Journal of Chemical Health Risks

www.jchr.org

JCHR (2024) 14(3), 2982-2993 | ISSN:2251-6727

Metabolite Profiling of Tomato (Solanum lycopersicum L.) Germplasms Using LC-MS Analysis

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(Received: 04 February 2024 Revised: 11 March 2024 Accepted: 08 April 2024)

Keywords:
Tomato, Metabolites, LCMS, Health benefits, Meghalaya.

ABSTRACT

Eleven tomato genotypes collected from different districts of Meghalaya were evaluated based on the analysis of metabolic characters of chemical parameters/constituents using Liquid Chromatography mass-spectrometry (LCMS) analysis. In the current study, a total of 19 primary metabolites, 2 common primary metabolites, 5 uncommon primary metabilotes, 24 secondary metabolites, 5 common secondary metabolites and 4 uncommon secondary metabolites were detected in 11 samples of tomato. It was observed that the detected primary metabolites and secondary metabolites of different tomato samples was found to have beneficial health effects. It was observed that the egg-shaped tomato genotype collected from Resubelpara (Sample No 3) contained two carcinogenic metabolites including five health-promoting metabolites. Accordingly, the 11 tomato genotypes have been arrranged in descending order based on their effects on human health as follows, Sample No-9 > sample No-5 > sample No-7 > sample No-4 > sample No-1 > sample No-8 > sample No-2 > sample No-6 > sample No-10 > sample No-11 > sample No-3. Based on the comparative study, it was concluded that the egg-shaped tomato genotype collected from Nongpoh (Sample No 9) contained twenty-one numbers of good metabolites with medicinal values and also it was observed that these metabolites was found very essential for human growth and development. As a result, the tomato genotype collected from Nongpoh (Sample No 9) was found to be the best among the other samples of tomato genotypes.

1. Introduction

A metabolite is an intermediate or final result of cellular metabolism; small molecules are commonly included in this term. Metabolites are used by the body for defence, signaling, catalytic action (usually as acofactor enzyme), promoting and inhibiting enzyme activity and ineracting with other organisms (pheromones, odorants and pigments). Metabolism is the process of transforming food into energy for cellular functions as well as building blocks for proteins, lipids, nucleic acids and carbohydrates (Mazzoccoli *et al.*, 2012). Metabolites are classified into two types: Primary and Secondary metabolites (Alamgir, 2017). Secondary metabolites are the by products of primary metabolism but do not form organism's basic molecular structure.

Tomato (*Solanum lycopersicum* L.) is a member of solanaceae family, can be consumed both as a fresh fruit and processed as food products like soups, sauces and juices (Li *et a.l,* 2018). It has been observed that the tomato is cultivated in India in an area of 812

thousand ha with an average annual production of 20573 thousand metric tones during 2019 - 2020 (National Horticulture Board, 2023). The metabolites present in tomatoes have a wide range of physiological properties, such as anti-inflammatory, antibacterial, anti-allergenic, vasodilatory, antithrombotic, cardio-protective, antioxidantetc (Raiola *et al.*, 2014). Carotenoids in tomatoes represent the major lycopeneof human diet (Viuda-Martos *et al.*, 2014).

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In addition to the nutritional value, it was reported that the carotenoids and polyphenolic compounds also improve the sensory properties like flavour, fragrance and texture of tomatoes (Tohge *et al.*, 2015). Vitamin C and E which are naturally occurring antioxidant found in tomatoes (Martí *et al*., 2016). A large number of metabolites namely sucrose, hexoses, citrate, malate and ascorbic acid are also present in tomatoes (Li *et al.*, 2018). The plant growing conditions affect the quality of tomato fruits and metabolite biosynthesis (Diouf *et al*., 2018). Tomatoes are considered as the most important vegetables worldwide because they possess several antioxidants and vitamins such as ascorbic acid and phenolic acids, tocopherols and carotenoids and addition of tomato to our diet promotehealth benefits (Weinert *et. al*., 2021). In this present study, the presence of common metabolites (primary and secondary) was investigated in tomato samples collected from different parts of Meghalaya with an objective to find out the presence or absence of any harmful/toxic substances to select the superior genotype.

2. Materialsand methods

2.1. Study Area

The state of Meghalaya is an upland area formed by a detached part of the Deccan plateau with an altitude range of 1220 to 1830m above sea level with geographical coordinates of latitude 20°1'N-26°5'N and longitude 85°49'E-92°52'E. In the present study, the tomato sample were randomly collected from different districts of Meghalaya for metabolite analysis.

2.2. Sampling locations

Half-ripened tomato fruit samples were collected from eleven locations of different districts of Meghalaya (Table 1).

