

FTIR and GCMS Studies in Phytochemical Characterization of *Physalis Angulata* and *Solanum Virgianum*

S. L. Chavan, S. M. Kurhade, R. G. Khose

New Arts Commerce and Science College, Ahmednagar, Maharashtra, India

ABSTRACT

The Present study focuses on analysis of phytochemicals present in various parts of *Solanum virgianum* and *Physalis angulata* (Solanaceae family) using GCMS and IR spectroscopy. The work also highlights the different phytochemicals present in various parts like fruits and leaves of the plants from Solanaceae family. The GCMS has identified 14 components each from *Physalis angulata* fruit and leaf extracts, and 13 from *Solanum virgianum* leaf extracts. However, 11 components were identified from *Solanum virgianum* fruit extracts. The FTIR spectrum confirmed the presence of functional groups like alcohol, phenol, alkene, alkanes, flavones, Azides, Arenes in the fruit and leaf extracts.

Keywords: *Solanum virgianum*, *Physalis angulata*, Solanaceae, GCMS, FTIR spectroscopy.

I. INTRODUCTION

Knowledge of the chemical constituents of plant is essential, for the discovery of therapeutic drugs as well as for finding new sources of such economic materials as tannins, oils, gums, precursors for the synthesis of complex chemical substances 3,12. A great variety of phytochemicals are synthesized and accumulated by woody plants in their cells, which include alkaloids, flavonoides, tannins, cyanogenic glycosides, phenolic compounds, saponins and lignin 17. Phytochemical which possess many economical and physiological roles are widely distributed as plant constituents

Physalis angulata and *Solanum virgianum* Dunal from the Solanaceae family are rich in secondary metabolites with specific pharmacological properties.

The metabolic constituents, particularly secondary metabolites differ with the variety of plant, tissue type and at times with the growth conditions²⁴. There is enormous difficulty in standardizing any formulation

if the exact composition of chemical constituents is not known 4,18. So there is a need to study the various chemicals present in different parts of plant to evaluate their potential as medicinal plants. With the advancement in analytical technology, details about metabolites present in plants can be identified with help of instruments like GCMS and IR spectroscopy 10,14,21. Present study deals with chemical screening of *Solanum virgianum* and *Physalis angulata* using Gas Chromatography-Mass Spectrometry (GCMS) and Infrared (IR) spectroscopy.

II. METHODS AND MATERIAL

2.1 Plant materials :

Solanum virgianum and *Physalis angulata* were collected from Ahmednagar district, Maharashtra state and identified 2. The leaves and fruits were isolated, dried and powdered. The samples were extracted with ethanol using Soxhlet apparatus. Analytical techniques GCMS and Fourier Transform Infrared (FT-IR)

spectroscopy were used for further phytochemical analysis^{5,16}.

III. RESULT AND DISCUSSION:

1. GCMS analysis: Identification of components detected by GCMS was based on direct comparison of the retention times and mass spectral data with those for standard compounds from National Institute of Standards and Technology (NIST) library. The GCMS identified 15 phytochemicals each from *Physalis angulata* fruit extract, *Physalis angulata* leaf extracts and *Solanum virgianum* leaf extracts, *Solanum virgianum* fruit extracts, however, showed the presence of 12 phytochemicals. The compounds, identified in the analysis and which are unique to particular extract are reported below with their retention times and area percentage.

1a. GCMS analysis of *Physalis angulata* fruit extract (PAF): The phytochemicals present in *Physalis angulata* fruit extract are shown in table no.1 and figure no.1 displays the GCMS chromatogram. Heptadecane, Octadecane, Dibutyl phthalate were present.

1b. GCMS analysis of *Physalis angulata* leaf extract (PAL): The phytochemicals present in *Physalis angulata* leaf extract are shown in table no 2 and figure no 2 displays the GCMS chromatogram. In the fruit and leaf extracts, octasiloxane and heptasiloxane were common.

1c. GCMS analysis of *Solanum virgianum* fruit extract (SVF): The phytochemicals present in *Solanum virgianum* fruit extract are shown in table no. 3 and figure no. 3 displays the GCMS chromatogram.

1d. GCMS analysis of *Solanum virgianum* leaf extract (SVL): The phytochemicals present in *Physalis*

angulata leaf extract are shown in table no. 4 and figure no. 4 displays the GCMS chromatogram.

