

# BIOFILES

FOR LIFE SCIENCE RESEARCH

2007  
Volume 2  
Number 2



DIETARY ANTIOXIDANTS

OMEGA-3 FATTY ACIDS  
AND HEART DISEASE

THE BIOACTIVE NUTRIENT  
EXPLORER

METABOLITE LIBRARIES

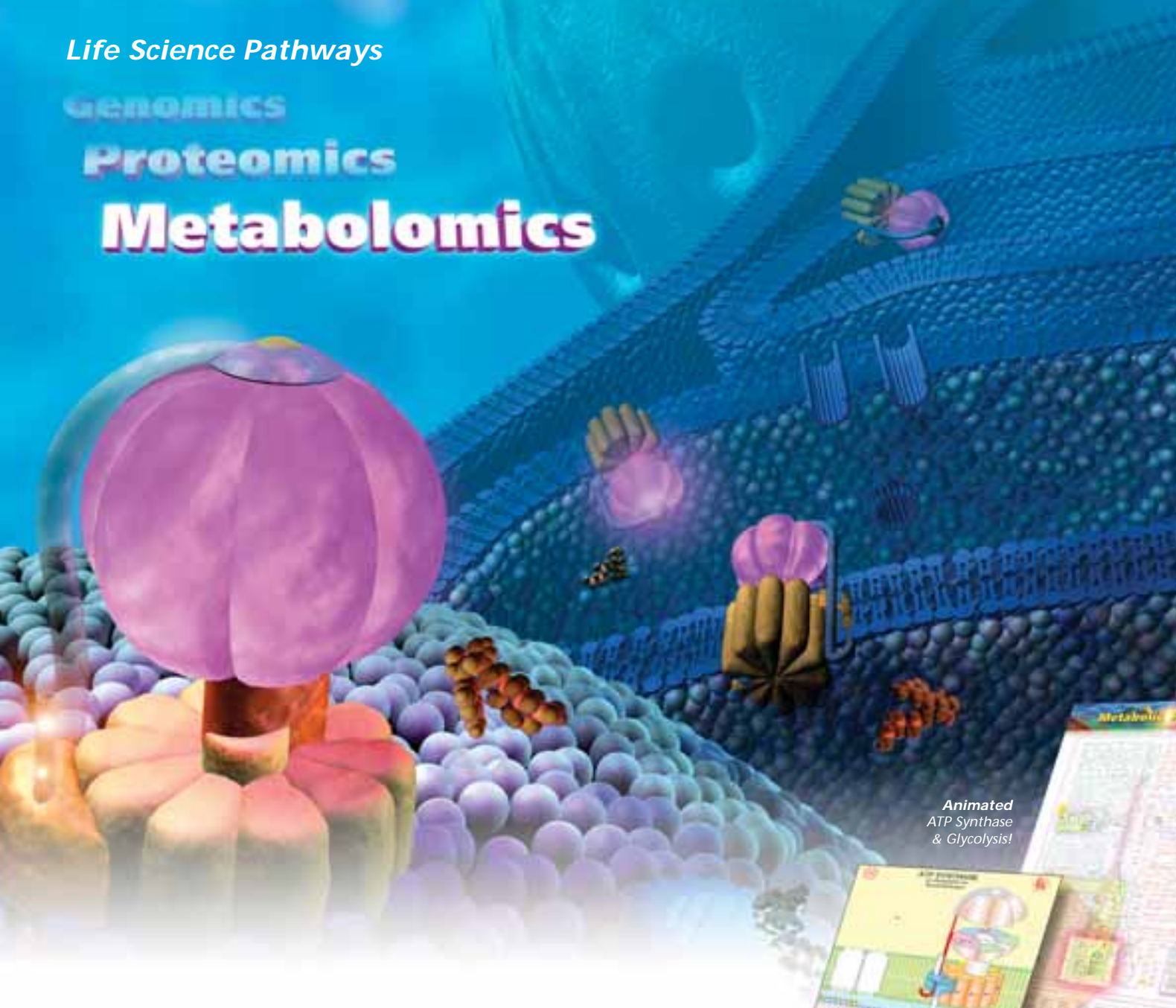
Examples of fruits and vegetables that contain antioxidants such as kaempferol, lycopene, and resveratrol.

## Nutrition Research

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## Introduction

For most of the world's population, foods and other plant and animal materials are consumed not only for their nutritional value, but also because they contain bioactive compounds that can prevent or treat diseases. Even in developed or rapidly developing economies, such as Japan, South Korea, China, and India, traditional medicines primarily derived from plant sources continue to be used along side, and often in preference to, modern pharmaceuticals. Throughout history, human populations have learned either by serendipity or by observation the properties of materials present in their environment. Even the most primitive societies, by modern standards, often had fairly sophisticated knowledge of the medicinal properties of local plants. This knowledge may have been passed down orally for centuries as the exclusive province of medicine men or shamans. Over time, this knowledge often became documented and codified, as in the Greco-Roman, Unani, Ayurvedic, or traditional Chinese pharmacopoeias and medical practices.

More recently, research interest in complementary and alternative medicine has surged as Western societies have embraced traditional herbal preparations and functional foods for their purported disease prevention and therapeutic properties. The global market for dietary supplements and functional foods was approximately \$145 billion in 2005, of which \$48 billion was within the U.S. Consumers perceive herbal source materials as safer than pharmaceuticals; in some cases there is research to support this view. Foods and herbs often contain several compounds with the same primary physiological effect but differing secondary actions. Thus, the beneficial effect is due to the combined action of several chemical entities, most of which are in low enough concentration to minimize secondary negative side effects.

From micronutrients to drugs of abuse, nutritionists, pharmacologists, and medical researchers are studying the physiological, therapeutic, and chemopreventive properties of foods and herbs and their constituents. This issue of BioFiles highlights some of the product groups available from Sigma-Aldrich to further this research, with special focus on omega-3 ( $\omega$ -3) fatty acids and antioxidant compounds such as carotenoids and polyphenols. We also introduce the Bioactive Nutrient Explorer, an interactive database on the Sigma-Aldrich web site that allows researchers to find plants of interest based on their physiological actions, plant constituents based on their chemical structure, and the chemical constituents of specific herbs and food plants.



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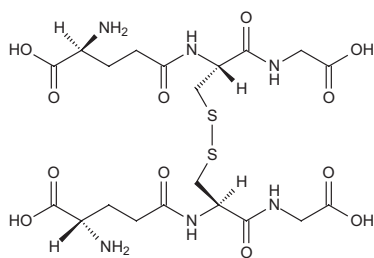
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## Dietary Antioxidants

### Dietary Antioxidants

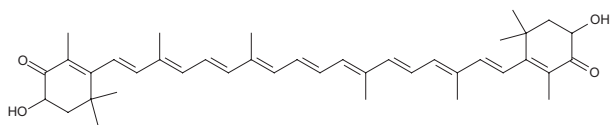
Antioxidants protect biological systems from oxidative damage produced by oxygen-containing free radicals and from redox-active transition metal ions such as iron, copper, and cadmium.<sup>1</sup> During the oxidative metabolism of glucose in the mitochondria, superoxide anions ( $O_2^-$ ) are produced as a by-product of the reduction of coenzyme Q complex III. The enzyme superoxide dismutase converts superoxide anions to hydrogen peroxide ( $H_2O_2$ ) that in turn can be converted to peroxy radicals ( $RO_2^-$ ), hydroxyl radicals ( $OH^\cdot$ ), or hypochlorite ( $ClO^-$ ) ions. Superoxide anions can also react with nitric oxide (NO) to form the highly reactive peroxynitrite ( $ONOO^-$ ).<sup>2</sup> Under normal conditions these cellular oxidants are reduced or scavenged by the intracellular antioxidants and antioxidant enzymes, the most important of which are glutathione, thioredoxin, superoxide dismutase, catalase, and peroxidase. Dietary antioxidants, such as ascorbic acid (vitamin C), vitamin E,  $\beta$ -carotene and other carotenoids, and selenium have been recognized as important contributors to the total antioxidant capacity of cells and plasma. The carotenoids lutein and zeaxanthin are important antioxidants in the eye and retina.<sup>3</sup> Vitamin E, a mixture of tocopherols and tocotrienols, of which  $\alpha$ -tocopherol is the major antioxidant,<sup>4</sup> is the major lipid soluble antioxidant in cells and plays a major role in protecting membrane lipids from peroxidation.<sup>2</sup> Low density lipoproteins (LDL) carry vitamin E into cells, which subsequently prevents the peroxidation of LDL by donating hydrogen to fatty peroxy radicals.<sup>5</sup> Polyphenolic compounds, especially the flavonoids, have recently been shown to be potent antioxidants in cultured cells. Human studies of flavonoids have also demonstrated effects that can in part be attributed to their antioxidant action.<sup>6</sup>

Antioxidants can act directly as reducing agents, donating protonic hydrogen to the unpaired oxygen electron or by stabilizing or relocating the free radical electron.<sup>7</sup> In the process the reducing agent becomes oxidized; for example, the cysteinyl sulfhydryl groups of two glutathione molecules are oxidized to form the intermolecular cystine of oxidized glutathione (see **Figure 1**).



**Figure 1.** Structure of oxidized glutathione

Lipoic acid is an endogenous antioxidant that has recently gained interest as a dietary supplement, since not only can it scavenge free radicals, but it is also a very effective reducing agent in its dihydrolipoate form. Lipoic acid reduces the oxidized forms of other antioxidants and ultimately can maintain the tissue concentrations of reduced glutathione.<sup>8</sup>



**Figure 2.** Structure of astaxanthin

Some antioxidants trap or scavenge the free radicals, and in the process become radicals themselves. When the carotenoids astaxanthin (see **Figure 2**), lutein, and zeaxanthin scavenge oxygen free radicals, the charge of the unpaired electron becomes delocalized over the entire polyene chain of the molecule.<sup>9</sup> The flavonol quercetin is oxidized to a quinone that can react with thiols.<sup>10</sup> Flavonoids are also excellent metal ion chelators and can prevent copper-catalyzed peroxidation of LDL.<sup>1,4,11</sup> The stilbene phytoalexin resveratrol is more potent than the flavonoids in chelating copper and preventing peroxidation of LDL.<sup>12</sup> This likely contributes to the antiatherosclerotic actions of resveratrol and the flavonoids.

Flavonoids and carotenoids, the major dietary antioxidants, are ubiquitous in fruits and vegetables. Epidemiological studies indicate that populations with diets high in these phytochemicals also have lower incidence rates of chronic diseases associated with oxidative stress, such as atherosclerosis, diabetes, neurodegenerative diseases, and cancer.<sup>8</sup> However, there is much disagreement concerning the mechanism of action of polyphenols *in vivo*. Polyphenols are treated as xenobiotics by the body and are rapidly metabolized and conjugated in the intestinal lining and liver. With the exception of the gallic acid conjugates of the catechins, such as epigallocatechin gallate,<sup>13</sup> most flavonoids in the blood are glucuronide, sulfate, or O-methylated conjugates.<sup>4,14</sup> These conjugates are essentially devoid of antioxidant activity.<sup>15</sup> Moskaug, et al., hypothesized that the flavonoids enhance cellular antioxidant systems by inducing a chronic, low level of oxidative stress in cells, thus boosting the cellular antioxidant defense system (the hormetic principle).<sup>15</sup> In contrast, Halliwell, et al., argued that micromolar concentrations of unabsorbed flavonoids and other phenolics remain in the small intestine and colon where their antioxidant, metal chelating, and other actions are protective against colorectal carcinogenesis.<sup>4</sup>

Recent studies confirm that the polyphenols have many intracellular effects beyond scavenging free radicals and chelating metal ions. Reactive oxygen species (ROS) and reactive nitrogen species (RNS) are also potential signaling molecules. They regulate gene expression via a class of redox-sensitive transcription factors that includes Nrf2, which induces expression of antioxidant/detoxifying enzymes, and NF $\kappa$ B and AP-1, which induce production of inflammatory cytokines, cell adhesion molecules, acute phase proteins, and are antiapoptotic.<sup>1,2,16</sup> These transcription factors are activated in response to oxidative stress; persistently elevated ROS levels activate NF $\kappa$ B by inducing the phosphorylation and disassociation of its inhibitory subunit, I $\kappa$ B. Silymarin and silybin (silibinin),<sup>17</sup> catechins and procyanidins,<sup>1,11</sup> and other flavonoids<sup>16</sup> have been reported to block the activation of NF $\kappa$ B.