Table 1. Sources of tomato samples for LCMS analysis

Sample No	Collection point Village(District)	Shape	Diameter (cm)	Latitude	Longitude
1	Ampati (South west Garo Hills)	Egg like	5.0	25˚27’49’’N	89˚55’46’’E
2	Dalu (West Garo Hills)	Round	5.1	25˚12’56’’N	90˚13’39’’E
3	Resubelpara (North Garo Hills)	Egg like	4.4	25˚90’41’’N	90˚60’62’’E
4	Tura (West Garo Hills)	Cherry like	1.9	25˚30’36’’N	90˚12’59’’E
5	Baghmara (South Garo Hills)	Round	4.9	25˚19’35’’N	90˚63’46’’E
6	Willaimnagar (East Garo hills)	Cherry like	2.0	25˚53’14’’N	90˚59’20’’E
7	Shillong (East khasi Hills)	Egg like	4.2	25˚57’88’’N	91˚89’33’’E
8	Jowai (West jaintia Hills)	Round	5.1	25˚30’00’’N	92˚15’00’’E
9	Nongpoh (Ri-bhoi)	Egg like	3.8	25˚86’99’’N	91˚83’37’’E
10	Mawkyrwat (South west khasi Hills)	Round	4.6	25˚36’25’’N	91˚45’56’’E
11	Khliehriat (East Jaintia Hills)	Egg like	4.3	25˚35’67’’N	92˚36’41’’E

2.3. Sample preparation

The fruit pericarp of tomato fruit was dried at room temperature for seven days. These were ground to obtain the powdered form. Added 10mL methanol to 1mg of powdered sample, kept it for 4hours and then the samples were centrifuged for 10 min at 5000 rpm. Centrifuged samples were performed for LCMS analysis.

2.4. Liquid chromatography mass-spectrometry analysis

The extraction was analysed using liquid chromatography mass spectrophotometry (LCMS) with a single quadruple LCMS system that was fitted with a capillary column. Each sample extract was centrifuged and separately diluted. The ion source was set to 230ºC withthe start time of (solvent delay) = 2 min (solvent cutting). The temperature was kept at 40ºC for 4 min and gradually increased to 280ºC at a rate of 20ºC/min.

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The overall run time was 30 min. The temperature at the LC and the trans-line sections was greater (280ºC) than that at the MS section (250ºC) to ensure that all ions have fully shifted to the MS section. Helium was used as the carrier gas at a constant flow rate of 1mL/min. The electron impact ionization voltage was 70eV. The compounds were analysed for constituent identification using total ion count (TIC) after being compared to a database known components available in the computer library attached to the LCMS instrument. The instrument was injected with 10µL of the sample in split mode. AnRtx5MS-30m column with 0.25-mm ID and 0.25µm df was used. Using a scanning range of 40 to 850 m/z, Mass spectra were obtained at 2 scan sec^{-1}. Each component's peak regions were quantified and normalization was conducted using internal standard. In the chromatograms the x-axis indicates the retention period while the y-axis represents the absorbance units AU (a signal corresponding to the detector's response) at 210 nm. The records were made in retention time of the first 10 min and absorbance units up to a maximum of 0.070. The chromatograms showed the components as functions of their retention period and mass-to-charge ratio by the mass relative abundance.

3. Results

3.1. Primary metabolites detected

In this present study, chromatograms of the tomato samples gave information on the presence of compounds. It was observed that an analyte has no effect on chromatogram; as a result, these can frequently be utilized as fingerprint for various molecules. It was also observed that there were several compounds found similar in the chromatograms. The chromatogram of LCMS spectra analysis showing peaks of the number of compounds from the LC fractions of the methanol extract of whole tomato is represented in the figures given below (Figure 1 to 11).

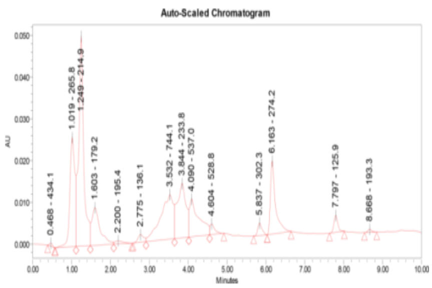
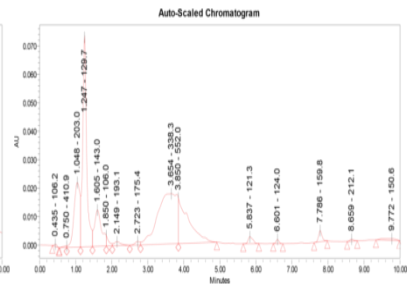
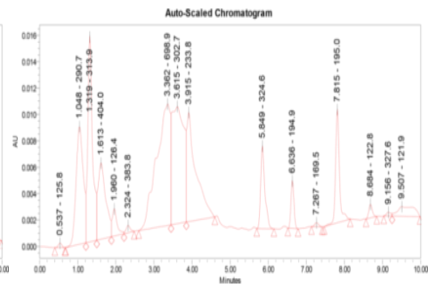

