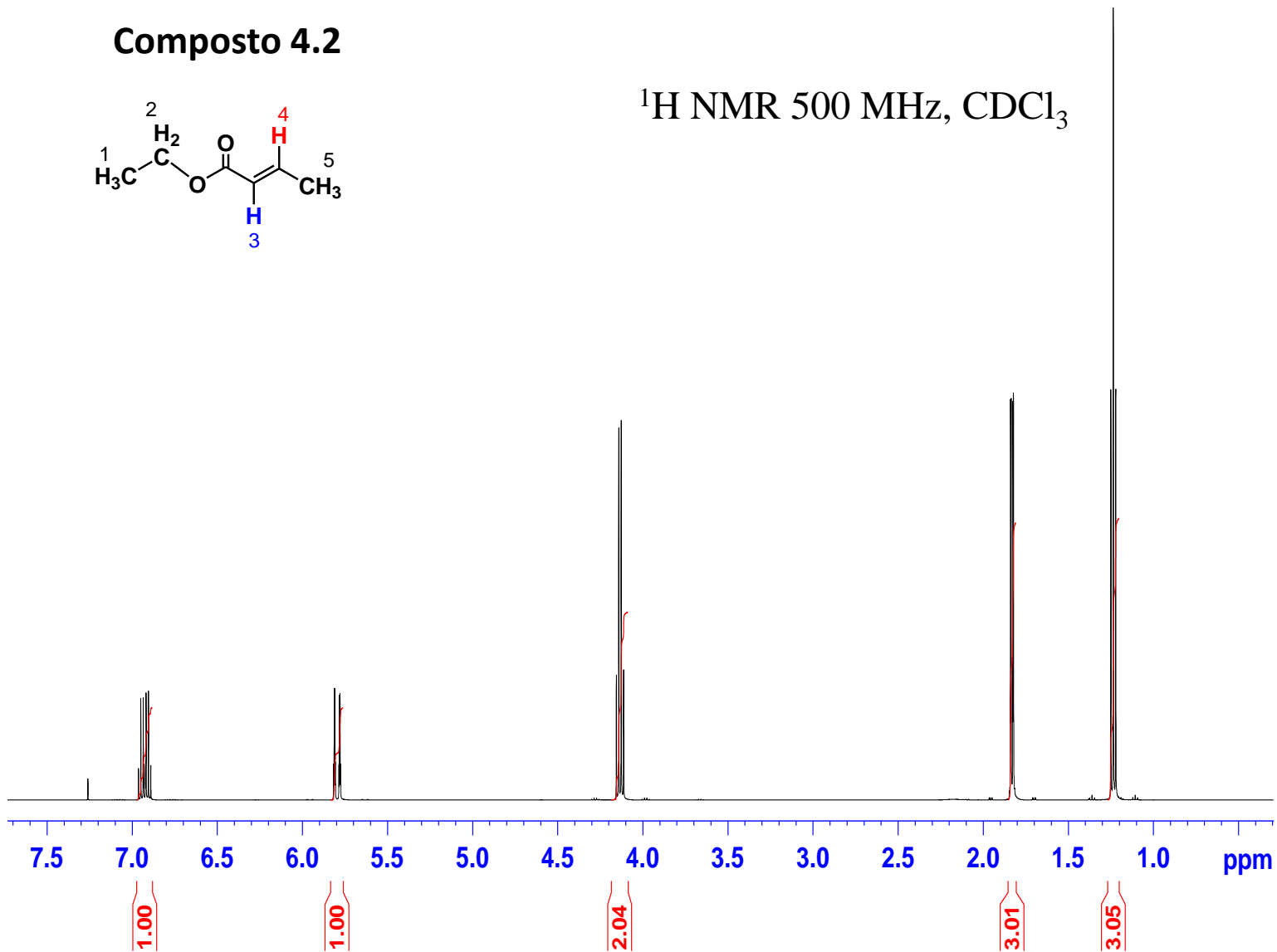


Peak	
ppm	Hz
8.3809	3353.45
8.3689	3348.65
7.0583	2824.24
7.0461	2819.36
6.4796	2592.68
6.4525	2581.84
6.4356	2575.08
6.4085	2564.23
5.7782	2312.03
5.7343	2294.47
5.2844	2114.45
5.2572	2103.56

Composto 4.2

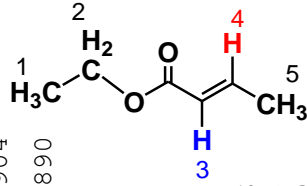


^1H NMR 500 MHz, CDCl_3



Composto 4.2 ¹H NMR -Expansões

500 MHz, CDCl₃



— 6.963
— 6.949
— 6.935
— 6.932
— 6.922
— 6.918
— 6.904
— 6.890

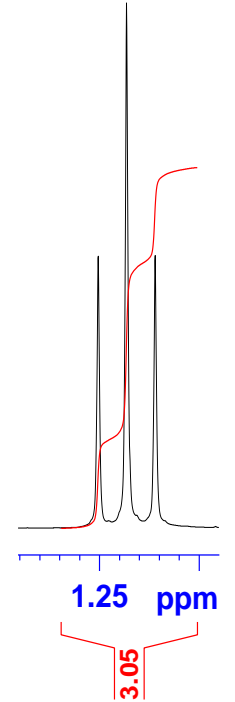
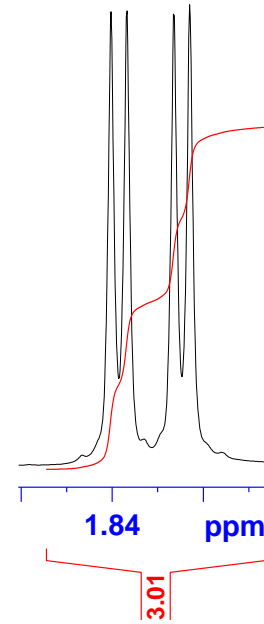
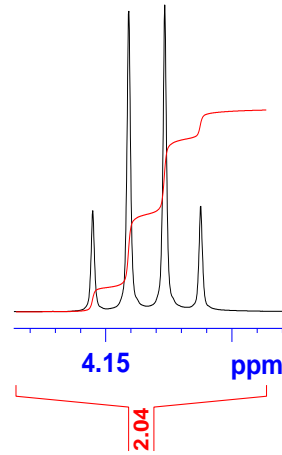
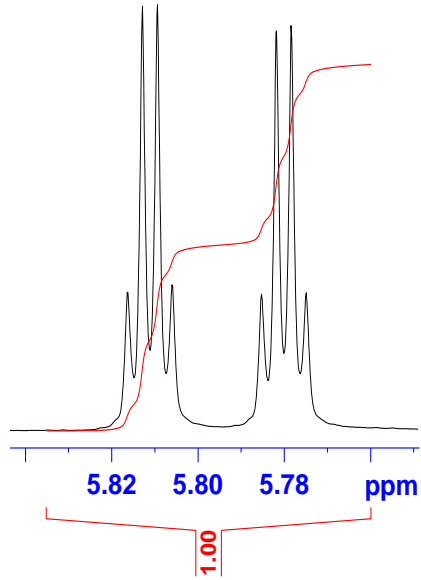
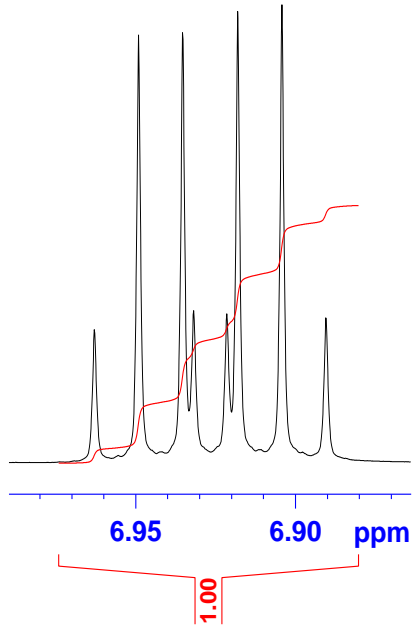
— 5.816
— 5.813
— 5.809
— 5.806

