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The mass spectral fragmentation of aciridinediones Derivatives

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Abstract: For all acridinediones compounds the electron ionization (EI) spectra are very clean, being dominated by loss of atoms or radicals such as CO,CH_3, ketene, isobutylene.In this paperwe would like to report the mass spectral fragmentation of 9-mono substituted acridinediones(**1a-g , 2a-h**).

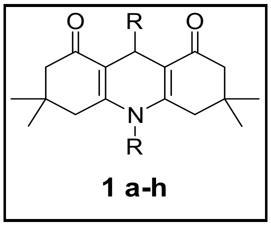
Key Words:Acridinedione, dihydroresorcinol, dimedone,ketene, isobutylene, methyl group.

Introduction

Mass spectrometry (MS) is unequivocally a powerful tool of characterization of organic compounds. Several series of acridinediones derivatives have been investigated by EI mass spectrometry because of due to their versatile wide applications such as laser dyes[1-8], OLED properties[9],solar cell[10],biological activities[11] and NLO properties[12]. The mass spectra of 9-substituted acridinediones in general shows very weak molecular ion. Almost most of the acridinediones compounds the electron ionization (EI) spectra are very clean, being dominated by loss of atoms or radicals such as CO,CH_3, ketene, isobutylene The base peak is invariably due to the ion obtained by loss of 9- substituents **(Scheme – I, Table –I).**Signal due to cleavages at α-bond and β-bond of the N-alkyl substituent have been observed **(b,c)** from the molecular ion. The fragmentations due to loss of CO and isobutylene from (**a**) have been observed (**d,e,f**). Another common fragment at m/z 272(or273) has also been recognized from acridinediones, by loss of the substituents at 9, 10 and gaining one H^+.

Experimental

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



1 a-h

Compound	R	**Compound**	R
1a	$C_6H_5CH_2$-	**1e**	$CH_3CH_2CH_2$-
1b	CH_2=CH-CH_2-	**1f**	$CH_3CH_2CH_2CH_2$-
1c	$CH_3COOCH_2CH_2$-	**1g**	Furfuryl
1d	$CH_3OCH_2CH_2CH_2$-	**1h**	P-NH_2SO_2-C_6H_4-

Common fragments (m/z 272 or 273) in most of the compounds observed wasgiven below.

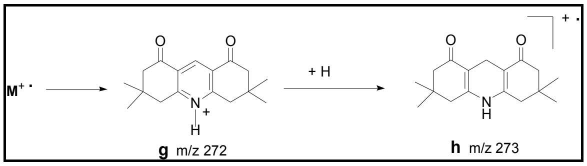
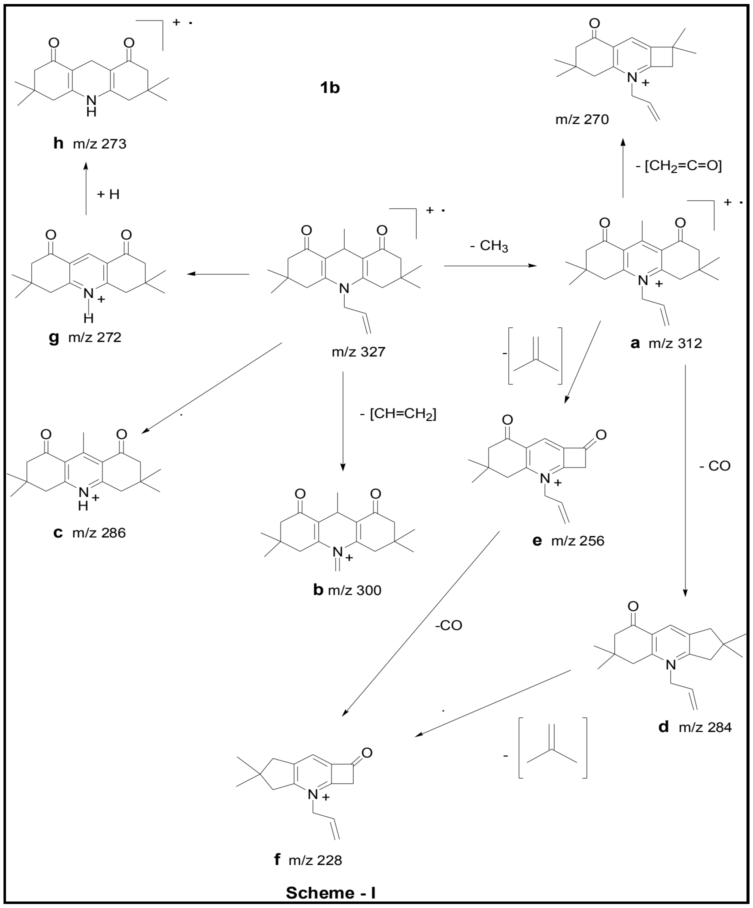


