

Αλογονοπαράγωγα.

Τα χλωρίδια και τα βρωμίδια εμφανίζουν τις χαρακτηριστικές $[M + 2]^+$ ισοτοπικές κορυφές. Στα αρωματικά, όταν υπάρχουν όλα τα αλογόνα, αποσπώνται κατά σειρά I, Br, Cl και τέλος το HF. Στα RX όσο μεγαλύτερο το μήκος του αλκυλίου τόσο πιο μικρό M^+ υπάρχει. Επίσης η ένταση του M^+ ελαττώνεται από το I προς Br, Cl, F.

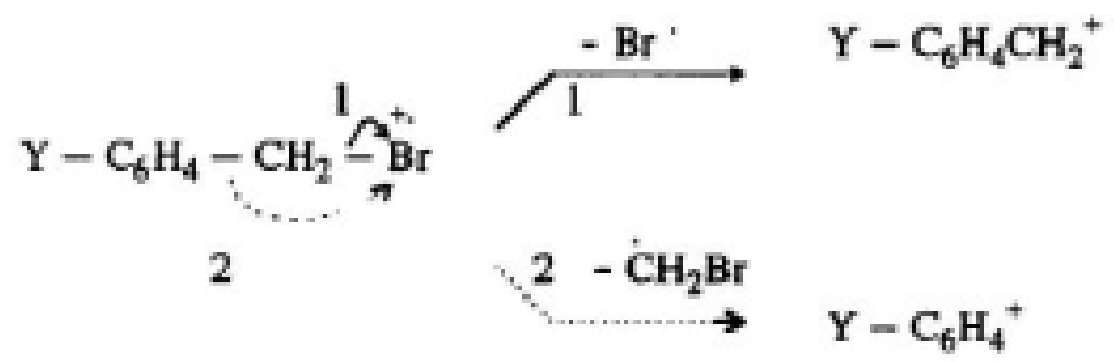
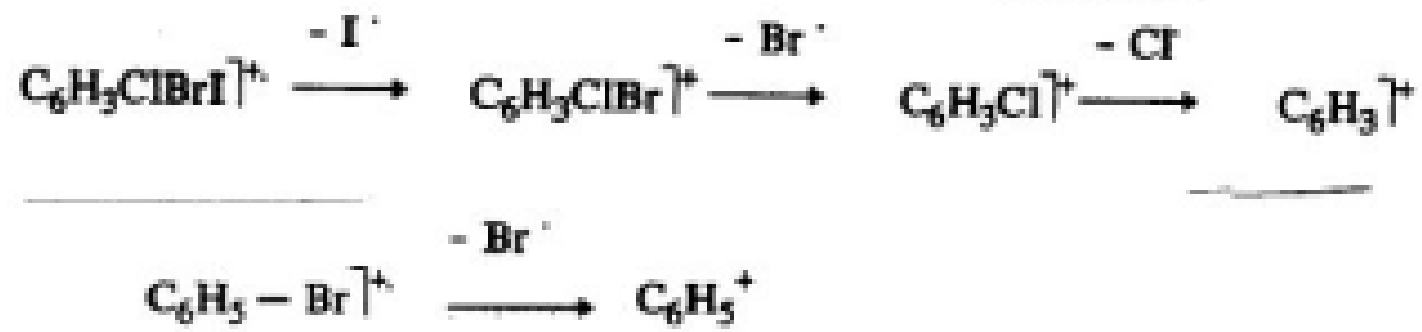
SPECTRAL ANALYSIS BOX — Alkyl Halides

MOLECULAR ION

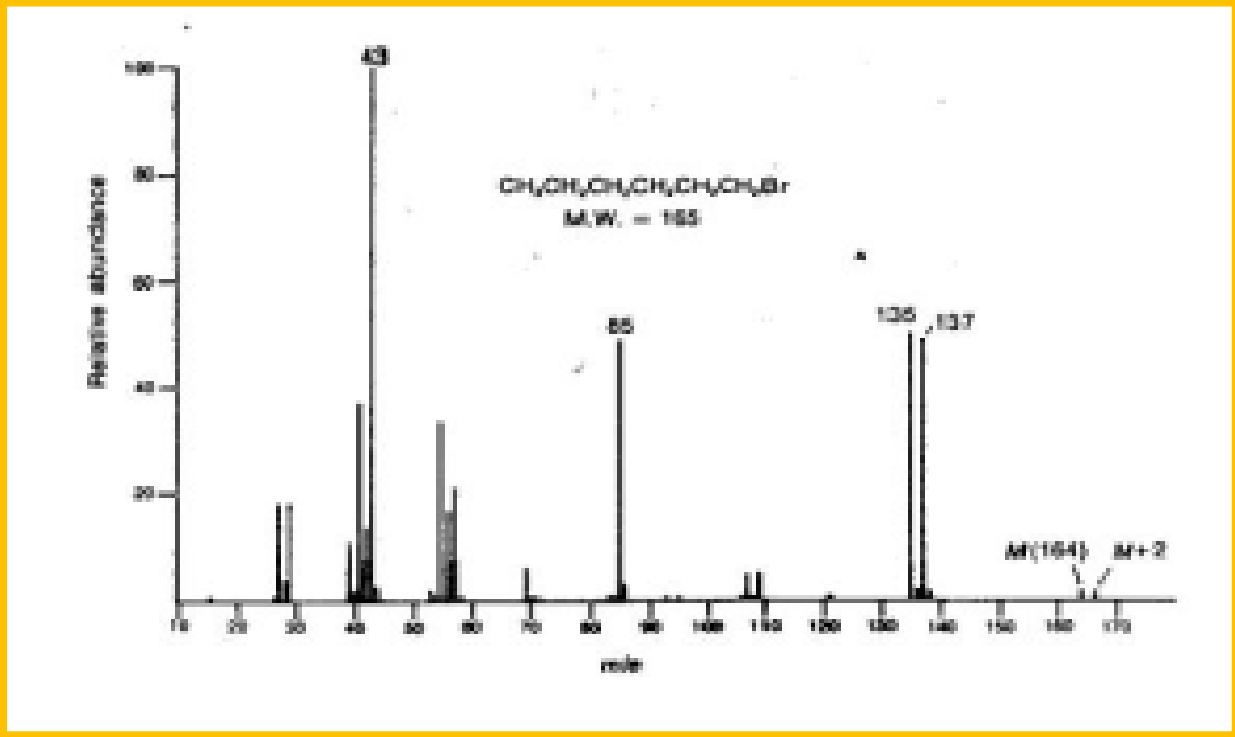
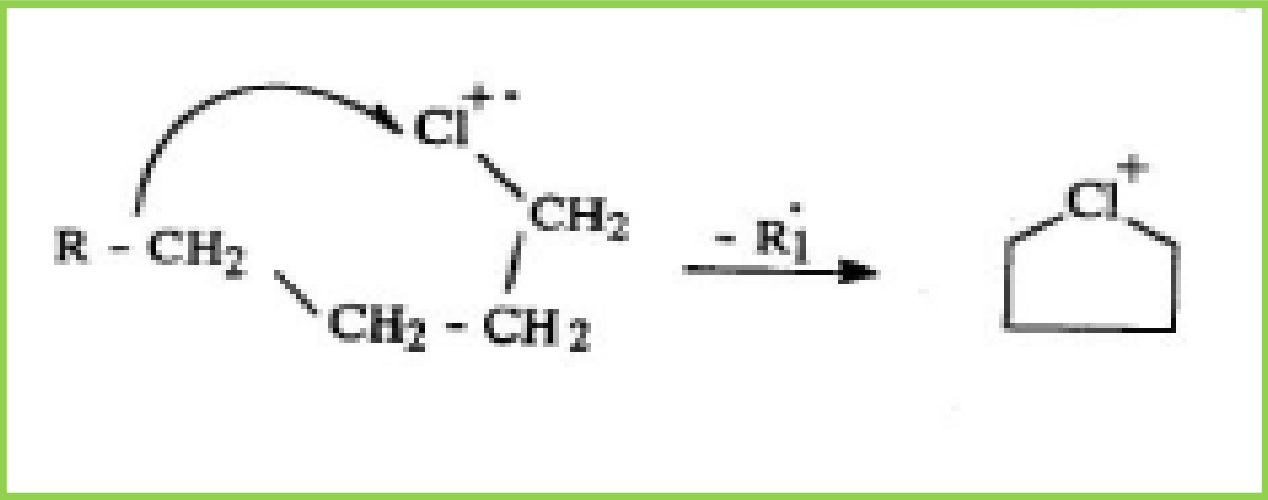
Strong $M + 2$ peak
(for Cl, $M/M + 2 = 3:1$;
for Br, $M/M + 2 = 1:1$)

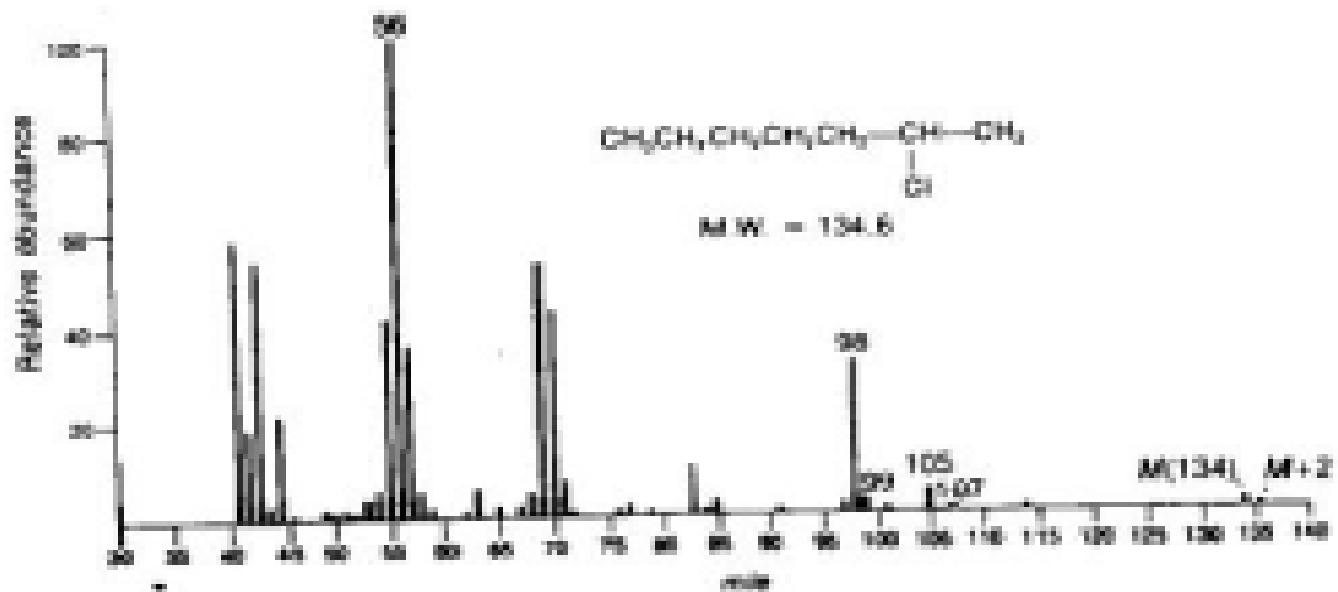
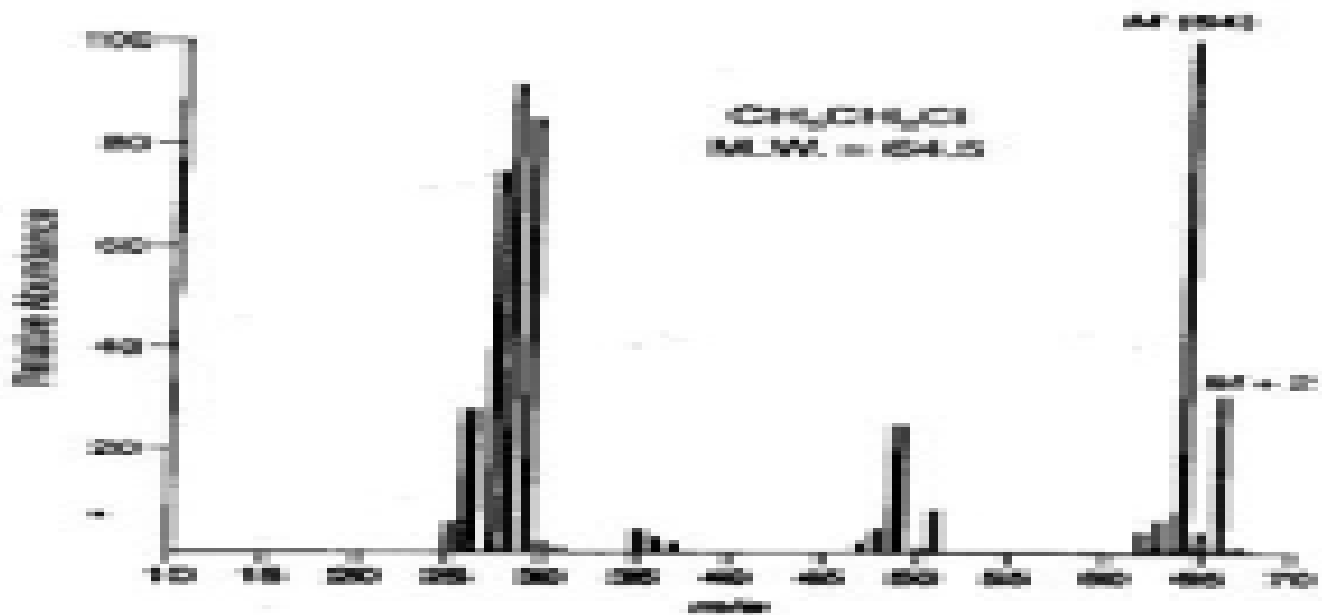
FRAGMENT IONS