— 5.785
— 5.782
— 5.778
— 5.775

— 4.155
— 4.141
— 4.127
— 4.112

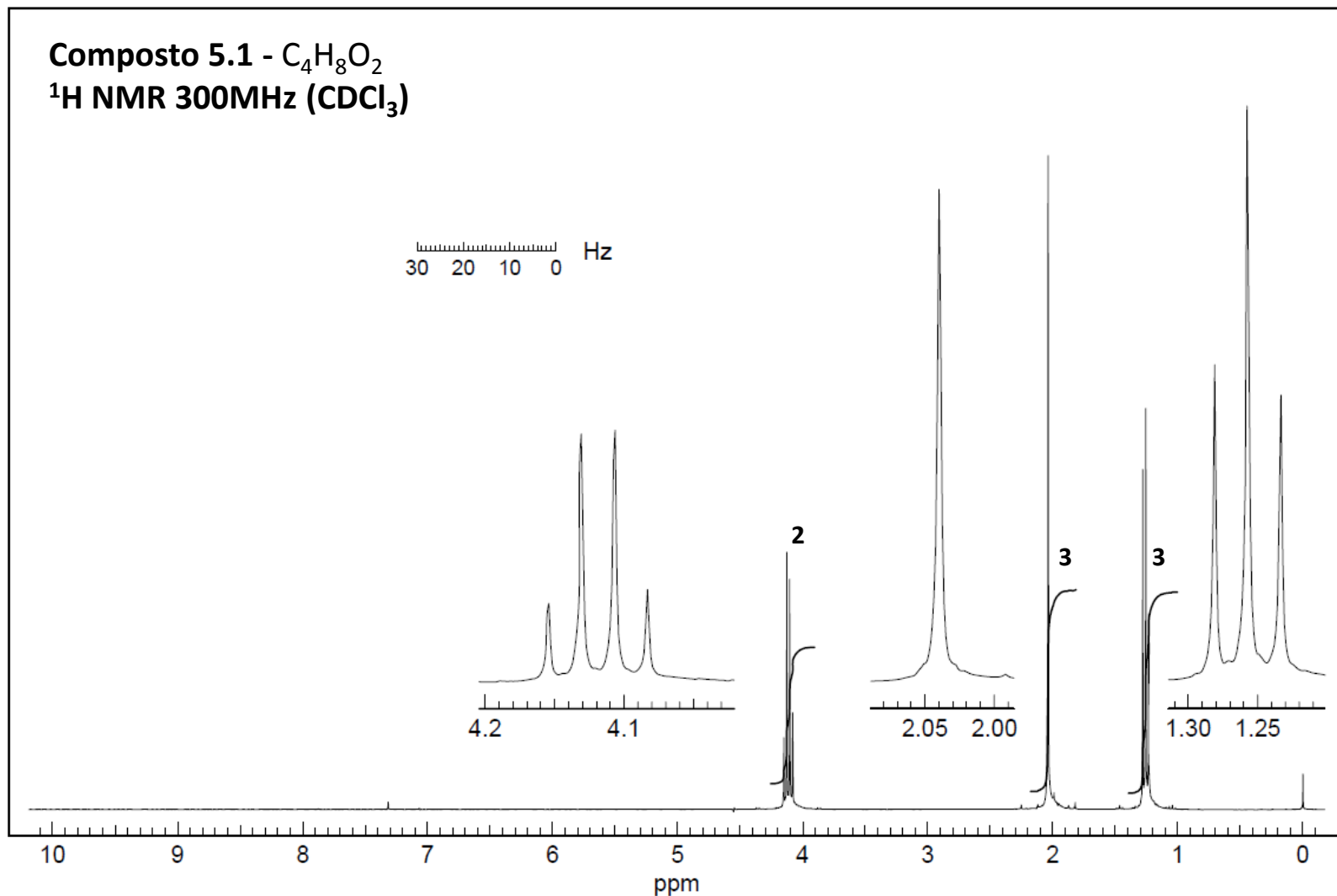
— 1.840
— 1.837
— 1.833
— 1.827
— 1.823

— 1.251
— 1.236
— 1.222

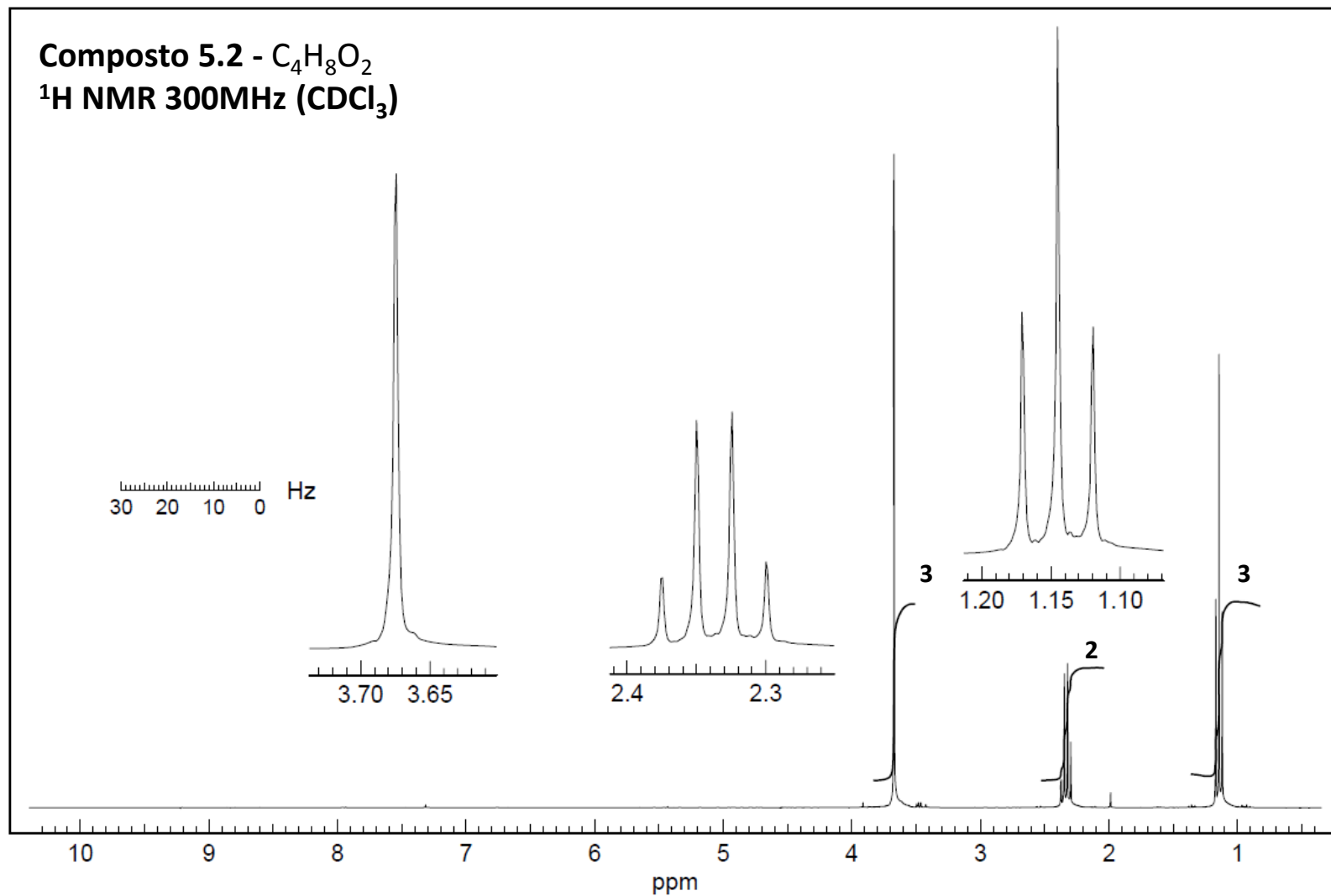


Spectrum from BRUKER topspin

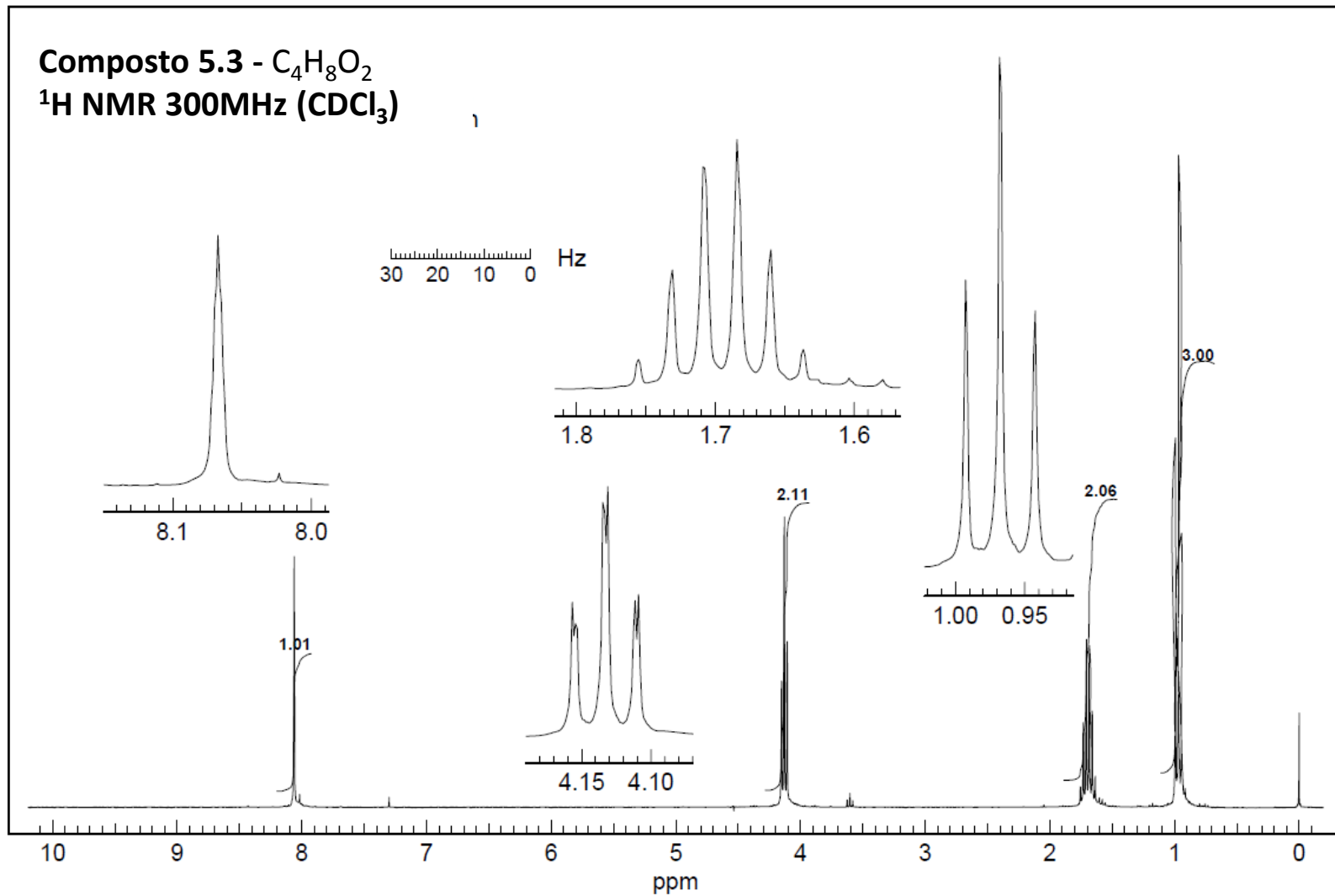
5- Determine a estrutura dos seguintes compostos a partir dos espectros de ^1H NMR.
 (sempre que possível apresente os sinais na forma δ 2.95, 1H, d, $J=2\text{Hz}$)



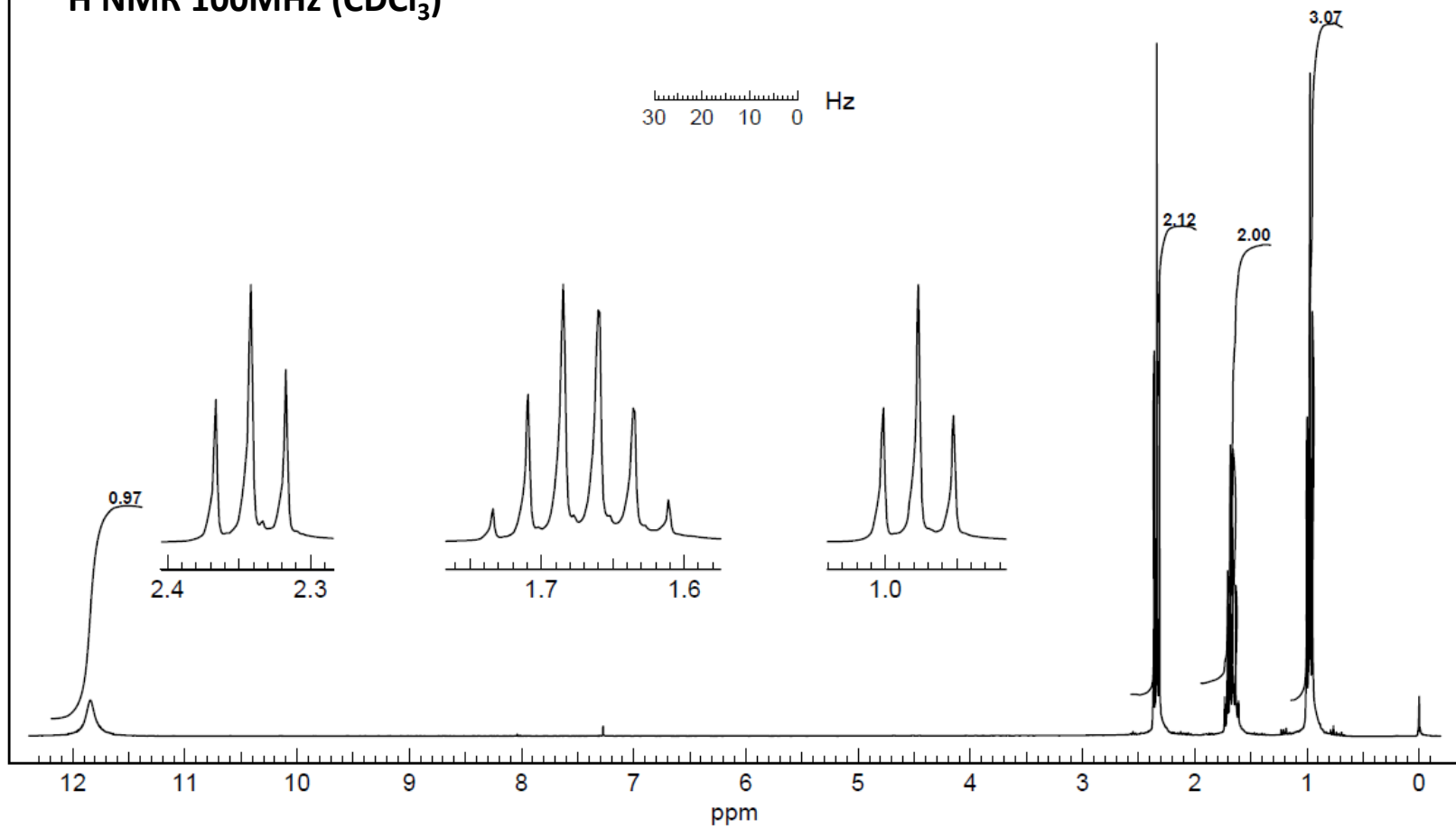
Composto 5.2 - C₄H₈O₂
¹H NMR 300MHz (CDCl₃)