Table - I

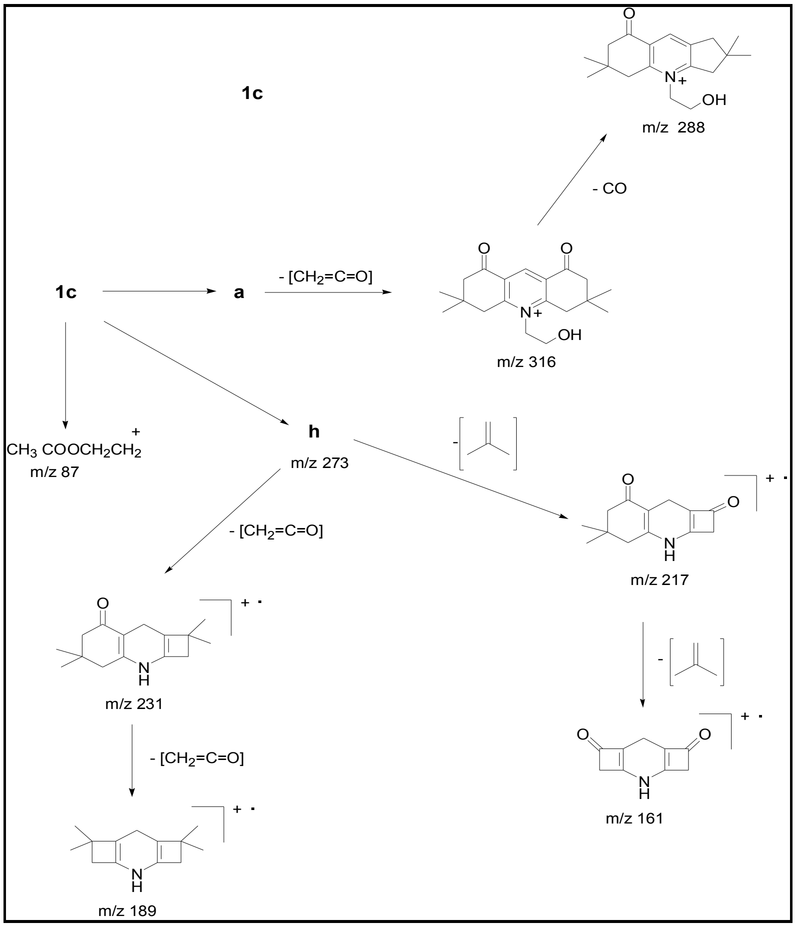
Compounds						
Compound Fragment	**1a**	**1b**	**1c**	**1d**	**1f**	**1g**
$M^{+\cdot}$	377 (0.1)	327(0.5)	374(M+1, 0.1)	359(1.5)	343(25)	368 (M+1, 20) 367(20) 366(35)
a	362(17.6)	312(100)	358(34.3)	344(100)	328(100)	352(70)
b	-	300(0.3)	300(0.5)	300(1.9)	300(10.0)	-
c	286(1.5)	286(2.5)	-	286(1.5)	286(20)	286(10)
d	-	284(3.4)	-	284(1.2)	284(1.2)	-
e	-	256(1.3)	-	256(1.7)		
f	-	228(1.9)	-	-	-	-
g	-	272(2.1)	272(1.2)	272(1.9)	272(90)	272(1)
h	273(1)	273(17.7)	-	-	-	-

