fermentasmania

SIPP Grant 2023

Polyphenolic Fruit Waste Valorisation Study

Stage 4 Report

Ecosystem Stress-Test Report

SUPPORTED BY

Tasmanian Government

PROJECT PARTNERS

Fruit Growers Tasmania

UNIVERSITY of TASMANIA

TIA

Tasmanian Institute of Agriculture

TIA is a joint venture of the University of Tasmania and the Tasmanian Government

Startupbootcamp FoodTech

the forager food co.

redefining the food experience

Clever intelligent fermentation

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Executive Summary

This **Ecosystem Stress Test Report** examines the feasibility of increasing the valorisation of Focus Fruit Waste in Tasmania. The study identified opportunities and challenges for new income streams for farmers, collaboration potential, infrastructure bottlenecks, and gaps in chemical testing and pilot/small-scale fermentation capabilities.

Key findings:

- **Existing Infrastructure:** Some underutilised facilities were discovered, but access to venture capital and market development remain challenges.
- **Chemical Testing:** Limited on-island testing capacity (particularly for bespoke analyses), making interstate labs more viable.
- **Polyphenolic Product:** High-value opportunity that requires precision fermentation for an optimised process, which is currently unavailable in Tasmania.
- **Piquette Wine Production:** Feasible and profitable using existing winery infrastructure.
- **Cherry Processing:** Infrastructure exists but requires automation and clear market demand.

Stakeholder Forums

- Forums held in **May and October 2024** brought together growers, infrastructure owners, and entrepreneurs. Key takeaways:
    - Collaboration increases viability but lacks formal mechanisms.
    - Market development is a major barrier to value-added products.
    - Awareness of funding and research opportunities is low.
    - Some new partnerships and products emerged as a direct result.

Ecosystem Stress-Test Results

Chemical Testing & New Product Development (Polyphenol Concentrate)

- Only **UTAS** had the potential for on-island testing, but lead times made it unviable.
- **Affinity Labs** (South Australia) was used for Focus Fruit chemical composition and fermentation trials.
- The study confirmed bioactivity and polyphenol profile changed as a result of fermentation , though methododology needs refining.

Processing Technologies

- **Pulverisation:** Alternative to freeze-drying was tested, but issues like enzyme interference and contamination limited success. Further research is needed.
- **Piquette Wine:** Trials at Swinging Gate Winery demonstrated profitability and ease of implementation.
- **Cherry Processing:** Challenges include limited automation and lack of domestic market for frozen/freeze-dried cherries.

Ecosystem Strengths, Bottlenecks, and Weaknesses

Strengths

- Clusters of Focus Fruit production around **Hobart and Launceston**.

- Opportunities for value-added products (e.g., fermented beverages, nutraceuticals). Dwayne – add the footnote here too please
- Some growers successfully increasing profits through product diversification.

Bottlenecks

- **Market Access:** Few Tasmanian businesses positioned to compete in national/international markets.
- **Funding Gaps:** Venture capital and angel investment in agriculture are scarce.
- **Regulatory Challenges:** Complex compliance requirements for new products.

Weaknesses

- Inconsistent access to **testing facilities** for chemical composition and fermentation trials.
- Logistical challenges for **fruit waste collection and distribution**.
- Lack of **precision fermentation** capacity within Tasmania.

Recommendations & Next Steps

- **Expand on-island chemical testing** capacity to reduce reliance on interstate labs.
- **Develop precision fermentation** infrastructure for high-value polyphenolic production.
- **Facilitate market development** for Tasmanian fruit waste products, particularly high-value exports.
- **Improve collaboration mechanisms** for growers, processors, and entrepreneurs.
- **Support investment in automation** for cherry processing and freeze-drying facilities.

Conclusion

This report highlights critical areas where Tasmania can improve waste valorisation, infrastructure, and market development.

"We are proud to be part of creating new income streams for Tasmanian farmers. We are equally proud to be diverting waste away from carbon emissions and into products that advance Tasmania's economy and global health"

Kim Seagram, fermentasmania Chair

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About fermentasmania

Fermentation is the delicious alchemy that transforms our food - grains into bread, cabbage into kraut, milk into cheese, grapes into wine.



At fermentasmania, we believe in the power of fermentation to transform our produce, our people, and our place. By connecting industry, educators, government, and consumers, we are cultivating a community of creative food lovers & innovators.

The word fermentation comes from the Latin verb "fervere" which means to boil. We believe fermentation can turn the heat up on Tasmania, creating new jobs and new businesses on our island and helping Tasmanian food reach new markets. Through fermentation, we can craft innovative, value-added food & drinks that take a taste of Tasmania to the world.

Human history is replete with examples of resourceful use of food ‘waste’ and also of making ‘hay’ (fermented food products) while the ‘sun’ shines (before foods are spoiled). Fermented foods formed part or the core of staple diets across global cultures; from kim chi in Korea, to Sauerkraut in Germany, to food produced by indigenous Australian cultures.

Fermentation is culture and in Tasmania our culture is alive. Join us on our journey, as we put Tasmania on the map as a unique global centre for excellence in fermentation.

The Fermentas Trade Network is your one-stop-shop for our island's premium fermentation businesses. Let us put you in touch with small and large producers alike to bring a taste of Tasmania to you.

Ask us if you want to know more about the value of fermented foods.

1. Defined Terms

Abbreviation	Term
CRC	Cooperative Research Centre
CAS	Controlled Atmosphere Storage
Focus Fruits	Apples, cherries and grapes
Focus Fruit Waste	Fruit and fruit by-products from the Focus Fruits that are diverted into landfill, compost or animal feed
Functional Drinks	A segment of the pre-packaged drinks market that includes non-alcoholic beverages that claim health benefits due to the inclusion of bioactive, biotic[1] or other compounds; includes energy/mood drinks, fermented drinks (kombucha, kefir and others), protein drinks and healthy 'shots' (Yakult, as one example)
Pét nat	Short for Pétillant Naturel, which means naturally bubbling, a type of wine produced from a secondary ferment of grape marc
Polyphenol Concentrate	A concentrated product high in polyphenol for use by the nutraceutical industry (may also be high in anthocyanins and antioxidants)
Target Fruits	Apples, blackcurrants, cherries, elderberries, grapes
Target Fruit Waste	Fruit and fruit by-products from the Target Fruits that are diverted into landfill, compost or animal feed
TIA	Tasmanian Institute of Agriculture
UTAS	University of Tasmania

[1] Including prebiotic, probiotic and postbiotic

2. Introduction

Fermentasmania received funds from the Tasmanian State Government through the SIPP Grant to research current uses of fruit seconds and by-products in Tasmania, and to investigate the viability of increasing the economic value derived by growers (and others).

This project follows other successful projects related to valorisation of food waste in Tasmania[2].

2.1 Project Stage 4

This report details:

- observations from forums conducted with key stakeholders about increasing valorisation of Focus Fruit Waste;
- stress-testing existing infrastructure to understand capacity and limits to accommodate a new ecosystem using Focus Fruit Waste; and
- results of bioavailability tests on certain Focus Fruits and Focus Fruit Waste to increase data needed for a new ecosystem.

2.2 Other Project Stages

The other stages of the Project have identified existing underutilised Focus Fruit Waste and products that might be viably produced in Tasmania. Infrastructure and funding sources for use in production have been identified.

This is Stage 4 of 6 stages in this Project and is a vital building block for the Project conclusions. For more details of each Stage see Appendix A.

Stage 1	Existing Ecosystem Report (complete)
Stage 2	Polyphenolic Fruit Byproduct / Waste Report
Stage 3	New Ecosystem Viability Report
Stage 4	***Ecosystem Trial Report (this Report)***
Stage 5	Funding Report
Stage 6	Fruit Waste Ecosystem Report

[2] Hort Innovation, 2008, *Innovative approaches to adding value to vegetable waste – Phase 2*, https://www.horticulture.com.au/growers/help-your-business-grow/research-reports-publications-fact-sheets-and-more/mt06053/

3. Focus Fruit Waste Forums

Forums were held in May and October 2024 to engage key stakeholders in the Project with Focus Fruit Waste as the central topic, and some reflections and observations from those forums have been included in this Report.

The forum held in May 2024 (May Forum) was a consultation on Focus Fruit Waste held in Launceston, including discussion of the content of Stage 1 and 2 Reports, and was a key input to the Stage 3 Report. The May Forum was composed of existing growers, infrastructure owners, representatives from industry groups and entrepreneurs who were involved in Focus Fruit production (including value-added products). The May Forum was attended by more than 30 people.

The second set of forums were held in October 2024 (October Forum) and were composed of:

- existing growers, infrastructure owners, representatives from industry groups and entrepreneurs who were involved in Focus Fruit production (including value-added products);
- FermenTasmania contacts interested in products from Focus Fruits and fermentation generally;
- Broader agriculture experts;
- Entrepreneurs from the agriculture sector; and
- Academics.

The October Forum included a presentation of Stage 3 and 5 reports, presentations from entrepreneurs, and facilitated panel discussions about a new ecosystem with a particular focus on infrastructure needs and developing markets and products. The October Forum was attended by more than 80 people.

3.1.1 Forum Reflections and Observations

Reflections and observations from the forums include:

1) Many participants met for the first time, including a notable number of growers meeting:
    a. other growers,
    b. infrastructure owners and
    c. entrepreneurs.

2) Existing infrastructure was identified that was previously unknown (particularly in the October Forum), and discussion of increased utilisation occurred at and after the Forums.

3) There was broad consensus that collaboration across ecosystem participants was likely to increase viability of Tasmanian production, noting that some ecosystem participants saw collaboration as a sub-optimal profit strategy for certain stakeholders.

4) Mechanisms for collaboration were under-identified by ecosystem participants. As Anna Barlow of Startupbootcamp observed, among several similar comments:

"Other regions, including several in New Zealand,
have remained viable and competitive
by ***collaborating and utilising collectives***

to take raw fruits and create valued-added products,
***increasing profit for all involved**."*

5) Many ecosystem participants noted lack of market development and identification as a barrier to value-added products, especially in national and international markets. As one grower put it:

"We need someone out there aggressively selling
high-value Tasmanian products."

6) Access to venture capital and angel investing in Tasmania and the agriculture sector more broadly was identified as a barrier to entrepreneurial activity for Focus Fruit Waste.

7) In the October Forum, participants were generally surprised at the amount of government funding available, including the number of programs available. There was scepticism from some participants about the value of government funding.

8) Awareness of Cooperative Research Centres remained low, other than those who were engaged with CRCs in their professional capacity.

9) New products and marketing approaches have resulted from participant who met for the first time at the May Forum and the October Forum, some of which have been highlighted in the Stage 3 Report.

These Forum reflections were used to inform the design of the Ecosystem Stress Test.

4. Ecosystem Stress-Test

Tasmanian production was identified as important due to the relatively high transport costs of shipping to and from Tasmania. The Project wanted to test the capabilities and capacities of Tasmanian providers to enable and support the proposed new ecosystem.

4.1 Stress-Test Elements

Stress testing was conducted to understand the following aspects to create a new ecosystem:

- Support services: Analytical services to conduct chemical testing on Focus Fruit Waste using Tasmanian providers
- New product development: shelf-stable powdered product using next-generation pulverisation
- New product development: creation of a concentrated polyphenolic product
- Viability assessment: Piquette (Pét nat-style) wine production

Details of the methodology for each detail is identified below.

4.1.1 Tasmanian Chemical Testing Capacity



New product development and innovative process development requires analytical testing beyond standard and regulatory parameters (e.g. alcohol and methanol testing). The Focus Fruits are high in polyphenols which are bioactive compounds that can form the basis for the development of functional ingredients and drinks (Stage 3 – New Ecosystem Report) Thus, bioactivity assessments and polyphenol profiling of Tasmanian-grown Focus Fruits and products made from the Fruits was determined to be a valuable input to a new ecosystem.

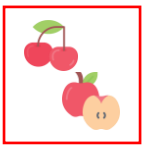
Desk-based research identified limit studies that detail the bioactivity of Tasmanian grown fruits. Peer-reviewed literature and industry journals identified broadly assumed that Tasmanian-grown Focus Fruits were of similar chemical composition and bioactivity to fruits grown in other Australian states, without sufficient scientific backing.

Web searches and direct calling of known Tasmanian chemical testing facilities was conducted to identify capacity to conduct bioactivity tests of Focus Fruits and Focus Fruit Waste on-island, (Appendix D).Several Tasmanian test labs were identified and only the University of Tasmania (UTAS) was a potential Tasmanian provider.

The Project invited collaboration with UTAS, including using the equipment of the Tasmanian Institute of Agriculture (TIA). After several enquiries and meetings, and identification of infrastructure that could have been used for chemical testing, it was concluded that without long lead times of 3 to 6 months, testing by UTAS would not be possible. That was due to UTAS's internal models that tended toward supporting research outcomes instead of commercial testing.

For entrepreneurs seeking time-sensitive chemical testing of Focus Fruits and Focus Fruit Waste, non-Tasmanian labs are currently the only viable option. Several laboratories in other States were identified as possibly suitable including NMI, BVAC, ACS Laboratories and ALS Global.

4.1.2 Powdered products



Preserving Focus Fruits and Focus Fruits Wastes is important to make valorisation more feasible and reduce the burden during harvest, as detailed in Stage 3 Report. Two methods to process Focus Fruits to shelf-stable powdered products were identified, and stress-tested: next-generation pulverisation and freeze-drying.

Only whole apples, apple pomace and frozen cherries were available for such testing, as detailed below.

4.1.2.1 Next-generation pulverisation



Project Partners were approached by FAPIC (Adelaide-based manufacturer) with a patented process (with related equipment) for pulverisation of fruit waste to a powdered product. Details of the equipment are in Appendix F. The potential suitability of innovative pulverisation technology and its potential as an alternative to freeze drying was investigated.

FAPIC's processes and equipment rely on low levels of moisture to produce a powdered product from food waste. Such powders are then usable for inputs to other forms of production including food products. FAPIC had successfully conducted tests on a variety of food wastes, including apples and apple pomace.

Apples, apple pomace and cherries were selected to submit to the pulverisation process.

Whole Apples

Whole apples were removed from Controlled Atmosphere Storage (CAS), packed into sealed containers, and shipped to FAPIC in Melbourne. Due to delays in shipping (5 business days, instead of 2) and FAPIC's production schedule, black-coloured mould was discovered on the apples so no processing was possible.

Apple Pomace

Apple pomace was sourced from a Tasmanian juice manufacturer. The apple pomace was waste from a second press after a primary press of apples for high quality juice. Juice from the second press was used for lower quality apple juice products and the apple pomace was typically discarded as compost.

FAPIC have previously successfully processed apple pomace. When they processed the apple pomace for this Project, an unexpected 'slimly goo' was produced instead of a fine powder. Estimates of moisture in the apple pomace were very low, so moisture content was ruled out as a cause. After further enquiries with the apple pomace provider, it was discovered that ~~certain~~ enzymes were added to first-press pomace at secondary pressing to increase juice extraction. The unanticipated result was that the enzymes continued to breakdown the apple pomace, even though there was no observable difference in the pomace. When pulverised, the apple pomace broke down to a 'goo' that indicates cellular destruction typical of enzymatic action. No further chemical testing was conducted on the 'goo'.

Further testing of apple pomace that hasn't undergone enzyme treatment is likely to yield different results.

Frozen cherries

Frozen cherries were sourced from a Tasmanian producer of high-value cherry products. The cherries were shipped in insulated containers via normal shipping methods, and delivery time was 4 business days, instead of the anticipated 2-3 business days.

FAPIC anticipated difficulty processing the due to high moisture content, and hoped that the production process would transform fruit flesh to powder and eject cherry pips. Fruits were processed at a relatively high rotation speed, and powder was produced after a secondary processing. However, the process also pulverised cherry pits, and due to the known ~~public~~ health risks of prussic acid, it was concluded that the powders were not suitable for use.

Indications are that de-pitted cherries, even with high moisture content, are suitable to pulverise into powders. Further optimisation of different operating speeds and techniques may result in effective separation of cherry pits from pulverised powders.

Conclusions on Pulverisation

Shipping times were an issue for an off-island pulverisation process, however pulverisation is worthy of further investigation, especially if a Tasmanian-based provider is available. There are no known plans for ownership of a FAPIC or FAPIC-type pulverising machine in Tasmania, and other emerging pulverisation techniques (such as sonic or microwave assisted) may yield powders that are usable in the ~~Tasmanian~~ production of high-value goods and products.

Project partners are grateful to FAPIC for agreeing to assist the Project, especially because outcomes were not anticipated, and because of the health risks discovered during testing.

4.1.2.2 Freeze-drying

Freeze-drying was identified as a way to produce high quality goods from 1st grade fruits, including apples and cherries; see Stage 3 Report.



The capacity of existing infrastructure to freeze and freeze dry increased quantities of cherries at harvesting times was on obvious opportunity to decrease the amount of cherry waste. Freeze-dried cherries could be used as a finished product, or powdered for use in other products including a concentrated polyphenolic powder or powders for use as an ingredient and food and beverage products.

It was identified that the only reasonable prospect of doing so was through Forager Foods, a Project Partner. Several meetings with Forager Foods revealed several barriers to increased harvesting and production of cherries:

- **Automated cherry de-pitting capability**. Forager Foods cherry de-pitting operations are not fully automated, and because Forager Foods runs multi-use production lines, line change times were a significant barrier to increased processing of cherries.
- **Logistical challenges during peak season:** cherry harvesting season in Tasmania is typically 8-10 weeks, and occurs at the same time as harvesting of other high value fruits that are faster and easier to process with existing equipment Investment in a larger cherry de-pitter would be viable if there was identifiable demand to contract for appropriate quantities. No potential buyers were identified through the project.
- **Frozen cherry market**. The frozen cherry market in Australia is dominated by cheap international imports and Tasmanian production could not compete on price. Only production for high-value products would create a viable market. The market for freeze dried cherries in Australia remains small, and arguably under-explored. Without

marketing to change consumer tastes, production of freeze dried cherries looks challenging. Export markets for high-quality products are periodically explored by the industry.

Through the October Forum, a high-volume cherry pitting machine was identified that remains almost unused, and with the right commercial stimulus may be available. Fermentasmania has identified a small commercial cherry de-pitter as an important assets for its Legana fermentation hub to support increased valorisation of fruit waste and the creation of high-value cherry-based products.

4.1.2.3 Bioactivity and polyphenol profiling of powdered products

These shelf-stable powdered products could then be sold as is, or potentially further processed, for example, through fermentation (see 4.1.3). Following the conclusions from 4.1.1, it was concluded that significant efficiencies (time and cost) could be gained by identifying laboratories that could simultaneously conduct freeze-drying, fermentation, and chemical testing. Affinity Labs (formerly the Australian Wine Research Institute) was chosen to investigate chemical composition of Tasmanian Fruits.

Availability of Focus Fruit Waste was limited at the time of testing, and whole apples, apple pomace and frozen whole cherries were sent for testing. Due to the results from the pulverisation tests, these powders were not included in this stress test of new product development. The results of bioactivity analysis of freeze-dried Focus Fruit Waste are summarised in Table 1 (below) and fully detailed in Appendix E – Affinity Labs Report

SmartBerries

Project Partners became aware of SmartBerries Test, an app-based fast-responding and commercially cheap polyphenolic test. The test, which is similar to a simple litmus test with specialised test strips and reagents, coupled with an app to interpret the results, has potential to speed development of Tasmanian products from Fruit Waste, and identify viability of Fruit Waste for use in production. The capability and limitations of the test and outputs was not further investigated.

4.1.3 Fermentation for Concentrated Polyphenolic Product

Through the Project, a concentrated polyphenolic product from Focus Fruit Waste was identified as the highest value item that might be produced in Tasmania, and worth further exploration. One way to produce such a product is through fermentation to increase bioactivity. Significant increases can be achieved through precision fermentation. However due to the lack of capability and capacity for producing products using precision fermentation in Tasmania currently, it was not considered in the stress test.

Desk-based identification of organisations with capacity to conduct fermentation trials was supplemented by industry contacts from Project Partners.

Formal approaches were made to:

- University of Tasmania (with support from TIA)
- Affinity Labs (an initiative of the Australian Wine Research Institute)

- ACS laboratories

As mentioned above (4.1.2), Affinity Labs was selected for their capability to conduct fermentation trials as well as the chemical testing and freeze-drying. The results of fermentation trials by Affinity Labs are summarised in Table 2, below and the full report is available in Appendix E.

Conclusions that can be drawn from the fermentation trials are limited in that the tests were not optimised or designed for extraction of particular polyphenols. The data forms a baseline for development of high-value fermentation products including concentrated polyphenol powders and functional drinks.

Some observations about the testing by Affinity are:

- Tasmanian fruits may have different polyphenolic content compared to the average of fruits grown in other States. If processing is to occur in non-Tasmanian facilities, processing of fruits and fruit waste to a shelf-stable form (such as freeze drying and powdering) would alleviate issues around shipping fresh produce observed in this stress test. Though it is likely to alter bioactivity and polyphenol content.
- Fermentation did appear to have an impact on polyphenol profiles.
- Affinity has expertise to further refine testing, and further research proposals will need to focus on product-driven actionable insights.
- Affinity has a team that are very keen to deliver relevant analysis for decision-making, with highly detailed analysis available.
- Results from analyses such as the polyphenol profiling are necessarily complex and require expert interpretation. In becoming a product development hub, Fermentasmania could add to Tasmanian expertise by identifying an expert panel with capability to quickly provide insights and a second opinion on testing results.
- Producers targeting the nutraceutical market will need to consider the expertise and testing required to back their claims for regulatory approvals.

Overall, Affinity Labs could function as a contract research service provider as well as an analytical service provider, along with other identified commercial labs. Affinity Labs' capacity to work to commercial timelines and terms for engagement means that they are positioned to support the development of the proposed new Ecosystem requiring capabilities that aren't currently available in Tasmania.

4.1.4 Piquette Wine Production



During the Fruit Waste research phase, it was identified that Swinging Gate Winery was considering re-commencing production of Piquette wines using the Pét nat method, after several years of not doing so. Previous successes were not repeated when the Winery purchased a new pressing machine that was able to extract more juice from the grapes, leaving grape marc that had much lower juice content. Swinging Gate Winery agreed to test the viability of Pét nat wine production using existing infrastructure common to such smale-scale wineries.

Production of Piquette wines (using the Pét nat method) by Swinging Gate Winery was possible with only small changes to existing production routines. A first press of grapes for full-alcohol wines was conducted as normal, at slightly lower pressing rates, and the resulting grape marc was used to make Pét nat wine (for more detail, see the Case Study in Stage 3

Report). The resulting increase in costs was in the range of 5-15% (mostly from water and labour costs), with the same volume of grapes resulting in increased revenue from sales of approximately 80% and a gross profit increase in the range of 65-85%.

Swinging Gate Winery, as a relatively small producer with limited production capacity, relies on selling all of its production to maximise profits. Evidence in the middle of summer 24/25 is that all of Swinging Gate's Pét nat production will sell out before the next season's production is sales-ready.

By increasing production and profit with no change to growing practices from the same production equipment, Swinging Gate has increased profitability, developed new revenue and gained access to the growing low alcohol market.

There were almost no barriers to a small winery producing piquette wines. Even large growers, who tend to send pressed grape juice to the mainland for processing, have easy access to grape marc and could use that to produce piquette wines and increase revenue and profit.

4.2 Other Opportunities Identified

Project Partners and growers were approached by several organisations about utilising Focus Fruit Waste. Such approaches were merely identified and were not included in the Ecosystem Stress Test.

4.2.1 Increased Cherry Harvesting

OzHarvest approached Project partners to assist with investigating the possibility of increased harvesting for diversion of 1st and 2nd grade cherries for use in OzHarvest's operations. Possible uses of such cherries included for food banks and as an ingredient for production of drinks or value-add food products.

OzHarvest could possibly supply volunteer pickers and transport, however growers identified liability and other management concerns about having additional people present at peak picking times such as biosecurity and safety concerns.

It is unclear whether negotiations will continue between OzHarvest and growers.

4.2.2 Organic Feedstock

Several entrepreneurs were interested in utilising Focus Fruit Waste as an input to production of biofuel, protein products and food production. Those entrepreneurs mostly preferred gathering organic food waste at a single source, and current streams of Focus Fruit Waste are largely distributed across Tasmania. In addition, centralised organic waste facilities in Tasmania tend toward using organic waste for energy and compost production, for example the commissioned facility owned by Dulverton Waste Management Group.

It is unclear whether such entrepreneurial products are viable while Focus Fruit Waste remains broadly distributed, although clusters of growers tend to be centralised around Hobart and Launceston.

5. Conclusions

Summarising all of the ecosystem stress-tests above, the following conclusions can be drawn.

5.1 New Ecosystem Strong Points

Strong points that support development of a New Ecosystem:

- Clusters of Focus Fruit production around Hobart and Launceston.
- Opportunities for value-added products (e.g., fermented beverages, functional foods and beverages, and nutraceuticals[3].
- Some growers successfully increasing profits through product diversification.
- Excess capacity for regular fermentation, such as that used in the wine and spirit manufacturing sector in Tasmania

5.2 New Ecosystem Bottlenecks

Bottlenecks to development of a New Ecosystem:

- **Market Access:** Few Tasmanian businesses positioned to compete in national/international markets.
- **Funding Gaps:** Venture capital and angel investment in agriculture are scarce.

5.3 New Ecosystem Weaknesses

Challenges to development of a New Ecosystem include:

- Small scale for proof of concept such as demonstrated here for New Product Development.
- Lack of **precision fermentation** capacity within Tasmania.
- Limited access to **testing facilities** for chemical composition and fermentation trials.
- Logistical challenges for **fruit waste collection and distribution**.

