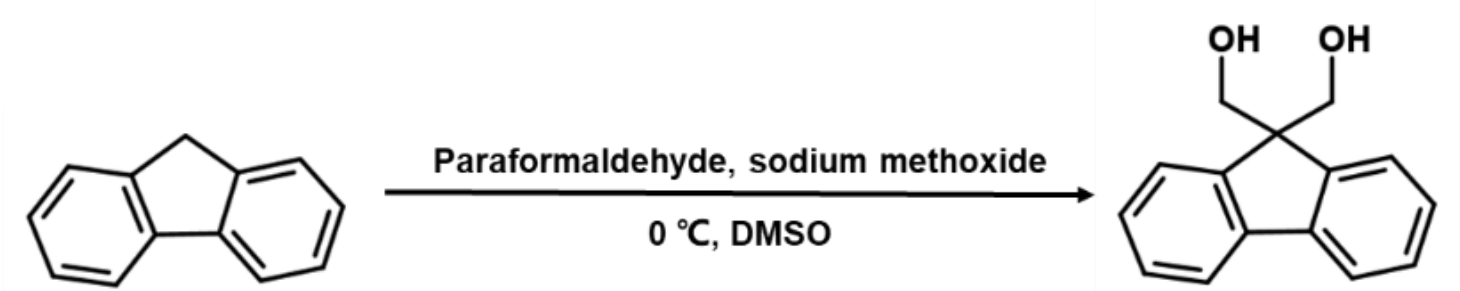
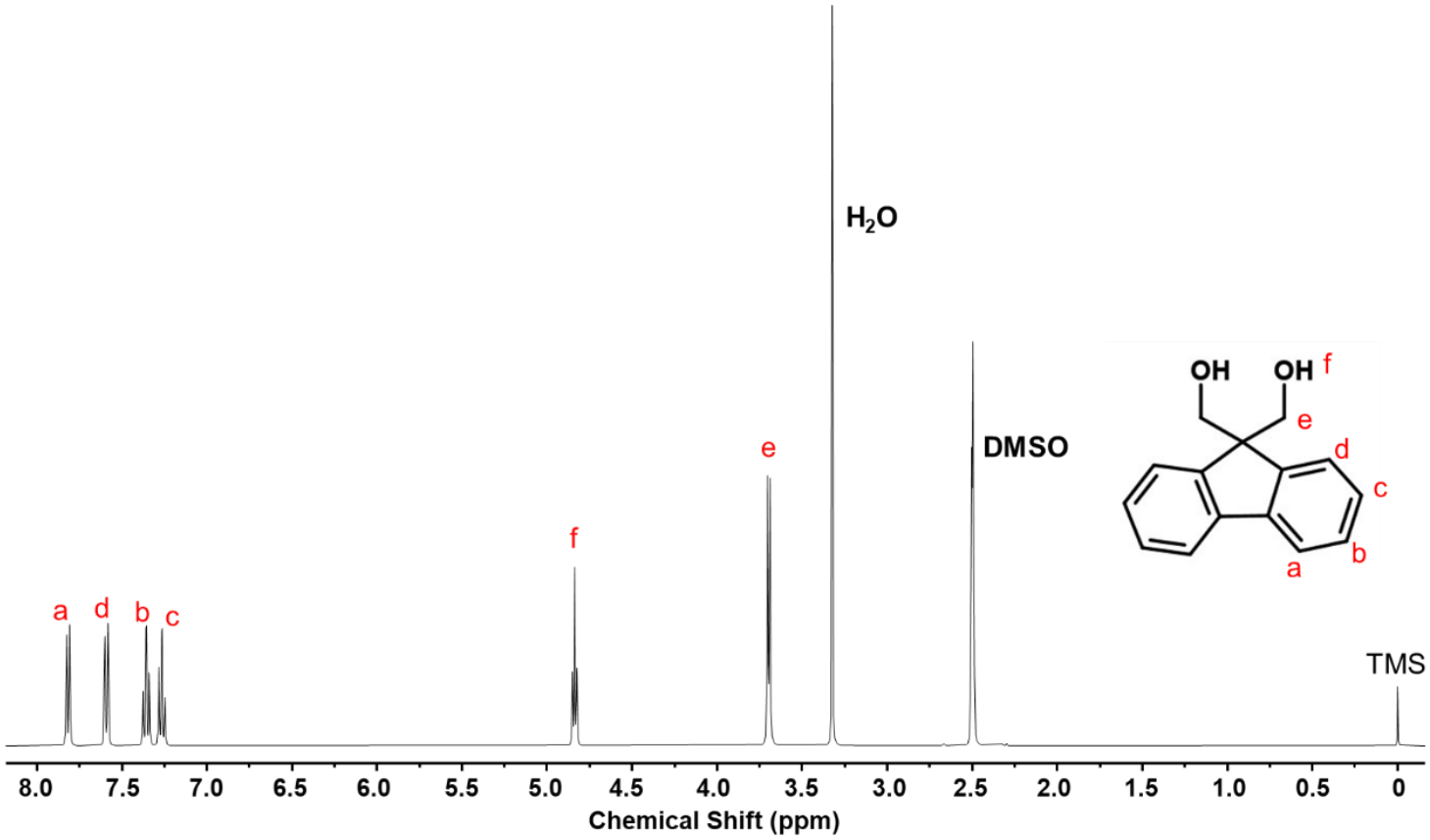
Spectroscopie de résonance magnétique nucléaire (RMN)

