

# 1. 茶 (*Camellia Sinensis*) の含有化合物の検索方法

## 検索フィールドのカスタマイズ

Dictionary of Food Compounds

1. クリック

➕ Add Properties

🗑️ Clear Properties

📄 Saved Searches

🌟 Customise Search Defaults

🔍 Start a New Search

Search Chemicals

🔍 Search

💾 Save Search

Tautomers:

Structure Matching: Substructure

Welcome!

🗑️ Clear Structure

Click to Draw  
Query Structure

2. 追加できる検索項目のリストが表示される。

検索項目の削除も可能

Add Properties

生物種(学名)の情報は  
Food Informationに  
収録されているため、  
その検索項目を追加する。

Boolean	Property	Value	Delete
AND	Chemical Name	<input type="text"/> [browse...] [clear]	<input type="button" value="✕"/>
AND	Molecular Formula	<input type="text"/> [browse...] [clear]	<input type="button" value="✕"/>
AND	Molecular Formula Element	<input type="text"/> [clear]	<input type="button" value="✕"/>
AND	CAS Registry Number	<input type="text"/> [browse...] [clear]	<input type="button" value="✕"/>
AND	All Text	<input type="text"/> [browse...] [clear]	<input type="button" value="✕"/>
AND	Melting Point	<input type="text"/> [browse...] [clear]	<input type="button" value="✕"/>
AND	Boiling Point	= <input type="text"/> [browse...] [clear]	<input type="button" value="✕"/>
AND	Food Information	<input type="text"/> [browse...] [clear]	<input type="button" value="✕"/>

Food Information 3. クリック

Close をクリックすることで、  
Add Properties を閉じる。

4. 検索項目 Food Information が  
追加される。

🔍 Search

💾 Save Search

# 生物種(学名)の入力

Dictionary of Food Compounds

Welcome! ?

Search Chemicals

Search Save Search Tautomers:  Structure Matching: Substructure Clear Structure

Click to Draw Query Structure

部分構造検索により類似骨格も検索可能

Boolean	Property	Comparison	Value	Delete
AND	Chemical Name		<input type="text"/> [browse...] [clear]	✕
AND	Molecular Formula		<input type="text"/> [browse...] [clear]	✕
AND	Molecular Formula by Element	= C	<input type="text"/> [clear]	✕
AND	CAS Registry Nos.		<input type="text"/> [browse...] [clear]	✕
AND	All Text		<input type="text"/> [browse...] [clear]	✕
AND	Melting Point	=	<input type="text"/> [browse...] [clear]	✕
AND	Boiling Point	=	<input type="text"/> [browse...] [clear]	✕
AND	Food Information		Camellia Sinensis [browse...] [clear]	✕

数値の範囲指定にも対応

Search Save Search

Search をクリックすることで、検索!