Forman, et al., cite evidence that hydrogen peroxide and superoxide anion exhibit the properties of second messengers by mediating redox signaling responses. They hypothesize that peroxides interact reversibly with critical cysteine thiolates that are present in the active site of signaling proteins.<sup>18</sup> Protein tyrosine phosphatase and thioredoxin are known to have active site cysteines in the thiolate form, while the transcription factors AP-1 and NFκB and some caspases have redox sensitive cysteines that may be in the thiolate form. Zinc-bound cysteines in the regulatory site of some protein kinase c isoforms may also be oxidized by hydrogen peroxide. The receptor-stimulated production of peroxide also leads to the activation of all mitogen activated protein kinase pathways (ERK, JNK, and p38 MAPK). Other signaling proteins and enzymes are targeted by nitric oxide, peroxide, or both oxidants (see **Table 1**). Therefore antioxidant polyphenols that scavenge reactive oxygen intermediates may have profound effects on intracellular signal transduction pathways that mediate cellular responses to oxidative stress.

Signaling Protein	Modulator Oxidant
PTP1B	NO, H <sub>2</sub> O <sub>2</sub>
SHP-2	H <sub>2</sub> O <sub>2</sub>
LMW-PTP	NO, H <sub>2</sub> O <sub>2</sub>
PTEN	H <sub>2</sub> O <sub>2</sub>
Trx	NO, H <sub>2</sub> O <sub>2</sub>
Src	H <sub>2</sub> O <sub>2</sub>
Ras	NO, H <sub>2</sub> O <sub>2</sub>
GSTp/JNK	H <sub>2</sub> O <sub>2</sub>
Gi/Go	H <sub>2</sub> O <sub>2</sub>
NMDA	NO

**Table 1.** Additional Targets of Redox Signaling

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## Amino Acids and Peptides

### N-Acetyl-L-cysteine

LNAC; NAC

HSCH<sub>2</sub>CH(NHCOCH<sub>3</sub>)CO<sub>2</sub>H FW 163.19 [616-91-1]

BRN 1724426

S: 22-24/25 EC No. 210-498-3 RTECS # HA1660000

#### ▶ Sigma Grade, ≥99% (TLC)

2-8°C	
A7250-5G	5 g
A7250-10G	10 g
A7250-25G	25 g
A7250-50G	50 g
A7250-100G	100 g
A7250-500G	500 g
A7250-1KG	1 kg

#### ▶ SigmaUltra, >99% (TLC)

Insoluble matter .....	≤0.1%
Phosphorus (P) .....	≤0.002%
ign. residue.....	≤0.5%
Al .....	≤0.0005%
Ca .....	≤0.0005%
Cu .....	≤0.0005%
Fe .....	≤0.0005%
K .....	≤0.005%
Mg .....	≤0.0005%
NH <sub>4</sub> <sup>+</sup> .....	≤0.05%
Na .....	≤0.1%
Pb.....	≤0.001%
Zn.....	≤0.0005%

2-8°C	
A8199-10G	10 g
A8199-25G	25 g
A8199-100G	100 g

## Dietary Antioxidants

### L-Cysteine

(R)-2-Amino-3-mercaptopropionic acid  
 $\text{HSCH}_2\text{CH}(\text{NH}_2)\text{CO}_2\text{H}$  FW 121.16 [52-90-4]  
 BRN 1721408

✗ R: 22 EC No. 200-158-2 RTECS # HA1600000

▶ **≥98%, from non-animal source, cell culture tested**

Endotoxin ..... tested

**C7352-10MG 10 mg**

**C7352-25G 25 g**

**C7352-100G 100 g**

**C7352-1KG 1 kg**

▶ **BioChemika Ultra, ≥99.5% (RT)**

foreign amino acids ..... ≤0.5%

insoluble matter ..... passes filter test

LOD ..... ≤0.05%, 20 °C (HV) K ..... ≤50 mg/kg

ign. residue ..... ≤0.05% (as  $\text{SO}_4$ ) Li ..... ≤5 mg/kg

chloride (Cl) ..... ≤100 mg/kg Mg ..... ≤5 mg/kg

sulfate ( $\text{SO}_4$ ) ..... ≤50 mg/kg Mn ..... ≤5 mg/kg

Al ..... ≤5 mg/kg Mo ..... ≤5 mg/kg

As ..... ≤0.1 mg/kg  $\text{NH}_4^+$  ..... ≤500 mg/kg

Ba ..... ≤5 mg/kg Na ..... ≤100 mg/kg

Bi ..... ≤5 mg/kg Ni ..... ≤5 mg/kg

Ca ..... ≤10 mg/kg Pb ..... ≤5 mg/kg

Cd ..... ≤5 mg/kg Sr ..... ≤5 mg/kg

Co ..... ≤5 mg/kg Zn ..... ≤5 mg/kg

Cr ..... ≤5 mg/kg  $\lambda$  ..... 1 M in 1 M HCl

Cu ..... ≤5 mg/kg 260 nm ..... ≤1.0

Fe ..... ≤5 mg/kg 280 nm ..... ≤0.2

**30089-25G 25 g**

**30089-100G 100 g**

**30089-500G 500 g**

### L-Cysteine hydrochloride monohydrate

$\text{HSCH}_2\text{CH}(\text{NH}_2)\text{COOH} \cdot \text{HCl} \cdot \text{H}_2\text{O}$  FW 175.63 [7048-04-6]  
 EC No. 2001577 BRN 5158059

✗ R: 36/37/38 S: 26

▶ **reagent grade, ≥98% (TLC)**

**C7880-100G 100 g**

**C7880-500G 500 g**

**C7880-1KG 1 kg**

**C7880-5KG 5 kg**

▶ **BioChemika Ultra, ≥99.0% (RT)**

insoluble matter ..... passes filter test

foreign amino acids ..... ≤0.5%

ign. residue ..... ≤0.05% (as  $\text{SO}_4$ ) Li ..... ≤5 mg/kg

sulfate ( $\text{SO}_4$ ) ..... ≤100 mg/kg Mg ..... ≤5 mg/kg

Al ..... ≤5 mg/kg Mn ..... ≤5 mg/kg

As ..... ≤0.5 mg/kg Mo ..... ≤5 mg/kg

Ba ..... ≤5 mg/kg  $\text{NH}_4^+$  ..... ≤500 mg/kg

Bi ..... ≤5 mg/kg Na ..... ≤50 mg/kg

Ca ..... ≤10 mg/kg Ni ..... ≤5 mg/kg

Cd ..... ≤5 mg/kg Pb ..... ≤5 mg/kg

Co ..... ≤5 mg/kg Sr ..... ≤5 mg/kg

Cr ..... ≤5 mg/kg Zn ..... ≤5 mg/kg

Cu ..... ≤5 mg/kg  $\lambda$  ..... 1 M in  $\text{H}_2\text{O}$

Fe ..... ≤5 mg/kg 260 nm ..... ≤1.0

K ..... ≤50 mg/kg 280 nm ..... ≤0.3

**30129-25G 25 g**

**30129-100G 100 g**

**30129-500G 500 g**

### L-Glutathione reduced

$\gamma$ -L-Glutamyl-L-cysteinyl-glycine: GSH

$\gamma$ -Glu-Cys-Gly

$\text{H}_2\text{NCH}(\text{CO}_2\text{H})\text{CH}_2\text{CH}_2\text{CONHCH}(\text{CH}_2\text{SH})\text{CONHCH}_2\text{CO}_2\text{H}$  FW 307.32

[70-18-8] BRN 1729812

EC No. 200-725-4 RTECS # MC0556000

▶ **≥99%**

2-8°C

**G4251-10MG 10 mg**

**G4251-300MG 300 mg**

**G4251-1G 1 g**

**G4251-5G 5 g**

**G4251-10G 10 g**

**G4251-25G 25 g**

**G4251-50G 50 g**

**G4251-100G 100 g**

**G4251-250G 250 g**

**G4251-500G 500 g**

▶ **SigmaUltra, 98-100%**

Phosphorus (P) ..... <0.005%

Insoluble matter ..... <0.1%

ign. residue ..... <0.1% K ..... <0.005%

sulfate ( $\text{SO}_4$ ) ..... <0.05% Mg ..... <0.0005%

Al ..... <0.0005%  $\text{NH}_4^+$  ..... <0.05%

Ca ..... <0.0005% Na ..... <0.005%

Cu ..... <0.0005% Pb ..... <0.001%

Fe ..... <0.0005% Zn ..... <0.0005%

2-8°C

**G6529-1G 1 g**

**G6529-5G 5 g**

**G6529-25G 25 g**

## Flavonoids

### Acacetin

5,7-Dihydroxy-4'-methoxyflavone

$C_{16}H_{12}O_5$  FW 284.26 [480-44-4] BRN 277879

**BioChemika,  $\geq 97.0\%$  (HPLC)**

✘ R: 36/37/38 S: 26-36 EC No. 207-552-3 Hygroscopic, Light sensitive  
RTECS # DJ3002000 [2-8°C]

00017-25MG 25 mg

00017-100MG 100 mg

### Amentoflavone

Didemethyl-ginkgetin

$C_{30}H_{18}O_{10}$  FW 538.46 [1617-53-4] BRN 380244

**$\geq 99.0\%$  (HPLC)**

S: 22-24/25 [2-8°C]

40584-1MG-F 1 mg

40584-5MG-F 5 mg

### Apigenin

4',5,7-Trihydroxyflavone

$C_{15}H_{10}O_5$  FW 270.24 [520-36-5] BRN 262620

✘ R: 36/37/38 S: 26-36 EC No. 208-292-3 RTECS # LK9276000

▶  **$\sim 95\%$  (TLC), from parsley**

[-20°C]

A3145-5MG 5 mg

A3145-25MG 25 mg

A3145-100MG 100 mg

▶ **BioChemika,  $\geq 95.0\%$  (HPLC)**

water ..... ~2%

[-20°C]

10798-25MG 25 mg

10798-100MG 100 mg

### Baicalein

5,6,7-Trihydroxyflavone

$C_{15}H_{10}O_5$  FW 270.24 [491-67-8] BRN 272683

**BioChemika,  $\geq 98.0\%$  (UV)**

✘ R: 36/37/38 S: 26-36 Light sensitive ◆ [2-8°C]

11712-100MG 100 mg

11712-500MG 500 mg

### Biochanin A

5,7-Dihydroxy-4'-methoxyisoflavone: Genistein 4'-methyl ether

$C_{16}H_{12}O_5$  FW 284.26 [491-80-5] BRN 278107

S: 22-24/25 EC No. 207-744-7

D2016-100MG 100 mg

D2016-250MG 250 mg

D2016-1G 1 g

### (+)-Catechin hydrate

(+)-Cyanidol-3: (2R,3S)-2-(3,4-Dihydroxyphenyl)-3,4-dihydro-1(2H)-benzopyran-3,5,7-triol

$C_{15}H_{14}O_6 \cdot xH_2O$  FW 290.27 (Anh) [225937-10-0] BRN 3595244

✘ R: 36/37/38 S: 26-36

▶ **puriss.,  $\geq 99.0\%$  (HPLC)**

EC No. 205-825-1 [2-8°C]

41343-1MG-F 1 mg

41343-5MG-F 5 mg

▶  **$\geq 98\%$  (TLC)**

C1251-5G 5 g

C1251-10G 10 g

### (-)-Catechin

(2S,3R)-2-(3,4-Dihydroxyphenyl)-3,4-dihydro-1(2H)-benzopyran-3,5,7-triol;

(+)-*trans*-3,3',4',5,7-Pentahydroxyflavane

$C_{15}H_{14}O_6$  FW 290.27 [18829-70-4]

▶  **$\geq 98\%$  (HPLC), from green tea**

EC No. 242-611-7 [2-8°C]

C0567-5MG 5 mg

▶ **puriss.,  $\geq 98.5\%$  (HPLC)**

[2-8°C]

51261-1MG-F 1 mg

### (-)-Catechin gallate

(2S,3R)-2-(3,4-Dihydroxyphenyl)-3,4-dihydro-1(2H)-benzopyran-3,5,7-triol  
3-(3,4,5-trihydroxybenzoate)

$C_{22}H_{18}O_{10}$  FW 442.37 [130405-40-2]

**$\geq 98\%$  (HPLC), from green tea**

✘ R: 36/37/38 S: 26-36 [2-8°C]

C0692-1MG 1 mg

C0692-5MG 5 mg

## Dietary Antioxidants

### Chrysin

5,7-Dihydroxyflavone  
 $C_{15}H_{10}O_4$  FW 254.24 [480-40-0] BRN 233276

**BioChemika,  $\geq 96.0\%$  (HPLC)**

S: 22-24/25 EC No. 207-549-7 RTECS # LK8329050

27214-5MG-F	5 mg
27214-100MG-F	100 mg

### Cyanidin chloride

3,3',4,5,7-Pentahydroxyflavylium chloride  
 $C_{15}H_{11}ClO_6$  FW 322.70 [528-58-5]