Fig 1.LCMS chromatogram of Sample no 1**Fig 2.**LCMS chromatogram of Sample no 2 **Fig 3.**LCMS chromatogram of Sample no 3

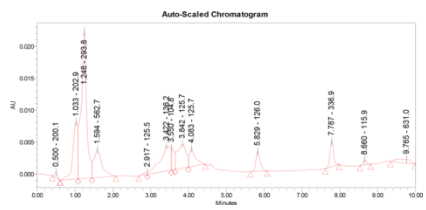
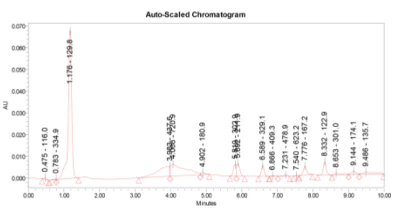
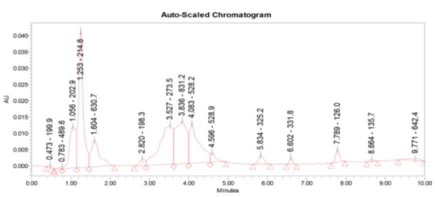

Fig 4.LCMS chromatogram of Sample no 4 **Fig 5.**LCMS chromatogram of Sample no 5 **Fig 6.**LCMS chromatogram of Sample no 6

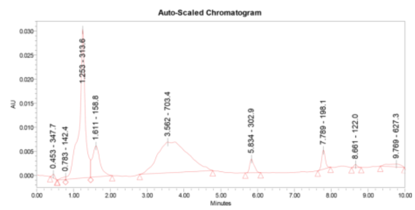
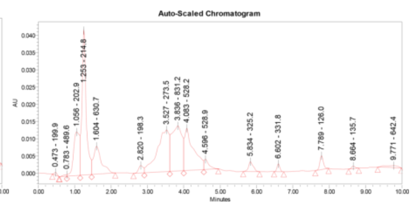
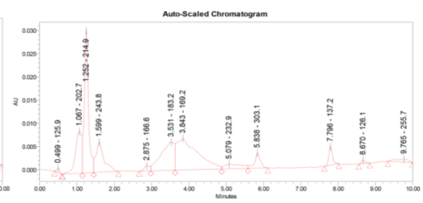

Fig 7. LCMS chromatogram of Sample no 7**Fig 8.**LCMS chromatogram of Sample no 8**Fig 9.**LCMS chromatogram of Sample no 9

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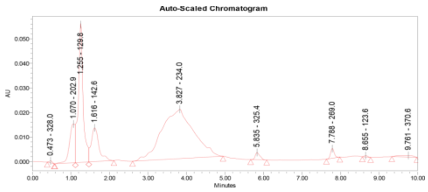

Fig 10. LCMS chromatogram of Sample no 10

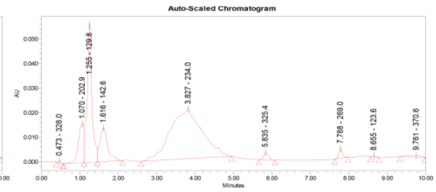

Fig 11. LCMS chromatogram of Sample no 11

A total of 19 primary metabolites was detected in the tomato samples. Most of the metabolites were detected in Sample No 3,7 and 2. Metabolite dected in Sample No 3 were Lignoceric acid ,cis-Aconitic acida, 3,5-Dimethoxycinnamic acid and Dicamba; Sample No 7 were 5-oxo-L-prolyl-glycine, Blasticidin Sand Cer[NS] d46:2; Sample No 2 were Safingol, D-erythro-Dihydrosphingosine and Dihydrosphingosine. Vitamin (Biotin) was also dected in Sample No 9. Compounds detected in the tomato samples has a wide array of properties like antibiotic, herbicide, lubricating agent, food additive, xenobiotic, antibacterial, cardio protective etc. Primary metabolites detected in the collected tomato samples in increasing order of retention times in the chromatograms along with their names, chemical composition, molecular mass, class and roles are litsed in Table 2.