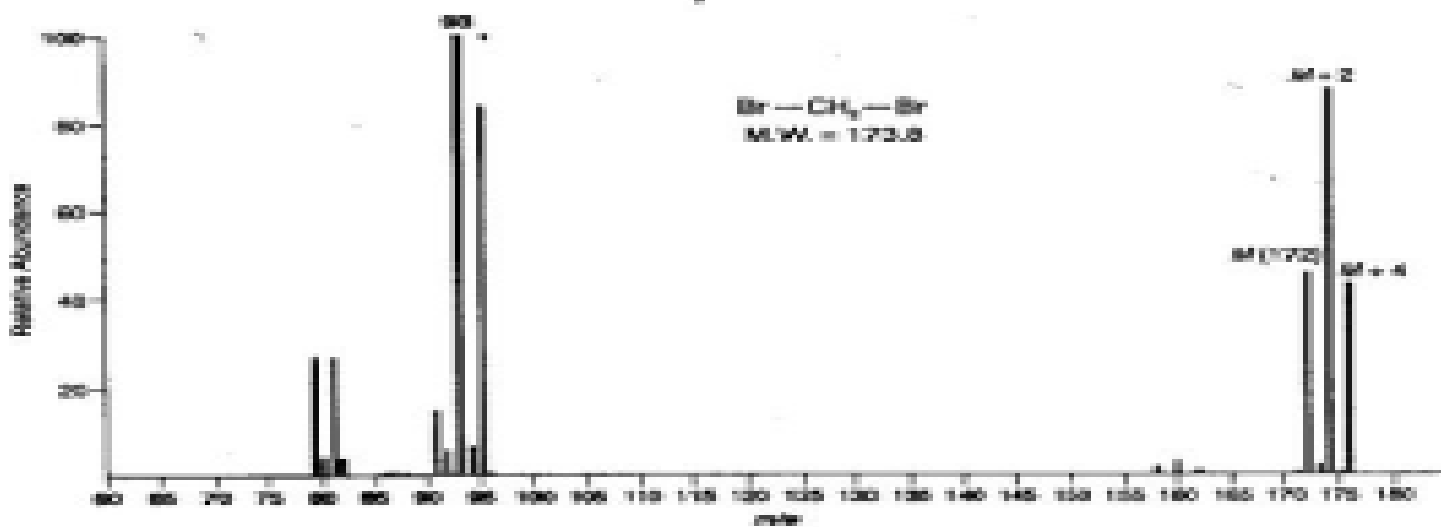
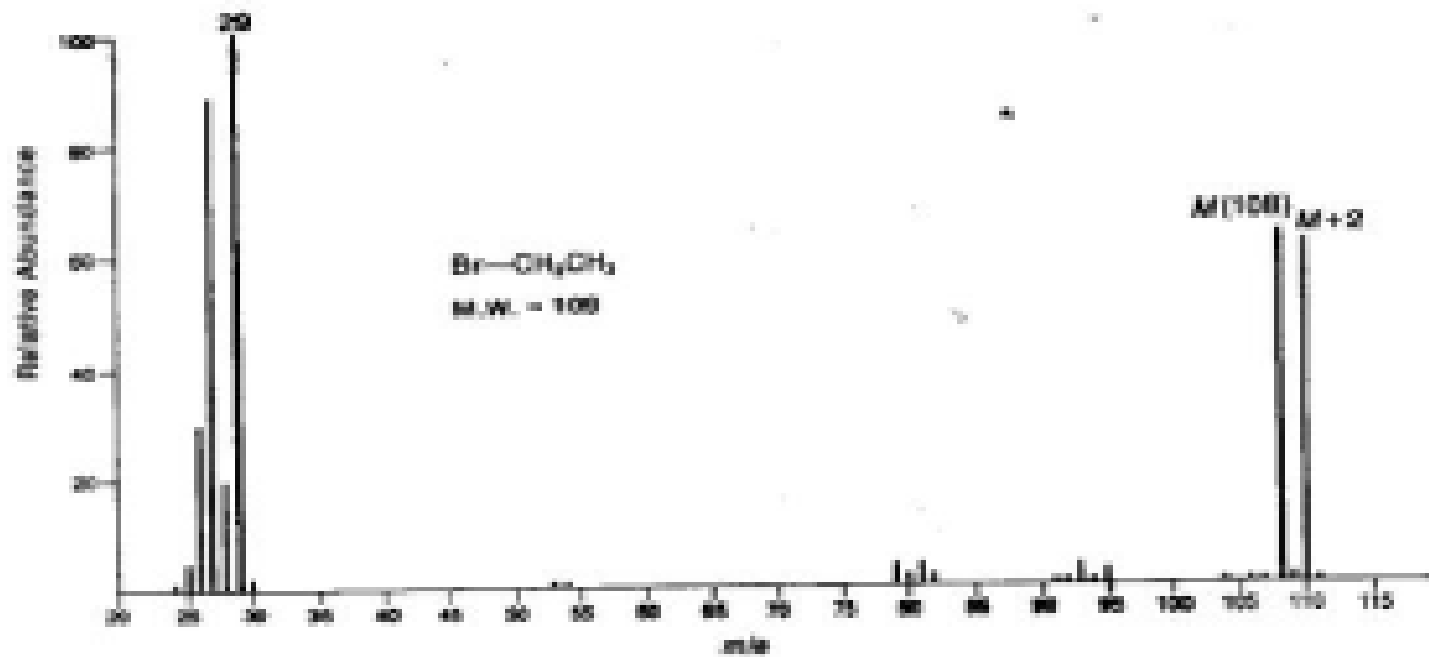
Loss of Cl or Br
Loss of HCl
 α -Cleavage

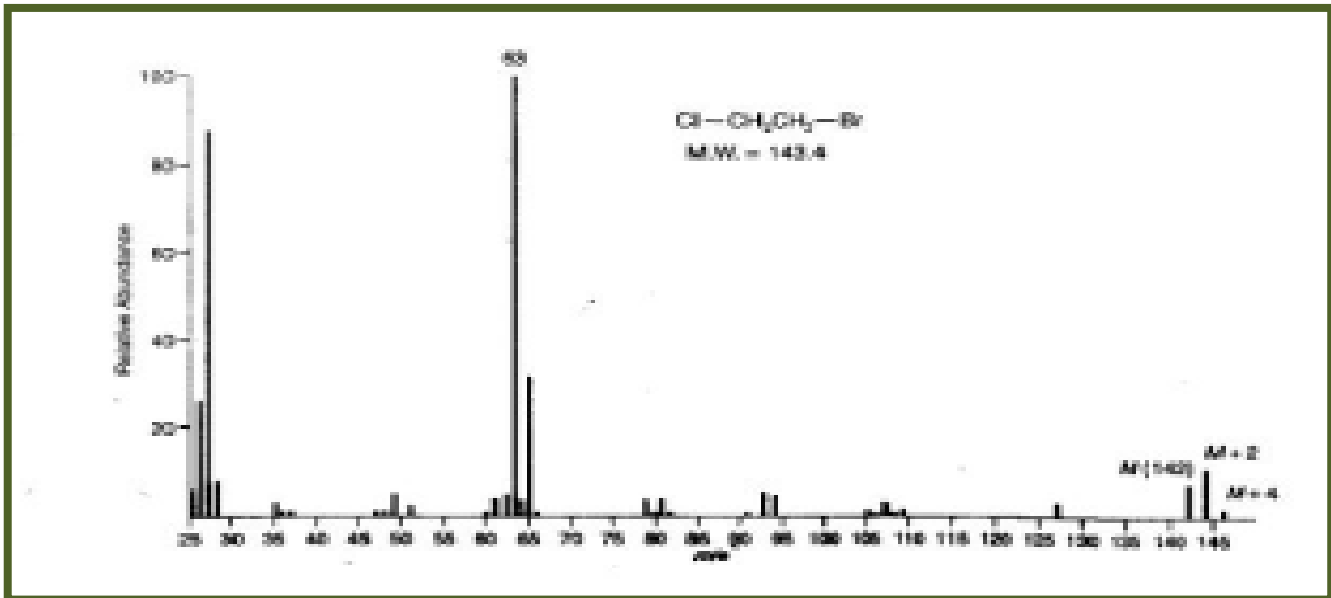
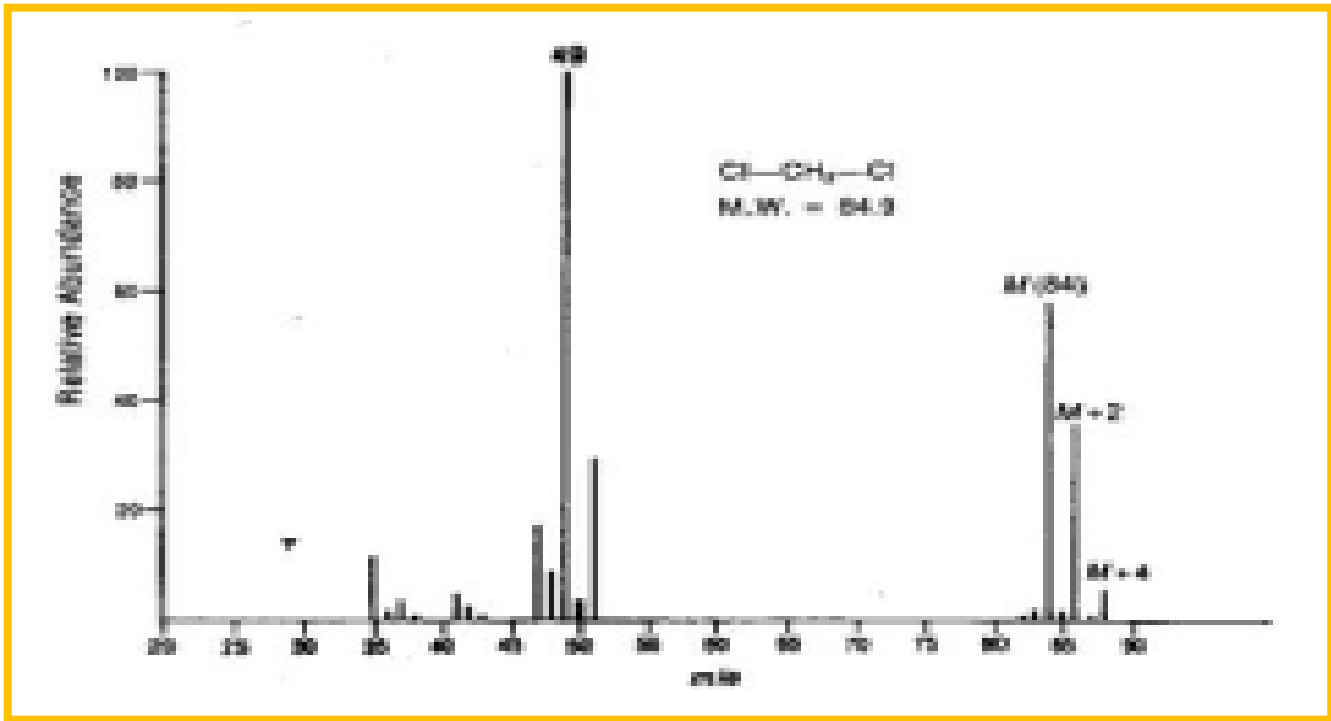


