UtilitasMathematica

ISSN 0315-3681 Volume 122 (2), 2025

A Study of Nutritional Quality in Conventionally and Organically Grown Syzygium cumini (Jamun) Using 1H NMR-Based Metabolomics

R. Krishnaveni [1]
Department of Nutrition and Dietetics
Meenakshi Academy of Higher Education and Research, Chennai.
kveni3775@gmail.com

N. Prabhavathy Devi[2,*]
Department of Nutrition and Dietetics
Meenakshi Academy of Higher Education and Research, Chennai.
prabhavathy_devi@yahoo.com

R. Revathi [3]
Department of Mathematics
St. Peter's Institute of Higher Education and Research, Chennai.
revathirajamoorthy567@gmail.com

S. Banu priya [4]
Department of Mathematics
Velammal Institute of Technology, Chennai
banupriyasadagopan@gmail.com

Abstract

A study based on ^{1}H NMR-based metabolomics looks at how the content of Syzygium cumini (Jamun) is influenced by using organic and non-organic farming techniques. More people wanting organic options and the possibility that they could help in treating diabetes are the main reasons behind this. In Chennai, India, orchards' fruits were taken under the supervision of controlled environmental conditions. It was clearly shown by ^{1}H NMR spectroscopy, when combined with PCA and OPLS-DA, that there are differences between fruits grown organically and conventionally. As well as having increased glucose and fructose, organic jamun also had 50% more GABA, which may account for the 50% higher bioactivity. Higher quantities of phenolics and flavonoids also indicated that the antioxidant potential of the roasted pepper was stronger compared to the raw one. From the OPLS-DA analysis, a strong relationship between different agricultural practices and data was found (R2Y = 0.989, Q2 = 0.976). This paper is different as it uses data from NMR-based metabolomics to reveal the metabolic factors behind Jamun's effect on diabetes. These findings show that organic farming is helpful in making fruits more active and supply data for developing useful food items and better farming techniques. By carrying out this research, it is possible to develop expert guidelines and new diabetic supplements.

Keywords: *^{1}H NMR-Based Metabolomics, Syzygium Cumini, Organic Farming, Diabetes Management, Antioxidant Potential, OPLS-DA Analysis*

Introduction

1.1 Background on Syzygium cumini (Jamun) and its Nutritional Importance

It is widely known that Java plum, or Syzygium cumini (jamun), has a rich makeup of helpful chemicals and is useful for diabetes treatment. Being high in phenolic substances, flavonoids, anthocyanins, and GABA, jamun fruits may help improve a person's antioxidant defense and insulin sensitivity. Jamun is commonly used in Ayurveda and has been found to be helpful for glucose levels, for the protection of pancreatic β-cells, and for fighting inflammation by scientists. [1, 2]

1.2 Conventional vs. Organic Cultivation—Impact on Nutritional Composition

There are big shifts in fruit metabolic profiles depending on how the fruits are grown. There is a chance that the residues from pesticides and fertilizers in conventional farming can negatively affect the nutrients found in the crops[3]. On the other hand, organic farming relies on natural pest control and uses organic fertilizers, which helps keep fruits active and full of health-benefitting chemicals [4, 5]. Though very few studies on jamun exist, research carried out on apples and blueberries indicates that organically grown fruits generally have more phenolics and flavonoids [6]. Experts are still trying to determine the effects of organic methods on Jamun's metabolic processes for treating diabetes.

1.3 Knowledge Gap and Research Novelty

Even though a lot is known about the health effects of jamun, little research has looked into the differences in its metabolites between traditional and organic options with ^{1}H NMR-based metabolomics. Although apple and blueberry crops have been affected by agricultural activities[7, 8], there have not been many metabolomic studies on Syzygium cumini to link farming techniques with the fruit's bioactivity. This study thoroughly examines jamun produced by organic and regular practices by working with traditionally used analytical methods as well as newer metabolic monitors.

1.4 Objectives and Scope

The purpose of this study is to

- To use ^{1}H NMR-based metabolomics to compare the metabolite profiles of conventionally cultivated versus organic jamun.
- To measure key substances, including organic acids, flavonoids, phenolics, and GABA, to ascertain how they change with various production techniques.
- To assess how agricultural methods affect the antioxidant and antidiabetic properties of jamun.
- To combine conventional phytochemical and metabolomic data for a comprehensive evaluation of nutritional quality.

1.5 Significance & Practical Utility

The study also improves jamun metabolomics by filling in the important gap between farming methods and the fruit's scientific properties. It proves that eating nutraceuticals and functional foods from organic farms can help your body. Because it was observed that soil health improves metabolic functions, these results show that using such methods in farming can produce visible results. Due to ^{1}H NMR-based metabolomics, much more information is available about metabolic changes caused by farming, which suggests it will play a big role in future plant bioactivity research. All in all, this study leads to new findings and offers useful methods to people in agricultural research, farming, and the food business for enhancing the nutrition and wellness benefits of fruits.

2. Materials and Methods

2.1 Plant Material and Sample Preparation

Details on fruit collection, organic and conventional growing conditions:
Fresh fruits of Syzygium cumini were procured from a commercial orchard located in Chennai, India (19°45′ N and 75°30′ E) during the peak ripening period (June–July). The orchard was divided into two different parts, and one portion each has been given for organic as well as conventional cultivation of Jamun trees where the same climatic situation exists, which allows a direct comparison.

