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# Untargeted metabolite profiling of *Aggregatum* onion cultivars: Insights from GC-MS based metabolomics studies

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### Abstract

*Allium cepa*, commonly known as onion, is renowned for its culinary and medicinal properties. This article investigates the phytochemical composition of four aggregatum onion varieties using preliminary phytochemical screening and gas chromatography-mass spectrometry (GC-MS) analysis. The study reveals diverse metabolites, including hydrocarbons, aldehydes, terpenoids, and organosulfur compounds, with variations observed among the onion varieties. Significant proportions of compounds such as diisooctyl phthalate, hexanol, and nobilitin, possessing various pharmacological activities like antimicrobial and antioxidant properties, were identified. The research emphasizes the importance of understanding onion phytochemistry, particularly given its widespread cultivation and consumption, notably in regions like Tamil Nadu, India. The identified bioactive compounds shed light on different onion varieties' unique attributes and potential health benefits. By elucidating onion bulb metabolite profiles using advanced techniques like GC-MS, this study contributes to understanding the phytochemical diversity within *Allium cepa* species. These findings lay the groundwork for future research into the medicinal and nutritional advantages of onions and support targeted breeding (selective breeding) programs to enhance health-promoting compounds in onion varieties. Overall, this study underscores onions' significance as a culinary staple and a valuable source of diverse bioactive compounds with pharmacological potential.

Key words: GC-MS, phytochemicals, secondary metabolites, retention time

## Introduction

Allium cepa, commonly known as onion, originates from Asia and belongs to the Alliaceae family. It is a biennial cool-season crop. In India, both common onion (Allium cepa var. cepa) and multiplier onion (Allium cepa var. aggregatum) are commercially cultivated and propagated by both seeds and bulbs. Aggregatum onion cultivars produce small bulb clusters with a strong flavor and aroma, while common onion cultivars yield large single bulbs with a milder flavor and poor storage ability. Aggregatum onion cultivars are primarily cultivated and consumed in southern parts of Tamil Nadu, known by various names such as small onion, ever-ready onion, underground onion, potato onion, shallots, nesting onions, multiplier onion, and Egyptian ground onion (Saraswathi et al., 2017). They thrive in tropical and subtropical regions, tolerate hot and humid conditions, and have gained widespread cultivation across various climates and soil types. Both the leaves and bulbs are used as raw vegetables and spice crops due to their pungency, attributed to compounds like allyl propyl disulfide (Farzaneh et al., 2021). Onions are commonly used in salads, soups, pickles, and curries. Moreover, onions possess numerous medicinal properties, including anticholesterol, anti-inflammatory, anticancer, appetizing, jaundice

remedy, blood-purifying, obesity-fighting, and respiratory ailment-relieving properties (Kumar *et al.*, 2010; Kusano *et al.*, 2016; Saviano *et al.*, 2019; Metrani *et al.*, 2020; Ren and Zhou, 2021). They are also used to alleviate earaches by applying warm onion juice and to prevent toothaches and oral infections (Chevallier, 2022). Onions are rich sources of polyphenols, flavonoids and volatile compounds, making them suitable as food supplements (Ramesh *et al.*, 2018).

Both onions contain a wide range of phytochemicals, such as phenols, flavonoids, anthocyanins, and organosulfur compounds (Golubev *et al.*, 2003). The composition of these compounds varies with the cultivars and environmental conditions, affecting the plant phenotype by accumulating phytochemicals at various growth stages (Roldan *et al.*, 2014; Dong *et al.*, 2015). These compounds can exist in plants in free, conjugated, or bound forms. Onions are cultivated during both the kharif and rabi seasons. Although these cultivars share similar morphological traits and are not easily differentiated, variations in metabolic compounds between them can differentiate cultivars (Hong *et al.*, 2016). Methods such as GC-MS, NMR, and thin-layer chromatography are commonly used to assess metabolite profiling and structure, effectively discriminating between varieties of various crops. GC-MS analysis has revealed various secondary metabolites

in onions, including organic acids, phenols, alkaloids, amino acids, ketones, and volatiles. Some varieties or cultivars have been found to have low sugar levels, as well as anticoagulant and anticarcinogenic properties, when grown in specific regional areas (Saviano *et al.*, 2019).