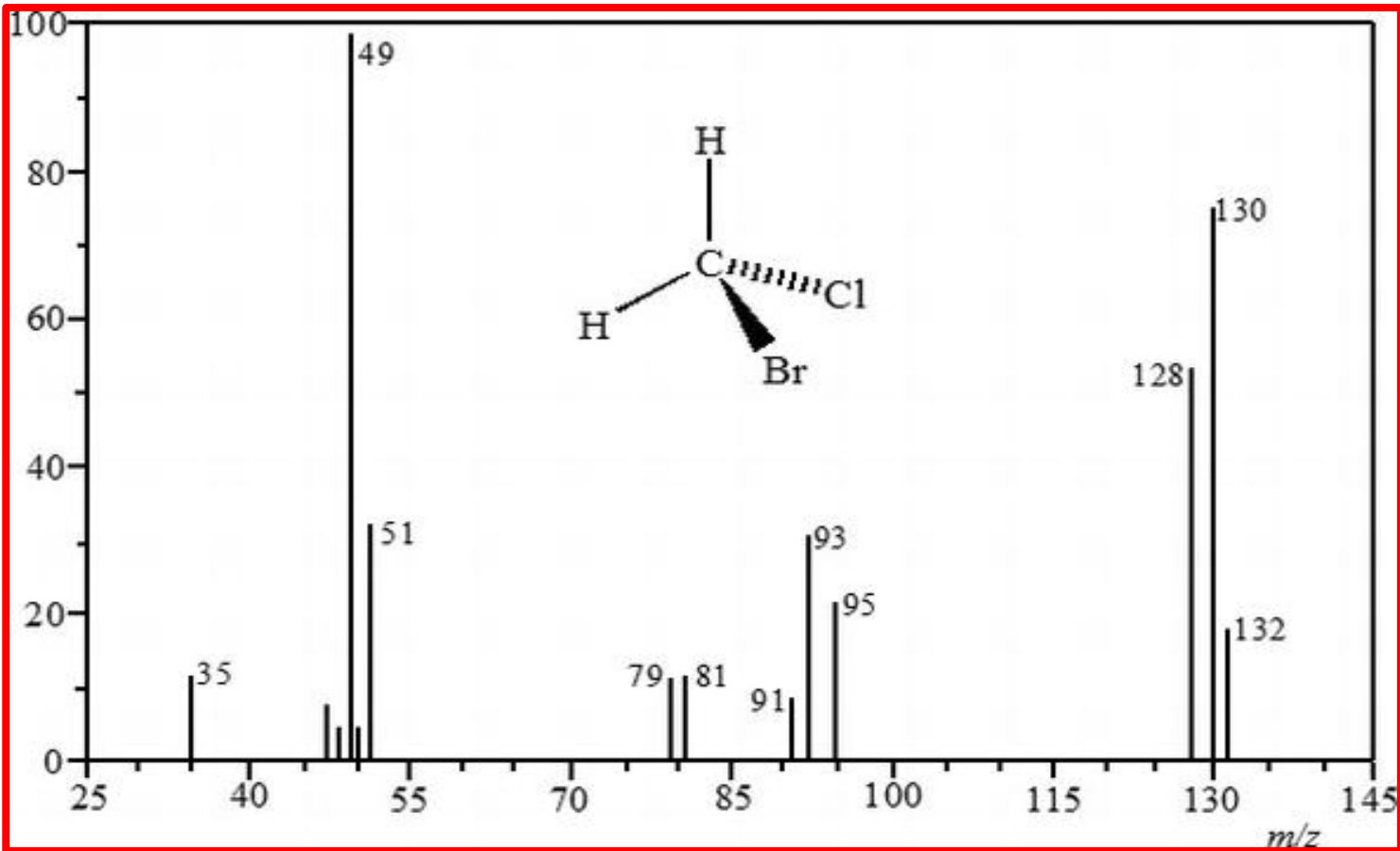




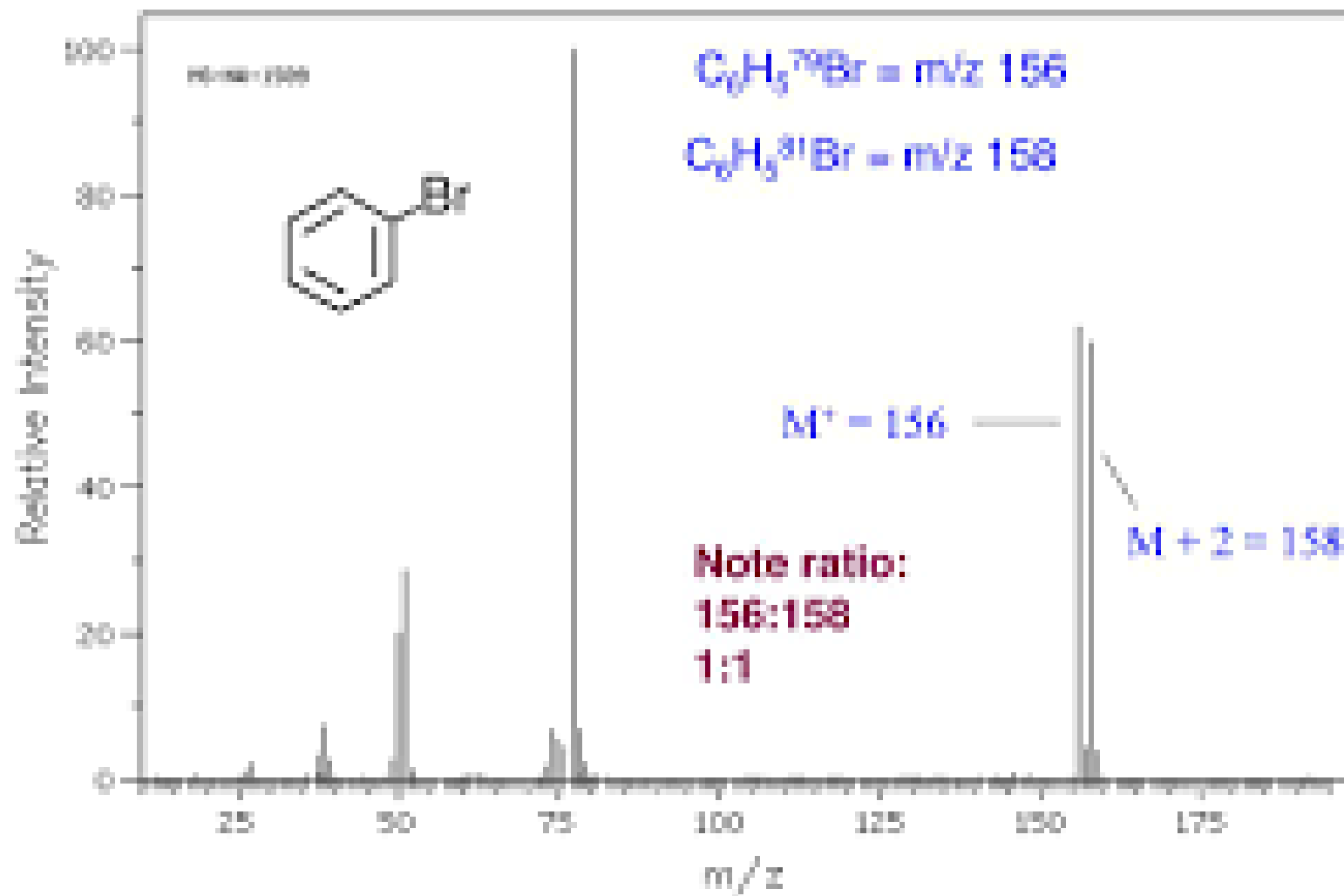




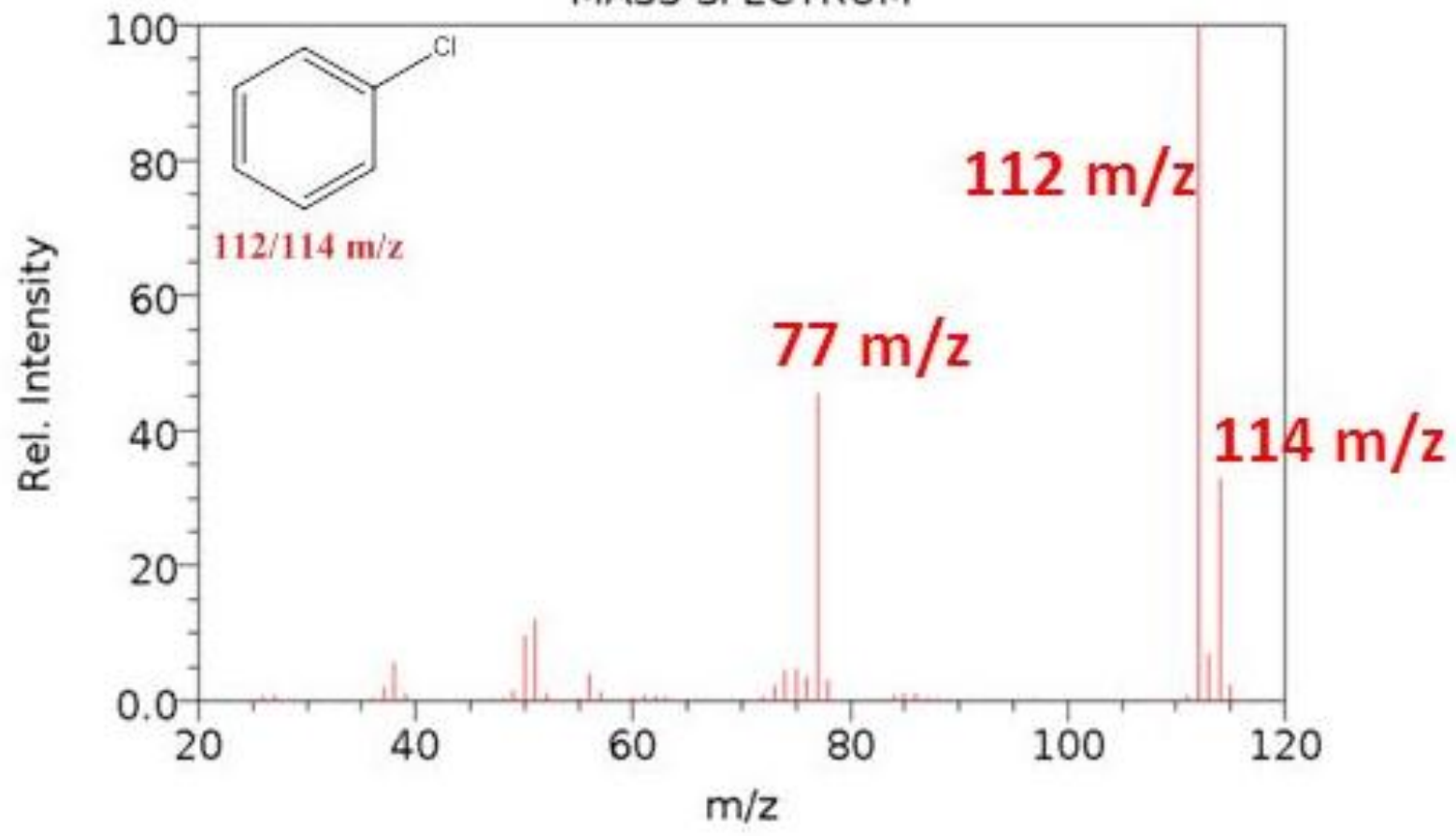


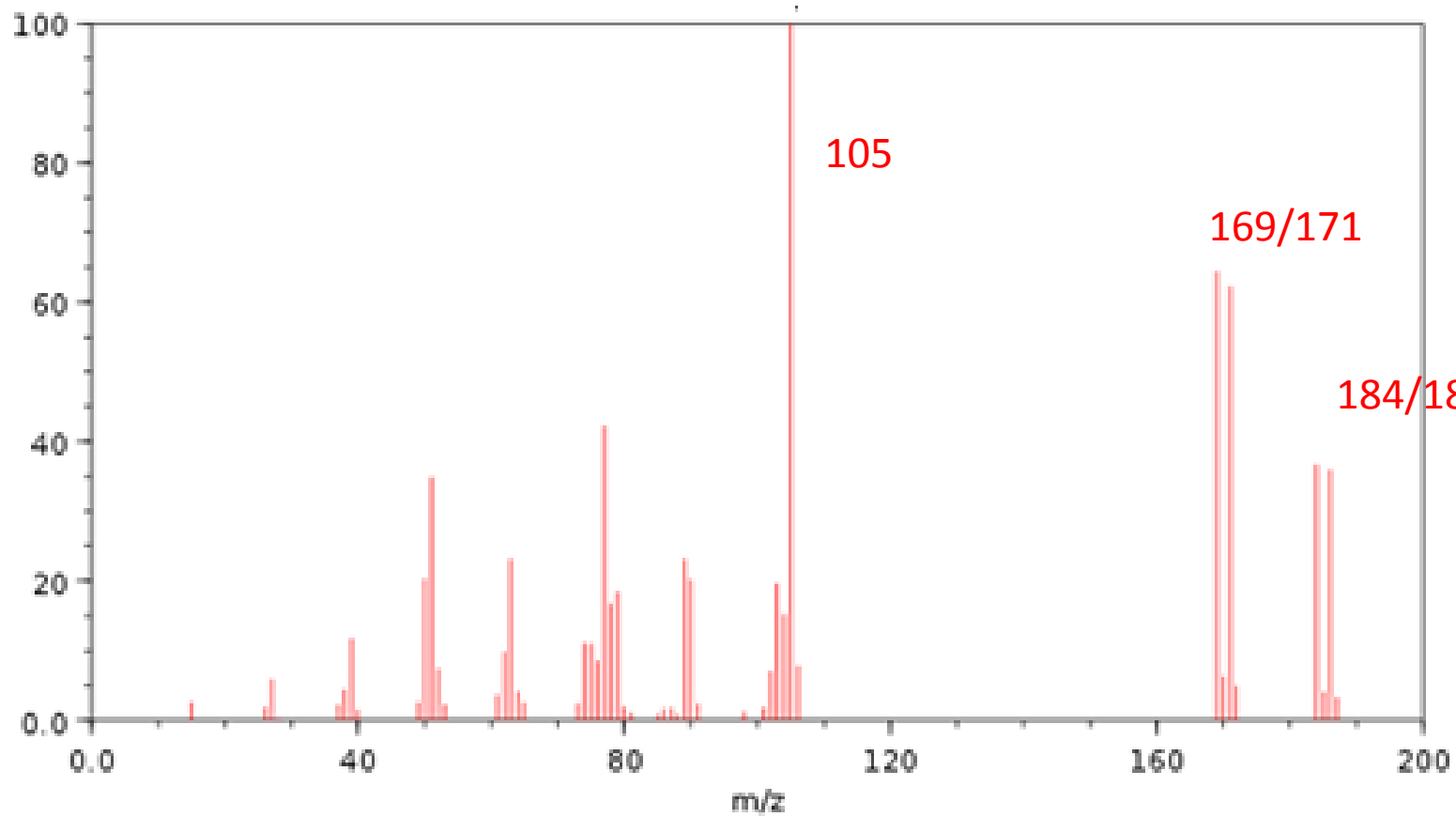
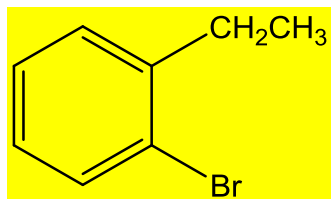


