

UNIVERSITY OF ESWATINI



MAIN EXAMINATION 2020/2021

TITLE OF PAPER: APPLIED SPECTROSCOPY

COURSE NUMBER: CHE602

TIME ALLOWED: THREE (3) HOURS

INSTRUCTIONS: THERE ARE SIX (6) QUESTIONS IN THIS PAPER. ANSWER ANY FOUR (4)

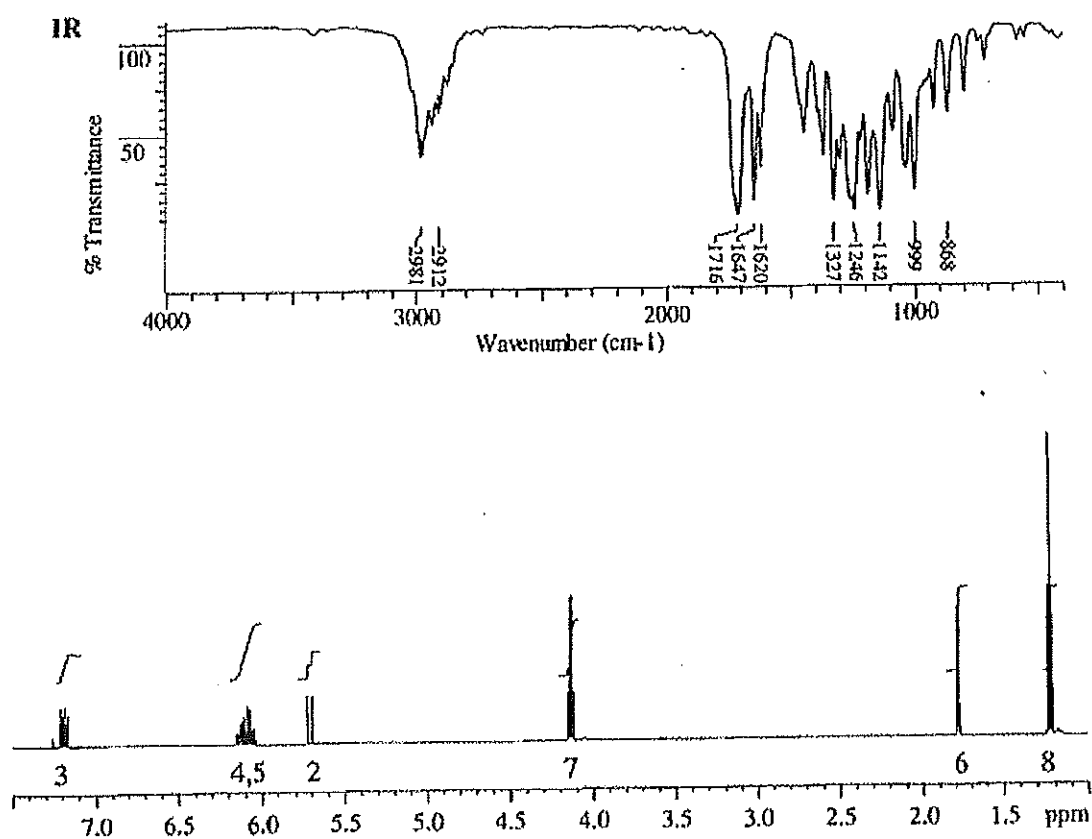
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Question 1

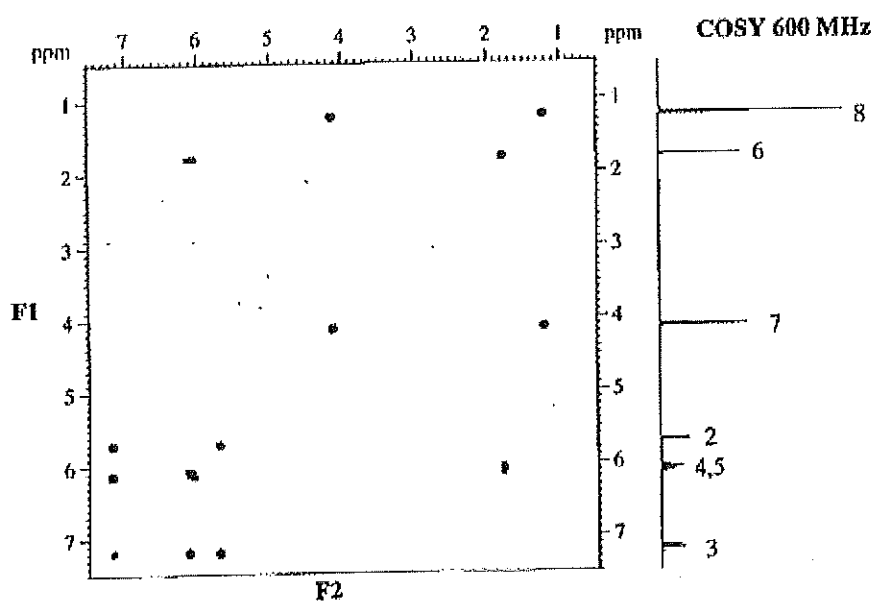
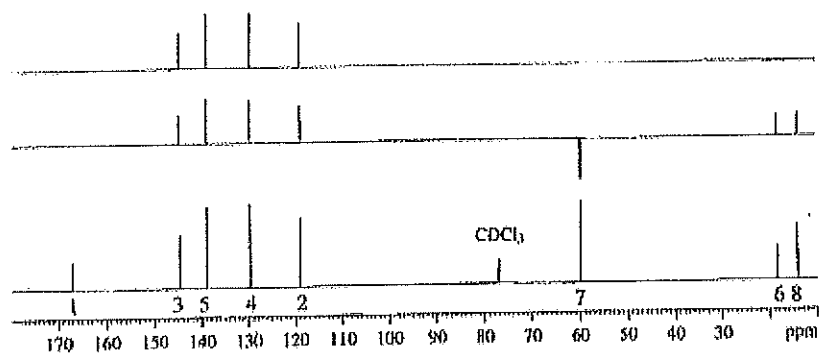
(a) Calculate the Index of Hydrogen deficiency of the following compounds. [10]