**BioChemika,  $\geq 95\%$  (HPLC)**

EC No. 208-438-6 RTECS # LK9824000  $-20^\circ\text{C}$

79457-1MG-F	1 mg
-------------	------

### Daidzein

4',7-Dihydroxyisoflavone: 7-Hydroxy-3-(4-hydroxyphenyl)-4H-1-benzopyran-4-one; 7-Hydroxy-3-(4-hydroxyphenyl)chromone  
 $C_{15}H_{10}O_4$  FW 254.24 [486-66-8] BRN 231523

$\geq 98\%$ , synthetic

**X** R: 36/38 S: 24-26 EC No. 207-635-4 RTECS # DJ3100040  $-20^\circ\text{C}$

D7802-25MG	25 mg
D7802-100MG	100 mg

### Datisctein

2',3,5,7-Tetrahydroxyflavone  
 $C_{15}H_{10}O_6$  FW 286.24 [480-15-9] BRN 39982

**BioChemika,  $\geq 99.0\%$  (HPLC)**

**X** R: 36/37/38 S: 26 EC No. 207-541-3  $\blacklozenge$

17801-10MG	10 mg
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### Delphinidin chloride

3,3',4',5,5',7-Hexahydroxyflavylium chloride  
 $C_{15}H_{11}ClO_7$  FW 338.70 [528-53-0]

**purum,  $\geq 95.0\%$  (HPLC)**

EC No. 208-437-0 RTECS # DK1310000  $-20^\circ\text{C}$

43725-1MG-F	1 mg
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### 4',7-Dimethoxyisoflavone

Daidzein dimethyl ether  
 $C_{17}H_{14}O_4$  FW 282.29 [1157-39-7] BRN 265550

**BioChemika,  $\geq 96.0\%$  (TLC)**

S: 22-24/25

38763-1MG	1 mg
38763-5MG	5 mg

### Diosmetinidin chloride

3',5,7-Trihydroxy-4'-methoxyflavylium chloride  
 $C_{16}H_{13}ClO_5$  FW 320.72 [64670-94-6]

$\geq 98.5\%$  (HPLC), purum

$-20^\circ\text{C}$

51702-1MG-F	1 mg
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### (-)-Epicatechin

(2R,3R)-2-(3,4-Dihydroxyphenyl)-3,4-dihydro-1(2H)-benzopyran-3,5,7-triol:  
 (-)-*cis*-3,3',4',5,7-Pentahydroxyflavane  
 $C_{15}H_{14}O_6$  FW 290.27 [490-46-0] BRN 92760

**X** R: 36/37/38 S: 26-36 EC No. 207-710-1 RTECS # KB3745000

$\blacktriangleright \geq 98\%$  (HPLC), from green tea

$-2-8^\circ\text{C}$

E4018-1MG	1 mg
E4018-5MG	5 mg

$\blacktriangleright$  purum,  $\geq 95.0\%$  (HPLC)

$-2-8^\circ\text{C}$

39263-1MG-F	1 mg
39263-5MG-F	5 mg

### (-)-Epicatechin gallate

(-)-*cis*-2-(3,4-Dihydroxyphenyl)-3,4-dihydro-1(2H)-benzopyran-3,5,7-triol  
 3-gallate; (-)-*cis*-3,3',4',5,7-Pentahydroxyflavane 3-gallate  
 $C_{22}H_{18}O_{10}$  FW 442.37 [1257-08-5]

$\geq 98\%$  (HPLC), from green tea

RTECS # DH9030000  $-2-8^\circ\text{C}$

E3893-10MG	10 mg
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### (-)-Epigallocatechin

(-)-*cis*-3,3',4',5,5',7-Hexahydroxyflavane; (-)-*cis*-2-(3,4,5-Trihydroxyphenyl)-  
 3,4-dihydro-1(2H)-benzopyran-3,5,7-triol  
 $C_{15}H_{14}O_7$  FW 306.27 [970-74-1]  
 RTECS # KB5100000

$\blacktriangleright \geq 95\%$  (HPLC), from green tea

$-2-8^\circ\text{C}$

E3768-5MG	5 mg
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$\blacktriangleright$  BioChemika,  $\geq 90\%$  (HPLC)

08108-1MG-F	1 mg
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**(-)-Epigallocatechin gallate**

EGCG: (-)-*cis*-3,3',4',5,5',7-Hexahydroxyflavane-3-gallate; (-)-*cis*-2-(3,4,5-Trihydroxyphenyl)-3,4-dihydro-1(2H)-benzopyran-3,5,7-triol 3-gallate

C<sub>22</sub>H<sub>18</sub>O<sub>11</sub> FW 458.37 [989-51-5]

Light sensitive RTECS # KB5200000

▶ **purum, ≥97.0% (HPLC)**

2-8°C

50299-1MG-F 1 mg

▶ **≥95%, from green tea**

2-8°C

E4143-50MG 50 mg

▶ **≥80% (HPLC), from green tea**

2-8°C

E4268-100MG 100 mg

**Eriodictyol**

(S)-3',4',5,7-Tetrahydroxyflavanone

C<sub>15</sub>H<sub>12</sub>O<sub>6</sub> FW 288.25 [552-58-9] BRN 5104930

**purum, ≥95.0% (HPLC)**

✗ R: 36/37/38 S: 26-37/39 EC No. 209-016-4

74565-5MG-F 5 mg

**Fisetin**

5-Deoxyquercetin; Natural Brown 1; 3,3',4',7-Tetrahydroxyflavone

C<sub>15</sub>H<sub>10</sub>O<sub>6</sub> · xH<sub>2</sub>O FW 286.24 (Anh) [345909-34-4]

BRN 292829

S: 22-24/25 EC No. 208-434-4 RTECS # LK9250000

-20°C

F4043-100MG 100 mg

F4043-500MG 500 mg

▶ **BioChemika, ≥99.0% (HPLC)**

46340-5MG 5 mg

46340-100MG 100 mg

**Formononetin**

7-Hydroxy-4'-methoxyisoflavone; 7-Hydroxy-3-(4-methoxyphenyl) chromone

C<sub>16</sub>H<sub>12</sub>O<sub>4</sub> FW 268.26 [485-72-3] BRN 237979

**BioChemika, ≥99.0% (TLC)**

✗ R: 36/37/38 S: 26-36 EC No. 207-623-9 N

47752-5MG-F 5 mg

47752-25MG-F 25 mg

**Galangin**

3,5,7-Trihydroxyflavone

C<sub>15</sub>H<sub>10</sub>O<sub>5</sub> FW 270.24 [548-83-4] BRN 272179

**BioChemika, ~95% (HPLC)**

✗ R: 36/37/38 S: 26-37/39 EC No. 208-960-4 RTECS # LK9275500

48291-1MG 1 mg

48291-5MG 5 mg

**(-)-Galocatechin**

(2S,3R)-2-(3,4,5-Trihydroxyphenyl)-3,4-dihydro-1(2H)-benzopyran-3,5,7-triol

C<sub>15</sub>H<sub>14</sub>O<sub>7</sub> FW 306.27 [3371-27-5]

**>98% (HPLC)**

✗ R: 36/37/38 S: 26-36 2-8°C

G6657-1MG 1 mg

G6657-5MG 5 mg

**(-)-Galocatechin gallate**

(2S,3R)-2-(3,4,5-Trihydroxyphenyl)-3,4-dihydro-1(2H)-benzopyran-3,5,7-triol 3-(3,4,5-trihydroxybenzoate)

C<sub>22</sub>H<sub>18</sub>O<sub>11</sub> FW 458.37 [4233-96-9]

**≥98% (HPLC), from green tea**

✗ R: 36/37/38 S: 26-36 RTECS # DH9000000 2-8°C

G6782-5MG 5 mg

**Genistein**

5,7-Dihydroxy-3-(4-hydroxyphenyl)-4H-1-benzopyran-4-one;

4',5,7-Trihydroxyisoflavone

C<sub>15</sub>H<sub>10</sub>O<sub>5</sub> FW 270.24 [446-72-0] BRN 263823

▶ **synthetic, ≥98% (HPLC)**

S: 22-24/25 EC No. 207-174-9 Light sensitive RTECS # NR2392000 B

G6649-5MG 5 mg

G6649-25MG 25 mg

G6649-100MG 100 mg

▶ **from *Glycine max* (soybean), ~98% (HPLC)**

✗ R: 36/38 S: 26 -20°C

G6776-5MG 5 mg

G6776-10MG 10 mg

**Genistein 4',7-dimethyl ether**

4',7-Dimethoxy-5-hydroxyisoflavone

C<sub>17</sub>H<sub>14</sub>O<sub>5</sub> FW 298.29 [34086-51-6] BRN 296689

**BioChemika, ~95% (TLC)**

48754-1MG 1 mg

48754-5MG 5 mg

## Dietary Antioxidants

### Glycitein

4',7-Dihydroxy-6-methoxyisoflavone; Glycitein  
 $C_{16}H_{12}O_5$  FW 284.26 [40957-83-3]

≥97% (HPLC)

[-20°C]

G2785-10MG	10 mg
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### Gossypin

3,3',4',5',7,8-Hexahydroxyflavone 8-glucoside  
 $C_{21}H_{20}O_{13}$  FW 480.38 [652-78-8]

≥90% (TLC), from *Hibiscus vitifolius*

✗ R: 36/37/38 S: 26-36 RTECS # DJ3009900

G1036-100MG	100 mg
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G1036-500MG	500 mg
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### Hesperetin

3',5,7-Trihydroxy-4-methoxyflavanone  
 $C_{16}H_{14}O_6$  FW 302.28 [41001-90-5]

≥95% (HPLC)

[2-8°C]

H4125-1G	1 g
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H4125-10G	10 g
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### Isorhamnetin

3'-Methoxy-3,4',5,7-tetrahydroxyflavone  
 $C_{16}H_{12}O_7$  FW 316.26 [480-19-3] EC No. 2075455 BRN 44723

BioChemika, ≥95.0% (HPLC)

17794-5MG	5 mg
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### Kaempferol

Robigenin; 3,4',5,7-Tetrahydroxyflavone; 3,5,7-Trihydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one  
 $C_{15}H_{10}O_6$  FW 286.24 [520-18-3] BRN 304401

✗ R: 36/37/38 S: 26-36 EC No. 208-287-6 RTECS # LK9275200

▶ BioChemika, ≥96% (HPLC)

water ..... ~6%

60010-25MG	25 mg
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60010-100MG	100 mg
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▶ ≥90% (HPLC)

[-20°C]

K0133-10MG	10 mg
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K0133-50MG	50 mg
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K0133-100MG	100 mg
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K0133-500MG	500 mg
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### Luteolin

3',4',5,7-Tetrahydroxyflavone  
 $C_{15}H_{10}O_6$  FW 286.24 [491-70-3] BRN 292084

≥98% (TLC)

✗ R: 36/37/38 S: 26-36 EC No. 207-741-0 RTECS # LK9275210 [2-8°C]

L9283-10MG	10 mg
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L9283-50MG	50 mg
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### Malvidin chloride

3,4',5,7-Tetrahydroxy-3',5'-dimethoxyflavylium chloride  
 $C_{17}H_{15}ClO_7$  FW 366.75 [643-84-5]

purum, ≥95.0% (HPLC)

EC No. 211-403-8 RTECS # LK9900000

68120-1MG-F	1 mg
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### Morin hydrate

2',3,4',5,7-Pentahydroxyflavone  
 $C_{15}H_{10}O_7 \cdot xH_2O$  FW 302.24 (Anh) [654055-01-3]

✗ R: 36/37/38 S: 26-36

M4008-2G	2 g
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M4008-5G	5 g
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M4008-10G	10 g
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### Myricetin

Cannabiscetin; 3,3',4',5,5',7-Hexahydroxyflavone  
 $C_{15}H_{10}O_8$  FW 318.24 [529-44-2] BRN 332331

BioChemika, ≥96.0% (HPLC)

EC No. 208-463-2 RTECS # LK8646000

70050-25MG	25 mg
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70050-100MG	100 mg
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### α-Naphthoflavone

7,8-Benzoflavone  
 $C_{19}H_{12}O_2$  FW 272.30 [604-59-1] BRN 210494  
 EC No. 210-071-1 RTECS # QL6250000 [2-8°C]

N5757-1G	1 g
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N5757-5G	5 g
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### β-Naphthoflavone

5,6-Benzoflavone  
 $C_{19}H_{12}O_2$  FW 272.30 [6051-87-2] BRN 18991

90-95%

S: 22-24/25 EC No. 227-958-4 RTECS # QL6200000 [2-8°C]

N3633-1G	1 g
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N3633-5G	5 g
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**(±)-Naringenin**

(±)-2,3-Dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one;  
4',5,7-Trihydroxyflavanone

C<sub>15</sub>H<sub>12</sub>O<sub>5</sub> FW 272.25 [67604-48-2]

