Data Article

Data on changes in the fatty acid composition during fruit development and ripening of three mango cultivars (Alphonso, Pairi and Kent) varying in lactone content

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ABSTRACT

Data in this article presents fatty acid composition of three mango cultivars: Alphonso, Pairi and Kent through fruit development and ripening. Change in the ω-6 and ω-3 fatty acids level during mango fruit development and ripening is depicted. Also, data on aroma volatile ‘lactones’ composition from pulp and skin tissues of these cultivars at their ripe stage, respectively is provided. Statistical data is also shown, which correlates modulation in lactone content with that of fatty acid composition and content during fruit development and ripening in all the three mango cultivars.

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Specifications Table

| Subject area       | Biology, Chemistry |
|--------------------|--------------------|
| More specific sub- | Fatty acid and lactone composition of mango fruit |
| ject area          | Table, graph, figure |

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How data was acquired
GC–MS: 7890B GC system Agilent Technologies coupled with Agilent 5977A MSD (Agilent technologies*, CA, U.S.A.)

Data format
Analyzed

Experimental factors
Pulp and skin tissues from fruits of three cultivars collected at various fruit development and ripening stages, tissue was snap frozen and stored at −80 °C.

Experimental features
Fatty acid methyl esters (FAMEs) were synthesized by transesterification and aroma volatiles were extracted in dichloromethane, identified and quantified by GC–MS

Data source location
Plant Molecular Biology Unit, Division of Biochemical Sciences, CSIR-National Chemical Laboratory, Pune 411008, (M. S.) India.

Data accessibility
Data is provided within this article

Value of the data
- Data from this research highlights the increase in the unsaturated fatty acid content in pulp and skin of mango with ripening and making ripened fruits more nutritious.
- Data signifies nutritionally important ω-3 fatty acid (α-linolenic acid) rich nature of mango skin for utilization by various industries.
- Investigated data from this article reveals probable fatty acid precursors for biosynthesis of lactones, which is useful to the researchers working in the area of flavor biochemistry.

1. Data

A total of 17 different fatty acids were identified and quantified from the pulp and the skin (Tables 1, 2 and Figs. 1, 2) at various stages of mango fruit development and ripening from three cultivars viz. Alphonso, Pairi and Kent with high, low and no lactone content at ripe stage, respectively (Table 3). Present analysis revealed the ratio of ω6/ω3 ≤ 1 at ripe stage (Table 4) suggesting ripened mango fruits as perfect source of essential fatty acids [1].

In the present data, a decrease in C16:0/C16:1 ratio and increase in the fatty acid derived flavor compounds, lactones, were evinced [2,3] from Alphonso pulp and skin and Pairi pulp (Table 4). Similarly, palmitoleic acid, 11-octadecenoic acid and 9, 15- octadecadienoic acid showed strong correlations with total lactone content from ripe pulp and skin of three cultivars (Table 5), whereas various unsaturated fatty acids showed strong correlation with content of all the eight lactones individually (Table 6).

2. Experimental design, materials and methods

2.1. Plant material

Fruits of cv. Alphonso and cv. Pairi were collected from the Mango Research Sub Centre, Deogad (16° 31’ N, 73° 20’ E) and of cv. Kent from the Regional Fruit Research Station, Vengurle (15° 51’ N, 73° 39’ E), both affiliated to Dr. Balasaheb Sawant Konkan Agricultural University, Dapoli, Maharashtra, India. Developing stages of all the three mango cultivars were collected at 15, 30 and 60 days after pollination (DAP) and at mature raw stage (90 DAP for cvs. Alphonso and Pairi, 110 DAP for cv. Kent). Fruits at these developing stages were harvested, pulp (mesocarp) and skin (exocarp) separated immediately, snap frozen in liquid nitrogen and stored at −80 °C until further use. A set of 12 fruits each for all the three cultivars were additionally harvested at their respective mature raw stage and kept in the hay containing boxes at ambient temperature for ripening. Three cultivars showed variation in the ripening duration, hence four ripening stages as table green, mid ripe, ripe and over ripe based on the skin color, aroma and fruit softness (each stage is represented by days after harvest i.e. DAH for cv. Alphonso as 5, 10, 15 and 20 days; for cv. Pairi as 4, 6, 8 and 10 days and for cv. Kent as...
Table 1
Fatty acid composition of pulp.
Fatty acid composition (μg g⁻¹ tissue) of pulp at various stages of fruit development and ripening from Alphonso, Pairi and Kent cultivars. Values shown are average of biological replicates sampled for the study. Difference between the stages was significant (p ≤ 0.05) if the alphabets (a, b, c...) after the quantity of the compounds are different. Difference between the cultivars for each compound at each stage was significant (p ≤ 0.05) if the alphabets (x, y, z) after the quantity of the compounds are different.