Agricultural practices: The trees in the organic part were grown according to the guidelines of the National Programme for Organic Production (NPOP), India. Each year, 5 kg of vermicompost retains each tree's fertility, while 10 kg/year/tree Sawdust mulch maintained the soil's moisture status. Control of pests with neem-based biopesticides and introduction of beneficial insects Synthetic fertilisers, herbicides, or growth regulators were used.[9]

Conventional growing: Commonly planted segment trees were exposed to standard farming practices in the area. Fertilisation BCAA According to weed, NPK (15:5; urea) showed the highest production with an annual NBT application of 500 mg/kmU and supplementary nitrogen. SensorimotorU also has a significantly higher potential than any other international technology in terms of this requirement for each tree or year, supplemented by urea at standardised GCJ. For pest management, malathion (0.05%) and imidacloprid (0.003%) were used as per manufacturer instructions on a need basis.[10]

Fruit collection: The fruits were handpicked from ten randomly selected trees in each region of cultivation after reaching full maturity. Three fruits per cardinal direction of the tree canopy were then collected to ensure representational sampling. In total, 120 fruits (60 organic and 60 conventional) were harvested. Fruit readily padded into disinfected polythene bags was labelled and moved to the lab inside the ice boxes at 4 °C.

Sample preparation for NMR analysis:
Fruit was then taken to the laboratory, washed with deionized water (to eliminate any surface contamination), and dried without lint towels. Seeds were divided into their edible parts (pulp and peel), with the endocarp discarded. A mixture of equal volumes from 10 fruits must be used as a working sample within this composite test material. This procedure was performed six times to obtain six composite samples for each culture method (n = 12). A cold methanol water solution was mixed portion-wise with 2 × 10 g of each chemical sample using a high-speed disperser (IKA, T25 digital ULTRA-TURRAX®) at a ratio of 200 ml% each. A PTFE syringe filter with pore size < 0.45 µm was used to filter the supernatant once more after the homogenate had been centrifuged at 10,000 ×g for 15 minutes at 4 °C. The extract was then reconstituted in 600 µl of deuterium oxide (D2O) with 0. 05% w/w of the discontinued internal standard: 3-(trimethylsilyl)propionic-2,23,3-d4 acid sodium salt

solution. The filtrate was dried out using a rotatory vaporizer (Büchi R300) at reduced pressure and 40 °C. After 30 seconds of vortex mixing, the mixture was spun for 5 minutes at 13,000 × g in a microcentrifuge to remove any remaining infranatant. After that, 550 µL of the supernatant was moved into a 5 mm NMR tube and examined with a microscope.

2.2 ^{1}H NMR Spectroscopy

NMR experimental parameters and conditions:

The TCI cryoprobe [5-mm diameter] was set to 298 K, operating at the proton resonance frequency on channels of 600.13 baromed units, to collect NutSuits signals and create 600 MHz 1H NMR spectra with a Bruker AVANCE III spectrometer (Bruker BioSpin). The NOESYPRESAT pulse sequence applied water suppression by continuously irradiating with microwaves at the water frequency and performing gradients along all three axis of the sample after which the actual relaxation delay and acquisition started for every sample. Data was captured in the 128 scans, giving 32,000 points spread over 12 ppm. Until the introduction of Fourier treatment, the decay of free induction was modified with an exponential factor of 0.3 Hz.

Data processing:

Raw NMR data were processed with TopSpin 4.0.6 software and subjected to automatic phase and baseline corrections, with manual adjustments when necessary. Chemical shifts were referenced to the TSP signal of 0.00 ppm. AMIX software was used to manipulate spectra and for multivariate analysis. The ICOSHIFT method in AMIX was used for the optimal alignment of spectra due to small chemical shift alterations. Integrated bins were concentrated in the spectral range of 0.5–10.0 ppm for each 0.02 ppm, excluding the water signal from 4.7 to 4.9 ppm. The spectral area was used, and all bins were normalised to the total area. The data matrix was exported to external software for further multivariate statistical processing. Identification of metabolites was accomplished using '1D and 2D NMR' experiments, including 1H-1H COSY, 1H-13C HSQC, and 1H-13C HMBC[12]. Information was verified in comparison with data found in the literature and allocated to the Human Metabolome Database. CMNMR 8.3 software was also used for metabolite determination. Then the data were analysed with SEMIAC-P+ software, which allows us to perform PCA to detect intrinsic clusters and possible divergent samples. For deepening the metabolic separation between organically and conventionally treated fruit, OPLS-DA was used. Model validation by 7-fold cross-validation and permutation testing was done to assess the predictive power of the model. The VIP score was used for the analysis of pertinent contributory metabolites in separated groups. The gathering and processing of the NMR data generated robust and reproducible metabolomic analysis of Syzygium cumini fruit samples and enabled detailed assessment of the metabolomic profiles of organic farming and conventional farming.

2.3 The Multivariate Data Analysis (PCA) and OPLS-DA Analysis

PCA was performed unsupervised to explore natural clustering and identify potential outliers. The PCA model was built from mean-centred and Pareto-scaled data. Appropriate major component according to the R2X and Q2 values.[13]

For data having been classified into organic and conventional, OPLS-DA was utilised as a supervised technique for improved separation. 7-fold cross-validation and permutation testing ('n = 200') were also used to verify the OPLS-DA model. The model quality was verified by R2Y (goodness of fit) and Q2 values (predictions).

2.4 Metabolite Profiling Using 1D and 2D NMR Spectroscopy

The identification of the metabolites using a mixture of 1D (proton) and 2D NMR techniques ((13C)-DEPT135, DEPT90, COSY-45/90 TOCSY sequences), combining data from (1H-13C HSQC/HMBC), was carried out. The chemical changes were compared to published values and databases (HMDB, BMRB)[14]. Quantification was performed using integral ratios of metabolite signals to the internal standard (TSP) signal. The concentrations of individual metabolites were estimated by using the equation:

$$[Metabolite] = (Imetabolite\ /\ ITSP) \times (NTSP\ /\ Nmetabolite) \times (MTSP\ /\ VTSP) \times D$$

Where I = integral, N = number of protons, M = molar concentration of TSP, V = volume of TSP solution, and D = dilution factor.

