Int J Ayu Pharm Chem
ISSN 2350-0204
www.ijapc.com

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LC-MS Profiling of Root and Stem Bark of Spathodea campanulata P. Beauv

Author: Vishwatej Parkhi[1]

Co Authors: Swati Dabhi[2], Vinay Shukla[3] and Bhupesh Patel[4]

[1-4]Dravyaguna Department, Institute of teaching and research in Ayurveda, Jamnagar, Gujarat, India

ABSTRACT

Plant based medicines are gaining popularity considering their safety and proven efficacy over the synthetic molecules being considerable toxic in profile. Many contemporary drug molecules which are in clinical practice today have herbal origin. Bridging the gap between existing ethnomedicinal knowledge and drug development field is the need of the hour. It can be achieved by effortful screening of potential herbs. *Spathodea campanulata* P. Beauv. from the family *Bignoniaceae* has been credited with numerous ethnomedicinal claims ranging from simplest skin disorders, sore throat to complex diseases like malaria, asthma. Contemporary research has also succeeded to identify some of its pharmacological activities like Analgesic and Anti-inflammatory, Antioxidant activity etc. Purpose of present attempt was to carry out screening, identification of bioactive compounds from methanolic extract of *Spathodea campanulata* P. Beauv. stem and root bark by Liquid chromatography and Mass spectroscopy (LC-MS). Including both the ionisation modes, root and stem bark revealed presence of 127 and 118 diversified compounds. Among them 5(S), 6(R)-Lipoxin A4-d5, Endomorphin-2, 6-Hydroxymethyletoricoxib, Carbenicillin, Levofuraltadone, Homostypolhydroperoxide, Coumeroic acid, 9(11)-Dehydroglycyrrhetic acid, Emedastine, Pranlukast, Muconic dialdehyde, Muconic dialdehyde, Medicagenic acid, Coumarin are major compounds having reported diverse pharmacological activities. Extracted information is useful for future perspective in drug development and understanding of its pharmacological actions

Key Words *LC-MS, Spathodea, Phytochemicals, Methanol extract, Bignoniaceae*

Received 23rd April 23 Accepted 18th May 23 Published 10th July 2023

INTRODUCTION

Plants are the soul of Ayurvedic system of medicine. Number of other alternative medicine systems like Chinese medicine, Homeopathy and Naturopathy incorporate plants or their derivatives to cure different ailments. Modern medicinal molecules like Digitalins, Artemisinin, Quinine, Reserpine, Atropine, Colchicine and Emetine are derived from the vegetative sources. Modern drug molecules make their way to drug development scenario through their traditional folklore and ethnomedicinal potential. Though synthetic products are popular and are in demand due to their cheap production cost, time effectiveness, easy quality control and quick effects but their safety and efficacy were always

the point of concern. This critical scenario brings us back to the natural products. In 21st century, 11% of the 252 drugs considered as basic and essential by the WHO were exclusively of flowering plant origin and 35000-70000 plant species have been screened for their medicinal use. The plant-derived compounds have a long history of clinical use, better patient tolerance and acceptance. The advancement in chemistry-allied sciences has helped isolation, identification, standardisation and pinpointing the pharmacological activity of the phytochemicals present in the plants[1].

Liquid chromatography-mass spectrometry (LC–MS) is one such powerful analytical technique used for separation, identification, and quantification of both unknown and known compounds, small molecules as well as to elucidate the structure and chemical properties of different molecules, multicomponent containing substances[2].

From the family Bignoniaceae, *Spathodea campanulata* P. Beauv. is the only monotypic genus species reported and seen in majority of floras. *Spathodea* though originated in Africa, it is very much naturalised in India since long time. Availability of *Spathodea campanulata* P. Beauv. in India is very widespread as it is evident in many floras of Botanical Survey of India. Eighteen floras of states like Gujarat, Maharashtra, Rajasthan etc. report *Spathodea campanulata* P. Beauv. in natural or cultivated-ornamental plant in sub-urban regions[3-5].

Medicinal potential of *Spathodea campanulata* P. Beauv[6,7].

Spathodea campanulata P. Beauv. reports almost 16 pharmacological activities like analgesic and anti-inflammatory activity, antioxidant activity, anticonvulsant activity, hepatoprotective activity, antimicrobial activity, antimalarial activity etc.

Ethnomedicinal claims of *Spathodea campanulata* P. Beauv-

Stem bark of *S. campanulata* is used in Africa to treat malaria. The leaves are used in India and Africa to treat skin disorders, epilepsy, liver disorder, asthma, measles and sore throat. The root is used for worm infections, stomach ache, dysentery and hallucination. Flower is used as an antidote against veterinary poison and cataract. Among the traditional uses cited, the most common conditions treated are malaria, gastrointestinal tract (GIT) problem, skin infections, wound healing and kidney diseases. The plant is used alone or in combination with other medicinal plants.

Purpose of the study- Considering all the above exceptional potential of this particular plant, LC-MS analysis was undertaken for its molecular screening to understand the probable rationality of its ethnomedicinal claims and pharmacological properties.

MATERIALS & METHODS

Drug collection & authentication - *Spathodea campanulata* P. Beauv. Stem & root barks were collected from Jamnagar suburban locality (near

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Gitamandir), Gujarat. Good collection practices advised by NMPB were followed throughout. Identification of plant specimen was confirmed by referring to various floras of Botanical Survey of India. Plant sample for experiment was authenticated by taxonomist Dr. Jadeja from Maharshi Dayanand Science College, Porbandar. Specimen was deposited at Pharmacognosy laboratory ITRA for future references.

Drug processing- Barks of stem and root were washed with water. They were dried in shade for 10 days. This dried stem and root barks were pulverized in mechanical grinder to prepare coarse powder. The powdered material obtained from stem and root bark was then stored in air tight containers made of polyethylene.