Limited research has utilized a metabolomics approach to distinguish different types of onion bulbs (Das *et al.*, 2016). The metabolite composition of 11 onion varieties was analyzed using GC-MS. Therefore, it would be intriguing to investigate the metabolites in the bulbs of seed-propagated onions, particularly due to their widespread cultivation and consumption in Tamil Nadu. Identifying important bioactive compounds in the bulb extract through GC-MS analysis could provide valuable insights into these onions' unique characteristics and potential health benefits.

#### **Materials and methods**

**Plant material:** The study utilized four aggregatum onion varieties: Co (On) 5, Co (On) 6 (from TNAU), Oriya (a local variety in Tamil Nadu), and Arka Ujjwal (from IIHR, Bangalore). Seedlings aged 45 days and measuring 10–15 cm in height were transplanted into the main field at the College Orchard, Department of Vegetable Science, TNAU, Coimbatore, between August and November 2022. Cultivation practices adhered to the guidelines outlined in the Crop Production Guide (CPG) of TNAU.

**Preliminary phytochemical screening:** Initial qualitative phytochemical investigations were carried out on the ethanolic extract of leaves using established procedures as outlined in standard references given by Junaid and Patil (2020).

**Preparation of extract:** The fresh bulbs were prepared by removing the outer layer, cutting them into small pieces, and then pulverizing them with a pestle and mortar to ensure homogenization. The resulting mixture was filtered using Whatman number 40 filter paper. The filtrate obtained was then centrifuged at 10,000 rpm for 20 min.. Subsequently, the extracts were concentrated using a rotary evaporator. For analysis, an aliquot of 2  $\mu$ L from each methanol-concentrated crude plant extract was injected into the split-less GC-MS apparatus.

**GC-MS analysis:** The GC-MS analysis of the extracts was conducted utilizing a Perkin Elmer Clarus Sq8c column equipped with a DB-5 MS capillary standard non-polar column. The column dimensions were 30 meters long, with an inner diameter (ID) of 0.25 mm and a film thickness of 0.25  $\mu$ m. Helium gas, with a purity of 99.999%, was employed as the carrier gas at a constant flow rate of 1 mL/min. The sample injection volume utilized was 1  $\mu$ L.

**Compound identification based on molecular mass and structure:** Data regarding the mass spectral range was obtained from the PubChem NIST Library. The molecular names, sizes, and structures of the compounds in the test material were identified by comparing them with entries in the library.

#### **Result and discussion**

**Preliminary Phytochemical screening of onion extract:** Phytochemical screening of allium extract revealed the presence of alkaloids, phenols, flavonoids, terpenoids, steroids, carbohydrates, proteins, amino acids and tannins. Notably, saponins were not detected. **Identification of compounds:** Extracts from the bulbs of four onion varieties using methanol revealed a diverse array of polar and non-polar compounds. A total of 40 metabolic compounds were identified across the different onion varieties, categorized into 11 classes. The most abundant class of metabolites was hydrocarbons, constituting 31% of the total, with 11 metabolites identified. Other prominent classes included aldehydes (18%), organosulfur compounds (12%), terpenoids (9%), steroids (6%), and benzenoids (13%). Minor classes such as amines, amino acids, flavonoids, lipids, lipid acyls, organic nitrogen compounds, and fatty acyls were also identified. These findings are visually represented in Fig. 1 and summarized in Table 1.