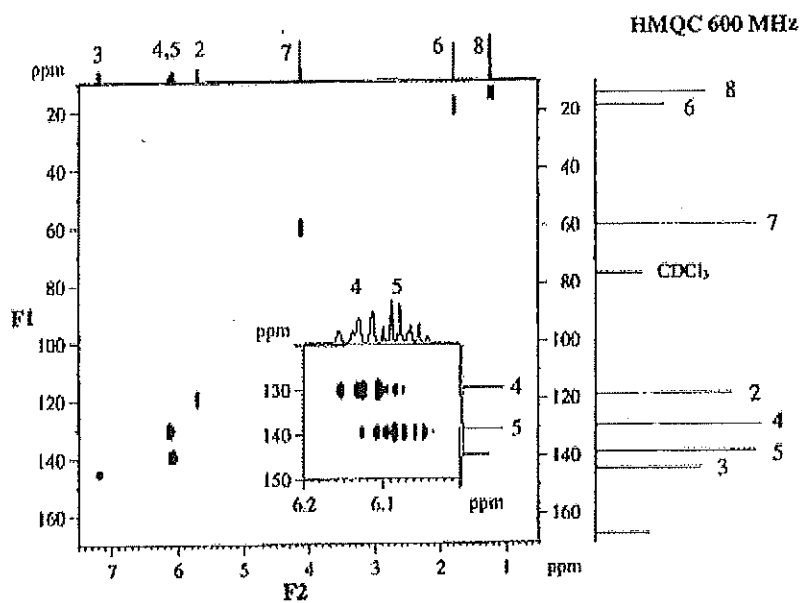
- (i) $C_6H_6N_2O$
- (ii) $C_{29}H_{50}O$
- (iii) C_4H_3IS
- (iv) $C_9H_{11}IN_2O_6$
- (v) $C_{11}H_{12}Cl_2N_2O_5$

(b) Predict the structure of the molecule represented by the following spectra i.e. IR, 1H , ^{13}C /DEPT, COSY, HMQC. [15]



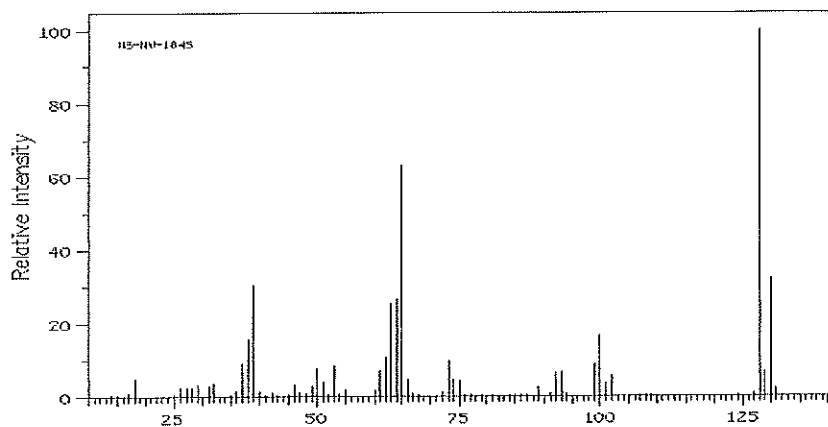
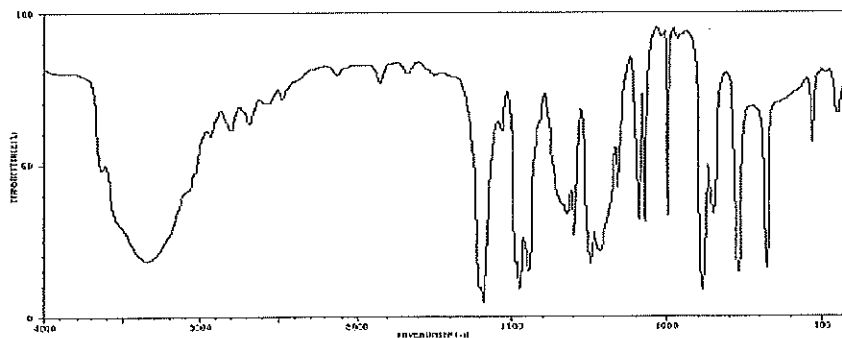
¹³C/DEPT NMR 150.9 MHz





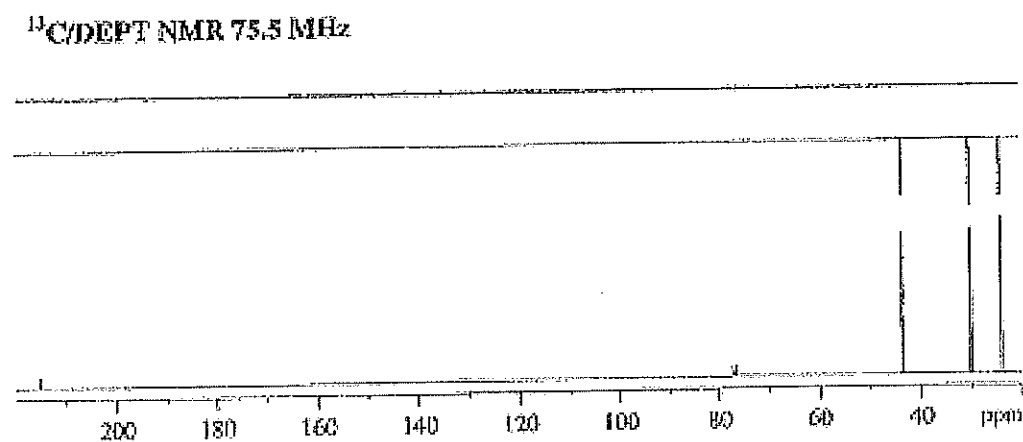
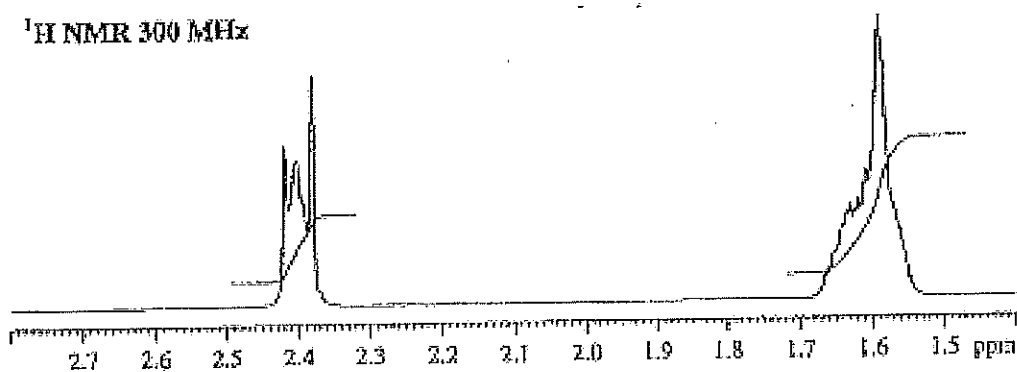
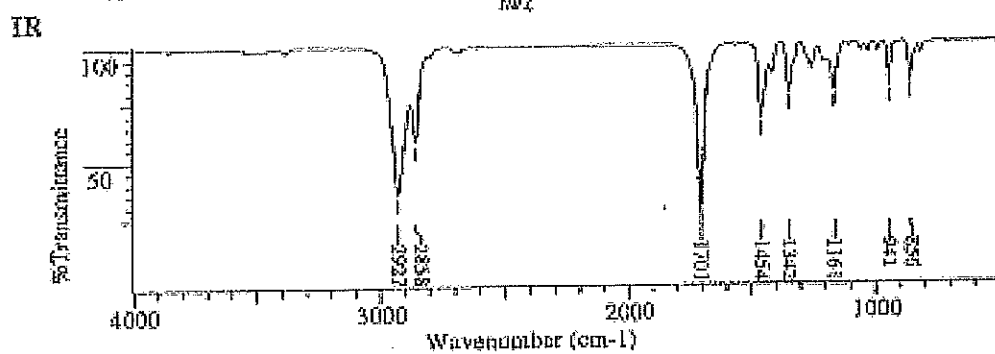
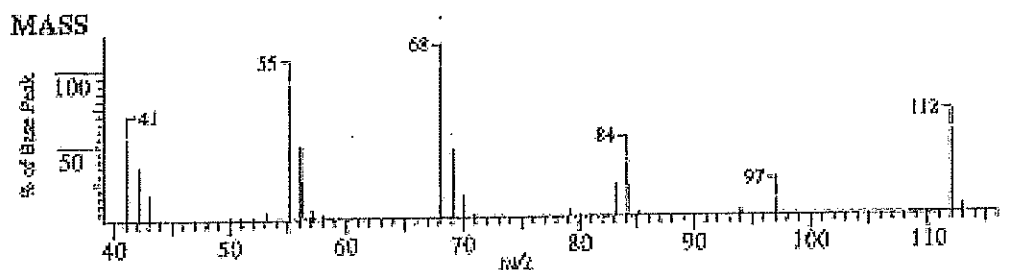
Question 2