01-11-2023

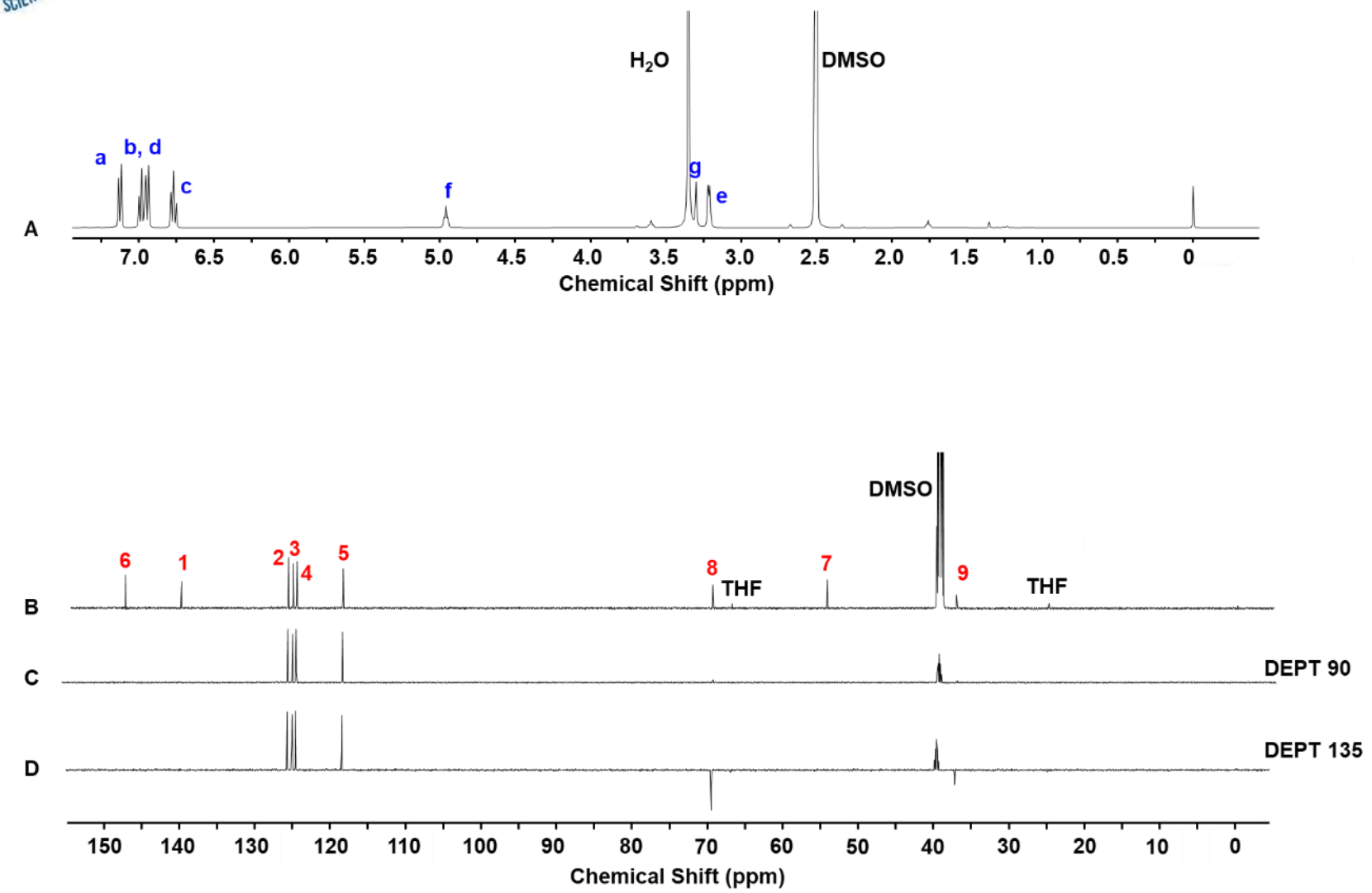
Lecture 8

Histoire Vraie…

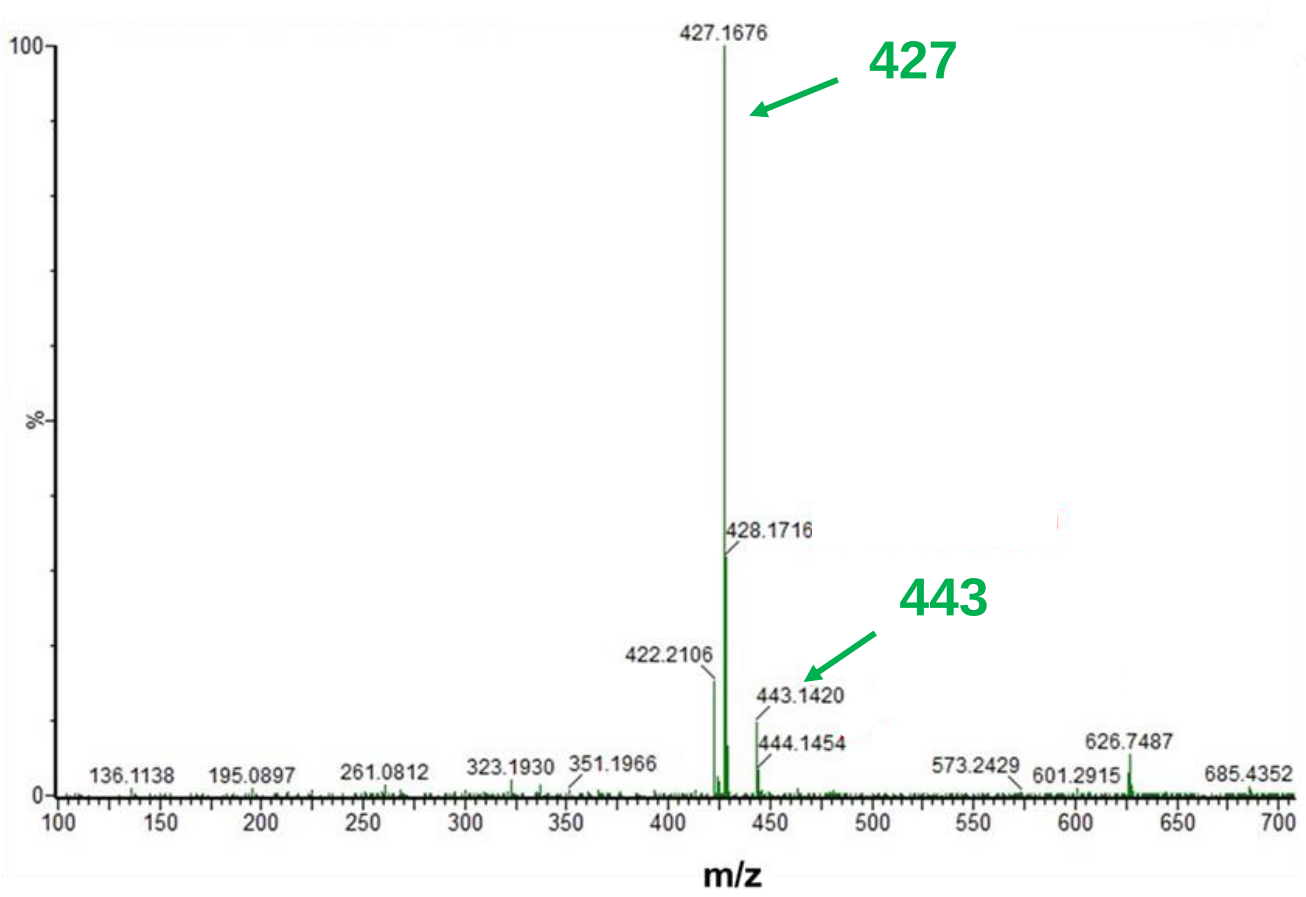




Spectres ^{1}H RMN et DEPT de l'impureté



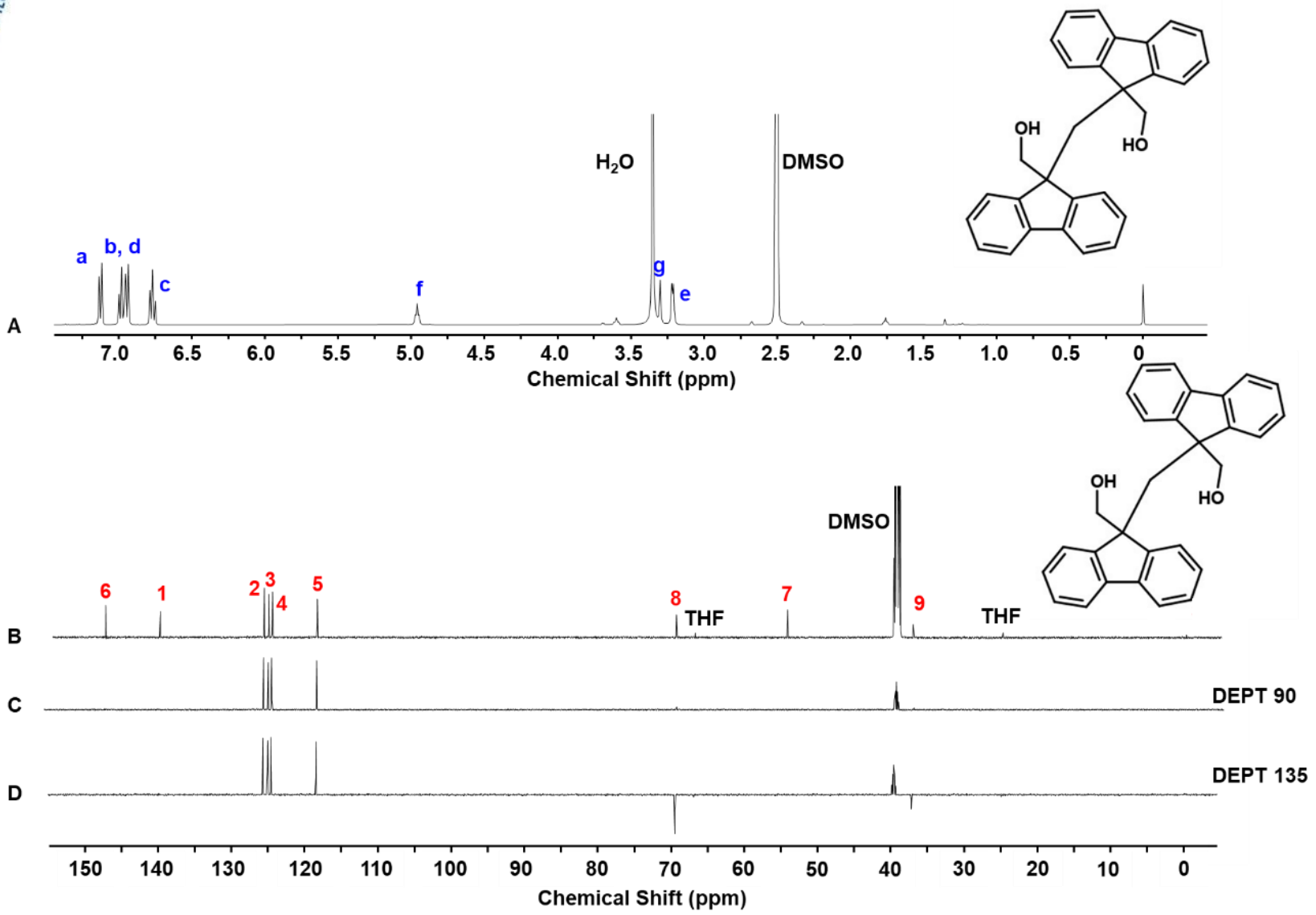
Spectre de masse de l'impureté



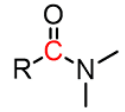
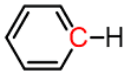
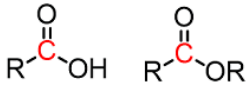
L'échantillon est incorporé dans une matrice qui contient des ions sodium (23 g/mol) et potassium (39 g/mol)