The phytochemical constituents obtained after GCMS of *Physalis angulata* fruit (PAF) and leaf (PAL) are shown in Table No.1 and 2 respectively. It shows presence of heptasiloxane monolinoleoyl glycerol trimethylsilyl ether and octasiloxane in both leaf and fruit extract. Present study also showed presence of compounds which are unique to fruit and leaf part of the plant. *Solanum virgianum* fruit extract contains 9,12- Octadecadienoic acid (Z,Z) methyl ester, tocopherol and carotene. *Solanum virgianum* leaf extract contains levoglucosenone, benzenetriol, heptadecane. The details about the retention time and area percentage of the compound indicated in the Table No.3 and 4.

2 FTIR analysis: The FTIR spectrum was used to identify the functional group of the active components based on the peak value in the region of infrared radiation

2a. FTIR analysis of PAF extract: The IR spectrum is shown in figure no.5. The PAF extract yielded maximum peak level 3600 cm^{-1} and minimum peak 783 cm^{-1} . FT-IR studies confirm the presence of functional groups in PAF extract and is listed in table no

5. Many of the functional present in *Physalis angulata* fruit and leaf extract are similar like aliphatic and carboxylic group but the fruit extract contains Arenes and *Physalis angulata* leaf contains flavones.

2b. FTIR analysis of PAL extract: The IR spectrum is shown in figure 6 and FT-IR studies confirm the presence of functional groups in PAF extract and is listed in table no

6. The PAL extract yielded maximum peak level 3600 cm⁻¹ and minimum peak 783cm⁻¹ .

2c. FTIR analysis of SVF extract: The IR spectrum is shown in figure 7 and FT-IR studies confirm the presence of functional groups in SVF extract and is listed in table no 7. The SVF extract yielded maximum peak level 3448 cm⁻¹ and minimum peak 723 cm⁻¹ . Many of the functional present in Solanum virgianum fruit and leaf extract are similar like aliphatic group ,alcohol group but the fruit extract contains azides ,arenes and Solanum virgianum leaf contains nitrile isocyanates and conjugated carbons.

2d. FTIR analysis of SVL extract: The IR spectrum is shown in figure 8 and FT-IR studies confirm the presence of functional groups in SVL extract and is listed in table no 8. The SVL extract yielded maximum peak level 3600 cm⁻¹ and minimum peak 715 cm⁻¹ .

IV. CONCLUSION

Phytochemical screening of plant extract is vital, as it helps us to verify the exact composition of metabolites in various plants .The research is helpful, in establishing relationship between the chemical and their biological, physiological roles. The study also emphasizes use of sophisticated instruments like GCMS and IR Spectroscopy in phytochemical research.

V. ACKNOWLEDGMENT

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Table No.1: Retention time, Area%, Molecular formula and Major peaks of chemicals detected by GCMS of Physalis angulata fruit extract (PAF).

Peak no.	Rt	Area %	Molecular formula	Compound
1	8.22	1.55	C10H30O5Si5	Cyclopentasiloxane
2	10.72	2.92	C14H44O6Si7	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13tetradecamethyl
3	13.95	3.85	C16H50O7Si8	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15 hexadecamethyl
4	14.95	4.52	C16H48O8Si8	Cyclooctasiloxane, hexadecamethyl
5	16.67	1.02	C16H48O6Si7	Heptasiloxane, hexadecamethyl
6	18.17	9.15	C16H22O4	Dibutyl phthalate
7	19.37	16.17	C19H34O2	9,12Octadecadienoic acid (Z,Z), methyl ester
8	19.97	5.85	C21H38O2	nPropyl 9,12octadecadienoate
9	23.21	3.66	C24H38O4	Diisooctyl phthalate
10	24.25	0.53	C20H60O10Si10	Cyclodecasiloxane, eicosamethyl
11	26.66	1.70	C28H39ClO9	9Desoxy9chloroingol 3,7,8,12tetraacetate
12	28.50	1.88	C23H48	Heptadecane, 9hexyl28
13	30.17	1.67	C26H54	Octadecane, 3ethyl15(2ethylbutyl)
14	33.07	2.56	C30H50O6	Olean12ene3,15,16,21,22,28hexol

