International Journal of ChemTech Research
CODEN (USA): IJCRGG ISSN: 0974-4290
Vol.8, No.4, pp 2241-2246, 2015

Mass spectral fragmentation analysis of some heterocyclic compounds

Periyasamy Murugan*

Department of Chemistry, Vel Tech University, Avadi, Chennai- 600 062, India.

Abstract: A number of heterocyclic compounds have been investigated by EI mass spectrometry because of due to their versatile wide applications such as laser dyes, OLED, liquid crystals, solar cells, NLO properties and biological applications. Mass spectral fragmentation of some heterocyclic compounds were thoroughly analyzed in this article.
Key words: Quinoacridine, quinoxanthene, pyridinedinitrile, pyranopyridine, quinoxaline.

Introduction

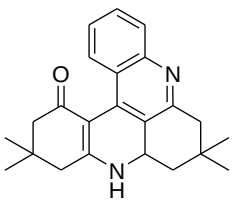
Mass spectrometry (MS) is unequivocally a powerful tool of characterization of organic compounds. In recent years, we have witnessed a significant development in the utilization of the Quinoacridine and quinoxanthene which are very useful in anti-HIV activity[1], Ca^{2+} release activity[2] and intercalation of DNA[3]. The substituted pyridinedinitrile and pyranopyridine derivatives are shows significant attention in the fields of electrical materials[4], biological activities[5] and quinoxalines show antimalarial activity against gallinaceum in chicks[6,7]. In this paper, we would like to report the mass spectral fragmentation pattern of quiniacridine (**1a)**,quinoxanthene **(1b)**, pyridinedinitrile compounds **(2 a-d)**, pyranopyridine derivatives (**3 a-c)** and quinoxaline derivatives(**4a-b, 5**) .The loss of H, isobutylene and ketene groups were observed in quinoacridine(**1a**). Similar loss of H,C_2H_2,NH_2, CN, groups were observed both pyridinedinitrile compounds **(2a-d)** and pyranopyridine derivatives (**3a-c**) .The common loss of H,CO,C_2H_4,HCN groups were observed in quinoxaline derivatives (**4a-b,5**).

Experimental

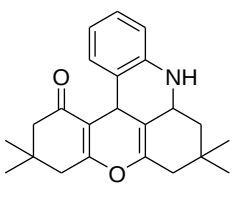
The mass spectra were recorded with Jeol-JMS-DX 303 HF and GCMS QP 5000 Shimadzu instruments.

Result and Discussion

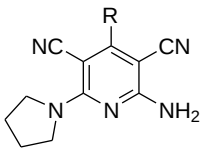
A successive loss of Hydrogen followed by loss of isobutylene, ketene and carbon monoxide groups were observed compound **1a** and fragmentation pattern depicted in **scheme** –I.



1a



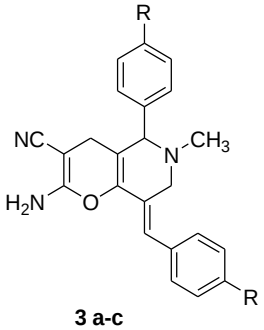
1b



2a-d

Table - I

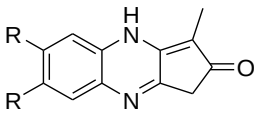
Compound	R
2a	p-OH-C_6H_4
2b	o-OH-C_6H_4
2c	p-NO_2-C_6H_4
2d	2-Thienyl



