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**KAMPOYAKI NATURAL  
PRODUCTS BIO-CHEMISTRY**

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## ATRARIC ACID

### Datasheet

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

### PRODUCT INFORMATION

**Name:** Atraric acid

**Catalog No.:** KRN98703

**Cas No.:** 4707-47-5

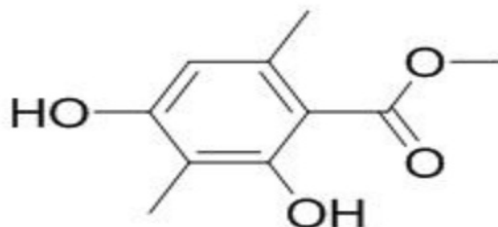
**Purity:** >= 95%

**M.F:** C<sub>10</sub>H<sub>12</sub>O<sub>4</sub>

**M.W:** 196.2

**Physical Description:** Powder

**Synonyms:** Methyl-2,4-dihydroxy-3,6-dimethylbenzoate.



### 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 *Vitis vinifera* L.

### BIOLOGICAL ACTIVITY OR INHIBITORS

Atraric acid (AA) isolated from bark material of *Pygeum africanum* has anti-androgenic activity, inhibiting the transactivation mediated by the ligand-activated human androgen receptor (AR); AA is able to efficiently repress the growth of both the androgen-dependent LNCaP and also the androgen-independent C4-2 Pca cells but not that of PC3 or CV1 cells lacking AR, AA also inhibits the expression of the endogenous prostate specific antigen gene in both LNCaP und C4-2 cells, suggests that AA can be used for prophylaxis or treatment of prostatic diseases. [1]

Protein tyrosine phosphatase 1B (PTP1B) is an attractive therapeutic target for diabetes, playing a major role in negative regulation of the insulin signaling pathway, atraric acid inhibits PTP1B activity in a dose-dependent manner with IC50 values of 51.5  $\mu$ M; suggest that atraric acid has potential to treat diabetes. [2]

## SOLVENT

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

## HPLC METHOD (2)

**Mobile phase:** 0.1% Formic acid in water- Methanol,gradient elution ;

**Flow rate:** 5.0 ml/min;

**Column temperature:** Room Temperature;

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

## STORAGE

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

## REFERENCES

[1] Papaioannou M, Schleich S, Prade I, et al. *J. Cell. Mol. Med.*, 2009, 13(8B):2210-23. [2] Changan Seo, Joung HanYim, Hong Kum Lee, et al. *Mycology An International Journal on Fungal Biology*, 2011, 2(1):18-23.



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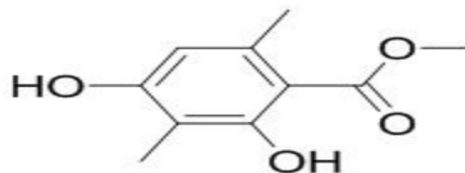
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## CERTIFICATE OF ANALYSIS

**Name:** Atraric acid  
**Catalog No.:** KRN98703  
**Cas No.:** 4707-47-5  
**Purity:** >= 98%  
**M.F:** C<sub>10</sub>H<sub>12</sub>O<sub>4</sub>



**Physical Description:** Powder

**Solvent:** Chloroform, Dichloromethane, Ethyl Acetate, DMSO, Acetone, etc.

**Weight** 20mg

**Lot No.** KRS201801

**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

Version 4.2

Revision Date 01/01/2018

Print Date 01/08/2019

## 1. PRODUCT AND COMPANY IDENTIFICATION

**GHS Product Name:** Atraric acid

**Product code:** KRN98703

**Company:** KAMPOYAKI HERS PTE LTD

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

**Tel:** +65-63833202

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## 2. HAZARDS IDENTIFICATION

### 2.1 GHS classification

**Physical Hazards:** Not classified

**Health Hazards:** Not classified

**Environmental Hazards:** Not classified

### 2.2 GHS label elements, including precautionary statements

**Pictograms or hazard symbols:** None

**Signal word:** No signal word

**Hazard statements:** None

**Precautionary statements:** None

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

**Chemical Name:** Atraric acid

**CAS#:** 4707-47-5

**Purity:**  $\geq 98\%$

**Formula:**  $C_{10}H_{12}O_4$

**Molecular Weight:** 196.2

**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

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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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**Acute Toxicity:** No data available

**Skin corrosion/  
irritation:** No data available

**Serious eye  
damage/irritation:** No data available

**Germ cell  
mutagenicity:** No data available

**Carcinogenicity:** ---

**IARC:** No data available

**NTP:** No data available

**Reproductive  
toxicity:** 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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