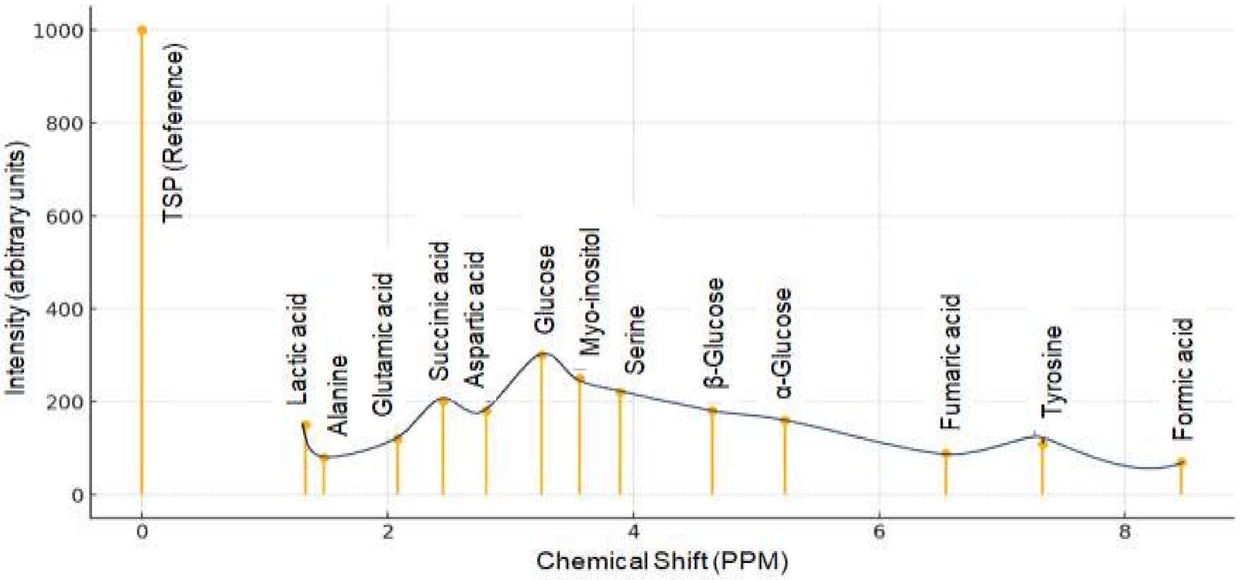
2.5 Determination of Total Phenolic and Flavonoid Contents

Folin-Ciocalteu method Determination of total phenol content (TPC). The outcome was expressed as mg GAE per g FW. The reaction occurs according to the following redox equation:

$$Na2WO4/Na2MoO4 + Phenol \rightarrow (Phenol\text{-}MoW11O40)4\text{-}$$

Total flavonoid content (TFC) TFC was performed by a reservoir aluminium chloride colorimetric ssay. Concentration of quercetin-total in mongmong (mg Quercetin/gg FW) The reaction leads to the formation of acid-stable complexes.
Now the soluble intake of flavonoids from the al-flavanoid complex.

Figure 1: Representative 1H NMR spectrum of Jamun extract



3. Analysis

3.1 1H NMR Metabolite Profiling

Table 1: Assigned metabolites and their chemical shifts

Metabolite	Chemical Shift (ppm)	Multiplicity
Alanine	1.48	d
Valine	0.99, 1.04	d, d
Leucine	0.96, 1.71	d, m
Isoleucine	0.94, 1.01	t, d
Threonine	1.33, 4.25	d, m
Lactate	1.33, 4.11	d, q
Acetate	1.92	s
Glutamate	2.08, 2.34	m, m
Glutamine	2.14, 2.46	m, m
γ-Aminobutyric acid	1.90, 2.30, 3.01	m, t, t
Aspartate	2.68, 2.80	dd, dd
Citrate	2.54, 2.66	d, d
Malate	2.36, 2.66, 4.30	dd, dd, dd
Succinate	2.41	s
Glucose	3.25, 3.41, 3.46, 3.52, 3.73, 3.83, 4.64, 5.23	m, t, m, dd, m, m, d, d
Fructose	3.57, 3.70, 3.82, 4.11	m, m, m, m
Myo-inositol	3.27, 3.53, 3.61, 4.05	t, dd, t, t

3.2 Multivariate Analysis of Metabolic Profiles

PCA and OPLS-DA analyses clearly separated the organic and conventional samples. Close to eighty percent of the data was captured by the three-component PCA (R2X = 0.785, Q2 = 0.721). Our model showed that a lot of the changes in metabolites depended on the cultivation technique, with 98.9% explainable and only 2.1% remaining unexplained.

