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# PASS-ASSISTED PREDICTION OF BIOLOGICAL ACTIVITY SPECTRA OF METHANOLIC EXTRACT OF *GYMNOPILUS JUNONIUS*, A WILD MUSHROOM FROM SOUTHERN WESTERN GHATS, INDIA

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#### ABSTRACT

*Gymnopilus junonius* was formerly known as *Gymnopilus spectabilis*, or *Pholiota spectabilis* v. *junonia*. This mushroom usually grows in clusters, but rarely grows solitary was collected from southern Western Ghats. This wild mushroom lacks evidence of scientific study and an attempt was made to identify the phytoconstituents present in it and their biological activity using PASS (Prediction of Activity Spectra for Substances). The most abundant constituents of this mushroom are Octadecanoic acid, 2,3-dihydroxypropyl ester, 1,4:3,6-Dianhydro-.alpha.-d-glucopyranose, Methyl stearate, 1,4:3,6-Dianhydro-.alpha.-d-glucopyranose, Benzeneacetic acid, D-Allose, Phenol, 2,4-bis (1,1-dimethylethyl), 1H-Imidazole, 4,5-dihydro-4-methyl-2-phenyl-, Octadecanoic acid, 2-hydroxy-1-(hydroxymethyl) ethyl ester and Octadecanoic acid. Our PASS-assisted prediction of biological activity spectra is the first report of this wild mushroom.

KEYWORDS: Biological activity, PASS, Western Ghats, Mushroom.

### INTRODUCTION

From time immemorial, wild mushrooms have been considered as highly nutritious tasty food items.<sup>[1,3]</sup> Besides nutritional importance wild edible mushrooms are now well known for their pharmaceutical constituents.<sup>[4,5]</sup> Currently, there are several mushroom species which have established therapeutic properties.<sup>[6,11]</sup> In addition, mushroom extract was considered as important remedies for the prevention and treatment of many diseases for thousands of years in several parts of the world.<sup>[12,13]</sup> Many traditionally used mushrooms from the genera, *Auricularia, Flammulina, Ganoderma, Grifola, Lentinus, Trametes (Coriolus)* and *Tremella* have been demonstrated to possess significant medicinal properties.<sup>[14,15]</sup>

From the dawn of civilization there have been references to mushrooms in the ancient Indian, Greek, Roman, Chinese, and other literature. Greek warriors regarded them as "strength food", Romans considered them as "food of Gods" whereas Chinese regarded mushrooms as "elixir of life". The Aztecs of South America referred mushrooms as "teo-nonacte" (God's flesh) and worshipped a group of mushrooms. In the Indian Rigveda and other ancient literature the much referred "somrus" was actually a decoction of mushroom that was known by different names as Ksumpa in Sanskrit, Kukurmutta, Kavaka, Chhatra, Khumbi, Bhoomi kavak and Bhustrna in Hindi.<sup>[16]</sup> There are approximately 700 species of higher Basidiomycetes that have been found to possess significant pharmacological activities.<sup>[17,14]</sup>

Considering the medicinal importance of the fungi, the methanolic extract of the Gymnopilus junonius, a wild mushroom from southern Western Ghats was studied for their biological activity spectra obtained by PASS (Prediction of Activity Spectra for Substances). This study will help to identify the bioactive compounds present in the extract that possess abundant therapeutic potential. PASS has been employed as a strong potential tool to predict the biological activity spectrum of synthetic substances for the discovery of new drugs. But the potential of PASS to predict the biological activity spectra of natural products are still underestimated.<sup>[18]</sup> Therefore, the present study was undertaken to investigate the biological activity spectrum of the methanol extract of wild mushroom. The present study is the first of its kind to employ PASS in mushrooms.

#### MATERIALS AND METHODS

**Collection of mushroom samples:** The general methodology and techniques for collection, preparation and preservation of specimens were followed.<sup>[19,20]</sup> Typical rainforest vegetation of south Western Ghats were surveyed for the present study. Survey was undertaken in the Fingerpost Reserve Forest of North Zone of Nilgiri, Tamilnadu in two consecutive years after the rainy days. Fruiting bodies of *Gymnopilus junonius* were collected in this vulnerable ecosystem. The collected samples were brought to the lab and preserved at 4°C for further studies.