Table 1. List of compounds identified in the onion bulb extract

	r	
S. No	Compound name (metabolite)	Group/class
1	Heptacosane	Hydrocarbons
2	Octadecane	Hydrocarbons
3	Hexadecane	Hydrocarbons
4	Dodecane	Hydrocarbons
5	Hentriacontane	Hydrocarbons
6	Tetratetracontane	Hydrocarbons
7	Tetracosane	Hydrocarbons
8	Eicosane	Hydrocarbons
9	Pentadecane	Hydrocarbons
10	Heptadecane	Hydrocarbons
11	Heneicosane	Hydrocarbons
12	2-Butanol	Aldehydes
13	3-Hexanol	Aldehydes
14	2-Pentanol	Aldehydes
15	1,5-Pentanediol	Aldehydes
16	1,2-Cyclooctanediol	Aldehydes
17	3-Pentanol	Aldehydes
18	Dimethyl trisulfide	Organo Sulfur Compounds
19	Methyl isopropyl disulphide	Organo Sulfur Compounds
20	(Z)-1-(Prop-1-en-1-yl)-2- propyldisulfane	Organo Sulfur Compounds
21	Diisooctyl phthalate	Benzenoids
22	Dibutyl phthalate	Benzenoids
23	Didodecyl phthalate	Benzenoids
24	Dibutyl phthalate	Benzenoids
25	11,14-Eicosadienoic acid	Fatty acyls
26	Geranyl isovalerate	Fatty acyls
27	Pentanoic acid	Fatty acyls
28	7-Methyl-Z-tetradecen-1-ol acetate	Fatty acyls
29	à-Hydroxybutyric acid	Acids
30	Acetic acid	Acids
31	á-Phellandrene	Terpenoids
32	à-Pinene	Terpenoids
33	Squalene	Terpenoids
34	Dexamethasone	Steroids
35	Estra-1,3,5(10)-trien-17á-ol	Steroids
36	1,2,3-Trimethyldiaziridine	Organic nitrogen compound
37	Nobiletin	Flavanoid
38	Linoleic acid ethyl ester	lipid acyls
39	2-Myristynoyl pantetheine	Amino acids
40	Cyclopentanamine	Amines

The bulb extract analysis revealed that the most abundant compound present was Diisooctyl phthalate, comprising 15.24% of the total peak area, followed by hexanol at 8.50%. Among the major phytochemicals identified in the allium extracts were



Fig. 1. Major proportions of phytoconstituents in onion bulb extract

diisooctyl phthalate (15.24%), Hexadecane (1.69%), dibutyl phthalate (1.51%), Squalane (1.78%), nobilitin (1.13%), 2-butanol (7.04%), 2-hexanol (8.50%), 3-pentanol (6.21%) and dimethyl trisulfides (0.54%).

A diverse range of metabolites were identified in the Co (On) 5, Co (On) 6, Arka Ujjwal, and Oriya varieties, each exhibiting varying retention times (Fig. 2). The number of metabolites observed was reduced to 18 in Co (On) 5 and Oriya, and 17 in Co (On) 6 and Arka Ujjwal, respectively. Few metabolites were commonly found across all the varieties, including Ecosane (6.09%) and heptacosane (0.4 – 0.7%). Additionally, 3-Hexanol compounds were detected in all the varieties except Co (On) 5, with a retention time of 3.26 min.

In the bulb extracts of Co (On) 5, a total of 18 bioactive compounds were identified. The most prominent was diisooctyl phthalate, constituting 15.24% of the total area with a retention time of 20.565 min. Additionally, 3 butanol (7.04% at 3.23 min),

Squalane (1.78% at 26.73 min), Hexadecane (1.69% at 20.85 min), Dibutyl phthalate (1.51% at 21.61 min), and nobilitin (1.131% at 29.70 min) were also detected (Table 2). In the bulb extracts of Co On 6, a total of 17 phytochemicals were identified (Table 3). Among these, 3 hexanol exhibited the highest area percentage at 8.50% with a retention time of 3.26 min. This was followed by 2 pentanol (0.88%), Piperidine (0.78%), tetracosane (0.65%), Eicosane (0.64%), and alpha phellandrene (0.51%) with retention times of 3.87 min, 5.19 min, 13.03 min, 17.46 min, and 5.04 min, respectively. Additionally, organosulphur compounds such as Dimethyl trisulfide and Methyl isopropyl disulphide were eluted at retention times of 4.21 min and 3.69 min.

The Oriya bulb extract exhibited a notable presence of aldehyde and hydroxyl group compounds. Notably, 3 hexanol and 1,5-Pentanediol demonstrated the highest area percentages, registering at 7.07% and 0.99%, respectively, with retention times of 3.26 min and 4.44 min (Table 4). Additionally, metabolites identified in the oriya bulb extract included 3 hexanol (8.11%), 3 pentanol (6.21%), heptacosane (1.52%), acetic acid (1.00%), Heneiocosane (0.80%), Eicosane (0.79%), cyclopentanamine (0.73%), Dimethyl trisulfide (0.67%), Methyl isopropyl disulphide (0.54%), and Dibutylphthalate (0.52%).