Preparation of extracts- The shade dried coarse powders of stem bark (5 gm) and root bark (5 gm) of *Spathodea campanulata* P. Beauv. were kept in methanol in conical flask (50 ml) for overnight with initial shaking up to 6 hours. After 24 hours, it was filtered and extracts were collected by evaporating them on water bath.

LC-MS setup specifications- Analysis was done at Sophisticated Analytical Instrument Facility (SAIF) IIT, Mumbai using TOF/Q-TOF mass spectrometer. Both methanol and acetonitrile are polar solvents. The rationale for selecting methanol-acetonitrile is higher solubility of most polar chemical compounds and their high miscibility with each other [8-10]. Absorbance of HPLC-grade acetonitrile is particularly low at short wavelengths. HPLC-grade acetonitrile is suited to high-sensitivity analysis with UV detection in the short-wavelength region. This acts to prevent background noise and faulty ghost peaks specific to LCMS analysis. This combination also has greater elution strength.

Brief system conditions are as follows-

Ionisation mode- Dual AJS ESI

Stop Time (min)- 30.00

Solvent Composition-

Channel A- 100.0 % Water+ 0.1% FA in Water

Channel B- 100.0 % Methanol+ 90% ACN +10% H2O+ 0.1% FA, 100.0 % Acetonitrile

Injection Volume- 5.00 µL

Flow rate- 0.300 mL/min

MS Scan Rate (spectra/sec)- 1.00

MS Min Range (m/z)- 120

MS Max Range (m/z)- 1200

High Pressure Limit- 1200.00 bar

Stop time- 35.00 min

Valve switch time- 0.01 min

Data reporting, identification of components and their activity- Software used for processing of mass spectra and chromatograms was Mass Hunter by Agilent technologies. Chemical constituents were identified by the chemical library at the IIT- Bombay. Databases used for characterisation various chemical compounds were HMP, KEGG, LMP, METLIN. The list of active chemical constituents with their molecular formulae, molecular weight, retention time and m/z ratio is prepared manually from the system generated files. Pharmacological activities of each chemical constituent and their classification in discussion section have been referred from PubChem database.

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RESULTS AND DISCUSSION

LC-MS analysis of *Spathodea campanulata* P. Beauv. root bark revealed presence of 78 and 49 number of phytochemicals respectively in positive and negative mode of ionisation as shown in tables 1, 2 and figures 1, 2.

Table 1 List of compounds identified in MeOH extract of *Spathodea campanulata* P. Beauv. Root bark- Positive mode

No.	Name	Formula	Mass	RT	m/z
1.	(22E)-(25R)-25-hydroxy-26-methyl-22,23-didehydrovitamin D3 / (22E)-(25R)-25-hydroxy-26-methyl-22,23-didehydrocholecalciferol	$C_{28}H_{44}O_2$	412.3341	8.233	435.3233
2.	(3S,5R,6R,7E)-3,5,6-Trihydroxy-7-megastigmen-9-one	$C_{13}H_{22}O_4$	242.152	4.906	265.1417
3.	(9R,13R)-1a,1b-dihomo-jasmonic acid	$C_{14}H_{22}O_3$	238.1558	10.462	239.163
4.	(S)-Nerolidol 3-O-[a-L-Rhamnopyranosyl-(1->4)-a-L-rhamnopyranosyl-(1->2)-b-D-glucopyranoside]	$C_{33}H_{56}O_{14}$	676.3651	12.466	699.3541
5.	11α-ethyl-1α,25-dihydroxyvitamin D3 / 11α-ethyl-1α,25-dihydroxycholecalciferol	$C_{29}H_{48}O_3$	444.3575	19.586	467.3467
6.	1α,25-dihydroxy-26,27-ethanovitamin D3 / 1α,25-dihydroxy-26,27-ethanocholecalciferol	$C_{29}H_{46}O_3$	442.3417	19.263	465.331
7.	1α,25-dihydroxy-2β-(3-hydroxypropoxy)vitamin D3 / 1α,25-dihydroxy-2β-(3-hydroxypropoxy)cholecalciferol	$C_{30}H_{50}O_5$	490.3658	15.579	513.3548
8.	2,6-Dihydroxy-4-methoxytoluene	$C_8H_{10}O_3$	154.0638	7.523	177.053
9.	20S-hydroxycholesterol	$C_{27}H_{46}O_2$	402.3506	19.299	425.3391
10.	22α-Hydroxy-5α-campestan-3-one	$C_{28}H_{48}O_2$	416.3653	18.107	439.3548
11.	24,24-difluoro-1α,25-dihydroxy-24a-homovitamin D3 / 24,24-difluoro-1α,25-dihydroxy-24a-homocholecalciferol	$C_{28}H_{44}F_2O_3$	466.3209	19.743	489.3101
12.	25-acetoxy-ergosta-3beta,5alpha,6beta-triol	$C_{30}H_{52}O_5$	492.3815	17.035	515.3706
13.	28:5(10Z,13Z,16Z,19Z,22Z)	$C_{28}H_{46}O_2$	414.3498	17.884	437.3392
14.	2-Butyl-3-phenyl-2-propen-1-al	$C_{13}H_{16}O$	188.1191	6.947	189.1264
15.	2-Propenal, 3-(1,3-benzodioxol-5-yl)-	$C_{10}H_8O_3$	176.0462	5.919	177.0531
16.	2-undecenal	$C_{11}H_{20}O$	168.1523	7.396	191.1416
17.	2α-methyl-1β,25-dihydroxyvitamin D3 / 2α-methyl-1β,25-dihydroxycholecalciferol	$C_{28}H_{46}O_3$	430.3443	8.195	453.3339
18.	3S-hydroxypalmitic acid	$C_{16}H_{32}O_3$	272.2359	14.286	295.2249
19.	4R-hydroxy-octanoic acid	$C_8H_{16}O_3$	160.1109	10.498	183.1002
20.	5-(2-Methylpropyl)tetrahydro-2-oxo-3-furancarboxylic acid	$C_9H_{14}O_4$	186.0901	5.282	209.0791
21.	5,6-Dimethoxyflavone	$C_{17}H_{14}O_4$	282.0879	9.037	283.095
22.	5-Amino-6-(4-hydroxy-2-butenoyl)-2,2-dimethyl-4-chromanone	$C_{15}H_{17}NO_4$	275.1164	6.091	298.1055
23.	5beta-cholestan-3-one	$C_{27}H_{46}O$	386.3554	19.554	409.344
24.	5-Methyl-2(3H)-furanone	$C_5H_6O_2$	98.0381	6.539	121.0274
25.	5-Nonyltetrahydro-2-oxo-3-furancarboxylic acid	$C_{14}H_{24}O_4$	256.1683	14.778	279.1575
26.	5-O-(Indol-3-ylacetyl-myo-inositol) D-galactoside	$C_{22}H_{29}NO_{12}$	499.1667	6.585	500.1736
27.	6alpha-hydroxycholestanol	$C_{27}H_{48}O_2$	404.3651	19.551	427.3541
28.	7-methyl-decanoic acid	$C_{11}H_{22}O_2$	186.163	11.18	209.1522
29.	8E-Tetradecenyl acetate	$C_{16}H_{30}O_2$	254.2254	14.26	277.2146
30.	8β-Hydroxycarapin, 3,8-hemiacetal	$C_{27}H_{32}O_8$	484.2181	6.396	485.2252
31.	9-hydroxy-hexadecan-1,16-dioic acid	$C_{16}H_{30}O_5$	302.2097	13.076	325.1989
32.	a-Asarone	$C_{12}H_{16}O_3$	208.1089	9.461	209.1162
33.	Araliacerebroside	$C_{40}H_{77}NO_{10}$	731.5519	20.282	732.5595
34.	Candimine	$C_{18}H_{19}NO_6$	345.1215	8.279	368.11
35.	Carminomycin	$C_{26}H_{27}NO_{10}$	513.1599	6.829	536.1499
36.	Carvyl propionate	$C_{13}H_{20}O_2$	208.1452	10.758	209.1524
37.	Coumeroic acid	$C_{17}H_{14}N_2O_7$	358.08	6.901	381.0711
38.	DG(16:1(9Z)/0:0/16:1(9Z)) (d5)	$C_{35}H_{59}D_5O_5$	569.4988	20.32	570.5061