**Extract preparation:** For the extraction procedure, fruiting bodies of the mushroom samples air-dried at 40°C and300mg were ground using the pestle and mortar with methanol and then filtered using WhatmanNo.1 filter paper. After that, the extract was centrifuged at 5000rpm for 15min and the supernatant was stored at 4°C for further experiment.

**Biological Activity:** The biological activity spectra of these phytochemical constituents were obtained by PASS version (version 9.1, http://195.178.207.233/PASS). This software estimates the predicted activity spectrum of a compound as probable activity (Pa) and probable inactivity (Pi). Prediction of this spectrum by PASS is based on qualitative structure-activity relationships (SAR) analysis of the training set containing more than 205,000 compounds exhibiting more than 3750 kinds of biological activities. Being probabilities, the Pa and Pi values vary from 0.000 to 1.000 and in general, Pa+Pi $\neq$ 1, since these probabilities are calculated independently. The PASS prediction results were interpreted and used in a flexible manner: (i) only activities with Pa>Pi are considered as possible for a particular compound; (ii) if Pa>0.7, the chance to find the activity experimentally is high; (iii) if 0.5<Pa<0.7, the chance to find the activity experimentally is high; (iii) if 0.5<Pa<0.7, the chance to find the activity experimentally is less, but the compound is probably not so similar to known pharmaceutical agents; (iv) if Pa<0.5, the chance to find the activity experimentally is less, but the chance to find a structurally new compound, that is, NCEs is more.<sup>[21,22,18]</sup>

#### **RESULTS AND DISCUSSION**

Gas chromatography and mass spectrometry (GC-MS) analyses of the Gymnopilus junonius extract lead to the identification of 33 components.<sup>[23]</sup> The prevalent compounds Octadecanoic acid, 2.3were dihydroxypropyl ester (21.5%), 1,4:3,6-Dianhydro-.alpha.-d-glucopyranose (8.44%) and Methyl stearate (8.19%). The biological activity spectrum of the 10 methanolic extract compounds chosen by their predominant area using GC-MS (Table 1) predicted by PASS is represented in the tables 2-10. Peak 3 and Peak 4 are similar compounds and hence, only 9 predominant compounds are taken for PASS assisted prediction of biological activity (Table 1).

Table 1: The predominant chemical compounds of methanolic extract of *Gymnopilus junonius*.

Peak	RT	Area %	Library/ID
28	23.63	21.5	Octadecanoic acid, 2,3-dihydroxypropyl ester
3	8.537	8.44	1,4:3,6-Dianhydroalphad-glucopyranose
18	18.88	8.19	Methyl stearate
4	8.707	7.08	1,4:3,6-Dianhydroalphad-glucopyranose
5	8.908	6.7	Benzeneacetic acid
7	12.05	6.23	D-Allose
8	12.47	4.84	Phenol, 2,4-bis (1,1-dimethylethyl)
6	11.86	4.38	1H-Imidazole, 4,5-dihydro-4-methyl-2-phenyl-
29	23.7	3.75	Octadecanoic acid, 2-hydroxy-1-(hydroxymethyl) ethyl ester
20	19.17	2.67	Octadecanoic acid

 Table 2: Octadecanoic acid, 2,3-dihydroxypropyl ester.