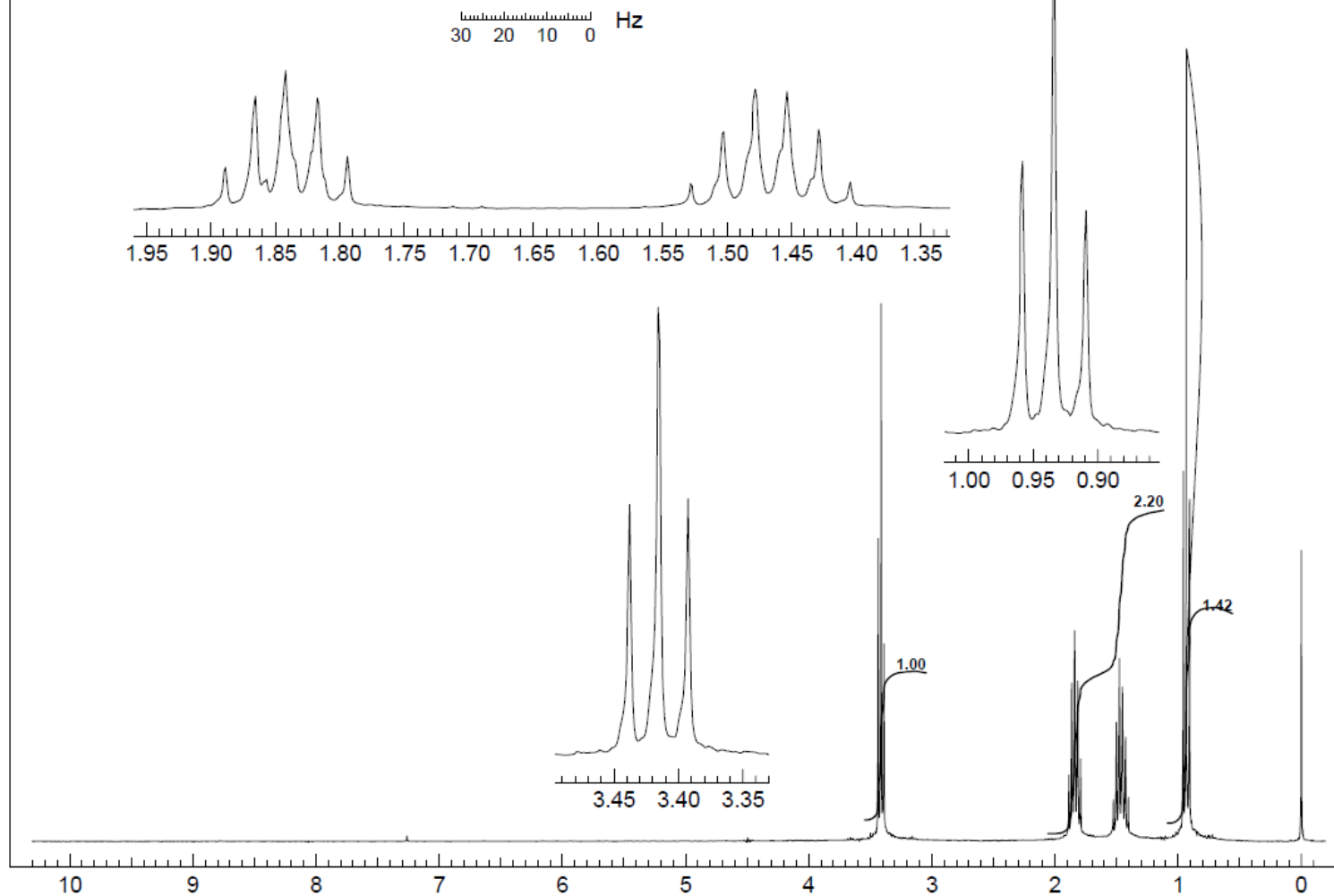
Composto 5.3 - C₄H₈O₂
¹H NMR 300MHz (CDCl₃)



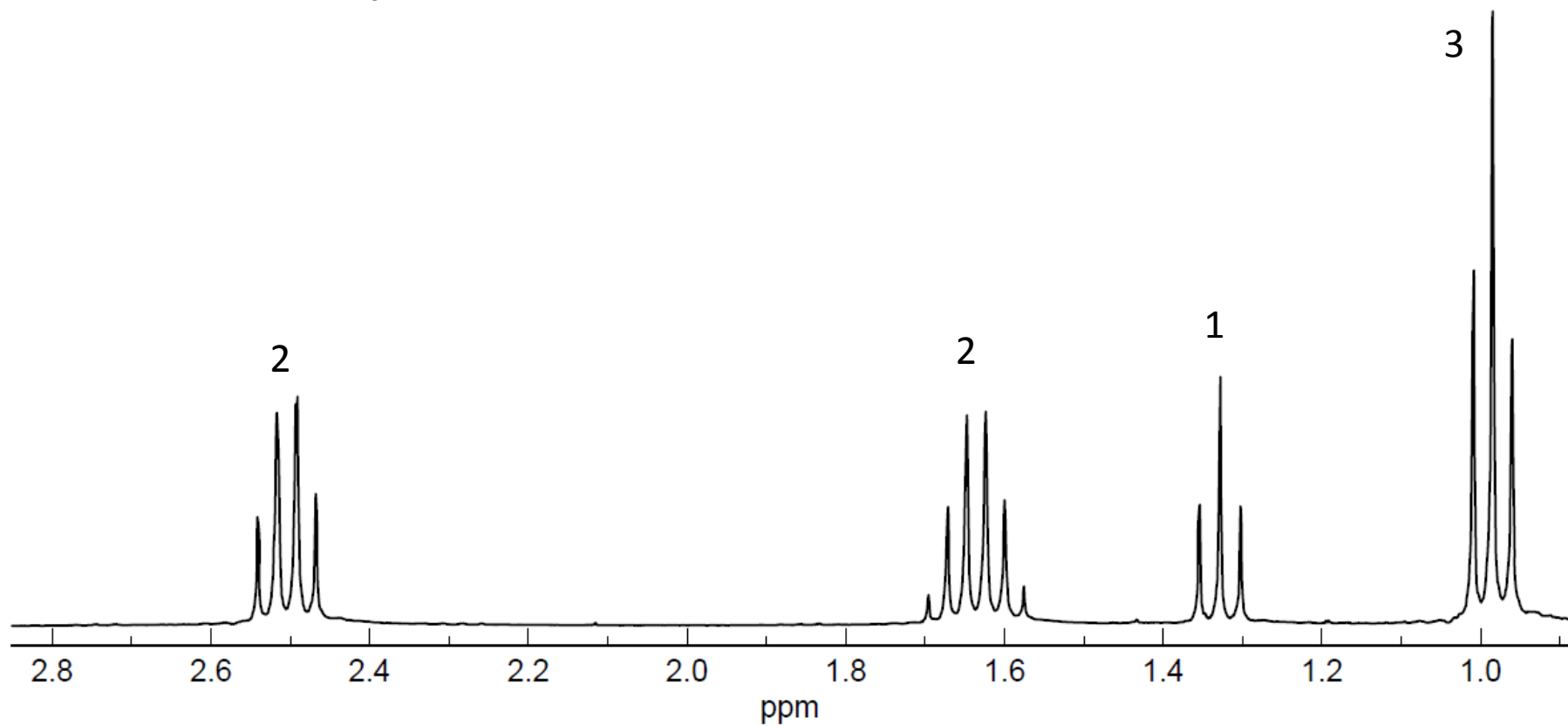
Composto 5.4 - C₄H₈O₂
¹H NMR 100MHz (CDCl₃)

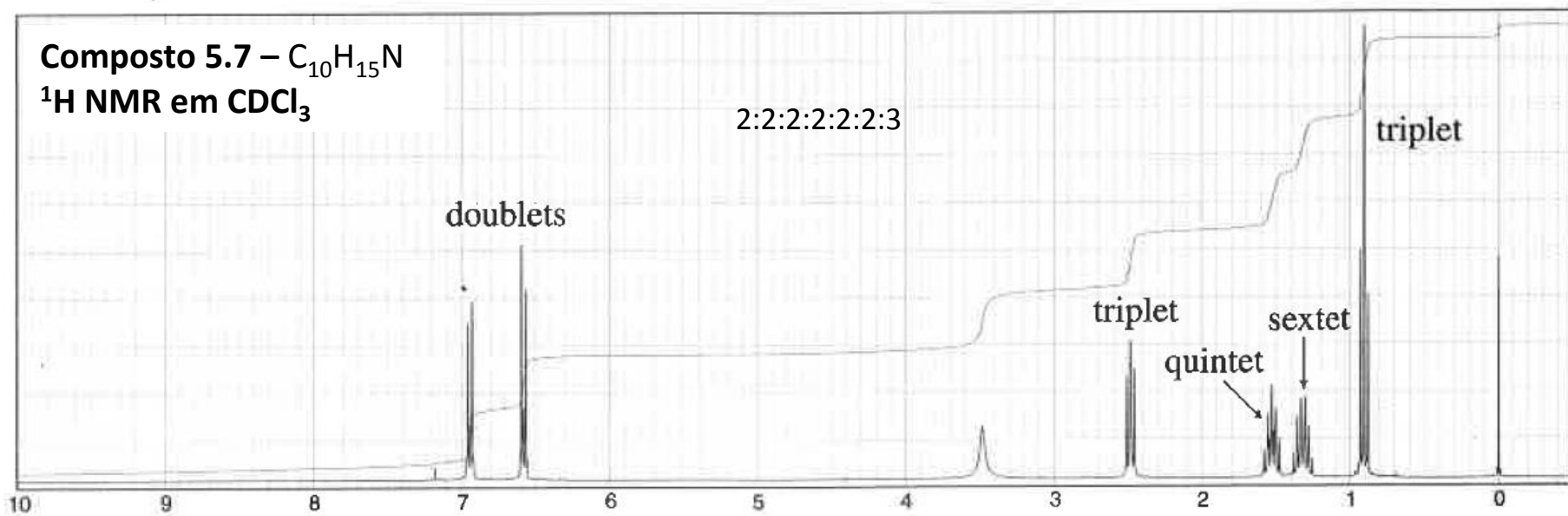


Composto 5.5 - C₄H₉Br
¹H NMR 300MHz (CDCl₃)