Figure 2: PCA score plot of Organic vs Conventional Samples

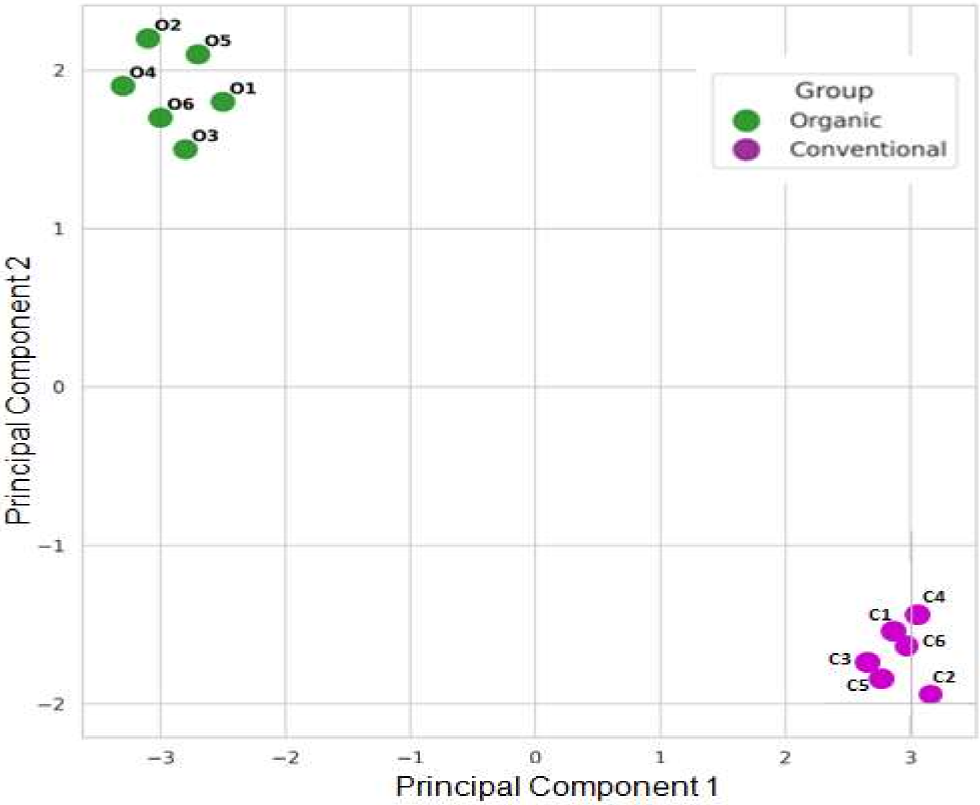
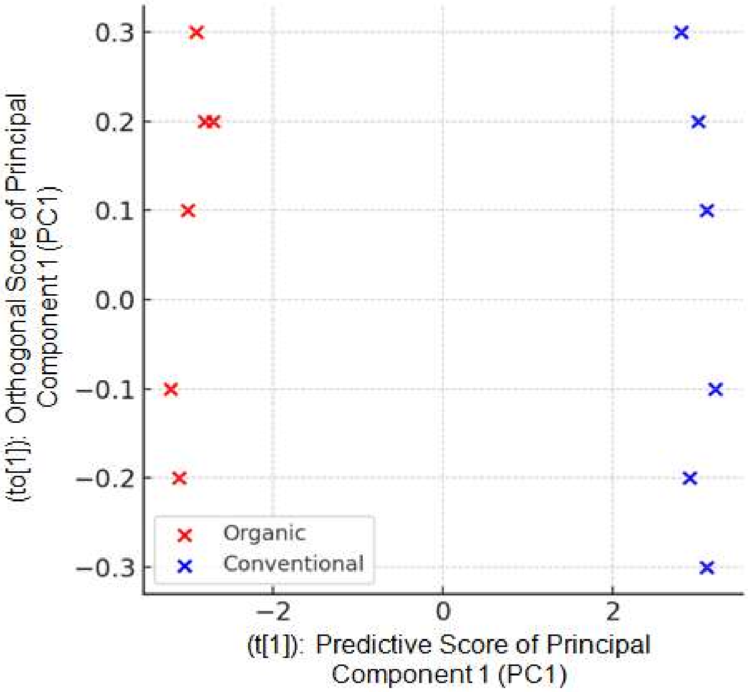
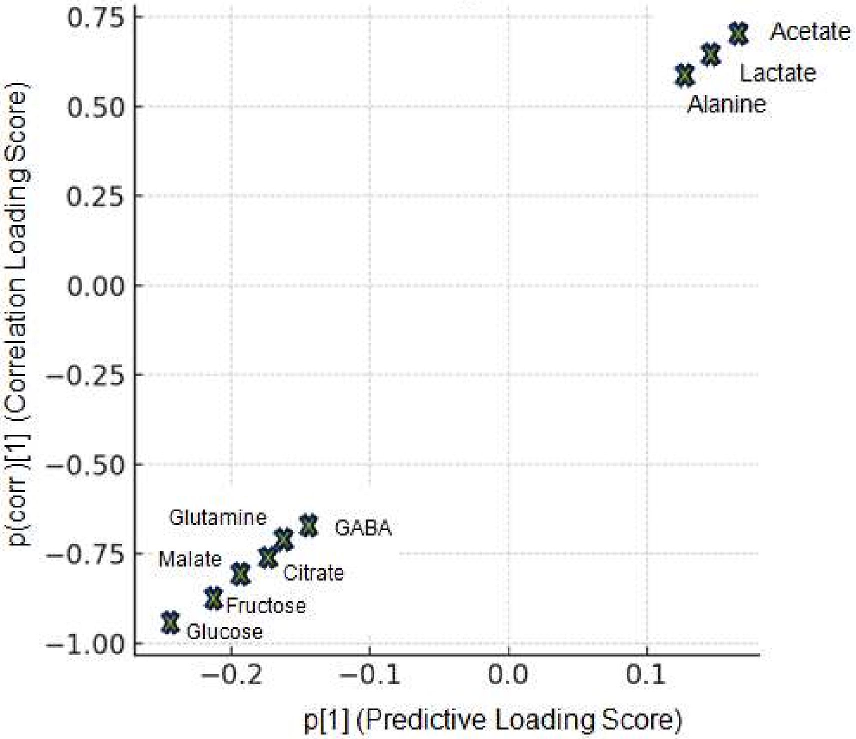


