université PARIS-SACLAY | GRADUATE SCHOOL Health and Drug Sciences

Sciences du Médicament et des Produits de Santé

MASTER 1
Development of Drug and Health Products

EXAMEN OTU 06: Basic structural elucidation applied to natural and synthetic compounds

Session: 1st (2021-2022)

May 11th, 2022
1 hour

NMR

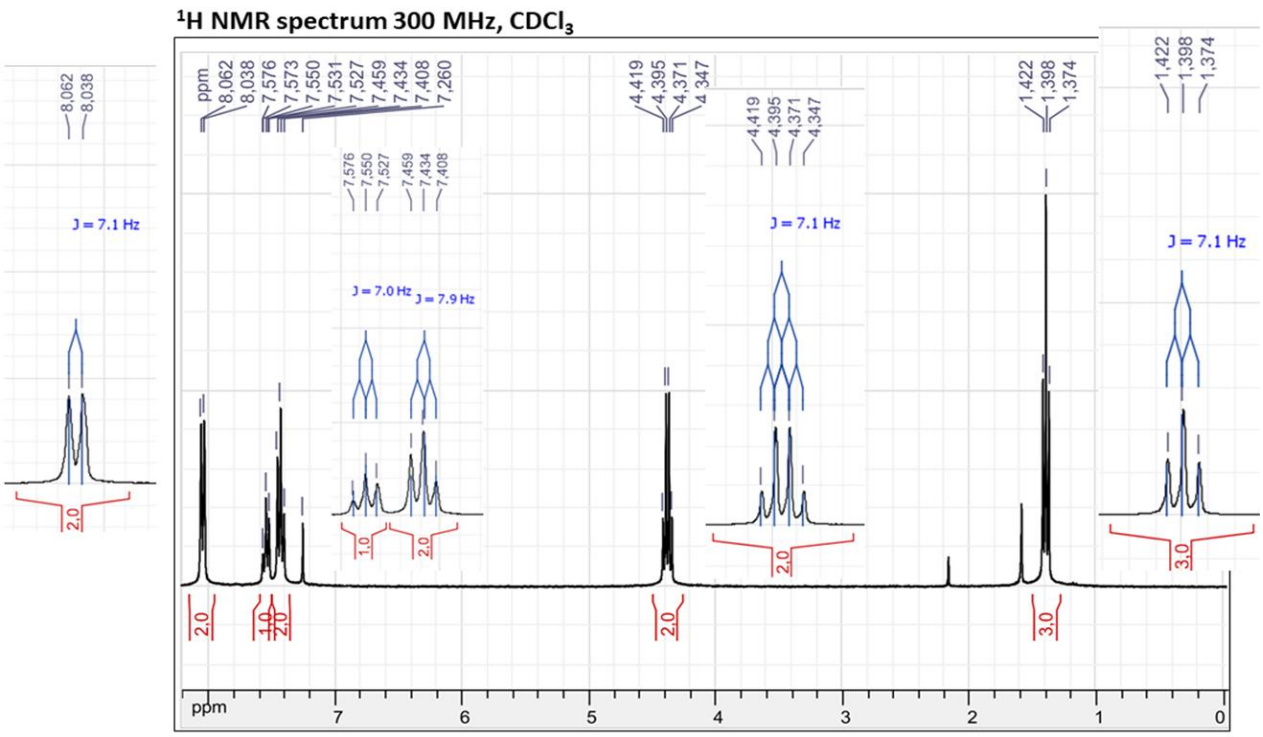
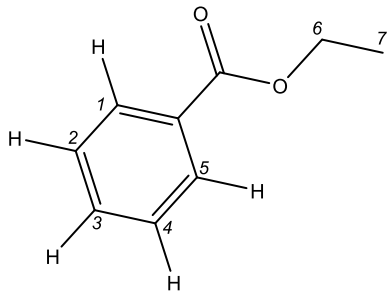


Figure 1: ^{1}H NMR spectrum of molecule A 300 MHz in $CDCl_3$ (peak-picking in ppm)

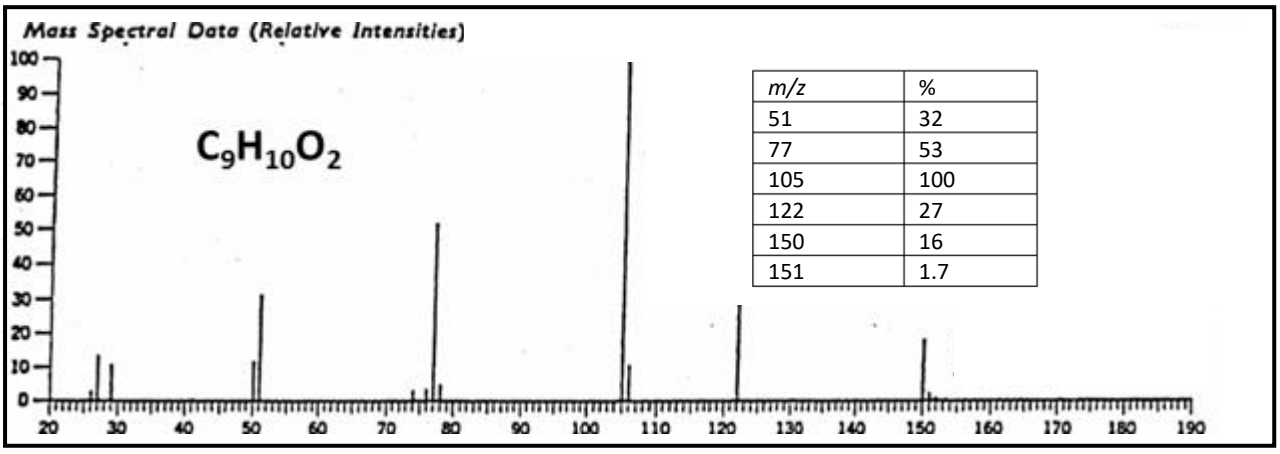
The provided ^{1}H NMR spectrum (Figure 1) is associated with the compound disclosed below.



Assign the ^{1}H NMR chemical shifts to the appropriate protons of the structure using the numbering system used above.
Summarize your data as a table compiling the integrations, multiplicities and different coupling constants.

MS

The electronic impact (EI) mass spectrum of molecule A is reported on the Figure 2.
As this spectrum is constituted of many fragments, this exercise will focus on the most important fragments that are reported in the table.



m/z	%
51	32
77	53
105	100
122	27
150	16
151	1.7

Figure 2: Mass spectrum of molecule A

1. Indicate which peak is the base peak and which is the molecular ion peak.

2. Indicate the nature of the ions at *m/z* = 105, 77 and 51 and detail the mechanism of their formation.

3. The formation of the ion at *m/z* = 122 is the result of a transposition mechanism, the neutral fragment having the chemical formula C_2H_4. Explain the mechanism of its formation.