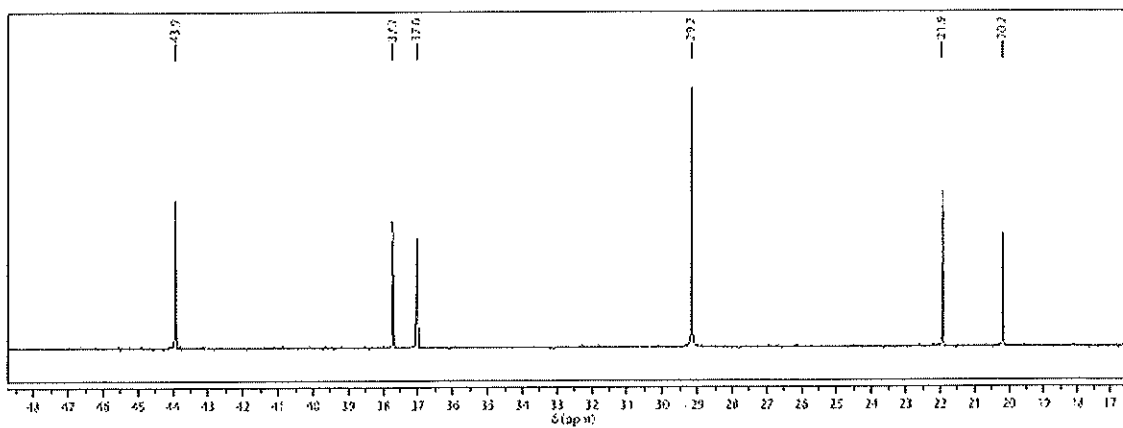
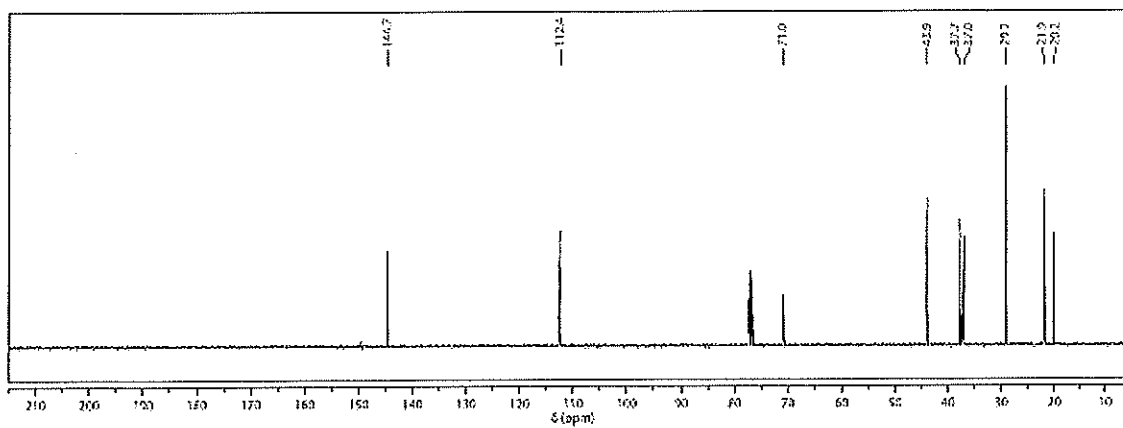
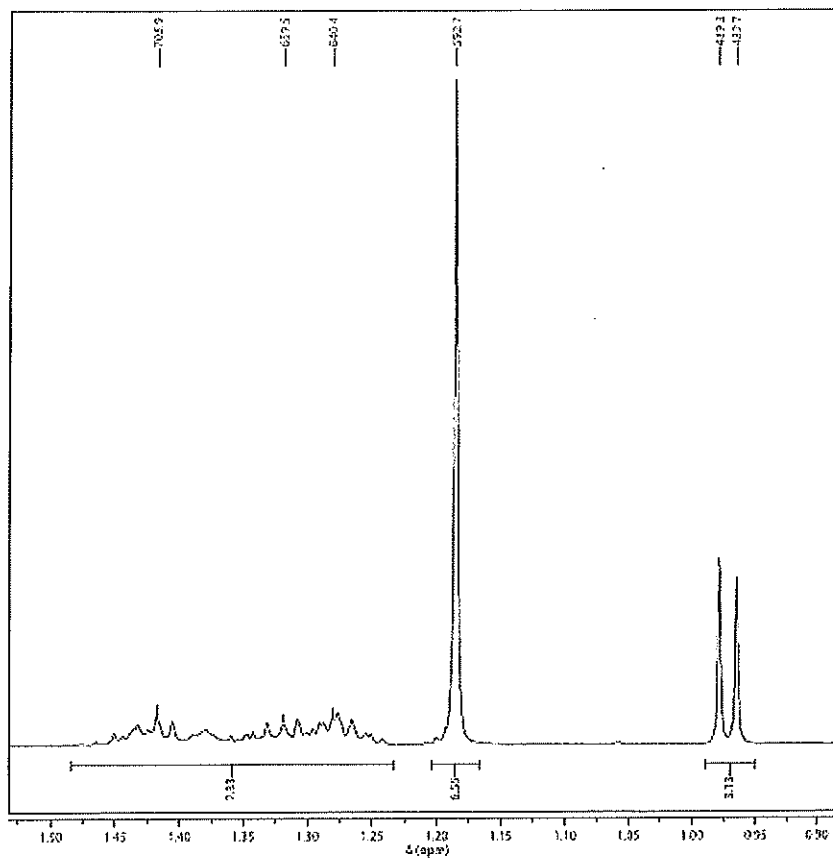
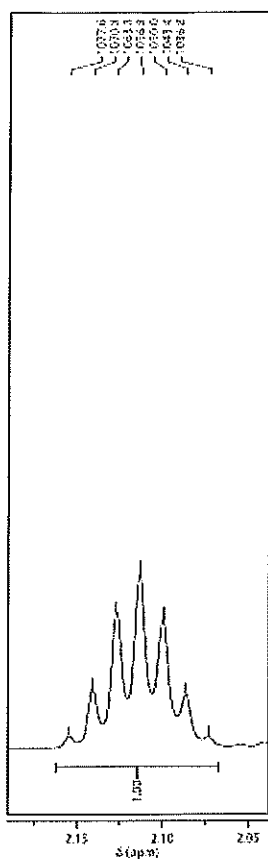
- (a) Compare and contrast CI ionization and EI ionization in mass spectrometry. [6]
- (b) What kind of information can you derive from DEPT (all DEPT experiments), COSY, HMQC and HMBC NMR experiments? [11]
- (c) Determine the molecular formula and possible structures based on the given IR & MS spectra. [8]



