1. 茶 (Camellia Sinensis) の含有化合物の検索方法

化合物大辞典にアクセス直後の画面

Combined Chemical Dictionary							
						• Welcome!	0
+ Add Properties	Search Chem	icals					
🥒 Clear Properties	Q Search	🖺 Save Search			Tautomers: Structure Matching: Substructure	🗸 🖉 🖉 Clear S	Structure
Saved Searches							
Customise Search Defaults					_		
🔅 Start a New Search			Cl	ick to	Draw		
			Qu	ery Su	uciure		
	Boolean	Property	Comparison		Value		Delete
	AND	Chemical Name			[browse] [clear]		×
	AND 🗸	Molecular Formula			[browse] [clear]		×
	AND -	Molecular Formula by Element	= V C V		[clear]		×
		CAS Registry Nos.			[browse] [clear]		×
	AND 🗸	All Text			[browse] [clear]		×
		Melting Point	=		[browse] [clear]		×
	AND 🗸	Boiling Point	=		[browse] [clear]		×
	Q Search	Save Search					

検索フィールドのカスタマイズ



生物種(学名)の入力

Combined Chemical	Dictiona	ry				60
						Welcome!
+ Add Properties	Search Chem	icals				
🥖 Clear Properties	Q Search	🖺 Save Search		Tautomers:	Structure Matching: Substructure	 Clear Structure
Saved Searches						
🔅 Customise Search Defaults						
🔅 Start a New Search			011	ick to Draw		
			Qu	cry oracture		
	Boolean	Property	Comparison		Value	Delete
	AND 🗸	Chemical Name			[browse] [clear]	×
	AND 🗸	Molecular Formula			[browse] [clear]	×
	AND 🗸	Molecular Formula by Element	= ~ C ~		[clear]	×
	AND 🗸	CAS Registry Nos.			[browse] [clear]	×
	AND 🗸	All Text			[browse] [clear]	×
	AND 🗸	Melting Point	= ~		[browse] [clear]	×
	AND 🗸	Boiling Point	= ~		[browse] [clear]	×
	AND	Biological Source		Camellia Sinensis	[browse] [clear]	×
7. Search をクリ	Q Search ックするこ	■ Save Search とで,検索!	6. B "Cal	iological Sou mellia Sinen	urce に sis"を入力	

検索結果(ヒットリスト)の表示

Combined Chemical Dictionary * 1 Welcome! 0 Search Chemicals Result Gack To Search Hits Per Page: 15 of 17 > Next Save Search Total Hits: 248 Page 1 Add/Remove Columns in Results 1 Molecular Formula Select Details 1 Chemical Name Sort This Table Acetophenone C₈H₈O Saved Searches Customise Column Defaults C₆H₇NO 2-Acetylpyrrole Reset Columns to Default View D Adenosine nucleosidase 🖻 Export the Data 8-C-Ascorbylepigallocatechin 3-O-gallate C28H24O17 クリック C44H36O22 Assamicain A ヒットリストを電子ファイル Ľ Assamicain A; 1'-Epimer C44H36O22 (CSV形式, Excel形式, HTML Assamicain C C44H36O22 形式)にエクスポート可能 Benzyl alcohol; O-[β -p-Xylopyranosyl-(1 \rightarrow 6)-p-glucopyranoside] C18H26O10 D 2,2',6,6'-Biphenyltetrol C12H10O4 2-Butyl-4,5-dimethyl-3(2H)-furanone; (ξ)-form C10H16O2 1(10),4-Cadinadiene; (6β,7β)-form C15H24 Chafuroside A C₂₁H₁₈O₉ Chafuroside B C21H18O9 2,7'-Cyclo-8,8'-lignan-3,3',4,4',5,5',9,9'-octol; (7'5,8R,8'R)-form, 3,3',5,5'-Tetra-Me ether, C39H48O17 9'-0-[4-hydroxy-3,5-dimethoxy-E-cinnamoyl-(→6) -β-D-glucopyranoside] Dehydrotheasinensin C C30H26O15 Hits Per Page: 15 🗸 Page of 17 Total Hits: 248 1