~95%

✗ R: 36/37/38 S: 26-36 EC No. 266-769-1

N5893-1G	1 g
N5893-5G	5 g
N5893-10G	10 g
N5893-25G	25 g

**Pelargonidin chloride**

3,4',5,7-Tetrahydroxyflavylium chloride

C<sub>15</sub>H<sub>11</sub>ClO<sub>5</sub> FW 306.70 [134-04-3] BRN 3922945

S: 22-24/25 EC No. 205-127-7 [2-8°C]

P1659-5MG	5 mg
P1659-10MG	10 mg

**Peonidin chloride**

3,4',5,7-Tetrahydroxy-3'-methoxyflavylium chloride

C<sub>16</sub>H<sub>13</sub>ClO<sub>6</sub> FW 336.72 [134-01-0]

BioChemika, ≥96.5% (HPLC)

EC No. 205-125-6 [20°C]

52527-1MG-F	1 mg
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**Pinocebrin**

C<sub>15</sub>H<sub>12</sub>O<sub>4</sub> FW 256.25

95% (TLC)

[2-8°C]

P5239-50MG	50 mg
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**Pinostrobin**

(S)-2,3-Dihydro-5-hydroxy-7-methoxy-2-phenyl-4H-1-benzopyran-4-one

C<sub>16</sub>H<sub>14</sub>O<sub>4</sub> FW 270.28 [480-37-5] BRN 270230

BioChemika, ≥99.0% (TLC)

✗ R: 36/37/38 S: 26-36 EC No. 207-548-1

80614-5MG	5 mg
80614-25MG	25 mg

**Procyanidin B1**

*cis,trans*-4,8"-Bi-(3,3',4',5,7-Pentahydroxyflavane)

C<sub>30</sub>H<sub>26</sub>O<sub>12</sub> FW 578.52 [20315-25-7]

BioChemika, ≥90% (HPLC)

[2-8°C]

19542-1MG-F	1 mg
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**Procyanidin B2**

4,8"-Bi-[(+)-epicatechin]; *cis,cis*-4,8"-Bi-(3,3',4',5,7-pentahydroxyflavane)

C<sub>30</sub>H<sub>26</sub>O<sub>12</sub> FW 578.52 [29106-49-8]

BioChemika, ≥90% (HPLC)

[2-8°C]

42157-1MG-F	1 mg
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**Quercetin dihydrate**

2-(3,4-Dihydroxyphenyl)-3,5,7-trihydroxy-4H-1-benzopyran-4-one dihydrate;

3,3',4',5,7-Pentahydroxyflavone dihydrate

C<sub>15</sub>H<sub>10</sub>O<sub>7</sub> · 2H<sub>2</sub>O FW 338.27 [6151-25-3]

BRN 317313

≥98% (HPLC)

☠ R: 25 S: 45 EC No. 204-187-1 RTECS # LK8950000

Q0125-10G	10 g
Q0125-25G	25 g
Q0125-100G	100 g

**Rhamnetin**

C<sub>16</sub>H<sub>12</sub>O<sub>7</sub> FW 316.26 [90-19-7] BRN 47741

BioChemika, ≥99.0% (HPLC)

✗ R: 36/37/38 S: 26-36/37 EC No. 201-974-1 RTECS # LK8748000 [2-8°C]

17799-1MG-F	1 mg
17799-5MG-F	5 mg

**Taxifolin**

(2R,3R)-Dihydroquercetin; (2R,3R)-3,3',4',5,7-Pentahydroxyflavanone

C<sub>15</sub>H<sub>12</sub>O<sub>7</sub> FW 304.25 [480-18-2] BRN 5299277

BioChemika, ≥85% (HPLC)

EC No. 207-543-4 RTECS # LK6920000

78666-25MG-F	25 mg
78666-100MG-F	100 mg

**(±)-Taxifolin**

Dihydroquercetin; 3,3',4',5,7-Pentahydroxyflavanone

C<sub>15</sub>H<sub>12</sub>O<sub>7</sub> FW 304.25 [24198-97-8]

≥85%

✗ R: 22 S: 36 [20°C]

T4512-25MG	25 mg
T4512-100MG	100 mg

## Dietary Antioxidants

### Coumarins, Lignins and Stilbenes

#### Resveratrol

5-[(1E)-2-(4-Hydroxyphenyl)ethenyl]-1,3-benzenediol; 3,4',5-Trihydroxy-*trans*-stilbene

C<sub>14</sub>H<sub>12</sub>O<sub>3</sub> FW 228.24 [501-36-0]

>99% (GC)

✘ R: 37/38-41 S: 26-3 9 RTECS # CZ8987000 -20°C

R5010-100MG	100 mg
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R5010-500MG	500 mg
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#### Silibinin

2,3-Dihydro-3-(4-hydroxy-3-methoxyphenyl)-2-(hydroxymethyl)-6-(3,5,7-trihydroxy-4-oxobenzopyran-2-yl)benzodioxin; Silybin

C<sub>25</sub>H<sub>22</sub>O<sub>10</sub> FW 482.44 [22888-70-6]

✘ R: 36/37/38 S: 26-37/39 EC No. 245-302-5 RTECS # DJ2981770 -20°C

S0417-1G	1 g
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S0417-10G	10 g
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#### Silymarin

Mixture of flavonolignans from *Silybum marianum*

S: 22-24/25 Light sensitive -20°C

S0292-10G	10 g
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S0292-50G	50 g
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### Isoprenoids and Carotenoids

#### Astaxanthin

3,3'-Dihydroxy-β,β-carotene-4,4'-dione

C<sub>40</sub>H<sub>52</sub>O<sub>4</sub> FW 596.84 [472-61-7]

≥98%

EC No. 207-451-4 -20°C

A9335-250MG	250 mg
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A9335-1G	1 g
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#### β-Carotene

β,β-Carotene; Provitamin A

C<sub>40</sub>H<sub>56</sub> FW 536.87 [7235-40-7] BRN 1917416

R: 44 S: 7-15-18 EC No. 230-636-6 Fp: 103 °C (218 °F) RTECS # FI0329500

▶ **Type I, synthetic, ~95% (UV)**

potency: ~1,600,000 units vitamin A per g

-20°C

C9750-5G	5 g
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C9750-10G	10 g
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C9750-25G	25 g
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▶ **Type II, synthetic, ≥95% (HPLC)**

€ <sup>1%</sup><sub>450nm</sub>, hexane .....2450-2590 (vs. 2590, lit.)

€ <sup>1%</sup><sub>478nm</sub>, hexane .....2160-2280 (vs. 2280, lit.)

α-carotene .....essentially free

-20°C

C4582-5MG	5 mg
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C4582-10MG	10 mg
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C4582-25MG	25 mg
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#### Carotene, mixed isomers

≥95% (HPLC), from carrots

Approx. 2:1 β:α

R: 44 S: 7-15-18 -20°C

C4646-5MG	5 mg
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#### Coenzyme Q<sub>10</sub>

Q-10; Ubiquinone10; Ubiquinone 50

C<sub>59</sub>H<sub>90</sub>O<sub>4</sub> FW 863.34 [303-98-0] BRN 1900141

≥98% (HPLC)

S: 22-24/25 EC No. 206-147-9 RTECS # DK3900000 -20°C

C9538-100MG	100 mg
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C9538-500MG	500 mg
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C9538-1G	1 g
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#### Lycopene

ψ,ψ-Carotene; 2,6,10,14,19,23,27,31-Octamethyl-dotriaconta-2,6,8,10,12,14,16,18,20,22,24,26,30-tridecaene

C<sub>40</sub>H<sub>56</sub> FW 536.87 [502-65-8]

≥90%, from tomato

EC No. 207-949-1 -70°C DRY ICE

L9879-1MG	1 mg
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L9879-5MG	5 mg
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L9879-10MG	10 mg
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#### (+)-α-Tocopherol

2,5,7,8-Tetramethyl-2-(4',8',12'-trimethyltridecyl)-6-chromanol; 5,7,8-Trimethyltolcol; Vitamin E

C<sub>29</sub>H<sub>50</sub>O<sub>2</sub> FW 430.71 [59-02-9] BRN 4712525

S: 23-24/25 EC No. 200-412-2 Fp: 110 °C (230 °F) RTECS # DJ2900000

▶ **from vegetable oil, Type V, activity: ~1000 IU/g**

Mixed isomers

Approx. 670 mg D-α-tocopherol per gram. The non-α content is 5-20 mg/g; remainder is soybean oil.

-20°C

T3634-10G	10 g
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T3634-25G	25 g
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T3634-100G	100 g
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▶ **BioChemika, ≥99.0% (UV)**

2-8°C

89550-25MG	25 mg
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89550-100MG	100 mg
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**(±)-α-Tocopherol**DL-all-*rac*-α-Tocopherol; Vitamin EC<sub>29</sub>H<sub>50</sub>O<sub>2</sub> FW 430.71 [10191-41-0] BRN 94012**synthetic, ~95% (HPLC)**

EC No. 233-466-0 Fp: 113 °C (235 °F) RTECS # GA8746000 E

T3251-5G	5 g
T3251-25G	25 g
T3251-100G	100 g
T3251-500G	500 g

**DL-α-Tocopherol acetate**all-*rac*-α-Tocopheryl acetate; Vitamin E acetateC<sub>31</sub>H<sub>52</sub>O<sub>3</sub> FW 472.74 [7695-91-2] BRN 97512

EC No. 231-710-0 Fp: 113 °C (235 °F) RTECS # GA8747000

**▶ BioChemika, ≥97.0% (HPLC), activity: 1 unit/mg**

1 unit corresponds to 1 USP unit acc. USP XXIII, 1631 (1995)

free tocopherol ..... ≤1.0%  
 heavy metals ..... ≤0.02%  
 ign. residue ..... ≤0.1%

◆ [2-8°C]

95250-25G	25 g
95250-100G	100 g

**▶ ≥96% (HPLC)**

[2-8°C]

T3376-5G	5 g
T3376-25G	25 g
T3376-100G	100 g

**(+)-α-Tocopherol acetate**

Vitamin E acetate

C<sub>31</sub>H<sub>52</sub>O<sub>3</sub> FW 472.74 [58-95-7]**activity: ~1360 IU/g, semisynthetic**

Synthesized from natural α-tocopherol

EC No. 200-405-4 Fp: 110 °C (230 °F) RTECS # GP8280000 [2-8°C]

T3001-10G	10 g
T3001-25G	25 g
T3001-100G	100 g

**(+)-α-Tocopherol acid succinate**

Vitamin E acid succinate

C<sub>33</sub>H<sub>54</sub>O<sub>5</sub> FW 530.78**semisynthetic, activity: ~1210 IU/g**

EC No. 224-403-8 RTECS # EJ9984000

T3126-5G	5 g
T3126-25G	25 g
T3126-100G	100 g

**(+)-γ-Tocopherol**

7,8-Dimethyltolcol; (R,R,R)-γ-Tocopherol

C<sub>28</sub>H<sub>48</sub>O<sub>2</sub> FW 416.68 [54-28-4] BRN 93072**≥96% (HPLC)**

EC No. 200-201-5 [2-8°C]

T1782-5MG	5 mg
T1782-25MG	25 mg
T1782-100MG	100 mg

**(+)-δ-Tocopherol**C<sub>27</sub>H<sub>46</sub>O<sub>2</sub> FW 402.65 [119-13-1]**-90%**

EC No. 204-299-0

T2028-25G	25 g
T2028-100G	100 g

**Xanthophyll**

α-Carotene-3,3'-diol; Lutein

C<sub>40</sub>H<sub>56</sub>O<sub>2</sub> FW 568.87 [127-40-2] BRN 2068547**from alfalfa**

Minimum 70% total carotenoids as xanthophyll.