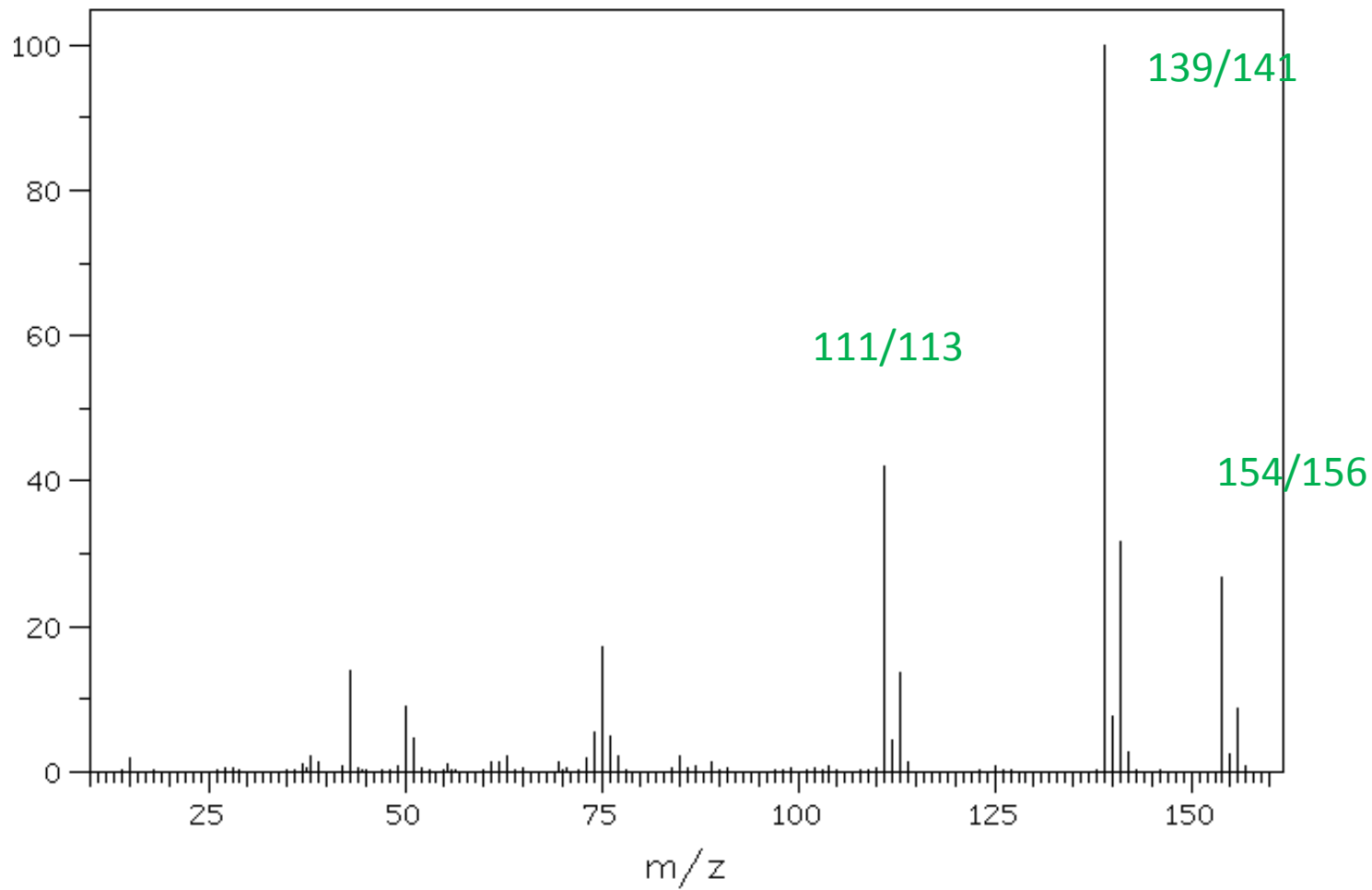
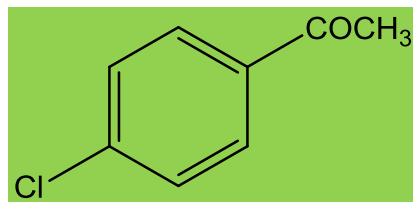
MS of Bromobenzene



MASS SPECTRUM



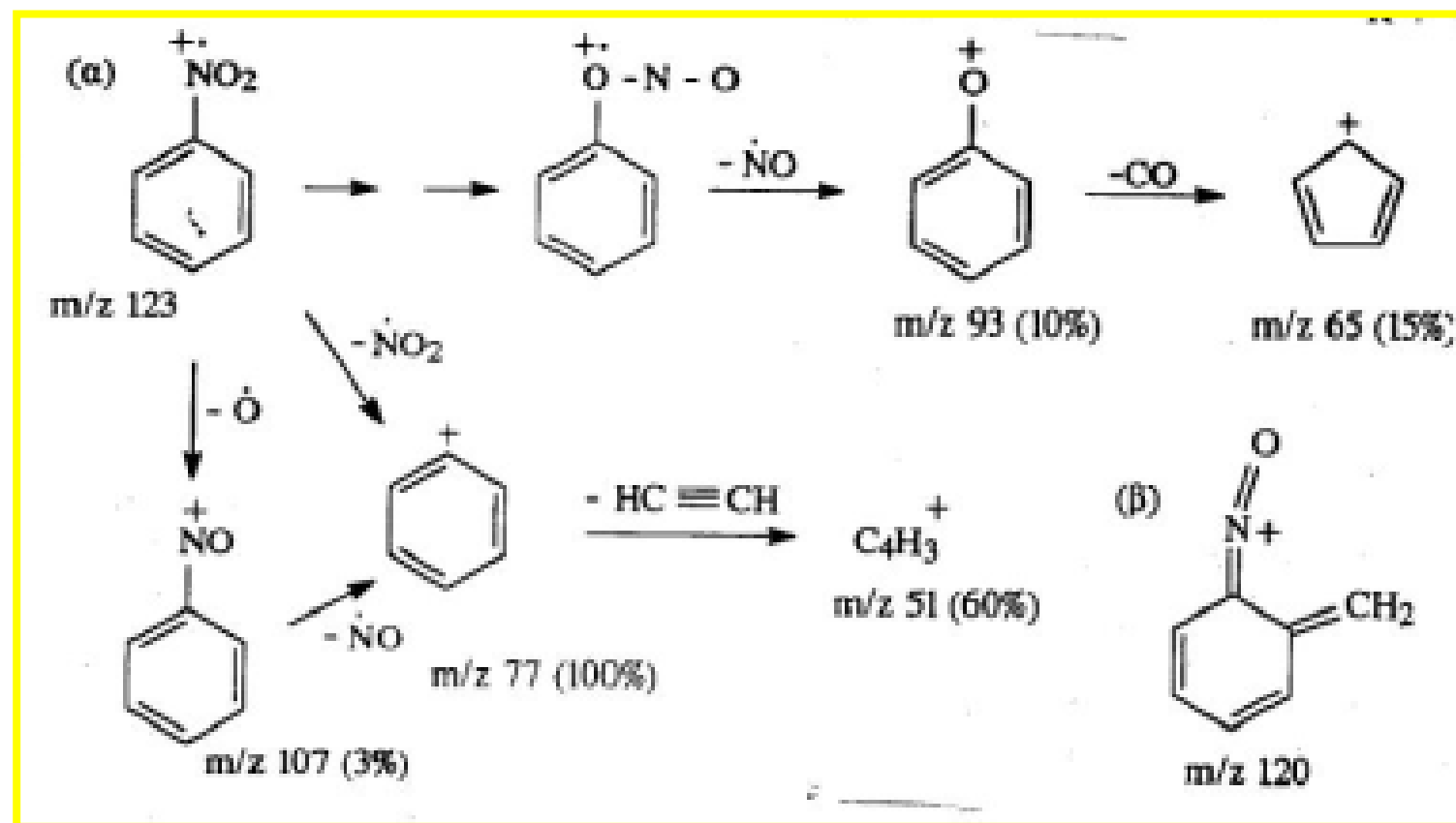
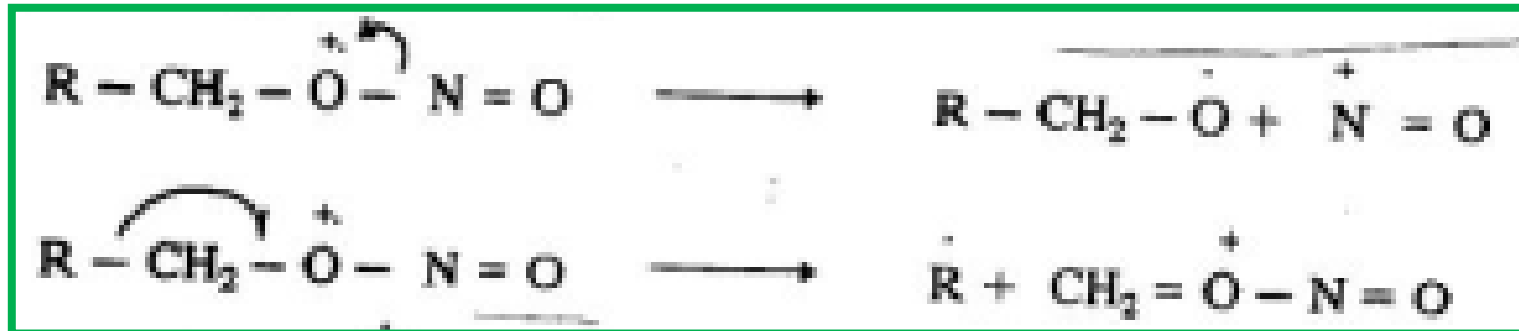


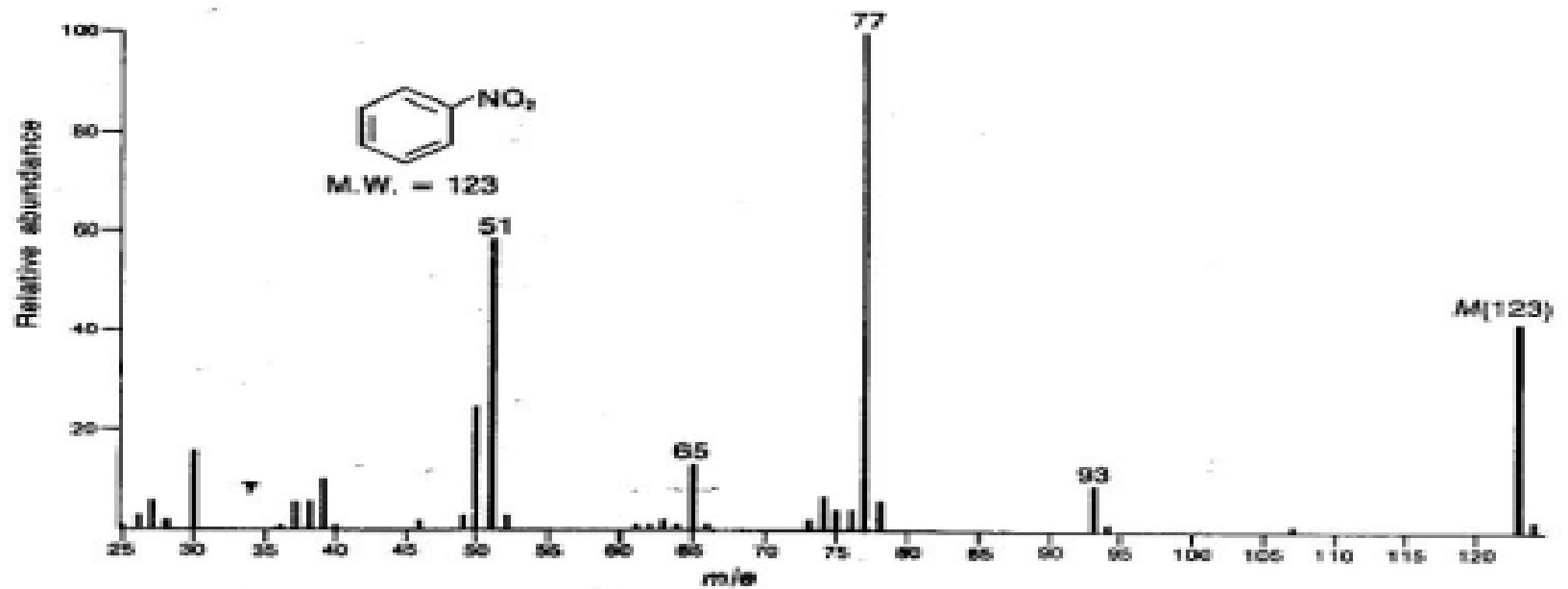
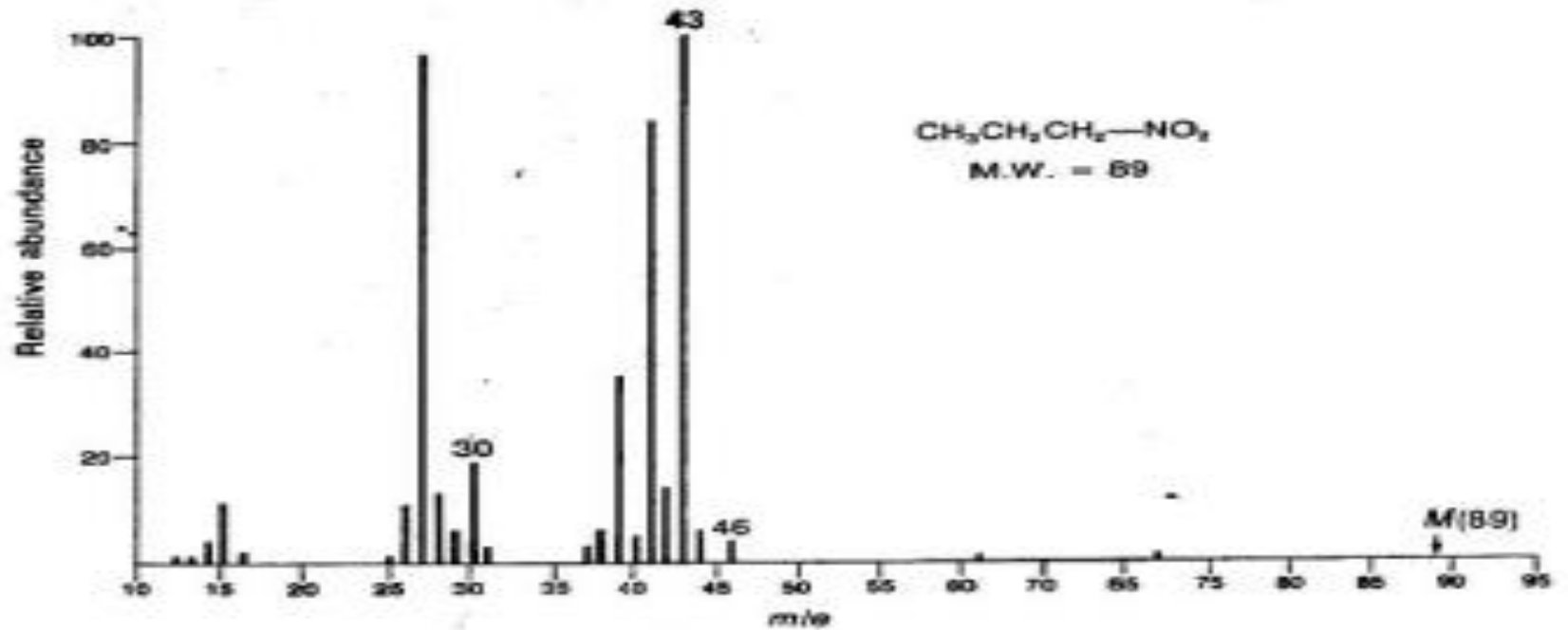