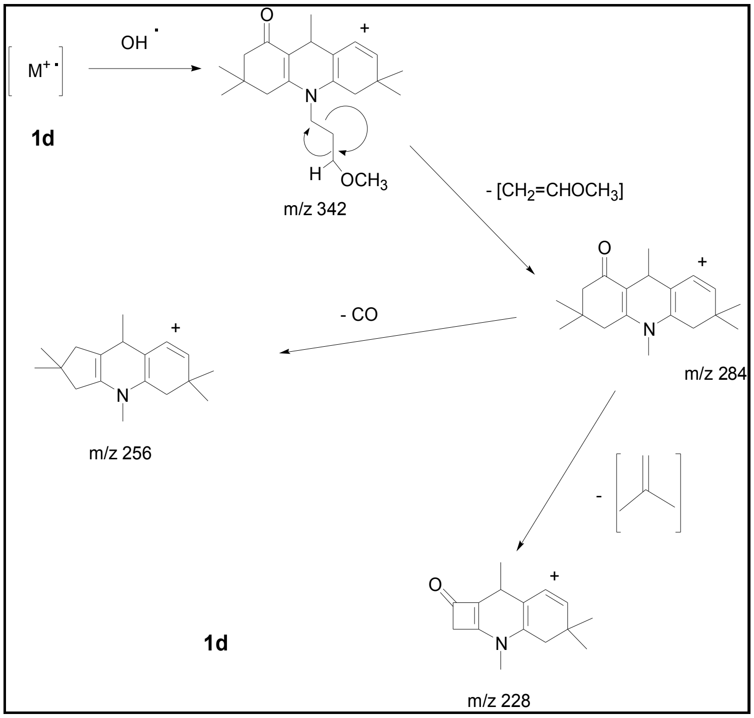
Compound **1b**shows loss of 9-substituted CH_3 group at m/z 312 and followed by loss of ketene at m/z 270, other major signals at m/z 300,284,256,228 may arise from fragment of ethylene, CO, isobutylene respectively. Other signals arising from the specific structural features have been recognized.



Scheme - I

Compound **1c**showed the loss of ketene from the acetoxy group followed by CO.Other major signals at m/z 231,189 may arise from fragment of ketene and m/z 217,161 may arise from fragment of isobutylene respectively.





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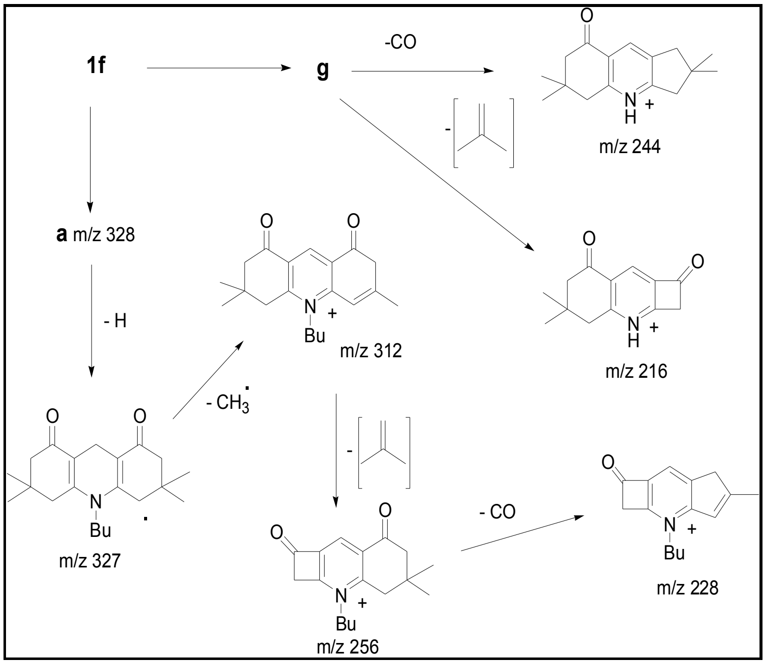
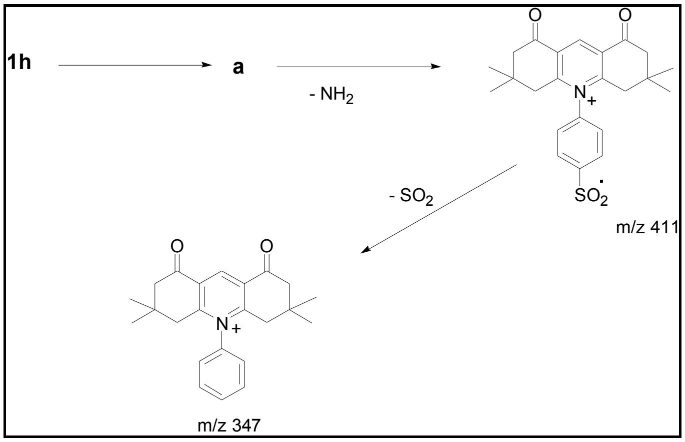
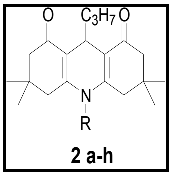


