

Supporting Information

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Saganhaematenones: Novel Bioactive Natural Products, Derived from *Haematococcus* (Chlorophyceae) dSgH-K1 Strain, that Inhibit Angiotensin-Converting Enzyme

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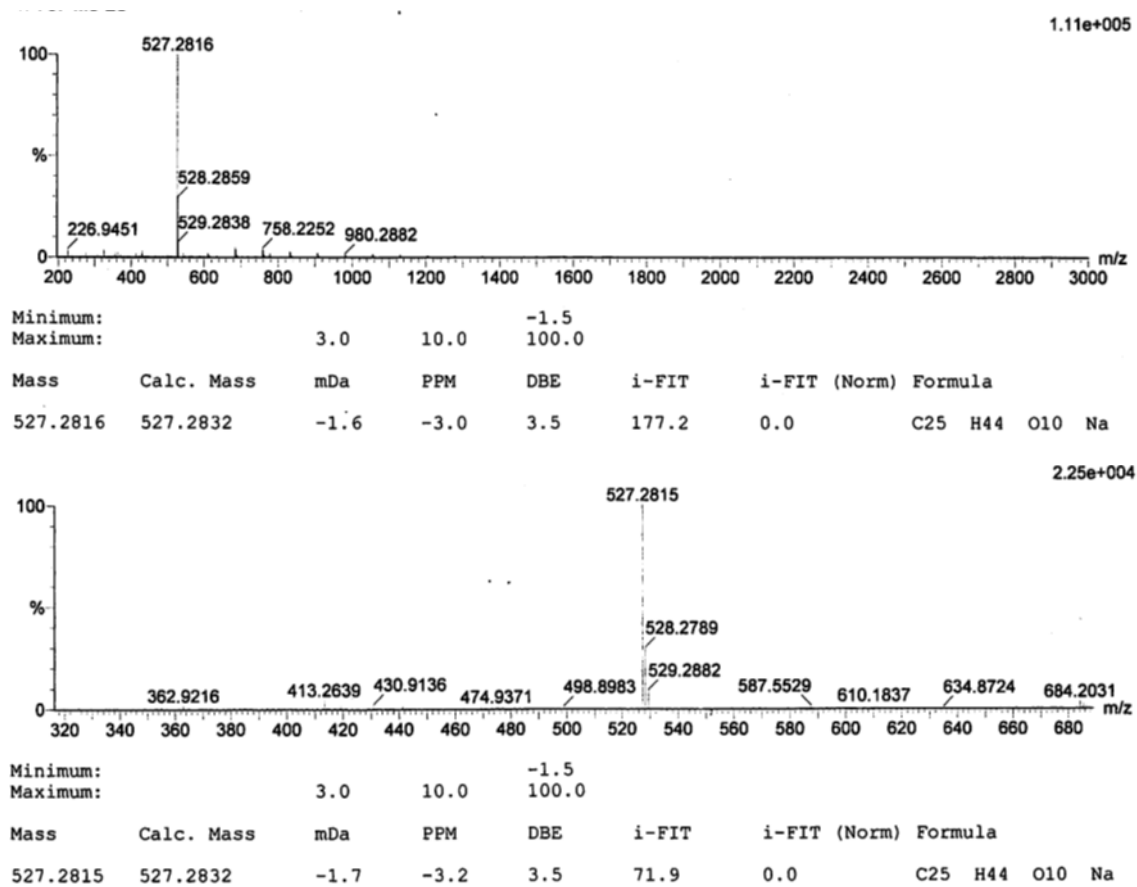


Figure S1: HRMS spectrum of saganhaematenone A (top) and saganhaematenone B (bottom)