5.4 New Ecosystem Support

The New Ecosystem could benefit from the following support.

- **Expand on-island chemical testing** capacity to reduce reliance on interstate labs.
- **Develop precision fermentation** infrastructure to produce high-value polyphenolic products.
- **Facilitate market development** for Tasmanian fruit waste products, particularly high-value exports (including to other States).
- **Improve collaboration mechanisms** for growers, processors, and entrepreneurs.

[3] Nutraceuticals are regulated by the TGA.

- **Support investment in automation** for cherry processing and freeze-drying facilities.

5.5 New Ecosystem Developments

Throughout the period of the Project, Fermentasmania has continued its plan to construct, develop and open a world-class fermentation hub in Tasmania. FermenTasmania have incorporated conclusions from the Project and have developed plans to:

- Increase Tasmanian chemical testing capacity.
- Develop Tasmanian capacity for fermentation, including precision fermentation.
- Acquire small-scale cherry de-pitting equipment.

Appendix A – Stages of this Project

Project Stages

Stage 1 – Existing Ecosystem Report
Identification of the existing Ecosystem in relation to Target Fruits.

Stage 2 – Polyphenolic Fruit Byproduct / Waste Report
A Report that identifies the Fruit Waste and by-products from Tasmanian Fruits.

Stage 3 – New Ecosystem Viability Report
Identification of opportunities from a new ecosystem that creates value from Fruit Waste and fruit by-products within Tasmania

Stage 4 – Ecosystem Trial Report
Trials will be conducted to test all elements of the fermentation ecosystem with a view to various scales of production.

Stage 5 – Funding Report
Details of sources and needs for additional capital and infrastructure investment needed to support a new ecosystem.

Stage 6 – Fruit Waste Ecosystem Report
A report that summarises the whole Project, including the value to Tasmania of creating new ecosystems that support maximisation of Tasmania's Fruits.

Project Timeline

2024

STAGE 1:
Existing Ecosystem Report
Identify the existing fruit ecosystem in Tasmania for Target Fruits

STAGE 2:
Fruit Waste Report
Report on the amounts of Fruit Waste in Tasmania for Target Fruits

STAGE 3:
New Ecosystem Viability Report
Identify existing capacity and additional capacity needed to make the new ecosystem

STAGE 4:
Ecosystem Trial Report

STAGE 5:
Funding Report
Detailing areas of investment needed

STAGE 6:
New Fruit Waste Ecosystem Report

Q1 Q2 Q3 Q4

Stakeholder Consultation

Market creation launch and events

Further stakeholder consultation

Identification of Innovative businesses

2025

Target Date for Launch of the world-class fermentasmania Fermentation Hub

Q1



Anticipated Project Outcomes

The Project Partners anticipate several outcomes for the Fruit Growing sector and from the creation of new products and sectors pursuing economic opportunities highlighted in this Project.

Anticipated Project Outcomes for growers

Tasmania's growers can expect to take their share of the creation of new economic opportunities that result in:

- Higher prices for fruits and fruit by-products at certain stages of the existing Target Fruit ecosystem
- Reduced costs in relation to disposal of fruit by-products and fruit waste
- Increased value from fruit by-product streams in new market opportunities
- Reputational benefits flowing from definable and measurable reductions in carbon emissions

It is anticipated that the final outputs of this project will be the identification of:

- Clearer categorisation of Target Fruit by-products and waste streams
- Better reporting of Target Fruit by-products and waste in certain stages of growth and production
- Viable uses of existing Target Fruit by-products and waste streams in the existing and in new ecosystems.
- Highest value uses for underutilised Target Fruit by-products and waste streams.
- Market value of changing farming practice and achieving higher price points for Target Fruit by-products and waste streams
- Job creation opportunities in the Tasmanian food and beverage sector
- Pinch-points of the existing ecosystem in order to identify growth points for an additional ecosystem
- Viability of new food and beverage sub-sectors in Tasmania
- Increased utilisation of existing Tasmanian infra-structure
- Gaps in understanding of the carbon emissions of the Fruit sector in Tasmania

Further, the outcomes of this project will be a necessary input to the successful launch of the Fermentation Hub, targeting:

- 650 new jobs for Tasmanians
- Leveraging Launceston's status as a UNESCO Creative City of Gastronomy
- Food Tourism to Tasmania
- Agri-Tourism to Tasmania

Project Limitations and Exclusions

This project is limited to analysis of Target Fruits, and in addition, the following limitations are expected:

- This Project is only relevant to the 2023 growing season (although may be informed by trends in the 2024 growing season)
- In several areas there aren't complete data sets to facilitate high-quality analysis and projection, including amounts of fruit in long-term storage at farm-level. Data

projections will need to be made from the available data, and it is difficult to know how accurate those projections will be

Appendix B - Reflections on this Report

fermentasmania Reflections

As identified in the McTAvish West report in 2020, growers are loathe to recognise and identify fruits and fruit by-products as 'waste'. Classification of fruit by-products

Project Partners Reflections

Global / Australia Wide

Specific to Tasmania

Other

Appendix C – Project Partners Background and Interested Parties

SUPPORTED BY

Tasmanian Government

Tasmanian Government Supported

In 2021 and 2022, the Launceston region and fermentasmania had watershed years. In no particular order, all of the following happened:

- Funding for building of a Launceston-based world class food hub was secured; including fermenting, distilling and chemical innovation facilities.
- Launceston was designated a UNESCO Creative City of Gastronomy, becoming Australia's second such city.
- fermentasmania successfully applied to the Strategic Industry Partnership Program for funding to engage in this Project.

In 2023, it was announced that fermentasmania had been awarded funding for this project to investigate the viability of using fruit waste as an input into a new and high-value ecosystem.

Fruit growers Tasmania Supported

Fruit growers Tasmania, as the second peak-industry body involved in guiding the Project, represents apple, pear, cherry, berry and stonefruit growers in Tasmania. It represents the interests of Tasmanian fruit growers and is by Tasmania's fruit growers, for Tasmania's fruit growers.

Fruit Growers Tasmania

Fruit growers Tasmania key focus areas are to support growers with matters of pest and disease management, strengthening of national and international trade and to support industry development. Fruit growers Tasmania:

- offers information and support services to make life easier for members as well as other Tasmanian fruit growers.
- organises industry information sharing activities, including orchard walks, field days, and the annual conference.
- ensures representatives and other industry leaders serve on industry Strategic Industry Advisory Panels, representing the State and their colleagues on the boards of national industry peak bodies.

- assists growers with navigating government export registrations and audit processes. Members can use our website to keep up to date with industry and government export information including audit scopes, work-plans, and other relevant information.
- assists growers meet the growing national and international food safety quality assurance certification auditing requirements by coordinating microbiological and residue testing services.

Partner Supported

In addition to Government support, and the peak industry bodies, fermentasmania and Fruit growers Tasmania, several other partners were strategically invited to join this Project. That's because we wanted this project to test the limits of the proposed ecosystem so that any interventions and supports to create new income streams can target the parts of the ecosystem that lack capacity.

Those partners are:

- **University of Tasmania** through **Tasmanian Institute of Agriculture**
  The Tasmanian Institute of Agriculture (TIA) has a mandate to deliver research, industry development and education for the agri-food industry of Tasmania.

  Our vision is to enable Tasmanian food producers and processors to accelerate primary sector productivity while maintaining and improving Tasmania's land and water quality for future generations.

  Close relationships across the agriculture and food value chain at a local, national and international level ensure we are connected with stakeholders and that our research and education priorities support industry needs and aspirations.

  Website: https://www.utas.edu.au/tia

- **Startupbootcamp**
  A global family of industry-focused programs that support early to growth stage food, aqua and agritech founders to rapidly scale their companies. We provide direct access to an international network of the most relevant mentors, corporate partners, and investors.

  We are working with startups with innovative technology, products, services or disruptive business models that solve problems or have solutions for the FoodTech, and Blue/AgriTech sectors.

All our programs align to the UN Sustainable Development Goals, continuing our focus on the Circular Economy, adding value to Australia's animal and horticultural produce as functional foods or ingredients, and finding innovative technologies to help our global food and beverage sector become more efficient and sustainable.

Website:

https://www.startupbootcamp.com.au/programs/foodtech-tasmania

- Clever Fermentation
  Clever develops fermented superfruit health ingredients for nutraceutical, supplemental and functional food brands.

  Website: https://cleverfermentation.com/

- **Forager Foods**
  Forager Food Co. is at the forefront of the Australian freeze-drying industry, offering a range of premium freeze-dried products, all expertly crafted using the finest ingredients and the latest in manufacturing facilities and technology. Commencing operations in 2009 we have quickly grown to be the largest and most advanced manufacturer of freeze-dried products in Australia.

  Forager Food Co. processes, dries, and package a diverse range of foods providing extended shelf life whilst protecting the most valuable and delicate ingredients, including vitamins, minerals, antioxidants, colours, and flavours.

  Our production facilities feature state-of-the-art freeze-drying capability and are supported by full-service manufacturing facilities, including ambient, chilled, and frozen storage, food processing, packing, despatch, and logistics services.

  Website: https://foragerfoods.com.au/about/

Interested Parties

In addition to the formal Project Partners, other parties we have identified with significant interest in the outcomes of this project, and the success of the fermentasmania hub, include:

- City of Gastronomy
- City of Launceston
- Enterprize
- Hort Innovation
- Northern Tasmania Development Corporation
- McTavish West
- Tasmanian Farmers and Graziers Association
- Tasmanian Food Cluster
- Tasmanian Fruit & Vegetable Export Facilitation Group
- Van Diemen Project
- West Tamar Council

Throughout the remainder of this project, we will add to the above list. If you would like to be kept informed of the progress of the project, please contact Dwayne Baraka by email, or on 0481 88 00 46.

Interested sub-sectors

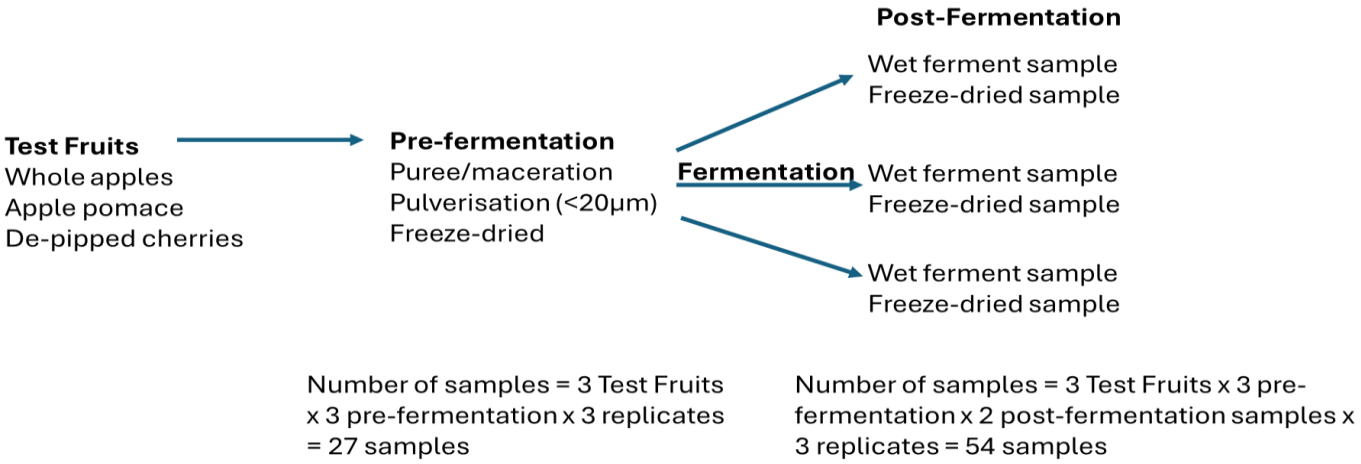
In investigating this report, the following sub-industries were identified:

- Grappa production
- Piquette production
- Polyphenol Concentrate production
- Haskap berry growers

Future parts of the study will try to identify interested parties from within those sub-sectors.

Appendix D – Brief to Testing / Fermenting Labs

The following flow diagram was provided to Testing / Fermenting labs as the basis for commercial discussion of the desired processes.



Appendix E – Affinity Labs Report

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Final Report

FermenTasmania Bioactivity Assessment of Apples and Cherries

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Contributors: Dr. Eva Sui
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Project Reference: PAF24144

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1. Introduction

FermenTasmania is currently undertaking research into the current uses of fruit seconds and by-products in Tasmania, to investigate the viability of increasing the economic value derived by growers (and others). Several main opportunities exist for Tasmanian fruit growers as have been established prior to engagement with Affinity Labs. On the basis of this preceding work, apples and cherries were shown to have annual waste streams high enough to explore viable alternative opportunities, and hence were selected for further profiling.

Affinity Labs were engaged by FermenTasmania to test the polyphenolic content of Tasmanian grown apples and cherries, including pre and post fermentation, in order to assist with the future development of a concentrated powder for sale into the nutraceutical market in Australia and globally. Early indications are that fermenting whole apples, and whole cherries into a concentrated powder may be a viable product for Tasmanian manufacturers, and this trial was established to enhance knowledge into this possible path to market.

For each of the desired test fruits; apples, and cherries the desired outcomes of the testing are to better understand:

- What are the baseline chemical profiles of polyphenols in the Test Fruits?
- Does fermentation change the bioactive / polyphenol / antioxidant content of raw fruits?
- Do different processing techniques change the bioactive / polyphenol / antioxidant content of fermented products?

This report details the outcomes of the testing, advising upon limitations brought about by fruit supply, fermentation and additional processing, and in turn presenting results of bioactivity and phenolic profiling.

2. Test Schedule

2.1 Proposed Test Schedule

Affinity Labs, through ongoing consultation with FermenTasmania, proposed the following test schedule (Table 1), whereby undertaking a series of different processing techniques on two identified test fruits, analysing the outputs through differing bioactivity assays (total phenolic content using Folin-Ciocalteu accompanied with MCP and antioxidant capacity using FRAP), and LCMS profiling of polyphenols.

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Table 1: Proposed test schedule

Test Fruits	Processing	Fermentation	Repetitions	Bioactivity Assay			LCMS Profiling
				Folin-Ciocalteu	FRAP	MCP	
Apple	Puree/Macerate		3	2	2	2	3
	Pulverisation		2	2	2	2	2
	Pulverisation + Fermentation (Bacteria 1)		2	2	2	2	2
	Freeze Dry + Grind + Fermentation (Bacteria 1)		2	2	2	2	2
	Freeze Dry + Grind		2	2	2	2	2
	Pulverisation + Fermentation (Bacteria 2)		2	2	2	2	2
	Freeze Dry + Grind + Fermentation (Bacteria 2)		2	2	2	2	2
Cherries	Puree/Macerate		3	2	2	2	3
	Pulverisation		2	2	2	2	2
	Pulverisation + Fermentation (Bacteria 1)		2	2	2	2	2
	Freeze Dry + Grind + Fermentation (Bacteria 1)		2	2	2	2	2
	Freeze Dry + Grind		2	2	2	2	2
	Pulverisation + Fermentation (Bacteria 2)		2	2	2	2	2
	Freeze Dry + Grind + Fermentation (Bacteria 2)		2	2	2	2	2
			TOTAL	28	28	28	30

2.1.1 Limiting Factors

Based on a series of limiting factors, the pulverization step as scoped initially was not followed throughout the trial. Affinity Labs was advised by the FermenTasmania team and Tom Debney, Chief Pulverisor at Food Application, Productivity, Innovation & Commercialisation (FAPIC) that there were extensive issues with pulverization of both cherries and apples. It is understood that excessive mould observed on test fruit proved preventative to pulverization. It is assumed that logistics and supply chain influences aided in this product deterioration.

A third test fruit, apple pomace, was initially discussed as a testing priority, however Affinity Labs was advised by FermenTasmania to remove this based on logistical challenges whereby the pomace appeared to be breaking down (enzymatically) throughout the supply chain.

2.2 Final Test Schedule

The final test schedule after removing the samples impacted by subsequent limiting factors is as per Table 2 below:

Table 2: Final test schedule

Test Fruits	Processing	Fermentation	Repetitions	Bioactivity Assay			LCMS Profiling
				Folin-Ciocalteu	FRAP	MCP	
Apple	Puree/Macerate		3	2	2	2	3
	Freeze Dry + Grind + Fermentation (Bacteria 1)		2	2	2	2	2
	Freeze Dry + Grind		2	2	2	2	2
	Freeze Dry + Grind + Fermentation (Bacteria 2)		2	2	2	2	2
Cherries	Puree/Macerate		3	2	2	2	3
	Freeze Dry + Grind + Fermentation (Bacteria 1)		2	2	2	2	2
	Freeze Dry + Grind		2	2	2	2	2
	Freeze Dry + Grind + Fermentation (Bacteria 2)		2	2	2	2	2
			TOTAL	16	16	16	18

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3. Materials and Method

3.1 Process Flow Map

Figure 1 represents a process flow map visualising the core project details. Each element within Figure 1 will be expanded upon with the following sub-sections of the report.

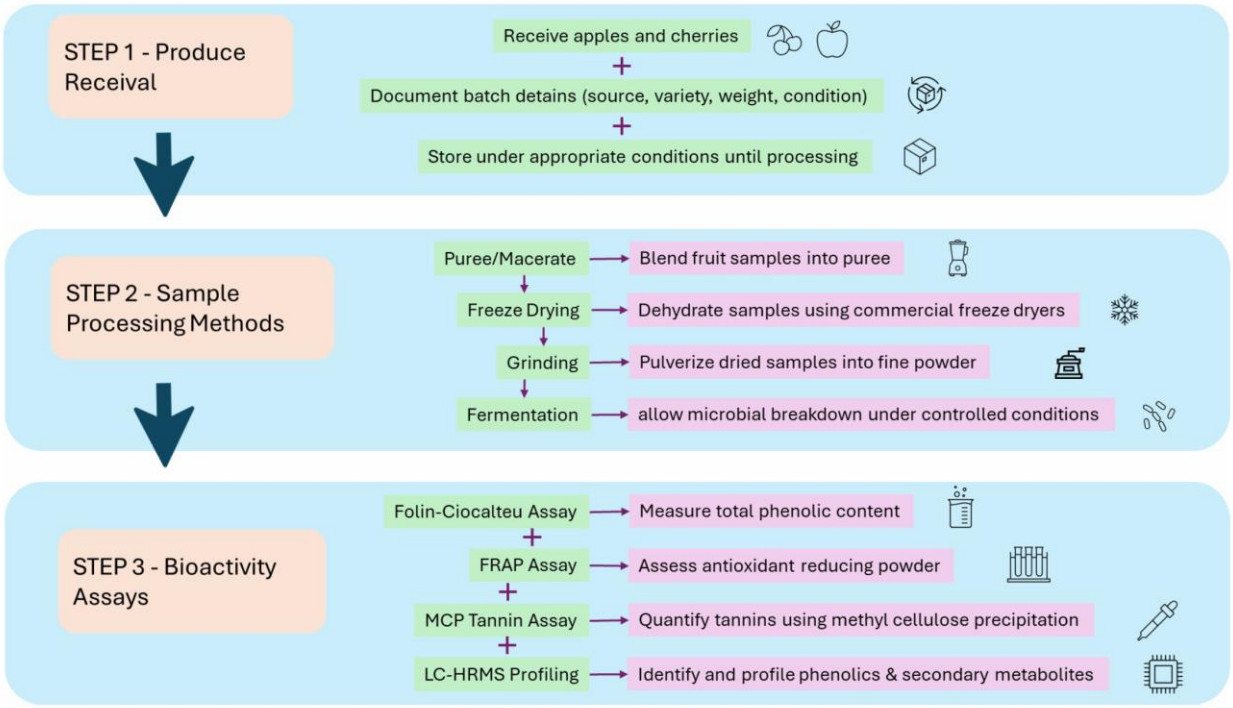


Figure 1: Process Flow Map

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3.2 Produce provided – Apple and Cherries

Approximately 15 kg of each test fruit (i.e. apples and cherries) were provided to Affinity Labs from Tasmanian producers identified through FermenTasmania. Samples arrived unfrozen and upon receipt of samples onsite at Affinity Labs they were placed in freezer storage, stored at -20°C prior to any processing to avoid degradation. Figure *2* depicts the apples as packaged and received onsite at Affinity Labs.



Figure 2: Test fruit (apples) upon receipt of delivery at Affinity Labs.

3.3 Processing methods

3.3.1 Purée/Macerate sample processing

Apple and cherry samples were defrosted overnight at 4°C prior to processing. Apples were cored and cut into eighths while cherries were pitted and halved before transferring to a Nutribullet for puréeing/macerating. All macerated samples were stored frozen at -20°C prior to subsequent analysis.

3.3.2 Commercial Scale Freeze Drying

Apple and cherry samples were defrosted overnight at 4°C prior to freeze drying in a commercial freeze drier hired through the South Australian Research and Development Institute - SARDI | Department of Primary Industries and Regions (Waite Campus, Adelaide). Apples were cored and cut into eighths while cherries were pitted and halved before transferring to the commercial freeze drier (Figure 3). Samples were freeze dried for seven (7) days.

3.3.3 Grinding

Freeze dried apples and cherries were ground into powder form using a Nutribullet. All freeze-dried samples were stored frozen at -20°C prior to subsequent analysis.

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Figure 3: Apples and cherries processed in bulk through SARDI commercial freeze drier.

3.3.4 Fermentation

Two commercial bacteria (Vegetable (V) culture and Yoghurt (Y) culture sourced from Mad Millie, QLD) were selected for use within the fermentation stage (Figure *4*). Bacteria selection stemmed from the consideration of undertaking a Lactic Fermentation (Liu, Z., et al 2023). Glass preservation jars were cleaned and autoclaved prior to fermentation. Caps/lids for the jars and other tools were UV light treated for 20 minutes. MilliQ water was used to rehydrate apple and cherry powders prior to fermentation. Two rehydration levels were chosen; 5% and 10% to achieve various sugar levels of the rehydrated apple or cherry mix. A 5% rehydration meant 10 g apple or cherry powder was added into 200 mL of MilliQ water. A 10% rehydration meant 20 g of apple or cherry powder was added into 200 mL of MilliQ water. Mixtures were stirred before inoculation with either V or Y culture mixes. Each fermentation treatment was prepared in duplicate (Figure *5*). The inoculation rate was 0.1 g of mixed V or Y culture into each 200 ml of ferment. All ferments were sealed and transferred to a 28°C incubator to engage fermentation for up to seven (7) days. Samples were monitored daily. Please refer to Table 3 for full sample list for the fermented samples. One of the apple fermentations (10% apple+ V rep2) was contaminated by mould during fermentation and hence was removed from the trial.



Figure 4: Vegetable culture and yoghurt culture sourced from Mad Millie, QLD to support Lactic fermentation

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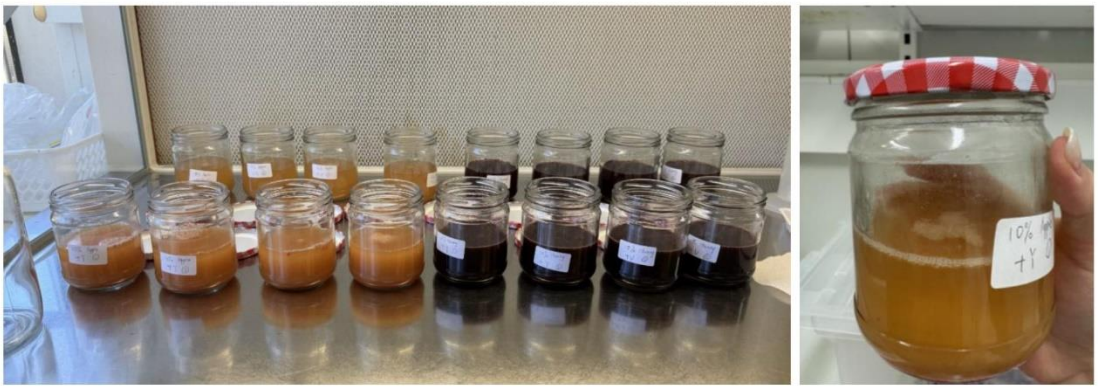


Figure 5: Lactic fermentation set up of test fruits.

Table 3: Final sample list for the fermented samples

Test Fruit: Apple Pre-fermentation processing: Freeze Dry and Grind	Test Fruit: Cherry Pre-fermentation processing: Freeze Dry and Grind
5% apple +V rep1	5% Cherry +V rep1
5% apple +V rep2	5% Cherry +V rep2
5% apple +Y rep1	5% Cherry +Y rep1
5% apple +Y rep2	5% Cherry +Y rep2
10% apple +V rep1	10% Cherry +V rep1
10% apple +Y rep1	10% Cherry +V rep2
10% apple +Y rep2	10% Cherry +Y rep1
	10% Cherry +Y rep2

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3.4 Bioactivity Assays

Fermented juice samples were stored in a -18°C freezer until use. Frozen samples were defrosted in the fridge and centrifuged at 3,500 rpm for 8 minutes. The supernatants were sub-sampled into 10 ml centrifuge tubes with minimal headspace and immediately frozen. The remaining samples were sub-sampled into multiple 1.5 ml PCR tubes and stored at -18°C until further analysis. Samples were defrosted as needed.

For purée and freeze-dried powder samples, 1 g of each homogenised sample was mixed with 10 ml of 50% (v/v) ethanol. The mixtures were placed on a roller mixer for one hour, then centrifuged. The extracts (supernatant) were sub-sampled into 1.5 ml PCR tubes and stored at -18°C for further testing.

