

# SciFinder<sup>®</sup>

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## 食品添加剂没食子酸丙酯的“前世今生”

您想了解没食子酸丙酯 (PG)吗？

您知道它是从何时开始被用做食品添加剂的吗？

您想知道它的最新检测手段吗？


您想知道没食子酸丙酯的最新应用前景吗？



A division of the American Chemical Society

[www.cas.org](http://www.cas.org)

# 没食子酸丙酯



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## Molecule of the Week


[Archive](#)

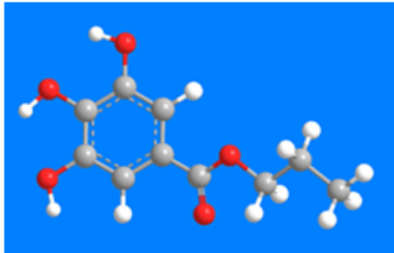
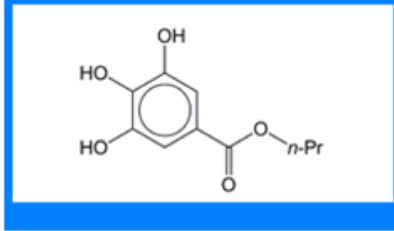
## Molecule of the Week

### *n*-Propyl gallate

**June 24, 2013**

*n*-Propyl gallate is an antioxidant for oils and fats that is used in foods, cosmetics, adhesives, and industrial lubricants. In 1983, M. A. Augustin and S. K. Berry were among the first researchers to study its antioxidant effectiveness. Recently, A. K. Franz and co-workers at the University of California, Davis, discovered a new property of *n*-propyl gallate: [It enhances the ability of microalgae to produce triacylglycerols](#). This finding may make it practical to use algae-derived lipids as biofuels.

 [More about this molecule](#) from CAS, the most authoritative and comprehensive source for chemical information.

近期, A. K. Franz 研究团队又发现了PG的特性: 它可促进微藻类生成三酰基甘油。此项发现使得利用藻类衍生物作为生物燃料变得实际可行。

## 到SciFinder中去检索更多关于PG的信息吧

The screenshot shows the SciFinder homepage with the 'SUBSTANCES: SUBSTANCE IDENTIFIER' search section. The search input field contains 'n-Propyl gallate'. Below the input field, there are examples of search terms: '50-00-0', '999815', and 'Acetaminophen'. A blue 'Search' button is visible. On the left sidebar, the 'SUBSTANCES' category is highlighted with a red circle, and its sub-options are listed: 'Chemical Structure', 'Markush', 'Molecular Formula', 'Property', and 'Substance Identifier'.

直接输入CAS号或英文名称、商品名、俗名等进行检索

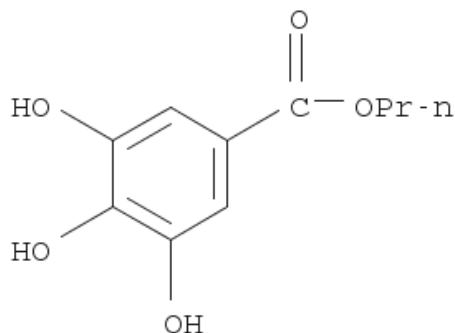
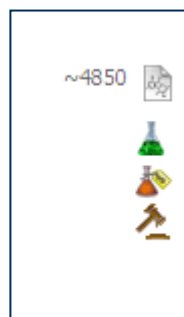
## CAS REGISTRY<sup>SM</sup>

数据库被誉为是世界上物质信息记录的“**黄金标准**”。通过SciFinder我们可以访问世界上最大最全的物质数据库。

物质检索的方式包括：

- 化学结构式
- 分子式
- 物质性质
- 物质名称
- CAS号

# SciFinder中关于PG的全面详尽物质信息



**CAS Registry Number:** 121-79-9

C<sub>10</sub> H<sub>12</sub> O<sub>5</sub>

Benzoic acid, 3,4,5-trihydroxy-, propyl ester

Gallic acid, propyl ester (6CI,8CI); Antioxidant PG; E 310; Gallic acid n-propyl ester; Hemostyptin; Marupi Gallate; NSC 2626; Nipa 49; Nipagallin P; Nipanox S 1; PG; Progallin P; Propyl 3,4,5-trihydroxybenzoate; Propyl gallate; Tenox PG; n-Propyl 3,4,5-trihydroxybenzoate; n-Propyl gallate