Secondary metabolites play a pivotal role in plants, with their production influenced by factors such as the growing environment, genotype, and phenotype (Eigenbrode *et al.*, 2002; Dudareva and Pichersky, 2008). Despite similar growing conditions, crops often exhibit distinct metabolite profiles, attributed to genetic makeup and sulfur uptake efficiency from the soil (Lanzotti, 2006). Enhancing onion flavour entails supplying sulfate and increased temperatures in dry climates (Packialakshmi *et al.*, 2014). Notably, Squalane, a triterpenoid compound abundant in the extract, finds applications in medicine, dietary supplements, and the cosmetic industry. It is known to lower cholesterol levels (Kumar *et al.*, 2014), exert anti-tumor and anticancer



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S.No	Retention time	Area percent	Compound name	Molecular formula	Molecular weight (g/mol)	Group/ class
1	3.238	7.043	2-Butanol	$C_4H_{10}O$	74.12	ALD
2	20.565	15.242	Diisooctyl phthalate	$C_{24}H_{38}O_4$	390.6	BNZ
3	21.616	1.511	Dibutyl phthalate	$C_{16}H_{22}O_4$	278.34	BNZ
4	29.764	0.563	11,14-Eicosadienoic acid	$C_{20}H_{36}O_2$	308.5	FTAs
5	29.704	1.131	Nobiletin	$C_{21}H_{22}O_8$	402.4	FL
6	12.992	0.427	Heptacosane	$C_{27}H_{56}$	380.07	HYC
7	17.439	0.53	Octadecane	$C_{18}H_{38}$	254.5	HYC
8	20.85	1.691	Hexadecane	$C_{16}H_{34}$	226.44	HYC
9	24.392	0.436	Dodecane	$C_{12}H_{26}$	170.33	HYC
10	24.807	1.185	Hentriacontane	$C_{31}H_{64}$	436.8	HYC
11	25.547	0.667	Tetratetracontane	C44H90	619.2	HYC
12	28.458	0.495	Tetracosane	$C_{24}H_{50}$	338.7	HYC
13	29.004	0.667	Eicosane	$C_{20}H_{42}$	282.5	HYC
14	26.588	0.596	Linoleic acid ethyl ester	$C_{20}H_{36}O_2$	308.5	LA
15	4.194	0.866	Dimethyl trisulfide	$C_2H_6S_3$	126.3	OSC
16	29.529	0.939	Dexamethasone	$C_{22}H_{29}FO_5$	392.5	ST
17	26.738	1.778	Squalene	C30H50	410.7	TER

Table 2. Metabolites identified in the bulb extract of Co (On) 5 using GC-MS

ALD: Aldehydes. BNZ: Benzenoids. FTA: Fatty acyls. FL: Flavanoid. HYC: Hydrocarbons. LA: Lipid acyls. OSC: Organosulphur compound. ST: Steroids. Ter: Terpenoids. FA: Fatty acids. ST: Steroids. ORA: Organoheterocyclic. AA: Amino acids. ONC: Organic nitrigen compound. HC: Hydrocarbon

Table 3. Metabolites identified in the bulb extract of Co (On) 6 using GC-MS

S. No	Retention time	Area percent	Compound name	Molecular formula	Molecular weight (g/mol)	Group/ class
1	3.263	8.50	3-Hexanol	C <sub>6</sub> H <sub>14</sub> O	102.17	ALD
2	3.874	0.88	2-Pentanol	$C_5H_{12}O$	88.15	ALD
3	19.815	0.44	Dibutyl phthalate	$C_{16}H_{22}O_4$	278.34	BNZ
4	7.015	0.45	trans-13-Octadecenoic acid	$C_{18}H_{34}O_2$	282.5	FA
5	12.707	0.42	Octanoic acid	$C_8H_{16}O_2$	144.21	FA
6	24.177	0.33	Geranyl isovalerate	$C_{15}H_{26}O_2$	238.37	FTA
7	8.626	0.42	Dodecane	$C_{12}H_{26}$	170.33	HYC
8	12.112	0.49	Tetratetracontane	C44H90	619.2	HYC
9	13.037	0.65	Tetracosane	C24H50	338.7	HYC
10	17.469	0.64	Eicosane	$C_{20}H_{42}$	282.5	HYC
11	28.468	0.52	Heptacosane	C27H56	380.07	HYC
12	29.014	0.39	Hexadecane	$C_{16}H_{34}$	226.44	HYC
13	5.199	0.78	Piperidine	$C_5H_{11}N$	85.15	ORA
14	3.659	0.48	Methyl isopropyl disulphide	$C_4H_{10}S_2$	122.3	OSC
15	4.219	0.36	Dimethyl trisulfide	$C_2H_6S_3$	126.3	OSC
16	5.044	0.51	á-Phellandrene	$C_{10}H_{16}$	136.23	TER