La masse molaire de l'impureté est donc de 427-23 = 443-39 = 404 g/mol

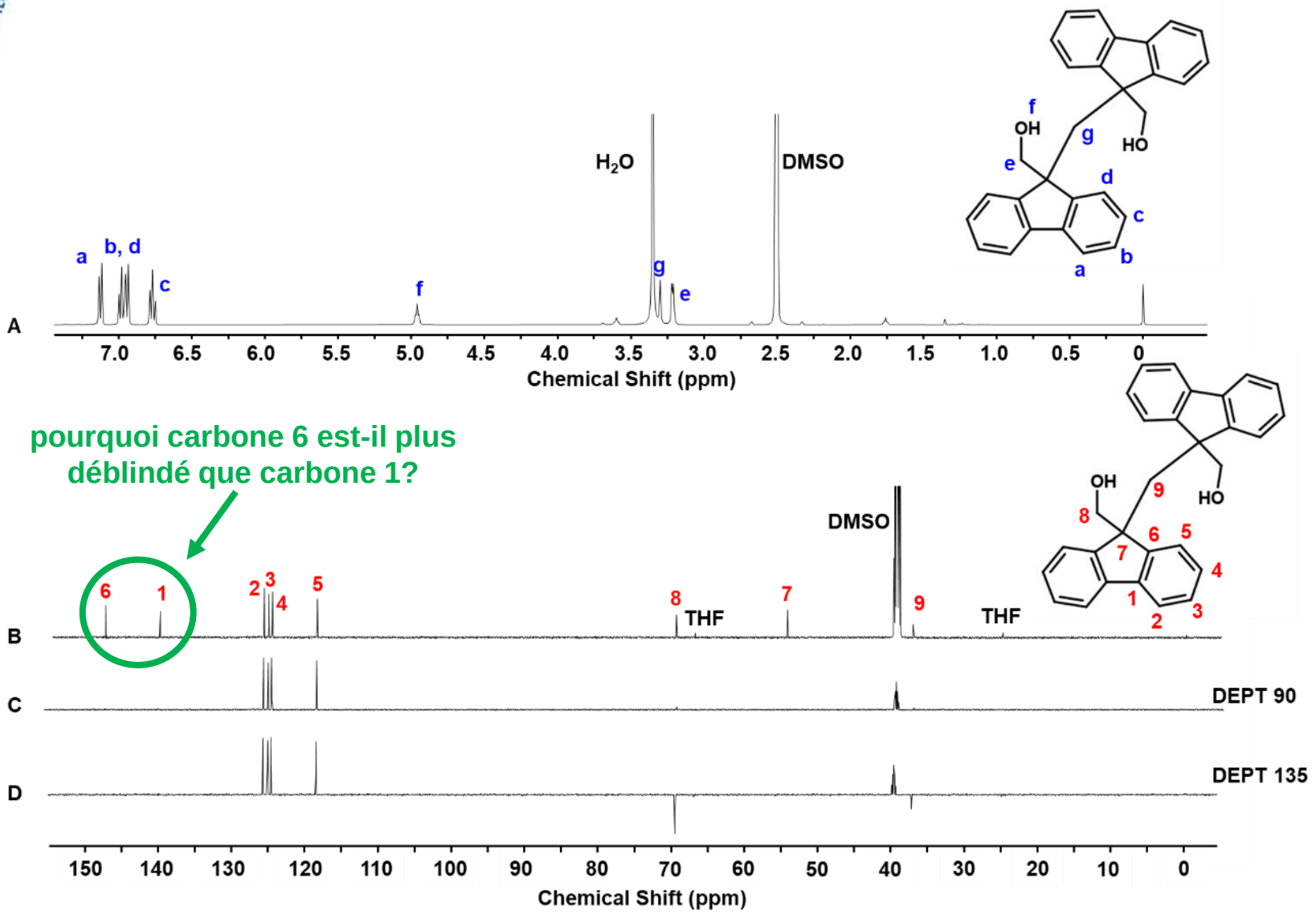
Spectres RMN ^{1}H et DEPT de l'impureté



Approximate Values of Chemical Shifts for ^{13}C NMR

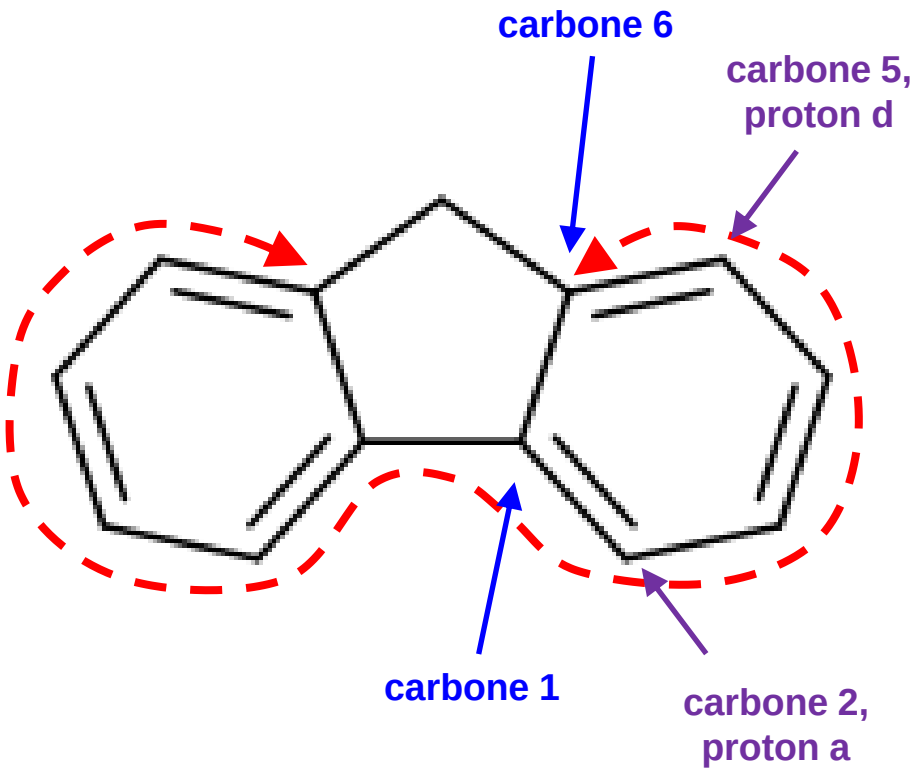
$(CH_3)_4Si$	0	*	I–C	-20 - 40		100 - 150	 155 - 185
R-CH_3	8 - 30		Br–C	25 - 65		110 - 170	 165 - 185
R-CH_2-R	15 - 55		Cl–C	35 - 80	C≡N	150 - 170	 190 - 220
R_3CH	20 - 60		O–C	40 - 80	C≡N	110 - 140	
R_4C	30 - 50		N–C	30 - 65			

Spectres RMN ^{1}H et DEPT de l'impureté



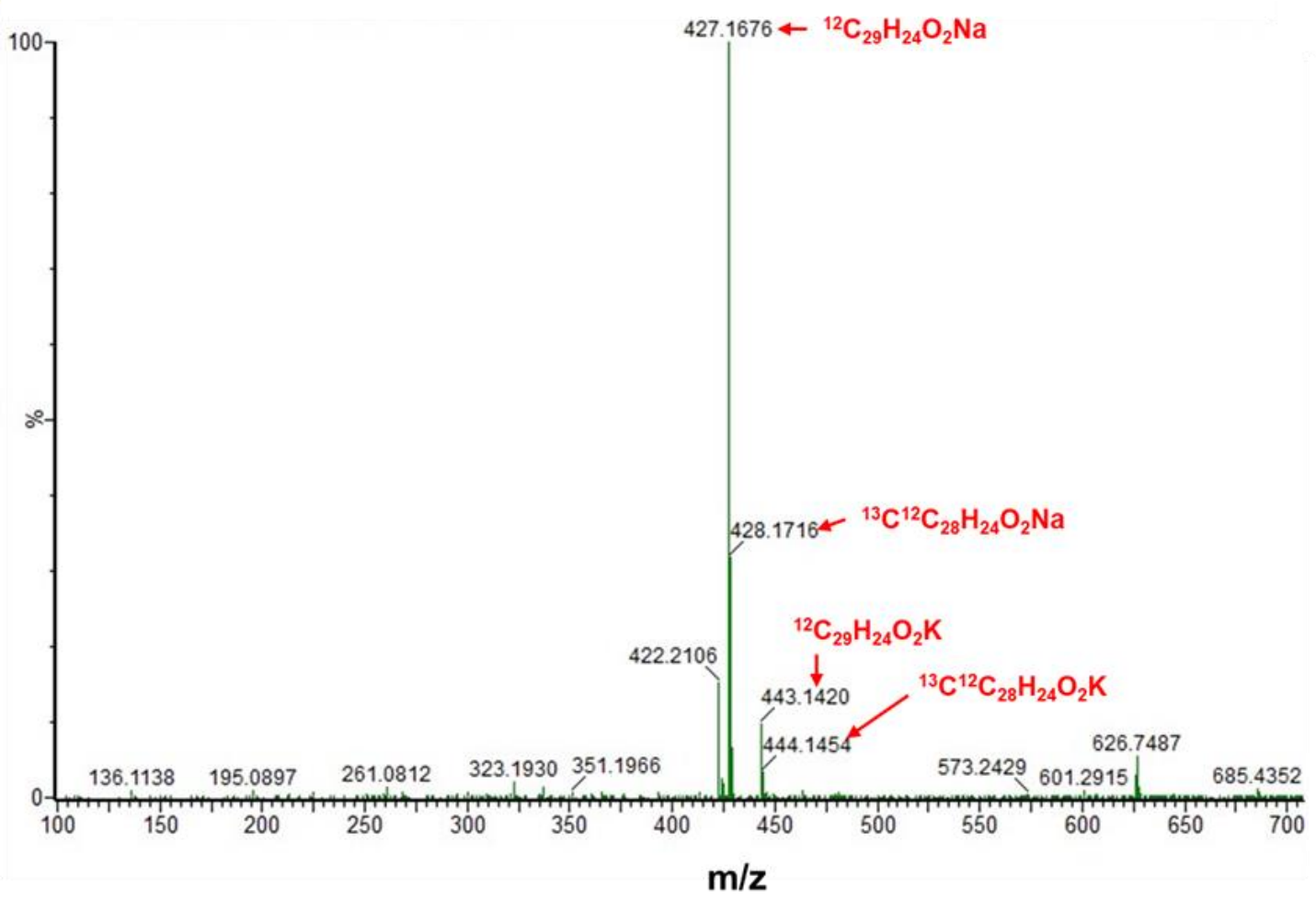
Pourquoi carbone 6 est plus déblindé que carbone 1?