**Deleted CAS Registry Numbers:** 56274-95-4

## Biological Properties

	Value
LD50	See full text
LD50	See full text
Median Lethal Dose(LD50)	2500 mg/kg
Minimum Inhibitory Concentration	See full text
Minimum Inhibitory Concentration	See full text
Minimum Inhibitory Concentration	See full text

## Lipinski and Related Properties

	Value
logP	See full text
logP	See full text

## Spectra Properties

	Value
Carbon-13 NMR Spectrum	See spectrum
Carbon-13 NMR Spectrum	See spectrum

# 全面的理化性质信息

Experimental Properties: [Biological Chemical Flow and Diffusion Lipinski and Related Spectra Structure-related Thermal](#)

Biological Properties	Value	Condition	Note
LD50	See full text		(14)CAS
LD50	See full text		(15)CAS
Median Lethal Dose(LD50)	2500 mg/kg	Organism: rat Route: oral	(2)CAS
Minimum Inhibitory Concentration	See full text		(28)CAS
Minimum Inhibitory Concentration	See full text		(29)CAS
Minimum Inhibitory Concentration	See full text		(12)CAS

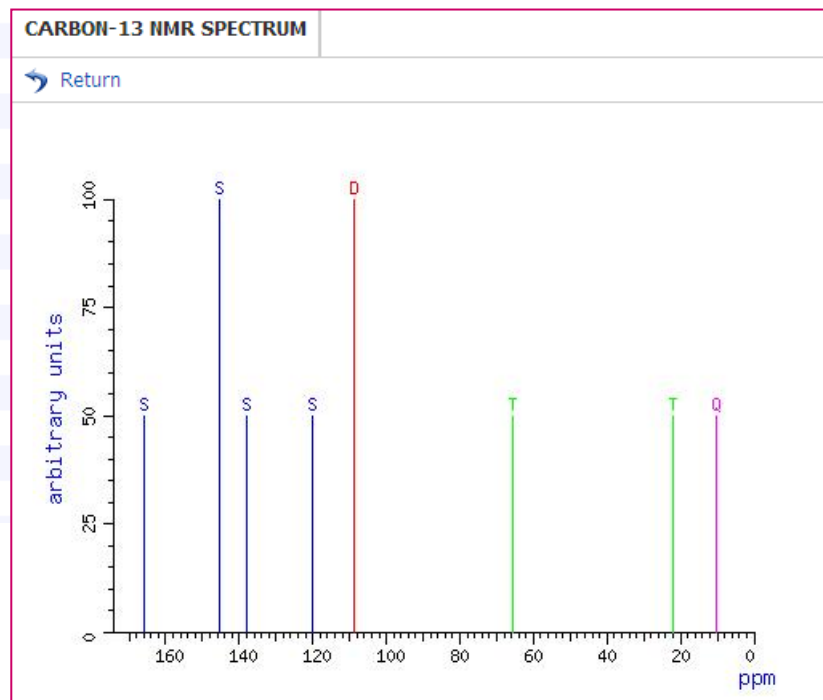
Chemical Properties	Value	Condition	Note
Acid/Base Dissociation Constant (Ka/Kb)	See full text		(1)CAS
Acid/Base Dissociation Constant (Ka/Kb)	See full text		(2)CAS
logP	See full text		(16)CAS
logP	See full text		(2)CAS
Partition Coefficient	See full text		(2)CAS
Potential of Electrode Reaction	See full text		(8)CAS
Potential of Electrode Reaction	See full text		(30)CAS
Potential of Electrode Reaction	See full text		(31)CAS
Potential of Electrode Reaction	See full text		(32)CAS
Solubility	See full text		(34)CAS