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39.	Dihydrocaffeic acid 3-O-glucuronide	$C_{15}H_{18}O_{10}$	358.0873	1.915	381.0768
40.	Dihydrodeoxystreptomycin	$C_{21}H_{41}N_7O_{11}$	567.287	9.79	568.294
41.	Dimethicone	$C_6H_{18}OSi_2$	162.0902	6.358	185.0793
42.	Diphenylcarbazide	$C_{13}H_{14}N_4O$	242.1164	6.19	265.1054
43.	EHNA	$C_{14}H_{23}N_5O$	277.1894	4.527	300.1785
44.	Ethyl 3-hydroxybutyrate	$C_6H_{12}O_3$	132.0799	4.991	155.0691
45.	Flavidulol C	$C_{34}H_{42}O_4$	514.3119	13.472	537.3011
46.	Flowerone	$C_{20}H_{20}O_6$	356.1248	8.748	357.132
47.	Gibberellin A 66	$C_{20}H_{26}O_7$	378.1681	8.401	401.158
48.	Gibberellin A76	$C_{19}H_{24}O_7$	364.153	8.623	387.1421
49.	Gingerglycolipid C	$C_{33}H_{60}O_{14}$	680.3955	14.069	703.3851
50.	Glucosyl (2E,6E,10x)-10,11-dihydroxy-2,6-farnesadienoate	$C_{21}H_{36}O_9$	432.2344	10.007	455.2236
51.	Gly Lys Gln	$C_{13}H_{25}N_5O_5$	331.1852	4.736	354.1744
52.	GW1843	$C_{27}H_{24}N_4O_6$	500.1691	8.876	523.1584
53.	Homotrypanothione	$C_{28}H_{51}N_9O_{10}S_2$	737.3106	6.125	760.2992
54.	Hydroxyhydroquinone	$C_6H_6O_3$	126.0329	14.739	149.0221
55.	Isohydrosorbic acid	$C_6H_{10}O_2$	114.0688	4.298	137.0581
56.	Isorhamnetin 3-[2"-(4'"-acetylrhamnosyl)-gentiobioside]	$C_{36}H_{44}O_{22}$	828.2478	6.691	851.2369
57.	Istamycin B1	$C_{18}H_{35}N_5O_6$	417.2574	7.967	440.2464
58.	JWH 018 N-(5-hydroxypentyl) metabolite-d5	$C_{24}H_{18}D_5NO_2$	362.2048	15.114	363.2122
59.	Leu Tyr Tyr	$C_{24}H_{31}N_3O_6$	457.2154	5.033	480.2046
60.	Linocinnamarin	$C_{16}H_{20}O_8$	340.1165	5.061	363.1052
61.	Lyngbic acid	$C_{15}H_{28}O_3$	256.205	14.465	279.1941
62.	Macrophylline	$C_{13}H_{21}NO_3$	239.1505	4.58	240.1577
63.	Mycinamicin VII	$C_{29}H_{47}NO_7$	521.3455	16.237	522.3528
64.	O-Acetylcyclocalopin A	$C_{17}H_{22}O_7$	338.1365	6.295	361.126
65.	Octadecyl fumarate	$C_{22}H_{40}O_4$	368.2931	19.501	391.282
66.	PA(O-20:0/0:0)	$C_{23}H_{49}O_6P$	452.3268	11.407	453.3342
67.	Palmitic amide	$C_{16}H_{33}NO$	255.2543	16.999	256.2616
68.	PE(17:0/20:2(11Z,14Z))	$C_{42}H_{80}NO_8P$	757.5589	18.411	758.5664
69.	PE(19:0/0:0)	$C_{24}H_{50}NO_7P$	495.3323	13.756	518.3213
70.	Pirbuterol	$C_{12}H_{20}N_2O_3$	240.1452	1.793	241.1525
71.	Propanoic acid, 2-(1-ethoxyethoxy)	$C_7H_{14}O_4$	162.0899	5.279	185.0791
72.	Senampeline A	$C_{25}H_{31}NO_8$	473.2104	5.316	496.1994
73.	Ser-Met-OH	$C_{14}H_{18}N_2O_7S$	358.0869	1.151	381.076
74.	Sulprostone	$C_{23}H_{31}NO_7S$	465.1819	4.863	466.1889
75.	Thr Asn Lys	$C_{14}H_{27}N_5O_6$	361.1954	4.192	384.1845
76.	trans,trans-hepta-2,4,6-trienoic acid	$C_7H_8O_2$	124.0536	7.377	147.0426
77.	trans-O-Methylgrandmarin	$C_{16}H_{18}O_6$	306.1113	7.43	329.1001
78.	Vicenistatin	$C_{30}H_{48}N_2O_4$	500.3688	18.356	523.3578