Pa	Pi	Biological Activity
0.973	0.002	Eye irritation, inactive
0.96	0.003	Skin irritation, inactive
0.956	0.003	Lipid metabolism regulator
0.953	0.002	Phosphatidate phosphatase inhibitor
0.937	0.002	Alkylacetylglycerophosphatase inhibitor
0.935	0.003	Acylcarnitine hydrolase inhibitor
0.934	0.002	All-trans-retinyl-palmitate hydrolase inhibitor
0.933	0.002	Fucosterol-epoxide lyase inhibitor
0.927	0.004	Sphinganine kinase inhibitor
0.925	0.001	Leukopoiesis stimulant
0.925	0.004	Acrocylindropepsin inhibitor
0.925	0.004	Chymosin inhibitor
0.925	0.004	Saccharopepsin inhibitor
0.924	0.002	Lipoprotein lipase inhibitor
0.923	0.004	Alkenylglycerophosphocholine hydrolase inhibitor
0.908	0.004	Sugar-phosphatase inhibitor
0.905	0.005	Polyporopepsin inhibitor
0.903	0.002	Alkanal monooxygenase (FMN-linked) inhibitor
0.9	0.003	Dextranase inhibitor

2152 possible activities at Pa>0.5%.

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Pa	Pi	Biological Activity
0.855	0.015	Phobic disorders treatment
0.835	0.002	2-Aminohexano-6-lactam racemase inhibitor
0.83	0.007	Nicotinic alpha2beta2 receptor antagonist
0.797	0.006	UDP-N-acetylglucosamine 4-epimerase inhibitor
0.786	0.014	Nicotinic alpha6beta3beta4alpha5 receptor antagonist
0.749	0.003	Antibiotic Glycopeptide-like
0.746	0.04	Testosterone 17beta-dehydrogenase (NADP+) inhibitor
0.745	0.003	Ornithine cyclodeaminase inhibitor
0.743	0.014	Acute neurologic disorders treatment
0.742	0.008	Pterin deaminase inhibitor
0.734	0.023	Glutamate-5-semialdehyde dehydrogenase inhibitor
0.711	0.019	Protein-disulfide reductase (glutathione) inhibitor
0.707	0.009	Chloride peroxidase inhibitor

1838 possible activities at Pa>0.9%.

## Table 4: Methyl stearate.

	Pa	Pi	Biological Activity
ļ	0.962	0.002	Acrocylindropepsin inhibitor
ļ	0.962	0.002	Chymosin inhibitor
	0.962	0.002	Saccharopepsin inhibitor
	0.942	0.003	Acylcarnitine hydrolase inhibitor
	0.942	0.003	Polyporopepsin inhibitor
ļ	0.926	0.003	Pro-opiomelanocortin converting enzyme inhibitor
ļ	0.922	0.002	All-trans-retinyl-palmitate hydrolase inhibitor
ļ	0.916	0.004	Phobic disorders treatment
	0.904	0.003	GST A substrate
ļ	0.903	0.005	Ubiquinol-cytochrome-c reductase inhibitor
ļ	0.9	0.004	Sugar-phosphatase inhibitor
	0.9	0.005	Alkenylglycerophosphocholine hydrolase inhibitor
	0.896	0.005	CYP2J substrate
	0.895	0.004	Alkylacetylglycerophosphatase inhibitor
	0.891	0.007	Mucositis treatment
	0.889	0.003	Fusarinine-C ornithinesterase inhibitor
	0.886	0.004	CYP2J2 substrate
	0.885	0.003	Cutinase inhibitor
	0.885	0.011	Aspulvinone dimethylallyltransferase inhibitor
	0.884	0.003	Sarcosine oxidase inhibitor
ļ	0.883	0.003	Carboxypeptidase Taq inhibitor
	0.882	0.002	Preneoplastic conditions treatment
ļ	0.864	0.004	Dextranase inhibitor
	0.862	0.004	Pullulanase inhibitor
ļ	0.854	0.009	Antieczematic
ļ	0.851	0.024	CYP2C12 substrate
ļ	0.847	0.004	Exoribonuclease II inhibitor
ļ	0.846	0.004	IgA-specific serine endopeptidase inhibitor
ļ	0.845	0.009	Sphinganine kinase inhibitor
ŀ	0.837	0.011	Mucomembranous protector
ļ	0.835	0.003	Glucan 1,4-alpha-maltotriohydrolase inhibitor
	0.834	0.004	Gluconate 5-dehydrogenase inhibitor
ļ	0.834	0.014	Methylenetetrahydrofolate reductase (NADPH) inhibitor
	0.832	0.015	Chlordecone reductase inhibitor
ļ	0.829	0.004	Poly(alpha-L-guluronate) lyase inhibitor
ļ	0.829	0.004	Skin irritation, inactive
	0.826	0.009	Taurine dehydrogenase inhibitor
ļ	0.825	0.004	Acetylesterase inhibitor
	0.821	0.003	Glutarate-semialdehyde dehydrogenase inhibitor
ļ	0.82	0.003	GABA aminotransferase inhibitor
	0.82	0.004	Xylan endo-1,3-beta-xylosidase inhibitor
	0.818	0.003	Poly(beta-D-mannuronate) lyase inhibitor
	0.811	0.002	Aspergillopepsin l inhibitor
	0.809	0.005	Lysine 2,3-aminomutase inhibitor
ŀ	0.807	0.004	Eye irritation, inactive
ļ	0.805	0.009	Membrane permeability inhibitor
ŀ	0.804	0.024	1 estosterone 1 / beta-dehydrogenase (NADP+) inhibitor
	0.8	0.008	Fucosterol-epoxide lyase inhibitor

