Electronic Supplementary Information (ESI):

Thaixylomolins O–R: Four New limonoids from the Trang mangrove,  

_Xylocarpus moluccensis_  

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$^{13}$C NMR (400 MHz) spectrum of Thaixylomolin P (2) in CDCl$_3$·

DEPT135 (400 MHz) spectrum of Thaixylomolin P (2) in CDCl$_3$·

$^1$H-$^1$H COSY (400 MHz) spectrum of Thaixylomolin P (2) in CDCl$_3$·

HSQC (400 MHz) spectrum of Thaixylomolin P (2) in CDCl$_3$·

HMBC (400 MHz) spectrum of Thaixylomolin P (2) in CDCl$_3$·

NOESY (400 MHz) spectrum of Thaixylomolin P (2) in CDCl$_3$·

HR-ESIMS of Thaixylomolin Q (3)·

$^1$H NMR (400 MHz) spectrum of Thaixylomolin Q (3) in CDCl$_3$·

$^{13}$C NMR (400 MHz) spectrum of Thaixylomolin Q (3) in CDCl$_3$·

DEPT135 (400 MHz) spectrum of Thaixylomolin Q (3) in CDCl$_3$·

$^1$H-$^1$H COSY (400 MHz) spectrum of Thaixylomolin Q (3) in CDCl$_3$·

HSQC (400 MHz) spectrum of Thaixylomolin Q (3) in CDCl$_3$·

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**Figure S2.** ECD spectra of thaixylomolins O (1) and P (2) measured in MeCN at the concentration of 250 μg/mL.
**Figure S3.** Comparison of the experimental ECD spectrum of thaixylomolin R (4) in MeCN with that calculated for 1R,5R,9S,10R,13R,15R,17R–4.
HR-ESIMS for compound 1
\(^1\)H NMR (400 MHz) spectrum of compound 1 in CDCl\(_3\)
$^1$H NMR (400 MHz) spectrum of compound 1 in CDCl$_3$
$^1$H NMR (400 MHz) spectrum of compound 1 in CDCl$_3$
$^{13}$C NMR (100 MHz) spectrum of compound 1 in CDCl$_3$
DEPT135 (100 MHz) spectrum of compound 1 in CDCl$_3$
DEPT135 (100 MHz) spectrum of compound 1 in CDCl₃
DEPT135 (100 MHz) spectrum of compound 1 in CDCl₃
DEPT135 (100 MHz) spectrum of compound 1 in CDCl₃

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![DEPT135 spectrum of compound 1 in CDCl₃]
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$^1$H-$^1$H COSY (400 MHz) spectrum of compound 1 in CDCl$_3$
$^1$H-$^1$H COSY (400 MHz) spectrum of compound 1 in CDCl$_3$
HSQC (400 MHz) spectrum of compound 1 in CDCl$_3$
HSQC (400 MHz) spectrum of compound 1 in CDCl₃
HSQC (400 MHz) spectrum of compound 1 in CDCl₃
HSQC (400 MHz) spectrum of compound 1 in CDCl₃
HMBC (400 MHz) spectrum of compound 1 in CDCl₃
HMBC (400 MHz) spectrum of compound 1 in CDCl₃
HMBC (400 MHz) spectrum of compound 1 in CDCl₃
HMBC (400 MHz) spectrum of compound 1 in CDCl$_3$
HMBC (400 MHz) spectrum of compound 1 in CDCl₃
HMBC (400 MHz) spectrum of compound 1 in CDCl₃
HMBC (400 MHz) spectrum of compound 1 in CDCl₃
NOESY (400 MHz) spectrum of compound 1 in CDCl₃
NOESY (400 MHz) spectrum of compound 1 in CDCl₃
NOESY (400 MHz) spectrum of compound 1 in CDCl₃
Mass Spectrum SmartFormula Report

Analysis Info
Analysis Name: D:\Data\MS\data\201609\liwanshan_dgy-3_pos_1_01_1849.d
Method: LC_Direct infusion_pos_100-1000m/z.m
Sample Name: liwanshan_dgy-3_pos
Comment:

Acquisition Info
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Operator: SCSIO
Instrument / Ser# m/zXis: 29

Acquisition Parameter
Source Type: ESI
Focus: Active
Scan Begin: 100 m/z
Scan End: 2000 m/z

Intensity x10^5
0.0 0.2 0.4 0.6 0.8 1.0 1.2
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M/z 659.2343 681.2165 1339.4448
Score 100.00 100.00 10.95