可链接到原始文献查看详细报导

Flow and Diffusion Properties	Value	Condition	Note
Diffusion Coefficient	See full text		(7)CAS
Diffusion Coefficient	See full text		(8)CAS

## 来源于文献报导的谱图信息

Spectra Properties	Value	Condition	Note
Carbon-13 NMR Spectrum	See spectrum		(4)AIST
Carbon-13 NMR Spectrum	See spectrum		(5)BIORAD
Carbon-13 NMR Spectrum	See spectrum		(6)WSS
IR Absorption Spectrum	See spectrum		(10)WSS
IR Absorption Spectrum	See spectrum		(10)WSS
IR Absorption Spectrum	See spectrum		(4)AIST
IR Absorption Spectrum	See spectrum		(4)AIST
IR Absorption Spectrum	See spectrum		(11)BIORAD
IR Absorption Spectrum	See spectrum		(11)BIORAD
IR Absorption Spectrum	See spectrum		(11)BIORAD
IR Absorption Spectrum	See spectrum		(11)BIORAD
IR Absorption Spectrum	See spectrum		(11)BIORAD
IR Absorption Spectrum	See spectrum		(11)BIORAD
IR Absorption Spectrum	See spectrum		(11)BIORAD
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IR Absorption Spectrum	See spectrum		(11)BIORAD
IR Absorption Spectrum	See spectrum		(11)BIORAD
IR Absorption Spectrum	See spectrum		(11)BIORAD
IR Absorption Spectrum	See spectrum		(11)BIORAD
IR Absorption Spectrum	See spectrum		(11)BIORAD
IR Absorption Spectrum	See full text		(11)BIORAD
IR Absorption Spectrum	See full text		(11)BIORAD
IR Spectrum	See full text		(12)CAS
IR Spectrum	See full text		(13)CAS
Mass Spectrum	See spectrum		(10)WSS



可直接点击查看谱图，也可回到原文中查看更详细谱图数据。

# PG的全球供应商信息

**COMMERCIAL SOURCES**

Analyze

Analyze by:

Sort by:

0 of 104 Commercial Sources Selected

- 1. **A Chemtek Product List**  
Supplier Name: A Chemtek, Catalog Publication Date: 13 Mar 2013  
Order Number: 031-20500  
Quantity: N/A  
121-79-9 Propyl gallate  
[Link](#)
- 2. **AAA Chemistry Stock Product List**  
Supplier Name: AAA Chemistry, Catalog Publication Date: 1 Mar 2013  
Order Number: AR-C1228  
Quantity: N/A  
121-79-9 Propyl Gallate  
[Link](#)
- 3. **ABCR Product List**  
Supplier Name: ABCR GmbH KG, Catalog Publication Date: 18 Dec 2012  
Order Number: AB120938  
Quantity: 500 g  
121-79-9 n-Propyl 3,4,5-trihydroxybenzoate, 98%  
[Link](#)

Supplier Name: Sigma-Aldrich 6  
TCI (Shanghai) Development Co., Ltd. 5  
TCI (Shanghai) Development Co., Ltd. (Beijing Branch) 5  
TCI America 5  
TCI America (East Coast Office) 5  
TCI Chemicals (India) Pvt. Ltd. 5  
TCI Deutschland GmbH 5