Mass- molecular mass, RT- Retention time, m/z- mass per charge ions

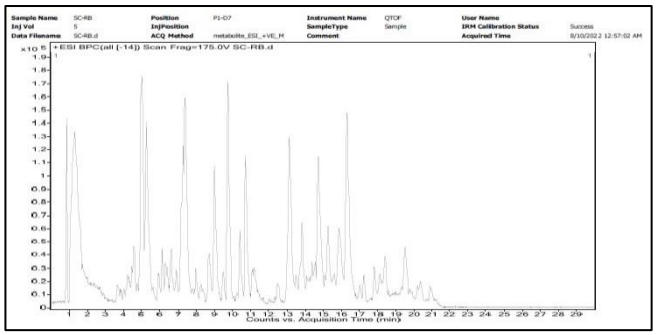

Figure 1 Positive mode LCMS chromatogram of *Spathodea campanulata* P. Beauv. root bark

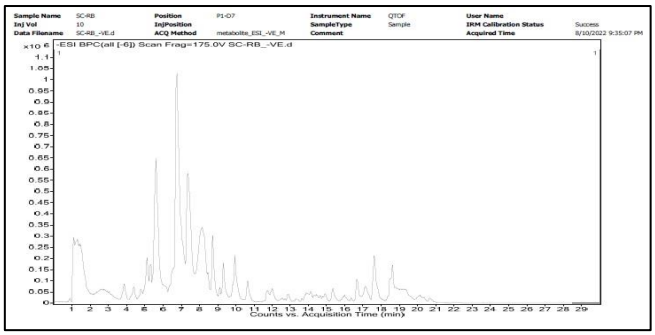

Figure 2 Negative mode LCMS chromatogram of *Spathodea campanulata* P. Beauv. root bark

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Table 2 List of compounds identified in MeOH extract of *Spathodea campanulata P. Beauv.* Root bark- Negative mode