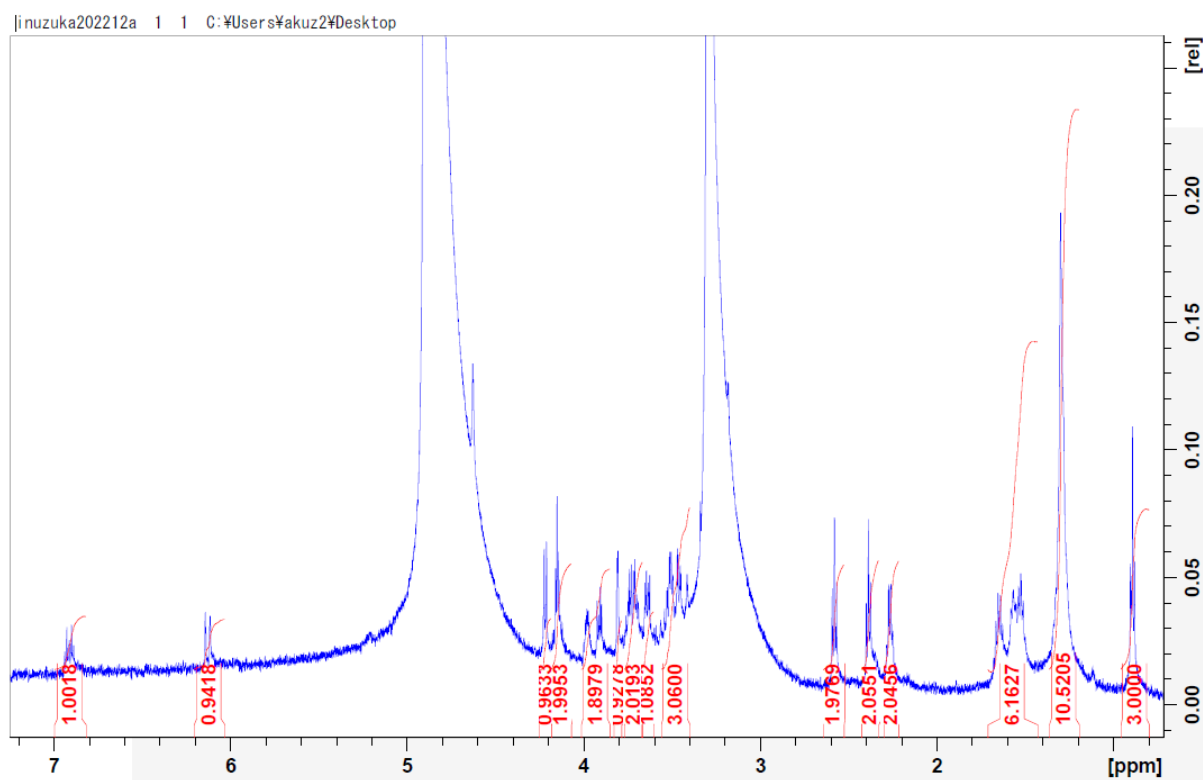


Figure S2: ^1H -NMR (600 MHz, CD_3OD) spectrum of saganhaemetone A

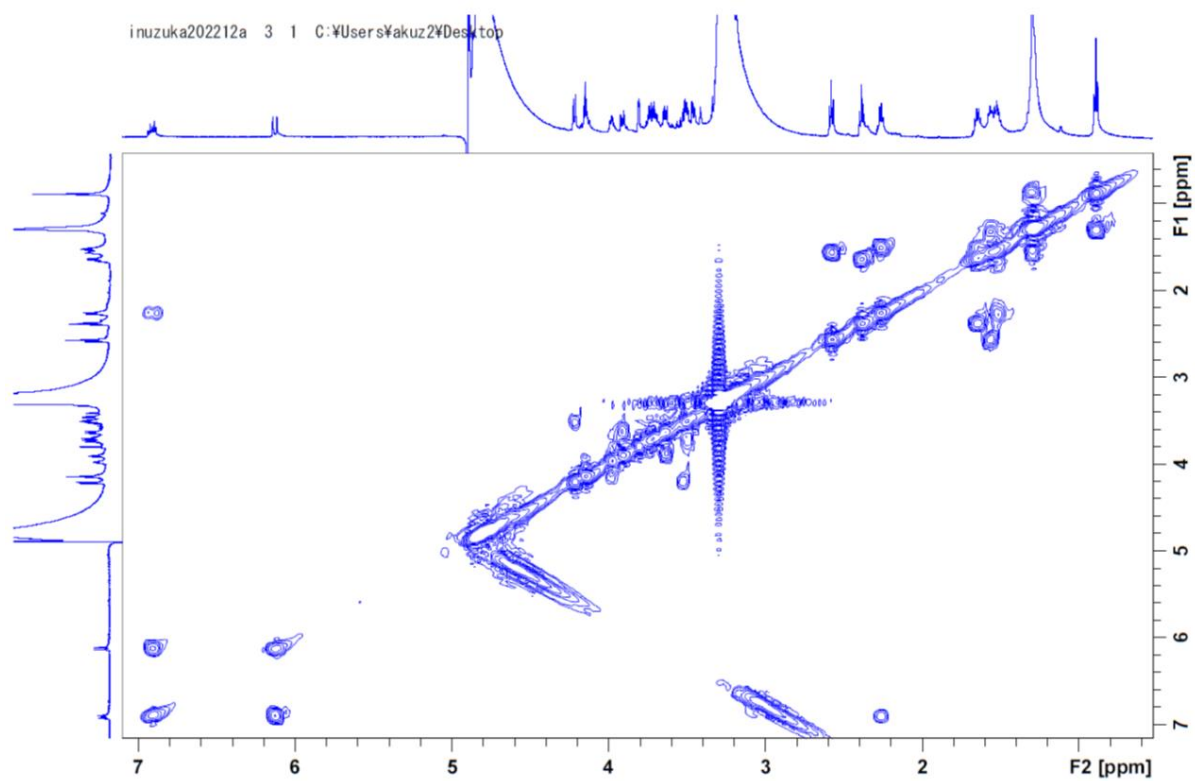


Figure S3: ^1H - ^1H COSY spectrum of saganhaematenone A

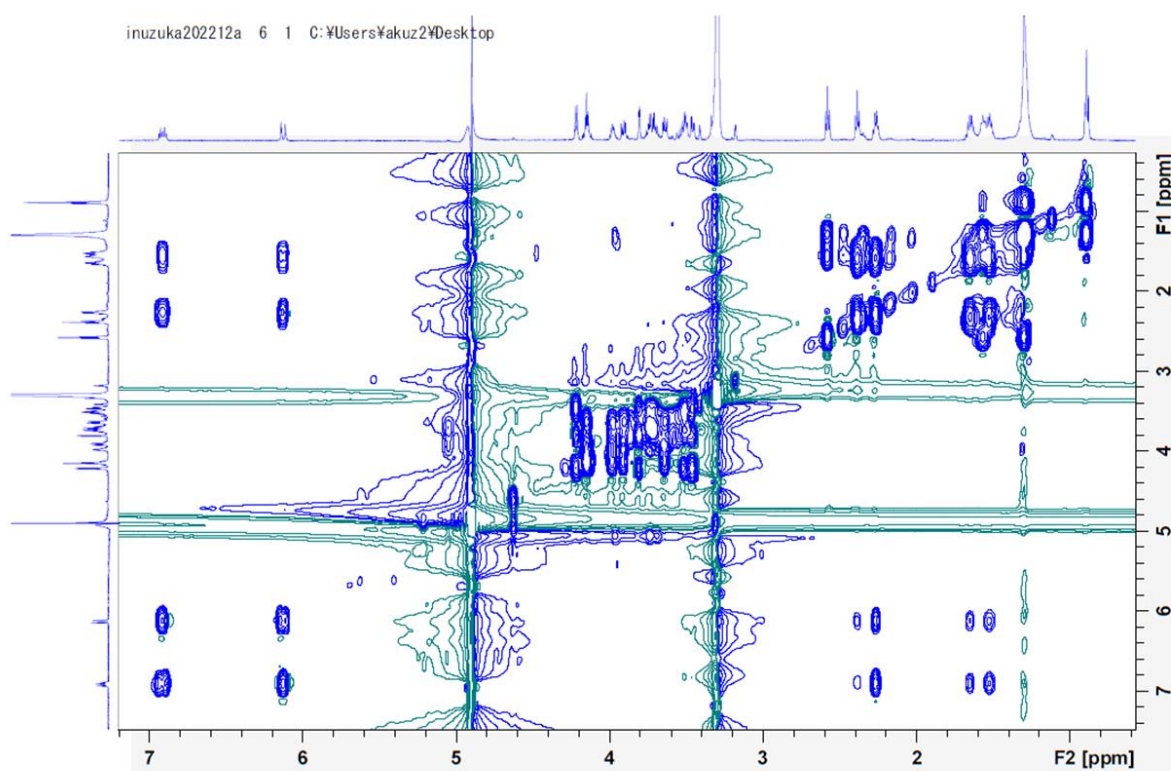


Figure S4: ^1H - ^1H TOCSY spectrum of saganhaematenone A

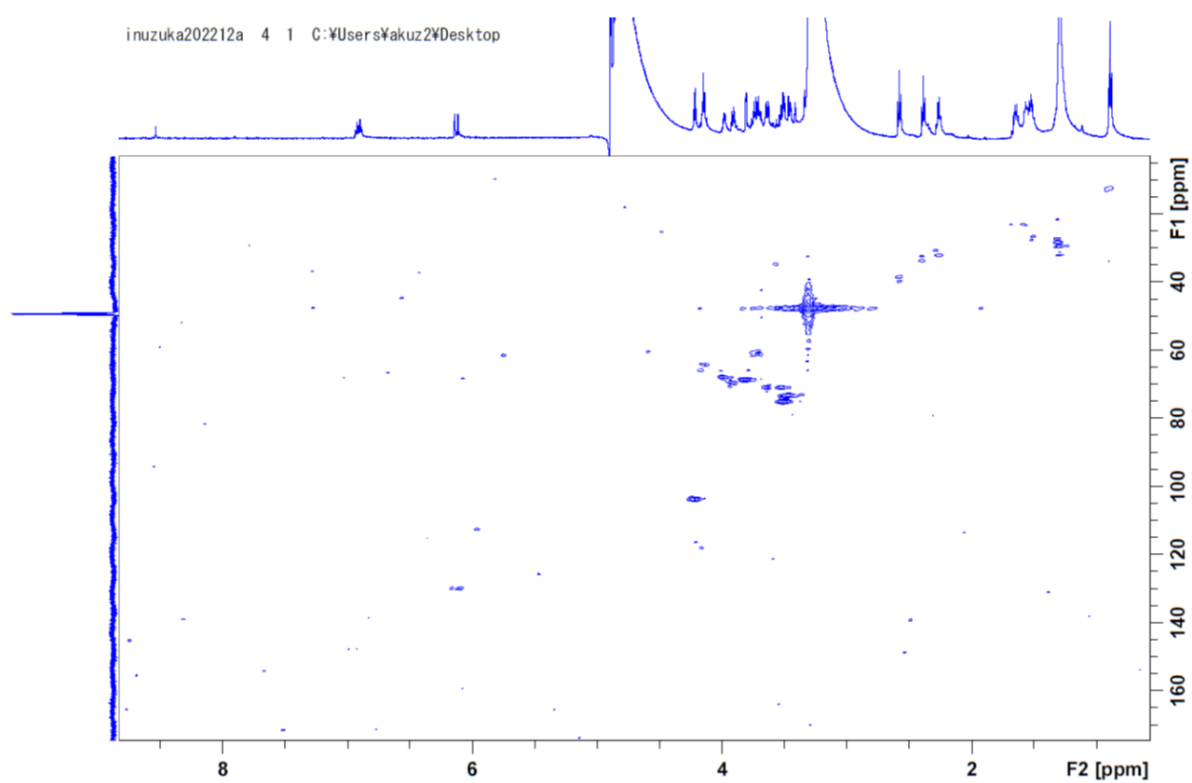


Figure S5: HMQC spectrum of sagahaematenone A

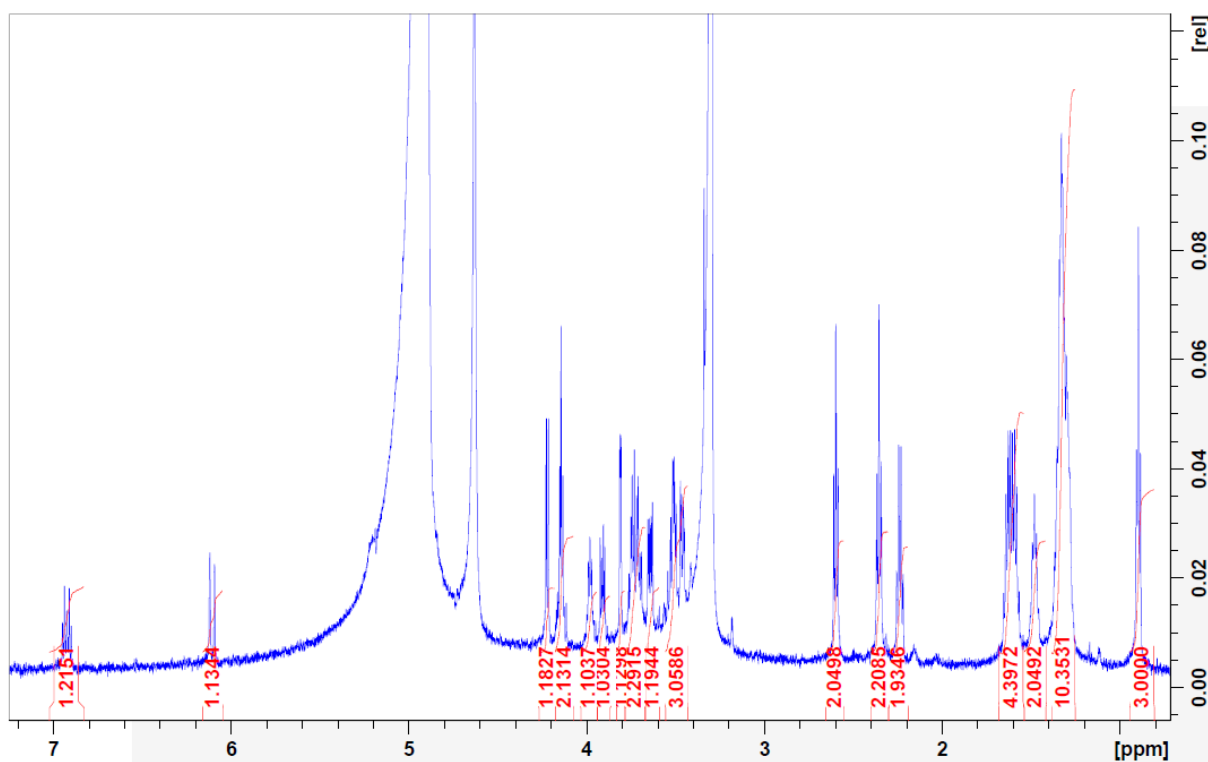