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effects, reduce cardiovascular disease risks, and improve skin flexibility and moisture retention, boost the absorption of other compounds (Cowan *et al.*, 2022). Geethanjali *et al.* (2023) reported the presence of this compound in Co 5 and Co 6 onion varieties, while Packialakshmi *et al.* (2014) identified it in the Vilathikulam onion variety.

GC-MS analysis of onion bulb extract revealed that hydrocarbons constitute the major phytonutrients. These hydrocarbons, predominantly alkanes, exhibit diverse pharmacological activities. For instance, Tetratetracontane demonstrates antibacterial properties (Gumgumjee*et al.*, 2015), Eicosane exhibits potent antioxidant activity (Vinjamuri and Achar, 2017), and Heneicosane possesses biopesticidal properties (Adesalu, 2016). Similar findings were reported by Eltayeb *et al.* (2017) in Acacia and Addai *et al.* (2022) in Opuntia.

Organosulfur compounds such as Dimethyl trisulfide and Methyl isopropyl disulfide serve as natural repellents against insects and herbivores, contributing to the higher pungency of onion bulbs and providing resistance against pest and disease attacks (Basundari *et al.*, 2021). This notion finds support in a study by Maranda *et al.* (2015), which identified 19 organosulfur compounds, including methyl propyl disulfide and propyl trisulfide. Another study by Manyar *et al.* (2020) found dipropyl disulfide and dipropyl trisulfide compounds in onion oil.

Nobilitin, a flavonoid compound in the Co 5 variety, is known to reduce the risk of coronary heart diseases. Terpenoids identified in the bulb extract play crucial roles in the plant defense system and abiotic stress management (Vickers *et al.*, 2009). They also act as signaling molecules to attract pollinators (Byers *et al.*, 2014) and serve as precursors for antifungal compounds (Fontana *et al.*, 2011).

Heat map analysis: The comparison of various metabolic compounds across different varieties was depicted using a heat map (Fig. 3), showcasing distinct colours for each compound. Among these, diisooctyl phthalate (15.24%) recorded the highest area percent in Co (On) 5, followed by 2-butanol (7.04%), represented in dark yellow and green colours, respectively. Conversely, the green coloration indicated that 2-hexanol emerged as the predominant compound in Co (On) 6, Arka Ujjwal, and Oriya varieties.

In summary, the wide range of phytochemicals present in onions highlights their remarkable health advantages and culinary adaptability. A diverse array of metabolites has been identified by applying GC-MS methodology, offering significant benefits such as antimicrobial, antibacterial, antifungal, and anticancer properties. Research findings strongly suggest that integrating onions into a balanced diet can enhance overall well-being and aid in disease prevention. Furthermore, onions hold potential applications in traditional medicine, drug

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Table 4. Metabolites identified in the bulb extract of Arka Ujjwal using GC-MS