Compound **(1g)** shows a strong M-1 signal in addition to many common fragments. The base peak is due to furfuryl ion (m/z 81). Compound **1a** also shows the base peak due to tropylium ion (m/z 91). This type of general observations reported in the earlier our report[1-8]. Further the absence of signal at m/z 300 (fragment **b**) due to the cleavage of the β – bond of the N-substituents resulting in the loss of unstable phenyl and furfuryl radical is notices for compounds **1a** and **1g**, supporting the fragmentation pathway.

Compound **1h** shows the loss of NH_2 and $SO_2$from sulfonamide group.





2 a-h

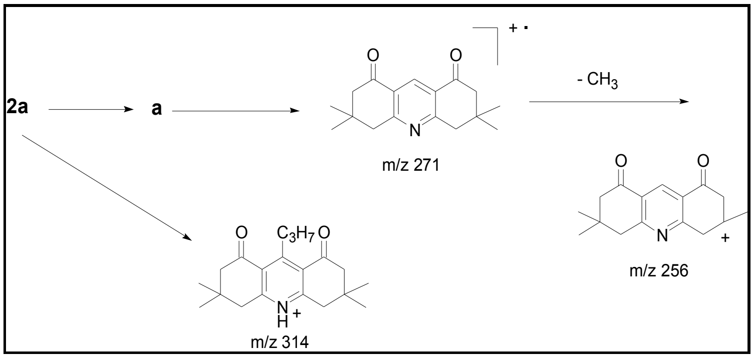
Compound	R	**Compound**	R
2a	$C_6H_5CH_2$-	**2e**	$CH_3CH_2CH_2$-
2b	CH_2=CH-CH_2-	**2f**	$CH_3CH_2CH_2CH_2$-
2c	$CH_3COOCH_2CH_2$-	**2g**	P – CH_3O-C_6H_4-
2d	$CH_3OCH_2CH_2CH_2$-	**2h**	H

The mass spectra of 9-propyl acridinediones in general show very weak molecular ion signals. The propyl group loss is highly facile to give the respective fragment **a**, as the base peak. Fragmentation, in general takes same mode as is observed in the 9-methyl analog. A detailed fragmentation is depicted for compound**2c** **(Scheme – II ; Table- II)**.

