

Supporting Information

Rec. Nat. Prod. 14:3 (2020) 195-200

Diterpenoids and Sesquiterpenoids from *Syzygium fluviatile*

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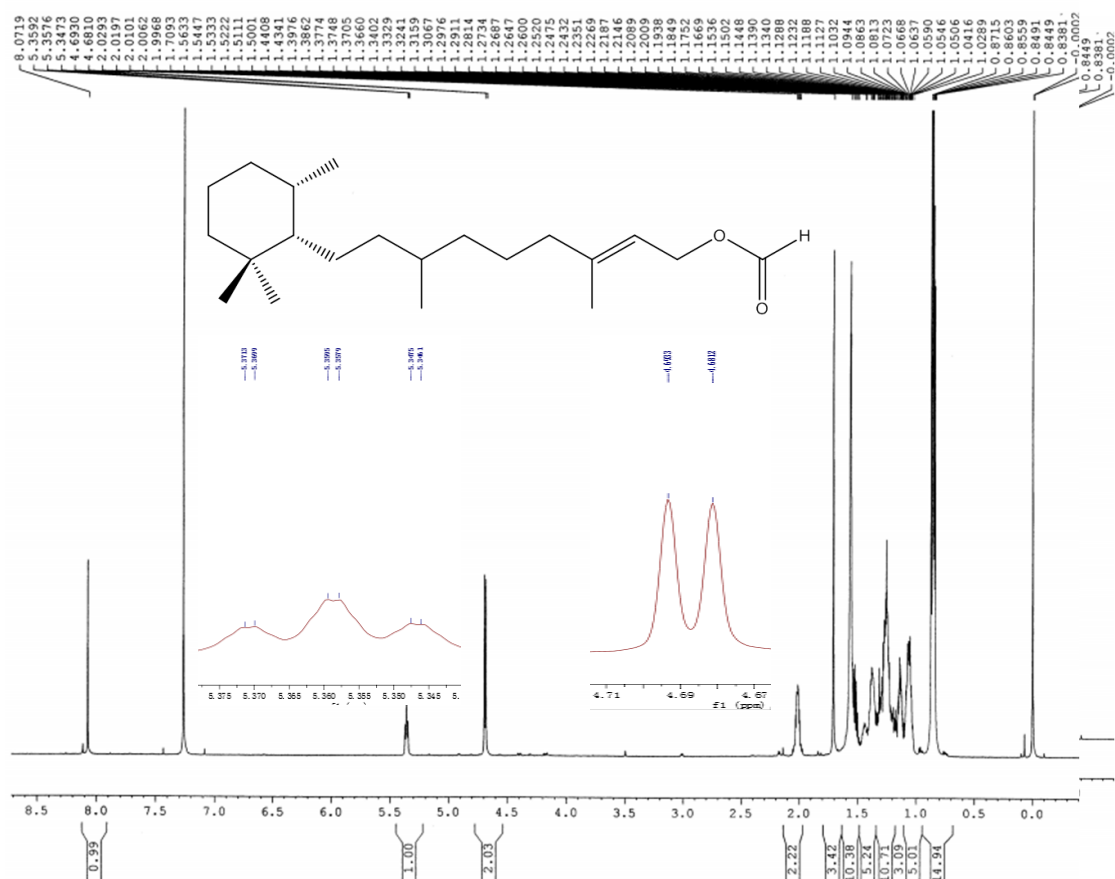