Food Information に "Camellia Sinensis" を入力

# 検索結果(ヒットリスト)の表示

## Dictionary of Food Compounds

← Back To Search

≡ Add/Remove Columns in Results

≡ Sort This Table

📄 Saved Searches

⚙️ Customise Column Defaults

↺ Reset Columns to Default View

📄 Export the Data

クリック

ヒットリストを電子ファイルに  
エクスポート可能

### Search Chemicals Result

📄 Save Search

Total Hits: 219
















< Prev

Page 1

of 15

> Next

Hits Per Page: 15

Select	Details	↑ Chemical Name	↕ Molecular Formula
<input type="checkbox"/>		8- <i>C</i> -Ascorbylepigallocatechin 3- <i>O</i> -gallate	C <sub>28</sub> H <sub>24</sub> O <sub>17</sub>
<input type="checkbox"/>		Assamicain A	C <sub>44</sub> H <sub>36</sub> O <sub>22</sub>
<input type="checkbox"/>		Assamicain A; 1'-Epimer	C <sub>44</sub> H <sub>36</sub> O <sub>22</sub>
<input type="checkbox"/>		Assamicain C	C <sub>44</sub> H <sub>36</sub> O <sub>22</sub>
<input type="checkbox"/>		Benzyl alcohol; <i>O</i> -[β- <i>D</i> -Xylopyranosyl-(1→6)- <i>D</i> -glucopyranoside]	C <sub>18</sub> H <sub>26</sub> O <sub>10</sub>
<input type="checkbox"/>		2,2',6,6'-Biphenyltetrol	C <sub>12</sub> H <sub>10</sub> O <sub>4</sub>
<input type="checkbox"/>		2-Butyl-4,5-dimethyl-3(2 <i>H</i> )-furanone; (5)-form	C <sub>10</sub> H <sub>16</sub> O <sub>2</sub>
<input type="checkbox"/>		Chafuroside A	C <sub>21</sub> H <sub>18</sub> O <sub>9</sub>
<input type="checkbox"/>		Chafuroside B	C <sub>21</sub> H <sub>18</sub> O <sub>9</sub>
<input type="checkbox"/>		2,7'-Cyclo-8,8'-lignan-3,3',4,4',5,5',9,9'-octol; (7' <i>S</i> ,8 <i>R</i> ,8' <i>R</i> )-form, 3,3',5,5'-Tetra-Me ether, 9'- <i>O</i> -[4-hydroxy-3,5-dimethoxy- <i>E</i> -cinnamoyl-(→6)-β- <i>D</i> -glucopyranoside]	C <sub>39</sub> H <sub>48</sub> O <sub>17</sub>
<input type="checkbox"/>		Dehydrotheasinensin C	C <sub>30</sub> H <sub>26</sub> O <sub>15</sub>
<input type="checkbox"/>		Delphinidin 3-glycosides; 3- <i>O</i> -[4-Hydroxy- <i>E</i> -cinnamoyl-(→6)-β- <i>D</i> -galactopyranoside]	C <sub>30</sub> H <sub>27</sub> O <sub>14</sub>
<input type="checkbox"/>		3,12-Dihydroxy-11,22-dioxo-12-ursen-24-oic acid; 3β-form	C <sub>30</sub> H <sub>44</sub> O <sub>6</sub>
<input type="checkbox"/>		4,8-Dihydroxy-2 <i>H</i> -furo[2,3- <i>h</i> ]-1-benzopyran-2-one; 8-Me ether	C <sub>12</sub> H <sub>8</sub> O <sub>5</sub>
<input type="checkbox"/>		3,7-Dimethyl-1,6-octadien-3-ol; ( <i>R</i> )-form, 3- <i>O</i> -[β- <i>D</i> -Xylopyranosyl-(1→6)-β- <i>D</i> -glucopyranoside]	C <sub>21</sub> H <sub>36</sub> O <sub>10</sub>

Total Hits: 219

<

Page 1

of 15

>

Hits Per Page:

15

# 表示項目の追加方法

## Dictionary of Food Compounds

クリック

← Back To Search

☰ Add/Remove Columns in Results

📄 Sort This Table

📄 Saved Searches

⚙️ Customise Column Defaults

🔄 Reset Columns to Default View

📄 Export the Data

Search Chemicals Result

📄 Save Search

Total Hits: 219

< Prev

Page 1

of 15

> Next

Hits Per Page: 15

Select	Details	↑ Chemical Name	↕ Molecular Formula
<input type="checkbox"/>		8- <i>C</i> -Ascorbyl-pigallocatechin 3- <i>O</i> -gallate	C <sub>28</sub> H <sub>24</sub> O <sub>17</sub>
<input type="checkbox"/>		Assamicain A	C <sub>44</sub> H <sub>36</sub> O <sub>22</sub>
<input type="checkbox"/>		Ass...	C <sub>44</sub> H <sub>36</sub> O <sub>22</sub>
<input type="checkbox"/>			C <sub>44</sub> H <sub>36</sub> O <sub>22</sub>
<input type="checkbox"/>			C <sub>18</sub> H <sub>26</sub> O <sub>10</sub>
<input type="checkbox"/>			C <sub>12</sub> H <sub>10</sub> O <sub>4</sub>
<input type="checkbox"/>			C <sub>10</sub> H <sub>16</sub> O <sub>2</sub>
<input type="checkbox"/>			C <sub>21</sub> H <sub>18</sub> O <sub>9</sub>
<input type="checkbox"/>			C <sub>21</sub> H <sub>18</sub> O <sub>9</sub>
<input type="checkbox"/>			C <sub>39</sub> H <sub>48</sub> O <sub>17</sub>
<input type="checkbox"/>			C <sub>30</sub> H <sub>26</sub> O <sub>15</sub>
<input type="checkbox"/>		Delphinidin 3-glycosides; 3- <i>O</i> -[4-Hydroxy- <i>E</i> -cinnamoyl-(→6)-β- <i>D</i> -galactopyranoside]	C <sub>30</sub> H <sub>27</sub> O <sub>14</sub>
<input type="checkbox"/>		3,12-Dihydroxy-11,22-dioxo-12-ursen-24-oic acid; 3β-form	C <sub>30</sub> H <sub>44</sub> O <sub>6</sub>
<input type="checkbox"/>		4,8-Dihydroxy-2 <i>H</i> -furo[2,3- <i>h</i> ]-1-benzopyran-2-one; 8-Me ether	C <sub>12</sub> H <sub>8</sub> O <sub>5</sub>
<input type="checkbox"/>		3,7-Dimethyl-1,6-octadien-3-ol; ( <i>R</i> )-form, 3- <i>O</i> -[β- <i>D</i> -Xylopyranosyl-(1→6)-β- <i>D</i> -glucopyranoside]	C <sub>21</sub> H <sub>36</sub> O <sub>10</sub>