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Bruker Compass DataAnalysis 4.0
printed: 5/19/2016 10:56:43 AM
$^1$H NMR (400 MHz) spectrum of compound 2 in CDCl$_3$
$^1$H NMR (400 MHz) spectrum of compound 2 in CDCl$_3$
$^1$H NMR (400 MHz) spectrum of compound 2 in CDCl$_3$
$^{13}$C NMR (100 MHz) spectrum of compound 2 in CDCl$_3$
DEPT135 (100 MHz) spectrum of compound 2 in CDCl₃
DEPT135 (100 MHz) spectrum of compound 2 in CDCl₃
DEPT135 (100 MHz) spectrum of compound 2 in CDCl₃
$^1$H-$^1$H COSY (400 MHz) spectrum of compound 2 in CDCl$_3$
$^1$H-$^1$H COSY (400 MHz) spectrum of compound 2 in CDCl$_3$
HSQC (400 MHz) spectrum of compound 2 in CDCl₃
HSQC (400 MHz) spectrum of compound 2 in CDCl₃
HSQC (400 MHz) spectrum of compound 2 in CDCl₃
HMBC (400 MHz) spectrum of compound 2 in CDCl₃
HMBC (400 MHz) spectrum of compound 2 in CDCl₃
HMBC (400 MHz) spectrum of compound 2 in CDCl₃
HMBC (400 MHz) spectrum of compound 2 in CDCl₃
HMBC (400 MHz) spectrum of compound 2 in CDCl$_3$
HMBC (400 MHz) spectrum of compound 2 in CDCl$_3$
NOESY (400 MHz) spectrum of compound 2 in CDCl₃
NOESY (400 MHz) spectrum of compound 2 in CDCl₃
NOESY (400 MHz) spectrum of compound 2 in CDCl₃
Mass Spectrum SmartFormula Report

Analysis Info
- Analysis Name: D:\Data\MS\data\201605\liwanshan_dgy-8_pos_3_01_1851.d
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- Sample Name: liwanshan_dgy-8_pos
- Comment:  

Acquisition Parameter
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- Ion Polarity: Positive
- Focus: Active
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$^1$H NMR (400 MHz) spectrum of compound 3 in CDCl$_3$
$^1$H NMR (400 MHz) spectrum of compound 3 in CDCl$_3$
$^1$H NMR (400 MHz) spectrum of compound 3 in CDCl$_3$
$^{13}$C NMR (100 MHz) spectrum of compound 3 in CDCl$_3$
DEPT135 (100 MHz) spectrum of compound 3 in CDCl₃
DEPT135 (100 MHz) spectrum of compound 3 in CDCl₃
DEPT135 (100 MHz) spectrum of compound 3 in CDCl₃
DEPT135 (100 MHz) spectrum of compound 3 in CDCl₃

ppm

-84.78  -80.52  -77.35  76.71  66.93  52.96  51.09  47.28  40.55  41.31  37.86  29.33  28.23  23.06  22.67  20.14  16.14  11.72
$^1$H-$^1$H COSY (400 MHz) spectrum of compound 3 in CDCl$_3$
**'H-'H COSY (400 MHz) spectrum of compound 3 in CDCl₃**

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- **PROCNO**: 1
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- **TD**: 2048
- **SOLVENT**: CDCl₃
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- **FIDRES**: 1.907349 Hz
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$^1$H-$^1$H COSY (400 MHz) spectrum of compound 3 in CDCl$_3$
HSQC (400 MHz) spectrum of compound 3 in CDCl₃
HSQC (400 MHz) spectrum of compound 3 in CDCl₃
HSQC (400 MHz) spectrum of compound 3 in CDCl₃
HSQC (400 MHz) spectrum of compound 3 in CDCl₃
HSQC (400 MHz) spectrum of compound 3 in CDCl₃

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**TD**  1024
**SOLVENT**  CDCl₃
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**DS**  16
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**RG**  208.5
**DE**  10.000 sec
**TE**  297.0 K
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**ND0**  2
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**P1**  12.00 usec
**P2**  24.00 usec
**P28**  0.00 usec
**ND0**  2
**TD**  256
**SF01**  100.6233 MHz
**SF**  400.1300079 MHz
**WDW**  QSINE
**SSB**  2
**LB**  0.00 Hz
**GB**  0
**PC**  1.40
**SI**  1024
**MC2**  echo-antiecho
**SF**  100.6127585 MHz
**WDW**  QSINE
**SSB**  2
**LB**  0.00 Hz
**GB**  0
HMBC (400 MHz) spectrum of compound 3 in CDCl₃
HMBC (400 MHz) spectrum of compound 3 in CDCl₃
HMBC (400 MHz) spectrum of compound 3 in CDCl₃
HMBC (400 MHz) spectrum of compound 3 in CDCl₃

NAME              dyg-8
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SOLVENT           CDCl₃
NS                  32
DS                  16
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RG                  208.5
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DE                  10.00 usec
TE                  297.0 K
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CNST13       10.0000000
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D2                0.00344828 sec
D6                0.00020000 sec
D16               0.00002080 sec