No.	Name	Formula	Mass	RT	m/z
1.	(22S)-1α,22,25-trihydroxy-26,27-dimethyl-23,23,24,24-tetradehydro-24a,24b,24c-trihomovitamin D3 / (22S)-1α,22,25-trihydroxy-26,27-dimethyl-23,23,24,24-tetradehydro-24a,24b,24c-trihomocholecalciferol	$C_{32}H_{50}O_4$	498.3735	18.526	497.3667
2.	(3beta,22R,23R,24S)-3,22,23-Trihydroxystigmastan-6-one	$C_{29}H_{50}O_4$	462.3726	19.62	461.3653
3.	(9R,13R)-1a,1b-dihomo-jasmonic acid	$C_{14}H_{22}O_3$	238.1582	10.678	237.1509
4.	17-Octadecynoic Acid	$C_{18}H_{32}O_2$	280.2411	15.255	279.2339
5.	3-hydroxy-2-methyl-3-phytyl-2,3-dihydro-1,4-naphthoquinone	$C_{31}H_{48}O_3$	466.3502	16.023	511.3448
6.	3-Hydroxybenzaldehyde	$C_7H_6O_2$	122.0368	4.102	167.0349
7.	3'-N-Acetyl-4'-O-(14-methylpentadecanoyl)fusarochromanone	$C_{33}H_{52}N_2O_6$	572.3898	18.314	631.4033
8.	4-Feruloyl-1,5-quinolactone	$C_{17}H_{18}O_8$	350.1025	6.206	349.0951
9.	6-Hydroxymethyletoricoxib	$C_{18}H_{15}ClN_2O_3S$	374.0545	1.795	433.0689
10.	7-Dehydrologanin tetraacetate	$C_{25}H_{32}O_{14}$	556.1824	6.771	555.1753
11.	8-Oxocoformycin	$C_{11}H_{14}N_4O_5$	282.0962	3.192	341.1099
12.	9(11)-Dehydroglycyrrhetic acid	$C_{30}H_{46}O_3$	454.3476	17.477	453.3403
13.	9,10-EOT	$C_{18}H_{28}O_3$	292.2048	13.083	291.1977
14.	Barbatoflavan	$C_{24}H_{28}O_{13}$	524.1574	6.665	523.1503
15.	Brompheniramine	$C_{16}H_{19}BrN_2$	318.0739	1.518	377.0879
16.	Caffeoquinone	$C_9H_6O_4$	178.027	5.458	177.0197
17.	Camelliagenin B	$C_{30}H_{48}O_5$	488.3519	12.534	487.3448
18.	cis-Piceid	$C_{20}H_{22}O_8$	390.1348	9.507	389.1276
19.	Cornuside I	$C_{24}H_{30}O_{14}$	542.1662	5.036	541.1591
20.	Dehydrogriseofulvin	$C_{17}H_{15}ClO_6$	350.0587	9.884	349.0516
21.	Dimethyl phthalate	$C_{10}H_{10}O_4$	194.0586	6.271	193.0512
22.	Ganoderic acid X	$C_{32}H_{48}O_5$	512.3523	15.857	511.345
23.	Halistanol sulfate	$C_{29}H_{52}O_{12}S_3$	688.2588	9.162	389.1276
24.	Hexazinone	$C_{12}H_{20}N_4O_2$	252.1563	16.748	297.1548
25.	His-Phe4Cl-OH	$C_{21}H_{19}ClN_4O_6$	458.101	6.633	517.1145
26.	Homostypolhydroperoxide	$C_{27}H_{40}O_4$	428.2866	17.657	473.2853
27.	Kelampayoside A	$C_{20}H_{30}O_{13}$	478.1707	5.279	523.1691
28.	m-Coumaric acid	$C_9H_8O_3$	164.0477	6.146	163.0403
29.	m-Hydroxyphenylpyruvic acid	$C_9H_8O_4$	180.0429	5.833	179.0356
30.	Muconic dialdehyde	$C_6H_6O_2$	110.037	4.315	109.0297
31.	N-Undecylbenzenesulfonic acid	$C_{17}H_{28}O_3S$	312.177	20.01	311.1697
32.	Oleanolic acid	$C_{30}H_{48}O_3$	456.3624	17.062	455.3553
33.	Patientoside A	$C_{19}H_{21}ClO_8$	412.0964	8.881	411.0892
34.	PI-103	$C_{19}H_{16}N_4O_3$	348.1238	7.038	393.1219
35.	Prunus inhibitor b	$C_{30}H_{24}O_{11}$	560.1313	6.77	559.1262
36.	Quercetin 3,5,3'-trimethyl ether	$C_{18}H_{16}O_7$	344.0927	8.282	343.0854
37.	Sebiferenic acid	$C_{30}H_{48}O_4$	472.3567	14.577	471.3498
38.	S-Formylmycothiol	$C_{18}H_{30}N_2O_{13}S$	514.1479	5.233	513.1414
39.	Syringic acid	$C_9H_{10}O_5$	198.0528	4.397	197.0455
40.	TGX-221	$C_{21}H_{24}N_4O_2$	364.192	9.938	363.1846
41.	Vanillic acid	$C_8H_8O_4$	168.0421	4.102	167.0348
42.	Compound 1	$C_7H_6O_2$	122.0368	4.102	167.0349
43.	Compound 2	$C_9H_6O_4$	178.0269	5.48	177.0197
44.	Compound 6	$C_{18}H_{30}O_3$	294.2206	14.624	293.2133
45.	Compound 11	$C_9H_{10}O_5$	198.0528	4.397	197.0455
46.	Compound 12	$C_{16}H_{18}O_9$	354.0941	4.632	353.0872
47.	Compound 16	$C_9H_6O_2$	146.0365	5.167	145.03
48.	Compound 17	C_7H_8O	108.058	6.359	167.0716
49.	Compound 19	$C_7H_6O_4$	154.0265	4.315	153.0192

Mass- molecular mass, RT- Retention time, m/z- mass per charge ions

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While that of stem bark showed 73 and 45 chemical constituents in dual mode respectively as depicted in tables 3, 4 and figures 3, 4. PubChem is free database of freely accessible chemical information. On PubChem, chemical molecules can be searched for their name, molecular formula, structure, chemical and physical properties, biological activities, safety and toxicity information, patents, literature citations etc. In all 8 compounds found to be unknown for available database of IIT, Mumbai. Molecule found as 5(S), 6(R)-Lipoxin A4-d5 is non-steroidal anti-inflammatory agent while Endomorphin-2 is from opioid analgesics class.

Table 3 List of compounds identified in MeOH extract of *Spathodea campanulata* P. Beauv. Stem bark- Positive mode