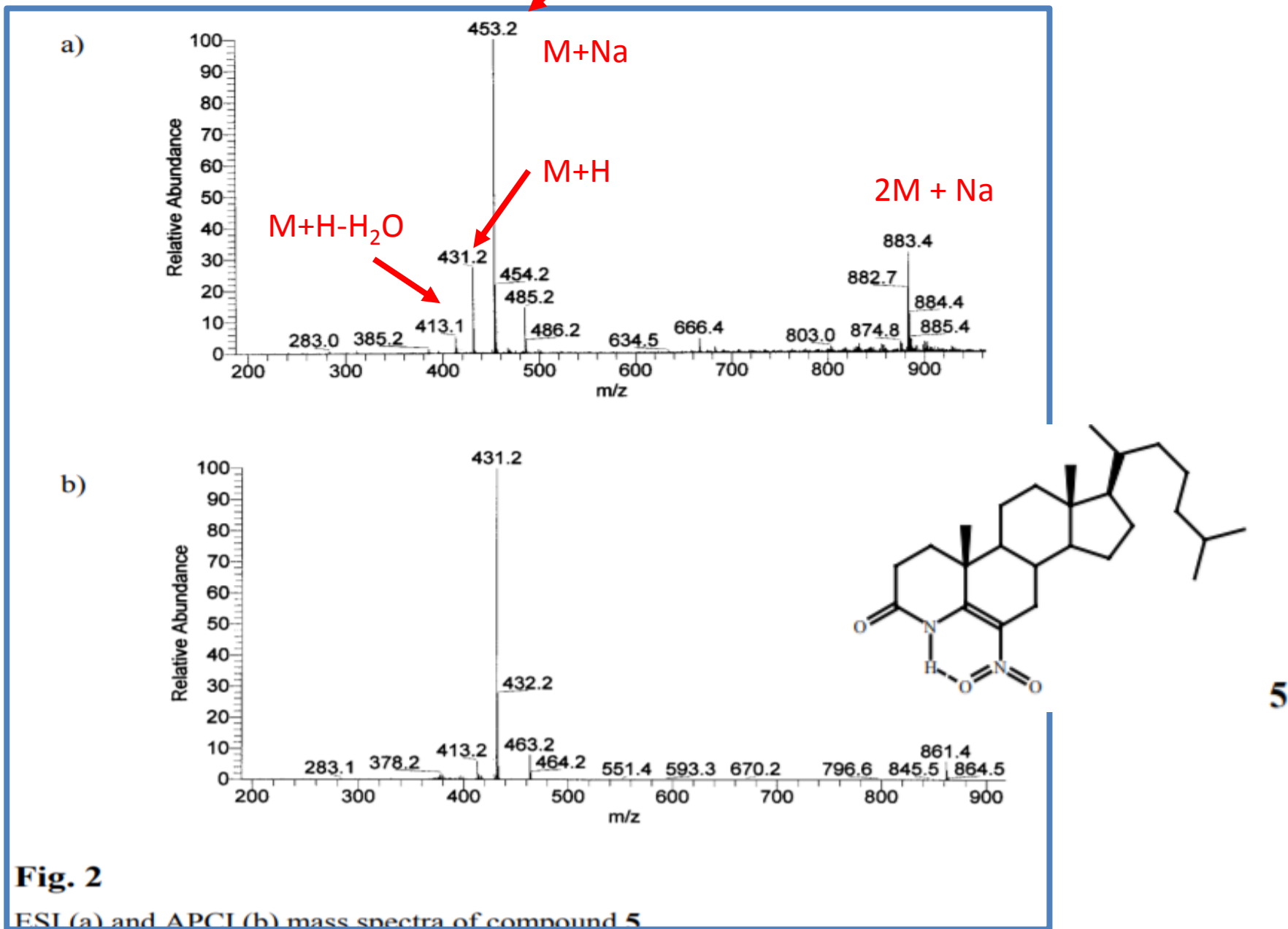
Νιτρο-ενώσεις.

Οι αλειφατικές δίνουν ασθενές M^+ . Οι αρωματικές δίνουν μεγάλο M^+ . Από τα αλειφατικά παράγωγα αποσπάται $\cdot\text{NO}_2$. Οι ισομερείς RONO εστέρες δίνουν β -απόσπαση. Οι αρωματικές χάνουν $\cdot\text{NO}_2$, $\cdot\text{NO}$, $\cdot\text{O}$. Τα ο-αλκυλοποκατεστημένα αρωματικά παράγωγα χάνουν $\cdot\text{OH}$ μέσω μετάθεσης McLafferty.







**Fig. 2**

ESI (a) and APCI (b) mass spectra of compound 5

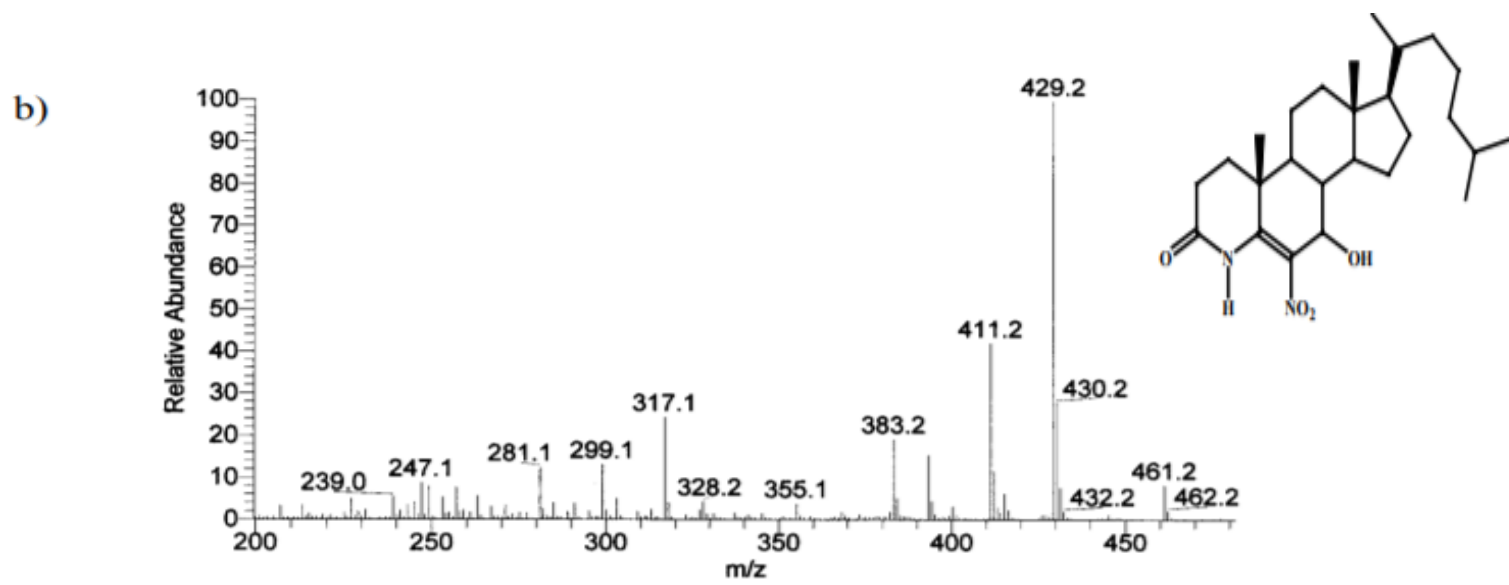
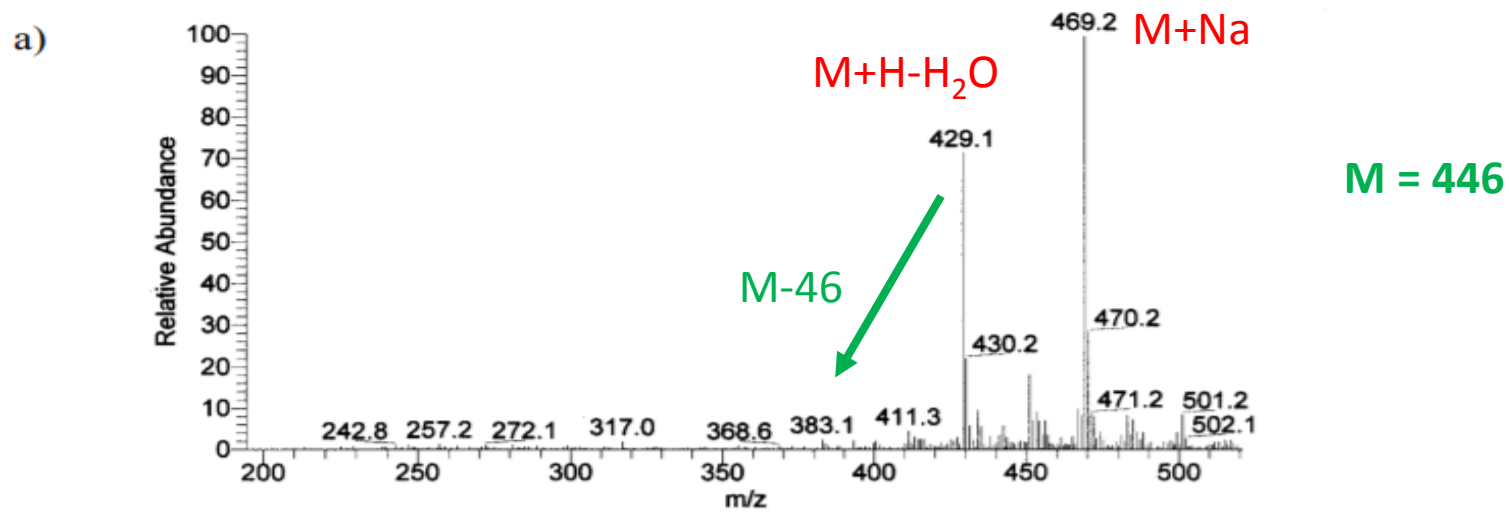


Fig. 3
ESI (a) and APCI (b) mass spectra of compound **8**

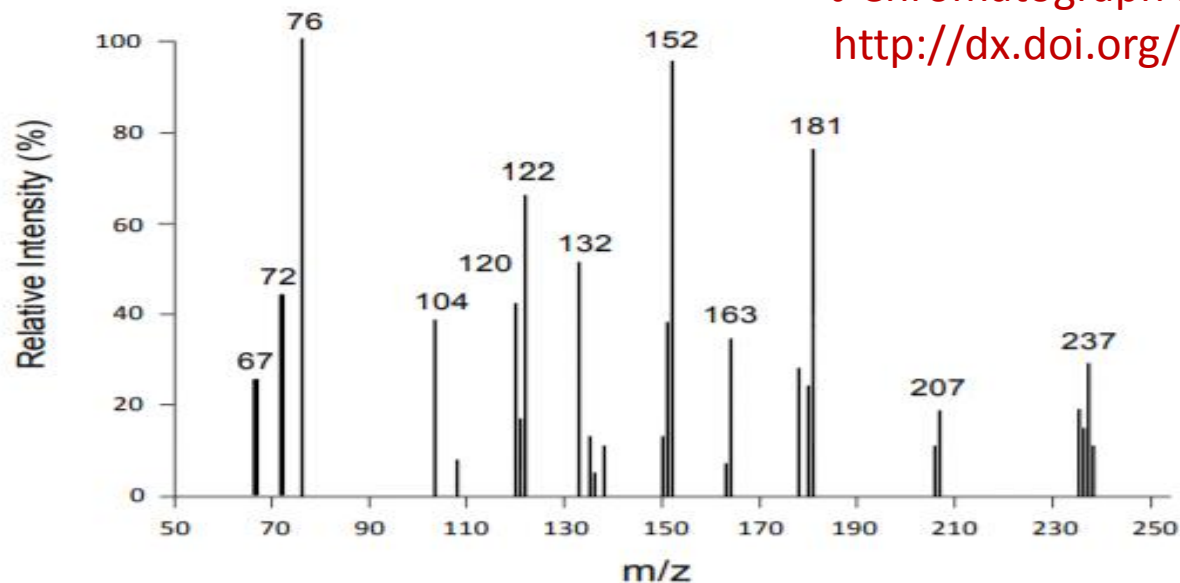


Figure 6: Proposed ESI negative mass spectrum fragmentation of propionaldehyde-DNPH.