2458 possible activities at Pa>0.5%.

## Table 5: Benzeneacetic acid.

Pa	Pi	Biological Activity
0.943	0.003	CYP2J substrate
0.942	0.002	CYP2J2 substrate
0.94	0.003	Chlordecone reductase inhibitor
0.934	0.001	Penicillin amidase inhibitor
0.925	0.002	L-glucuronate reductase inhibitor
0.92	0.001	N-formylmethionyl-peptidase inhibitor
0.92	0.003	Linoleate diol synthase inhibitor
0.916	0.002	NADPH-cytochrome-c2 reductase inhibitor
0.914	0.003	Pullulanase inhibitor
0.912	0.001	Arylesterase inhibitor
0.912	0.004	Phobic disorders treatment
0.91	0.002	Mitochondrial processing peptidase inhibitor
0.91	0.003	Glutamyl endopeptidase II inhibitor
0.909	0.005	Testosterone 17beta-dehydrogenase (NADP+) inhibitor
0.904	0.001	Benzoylformate decarboxylase inhibitor
0.903	0.005	Alkenylglycerophosphocholine hydrolase inhibitor

2689 possible activities at Pa>0.5%.

# Table 6: D-Allose.

Pa	Pi	Biological Activity
0.986	0.001	Sugar-phosphatase inhibitor
0.98	0.001	Alkenylglycerophosphocholine hydrolase inhibitor
0.975	0.001	UDP-N-acetylglucosamine 4-epimerase inhibitor
0.975	0.001	Glucan endo-1,3-beta-D-glucosidase inhibitor
0.971	0.001	Fructan beta-fructosidase inhibitor
0.971	0.001	Exoribonuclease II inhibitor
0.97	0.001	Beta-mannosidase inhibitor
0.968	0.002	CDP-glycerol glycerophosphotransferase inhibitor
0.967	0.001	Fucosterol-epoxide lyase inhibitor
0.966	0.001	Lactose synthase inhibitor
0.965	0.001	Levanase inhibitor
0.963	0	Osmotic diuretic
0.963	0.001	IgA-specific metalloendopeptidase inhibitor
0.963	0.002	Benzoate-CoA ligase inhibitor
0.962	0.001	D-threo-aldose 1-dehydrogenase inhibitor
0.96	0.001	Anthranilate-CoA ligase inhibitor
0.958	0.001	Mucinaminylserine mucinaminidase inhibitor
0.956	0	Xylose isomerase inhibitor
0.956	0.001	Manganese peroxidase inhibitor
0.951	0.001	Ribulose-phosphate 3-epimerase inhibitor
0.948	0.003	Beta-adrenergic receptor kinase inhibitor
0.948	0.003	G-protein-coupled receptor kinase inhibitor
0.947	0.001	N-acylmannosamine kinase inhibitor
0.946	0	Beta-amylase inhibitor
0.946	0.001	3-Phytase inhibitor
0.945	0.001	Peptide-N4-(N-acetyl-beta-glucosaminyl)asparagine amidase inhibitor
0.943	0.001	Aldose reductase substrate
0.939	0.001	Licheninase inhibitor
0.937	0	Riboflavin phosphotransferase inhibitor
0.936	0.002	Glucan endo-1,6-beta-glucosidase inhibitor
0.935	0.001	Alkenylglycerophosphoethanolamine hydrolase inhibitor
0.934	0.001	Phosphatidylglycerophosphatase inhibitor
0.933	0.005	Membrane integrity agonist
0.931	0.001	Mannosidase inhibitor
0.931	0.001	Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
0.931	0.003	Anaphylatoxin receptor antagonist

