



**ISO 9001:2015**  
Certification  
ISO 16128-1 ISO 16128-2-2017 EPA www.epa.gov/greenchemistry

**KAMPOYAKI NATURAL  
PRODUCTS BIO-CHEMISTRY**

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## 3-O-FERULOYLQUINIC ACID

### Datasheet

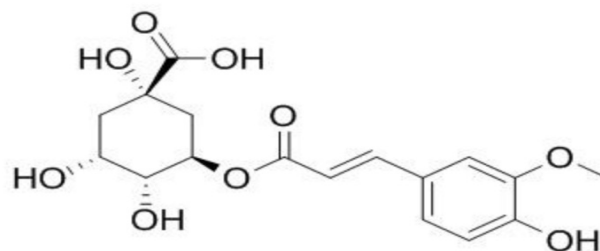
Kampoyaki Novo-Drug Screening Libraries 4<sup>th</sup> Edition (Revised in July, 2016)

### PRODUCT INFORMATION

**Name:** 3-O-Feruloylquinic acid  
**Catalog No.:** KRN92393  
**Cas No.:** 1899-29-2  
**Purity:** >=98%  
**M.F:** C<sub>17</sub>H<sub>20</sub>O<sub>9</sub>  
**M.W:** 368.3

**Physical Description:** Powder

**Synonyms:** (1S,3S,4S,5S)-1,3,4-trihydroxy-5-[(E)-3-(4-hydroxy-3-methoxyphenyl)-1-oxoprop-2-enoyl]-1-cyclohexanecarboxylic acid



### POTENTIAL USES

**1.** Reference standards; **2.** Pharmacological research; **3.** Food and cosmetic research;  
**4.** Synthetic precursor compounds; **5.** Active Pharmaceutical Intermediates (API) & Fine Chemicals; **6.** Ingredient in supplements, beverages; **7.** Agricultural research; **8.** Botanical Bio- Allelopathy, **9.** Natural Botanical Molecules as Botanical Bio-Herbicides **10.** As Botanical Bio- Anti-Blight Fungicides

### SOURCE

The fruits of *Coffea canephora* var. *Robusta*

### BIOLOGICAL ACTIVITY OR INHIBITORS

3-O-Feruloylquinic acid could be a starting basis for new Microsomal prostaglandin E synthase-1 (mPGES-1) inhibitors.[1]

3-O-Feruloylquinic acid, is a secondary-metabolic compound isolated from winter wheat (*Triticum aestivum* L. cv Chihokukomugi), exhibits antioxidative activity.[2]

## SOLVENT

Chloroform, Dichloromethane, Ethyl Acetate, DMSO, Acetone, etc.

## HPLC METHOD (3)

**Mobile phase:** Methanol-H<sub>2</sub>O gradient elution;

**Flow rate:** 1.0 ml/min;

**Column temperature:** 30 °C;

**The wave length of determination:** 254 nm.

## STORAGE

2-8°C, Protected from air and light, refrigerate or freeze.

## REFERENCES

[1] Li CH, Chang TT, Sun F, et al. Mol. Simulat., 2011, 37(3):226-36.

[2] Jin, Shigeki, Yoshida, Midori. Biotechnology Society of hypothermia, 2005, 51:57-62.

[3] Chen F, Long X, Liu Z, et al. Sci. World J., 2014:568043.



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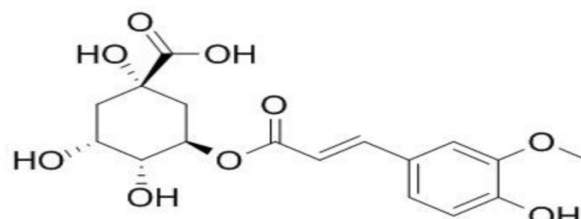
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## CERTIFICATE OF ANALYSIS