Table2. Primary metabolites detected in the tomato samples in increasing order of retention times in the chromatograms along with their roles

Sl No	**Sample No**	**RT (min)**	**m/z value**	**Name of the compound, chemical composition and molecular mass(g/mol)**	**Class**	**Roles**
1	3	0.435	106.2	Lignoceric acid (or Tetracosanoic acid) $C_{24}H_{48}O_2$, 368.63	Long-chain fatty acids.	It plays a role as a volatile oil component.
2	10	0.473	328.0	Mefenpyr-diethyl $C_{16}H_{18}Cl_2N_2O_4$, 373.23	Amino acids	Mefenpyr-diethyl is a herbicide safener that protects crops against herbicide damage.
3	8	0.750	284.5	Stearic acid $C_{18}H_{36}O_2$, 284.48	Long-chain fatty acids.	Stearic acid is a lubricating agent and food additive.
4	7	0.783	142.4	5-oxo-L-prolyl-glycine $C_7H_{10}N_2O_4$, 186.165	α amino acids	Protect the kidneys from bad side effects of some medicines, as well as the liver from the hamful effects of alcohol.
5	3	1.247	129.7	cis-Aconitic acid $C_6H_6O_6$, 174.11	Carboxylic acid	Glutaminolysis is a metabolic disease that is associated with the cancer pathway
6	7	1.253	313.6	Blasticidin S $C_{17}H_{26}N_8O_5$, 422.4	Amino acids	It is an antibiotic that is used in biology research for selecting cells for cell culture.

7	4	1.428	293.8	6:2fluorotelomer unsaturated carboxylic acid.$C_8H_2F_{12}O_2$,358.08	Carboxylic acid	It has a role as a xenobiotic and a persistent organic pollutant.
8	9	1.599	243.8	Biotin, $C_{10}H_{16}N_2O_3S$, 244.31	Vitamin B7	Often used as a therapy for hair loss and to maintain healthy hair, skin, and nails.
9	7	1.611	158.8	5-oxo-L-prolyl-glycine $C_7H_{10}N_2O_4$,186.165	α amino acids	Protect the kidneys from the detrimental effects of certain medications as well as the liver from the damaging effects of alcohol.
10	10	1.616	142.6	N-Methylglutamic acid $C_6H_{11}NO_4$, 161.156	Amino acids	It plays a role as a bacterial xenobiotic metabolite
11	8	1.619	241.4	Lauramidopropyl betaine $[C_{19}H_{39}N_2O_3]^+$, 343	Amino acids	It helps to keep the skin clean and dirt-free.
12	3	1.850	106.03	3,5-Dimethoxycinnamic acid, $C_{11}H_{12}O_4$,208.21	Carboxylic acid	Used as a herbicide.
13	11	1.938	179.5	Hippuric acid $C_9H_9NO_3$, 179.17	Carboxylic acid	It has antibacterial activity.
14	3	2.723	175.45	Dicamba $C_8H_6Cl_2O_3$, 221.03	Benzoic acid or chlorophenoxy herbicide	Primarily used as a herbicide.
15	11	2.903	142.3	Gabapentin Related Compound E. $C_9H_{14}O_4$,186.205	Anticonvulsants	Acts as an anticonvulsant, calcium channel blocker, environmental contaminant, and xenobiotic.
16	7	3.562	703.39	Cer[NS] d46:2 $C_{46}H_{89}NO_3$,703	Lipid	Helps to moisturize and strengthen the protective skin barrier and protects against skin pollution.
17	2	3.615	302.7	Safingol(IUPAC- 2-aminooctadecane-1,3-diol), $C_{18}H_{39}NO_2$,301.52	Amino diol	Involved in functions such as cell growth, differentiation, and apoptosis. Use for cancer treatment.
18	2	3.615	302.7	D-erythro-Dihydrosphingosine $C_{18}H_{39}NO_2$,301.51	Amino alcohols	It is used as a standard lipid in quantification and kinetics assay to determine serine palmitoyl transferase activity.
19	2	3.615	302.7	Dihydrosphingosine $C_{18}H_{39}NO_2$,301.51	Amino alcohols	Used for cardiovascular disease, cancer, and lung, liver, and kidney diseases.

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JCHR (2024) 14(3), 2982-2993 | ISSN:2251-6727

3.2. Common primary metabolites detected

Two common primary metabolites were detected from the tomato samples namely Fenofibric acid (in Sample No 1 and 2) and 5-L-Glutamyl-L-cysteine (in Sample No 2 and 5). Common primary metabolites detected in the tomato samples along with roles are litsed in Table 3.

Table 3. Common primary metabolites detected in the tomato samples along with their roles

Sl No	Sample No	Name of the compound	Roles
1	1, 2	Fenofibric acid	It is used in conjunction with a diet to treat high blood cholesterol and triglyceride levels in blood. It also prevents pancreatitis, which is caused by excessive blood triglycerides.
2	2, 5	5-L-Glutamyl-L-cysteine	It has an antioxidant properties that protect cells against oxidative injury.

3.3. Uncommon primary metabolites detected

Five uncommon primary metabolites were detected from the tomato samples namely Lignoceric acid, 3,5-Dimethoxycinnamic acid, Dicamba (in Sample No 3); 5-oxo-L-prolyl-glycine (in Sample No 7); and Biotin (in Sample No 9). Uncommon primary metabolites detected in the tomato samples along with roles are litsed in Table 4.

