# PARIPEX - INDIAN JOURNAL OF RESEARCH

Journal or p OR		RIGINAL RESEARCH PAPER	Medical Science
Indian	PARIPET AL	ENTIFICATION AND PREDICTION OF ACTIVITY ECTRUM OF CHEMICAL CONSTITUENTS FROM LIUM SATIVUM LINN	<b>KEY WORDS:</b> Allium Sativum, Garlic, Chromatography,
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RACT	The current investigation subjected for identification and prediction of activity spectrum of chemical composition from Allium sativum Linn by liquid chromatography and mass spectroscopy. The garlic extract was then subjected to preliminary		

phytochemical screening for the detection of class of compounds. The extract contain a variety compounds, in which

organosulfur compounds have high anti angiogenic activity which was already done by authors [1, 2]

INTRODUCTION

ABSTR

Garlic (Allium sativum. L) belongs to Liliaceae family .It is root vegetables cultivates throughout the world, originated from Central Asia .Since ancient times garlic plant employed for treatment of disease and various purposes .Garlic contains sulfur compounds,17 amino acids , enzymes, vitamins, antioxidants, flavanoids and minerals such as selenium .Higher concentration of sulfur compounds is one of the feature of all Allium species Organosulfur compounds in garlic cause pungent odor , many of its medicinal effects .Allicin is the organosulfur compound (diallyl thiosulfinate or diallyl disulfide) which is the most biological active compound<sup>[3]</sup>.Garlic is considered as a spice, medicine and food additive .When garlic powder given with common salt, it relives from colic pain and nervous headache, also used as vermifuge to expel round worm. Recent research studies have been proved that garlic show antidiabetic, antimicrobial, antihypertensive, and hepatoprotective, insecticidal and antiangiogenic properties. It is found that Garlic extract can reduce serum cholesterol level in human body. Antifungal activity of garlic extract and its constituents extensively studied. Garlic treatment is effective for chicken infected with 'Candida albicans' and species Cryptococcus present in human serum<sup>[4]</sup>.

Chemical constituents are vary in garlic oil, garlic extract, fresh leaves and dried cloves. Sulfur containing non-volatile amino acids, among which allin or S-allyl-cysteine sulfoxide compounds are responsible for that flavor producing in garlic. Therapeutic and medical uses in both traditional and modern medical research make garlic is one of the important vegetable<sup>15</sup>. In this study we subjected Garlic extract to liquid chromatography and mass spectroscopy

## MATERIALS AND METHODS

The liquid Chromatographic column which we used was RP-C18 with a pump of spd-10 AVP. After different trials the solvent system was fixed at the ratio 50:50 with Water: Methanol. The ionization mode which we used was electronic spray ionization in both the positive and negative mode. The injection volume was 10 microlitre with a flow rate of 2 ml/min and the column temperature maintained at 25<sup>c</sup>C.The specifications of the column is as below.

Column: phenomenex rp 18 Column dimension: 25 cm x2.5 mm Lc detection : 254 nm M/z range: 50-800 for neg and 50-950 for pos Soft ware: class v p integrated. Library: Metwin 2.0

#### PROCEDURE

10 ul of the filtered samples were then injected to the automatic injector using a Micro syringe (1-20ul, Shimadzu). The mobile phase as per the above in an isocratic mode. The column used was RP.C-18 (phenomenex). The flow rate was maintained to 2.0

ml/mn with a column temperature of 25+ 2 0C. The class VP integration software was used for the data analysis.



#### LCMS LIBRARY SEARCH [INTEGRATED]

SL NO	COMPOUND NAME	LIB;SQ;NO	MOLECULAR MASS
1	VALINE	MTW/UM/2.1/4654/10	117.05
2	VANILLIN	MTW/UM/2.1/3564/10	152.15
3	OCIMENE	MTW/UM/2.1/8796/10	136.24
4	MYRCENE	MTW/UM/2.1/9765/10	136.23
5	FLAVIDIN	MTW/UM/2.1/4667/10	240.26
6	GERMACRENE	MTW/UM/2.1/4488/10	204.35
7	CYCLOEUDESMOL	MTW/UM/2.1/9958/10	222.37
8	ALANINE	MTW/UM/2.1/8757/10	89.09
9	METHYL PHENOL	MTW/UM/2.1/6666/10	108.14
10	PASORBIC ACID	MTW/UM/2.1/8907/10	112.13
11	ASPARATIC ACID	MTW/UM/2.1/2345/10	133.11
12	PARTHENIN	MTW/UM/2.1/7654/10	262.305
13	METHYL N- METHYLANTHRANI LATE	MTW/UM/2.1/2345/10	165.19
14	LINALOOL	MTW/UM/2.1/9087/10	154.25
15	TRIGONELLINE CHLORIDE	MTW/UM/2.1/4637/10	173.60
16	AMINO-B- OXALYLAMINOPR OPIONIC ACI	MTW/UM/2.1/3554/10	176.13