SciFinder中可查找到来自全球供应商信息。

查询结果可导出，方便根据需要寻求试剂级或工业级供应商

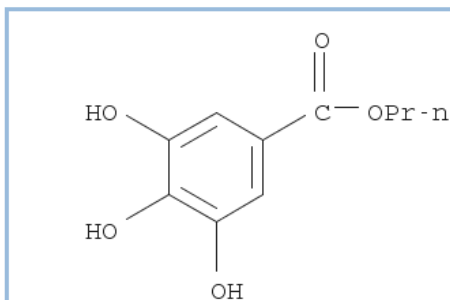
D	E	F

供应商也可能是是竞争对手？合作伙伴？

Catalog Name	Supplier Name	Street Address	City	Additional Company Contact Info	Publication Date
5 A Chemtek Product List	<a href="#">A Chemtek</a>	100 Barber Av.	Worcester	Phone: 508-471-4121 Fax: 508-845-9201 Email: sales@achemtek.com	13 Mar 2013
6 AAA Chemistry Stock Product List	<a href="#">AAA Chemistry</a>	4/F, Silvercord Centre Tower One 30 Canton Road	TST, KLN	Phone: 0085281916999 Fax: 00862584637266 Email: contact@aaa-chem.com	1 Mar 2013
7 ABCR Product List	<a href="#">ABCR GmbH KG</a>	Im Schleiert 10	Karlsruhe	Phone: ++49-(0)721-95061-0 Fax: ++49-(0)721-95061-80 Email: info@abcr.de	18 Dec 2012
8 ABI Chem Stock Building Blocks	<a href="#">ABI Chem</a>	Samoa Strasse 79	Munich	Phone: +49 89 1298 7050 Email: sales@abichem.com Phone: 800-368-1131 Fax: 800-410-2577 Email:	19 Apr 2013

# PG的合成方法

## 1. Substance Detail 121-79-9



**C<sub>10</sub> H<sub>12</sub> O<sub>5</sub>**  
Benzoic acid, 3,4,5-trihydroxy-, propyl ester

~4850 CAS Registry Number: 121-79-9

- >> View Substance Detail
- 🔍 Explore by Structure
- Synthesize this...**
- Get Reactions where Substance is a ▶
- Get Commercial Sources
- Get Regulatory Information
- Get References
- Export as Image
- Export as molfile
- Send to SciPlanner

SciFinder中的物质标准菜单整合了物质相关的所有信息。

做为权威领先的电子检索工具，SciFinder致力于提供高水准的便捷工具，让检索更轻松更愉悦！

~4854

### Get Reactions

**Limit results by reaction role:**

- Product**
- Reactant
- Reagent
- Reactant or reagent
- Catalyst
- Solvent
- Any role

Get Cancel

### Get References

**Limit results to:**

<input type="checkbox"/> Adverse Effect, including toxicity	<input type="checkbox"/> Prophetics in Patents
<input type="checkbox"/> Analytical Study	<input checked="" type="checkbox"/> Preparation
<input type="checkbox"/> Biological Study	<input type="checkbox"/> Process
<input type="checkbox"/> Combinatorial Study	<input type="checkbox"/> Properties
<input type="checkbox"/> Crystal Structure	<input type="checkbox"/> Reactant or Reagent
<input type="checkbox"/> Formation, nonpreparative	<input type="checkbox"/> Spectral Properties
<input type="checkbox"/> Miscellaneous	<input type="checkbox"/> Uses
<input type="checkbox"/> Occurrence	

**For each sequence, retrieve:**

Additional related references, e.g., activity studies, disease studies.

Get Cancel

物质相关的反应和文献依据CAS Roles做了详细分类！



# PG的合成路线、文献出处、实验步骤、反应信息等

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Substance Identifier "n-Propyl gallate" > substances (1) > get reactions (45)

REACTIONS

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Analyze | Refine

Group by: Document | Sort by: Experimental Procedure

Answers per Page [50] | Display: [Icons]

Analyze by: Catalyst

Author Name  
Catalyst  
Company-Organization  
Document Type  
Experimental Procedure  
Journal Name  
Language  
Number of Steps  
Product Yield  
Publication Year  
Solvent

No Grouping  
Document  
Transformation

Accession Number  
Experimental Procedure  
Number of Steps  
Product Yield  
Publication Year

multaneous production of tannase and gallic acid by marine *Aspergillus awamori* BTMF032

Full Text  
Reaction Similar Reaction

Single Step Hover over any structure for more options.