**Name:** 3-O-Feruloylquinic acid  
**Catalog No.:** KRN92393  
**Cas No.:** 1899-29-2  
**Purity:** >= 98%  
**M.F.:** C<sub>17</sub>H<sub>20</sub>O<sub>9</sub>  
**Physical Description:** Powder



**Solvent:** Chloroform, Dichloromethane, Ethyl Acetate, DMSO, Acetone, etc.  
**Weight** 5mg  
**Lot No.** KRS201802  
**Storage** Protected from air and light, refrigerate or freeze (2-8 °C)  
**Intended Use** For laboratory use only  
**Shelf Life** 2 years

## CHARACTERIZATION DATA SUMMARY

### Analytical Test

Identification by , 1H-NMR , HPLC  
Purity tested

### Results

Consistent with the above structure  
>= 98%



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## GHS SAFETY DATA SHEET

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**Version 4.2**  
**Revision Date 01/01/2018**  
**Print Date 01/08/2019**

## 1. PRODUCT AND COMPANY IDENTIFICATION

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**GHS Product Name:** 3-O-Feruloylquinic acid

**Product code:** KRN92393

**Company:** KAMPOYAKI HERS PTE LTD

**Address:** 16 New Industrial Road, #05-05 Hudson Techno Centre Singapore 536204

**Tel:** +65-63833202

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**Website:** www.kampoyaki-research.com

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## 2. HAZARDS IDENTIFICATION

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### 2.1 GHS classification

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**Physical Hazards:** Not classified

**Health Hazards:** Not classified

**Environmental Hazards:** Not classified

### 2.2 GHS label elements, including precautionary statements

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**Pictograms or hazard symbols:** None

**Signal word:** No signal word

**Hazard statements:** None

**Precautionary statements:** None

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

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**Chemical Name:** 3-O-Feruloylquinic acid

**CAS#:** 1899-29-2

**Purity:** >=98%

**Formula:** C<sub>17</sub>H<sub>20</sub>O<sub>9</sub>

**Molecular Weight:** 368.3

**Hazard Symbols:** ----

**Risk Phrases:** ----

## 4. FIRST AID MEASURES

### 4.1 Description of first aid measures

**Eyes:** Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Consult a doctor.

**Skin:** Flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Consult a doctor.

**Ingestion:** Do NOT induce vomiting. If conscious and alert, rinse mouth and drink 2-4 cupfuls of milk or water. Consult a doctor.

**Inhalation:** Remove from exposure and move to fresh air immediately. Consult a doctor.

### 4.2 Indication of immediate medical attention and special treatment needed

Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.

## 5. FIRE FIGHTING MEASURES

### 5.1 Suitable extinguishing

**Media:** Dry chemical, foam, water spray, carbon dioxide.

**Precautions for firefighters:** Fire-extinguishing work is done from the windward and the suitable fire-extinguishing method according to the surrounding situation is used. Uninvolved persons should evacuate to a safe place. In case of fire in the surroundings: Remove movable containers if safe to do so.

### 5.2 Special protective

**Equipment for firefighters:** When extinguishing fire, be sure to wear personal protective equipment.

## 6. ACCIDENTAL RELEASE MEASURES

### 6.1 Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing vapors, mist or gas.

### 6.2 Environmental precautions

Do not let product enter drains.

### 6.3 General Information

Use proper personal protective equipment as indicated in Section 8.

## 6.4 Spills/Leaks

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Clean up spills immediately, observing precautions in the Protective Equipment section. Sweep up, then place into a suitable container for disposal. Decontaminate spill site with 10% caustic solution and ventilate area until after disposal is complete

## 7. HANDLING AND STORAGE

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### 7.1 Precautions for safe handling:

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Wash thoroughly after handling. Remove contaminated clothing and wash before reuse. Avoid contact with eyes, skin, and clothing. Avoid ingestion and inhalation. Keep away from sources of ignition. Avoid prolonged or repeated exposure.

### 7.2 Storage

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Store in a well closed container. Protected from air and light, refrigerate or freeze.(2-8°C)

### 7.3 Specific end uses

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Use in a laboratory fume hood where possible. Refer to employer is COSHH risk assessment.