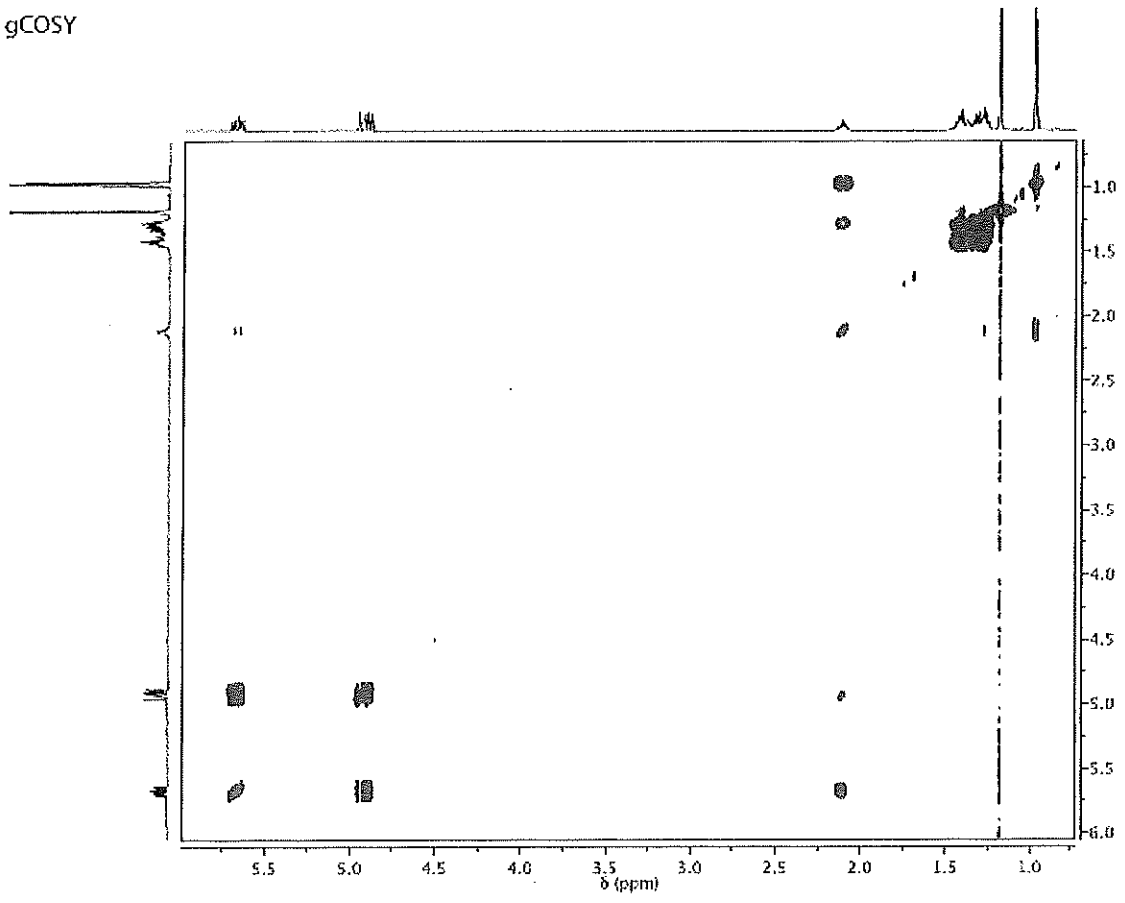
Question 3

Determine the structure of the compound best represented by the following spectral information (MS, IR, ^1H NMR, ^{13}C /DEPT). [25]

