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## Isolation and structure elucidation of Scopoletin from *Ipomoea reniformis* (Convolvulaceae)

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### ABSTRACT

Besides a known Coumarin derivative, Scopoletin, the iridoids gardenoside was isolated for the first time from an *Ipomoea* species, namely *Ipomoea reniformis* (Convolvulaceae). Its structure was established on the basis of its spectroscopic data.

**Key words:** *Ipomoea reniformis*, Convolvulaceae, Mass, NMR, UV, IR, Melting point, Coumarin.

### INTRODUCTION

*Ipomoea reniformis* chois (Convolvulaceae) is a perennial, much branched herb (creeper). It is found widely distributed all over India, especially in damp places in upper Gangetic plain, Gujarat, Bihar, West Bengal, Western Ghats ascending up to 900 metres in the hills, Goa & Karnataka in India & Ceylon & Tropical Africa (Kirtikar and Basu., 1935), (Shah., 1987), (Ansari., 2006), (Agarwal., 1997), (Satyvati and Gupta., 1987), (Backer., 2002), (Chattertee., 2003), (Agarwal., 1947). In India it is known by different names in different regions, viz. Mooshakarni in Sanskrit, Underkani in Mumbai, Indurkani in Telugu, Chukakani in Urdu, Goromusha in Persian, mushkani in Hindi, Paerattae-kirae in Tamil and Yellikkadukirai in Chennai (Nadkarni., 2000), (Warden and Hooper., 1890).

In the Indigenous system of Medicine, *Ipomoea reniformis* has been claimed to be useful for cough, headache, neuralgia, rheumatism, diuretic & inflammation and troubles of nose & kidney diseases. The powder of leaves acts as a purgative and the root has diuretic, laxative and applications in the eyes & gums diseases. The whole plant decoction is mainly responsible for its medicinal uses (Nadkarni., 2000).

The course of our search for secondary metabolites in this species led us to the isolation and characterization of Scopoletin from the methanolic extract of the whole herb of *Ipomoea reniformis*.

### EPERIMENTAL

#### Authentification and Collection of plant

Fresh & entire plant of *Ipomoea reniformis* was collected in the month of August – September from the Bio-Science department, Vallabh Vidyanagar, Anand district of Gujarat state. This was identified, confirmed and authenticated by taxonomist of Bioscience Department, Sardar Patel University, Vallabh vidyanagar. A voucher specimen of plant (Voucher No. MKB/Ir-1/15/ARGH-10) is deposited in Departmnet of Pharmacognosy, A. R. College of pharmacy,

Vallabh Vidyanagar, for future reference.

## Extraction and isolation

### Preparation of sample

100gm of dried whole herb powder of *Ipomoea reniformis* was treated with petroleum ether to remove fatty materials. The defatted powder is then extracted with methanol exhaustively. The Methanolic extract was concentrated and it has been taken for preparative Thin Layer Chromatography.

In Preparative thin layer chromatography, the substance of interest was scrapped from the layer after detection and subsequently examining it with aid of suitable analytical technique. The mobile phase used was Toluene: Ethyl acetate: Formic acid (5:4:1). After spotting and developing the plate in the solvent system, it was dried and then observed under UV light at 366nm in UV cabinet. Four spots at  $R_f$  value 0.47, 0.6, 0.88, 0.95 were observed. One spot of  $R_f$  value 0.47 was scrapped and put in Petri dish and methanol was added and filtered. The filtrate was evaporated to obtain one sample i.e. Isolated compound V ( $R_f$ : 0.47), may be Scopoletin. The sample was then subjected to Co-TLC, chemical test and spectroscopic studies for further identification and confirmation.

## RESULTS AND DISCUSSION

### Characterization and confirmation of isolated compound

Compound V ( $R_f$ : 0.47) Scopoletin, was isolated by the preparative thin layer chromatography using Silica Gel G as adsorbant. The solvent system used was Toluene: Ethyl acetate: Formic acid (5:4:1).