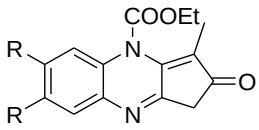
3 a-c

Table –II

COMPOUND	R
3a	CH_3
3b	CH_3
3c	OCH_3

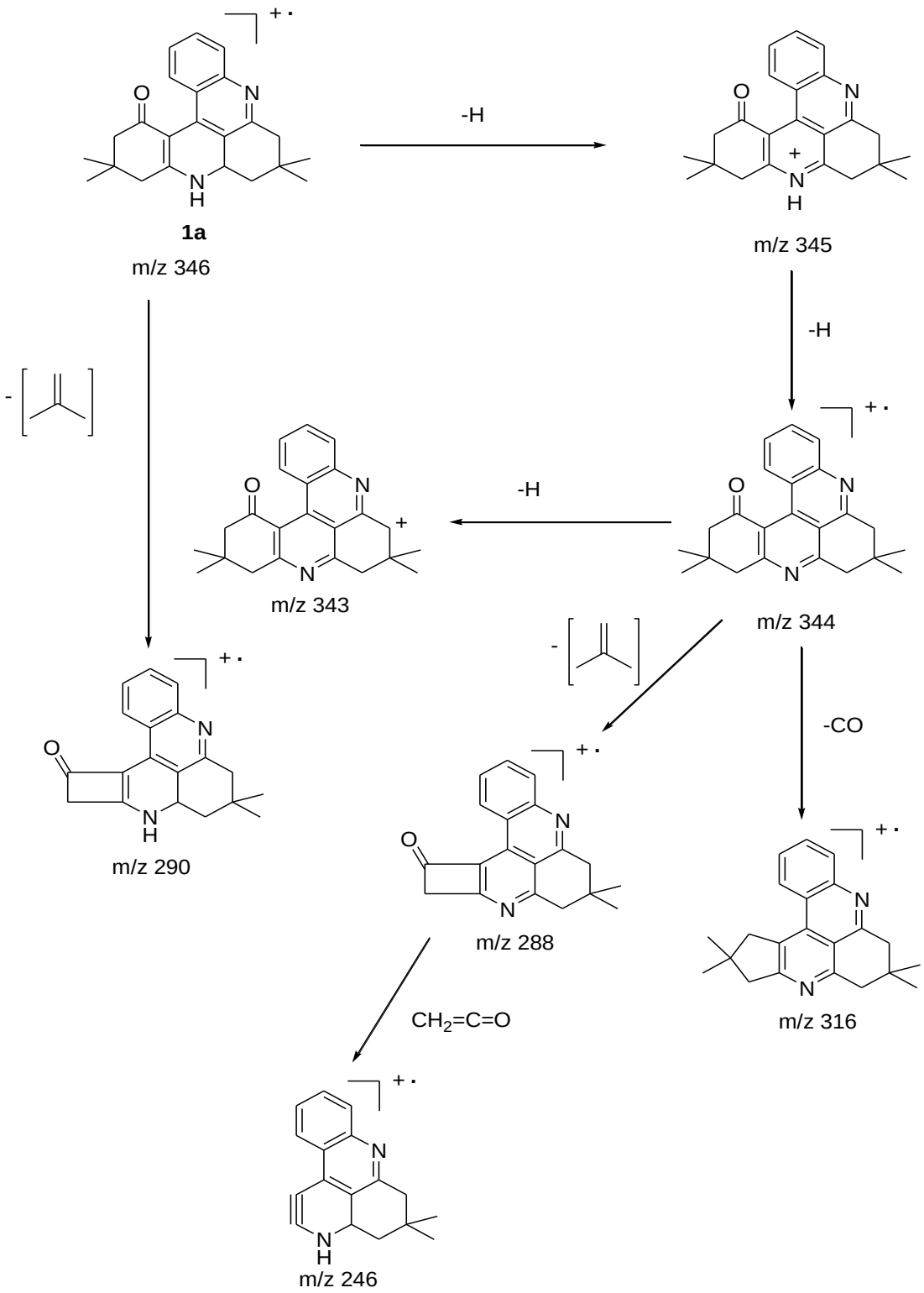


4a = R= H
4b = R = CH_3

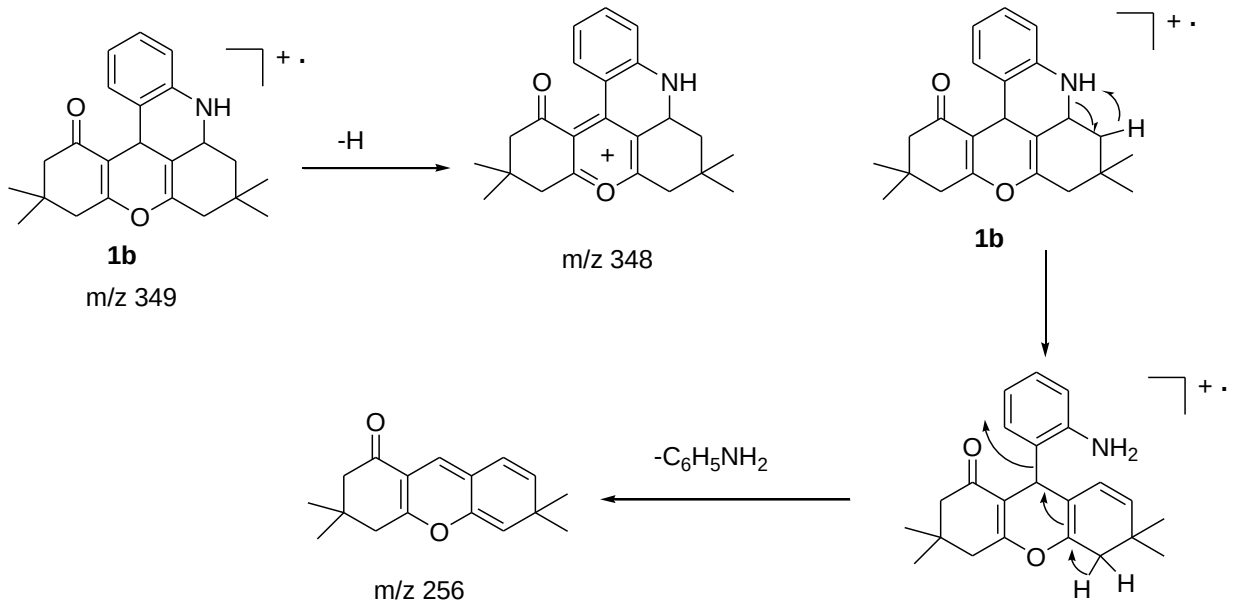


5

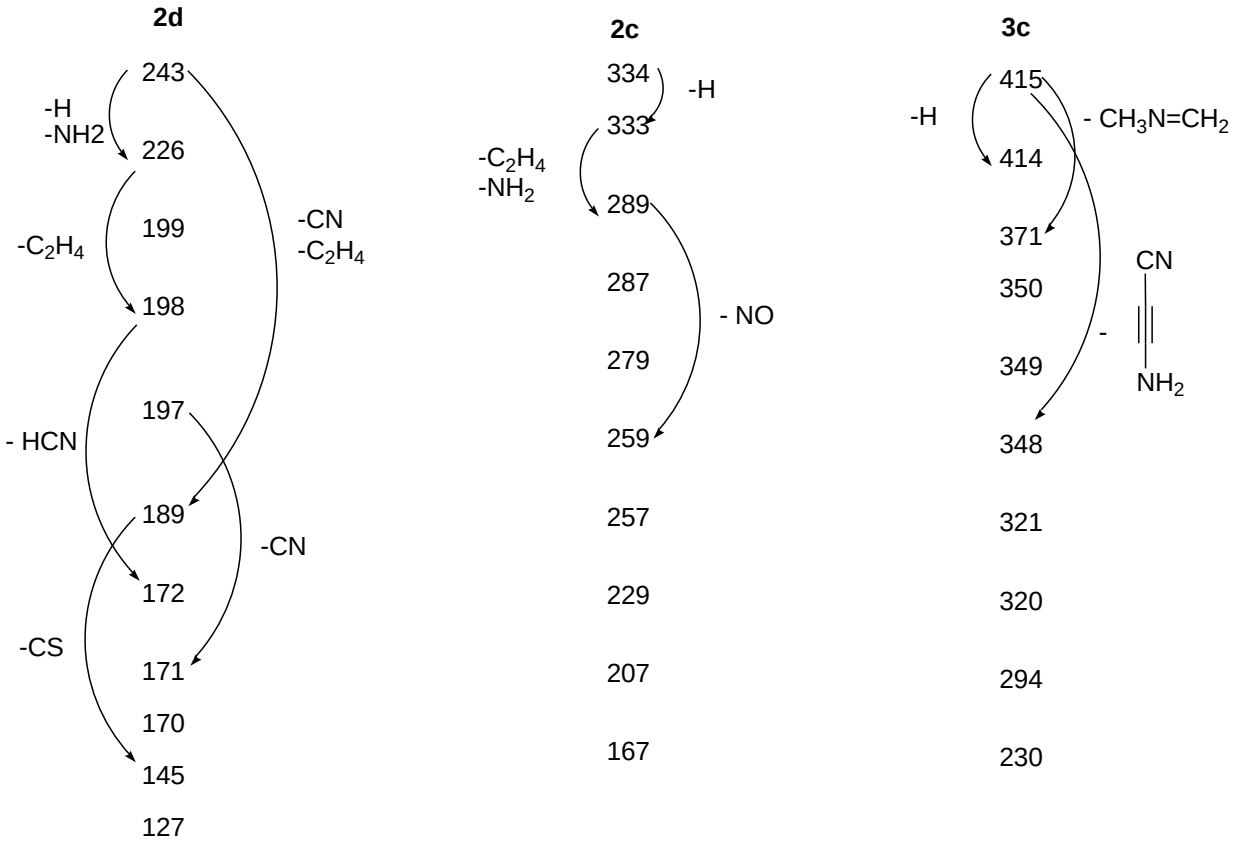
The loss of hydrogen and followed by cleavage of benzylamine groups was observed in compound **1b**and the fragmentation pattern shown in **Scheme-II**. The almost similar loss of H , C_2H_4, CN, NH_2 groups was observed in compounds **2a-d**and the characteristic loss of Hydrogen, Schiff's base and substituted acetylene moiety groups was observed in compounds **3a-c**and the schematic fragmentation pattern is depicted in **scheme-III**.The common loss of H,CO,C_2H_4,HCN groups were observed in quinoxaline derivatives (**4a-b,5**) and the fragmentation pattern is depicted in **Scheme-IV.**


-H
1a
m/z 346
m/z 345
-H
-
-H
m/z 343
m/z 344
-
-CO
m/z 290
m/z 288
m/z 316
CH2=C=O
m/z 246