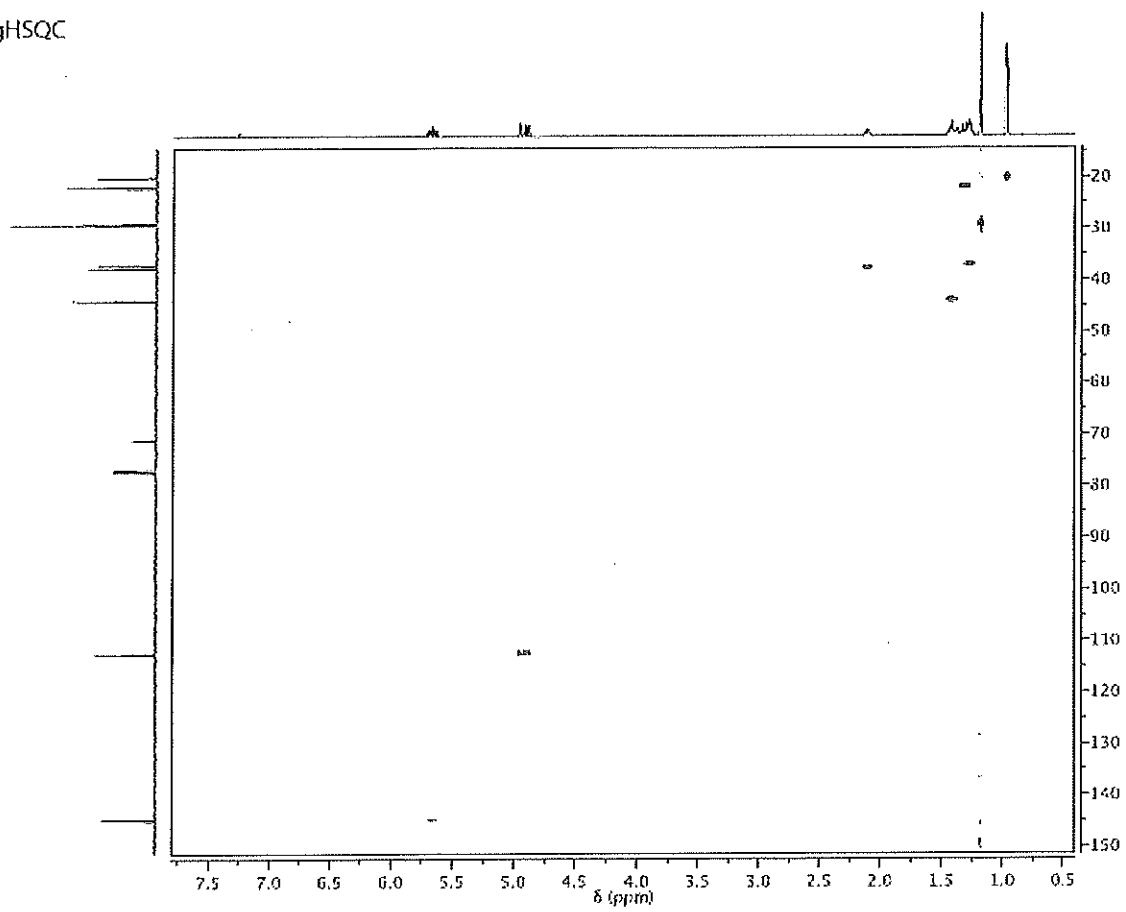




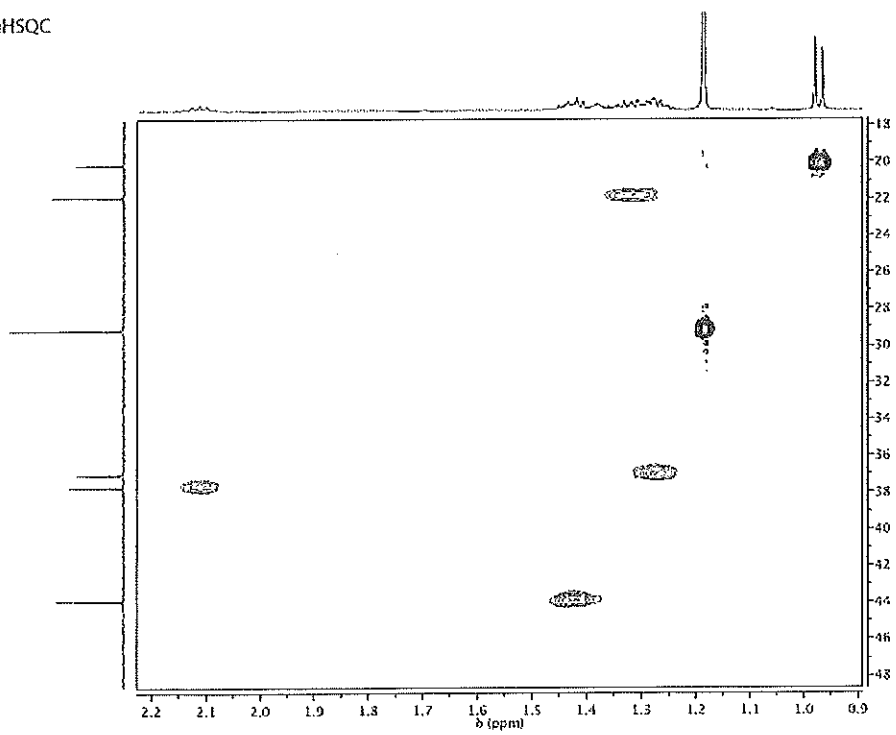
gCOSY



gHSQC

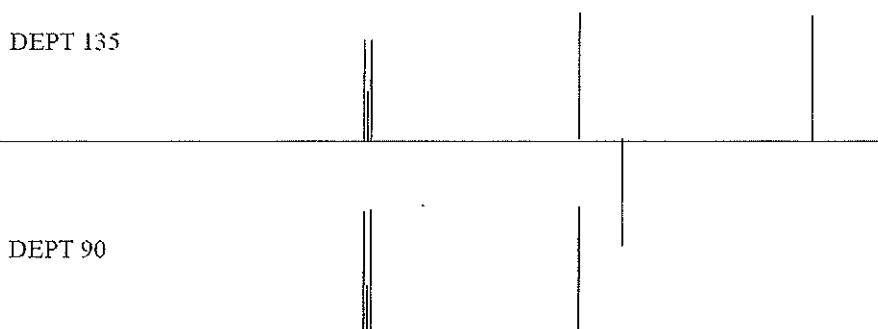
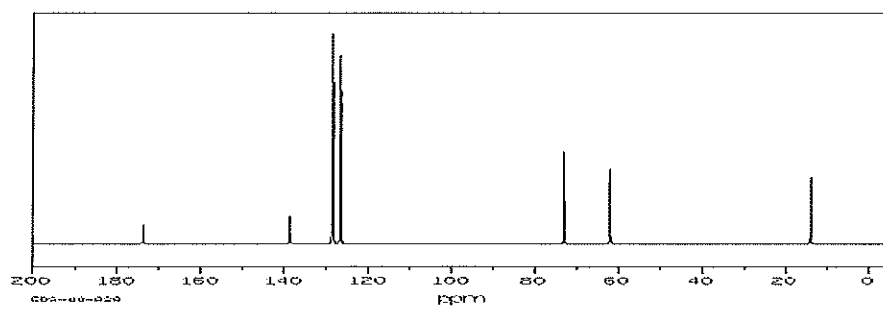