No.	Name	Formula	Mass	RT	m/z
1.	(10S)-Juvenile hormone III acid diol	$C_{15}H_{26}O_4$	270.1837	14.567	293.1729
2.	(7R)-7-(5-Carboxy-5-oxopentanoyl)aminocephalosporinate	$C_{16}H_{18}N_2O_9S$	414.067	1.95	437.057
3.	14,14,14-Trifluoro-11E-tetradecenyl acetate	$C_{16}H_{27}F_3O_2$	308.1968	14.705	331.1863
4.	14,15-LTE4	$C_{23}H_{37}NO_5S$	439.2395	7.956	440.2467
5.	17-phenoxy trinor PGF2α ethyl amide	$C_{25}H_{37}NO_5$	431.2696	5.814	432.2768
6.	1α,25-Dihydroxy-2α-(3-hydroxypropyl)vitamin D3	$C_{30}H_{50}O_4$	474.371	17.781	497.3602
7.	1α,25-dihydroxy-2β-(3-hydroxypropoxy)vitamin D3 / 1α,25-dihydroxy-2β-(3-hydroxypropoxy)cholecalciferol	$C_{30}H_{50}O_5$	490.3654	15.663	513.354
8.	2,4,12-Octadecatrienoic acid isobutylamide	$C_{22}H_{39}NO$	333.3012	18.043	334.3085
9.	2',5'-Dihydroxy-4-methoxychalcone	$C_{16}H_{14}O_4$	270.0899	6.028	293.0791
10.	2,6-Dihydroxy-4-methoxytoluene	$C_8H_{10}O_3$	154.0638	5.997	177.053
11.	22α-Hydroxy-5α-campestan-3-one	$C_{28}H_{48}O_2$	416.366	18.328	439.3547
12.	24,24-difluoro-1α,25-dihydroxy-24a-homovitamin D3 / 24,24-difluoro-1α,25-dihydroxy-24a-homocholecalciferol	$C_{28}H_{44}F_2O_3$	466.3211	19.722	489.31
13.	24:3(5Z,9Z,17Z)(11Me,15Me,19Me,23Me)	$C_{28}H_{50}O_2$	418.3811	17.507	441.3707
14.	25-acetoxy-ergosta-3beta,5alpha,6beta-triol	$C_{30}H_{52}O_5$	492.3809	17.068	515.3701
15.	28:5(10Z,13Z,16Z,19Z,22Z)	$C_{28}H_{46}O_2$	414.3489	15.818	437.3382
16.	2-amino-14,16-dimethyloctadecan-3-ol	$C_{20}H_{43}NO$	313.3339	19.07	336.3231
17.	2R-hydroxylauric acid	$C_{12}H_{24}O_3$	216.1733	10.48	239.1625
18.	3(4->5)-Abeo-4,11:4,12-diepoxy-3-eudesmanol	$C_{15}H_{24}O_3$	252.1734	13.076	275.1623
19.	3-Methyladipic acid	$C_7H_{12}O_4$	160.0739	1.823	183.0631
20.	4'-Apo-beta,psi-caroten-4'-al	$C_{35}H_{46}O$	482.3578	18.4	483.3656
21.	4R-hydroxy-octanoic acid	$C_8H_{16}O_3$	160.1108	10.418	183.1001
22.	5(S),6(R)-Lipoxin A4-d5	$C_{20}H_{27}D_5O_5$	357.2495	15.336	358.2569
23.	5-Methyl-2(3H)-furanone	$C_5H_6O_2$	98.0383	6.579	121.0274
24.	5-Nonyltetrahydro-2-oxo-3-furancarboxylic acid	$C_{14}H_{24}O_4$	256.1681	14.76	279.1574
25.	5-O-(Indol-3-ylacetyl-myo-inositol) D-galactoside	$C_{22}H_{29}NO_{12}$	499.1657	6.544	500.173
26.	7-Decynoic acid, 5-oxo-	$C_{10}H_{14}O_3$	182.0951	14.8	205.0841
27.	7-methyl-decanoic acid	$C_{11}H_{22}O_2$	186.1629	11.19	209.1521
28.	Araliacerebroside	$C_{40}H_{77}NO_{10}$	731.5522	20.229	732.559
29.	C10:1n-7	$C_{10}H_{18}O_2$	170.1314	15.283	193.1211
30.	C11:1n-3	$C_{11}H_{20}O_2$	184.1466	5.633	207.1361
31.	Candimine	$C_{18}H_{19}NO_6$	345.1214	8.356	368.1105
32.	Carbenicillin	$C_{17}H_{18}N_2O_6S$	378.0926	1.239	401.0802
33.	Cathasterone	$C_{28}H_{48}O_3$	432.3604	15.894	455.35
34.	Citrusin D	$C_{16}H_{22}O_8$	342.1307	4.394	365.1199
35.	Convolvulinolic acid	$C_{15}H_{30}O_3$	258.22	14.578	281.2091
36.	Coumarin	$C_9H_6O_2$	146.0355	7.341	147.0427

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37.	Coumeroic acid	$C_{17}H_{14}N_2O_7$	358.08	6.929	381.0707
38.	Dihydrodeoxystreptomycin	$C_{21}H_{41}N_7O_{11}$	567.2861	9.793	568.2931
39.	Dipiperamide A	$C_{34}H_{38}N_2O_6$	570.2699	13.028	571.2769
40.	Docosanamide	$C_{22}H_{45}NO$	339.3505	19.193	362.3399
41.	Emedastine	$C_{17}H_{26}N_4O$	302.2099	13.115	325.199
42.	Endomorphin-2	$C_{32}H_{37}N_5O_5$	571.2737	14.067	572.2804
43.	Euphornin	$C_{33}H_{44}O_9$	584.2992	18.745	607.2884
44.	Gingerglycolipid C	$C_{33}H_{60}O_{14}$	680.3952	14.06	703.3841
45.	GlcCer(d18:0/14:0)	$C_{38}H_{75}NO_8$	673.5487	20.837	696.5376
46.	Homotrypanothione	$C_{28}H_{51}N_9O_{10}S_2$	737.3089	6.131	760.2972
47.	Hydralazine	$C_8H_8N_4$	160.0747	6.677	183.0638
48.	Hydroxyhydroquinone	$C_6H_6O_3$	126.0329	14.752	149.0221
49.	Idebenone Metabolite (QS-4)	$C_{13}H_{16}O_6$	268.0938	4.651	291.0835
50.	Isochamanetin	$C_{22}H_{18}O_5$	362.1169	2.545	385.1059
51.	Isohydrosorbic acid	$C_6H_{10}O_2$	114.0687	4.827	137.0579
52.	JWH 018 N-(5-hydroxypentyl) metabolite-d5	$C_{24}H_{18}D_5NO_2$	362.2043	15.291	363.2116
53.	Leu Tyr Tyr	$C_{24}H_{31}N_3O_6$	457.2146	5.071	480.2038
54.	Leukotriene F4	$C_{28}H_{44}N_2O_8S$	568.2822	3.881	591.2711
55.	Linocinnamarin	$C_{16}H_{20}O_8$	340.1162	5.685	363.1046
56.	Met Met	$C_{10}H_{20}N_2O_3S_2$	280.093	5.269	281.1001
57.	Mycinamicin VII	$C_{29}H_{47}NO_7$	521.3455	16.308	522.3526
58.	Naphthofluorescein	$C_{28}H_{16}O_5$	432.0991	2.048	433.1064
59.	N-linoleoyl taurine	$C_{20}H_{37}NO_4S$	387.244	5.561	388.2509
60.	Occidentoside	$C_{36}H_{32}O_{15}$	704.1714	1.139	705.1791
61.	Octadecyl fumarate	$C_{22}H_{40}O_4$	368.2931	19.484	391.2821
62.	Oleic Acid-biotin	$C_{28}H_{50}N_4O_3S$	522.3514	18.435	523.3584
63.	Otonecine	$C_9H_{15}NO_3$	185.1055	4.53	208.0949
64.	Palmidin C	$C_{30}H_{22}O_7$	494.1386	5.333	517.1279
65.	PE(19:0/0:0)	$C_{24}H_{50}NO_7P$	495.3303	15.945	496.3368
66.	p-Hydroxymeperidine	$C_{15}H_{21}NO_3$	263.1528	11.641	286.1419
67.	Quercetin 5,7,3',4'-tetramethyl ether 3-rutinoside	$C_{31}H_{38}O_{16}$	666.2153	1.183	689.2047
68.	Rugulosin	$C_{30}H_{22}O_{10}$	542.119	1.493	543.1267
69.	Senampeline A	$C_{25}H_{31}NO_8$	473.2097	5.326	496.1989
70.	Ser-Met-OH	$C_{14}H_{18}N_2O_7S$	358.0864	1.138	381.0755
71.	Sulprostone	$C_{23}H_{31}NO_7S$	465.1815	4.954	466.1888
72.	trans-O-Methylgrandmarin	$C_{16}H_{18}O_6$	306.1107	7.886	329.0999
73.	Trp Trp Pro	$C_{27}H_{29}N_5O_4$	487.2247	5.378	510.214