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17		N	1TW/UM/2.1/5554/10	176.17	
10	IVIET HOAT COUVIARIN				
18	METHYL LINOLEATE		MTW/UM/2.1/3545/10 294		
19	GERMACRENE		1TW/UM/2.1/8988/10	204.35	
20	METHYL STEARATE	N	1TW/UM/2.1/3990/10	298.51	
21	ALLICIN	MTW/UM/2.1/6621/10 162.27		162.27	
UNK	NOWN MASSES				
187			875		
345			900		
675			555		
890			777		
678			240		
987		872			
1098		982			
456		567			
789		355			
987		092			
345					
567					
164					
198					
902					
576					

# PASS ANALYSIS

## ALLICIN

0,998	0,000	Inflammatory Bowel disease treatment
0,998	0,001	Platelet antagonist
0,997	0,001	Atherosclerosis treatment
0,996	0,000	Antioxidant
0,997	0,001	Lipoprotein disorders treatment
0,996	0,001	Platelet aggregation inhibitor
0,995	0,001	Antileukemic
0,996	0,002	Antidiabetic
0,986	0,004	Antineoplastic
0,984	0,001	CYP2E1 inhibitor
0,980	0,001	Antiprotozoal
0,942	0,004	Apoptosis agonist
0,942	0,003	Lipid metabolism regulator
0,935	0,002	Antiprotozoal (Amoeba)
0,913	0,001	TRPA1 agonist
0,854	0,001	Chemoprotective
0,838	0,004	Antihypercholesterolemic
0,832	0,025	Aspulvinone dimethylallyltransferase inhibitor
0,751	0,019	NADPH peroxidase inhibitor
0,741	0,011	Hypolipemic
0,730	0,007	Chloride peroxidase inhibitor
0,722	0,010	Fatty-acyl-CoA synthase inhibitor
0,733	0,042	Mucomembranous protector

# GERMACRENE

0,005	Ubiquinol-cytochrome-c reductase inhibitor
0,002	Carminative
0,006	Antieczematic
0,017	CYP2C12 substrate
0,015	Testosterone 17beta-dehydrogenase (NADP+) inhibitor
0,013	CYP2J substrate
0,014	Alkenylglycerophosphocholine hydrolase inhibitor
0,005	Phosphatidylcholine-retinol O-acyltransferase inhibitor
0,005	Fibrinolytic
0,010	Glutamyl endopeptidase II inhibitor
0,005	All-trans-retinyl-palmitate hydrolase inhibitor
0,012	Alkylacetylglycerophosphatase inhibitor
0,011	5-O-(4-coumaroyl)-D-quinate 3'-monooxygenase inhibitor
	0,005 0,002 0,006 0,017 0,013 0,013 0,014 0,005 0,005 0,010 0,005 0,012 0,011

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0,784	0,038	Aspulvinone dimethylallyltransferase inhibitor
0,759	0,018	Acylcarnitine hydrolase inhibitor
0,780	0,041	Phobic disorders treatment
0,732	0,002	NF-E2-related factor 2 stimulant
0,760	0,031	Mucomembranous protector
0,728	0,005	Adenomatous polyposis treatment
0,726	0,016	Ribulose-phosphate 3-epimerase inhibitor
0,735	0,027	Sugar-phosphatase inhibitor
0,707	0,004	H+-exporting ATPase inhibitor
0,721	0,030	Membrane permeability inhibitor
0,709	0,031	CYP2J2 substrate
0,701	0,034	Nicotinic alpha6beta3beta4alpha5 receptor
		antagonis

## CONCLUSION

From the present study we conclude that the garlic extract contains a variety of promising compounds which is highly potential in terms of biological activity. The activity spectrum which we sketched showed that the identified compounds are very significant. The PASS analysis which we carried out in the promising compounds needs further studies like molecular docking and in-vivo works which will be a boon for the entire drug industry as the source for the compounds are cheap and easily available in whole over the world. More than twenty un-known compounds are found in the LCMS analysis of Allium sativum so we recommend and more than we are proceeding for the identification of the unknown compounds.

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