表示項目の追加・削除が可能

Select Hit Columns

追加可能な項目

現在の表示項目

Available

Accurate Mass  
Boiling Point  
CAS Registry Nos.  
CRC Number  
Density  
Dissociation Const.  
General Statement  
Hazard and Toxicity

>  
>  
<  
<

Columns Displayed

Chemical Name  
Molecular Formula  
Molecular Weight  
Food Information

^  
^  
v  
v

この項目を追加

OK

Close

Total Hits: 219

<

Page 1

of 15

>

Hits Per Page:

15

# 項目追加後のヒットリスト

## Dictionary of Food Compounds

- ← Back To Search
- ≡ Add/Remove Columns in Results
- ≡ Sort This Table
- 📄 Saved Searches
- ⚙️ Customise Column Defaults
- ↺ Reset Columns to Default View
- 📄 Export the Data**

クリック

ヒットリストを電子ファイルに  
エクスポート可能

### Search Chemicals Result

Save Search

Total Hits: 219

← Prev

Page 14

of 15

Next >

Hits Per Page: 15

Select	Details	↑ Chemical Name	↕ Molecular Formula	↕ Molecular Weight	↕ Food Information
<input type="checkbox"/>		Theaflavic acid	C <sub>21</sub> H <sub>16</sub> O <sub>10</sub>	428.351	Isol. from <i>Camellia sinensis</i> (black tea)
<input type="checkbox"/>		Theaflavic acid; 3-Epimer	C <sub>21</sub> H <sub>16</sub> O <sub>10</sub>	428.351	Isol. from <i>Camellia sinensis</i> (black tea)
<input type="checkbox"/>		Theaflavic acid; 3-Epimer, 3- <i>O</i> -(3,4,5-trihydroxybenzoyl)	C <sub>28</sub> H <sub>20</sub> O <sub>14</sub>	580.458	Isol. from <i>Camellia sinensis</i> (black tea)
<input type="checkbox"/>		Theaflavin	C <sub>28</sub> H <sub>24</sub> O <sub>12</sub>	564.501	Constit. of <i>Camellia sinensis</i> (black tea)
<input type="checkbox"/>		Theaflavin; 3- <i>O</i> -(3,4-Dihydroxy-5-methoxybenzoyl)	C <sub>37</sub> H <sub>30</sub> O <sub>16</sub>	730.634	Constit. of black tea ( <i>Camellia sinensis</i> )
<input type="checkbox"/>		Theaflavin; 3- <i>O</i> -(3,4-Dihydroxy-5-methoxybenzoyl), 3'- <i>O</i> -(3,4,5-trihydroxybenzoyl)		922.741	Constit. of black tea ( <i>Camellia sinensis</i> )
<input type="checkbox"/>		Theanine; (5)-form			Constit. of tea ( <i>Camellia sinensis</i> ) and of the fungus <i>Xerocomus badius</i> (kostenjevka)
<input type="checkbox"/>		Theasinensin C			Isol. from <i>Camellia sinensis</i> var. <i>viridis</i> (oolong tea)
<input type="checkbox"/>		Theasinensin C; Atropisomer		610.527	Isol. from <i>Camellia sinensis</i> var. <i>viridis</i> (oolong tea)
<input type="checkbox"/>		Theasinensin C; Atropisomer, 3,3'-bis- <i>O</i> -(3,4,5-trihydroxybenzoyl)	C <sub>44</sub> H <sub>34</sub> O <sub>22</sub>	914.739	Isol. from <i>Camellia sinensis</i> var. <i>viridis</i> (oolong tea)
<input type="checkbox"/>		Theasinensin C; Atropisomer, 3''-deoxy, 3,3'-bis- <i>O</i> -(3,4,5-trihydroxybenzoyl)	C <sub>44</sub> H <sub>34</sub> O <sub>21</sub>	898.740	Isol. from <i>Camellia sinensis</i> var. <i>viridis</i> (oolong tea)
<input type="checkbox"/>		Theasinensin C; 3''-Deoxy, 3,3'-bis- <i>O</i> -(3,4,5-trihydroxybenzoyl)	C <sub>44</sub> H <sub>34</sub> O <sub>21</sub>	898.740	Isol. from <i>Camellia sinensis</i> var. <i>viridis</i> (oolong tea)
<input type="checkbox"/>		Theatribenzotropolone A	C <sub>71</sub> H <sub>52</sub> O <sub>30</sub>	1385.174	Constit. of <i>Camellia sinensis</i> (black tea)
<input type="checkbox"/>		3,11,13-Trihydroxy-12,22-dioxo-23-oleananoic acid; (3β,11α)-form	C <sub>30</sub> H <sub>46</sub> O <sub>7</sub>	518.689	Constit. of roots of <i>Camellia sinensis</i> (black tea)
<input type="checkbox"/>		4',5,7-Trihydroxyflavanone; (5)-form, <i>O</i> -Fructoside	C <sub>21</sub> H <sub>22</sub> O <sub>10</sub>	434.399	Isol. from <i>Camellia sinensis</i> (tea)