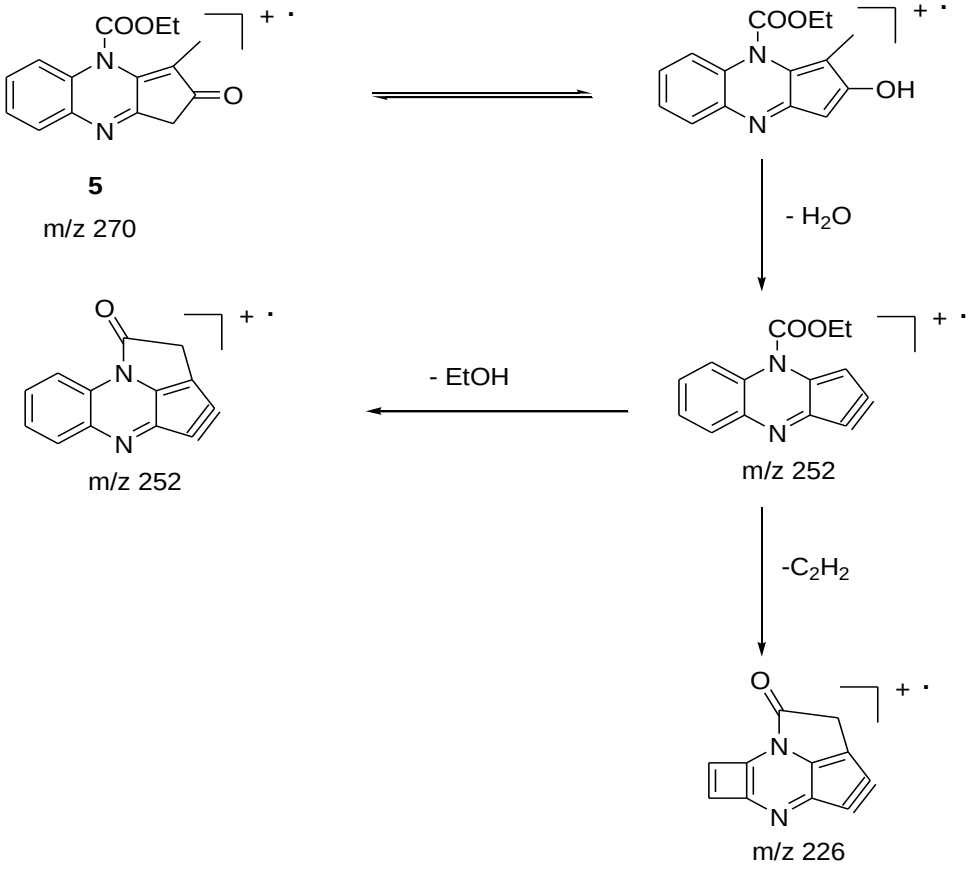
Scheme –I

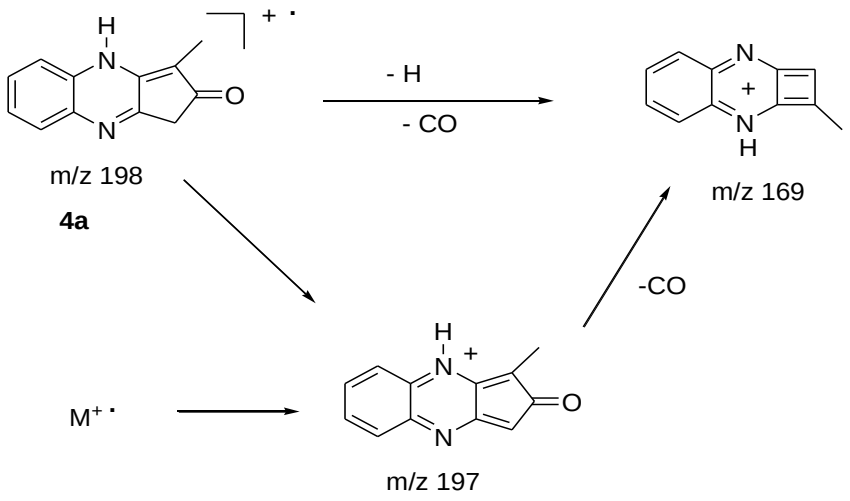


Scheme –II



Scheme- III





Scheme- IV

Compound **4a** loss of H,CO groups in two different routes was observed and showed in **Scheme-IV**.

Conclusion

Totally **10**heterocyclic compounds were studied for their mass spectral fragmentation pattern. Molecular mass information and fragmentation pattern are easily obtained under the electron ionization (EI) condition. The loss of H, isobutylene and ketene groups were observed in quinoacridine(**1a**). Similar loss of H,C_2H_2,NH_2,CN,groups were observed both pyridinedinitrile compounds **(2a-d)** and pyranopyridine derivatives (**3a-c**) .The common loss of H,CO,C_2H_4,HCN groups were observed in quinoxaline derivatives (**4a-b,5**).

Acknowledgment

We thank the DST, India for the financial support of this work and Prof V.T. Ramakrishnan for generous support for all my work.

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