Oc1c(O)c(O)c(C(=O)O)c1.OCCCO>>Oc1c(O)c(O)c(C(=O)OCC)c1

444335-74-4 1  
80997-96-2 1  
856163-48-9 1

Show More

Overview

Experimental Procedure

Springer

Synthesis of Propyl Gallate. Propyl gallate was synthesized by transesterification of tannic acid in the presence of purified acidophilic tannase, produced by marine *A. awamori* BTMF032. Two millilitres of the tannase enzyme (699 U/ml) was added to 10 ml of 10 mM tannic acid in n-propanol and shaken at 100 rpm for 72 h. After incubation, the content was extracted with double-fold volume of ethyl acetate and separated using a separating funnel. Ethyl acetate was evaporated to recover propyl gallate in powder form. This powder was further analyzed for the presence of propyl gallate by thin layer chromatography (TLC) with silica gel G-60 F<sub>254</sub> (E. Merck, Mumbai, India). The solvent system consisted of ethyl acetate, chloroform and formic acid (4:4:1, v/v/v). After drying, the plates were developed by spraying a solution of FeCl<sub>3</sub>. Standard propyl gallate (Merck, Germany) and samples were run in

无需原文，合成化学家可立即开始实验工作！

# 关于PG抗氧化性能的最早研究报导可追溯到1943年

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Substance Identifier "n-Propyl gallate" > substances (1) > get references (4976) > keep analysis "Index Term" (1962)

REFERENCES

Get Substances | Get Reactions | Get Related Citations | Get Full Text | Tools

Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine | Categorize

Sort by: Publication Year

Answers per Page [20] Display: [ ] [ ] [ ]

0 of 1962 References Selected

Page: 1 of 99

Analyze by:

- Index Term
- Antioxidants 1962
- Tocopherols 283
- Drug delivery systems 187
- Fats and Glyceric oils 182
- Surfactants 166
- Polyoxyalkylenes 162
- Fatty acids 151
- Soybean oil 148
- Lecithins 144
- Human 139

Show More

- Study of the inhibiting actions of propyl gallate (propyl trihydroxy benzoate) and certain other trihydric phenols on the autoxidation of animal and vegetable oils**

By Boehm, Erich; Williams, Reginald  
From Quarterly Journal of Pharmacy and Pharmacology (1943), 16, 232-43. | Language: Unavailable, Database: CAPLUS

See C. A. 37, 6087.7.
- Action of propyl gallate in the autoxidation of oils**

By Boehm, E.; Williams, R.  
From Pharmaceutical Journal (1943), 151, 53. | Language: Unavailable, Database: CAPLUS

This compd. was found to be less effective as an antioxidant than pyrogallol, which, however, turns lard brown, and more effective than gallic acid, 10 times more effective than Siam benzoin and more than 30 times more effective than Sumatra benzoin. Lard treated with 0.05% nronyl gallate is adequately preserved.
- Action of propyl gallate in the**

By Boehm, E.; Williams, R.  
From Chemist and Druggist (1943), 140, 146. | Language: Unavailable, Database: CAPLUS

This compd. was found to be less effective as an antioxidant than pyrogallol, which, however, turns lard brown, and more effective than gallic acid, 10 times more effective than Siam benzoin and more than 30 times more effective than Sumatra benzoin. Lard treated with 0.05% propyl gallate is adequately preserved.
- Protection of ether against peroxide formation**

By Boehm, Erich; Williams, Reginald  
From Quarterly Journal of Pharmacy and Pharmacology (1944), 17, 171-7. | Language: Unavailable, Database: CAPLUS

The disadvantageous effects of the products formed in the autoxidation of Et<sub>2</sub>O have been briefly surveyed. Tests for the detection of peroxides in Et<sub>2</sub>O have been enumerated. The efficiencies of pyrogallol, hydroquinone, propyl and butyl gallates as antioxidants for Et<sub>2</sub>O have been compared in sunlight. Minute traces of propyl gallate have been found to exert a considerable inhibition on the autoxidation of Et<sub>2</sub>O, when exposed to diffused light, and at this low concn. the ester does