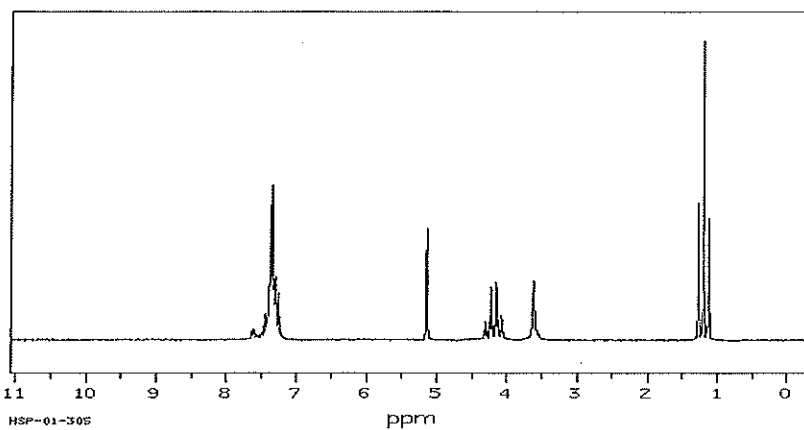
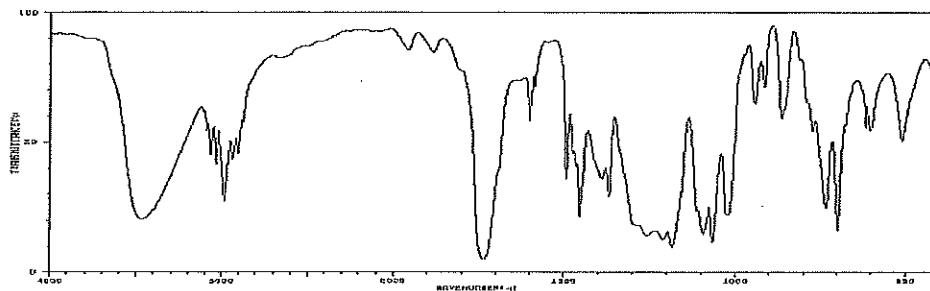


gHSQC



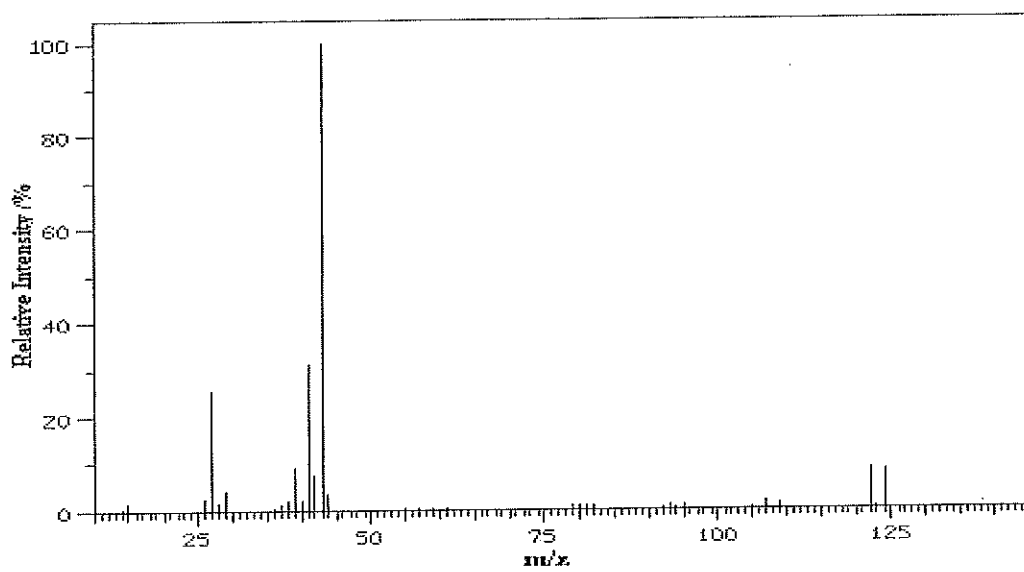
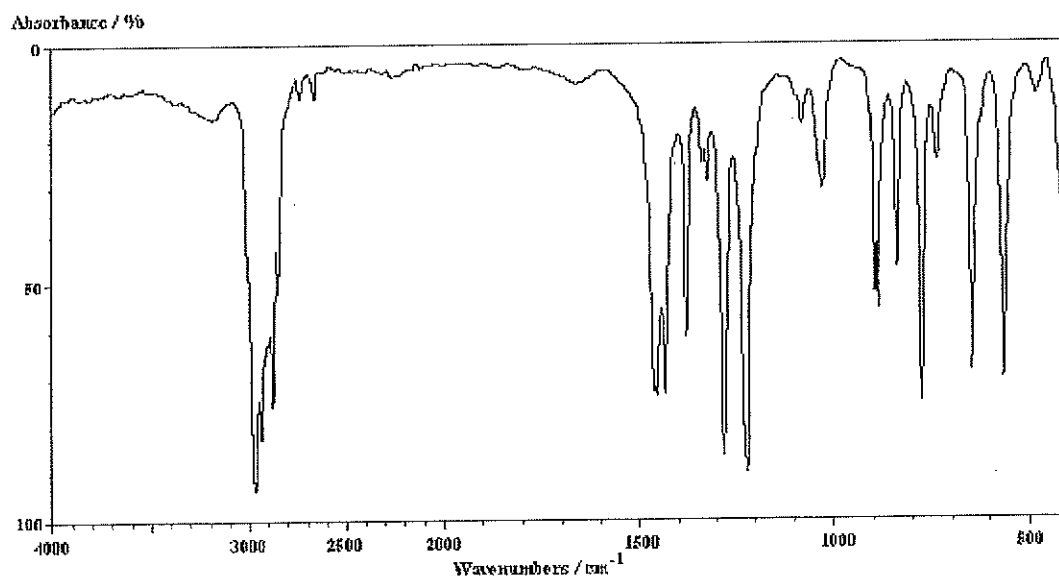
Question 5