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P2                24.00 usec
TD                 128
SF01       100.6233 MHz
FIDRES       187.800476 Hz
SM              238.896 ppm
FnMODE        QF
SI                2048
SF     400.1300078 MHz
WGM           SINE
SBB               0
LB                 0.00 Hz
GB                1.40
SI                1024
MCFT         QF
SF     100.6127685 MHz
WGM           SINE
SBB               0
LB                 0.00 Hz
GB                0
HMBC (400 MHz) spectrum of compound 3 in CDCl₃
HMBC (400 MHz) spectrum of compound 3 in CDCl₃
NOESY (400 MHz) spectrum of compound 3 in CDCl₃
NOESY (400 MHz) spectrum of compound 3 in CDCl₃
NOESY (400 MHz) spectrum of compound 3 in CDCl₃
NOESY (400 MHz) spectrum of compound 3 in CDCl₃
Mass Spectrum SmartFormula Report

Analysis Info
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Sample Name: iwanshan_dgy-21_pos
Comment:

Acquisition Date: 5/19/2016 8:44:40 AM
Operator: SCSIO
Instrument / Ser#: maxXis

Source Type: ESI
Focus: Active
Scan Begin: 100 m/z
Scan End: 2000 m/z

Ion Polarity: Positive
Set Capillary: 4500 V
Set End Plate Offset: -500 V
Set Collision Cell RF: 800.0 Vpp
Set Divert Valve: Waste
Set Nebulizer: 0.4 Bar
Set Dry Heater: 180 °C
Set Dry Gas: 4.0 l/min

+MS, 0.4min #25

Meas. m/z # Formula Score m/z err [ppm] err [mDa] mSigma rdb e Conff N-Rule
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451.2091 1 C 25 H 32 Na O 6 100.00 451.2091 1.0 0.4 28.6 9.5 even ok
879.4295 1 C 50 H 64 Na O 12 100.00 879.4290 -0.6 -0.5 17.5 16.5 even ok

Bruker Compass DataAnalysis 4.0 printed: 5/19/2016 11:26:25 AM Page 1 of 1
$^1$H NMR (400 MHz) spectrum of compound 4 in CDCl$_3$
$^1$H NMR (400 MHz) spectrum of compound 4 in CDCl$_3$
$^1$H NMR (400 MHz) spectrum of compound 4 in CDCl$_3$
$^{13}$C NMR (100 MHz) spectrum of compound 4 in CDCl$_3$
DEPT135 (100 MHz) spectrum of compound 4 in CDCl₃
DEPT135 (100 MHz) spectrum of compound 4 in CDCl₃
$^1$H-$^1$H COSY (400 MHz) spectrum of compound 4 in CDCl$_3$
$^1$H-$^1$H COSY (400 MHz) spectrum of compound 4 in CDCl$_3$
HSQC (400 MHz) spectrum of compound 4 in CDCl₃
HSQC (400 MHz) spectrum of compound 4 in CDCl₃
HSQC (400 MHz) spectrum of compound 4 in CDCl₃
HMBC (400 MHz) spectrum of compound 4 in CDCl₃
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HMBC (400 MHz) spectrum of compound 4 in CDCl₃
HMBC (400 MHz) spectrum of compound 4 in CDCl$_3$
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HMBC (400 MHz) spectrum of compound 4 in CDCl₃
NOESY (400 MHz) spectrum of compound 4 in CDCl₃
NOESY (400 MHz) spectrum of compound 4 in CDCl₃
NOESY (400 MHz) spectrum of compound 4 in CDCl₃
NOESY (400 MHz) spectrum of compound 4 in CDCl₃

NAME             dyg-21
EXPNO              7
PROCNO              1
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Time              8.06
INSTRUM            spect
PULPROG          noesygpphpp
TD                2048
SOLVENT           CDCl₃
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DS              32
SNH           4000.000 Hz
FIDRES        1.953125 Hz
AQ            0.2560500 sec
RG              208.5
DM              125.000 usec
DE              10.000 usec
TE              297.0 K
D0        0.00010972 sec
D1     1.99385595 sec
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D12    0.00002000 sec
D16   0.00020000 sec
INO   0.00025000 sec

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NUC1              1H
P1            12.000 usec
P2             24.000 usec
P17         2500.0000 usec
ND0             1
TD             256
FIDRES       15.625000 Hz
SNH           9.997 Ppm
FmMODE        States-TPPI
SI              1024
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WDM        QSINE
SSB             2
LB              0.00 Hz
GB             0
PC            1.00
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MCC2 States-TPPI
SF   400.1300098 MHz
WDM        QSINE
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