EC No. 204-840-0 [70°C] DRY ICE

X6250-1MG	1 mg
X6250-5MG	5 mg

**Zeaxanthin**

β,β-Carotene-3,3'-diol

C<sub>40</sub>H<sub>56</sub>O<sub>2</sub> FW 568.87 [144-68-3] EC No. 205 636 4**purum p.a., ≥95.0% (TLC)**

[-20°C]

14681-1MG-F	1 mg
14681-5MG-F	5 mg

## Dietary Antioxidants

### Minerals

#### Sodium selenite

Na<sub>2</sub>SeO<sub>3</sub> FW 172.94 [10102-18-8]



R: 23-28-31-43-51/53 S: 28-36/37-45-61 EC No. 233-267-9

Moisture sensitive RTECS # VS7350000

TSCA ◆

▶ 99%

214485-5G	5 g
214485-100G	100 g
214485-500G	500 g

▶ ~98%, cell culture tested

S5261-10G	10 g
S5261-25G	25 g
S5261-100G	100 g

#### Sodium selenite pentahydrate

Na<sub>2</sub>SeO<sub>3</sub> · 5H<sub>2</sub>O FW 263.01 [26970-82-1]



R: 23-28-31-43-51/53 S: 28-36/37-45-61 EC No. 233-267-9

RTECS # VS7420000 ◆

▶ puriss. p.a., ≥99.0% (RT)

00163-25G	25 g
00163-100G	100 g

▶ purum p.a., ≥97.0% (RT)

71955-25G	25 g
71955-100G	100 g

#### Seleno-L-methionine

(S)-2-Amino-4-(methylseleno)butyric acid

CH<sub>3</sub>SeCH<sub>2</sub>CH<sub>2</sub>CH(NH<sub>2</sub>)CO<sub>2</sub>H FW 196.11 [3211-76-5]

≥98% (TLC)



R: 23/25-33-50/53 S: 20/21-28-45-60-61 RTECS # EK7713840 [−20°C]

S3132-25MG	25 mg
S3132-100MG	100 mg
S3132-500MG	500 mg

#### Se-(Methyl)selenocysteine hydrochloride

C<sub>4</sub>H<sub>9</sub>NO<sub>2</sub>Se · HCl FW 218.54 [26046-90-2]

≥95% (TLC)



R: 23/25-33-50/53 S: 20/21-28-45-60-61 [−20°C]

M6680-100MG	100 mg
-------------	--------

#### Ebselen

2-Phenyl-1,2-benzisoselenazol-3(2H)-one

C<sub>13</sub>H<sub>9</sub>NOSe FW 274.18 [60940-34-3]



R: 23/25-33-50/53 S: 20/21-28-45-60-61 RTECS # DE4140750 [2-8°C]

E3520-25MG	25 mg
E3520-100MG	100 mg

### Additional Antioxidants

#### L-Ascorbic acid

Antiscorbutic factor; L-Threoascorbic acid; Vitamin C

C<sub>6</sub>H<sub>8</sub>O<sub>6</sub> FW 176.12 [50-81-7] BRN 84272

EC No. 200-066-2 Light sensitive RTECS # CI7650000

▶ reagent grade, ~325 mesh

A7506-25G	25 g
A7506-100G	100 g
A7506-500G	500 g
A7506-1KG	1 kg
A7506-5KG	5 kg

▶ reagent grade, 20-200 mesh

A0278-25G	25 g
A0278-100G	100 g
A0278-500G	500 g
A0278-1KG	1 kg

▶ SigmaUltra, ≥99.0%

Insoluble matter.....	<0.1%
Phosphorus (P).....	<0.0005%
ign. residue.....	<0.1%
sulfate (SO <sub>4</sub> ).....	<0.05%
Al.....	<0.0005%
Ca.....	<0.0005%
Cu.....	<0.0005%
Fe.....	<0.0005%
K.....	<0.005%
Mg.....	<0.0005%
NH <sub>4</sub> <sup>+</sup> .....	<0.05%
Na.....	<0.005%
Pb.....	<0.001%
Zn.....	<0.0005%

A5960-10MG	10 mg
A5960-25G	25 g
A5960-100G	100 g
A5960-500G	500 g

#### Linoleic acid, conjugated

CLA; Octadecadienoic acid, conjugated

A mixture of *cis*- and *trans*-9,11- and -10,12-octadecadienoic acids. Isomer ratio may vary from lot to lot.

Linoleic acid ..... <1%  
[−20°C]

O5507-250MG	250 mg
O5507-1G	1 g

**(±)-α-Lipoic acid**

(±)-1,2-Dithiolane-3-pentanoic acid; 6,8-Dithiooctanoic acid; DL-α-Lipoic acid; Lip(S2); DL-6,8-Thioctic acid

C<sub>8</sub>H<sub>14</sub>O<sub>2</sub>S<sub>2</sub> FW 206.33 [1077-28-7] BRN 81853

✗ R: 22 EC No. 214-071-2 RTECS # JP1192000

▶ **synthetic, ≥99% (titration)**

Oxidized form

<b>T5625-500MG</b>	<b>500 mg</b>
<b>T5625-1G</b>	<b>1 g</b>
<b>T5625-5G</b>	<b>5 g</b>
<b>T5625-25G</b>	<b>25 g</b>
<b>T5625-50G</b>	<b>50 g</b>

▶ **BioChemika, ≥98.0% (HPLC)**

Loss on drying ..... ≤0.1%, 20 °C (HV)  
ign. residue ..... ≤0.1%

**2-8°C**

<b>62320-5G-F</b>	<b>5 g</b>
<b>62320-25G-F</b>	<b>25 g</b>

**Magnolol**

**NEW**

5,5'-Diallyl-2,2'-biphenyldiol

C<sub>18</sub>H<sub>18</sub>O<sub>2</sub> FW 266.33 [528-42-8]

≥98% (HPLC), from plant

✗ R: 37/38-41-51/53 S: 26-39-61 RTECS # DV5105500 **2-8°C**

<b>M3445-10MG</b>	<b>10 mg</b>
-------------------	--------------

**(+)-Sodium L-ascorbate**

L(+)-Ascorbic acid sodium salt; Vitamin C sodium salt

C<sub>6</sub>H<sub>7</sub>NaO<sub>6</sub> FW 198.11 [134-03-2] BRN 3767246

EC No. 205-126-1 Light sensitive RTECS # CI7671000

▶ **≥98%**

<b>A7631-25G</b>	<b>25 g</b>
<b>A7631-100G</b>	<b>100 g</b>
<b>A7631-500G</b>	<b>500 g</b>
<b>A7631-1KG</b>	<b>1 kg</b>

▶ **BioChemika, ≥99.0% (NT)**

Loss on drying ... ≤0.2%, 110 °C	Fe ..... ≤5 mg/kg
chloride (Cl) ..... ≤50 mg/kg	K ..... ≤50 mg/kg
sulfate (SO <sub>4</sub> ) ..... ≤50 mg/kg	Mg ..... ≤5 mg/kg
Ca ..... ≤50 mg/kg	Mn ..... ≤5 mg/kg
Cd ..... ≤5 mg/kg	Ni ..... ≤5 mg/kg
Co ..... ≤5 mg/kg	Pb ..... ≤5 mg/kg
Cr ..... ≤5 mg/kg	Zn ..... ≤5 mg/kg
Cu ..... ≤5 mg/kg	

◆

<b>11140-50G</b>	<b>50 g</b>
<b>11140-250G</b>	<b>250 g</b>
<b>11140-1KG</b>	<b>1 kg</b>



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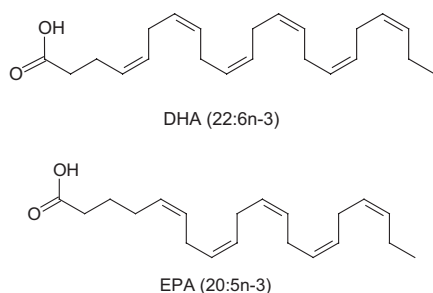
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## Omega-3 Fatty Acids and Heart Disease

### EPA and DHA

The potential for the prevention and treatment of cardiovascular disease through increased dietary intake of omega-3 ( $\omega$ -3) fish oils is not a recent scientific discovery. A historically important study in 1980 reported that high levels of omega-3 fatty acids in the diet of the Inuit people of Greenland were linked to a lower rate of death from acute myocardial infarction compared to the Danish population.<sup>1,2</sup> An abundance of ensuing clinical trials supported the benefit of the omega-3 polyunsaturated fatty acids *cis*-5,8,11,14,17-eicosapentaenoic acid (EPA) and *cis*-4,7,10,13,16,19-docosahexaenoic acid (DHA) (see **Figure 1**). EPA and DHA have demonstrated many cardioprotective effects including antiarrhythmic, blood triglyceride-lowering, and antithrombotic effects, as well as improving endothelial relaxation and inhibiting both atherosclerosis and inflammation.



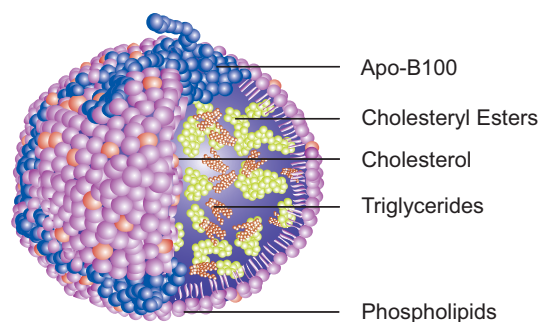
**Figure 1.** Structures of EPA and DHA.

The primary dietary source of EPA (20:5n-3) and DHA (22:6n-3) is fish products.  $\alpha$ -Linolenic acid (18:3n-3) is also an omega-3 fatty acid but is found in plant foods and vegetable oils rather than fish products. Additionally, vegetable oils provide high levels of the omega-6 fatty acid linoleic acid (18:2n-6).  $\alpha$ -Linolenic acid is a precursor to EPA and DHA.<sup>1</sup> The combined level of EPA and DHA in a typical U.S. diet is only 100-150 mg per day compared to 1-3 g per day for  $\alpha$ -linolenic acid and 12-15 g per day for linoleic acid.<sup>3,4</sup> Since linoleic is not an EPA or DHA precursor, the World Health Organization and Health Canada have recommended lowering the dietary intake ratio of linoleic acid to  $\alpha$ -linolenic acid.<sup>5,6</sup> However,  $\alpha$ -linolenic acid normally does not accumulate to high concentrations even with increased dietary intake levels due to extensive  $\beta$ -oxidation *in vivo*. The  $\beta$ -oxidation effect compounded with the limited conversion effectiveness of dietary  $\alpha$ -linolenic acid to DHA strongly suggests that the direct intake of EPA and DHA is a potent way to enhance the levels of circulating omega-3 fatty acids in human serum.

### Lipid Metabolism

Free fatty acids circulate in plasma with the aid of albumin while triglycerides, phospholipids, and cholesterol are transported as lipoproteins. Lipoprotein cores consist of triglycerides and cholesterol esters while the surface consists of free cholesterol, phospholipids, and apoproteins (see **Figure 2**). The positive effect of omega-3 fish oils is linked to very low density lipoprotein (VLDL) levels while the relationship between omega-3 fish oils and low density lipoprotein (LDL) and high density lipoprotein (HDL) levels has not been fully characterized.

#### Low Density Lipoprotein



**Figure 2.** Schematic drawing of the structure of low density lipoprotein.

The metabolomic outcome of circulating omega-3 fish oils is lower plasma triglyceride levels. Omega-3 fish oils consistently lower plasma triglyceride levels by decreasing VLDL-triglycerides, VLDL-cholesterol, and VLDL-apolipoprotein B (Apo-B). This beneficial influence of omega-3 fish oils on triglyceride levels is observed in the regulation of the hepatic production of VLDL. Circulating fish oils reduce VLDL production by inhibiting fatty-acid synthesis, increasing oxidation, decreasing triglyceride and cholesteryl production, and increasing the degradation of the obligatory VLDL production protein Apo-B. Since VLDL carries primarily triglycerides, the end result is a decreased plasma concentration of triglycerides.<sup>7</sup>

The correlation between omega-3 fish oils and decreased secretion rates of triglycerides and Apo-B100 in VLDL has been demonstrated in several studies on humans and primates.<sup>8,9</sup> Scientific observations have revealed that omega-3 fish oils suppress lipogenesis by down regulating the transcription of fatty acid synthase.<sup>10,11</sup> Fish oils increase oxidation by diverting fatty acids into peroxisomal or mitochondrial oxidation<sup>12-15</sup> and inducing the transfer of long-chain fatty acids into the mitochondria by carnitine palmitoyl transferase I.<sup>16,17</sup> Since fish oils are poor substrates for diacylglycerol transferase (DAG), DAG metabolism is diverted from triglycerides to phospholipids synthesis.<sup>18,19</sup> Additionally, they are poor substrates for cholesterol esterification. Furthermore, fish oils reduce VLDL production by increasing proteolytic degradation of Apo-B in the novel, post-ER presecretory pathway.<sup>20</sup>

Additional effects of omega-3 fish oils during lipid metabolism include the acceleration of chylomicron triglyceride clearance due to increased lipoprotein lipase activity<sup>21</sup> and the lipolysis of VLDL triglyceride in the peripheral liver tissue.<sup>11,22</sup> However, hypotheses regarding both lipolysis pathways are still being tested.