Notez que le carbone 6 se trouve à l'extrêmité de la délocalisation (flèche rouge), ce qui amplifie le déblindage



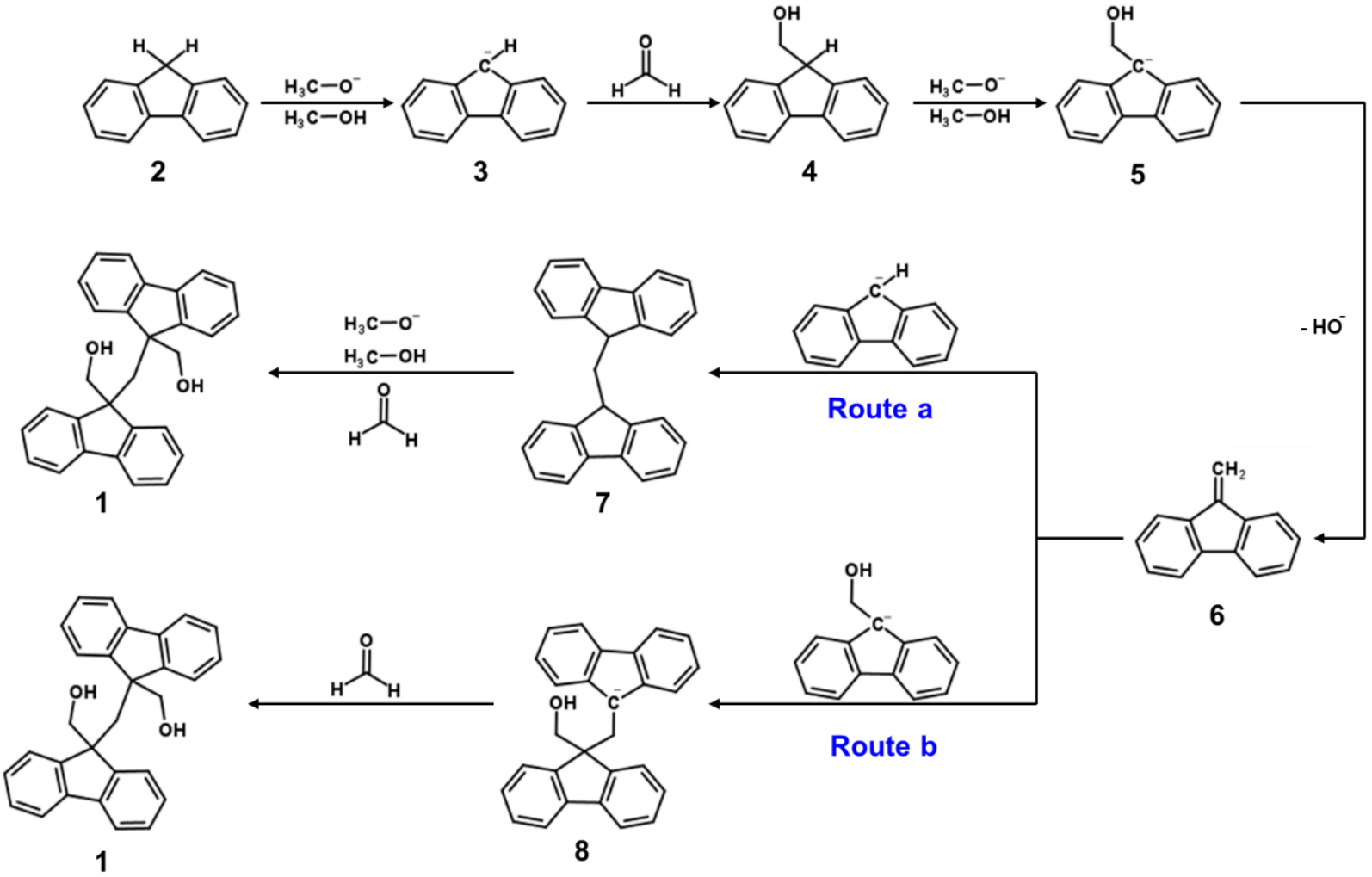
Notez aussi que les protons a et d sont placés sur les carbones 2 et 5 (respectivement), et pas sur les carbones 1 et 6.

Spectre de masse de l'impureté



On retrouve bien la valeur de 404 g/mol

Origine de l'impureté



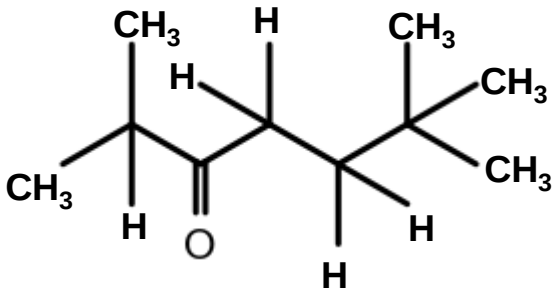
Exercice 1

a) Donnez le nombre de groupes de protons différents (non équivalents)

b) Indiquez la multiplicité correspondant à chaque groupe

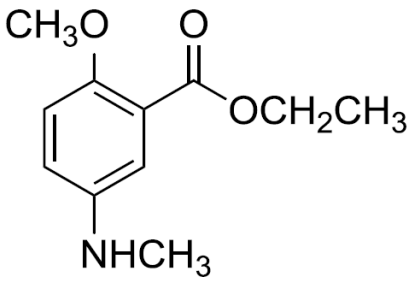
1) $CH_3 - CH_2 - CH_2 - CH_2 - CH_2 - CH_3$

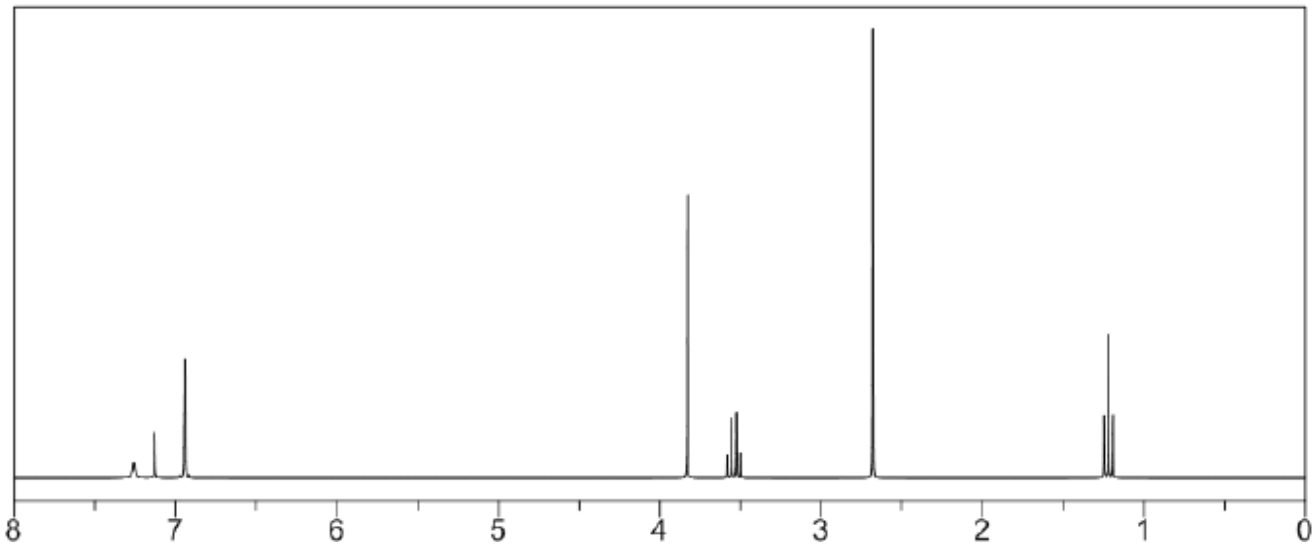
2)