| Compound | 15 DAP | 30 DAP | 60 DAP | Mature raw | Table green | Mid ripe | Ripe | Over ripe |
|----------|--------|--------|--------|------------|-------------|----------|------|----------|
| **Saturated fatty acids** | | | | | | | | |
| Myristic acid* (C14:0) | Alphonso 8.41 | Pairi 7.2 | Kent 4.2 | | | | | |
| | 5.95 | 7.73 | 3.8 | | | | | |
| Palmitic acid* (C16:0) | Alphonso 1186.8 | Pairi 1534.9 | Kent 830.6 | | | | | |
| | 1302.7 | 1347.6 | 456.0 | | | | | |
| Stearic acid* (C18:0) | Alphonso 679.7 | Pairi 84.9 | Kent 57.2 | | | | | |
| | 61.2 | 8.1 | 19.2 | | | | | |
| Arachidic acid* (C20:0) | Alphonso 32.6 | Pairi 43.6 | Kent 19.9 | | | | | |
| | 33.6 | 47.1 | 7.9 | | | | | |
| **Mono-unsaturated fatty acids** | | | | | | | | |
| Palmitoleic acid* (C16:1, n-7) | Alphonso 11.7 | Pairi 15.0 | Kent 13.5 | | | | | |
| | 9.1 | 15.7 | 8.1 | | | | | |
| 11-Hexadecenoic acid* (C16:1, n-5) | Alphonso n.d. | Pairi n.a. | Kent n.a. | | | | | |
| | n.d. | n.a. | n.a. | | | | | |
| 10-Heptadecenoic acid* (C17:1, n-7) | Alphonso n.d. | Pairi n.a. | Kent n.d. | | | | | |
| | n.d. | n.a. | n.d. | | | | | |
| Oleic acid* (C18:1, n-9) | Alphonso 271.5 | Pairi 328.4 | Kent 255.2 | | | | | |
| | 222.8 | 365.7 | 133.6 | | | | | |
| 11-Octadecenoic acid* (C18:1, n-7) | Alphonso 29.0 | Pairi 112.8 | Kent 46.4 | | | | | |
| | 32.8 | 103.0 | 45.2 | | | | | |
| 11-Eicosenoic acid* (C20:1, n-9) | Alphonso 6.5 | Pairi 6.9 | Kent 5.8 | | | | | |
| | 6.0 | 6.9 | 6.0 | | | | | |
| **Poly-unsaturated fatty acids** | | | | | | | | |
| 9,12 Hexadecadienoic acid* (C16:2, n-4) | Alphonso n.d. | Pairi n.d. | Kent n.d. | | | | | |
| | n.d. | n.d. | n.d. | | | | | |
| Linoleic acid* (C18:2, n-6) | Alphonso 1425.0 | Pairi 1698.9 | Kent 1178.9 | | | | | |
| | 1707.6 | 1575.4 | 546.5 | | | | | |
| 9,15 Octadecadienoic acid* (C18:2, n-3) | Alphonso n.d. | Pairi n.d. | Kent n.d. | | | | | |
| | n.d. | n.d. | n.d. | | | | | |
| Hepta-2,4(E,E)-dienoic acid* (C7:2, n-3) | Alphonso 79.5 | Pairi 167.6 | Kent 215.1 | | | | | |
| | 54.8 | 196.3 | 233.3 | | | | | |
| Linolenic acid* (C18:3, n-3) | Alphonso 454.0 | Pairi 394.5 | Kent 326.2 | | | | | |
| | 443.3 | 301.4 | 142.5 | | | | | |

n.d.: not detected.