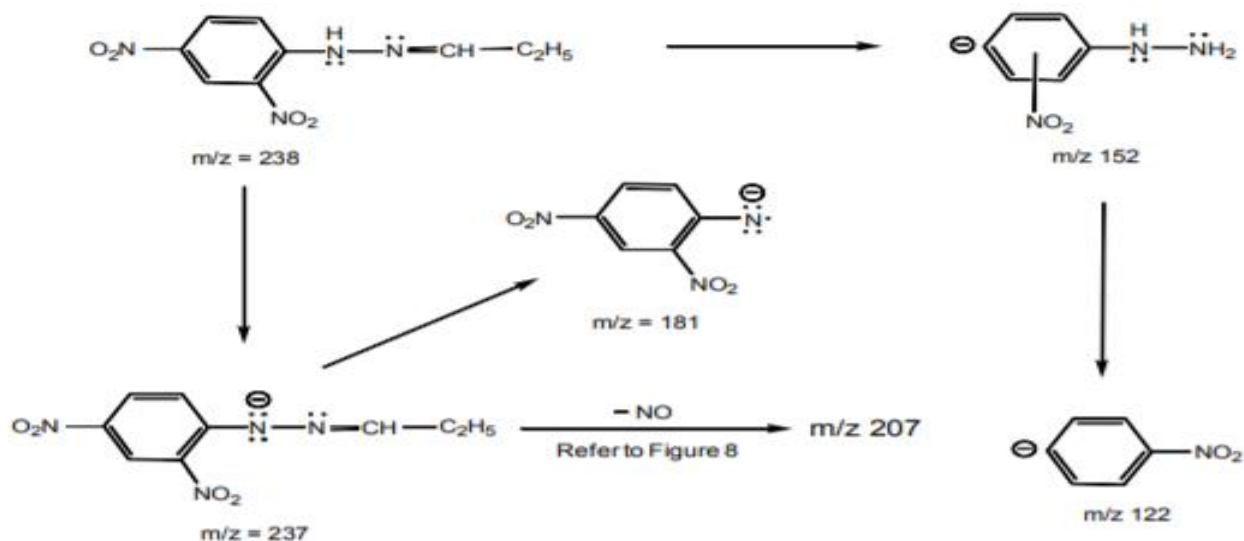


Figure 7: Proposed formation of the fragments from propionaldehyde-DNPH.

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Application of Spectra Accuracy for Analysis of Organic Explosive: 2,4,6-trinitrotoluene by AccuTOF-DART (Direct Analysis in RealTime)

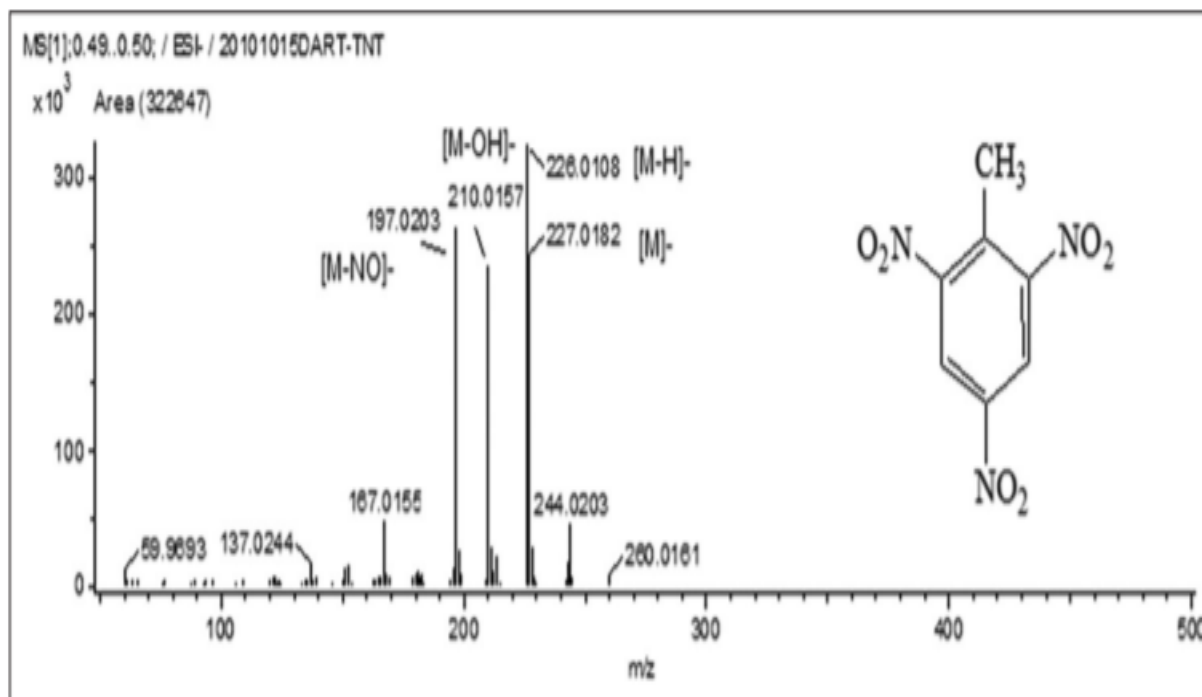


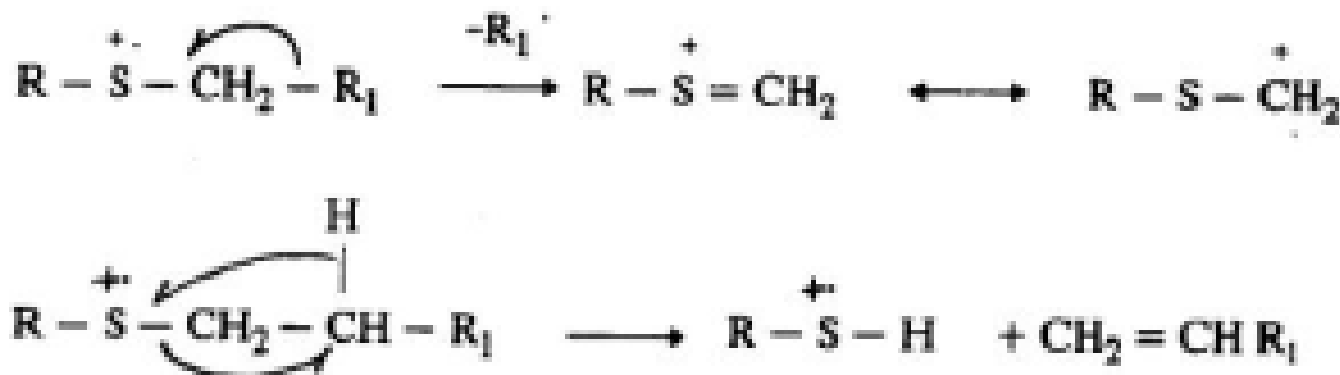
Figure 1: 2,4,6-trinitrotoluene standard substance mass spectra obtained from direct analysis in real-time time-of-flight mass spectrometer

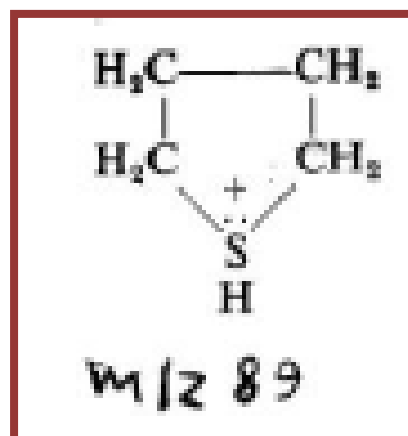
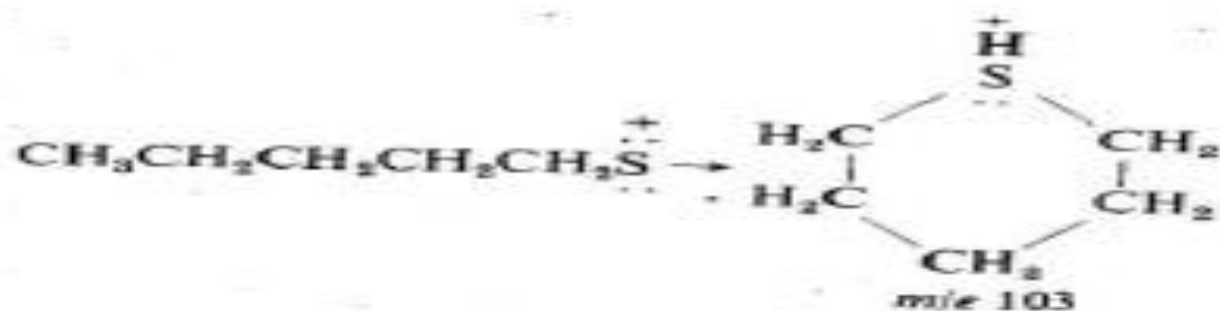
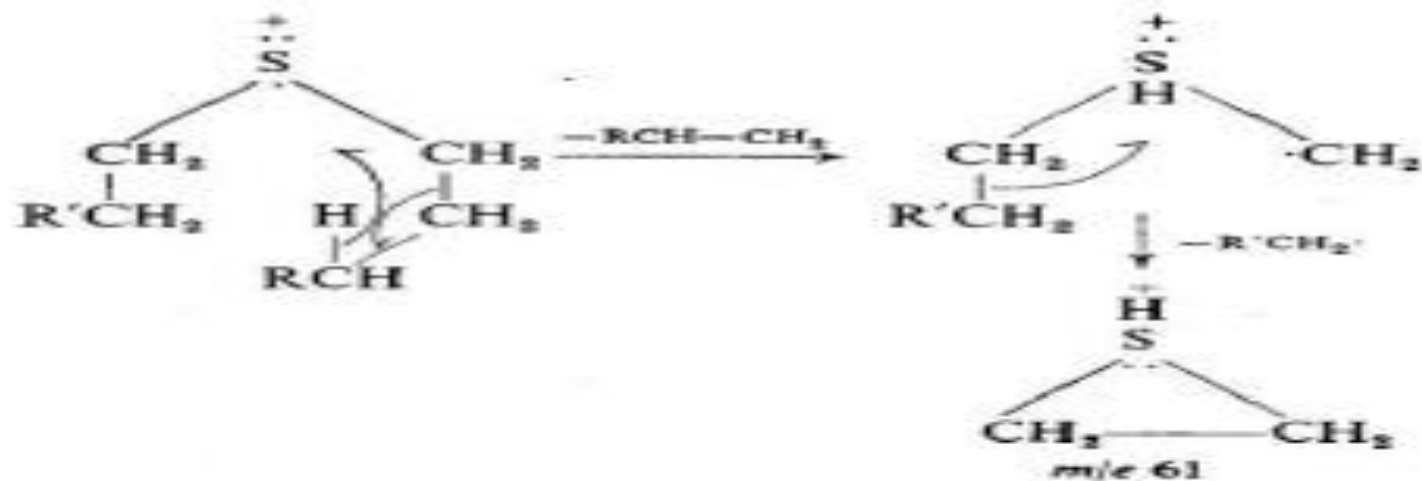
Θειούχες Ενώσεις.