Figure S1: ¹H NMR spectrum of compound **1** recorded in CDCl₃ at 600 MHz

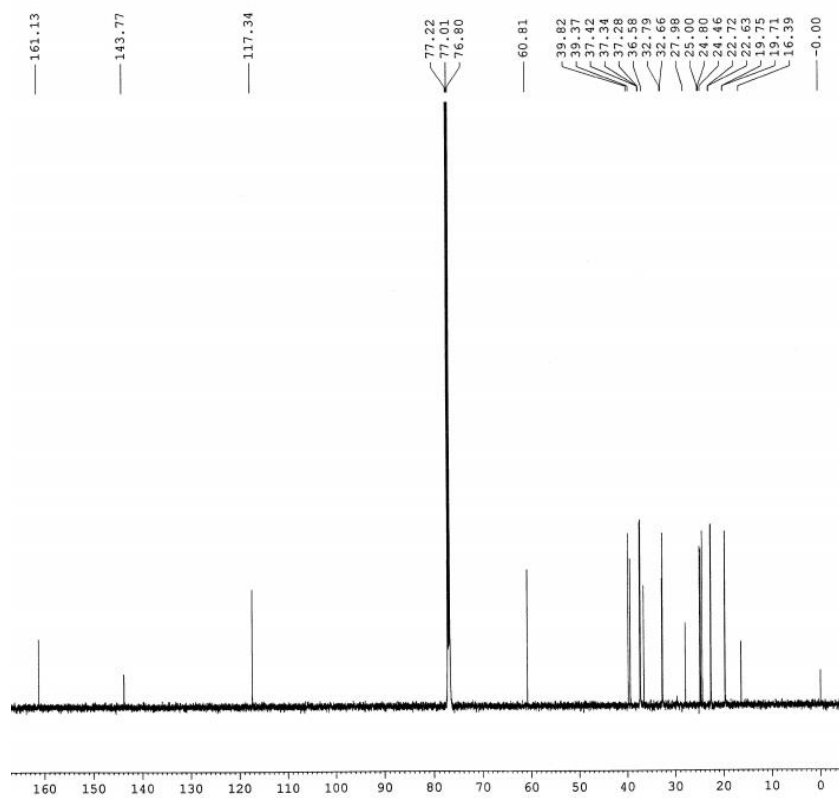


Figure S2: ¹³C NMR spectrum of compound **1** recorded in CDCl₃ at 150 MHz

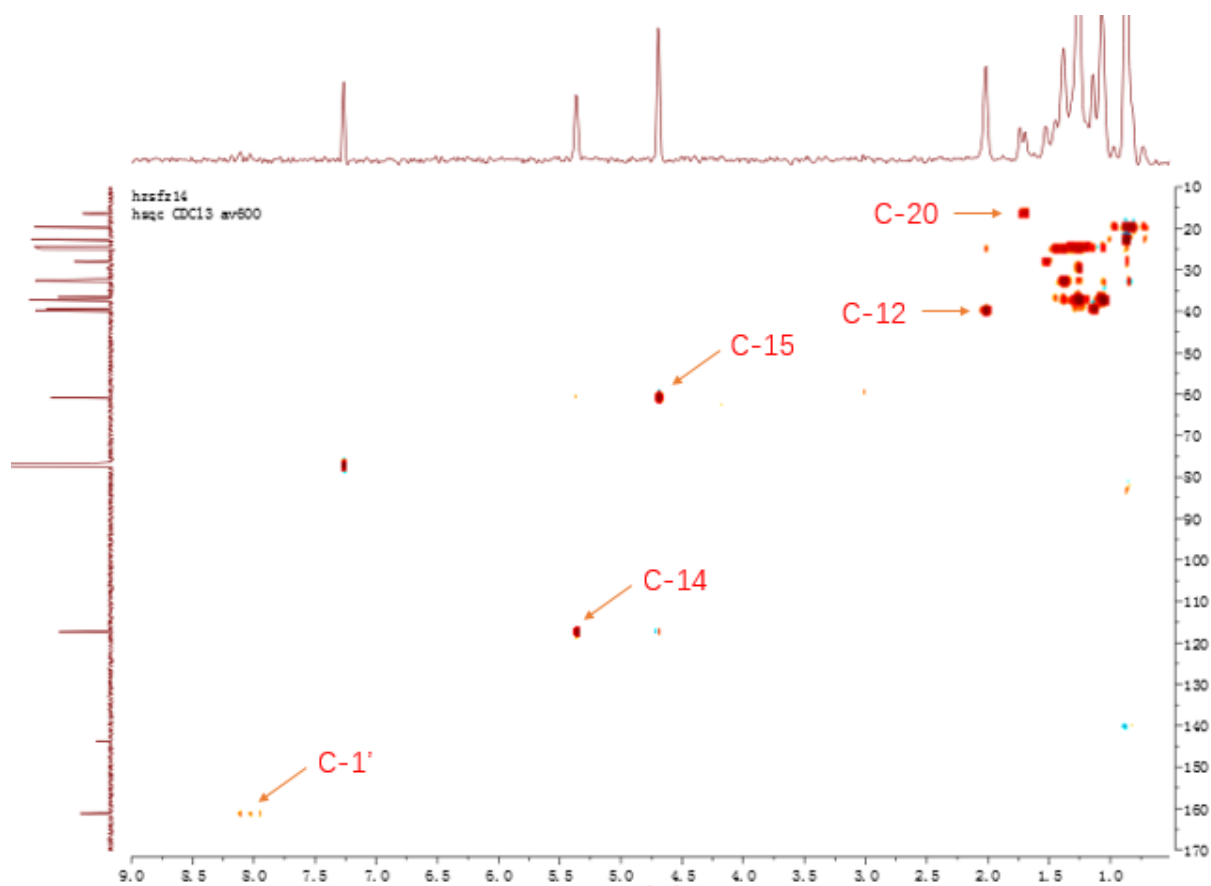


Figure S3: HSQC spectrum of compound **1** recorded in CDCl₃

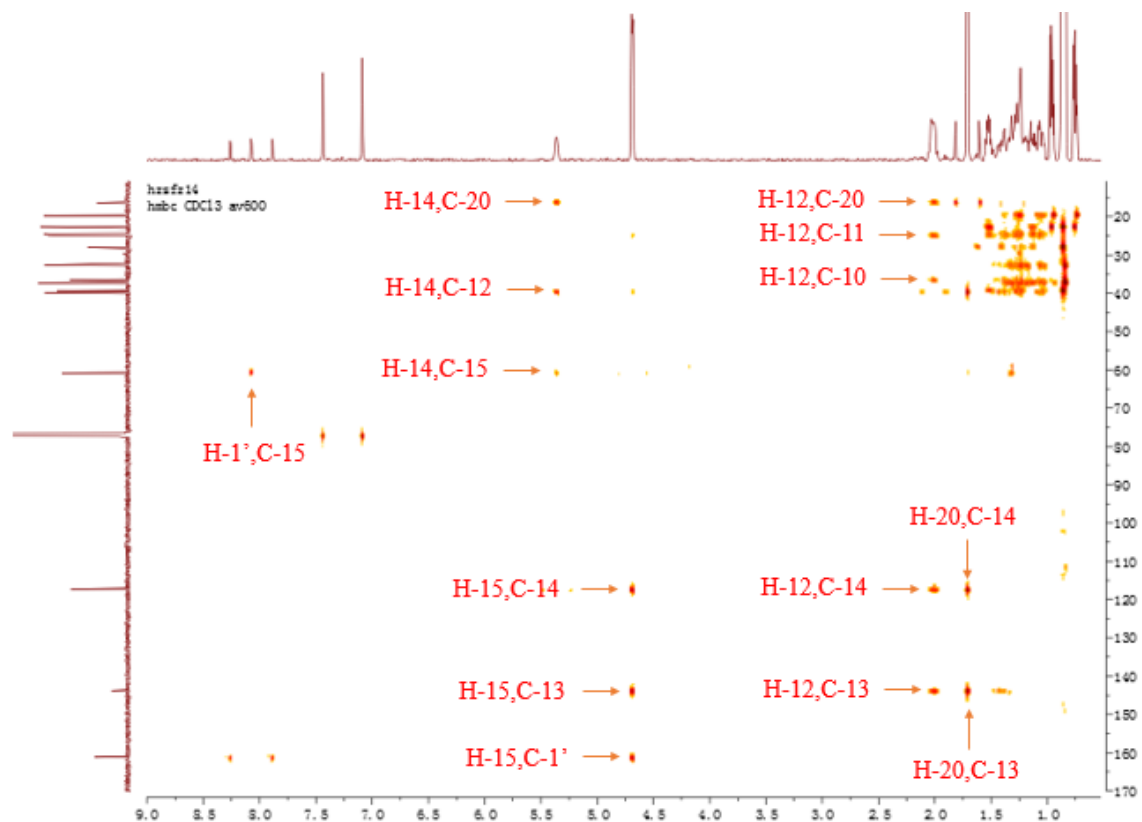


Figure S4. HMBC spectrum of compound **1** recorded in CDCl₃