0.928	0.001	Galacturan 1,4-alpha-galacturonidase inhibitor
0.927	0.001	Endo-1,3(4)-beta-glucanase inhibitor
0.927	0	Glucan 1,3-alpha-glucosidase inhibitor
0.927	0.001	Phenylacetate-CoA ligase inhibitor
0.926	0.001	Alpha-N-acetylglucosaminidase inhibitor
0.925	0.001	Beta-glucosidase inhibitor
0.924	0.001	Glucan 1,3-beta-glucosidase inhibitor
0.924	0.001	Lactase inhibitor
0.921	0	Beta-D-fucosidase inhibitor
0.919	0	Alpha-L-rhamnosidase inhibitor
0.916	0	Sucrose alpha-glucosidase inhibitor
0.916	0.001	Laminaribiose phosphorylase inhibitor
0.914	0.001	Mycothiol-S-conjugate amidase inhibitor
0.911	0.001	Cyclomaltodextrinase inhibitor
0.909	0	Maltose-transporting ATPase inhibitor
0.909	0	Alternansucrase inhibitor
0.908	0	Mannosyl-oligosaccharide 1,2-alpha-mannosidase inhibitor
0.908	0.001	Alpha-mannosidase inhibitor
0.908	0.001	Lipotropic
0.907	0.002	Glucan 1,4-alpha-maltotriohydrolase inhibitor
0.905	0.001	GDP-mannose 6-dehydrogenase inhibitor
0.904	0.003	Pullulanase inhibitor
0.904	0.004	NAD(P)+-arginine ADP-ribosyltransferase inhibitor
0.902	0	1,4-Alpha-glucan branching enzyme inhibitor
0.9	0.001	Glucan 1,6-alpha-glucosidase inhibitor

1897 possible activities at Pa>0.4%.

## Table 7: Phenol, 2,4-bis (1,1-dimethylethyl).

Pa	Pi	Biological Activity
0.922	0.005	Aspulvinone dimethylallyltransferase inhibitor
0.917	0.004	Ubiquinol-cytochrome-c reductase inhibitor
0.91	0.004	Alkenylglycerophosphocholine hydrolase inhibitor
0.881	0.004	Dehydro-L-gulonate decarboxylase inhibitor
0.88	0.009	Testosterone 17beta-dehydrogenase (NADP+) inhibitor
0.88	0.017	CYP2C12 substrate
0.874	0.004	Linoleate diol synthase inhibitor
0.869	0.001	SULT1A2 substrate
0.86	0.004	Dextranase inhibitor
0.859	0.008	Sphinganine kinase inhibitor
0.857	0.004	Glutathione thiolesterase inhibitor
0.856	0.005	Superoxide dismutase inhibitor
0.85	0.01	Antiseborrheic
0.847	0.009	Mucomembranous protector
0.843	0.005	Glucan endo-1,6-beta-glucosidase inhibitor
0.843	0.008	Feruloyl esterase inhibitor
0.842	0.003	Long-chain-aldehyde dehydrogenase inhibitor
0.842	0.013	Chlordecone reductase inhibitor
0.832	0.005	N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor
0.827	0.004	Lipoprotein lipase inhibitor
0.826	0.005	Alkane 1-monooxygenase inhibitor
0.824	0.013	Sugar-phosphatase inhibitor
0.82	0.002	SULT1A3 substrate
0.819	0.004	UGT1A6 substrate
0.809	0.019	CYP2J substrate
0.808	0.004	Reductant
0.805	0.006	NADPH-cytochrome-c2 reductase inhibitor
0.803	0.013	Beta-adrenergic receptor kinase inhibitor
0.803	0.013	G-protein-coupled receptor kinase inhibitor

2328 possible activities at Pa>0.9%.