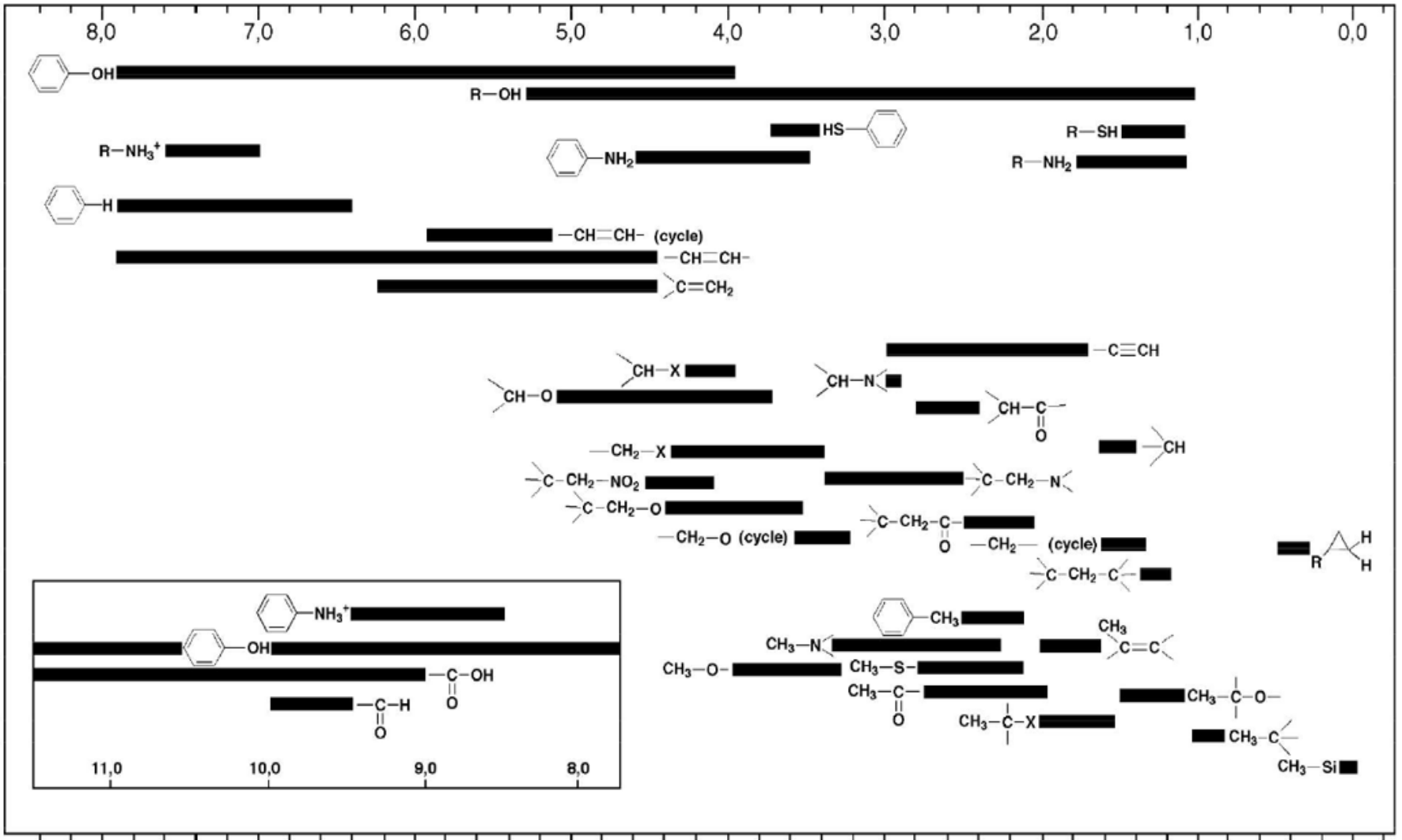
Exercice 2

Associez chaque signal du spectre RMN ^1H au groupe de protons de la molécule ci-dessous :

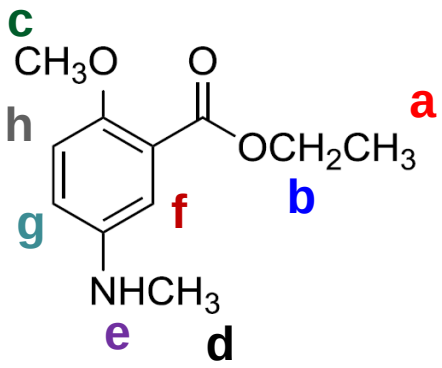


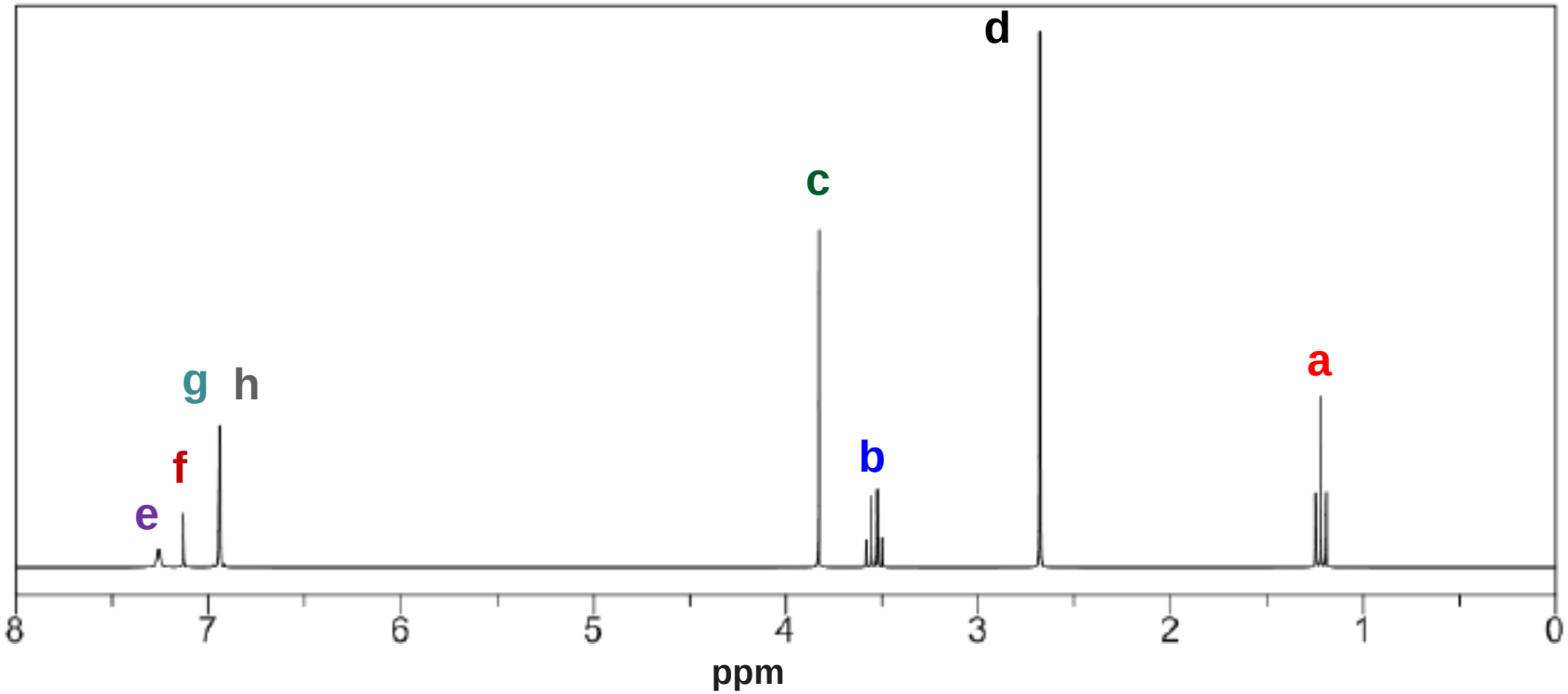


Déplacements chimiques typiques de protons.