Figure S6: ^1H -NMR (600 MHz, CD_3OD) spectrum of saganhaemetone B

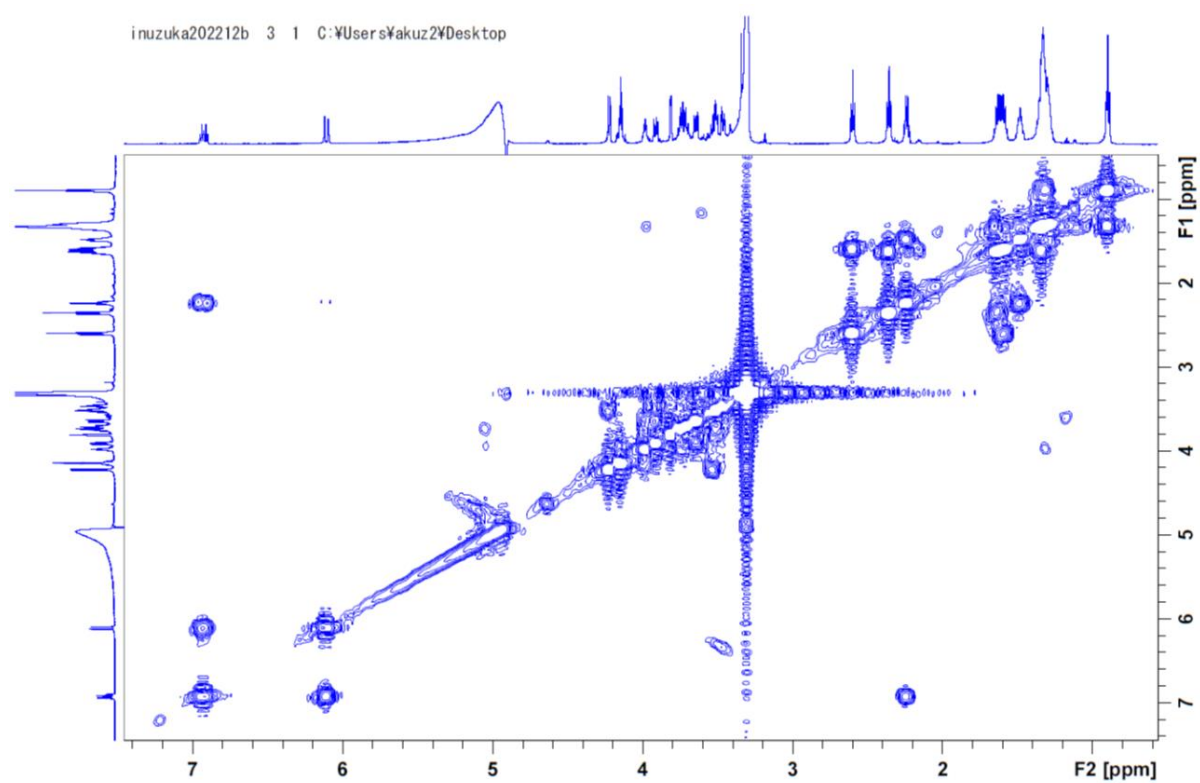


Figure S7: ^1H - ^1H COSY spectrum of saganhaematenone B

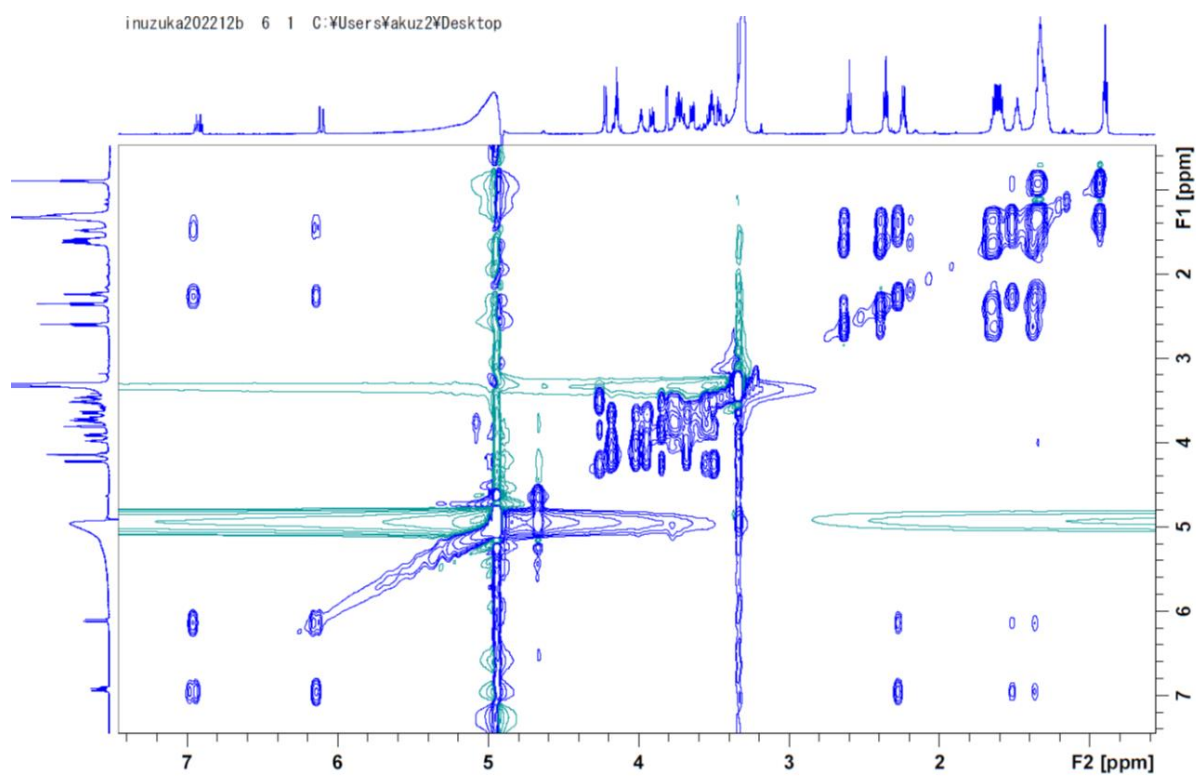


Figure S8: ^1H - ^1H TOCSY spectrum of saganhaematenone A

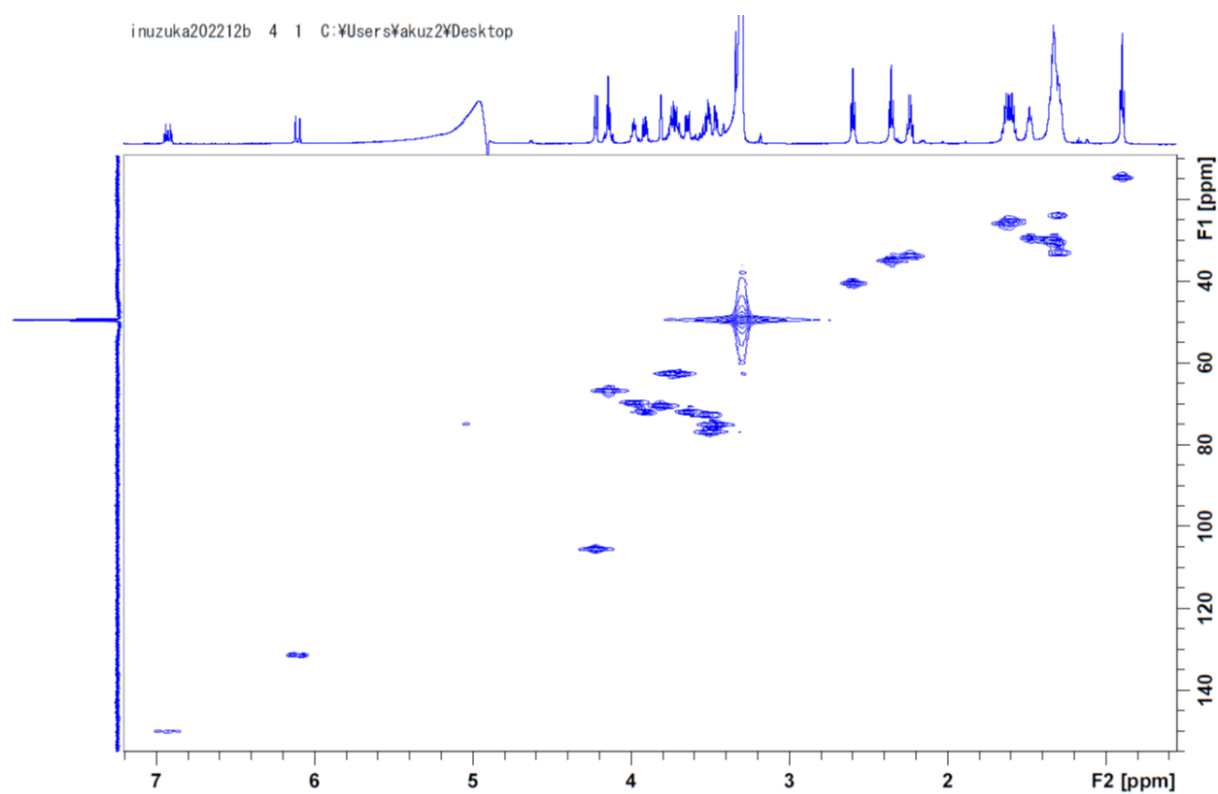


Figure S9: HMQC spectrum of sagahaematenone B

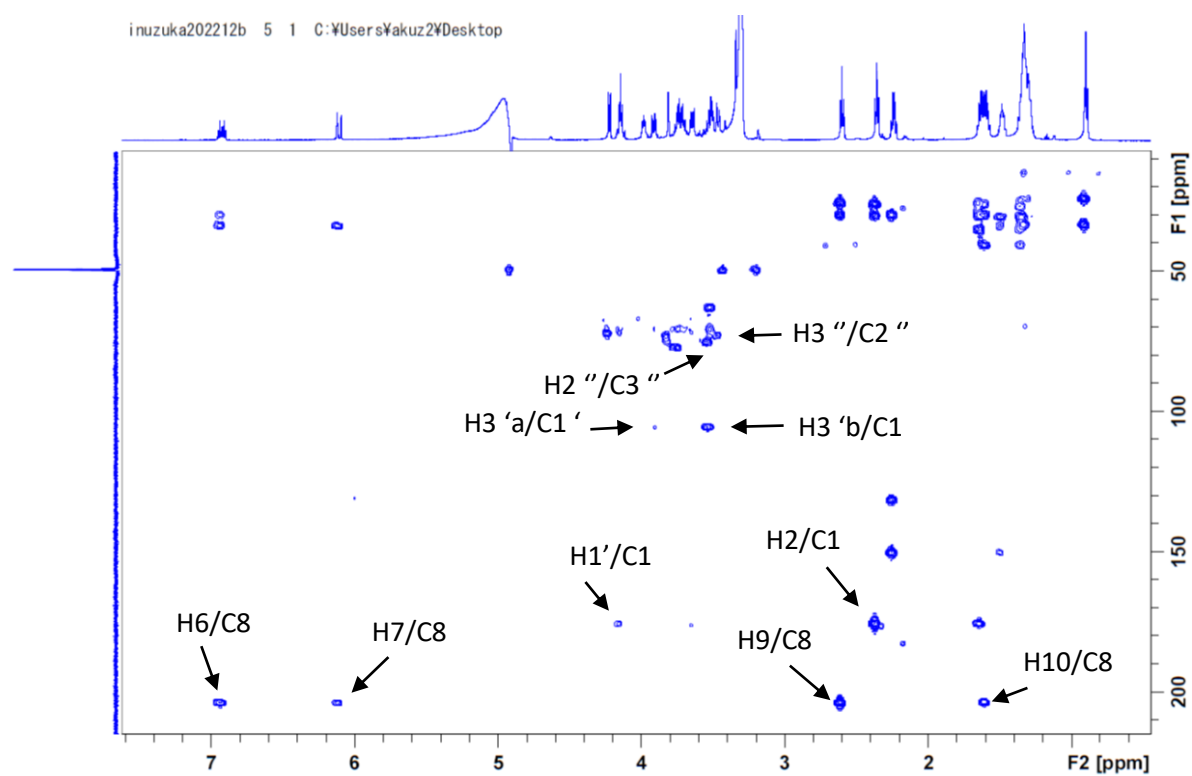


Figure S10: HMBC spectrum of saganhaematenone B