### Spectroscopic studies

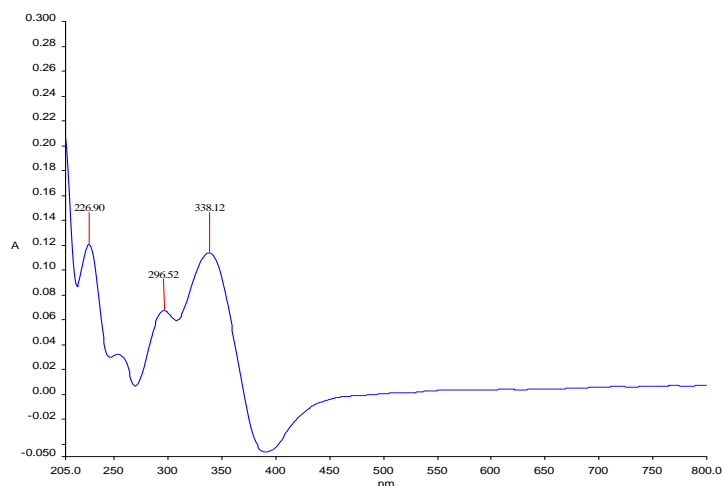
#### UV-Visible spectroscopy

The results obtained by UV spectroscopy of isolated compound V ( $R_f$ : 0.47) & Standard Scopoletin, in methanol and after addition of 2-4 drops of 2M NaOH indicate the  $\lambda_{max}$  value as given in Table-1.

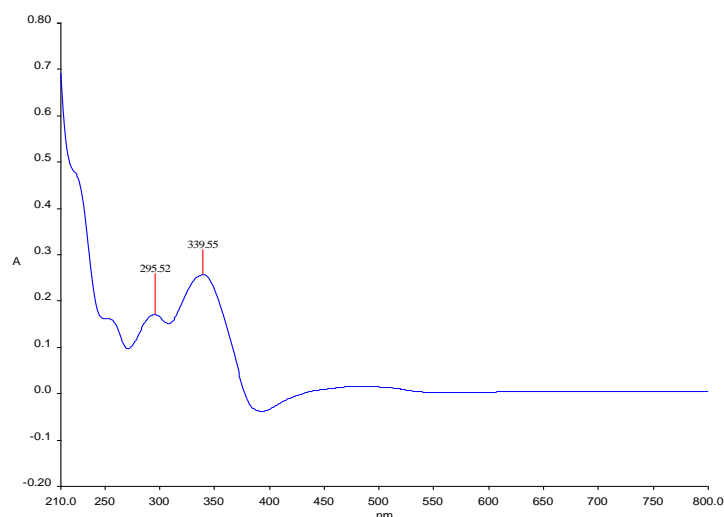
**Table 1:** The data from UV spectrum of isolated compound V and standard Scopoletin.

Sample	$\lambda_{max}$ (nm)		Inference
Standard Scopoletin	Before addition of NaOH	After addition of NaOH	Isolated Compound V is Scopoletin
	338.12 296.52 226.90	390.29	
Isolated Compound V	339.55 295.52	389.75	

The UV spectrums of the Methanolic solution of Standard Scopoletin and Isolated Compound V have characteristic bands at 338.12nm, 296.52nm, 226.90nm, and 339.55nm, 295.52nm respectively. This leads to the conclusion that the Isolated Compound V is Scopoletin. (Figures 1 &2).