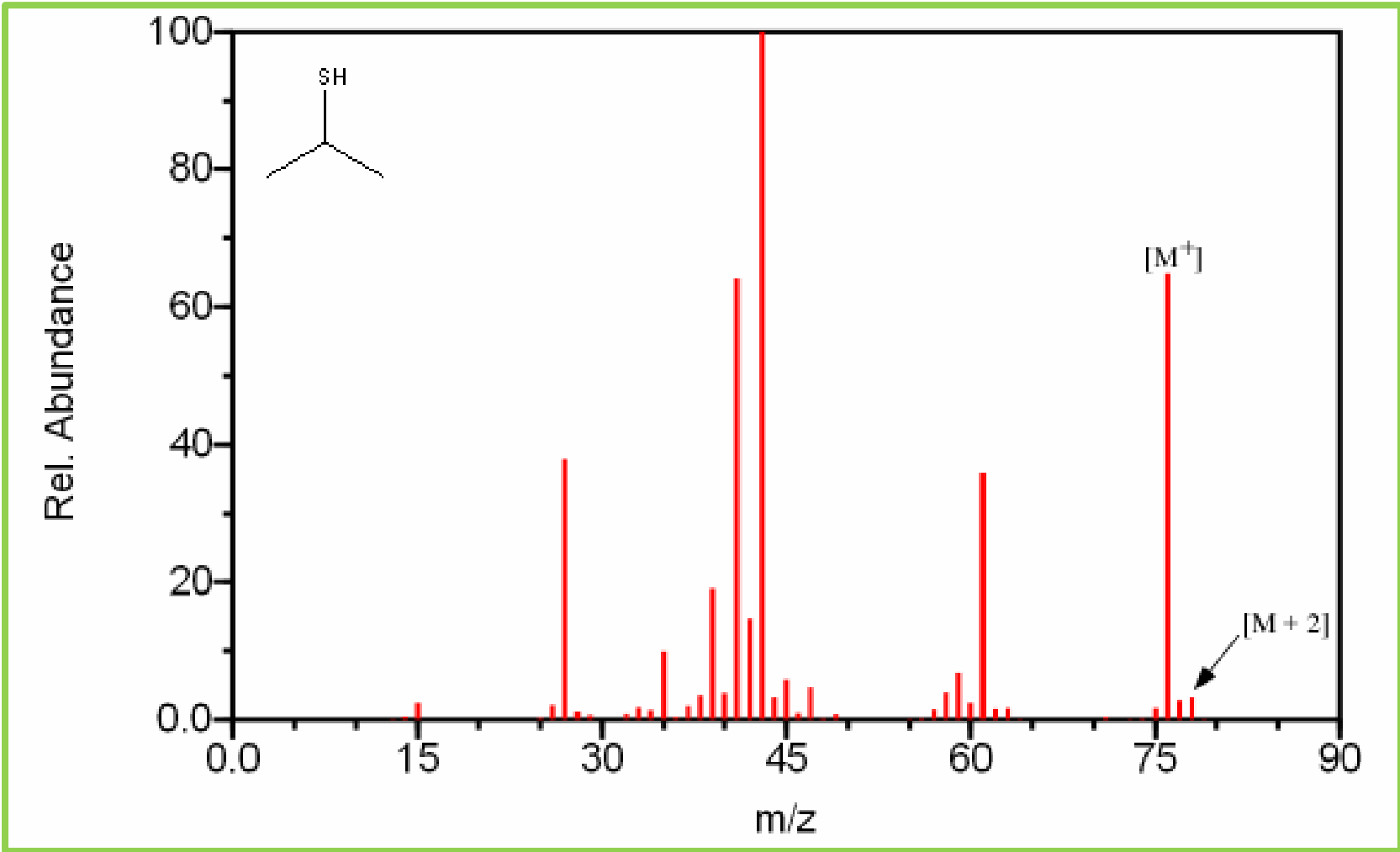
Εμφανίζουν την χαρακτηριστική κορυφή $M + 2$ λόγω του ισότοπου ^{34}S (4.2 %).

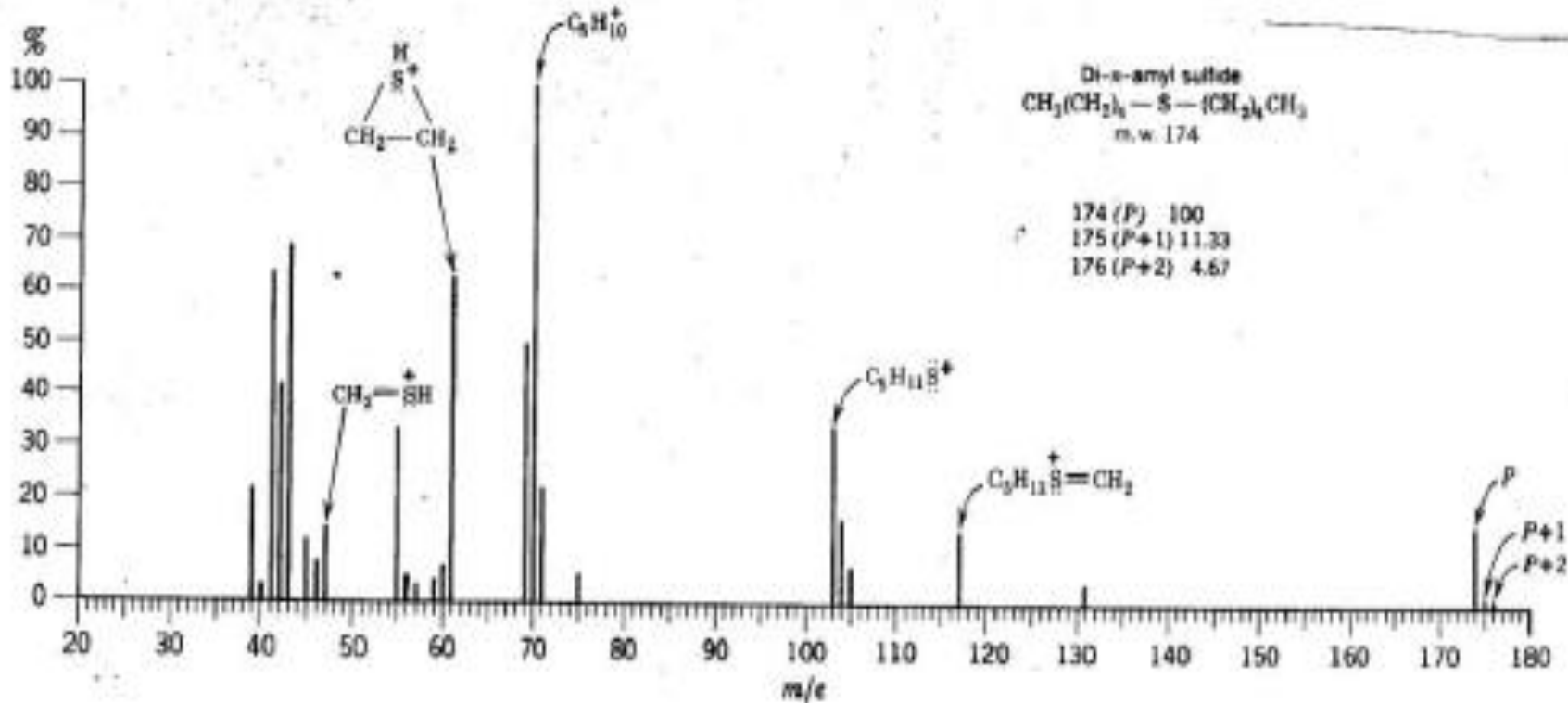
Οι θειόλες δίνουν εντονότερα M^+ από τις ROH, με παρόμοιο τρόπο διάσπασης. Έτσι χάνουν H_2S ($M - 34$) και SH ($M - 33$). Δίνουν χαρακτηριστικές κορυφές σε m/z 47 ($\text{CH}_2=\text{S}^+\text{H}$), 61, 75, 89 λόγω α -, β -, γ -, δ -διασπάσεων. Σε μακράς αλυσίδας αλειφατικές θειόλες υπάρχουν κορυφές λόγω των αλκυλίων (m/z 43, 57, 71,...) και ολεφινικών κατιόντων ($m.z$ 41, 55, 69,...).

Τα σουλφίδια δίνουν πιο έντονο M^+ από τους αιθέρες με παρόμοιο τρόπο διάσπασης. Δίνουν α -διάσπαση με απόσπαση του μεγαλύτερου αλκυλίου. Εμφανίζουν ιόντα $\text{RCH}=\text{S}^+\text{H}$ χωρίς τις αποσπάσεις $M-\text{H}_2\text{S}$ και $M-\text{HS}$.

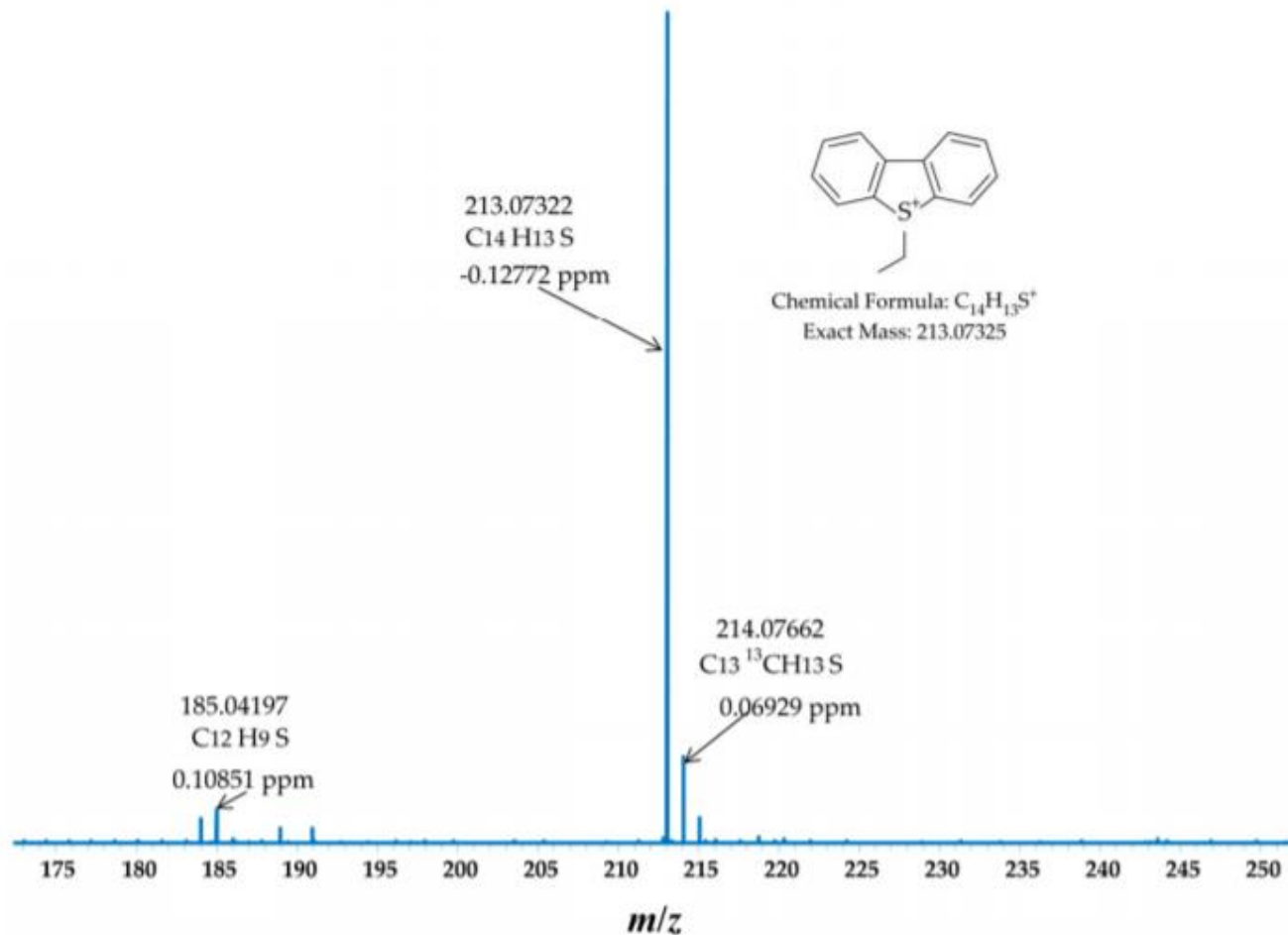








Selective Analysis of Sulfur-Containing Species in a Heavy Crude Oil by Deuterium Labeling Reactions and Ultrahigh Resolution Mass Spectrometry



HRMS (electrospray ionization Fourier transform ion cyclotron resonance mass spectrometry (ESI FT-ICR MS)) spectra (bottom) of 5-ethyldibenzo[b,d] thiophenium tetrafluoroborate.