3.4.1 Folin-Ciocalteu Assay

The Folin-Ciocalteu assay uses Folin-Ciocalteu's phenol reagent to quantify antioxidant content in samples. The reagent consists of a mixture of phosphomolybdate and phosphotungstate. This assay is a colorimetric measurement of antioxidants, including flavonoids, anthocyanins, and non-flavonoid phenolic compounds.

All standards and extracts were brought to room temperature before analysis. 100 µL of the sample was transferred into a 1.5 ml PCR tube. 200 µL of Folin-Ciocalteu reagent and 800 µL of 20% Na_2CO_3 were added to the tube. The mixture was heated at 37°C for 30 minutes using a heating block, then cooled on ice. The tubes were centrifuged at 10,000 rpm for 2.5 minutes. 100 µL of the supernatant was transferred into a well of a 96-well plate. A blank measurement of the 96-well plate was taken prior to adding the samples.

A standard curve was prepared using 1,000 mg/L gallic acid standards. The primary stock solution was further diluted to produce working standards at six concentration levels: 0, 43.75, 87.5, 175, 250, 500, and 700 mg/L. The resulting equation was:

$$\frac{\text{Abs765nm (gallic acid)} + 0.2766)}{0.005}$$

with an R^2 value of 0.9917 (Figure *6*).

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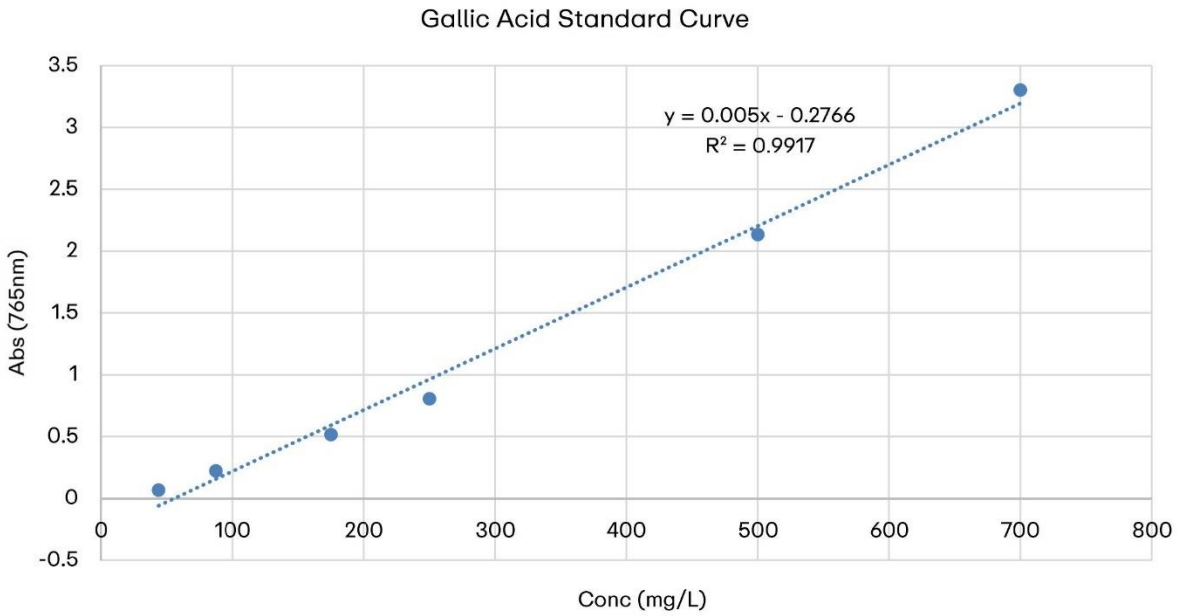


Figure 6: Gallic Acid Standard Solution Calibration Curve

3.4.2 Ferric reducing antioxidant power (FRAP) assay

The FRAP (Ferric Reducing Antioxidant Power) assay measures the reducing power of antioxidants in a sample by monitoring the reduction of Fe(III) to Fe(II). This reaction changes the colour from colourless to blue, which can be quantified by measuring absorbance at 594 nm. The absorbance readings correlate with the electron-donating ability of antioxidants, allowing the assay to rank reducing power and antioxidant potential across a variety of compounds.

The FRAP reagent was prepared fresh daily and stored in the fridge until use. The reagent was brought to room temperature before use. Standards were also prepared fresh daily. The entire reaction was performed in a 96-well plate. Two FRAP assays were performed on two different dates on freshly defrosted samples.

Each well contained 10 µL of the sample + 190 µL of FRAP reagent. Each sample also had a background mix scan (10 µL sample +190 µL of background mix solution). After adding the FRAP reagent and background mix to each sample well, the plate was measured in dark using kinetic mode.

Absorbance was recorded at 594 nm at 37°C. Readings were taken every 10 minutes for 60 minutes, resulting in a total of six measurements. 0 minute was also taken as reference. Absorbance values at 60 minutes were used for calculations.

A standard curve was prepared and plotted using 5 mM ferrous ammonium sulphate, with concentration range from 0.2 to 5 mM. The resulting equation was

$$\frac{\text{Abs 594nm (Ferrous ammonium sulphate)} + 0.0324)}{0.6753}$$

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with an R^2 value of 0.9994. (Figure 7)

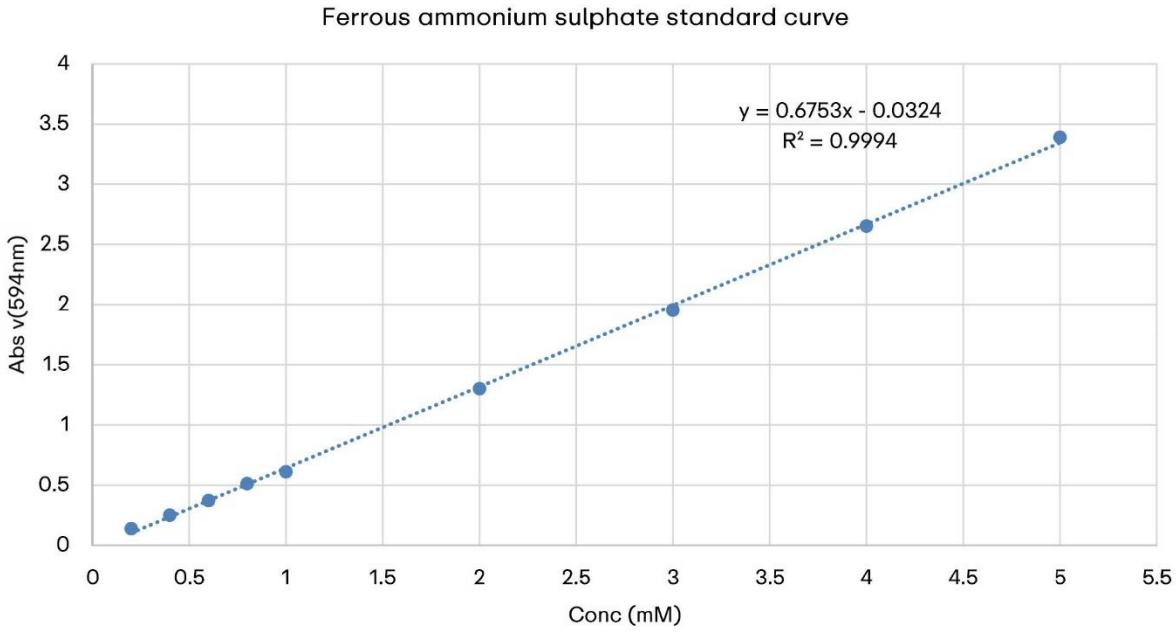


Figure 7: Ferrous ammonium sulphate solution calibration curve

3.4.3 Methyl cellulose precipitable (MCP) tannin assay

The MCP assay is a simple and robust method for measuring total tannin content in red grape homogenate extracts, red wine, and other aqueous solutions (Sarneckis et al., 2005; Smith, 2005; Mercurio & Smith, 2006). The assay is based on polymer-tannin interactions, resulting in the formation of insoluble polymer-tannin complexes that then precipitate.

1 ml of each fermented juice sample and extract was mixed with 3 ml of 0.04% methyl cellulose solution. Then, 2 ml of saturated ammonium sulphate was added to precipitate protein molecules. Distilled water was added to each test tube to bring the total volume to 10 ml. The solutions were left to settle for 12 minutes before centrifugation. The supernatant was measured using UV-Vis spectrophotometry at 280 nm.

A standard curve was prepared using 3 mg/L tannic acid at five concentration levels: 0, 0.0075, 0.015, 0.03, 0.045, and 0.075 mg/L. The resulting equation was:

$$\frac{\text{Abs280nm (Tannin)} - 0.0268)}{4.0995}$$

with an R^2 value of 0.9981 (Figure 8)

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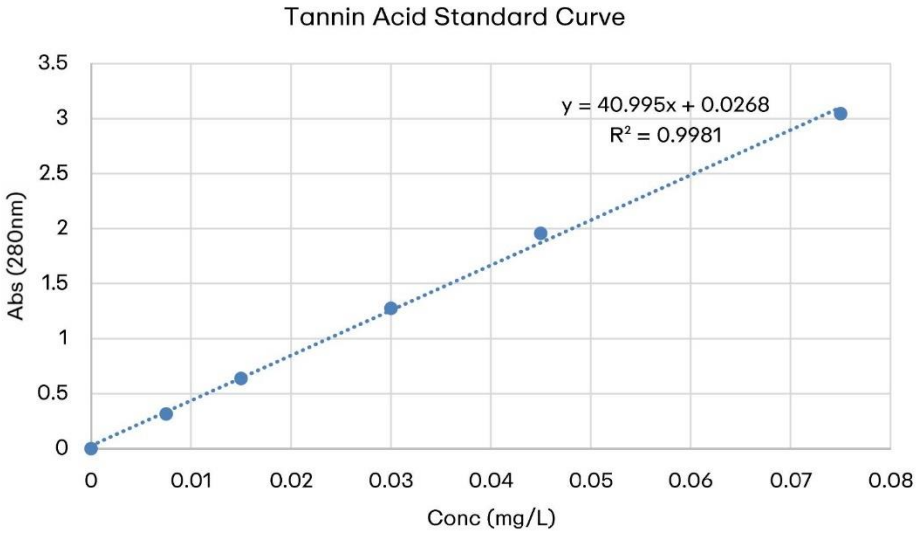


Figure 8: Tannin Standard Solution Calibration Curve

3.4.4 Profiling of phenolics using LC-HRMS (secondary metabolites)

The profiling of phenolics was outsourced to Metabolomics SA, their analysis specifically characterized non-polar secondary analytes. The methodology used is outlined below. The samples provided for analysis and the recorded weights of freeze dried material provided is as per Table 4 and Table 5 .

Table 4: Test fruit (apples) sample list for profiling of phenolics through Metabolomics SA.

Sample	Class	Weight (mg)
10% apple +V rep1	10% apple+V	392.4
10% apple +Y rep1	10% apple+Y	194.1
10% apple +Y rep2	10% apple+Y	328.5
5% apple +V rep1	5% apple +V	96.3
5% apple +V rep2	5% apple +V	108.8
5% apple +Y rep1	5% apple +Y	184.7
5% apple +Y rep2	5% apple +Y	120.7
Apple FD+G rep1	Apple FD+G	500.7
Apple FD+G rep2	Apple FD+G	499.7
Apple purée rep1	Apple purée	500.6
Apple purée rep2	Apple purée	499.8
Apple purée rep3	Apple purée	499.2

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Table 5: Test fruit (cherries) sample list for profiling of phenolics through Metabolomics SA.

Sample	Class	Weight (mg)
10% Cherry +V rep1	10% Cherry +V	235.6
10% Cherry +V rep2	10% Cherry +V	251.5
10% Cherry +Y rep1	10% Cherry +Y	242.5
10% Cherry +Y rep2	10% Cherry +Y	217
5% Cherry +V rep1	5% Cherry +V	81.1
5% Cherry +V rep2	5% Cherry +V	63.2
5% Cherry +Y rep1	5% Cherry +Y	75.6
5% Cherry +Y rep2	5% Cherry +Y	65.7
Cherry FD+G rep1	Cherry FD+G	500.2
Cherry FD+G rep2	Cherry FD+G	499.3
Cherry purée rep1	Cherry purée	500.2
Cherry purée rep2	Cherry purée	500.6
Cherry purée rep3	Cherry purée	500.1

3.4.4.1 Sample preparation

Samples were received by Metabolomics SA as freeze-dried material. The amount of freeze-dried material varied across samples. When possible 500 mg of each sample was used, otherwise the entire mass submitted was used. Recorded weights can be found in Table 4 and Table 5.

Freeze-dried material was weighed in a 10 mL tube, into which 5 mL of a water/chloroform/methanol mixture (1:2:2) was added. The samples were vortexed for 1 minute and extracted using an orbital shaker for 15 minutes.

Samples were then centrifuged at 4,500 rpm for 25 minutes at 4 °C and the supernatant collected. The pellet was re-extracted by adding 1 mL of water and 2 mL of methanol, vortexed and extracted using an orbital shaker for 15 min.

Centrifugation at 4,500 rpm for 25 minutes at 4 °C was repeated and the supernatant was combined with the one obtained from the first extraction.

The samples were dried using a nitrogen evaporator, using a flow of 3.5 mL/mins at 30 °C. The dried samples were reconstituted using 8 mL of MilliQ water and vortexed for 30 seconds.

SPE extraction was then performed using Phenomenex Strata-X polymeric RP SPE cartridges (60 mg/3mL). The cartridges were conditioned using 1 mL methanol and 1 mL Milli-Q water. The reconstituted sample extract (8 mL) was loaded, and cartridges were washed with 2% methanol (1 mL) and dried under vacuum (5min).

Sample analytes were eluted with 1 mL of methanol and extract collected. The extracts were dried using a nitrogen evaporator using 3.5 mL/min nitrogen flow and a water bath held at 30°C.

The dried samples were resuspended in 50uL solvent A (0.5% MeOH and 0.1% formic acid in MilliQ water) then vortexed for 20 seconds. Following this, 50µL of solvent B was added (40% acetonitrile,2% MilliQ water and 0.1% formic acid in MeOH) before being vortexed for 20 seconds. The samples were centrifuged, and supernatant transferred into the 250 µL insert of a 2 mL HPLC vial for analysis.

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Prior to analysis the vial inserts containing the sample extract were further centrifuged into Eppendorf tubes for 4 min at 3,800 rpm due to the presence of precipitate. The supernatant was collected for all samples and transferred into new inserts for analysis.

A PBQC (Pooled Biological Quality Control) for each sample type (apple and cherry) was prepared by mixing equal aliquots from individual samples. PBQC analytical replicates were analysed along the sequence and used as QC steps to monitor the instrument performance (data not reported).

3.4.4.2 Chemical analysis.

Separation was performed on a Thermo Vanquish horizon LC system coupled to a Thermo Orbitrap Tribrid IDX. Samples were acquired in MS and MS/MS negative mode. The operating conditions are listed in Table 6, Table 7, and Table 8. The HPLC method and MS conditions used, capture a wide range of molecules with molecular weights in the range 50-1000 amu.

Table 6: Operating conditions of LC system

Injection Volume	**4 µL MS, 8 µL MS/MS**
Flow rate	0.4 mL/min
Solvent A	0.1% formic acid, 0.5% Methanol in Milli-Q water
Solvent B	0.1% formic acid, 2% MilliQ water 40% Acetonitrile in Methanol
Column	Phenomenex Kinetex F5 2.6 µm 150mm x 2.1mm ID
Column oven temperature	30°C
LC runtime	42 min

Table 7: Solvent table

Time (min)	Flow Rate (ml/min)	% Solvent B
0.00	0.4	0.0
6.25	0.4	1.0
20.00	0.4	7.5
30.00	0.4	60.0
33.00	0.4	90.0
38.00	0.4	90.0
38.20	0.4	0.0
38.40	0.4	90.0
38.60	0.4	0.0
38.80	0.4	90.0
39.00	0.4	0.0
42.00	0.4	0.0

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Table 8: Operating conditions of MS

	H-ESI negative mode
Spray Voltage	3400 V
Sheath Gas	25
Aux Gas	7
Sweep Gas	1
Ion transfer Tube Temperature	275 °C
Vaporiser Temperature	300 °C

3.4.4.3 Data processing

Raw data was exported and processed using Thermo Compound Discoverer version 3.3 SP2. The exported files of MS data were organised in classes according to Variety and Planting Site. Each class included the analyses of the 3 biological replicates. In addition, a sample class for each pooled sample (containing 6 replicates for each variety) was created. Pooled samples were analysed to allow for comparisons among varieties regardless of planting site. MS/MS data was used for compound identification purposes only.

Procedural blanks and several QC samples were also acquired to monitor instrument performance along the acquisition sequence.

The selected workflow included the following steps:

- Compound and adduct detection
- Retention time alignment
- Background Noise filtering
- Compound formula assignation based on detected accurate mass
- Putative identification based on Chem Spider Databases
- Putative identification based on spectral libraries (in house built and on-line)

After the processing was concluded, the data was manually inspected to remove compounds that did not satisfy the minimum area value criteria and/or minimum peak shape quality.

The relative abundance of each compound in the samples is reported as normalised area (areas were normalised on sample weights). ***Samples are to be qualitatively compared based on relative abundances.***

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4. Results and Discussion

For the purposes of the bioactivity assay comparisons, ideally, a 5% and 10% rehydrated sample would have been available as a control. Given this limitation, we are still in a position to compare based on fruit concentration:

- Puree: 1g in 10 ml = 100g/L
- Grind: 1g in 10ml = 100g/L
- 5%: 10g in 200ml = 50g/L
- 10%: 20g in 200ml = 100g/L

To normalise the data, the 5% ferment outcome has been result by 2 to bring the concentration to 100g freeze-dried grind/L.

The results for each assay were divided into two tables. **Table A** presents the raw data based on test volume (1 gram of puree and 1 gram of freeze-dried grind). **Table B** adjusts the results to correlate with the fruit's dry weight (DW), where apple and cherry puree have a DW of approximately 30% and 20%, respectively, while the corresponding freeze-dried grind has a DW of approximately 95%.

4.1 Apples

4.1.1 Folin-Ciocalteu Assay

Among all treatments, the freeze-dried grind exhibited the highest phenolic content, measuring more than three times greater than the macerate (control) treatment (Table 9a). In the fermentation trials, 5% samples fermented with Bacteria V and Y retained more phenolic content than those fermented with 10% fruit contents with Bacteria V and Y.

The dry weight-adjusted total phenolic content results (Table 9b) indicate that the freeze-dried grind exhibited a 10% higher phenolic content compared to the purée/macerate (control). This suggests that the freeze-drying process helps retain more phenolic compounds relative to the purée,

Table 9a: Total Phenolic Content (expressed in gallic acid equivalents) in Different Apple Treatments, measured by the Folin-Ciocalteu Assay.

		Unit	Rep 1	Rep 2	Average	Total phenolic content difference in % compared to Purée (control)
Purée/ Macerate		mg/L	120.5	114.0	117.2	
Ferment*^	V + 5%	mg/L	208.9	209.3	209.1	+78%
	Y + 5%	mg/L	234.1	256.0	245.0	+109%
	V + 10%	mg/L	150.2	N/A	150.2	+28%
	Y + 10%	mg/L	127.5	178.9	153.2	+31%
Freeze Dried Grind		mg/L	425.5	388.7	407.1	+247%

*: V =vegetable culture, and Y = yoghurt culture; ^: 5% = 10 g freeze-dried ground apple added into 200 mL of MilliQ water, and 10% =20 g of freeze-dried apple grind added into 200 mL of MilliQ water.

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Table 10b: Dry Weight-Adjusted Total Phenolic Content (Extension of Table 9a)

	Unit	Rep 1	Rep 2	Average	Total phenolic content difference in % compared to Purée (control)
Purée/ Macerate	mg/L	401.5	380.0	390.7	
Freeze Dried Grind	mg/L	447.9	409.2	428.5	10%

4.1.2 Ferric reducing antioxidant ability (FRAP) assay

The FRAP assay has a detection limit of 3.5 absorbance units, which was reached by the freeze-dried grind at 60 minutes, indicating a high antioxidant capacity. The intensity of the blue complex formed in the assay is proportional to the ability of the sample to reduce Fe^{3+} ions, with darker blue indicating stronger electron-donating potential and higher antioxidant capacity. As shown in Table 11a, the 5% fermentation treatment exhibited the lowest antioxidant capacity, while the freeze-dried and ground had the highest. The 10% ferments demonstrated greater antioxidant capacity than both the macerate and 5% ferment samples; however, the available data is insufficient to establish a clear correlation between fruit content percentage and antioxidant capacity.

The dry weight-adjusted antioxidant capacity results (Table 10b) show that the freeze-dried grind had a saturated FRAP reading (>5 mM) in all replicates, indicating a significantly higher antioxidant capacity compared to the purée/macerate (control), which averaged 3.4 mM. Due to the saturation of the measurement, the exact percentage difference could not be determined, but the results suggest that freeze-drying preserves or enhances antioxidant activity more effectively than the purée treatment in apple.

Table 11a: Antioxidant capacity in Different Apple Treatments, measured by the FRAP Assay.

			FRAP 1		FRAP 2			
		Unit	Rep 1	Rep 2	Rep 1	Rep 2	Average	Antioxidant capacity difference in % compared to Purée (control)
Purée/ Macerate		mM	1.3	1.2	1.1	1.0	1.1	
Ferment*^	V + 5%	mM	2.2	2.1	1.3	1.7	1.8	+60%
	Y + 5%	mM	2.3	2.1	1.8	1.7	2.0	+73%
	V + 10%	mM	1.8	N/A	1.6	N/A	1.7	+48%
	Y + 10%	mM	1.7	1.8	1.4	1.4	1.6	+38%
Freeze Dried Grind		mM	>5	>5	>5	>5	>5	-

Table 12b: Dry Weight-Adjusted Total Phenolic Content (Extension of Table 10a)

		FRAP 1		FRAP 2			
	Unit	Rep 1	Rep 2	Rep 1	Rep 2	Average	Antioxidant capacity difference in % compared to Purée (control)
Purée/ Macerate	mM	4.3	4.0	3.6	3.3	3.4	
Freeze Dried Grind	mM	>5	>5	>5	>5	>5	-

4.1.3 Methyl cellulose precipitable (MCP) tannin assay

All treatments resulted in a reduction of tannic acid or other precipitable phenolic content compared to the control (Table 13a). The freeze-dried grind showed the smallest reduction (6%), while the 5% and 10% ferments

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with Bacteria Y exhibited a 43 and 45% reduction, respectively. The remaining treatments achieved tannic acid reductions exceeding 50%.

The dry weight-adjusted total tannic acid content results (Table 11b) show that the freeze-dried grind had a significantly lower tannic acid concentration (26.0 mg/L) compared to the purée/macerate (87.2 mg/L). This represents a 70% reduction in tannic acid content in the freeze-dried grind, suggesting that the freeze-drying process may lead to reduced extractability or tannin (or polyphenols) degradation.

Table 13a: Total Phenolic Content (expressed in tannic acid equivalents) in Different Apple Treatments, Measured by the MCP Assay.

		Unit	Rep 1	Rep 2	Average	Total tannic acid difference in % compared to Purée (control)
Purée/ Macerate		mg/L	27.2	25.1	26.2	
Ferment*^	V + 5%	mg/L	11.9	7.4	9.6	-63%
	Y + 5%	mg/L	10.8	18.9	14.8	-43%
	V + 10%	mg/L	17.0	0.09	8.5	-67%
	Y + 10%	mg/L	14.9	14.1	14.5	-45%
Freeze Dried Grind		mg/L	24.6	24.7	24.7	-6%

Table 14b: Dry Weight-Adjusted Total Phenolic Content (Extension of Table 11a),

	Unit	Rep 1	Rep 2	Average	Total tannic acid difference in % compared to Purée (control)
Purée/ Macerate	mg/L	90.7	83.7	87.2	
Freeze Dried Grind	mg/L	25.9	26.0	26.0	-70%

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4.2 Cherries

4.2.1 Folin-Ciocalteu Assay

Among all treatments, the freeze-dried grind once again exhibited the highest phenolic content, measuring at least twice as much as the macerate (control) treatment (*Table 15a*). In the fermentation trials, samples fermented with both bacterial strains produced similar results, while lower fruit content percentages were associated with lower total phenolic content.

The dry weight-adjusted total phenolic content results (Table 12b) indicate that the freeze-dried grind (434.8 mg/L) contained 45% less total phenolics compared to the purée/macerate (783.4 mg/L). This suggests that while freeze-drying cherries preserves some phenolic compounds, there may be losses due to degradation, oxidation, or reduced extractability in the dried form.

Table 15a: Total Phenolic Content (expressed in gallic acid equivalents) in Different Cherry Treatments, Measured by the Folin-Ciocalteu Assay.

		unit	Rep 1	Rep 2	Average	Total phenolic content difference in % compared to Purée (control)
Purée/ Macerate		mg/L	161.4	152.0	156.7	
Ferment*^	V + 5%	mg/L	328.9	292.1	310.5	+98%
	Y +5%	mg/L	330.0	265.8	297.9	+90%
	V +10%	mg/L	375.5	336.1	355.8	+127%
	Y +10%	mg/L	324.4	347.1	335.7	+114%
Freeze Dried Grind		mg/L	404.5	421.6	413.1	+164%

*: V for vegetable culture and Y for yoghurt culture; ^: 5% = 10 g freeze-dried cherry grind added into 200 mL of MilliQ water, and 10% =20 g of freeze-dried cherry grind added into 200 mL of MilliQ water.