* Compounds identified by matching mass spectrum from NIST2011 and Wiley 10th edition mass spectral libraries and retention time and mass spectrum of authentic standard; remaining compounds were identified by matching mass spectrum from NIST2011 and Wiley 10th edition mass spectral libraries. MS spectra for odd chain and unusual poly-unsaturated FAMEs has been provided as Fig. 4.

Unusual fatty acids.
Table 2
Fatty acid composition of skin.
Fatty acid composition (μg g⁻¹ tissue) of skin at various stages of fruit development and ripening from Alphonso, Pairi and Kent cultivars. Values shown are average of biological replicates sampled for the study. Difference between the stages was significant (p ≤ 0.05) if the alphabets (a, b, ...) after the quantity of the compounds are different. Difference between the cultivars for each compound at each stage was significant (p ≤ 0.05) if the alphabets (x, y, z) after the quantity of the compounds are different.

| Compound | 15 DAP | 30 DAP | 60 DAP | Mature raw | Table green | Mid ripe | Ripe | Over ripe |
|----------|--------|--------|--------|------------|------------|---------|------|-----------|

**Saturated fatty acids**

| Compound | Alphonso | Pairi | Kent |
|----------|----------|-------|------|
| Oleic acid | 17.47²| 19.58 | 9.96³ |
| Palmitic acid | 173.73⁴| 265.33 | 194.53 |
| Stearic acid | 120.07| 172.83 | 130.25 |
| Arachidic acid | 58.52| 80.59 | 61.9 |
| Behenic acid | 90.76| 94.21 | 80.13 |
| Lignoceric acid | 110.84| 115.19 | 76.08 |

**Mono-unsaturated fatty acids**

| Compound | Alphonso | Pairi | Kent |
|----------|----------|-------|------|
| Palmitoleic acid | 32.95| 50.48 | 48.93 |
| 11-Hexadecenoic acid | n.d.| n.d.| n.d. |
| 10-Heptadecenoic acid | n.d.| n.d.| n.d. |
| Oleic acid | 299.97| 394.18 | 343.36 |
| 11-Octadecenoic acid | 43.86| 341.82 | 243.86 |
| 11-Eicosenoic acid | 3.71| 6.65 | 4.78 |

**Poly-unsaturated fatty acids**

| Compound | Alphonso | Pairi | Kent |
|----------|----------|-------|------|
| 9,12 Hexadecadienoic acid | n.d.| n.d.| n.d. |
| Linoleic acid | 2054.46| 3104.44 | 2749.59 |
| 9,15 Octadecadienoic acid | n.d.| n.d.| n.d. |
| Hepta-2,4(E,E)-dienoic acid | 29.95| 19.06 | 158.38 |
| Linolenic acid | 938.51| 866.49 | 918.68 |

n.d.: not detected.

a Compounds identified by matching mass spectrum from NIST2011 and Wiley 10th edition mass spectral libraries and retention time and mass spectrum of authentic standard; remaining compounds were identified by matching mass spectrum from NIST2011 and Wiley 10th edition mass spectral libraries.

b Unusual fatty acids.
Fig. 1. Fatty acid column chart—Content (μg g⁻¹) of individual fatty acid from pulp and skin through various developing and ripening stages of Alphonso, Pairi and Kent mango cultivars. Vertical bars at each data point represent standard error of measurement calculated for the biological replicates used in the study.
Fig. 2. Radar plot representing contribution (mg g⁻¹) of total fatty acids. Total saturated fatty acids from pulp (a), total saturated fatty acids from skin (b), total unsaturated fatty acids from pulp (c) and total unsaturated fatty acids from skin (d) at various developing and ripening stages of Alphonso, Pairi and Kent mango cultivars.