Table 4. Uncommon primary metabolites detected in the tomato samples along with their roles

SL. No	RT (min)	m/z value	Sample No.	Name of the compound, chemcial formula and molecular mass(g/mol)	Class	Roles in tomatoes/ humans
1	0.43 5	106.2	3	Lignoceric acid (or Tetracosanoic acid) $C_{24}H_{48}O_2$, 368.63	Long-chain fatty acids	It plays a role as a volatile oil component.
2	0.78 3	142.4	7	5-oxo-L-prolyl-glycine $C_7H_{10}N_2O_4$*186.165*, .	α amino acids	Prevent liver from the damaging effects of alcohol and kidneys from the negative side effects some medications.
3	1.59 9	243.8	9	Biotin, $C_{10}H_{16}N_2O_3S$ 244.31	Vitamin B7	Often used for hair loss treatment and also promotes healthy hair, skin, and nails.
4	1.85 0	106.0 3	3	3,5-Dimethoxycinnamic acid, $C_{11}H_{12}O_4$, 208.21	Carboxylic acid	It helps to control nutrient use and metabolism
5	2.72 3	175.4 5	3	Dicamba $C_8H_6Cl_2O_3$, 221.03	Benzoic acid or chlorophenoxy herbicide	Primarily used as a herbicide.

3.4. Secondary metabolites detected

A total of 24 secondary metabolites was detected in the tomato samples through LCMS analysis. Most of the metabolites were detected in Sample No 3, 4, 5, 6, and 11. Metabolite dected in Sample No 3 were Tetracycline, Thiabendazole and Tropine; Sample No 4 were 9-Amino-1,2,3,4-tetrahydroacridine, Thiabendazole and Bovoside; Sample No 5 were

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Deprenyl, Seneciphylline and 5-Fluorouracil; Sample No 6 were Harmine, Thiabendazole and Ecdysterone 22-O-benzoate; and in Sample No 11 were Isonicotinic acid, Bioguard and 5-Fluorouracil. Most of the comounds detected were from the benzimidazole group. Compounds detected in tomato samples has a wide array of properties like antimicrobial, antifungal, antitumor, antiplasmodial, antioxidant, Anti-tuberculosis, antihistamine, anti-malarial, antidiabetic, anticancer, antiviral, anti-HIV, anti-inflammatory, analgesic etc. Secondary metabolites detected in the tomato samples in increasing order of retention times in the chromatograms along with their names, chemical composition, molecular mass, class and roles are litsed in Table 5.

Table5. Secondary metabolites detected in the tomato samples in increasing order of retention times in the chromatograms along with their roles

Sl No	Sample No	RT (min)	m/z value	Name of the compound, chemical formula and molecular mass(g/mol)	Class	Roles
1	7	0.453	347.7	5'-inosinate or 5'-IMP Or Inosinic acid or inosine monophosphate $C_{10}H_{13}N_4O_8P$, 348.206	purine ribonucleoside monophosphates.	Widely used as a flavor enhancer
2	1	0.468	434.1	Apigenin 7-O-rutinoside. $C_{27}H_{30}O_{14}$, 578	8-O-methylated flavonoids	It causes autophagy in leukemia cells. It function as a metabolite and an anti-cancer agent.
3	8	0.473	199.9	Carbendazim $C_9H_9N_3O_2$,191.187	Benzimidazole	Used against various fungal diseases in agricultural products.
4	6	0.473	199.9	Harmine $C_{13}H_{12}N_2O$, 212.25	Alkaloids	Harmine has antimicrobial, antifungal, antitumor, cytotoxic, antiplasmodial, and antioxidant properties.
5	5	0.475	116.0	Deprenyl $C_{13}H_{17}N$,187.2808	phenethylamine and amphetamine	It is used to treat Parkinson's disease and serious depression.
6	9	0.499	125.9	Thymine $C_5H_6N_2O_2$, 126.1133	pyrimidines	Thymine has a higher resistance to photochemical mutations and makes the genetic code more durable.
7	4	0.500	200.1	9-Amino-1,2,3,4-tetrahydroacridine $C_{13}H_{14}N_2$, 198.26	Acridine	An allegedly effective drug for Alzheimer's disease.
8	2	0.537	125.8	cis-Cinnamic acid $C_9H_8O_2$,148.17	phenylpolypropanoids	Cinnamic acid derivatives are used to treat cancer, bacterial infections, diabetes, and neurological disorders.
9	11	0.750	125.6	Isonicotinic acid $C_6H_5NO_2$, 123.11	Pyridine carboxylic	Acts as an antibacterial drug for treating tuberculosis,