## 没食子酸丙酯在油脂中的抗氧化性作用

# PG在食品等中的最新检测方法

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0 of 117 References Selected | Page: 1 of 6

1. **Development of a generic assay for the determination of total trihydroxybenzoate derivatives based on gold-luminol chemiluminescence** [Full Text](#)

By Giokas, Dimosthenis L.; Christodouleas, Dionysios C.; Vlachou, Ioanna; Vlessidis, Athanasios G.; Calokerinos, Antony C.  
From Analytica Chimica Acta (2013), 764, 70-77. | Language: English

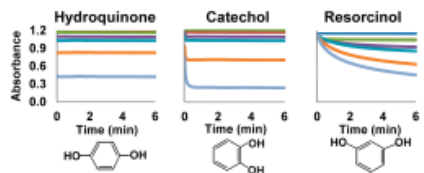
A selective assay for the detn. of one of the most imp. (at least one gallate moiety) based on their enhancing eff. In the presence of trihydroxybenzoate derivs., the light emission generated when alk. luminol is oxidized by gold ions is amplified several orders of magnitude compared to other common phenolic compds. which exhibit minor reactivity or no reactivity at all (e.g. hydroxycinnamates, flavo...

**没食子酸衍生物的通用快速检测方法**

2. **Effects of Molecular Structure on Kinetics and Dynamics of the Trolox Equivalent Antioxidant Capacity Assay with ABTS+•** [Full Text](#)

By Tian, Xin; Schaich, K. M.  
From Journal of Agricultural and Food Chemistry (2013), 61(23), 5511-5519. | Language: English, Database: CAPLUS

Reaction kinetics in the Trolox equiv. antioxidant capacity (TEAC) assay between ABTS+• [2,2'-azinobis(3-ethylbenzothiazoline-6-sulfonic acid) cation radical] and compds. with different structure, mol. wt., no. of OH groups, and redox potential were investigated by recording loss of ABTS+• absorbance (734 nm) continuously over time. Curves showed six distinguishable kinetic patterns, including both immediate and extended reaction components. Radical quenching rates in the immediate component most relevant to reactions in foods and tissues depended on phenol structure and steric accessibility...



3. **Rapid detection method of propylgallate in edible grease food** [Full Text](#)

By Yang, Yaling; Li, Yingtang; Jiao, Yang  
From Faming Zhuanli Shenqing (2013), CN 103105393 A 20130515. | Language: C

The title detection method includes the steps of extg. the propylgall out liq.-liq. micro-extn. for the color developed soln. by alc. org. solvent and surface active agent, centrifuging and sepg. the phases, and comparing with std. PG soln. to identify the content. The org. solvent for extg. PG in edible grease food is one or more of acetonitrile, methanol, acetone, ethanol, ethylene glycol. The developer is one or more of ammonium acetate, diethylamine, ammonium sulfate, ferrous sulfate, sodiu...

**食用油脂中PG的快速检测方法**

# PG作为油脂抗氧化剂广泛应用于食品、化妆品、粘合剂、工业润滑剂中

**Categorize** ?

1. Select a heading and category.      2. Select index terms of interest.

Category Heading	Category	Index Terms	Selected Terms
All	Substances in technology (14934)	Page: 1 of 7 Select All   Deselect All	Click 'x' to remove the category from 'Selected Terms'
General chemistry	<b>Materials &amp; products (607)</b>	Antioxidants 2019	Technology > Materials & products (1 Terms)
Biotechnology	Metallurgy (464)	Soybean oil 247	
Biology	Processes & apparatus (417)	Surfactants 246	
<b>Technology</b>	Formed, removed, & other substances (347)	Tannins 214	
Physical chemistry	Imaging & recording (83)	Stabilizing agents 169	
Polymer chemistry	Construction (35)	Oxygen 156	
Synthetic chemistry	Ceramics (29)	Preservatives 145	
Genetics & protein chemistry	Power & fuel topics (32)	Solvents 134	
Analytical chemistry		Antibacterial agents 133	
Environmental chemistry		Emulsifying agents 123	
Catalysis		Xanthan gum 116	
		Cosmetics 108	
		Fungicides 96	
		Gum arabic 86	
		Paraffin oils 84	