Table 3
Lactone content of ripe fruit.
Lactone content (µg g⁻¹ tissue) of pulp and skin of Alphonso, Pairi and Kent at ripe stage.

| Lactone        | Alphonso pulp | Alphonso skin | Pairi pulp | Pairi skin | Kent pulp | Kent skin |
|----------------|---------------|---------------|------------|------------|-----------|-----------|
| γ-Butyrolactone| 1.39 ± 0.16   | 0.17 ± 0.01   | 0.30 ± 0.03| 0.09 ± 0.01| Trace*    | Trace*    |
| γ-Hexalactone  | 1.45 ± 0.16   | 0.28 ± 0.01   | 0.12 ± 0.04| n.d.       | n.d.      | n.d.      |
| δ-Hexalactone  | 1.27 ± 0.20   | 1.49 ± 0.09   | 0.07 ± 0.01| 0.28 ± 0.03| n.d.      | n.d.      |
| γ-Octalactone  | 0.65 ± 0.05   | 0.15 ± 0.006  | 0.11 ± 0.03| 0.14 ± 0.01| n.d.      | n.d.      |
| γ-Decalactone  | 0.32 ± 0.28   | 0.33 ± 0.04   | n.d.       | 0.35 ± 0.06| n.d.      | n.d.      |
| δ-Decalactone  | 0.09 ± 0.01   | 0.61 ± 0.20   | n.d.       | n.d.       | n.d.      | n.d.      |
| Total          | 7.12          | 3.16          | 1.3        | 1.12       | n.d.      | n.d.      |

* Compound detected in traces in GC–MS analysis but not detected in GC–FID analysis.
Table 4
Flavor and nutritional perspective of fatty acids.
Table representing total lactone content (μg g⁻¹), palmitic acid/palmitoleic acid (16:0/C16:1) ratio and linoleic acid/linolenic acid (ω6/ω3) in pulp and skin at ripe stage of Alphonso, Pairi and Kent mango cultivars. Values shown are average of biological replicates sampled for the study. Difference between the tissues was significant (p ≤ 0.05) if the alphabets (a, b, c,…) after the quantity of the lactone are different.

| Ripe tissue     | Flavor   | Nutrition          |
|-----------------|----------|--------------------|
|                 | Total lactone content | C16:0/C16:1 | LA/ALA (ω6/ω3) |
| Alphonso pulp   | 7.12d    | 0.67               | 0.1            |
| Pairi pulp      | 1.30b    | 1.49               | 0.27           |
| Kent pulp       | nd⁴      | 1.78               | 0.2            |
| Alphonso skin   | 3.16c    | 1.35               | 0.37           |
| Pairi skin      | 1.12b    | 6.48               | 0.98           |
| Kent skin       | nd⁴      | 1.89               | 1.06           |

Table 5
Correlation analysis.
Correlation analysis of total lactone content (μg g⁻¹ tissue) and individual fatty acid content from the pulp and the skin tissues of Alphonso, Pairi and Kent cultivars at ripe stage. Values represent correlation coefficient (r), Values in bold represents strong positive correlation (0.7 ≤ r) between fatty acid and lactone.

| Fatty acid   | Correlation coefficient |
|--------------|-------------------------|
| Myristic acid| -0.008                  |
| Palmitic acid| 0.064                   |
| Stearic acid | -0.064                  |
| Arachidic acid| -0.043                  |
| Behenic acid | 0.027                   |
| Lignoceric acid| -0.144                 |
| Palmitoleic acid| 0.847                  |
| 11-Hexadecenoic acid| 0.547              |
| 10-Heptadecenoic acid| 0.633            |
| Oleic acid | 0.078                   |
| 11-Octadecenoic acid| **0.954**          |
| 11-Eicosenoic acid| 0.477                 |
| 9,12-Hexadecadienoic acid| 0.645              |
| Linoleic acid | -0.385                  |
| 9,15-Octadecadienoic acid| **0.76**            |
| 2,4-Heptadienoic acid| -0.099               |
| Linolenic acid| -0.053                  |