					acid	psoriasis, and arthritis.
10	3	0.750	410.9	Tetracycline $C_{22}H_{24}N_2O_8$,444.435	Tetracycline	It is an anticancer agent.
11	5	0.783	334.9	Seneciphylline $C_{18}H_{23}NO_5$, 333.37	Pyrrolizidine alkaloids	It is used to externally treat bruises and joint injuries with tinctures and ointments,
12	4	1.033	202.9	Thiabendazole $C_{10}H_7N_3S$, 201.25	Benzimidazole	Antifungal agent and antiparasitic agent
13	3	1.048	203.0	Thiabendazole $C_{10}H_7N_3S$, 201.25	Benzimidazole	Antifungal agent and antiparasitic agent
14	6	1.056	202.9	Thiabendazole $C_{10}H_7N_3S$, 201.25	Benzimidazole	Antifungal agent and antiparasitic agent
15	11	1.060	202.7	Bioguard. $C_{10}H_7N_3S$, 201.25	Benzimidazole	Anti-tuberculosis, antihistamine, antimicrobial, anti-malarial, antidiabetic, anticancer, antiviral, antifungal, aanti-HIV, annti-inflammatory, analgesic
16	9	1.067	202.7	Bovizole $C_{10}H_7N_3S$, 201.25	Benzimidazole	Anti-HIV antihistamine, antiviral, antidiabetic, anticancer, antimicrobial, anti-tuberculosis, antifungal, anti-inflammatory and antimalarial
17	10	1.070	202.9	Thiabendazole $C_{10}H_7N_3S$, 201.25	Benzimidazole	Antifungal agent and antiparasitic agent
18	5	1.176 ,	129.8	5-Fluorouracil $C_4H_3FN_2O_2$, 130.078	anti-metabolites (Chemotherapy drugs)	It is an antimetabolite drug widely used for the treatment of cancer.
19	1	1.249	214.9	Niflumic acid $C_{13}H_9F_3N_2O_2$, 282.21	pyridines	Niflumic acid is a drug used to relieve joint and muscular pain.
20	11	1.257	129.9	5-Fluorouracil $C_4H_3FN_2O_2$,130.078	anti-metabolites (Chemotherapy drugs)	It is an anti metabolite drug widely used for the treatment of cancer.
21	2	1.319	313.9	Norclozapine $C_{17}H_{17}ClN_4$, 312.8	Dibenzodiazepine	It combines an a typical antipsychotic effectiveness profile with the potential advantage of improved cognition, addressing one of Schizoprenia’s main problem.
22		1.594	562.7	Bovoside	Carbaldehyde	It is used to reduce pain and

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	4			$C_{31}H_{44}O_{9}$, 560.7		inflammation in conditions such as rheumatoid arthritis.
23	6	1.604	630.7	Ecdysterone 22-O-benzoate, $C_{34}H4_{8}O_{8}$, 584.7	Steroids	Ecdysterone is used to increase muscle mass and improve athletic performance.
24	3	1.605	143.01	Tropine $C_{8}H_{15}NO$ 141.21	Anticholinergics (alkaloids)	Helps restore normal heartbeat in cardiac arrest cases

3.5. Common secondary metabolites detected

Five common secondary metabolites were detected from the tomato samples namely Thiabendazole (in Sample No 3, 4, 6, 9,10, 11); Dihydrocodeine (in Sample No 5, 7, 8, 9, 10); Cis-Cinnamic acid (in Sample No 2, 4, 6); Harmol (in Sample No 9, 11); and Isonicotinic acid (in Sample No 4, 11). Common secondary metabolites detected in the tomato samples along with roles are litsed in Table 6.

Table 6. Common secondary metabolites detected in the tomato samples along with their roles

SlNo	**Name of the metabolites**	**Sample number**	**Roles in tomatoes/humans**
1	Thiabendazole	3,4,6,9, 10,11	Thiabendazole is a fungicide and parasiticide and is also a chelating agent that binds metals in cases of lead poisoning, mercury poisoning, or antimony poisoning. It is also used as a food additive, antifungal and for treating aspergillosis.
2	Dihydrocodeine	5,7,8,9,10	Dihydrocodeine is an opioid pain reliever. It is used to relieve moderate to severe pain, such as after an surgery or a traumatic injury.
3	Cis-Cinnamic acid	2,4,6	Cinnamic acid is extensively utilized as aflavorin grdient in foods and drinks, and for its fragrance in perfumes and cosmetics, it also used as a sunscreen agent as it reduces UV-A and UV-B and thus prevents skin damage.
4	Harmol	9,11	Traditional use of harmol as an, anti-inflammatory,analgesic, and anti-erythematous substance.
5	Isonicotinic acid	4,11	It is used to treat tuberculosis and HIV infection.

3.6. Uncommon secondary metabolites detected

Four uncommon secondary metabolites were detected from the tomato samples namely Apigenin 7-O-rutinoside(in Sample No 1); Harmine(in Sample No 6); 5'-inosinate (in Sample No 7); and Carbendazim (in Sample No 8). Uncommon secondary metabolites detected in the tomato samples along with roles are litsed in Table 7.