生物種(学名)の情報は  
Food Informationの項目に  
収録されている。

Total Hits: 219

←

Page

14

of 15

>

Hits Per Page:

15

前後のページに移動可能

## 2. 化合物のレコード表示方法

Dictionary of Food Compounds

Search Chemicals Result

Save Search Total Hits: 219

Select	Details	Chemical M
<input type="checkbox"/>		Theaflavic acid
<input type="checkbox"/>		Theaflavic acid; 3-Epimer
<input type="checkbox"/>		Theaflavic acid; 3-Epimer, 3-O-(3,4,5-trihydroxybenzoyl)
<input type="checkbox"/>		Theaflavin
<input type="checkbox"/>		Theaflavin; 3-O-(3,4-Dihydro methoxybenzoyl)
<input type="checkbox"/>		Theaflavin; 3-O-(3,4-Dihydro methoxybenzoyl), 3'-O-(3,4,5-trihydroxybenzoyl)
<input type="checkbox"/>		Theanine; (S)-form
<input type="checkbox"/>		Theasinensin C
<input type="checkbox"/>		Theasinensin C; Atropisomer
<input type="checkbox"/>		Theasinensin C; Atropisomer, bis-O-(3,4,5-trihydroxybenzoyl)
<input type="checkbox"/>		Theasinensin C; Atropisomer, bis-O-(3,4,5-trihydroxybenzoyl)
<input type="checkbox"/>		Theasinensin C; 3"-Deoxy, 3; bis-O-(3,4,5-trihydroxybenzoyl)
<input type="checkbox"/>		Theatribenzotropolone A
<input type="checkbox"/>		3,11,13-Trihydroxy-12,22-dioleanoic acid; (3β,11α)-form
<input type="checkbox"/>		4',5,7-Trihydroxyflavanone; O-Fructoside

Click

Entry

クリックすることで、印刷用画面に切り替え.

Printable Expand All Collapse All

Theaflavin

Entry Name: Theaflavin

Synonym(s): 1,8-Bis(3,4-dihydro-3,5,7-trihydroxy-2H-1-benzopyran-2-yl)-3,4,6-trihydroxy-5H-benzocyclohepten-5-one, CAS.

Relative Configuration

CRC Number: HHP83-R

CAS Registry Number: 4670-05-7

Type of Compound Code(s): V.G.98000 V.K.11000 W.A.10000 W.I.46000 Z.Q.66800

Molecular Formula: C<sub>29</sub>H<sub>24</sub>O<sub>12</sub>

Molecular Weight: 564.501

Accurate Mass: 564.12678

Percentage Composition: C 61.70%; H 4.29%; O 34.01%

Food Information: Constit. of *Camellia sinensis* (black tea)

Physical Description: Cryst. + 4H<sub>2</sub>O (H<sub>2</sub>O, MeOH or MeOH aq.)

Melting Point: Mp 237 - 240° dec.

Solubility: Poorly sol. hexane

UV: [neutral] $\lambda_{max}$  216 ( $\epsilon$ 35000); 271 ( $\epsilon$ 19500); 384 ( $\epsilon$ 8700); 470 ( $\epsilon$ 3600)(EtOH)

RTECS Accession Number: DE8382900

InChi Key: IPMYMEWFZKHXGAX-UHFFFAOYSA-N

生物種(学名)の情報は Food Information の項目に収録されている。