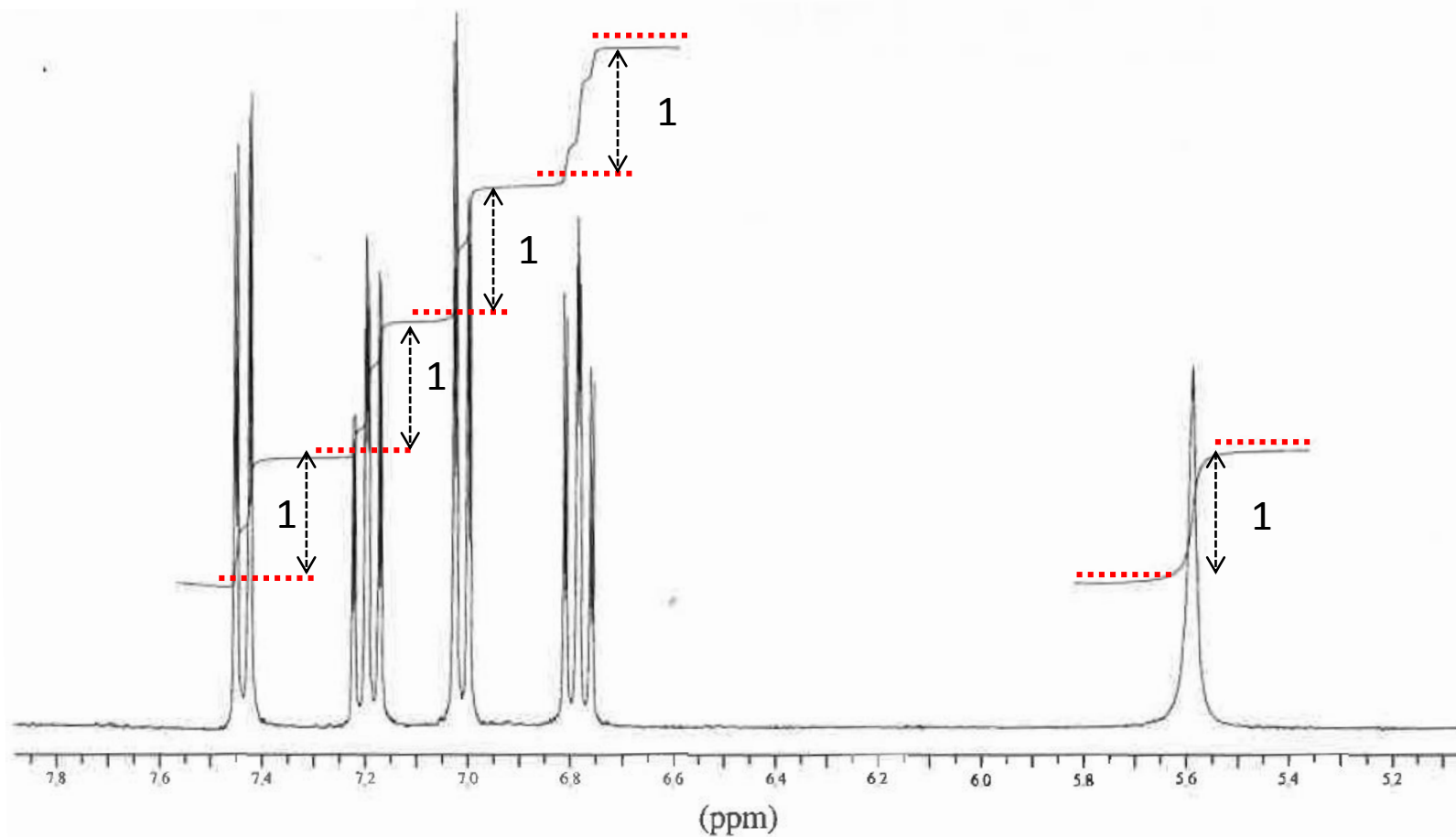
Composto 5.6 - C₃H₈S
¹H NMR 300MHz (CDCl₃)