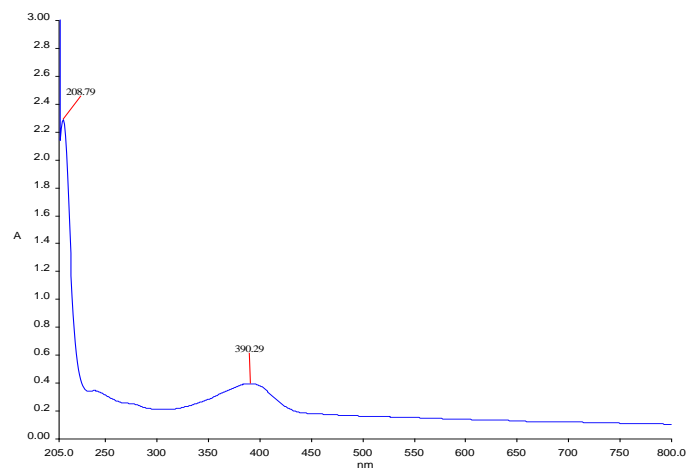


**Fig 1** UV Spectra of Standard Scopoletin in Methanol

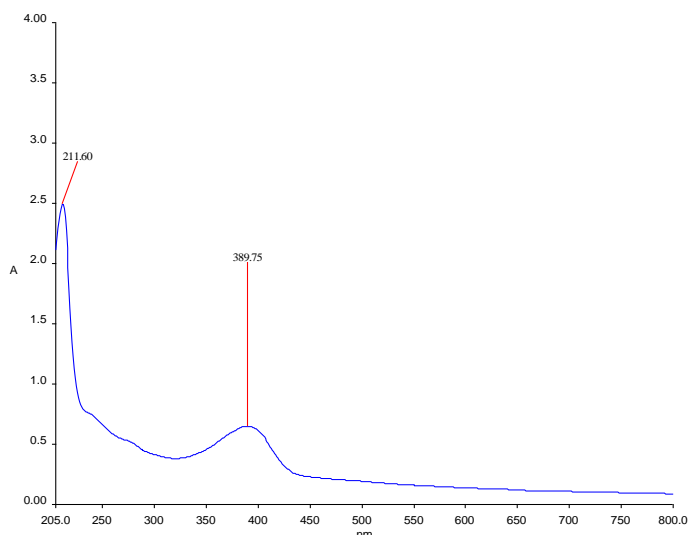


**Fig 2** UV Spectra of Isolated Compound V in Methanol.

After addition of 2-4 drops of 2M NaOH in Methanolic solution of Standard Scopoletin & Isolated Compound V, bathochromic shift was observed which also confirms that Isolated Compound V is Scopoletin. (Figures 3&4).



**Fig 3** UV Spectra of Standard Scopoletin in Methanol after addition 2M NaOH



**Fig 4** UV Spectra of Isolated Compound V in Methanol after addition 2M NaOH.

### IR Spectroscopy

Table 2 shows the data obtained from FTIR Spectroscopy and possible functional groups present.

In the IR spectral analysis, the Peak at 3337.44 & 3341.44  $\text{cm}^{-1}$ , a broad band is most probably the result of O-H stretching vibrations of phenol OH group. The peak at 2850.97 & 2875.05  $\text{cm}^{-1}$  showed C-H Stretching due to  $-\text{CH}_3$ . The peak at 1702.90 & 1703.42 indicates the presence of  $-\text{C}=\text{O}$ , Carbonyl group. The peak at 1628.09 & 1606.75 showed the presence of  $-\text{CH}=\text{CH}$  group. The peak at 1565.06, 1510.53 & 1568.83, 1511.16 indicates the presence of benzene ring. The peak at 861.46 & 861.50 showed the presence of disubstitution of benzene ring in both standard Scopoletin and isolated compound V respectively. The above Comparison with standard confirms that isolated compound V is Scopoletin (Figures 5&6).

**Table 2:** The data from FTIR spectrum of standard Scopoletin and isolated compound V.

Peaks ( $\text{cm}^{-1}$ )		Functional group
Standard Scopoletin	Isolated Compound V	
3337.44	3341.44	O-H Alcohol group present
2850.97	2875.05	C-H group present
1702.90	1703.42	Carbonyl C=O group present
1628.09	1606.75	CH=CH group present
1565.06	1568.83	Benzene ring present
1510.53	1511.16	Benzene ring present
861.46	861.50	Due to disubstitution of benzene

### NMR spectroscopy

Table 3 shows the data obtained from NMR Spectroscopy. The  $^1\text{H}$  NMR spectrum of standard Scopoletin and Isolated Compound V showed two doublets with coupling constant of 9.2 Hz at  $\delta$  6.23, 6.22 and 7.88 ppm, which were assigned as H-

3 and H-4, respectively in standard Scopoletin and isolated compound V, characteristic for coumarins.