Table 16b: Dry Weight-Adjusted Total Phenolic Content (Extension of Table 12a).

	unit	Rep 1	Rep 2	Average	Total phenolic content difference in % compared to Purée (control)
Purée/ Macerate	mg/L	806.9	759.9	783.4	
Freeze Dried Grind	mg/L	425.8	443.8	434.8	-45%

4.2.2 Ferric reducing antioxidant ability (FRAP) assay

Similar to apples, the freeze-dried grind displayed the highest antioxidant capacity, with absorbance readings reaching saturation before the final plate reading at 60 minutes. The 10% ferments demonstrated greater antioxidant capacity than both the macerate and 5% ferment samples (*Table 17a*). However, a clear correlation between fruit content percentage and antioxidant capacity has yet to be established due to limited data.

The dry weight-adjusted antioxidant capacity results (Table 13b) show that the freeze-dried grind reached the upper detection limit of the FRAP assay (>5 mM), preventing precise quantification. In contrast, the purée/macerate had an average antioxidant capacity of 9.6 mM. This suggests that while freeze-dried samples may still retain antioxidant activity, the FRAP assay's limitations make direct comparison difficult. Further refinement of the assay method or dilution of freeze-dried samples may be necessary for more accurate assessment.

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Table 17a: Antioxidant capacity in Different Cherry Treatments, Measured by the FRAP Assay.

			FRAP 1		FRAP 2		Average	Antioxidant capacity difference in % compared to Purée (control)
		unit	Rep 1	Rep 2	Rep 1	Rep 2		
Purée/ Macerate		mM	2.2	2.2	1.9	1.9	2.1	
Ferment^^	V + 5%	mM	4.1	3.6	3.0	2.9	3.4	+65%
	Y +5%	mM	3.2	3.8	2.6	2.3	3.0	+44%
	V +10%	mM	4.6	4.6	3.0	2.7	3.7	+81%
	Y +10%	mM	4.0	4.4	2.7	2.4	3.4	+64%
Freeze Dried Grind		mM	>5	>5	>5	>5	>5	

Table 18b: Dry Weight-Adjusted Total Phenolic Content (Extension of Table 13a).

		FRAP 1		FRAP 2		Average	Antioxidant capacity difference in % compared to Purée (control)
	unit	Rep 1	Rep 2	Rep 1	Rep 2		
Purée/ Macerate	mM	11.0	11.1	9.5	9.6	9.6	
Freeze Dried Grind	mM	>5	>5	>5	>5	>5	-

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4.2.3 Methyl cellulose precipitable (MCP) tannin assay

All treatments resulted in a reduction of tannic acid or other precipitable phenolic content compared to the control. All fermented samples exhibited a 90% reduction in precipitable phenolic content relative to the control, except for the 10% ferment with Bacteria V, which showed an 85% reduction (Table 19a).

The dry weight-adjusted total tannic acid results (Table 14b) indicate that the freeze-dried grind had a lower tannic acid content (103.1 mg/L), representing an 83% reduction compared to the purée/macerate (601.8 mg/L). This suggests that the freeze-drying process may lead to substantial tannin degradation or reduced extractability. Further studies could investigate whether this reduction is due to structural changes in the tannins (or polyphenols) or interactions with other compounds during processing.

Table 19a: Total Phenolic Content (expressed in tannic acid equivalents) in Different Cherry Treatments, Measured by the MCP Assay.

		unit	Rep 1	Rep 2	Average	Total tannic acid difference in % compared to Purée (control)
Purée/ Macerate		mg/L	119.4	121.3	120.36	
Ferment*^	V + 5%	mg/L	12.5	23.2	17.86	-85%
	Y +5%	mg/L	12.7	14.2	13.49	-89%
	V +10%	mg/L	14.2	22.0	18.12	-85%
	Y +10%	mg/L	11.8	9.5	10.65	-91%
Freeze Dried Grind		mg/L	99.9	95.9	97.90	-19%

Table 20b: Dry Weight-Adjusted Total Phenolic Content (Extension of Table 14a)

	unit	Rep 1	Rep 2	Average	Total tannic acid difference in % compared to Purée (control)
Purée/ Macerate	mg/L	597.0	606.5	601.8	
Freeze Dried Grind	mg/L	105.2	100.9	103.1	-83%

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4.3 Phenolic Profiling of Apples and Cherries

Putative identification of compounds reported as a result of the non-polar metabolite profiling of apple and cherry samples by reverse phase HPLC HRFTMS was achieved utilising two (2) different approaches described below. The first approach provides the highest level of confidence in compound annotation by comparing the detected MS/MS spectra with the MS/MS spectra present in the Metabolomics SA internal database and an online spectral database (mzCloud, Thermo Scientific). The algorithm used for comparison was Thermo's "HighChem HighRes" and similarity was expressed as percentage. Values below 50% of spectra similarity were discarded because they are considered unreliable.

The second approach of compound identification is applied for compounds where no MS/MS spectra match could be assigned but the identification is based on the compatibility of molecular formula with the compounds present in databases. Specific databases were utilised for the compound assignment in this approach, including those specific for plant metabolites and phenolic compounds. The following databases were included in the search: "Phenol Explorer", "Small Molecules", "Kegg", "Nature Chemistry" and "Natural Products".

The relative abundance of each compound in the samples is reported as normalised area (areas were normalised on sample weights). Full data outputs are presented in Appendix A.

By way of a quick summary, for apple samples a series of 170 compounds were detected. The most abundant throughout were as shown in Table 15. Table 15 further provides details as to key potential characteristics of each of the most phenolic compound:

Table 21: Most abundant phenolic compounds identified in apples and their key potential characteristics

Phenolic Compound	Key potential characteristics
2-Isopropylmalic acid	A metabolic intermediate involved in amino acid biosynthesis, contributing to cellular energy production and potentially supporting metabolic health.
DL-4-Hydroxyphenyllactic acid	Exhibits antimicrobial and antioxidant properties, with potential applications in natural food preservation and skincare formulations.
Caffeic acid	A potent antioxidant with anti-inflammatory, anti-cancer, and neuroprotective properties, often utilized in nutraceuticals and functional foods.
Epicatechin	A flavanol with cardiovascular benefits, improving blood circulation, reducing oxidative stress, and supporting cognitive health.
Chlorogenic acid	Known for its anti-diabetic properties, aiding glucose metabolism, weight management, and liver protection.
Catechin	Offers strong antioxidant activity, promoting heart health, reducing inflammation, and supporting neuroprotection.
Rutin	A flavonoid with vascular-protective effects, strengthening blood vessels, reducing hypertension, and exhibiting anti-inflammatory and anti-allergic benefits.
Astragalin	A bioactive flavonoid with anti-inflammatory, anti-allergic, and neuroprotective properties, used in pharmaceutical and skincare products.
Phloridzin	Unique to apples, this compound regulates glucose absorption, making it valuable for managing diabetes and metabolic disorders.

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Quercetin	A powerful antioxidant with anti-cancer, immune-boosting, and cardiovascular benefits, frequently used in dietary supplements.

For cherry samples a series of 332 compounds were detected. The most abundant throughout were as follows. The most abundant throughout were as shown in Table 16. Table 16 further provides details as to key potential characteristics of each of the most phenolic compound::

Table 22: Most abundant phenolic compounds identified in cherries and their key potential characteristics

Phenolic Compound	Key potential characteristics
2-Isopropylmalic acid	Functions as a key intermediate in metabolic pathways, contributing to amino acid biosynthesis and energy production.
DL-4-Hydroxyphenyllactic acid	Displays antimicrobial and antioxidant effects, beneficial in functional foods and probiotic formulations.
2-Hydroxycaproic acid	Supports metabolic health and is linked to skin and cellular repair mechanisms, useful in cosmetic applications.
Neochlorogenic acid	A powerful antioxidant that protects against oxidative stress, inflammation, and age-related diseases.
2-Hydroxy-4-(4-hydroxyphenyl)butanoic acid	Potential neuroprotective compound with anti-inflammatory and free-radical scavenging properties.
L-(-)-3-Phenyllactic acid	Known for its antimicrobial properties, supporting gut health and probiotic efficacy in functional foods.
Quercetin	A powerful antioxidant with anti-cancer, immune-boosting, and cardiovascular benefits, frequently used in dietary supplements.
(15Z)-9,12,13-Trihydroxy-15-octadecenoic acid	A bioactive lipid with anti-inflammatory and cardioprotective properties, potentially beneficial in skincare and cardiovascular supplements

Replicate consistency was observed in cherry samples however significant variability was observed in apple replicates.

Data visualisation for both test fruits is represented in Appendix B, where heat maps have been provided. The provided heat maps are a graphical representation of the phenolic composition data where individual values are depicted using colour gradients.

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5. Summary

Among all treatments, freeze-dried powder exhibited the highest antioxidant activity and total phenolic content, followed by the purée/macerate treatment. Fermented juice (both 5% and 10%) contained the lowest levels of phenolic compounds and antioxidant activity. However, these results are specific to the preparation methods and bacterial strains used in this study.

The use of only two dilution levels (5% and 10% fruit content) was insufficient to determine the factors contributing to the decrease or increase in total phenolic compounds and antioxidant activity. Additionally, multiple variables were present in the fermentation trials, introducing unknown factors that may have influenced the results (see the next section for further discussion).

As a result, no definitive conclusions can be drawn at this stage, except that some levels of phenolic compounds and antioxidants remain present in 5% and 10% fermented juice. Future studies should explore variables such as rehydration levels, bacterial strains, fermentation duration, and temperature to better understand the relationship between fermentation and phenolic/antioxidant retention.

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6. Limitations and Further recommendations

6.1 Control and variables

6.1.1 Microbial diversity

Microbial loads were high in freeze-dried samples prior to the fermentation trial. As a result, this study lacked full control over the microbial composition present in the glass jar, leading to a limited understanding of how these various microorganisms may have influenced total phenolic content and antioxidant activity.

Following fermentation, ferments were individually plated on WL plates to determine presence of bacteria. By appearance, not much consistency in colony presence was achieved between replicates. Some samples appeared to have large satellite colonies and thus difficulty lies in understanding which of the identified strains were influencing product change through fermentation. This influence could be responsible for variations observed throughout data processing and in future applications needs to be better understood to ensure the final product is as desired based on the necessary function of the ferment.

6.1.2 Growing conditions for bacteria

To replicate a real-world fermentation environment for the selected bacterial strains, sugar levels were considered when determining the fruit content percentages for fermentation trials. The sugar content of dissolved freeze-dried powder in water was measured and compared to the sugar levels present in the recommended quantity of fruit pulp, as specified by the commercial bacterial culture supplier. However, this approach introduced additional variables, including differences in moisture content, water activity, pH levels, and the original microbiome in fresh or frozen fruit pulp, juice and/or purée.

6.1.3 Bioactivity Screening

In this study, the bioactivity assays and LC-MS profiling served as a screening tool to analyse the end products of each treatment. These results provide insights into selecting the most appropriate treatment based on the intended purpose of the final product. For instance, freeze-dried powder exhibited the highest antioxidative activity, whereas 5% fermented juice contained a broader range of phenolic compounds. This suggests that phenolics and antioxidants may be more stable in freeze-dried form, while rehydration and fermentation could facilitate the release of certain phenolics into the liquid phase through interactions with water and bacteria.

6.2 Future study directions

Rather than attempting to measure all potential phenolic compounds and bioactive components, future studies should focus on specific groups of compounds and their functionality. Investigating factors such as rehydration methods, aqueous-to-solid ratios, pH levels, and conductivity could add further value to this research by identifying optimal treatment methods for apples and cherries.

Based on comparisons to a peer reviewed study undertaken assessing phenolic composition of different apple varieties across South Australia (Bindon et al. 2023), evidence suggests that the environment may influence phenolic composition more significantly than the genotype, and based on findings within this report, some differing phenolic compounds were identified at higher relative abundances in Tasmanian apples compared to South Australian apples hence further work to classify these differences is required.

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7. References

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8. Appendix A: Non-polar metabolite profiling of apple and cherry samples by reverse phase HPLC HRFTMS

Results are summarised in the tables below. Results for apple and cherry samples are reported separately within the tables below. The relative abundance of each compound in the samples is reported as normalised area (areas were normalised on sample weights).

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Test Fruit: Apples

Name	Formula	Calc. MW	10% apple +V rep1	10% apple +Y rep1	10% apple +Y rep2	5% apple +V rep1	5% apple +V rep2	5% apple +Y rep1	5% apple +Y rep2	Apple FD+G rep1	Apple FD+G rep2	Apple purée rep1	Apple purée rep2	Apple purée rep3
Gluconic acid	C6 H12 O7	196.0582	760470	1967662	1073020	1195699	942955	1164994	2166361	11533	5116	7520	4622	11266
β-D-Glucopyranuronic acid	C6 H10 O7	194.043	334130	156631	489928	110390	1238160	1060266	807444	5620	5552	4079	4338	12878
Sucrose	C12 H22 O11	342.1163	1592	50429	1866	24698	2598	11951	4083	61733	116284	120631	135028	155002
D-(-)-Quinic acid	C7 H12 O6	192.0635	14278	83174	15622	56369	24136	14178	39741	27692	33033	373	21226	710
2-deoxyglucose	C6 H12 O5	164.0686	101	5104	192	524	104	427	404	2270	1678	1436	1559	8056
3-Hydroxyglutaric Acid	C5 H8 O5	148.0372	2496	8747	4954	7340	6719	21155	9159	6018	5435	4552	5617	26491
Galacturonic acid	C6 H10 O7	194.0427	28190	9620	489962	30964	115494	70007	78897	1080	1761	5076	5219	5690
Succinic acid	C4 H6 O4	118.0263	26050	1155144	537365	1586561	1673148	7297	321820	2975	2522	7010	2992	1612
Mevalonic acid	C6 H12 O4	148.0734	3359	287018	10505	206497	28854	749	30131	411	279	651	786	428
Adenosine	C10 H13 N5 O4	267.0967	23	463	28	934	68	38	163	10978	9514	15727	17092	114
Guanosine	C10 H13 N5 O5	283.0918	73	855	59	70	109	36	701	9820	11878	9752	9335	5726
2-Hydroxyvaleric acid	C5 H10 O3	118.0626	57561	450526	78054	869122	535436	3973	366915	519	782	3376	2277	1256
Sarmentosin	C11 H17 N O7	275.1006	19850	18375	3173	42293	42210	125	1334	214	225	142	93	39
Pantothenic acid	C9 H17 N O5	219.1106	197139	346994	285864	488454	516056	918	572573	106388	114202	134839	141653	742
Procyanidin A2	C30 H24 O12	576.1268	176	699	143	565	222	77	269	18646	17427	12441	33993	1490
8-Epideoxyloganic acid	C16 H24 O9	360.1423	13260	29830	10905	26580	20992	156	13769	6513	7070	6707	5194	406
1-O-[(2E)-3-(3,4-Dihydroxyphenyl)-2-propenoyl]-β-D-glucopyranuronic acid	C15 H16 O10	356.0746	35995	91320	41115	62860	67614	3794	54163	26946	27124	27865	27920	5125
N-Acetylnorvaline	C7 H13 N O3	159.0895	1028	12154	1880	17881	65777	71	3608	98	104	92	139	25
2-Isopropylmalic acid	C7 H12 O5	176.0682	424692	10359131	531676	8760929	941241	32288	2381185	59498	54836	75497	79163	2963
DL-4-Hydroxyphenyllactic acid	C9 H10 O4	182.0577	200796	5070627	236575	3559916	535018	12908	823308	9056	7224	7331	4458	3829
D-(−)-Salicin	C13 H18 O7	286.1053	26362	22329	21840	49113	35413	988	32290	25089	28642	22009	22618	1400
N-[(2S)-2-Hydroxypropanoyl]-L-tyrosine	C12 H15 N O5	253.0952	5446	239	2289	237	1729	75	480	23199	26541	10350	11221	4535
2-hydroxy-5-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxybenzoic acid	C13 H16 O9	316.0796	19144	30767	22236	31362	32433	750	30898	11178	12926	8556	7903	988
3-[3-(beta-D-Glucopyranosyloxy)-2-hydroxyphenyl]propanoic acid	C15 H20 O9	344.1108	107547	139979	74648	203213	95829	10772	105372	42540	40396	35973	33970	5069
1-(3-Acetyl-2,4,6-trihydroxyphenyl)-1,5-anhydrohexitol	C14 H18 O9	330.0952	62421	136904	76060	79245	132131	2864	126741	55470	56068	79793	97829	7282
5-[(E)-2-Carboxyvinyl]-2-hydroxyphenyl β-D-glucopyranosiduronic acid	C15 H16 O10	356.0746	15776	38836	16698	27255	25903	1763	21139	15125	15205	14985	17101	1844
Norsanguinarine	C19 H11 N O4	317.0689	1627	4156	1959	13980	14556	46	16693	30	26	28	39	17
5-(5-Methyl-2-furyl)-3,4-dihydro-2H-pyrrole	C9 H11 N O	149.084	9348	11938	9785	18721	14354	64	15264	7230	7570	6437	6796	32
dehypoxanthine futalosine	C14 H16 O7	296.0897	23653	43902	23994	37087	36451	200	32151	14486	14508	13009	10330	227
Neochlorogenic acid	C16 H18 O9	354.0952	225706	512449	241604	366185	329537	22824	334483	166862	189941	177752	159625	22358
2-(E)-O-feruloyl-D-galactaric acid	C16 H18 O11	386.085	8736	23299	9532	15710	11584	192	12449	3281	5023	5498	4586	288
N-Acetyl-L-tyrosine	C11 H13 N O4	223.0845	3013	3183	2279	23284	9249	71	4190	225	243	196	229	30
Deutzioside	C15 H22 O9	346.1263	39304	43117	26713	71615	44834	867	45407	32036	31883	28614	50833	1770
3-(4,7-Dimethoxy-1,3-benzodioxol-5-yl)acrylic acid	C12 H12 O6	252.0635	11774	30280	13478	25381	19585	440	20771	9808	8807	6321	5413	459
3-p-coumaroylquinic acid	C16 H18 O8	338.1005	81916	194717	76026	137393	106036	4552	115667	60921	63627	37648	42274	3600
(2E,4Z)-2-Hydroxy-6-(2-hydroxyphenoxy)-6-oxo-2,4-hexadienoic acid	C12 H10 O6	250.0478	17027	48205	19803	27897	27144	1439	28851	7277	5696	3588	3272	495
6β-hydroxygeniposide	C17 H24 O11	404.132	37129	72400	36361	57324	64291	2290	56936	42705	39247	47466	45036	2487
4-Acetyl-3-hydroxy-5-methylphenyl β-D-glucopyranoside	C15 H20 O8	328.1159	844617	1908258	961218	1883635	1302304	54085	1449562	819398	848386	627790	640243	61586
5,8,12-Trihydroxy-2-oxododecanoic acid	C12 H22 O6	262.1417	75461	182909	76785	150735	126794	756	126261	77133	60814	50769	51918	165
α-Cyano-3-hydroxycinnamic acid	C10 H7 N O3	189.0427	7755	26933	9349	23209	16615	69	15253	154	138	129	142	21
1-Caffeoyl-β-D-glucose	C15 H18 O9	342.0951	450954	1424540	480411	817445	666685	81722	667495	413365	429593	302070	250475	36338
Deoxyanisatin	C15 H20 O7	312.1209	243706	614783	254004	498374	324725	3320	347776	243518	242048	213897	238552	4981

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Test Fruit: Apples

Name	Formula	Calc. MW	10% apple +V rep1	10% apple +Y rep1	10% apple +Y rep2	5% apple +V rep1	5% apple +V rep2	5% apple +Y rep1	5% apple +Y rep2	Apple FD+G rep1	Apple FD+G rep2	Apple purée rep1	Apple purée rep2	Apple purée rep3
Neochlorogenic acid	C16 H18 O9	354.0951	673024	1562217	651547	1436823	947415	50871	1082224	516369	502132	267544	316057	32649
sec-Butyl 6-O-[(2R,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)tetrahydro-2-furanyl]-D-glucopyranoside	C15 H28 O10	368.1685	16541	40803	19058	31229	21789	2743	23514	17852	18598	16051	15075	1579
N-Acetyl-L-leucine	C8 H15 N O3	173.1052	4028	38175	5528	40285	10826	124	3787	1341	1364	1272	1265	19
N-Malonylanthranilic acid	C10 H9 N O5	223.0481	9649	44442	8414	53802	23692	84	18537	139	128	113	99	32
2-Hydroxyhippuric acid	C9 H9 N O4	195.0532	7081	33450	6253	39757	17307	128	14107	140	129	113	111	32
Leiocarposide	C27 H34 O16	614.1851	707	4219	3974	2282	5185	212	2150	31475	37320	49939	58450	3647
L-Tyrosine	C9 H11 N O3	181.0739	200	58959	136	221084	189	51	213	140	122	136	141	20
N-(2-Hydroxy-4-methoxybenzoyl)glycine	C10 H11 N O5	225.0638	540	142047	218	526566	181	49	535	134	117	130	136	19
p-Coumaric acid glucoside	C15 H18 O8	326.1003	381772	334566	406441	430709	559206	35665	495714	424773	400551	360117	353621	12549
6-Methoxy-4-oxo-3-(2,4,5-trimethoxyphenyl)-4H-chromen-7-yl 6-O-[(2R,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)tetrahydro-2-furanyl]-α-L-idopyranoside	C30 H36 O16	652.201	36603	44300	35568	24991	17202	34	18933	51521	42979	36441	48999	153
Phenylacetaldehyde	C8 H8 O	120.0574	3447	57791	2076	56636	8989	444	18834	334	318	692	661	51
3-[5-(2-methylpropyl)-3,6-dioxopiperazin-2-yl]propanoic acid	C11 H18 N2 O4	242.1267	8386	182	2911	3612	18546	43	5220	323	676	41	42	17
Aucubin	C15 H22 O9	346.1265	5913	16636	5841	11443	5785	90	7839	3067	8156	5303	6106	30
2-(Acetylamino)hexanoic acid	C8 H15 N O3	173.1052	3361	25650	3230	21491	7823	42	3015	950	885	738	796	16
4-Acetyl-3-hydroxy-5-methylphenyl β-D-glucopyranoside	C15 H20 O8	328.1157	122996	400910	145736	296252	251148	6982	253751	135360	108556	80652	69697	7832
2-(5-benzyl-3,6-dioxopiperazin-2-yl)acetic acid	C13 H14 N2 O4	262.0954	44653	86172	42467	126958	87902	1809	95304	93562	92997	95100	108779	5751
4-Hydroxy-5-(3′,4′-dihydroxyphenyl)-valeric acid-O-glucuronide	C17 H22 O11	402.1163	5088	17426	2389	25315	17993	2074	20102	29461	22875	45001	57695	7791
N-4-hydroxyphenylacetylglutamic acid	C13 H15 N O6	281.09	11028	215	9848	166	13455	42	3023	20311	18694	21785	24837	177
Esculin	C15 H16 O9	340.0797	12349	28880	14035	21514	19280	1312	22083	7866	4763	3154	3382	632
Caffeic acid	C9 H8 O4	180.0422	1418455	3383491	1061543	3279321	2130013	513280	2005891	56951	50141	30209	28125	6665
dehypoxanthine futalosine	C14 H16 O7	296.0897	14462	41454	14622	25695	19470	53	20029	14415	13009	9417	11664	60
Methyl 5,7,11-trihydroxy-2-methyl-2′,10-dioxospiro[9-oxatricyclo[6.3.1.0^1,5^]dodecane-6,3′-oxetane]-7-carboxylate	C16 H20 O9	356.111	5383	11394	4411	10595	5219	63	6189	9593	8200	10654	10688	497
Sweroside	C16 H22 O9	358.1266	176099	395767	178029	419112	264209	3694	267081	176224	170113	148924	161775	11442
(1S,2R,4R,5R,6S,7R,8S,11R)-4,5,7,11-Tetrahydroxy-2,7-dimethyl-10H-spiro[9-oxatricyclo[6.3.1.0^1,5^]dodecane-6,3′-oxetane]-2′,10-dione	C15 H20 O8	328.116	8017	16267	7771	16990	9602	308	10827	5753	4989	5255	6266	221
(1ξ)-1,5-Anhydro-1-[(2R,3R)-2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-3,4-dihydro-2H-chromen-6-yl]-D-glucitol	C21 H24 O11	452.1322	17589	15502	20306	30439	36173	4857	41299	25707	26509	24873	26274	5460
N5-Dinitrophenyl-L-ornithine methyl ester	C18 H20 N4 O6	388.1371	293193	685300	330076	713025	413854	8167	427719	274719	276919	293223	287099	6315
(1Z,2E)-1-({[(2R,3S,4S,5R,6S)-6-{[2-(3,4-Dihydroxyphenyl)-7-hydroxy-5-oxo-5H-chromen-3-yl]oxy}-3,4-dihydroxy-5-{[(2S,3R,4S,5R)-3,4,5-trihydroxytetrahydro-2H-pyran-2-yl]oxy}tetrahydro-2H-pyran-2-yl]methyl}oxonio)-3-(4-hydroxyphenyl)-2-propen-1-olate (non-preferred name)	C35 H34 O17	726.18	21258	44423	27142	29871	18396	1381	33002	1286	2791	14956	16982	1575
Gambiriin A1	C30 H28 O12	580.1583	449581	318629	316132	322939	296719	19272	393303	1359317	992950	1148023	1282573	103448

