Supporting Information

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Isolation of New Secondary Metabolites from Kedrostis gijef and

Evaluation of Their α-Glucosidase Inhibitory Activity

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Figure S1: Negative HRESIMS for compound 4



Figure S3: Expanded ¹H- NMR of compound 4 (in CD₃OD, 600 MHz)



Figure S4: APT-NMR of compound 4 (in CD₃OD, 150 MHz)



Figure S5: Expanded APT-NMR of compound 4 (in CD₃OD, 150 MHz)



Figure S7: Expanded HSQC spectrum of compound 4



Figure S8: HMBC spectrum of compound 4



Figure S9: Expanded HMBC spectrum of compound 4



Figure S10: 1H-1H-COSY spectrum of compound 4



Figure S11: Expanded ¹H-¹H-COSY spectrum of compound 4



Figure S12: NOESY spectrum of compound 4





Figure S14: Negative HRESIMS for compound 5



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S17: APT-NMR of compound 5 (in CD₃OD, 150 MHz)



Figure S18: Expanded APT-NMR of compound 5 (in CD₃OD, 150 MHz)



Figure S20: Expanded HSQC spectrum of compound 5





Figure S22: Expanded HMBC spectrum of compound 5

f1 (ppm)



Figure S23: ¹H-¹H-COSY spectrum of compound 5



Figure S24: Expanded ¹H-¹H-COSY spectrum of compound 5





Figure S26: Expanded NOESY spectrum of compound 5



Figure S27: Negative HRESIMS for compound 6



Figure S28: ¹H- NMR of compound 6 (in CD₃OD, 600 MHz)



Figure S29: Expanded ¹H- NMR of compound 6 (in CD₃OD, 600 MHz)



Figure S31: Expanded APT-NMR of compound 6 (in CD₃OD, 150 MHz)



Figure S33: Expanded HSQC spectrum of compound 6



Expanded HMBC spectrum of compound 5

23





S38: NOESY spectrum of compound **6**



Figure S39: Expanded NOESY spectrum of compound 6



Figure S40: Positive HRESIMS for compound 7



Figure S42: Expanded ¹H- NMR of compound 7 (in CD₃OD, 600 MHz)



Figure S43: APT-NMR of compound 7 (in CD₃OD, 150 MHz)



Figure S44: Expanded APT-NMR of compound 7 (in CD₃OD, 150 MHz)



Figure S46: Expanded HSQC spectrum of compound 7

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Figure S48: Expanded HMBC spectrum of compound 7



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Figure S51: NOESY spectrum of compound 7



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SciFinderⁿ®

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Search Tasks

TaskSearch TypeViewExported: Returned Substance Results + Filters (1)SubstancesView Results

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Figure S53: Sci-Finder search for compound 4

CAS 🐞 SciFinderⁿ

Subs	tances (1)			View in SciFinder
1					Similarity Score: 99
405281-91-	6		Key Physical Properties	Value	Condition
	Ħ		Molecular Weight	652.86	۰. ۵
Absolute stereochemistry shown,		×	Melting Point (Experimental)	124-156 °C	12.
		Boiling Point (Predicted)	772.4±60.0 °C	Press: 760 Torr	
		Density (Predicted)	1.27±0.1 g/cm ³	Temp: 20 °C; Press: 760 Torr	
	Kotation (+)		pKa (Predicted)	12.91±0.70	Most Acidic Temp: 25 °C
C ₃₆ H ₆₀ O ₁₀ 19-Norlanosta glucopyranosy methyl-, (3β,6c	n-11-one, 5,6-e doxy)-24,25-dihy ι,9β,10α,24 <i>R</i>)-	poxy-3-(β-D- ydroxy-9-	Experimental Properties Spe	ectra	
1 Reference	■ 0 Reactions	Description: Note: N			

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Figure S54: Sci-Finder similarity report for compound 4

SciFinderⁿ®

CAS 🌼 SciFinderⁿ

Initiating Search

Task History

Page 1

June 21, 2024, 3:13 PM



Structure Match: Similarity

Search Tasks

Task	Search Type	View
Exported: Returned Substance Results + Filters (2)	Substances	View Results

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Figure S55: Sci-Finder search for compound 5