Mass- molecular mass, RT- Retention time, m/z- mass per charge ions

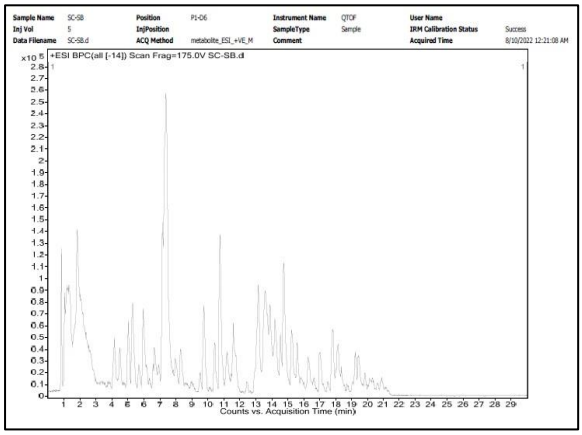

Figure 3- Positive mode LCMS chromatogram of *Spathodea campanulata* P. Beauv. stem bark

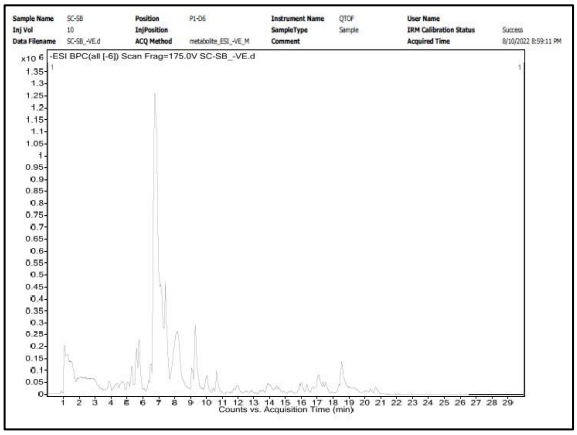

Figure 4 Negative mode LCMS chromatogram of *Spathodea campanulata* P. Beauv. stem bark

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Table 4 List of compounds identified in MeOH extract of *Spathodea campanulata* P. Beauv. Stem bark-negative mode

