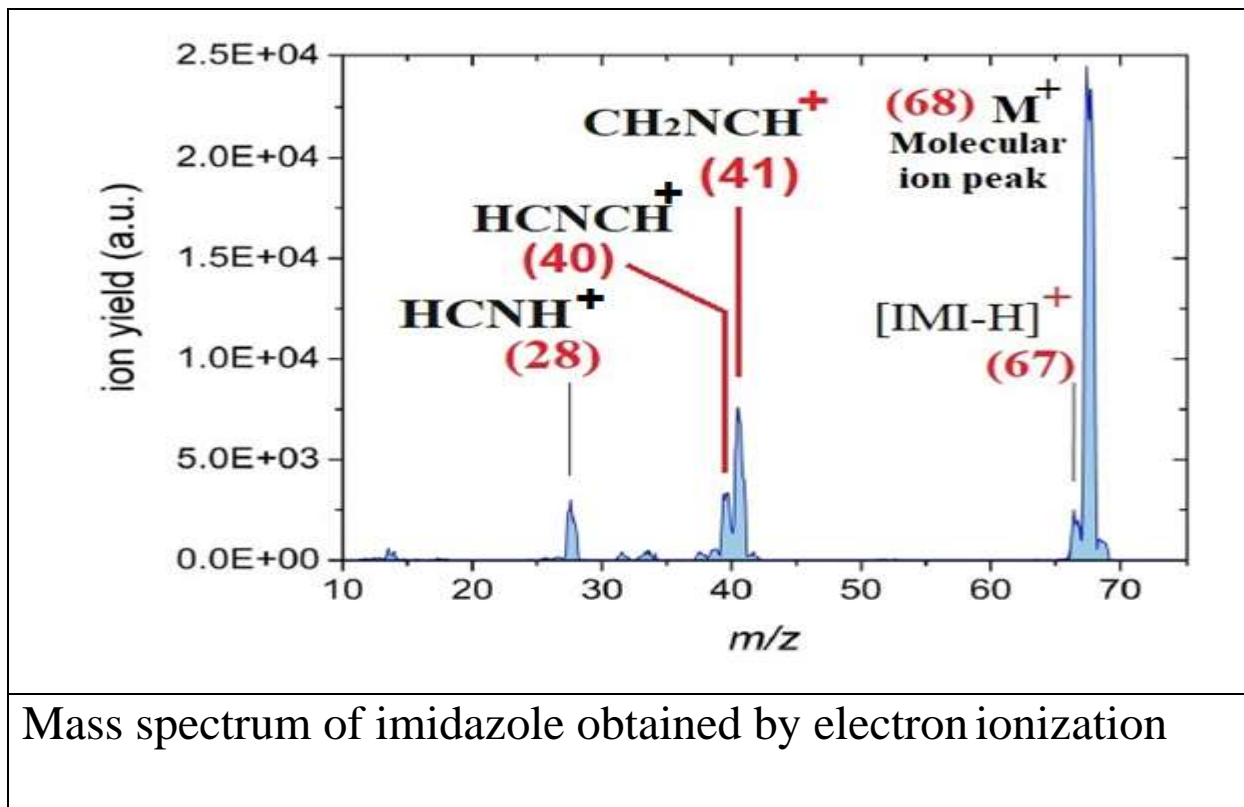
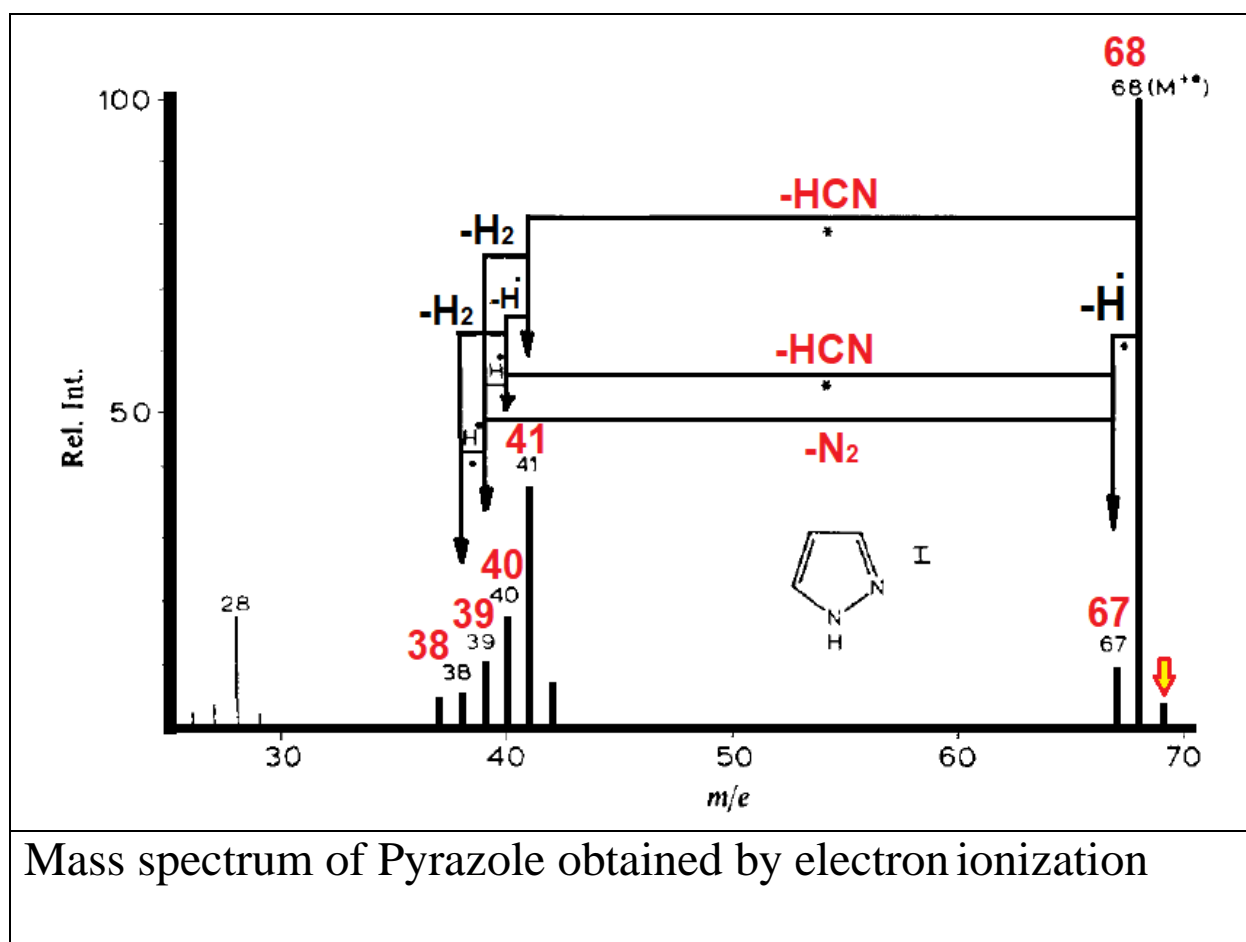
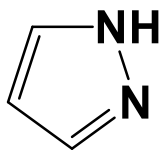