Table 6
Correlation analysis.
Correlation analysis of individual lactone and individual fatty acid content from the pulp and the skin tissues of Alphonso, Pairi and Kent cultivars at ripe stage. Values represent correlation coefficient (r), Values in bold represents strong positive correlation (0.7 ≤ r) between fatty acid and lactone content.

| Lactone        | Palmitoleic acid | 10-Heptadecenoic acid | 11-Octadecenoic acid | 11-Eicosenoic acid | 9,12-Hexadecadienoic acid | 9,15-Octadecadienoic acid |
|----------------|------------------|-----------------------|----------------------|--------------------|----------------------------|---------------------------|
| γ-Butyrolactone| 0.752            | 0.813                 | 0.828                | 0.229              | **0.823**                  | 0.91                      |
| γ-Hexalactone  | 0.832            | 0.73                  | 0.885                | 0.259              | **0.77**                   | 0.878                     |
| δ-Hexalactone  | 0.487            | 0.9                   | 0.622                | 0.202              | **0.808**                  | 0.825                     |
| γ-Octalactone  | 0.888            | 0.416                 | 0.974                | 0.566              | 0.457                      | 0.592                     |
| δ-Octalactone  | 0.77             | 0.706                 | 0.893                | 0.405              | **0.724**                  | **0.836**                 |
| γ-Decalactone  | 0.496            | -0.058                | 0.748                | 0.953              | -0.035                     | 0.118                     |
| δ-Decalactone  | 0.452            | -0.283                | 0.472                | 0.558              | -0.287                     | -0.22                     |
5, 8, 10 and 13 days, respectively) were used for further analysis. At each ripening stage fruits for each cultivar were removed from the box, pulp and skin were separated, frozen in liquid nitrogen and stored at \(-80^\circ\text{C}\) till further use.

2.2. Transesterification of fatty acids

Fatty acid methyl esters (FAMEs) were synthesized by transesterification reaction in methanolic HCl. 500 mg of the tissue was finely crushed in liquid nitrogen and added to the 5 ml methanol containing 3 M HCl, 25 μg butylated hydroxytoluene (BHT) as an antioxidant and 250 μg tridecanoic acid as an internal standard. Transesterification was carried out at 80 °C in water bath for 2 h to synthesize FAMEs. After incubation reaction mixture was cooled on ice and FAMEs were extracted twice in 2 ml n-Hexane. n-Hexane layer was completely evaporated in vacuum evaporator, FAMEs were reconstituted in 250 μl chloroform and used for Gas Chromatography-Mass Spectrometry (GC–MS) and GC–Flame Ionization Detector (FID) analysis.

2.3. Extraction of aroma volatiles

Aroma volatiles were extracted from 2 g pulp and skin of completely ripe fruits of all the 3 cultivars by solvent extraction method using dichloromethane with appropriate concentration of nonyl acetate as an internal standard. Procedures for dehydration of dichloromethane, removal of fats and concentrating extracts were carried out as described earlier [4,5].
2.4. Gas chromatography analysis