No.	Name	Formula	Mass	RT	m/z
1.	(+)-7-epi-Syringaresinol 4'-glucoside	$C_{28}H_{36}O_{13}$	580.2189	7.06	579.2123
2.	(+)-Plicamine	$C_{26}H_{26}N_2O_6$	462.1773	5.182	507.1756
3.	(2S,2"S,3S,3"R,4S)-3,4',5,7-Tetrahydroxyflavan(2->7,4->8)-3,4',5,7-tetrahydroxyflavan	$C_{30}H_{24}O_{10}$	544.1373	7.327	543.1319
4.	10E,12E-Hexadecadienyl acetate	$C_{18}H_{32}O_2$	280.2443	17.279	279.2369
5.	13,14-dihydro-16,16-difluoro Prostaglandin E1	$C_{20}H_{34}F_2O_5$	392.2391	14.163	451.2527
6.	2E,4E,6Z,8Z-Decatetraenedioic acid	$C_{10}H_{10}O_4$	194.0592	6.569	193.0518
7.	3-Dehydro-L-threonate	$C_4H_6O_5$	134.0226	1.203	133.0153
8.	3-Fucosyllactose	$C_{18}H_{32}O_{15}$	488.1777	1.521	533.176
9.	5-[4,5-Dihydroxy-6-(hydroxymethyl)-3-(3,4,5-trihydroxyoxan-2-yl)oxyoxan-2-yl]oxy-7,8-dimethoxy-3-(4-methoxyphenyl)chromen-4-one	$C_{29}H_{34}O_{15}$	622.1945	6.836	621.1871
10.	5Z-octadecenoic acid	$C_{18}H_{34}O_2$	282.2602	18.293	281.2528
11.	6-HODE	$C_{18}H_{32}O_3$	296.2387	13.633	295.2314
12.	6'-O-E-Caffeoyl-mussaenosidic acid	$C_{25}H_{30}O_{13}$	538.1731	7.608	537.1658
13.	9R-HOME(10E)	$C_{18}H_{34}O_3$	298.2551	14.619	297.2478
14.	Antibiotic X 14889D	$C_{33}H_{58}O_7$	566.4167	20.087	611.4164
15.	Barbatoflavan	$C_{24}H_{28}O_{13}$	524.1571	6.655	523.1492
16.	Camelliagenin B	$C_{30}H_{48}O_5$	488.3543	11.573	487.3473
17.	Formimidoyl-fortimicin A	$C_{18}H_{36}N_6O_6$	432.2769	8.672	491.2906
18.	Glu Trp Glu	$C_{21}H_{26}N_4O_8$	462.177	4.509	461.1702
19.	Glyinflanin H	$C_{19}H_{16}O_4$	308.1081	9.917	307.1008
20.	Hexazinone	$C_{12}H_{20}N_4O_2$	252.159	18.556	311.1731
21.	Idebenone Metabolite (Benzenedecanoic acid, 2-hydroxy-3,4-dimethoxy-6-methyl-5-(sulfooxy)-)	$C_{19}H_{30}O_9S$	434.1608	7.436	433.1533
22.	Isoacteoside	$C_{29}H_{36}O_{15}$	624.2099	6.61	623.2029
23.	Isophylloflavanine	$C_{35}H_{32}O_{13}$	660.1862	6.891	659.1791
24.	Istamycin KL1	$C_{13}H_{28}N_4O_6$	336.2007	8.726	395.2147
25.	Kelampayoside A	$C_{20}H_{30}O_{13}$	478.1708	5.822	537.1855
26.	Lamprolobine	$C_{15}H_{24}N_2O_2$	264.1804	17.815	309.1787
27.	Lauryl hydrogen sulfate	$C_{12}H_{26}O_4S$	266.1592	15.756	265.152
28.	Levofuraltadone	$C_{13}H_{16}N_4O_6$	324.1085	1.52	383.1223
29.	Medicagenic acid	$C_{30}H_{46}O_6$	502.3338	12.409	501.327
30.	Momordol	$C_{26}H_{48}O_5$	440.3562	18.619	499.3703
31.	Muconic dialdehyde	$C_6H_6O_2$	110.0377	4.29	109.0304
32.	Norswertianolin	$C_{19}H_{18}O_{11}$	422.0849	1.113	421.0781
33.	octadeca-9Z,11E,15Z-trienoic acid	$C_{18}H_{30}O_2$	278.2285	16.413	277.2212
34.	Phylloflavan	$C_{26}H_{26}O_{10}$	498.1517	4.933	497.1466
35.	Pranlukast	$C_{27}H_{22}N_5O_4$	480.1668	5.554	525.165
36.	Proparacaine	$C_{16}H_{26}N_2O_3$	294.1908	19.996	293.1839
37.	Pteridine	$C_6H_4N_4$	132.0442	1.108	191.058
38.	Scutellarioside II	$C_{24}H_{28}O_{12}$	508.1622	7.372	507.1549
39.	S-methylcaptopril	$C_{11}H_{18}O_3S$	230.0976	8.267	275.0955
40.	Sodium Tetradecyl Sulfate	$C_{14}H_{30}O_4S$	294.1914	18.619	353.2051
41.	SSR 125543	$C_{27}H_{28}ClFN_2OS$	482.1596	5.19	527.1578
42.	Thr Pro Arg	$C_{15}H_{28}N_6O_5$	372.2125	17.52	431.2261
43.	Trp Glu Glu	$C_{21}H_{26}N_4O_8$	462.1772	4.898	507.1754
44.	Trp Ser Gly	$C_{16}H_{20}N_4O_5$	348.1449	4.489	347.1374
45.	TyrMe-HoPhe-OH	$C_{26}H_{26}N_2O_7$	478.1727	5.156	537.1867

Mass- molecular mass, RT- Retention time, m/z- mass per charge ions

Chemical entity 6-Hydroxymethyletoricoxib is human metabolite of Etoricoxib molecule. Carbenicillin is semisynthetic penicillin having substantial in vitro activity against a variety of both gram-positive, gram-negative microorganisms and have antipseudomonal and antiproteal activity. Levofuraltadone is anti-infective, antibacterial agent. Homostypolhydroperoxide is one of the local anti-infective agent. Coumeroic acid is having free radical scavenging, antioxidant and anti-infective activity. Derivative of glycyrrhizic acid is 9(11)-dehydroglycyrrhetic acid. Glycyrrhizic acid was reported to present anti-allergic, antiviral and anti-inflammatory activities as well as improvements in glucose tolerance. Brompheniramine and Emedastine are histamine H1 antagonist while Pranlukast is anti-asthmatic agent and Leukotriene antagonist. Muconic dialdehyde, Muconic dialdehyde are antifungal agents while Medicagenic acid have fungistatic & haemolytic activity. Coumarin acts as anticoagulant agent while Hydralazine shows antihypertensive activity[11].

CONCLUSION

These separated chemical compounds help us to understand possible mechanism behind ethno-medicinal claims and pharmacological activities of plant. Inferred information will be useful for stakeholders in the drug development sector for future research and scientific aspects. Information can be used as reference guidance for the quality control studies involving this plant species. Future works regarding specific activity of screened compounds may provide more insight about the use of the plant. Generated data surely adds valuable scientific information to the present literature status of *Spathodea campanulata* P. Beauv.

ACKNOWLEDGMENT

Authors are thankful to Dean, Director, Head of Pharmaceutical chemistry Laboratory-ITRA for preliminary research facilities and extract preparation, SAIF-IIT Mumbai for carrying out LC-MS analysis and Dr. Jadeja for providing authentication of the plant specimen.

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