Composto 5.8 – C₆H₅BrO

¹H NMR

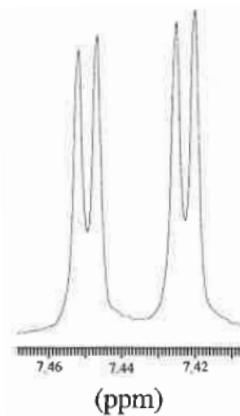


Composto 5.8 – C₆H₅BrO

¹H NMR -Expansões

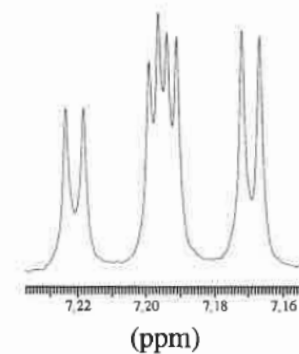
Peak Hz

2236.67
 2235.06
 2228.58
 2227.05



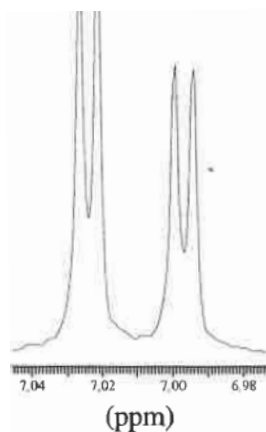
Peak Hz

2168.00
 2166.47
 2160.68
 2159.15
 2158.31
 2152.59
 2152.99



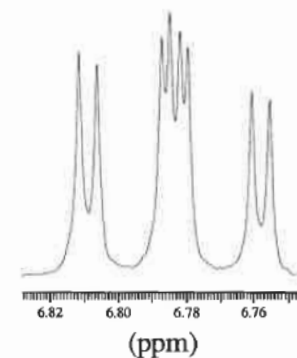
Peak Hz

2108.95
 2107.42
 2100.79
 2099.26



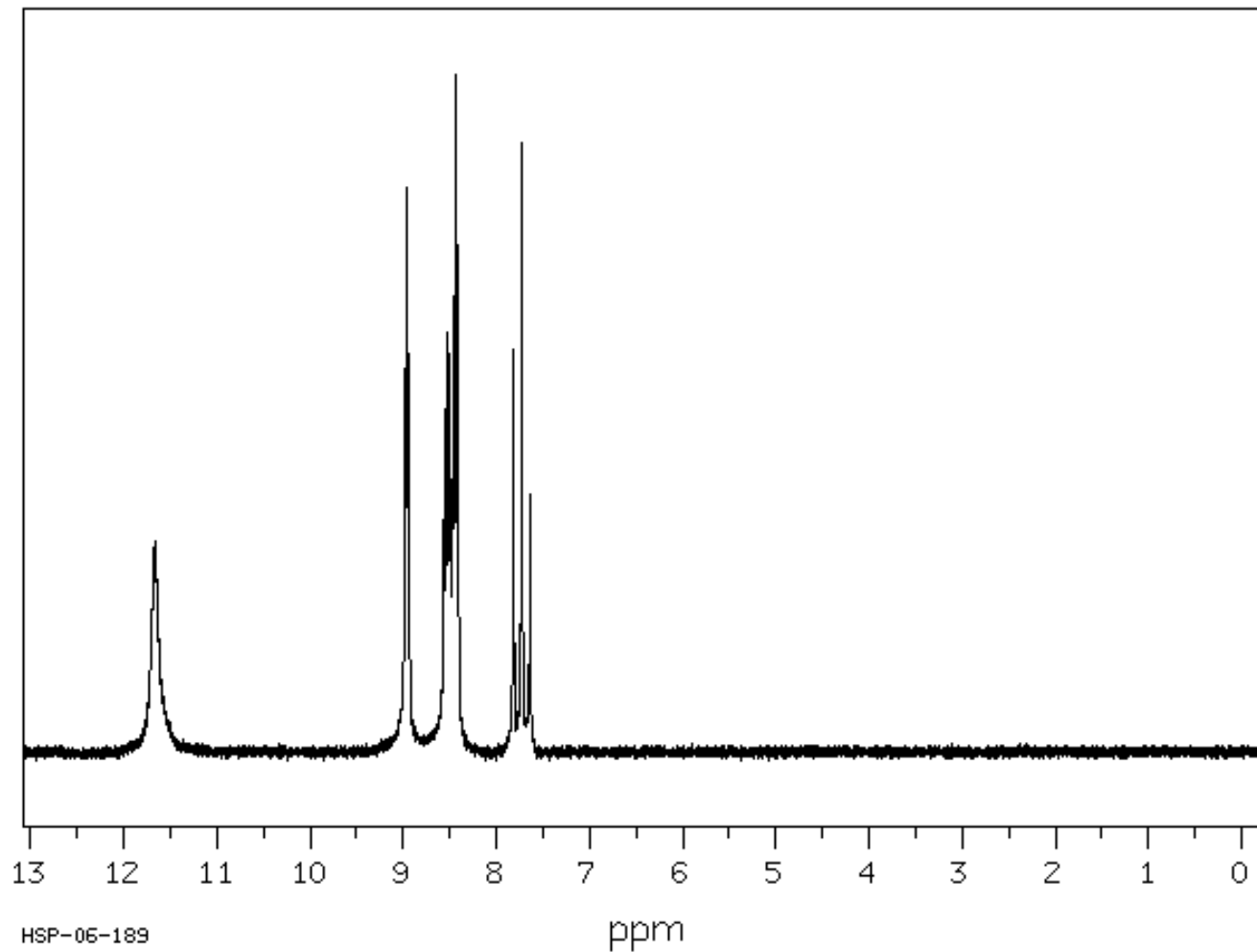
Peak Hz

2044.48
 2042.88
 2037.16
 2036.47
 2034.87
 2029.15
 2027.54

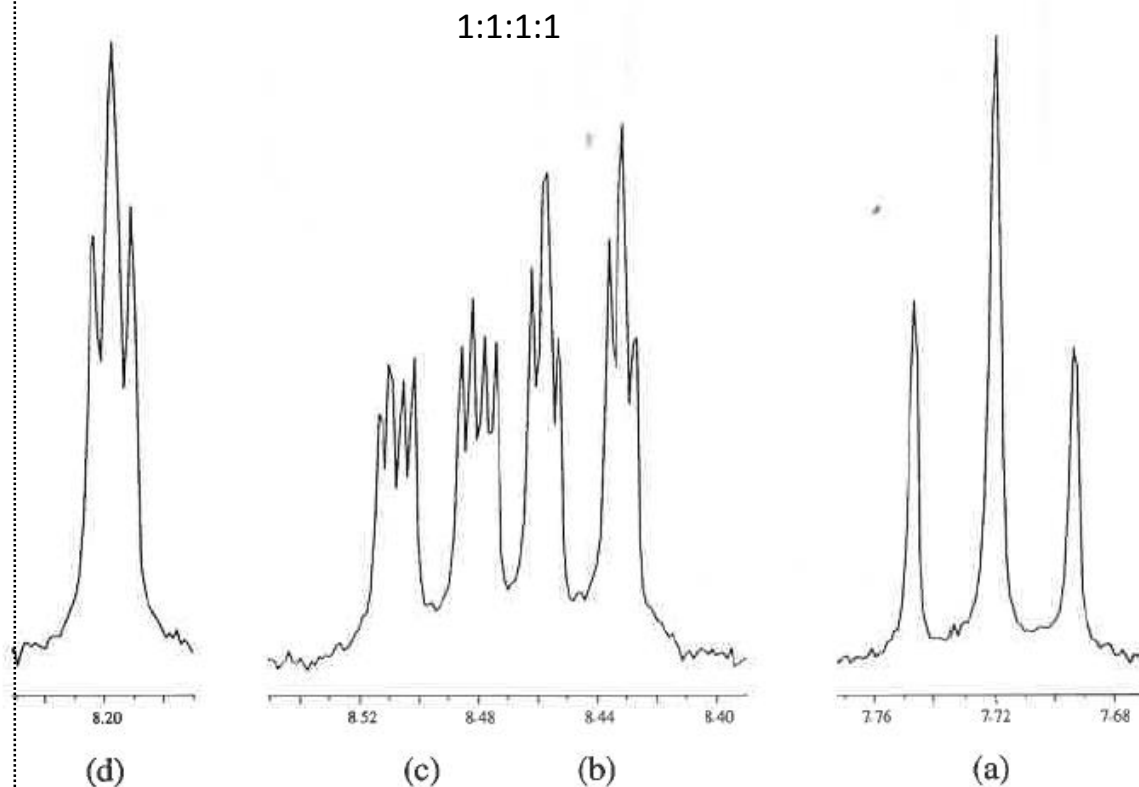


Composto 5.9 – C₇H₅NO₄

¹H NMR em CDCl₃

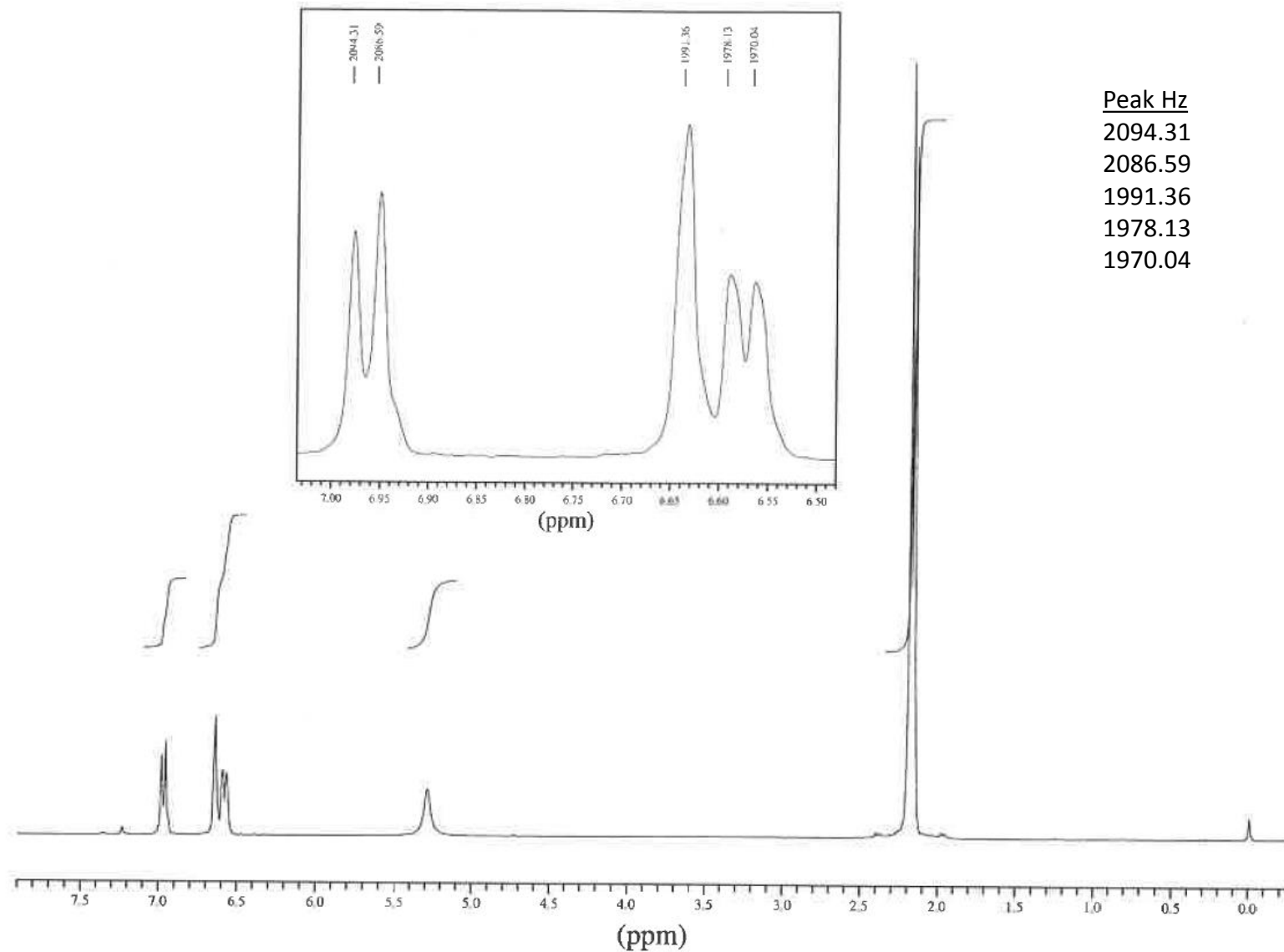


Composto 5.9 – C₇H₅NO₄
¹H NMR 300MHz (CDCl₃) - Expansão



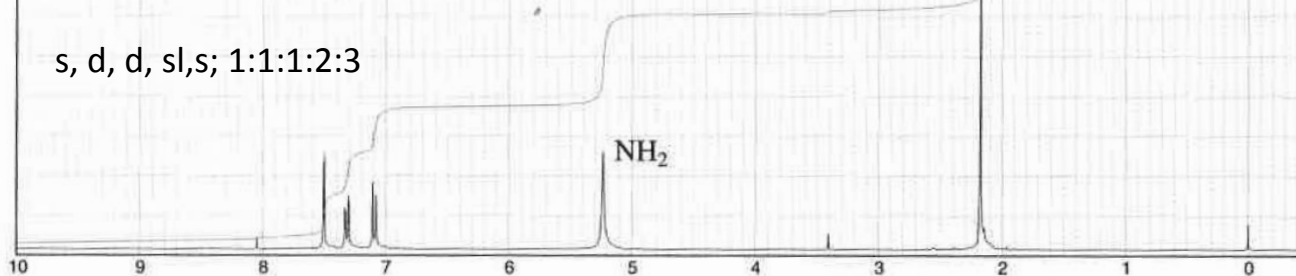
Peak Hz
2690.33
2688.49
2686.65
2555.39
2554.28
2552.81
2551.71
2546.93
2545.83
2544.73
2543.62
2539.95
2538.47
2537.37
2532.22
2530.75
2529.28

Composto 5.10 – C₈H₁₀O
¹H NMR (CDCl₃)



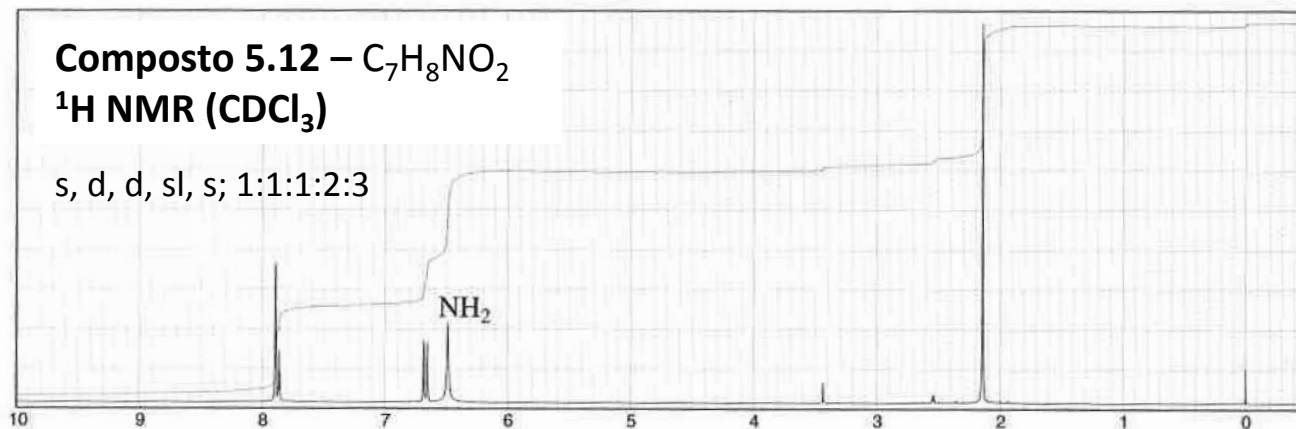
Composto 5.11 – C₇H₈NO₂
¹H NMR (CDCl₃)

s, d, d, sl,s; 1:1:1:2:3



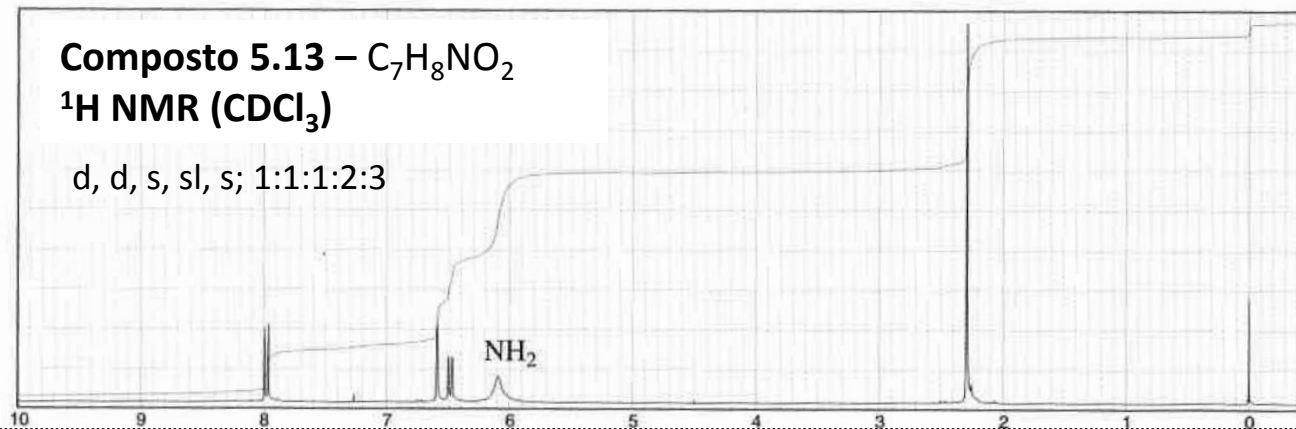
Composto 5.12 – C₇H₈NO₂
¹H NMR (CDCl₃)