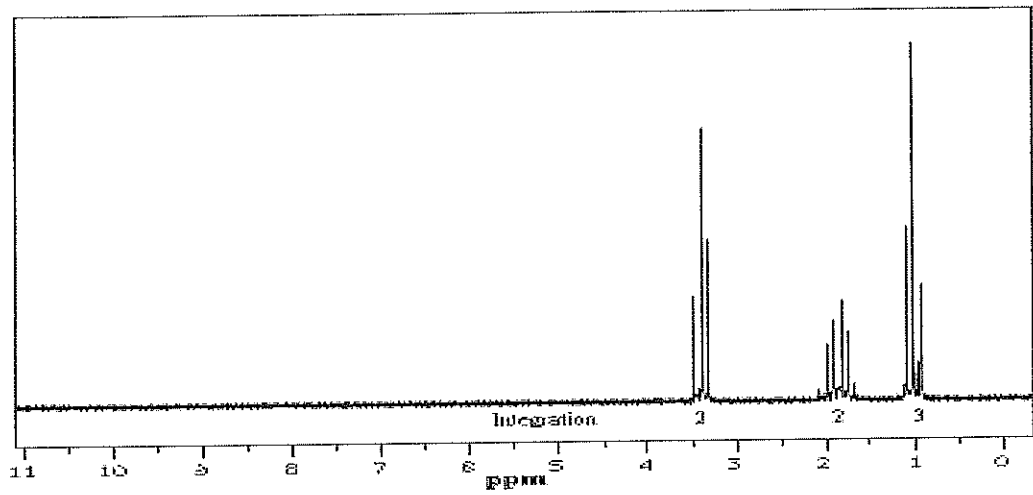
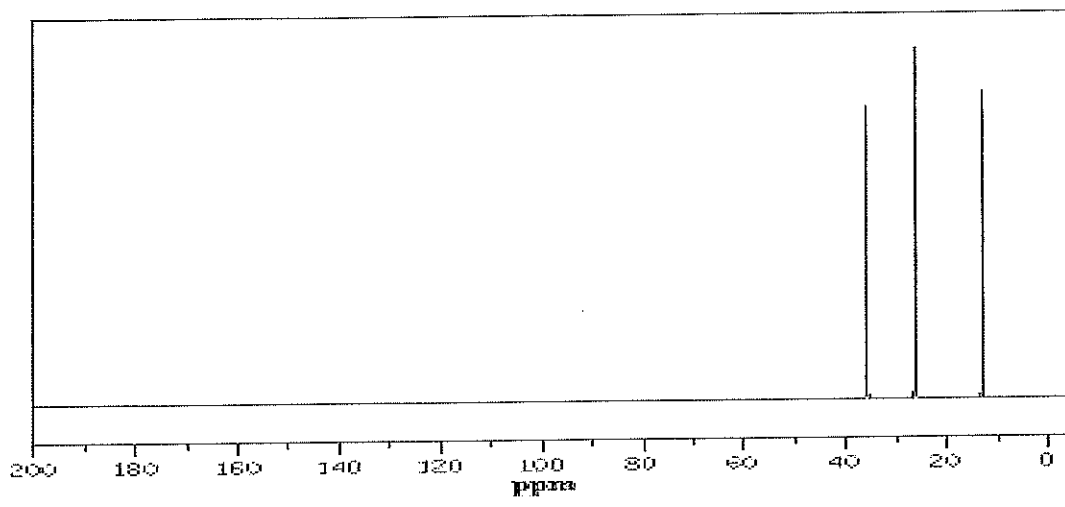
- (a) Compound X has an empirical formula of $C_{10}H_{12}O_3$. Given the following spectra. [15]
- Determine the degree of unsaturation for the compound.
 - Assign the pertinent IR peaks.
 - Show all your work clearly and draw the structure.



(b) Draw the structure that fits the following spectra.

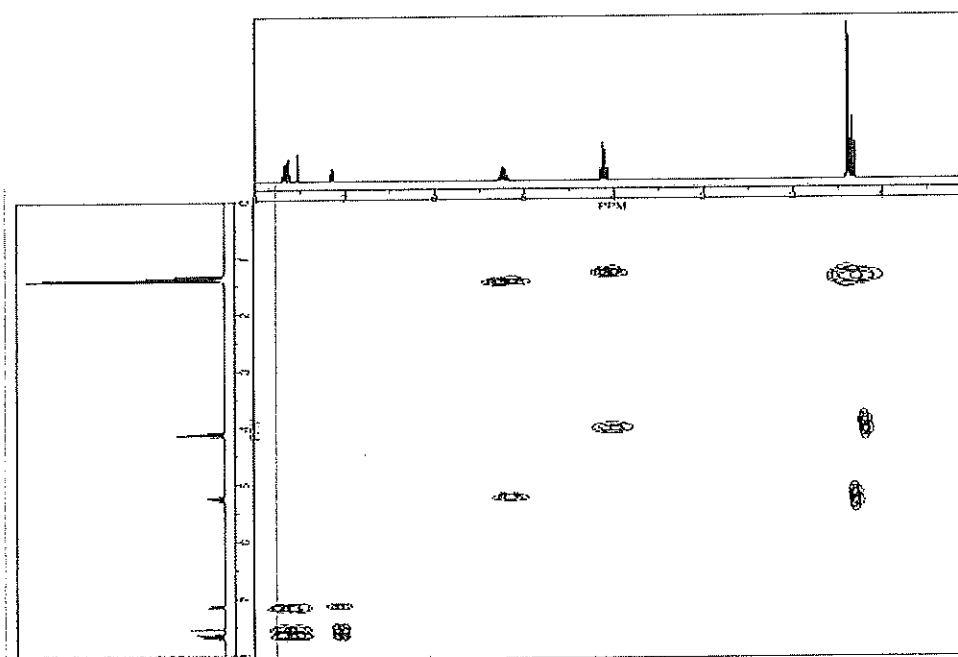
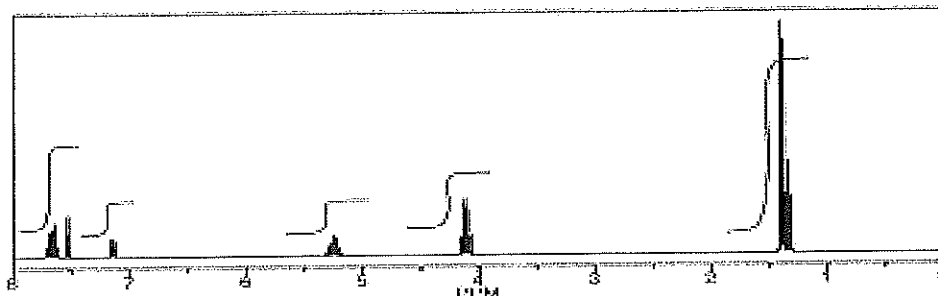
[10]