## Imidazole

1. The most intense ion has been ascribed to the parent cation at  $m/z$  68.
- 2- The peak at  $m/z$  67 assigned to  $[\text{IMI} - \text{H}]^+$ , which corresponds to the dehydrogenated parent cation.
- 3 - The fragment at  $m/z$  41 is assigned to  $\text{CH}_2\text{NCH}^+$  or  $\text{CH}_2\text{CNH}^+$  cation is formed by  $\text{HCN}$  loss.
- 4- The fragment at  $m/z$  40 is assigned to  $\text{HCNCH}^+$  cation is formed by  $\text{HCN} + \text{H}$  loss.
- 5- The fragment at  $m/z$  28 is assigned to  $\text{HCNH}^+$  cation is formed by  $\text{CH}_2\text{CN}$  loss.

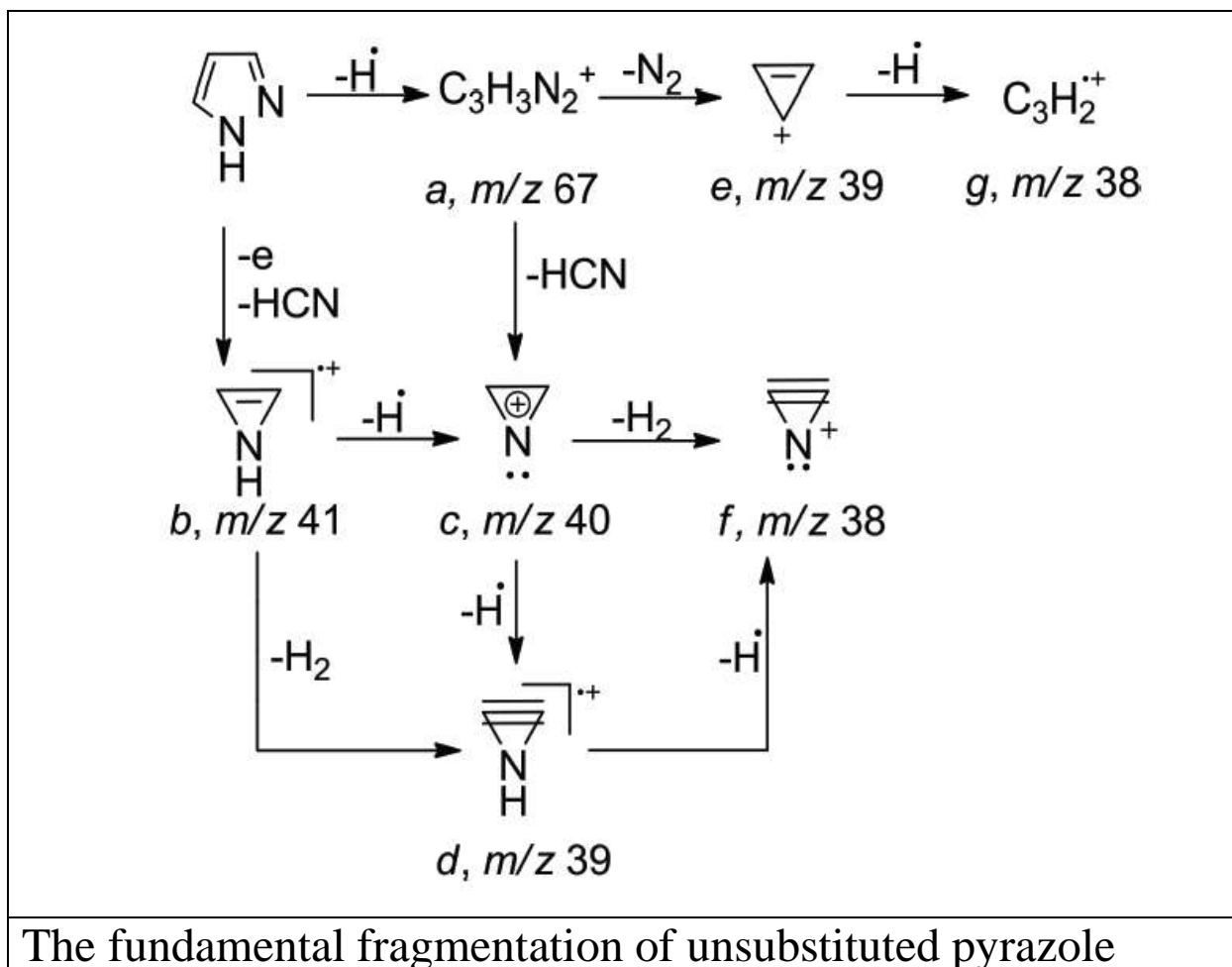


Pyrazole

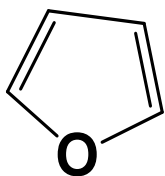


The fragmentation of pyrazole (I, Fig. 1) follows two distinct routes. The predominant feature, also observed in imidazole, is expulsion of HCN from  $[M]^+$  and  $[M-H]^+$  ( $m/e$  67), leading to  $[C_2H_3N]^+$  ( $m/e$  41) and  $[C_2H_2N]^+$  ( $m/e$  40) respectively.

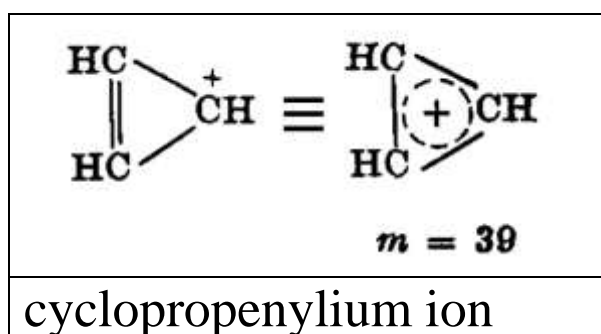
The second process is loss of a nitrogen molecule from  $[M-H]^+$  giving the cyclopropenyl ion  $[C_3H_3]^+$  ( $m/e$  39), which is the most abundant fragment ion in pyrrole.