## Lipid Mediators: Resolvins, Protectins, and Neuroprotectins

Current research has begun to reveal the structure and function of small bioactive molecules critical to the cell-cell interactions that provide anti-inflammatory actions and promote inflammation resolution. Novel lipid mediators that display these potent anti-inflammatory and proresolving actions have recently been identified as oxygenated metabolites of EPA and DHA. These local-acting lipid mediators derived from EPA and DHA are referred to as resolvins (i.e., **resolution-phase interaction products**). The bioactive products of EPA are designated resolvins of the E series (RvE1), while those derived from DHA are designated resolvins of the D series (RvD). A second family of anti-inflammatory lipid mediators is the protectin family, which includes the immunoregulatory and neuroprotective neuroprotectins.<sup>23,24</sup> The protectins are derived from docosatrienes, bioactive lipids related to DHA containing conjugated triene structures.<sup>25,26</sup>

Lipid mediators, including resolvins, play an important role during the intimate cell-cell interactions within vessel walls. Emerging evidence suggests that acute inflammation normally resolves by an active, coordinated program that begins in the first few hours following the initiation of the inflammatory response. Polymorphonuclear leukocytes (PMN) move into the inflamed tissue and promote the switch from the arachidonic acid-derived prostaglandins and leukotrienes to lipoxins, which initiate the termination series of the resolution program. The coinciding biosynthesis of the anti-inflammatory resolvins and protectins leads to the regulation of PMNs by inhibition of infiltration and transmigration. Prostaglandins, leukotrienes, and lipoxins are classified as proinflammatory lipid mediators, while the resolvins and protectins are anti-inflammatory lipid mediators. Accordingly, PMN clearance leads to the release of anti-inflammatory and reparative cytokines.<sup>27</sup>

Aspirin (acetylsalicylic acid) treatment results in the endogenous formation of the 17R-D series resolvins and docosatrienes, denoted as aspirin-triggered (AT)-RvD and (AT)-DT. During PMN-endothelial and/or PMN-epithelial interactions, aspirin initiates the production of 15-epilipoxins (i.e. aspirin-triggered lipoxin [ATL]) via acetylated cyclooxygenase-2 (COX-2).<sup>25</sup> Inflammation is not a requirement for the biosynthesis of (AT)-RvD. Lipoxin is a potent regulator of transendothelial-transepithelial migration of PMN.<sup>28-30</sup> *In vivo* studies have confirmed RvE1 and AT-RvDs inhibition of PMN transmigration or PMNs infiltration in murine exudates,<sup>31,32</sup> along with RvE1 and RvD2-4 inhibition of PMN infiltration in human blood.<sup>33,34</sup> Inhibition of PMN infiltration by RvE1 during the down-regulation of NF- $\kappa$ B activation through a G protein-coupled receptor concludes in a fluctuation of blood-based cells into the inflammation location.<sup>28</sup>

It has been proposed that new therapeutic approaches based on the signaling pathways of endogenous resolvins, protectins, and neuroprotectins will be effective in dampening inflammatory responses. Understanding the mechanism of inflammation resolution will aid in the development of novel drugs for the treatment of human disorders linked with inflammation including cardiovascular heart disease.<sup>35</sup> As research continues to elucidate this relationship, the question to be answered is: can the inflammatory response become deregulated by novel drugs without injurious consequences to the patient? Upsetting the delicate balance of interactions between proinflammatory lipid mediators and anti-inflammatory mediators could lead to dramatic responses more severe than the natural resolution of inflammation.<sup>36</sup>

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## Omega-3 Fatty Acids and Heart Disease



### Omega-3 Polyunsaturated Fatty Acids and Precursor

#### $\omega$ -3 Arachidonic acid

NEW

C<sub>20</sub>H<sub>32</sub>O<sub>2</sub> FW 304.47

concentration .....5 mg/mL in ethanol

 R: 11 S: 7-16 Fp: 14 °C (57 °F)   WET ICE



A8105-1MG	1 mg
A8105-5MG	5 mg

#### *cis*-4,7,10,13,16,19-Docosahexaenoic acid

DHA

C<sub>22</sub>H<sub>32</sub>O<sub>2</sub> FW 328.49 [6217-54-5] BRN 1715505

≥98%

S: 23-24/25 Fp: 62 °C (144 °F)   DRY ICE

D2534-25MG	25 mg
D2534-100MG	100 mg
D2534-1G	1 g

#### *cis*-4,7,10,13,16,19-Docosahexaenoic acid-1-<sup>14</sup>C





DHA

CH<sub>3</sub>[CH<sub>2</sub>CH=CH]<sub>6</sub>CH<sub>2</sub>CH<sub>2</sub><sup>14</sup>CO<sub>2</sub>H FW 328.49

≥95% (HPLC, Radiochemical Purity), ethanol solution

Combi-vial

extent of labeling..... 40-60 mCi per mmol

  R: 36/37/38 S: 16-26-36 Fp: 14 °C (57 °F)  

D4685-10UCI	10 μCi
D4685-50UCI	50 μCi

#### *cis*-4,7,10,13,16,19-Docosahexaenoic acid sodium salt

DHA sodium salt

C<sub>22</sub>H<sub>31</sub>O<sub>2</sub>Na FW 350.47 [81926-93-4]

≥95%, from cod liver oil



D8768-5MG	5 mg
D8768-25MG	25 mg

#### *cis*-4,7,10,13,16,19-Docosahexaenoic acid ethyl ester

DHA ethyl ester

C<sub>24</sub>H<sub>36</sub>O<sub>2</sub> FW 356.54 [84494-72-4]

~99%



D2661-10MG	10 mg
D2661-100MG	100 mg

#### *cis*-4,7,10,13,16,19-Docosahexaenoic acid methyl ester

Methyl 4,7,10,13,16,19-docosahexaenoate: DHA methyl ester

CH<sub>3</sub>(CH<sub>2</sub>CH=CH)<sub>6</sub>CH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>CH<sub>3</sub> FW 342.51 [301-01-9]

≥98%

S: 23-24/25 Fp: 93 °C (200 °F) 




D2659-10MG	10 mg
D2659-50MG	50 mg
D2659-100MG	100 mg
D2659-1G	1 g

#### *cis*-5,8,11,14,17-Eicosapentaenoic acid

EPA; Timnodonic acid

CH<sub>3</sub>(CH<sub>2</sub>CH=CH)<sub>5</sub>(CH<sub>2</sub>)<sub>3</sub>CO<sub>2</sub>H FW 302.45 [10417-94-4] BRN 1714433

≥99%

 R: 34 S: 26-36/37/39-45 Fp: 93 °C (200 °F)  

E2011-10MG	10 mg
E2011-25MG	25 mg
E2011-50MG	50 mg
E2011-100MG	100 mg

#### *cis*-5,8,11,14,17-Eicosapentaenoic acid sodium salt

EPA sodium salt

CH<sub>3</sub>(CH<sub>2</sub>CH=CH)<sub>5</sub>(CH<sub>2</sub>)<sub>3</sub>CO<sub>2</sub>Na FW 324.43 [73167-03-0]

~99% (capillary GC)

  DRY ICE

E6627-5MG	5 mg
E6627-10MG	10 mg
E6627-25MG	25 mg

#### Methyl all-*cis*-5,8,11,14,17-eicosapentaenoate

*cis*-5,8,11,14,17-Eicosapentaenoic acid methyl ester; EPA methyl esterCH<sub>3</sub>(CH<sub>2</sub>CH=CH)<sub>5</sub>(CH<sub>2</sub>)<sub>3</sub>CO<sub>2</sub>CH<sub>3</sub> FW 316.48 [2734-47-6] BRN 1914828

~99% (capillary GC)

S: 24/25 Fp: 104 °C (219 °F) 

E2012-1MG	1 mg
E2012-5MG	5 mg
E2012-10MG	10 mg
E2012-50MG	50 mg
E2012-100MG	100 mg

#### Linolenic acid

α-Lnn; *cis,cis,cis*-9,12,15-Octadecatrienoic acidCH<sub>3</sub>(CH<sub>2</sub>CH=CH)<sub>3</sub>(CH<sub>2</sub>)<sub>7</sub>CO<sub>2</sub>H FW 278.43 [463-40-1]

BRN 1727693

≥99%

EC No. 207-334-8 Fp: 113 °C (235 °F) 

L2376-500MG	500 mg
L2376-5G	5 g
L2376-10G	10 g

## Omega-6 Polyunsaturated Fatty Acids

### Linoleic acid

*cis*-9, *cis*-12-Octadecadienoic acid

CH<sub>3</sub>(CH<sub>2</sub>)<sub>4</sub>CH=CHCH<sub>2</sub>CH=CH(CH<sub>2</sub>)<sub>7</sub>CO<sub>2</sub>H FW 280.45 [60-33-3]  
BRN 1727101

≥99%

EC No. 200-470-9 Fp: 113 °C (235 °F) RTECS # RF9990000 [-20°C]

L1376-10MG	10 mg
L1376-500MG	500 mg
L1376-1G	1 g
L1376-5G	5 g
L1376-10G	10 g
L1376-25G	25 g

### Linoleic acid-1-<sup>14</sup>C

CH<sub>3</sub>(CH<sub>2</sub>)<sub>4</sub>CH=CHCH<sub>2</sub>CH=CH(CH<sub>2</sub>)<sub>7</sub><sup>14</sup>CO<sub>2</sub>H FW 280.45

≥95% (HPLC, Radiochemical Purity)

extent of labeling..... 40-60 mCi per mmol

 R: 11-36/37/38 S: 16-26-36 Fp: 14 °C (57 °F)  WET ICE

L6277-50UCI	50 µCi
L6277-100UCI	100 µCi
L6277-250UCI	250 µCi

## Lipid Metabolism Related Products

### Apolipoprotein B from human plasma

~95%

Lyophilized from buffer containing 10 mM sodium deoxycholate, 0.05 M sodium carbonate, and 0.05 M sodium chloride, pH 10.0. Delipidated with sodium deoxycholate.

 R: 22-36/37 S: 22-26-36 [-20°C]

A5353-.5MG	0.5 mg
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### Lipoprotein Lipase from bovine milk

Diacylglycerol acylhydrolase; Diacylglycerol lipase  
[9004-02-8] E.C. 3.1.1.34

activity: 2,000-6,000 units/mg protein (BCA)

Suspension in 3.8 M ammonium sulfate, 0.02 M Tris HCl, pH 8.0

Affinity purified

One unit will release 1.0 nmole of p-nitrophenol per min at pH 7.2 at 37 °C using p-nitrophenyl butyrate as substrate.

EC No. 232-669-1 [-2-8°C]


L2254-1KU	1,000 units
L2254-5KU	5,000 units

### Lipoprotein, high density from human plasma

HDL; High density lipoprotein; α-Lipoprotein

>95% (SDS-PAGE)

Solution in 150 mM NaCl, pH 7.4, 0.01% EDTA

 EC No. 235-824-1 [-2-8°C] WET ICE


L8039-10MG	10 mg
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### Lipoprotein, low density from human plasma

LDL; β-Lipoprotein; Low density lipoprotein

≥95% (SDS-PAGE)

Solution in 150 mM NaCl, pH 7.4, and 0.01% EDTA

 EC No. 2944-82-1 S: 23-24/25 [-2-8°C] WET ICE


L7914-5MG	5 mg
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### Lipoprotein, very low density from human plasma

Pre-β-lipoprotein; Very low density lipoprotein; VLDL

≥95% (SDS-PAGE)

Solution in 150 mM NaCl, pH 7.4, and 0.01% EDTA

 EC No. 2944-82-1 [-2-8°C]

L7527-1MG	1 mg
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### Serum Triglyceride Determination Kit


1 kit sufficient for 250 tests

The Serum Triglyceride Determination Kit can be used for the measurement of glycerol, true triglycerides, or total triglycerides in serum or plasma. The procedure involves enzymatic hydrolysis by lipase of the triglycerides to glycerol and free fatty acids. The glycerol produced is then measured by coupled enzyme reactions. The kit also includes sufficient reagent for an additional 250 free glyceride tests for true triglyceride determination. In addition to kits, the individual reagents and glycerol standard are available separately when fewer reactions are needed.

#### Components

Free Glycerol Reagent (Sigma F6428) 10X40 ML

Triglyceride Reagent (Sigma T2449) 5X10 ML

 R: 5-23/24/25-32-52/53 S: 28-36/37-45-7/9 [-2-8°C]

TR0100-1KT	1 kit
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## Lipid Mediator Related Products

### Cyclooxygenase 2 human

COX-2; Prostaglandin H synthase 2

≥70% (SDS-PAGE), recombinant, expressed in Sf21 cells, activity: ≥8000 units/mg protein

Tagged with a six-residue histidine sequence near the N-terminus.

Solution in 80 mM Tris-HCl, pH 8, with 0.1% TWEEN® 20 and 300 µM diethyldithiocarbamate.

Homodimer subunit mol. wt. 70-74 kDa.

One unit consumes one nanomole of oxygen per minute at 37 °C in 0.1 M Tris-HCl buffer, pH 8, containing 100 µM arachidonate, 5 mM EDTA, 2 mM phenol, and 1 µM hematin.