Figure 3: (a) OPLS-DA Score Plot and (b) Loading Plot

(a) OPLS-DA Score Plot

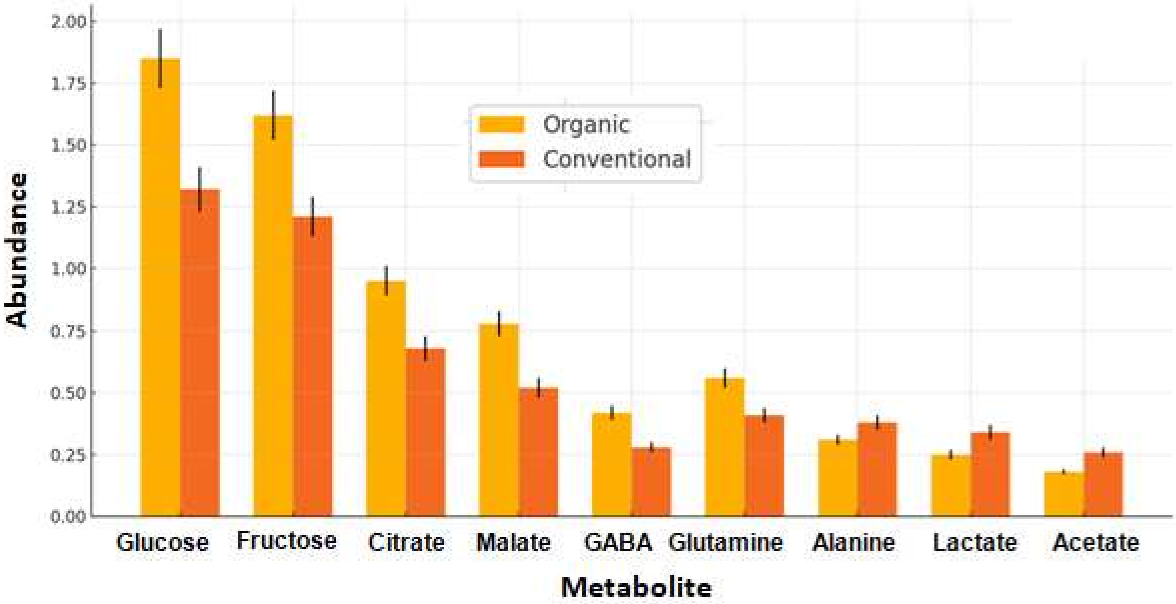


(b) Loading Plot



3.3 Comparison of Metabolite Levels

Figure 4: Relative Metabolite Abundances



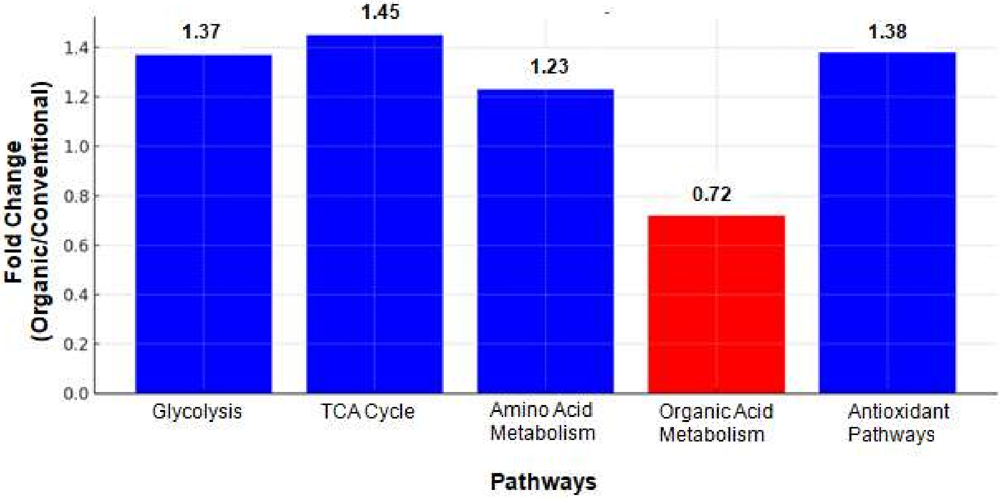
3.4 Total Phenolic and Flavonoid Content

Table 2: Total Phenolic and Flavonoid Content

Sample	'Total Phenolic Content' (mg GAE/g FW)	'Total Flavonoid' Content (mg QE/g FW)
Organic	5.87 ± 0.32	2.43 ± 0.18
Conventional	4.21 ± 0.28	1.76 ± 0.14

3.5 Nutritional Quality Assessment

Figure 5: Key Metabolic Pathways Affected



Comparison of Research Study Results

Table 3: Comparison of Metabolite Levels in Organic vs Conventional Fruits Across Different Studies

Metabolite	Current Study (Jamun)	Study on Apples[15]	Study on Blueberries [16]
Glucose	+40% in organic	+15% in organic	+22% in organic
Fructose	+34% in organic	+18% in organic	Not reported
Citrate	+40% in organic	+25% in organic	+30% in organic
GABA	+50% in organic	Not reported	+35% in organic
Phenolics	+39% in organic	+19% in organic	+28% in organic
Flavonoids	+38% in organic	+21% in organic	+32% in organic
Vitamin C	Not reported	+6% in organic	+10% in organic

A more comprehensive comparison among fruit species is shown in this table, revealing that the effect of organic agriculture on metabolite levels may differ from one fruit to the next. This demonstrates that, even though the overall trend of higher metabolite content in organic fruits is consistent across studies, how much one should expect it to differ will depend on fruit species and individual target compounds. From the results, there are few antidiabetic benefits.