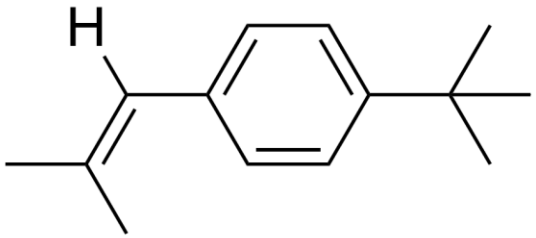
Exercice 2

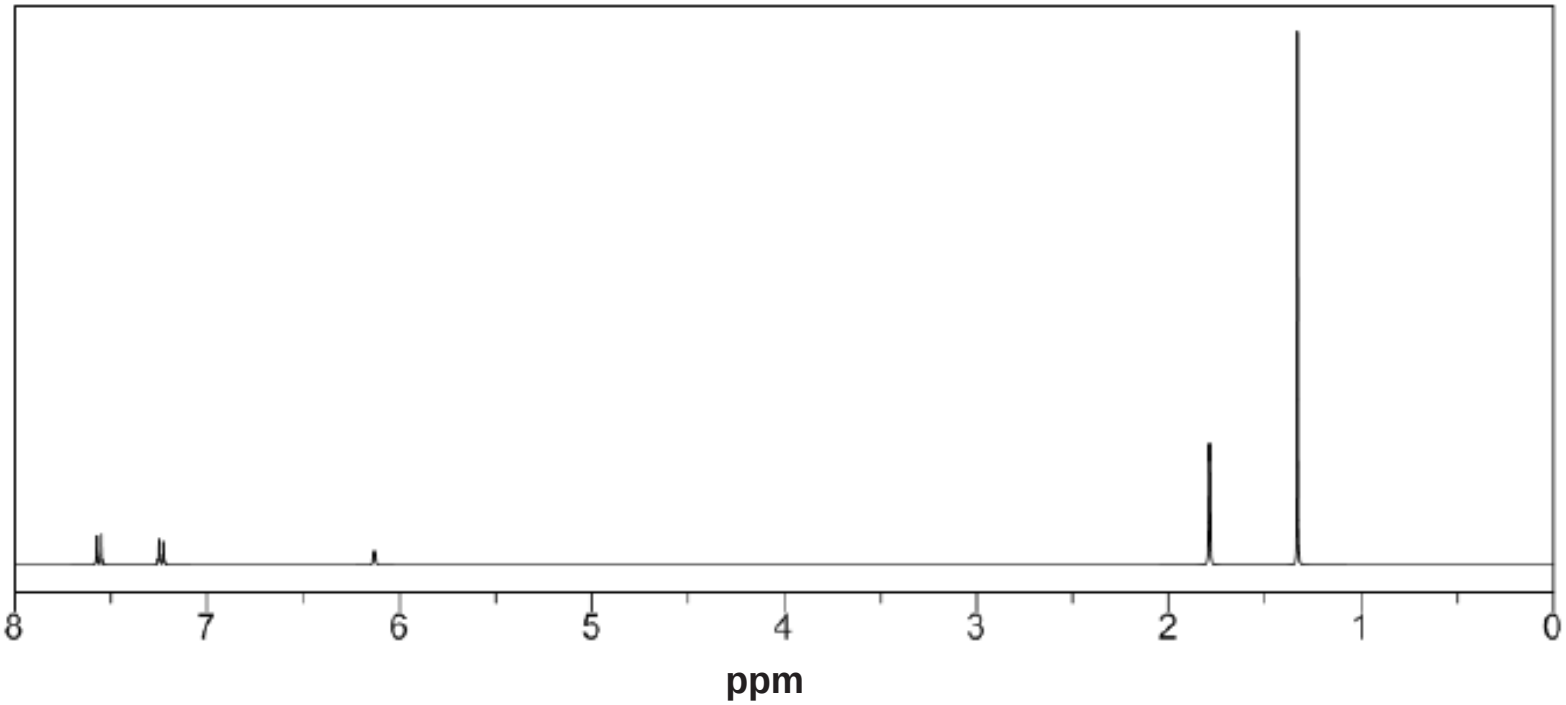




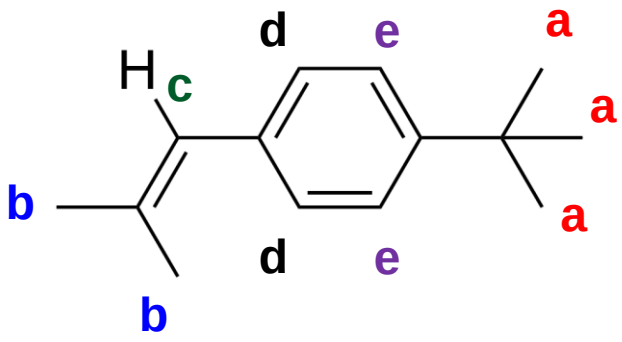
Exercice 3

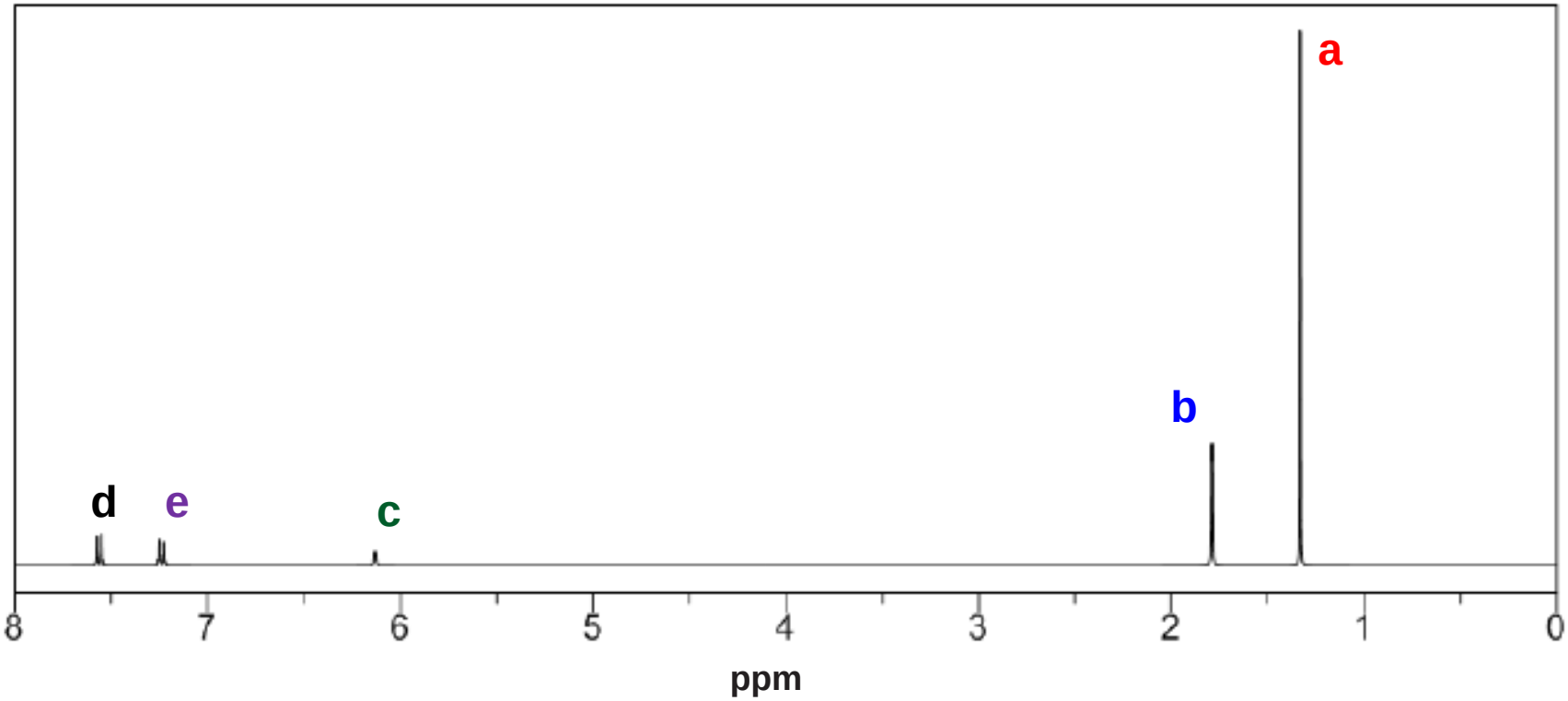
Associez chaque signal du spectre RMN ^{1}H au groupe de protons de la molécule ci-dessous :



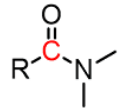
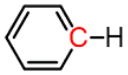
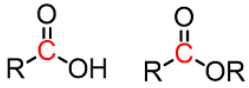