Figure 1 : GCMS chromatogram of Physalis angulata fruit (PAF)

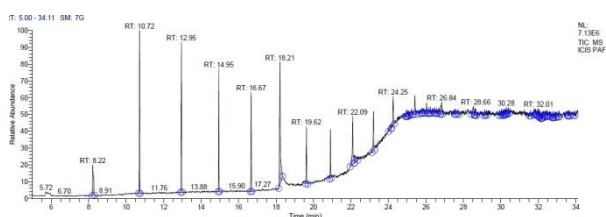


Figure 2: GCMS chromatogram of Physalis angulata leaf (PAL)

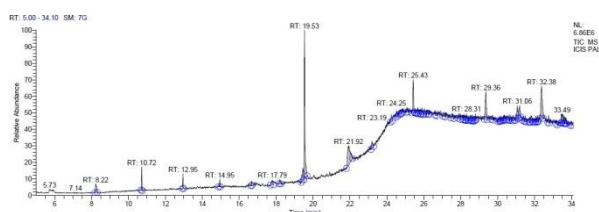


Table no 2: Retention time, Area%, Molecular formula and Major peaks of chemicals detected by GCMS of Physalis angulata leaf extract (PAL).

Peak no.	Rt	Area %	Molecular formula	Compound
1	8.22	1.55	C ₁₀ H ₃₀ O 5Si ₅	Cyclopentasiloxane
2	10.72	2.92	C ₁₄ H ₄₄ O 6Si ₇	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13tetradecamethyl
3	12.95	3.85	C ₁₆ H ₅₀ O 7Si ₈	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15hexadecamethyl
4	14.95	1.63	C ₁₆ H ₄₈ O 8Si ₈	Cyclooctasiloxane, hexadecamethyl
5	16.67	1.02	C ₁₆ H ₄₈ O 6Si ₇	Heptasiloxane, hexadecamethyl
6	18.21	10.43	C ₂₀ H ₃₀ O 4	1,2Benzenedicarboxylic acid, butyl 2ethylhexyl ester

7	19.62	3.78	C ₂₀ H ₆₀ O 10Si ₁₀	BenzoicCyclodecasiloxane, eicosamethyl
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8	22.09	3.68	C ₂₄ H ₇₂ O 12Si ₁₂	Tetracosamethylcyclododecasiloxane
9	22.88	0.65	C ₂₇ H ₅₄ O 4Si ₂	Monolinoleoylglycerol trimethylsilyl ether
10	23.32	1.06	C ₂₇ H ₅₄ O 4Si ₂	1Monolinoleoylglycerol trimethylsilyl ether
11	24.25	0.53	C ₂₀ H ₆₀ O 10Si ₁₀	Cyclodecasiloxane, eicosamethyl
12	27.14	1.52	C ₁₂ H ₃₈ O 5Si ₆	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15tetradecamethyl
13	28.92	0.70	C ₂₈ H ₃₈ O 10	3Desoxo3,16dihydroxy12desoxyphorbol 3,13,16,20tetraacetate
14	29.06	2.11	C ₁₄ H ₄₄ O 6Si ₇	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13tetradecamethyl

Peak no.	Rt	Area %	Molecular formula	Compound
1	5.89	1.09	C ₈ H ₂₄ O ₄ Si ₄	Cyclotetrasiloxane, octamethyl
2	10.72	4.08	C ₁₄ H ₄₄ O ₆ Si ₇	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl
3	12.95	2.41	C ₁₆ H ₅₀ O ₇ Si ₈	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl
4	16.67	0.84	C ₁₈ H ₅₄ O ₉ Si ₉	Cyclononasiloxane, octadecamethyl
5	19.42	10.06	C ₁₉ H ₃₄ O ₂	9,12-Octadecadienoic acid (Z,Z), methyl ester
6	23.21	0.75	C ₂₇ H ₅₄ O ₄ Si ₂	Monolinoleoyl glyceroltrimethylsilyl ether