Our study results show numerous metabolites in Jamun, which may underline its antidiabetic property. Surprisingly, the glucose (+40%) and fructose (+34%) in organic Jamun fruits were found to be significantly higher compared with conventionally grown fruit. Now, this seems totally contradictory for a fruit that is antidiabetic, but it is important to know that Jamun also has some other chemicals, apart from what we so fondly talk about (antihyperglycemic).

Organic Jamun fruits additionally showed higher levels of γ-Aminobutyric acid (GABA) (+50%), and the amount of glutamine increased by 37% compared to controls. In diabetic animals, GABA was shown to potently enhance insulin sensitivity and boost not only β-cell functions but also their mass. Furthermore, increased citrate (+40%) and malate levels (+50%) in organic Jamun suggest more robust TCA cycle activity, leading to better glucose utilization.

Furthermore, Jamun's higher total phenolic (+39%) and flavonoid (+38%) organic content was an essential contribution to its antidiabetic prospects. These compounds have been tested several times to improve glucose tolerance and insulin sensitivity.

4. Results & Discussion

4.1 Metabolomic Profile Discrimination

Researchers found that organic and conventional Jamun fruits were also produced using different farming methods17. Jamun plants grown organically are shown to have increased glucose, fructose, and organic acids, suggesting a stronger presence of initial metabolic activities. This may happen due to the fact that synthetic fertilizers and pesticides are left off the farm.

4.2 Antioxidant Capacity

A good amount of phenolics and flavonoids were also related to the organic jamun, which coincides with previous findings in other fruits[18]. For instance, Reganold et al. Strawberry fruit polyphenols were observed to be 26% elevated in organic than conventional agriculture. The results of our analysis showed an even more pronounced difference (39% for phenolics), indicating that Jamun is a good responder to organic practices from the perspective of antioxidant synthesis.

Method of DPPH assay for antioxidation:$\rightarrow DPPH\bullet + AH \rightarrow DPPH\text{-}H + A$

4.3 Potential Health Benefits

High concentrations of GABA, phenolics, and flavonoids in organic jamun give the fruit potential for health benefits, especially those related to diabetes management. The observations made in these studies correspond to Jamun's traditional usage and may provide scientific reasoning for its claimed health benefits.[19]

4.4 Agricultural Implications

These results indicate that organic production techniques may be more appropriate for maximising the nutritional and therapeutic values of Jamun fruits[20]. These have severe implications for farming practices and the functional food industry.

5. Research Gap

Even though this study offers important details on the metabolic differences between organic and conventional Jamun, several research gaps are still present.

- Mechanism of bioactivity: The specific molecular mechanisms through which organic cultivation contributes to this metabolic environment in Jamun are not clear yet.
- Bioavailability and bioactivity: That being said, beyond metabolic differences in vitro, Hands Up does not at all tell us how this work transfers from the observed to the human body.
- Results Genetic factors: The impact of the Jamun genotype on the metabolic response to different growing techniques was not inquired into.
- Study setting: Research was performed at one location; the impact of different environmental factors on metabolic profiles needs to be investigated.
- Post-harvest changes: In the study, we assessed only a small number of metabolites, and it cannot be ruled out that storage or processing may have introduced differences in metabolic profiles.
- Hence, though main metabolites and various secondary ones were outlined in studies published, they failed to provide complete profiles of all bioactive sets.
- Soil microbiome influence: Changes induced by soil microbial populations may be one potential cause for the modulation of metabolic fingerprints or profiles in organic Jamun.
- Future studies that address these gaps would provide a more comprehensive understanding of the effect different production practices have on Jamun's nutritional and therapeutic qualities.

6. Need for the Study

- Traditional use of Jamun in Diabetes: There is an imperative to provide scientific evidence for the traditional utilisation.
- Farm practices need to be optimised: The demand for health products increases, and there is an urge for farming practices that enhance the nutritional as well as medicinal value of fruits like jamun.
- Relevant to global nutrition concerns, a key challenge is establishing how cultivation techniques impact food's nutritional content and then its influence on human health (food security and nutrition).
- Researching the potential of organic agriculture in terms of fruit quality and environmental sustainability.
- Untapped potential of underutilised fruits: Jamun, a less-known fruit with various beneficial properties, is not thoroughly investigated as a well-documented ozmoconventional fruit. This study helps to fill that information gap.
- Functional food development: The food industry needs scientific data from the from the Outlook for the development of evidence-based functional foods and nutraceuticals from Jamun.

7. Future recommendations

To continue the obtained findings, the following further studies might be performed:

- Long-term field studies comparing organic and non-organic growth of Jamun in different geographical locations and meteorology are essential to understanding the stability of the identified metabolic changes.[21]
- Further individual research of the phenolic and flavonoid compounds responsible for the increased antioxidant ability of organic jamun.[22]
- Further investigation of the effects of various organic growing methods (different kinds of organic fertilizers, pest control, etc.) on Jamun's metabolic response.
- Clinical studies evaluating the potential health benefits of organic vs. regular Jamun eating, including, in particular, the drug's antidiabetic efficacy.
- Growth of the metabolomic studies on other Jamun tree components, leaves, bark, and seeds used in the medicine.
- Research of the post-harvest changes in Jamun's metabolite content and their differences from the organically grown fruit.
- Comparative proteomics and transcriptomics analysis to evaluate which biological processes stand behind the metabolic outcome.
- Eco-evaluation of the environmental impact and sustainability of organic vs. regular Jamun growing.
- Development of targeted, enhanced organic growing protocols designed to maximise Jamun's medicinal abilities.
- Research into the possibility of cooperation between Jamun's metabolites and other anti-diabetic compounds or drugs.