[-70°C] DRY ICE

C0858-1000UN	1,000 units
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### Lipoxin A4

(5S,6R,15S)-Trihydroxy-(7E,9E,11Z,13E)-Eicosatetraenoic acid

C<sub>20</sub>H<sub>32</sub>O<sub>5</sub> FW 352.47 [89663-86-5]

#### Ethanol solution

 R: 11 S: 7-16  DRY ICE

L0521-25UG	25 µg
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## Bioactive Nutrient Explorer

### Helping Scientists Connect Bioactives to Botanicals

#### The Bioactive Nutrient Explorer

Passage of the Dietary Supplement Health and Education Act in the United States in 1994 sparked consumer interest in the health benefits of herbal preparations and non-vitamin dietary supplements. As usage of these products increased, the U.S. scientific community joined with scientists throughout Asia, Europe, and Africa in recognizing the necessity of determining the physiological actions of these substances, their roles in disease prevention and therapy, and the connection between nutrition and health. In the United States, the National Institute of Health has established the Office of Dietary Supplements and the National Center for Complementary and Alternative Medicine. Globally, university food science departments are teaming up with associated medical schools and agriculture departments to conduct interdisciplinary research on human nutrition.

In 2004, Dr. Libby Yunger of Sigma-Aldrich identified a group of roughly 1,200 chemicals that were of interest to nutritional researchers as chemical constituents of herbal supplements or purified compounds present in dietary supplements. These chemicals were assigned classifications based on their organic structure. In addition, Dr. Yunger prepared an information matrix showing which of these chemicals are found in specific plants. To expand the information matrix, Dr. Yunger began reviewing scientific sources for documented physiological actions of herbs that were associated with disease intervention or prevention. The main technical resource used was the U.S. National Library of Medicine/National Institute of Health Web site ([www.ncbi.nlm.nih.gov](http://www.ncbi.nlm.nih.gov)) with additional information obtained from The Complete German Commission E Monographs: Therapeutic Guide to Herbal Medicines (American Botanical Council, 1998), PDR for Herbal Medicines, 3rd edition (2004), Consumer Lab monographs ([www.consumerlab.com](http://www.consumerlab.com)), and other research-based sources.

The resulting database forms the basis of an internet tool called the Bioactive Nutrient Explorer that uses Adobe® Macromedia® Flash® software. The initial version of the Bioactive Nutrient Explorer was demonstrated at the Experimental Biology conference in San Diego, March, 2005, and added to the Sigma-Aldrich web site in July, 2005. The revised Bioactive Nutrient Explorer was subsequently launched in November, 2006.

Today, the Bioactive Nutrient Explorer contains ~5,000 products representing ~1,400 chemicals, as well as over 500 plant listings. The Bioactive Nutrient Explorer program includes a straightforward Quick Search method to find chemicals, plants, and Sigma-Aldrich catalog numbers, and a Guided Search function that uses a stepwise approach, leading the customer through a selection of terms until the desired product or plant is identified.



The **Quick Search** allows customers to search for chemicals and plants by common names. The database includes synonyms for chemicals and Latin names for plants as well as a 2-character search term minimum, so an exactly matching term is not required for searching.



The **Guided Search** assists researchers in finding chemicals by structural families and classes. Each selection guides the user closer to the desired list of products while showing alternative selections for backtracking or additional searches.

[sigma-aldrich.com/nutrition](http://sigma-aldrich.com/nutrition)

# BIOACTIVE NUTRIENT

explorer



## Metabolite Libraries

Most metabolites are individually packaged standards in convenient autosampler vials for metabolomic analysis. Choose your own components, and build a custom library online using the Sigma-Aldrich Metabolomics Web Resource.

### Libraries Available:

- 70 Amino Acids and Metabolic Intermediates
- 73 Carbohydrates and Metabolic Intermediates
- **New!** 78 Lipids and Metabolic Intermediates

### Currently in Development:

- Nucleotide Library
- Vitamin/Cofactor Library

Hundreds of metabolites are available in standard packaging and can be found in the Sigma General Catalog or online at [sigma-aldrich.com/metpath](http://sigma-aldrich.com/metpath).

### Custom Packaging Capabilities

Sigma Aldrich offers custom packaging of metabolite standards with vial content and container specifications to fit your requirements. Contact your local sales office for more details.



### Amino Acid Metabolite Library

Metabolite	Cat. No.
Acetyl-L-carnitine hydrochloride	A6706-10MG
O-Acetyl-L-serine hydrochloride	A6262-10MG
Adenosine 5'-phosphosulfate sodium salt *	A5508-5MG
S-(5'-Adenosyl)-L-homocysteine	A9384-10MG
L-Alanine	A7469-10MG
β-Alanine	A9920-10MG
γ-Aminobutyric acid	A5835-10MG
5-Aminolevulinic acid hydrochloride	A7793-10MG
Anthranilic acid	A89855-10MG
L-Arginine	A8094-10MG
Argininosuccinic acid disodium salt	A5707-10MG
L-Asparagine	A0884-10MG
L-Aspartic acid	A8949-10MG
Betaine aldehyde chloride	B3650-10MG
Betaine hydrochloride	B7045-10MG
L-Carnitine hydrochloride	C0283-10MG
L-Carnosine	C9625-10MG
Choline chloride	C7017-10MG
Chorismic acid	C1761-10MG
L-Citrulline	C7629-10MG
Creatine	C0780-10MG
Creatinine	C4255-10MG
L-Cystathionine	C7505-10MG
Cysteamine	M9768-10MG
L-Cysteine	C7352-10MG
Cystine	C7602-10MG
N,N-Dimethylglycine	D1156-10MG
N-Formyl-L-methionine	F3377-10MG
L-Glutamic acid	G8415-10MG
L-Glutamine	G8540-10MG
L-Glutathione, reduced	G4251-10MG
Glycine	G7126-10MG
Histamine dihydrochloride	H7250-10MG
L-Histidine	H6034-10MG
L-Histidinol dihydrochloride	H6647-10MG
DL-Homocysteine	H4628-10MG
DL-Homocystine	H0501-10MG

Metabolite	Cat. No.
Homogentisic acid	H0751-10MG
L-Homoserine	H6515-10MG
cis-4-Hydroxy-D-proline	H5877-10MG
trans-4-Hydroxy-L-proline	H5534-10MG
Hypotaurine	H1384-10MG
L-Isoleucine	I7403-10MG
α-Keto-γ-(methylthio)butyric acid sodium salt	K6000-10MG
L-Leucine	L8912-10MG
Lithium carbamoylphosphate dibasic	C5625-10MG
L-Lysine	L5501-10MG
L-Methionine	M5308-10MG
L-Methionine sulfoxide	M1126-10MG
L-Ornithine monohydrochloride	O2375-10MG
L-Phenylalanine	P5482-10MG
Phosphocholine chloride calcium salt tetrahydrate	P0378-10MG
Phosphocreatine disodium salt hydrate	P7936-10MG
O-Phospho-L-serine	P0878-10MG
Prephenic acid barium salt	P2384-10MG
L-Proline	P0380-10MG
Sarcosine	S7672-10MG
L-Serine	S4500-10MG
Shikimic acid	S5375-10MG
Sodium 2-oxobutyrate	K0875-10MG
Sodium phenylpyruvate	P8001-10MG
O-Succinyl-L-homoserine *	S7129-25MG
Taurine	T0625-10MG
L-Threonine	T8441-10MG
N,N,N-Trimethyllysine *	T1660-25MG
Tryptamine	T2891-10MG
L-Tryptophan	T8941-10MG
Tyramine hydrochloride	T2879-10MG
L-Tyrosine	T8566-10MG
L-Valine	V0513-10MG

\* NOT currently available in Autosampler vials

## Carbohydrate Metabolite Library

Metabolite	Cat. No.
N-Acetyl-D-galactosamine	A2795-10MG
N-Acetyl-D-glucosamine	A8625-10MG
N-Acetyl-D-lactosamine	A7791-10MG
N-Acetyl-D-mannosamine	A8176-10MG
N-Acetyl-neuraminic acid *	A2388-10MG
Adenosine-5'-diphosphoglucose disodium salt	A0627-10MG
Adonitol	A5502-10MG
D-Allose	A6390-10MG
L-(+)-Arabinose	A3256-10MG
L-(-)-Arabitol	A3506-10MG
L-Ascorbic acid	A5960-10MG
D-(+)-Cellobiose	C7252-10MG
2-Deoxy-D-glucose	D8375-10MG
6-Deoxy-D-glucose	D9761-10MG
2-Deoxy-D-ribose	D5899-10MG
2-Deoxyribose 5-phosphate sodium salt *	D3126-25MG
Dihydroxyacetone phosphate dillithium salt	D7137-10MG
2,3-Diphospho-D-glyceric acid pentasodium salt *	D5764-25MG
Dulcitol	D0256-10MG
D-Erythrose 4-phosphate sodium salt	E0377-10MG
D-(-)-Fructose	F0127-10MG
D-Fructose 1,6-bisphosphate trisodium salt	F6803-10MG
D-Fructose 1-phosphate sodium salt	F1127-10MG
D-Fructose 6-phosphate disodium salt dihydrate	F3627-10MG
L-(-)-Fucose	F2252-10MG
$\alpha$ -D-Galactosamine 1-phosphate *	G5134-25MG
D-(+)-Galactosamine hydrochloride	G0500-10MG
D-(+)-Galactose	G0750-10MG
$\alpha$ -D-Galactose 1-phosphate dipotassium salt pentahydrate	G0380-10MG
D-Gluconic acid sodium salt	G9005-10MG
D-Glucosamine 6-phosphate	G5509-10MG
D-(+)-Glucosamine hydrochloride	G4875-10MG
D-(+)-Glucose	G7528-10MG
$\alpha$ -D-Glucose 1-phosphate disodium salt hydrate	G7018-10MG
D-Glucose 6-phosphate disodium salt hydrate	G7250-10MG
D-Glucuronic acid	G5269-10MG
Guanosine 5'-diphosphoglucose sodium salt	G7502-10MG
myo-Inositol	I5125-10MG
Isomaltose *	I7253-100MG

Metabolite	Cat. No.
D-Lactose monohydrate	L8783-10MG
D(-)-Lyxose *	220477-1G
D-(+)-Maltose monohydrate	M9171-10MG
D-Mannitol	M4125-10MG
D-Mannosamine hydrochloride	M4670-10MG
D-(+)-Mannose	M8296-10MG
$\alpha$ -D-(+)-Mannose 1-phosphate dipotassium salt	M2152-10MG
D-Mannose 6-phosphate disodium salt hydrate	M6876-10MG
Melibiose	M5500-10MG
N-Acetylneuraminic acid	A2388-10MG
Palatinose	P2007-10MG
Phospho(enol)pyruvic acid monopotassium salt	P7127-10MG
6-Phosphogluconic acid trisodium salt	P6888-10MG
D-(-)-3-Phosphoglyceric acid disodium salt	P8877-10MG
D-Psicose	P8043-10MG
D-(+)-Raffinose pentahydrate	R0514-10MG
L-Rhamnose monohydrate	R3875-10MG
D-(-)-Ribose	R7500-10MG
D-Ribose 5-phosphate disodium salt hydrate	R7750-10MG
D-Ribulose *	R2762-100MG
D-Ribulose 1,5-bisphosphate sodium salt hydrate	R0878-10MG
D-Ribulose 5-phosphate sodium salt	R9875-10MG
Sodium pyruvate	P2256-10MG
D-Sorbitol	S1876-10MG
Stachyose hydrate	S4001-10MG
Sucrose	S9378-10MG
D-(-)-Tagatose	T2751-10MG
Trehalose 6-phosphate dipotassium salt	T4272-10MG
D-(+)-Trehalose dihydrate	T9531-10MG
Uridine 5'-diphosphogalactose disodium salt	U4500-10MG
Uridine 5'-diphosphoglucose disodium salt	U4625-10MG
Uridine 5'-diphosphoglucuronic acid trisodium salt	U6751-10MG
Xylitol	X3375-10MG
D-(+)-Xylose	X1500-10MG
D-Xylulose	X4625-10MG

### Your New Metabolomics Resource Center at: [sigma-aldrich.com/metpath](http://sigma-aldrich.com/metpath)

Sigma-Aldrich is proud of our continuing alliance with the International Union of Biochemistry and Molecular Biology. Together we produce, animate, and publish the Nicholson Metabolic Pathway Charts, created and continually updated by Dr. Donald Nicholson. These classic resources can be downloaded from the Sigma-Aldrich Web site as PDF or GIF files at no charge. This site also features our metabolite libraries and kits for metabolite and dietary analysis.