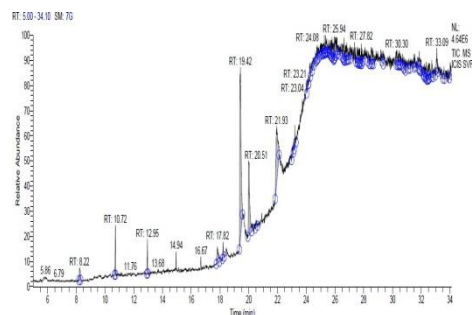


Figure no 3: GCMS chromatogram of Solanum virgianum fruit (SVF)

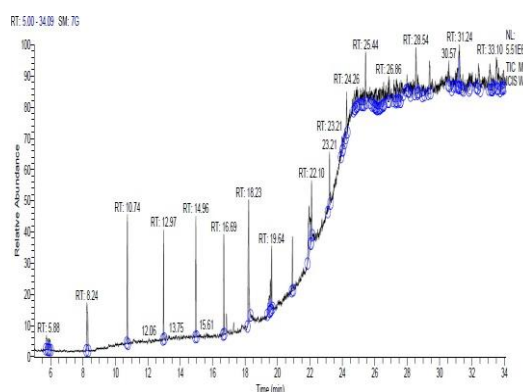


Figure no 4: GCMS chromatogram of Solanum virgianum (SVL)

Table no 4 : Retention time, Area%, Molecular formula and Major peaks of chemicals detected by GCMS of Solanum virgianum leaf extract (SVL).

8	26.84	0.94	C ₂₈ H ₅₃ NO ₅ Si ₂	Pregnan-20-one, 3,11-dihydroxy-17,21-bis[(trimethylsilyloxy)], Omethylloxim,
9	29.39	4.41	C ₂₉ H ₅₀ O ₂	dl-α-Tocopherol
10	31.87	1.33	C ₄₂ H ₆₄ O ₂	psi., psi. Carotene, ,1',2,2'tetrahydro-1,1'dimethoxy
11	33.55	3.31	C ₃₀ H ₄₂ O ₁₁	9-Desoxy-9-hydroxy-3,7,8,9,12-pentaacetate Ingot

Peak no.	Rt	Area%	Molecular formula	Compound
1	8.24	3.55	C ₁₀ H ₃₀ O ₅ Si ₅	Cyclopentasiloxane decamethyl
2	10.74	3.90	C ₆ H ₆ O ₃	Levoglucosenone
3	12.97	2.85	C ₁₆ H ₅₀ O ₇ Si ₈	Octasiloxane,1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15 hexadecamethyl
4	14.95	4.52	C ₆ H ₆ O ₃	2-Furancarboxaldehyde, 5-(hydroxymethyl)-
5	16.67	1.02	C ₁₆ H ₄₈ O ₆ Si ₇	Heptasiloxane, hexadecamethyl
6	18.23	7.40	C ₁₇ H ₂₀ O ₂	2-(4'-Methoxyphenyl)-2-(2'-methoxyphenyl)propane
7	19.64	2.22	C ₆ H ₆ O ₃	1,2,3-Benzenetriol
8	22.10	2.30	C ₂₄ H ₇₂ O ₁₂ Si ₁₂	Tetracosamethylcyclododecasiloxane
9	23.21	2.06	C ₆ H ₁₀ O ₅	1,6-Anhydro-α-D-galactofuranose
10	24.26	1.84	C ₂₀ H ₆₀ O ₁₀ Si ₁₀	Cyclodecasiloxane, eicosamethyl
11	25.44	2.58	C ₂₇ H ₅₄ O ₄ Si ₂	1Monolinoleoylglyceroltrimethylsilyl ether
12	28.54	3.35	C ₂₆ H ₅₄	Heptadecane, 9hexyl28
13	31.24	2.44	C ₃₄ H ₅₂ O ₄	Lanosta7,9(11),20(22)triene3á, 18diol, diacetate

Table no 5: FTIR Result for Physalis angulata Fruit extract (PAF)

Wavelength in cm-1	Functional groups	Name of the Functional groups
3600-3000	O-H	Alcohol
2926 , 2854	C-H	Aliphatic
1745	C=O	Carboxylic acid
1643	C=C	Arenes
1159 ,1097	C-O	Alcohols/ Phenols
715	=C-H bending	(out-of-plane bending) cis -RCH=CHR

Figure no 5: FTIR spectrum of Physalis angulata Fruit extract (SNF)