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Test Fruit: Apples

Name	Formula	Calc. MW	10% apple +V rep1	10% apple +Y rep1	10% apple +Y rep2	5% apple +V rep1	5% apple +V rep2	5% apple +Y rep1	5% apple +Y rep2	Apple FD+G rep1	Apple FD+G rep2	Apple purée rep1	Apple purée rep2	Apple purée rep3
Epicatechin	C15 H14 O6	290.0791	1750322	2126731	1592753	3031359	3049667	545244	3323610	2840591	2377294	2603009	2800613	889473
(+)-Syringaresinol	C22 H26 O8	418.1609	24820	75496	30057	76612	44781	2290	54376	18964	16532	18765	14019	4137
granaticin	C22 H20 O10	444.1059	12818	21601	9596	35157	34393	7484	25064	5104	6257	2477	1855	5012
ISOEUGENITOL	C11 H10 O4	206.058	11794	35589	13715	24087	18367	745	18581	12521	12052	10099	10476	1214
2-(4-Hydroxyphenyl)ethyl 6-O-[(2R,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)tetrahydro-2-furanyl]-beta-D-glucopyranoside	C19 H28 O11	432.1634	8264	21746	8844	16063	11285	1847	11515	8859	5424	6704	7828	1520
Methyl 4,5,7,11-tetrahydroxy-2-methyl-2',10-dioxospiro[9-oxatricyclo[6.3.1.0~1,5~]dodecane-6,3'-oxetane]-7-carboxylate	C16 H20 O10	372.1059	69429	148654	65051	146158	107270	5472	105867	63617	65383	44669	43449	6641
Isopropyl (4S)-4-(2,1,3-benzoxadiazol-4-yl)-2,6-dimethyl-5-nitro-1,4-dihydro-3-pyridinecarboxylate	C17 H18 N4 O5	358.1263	407619	909242	438047	1012315	722397	3518	717554	383337	381334	306374	330160	8683
Lusitanicoside	C21 H30 O10	442.1841	8188	20449	8710	19678	12237	76	13625	9119	8779	6181	7120	30
trans-isoeugenol-O-glucuronide	C16 H20 O8	340.116	15889	34558	14760	31215	20421	135	21287	16207	18037	12033	13450	39
Irisxanthone	C20 H20 O11	436.1008	85214	202165	103804	137199	97750	33404	96609	3619	3928	32320	33350	8332
Orthosporin	C12 H12 O5	236.0686	45914	113983	40228	64496	46906	1389	58730	33702	29804	20458	17115	761
1-O-(4-coumaroyl)-β-D-glucose	C15 H18 O8	326.1002	418155	1051228	426119	866461	613957	37403	608519	523418	499603	436848	470756	47642
Caffeic acid 3-glucoside	C15 H18 O9	342.0952	29695	19500	32661	17845	32430	4115	46898	1348	486	842	559	57
Lamioside	C18 H28 O11	420.1634	7421	16721	7206	16887	12150	174	11678	6754	7204	4085	4787	19
1-O-feruloyl-β-D-glucose	C16 H20 O9	356.1107	586574	1396797	706422	2011301	1769182	30525	1565567	732791	821354	646240	602837	32971
Chlorogenic acid	C16 H18 O9	354.0955	3210205	6483307	3309942	10749574	8496098	598197	8510463	3027565	2936583	2530746	2714680	486918
Benzoyl glucuronide	C13 H14 O8	298.069	8593	23065	11118	23326	15725	1285	15612	3438	1515	4792	4755	508
Salicylic acid	C7 H6 O3	138.0317	18312	8040	13340	45389	42550	9117	41072	874	971	1016	970	717
(+)-geniposide	C17 H24 O10	388.1372	111014	244779	111148	436915	367099	2039	305797	200045	153343	112857	135539	1773
3,7,15-Trihydroxy-12,13-epoxytrichothec-9-en-8-one	C15 H20 O6	296.126	181577	452812	216755	415608	333096	6230	328454	144206	147979	110870	118982	914
Methyl 4,5,7,11-tetrahydroxy-2-methyl-2',10-dioxospiro[9-oxatricyclo[6.3.1.0~1,5~]dodecane-6,3'-oxetane]-7-carboxylate	C16 H20 O10	372.1058	72237	177597	74401	162193	127665	6333	127359	53029	51995	49876	52501	12212
4'-METHYL-EPIGALLOCATECHIN-3'-GLUCURONIDE	C22 H24 O13	496.1222	2625	358	111	7880	16992	6925	17402	29021	28138	18624	20890	7593
Oxagrelate	C14 H16 N2 O4	276.1111	5396	187	2220	1078	9843	30	4728	190	138	215	87	33
Plantagoside	C21 H22 O12	466.1115	17780	18789	14270	38762	37086	14822	61699	98428	146165	50924	52080	39281
sinapoylglucose	C17 H22 O10	386.1215	63957	128294	75851	209530	172218	3221	160169	50670	58189	54267	54255	10920
Indole-3-lactic acid	C11 H11 N O3	205.0738	42979	188699	134690	123748	183903	8617	182479	2141	2088	5055	2182	953
Catechin	C15 H14 O6	290.0792	2473758	3394894	2419605	6298971	6863707	2218117	6717384	1529571	3098578	2996048	3433091	1723119
myricetin	C15 H10 O8	318.0377	77451	265970	79247	137817	103195	94094	114102	6336	6813	4892	4828	7660
Paeonolide	C20 H28 O12	460.1584	5265	14075	5946	14520	12887	544	10120	5161	5463	2999	3238	1138
Methyl {2-[(2E)-5-(hexopyranosyloxy)-2-penten-1-yl]-3-oxocyclopentyl}acetate	C19 H30 O9	402.1892	2575	5396	2861	6048	5891	579	5388	1741	1810	1421	1568	740
Robinetinidol-(4α->8)-catechin-(6->4α)-robinetinidol	C45 H38 O18	866.2055	124090	70971	45229	48941	13130	14152	13764	759709	487073	726459	717128	406933
5,6,7,8,4'-Pentahydroxyflavone	C15 H10 O7	302.0429	2367	5175	3030	8797	14777	8824	12757	25446	28296	18383	20316	11849
4-(4,7-Dihydroxy-6-methoxy-3,4-dihydro-2H-chromen-3-yl)-1,2,3,5-benzenetetrol	C16 H16 O8	336.0847	33844	65459	37364	80767	65341	15672	65379	76786	62685	91829	89621	21506
1,3,5-trihydroxy-4-{[(2E)-3-(3-hydroxy-4-methoxyphenyl)prop-2-enoyl]oxy}cyclohexane-1-carboxylic acid	C17 H20 O9	368.111	3901	9554	4924	6565	7823	642	5947	500	1412	1410	1570	80

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Test Fruit: Apples

Name	Formula	Calc. MW	10% apple +V rep1	10% apple +Y rep1	10% apple +Y rep2	5% apple +V rep1	5% apple +V rep2	5% apple +Y rep1	5% apple +Y rep2	Apple FD+G rep1	Apple FD+G rep2	Apple purée rep1	Apple purée rep2	Apple purée rep3
{4,6-Dihydroxy-2-methoxy-3-[(2E)-3-methyl-4-(sulfooxy)-2-buten-1-yl]phenyl}acetic acid	C14 H18 O9 S	362.0674	6341	16278	10123	19225	15245	684	14639	10359	7680	9872	10489	873
3-hydroxy-3-methyl-5-oxo-5-[(3,4,5-trihydroxy-6-propan-2-yloxyoxan-2-yl)methoxy]pentanoic acid	C15 H26 O10	366.1527	26563	106610	48384	169289	120767	6578	50095	122561	108097	97583	105715	29361
Baicalin	C21 H18 O11	446.0852	1100	4312	1787	4604	1169	1274	980	2123	3414	58036	3969	3880
(1R,3R,4R,5R)-1,4-Dihydroxy-7-oxo-6-oxabicyclo[3.2.1]oct-3-yl (2E)-3-(4-hydroxyphenyl)acrylate	C16 H16 O7	320.0898	2289	9864	4785	9085	3618	837	6840	2637	2262	6087	6276	1352
3-Hydroxytetradecanedioic acid	C14 H26 O5	274.1781	19160	33881	33403	49831	40442	972	33197	11317	2523	735	434	112
Piceid	C20 H22 O8	390.1317	2078	6596	3104	8371	8129	552	6013	1227	1976	1669	1924	207
7-Ethoxycoumarin	C11 H10 O3	190.063	195	51256	205	29184	1743	263	260	134	715	147	246	120
thioinosine	C10 H12 N4 O4 S	284.0567	4109	13829	7200	12664	9743	55	8496	4497	7813	4804	5025	1545
Quercetin 3-O-sambubioside	C26 H28 O16	596.1383	9384	29607	18742	42276	30005	4627	33673	12664	17638	19300	17178	7747
4H-1-Benzopyran-4-one, 6-β-D-glucopyranosyl-2,3-dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-, (S)-	C21 H22 O10	434.1215	19247	61213	32974	57275	45884	3066	49283	5550	27498	45077	33921	8777
Astragalin	C21 H20 O11	448.1009	12722	56449	29292	50370	41871	7332	39323	9789	15921	9647	11206	4171
2-(5,6-Dihydroxy-1,1,3a-trimethyl-1a,2,3,3a,8b,8c-hexahydro-1H-4-oxabenzo[f]cyclobuta[cd]inden-7-yl)-7-hydroxy-4-oxo-3,4-dihydro-2H-chromen-5-yl hexopyranosiduronic acid	C31 H34 O13	614.2001	1545	8362	3239	6869	4117	886	4085	2482	3445	2454	3686	1990
Rutin	C27 H30 O16	610.1535	435449	1000759	829304	2698745	2446326	388345	2053524	433307	639840	635689	621980	777316
6-Methoxytaxifolin	C16 H14 O8	334.0691	304	486	378	1226	1156	759	650	2753	4285	2994	2033	6915
p-Cresol glucuronide	C13 H16 O7	284.0899	24721	63028	37231	59973	36604	12095	78253	36546	132	506	163	114
4,5-Dicaffeoylquinic acid	C25 H24 O12	516.1271	9811	22984	16071	27691	26461	11892	22345	16241	22698	22611	21879	21528
Furcatin	C20 H28 O10	428.1685	3256	11263	5857	11696	8840	514	9678	647	1194	377	651	394
(E)-3-[3-(hydroxymethyl)-7-methoxy-2-[3-methoxy-4-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenyl]-2,3-dihydro-1-benzofuran-5-yl]prop-2-enoic acid	C26 H30 O12	534.1741	5275	12738	9213	31543	29335	1607	26199	2198	1380	673	9125	4020
Barpisoflavone A	C16 H12 O6	300.0635	11994	29796	17021	47167	25190	2739	25268	690	408	558	504	271
3,5-Dihydroxy-2-(4-hydroxyphenyl)-4-oxo-3,4-dihydro-2H-chromen-7-yl hexopyranoside	C21 H22 O11	450.1164	7211	19411	10735	21073	19007	5917	19521	5710	7276	6816	7271	4583
2-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-4-oxo-4H-chromen-3-yl β-L-arabinofuranoside	C20 H18 O11	434.085	282659	591103	395439	1135132	1076992	605474	998013	208615	204856	254653	243866	257534
Kaempferol-3-O-glucorhamnoside	C27 H30 O15	594.159	24889	56326	34594	72470	66528	13972	55570	19005	24517	35373	32678	32532
luteolin 7-O-glucuronide	C21 H18 O12	462.0797	29912	83892	36838	50168	33204	16994	53331	63043	57327	60203	63509	28197
naringenin chalcone	C15 H12 O5	272.0686	9839	12713	12467	18667	24824	30990	16707	281	210	250	163	233
Astragalin	C21 H20 O11	448.1007	1725692	3085644	1981834	6025659	5864935	3077983	5193527	1200945	1086234	1085244	1024256	1018821
Phloridzin	C21 H24 O10	436.1371	1093231	1942576	1213429	3675482	3326419	1595272	3221460	366027	959825	630452	1127783	944273
6-O-[(2E)-3-(4-Hydroxyphenyl)-2-propenoyl]-1-O-(3,4,5-trihydroxybenzoyl)hexopyranose	C22 H22 O12	478.1114	32438	60463	38590	78629	65904	13908	58327	28478	27105	24698	24619	15890
Medicarpin 3-O-glucoside-6′-malonate	C25 H26 O12	518.1429	4925	11613	5811	10863	9285	3091	8105	5298	4361	2475	2417	1446
6-O-[(2E)-3-Phenyl-2-propenoyl]-1-O-(3,4,5-trihydroxybenzoyl)-β-D-glucopyranose	C22 H22 O11	462.1166	3470	7872	3859	6873	5154	1847	4791	4076	4093	3584	3904	1329
8,10-Dihydroxy-6-methoxy-1,2,3a,12c-tetrahydro-7H-furo[3′,2′:4,5]furo[2,3-c]xanthen-7-one	C18 H14 O7	342.0742	14605	33290	16464	32560	21576	19120	21780	7366	7656	8941	8801	7516

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Test Fruit: Apples

Name	Formula	Calc. MW	10% apple +V rep1	10% apple +Y rep1	10% apple +Y rep2	5% apple +V rep1	5% apple +V rep2	5% apple +Y rep1	5% apple +Y rep2	Apple FD+G rep1	Apple FD+G rep2	Apple purée rep1	Apple purée rep2	Apple purée rep3
Aurantio-obtusin β-D-glucoside	C23 H24 O12	492.1271	18829	39083	20814	33906	27717	15601	26748	23738	24300	14641	14648	8871
ACETYLGLYCITIN	C24 H24 O11	488.1321	5390	13493	6646	10170	8579	7937	8385	8603	7176	6574	5557	5925
Iridodial glucoside tetraacetate	C24 H34 O11	498.2104	8536	22155	8615	19489	12959	1620	15079	8322	10336	6933	744	4915
1,2,4-Trihydroxyanthraquinone	C14 H8 O5	256.0373	6798	13434	8516	11385	9027	6479	10177	10499	9374	9019	8352	7389
Luteolin 7-O-malonylglucoside	C24 H22 O14	534.1014	2435	8751	6799	6019	3993	2410	6234	15173	21358	32153	27455	13148
Ethylvanillin propylene glycol acetal	C12 H16 O4	224.1049	1792	8887	4727	9425	7682	4287	6632	1919	4345	1876	2396	1063
(−)-Epiafzelechin 3-O-gallate	C22 H18 O9	426.0953	164	542	521	525	689	498	883	4834	5131	2095	2130	2310
Juglalin	C20 H18 O10	418.0901	98164	548085	299921	620319	485270	176655	513001	145646	240021	244084	234533	221402
streptonigrin	C25 H22 N4 O8	506.1428	10822	74149	37379	69092	55713	9223	55542	13100	33065	25889	25476	13513
(−)-Epiafzelechin 3-O-gallate	C22 H18 O9	426.0954	436	3590	708	3224	1131	411	989	1961	5303	2918	2751	2861
Afzelin	C21 H20 O10	432.1057	66808	386086	201527	353127	271248	95285	287942	70016	151473	143280	152279	89043
ISORHAMNETIN-3-GLUCOSIDE	C22 H22 O12	478.1113	24190	181787	97766	168067	127688	10195	134053	33683	75233	70067	72173	43212
1,5-Anhydro-1-[5-hydroxy-2-(4-hydroxy-3-methoxyphenyl)-7-methoxy-4-oxo-4H-chromen-8-yl]hexitol	C23 H24 O11	476.1322	1250	6527	3874	5839	3901	2269	4127	1481	3981	3020	2743	2008
(−)-Pinoresinol glucoside	C26 H32 O11	520.1947	6199	33315	15535	26709	19025	3341	19430	4867	19913	12891	14399	9745
(2R,3R)-5,7-Dihydroxy-2-(3,4,5-trihydroxyphenyl)-3,4-dihydro-2H-chromen-3-yl (2E)-3-phenylacrylate	C24 H20 O8	436.116	18663	72291	35191	58548	50872	58571	45431	27411	59630	49424	58016	69399
1,6-Bis-O-[(2E)-3-(4-hydroxyphenyl)-2-propenoyl]-β-D-glucopyranose	C24 H24 O10	472.1372	2040	8956	3737	7386	5336	2019	5751	1915	3888	4722	5432	2695
Eriodictyol	C15 H12 O6	288.0635	3739	15589	7230	8307	6815	7444	8660	194	779	701	766	685
puerarin	C21 H20 O9	416.111	2927	12968	6435	11130	8367	2086	9248	2399	5345	4739	4693	3136
3,5-Dihydroxy-2-(4-hydroxyphenyl)-3,4-dihydro-2H-chromen-7-yl pentofuranoside	C20 H22 O9	406.1266	1493	6046	2509	4693	3481	1736	4209	2837	5033	9080	9416	5440
1,2-Diacetoxy-4,7,8-trihydroxy-3-(4-hydroxyphenyl)dibenzofuran	C22 H16 O9	424.0798	7003	20626	10660	10660	10228	6765	11438	4138	8253	9941	12153	12213
2,4,5,6-Phenanthrenetetrol	C14 H10 O4	242.058	6871	23933	14882	13189	13567	26890	14289	1097	2167	544	635	759
(3α,4β,8α)-4,15-Diacetoxy-3-hydroxy-12,13-epoxytrichothec-9-en-8-yl butyrate	C23 H32 O9	452.2049	2624	8397	3907	7040	4053	1317	5059	2544	3838	3036	3643	1729
2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4-oxo-4H-chromen-3-yl 6-O-[(2E)-3-(4-hydroxyphenyl)prop-2-enoyl]-β-D-glucopyranoside	C30 H26 O14	610.1324	19863	46098	34007	25903	18599	22183	23203	20850	34154	43043	45210	43761
3-(2,6-Dihydroxyphenyl)-4-hydroxy-6-methyl-2-benzofuran-1(3H)-one	C15 H12 O5	272.0686	12104	24833	11397	12806	11293	10717	14908	870	1127	761	865	579
Quercetin	C15 H10 O7	302.0428	1092450	3688108	2686725	4358188	4961688	3364989	4880725	230536	204209	177496	142845	113482
Naringenin	C15 H12 O5	272.0686	7504	19459	9851	9765	10130	13423	10738	435	848	998	1318	1079
Eldecalcitol	C30 H50 O5	490.3663	4997	7665	5211	1940	2624	10179	2633	13144	11936	10358	10616	17518
2,3-Dihydroxyolean-12-ene-23,28-dioic acid	C30 H46 O6	502.3301	3280	8212	3240	2075	3795	8196	2560	4625	3523	4478	6180	9574
(2α,3β,19α)-2,3,19-Trihydroxyolean-12-en-28-oic acid	C30 H48 O5	488.3503	38990	71673	40315	14954	24834	77586	18582	72079	69053	36122	49267	78352
(2R)-1-{[(2-Aminoethoxy)(hydroxy)phosphoryl]oxy}-3-hydroxy-2-propanyl (9Z,12Z,15Z)-9,12,15-octadecatrienoate	C23 H42 N O7 P	475.2701	23839	2516	29923	2481	36705	13818	6758	9671	15160	3408	1906	2808
3-{[(2E)-3-(3,4-Dihydroxyphenyl)-2-propenoyl]oxy}-2,19-dihydroxyurs-12-en-28-oic acid	C39 H54 O8	650.3822	42169	7633	30289	28562	71878	100649	42977	53025	21584	12413	7818	15635
18-β-Glycyrrhetinic acid	C30 H46 O4	470.34	3129	3071	4154	2613	8902	10226	7513	5308	4563	4435	1831	5196

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Test Fruit: Apples

Name	Formula	Calc. MW	10% apple +V rep1	10% apple +Y rep1	10% apple +Y rep2	5% apple +V rep1	5% apple +V rep2	5% apple +Y rep1	5% apple +Y rep2	Apple FD+G rep1	Apple FD+G rep2	Apple purée rep1	Apple purée rep2	Apple purée rep3
3-{[(2E)-3-(3,4-Dihydroxyphenyl)-2-propenoyl]oxy}-2-hydroxylup-20(29)-en-28-oic acid	C39 H54 O7	634.3871	68132	74236	59461	52193	125159	249431	159350	95618	50738	24484	36941	31881
(6Z,9Z,21R)-27-Amino-24-hydroxy-24-oxido-18-oxo-19,23,25-trioxa-24λ~5~-phosphaheptacosa-6,9-dien-21-yl (6Z,9Z,12Z)-6,9,12-octadecatrienoate	C41 H72 N O8 P	737.5003	41549	4388	18109	3279	88458	51450	82294	41611	24394	28354	58995	56372
1-Palmitoyl-2-linoleoyl PE	C39 H74 N O8 P	715.5158	84854	12357	70204	12849	163261	103744	170910	76541	41610	67697	123749	66938
O-{[(2R)-3-[(13Z,16Z)-13,16-Docosadienoyloxy]-2-(pentadecanoyloxy)propoxy](hydroxy)phosphoryl}-L-serine	C43 H80 N O10 P	801.5526	66386	5016	53151	4494	133803	117953	137453	87503	48605	38576	83586	82647

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Test Fruit: Cherries

Name	Formula	Calc. MW	10% Cherry +V rep1	10% Cherry +V rep2	10% Cherry +Y rep1	10% Cherry +Y rep2	5% Cherry +V rep1	5% Cherry +V rep2	5% Cherry +Y rep1	5% Cherry +Y rep2	Cherry FD+G rep1	Cherry FD+G rep2	Cherry purée rep1	Cherry purée rep2	Cherry purée rep3
3-Methyl-2-buten-1-yl hydrogen sulfate	C5 H10 O4 S	166.02994	2978	4364	4703	10447	25197	24677	28277	44254	7	7	8	7	7
methyl 2-O-α-L-fucopyranosyl-β-D-galactoside	C13 H24 O10	340.13728	4239	4056	3106	2551	13055	20059	11655	24984	2607	2177	3028	2037	2647
N-Acetyl-S-2-hydroxyethyl-L-cysteine	C7 H13 N O4 S	207.05652	3599	5554	4448	5149	32053	22520	34093	39227	15	25	17	15	15
Adenine	C5 H5 N5	135.05443	399	586	369	772	4012	8903	3963	11958	10284	17695	9291	13325	9751
1-Pentofuranosyl-2,4(1H,3H)-pyrimidinedione	C9 H12 N2 O6	244.06964	3327	1078	1461	3510	9546	3483	10691	10983	4942	9885	2428	6230	3361
shanzhiside	C16 H24 O11	392.13227	2464	3646	2410	4196	42619	44114	51809	59014	16766	26929	8073	24397	13439
auculin	C15 H22 O9	346.12668	1431	2129	1495	2464	25182	24794	28741	33398	8844	15440	4455	12431	6939
6-Hydroxy-7-methoxy-1,3-benzodioxole-5-carboxylic acid	C9 H8 O6	212.03211	14504	9857	5401	12833	14103	7344	8662	2574	504	356	429	485	465
N-(β-D-glucosyl)nicotinate	C12 H15 N O7	285.08508	974	1344	1096	1672	17179	18389	13477	20742	6780	8025	4566	8811	7137
Mevalonic acid	C6 H12 O4	148.07336	6209	3219	4890	10266	642711	299179	902745	359128	1086	1073	759	1360	1154
Ranunculin	C11 H16 O8	276.08468	102	172	116	486	15810	5115	16736	2043	139	211	113	302	258
Rhimantin	C15 H22 O9	346.12665	973	1603	1191	2489	14309	21101	22389	27017	6619	11786	3981	10152	5410
2-Acetyl-4,7,8-trihydroxy-6-methoxy-3-methyl-1,5-naphthalenedione	C14 H12 O7	292.05848	793	1139	780	1413	27835	33849	35800	52454	884	2040	1201	1763	1190
Methyl tyrosinate	C10 H13 N O3	195.08954	4901	4921	4393	6010	4820	3051	5246	2477	7382	10901	5737	9071	5565
5'-Dehydroinosine	C10 H10 N4 O5	266.06388	7895	10100	5218	8672	108904	38195	77932	11789	231	173	239	146	170
loganate	C16 H24 O10	376.13727	2577	4030	2574	4895	64024	77435	77287	104407	20786	35067	12575	31447	19860
Metirosine	C10 H13 N O3	195.08954	7265	8160	7139	8387	6953	6685	11880	5265	9643	12774	8507	15001	7635
5-(2-Carboxyethyl)-4-hydroxy-6-oxo-1,6-dihydro-2-pyridinecarboxylic acid	C9 H9 N O6	227.0431	1879	15188	7449	13870	59080	7093	44508	951	37	43	37	43	37
Ethyl lactate	C5 H10 O3	118.06265	59325	88378	97814	220879	1602678	1519039	1890652	1601804	6958	8004	3369	5056	5313
L-γ-Glutamyl-L-valine	C10 H18 N2 O5	246.12162	3621	2659	2069	3831	24953	10012	30462	14650	44	81	42	105	54
DL-Ala-DL-Leu	C9 H18 N2 O3	202.13183	10821	6073	4066	8667	34956	13566	33145	21127	48	130	47	117	60
leu-gln	C11 H21 N3 O4	259.15327	6157	4415	1539	5708	25370	16410	30467	14562	37	171	33	59	34
Threonylleucine	C10 H20 N2 O4	232.14238	15450	9291	5933	9003	35553	20415	36141	31952	90	135	62	112	53
glu-leu	C11 H20 N2 O5	260.13723	17563	10903	8272	16155	86280	37162	99352	56246	187	467	122	192	124
N-Acetylneuraminic acid	C11 H19 N O9	309.10619	975	2360	1251	3758	24355	36246	26376	22232	4058	9447	1967	6471	4038
2-oxo-3-(5-oxofuran-2-ylidene)propanoic acid	C7 H4 O5	168.00583	6406	6470	4743	8008	21343	27276	25573	42457	919	1149	917	842	765
Tyrosylalanine	C12 H16 N2 O4	252.11111	21769	15818	10859	16523	94296	52729	121802	91048	310	643	103	195	115
8-Hydroxy-6-methoxy-2-oxo-2H-chromen-7-yl β-D-glucopyranoside	C16 H18 O10	370.09012	167228	269558	125392	148597	1607728	1572023	1511692	1641583	34722	47010	22954	59088	35335
N-Acetylvaline	C7 H13 N O3	159.08956	4756	6584	3150	8097	69615	25185	56150	17482	1392	2722	588	1591	1344
Benzoic acid + 2O, O-Hex	C13 H16 O9	316.07954	40722	49348	58873	45756	252247	281857	301604	301917	78994	119089	138313	192375	139408
asn-phe	C13 H17 N3 O4	279.12203	15723	8307	6733	10296	63463	33569	62815	48243	315	724	100	211	122
1-Isopropyl citrate	C9 H14 O7	234.07401	752	4414	2948	1114	30910	34802	23962	40055	292	608	399	476	405
N-Acetylnorvaline	C7 H13 N O3	159.08952	2717	8371	4968	6124	63645	50780	63885	49430	207	318	96	173	126
Leu-Val	C11 H22 N2 O3	230.1631	15648	8346	5253	10588	100961	43502	92172	92805	290	355	115	133	129
Avenein	C14 H18 O8	314.10037	12602	24547	12605	26268	123871	61017	117754	43722	9225	39008	10210	38246	9631
3-(4-Hydroxy-3,5-dimethoxyphenyl)-2-oxiranecarboxylic acid	C11 H12 O6	240.06351	13420	15057	13509	13062	33800	38365	37871	49022	21422	23205	23397	26739	23271
2-Isopropylmalic acid	C7 H12 O5	176.06822	741884	754316	579202	959800	13634241	12109565	15367471	12341923	179626	351437	77953	267400	160876
2,3-Dihydroxypropyl 3,4,5-trihydroxybenzoate	C10 H12 O7	244.05838	4849	5636	6891	11036	50604	78421	51365	84213	548	645	360	129	400
DL-4-Hydroxyphenyllactic acid	C9 H10 O4	182.05785	864049	1067972	1604325	1973511	9157060	13221508	10394772	15294269	4998	6704	4056	3335	3607
γ-glutamyltyramine	C13 H18 N2 O4	266.12677	21830	14117	9683	12584	70950	39910	77375	53629	565	1151	202	416	250
Neochlorogenic acid	C16 H18 O9	354.09523	186214	209401	170075	180820	379817	418132	387869	463591	167420	180129	199811	301488	202810
L-Glutaminyl-L-Leucine	C11 H21 N3 O4	259.15328	7948	5944	3956	5271	31983	9390	32576	13114	113	244	50	96	58
2-Hydroxycaproic acid	C6 H12 O3	132.07822	508480	570907	695528	882313	3873554	4070292	4165874	5956951	41433	50680	33530	20205	38729
4-Pyridoxate	C8 H9 N O4	183.05316	12261	54333	33676	21053	168218	61948	166783	17286	98	102	38	92	47
Norsanguinarine	C19 H11 N O4	317.06888	6459	9447	10975	10527	35735	51371	41327	66064	23	41	23	23	42
5-(5-Methyl-2-furyl)-3,4-dihydro-2H-pyrrole	C9 H11 N O	149.08406	73933	84269	74417	78864	167017	140022	163946	135322	12679	23906	10504	30073	20824
Diphenol glucuronide	C12 H14 O8	286.06902	12030	8741	18832	11572	29005	16245	30300	36944	16055	20266	16148	18828	16038
(3E)-4-(pyridin-3-yl)but-3-enoic acid	C9 H9 N O2	163.06339	8436	20928	4677	5916	17931	10175	28602	12198	866	816	893	1019	817