**Table 3:** The data from NMR spectrum of standard Scopoletin and isolated compound V.

No. of H atom	Standard Scopoletin		Isolated Compound V	
	$\delta$ value, ppm	Integration, Multiplicity (J, HZ)	$\delta$ value, ppm	Integration, Multiplicity (J, HZ)
3	6.23	1H, d(9.2)	6.22	1H, d(9.2)
4	7.88	1H, d(9.6)	7.88	1H, d(9.2)
5	7.14	1H, S	7.13	1H, S
8	6.79	1H, S	6.79	1H, S
C-6-OMe	3.93	3H, S	3.93	3H, S

**Table 4:** The molecular weight data from mass spectrum of standard Scopoletin and isolated compound V.

No. Sample	M-1 Peak	Molecular weight
Standard Scopoletin	191.10	192.10
Isolated Compound V	191.10	192.10

**Table 5:** Melting point.

Compound	Melting Point $^{\circ}\text{C}$
Scopoletin (Standard)	200-207
Isolated Compound V	206.2

The  $^1\text{H}$  NMR spectrum of Scopoletin showed a methoxyl group singlet at  $\delta$  3.93 ppm and two aromatic singlets at  $\delta$  7.14, 7.13 & 6.79 respectively in standard Scopoletin and isolated compound V which were explained by 6,7-disubstitution. So it confirms that isolated compound V is Scopoletin (Figures 7&8).

### Mass spectroscopy

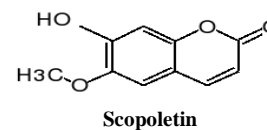
Mass spectra of both standard Scopoletin and isolated Compound V shows M-1 peak at 191.10 which indicate that their molecular weight is same, 192.10. So it confirms that isolated compound V is Scopoletin (Figures 9&10).

### Melting point

Table-5 shows the data obtained from the melting point determination of standard & isolated compound V. Melting Point of Isolated Compound V and Standard Scopoletin are same.

### CONCLUSION

From above spectroscopic studies, we have concluded that the isolated compound V, from the methanolic extract of *Ipomoea reniformis* is Scopoletin.



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Sophisticated Instrumentation Centre for Applied Research & testing  
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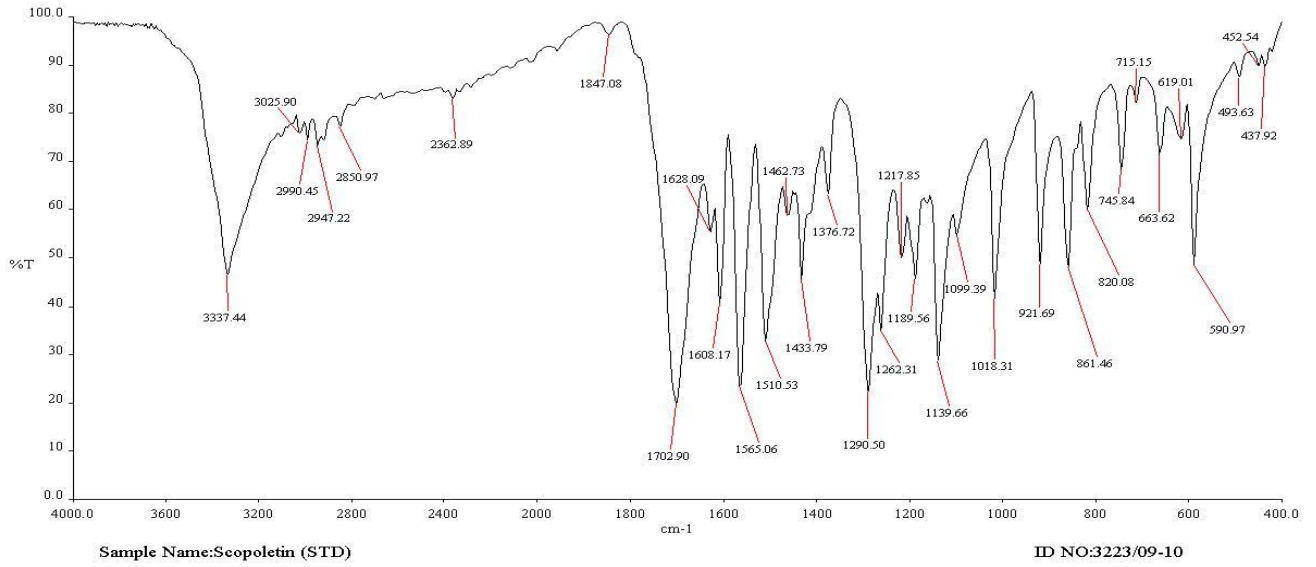


Fig 5 IR spectrum of standard Scopoletin.