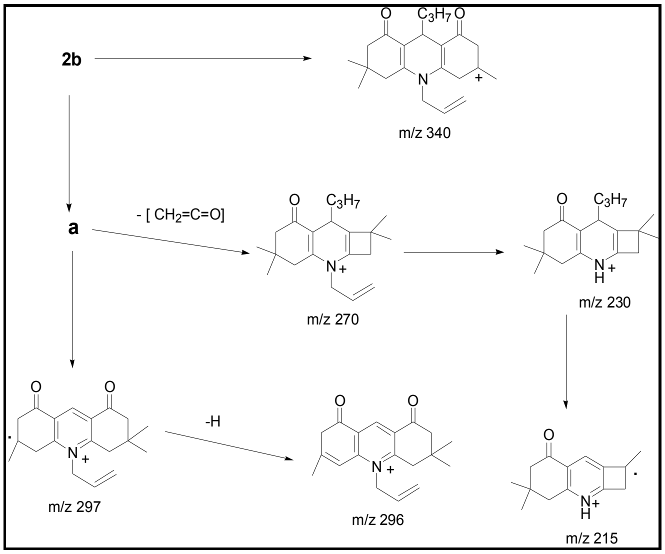
Table - II

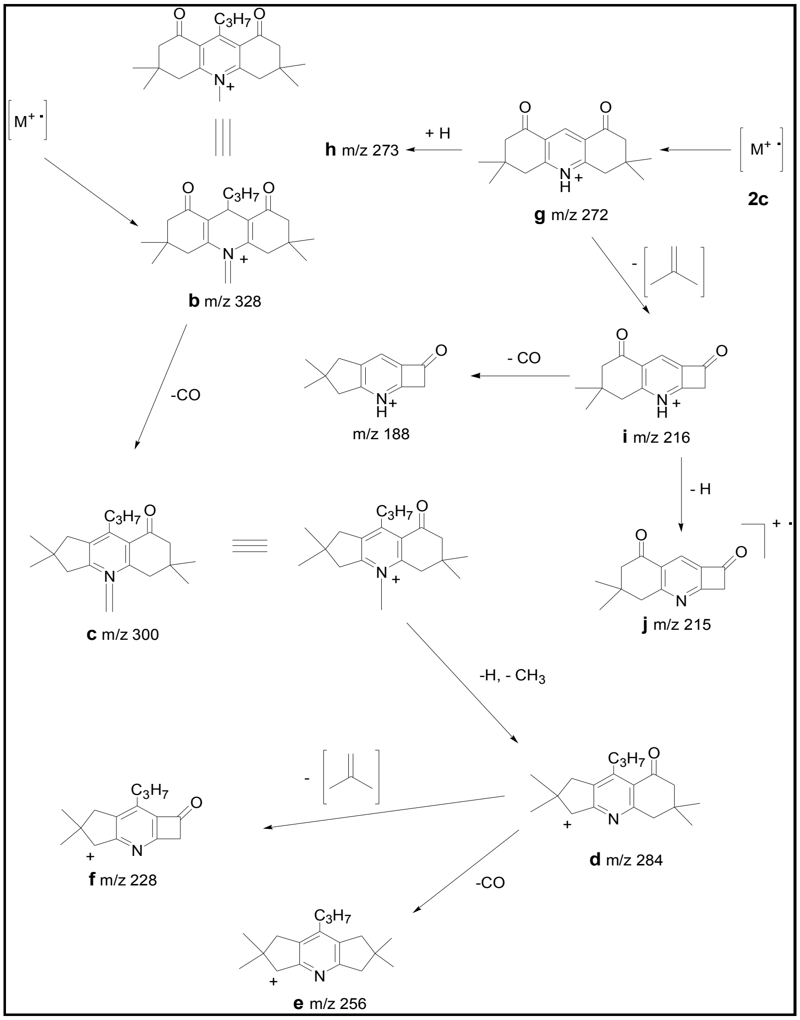
	Compounds						
Compound Fragment	**2a**	**2b**	**2c**	**2e**	**2f**	**2g**	**2h**
$M^{+\cdot}$	405 (0.12)	-	401 (0.07)	-	371 (0.06)	422 (M+1,10.9)	314 (M-1,1.2)
a	362 (79.8)	312 (100)	358 (100)	314 (100)	328 (100)	378 (100)	272 (100)
b	-	284 (0.6)	328 (0.45)	-	-	-	-
c	-	-	300 (2.5)	-	-	-	-
d	-	-	284 (1.8)	-	-	-	-
e	-	-	256 (0.8)	-	-	-	-
f	-	-	228 (0.8)	-	-	-	-
g	272 (4.8)	272 (2.6)	272 (2.9)	-	272 (8.8)	272 (100)	-
h	273 (6.0)	273 (6.0)	273 (2.3)	-	273 (5.1)	-	-
i	-	-	-	-	216 (1.6)	-	216 (4.1)
j	-	-	-	-	215 (1.0)	-	215 (2.2)

Signals characteristic of the N-substituents are also observed. Compound **2a** gives tropylium ion as the base peak at m/z 91. Benzyl grouploss from $\mathbf{M}^{+\cdot}$as well as from fragment give signals at m/z 314 and m/z 271 respectively.