前後のページに移動可能

表示項目の追加方法

クリック



項目追加後のヒットリスト

Combined Chemical Dictionary 検索画面に戻る

l							Welcome		
クリ	ック 🖕 Back To Search	Search	Search Chemicals Result						
	Add/Remove Columns in	🖹 Si	ave Search	Total Hits: 248	Prev Page 1 of 17 > Next		Hits Per Page: 15 🗸		
	Results	Select	Details	1 Chemical Name	🗘 Molecular Formula	Ø Molecular Weight	Biological Source		
	 Saved Searches Customise Column Defaults 		۵	Acetophenone	C _a H _a O	120.151	Isol. from essential oils. Constit. of the flowers of <i>Camellia sinensis</i> . Obt. comly as byprod. in the Hock phenol synthesis		
	 Reset Columns to Default View Export the Data 			2-Acetylpyrrole	C ₆ H ₇ NO	109.128	Found in Valeriana officinalis, Camellia sinensis, Paeonia moutan (Chinese drug Botanpi) and Lycium chinense. Prod. by Streptomyces sp. A-5071		
Γ.	クリック		D	Adenosine nucleosidase			Isol. from plant tissues, e.g. <i>Helianthus tuberosus, Triticum</i> aestivum, Camellia sinensis, Hordeum vulgare, Coffea arabica		
	Cジトリストを電子ファイル (CSV形式, Excel形式, HTML		D	8-C-Ascorbylepigallocatechin 3-O-gallate		632.483	Constit. of commercial oolong tea (<i>Camellia sinensis</i> var. <i>viridis</i>) and Pu-erh tea (<i>Camellia sinensis</i> var. <i>assamica</i>)		
	形式)にエクスポート可能			Assamicain A	物種(学名)の情報は	6.75	Isol. from the leaves of <i>Camellia sinensis</i> var. <i>assamica</i> (Assam tea)		
			Ľ	Assamicain A; 1'-Epimer	ological Source の項	目に 16.75	Isol. from leaves of <i>Camellia sinensis</i> var. <i>assamica</i> (Assam tea)		
				Assamicain C	(球されている.		Derived from the leaves of Camellia sinensis var. assamica		
			D	Benzyl alcohol; <i>O</i> -[β-ɒ-Xylopyranosyl-(1→6) -ɒ-glucopyranoside]	Стандаюто	402.396	Constit. of Alangium platanifolium, Camellia sinensis, Panax ginseng and Prunus laurocerasus		
			D	2,2',6,6'-Biphenyltetrol	C ₁₂ H ₁₀ O ₄	218.208	Isol. from Pu-erh tea obt. from <i>Camellia sinensis</i> var. assamica		
				2-Butyl-4,5-dimethyl-3(2 <i>H</i>)-furanone; (ξ)-form	C ₁₀ H ₁₆ O ₂	168.236	Isol. from green tea (<i>Camellia sinensis</i>)		
				1(10),4-Cadinadiene; (6β,7β)-form	C ₁₅ H ₂₄	204.357	Constit. of ylang-ylang, citronella, cubebs, sweetflag and cade. Also in <i>Camellia sinensis, Xylopia</i> sp., <i>Gossypium hirsutum</i> and others		
			D	Chafuroside A	C ₂₁ H ₁₈ O ₉	414.366	Constit. of tea leaves (<i>Camellia sinensis</i>)		

2. 化合物のレコード表示方法



3. 部分構造検索の方法

検索画面



Boolean	Property	Comparison	Value	Delete
AND	Chemical Name		[browse] [clear]	×
AND	Molecular Formula		[browse] [clear]	×
AND	Molecular Formula by Element	= ~ C ~	[clear]	×
AND	CAS Registry Nos.		[browse] [clear]	×
AND	All Text		[browse] [clear]	×
AND	Melting Point	- ~	[browse] [clear]	×
AND	Boiling Point	=	[browse] [clear]	×
Q Search	B Save Search			

部分構造式の作図

Combined Chemical	Dictionary			
				Welcome!
😌 Add Properties	Search Chemicals			
🥒 Clear Properties	Q Search 🗈 Save Search		Tautomers: Structure Matching: Substructure	✓
Saved Searches				
Customise Search Defaults				
💠 Start a New Search		Click to Draw		
			X	
		D D D C X D D & @ 0		
			р ^и ц	
			c	
	Boolean Property	47	N	Delete
	AND Chemical Name	+ / H	0	×
	AND 🗸 Molecular Formula	-	S	×
	AND Molecular Formula by Element		F	×
[Import ボタンをクリ	ックすることで		P	
構造式ファイルのイン	ポート画面(最終ページ)		Br	
が開き、他社構造式指	描画ソフト(ChemDraw等)	→ 2. 構造式描画ソフト Marvin JS ; ク 問くので 部分構造式を作回する		×
にて作成したファイル	のインポートが可能.	開いて、即り構造式を作らす。	*	×
	AND Boiling Point		A	×
	Q Search 🖹 Save Search	1 Import		
		+ Click to add structure to search query 3. クリック	_	
		× Close		

部分構造式の入力と検索

Combined Chemical Dictionary Welcome! 0 Search Chemicals + Add Properties Clear Properties Q Search Save Search Tautomers: Structure Matching: Substructure Clear Structure 😑 Saved Searches OH $\hat{\rho}$ Customise Search Defaults Start a New Search 4. 化学構造式が入力される. Boolean Property Comparison Value Delete Chemical Name AND \sim [browse...] [clear] × \sim AND Molecular Formula [browse...] [clear] × ✓ C \sim AND \sim Molecular Formula by Element = [clear] × \sim AND CAS Registry Nos. [browse...] [clear] × \sim AND All Text [browse...] [clear] × ~ AND \sim Melting Point [browse...] [clear] = × \sim \sim **Boiling Point** AND = [browse...] [clear] Save Search 5. Searchをクリックすることで、検索!