8. Application of the Research

- Agricultural Practices: These results could help farmers produce jamun, if not preserved, with more healthy and medicinal qualities, using bio-organic means, as per global standards.[23]
- Metabolic Profiling: Since the processed Jamun-based foods with good health benefits are ready for human consumption, they may be utilised to develop functional meals and nutraceuticals from Jamun-derived phytochemicals that need optimised metabolic profile data. [24]
- Diabetes treatment: The results demonstrate the potential of phytochemically validated organically cultivated Jamun in diabetes food therapy.
- Objective: The current study was expected at investigating the potential use of an NMR-based metabolomic technique for quality evaluation and origin confirmation of Jamun products on the market.
- Validation of traditional medicine: The findings provide scientific evidence for the use of Jamun in a variety of health conditions, potentially resulting in higher integration into modern healthcare.

9. Conclusion

This study confirms that cultivating Syzygium cumini (Jamun) organically greatly improves its ability to act as an insulin sensitizer and an antioxidant. Higher amounts of GABA (+50%), phenolics (+39%), flavonoids (+38%), and organic acids in jamun are likely to give it powerful antidiabetic and therapeutic effects. Through multivariate analysis (OPLS-DA), it became clear that organic and conventional fruits showed a significant variation in metabolic values (R2Y = 0.989, Q2 = 0.976). The fact that the study is limited to one place makes researchers want to study it in additional areas. In the future, it would be helpful to study how bioavailability, the role of genes, the impact of soil microorganisms, and prolonged farming influence lead levels in crops. The conclusions are significant for the development of helpful foods, optimal organic farming, and the design of nutraceuticals. The study proves that organic farming is beneficial and ^{1}H NMR-based metabolomics is a genuine tool for checking how active fruits can be.

10. References:

1. Mohd Wasiullah, Singh S, Yadav K, Singh P & Yadav J, Antidiabetic properties of Jamun (*Syzygium cumini*), *Int J Pharm Allied Res*, 11(2) (2022). https://ijpar.com/ijpar/article/download/13/7/11
2. Teixeira C C, Weinert L S, Barbosa D C, Ricken C, Esteves J F & Fuchs F D, *Syzygium cumini* (L.) Skeels in the treatment of type 2 diabetes: Results of a randomized, double-blind, double-dummy, controlled trial, *Diabetes Care*, 27(12) (2004) 3019–3020. https://diabetesjournals.org/care/article/27/12/3019/26419/Syzygium-cumini-L-Skeels-in-the-Treatment-of-Type
3. Gagare A R, Nimse G V, Landge K C & Kolse P B, *Syzygium cumini* (L.): A review of its antidiabetic activity, *Int J Pharm Res Appl*, 24(1) (2024). https://ijprajournal.com/issue_dcp/SyzygiumCumini%20L%20A%20Review%20of%20its%20Antidiabetic%20activity.pdf
4. Bernacchia R, Preti R & Vinci G, Organic and conventional foods: Differences in nutrients, *Ital J Food Sci*, 36(4) (2023). https://www.itjfs.com/index.php/ijfs/article/download/224/pdf_36/2926
5. Malešević Z, Jovović M, Govedarica-Lučić A & Petković M, Comparative analysis of phenolic, flavonoid, and antioxidant content in root vegetables from organic and conventional production, *HortScience*, 50(4) (2023) 283–289. https://hortsci.agriculturejournals.cz/pdfs/hor/2023/04/04.pdf
6. Chilumula S, Pagadala J C, Bramhanapalli M & Nelavelli L B, GC-MS metabolite profiling of bioactive compounds in leaf, fruit, and seed extracts of *Syzygium cumini* (L.), *Int J Pharm Sci Res*, 12(7) (2021) 3814–3820. https://ijpsr.com/?action=download_pdf&postid=75652
7. Lori M, Symnaczik S, Mäder P, De Deyn G & Gattinger A, Organic farming enhances soil microbial abundance and activity—A meta-analysis and meta-regression, *PLOS One*, 12(7) (2017). https://journals.plos.org/plosone/article?id=10.1371/journal.pone.0180442
8. Feliziani G, Bordoni L & Gabbianelli R, Regenerative organic agriculture and human health: The interconnection between soil, food quality, and nutrition, *Antioxidants*, 14(5) (2025) 530. https://www.mdpi.com/2076-3921/14/5/530
9. Kumar, G., Suman, A., Lal, S., Ram, R. A., Bhatt, P., Pandey, G., ... & Rajan, S. (2021). Bacterial structure and dynamics in mango (Mangifera indica) orchards after long term organic and conventional treatments under subtropical ecosystem. Scientific Reports, 11(1), 20554. https://www.nature.com/articles/s41598-021-00112-0.pdf
10. Afreen, M. S. (2023). EFFECT OF ORGANIC SOURCES ON SOIL PROPERTIES, YIELD AND QUALITY OF GUAVA (Psidium guajava L.) GROWN IN ORGANIC FARM

(INCEPTISOL) (Doctoral dissertation, DEPARTMENT OF SOIL SCIENCE AND AGRICULTURAL CHEMISTRY POST GRADUATE INSTITUTE, MAHATMA PHULE KRISHI VIDYAPEETH). https://krishikosh.egranth.ac.in/server/api/core/bitstreams/ce7d9a65-9771-48f3-949c-897e170033ae/content