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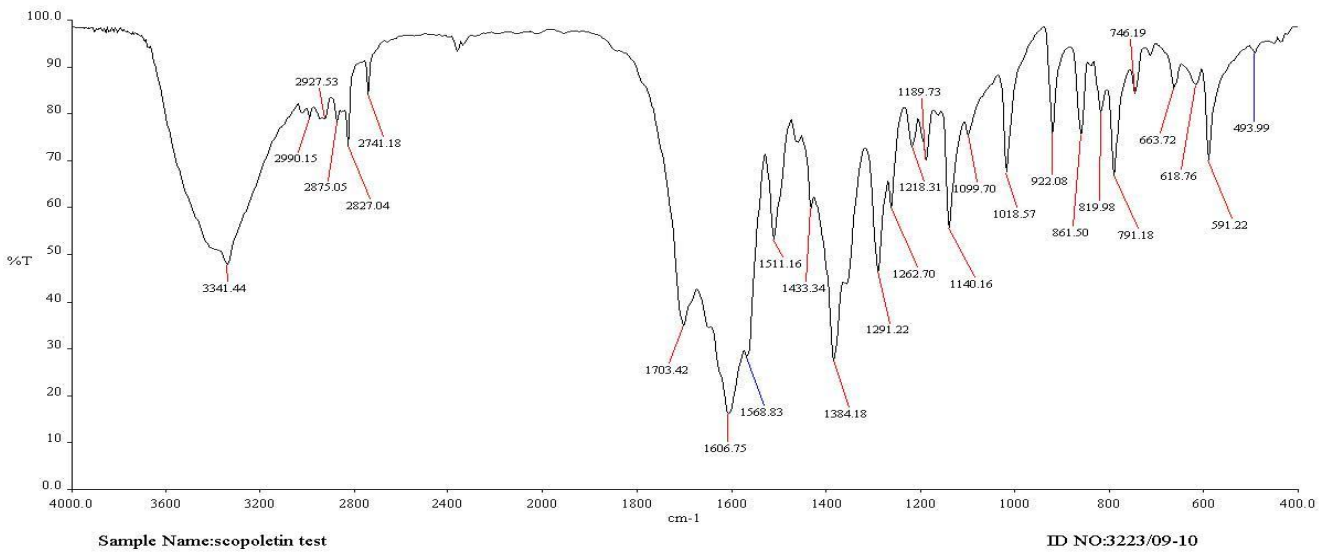


Fig 6 IR spectrum of Isolated Compound V.

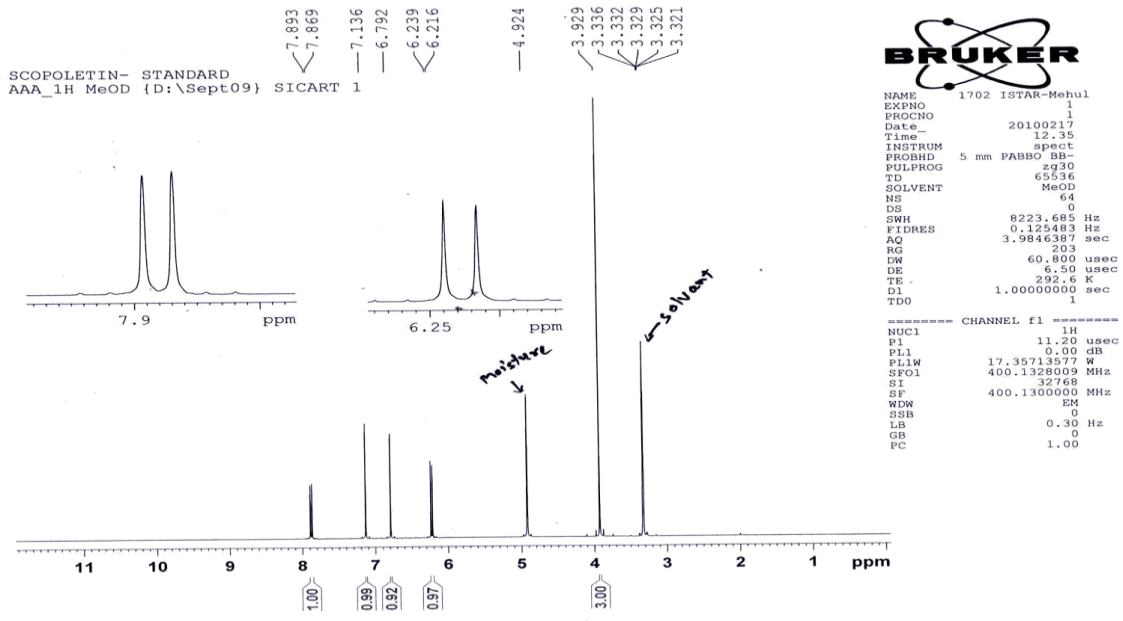


Fig 7: NMR spectrum of Standard Scopoletin.