検索結果(ヒットリスト)の表示

Combined Chemical Dictionary

🔶 Back To Search

■ Add/Remove Columns in Results
▲ Sort This Table

- Saved Searches
- 💠 Customise Column Defaults
- Reset Columns to Default View
- 🕝 Export the Data

earch Chen	nicals Result		Welcome
🖺 Save S	Search Tota	Hits: 18 Prev Page 1 of 2 Next	Hits Per Page: 15
Select	Details	Î Chemical Name	Molecular Formula
	٥	3,9-Dihydroxy-7-illuden-1-one	C ₁₅ H ₂₂ O ₃
		3,9-Dihydroxy-7-illuden-1-one; (2β,3β,9β)-form	C ₁₅ H ₂₂ O ₃
		3,9-Dihydroxy-7-illuden-1-one; (2β,3β,9β)-form, 9-(2- <i>O</i> -Acetyl-β-D-glucopyranoside)	C ₂₃ H ₃₄ O ₉
		3,9-Dihydroxy-7-illuden-1-one; (2β,3β,9β)-form, 9-[2- <i>O</i> -Acetyl-4-(<i>ρ</i> -hydroxy- <i>E</i> -cinnamoyl)-β-p-glucopyranoside]	C ₃₂ H ₄₀ O ₁₁
		3,9-Dihydroxy-7-illuden-1-one; (2β,3β,9β)-form, 9-[2- <i>O</i> -Acetyl-4-(<i>p</i> -hydroxy- <i>Z</i> -cinnamoyl)-β-p-glucopyranoside]	C ₃₂ H ₄₀ O ₁₁
		Ptaquiloside	C ₂₀ H ₃₀ O ₈
		Ptaquiloside; 3-Epimer	C ₂₀ H ₃₀ O ₈
		Ptaquiloside; Tetra-Ac	
		Ptaquiloside Z	C ₂₁ H ₃₂ O ₈
		3,9,13-Trihydroxy-7-illuden-1-one	C ₁₅ H ₂₂ O ₄
		3,9,13-Trihydroxy-7-illuden-1-one; (2β,3α,9β)-form	C ₁₅ H ₂₂ O ₄
		3,9,13-Trihydroxy-7-illuden-1-one; (2β,3α,9β)-form, 9- <i>Ο</i> -β-ε-Glucopyranoside	C ₂₁ H ₃₂ O ₉
		3,9,13-Trihydroxy-7-illuden-1-one; (2β,3β,9β)-form	C ₁₅ H ₂₂ O ₄
		3,9,13-Trihydroxy-7-illuden-1-one; (2β,3β,9β)-form, 9- <i>Ο</i> -(2- <i>Ο</i> -Acetyl-β-ɒ-glucopyranoside)	C ₂₃ H ₃₄ O ₁₀
		3,9,13-Trihydroxy-7-illuden-1-one; (2β,3β,9β)-form, 9-∂-[2-∂-Acetyl-[4-hydroxy- <i>E</i> -cinnamoyl-(→4)]-β-o-glucopyranoside]	C ₃₂ H ₄₀ O ₁₂
		Total Hits: 18 Page 1 of 2 Hits Per Page: 15	

構造式ファイルのインポート画面

Search Chemi	icals				
Q Search	Save Search		Tautomers: Structure Matching:	Substructure 🖌	Clear Structure
		Import OH //	x		
		Import a structure from a file or paste an InChI, SMILES or SMARTS File Import	lin ⁿⁱ H		
Boolean	Prop	select from the following file types: cax, caxmi, cmi, csmoi, csraf, csrgf, cssaf, cube, cxsmiles, inchi, mol, mol2, mrv, pdb, rdf, rgf, sdf, smarts, smiles, xyz	N		Delete
AND ~	Chemical Name Molecular Formula	+ Select File 他社構造式描画ソフト(ChemDraw等)に 作成したファイルのインポートが可能.	ст о s		×
AND ~	Molecular Formula b	Paste InChl, SMILES or SMARTS	F		×
AND ~	CAS Registry Nos.	Select Format to Import:	a		×
AND ~	All Text	Paste the Structure text below (importing may take a few moments)	Br		×
AND ~	Melting Point				×
AND	Boiling Point	+ Load Structure	A		×
Q Search	Save Search	× Close			