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Test Fruit: Cherries

Name	Formula	Calc. MW	10% Cherry +V rep1	10% Cherry +V rep2	10% Cherry +Y rep1	10% Cherry +Y rep2	5% Cherry +V rep1	5% Cherry +V rep2	5% Cherry +Y rep1	5% Cherry +Y rep2	Cherry FD+G rep1	Cherry FD+G rep2	Cherry purée rep1	Cherry purée rep2	Cherry purée rep3
2-(E)-O-feruloyl-D-galactaric acid	C16 H18 O11	386.08519	12771	13735	12594	10417	29208	25968	27605	24208	2771	2939	4691	5464	5113
Neochlorogenic acid	C16 H18 O9	354.09528	2497537	2448289	2543222	2407124	3458833	2095535	3166175	3819606	3670176	3697229	3233707	4267469	3641098
N-Acetyl-L-tyrosine	C11 H13 N O4	223.08452	9651	9891	20344	9449	114068	107077	109172	147947	827	779	815	973	780
Agnuside	C22 H26 O11	466.14781	40795	50930	38510	34718	98444	111646	122654	120783	131223	191317	64439	186004	111523
2-Hexenoic acid	C6 H10 O2	114.06798	22140	26803	16864	22663	134089	144929	145084	152474	19977	32495	9252	25730	17744
8-Epideoxyloganic acid	C16 H24 O9	360.14213	7137	6904	7723	7240	28231	31819	28368	36812	63105	67674	64964	67585	67981
2-Aminooctanedioic acid	C8 H15 N O4	189.10012	62207	94765	76520	107667	238327	271914	171975	304225	55	378	37	138	116
4-(4-Hydroxyphenyl)-2-butanyl 6-O-[(4ξ)-α-L-threo-pentofuranosyl]-β-D-glucopyranoside	C21 H32 O11	460.19506	1525	2248	1548	2513	13924	11278	11103	18027	130	452	125	304	180
2-Hydroxy-4-(4-hydroxyphenyl)butanoic acid	C10 H12 O4	196.07354	573151	772093	629048	890240	6252514	5913393	4957270	8304349	14746	40274	7652	22237	13755
2-Hydroxy-3-{[(2Z)-3-(4-hydroxyphenyl)-2-propenoyl]oxy}succinic acid	C13 H12 O8	296.0534	107758	79901	38958	66506	36110	30528	35509	16841	1072	1246	1698	2623	2280
D-ribosylnicotinate	C11 H13 N O6	255.07448	5658	11025	5180	5662	30024	15873	6287	16100	176	311	127	237	219
Alanyltryptophan	C14 H17 N3 O3	275.12713	38589	36609	20390	29632	192812	136714	310714	303603	925	1838	479	511	446
3-p-coumaroylquinic acid	C16 H18 O8	338.10033	1408325	1538419	1382098	1387148	2905781	2875740	3051859	3561585	985852	963687	1000977	1205508	1080333
4-Acetyl-3-hydroxy-5-methylphenyl β-D-glucopyranoside	C15 H20 O8	328.11599	14450	7396	15834	8560	33986	32677	45538	38480	117641	141091	80620	105281	94500
2-Hydroxy-3-(2,4,5-trihydroxyphenyl)propanoic acid	C9 H10 O6	214.04785	63683	49986	20728	24765	86458	45266	64129	12876	677	728	535	662	681
4-hydroxy-4-(indol-3-ylmethyl)glutamic acid	C14 H16 N2 O5	292.10606	39573	56839	25900	30789	223985	133115	175672	157067	502	734	563	697	687
Valyl-4-hydroxyproline	C10 H18 N2 O4	230.12669	807	2465	7333	5096	4516	7316	3910	14976	41	63	41	73	54
N-Isovalerylglycine	C7 H13 N O3	159.08954	2890	3333	3639	4086	38133	26215	33411	12930	131	181	81	114	157
3-(3,4-dihydroxyphenyl)lactamide	C9 H11 N O4	197.06883	13667	11665	10312	12532	73598	37521	62308	33266	264	204	419	341	425
5-(tert-butyl)-2-methyl-N-(5-methyl-3-isoxazolyl)-3-furamide	C14 H18 N2 O3	262.13192	23771	18733	8441	10775	80255	41997	60692	66579	518	682	526	495	557
4-Acetyl-3-hydroxy-5-methylphenyl β-D-glucopyranoside	C15 H20 O8	328.11598	87929	90892	96360	94073	413531	482852	428021	555678	437911	506203	529823	611388	216675
(5E)-2-[(Carboxymethyl)amino]-5-octenoic acid	C10 H17 N O4	215.11583	8524	9536	8003	8457	22914	21632	16995	22235	19386	12013	3267	5838	3132
1,2,3,4-tetrahydro-β-carboline-3-carboxylic acid	C12 H12 N2 O2	216.08993	15851	15869	17068	14344	25495	32225	27263	34401	6521	7798	5982	8586	7793
4-Hydroxy-5-(phenyl)-valeric acid-O-glucuronide	C17 H22 O9	370.12657	8608	11691	9175	9976	21595	21074	21029	25175	8401	9122	9306	9271	8993
Deoxyanisatin	C15 H20 O7	312.12105	302467	319276	313491	296464	811343	830706	856903	1009292	152220	208058	184421	214381	185598
N-Acetylvanilalanine	C12 H15 N O5	253.09509	110681	177021	177830	174344	280488	388325	211894	492740	346	377	275	371	358
N-Acetyl-D-alloisoleucine	C8 H15 N O3	173.1052	37733	62802	76041	66042	220857	241106	246478	350435	8342	12094	4954	11534	7826
glu-leu	C11 H20 N2 O5	260.13729	22861	27770	27280	30250	89397	78267	83730	120438	305	524	71	238	111
Leu-Gly-Pro	C13 H23 N3 O4	285.16899	19446	19249	13859	11706	50081	23544	45154	30294	82	284	69	99	89
Phenylacetaldehyde	C8 H8 O	120.05734	24264	23733	33792	37078	112685	111186	133409	106036	608	617	788	668	673
1-(3,6-Dihydroxy-2,4-dimethoxyphenyl)-3-(4-methoxyphenyl)-1-propanone	C18 H20 O6	332.1261	312128	312790	483180	128292	1694872	1612171	2144775	2611071	822	993	757	1075	998
L-(-)-3-Phenyllactic acid	C9 H10 O3	166.06285	3502365	3409523	4898801	5393115	16247988	16022991	19011375	22833173	19658	26403	10342	13569	14024
D-(−)-Salicin	C13 H18 O7	286.1054	41632	44209	36241	36635	71865	81076	72813	79834	41927	54696	40557	56469	51292
Benzyl 6-O-beta-D-glucopyranosyl-beta-D-glucopyranoside	C19 H28 O11	432.16309	200138	214654	190909	178833	416249	430557	450002	503184	167424	200415	177122	212672	210409
Ethyl malate	C8 H14 O5	190.08418	238532	280595	234401	230943	769851	808031	808248	1042468	75961	107519	88016	118054	93657
L-γ-Glutamyl-L-leucine	C11 H20 N2 O5	260.1373	16878	14791	23937	26258	35910	33348	26545	39227	33	33	44	49	41
Luteolin 7-O-malonylglucoside	C24 H22 O14	534.10176	24521	27875	17239	26108	36797	41460	40433	44954	5665	5835	5983	6407	6347
N-CAFFEOYL-L-ASPARTIC ACID	C13 H13 N O7	295.06936	9268	9759	7454	9032	17861	12516	16053	13084	2636	3214	2579	3273	2723
2,6-Dimethyl-5-(4-methylphenoxy)pyrimidin-4-ol	C13 H14 N2 O2	230.10557	62074	110172	186330	48438	69694	194879	71678	83666	26311	28610	25163	40178	35357
N-Acetyl-L-leucine	C8 H15 N O3	173.10515	46644	85561	146749	109386	286042	333749	306032	517384	731	1003	536	644	591
Sibiricose A3	C19 H26 O13	462.13783	14065	13192	14506	11940	14037	26614	24747	27574	24386	24852	21872	23595	28460
geniposidic acid	C16 H22 O10	374.12158	74245	69335	65181	59938	136256	126547	127664	140598	40672	48086	37987	50048	41617
N-4-hydroxyphenylacetylglutamic acid	C13 H15 N O6	281.09005	10690	10284	9389	7966	19161	12170	16175	13588	7195	5843	6166	10102	7631
Scopoletin acetate	C12 H10 O5	234.05289	32707	29558	19118	20855	59854	47271	58937	56426	325	333	3376	4622	3553
Esculin	C15 H16 O9	340.0796	9116	9571	9363	8016	12072	15154	16352	17735	2477	2991	2171	2737	2520
Paeonoside	C15 H20 O8	328.116	42796	61261	50734	46355	325801	292595	290466	502184	60097	86419	53256	104679	81920
N-[(6-Hydroxy-7-methoxy-1,3-benzodioxol-5-yl)carbonyl]glycine	C11 H11 N O7	269.05367	7858	26552	4555	10074	73294	15120	66045	5329	295	328	327	353	298

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Test Fruit: Cherries

Name	Formula	Calc. MW	10% Cherry +V rep1	10% Cherry +V rep2	10% Cherry +Y rep1	10% Cherry +Y rep2	5% Cherry +V rep1	5% Cherry +V rep2	5% Cherry +Y rep1	5% Cherry +Y rep2	Cherry FD+G rep1	Cherry FD+G rep2	Cherry purée rep1	Cherry purée rep2	Cherry purée rep3
1,5,8-Trihydroxy-2,3,4-trimethoxy-6-methyl-9,10-anthraquinone	C18 H16 O8	360.08483	109580	65099	112950	92927	21429	54584	17721	67351	5805	6579	3000	3155	3178
1-O-(2-Hydroxybenzoyl)-β-D-glucopyranose	C13 H16 O8	300.08467	36621	56193	46550	31190	115813	103380	120354	191561	5581	9372	2161	10831	8227
1-(3-Acetyl-2,4,6-trihydroxyphenyl)-1,5-anhydrohexitol	C14 H18 O9	330.09526	181575	227933	193964	195520	437068	455404	475608	555983	226854	268140	268222	359243	326928
p-Cresol glucuronide	C13 H16 O7	284.08979	16956	24210	20666	18419	43908	44702	40279	49474	19599	24148	23397	38607	32156
6-[(6-Aminohexanoyl)amino]hexanoic acid	C12 H24 N2 O3	244.17876	36238	18810	20817	31834	222267	128029	232343	269486	1578	2603	1032	1175	956
4-Hydroxyprolylleucine	C11 H20 N2 O4	244.1424	20790	22607	21543	24350	62222	36692	48790	39459	1366	1652	1068	1131	939
1-Caffeoyl-β-D-glucose	C15 H18 O9	342.0952	214557	218730	240652	237279	616911	535640	610938	588453	409035	455628	491748	586299	569146
N-(3,5-Dimethoxybenzoyl)glycine	C11 H13 N O5	239.07949	34237	18210	35154	50537	16272	3104	6728	645	65	86	78	103	78
Methyl 2,3-dihydro-3-hydroxy-2-oxo-1H-indole-3-acetate	C11 H11 N O4	221.06886	4165	8191	8842	8029	21140	20919	30444	29780	115	102	103	121	107
2,6-Dideoxy-3-O-methyl-L-arabino-hexopyranose	C7 H14 O4	162.08923	12099	14843	12532	12360	19618	15691	18202	14190	5566	7152	5072	6773	5394
6-(5-Hydroxy-3,7-dimethoxy-4-oxo-4H-chromen-2-yl)-2,3-dimethoxyphenyl β-D-glucopyranoside	C25 H28 O13	536.15354	23623	27441	23882	22147	35180	30613	30771	42862	13393	19610	12365	20178	17425
Catechin	C15 H14 O6	290.07918	5370	7599	4422	4391	7344	21784	18126	48592	112517	103537	96021	147664	132645
2-Acetyl-5-hydroxy-3-methoxyphenyl hexopyranoside	C15 H20 O9	344.11091	65302	81033	62561	58087	121164	102861	104806	88007	38064	45286	45316	56561	48254
(R)-2-propylmalic acid	C7 H12 O5	176.06856	264380	343394	243659	231344	536579	429101	446011	447407	177749	211133	166633	231558	114517
2-[4-(Hydroxymethyl)cyclohexyl]-2-propanyl hexopyranoside	C16 H30 O7	334.19936	11841	13131	15480	34785	30874	31301	33282	35291	10052	9723	8523	9713	8872
4-(2-Carboxyethyl)-2-methoxyphenyl β-D-glucopyranosiduronic acid	C16 H20 O10	372.10587	53244	55570	55392	50019	115139	116610	112514	112397	40016	46027	35108	44654	42779
Dihydromyricetin	C15 H12 O8	320.05336	25787	30218	22143	20166	44727	48490	87096	317297	16506	15276	11740	12288	12461
Phe-glu	C14 H18 N2 O5	294.12173	9446	9748	8407	11151	69305	53969	70449	75346	478	914	212	303	253
5-p-Coumaroylquinic acid	C16 H18 O8	338.10033	662701	734139	675825	679954	1067727	1018340	1162386	1250065	544445	495688	554831	705024	628009
(3R,5R)-1,3,5-Trihydroxy-4-{[(2E)-3-(4-hydroxy-3-methoxyphenyl)-2-propenoyl]oxy}cyclohexanecarboxylic acid	C17 H20 O9	368.1108	770954	894666	776683	784299	1341593	1187853	1549512	1843653	690001	730698	799090	878609	836213
N-feruloylglycine	C12 H13 N O5	251.07937	266383	336440	203673	279562	1198946	958948	962853	1209884	2784	5901	1919	2326	1868
N-Acetyl-L-phenylalanine	C11 H13 N O3	207.0895	84146	124580	157861	145853	511584	471824	516961	597035	954	1154	508	595	542
Tyr-Phe	C18 H20 N2 O4	328.14249	49596	34460	31392	30820	132334	57852	146697	134502	972	1382	225	308	286
2-(3,4-dihydroxyphenyl)-5-hydroxy-7-[3,4,5-trihydroxy-6-[(3,4,5-trihydroxy-6-methyloxan-2-yl)oxymethyl]oxan-2-yl]oxy-2,3-dihydrochromen-4-one	C27 H32 O15	596.17497	13084	18809	13718	6931	32225	54695	34621	42914	58677	49953	32828	20570	38211
1-O-(4-coumaroyl)-β-D-glucose	C15 H18 O8	326.10043	6095	8632	7249	5839	10243	13107	11451	10883	15980	15027	21911	37006	30001
(2S,3S)-2-hydroxytridecane-1,2,3-tricarboxylic acid	C16 H28 O7	332.18368	8527	8963	9063	8568	23901	24458	25504	31573	8596	8285	9218	11562	10083
Irisxanthone	C20 H20 O11	436.10064	55239	52317	66585	64310	138232	164352	182702	216148	8417	7697	22810	26518	27240
{(1R,2R)-2-[(2Z)-5-(Hexopyranosyloxy)-2-penten-1-yl]-3-oxocyclopentyl}acetic acid	C18 H28 O9	388.1735	82057	90333	93055	80497	168239	179384	170964	259842	87111	103091	85364	98741	94309
6-Methoxy-2-oxo-2H-1-benzopyran-7-yl 6-O-(6-deoxyhexopyranosyl)hexopyranoside	C22 H28 O13	500.15363	22705	26498	26835	23506	28243	70272	61037	119351	4808	4687	4379	5305	5016
3,4-Methylenesebacic acid	C12 H18 O4	226.12054	46255	56540	46813	47451	94194	105679	102830	179236	24561	27300	23964	21848	22030
Bergenin	C14 H16 O9	328.07971	6198	7751	6691	6220	11919	11429	12203	15173	1681	2753	2245	2765	2309
3,7,15-Trihydroxy-12,13-epoxytrichothec-9-en-8-one	C15 H20 O6	296.12604	86984	103854	88727	98978	195188	208380	202453	275840	75847	82245	74041	86368	81681
Methyl 4,5,7,11-tetrahydroxy-2-methyl-2',10-dioxospiro[9-oxatricyclo[6.3.1.0~1,5~]dodecane-6,3'-oxetane]-7-carboxylate	C16 H20 O10	372.10578	149634	166267	65258	153856	318711	345762	355326	464708	137498	149183	111538	148850	128524
Lusitanicoside	C21 H30 O10	442.18433	2928	3188	3623	2813	5870	6736	6328	9752	3086	3661	2676	4046	3664
4-Hydroxy-5-(3',4'-dihydroxyphenyl)-valeric acid-O-glucuronide	C17 H22 O11	402.11644	2135	2327	2781	2472	6941	7553	6935	9366	4725	5435	4159	6100	5257
N-[(2S)-2-Hydroxypropanoyl]-L-tryptophan	C14 H16 N2 O4	276.11107	65166	57095	41985	45519	252595	173477	238192	287348	156	166	111	142	83
Val-Trp	C16 H21 N3 O3	303.15845	30272	20286	18579	18008	83110	73307	115341	134995	948	1310	146	224	183
4,7-Dihydroxy-2,2-dimethyl-3,4-dihydro-2H-chromen-5-yl hexopyranosiduronic acid	C17 H22 O10	386.12152	111388	122837	132896	114689	255906	287765	275688	358971	103669	113040	114185	148823	130048
[3-(Hydroxymethyl)-3-methyl-2-oxobicyclo[2.2.1]hept-1-yl]methyl hexopyranoside	C16 H26 O8	346.16293	61065	62839	72176	66288	212321	225312	226585	223462	118278	126789	111743	186964	168316
3-[(1E)-3-Hydroxy-1-propen-1-yl]phenyl hexopyranosiduronic acid	C15 H18 O8	326.10029	2290	2835	2662	2600	5676	6443	5563	8268	1248	1499	2658	2995	2740

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Test Fruit: Cherries

Name	Formula	Calc. MW	10% Cherry +V rep1	10% Cherry +V rep2	10% Cherry +Y rep1	10% Cherry +Y rep2	5% Cherry +V rep1	5% Cherry +V rep2	5% Cherry +Y rep1	5% Cherry +Y rep2	Cherry FD+G rep1	Cherry FD+G rep2	Cherry purée rep1	Cherry purée rep2	Cherry purée rep3
2-Phenylethyl 6-O-β-D-xylopyranosyl-β-D-glucopyranoside	C19 H28 O10	416.16859	3321	3915	3574	3534	6924	7368	7437	12806	2175	2634	3718	5066	4418
1,5-Anhydro-1-(2,4,6-trihydroxyphenyl)hexitol	C12 H16 O8	288.08465	17152	19577	16748	17369	38145	29472	35291	41939	379	358	7134	15729	697
2-Hydroxy-3-{[5-hydroxy-3-(4-hydroxyphenyl)-4-oxo-4H-chromen-7-yl]oxy}succinic acid	C19 H14 O10	402.059	7322	8198	7199	5657	12113	17247	17473	21348	2298	2344	4118	4873	4623
2-Hydroxy-3-{[3-(4-hydroxyphenyl)-4-oxo-4H-chromen-7-yl]oxy}succinic acid	C19 H14 O9	386.06408	15009	17514	17480	17161	34800	44837	37282	44213	342	425	550	421	420
4-(3-Butoxy-4-methoxybenzyl)imidazolidin-2-one	C15 H22 N2 O3	278.16314	87469	60255	54132	62887	278737	172115	330804	338867	1910	507	235	670	356
Ethyloctanedioic acid	C10 H18 O4	202.1206	166110	177823	155895	164478	299441	318357	359973	441504	79289	96116	76476	92068	81728
2-[(8Z,11Z,14Z,17Z)-8,11,14,17-Icosatetraenoyloxy]-3-[(9Z,12Z)-9,12-nonadecadienoyloxy]propyl (4Z,7Z,10Z,13Z,16Z,19Z)-4,7,10,13,16,19-docosahexaenoate	C64 H100 O6	964.7502	11579	11627	12301	11028	4745	27482	9508	41655	1391	1189	2401	570	1738
5,8,12-Trihydroxy-2-oxododecanoic acid	C12 H22 O6	262.14171	166110	177823	155895	164478	299441	318357	359973	463688	79289	96116	76476	92068	81728
(−)-Riboflavin	C17 H20 N4 O6	376.1385	5253	5943	4801	3925	15469	20398	22571	18387	275	323	180	203	231
(1R)-6-Hydroxy-7-methoxy-1-methyl-1,2,3,4-tetrahydro-1-isoquinoliniumcarboxylate	C12 H15 N O4	237.09987	156741	182582	217406	239225	305770	370778	261571	624418	303	216	200	337	254
Indole-3-lactic acid	C11 H11 N O3	205.07355	125590	276048	325187	267344	861748	1379316	1141836	1642860	358	240	405	398	300
3-(6,7-Dimethoxy-1,3-benzodioxol-5-yl)-2-oxiranecarboxylic acid	C12 H12 O7	268.05827	23646	25399	23648	24413	44323	45244	49940	52062	6269	6172	9582	9449	7946
Dibutyl malate	C12 H22 O5	246.14677	156891	152083	140189	142624	263969	231657	135385	121877	4282	4226	6375	19220	10530
(2E)-3-(3,4-Dimethoxyphenyl)acrylic acid	C11 H12 O4	208.07367	17660	20702	18728	17633	45434	54246	39261	67124	6741	8309	6112	7759	7214
2-[(2R)-1-Hydroxy-3-(4-hydroxy-3-methoxyphenyl)-2-propanyl]-4-[(1E)-3-hydroxy-1-propen-1-yl]-6-methoxyphenyl β-D-glucopyranoside	C26 H34 O11	522.21064	12050	12537	12645	11178	29468	39444	37007	45690	8084	8586	7828	10085	9327
P-COUMARYL ALCOHOL 4-GLUCOSIDE	C15 H20 O7	312.12106	563	699	765	660	1247	1217	1321	1153	16966	16778	13768	15235	14791
1-O-feruloyl-β-D-glucose	C16 H20 O9	356.11094	61632	62131	61437	66573	142459	185884	150044	219164	46916	57871	39569	51559	49807
4-(1,2-Dihydroxypropan-2-yl)-1-methylcyclohexane-1,2-diol	C10 H20 O4	204.13604	7643	8177	7365	7990	12199	15606	10729	18954	220	288	170	225	214
2-(Benzoyloxy)succinic acid	C11 H10 O6	238.0478	22584	24853	22899	25762	50626	54346	60678	68751	16969	22233	14221	23479	17496
(2E)-5-hydroxy-N-[3-(5-{3-[(2E)-5-hydroxy-3-methylpent-2-enamido]propyl}-3,6-dioxopiperazin-2-yl)propyl]-3-methylpent-2-enamide	C22 H36 N4 O6	452.26275	2287	2264	2387	2323	4601	4995	4992	7018	1804	908	1606	2425	2146
Fraxin	C16 H18 O10	370.09024	7009	7658	7110	4697	10047	11493	11194	21535	5054	5173	4717	6053	5701
5-carboxyvanillic acid	C9 H8 O6	212.03215	5495	8068	6547	6007	25203	30306	36368	38053	1506	1471	657	989	896
Isorhamnetin 3-neohesperidoside	C28 H32 O16	624.16965	14931	18271	13663	13509	31356	47654	39771	55642	7020	8636	6257	7722	7695
(Z)-N-[(2S)-2-Amino-1-hydroxy-3-{(Z)-[(2E)-1-hydroxy-4-methoxy-4-oxo-2-buten-1-ylidene]amino}propylidene]-L-phenylalanine	C17 H21 N3 O6	363.14332	3052	3460	4810	5816	4164	4758	3299	3058	247	218	203	238	195
4-Methoxy-6H-[1,3]dioxolo[4,5-g]chromen-6-one	C11 H8 O5	220.03725	5705	6664	8714	7884	26293	73045	51795	88044	24781	31011	28993	39943	36898
(2E)-3-(7-Hydroxy-6-methoxy-1,3-benzodioxol-5-yl)acrylic acid	C11 H10 O6	238.04782	5705	6664	8714	7884	26293	73045	51795	88044	24781	31011	28993	39943	36898
4-Indolecarbaldehyde	C9 H7 N O	145.05272	5409	7484	5311	6625	24333	40131	29549	32686	1277	2398	1664	2860	2142
8-Hydroxy-6-methoxy-7-oxo-3a,12c-dihydro-7H-furo[3',2':4,5]furo[2,3-c]xanthen-9-yl hexopyranosiduronic acid	C24 H20 O13	516.09073	4801	6270	7422	5360	27726	50193	42356	45371	6482	6451	5233	7769	6916
3,5,6,7-Tetrahydroxy-2-(3-hydroxyphenyl)-2,3-dihydro-4H-chromen-4-one	C15 H12 O7	304.05843	6219	8762	10071	5729	54876	269429	160408	358851	115789	130057	50072	72722	66686
N-(4-Hydroxy-3,5-dimethoxybenzoyl)glycine	C11 H13 N O6	255.07435	105886	153226	65122	159634	458828	195850	439722	50204	229	223	169	205	172
Paeonolide	C20 H28 O12	460.15862	17195	18964	21009	18581	48129	51844	51773	71025	11407	12096	12292	14251	14487
N-{(2R,4S,5R)-5-[3-(3,4-Dimethoxyphenyl)-1-methyl-1H-pyrazol-5-yl]-1-azabicyclo[2.2.2]oct-2-yl}methyl)-2-thiophenecarboxamide	C25 H30 N4 O3 S	466.20539	8466	10289	8540	7806	15620	13902	15287	21345	8517	8843	8137	9656	9080
(3S)-3-{(Z)-[(3S)-3-{(Z)-[(3R)-3-Amino-1-hydroxy-4-methylpentylidene]amino}-1-hydroxybutylidene]amino}-5-methylhexanoic acid	C17 H33 N3 O4	343.24733	10577	8285	8160	8607	27682	17597	28195	31534	108	94	67	132	81
Eriodictyol 7-O-rutinoside	C27 H32 O15	596.17494	441	1029	838	581	3093	5762	3958	7984	30996	33967	15509	21256	22368
N-Acetyl-DL-tryptophan	C13 H14 N2 O3	246.10049	18484	19741	45272	36248	86200	107558	94941	152432	2773	5609	49	147	1316