Technology > Materials & products > 1 Index Term(s) Selected

OK   Cancel

PG在大豆油、表面活性剂、化妆品、石蜡油、等各种产品中的应用文献分类。

**Categorize系统分类功能，基于索引词根据学科方向对文献做出精准分类！**

# PG最新报导的应用前景

REFERENCE DETAIL

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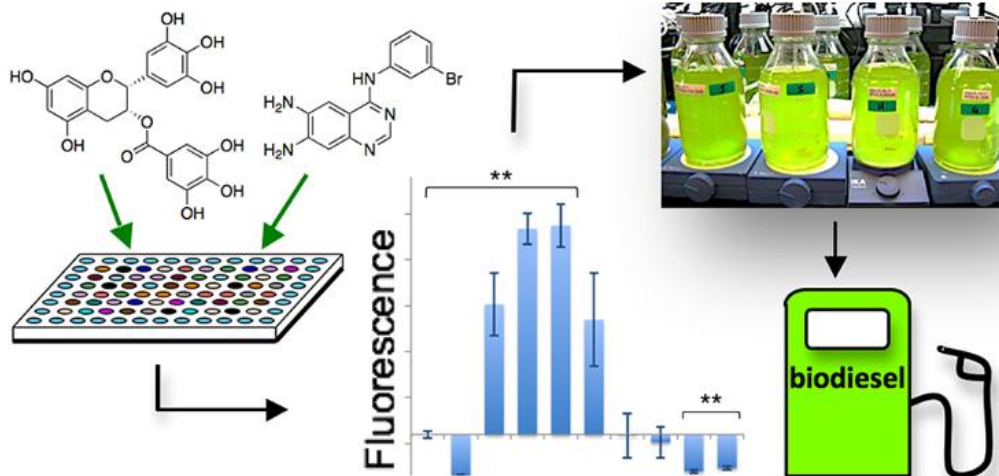
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Return

## Phenotypic Screening with Oleaginous Microalgae Reveals Modulators of Lipid Productivity

By: Franz, Annaliese K.; Danielewicz, Megan A.; Wong, Diana M.; Anderson, Lisa A.; Boothe, Jordan R.

Here we describe the first phenotypic screening with microalgae to study lipid metab. and to discover org. small mol. as chem. triggers that increase growth and lipid prodn. A microplate assay has been developed for anal. of intracellular lipids using Nile Red fluorescence in order to screen a collection of diverse bioactive org. mol. (e.g., kinase inhibitors) with four strains of oleaginous microalgae (*Nannochloropsis salina*, *Nannochloropsis oculata*, *Nannochloris* sp., and *Phaeodactylum tricornutum*). Several small mol. identified in microplate screening increased lipid productivity >200% without decreasing growth and biomass prodn. Selected compds. were further investigated in the context of larger batch culture expts. (e.g., 500 mL) and demonstrated to increase lipid levels (up to 84%) while maintaining or increasing the specific growth rate. Bioactive mol. such as forskolin and quinacrine were identified as promising probes of microalgae lipid pathways. We have also detd. that common antioxidants such as epigallocatechin gallate and butylated hydroxyanisole (BHA) increase lipid productivity and may represent new probes of oxidative signaling pathways for photooxidative protection.