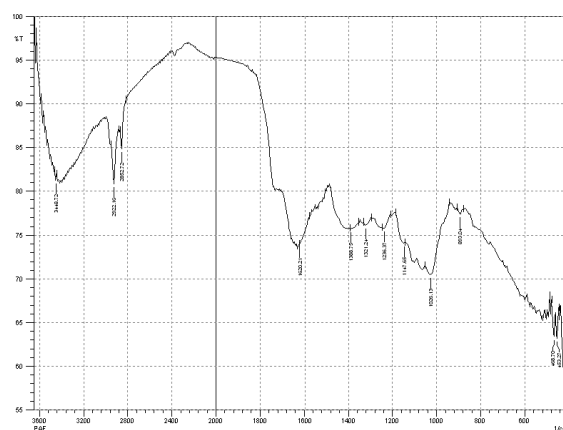


Table no 6: FTIR Result for Physalis angulata Leaf extract (PAL)

Wavelength in cm-1	Functional groups	Name of the Functional groups
3600-3000	O-H	Alcohol
2931	C-H	Aliphatic
1745	C=O	Carboxylic acid
1651	C=C	Conjugated carbonyl (may be flavone)
1159, 1097	C-O	Alcohols/ Phenols
783	=C-H bending	(out-of-plane bending) cis – RCH=CHR

Figure no 7: FTIR spectrum of Withania somnifera Fruit extract (SVF)

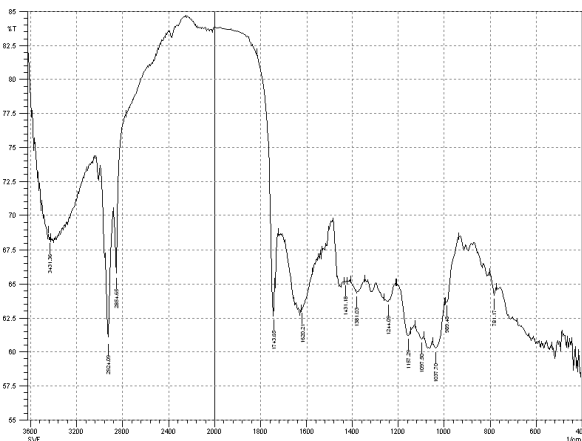


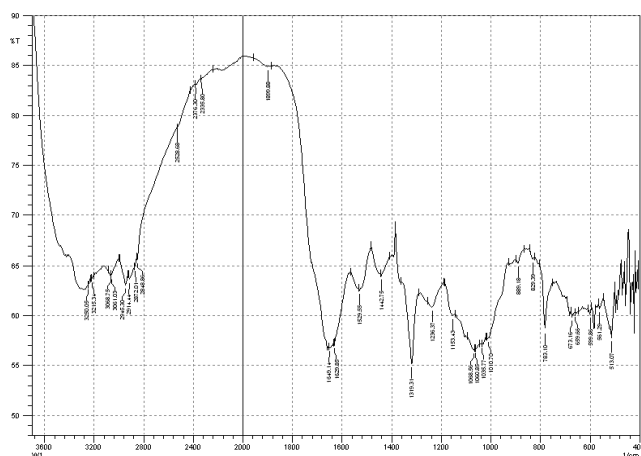
Table no7 :FTIR Result for Solanum virgianum Fruit extract (SVF)

Wavelength in cm-1	Functional groups	Name of the Functional groups
3600-3000	O-H	Alcohol
2924, 2854	C-H	Aliphatic
2100-2270	-N=C=N,-N3,-N=C=O	Azides and ketones
1629	C=C	Arenes
1163,1103,1031	C-O	Alcohols/ Phenols
898,723	=C-H bending	(out-of-plane bending) cis – RCH=CHR

Table no8 :FTIR Result of Solanum virgianum Leaf extract(SVL)

Wavelength in cm-1	Functional groups	Name of the Functional groups
3600-3000	O-H	Alcohol
2945, 2914	C-H	Aliphatic
2240-2260	-N=C=O	Nitrile isocyanates
1629	C=C	Conjugated
1068,1060	C-O	Alcohols/ Phenols
783	=C-H bending	(out-of-plane bending) cis – RCH=CHR

Figure no 8: FTIR spectrum of Solanum virgianum Leaf extract(SVL)



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