Pa	Pi	Biological Activity
0.809	0.01	Nicotinic alpha6beta3beta4alpha5 receptor antagonist
0.786	0.012	Nicotinic alpha2beta2 receptor antagonist
0.704	0.074	Phobic disorders treatment
0.696	0.008	Centromere associated protein inhibitor
0.692	0.004	Imidazoline I1 receptor agonist
0.692	0.004	Imidazoline receptor agonist
0.67	0.065	Testosterone 17beta-dehydrogenase (NADP+) inhibitor
0.65	0.022	Kidney function stimulant
0.648	0.011	Leukopoiesis stimulant
0.635	0.019	Chloride peroxidase inhibitor
0.635	0.035	Omptin inhibitor
0.624	0.001	Imidazoline receptor antagonist
0.621	0.047	Glutamyl endopeptidase II inhibitor
0.619	0.091	Aspulvinone dimethylallyltransferase inhibitor
0.618	0.012	Insulin promoter
0.611	0.036	Complement factor D inhibitor
0.604	0.045	Pseudolysin inhibitor
0.602	0.055	Taurine dehydrogenase inhibitor
0.6	0.038	5 Hydroxytryptamine release stimulant

## Table 8: 1H-Imidazole, 4,5-dihydro-4-methyl-2-phenyl.

1367 possible activities at Pa>1.2%.

## Table 9: Octadecanoic acid, 2-hydroxy-1-(hydroxymethyl) ethyl ester.

Pa	Pi	Biological Activity
0.961	0.001	All-trans-retinyl-palmitate hydrolase inhibitor
0.954	0.003	Lipid metabolism regulator
0.936	0.003	Eye irritation, inactive
0.933	0.003	Antieczematic
0.928	0.003	CYP2J substrate
0.926	0.003	Acylcarnitine hydrolase inhibitor
0.925	0.003	CYP2J2 substrate
0.916	0.003	Linoleate diol synthase inhibitor
0.909	0.003	Lipoprotein lipase inhibitor
0.905	0.003	GST A substrate
0.902	0.002	Macrophage colony stimulating factor agonist
0.902	0.005	Alkenylglycerophosphocholine hydrolase inhibitor
0.9	0.002	Phosphatidylglycerophosphatase inhibitor

1953 possible activities at Pa>0.8%.

#### Table 10: Octadecanoic acid.

Pi	Biological Activity
0.001	Acylcarnitine hydrolase inhibitor
0.001	Alkylacetylglycerophosphatase inhibitor
0.002	Alkenylglycerophosphocholine hydrolase inhibitor
0.002	CYP2J substrate
0.001	CYP2J2 substrate
0.002	Acrocylindropepsin inhibitor
0.002	Chymosin inhibitor
0.002	Saccharopepsin inhibitor
0.001	Dextranase inhibitor
0.001	Carboxypeptidase Taq inhibitor
0.003	Polyporopepsin inhibitor
0.002	Glucan endo-1,3-beta-D-glucosidase inhibitor
0.002	Sugar-phosphatase inhibitor
0.002	Pullulanase inhibitor
0.002	Sarcosine oxidase inhibitor
0.003	Pro-opiomelanocortin converting enzyme inhibitor
	Pi           0.001           0.002           0.002           0.001           0.002           0.001           0.002           0.002           0.002           0.002           0.002           0.002           0.001           0.001           0.003           0.002           0.002           0.002           0.002           0.002           0.002           0.002           0.003