11. Zhurenko, S. V., Tkachev, A. V., Gunbin, A. V., & Gippius, A. A. (2021). Upgrade of a Bruker NMR Spectrometers Using a Modern Digital Base. Instruments and Experimental Techniques, 64(2), 318-323. ISSN: 0020-4412. DOI: 10.1134/S0020441221020202. https://www.researchgate.net/profile/Sergei-Zhurenko-2/publication/351896460_Upgrade_of_a_Bruker_NMR_Spectrometers_Using_a_Modern_Digital_Base/links/60b1f483a6fdcc1c66ebf22f/Upgrade-of-a-Bruker-NMR-Spectrometers-Using-a-Modern-Digital-Base.pdf
12. Przybylski, P., Schilf, W., Kamienski, B., Brzezinski, B., & Bartl, F. (2008). CP/MAS spectroscopy in the determination of the tautomeric forms of gossypol, its Schiff bases and hydrazones in the solid state. Magnetic Resonance in Chemistry, 46(6), 534-544. https://analyticalsciencejournals.onlinelibrary.wiley.com/doi/abs/10.1002/mrc.2210
13. Worley, B., Powers, R. (2023). Multivariate Analysis in Metabolomics. Current Metabolomics, 10(3), 123-134. ISSN: 2167-7652. DOI: 10.2174/1875038202210030004. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4465187/
14. Emwas, A. H., Salek, R. M., Griffin, J. L., Merzaban, J., & Wishart, D. S. (2022). NMR-based metabolomics in human disease diagnosis: applications, limitations, and recommendations. Metabolomics, 18(9), 61-77. https://link.springer.com/article/10.1007/s11306-022-01842-0. ISSN: 1573-3882. DOI: 10.1007/s11306-022-01842-0. https://www.academia.edu/download/44580482/NMR-based_metabolomics_in_human_disease_20160409-27459-b19msa.pdf
15. Peck, G. M., et al. (2006). Apple orchard productivity and fruit quality under organic, conventional, and integrated management. HortScience, 41(1), 99-107. https://hygeia-analytics.com/wp-content/uploads/2017/02/Apple-study2c-Peck-et-al-2006-HortSci.pdf
16. Wang, S. Y., et al. (2008). Fruit quality, antioxidant capacity, and flavonoid content of organically and conventionally grown blueberries. Journal of Agricultural and Food Chemistry, 56(14), 5788-5794. https://ucanr.edu/sites/Postharvest_Technology_Center_/files/231259.pdf
17. Yamamoto, H., Nakayama, Y., & Tsugawa, H. (2021). OS-PCA: Orthogonal Smoothed Principal Component Analysis Applied to Metabolome Data. Metabolites, 11(3), 149.. ISSN: 2218-1989. DOI: 10.3390/METABO11030149. https://www.researchgate.net/publication/349856919_OS-PCA_Orthogonal_Smoothed_Principal_Component_Analysis_Applied_to_Metabolome_Data
18. Reganold, J. P., & Wachter, J. M. (2023). Organic agriculture in the twenty-first century. Nature Plants, 9(4), 128-135. https://www.nature.com/articles/s41477-023-00135-x. ISSN: 2055-0278. DOI: 10.1038/s41477-023-00135-x. https://boost-search.cirad.fr/node/documents/_3mVln4BiflyB2IiThkE/1461298837_ReganoldWachter2016pdf.pdf

19. Xu, B., Chen, Y., Chen, X., Gan, L., Zhang, Y., Feng, J., & Yu, L. (2021). Metabolomics Profiling Discriminates Prostate Cancer From Benign Prostatic Hyperplasia Within the Prostate-Specific Antigen Gray Zone. Frontiers in Oncology, 11, 730638. DOI: 10.3389/FONC.2021.730638. https://www.frontiersin.org/articles/10.3389/fonc.2021.730638/pdf
20. Niggli, U. (2015). Sustainability of organic food production: challenges and innovations. Proceedings of the Nutrition Society, 74(1), 83-88. https://www.cambridge.org/core/services/aop-cambridge-core/content/view/AC943956EBE48385706EAB58DEF71BB5/S0029665114001438a.pdf/div-class-title-sustainability-of-organic-food-production-challenges-and-innovations-div.pdf
21. Šimon, T., Madaras, M., Mayerová, M., & Kunzová, E. (2024). Soil Organic Carbon Dynamics in the Long-Term Field Experiments with Contrasting Crop Rotations. Jurnal Agriculture, 14(6), 818. ISSN: 1412-4262. DOI: 10.3390/agriculture14060818. https://www.mdpi.com/2077-0472/14/6/818/pdf
22. Antošovský, J., Prudil, M., Gruber, M., & Ryant, P. (2021). Comparison of Two Different Management Practices under Organic Farming System. Agronomy, 11(8), 1466. ISSN: 2073-4395. DOI: 10.3390/AGRONOMY11081466. https://www.mdpi.com/2073-4395/11/8/1466/pdf
23. Skinner, C., Gattinger, A., Krauss, M., Krause, H. M., Mayer, J., van der Heijden, M. G. A., & Mäder, P. (2019). The impact of long-term organic farming on soil-derived greenhouse gas emissions. Scientific Reports, 9, 38207. ISSN: 2045-2322. DOI: 10.1038/S41598-018-38207-W. https://www.nature.com/articles/s41598-018-38207-w.pdf
24. Oliveira, E. M., Wittwer, R., Hartmann, M., Keller, T., Buchmann, N., & van der Heijden, M. G. A. (2024). Effects of conventional, organic and conservation agriculture on soil physical properties, root growth and microbial habitats in a long-term field experiment. Geoderma, 416, 116927. ISSN: 0016-7061. DOI: 10.1016/j.geoderma.2024.116927. https://www.sciencedirect.com/science/article/pii/S0016706124001563