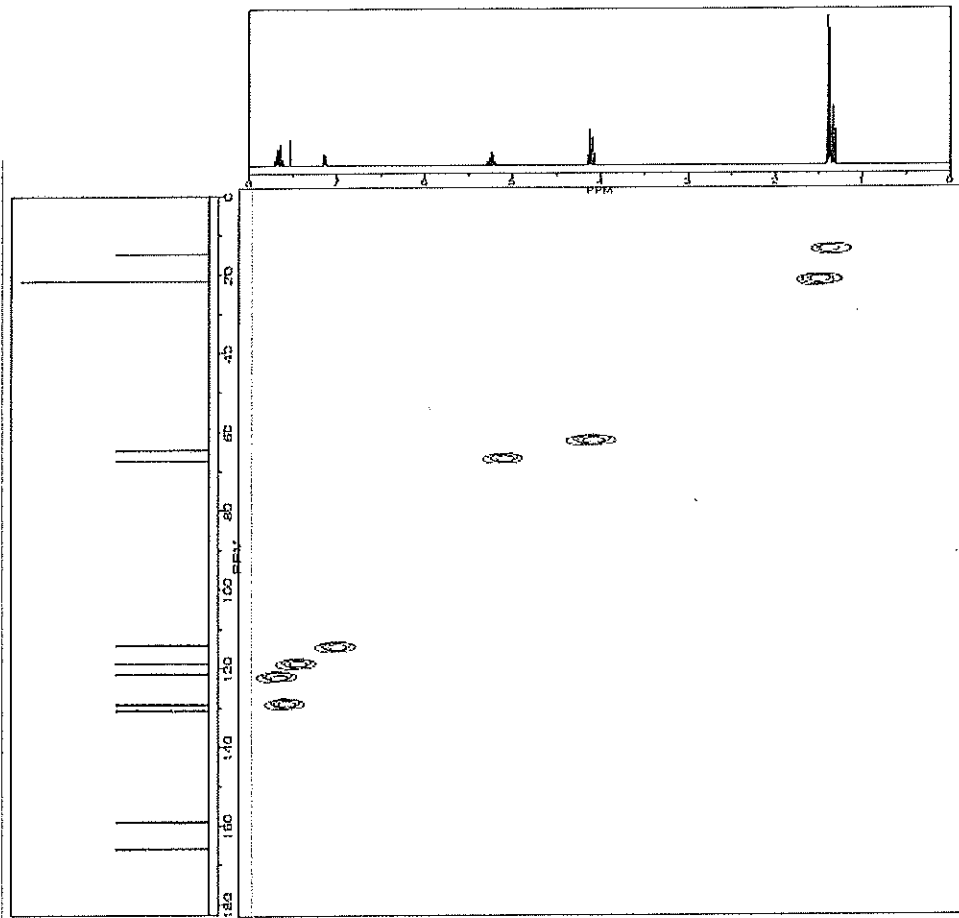
Question 6

- (a) Suggest how pentan-2-one and pentan-3-one could be distinguished in a mass spectrum. Write equations and m/z values for the formation of any important fragment ions. [5]
- (b) Analyse the data to determine the structure of the compound with the molecular formula $C_{12}H_{16}O_3$. [20]

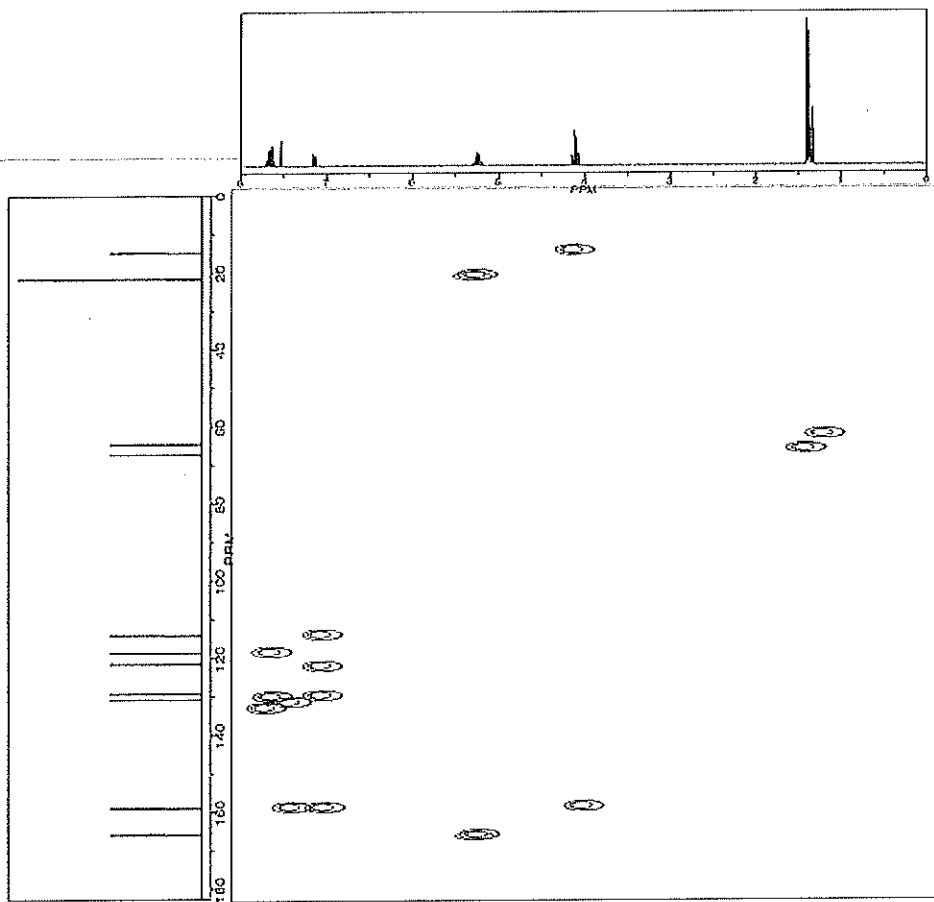


COSY

HMQC



HMBC



---The End---