Exercice 3



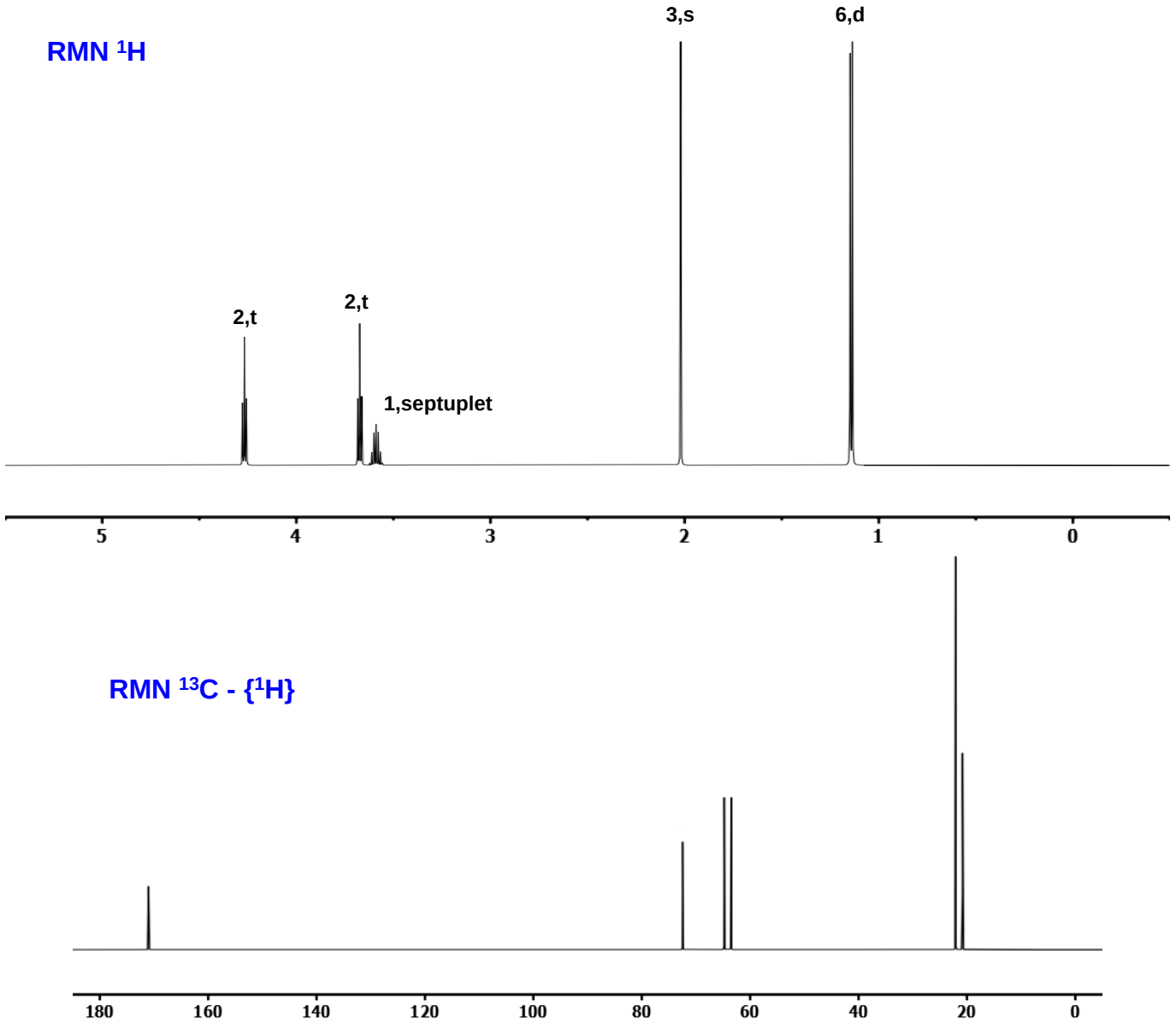


Approximate Values of Chemical Shifts for ^{13}C NMR

$(CH_3)_4Si$	0	*	I–C	-20 - 40		100 - 150	 155 - 185
R-CH_3	8 - 30		Br–C	25 - 65		110 - 170	 165 - 185
R-CH_2-R	15 - 55		Cl–C	35 - 80	C≡N	150 - 170	 190 - 220
R_3CH	20 - 60		O–C	40 - 80	C≡N	110 - 140	
R_4C	30 - 50		N–C	30 - 65			

Exercice 4

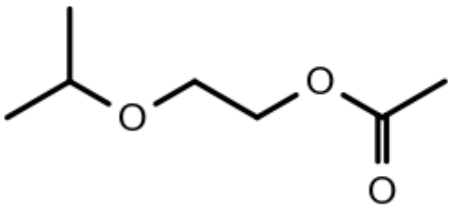
Déterminez la structure de formule moléculaire $C_7H_{14}O_3$ à l'aide des spectres RMN ^1H et RMN ^{13}C ci-dessous :