## Furan



1- The spectrum of furan shows, besides the molecular ion peak ( $M^+$ ), a very pronounced peak of the cyclopropenylum ion at mass 39. Another fragment of higher intensity corresponds to the well-stabilized  $H-C=O^+$  ion of mass 29.

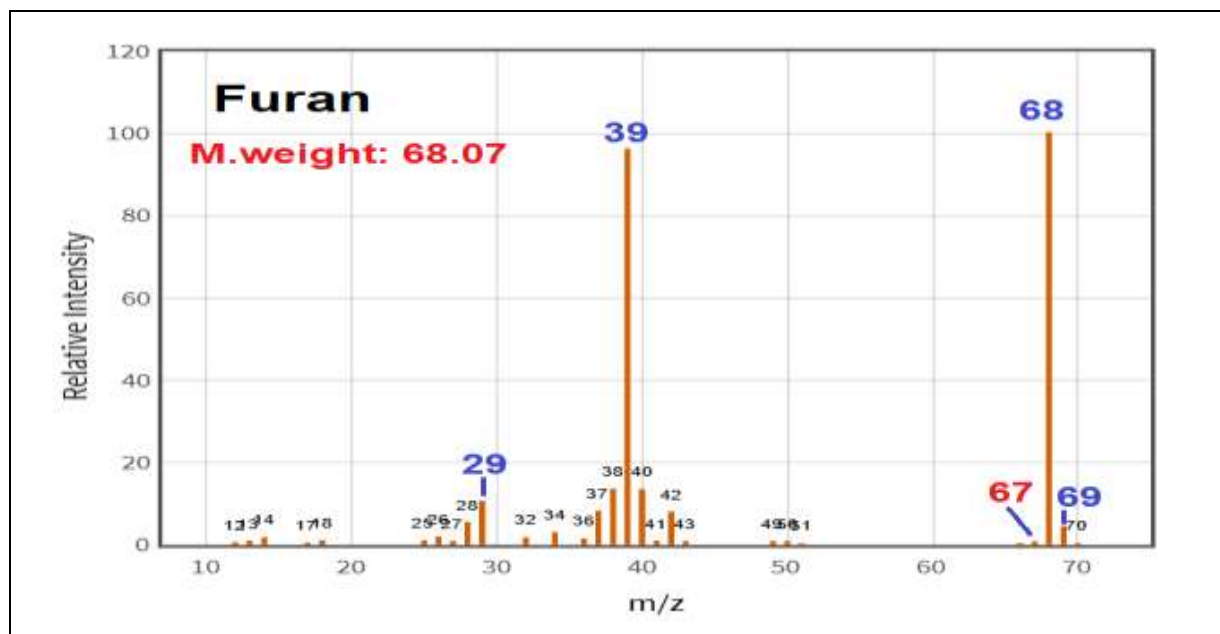


2- The peak at 68 amu in the mass spectrum corresponds to the stable  $C_4H_4O^+$  cation, while those at 69 and 70 amu to its  $^{13}C_{12}C_3H_4O^+$  and  $^{13}C_2^{12}C_2H_4O^+$  isotopes, respectively.