s, d, d, sl, s; 1:1:1:2:3



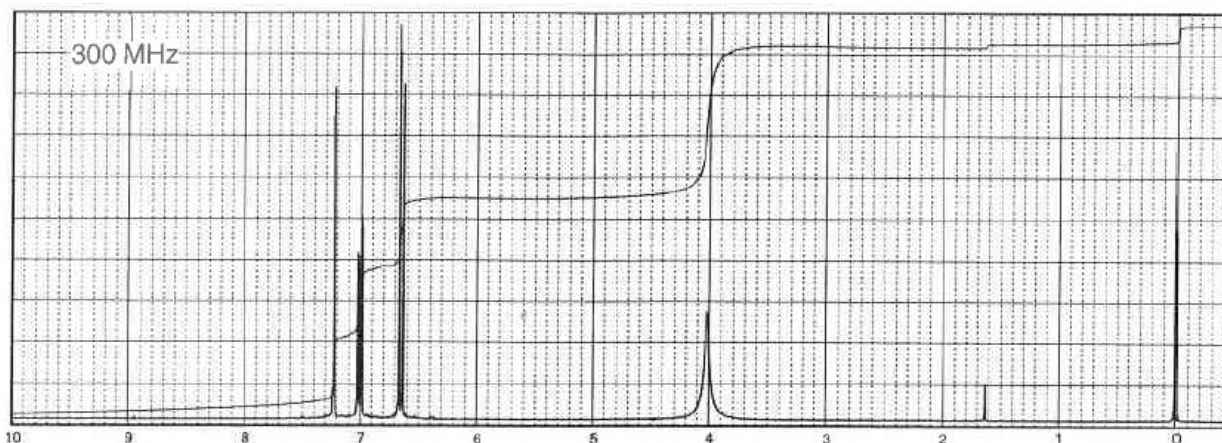
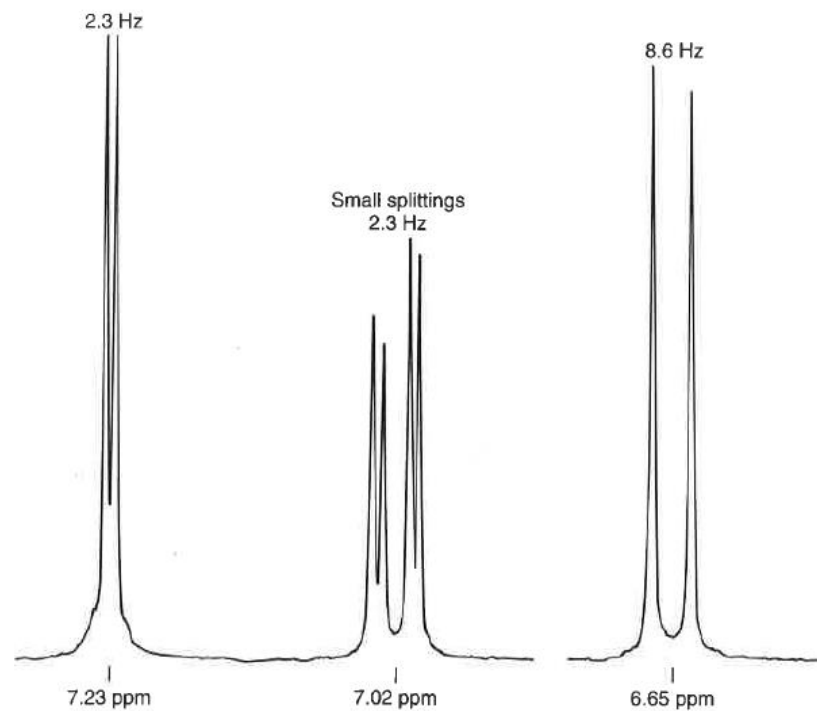
Composto 5.13 – C₇H₈NO₂
¹H NMR (CDCl₃)

d, d, s, sl, s; 1:1:1:2:3

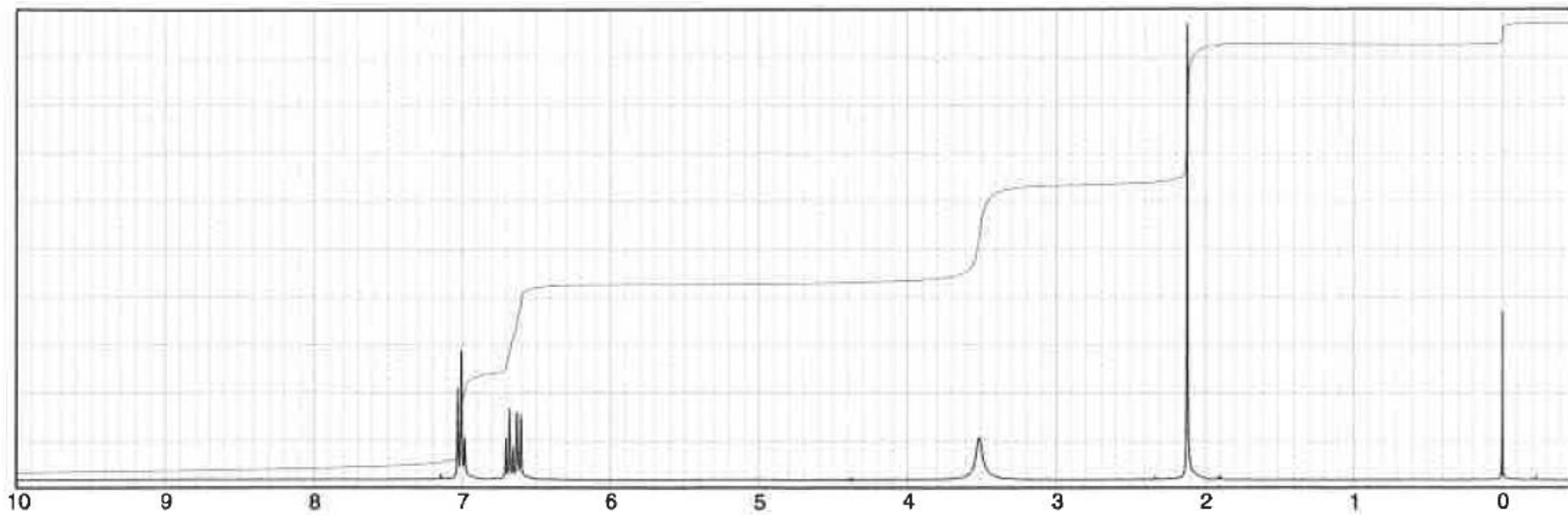
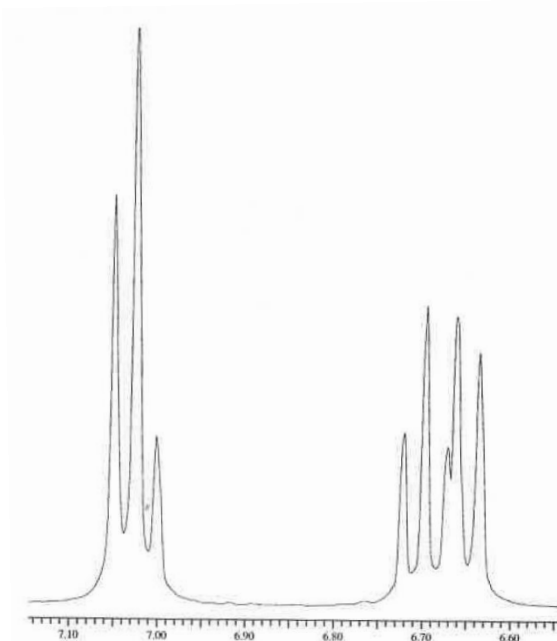




Composto 5.14 – C₆H₅NO₂
¹H NMR 300MHz



Composto 5.15 – C₇H₉N
¹H NMR 300MHz



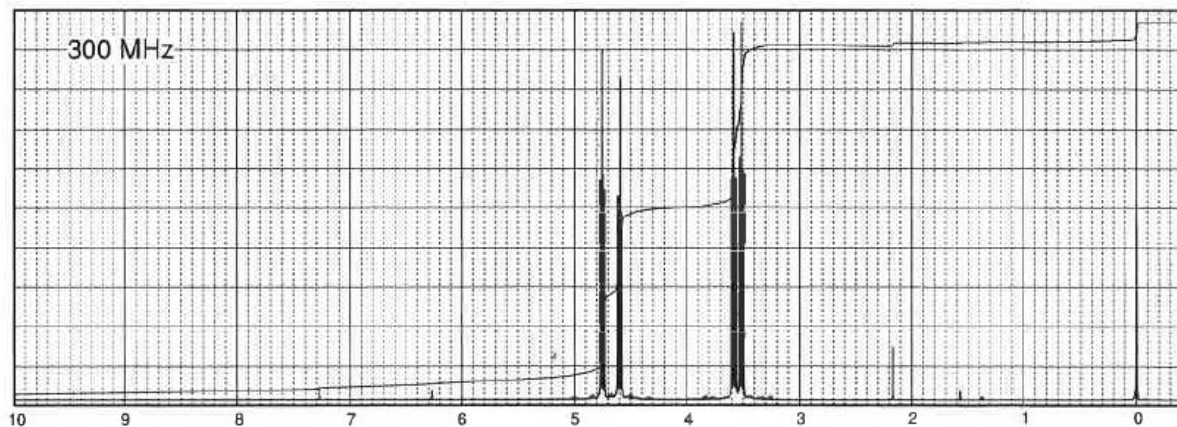
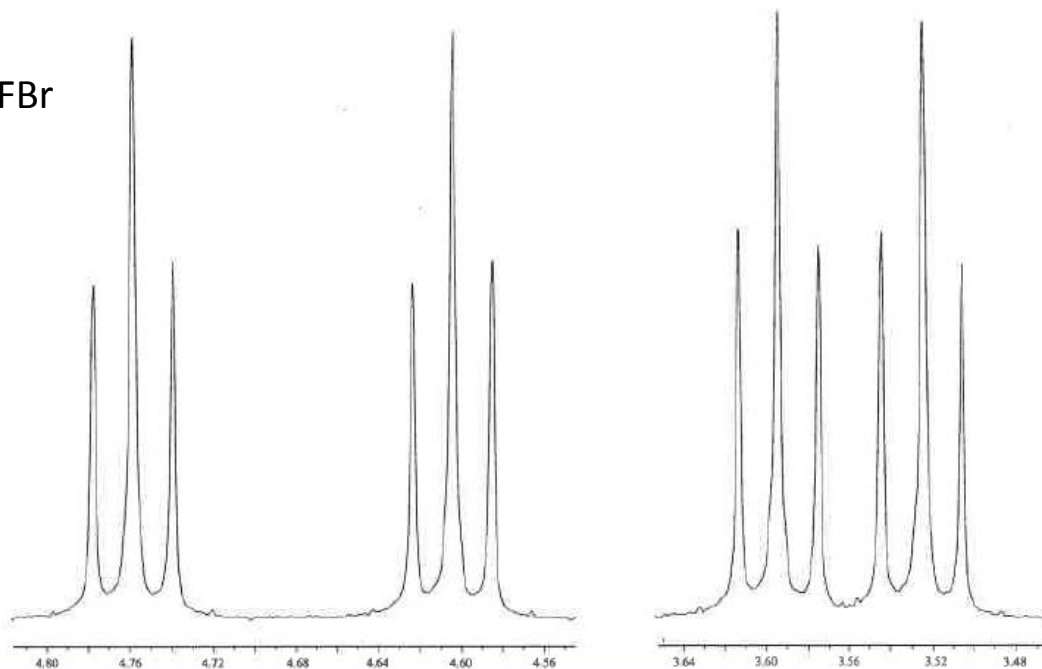
Composto 5.16 – C₂H₄FBr
¹H NMR 300MHz