## Metabolite Libraries

### Lipid Metabolite Library

Metabolite	Cat. No.
Acetoacetyl coenzyme A sodium salt hydrate *	A1625-10MG
Acetyl coenzyme A sodium salt *	A2056-10MG
Acetyl coenzyme A trillithium salt *	A2181-10MG
Arachidonoyl coenzyme A lithium salt *	A5837-10MG
O-Acetyl-L-carnitine hydrochloride *	A6706-10MG
Arachidonic acid *	A9673-10MG
Butyryl coenzyme A dilithium salt hydrate *	B1508-10MG
Benzoyl coenzyme A lithium salt *	B1638-5MG
Cytidine 5'-diphosphoethanolamine sodium salt *	C0456-10MG
Cardiolipin from bovine heart solution *	C1649-10MG
Coenzyme A trillithium salt *	C3019-10MG
Coenzyme A sodium salt hydrate *	C3144-10MG
Coenzyme A hydrate *	C4282-10MG
2-Butenoyl Coenzyme A lithium salt *	C6146-10MG
Choline chloride *	C7017-10MG
3'-Dephosphocoenzyme A *	D3385-5MG
$\gamma,\gamma$ -Dimethylallyl pyrophosphate ammonium salt *	D4287-1VL
Decanoyl coenzyme A monohydrate *	D5269-5MG
Desmosterol *	D6513-10MG
DL-erythro-Dihydrosphingosine *	D6908-10MG
Farnesyl pyrophosphate ammonium salt *	F6892-1VL
Geranylgeranyl pyrophosphate ammonium salt *	G6025-1VL
Geranyl pyrophosphate ammonium salt *	G6772-1VL
DL- $\beta$ -Hydroxybutyryl coenzyme A lithium salt *	H0261-10MG
n-Heptadecanoyl coenzyme A lithium salt *	H1385-5MG
Hexanoyl coenzyme A trillithium salt trihydrate *	H2012-10MG
DL-3-Hydroxy-3-methylglutaryl coenzyme A sodium salt *	H6132-10MG
Isobutyryl coenzyme A lithium salt *	I0383-10MG
Isopentenyl pyrophosphate ammonium salt solution *	I0503-1VL
Isovaleryl coenzyme A lithium salt *	I9381-10MG
Leukotriene B <sub>4</sub> *	L0517-50UG
L- $\alpha$ -Lysophosphatidylcholine from bovine brain *	L1381-5MG
Lauroyl coenzyme A lithium salt *	L2659-5MG
Lanosterol *	L5768-5MG
Linoleoyl coenzyme A lithium salt *	L9754-10MG
Methylmalonyl coenzyme A tetralithium salt hexahydrate *	M1762-5MG
$\beta$ -Methylcrotonyl coenzyme A lithium salt *	M3013-10MG
Malonyl coenzyme A lithium salt *	M4263-10MG
Myristoyl coenzyme A lithium salt *	M4414-5MG
Octanoyl coenzyme A lithium salt monohydrate *	O6877-10MG

Metabolite	Cat. No.
Oleoyl coenzyme A lithium salt *	O1012-10MG
Phosphocholine chloride calcium salt tetrahydrate *	P0378-10MG
L- $\alpha$ -Phosphatidylinositol ammonium salt solution *	P2517-10MG
n-Propionyl coenzyme A lithium salt *	P5397-10MG
Prostaglandin E <sub>2</sub> *	P5640-10MG
3-sn-Phosphatidyl-L-serine sodium salt *	P5660-5MG
Palmitoleoyl coenzyme A lithium salt *	P6775-10MG
3-sn-Phosphatidylethanolamine from bovine brain *	P7693-5MG
Psychosine from bovine brain *	P9256-10MG
Palmitoyl coenzyme A lithium salt *	P9716-10MG
3-sn-Phosphatidic acid sodium salt from egg yolk lecithin *	P9511-10MG
Stearoyl coenzyme A lithium salt *	S0802-10MG
Succinyl coenzyme A sodium salt *	S1129-5MG
Squalene *	S3626-10ML
Sphingomyelin from bovine brain *	S7004-10MG
Thromboxane B <sub>2</sub> *	T0516-1MG
3-sn-Phosphatidic acid sodium salt from egg yolk lecithin *	P9511-10MG
Acetylcholine chloride	A6625-10MG
Lithium acetoacetate	A8509-10MG
Cytidine 5'-diphosphocholine sodium salt dihydrate *	C0256-10MG
Ethanolamine	E9508-10UL
Glyoxylic acid solution	G1134-20UL
rac-Glycerol 3-phosphate disodium salt hexahydrate	G2138-10MG
Glycolaldehyde dimer *	G6805-1G
Glycolic acid	G8284-10MG
$\gamma$ -Hydroxybutyric acid sodium salt *	H3635-10MG
Linoleic acid	L1376-10MG
$\gamma$ -Linolenic acid	L2378-10MG
( $\pm$ )-Mevalonolactone *	M4667-1G
Oxalic acid dihydrate	O0376-10MG
Progesterone *	P0130-25G
O-Phosphorylethanolamine	P0503-10MG
L- $\alpha$ -Phosphatidylcholine	P3841-10MG
L- $\alpha$ -Phosphatidyl-DL-glycerol sodium salt	P8318-10MG
5-Pregnen-3 $\beta$ -ol-20-one	P9129-10MG

\* NOT currently available in Autosampler vials



## FTA® Cards for Plant DNA Acquisition and Storage in the Field

Conventional methods for plant DNA acquisition and storage are not suited for field experiments. Expensive or cumbersome equipment is often necessary to preserve plant DNA. These methods may include grinding samples with a mortar and pestle, blending samples with a commercial homogenizer, or freezing samples with liquid nitrogen. Conventional methods also require large amounts of fresh plant tissue. Clearly, it is difficult for scientists to bring this equipment with them to remote locations where field experiments may be conducted. Whatman FTA Cards are a great alternative to conventional methods of DNA acquisition and storage, because they are designed for simple collection in the field and room temperature storage. The FTA Card is a small paper card impregnated with a patented

chemical formula that lyses cell membranes and denatures proteins upon contact. Nucleic acids are immobilized and protected from UV damage and microbial attack. Plant DNA is acquired by direct leaf press, where the plant sample is pressed or pounded directly onto the FTA Card. A coring device, such as the Harris Micro-punch, used to remove a disc of paper containing the isolated DNA. That disc is used for sample analysis.

*"I collect samples by squashing leaves on the FTA Card"—Hirokazu Tsukaya, Ph.D. National Institute for Basic Biology, Japan*

## FTA Technology in Plant Research Studies

Some common research studies requiring the acquisition and storage of plant DNA include Marker Selected Breeding, Varietal Identification, Phylogeny Analysis, and Transgenic Identification. This can be a challenge when only small amounts of DNA are readily available. FTA technology, however, has proven to be a vital tool for many researchers. For example, during studies of transgenic maize development at Kenya Agricultural Research Institute, Jedida Wamuyu Danson, Ph.D., has documented his success with this cutting-edge technology. In his research, Danson was challenged with collecting enough DNA from maize leaves where

*"...able to do PCR reactions with samples taken from any growth stage..."*

only a small amount of sap was present. "As you may know, it is always recommended to use young leaves," Danson said. "But, with FTA, researchers are able to perform PCR reactions with samples taken from any growth stage where only small amounts of sap can be obtained." By winding the old leaves around the card and applying pressure with pliers, Danson was able to collect the DNA he needed. This technique was a time-saver for him, because he did not require a pounding step with a pestle and table. "One person could perform an average of 100 samples per day," Danson added. FTA enabled Danson to collect leaf samples quickly and has been critical for success of his project.

### REFERENCES

Detection of *Bacillus thuringiensis* genes in transgenic maize by the PCR method and FTA paper technology, Jedidah W. Danson, Michael Kimani, and Mercy Mbogori, *African Journal of Biotechnology* Vol. 5 (22), pp. 2345-2349, 16 November 2006.

Large-scale general collection of wild-plant DNA in Mustang, Nepal, Hirokazu Tsukaya, Yu Iokawa, Makiko Kondo, Hideaki Ohba, *J Plant Res* (2005) 118:57-60.

Optimization of FTA technology for large scale plant DNA isolation for use in marker assisted selection, Mbogori MN, Kimani M, Lagat M, Danson, JW, *African Journal of Biotechnology* Vol. 5 (9), pp 693-696, 2 May 2006.

## Featured Products

Plant-friendly FTA Card, in a Classic Card format features a laminated flap that enables you to vigorously pound the plant sample into the FTA matrix without damaging the FTA Card.

- Capture nucleic acid in one easy step
- Captured nucleic acid is ready for downstream applications in less than 30 minutes
- Nucleic acids collected on FTA Cards are stable for years at room temperature
- FTA Cards are stored at room temperature before and after sample application, reducing the need for laboratory freezers
- Suitable for virtually any cell type
- Indicating FTA Cards change color upon sample application to facilitate handling of colorless samples



Whatman® FTA® Technology PlantSaver FTA Card, Z719811

Harris Micro-punch is a multi-purpose sampling tool for standardizing sample sizes of DNA cards to 1.2 mm in diameter. This is a coring tool designed for simultaneous sample extraction, collection and storage in one operation.



Harris Micro-punch, 1.2 mm, Z708658

Rockwell hardened, hand sharpened tips are designed for long shelf-life and delivering precise repeatable samples with accurate placement.

For information about Extract-N-Amp Plant PCR Kits for rapid extraction and PCR amplification of genomic DNA from plant leaves, go to [sigma-aldrich.com/extract-n-amp](http://sigma-aldrich.com/extract-n-amp).

## Paula's Pointers

- L**eaf Sampling with a Harris Uni-Core Punch
1. Place the leaf on a Harris self-healing cutting mat.
  2. Grip the Uni-Core between the thumb and index fingers and position the tip at a right angle above the target area.
  3. Apply gentle, but firm, downward pressure as the cutting tip passes through the leaf and makes contact with the mat.
  4. Lift the Uni-Core away from the leaf and mat with a disc firmly stored in the cutting tip. Do not depress the plunger until you are ready to transfer the leaf sample.
  5. Eject the disc by depressing the plunger.



Z708828 Harris Uni-core 1.25 mm

**Remember! Never depress the plunger while you are extracting your leaf sample!**

For more protocols for the Harris Uni-Core, go to our Web site at [sigma-aldrich.com/labwarenotes](http://sigma-aldrich.com/labwarenotes).

"Congratulations on having your own separate catalog! It looks great and is easy to use."

- Susan Gitelson, Pres, Magic Touch Icewares International Corp.

"...the new two-volume format is beautifully done."

-David Kasman, Lab Devices

"(The catalog) looks great."

-Joe Kumpel, Ace Glass Inc.



## Latest News

**T**he 2007-2008 Labware Catalog and Aldrich Handbook of Fine Chemicals set is now available! The new Labware catalog contains:

- Approximately 1,300 pages showing 17,000 products carefully selected to support Chemistry and Life Science customers and applications
- Comprehensive 40 page index and thumbnail pictures for easy navigation
- More photos and section tables

To request your 2007-2008 Labware Catalog and Aldrich Handbook of Fine Chemicals set, please go to our Web site at [sigma-aldrich.com/handbook33](http://sigma-aldrich.com/handbook33). Please continue to send us your comments at [labware@sial.com](mailto:labware@sial.com).

**Research is easier when you use the right tools!**

## Labware Listens

**V**ickie Langer of Dow Chemical suggested that we offer a disposable micro-spatula. In response we have introduced a new line of products called smartSpatula™.

The smartSpatula is a clean, economical, and disposable spatula for chemical and biological material transfer, collection and manipulation. The double-ended design has a spoon or spatula on one end and a pick to break up clumps at the other. The flexible spatula ends are shatter-resistant after liquid nitrogen freezing, and readily form to an object to scrape or collect samples. These convenient spatulas are made of polypropylene and are autoclavable.

**If you have any suggestions, please contact us at [labware@sial.com](mailto:labware@sial.com).**

Z560057 smartSpatula, L 310 mm, green  
Z560030 smartSpatula, L 210 mm, blue  
Z560049 smartSpatula, L 210 mm, white  
Z561762 smartSpatula, L 140 mm, micro white

## Further Reading

*IGF and Nutrition in Health and Disease* – a review of specific nutrients that impact the Insulin-like Growth Factor system, thus affecting human health and disease. This volume includes topics such as nutrition and the IGF system in reproduction, adulthood and aging in relation to bone health, nervous systems disorders, gastrointestinal disease, kidney function and cancer.



Z705756 IGF and Nutrition in Health and Disease

## Down Time

Sudoku was published by Nicoli in 1986. The name Sudoku is an abbreviation of the Japanese phrase "suji wa dokushin ni kagiru," meaning "digits must occur only once." Fill in all squares in the grid so that each row, each column and each of the 3x3 squares contain all digits from 1 to 9. Answers can be found at [sigma-aldrich.com/labwarenotes](http://sigma-aldrich.com/labwarenotes).

		8			7		3	
4	3							
		5	6	2		4		
		9		6		1		
3			9	4				
	2					6		
5			1		9		2	
	8		5					
	6	3						

## Labware Links

For more information on the products featured in this newsletter, protocols and many useful Labware Web links, please visit [sigma-aldrich.com/labwarenotes](http://sigma-aldrich.com/labwarenotes).

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