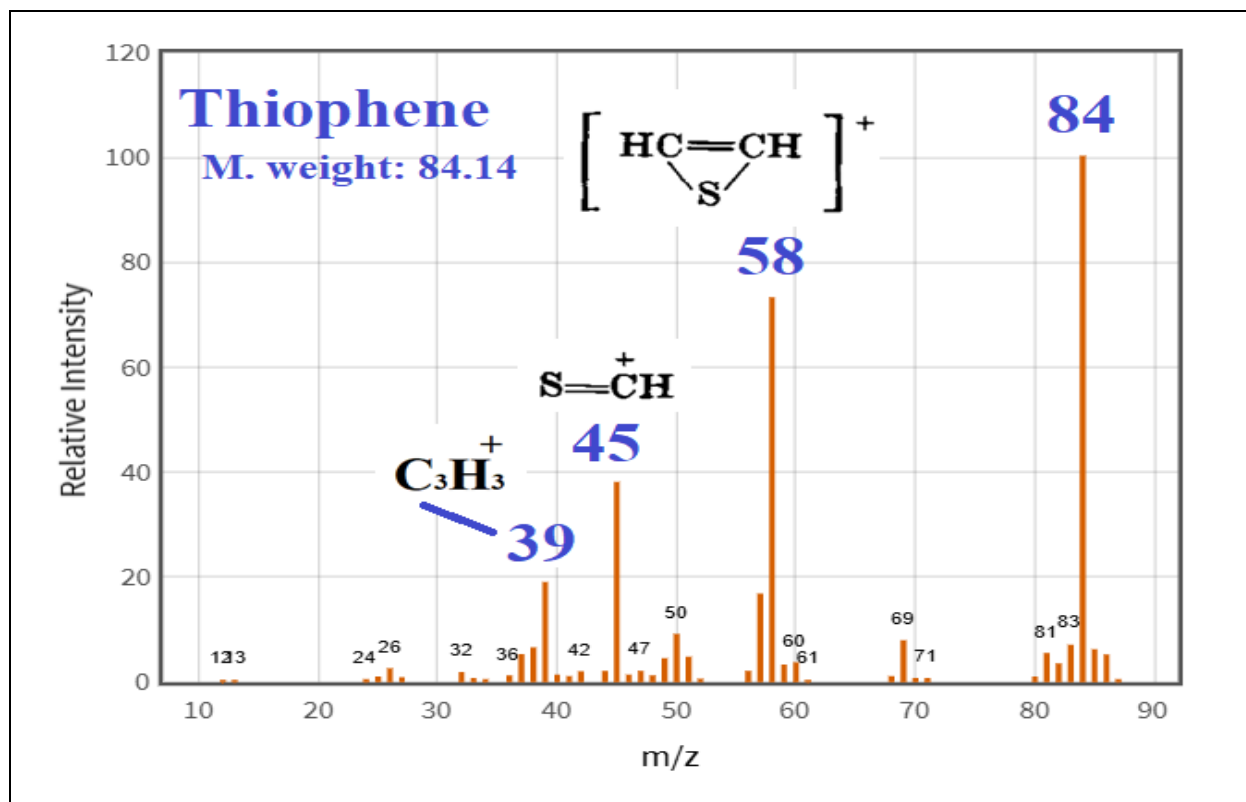
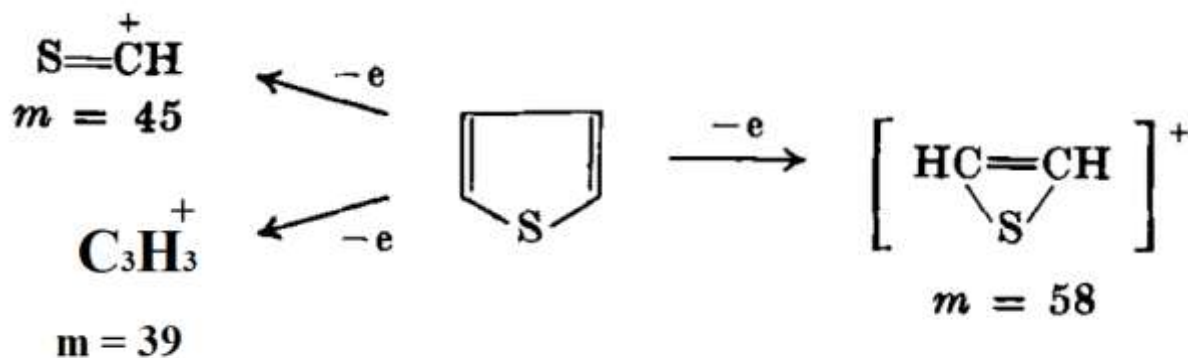
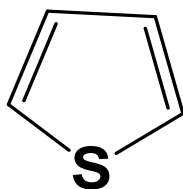
3- The  $C_3H_3^+$  cation ( $m=39$  amu), which gives the highest intensity peak in the mass spectrum is produced in a reaction that provides the HCO molecule:

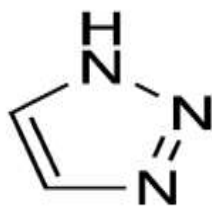


4- The intense peak in this mass region at  $m=29$  amu belongs to the  $\text{HCO}^+$  cation released in the reaction:



# Thiophene

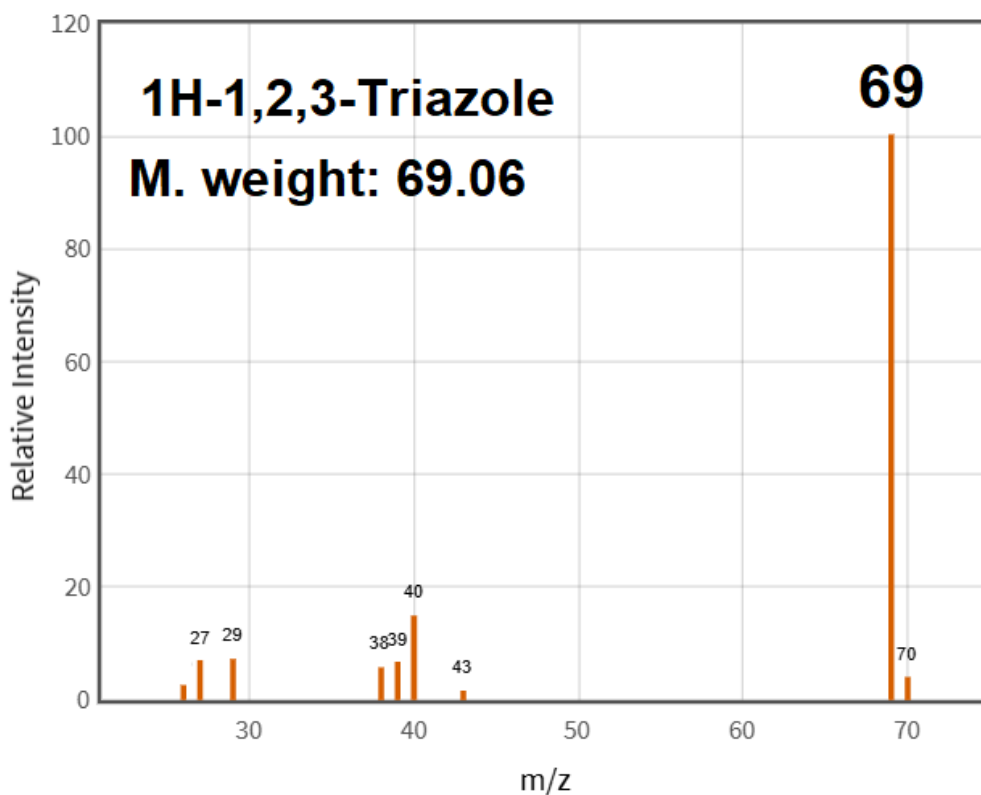




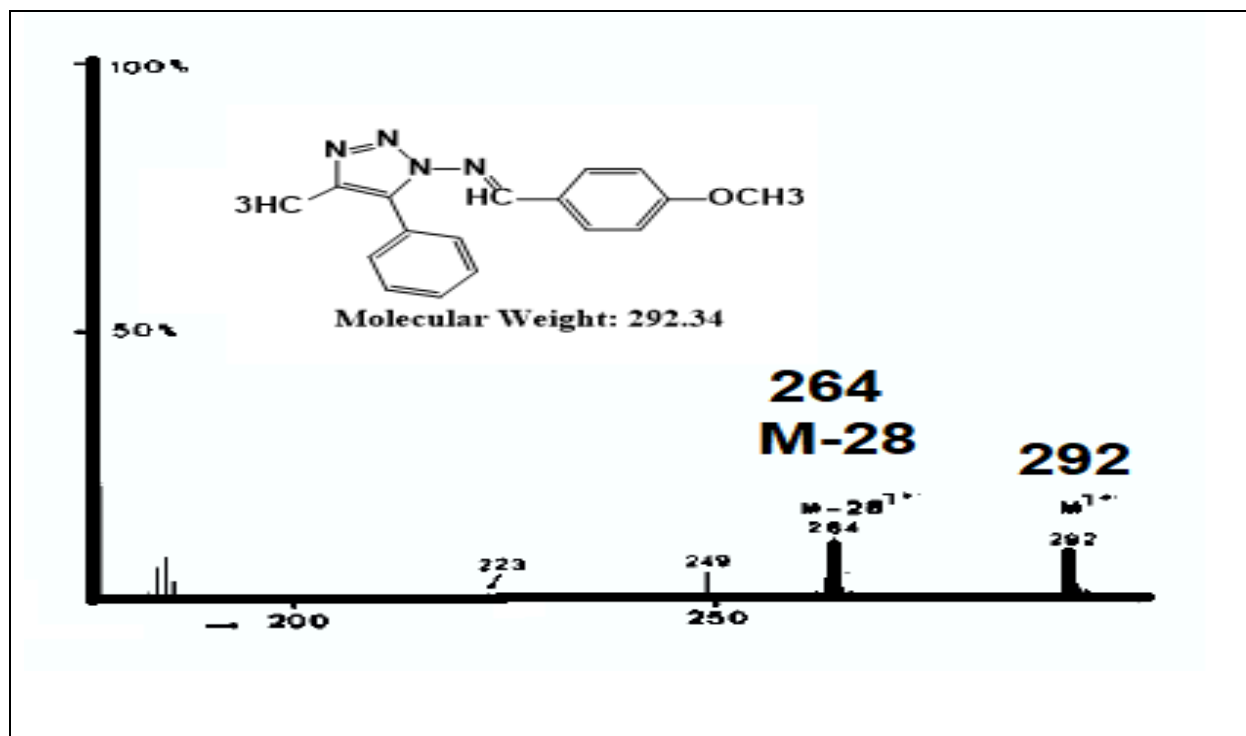
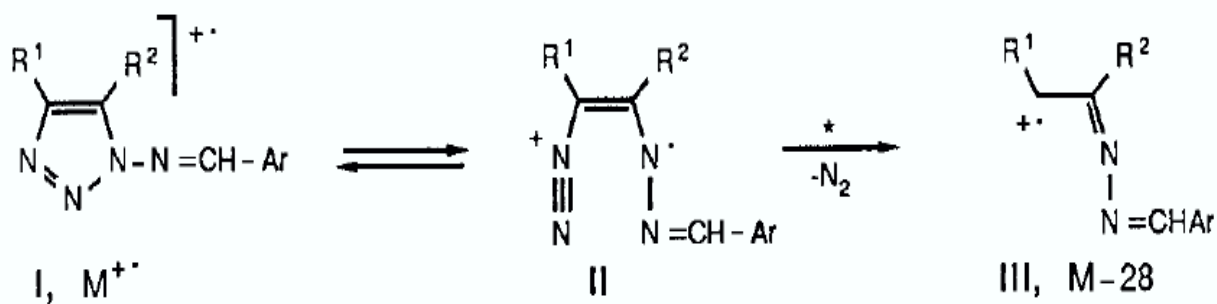
## 1,2,3-Triazole

The EI mass spectrum of 1,2,3-triazole typically shows a strong molecular ion peak at  $m/z$  69.