Peak Hz
1433.66
1427.91
1422.16

1387.00
1381.25
1375.50

1084.59
1078.73
1072.98

1063.58
1057.83
1052.08





Composto 5.17 – $C_{10}H_{10}O_3$

1H NMR 300MHz

1:1:1:1:1:1

Peak Hz

2338.83

2322.87

2207.15

2199.33

2191.35

2151.23

2143.56

Peak Hz

2122.81

2097.40

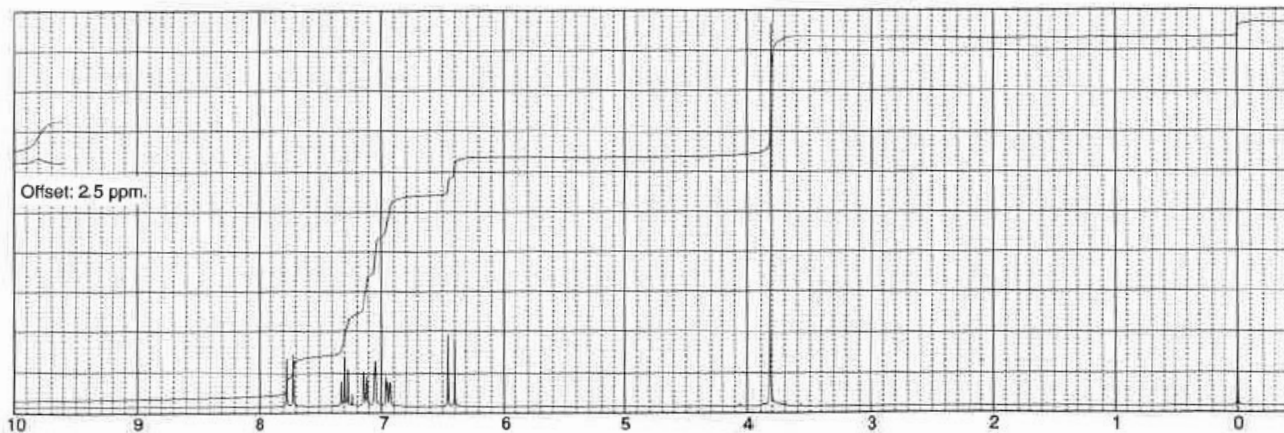
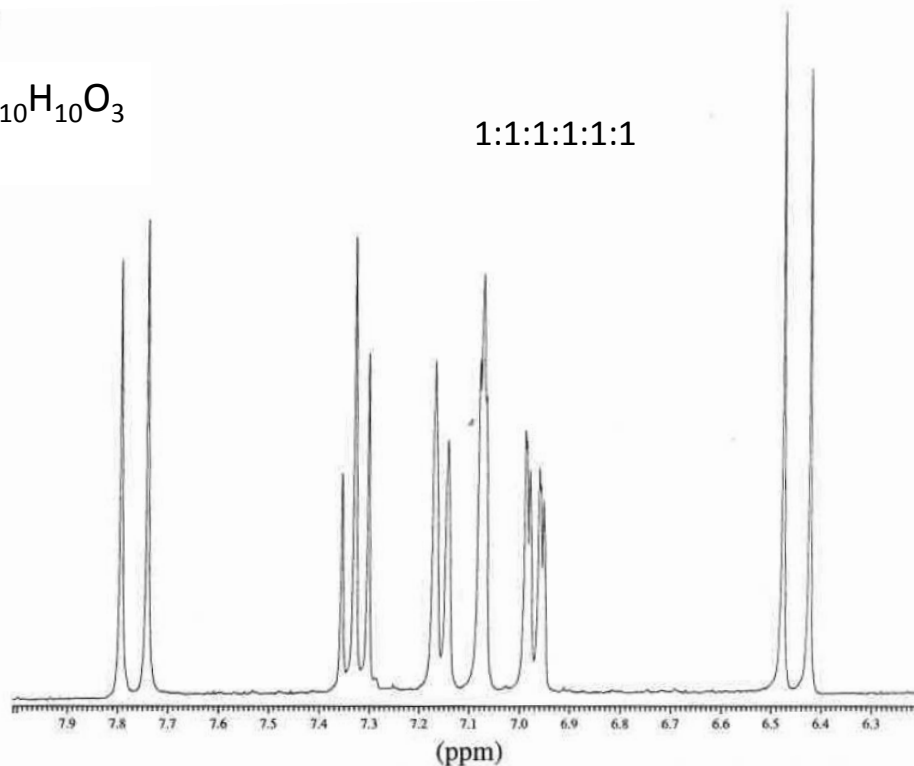
2094.84