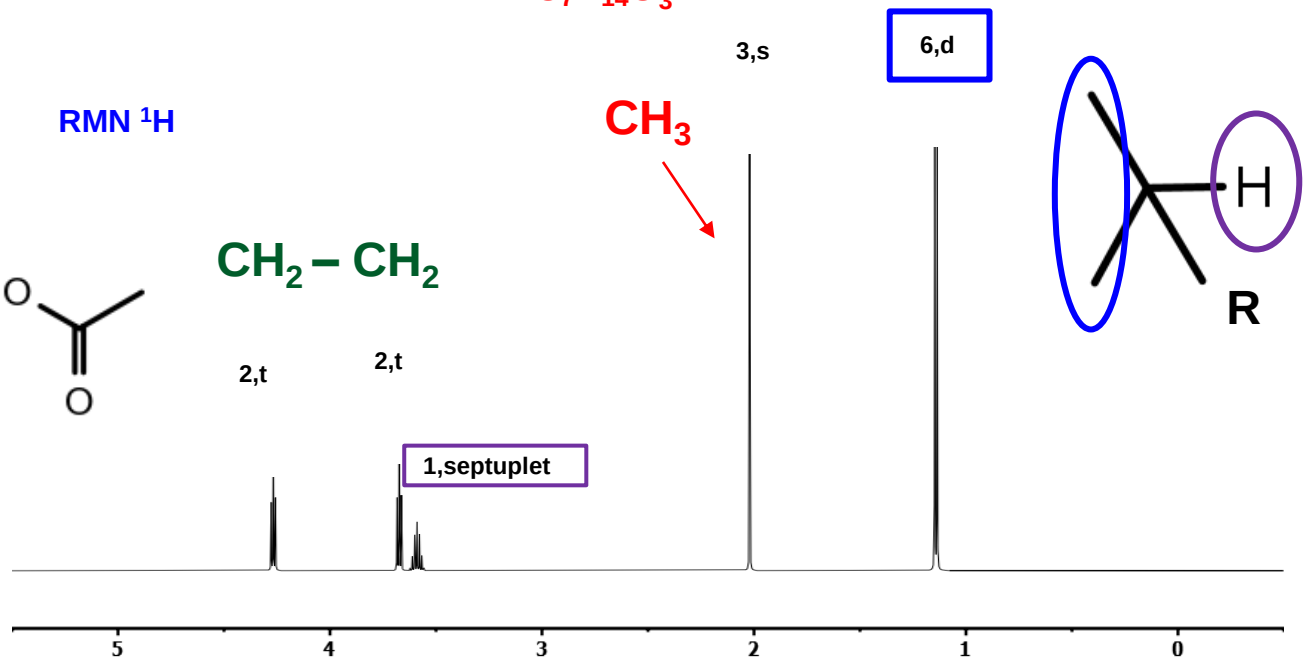


Exercice 4

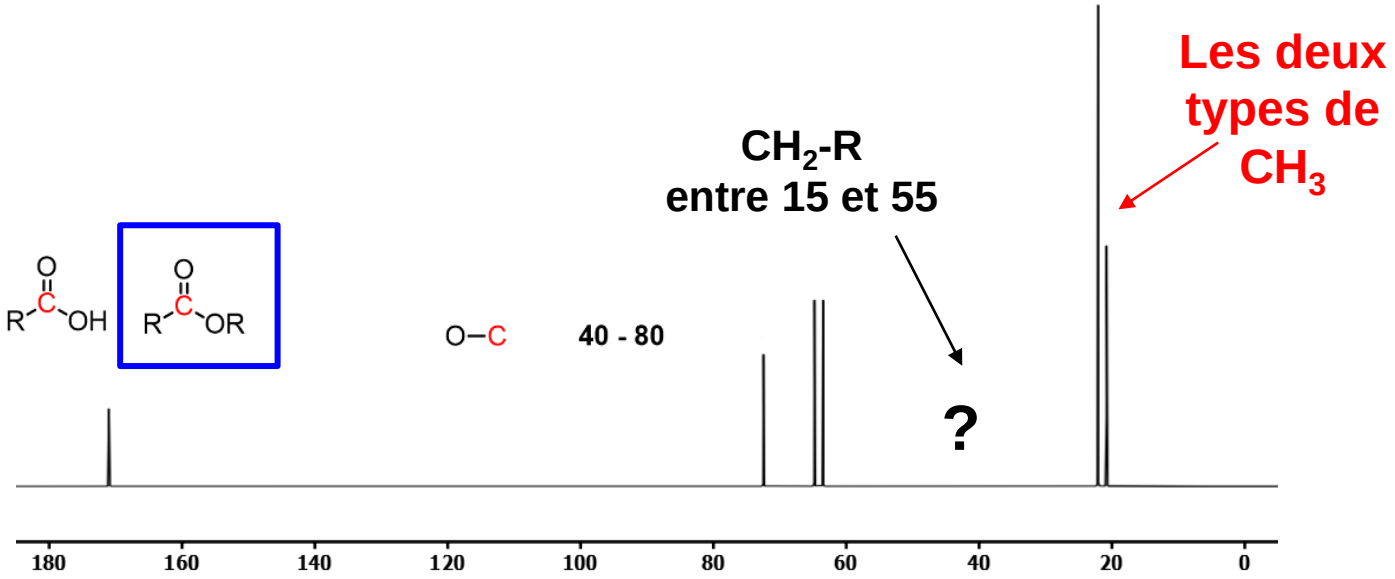
$C_7H_{14}O_3$

RMN ^1H





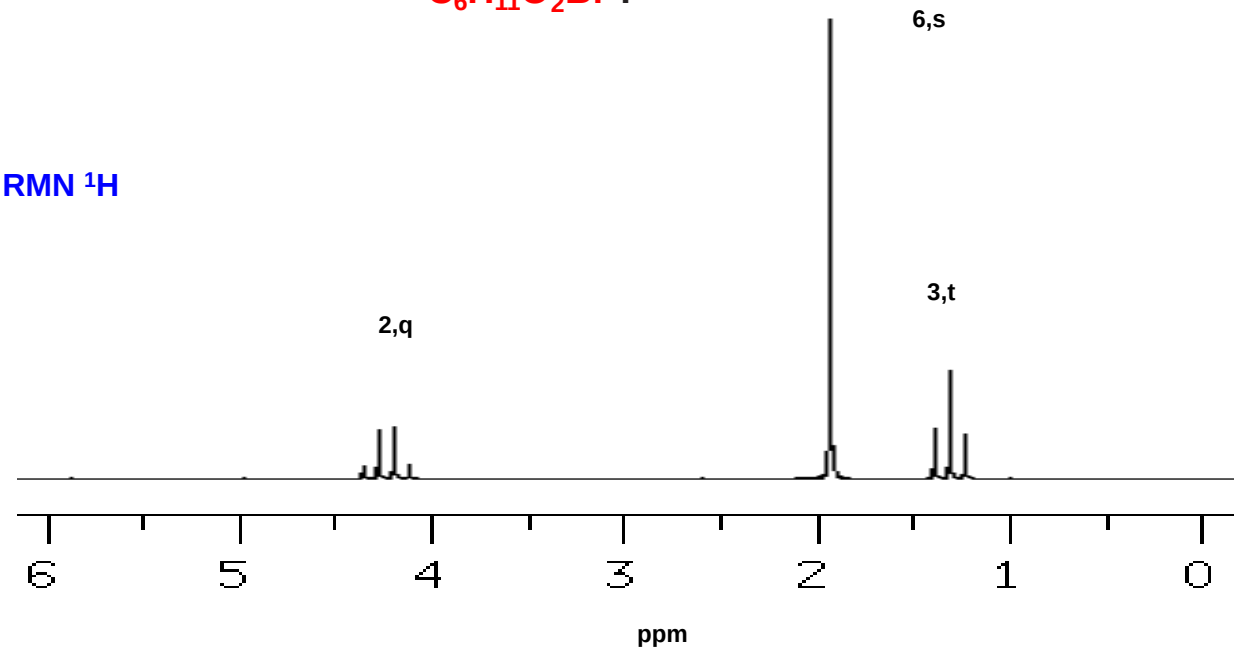
RMN ^{13}C - $\{^1H\}$



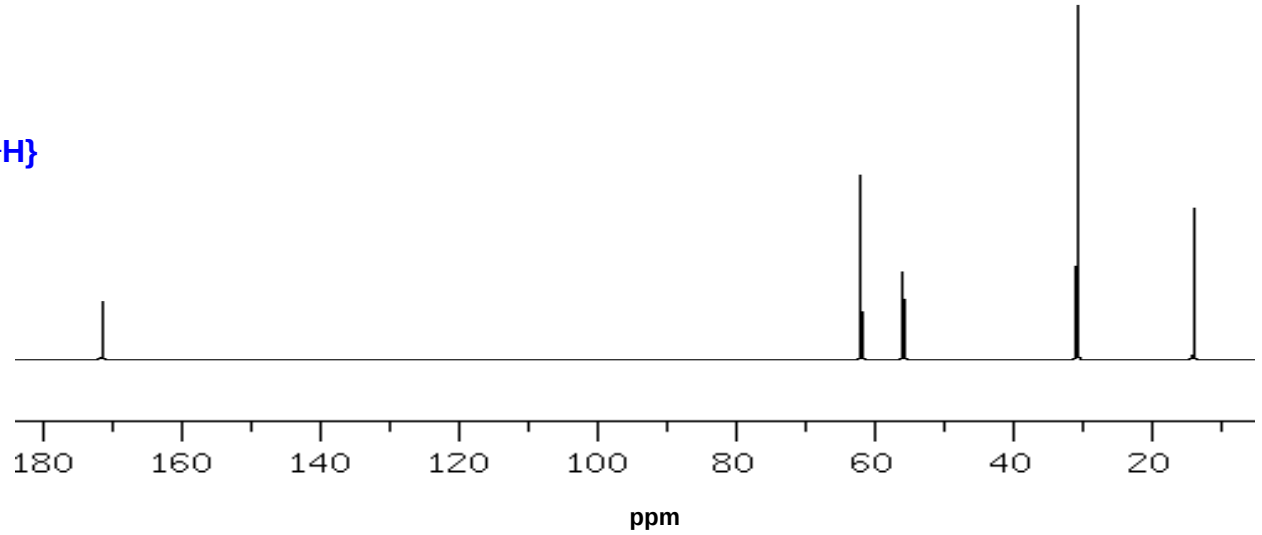
Exercice 5

$C_6H_{11}O_2Br$:

RMN ^1H



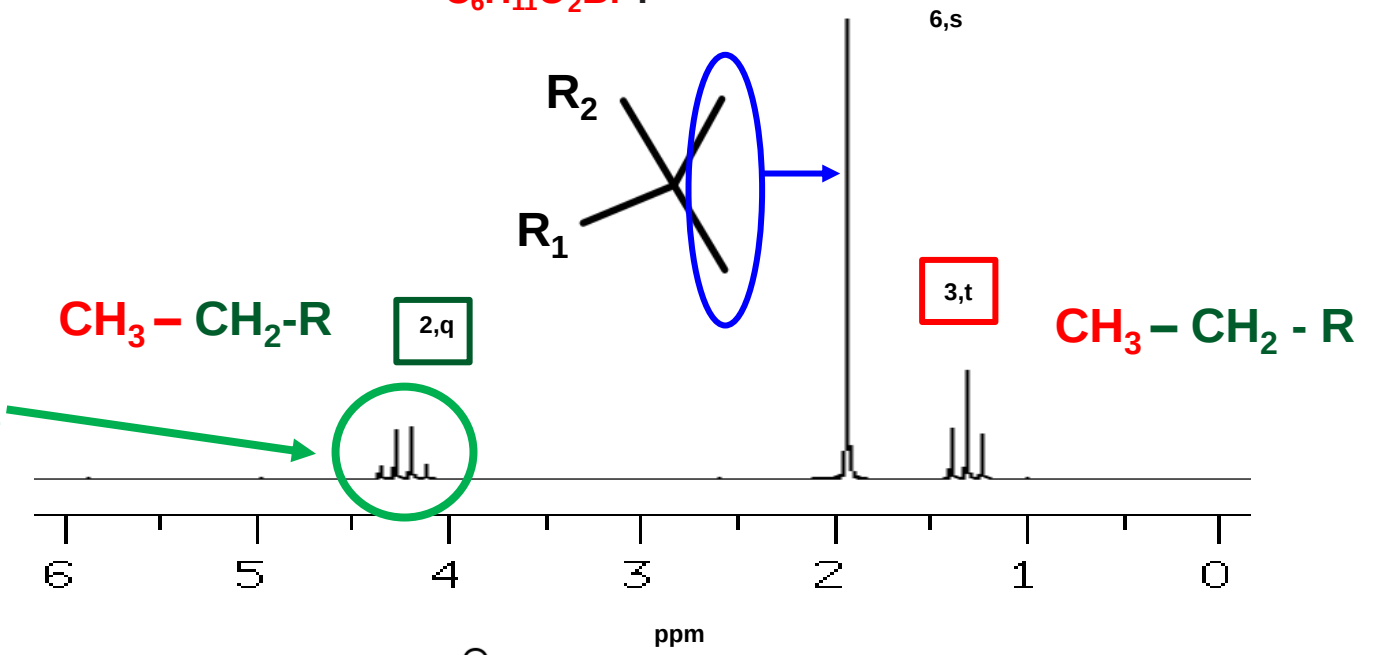
RMN ^{13}C - $\{^1H\}$



Exercice 5

$C_6H_{11}O_2Br$:

RMN ^1H



Notez que le déblindage assez important indique que le CH2 est proche d'un oxygène

RMN ^{13}C - {^1H}