2.4.1. Identification and quantification of FAMEs

Gas chromatographic analysis was carried out on 7890B GC system Agilent Technologies coupled with Agilent 5977 A MSD (Agilent technologies®, CA, U.S.A.). 1 µl chloroform reconstituted FAMEs were injected for GC–MSD analysis. Method for the gas chromatographic separation of fatty acid
Fig. 5. Loading plot (a) and Score plot (b) of principle component analysis of 17 different fatty acids contributing to pulp and skin through various stages of fruit development and ripening from three mango cultivars, Alphonso, Pairi and Kent. Average values from biological replicates for each fatty acid were considered for the analysis. For the score plot (b) data labels represents, cultivars as A: Alphonso, P: Pairi and K: Kent, tissues as p: pulp and s: skin and stages as 15: 15DAP, 30: 30DAP, 60: 60DAP, MR: mature raw, TG: table green, MDR: mid ripe, R: ripe and OR: over ripe.
structural isoforms was standardized, for better resolution of fatty acids 75 m long SP™ 2560 (Supelco, Bellefonte, Pennsylvania, U.S.A.) column with 0.18 mm i.d. and 0.14 μm film thickness was used (Fig. 3). Helium was used as the carrier gas with 1 ml min⁻¹ flow. Initial oven temperature was kept at 130 °C and held for 5 min, followed by a ramp of 10 °C min⁻¹ till 230 °C with hold at 230 °C for 20 min. Injector temperature was maintained at 250 °C, source, quadrupole and transfer line temperatures were 150 °C, 180 °C and 250 °C, respectively. Mass spectra were obtained by Agilent MSD at 70 eV on scan mode with scanning time of 0.2 s for range of m/z 30–400. FAMEs were identified by matching generated spectra with NIST 2011 and Wiley 10th edition mass spectral libraries (Fig. 4). Identified compounds were confirmed by matching retention time and spectra of authentic standards procured from Sigma Aldrich (St. Louis, MO, USA). Identified compounds were quantified by GC–FID. Similar chromatographic conditions were maintained for GC–FID with detector temperature at 250 °C. Absolute quantification was done using internal standard by normalizing concentrations of all the FAMEs with that of tridecanoic acid methyl ester.

2.4.2. Qualitative and quantitative analysis of lactones

GC-MSD and GC-FID analysis for lactones was carried out on similar instrument used for analysis of FAMEs. Aroma volatiles were separated on GsBP-5MS™ (GeneralSeparation Technologies, Newark, DE, U.S.A.) capillary column (30 m × 0.32 mm i.d. × 0.25 μm film thickness). Other chromatographic conditions were maintained as mentioned previously [6]. Since fatty acids are known to be the precursors for lactone biosynthesis, qualitative and quantitative analysis for lactones alone was carried out in the present study. Lactones were identified by matching generated spectra with NIST 2011 and Wiley 10th edition mass spectral libraries. Identified compounds were confirmed by matching retention time and spectra of authentic standards procured from Sigma Aldrich (St. Louis, MO, U.S.A.). Absolute quantification was done using internal standard by normalizing concentrations of all the lactones with that of known concentration of nonyl acetate.

2.5. Statistical analysis

To validate data statistically tissue for each developing and ripening stages were collected from fruits of 3 independent trees for cv. Alphonso and 2 independent trees each for cv. Pairi and cv. Kent. These were considered as biological replicates. Extraction of FAMEs and volatiles was carried out twice for each tissue as technical replicates followed by duplicate GC–FID runs of each extracts as analytical replicates. Fisher’s LSD test was performed separately for pulp and skin at p ≤ 0.05 by ANOVA for comparative analysis of quantity of each fatty acid during various developing and ripening stages from each cultivar. Also comparison was done for each fatty acid at individual stage among the three cultivars using StatView® software, version 5.0 (SAS Institute Inc., Cary, NC, U.S.A.). Similarly ANOVA was carried out for lactone content of ripe pulp and skin from the three cultivars. Correlation analysis of total lactone content with individual fatty acid content and individual lactone content with individual fatty acid content from the pulp and the skin of three cultivars at ripe stage was studied using StatView software. Principle component analysis for whole data set (Fig. 5) of fatty acid content was carried out using Systat® statistical software (Version11, Richmond, CA, U.S.A.).

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Transparency document. Supplementary material

Transparency data associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.dib.2016.09.018.

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