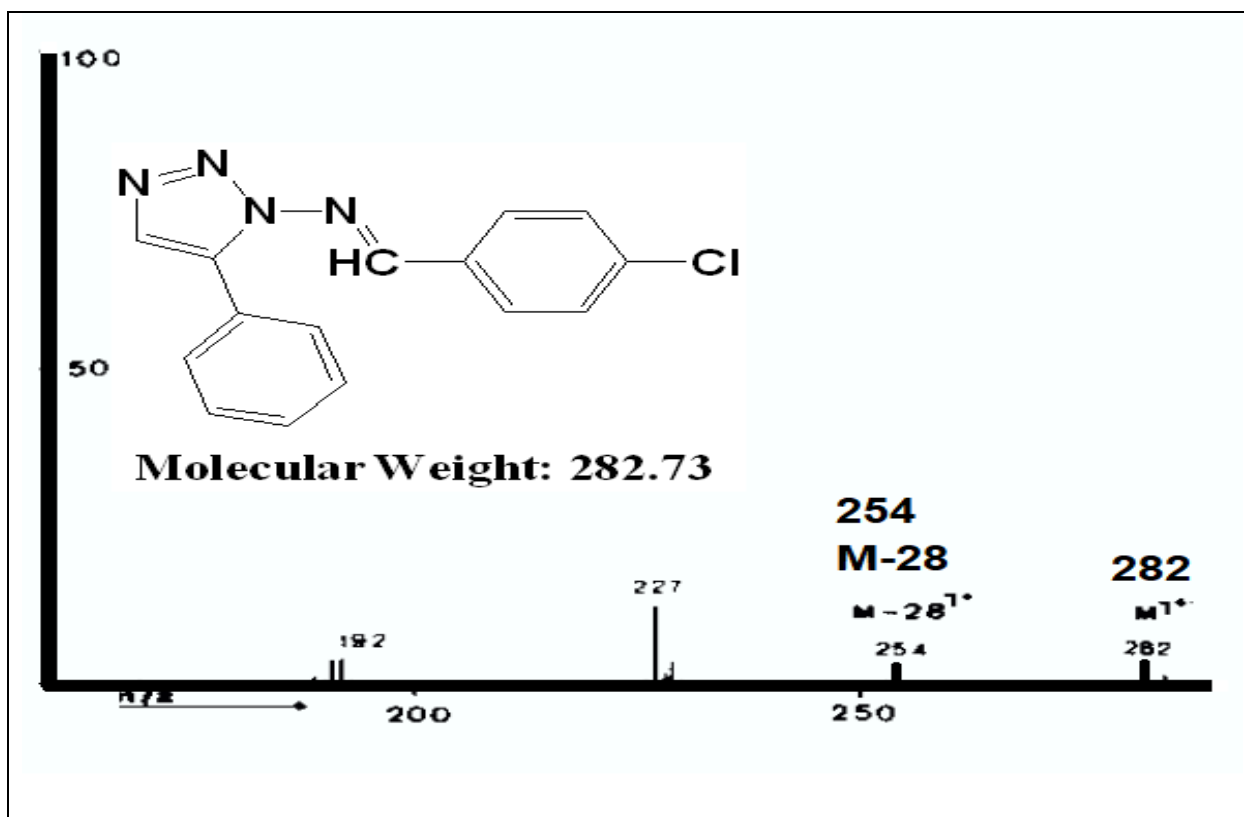
The peak at 69 amu in the mass spectrum corresponds to the stable  $C_2H_2N_3^+$  cation. The peak at 70 amu in the mass spectrum corresponds to the  $^{13}C^{12}CH_2N_3^+$



The most prominent fragmentation pathway involves the loss of a nitrogen molecule ( $N_2$ ) from the molecular ion ( $M^+$ ).

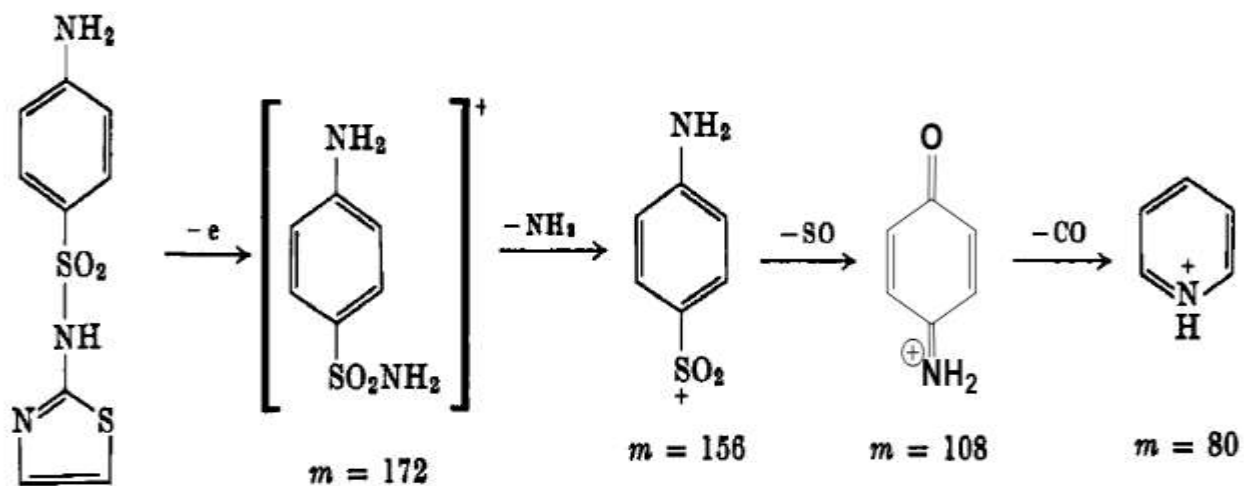






## Sulfonamides

The expulsion of  $\text{SO}_2$  (M-54) is a favored process if the amide nitrogen is connected to a carbon having a partial positive charge. The elimination probability of  $\text{SO}_2$  increases with increasing positive charge at this carbon.



**M = 255**

