Supporting Information:

A tirucallane and two pairs of tetranortriterpene 23-epimers from the Thai mangrove, *Xylocarpus moluccensis*

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HR-ESI-MS, HR-TOF-MS, 1D and 2D NMR spectra of (1-3)

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HR-ESI-MS of 3 β -hydroxy-3-decarbonyl-24-epi-piscidinol A (1)

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\MS\data\201407\liwanshan_NK-5_pos.d
 Method POS_100-2000_Direct Infusion.m
 Sample Name SCSIO
 Comment

Acquisition Date 7/2/2014 4:16:24 PM
 Operator BDAL@DE
 Instrument / Ser# maXis 29

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	2000.0 Vpp	Set Divert Valve	Waste

Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e ⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNo	Std m/z Diff	Std Comb Dev
499.3757	1	C 30 H 52 Na O 4	499.3758	0.1	0.4	4.5	ok	even	16.6	24.5	0.4	8.1	0.6	842.7
975.7623	1	C 60 H 104 Na O 8	975.7623	0.0	0.6	8.5	ok	even	10.7	11.5	2.0	3.7	1.3	842.7

^1H NMR (500 MHz) spectra of 3 β -hydroxy-3-decarbonyl-24-epi-piscidinol A (**1**) in CDCl_3

^{13}C NMR (125 MHz) spectrum of 3β -hydroxy-3-decarbonyl-24-epi-piscidinol A (**1**) in CDCl_3

DEPT135°(125 MHz) spectra of 3 β -hydroxy-3-decarbonyl-24-epi-piscidinol A (**1**) in CDCl₃

13c dept135 nmr of sample nk-5

^1H - ^1H COSY(400 MHz) spectra of 3 β -hydroxy-3-decarbonyl-24-epi-piscidinol A (**1**) in CDCl_3

S10

HSQC(400 MHz) spectra of 3 β -hydroxy-3-decarbonyl-24-epi-piscidinol A (**1**) in CDCl₃

S12

HMBC (400 MHz) spectra of 3 β -hydroxy-3-decarbonyl-24-epi-piscidinol A (**1**) in CDCl₃

S14

S15

NOESY (400 MHz) spectra of 3 β -hydroxy-3-decarbonyl-24-epi-piscidinol A (**1**) in CDCl₃

S17

HR-ESI-MS of Thaimoluccepimer A (2)

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\MS\data\201406\liwanshan_nk-11_pos.d
 Method POS_100-2000_Direct Infusion.m
 Sample Name SCSIO
 Comment

Acquisition Date 6/17/2014 2:58:44 PM
 Operator BDAL@DE
 Instrument / Ser# maXis 29

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	2000.0 Vpp	Set Divert Valve	Waste

Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-Rule	e ⁻ Conf	mSig	Std I	Std Mean m/z	Std VarNo	Std m/z Diff	Std Comb Dev
559.2158	1	C ₂₉ H ₃₅ O ₁₁	559.2174	2.8	3.0	12.5	ok	even	6.5	12.0	1.7	4.3	0.8	842.7
581.1982	1	C ₂₉ H ₃₄ NaO ₁₁	581.1993	1.9	2.1	12.5	ok	even	5.3	10.3	1.3	4.0	1.0	842.7

^1H NMR (400 MHz) spectra of Thaimoluccepimer A (**2**) in CDCl_3

^{13}C NMR (100 MHz) spectra of Thaimoluccepimer A (2) in CDCl_3

DEPT135° (100 MHz) spectra of Thaimoluccepimer A (2) in CDCl₃

```

NAME          NK-11
EXPNO          3
PROCNO         1
Date_         20141218
Time          23.25
INSTRUM        spect
PROBHD         5 mm CFPBBO BB
PULPROG        deptapl35
TD             65536
SOLVENT        CDCl3
NS             300
DS             4
SWH            24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG             130.26
DW             20.800 usec
DE             18.00 usec
TE             297.0 K
CNST2          145.0000000
D1             2.00000000 sec
D2             0.00344828 sec
D12            0.00002000 sec
TD0            1

===== CHANNEL f1 =====
SFO1          100.6233324 MHz
NUC1           13C
P1             10.00 usec
P13            2000.00 usec
SI             32768
SF             100.6127685 MHz
WDW            EM
SSB            0
LB             1.00 Hz
GB             0
PC             1.40
    
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^1H - ^1H COSY (400 MHz) spectrum of Thaimoluccepimer A (**2**) in CDCl_3

HSQC (400 MHz) spectra of Thaimoluccepimer A (**2**) in CDCl₃

HMBC (400 MHz) spectra of Thaimoluccepimer A (**2**) in CDCl₃

S30

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NOESY (400 MHz) spectra of Thaimoluccepimer A (**2**) in CDCl₃

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HR-TOF-MS of Thaimoluccepimer B (3)

<div><div><div><div><div></div><div></div><div></div><div></div><div></div></div></div><div><div><div>✓</div><div>✓</div><div>✓</div><div>✓</div><div>✓</div></div></div></div></div>	Compound Name (Library Hit)	Formula	Intensity	Threshold	Expected m/z	Found at m/z	Error (ppm)	Expected RT (min)	Found RT (min)	RT Delta (min)	Isotope Diff (%)	Purity (%)
<div><div><div><div><div></div><div></div><div></div><div></div><div></div></div></div><div><div><div>✓</div><div>●</div><div>●</div><div>●</div><div>▲</div></div></div></div></div>	470.19406832 (No Match)	C ₂₆ H ₃₀ O ₈	553279	50	471.2013	471.2015	0.3	0.00	0.11	0.11	21.8%	0.0%

● Spectrum from sample nk.wiff (sample 1) - Sample nk, Experiment 1, +TOF MS (100 - 1000) from 0.086 to 0.119 min
● C₂₆H₃₀O₈ +H

^1H NMR (400 MHz) spectra of Thaimolucceperimer B (**3**) in CDCl_3

^{13}C NMR (100 MHz) spectra of Thaimoluccepimer B (**3**) in CDCl_3

DEPT135° (100 MHz) spectra of Thaimoluccepimer B (**3**) in CDCl₃

^1H - ^1H COSY (400 MHz) spectra of Thaimoluccepimer B (**3**) in CDCl_3

S45

S46

HSQC (400 MHz) spectra of Thaimoluccepimer B (**3**) in CDCl₃

S48

HMBC (400 MHz) spectra of Thaimoluccepimer B (**3**) in CDCl₃

S50

S51

S52

NOESY (400 MHz) spectra of Thaimoluccepimer B (**3**) in CDCl₃

S53

S54

S55