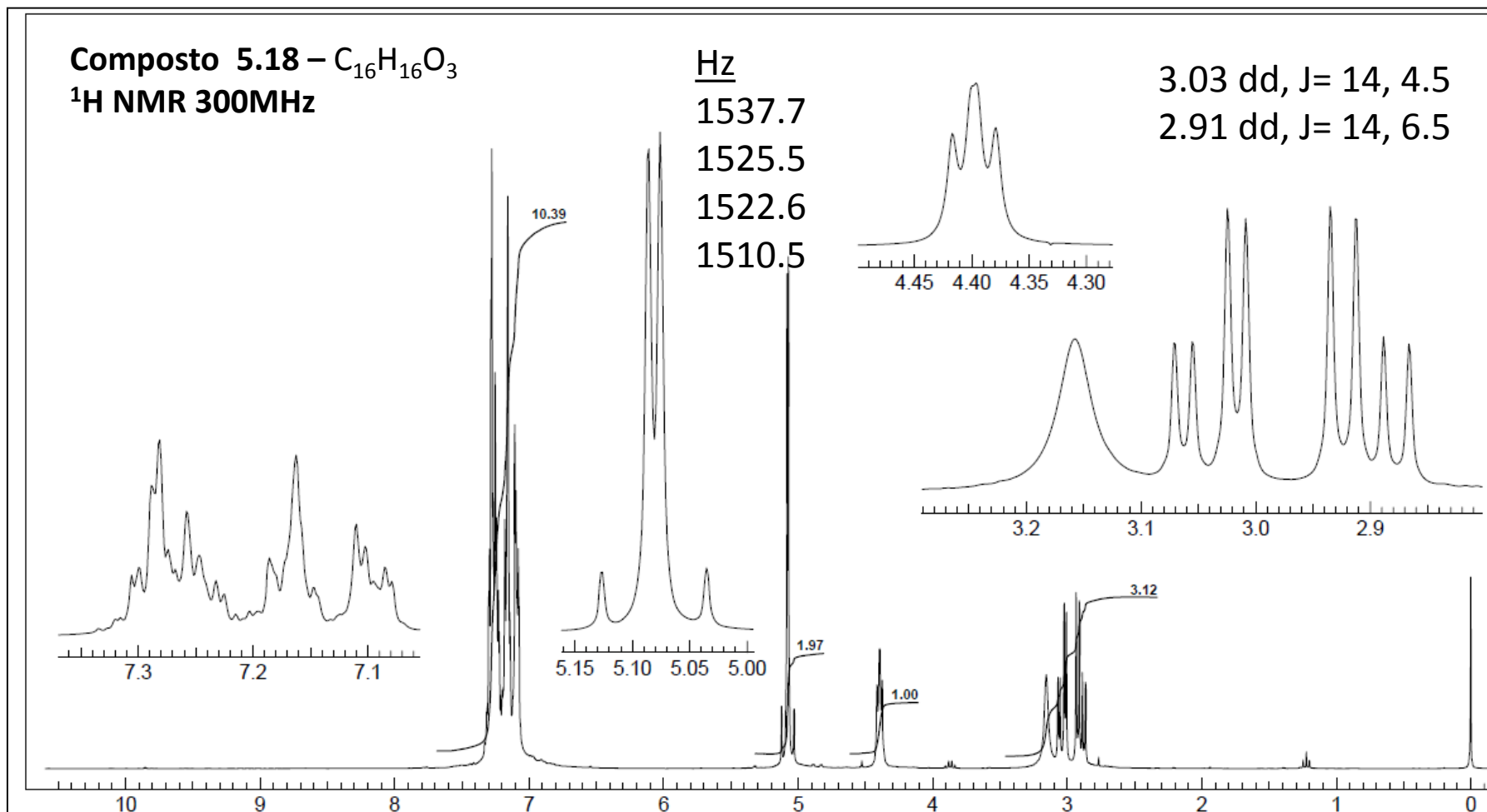
2089.19

2086.71

1943.42

1927.46

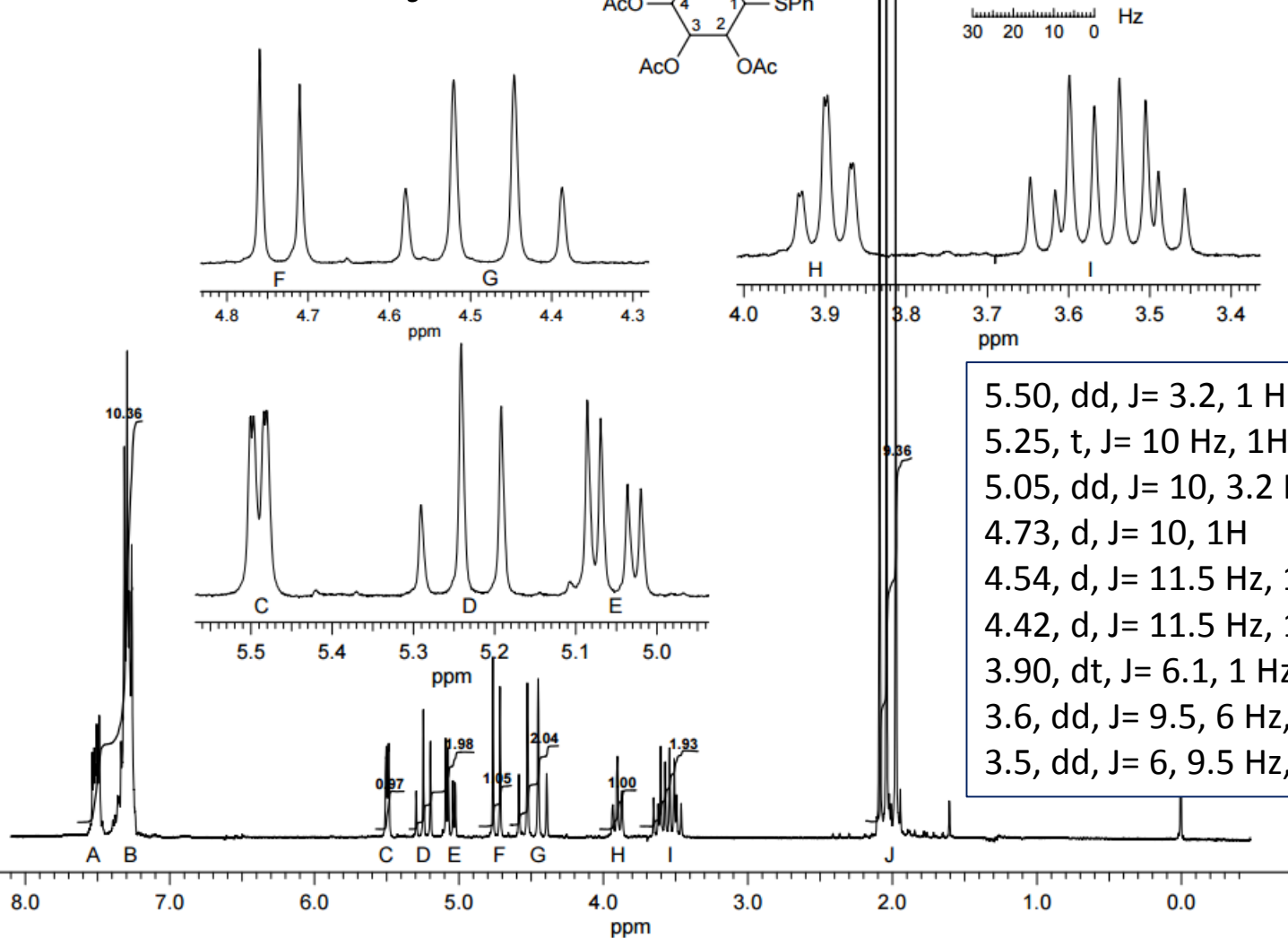
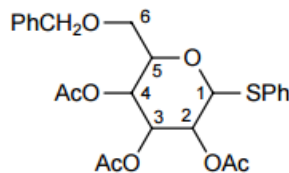




6. Determinar a estereoquímica dos seguintes compostos:

Composto 6.1

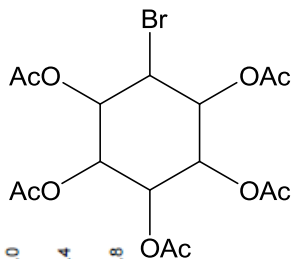
^1H NMR 200MHz em CDCl_3



- 5.50, dd, $J = 3.2, 1$ Hz, 1H
- 5.25, t, $J = 10$ Hz, 1H
- 5.05, dd, $J = 10, 3.2$ Hz, 1H
- 4.73, d, $J = 10$, 1H
- 4.54, d, $J = 11.5$ Hz, 1H
- 4.42, d, $J = 11.5$ Hz, 1H
- 3.90, dt, $J = 6.1, 1$ Hz, 1H
- 3.6, dd, $J = 9.5, 6$ Hz, 1H
- 3.5, dd, $J = 6, 9.5$ Hz, 1H

Composto 6.2

¹H NMR



1544.3
1541.1
1534.3
1530.9

1512.6
1511.3
1508.4
1506.0
1501.8

1492.1

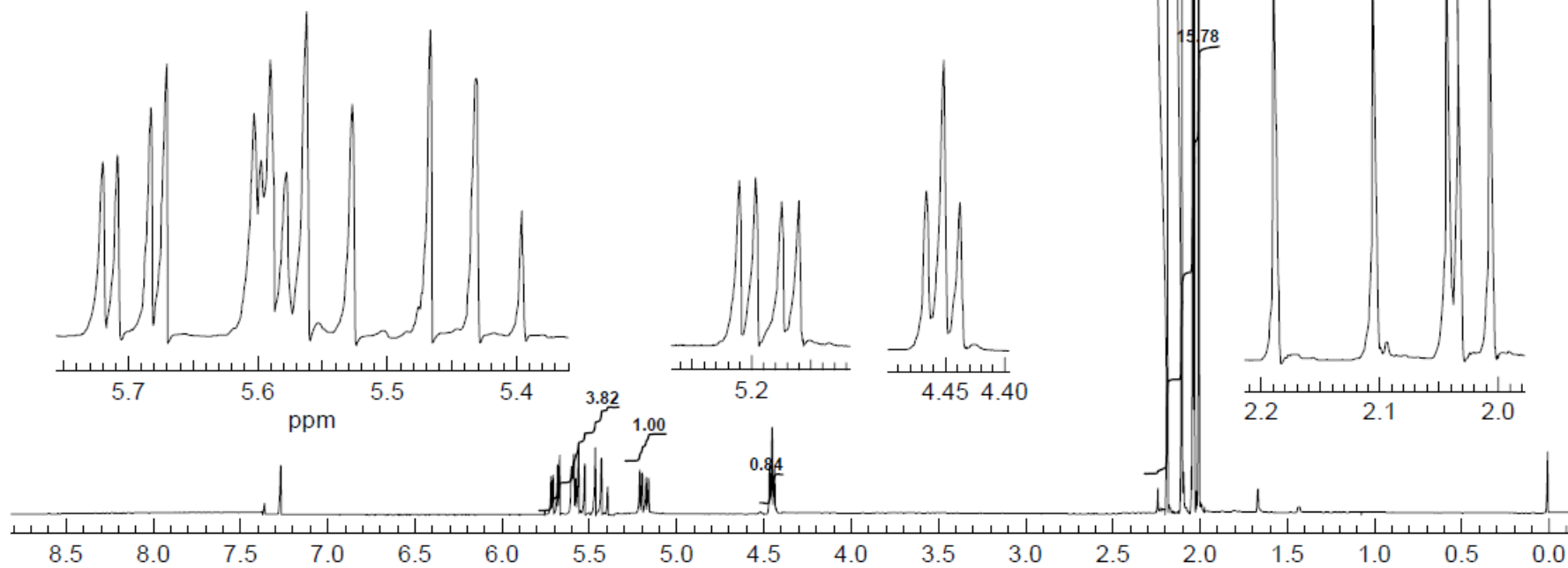
1476.0

1466.4

1456.8

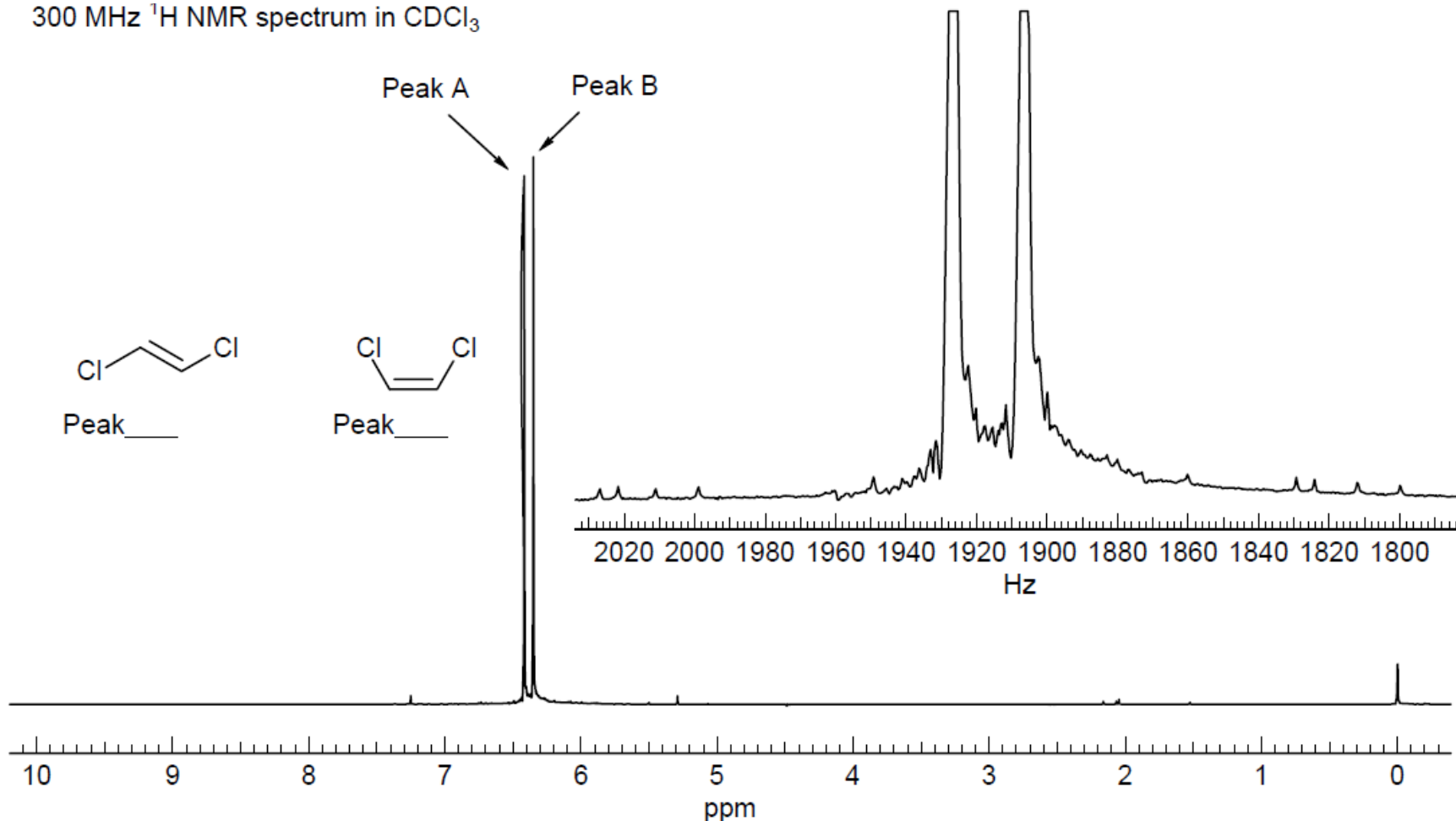
4.5, t, J= 4 Hz
 5.2, dd, J= 10, 4 Hz, 1H
 5.43, t, J= 10 Hz, 1H
 5.56, t, J= 10 Hz, 1H
 5.59, t, J= 3.5 Hz, 1H
 5.70, dd, J= 10, 3.3 Hz

2.19, s
 2.11, s
 2.04, s
 2.03, s
 2.00, s



7. Atribuir aos isómeros *cis* e *trans* do 1,2-dicloroeteno os respectivos sinais de H.

300 MHz ^1H NMR spectrum in CDCl_3



8. Atribuir todos os sinais de próton presentes no espectro de ^1H RMN do ácido fumárico em DMSO- d_6 (400.13MHz), indicando os sinais dos isotopomeros e as constantes de acoplamento $^1J_{\text{HC}}$ e $^3J_{\text{HH}}$.