## 8. EXPOSURE CONTROLS / PERSONAL PROTECTION

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### 8.1 Engineering controls

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Use adequate general or local exhaust ventilation to keep airborne concentrations below the permissible exposure limits. Use process enclosure, local exhaust ventilation, or other engineering controls to control airborne levels.

**Control parameters:** Not set up

### 8.2 Personal protective equipment

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**Respiratory protection:** Dust respirator. Follow local and national regulations.

**Hand protection:** Protective gloves.

**Eye protection:** Wear safety glasses and chemical goggles if splashing is possible.

**Skin and body protection:** Wear appropriate protective gloves and clothing to prevent skin exposure.

## 9. PHYSICAL AND CHEMICAL PROPERTIES

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- a) Appearance Yellow powder
- b) Odour no data available
- c) Odour Threshold no data available
- d) pH no data available
- e) Melting point/freezing point no data available
- f) Initial boiling point and boiling range no data available
- g) Flash point no data available
- h) Evaporation rate no data available
- i) Flammability (solid, gas) no data available
- j) Flammability or explosive limits no data available
- k) Vapour pressure no data available
- l) Vapour density

- m) Relative density no data available
- n) Water solubility no data available
- o) Partition coefficient: no data available
- p) Autoignition temperature no data available
- q) Decomposition temperature no data available
- r) Viscosity no data available
- s) Explosive properties no data available
- t) Oxidizing properties no data available

## 10 - STABILITY AND REACTIVITY

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### 10.1 Reactivity

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Stable under recommended transport or storage conditions.

### 10.2 Chemical Stability

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Stable under normal temperatures and pressures.

### 10.3 Conditions to Avoid

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Incompatible materials, strong oxidants, heat.

### 10.4 Incompatibilities with Other Materials

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Strong oxidising/reducing agents, strong acids/alkalis.

### 10.5 Hazardous Decomposition Products

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Nitrogen oxides, carbon monoxide, irritating and toxic fumes and gases, carbon dioxide, nitrogen.

### 10.6 Hazardous Polymerization

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Has not been reported.

## 11. TOXICOLOGICAL INFORMATION

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<b>Acute Toxicity:</b>	No data available
<b>Skin corrosion/irritation:</b>	No data available
<b>Serious eye damage/irritation:</b>	No data available
<b>Germ cell mutagenicity:</b>	No data available
<b>Carcinogenicity:</b>	---
<b>IARC:</b>	No data available
<b>NTP:</b>	No data available
<b>Reproductive toxicity:</b>	No data available

## 12. ECOLOGICAL INFORMATION

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<b>Toxicity:</b>	No data available
<b>Persistence and degradability:</b>	No data available
<b>Bioaccumulative potential:</b>	No data available
<b>Mobility in soil:</b>	No data available
<b>Results of PBT and vPvB assessment:</b>	No data available
<b>Other adverse effects:</b>	May be harmful to the aquatic environment.

### 13. DISPOSAL CONSIDERATIONS

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Dispose of in a manner consistent with federal, state, and local regulations.

### 14. TRANSPORT INFORMATION

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#### 14.1 Hazards Class:

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Does not meet the criteria for classification as hazardous for transport

#### 14.2 UN proper shipping name

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**ADR/RID:** Not dangerous goods

**IMDG:** Not dangerous goods

**IATA:** Not dangerous goods

#### 14.3 Transport hazard class(es)

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Does not meet the criteria for classification as hazardous for transport.

### 15. REGULATORY INFORMATION

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#### 15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

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No data available

#### 15.2 Chemical Safety Assessment

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No data available

### 16. ADDITIONAL INFORMATION

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This GHS SDS above is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes. In no way shall the company be liable for any claims, losses, or damages of any third party or for lost profits or any special, indirect, incidental, consequential or exemplary damages, howsoever arising, even if the company has been advised of the possibility of such damages.



End of GHS safety data sheet



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