0.939	0.003	Phobic disorders treatment
0.938	0.001	Phosphatidylglycerophosphatase inhibitor
0.935	0.002	Poly(alpha-L-guluronate) lyase inhibitor
0.935	0.001	Xylan endo-1,3-beta-xylosidase inhibitor
0.935	0.003	Sphinganine kinase inhibitor
0.933	0.002	Exoribonuclease II inhibitor
0.933	0.004	Mucomembranous protector
0.932	0.002	D-lactaldehyde dehydrogenase inhibitor
0.931	0.001	Poly(beta-D-mannuronate) lyase inhibitor
0.931	0.002	Levanase inhibitor
0.929	0.001	Glutarate-semialdehyde dehydrogenase inhibitor
0.929	0.002	Methylamine-glutamate N-methyltransferase inhibitor
0.927	0.001	Phenylacetate-CoA ligase inhibitor
0.921	0.001	Prostaglandin-A1 DELTA-isomerase inhibitor
0.92	0.002	Peptide-N4-(N-acetyl-beta-glucosaminyl)asparagine amidase inhibitor
0.92	0.002	L-glucuronate reductase inhibitor
0.92	0.004	Antieczematic
0.919	0.003	Fucosterol-epoxide lyase inhibitor
0.914	0.002	IgA-specific metalloendopeptidase inhibitor
0.914	0.003	Superoxide dismutase inhibitor
0.911	0.002	Gluconate 5-dehydrogenase inhibitor
0.91	0.002	Lysine 2,3-aminomutase inhibitor
0.91	0.003	Lipoprotein lipase inhibitor
0.91	0.006	Methylenetetrahydrofolate reductase (NADPH) inhibitor
0.907	0.001	(S)-2-hydroxy-acid oxidase inhibitor
0.907	0.005	Ubiquinol-cytochrome-c reductase inhibitor
0.906	0.002	Acetylesterase inhibitor
0.904	0.001	Pectin lyase inhibitor
0.902	0.002	Aminoacylase inhibitor
0.902	0.003	GST A substrate
0.901	0.005	Prostaglandin-E2 9-reductase inhibitor
0.9	0.003	Arginine 2-monooxygenase inhibitor

2712 possible activities at Pa>0.3%.

The various volatile compounds from these selected mushrooms were reported earlier from fungi and plants. Dimethylsilane group of compounds have potential as anticancer drugs.<sup>[24,25]</sup> Stearic acid, methyl ester or stearate is a saturated 19 carbon-chained compound and it is also known as octadecanoic acid methyl ester (OA).<sup>[26]</sup> OA is classified as fatty acid methyl ester (FAMEs) and has been shown to have antimicrobial<sup>[27]</sup> and potential anticancer<sup>[28]</sup> properties. There are various antiviral activities from fatty acids against viruses. Fatty acid was able to inhibit the replication of HCV and synergistic effect with IFN- $\alpha$  was observed.<sup>[29]</sup>

The GC-MS analyses of *Moringa oleifera* extracts revealed numerous known anti-cancer compounds, namely eugenol, isopropyl isothiocynate, D-allose, and hexadeconoic acid ethyl ester, all of which possess long chain hydrocarbons, sugar moiety and an aromatic ring. This suggests that the anti-cancer properties of *Moringa oleifera* could be attributed to the bioactive compounds present in the extracts from this plant.<sup>[30]</sup> Since the bioactivity is attributed to the presence of various chemicals present in the methanolic extract of wild mushroom there is a need to understand the various

chemical structures and their possible bioactivity in the metabolic pathways.<sup>[18]</sup>

#### CONCLUSION

Our systematic investigation reveals the potential of *Gymnopilus junonius* collected from Western Ghats, Tamil Nadu, India as a good source of bioactive compounds such as alkanes, alkenes and hydrocarbons. The PASS study reveals that compounds identified from the present study have various potential biological activities. Further studies are needed to validate these predictions. However, our study also gives a better understanding for identification and comparison of volatile and non-volatile compounds in mushroom extract by GC-MS and further interest to researchers for the study and isolation of bioactive compounds.

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