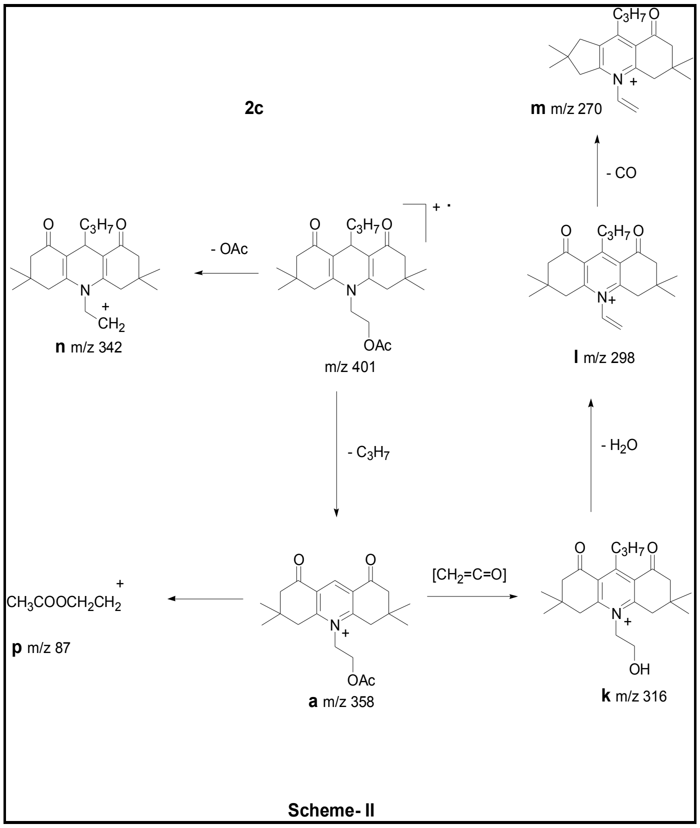


Compound **2b**shows also loss of CH_3 at m/z 340; other signals at m/z 297, 296,270,230,215 may arise from fragment**a** as depicted follows.



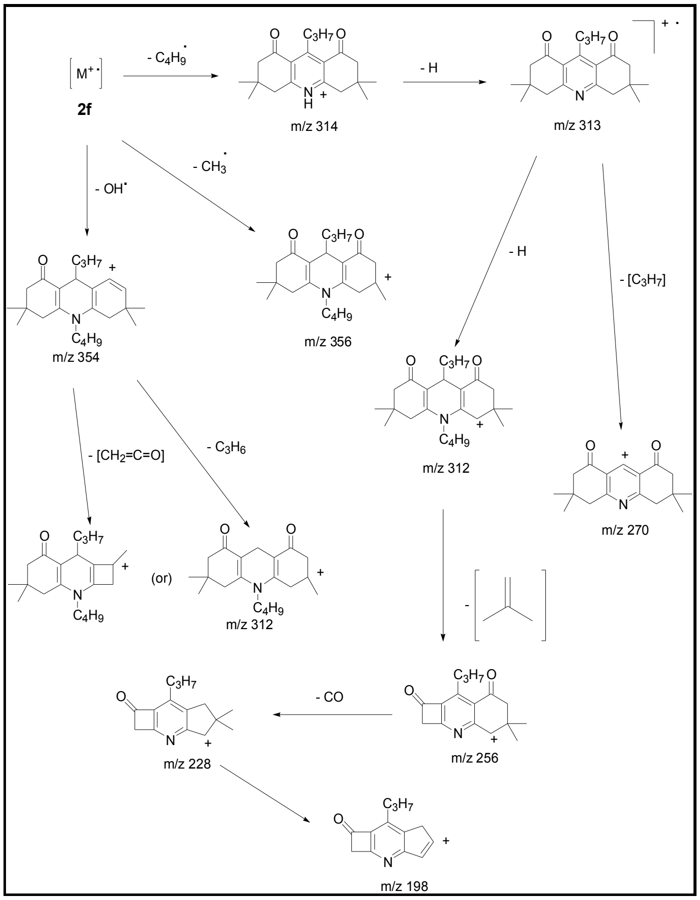


Compound **2c** shows OAc, CO loss as well as the characteristic propyl loss, followed by other fragmentations as depicted as follows.