S. No	Retention time	Area percent	Compound name	Molecular formula	Molecular weight (g/ mol)	Group/ class
1	7.075	0.36	à-Hydroxybutyric acid	$C_4H_8O_3$	104.1	Acids
2	4.599	0.38	1,2-Cyclooctanediol	$C_8H_{16}O_2$	144.21	ALD
3	4.444	0.99	1,5-Pentanediol	$C_5H_{12}O_2$	104.15	ALD
4	3.269	7.07	3-Hexanol	$C_{6}H_{14}O$	102.17	ALD
5	3.884	0.95	4-Oxopentyl formate	$C_{6}H_{10}O_{3}$	130.139	CAE
6	7.015	0.65	Octanoic acid	$C_8H_{16}O_2$	144.21	FA
7	18.164	0.36	7-Methyl-Z-tetradecen- 1-ol acetate	$C_{17}H_{32}O_2$	268.4	FTA
8	5.549	0.34	Pentanoic acid	$C_5H_{10}O_2$	102.13	FTA
9	20.885	0.86	Eicosane	C20H42	282.5	HYC
10	13.032	0.93	Heptacosane	C27H56	380.07	HYC
11	13.438	0.30	Pentadecane	$C_{15}H_{32}$	212.41	HYC
12	29.214	0.46	Tetratetracontane	C44H90	619.2	HYC
13	3.404	0.43	1,2,3- Trimethyldiaziridine	$C_4H_{10}N_2$	86.14	ONC
14	5.204	0.63	Piperidine	$C_5H_{11}N$	85.15	ONC
15	6.325	0.38	(Z)-1-(Prop-1-en-1-yl)- 2-propyldisulfane	$C_6H_{12}S_2$	148.3	OSC
16	3.664	0.38	Methyl isopropyl disulphide	$C_4H_{10}S_2$	122.3	OSC
17	5.059	0.71	à-Pinene	$C_{10}H_{16}$	136.23	TER

ALD: Aldehydes. BNZ: Benzenoids. FTA: Fatty acyls. FL: Flavanoid. HYC: Hydrocarbons. LA: Lipid acyls. OSC: Organosulphur compound. ST: Steroids. Ter: Terpenoids. FA: Fatty acids. ST: Steroids. ORA: Organoheterocyclic. AA: Amino acids. ONC: Organic nitrigen compound. HC: Hydrocarbon

Table 5. Metabolites	identified in the	e bulb extract of	Oriva using GC-MS
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S. No	Retention time	Area percent	Compound name	Molecular formula	Molecular weight (g/ mol)	Group/ class
1	9.361	0.32	2-Myristynoyl pantetheine	C25H44N205S	484.7	AA
2	3.263	8.11	3-Hexanol	$C_{6}H_{14}O$	102.17	ALD
3	3.494	6.21	3-Pentanol	$C_5H_{12}O$	88.15	ALD
4	4.434	1.00	Acetic acid	$C_2H_4O_2$	60.05	Acids
5	5.049	0.45	à-Pinene	C10H16	136.23	TER
6	4.479	0.73	Cyclopentanamine	$C_5H_1N_1$	85.15	Amine
7	19.83	0.52	Dibutyl phthalate	$C_{16}H_{22}O_4$	278.34	BNZ
8	14.238	0.30	Didodecyl phthalate	C32H54O4	502.8	BNZ
9	4.219	0.67	Dimethyl trisulfide	$C_2H_6S_3$	126.3	OSC
10	17.479	0.79	Eicosane	$C_{20}H_{42}$	282.5	HC
11	21.561	0.29	Estra-1,3,5(10)-trien-17á-ol	C <sub>18</sub> H <sub>24</sub> O	256.39	ST
12	20.875	0.80	Heneicosane	C21H44	296.6	HYC
13	21.691	1.52	Heptacosane	C27H56	380.07	HYC
14	13.027	0.67	Heptadecane	C17H36	240.5	HYC
15	3.664	0.54	Methyl isopropyl disulphide	$C_4H_{10}S_2$	122.3	OSC
16	7.025	0.30	Octanoic acid	C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>	144.21	FA

ALD: Aldehydes. BNZ: Benzenoids. FTA: Fatty acyls. FL: Flavanoid. HYC: Hydrocarbons. LA: Lipid acyls. OSC: Organosulphur compound. ST: Steroids. Ter: Terpenoids. FA: Fatty acids. ST: Steroids. ORA: Organoheterocyclic. AA: Amino acids. ONC: Organic nitrigen compound. HC: Hydrocarbon

development, and the cosmetic industry. Moreover, specific onion varieties contain unique metabolites like nobilitin (a flavonoid), which could prove invaluable for enhancing onion varieties through targeted breeding and improvement efforts.

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Fig. 3. Heat map based on the area percent. The metabolites were compared with colours. S1. Co (On) 5 S2. Co (On) 5 S3. Oriya S4. Arka ujjwal

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