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Test Fruit: Cherries

Name	Formula	Calc. MW	10% Cherry +V rep1	10% Cherry +V rep2	10% Cherry +Y rep1	10% Cherry +Y rep2	5% Cherry +V rep1	5% Cherry +V rep2	5% Cherry +Y rep1	5% Cherry +Y rep2	Cherry FD+G rep1	Cherry FD+G rep2	Cherry purée rep1	Cherry purée rep2	Cherry purée rep3
3-O-(3-Methylbutanoyl)-β-D-fructofuranosyl 4-O-(3-methylbutanoyl)-α-D-glucopyranoside	C22 H38 O13	510.2317	7328	8339	7766	7137	14342	18878	16837	24537	4773	4330	4691	5954	5678
5,6,7-Trihydroxy-2-(3,4,5-trihydroxyphenyl)-2,3-dihydro-4H-chromen-4-one	C15 H12 O8	320.05343	29023	23786	30013	27939	100289	94941	116159	135995	158756	167719	79892	105152	97565
Adenosine monophosphate	C10 H14 N5 O7 P	347.06431	6196	7279	4900	9421	14528	2560	15507	731	151	181	192	188	181
(+)-abscisic acid β-D-glucopyranosyl ester	C21 H30 O9	426.18913	460559	519130	483908	509243	898152	1007276	941841	1301568	299631	319187	347645	429915	396534
4-[(1S,3aS,4R,6aR)-3a-Hydroxy-4-(4-hydroxy-3-methoxyphenyl)tetrahydro-1H,3H-furo[3,4-c]furan-1-yl]-2-methoxyphenyl β-D-glucopyranoside	C26 H32 O12	536.18995	2135	2180	2274	2320	5548	6146	6354	7810	2595	3112	3236	3954	3789
3-Hydroxyoctyl 4-deoxy-2-O-[3-hydroxy-4-(hydroxymethyl)-4-methyltetrahydro-2-furanyl]-4-methylhexopyranoside	C21 H40 O9	436.26751	8875	9322	8943	10368	19954	22444	17101	28507	6399	6962	6616	6817	8073
(1'S,2'S)-3',11'-dihydroxy-1',2',5'-trimethyl-8'-oxaspiro[oxirane-2,12'-tricyclo[7.2.1.0Â?,â?·]dodecan]-5'-en-4'-one	C15 H20 O5	280.13117	16471	16587	16380	16863	30659	40402	31349	55040	7133	10263	9985	12271	11050
2,3-Bis(4-hydroxy-3-methoxybenzyl)-1,2,4-butanetriol	C20 H26 O7	378.16825	8680	9519	8024	9621	15762	19596	14092	21997	2117	2668	2261	2660	2744
(2E)-1-(2,4,6-trihydroxyphenyl)-3-(3,4,5-trihydroxyphenyl)prop-2-en-1-one	C15 H12 O7	304.05848	29141	29582	29797	28183	37111	57797	14883	64575	19920	18272	13667	17268	16714
Astilbin	C21 H22 O11	450.11666	2931	3329	3111	3031	5485	8562	7654	10020	4046	1937	2642	3917	3565
Epidihydrophaseic acid	C15 H22 O5	282.14687	23042	24993	24252	22144	40736	46678	48241	58562	13303	16672	16416	20019	18844
(2E,4Z)-2-Hydroxy-6-(2-hydroxyphenoxy)-6-oxo-2,4-hexadienoic acid	C12 H10 O6	250.04805	19141	17813	18887	18505	30879	35391	34441	29605	5276	5663	7729	6725	7553
Lariciresinol 4-O-glucoside	C26 H34 O11	522.21064	8340	8945	9425	7941	16259	23172	18991	26751	9055	9292	8418	11939	11005
Oxagrelate	C14 H16 N2 O4	276.11107	4698	6834	6214	5471	7794	19658	6688	26594	54	35	47	40	59
(+)-sesamin dicatechol	C18 H18 O6	330.11053	51851	58578	117946	47377	15781	34002	12521	16327	731	815	705	57	867
4,8-Dihydroxy-2H-furo[2,3-h]chromen-2-one	C11 H6 O5	218.02156	30019	19935	35901	37803	64735	73899	99652	107534	1285	967	569	658	734
2-(4-Methyl-3-cyclohexen-1-yl)-2-propanyl 6-O-(6-deoxy-α-L-mannopyranosyl)-β-D-glucopyranoside	C22 H38 O10	462.24692	8415	9388	9316	8995	14135	14748	14790	19695	6757	6605	6761	7824	8323
5-(5,7-Dihydroxy-3-{[2-O-(β-D-xylopyranosyl)-β-D-galactopyranosyl]oxy}-2-chromeniumyl)-2-hydroxyphenolate	C26 H28 O15	580.14357	14893	15638	15047	17322	25303	26298	30747	31020	16253	18357	15874	18766	19049
Quercetin 3-O-sophoroside	C27 H30 O17	626.14903	74	165	72	94	153	153	254	364	5963	6199	4560	7559	7023
Leucyl-leucyl-norleucine	C18 H35 N3 O4	357.26308	12703	11049	10631	10107	48220	23764	45850	51068	263	375	103	222	81
Taxifolin	C15 H12 O7	304.05848	13239	15791	13938	12991	54903	38681	65151	42608	13650	13351	11238	14891	12752
Isorhapontin	C21 H24 O9	420.14237	7514	8299	7413	8118	16532	18027	15428	21505	5861	5850	6035	7724	6626
5-Hydroxy-6-methylene-16-oxo-15-oxapentacyclo[9.3.2.1~5,8~.0~1,10~.0~2,8~]heptadec-12-ene-9,11-dicarboxylic acid	C19 H20 O7	360.12116	7514	8299	7413	8118	16532	18027	15428	21505	5861	5850	6035	7724	6626
Ethyl {2-[(2E)-5-(hexopyranosyloxy)-2-penten-1-yl]-3-oxocyclopentyl}acetate	C20 H32 O9	416.20466	87935	84376	93304	81042	185448	210745	193308	242526	82930	95452	91279	120832	111642
(E)-3-Nonen-2-one	C9 H16 O	140.12008	6740	14345	9213	5458	13949	21342	14468	19194	79	73	89	85	130
5,7-Dihydroxy-4-methylcoumarin	C10 H8 O4	192.04229	68572	72122	68545	67915	130061	163270	144548	202677	38596	48105	38651	44312	43882
4-{[(1R,3aR,4S,6aR)-4-(1,3-Benzodioxol-5-yl)tetrahydro-1H,3H-furo[3,4-c]furan-1-yl]oxy}-2-methoxyphenyl 6-O-β-D-glucopyranosyl-β-D-glucopyranoside	C32 H40 O17	696.22685	9845	14420	19382	10428	57633	80135	25462	310023	73	129	26	193	100
4-[5,7-Dihydroxy-3-({6-O-[(1R,2R,3R,4S,5R)-2,3,4-trihydroxy-5-methylcyclohexyl]-β-D-glucopyranosyl}oxy)-2-chromeniumyl]-2,6-dimethoxyphenolate	C30 H36 O15	636.20595	9845	14420	19382	10428	57633	80135	25462	310023	73	110	26	193	103
Methyl {2-[(2E)-5-(hexopyranosyloxy)-2-penten-1-yl]-3-oxocyclopentyl}acetate	C19 H30 O9	402.18922	21138	22924	19206	20093	30820	31223	31503	36719	4511	5705	4285	5555	4961
6-Hydroxy-1a,5,7a-trimethyl-2,2a,6,6a,7a,8,9,9a-octahydrobisoxireno[4,5:8,9]cyclodeca[1,2-b]furan-4(1aH)-one	C15 H20 O5	280.13121	23155	24080	22775	21461	43447	50349	42931	59449	14904	16156	16617	21083	19066
Patuletin	C16 H12 O8	332.05343	3851	4173	4153	4464	9184	10065	10592	2404	2353	2899	550	2504	2591

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Test Fruit: Cherries

Name	Formula	Calc. MW	10% Cherry +V rep1	10% Cherry +V rep2	10% Cherry +Y rep1	10% Cherry +Y rep2	5% Cherry +V rep1	5% Cherry +V rep2	5% Cherry +Y rep1	5% Cherry +Y rep2	Cherry FD+G rep1	Cherry FD+G rep2	Cherry purée rep1	Cherry purée rep2	Cherry purée rep3
1,5-Anhydro-6-O-(4-carboxy-3-hydroxy-3-methylbutanoyl)-1-[5,7-dihydroxy-2-(4-hydroxyphenyl)-4-oxo-4H-chromen-8-yl]hexitol	C27 H28 O14	576.1488	6283	5216	5128	4259	10147	11616	11036	11795	11787	10688	11553	12297	12978
N-Phenyl-β-D-glucopyranosylamine	C12 H17 N O5	255.11093	50471	46588	46287	25058	54990	31263	21898	12293	388	323	360	414	330
Benzyl 6-O-β-D-xylopyranosyl-β-D-glucopyranoside	C18 H26 O10	402.15292	78174	79869	74397	76251	125575	129468	126670	142982	18237	19734	15337	18694	16664
Maclurin	C13 H10 O6	262.04795	7523	7955	8034	7936	17549	15062	19360	15144	7362	9094	8234	8907	8390
(E,Z)-2,6-Nonadienal	C9 H14 O	138.10453	66642	66716	64568	62490	117814	141493	125777	173080	24644	40446	33193	37758	35764
Fraxetin	C10 H8 O5	208.0372	22964	33725	2370	4205	65089	63447	69616	71323	28160	28673	22932	23528	23506
Apigetrin	C21 H20 O10	432.10613	8391	9278	9997	8695	15996	23027	21044	25515	4975	5547	7355	12149	10399
Trp-Phe	C20 H21 N3 O3	351.15862	7035	4655	4838	5431	15079	8074	20296	20248	61	58	40	43	44
Leucyl-leucyl-norleucine	C18 H35 N3 O4	357.26314	15278	11105	11179	10848	48685	22136	49079	46993	215	250	106	196	164
6,8-Dihydroxy-3-[(2S)-2-hydroxy-4-oxopentyl]-1H-isochromen-1-one	C14 H14 O6	278.07914	45314	41990	53720	44378	72172	85785	86527	106285	13976	26759	9472	21264	14931
3,8,9-trihydroxy-10-propyl-3,4,5,8,9,10-hexahydro-2H-oxecin-2-one	C12 H20 O5	244.13108	222309	218002	227121	196050	373991	418705	381869	521059	136996	154161	141064	177571	162225
(5R)-5-Isopropyl-2-methyl-1-nitro-1,3-cyclohexadiene	C10 H15 N O2	181.11033	4107	5197	2435	4944	19439	9628	16555	3414	167	41	42	50	47
5-(5-Hydroxy-3,6,7-trimethoxy-4-oxo-4H-chromen-2-yl)-2-methoxyphenyl β-D-glucopyranoside	C25 H28 O13	536.154	12501	13906	12345	12285	23321	29513	22826	35738	7629	8198	4764	10065	9197
4-[4-(4-Hydroxy-3-methoxyphenyl)tetrahydro-1H,3H-furo[3,4-c]furan-1-yl]-2-methoxyphenyl hexopyranoside	C26 H32 O11	520.19487	37063	36927	43926	39902	113130	133349	125540	146624	12814	11553	17498	17790	17300
N-(2,3,4-Trimethoxybenzoyl)glycine	C12 H15 N O6	269.09004	294712	367900	204641	391649	1082804	488154	977559	141517	684	751	650	771	612
Gallic acid	C7 H6 O5	170.02158	120287	16071	37204	53366	104636	22088	193615	265954	11546	13243	8036	19185	13867
N-Phenylacetyl pyroglutamic acid	C14 H15 N O3	245.10529	3999	4116	3758	5445	3079	1069	1262	1035	437	601	520	617	490
β-Fagarine	C14 H13 N O4	259.08454	37760	48836	23772	50472	253339	135395	231270	41931	326	591	341	364	401
Versicolorin B	C18 H12 O7	340.0585	1147	1331	1562	1351	7910	64554	13862	61963	206	156	159	209	254
Hesperetin 7-glucoside	C22 H24 O11	464.13225	467	406	544	473	1049	1235	841	1348	3926	4743	4055	6658	5857
QUERCETIN-3'-GLUCURONIDE	C21 H18 O13	478.07517	107	737	116	503	6110	682	25302	865	210	143	3675	994	164
Norathyriol	C13 H8 O6	260.03218	7430	6639	7847	7817	10825	14727	15483	14840	1485	1533	1374	1396	1514
8-Hydroxy-4-methoxy-7-methyl-7,8-dihydro-5H-furo[2,3-g]isochromen-5-one	C13 H12 O5	248.06858	12449	11326	14593	13963	19872	22794	25611	22919	2320	4146	1522	3527	2550
(2Z)-3-(3,4,5-Trimethoxyphenyl)-2-propen-1-yl acetate	C14 H18 O5	266.11552	6731	7014	6504	6840	11484	12141	10995	13994	2031	2833	3130	3791	3471
alternarian acid	C15 H12 O8	320.05335	129905	121690	8973	146711	6085	9538	272627	243232	24929	45431	16708	38238	27431
Quercetin-3β-D-glucoside	C21 H20 O12	464.09574	16043	12431	3340	5755	28359	32568	54552	31537	280681	322574	234459	327556	313774
(2E)-2-(hydroxymethyl)-3-[3-oxo-5-(propan-2-yl)-1,3,4,5,6,7-hexahydro-2-benzofuran-4-yl]prop-2-enoic acid	C15 H20 O5	280.13119	31863	34226	32492	32893	58169	62826	58910	70928	14660	20650	19315	26734	24072
Eugenyl glucoside	C16 H22 O7	326.13671	12788	13896	13622	12974	23073	26205	25198	30212	6144	8472	8395	10950	10048
Etilevodopa	C11 H15 N O4	225.10018	5337	6789	3441	9045	42938	18087	34036	6637	187	252	213	219	254
Ambrosic acid	C15 H20 O4	264.13627	12703	12345	11281	13240	20711	24352	19633	27438	3960	4960	5299	4894	4775
4H-1-Benzopyran-4-one, 6-β-D-glucopyranosyl-2,3-dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-, (S)-	C21 H22 O10	434.12154	8958	8059	8713	10017	25602	27289	28286	28651	41289	38893	66213	90514	83121
4,5-Dicaffeoylquinic acid	C25 H24 O12	516.12713	31662	30343	29788	32649	36028	44604	50886	50586	222917	179016	112289	134094	137640
Luteolin	C15 H10 O6	286.04815	40376	44474	40055	42548	64606	89739	83363	98462	14022	15089	12355	15953	14481
1,5-Anhydro-6-O-(4-carboxy-3-hydroxy-3-methylbutanoyl)-1-[5,7-dihydroxy-2-(4-hydroxyphenyl)-4-oxo-4H-chromen-8-yl]hexitol	C27 H28 O14	576.14873	3807	3759	4509	3356	6006	5698	6052	6616	2464	2336	1929	2198	2144
Poncirin	C28 H34 O14	594.19547	359	504	812	303	728	1720	1408	2319	1143	1857	2020	2414	2072
6-Hydroxy-7-oxo-1,2,3a,12c-tetrahydro-7H-furo[3',2':4,5]furo[2,3-c]xanthen-8-yl hexopyranosiduronic acid	C23 H20 O12	488.09598	6520	7672	7461	5974	13956	16885	16832	15774	2020	2441	1923	2643	2308
N-[4-(5-Amino-2,2-dimethyl-4-oxo-3,4-dihydro-2H-chromen-6-yl)-1-hydroxy-4-oxo-2-butanyl]formamide	C16 H20 N2 O5	320.13733	4475	3771	2287	2870	24917	23477	18900	35358	271	340	105	318	201
1-(4-Hydroxy-3,5-dimethoxyphenyl)-1,2,3-propanetriol	C11 H16 O6	244.09494	13994	13753	10929	12816	16352	14882	13632	17384	5168	5964	6146	6907	6289
6-Hydroxypentadecanedioic acid	C15 H28 O5	288.19378	8282	9613	8214	8795	18195	22535	20104	25856	985	1210	909	710	1013

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5,7-Dihydroxy-2-(4-hydroxyphenyl)-4-oxo-4H-chromen-3-yl 6-O-(6-deoxyhexopyranosyl)hexopyranoside	C27 H30 O15	594.15884	2271	2070	2082	3601	5734	17101	13583	9841	627071	621378	471539	580840	652461
Piceid	C20 H22 O8	390.13175	65388	81500	916	1009	71706	111901	76455	121448	3913	4077	3554	4722	4545
3,5-Dihydroxy-2-(4-hydroxyphenyl)-4-oxo-3,4-dihydro-2H-chromen-7-yl hexopyranoside	C21 H22 O11	450.1165	144649	160796	143214	139155	242969	277799	272426	320138	89307	140689	117836	139436	134902
5,7-Dimethoxy-1a,2a,11c,11d-tetrahydro-6H-oxireno[4',5']furo[3',2':4,5]furo[2,3-c]xanthen-6-one	C19 H14 O7	354.07425	23462	24410	23133	21975	41871	49973	48492	49960	9725	9951	10978	10850	11458
Monoxerutin	C29 H34 O17	654.18028	347	477	328	316	713	664	484	852	21470	25347	19763	25866	23101
2-(4-Methyl-3-cyclohexen-1-yl)-2-propanyl 6-O-(6-deoxy-α-L-mannopyranosyl)-β-D-glucopyranoside	C22 H38 O10	462.24685	268268	290705	273616	250102	462219	469567	429448	574619	122178	154476	161922	214757	188864
tutin	C15 H18 O6	294.11051	122402	54047	52092	114798	114878	57630	79876	70909	53357	48169	5794	20168	11217
(E)-3-(2-carboxyacetyl)oxy-10-hydroxy-4,9-dimethyldodec-6-enedioic acid	C17 H26 O9	374.15789	150583	156223	141402	142000	220076	211984	221119	267844	70783	82157	88494	91415	88137
2-(3,4-Dihydroxyphenyl)-5-hydroxy-6,7-dimethoxy-4-oxo-4H-chromen-3-yl β-D-glucopyranoside	C23 H24 O13	508.12235	3313	2950	1886	2373	4755	4949	4696	4050	9745	12020	10116	12103	11709
4-Allyl-2-methoxyphenyl 4-(sulfooxy)benzoate	C17 H16 O7 S	364.06171	4239	4893	4988	3932	9607	11266	9950	13774	2623	3725	3598	5046	5041
(±)-Abscisic acid	C15 H20 O4	264.13621	279124	303947	281041	264555	528000	562199	534098	674079	151308	226738	220480	265306	248163
2-(3-Hydroxybenzyl)heptanal	C14 H20 O2	220.1464	5805	6048	5550	5450	10590	11238	10814	13493	2979	4498	4460	5259	4962
CALENDOFLAVOSIDE	C28 H32 O16	624.16945	567	663	612	676	999	1848	1818	1913	132620	141184	113608	147138	140031
Aloin B	C21 H22 O9	418.12672	13599	12987	16090	16640	38254	35740	41060	29359	34092	41485	77978	104318	79257
8,10-Dihydroxy-6-methoxy-1,2,3a,12c-tetrahydro-7H-furo[3',2':4,5]furo[2,3-c]xanthen-7-one	C18 H14 O7	342.07418	6310	6561	7029	6074	10592	12964	12741	13622	4900	5032	5174	6597	6128
(±)-(2E)-Abscisic acid	C15 H20 O4	264.13624	4402	4370	3704	5220	8584	9486	9681	10140	2496	3462	3904	3536	3451
(9α,11α,13E,15S)-5,6,9,11,15-Pentahydroxyprost-13-en-1-oic acid	C20 H36 O7	388.24637	5056	5869	5383	4743	8275	8953	8552	11014	3127	4260	3822	4800	4889
6-Methoxytaxifolin	C16 H14 O8	334.06903	2092	2156	2073	2110	3864	3531	5020	1049	1468	1716	2675	3343	2945
3,4-di-o-methylellagic acid	C16 H10 O8	330.03776	2502	1962	2396	2499	27927	14313	54209	15632	482	556	488	391	420
8-Hydroxyquercetagetin	C15 H10 O9	334.03271	28829	35367	23901	27517	119355	136772	148596	129888	318	281	190	320	266
(2R,3R)-5,7-Dihydroxy-2-(3,4,5-trihydroxyphenyl)-3,4-dihydro-2H-chromen-3-yl (2E)-3-(4-hydroxyphenyl)acrylate	C24 H20 O9	452.11123	6568	7374	7343	5798	11217	12526	11755	11589	16365	18302	11122	15286	13842
Methyl 2-(6-methylheptyl)-4,6-dinitrophenyl carbonate	C16 H22 N2 O7	354.14299	2734	2263	1219	2914	22015	4611	15422	1483	29	43	56	99	50
Nigakilactone E	C24 H34 O8	450.22734	4241	4438	2237	2561	3349	2367	3238	2465	457	502	479	754	599
Eugenol	C10 H12 O2	164.08383	391	425	331	383	736	804	598	760	5708	6070	6094	5105	5448
myricetin	C15 H10 O8	318.03775	25053	23265	11090	14933	12050	18997	15156	17938	636	602	256	363	369
Eriodictyol	C15 H12 O6	288.06357	18762	20783	19355	21642	23496	38711	26454	50234	17213	16988	14412	15456	15555
7-Hydroxyhexadecanedioic acid	C16 H30 O5	302.20945	12391	12993	11630	11863	23405	25141	20832	28945	4274	6841	4306	13017	6483
13-oxotrideca-9,11-dienoic acid	C13 H20 O3	224.14129	6250	6532	6344	5889	10659	11564	11166	13272	2628	3423	3501	4200	4179
1-O-(indol-3-ylacetyl)-β-D-glucose	C16 H19 N O7	337.11633	10429	7401	2602	8064	35450	10722	15331	311	31	27	29	28	39
6-Hydroxyluteolin	C15 H10 O7	302.04284	16938	21972	18951	16993	98700	175824	125153	206113	423409	452787	329643	341842	319594
(2S)-7-Hydroxy-2-(4-hydroxyphenyl)-4-oxo-3,4-dihydro-2H-chromen-5-yl 6-deoxy-α-L-mannopyranoside	C21 H22 O9	418.12678	31459	34979	30039	29976	57690	57161	56180	68501	453	500	603	28856	22595
NERIIFOLIN	C30 H46 O8	534.31994	105055	110157	95147	101506	177925	163092	144275	204883	52438	53184	41900	54256	48843
Hematoxylin	C16 H14 O6	302.07913	43087	40224	39884	44062	74717	78365	85385	88861	15095	29658	31493	45815	39883
Hispidulin	C16 H12 O6	300.0636	6402	4438	4861	5631	6412	6143	5637	5703	2726	1321	313	510	422
Iridodial glucoside tetraacetate	C24 H34 O11	498.21057	353	149	141	536	614	677	304	435	8146	8565	8985	7989	8859
(1S)-1,5-Anhydro-1-[5,7-dihydroxy-2-(4-hydroxyphenyl)-4-oxo-3,4-dihydro-2H-chromen-8-yl]-D-glucitol	C21 H22 O10	434.12147	269725	311782	275629	252893	453762	484976	465301	577505	181982	223631	223663	299874	266516
Mono(5-carboxy-2-ethylpentyl) phthalate	C16 H20 O6	308.12605	877	932	1096	933	2236	3018	1906	2692	3298	3764	3766	4046	4148
2,4,6-Trihydroxy-2-(4-hydroxybenzyl)-1-benzofuran-3(2H)-one	C15 H12 O6	288.06358	33948	34325	31061	28467	33507	43838	46625	58552	10362	12567	7980	9411	8922
Puerarin	C21 H20 O9	416.111	41636	44059	39348	38512	79113	81238	92890	87552	24110	28463	63499	94577	82130