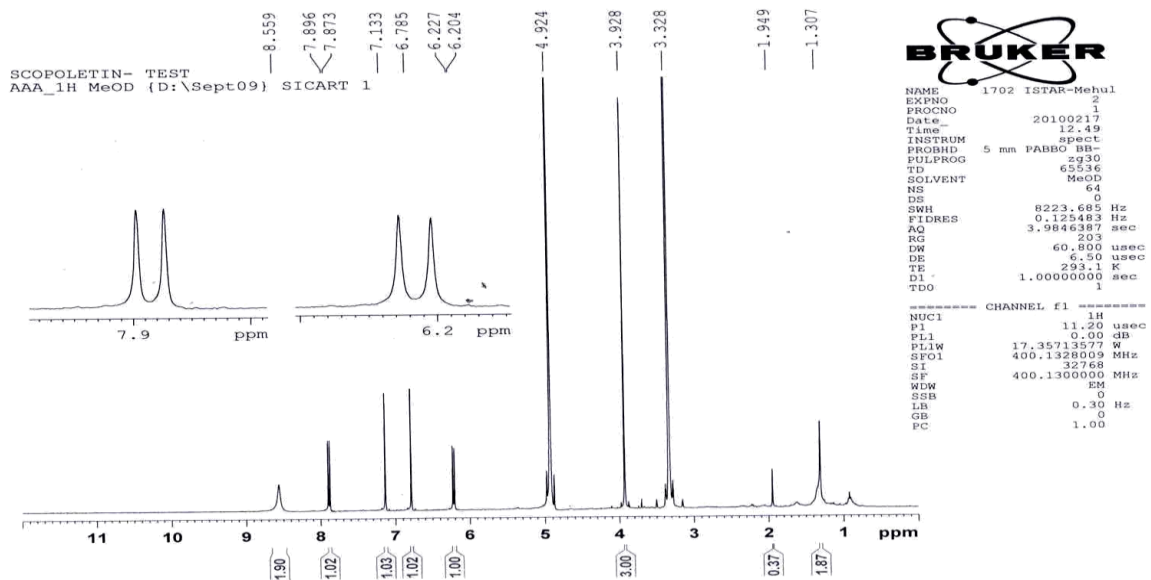


Fig 8 NMR spectrum of Isolated Compound V.