SciFinder®



Substances (2) View in SciFinderⁿ 1 Similarity Score: 99 Key Physical Properties 1283586-92-4 Value Condition Molecular Weight 654.87 Press: 760 Torr Boiling Point (Predicted) 773.2±60.0 °C Density (Predicted) 1.27±0.1 g/cm³ Temp: 20 °C; Press: 760 Torr Most Acidic Temp: 25 °C pKa (Predicted) 12.92±0.70 Absolute stereochemistry shown C36H62O10 5*R*,6*R*-Epoxymogroside 1 E₁ 1 0 0 Reference Reactions Suppliers Similarity Score: 99 2 Key Physical Properties Value Condition 476468-77-6 Molecular Weight 654.87 Boiling Point (Predicted) 773.2±60.0 °C Press: 760 Torr Density (Predicted) 1.27±0.1 g/cm³ Temp: 20 °C; Press: 760 Torr pKa (Predicted) 12.92±0.70 Most Acidic Temp: 25 °C Absolute stereochemistry shown C₃₆H₆₂O₁₀ β-D-Glucopyranoside, (3β,6α,9β,10α,11α,24*R*)-5,6-epoxy-11,24,25-trihydroxy-9-methyl-19norlanostan-3-yl 4 0 д 0 References Reactions Suppliers

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Figure S56: Sci-Finder similarity report for compound 5

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SciFinderⁿ®

Page 1

CAS 🌼 SciFinder[®]

Task History

June 21, 2024, 3:22 PM

Initiating Search

Substances:
 Filtered By:
 Similarity: 95-98
 Number of Components: 1



Structure Match: Similarity

Search Tasks

Task	Search Type	View
Exported: Returned Substance Results + Filters (1)	Substances	View Results

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Figure S57: Sci-Finder search for compound 6

SciFinderⁿ®

Page 2

CAS DiFinder

Substances (1)

Violar	in	COL	inc	lor
VIEW		SULL		EL.

1					Similarity Score: 97
405281-91-	6		Key Physical Properties	Value	Condition
	ŧ.		Molecular Weight	652.86	
19. al	XXX	с. он	Melting Point (Experimental)	124-156 °C	3
Absolute stereochemistry shown,			Boiling Point (Predicted)	772.4±60.0 °C	Press: 760 Torr
		Density (Predicted)	1.27±0.1 g/cm ³	Temp: 20 °C; Press: 760 Torr	
	Rotation (+)		pKa (Predicted)	12.91±0.70	Most Acidic Temp: 25 °C
C ₃₆ H ₆₀ O ₁₀ 19-Norlanosta glucopyranosy methyl-, (3β,6c	n-11-one, 5,6-e (loxy)-24,25-dih 1,9β,10α,24 <i>R</i>)-	poxy-3-(β-D- ydroxy-9-	Experimental Properties Spe	ectra	
1 Reference	■ 0 Reactions	📜 0 Suppliers			

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Figure S58: Sci-Finder similarity report for compound 6

SciFinder®

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Search Tasks

Task	Search Type	View
Exported: Returned Substance Results + Filters (2)	Substances	View Results

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Figure S59: Sci-Finder search for compound 7

CAS 🗱 SciFinderⁿ

Substances (2)

Vi	ew	in	Sci	Finc	ler ⁿ

1			
1283586-92-4	Key Physical Properties	Value	Condition
	Molecular Weight	654.87	-
VICE -	Boiling Point (Predicted)	773.2±60.0 °C	Press: 760 Torr
	Density (Predicted)	1.27±0.1 g/cm ³	Temp: 20 °C; Press: 760 Torr
Absolute stereochemistry shown	pKa (Predicted)	12.92±0.70	Most Acidic Temp: 25 °C
C ₃₆ H ₆₂ O ₁₀ 5 <i>R</i> ,6 <i>R</i> -Epoxymogroside 1 E ₁ 1 A 0 0 0 Reference Reactions Suppliers			
2			
476468-77-6	Key Physical Properties	Value	Condition
¥	Molecular Weight	654.87	-
LAXX.	Boiling Point (Predicted)	773.2±60.0 °C	Press: 760 Torr
	Density (Predicted)	1.27±0.1 g/cm ³	Temp: 20 °C; Press: 760 Torr
Absolute stereochemistry shown	pKa (Predicted)	12.92±0.70	Most Acidic Temp: 25 °C
$\begin{array}{c} \textbf{C}_{36}\textbf{H}_{62}\textbf{O}_{10}\\ \beta\text{-D-Glucopyranoside, }(3\beta,6\alpha,9\beta,10\alpha,11\alpha,24\textit{R})\text{-}5,6\text{-}epoxy\text{-}11,24,25\text{-}trihydroxy\text{-}9\text{-}methyl\text{-}19\text{-}norlanostan\text{-}3\text{-}yl\\ \hline \hline \end{tabular}$			