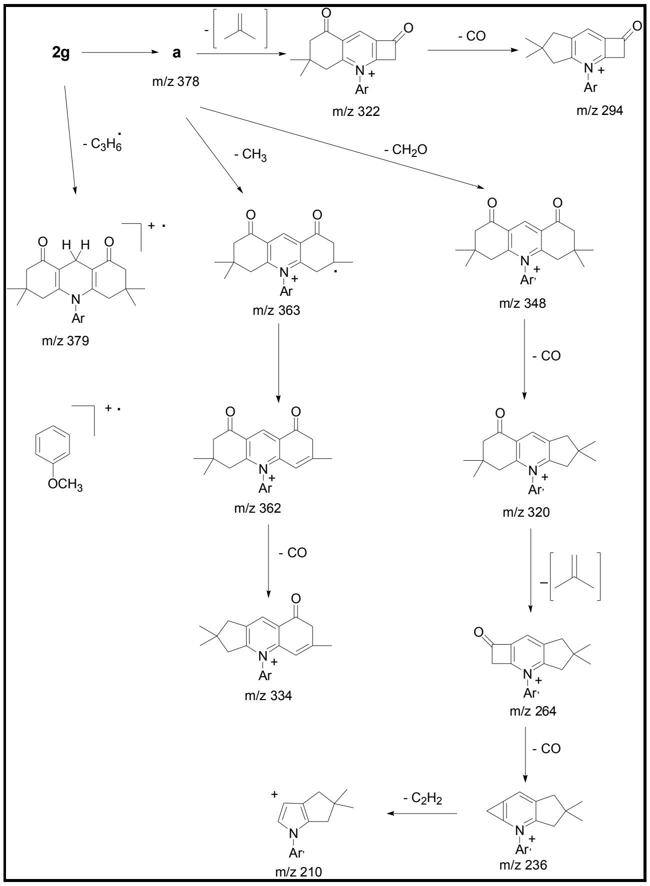


Scheme- II

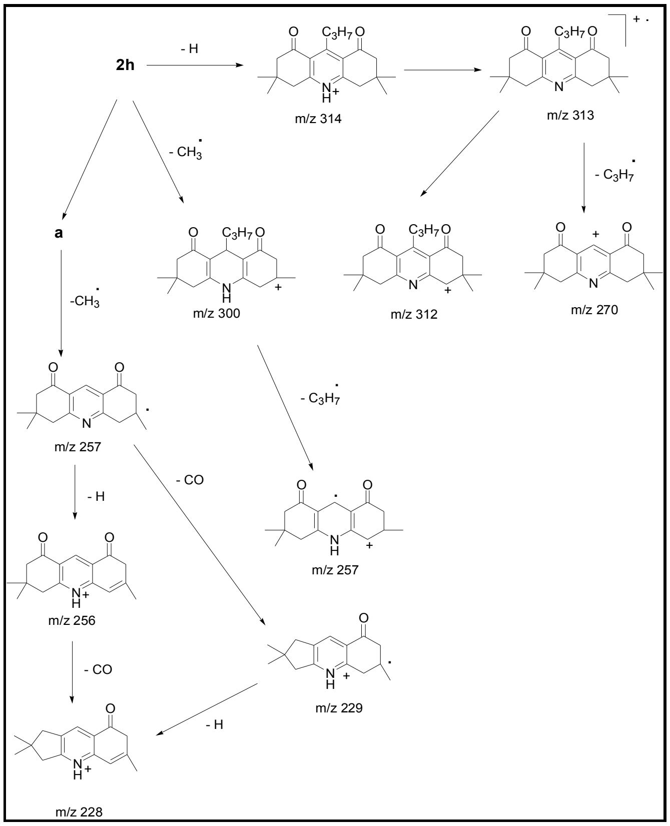
Compound **2f** shows $(M\text{-}CH_3)^+$, $(M\text{-}OH)^+$, $(M\text{-}C_4H_9)^+$ and other derived signals as follow



Compound**2g**shows many peaks arising from fragments**a** and through the loss of CH_2O from **a**.



Compound **2h**shows H and CH_3lossas well as the characteristic propyl loss, followed by other fragmentations as depicted.



Conclusion

Totally **16** acridinediones derivatives were studied for their mass spectral fragmentations. Molecular mass information and fragmentation pattern are easily obtained under the electron ionization (EI) condition. Common fragment at m/z 272 (or 273) has also been recognized from most of the acridinediones, by loss of substituents at 9, 10 and gaining one H^+. Almost all acridinediones compounds the electron ionization (EI) spectra are very clean, being dominated by loss of atoms or radicals such as CO,CH_3, ketene, isobutylene.

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