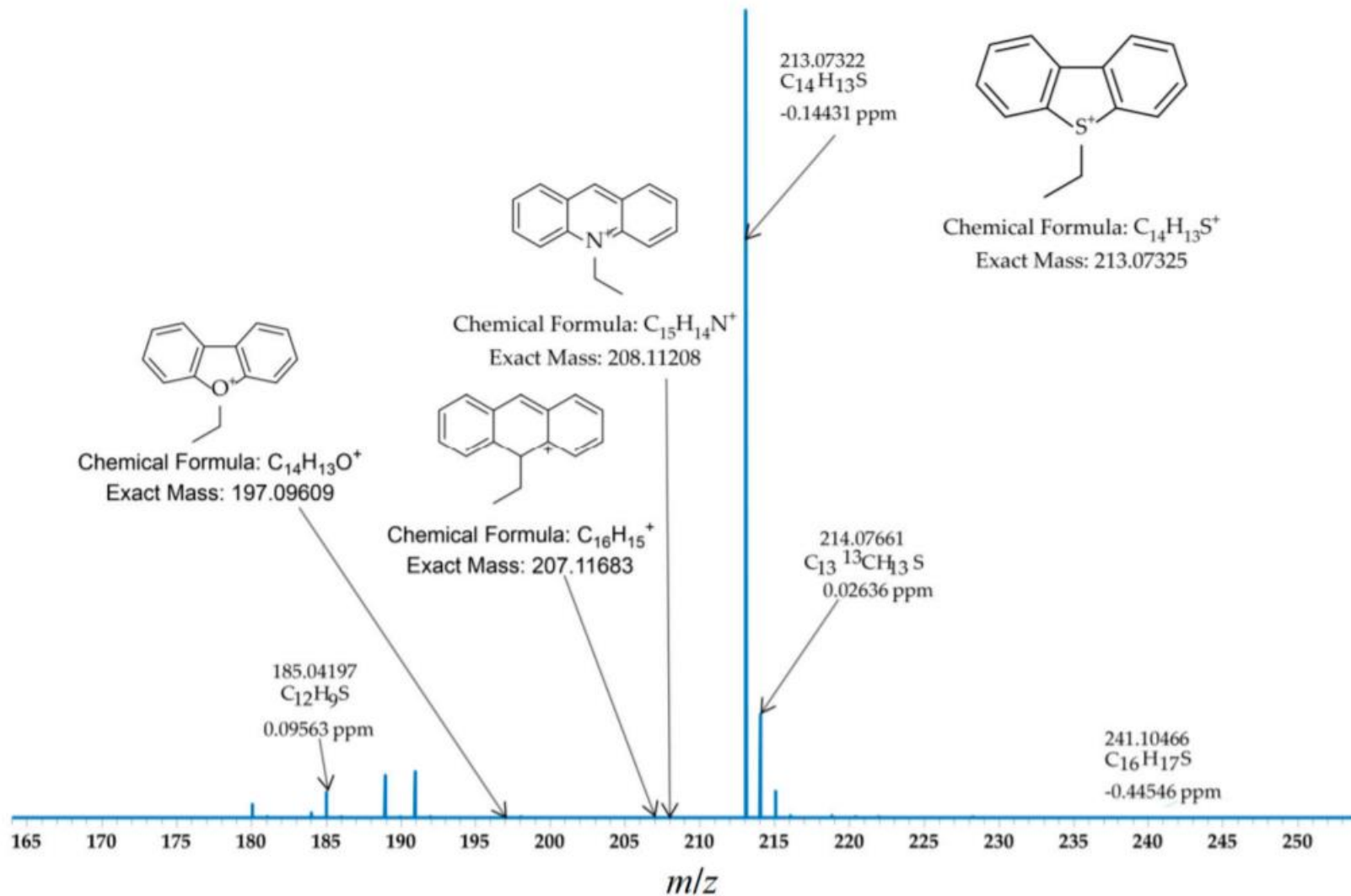
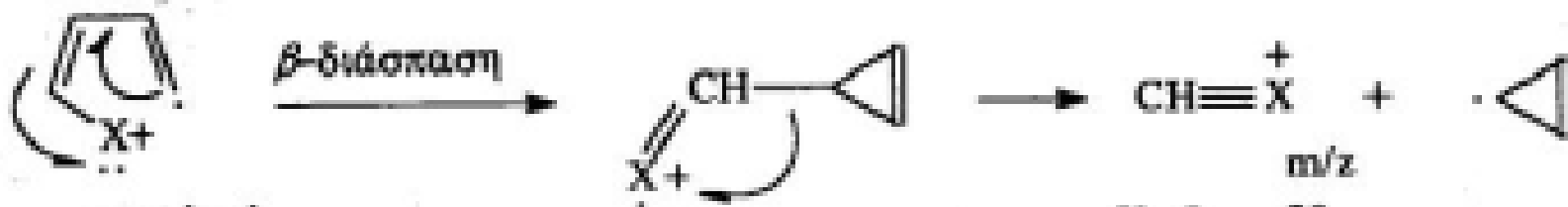


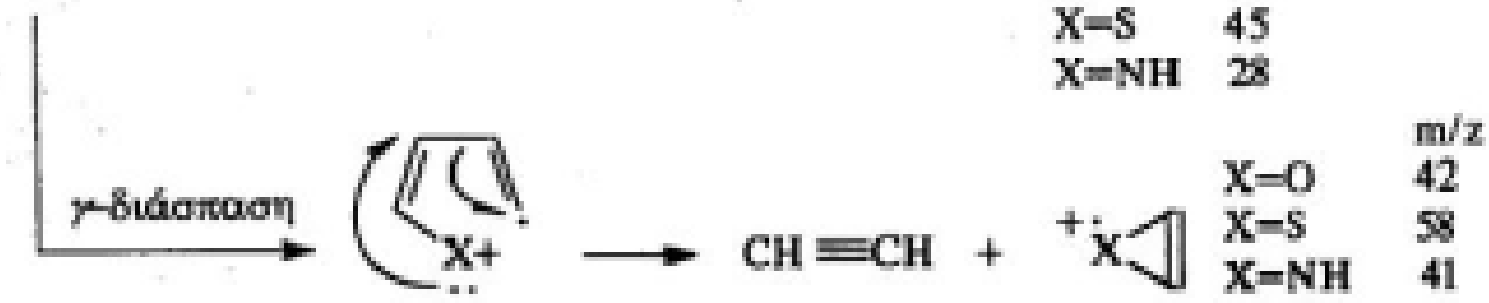
Figure 2. ESI FT-ICR MS spectrum of a mixture of the ethylated standards (anthracene (ANTH), DBT, acridine (ACR) and dibenzofuran (DBF)).

Διασπάσεις Ετεροκυκλικών Ενώσεων.

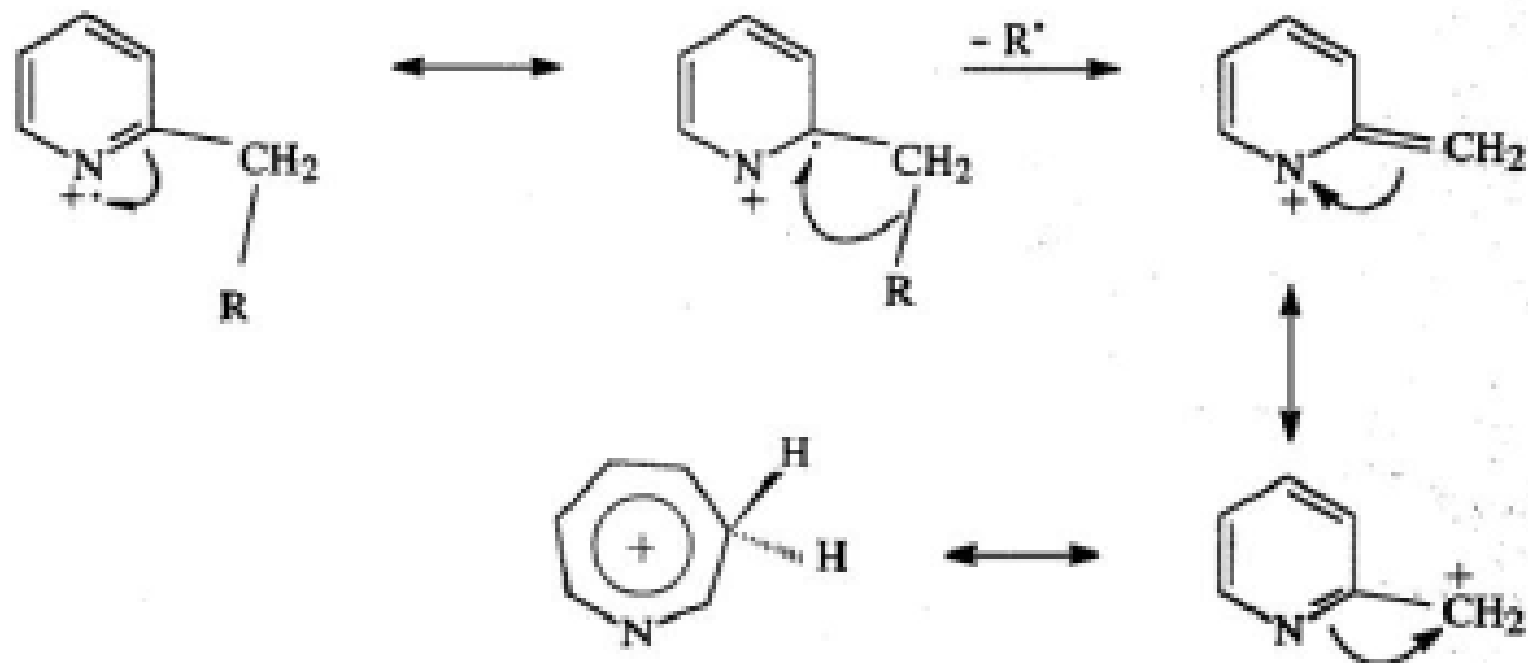
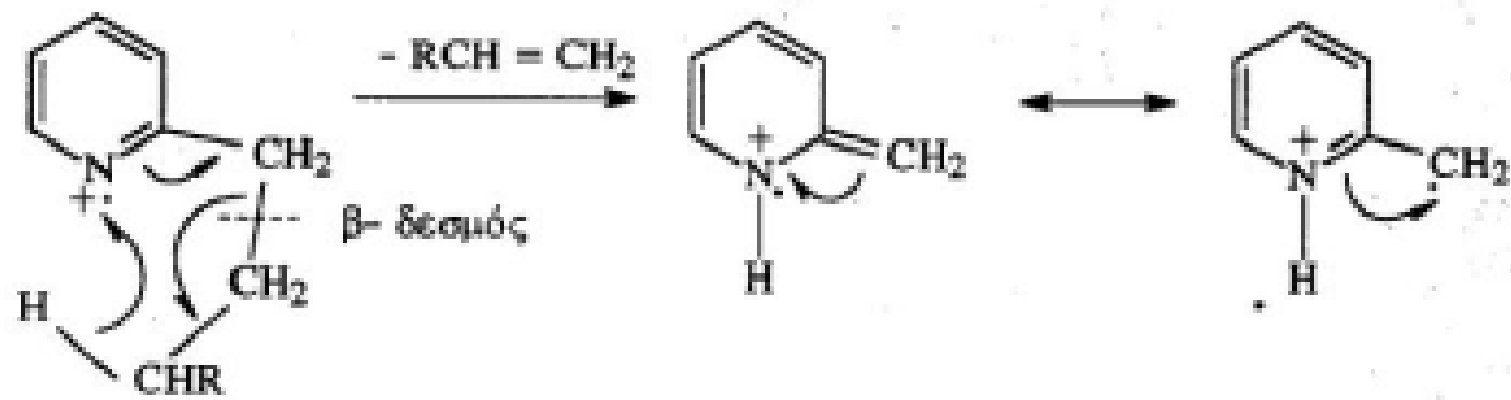
Διασπώνται στον ετεροκυκλικό δακτύλιο είτε στην πλευρική αλυσίδα.

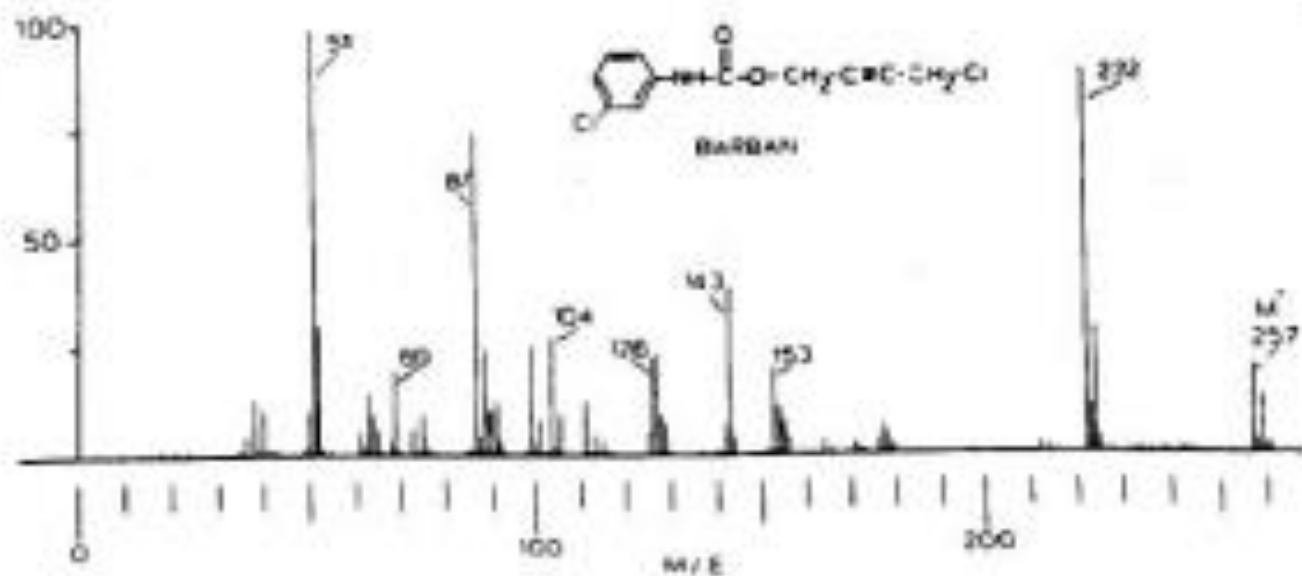


X=O	29
X=S	45
X=NH	28



X=O	42
X=S	58
X=NH	41





Σχήμα 16.20 Φάσμα μαζών (EI) του εντομοκτόνου barban.