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Table7. Uncommon secondary metabolites detected in the tomato samples along with their roles

SlNo	RT (min)	m/z value	Sample No	Name of the constituent, chemical formula and molecular mass(g/mol)	Class	Roles
1	0.453	347.7	7	5'-inosinate or 5'-IMP or Inosinic acid or inosine monophosphate $C_{10}H_{13}N_4O_8P$,348.206	Purine ribonucleoside monophosphates	Widely used as a flavor enhancer
2	0.468	434.1	1	Apigenin 7-O-rutinoside $C_{27}H_{30}O_{14}$, 578	8-O-methylated flavonoids	It causes autophagy in leukemia cells. It acts as both a metabolite and an antineoplastic agent
3	0.473	199.9	8	Carbendazim $C_9H_9N_3O_2$,191.187	Benzimidazole	Used against various fungal diseases in agricultural products.
4	0.473	199.9	6	Harmine $C_{13}H_{12}N_2O$, 212.25	Alkaloids	Harmine has antimicrobial, antifungal, antitumor, cytotoxic, antiplasmodial and antioxidant properties.

4. Discussion

In the present study, a total of 19 primary metabolites, 2 common primary metabolites, 5 uncommon primary metabilotes, 24 secondary metabolites, 5 common secondary metabolites and 4 uncommon secondary metabolites were found in 11 samples of tomato genotype. Based on these result, the19 primary metabolites were divided into 9 classes, including 2 long-chain fatty acids, 6 amino acids, 4 carboxylic acids, 1 vitamins, 1 benzoic acid, 1 anticonvulsants, 1 lipid, 1 amino diol, 2 amino alcohol. Twenty four secondary metabolites were devided into 17 classes, including 1 purine, 1 8-O-methylated flavonoids, 7 benzimidazole, 1 alkaloid, 1 phenethylamine, 1 pyrimidine, 1 acridine, 1 phenylpolypropanoids, 1 pyridine carboxylic acid, 1 tetracycline, 1 pyrrolizidine, 2 anti-metabolites, 1 pyridines, 1 dibenzodiazepine, 1 carbaldehyde, 1 steroid, and 1 anticholinergics. The reports are in line with the findings of Moco *et. al.* (2006) who detected several compounds in tomato though LCMS analysis. In this present study, it was found that the detected primary metabolites and secondary metabolites of different tomato samples was found to have beneficial health effects. Amino acid has been reported as building blocks of proteins which required for all living things to make protein to perform many biological and chemical functions in various regions of our body, such as tissue growth and repair, role of enzymes, transportation of molecules, and food digestionetc (Bruce *et. al.*, 2002).In this study, it was found that the presence of amino alcohols (organic substances having both an alcohol and an amino group) may be used to create medicines, agrochemicals, surfactants and solvents etc. It was also reported that a variety of biological and therapeutic processes can use amino alcohols as ligands or catalysts(Francisco and Gregory 2006). It has been reported that carboxylic acidsare excellent for human health and they consists a sequence of fatty acids thataid in protecting the cell membrane and regulating the uptake of nutrients and metabolism likeomega-6 and omega-3 fatty acids(Silva *et. al.*, 2017). Lipidsare responsible for absorbing vitamins and producing hormones. It was found that lipidsacts as a source of storing energy that can be used during fasting (Luke *et. al*., 2021). It was reported that alkaloids are toxic and plants, herbivores and insects use it as a defence mechanism to protect themselves from the predators or ensure their survival in the environment. It was found that alkaloids are substances that required for gene code realization in the genotype and cell activity (Goyal,2013).

5. Conclusion

In this present study, it was observed that the detected primary metabolites and secondary metabolites of different tomato samples was found to have beneficial health effects. It was observed that the egg-shaped tomato genotype collected from Resubelpara (Sample No 3) contained two carcinogenic metabolites including five health-promoting metabolites. Accordingly, the 11 tomato genotypes have been arrranged in descending order based on their effects on human health as follows, Sample No-9 > sample No-5 > sample No-7 > sample No-4 > sample No-1 > sample No-8 > sample No-2 > sample No-6 > sample No-10 > sample No-11 > sample No-3.Based on the comparative study, it was concluded that the egg-shaped tomato genotype collected from Nongpoh (Sample No 9) contained twenty-one numbers of good metabolites with medicinal values and also it was observed that these metabolites was found very essential for human growth and development. As a result, the tomato genotype collected from Nongpoh (Sample No 9) was found to be the best among the other samples of tomato genotypes.

Acknowledgment

Authors are thankful to Cotton University, Guwahati and DBT, New Delhi for providing the support for research.