re Substance Se: x +

scifinder-n.cas.org/search/substance/688ee594f826df4a20b5ab6b/1

CAS SciFinder Substances Enter a query...

Return to Home

Substances search for drawn structure

View Related Results

Filter Results

Structure Match

As Drawn (1)

Substructure (3)

Similarity (205K)

Analyze Structure Precision

Behavior

Filter by Exclude

Search Within Results

Reference Role

Biological Study (1)

Food or Feed Use (1)

Pharmacological Activity (1)

Preparation (1)

Properties (1)

View All

Commercial Availability

1 Result

2991917-54-3

C23H44O10

1 0 0

View: Partial

CAS SciFinder References Enter a query...

Draw

Return to Home

References for 2991917-54-3

View Related Results

Filter Results

Behavior

Filter by Exclude

Search Within Results

Document Type

Patent (1)

Substance Role

Biological Study (1)

Preparation (1)

Properties (1)

Substance Claimed (1)

Uses (1)

View All

Language

Japanese (1)

Publication Year

1 Result

View: Partial Abstract

A novel cyclic compound, an angiotensin converting enzyme inhibitor, its manufacturing method, and its use

Assignees: Saga University; Saga Sorui Biomass Kyogikai
Japan, JP2023143827 A 2023-10-06 | Language: Japanese, Database: CApius

To provide an angiotensin converting enzyme inhibitor containing a new cyclic compound which has a low environmental load, can be produced at a low cost, can be used for pharmaceuticals, functional foods and the like, and a use thereof. For example, the following compound 3153 a or 3154 a, a salt thereof, or a solvate thereof is provided.

PatentPak Full Text 7 0 0 0

Figure S11: SciFinder Exact Match Reports of saganhaematenones

scifinder-n.cas.org/search/substance/688eebc5f828df4a20b5d329/1

CAS SciFinder Substances Enter a query...