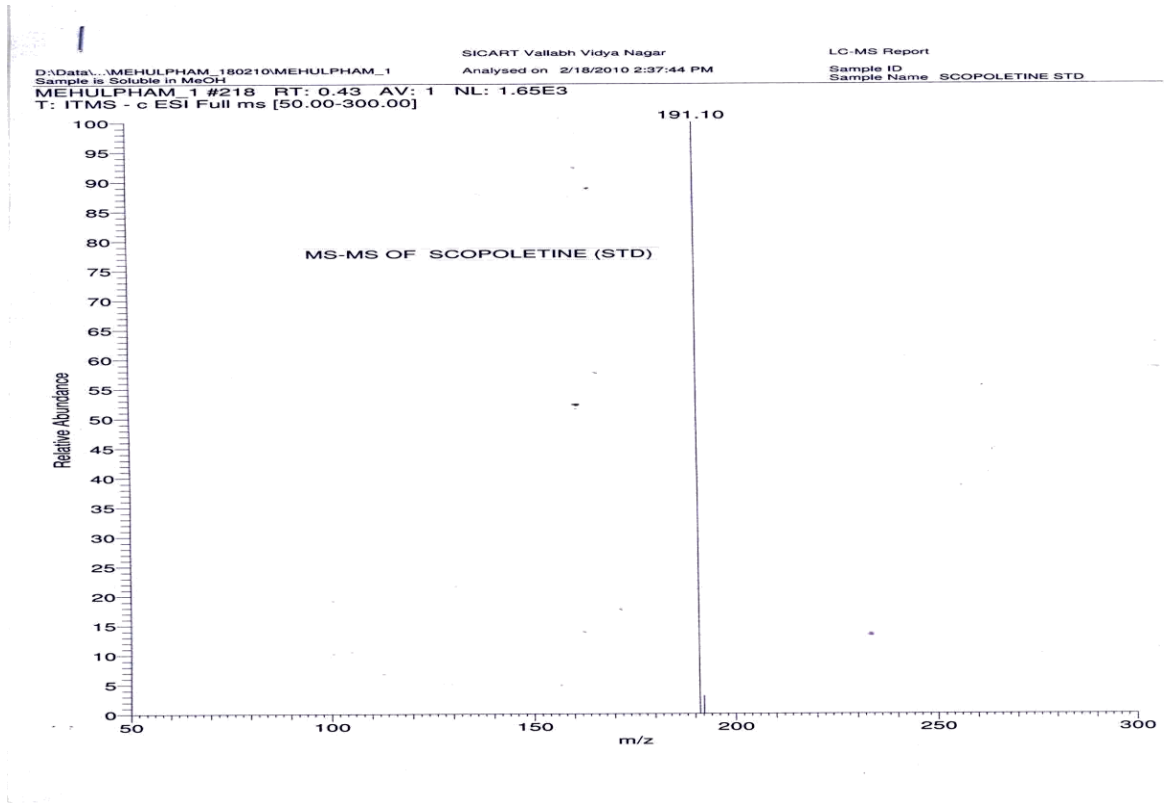


Fig 9 Mass spectrum of standard Scopoletin.

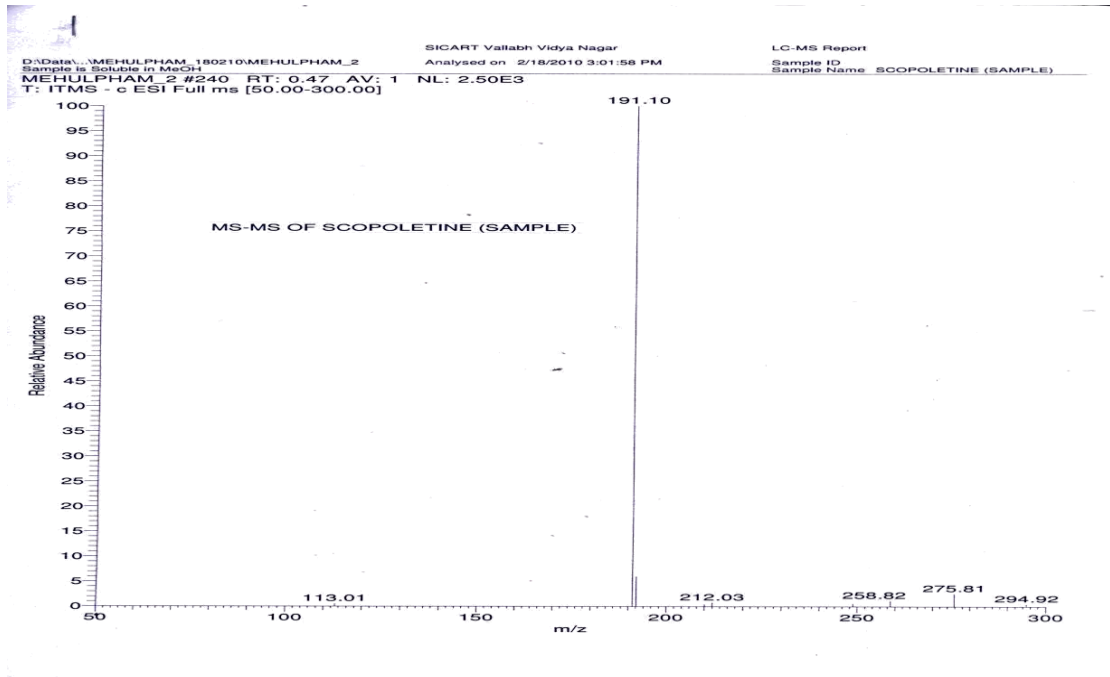


Fig 10: Mass spectrum of Isolated Compound V.

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