References

1. Alamgir A.N.M., 2017. Pharmacognostical Botany: Classification of medicinal and aromaticplants (MAPs), Botanical taxonomy, morphology, and anatomy of drug plants. In: Therapeutic Use of Medicinal Plants and Their Extracts: Progress in Drug Research Volume 1, pp 177-293.
2. Bruce A., Johnson A., Lewis J., Raff M., Roberts K., Walter P., 2002. Molecular Biology of the Cell. 4th edition. New York: Garland Science. Available from:https://www.ncbi.nlm.nih.gov/books/NBK21054/.
3. Diouf I.A., Derivot L., Bitton F., Pascual L., Causse M., 2018. Water deficit and salinity stress reveal many specific QTLs for plant growth and fruit quality traits in tomatoes. Front Plant Sci. 9,279.doi: 10.3389/fpls.2018.00279.
4. Francisco G., Gregory F., 2006. Amino Alcohols as Ligands for Nickel-Catalyzed Suzuki Reactions of Inactivated Alkyl Halides, Including Secondary Alkyl Chlorides, with Acrylboronic Acids. J Am. Chem. Soc. 128(16), 5360-5361. https://doi.org./10.1021/ja0613761.
5. Goyal S., 2013. Ecological role of alkaloids. Natural products. pp-149-179. https://doi.org./10.1007/978-3-642-22144-6_98.
6. Li Y., Wang H., Zhang Y., Martin C., 2018. Can the world's favorite fruit, tomato, provide an effective biosynthetic chassis for high-value metabolites? Plant Cell Rep. 37(10), 1443–1450. doi: 10.1007/s00299-018-2283-8.
7. Olsen L., Thum E., Rohner N., 2021. Lipid metabolism in adaptation to extreme nutritional challenges. Dev. Cell. 56(10),1417-1429. https://doi.org/10.1016/j.devcel.2021.02.024.
8. Martí R., Roselló S., Cebolla-Cornejo J., 2016. Tomato is a source of carotenoids and polyphenols targeted to cancer prevention. Cancers (Basel). 8(6), 58. doi:10.3390/cancers8060058.
9. Mazzoccoli G., Pazienza V.,Vinciguerra M., 2012. Clock genes and clock-controlled genes in the regulation of metabolic rhythms. Chronobiology International. 29(3), 227-251. https://doi.org/10.3109/07420528.2012.658127.
10. NBH (National Horticulture Board) 2023. Horticultural Crops 2019-20 (First Advance Estimates). National Horticulture Board, Ministry of Agriculture, Government of India. https://nhb.gov.in/StatisticsViewer.aspx?enc=FdhWKi1URA5yNAM+4mV5hQpJDviTxMmPkSfD97hsCEQ+Z+J1lzLFolcG88JyPsUQ.
11. Raiola A., Rigano M.M., Calafiore R., Frusciante L., Barone A., 2014. Enhancing the health-promoting effects of tomato fruit for biofortified food. Mediators Inflamm. Doi. 10.1155/2014/139873.
12. Silva F. P., Carla I. A., Marcelino G., Maiara Lopes Cardozo C., de Cassia Freitas K., de Cassia Avellaneda Guimaraes R., Pareira de Castro A., Aragao do Nascimento V., Aiko Hiane P., 2017. Fatty Acids Consumption: The Role Metabolic Aspects Involved in Obesity and Its Associated Disorders. Nutri. 9(10), 1158. doi: 10.3390/nu9101158.

Journal of Chemical Health Risks

www.jchr.org

JCHR (2024) 14(3), 2982-2993 | ISSN:2251-6727

13. Moco S., Bino R.J., Vorst O., Verhoeven H.A., de Groot J., van Beek T.A., de Vos C.H., 2006. A Liquid Chromatography-Mass Spectrometry-Based Metabolome Database for Tomato. Plant Physiol. 141(4), 1205-1218. doi: 10.1104/pp.106.078428
14. Tohge T., Fernie A.R., 2015. Metabolomics-inspired insight into developmental, environmental, and genetic aspects of tomato fruit chemical composition and quality. Plant Cell Physiol.56(9), 1681–1696.doi: 10.1093/pcp/ pcv093.
15. Viuda-Martos M., Sanchez-Zapata E., Sayas-Barberá E., Sendra E., Perez-Alvarez J.A., Fernandez-Lopez J., 2014. Tomato and tomato by products. Human health benefits of lycopene and its application to meat products: a review. Crit. Rev. Food Sci. Nutr.54(8), 1032–1049. doi: 10.1080/ 10408398.2011.623799.
16. Weinert C.H., Frederike S., Bj¨orn E., Elke P., Sabine E., Kulling I.S., 2021. The effect of potassium fertilization on the metabolite profile of tomato fruit (*Solanum lycopersicum* L.) www.elsevier.com/locate/plaphy.159,89-99. Doi.10.1016/j.plaphy.2020.12.010.