Return to Home

Substances search for drawn structure

View Related Results

Filter Results

Structure Match

As Drawn (1)

Substructure (3)

Similarity (205K)

Behavior

Filter by Exclude

Search Within Results

Similarity

>=99 (1)

90-94 (90)

85-89 (865)

80-84 (3,319)

75-79 (9,824)

View All

Reaction Role

Product (36)

Reactant (6)

Reference Role

Preparation (71)

Biological Study (66)

Uses (45)

Synthetic Preparation (38)

Therapeutic Use (34)

View All

Life Science Data

Commercial Availability

Available (6)

Not Available (85)

Number of Components

1 (91)

Molecular Weight

1-100

Filtering: Similarity: 2 Selected

91 Results

Sort: Relevance View: Partial

1 2 3 4 5 6 7 8 9

2991917-54-3

$C_{25}H_{44}O_{10}$

3081458-98-9

$C_{25}H_{46}O_{11}$

Compound 1

145014-07-9

$C_{27}H_{46}O_9$

(2S)-2-Hydroxy-3-[[[(9Z)-1-oxo-9-octadecen-1-yl]oxy]propyl] β -D-galactopyranoside

176966-09-9

$C_{27}H_{46}O_9$

(1S)-1-(Hydroxymethyl)-2-[[[(9Z)-1-oxo-9-octadecen-1-yl]oxy]ethyl] β -D-glucopyranoside

155156-06-2

$C_{27}H_{46}O_9$

2-Hydroxy-3-[[[(9Z)-1-oxo-9-octadecen-1-yl]oxy]propyl] β -D-glucopyranoside

2245941-29-9

$C_{33}H_{56}O_{14}$

1322574-32-2

$C_{27}H_{46}O_9$

(2S)-2-Hydroxy-3-[[[(9Z)-1-oxo-9-octadecen-1-yl]oxy]propyl] α -D-galactopyranoside

662143-90-0

$C_{29}H_{48}O_9$

(2R)-3-Hydroxy-2-[[[(9Z)-1-oxo-9-eicosen-1-yl]oxy]propyl] β -D-galactopyranoside

660831-38-9

$C_{27}H_{46}O_9$

(2R)-3-Hydroxy-2-[[[(9Z)-1-oxo-9-octadecen-1-yl]oxy]propyl] β -D-galactopyranoside

Figure S12: SciFinder Similarity report of saganhaematenones

Table S1: Comparison of NMR data between saganhaematenone A and its most closely related compound 1

Compound 1 [†]			Saganhaematenone A [‡]		
Position	δ H (ppm, J in Hz)	δ C, (ppm, Type)	Position	δ H (ppm, J in Hz)	δ C, (ppm)
1'	4.26, d (7.2)	105.2, CH	1'	4.22, d (7.7)	105.7
2'	3.53, overlap	72.5, CH	2'	3.52, m	72.7
3'	3.51, dd (9.3, 2.8)	74.7, CH	3'	3.45, dd (9.5, 3.1)	74.9
4'	3.88, brs	69.9, CH	4'	3.81, brd (3.2)	70.6
5'	3.55, m	76.3, CH	5'	3.52, m	77.2
6'	3.76, m	62.4, CH ₂	6'a	3.75, m	62.8
			6'b	3.70, m	
1	4.12, d (5.4)	66.1, CH ₂	1	4.15, m	66.8
2	3.94, m	69.3, CH	2	3.98, m	69.9
3a	3.66, dd (10.7, 4.8)	72.1, CH ₂	3a	3.64, dd (10.7, 4.6)	72.2
3b	3.82, dd (10.7, 5.5)		3b	3.91, dd (10.7, 4.7)	
1''		173.7, C	1''		175.8
2''	2.33, t (7.4)	34.4, CH ₂	2''	2.39, t (7.4)	33.7
3''	1.62, overlap	25.1, CH ₂	3''	1.66, m	25.6
4''	1.44, m	29.3, CH ₂	4''	1.52, m	25.6
5''	2.07, overlap	32.6 a, CH ₂	5''	2.26, dt (6.6, 6.6)	33.3
6''	5.68, dt (15.4, 6.5)	134.6, CH	6''	6.91, dt (15.8, 6.6)	149.4
7''	5.41, ddt (15.4, 7.9, 1.5)	131.2, CH	7''	6.13, d (15.8)	129.9
8''	4.19, m	86.6, CH	8''		204.2
9''a	1.41, m	33.6, CH ₂	9''	2.57, t (7.3)	38.7
9''b	1.63, overlap				
10''	1.23–1.37, m	26.1, CH ₂	10''	1.56, m	23.2
11''	1.23–1.37, m	30.0 b, CH ₂	11''	1.30-1.33	24.2-33.3
12''	1.23–1.37, m	30.3 b, CH ₂	12''	1.30-1.34	24.2-33.4
13''	1.23–1.37, m	30.4 b, CH ₂	13''	1.30-1.35	24.2-33.5
14''	1.23–1.37, m	32.7 a, CH ₂	14''	1.30-1.36	24.2-33.6
15''	1.23–1.37, m	23.3, CH ₂	15''	1.30-1.37	24.2-33.7
16''	0.88, t (6.8)	14.4, CH ₃	16''	0.89, t (6.9)	14.9
8''-OOH	10.31, s				

[†]¹H (600 MHz) and ¹³C NMR (150 MHz) spectroscopic data for compound 1 in acetone-d₆.

[‡]¹H (600 MHz) and ¹³C NMR (based on the HMBC and HMQC spectra) spectroscopic data for saganhaematenone A in CD₃OD.