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Test Fruit: Cherries

Name	Formula	Calc. MW	10% Cherry +V rep1	10% Cherry +V rep2	10% Cherry +Y rep1	10% Cherry +Y rep2	5% Cherry +V rep1	5% Cherry +V rep2	5% Cherry +Y rep1	5% Cherry +Y rep2	Cherry FD+G rep1	Cherry FD+G rep2	Cherry purée rep1	Cherry purée rep2	Cherry purée rep3
Visnagin	C13 H10 O4	230.05805	12272	11006	10799	10651	15138	16242	11106	20469	4731	4869	963	5010	2587
Epicatechin	C15 H14 O6	290.0792	12272	11006	10799	10651	15138	16242	11106	20469	4731	4869	963	5010	2587
1,2-Diacetoxy-4,7,8-trihydroxy-3-(4-hydroxyphenyl)dibenzofuran	C22 H16 O9	424.07984	27078	25585	23925	23995	35046	44987	47948	42512	16393	20055	15894	18013	18218
6,8,9-Trihydroxy-3a,12c-dihydro-7H-furo[3',2':4,5]furo[2,3-c]xanthen-7-one	C17 H10 O7	326.04286	47090	45691	44755	51581	79436	109502	140373	124468	3062	1854	2776	2374	1467
1,3,9-Trihydroxy-8-methoxy-6H-[1]benzofuro[3,2-c]chromen-6-one	C16 H10 O7	314.04281	2582	2699	2698	2738	52921	19917	80055	26585	1359	1312	555	760	47
3-[2-(2,4-Dihydroxy-6-methylphenyl)-2-oxoethyl]-6,8-dihydroxy-1H-isochromen-1-one	C18 H14 O7	342.07418	1288	2113	3782	2447	33888	69405	51561	300006	24	34	27	43	35
Isoscoparin	C22 H22 O11	462.1167	1256	1052	1270	1163	3022	3035	3350	3387	7812	8717	22288	35557	31676
Arjungenin	C30 H48 O6	504.34591	4412	4273	3926	3674	6466	6578	5449	6220	3668	5031	4011	4793	4767
8-hydroxybergapten	C12 H8 O5	232.03737	4193	3724	3696	3627	4358	4982	5936	4442	2683	3279	2413	2292	2379
Phloretin	C15 H14 O5	274.08422	6426	5451	5321	4769	4288	5606	4762	8300	455	319	120	122	137
Swertianin	C14 H10 O6	274.04778	5711	5415	5353	5852	9777	11954	11345	12821	2845	2816	2311	2758	2609
3-(2,6-Dihydroxyphenyl)-4-hydroxy-6-methyl-2-benzofuran-1(3H)-one	C15 H12 O5	272.0686	280473	274950	250036	244010	362908	450504	445877	460130	167182	194573	165766	180172	179315
1-(6-Hydroxy-1,3-benzodioxol-5-yl)-3-(4-methoxy-1-benzofuran-5-yl)-1,3-propanedione	C19 H14 O7	354.07421	11260	11584	10343	10321	17329	21274	20689	22063	1102	1260	829	888	935
6,8,9-Trihydroxy-3a,12c-dihydro-7H-furo[3',2':4,5]furo[2,3-c]xanthen-7-one	C17 H10 O7	326.04287	6551	6170	5811	5435	10153	13449	15274	11767	1433	1425	1079	1179	1094
Quercetin	C15 H10 O7	302.04293	2964917	2672956	2756639	2889468	3313965	4399235	4331156	4221037	254974	251134	159363	203985	183161
6-[(1S,3aR,4S,6aR)-4-(1,3-Benzodioxol-5-yl)tetrahydro-1H,3H-furo[3,4-c]furan-1-yl]-1,3-benzodioxol-5-yl β-D-glucopyranoside	C26 H28 O12	532.15875	2835	2916	2697	2530	4596	4260	4261	5249	3382	3035	3108	3544	3269
(±)-Hesperetin	C16 H14 O6	302.07905	218622	214654	205150	205653	424563	475617	456747	468176	78680	117299	100815	107646	102813
14-Ethoxy-5,15-dihydroxy-2,9,26-trimethyl-3,19,23,28-tetraoxaoctacyclo[16.9.1.1~18,27~.0~1,5~.0~2,24~.0~8,17~.0~9,14~.0~21,26~]nonacos-11-ene-4,10,22,29-tetrone	C30 H36 O11	572.22641	3916	4103	4285	2641	9456	9095	8461	6690	1467	2593	2212	2846	2852
Naringenin	C15 H12 O5	272.06857	516495	521133	481022	464891	703472	866210	814593	946775	131196	153045	127543	143416	139106
Kolaflavanone	C31 H24 O12	588.1276	213	140	114	140	473	1430	1273	2844	9878	12256	8521	10852	10004
3-Methoxyluteolin	C16 H12 O7	316.05841	3262	3730	3486	3192	15366	27237	24594	49579	141711	171121	133641	158322	151076
1,2,4-Trihydroxyanthraquinone	C14 H8 O5	256.03728	3262	3730	3486	3192	15366	27237	24594	49579	141711	171121	133641	158322	151076
Sulochrin	C17 H16 O7	332.08966	4490	3602	4078	4211	7535	7641	7345	6302	1544	2463	1747	1070	1896
1-O-[(2α,3β,5ξ,9ξ,18ξ,19α)-2,3,19,23-Tetrahydroxy-28-oxoolean-12-en-28-yl]-β-D-glucopyranose	C36 H58 O11	666.39878	8060	8279	12263	6860	10237	10296	9508	4456	5461	5526	4921	6004	5301
Naringenin	C15 H12 O5	272.06859	24048	20703	17280	24808	24330	41175	28305	29528	4871	9051	8373	9875	8866
(15Z)-9,12,13-Trihydroxy-15-octadecenoic acid	C18 H34 O5	330.24082	5339449	5308329	5188304	5366278	13552401	14907891	12941298	14961806	526722	1620905	1518024	1869907	1703773
5,5',7,7'-Tetrahydroxy-2-(4-hydroxyphenyl)-2,3-dihydro-4H,4'H-3,8'-bichromene-4,4'-dione	C24 H16 O9	448.07986	92636	88599	35096	79948	147911	178672	152240	94199	46142	46519	50421	49001	40775
Jasmonic acid	C12 H18 O3	210.12577	2503	4376	1408	1829	6010	6309	4650	5468	581	1323	2578	4361	3315
14,18-Dihydroxy-12-oxo-9,13,15-octadecatrienoic acid	C18 H28 O5	324.19399	23256	18003	21922	21623	54851	62069	69676	75469	7979	21182	13892	17918	15818
3,7,8,9-Tetrahydroxy-6H-[1]benzofuro[3,2-c]chromen-6-one	C15 H8 O7	300.02717	60555	55499	60280	68210	152692	162211	186014	137983	5818	6605	4390	4398	5171
2,3,9-Trihydroxy-6-oxo-6H-[1]benzofuro[3,2-c]chromen-8-yl acetate	C17 H10 O8	342.03769	6104	5033	5328	5477	6095	6024	7588	4684	42	47	123	47	49
Rhapontigenin	C15 H14 O4	258.08933	5706	5384	4560	4480	4101	4528	4141	4791	3227	3040	1571	1430	1570
3-Methyl-5-pentyl-2-furanpentanoic acid	C15 H24 O3	252.17283	6479	5014	4143	4633	7607	7224	6510	7034	2265	3502	3218	3538	3646
Apigenin	C15 H10 O5	270.05295	43049	43660	38878	35530	35744	44908	56162	45398	2510	2995	3830	4276	4240
Phloionolic acid	C18 H36 O5	332.25632	6244	12108	9393	59249	9052	10384	9150	10608	583	1928	367	564	724
(5Z,9α,11α,13E,15S)-9,11,15,20-Tetrahydroxyprosta-5,13-dien-1-oic acid	C20 H34 O6	370.23571	15510	10543	10390	17087	47744	39056	39840	38277	143	207	127	415	279
2,3,8,9-Tetrahydroxybenzo[b][1]benzofuro[2,3-f][1]benzofuran-6,12-dione	C18 H8 O8	352.02212	2672	2514	2381	2211	4479	3991	7314	5116	3149	3676	3953	4106	4203
Syringetin	C17 H14 O8	346.06903	56556	48369	50822	52984	112285	95288	106074	92447	938	79	592	1108	916

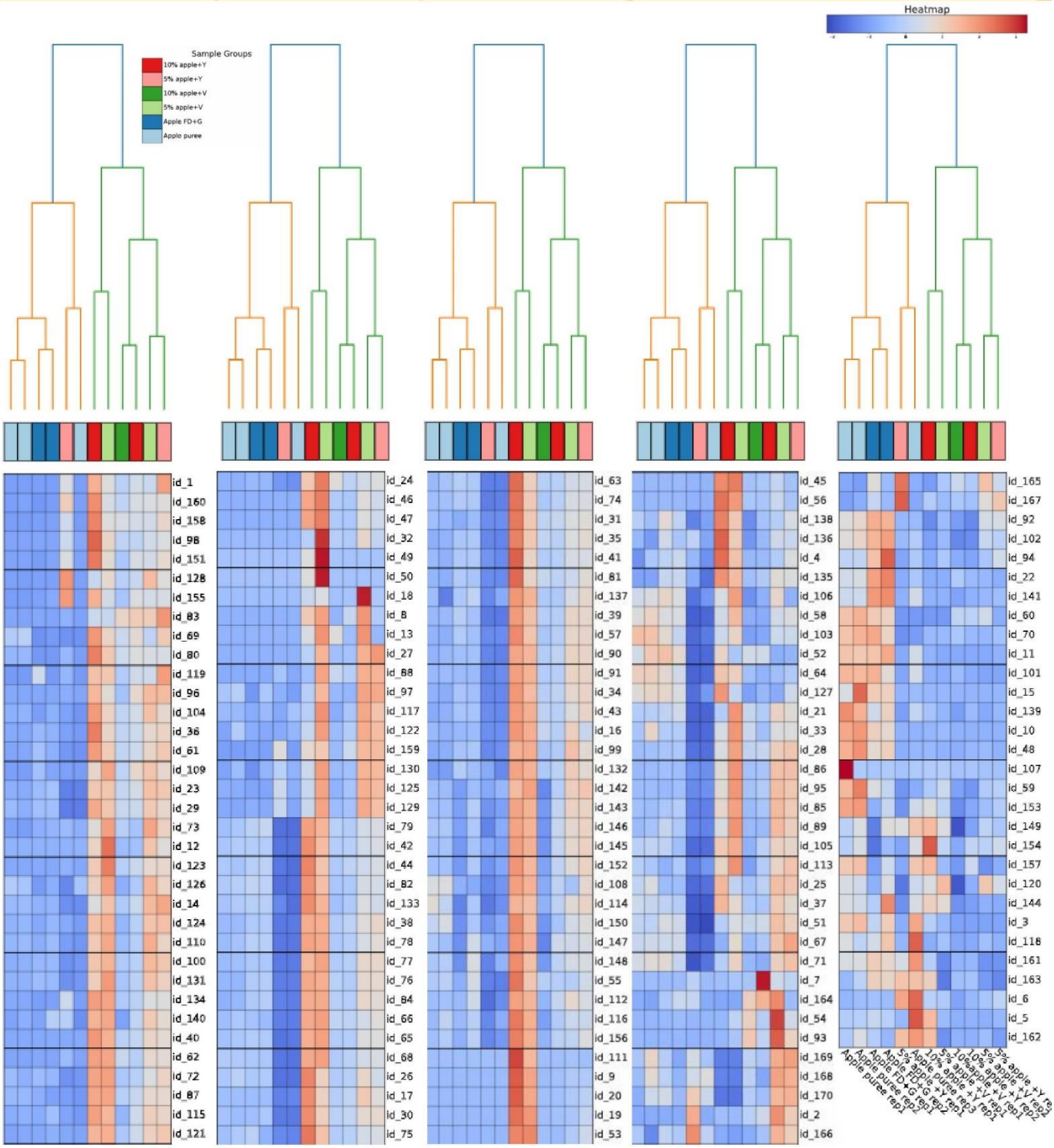
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Test Fruit: Cherries

Name	Formula	Calc. MW	10% Cherry +V rep1	10% Cherry +V rep2	10% Cherry +Y rep1	10% Cherry +Y rep2	5% Cherry +V rep1	5% Cherry +V rep2	5% Cherry +Y rep1	5% Cherry +Y rep2	Cherry FD+G rep1	Cherry FD+G rep2	Cherry purée rep1	Cherry purée rep2	Cherry purée rep3
3-Methoxy-5,7,3',4'-tetrahydroxy-flavone	C16 H12 O7	316.05843	310990	298857	269305	287058	273869	262208	277994	283976	40232	53787	36472	35662	34786
(2R,3aS,5aR,5bS,9S,13S,14R,16aS,16bR)-9-Ethyl-13-hydroxy-14-methyl-7,15-dioxo-2,3,3a,5a,5b,6,7,9,10,11,12,13,14,15,16a,16b-hexadecahydro-1H-as-indaceno[3,2-d]oxacyclododecin-2-yl 6-deoxy-2-O-methyl-al pha-L-mannopyranoside	C31 H46 O9	562.31446	129195	112680	101573	112816	226160	204993	129322	169027	31247	27242	21317	2994	21602
Pentosidine	C17 H26 N6 O4	378.20207	1022	1088	1043	1252	4061	6440	4333	5033	2571	5093	2805	3594	3394
Methyl (3aR,5Z,9E,11aS)-10-methyl-3-methylene-2-oxo-2,3,3a,4,7,8,11,11a-octahydrocyclodeca[b]furan-6-carboxylate	C16 H20 O4	276.13617	26840	19091	23335	24672	70204	109509	68557	70690	390	1083	967	1355	1474
1,4,9-Trihydroxy-9-methyl-5,8,10-trioxo-5,8,9,10-tetrahydro-2-phenanthrenecarboxylic acid	C16 H10 O8	330.03792	17412	14533	10284	10720	24553	17519	41792	29213	10844	10985	5299	4650	5055
Pinocembrin	C15 H12 O4	256.07386	131111	114675	105821	119756	180942	246275	212326	261129	45693	50456	44347	44415	35133
Gentiin	C14 H10 O5	258.05294	487595	378058	420666	460354	775804	1093497	820123	1657320	472589	367272	65915	326863	200478
N-[[(2R,4S,5R)-5-(3-Cyclopentyl-1-methyl-1H-pyrazol-5-yl)-1-azabicyclo[2.2.2]oct-2-yl]methyl]-4-methoxybenzamide	C25 H34 N4 O2	422.26719	5276	5096	4241	5034	11566	9989	6312	11486	85	76	62	76	90
(±)9-HpODE	C18 H32 O4	312.2302	104402	106006	93576	209723	223369	281327	199861	217870	11406	20895	11348	9106	13243
3-(3,4-Dihydroxyphenyl)-2,7,8-trihydroxy-1,4-dibenzofurandione	C18 H10 O8	354.03787	11452	12058	11321	10274	10920	10419	13212	9993	1621	1480	1370	1311	1359
(6E)-6-(3,4-Dihydroxybenzylidene)-4-(2,5-dihydroxyphenyl)-3-hydroxy-2H-pyran-2,5(6H)-dione	C18 H12 O8	356.05347	5403	4163	4052	3903	6128	5220	9099	6004	1366	1207	1127	738	1027
9(S)-HpOTrE	C18 H30 O4	310.21442	113958	74887	75012	97070	256067	274308	243664	234199	49096	67712	98240	84322	120217
GENTISEIN	C13 H8 O5	244.03724	20083	16059	15988	20329	7400	12142	4504	2959	75	62	45	48	52
Chrysin	C15 H10 O4	254.05798	77829	61742	58810	57160	98535	103360	86046	81694	3941	5813	15343	18769	18165
(9Z,12Z)-6,8-Dihydroxy-9,12-octadecadienoic acid	C18 H32 O4	312.23008	1171373	826504	799473	954300	1651061	2247746	1061532	1286994	90542	53351	113793	157239	134361

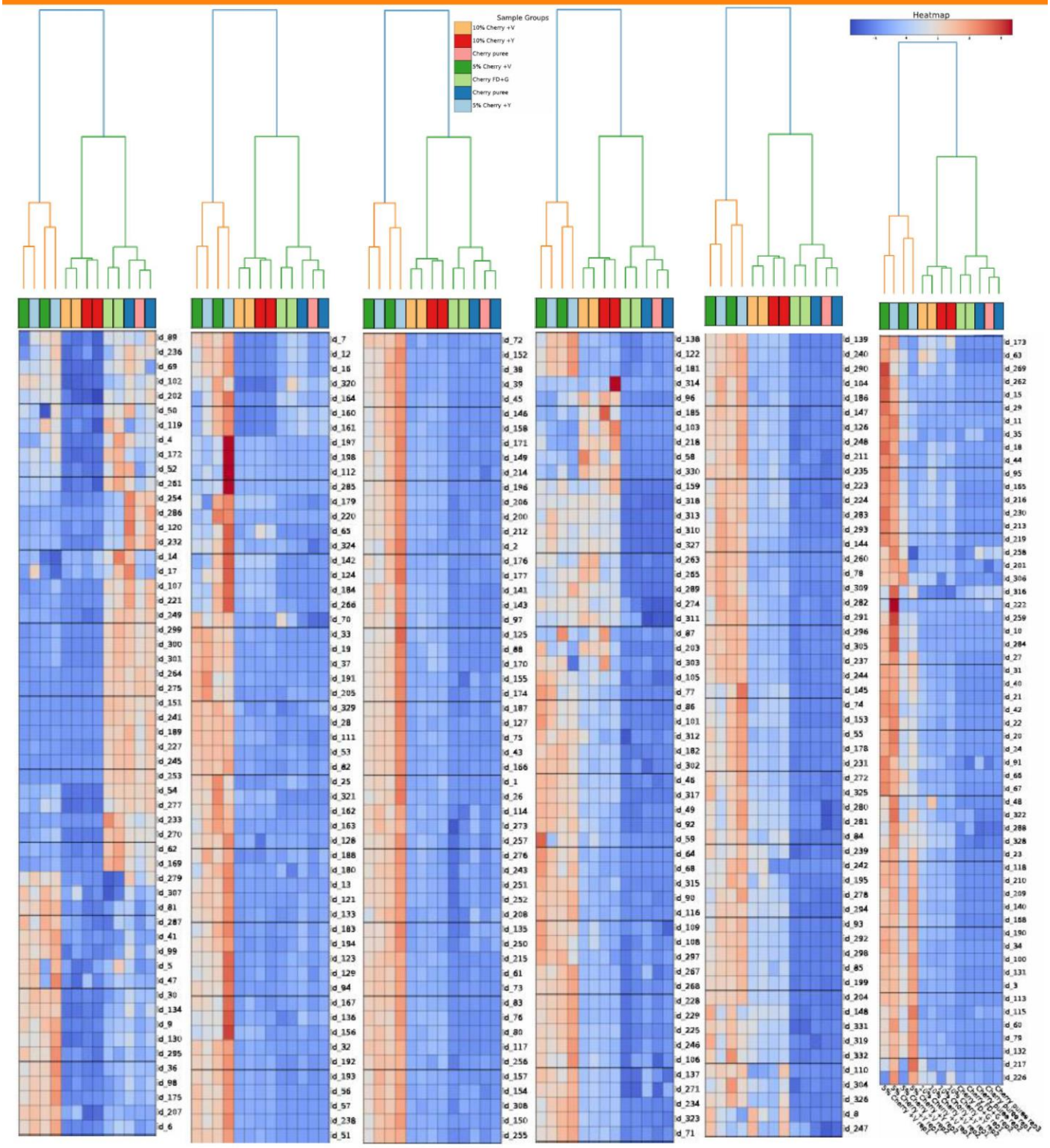
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Appendix B: Non-polar metabolite profiling of apples and cherries samples by reverse phase HPLC HRFTMS – heat map visualisation



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Appendix B: Non-polar metabolite profiling of apples and cherries samples by reverse phase HPLC HRFTMS – heat map visualisation



Appendix F – Pulverisation Equipment

VORTAIR
Super Fine Autogenous Grinder

WASTE RECOVERY

WASTE REDUCTION

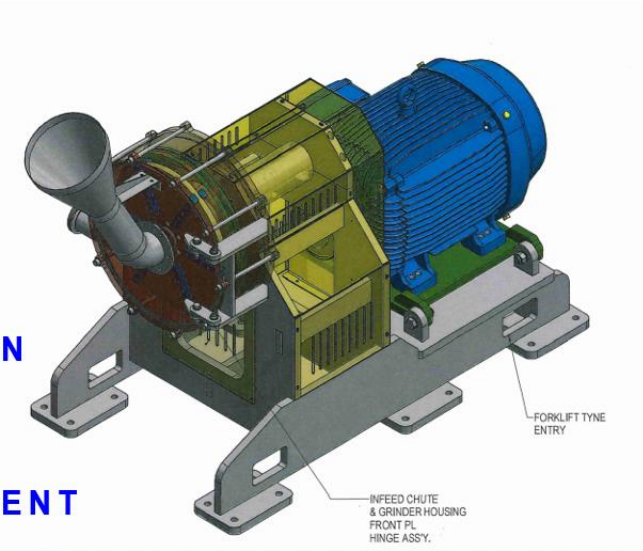
SIZE REDUCTION

MOISTURE REDUCTION

MINERAL GRINDING

PRODUCT ENHANCEMENT

POWDER DOWN TO 10µM



- ✓ **Conversion of vegetable products – carrot, beetroot etc to low moisture powders for long term non-refrigerated storage and later reconstitution, local and export markets.**
- ✓ **Fine grinding of food waste, damaged product, off spec product, for incorporation into front end processing or diversion to pet foods or compost.**
- ✓ **Fine slurry grinding of soup stock bones for incorporation into front end processing or pet food with zero waste and recovery of valuable minerals and proteins.**
- ✓ **Fine grinding of flax, hemp and sugar cane into fine fibres for incorporation into drinks and dessert mixes to increase fibre content.**

MADE IN AUSTRALIA
FAPIC

Vortair Pty Ltd

Contact:

FAPIC Pty Ltd, P. O. Box 343 Vermont, Victoria, 3133 Australia
Telephone : 61-417 568 423 Email : fapic@fapicglobal.com
Website: www.fapicglobal.com

APPLICATIONS

- ✓ **Grains Seed and Pulses** Wheat, Rice, Soy Bean, Oats, Barley, Corn, Linseed, Hemp, Cocoa, Almond, Peas, Lentils, Sugar Cane, Nuts, Eucalypt, Sunflower, Coffee, Quinoa, Chia, Chick Pea
- ✓ **Herbs and Spices** Cinnamon, Parsley, Chives, Leafy Herbs, Chilli, Mint, Rosemary
- ✓ **Root Vegetables** Carrot, Swede, Beetroot, Turnip, Pumpkin, Brocolli, Ginger, Silverbeet
- ✓ **Fruits** Plum, Apple Pomace, Pear Pomace Orange, Lemon, Grape Marc, Avocado
- ✓ **Oils and fats** Fish oil recovery, Coffee Whitener, Vegetable Oils, Seaweed (kelp), Cocoa , Chocolate, meat wastes
- ✓ **Textiles** Wool & Polyester Recovery, Component Separation, Waste Garment Reduction
- ✓ **Building Construction** Building Scrap Waste, Offcut Processing, Plasterboard recovery
- ✓ **Minerals** Zeolite, Lime Recovery



CONSTRUCTION

- ✓ All stainless steel, finished to food industry standards.
- ✓ Rotational speeds up to 10,000 RPM
- ✓ Fully balanced machine rotor
- ✓ Non-contact labyrinth seals
- ✓ Clean in Place
- ✓ VSD for continuous control of power, speed, frequency and temperature
- ✓ Includes MCC and vibration sensing
- ✓ Patent Pending
- ✓ Designed and manufactured in Australia
- ✓ Service and spare parts readily available

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