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Figure S60: Sci-Finder similarity report for compound 7

No. Bryonioside D			3-O-β-D-allopyranosyl-25-O-β-D-gl 5β,19-epoxycucurbita-6-ene-23(R	ucopyranosyl- R),24(S)-diol	Bryonioside F	
	δн	δc	δн	δc	δн	δc
1	1.60, 2.23	20.5	1.31, 1.72	18.5	1.52, 1.92	22.1
2	1.88, 2.42	29.7	1.74, 2.32	27.2	1.80, 2.39	28.5
3	3.71 (br si	86.4	3.64 br s	85.2	3.65 (br s)	87.2
		41.0		38.6		42.0
		64.8		85.8		141.2
6	3.16 (br d, 5.3)	51.5	6.14 dd (1.3 8.3)	133.8	5.53 (br d, 6.0)	118.5
7	1.73, 2.15	23.1	5.5 dd (3.3 9.8)	130.1	1.76, 2.17	24.1
8	1.77	42.7	2.26	51.9	1.80	43.9
		48.6		44.9		49.0
10	2.42	33.7	2.24	39.7	2.46	35.9
		213.8	1.29, 1.58	23.5		213.6
	2.93 (d, 15.0), 2.48 (d, 15.0)	48.7	1.44, 1.54	30.7	2.92 (d, 14.4), 2.46 (d, 14.4)	48.7
		49.1		45.2		49.1
		49.1		48.6		49.6
15	1.11, 1.30	34.5	1.09, 1.14	32.9	1.17, 1.27	34.5
16	1.76, 1.85	28.7	1.36, 1.86	28.1	1.35, 1.96	27.9
17	1.70	50.2	1.44	51.2	1.68	49.7
18	0.66 (s)	16.7	0.74 s	14.6	0.70 (s)	16.9
19	1.37 (s)	19.4	3.56 d (7.7) 3.74 d (7.7)	79.8	1.16 (s)	20.3
20	1.50	36.0	2.04	32.3	1.40	35.8
21	0.92 (d, 6.4)	18.6	1.06 d (6.0)	18.5	0.86 (d, 6.4)	18.4
22	1.67, 1.79	34.0	1.14, 2.26	42.3	1.40, 1.96	30.4
23	1.33, 2.01	27.7	4.48	66.6	2.92, 2.98	33.3
24	3.77 (d, 9.8)	79.1	3.61	79.7		216.4
		72.2	1.72 s	81.0		76.8
26	1.56 (s)	26.0	1.73 s	23.0	1.58 (s)	27.3
27	1.54 (s)	26.2	1.45 s	24.6	1.58 (s)	27.3
28	1.19 (s)	20.8	0.86 s	20.5	1.12 (s)	28.3
29	1.25 (s)	25.4	0.83 s	25.2	1.56 (s)	25.9
30	1.03 (s)	19.8	1.06 d (6.0)	19.8	0.96 (s)	18.2
1'	4.88 (d, 7.8)	106.8	5.34 d (7.7)	104.0	4.88 (d, 7.8)	107.4
2'	3.99	75.6	3.92	72.7	3.96	75.5
3'	4.23	78.6	4.67	72.3	4.19	78.8
4'	4.22	71.7	4.14	68.9	4.22	71.8
5'	3.95	78.5	4.44	75.8	3.96	78.3
6'	4.41, 4.55	62.9	4.32 4.50	62.9	4.40, 4.55	63.0
1"			5.21 d (7.8)	98.5		
2"			3.96	75.0		
3"			4.22	78.5		
4"			4.16	71.5		
5"			3.93	78.0		
6"			4.32 4.52	62.5		

 Table S1: The NMR data of similar compounds



R= β-D-glucopyranosyl, R1=β-D-allopyranosyl



References

- [1] M. Ukiya, T. Akihisa, K. Yasukawa, H. Tokuda, M. Toriumi, K. Koike, Y. Kimura, T. Nikaido, W. Aoi and H. Nishino (2002). Anti-inflammatory and anti-tumor-promoting effects of cucurbitane glycosides from the roots of *Bryonia dioica*, J. Nat. Prod. 65, 179-183.
- [2] M.-J. Tan, J.-M. Ye, N. Turner, C. Hohnen-Behrens, C.-Q. Ke, C.-P. Tang, T. Chen, H.-C. Weiss, E.-R. Gesing and A. Rowland (2008). Antidiabetic activities of triterpenoids isolated from bitter melon associated with activation of the AMPK pathway, *Chem. Biol.* 15, 263-273.