### QUICK LINKS

0 Tags, 0 Comments

### SOURCE

*ACS Chemical Biology*  
Volume 8  
Issue 5  
Pages 1053-1062  
Journal; Online Computer File  
2013  
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ISSN: 1554-8929  
DOI: 10.1021/cb300573r

### COMPANY/ORGANIZATION

Department of Chemistry  
University of California  
Davis, CA, USA 95616

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2013:448054  
CAN158:605047  
CAPLUS

### PUBLISHER

American Chemical Society

### LANGUAGE

English

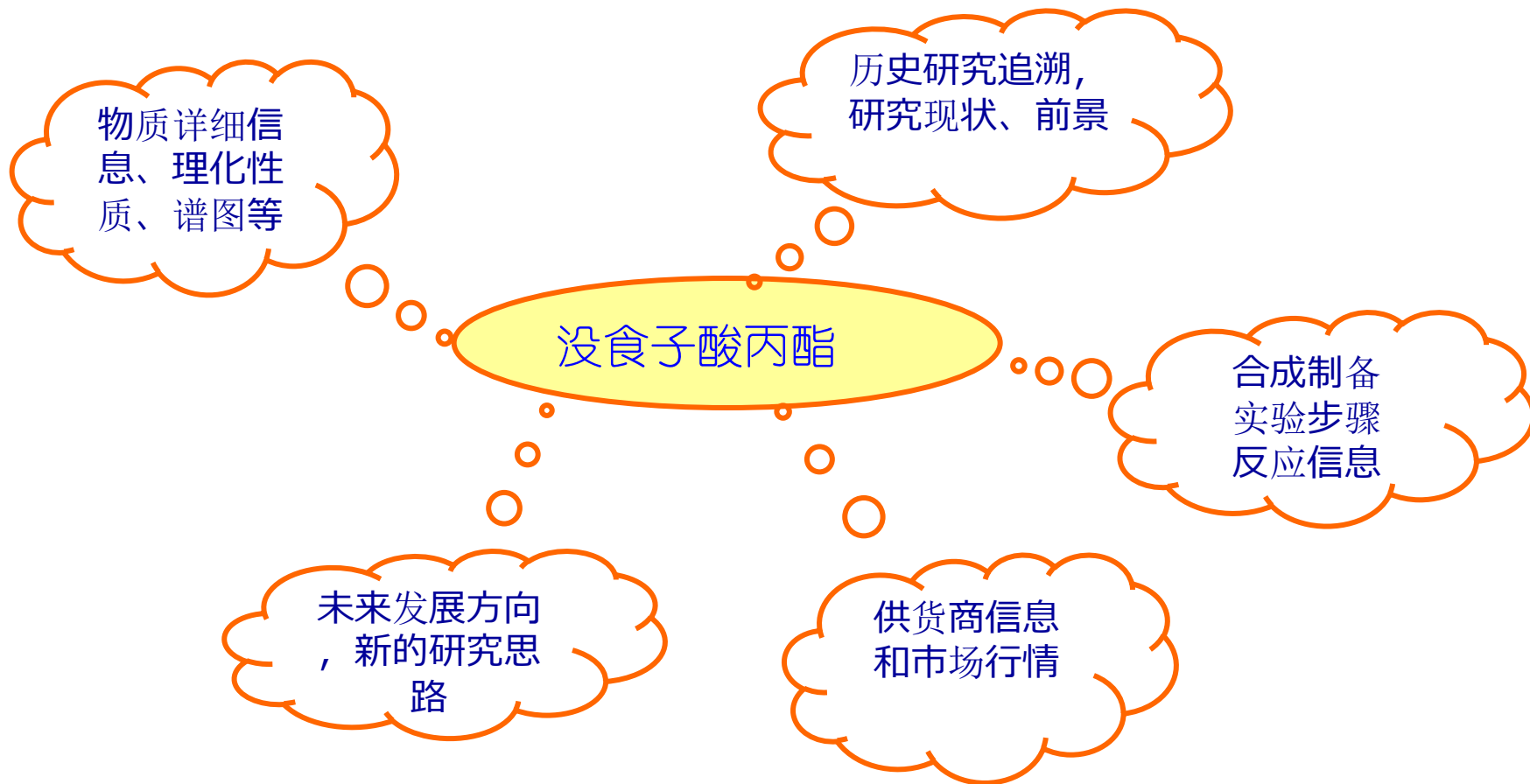
### Indexing

Fermentation and Bioindustrial Chemistry (Section 16-1)

常见抗氧化剂没食子酸酯类可促进微藻类转化成生物柴油



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