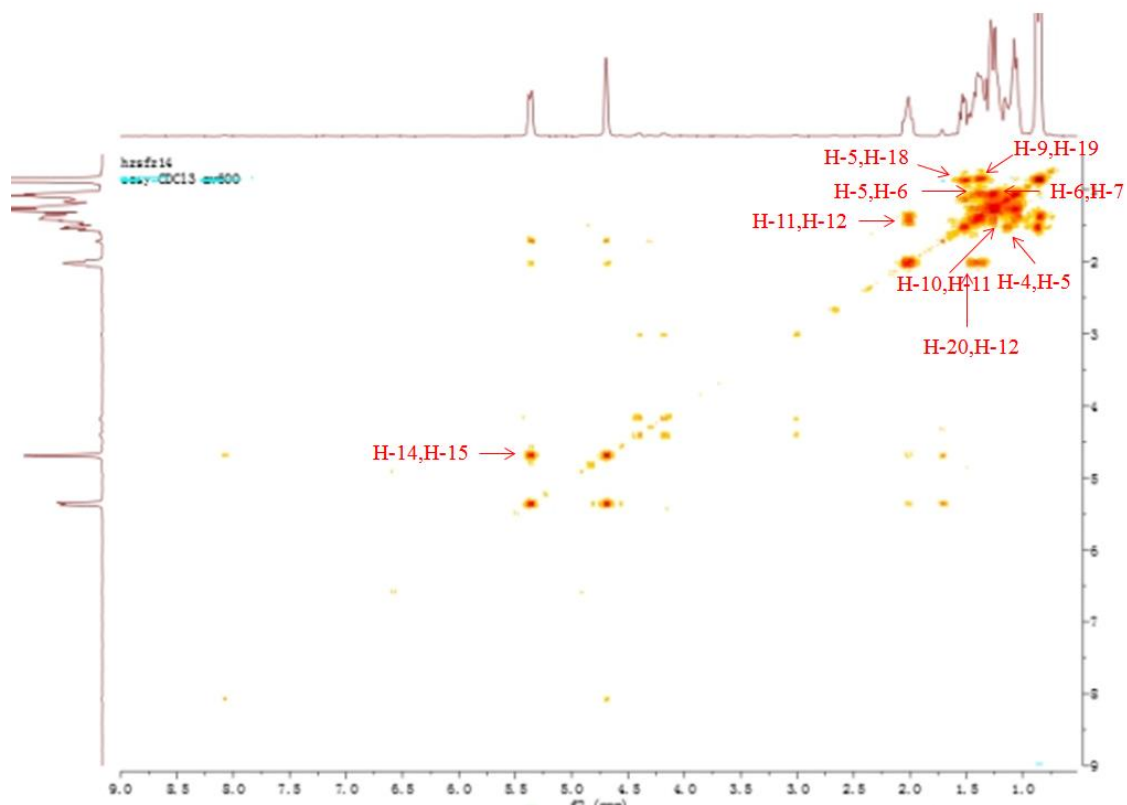


Figure S5. ^1H - ^1H COSY spectrum of compound **1** recorded in CDCl_3

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

17 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

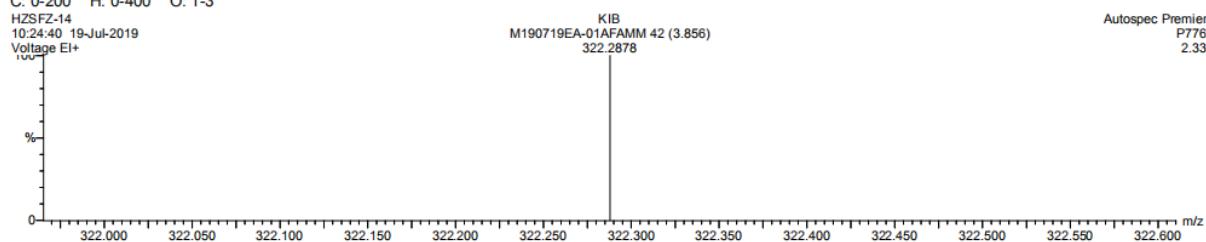
Elements Used:

C: 0-200 H: 0-400 O: 1-3

HZSFZ-14

10:24:40 19-Jul-2019

Voltage EI+



Minimum: -10.0
Maximum: 120.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
322.2878	322.2872	0.6	1.9	3.0	5546025.5	C ₂₁ H ₃₈ O ₂

Figure S6: HR-EI-MS spectrum of compound **1**

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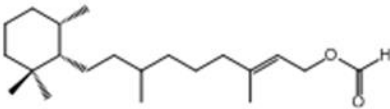
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Chemical Structure exact:

SUBSTANCES
No candidates available



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Figure S7. Scifinder new compound report

Table S1. ¹³C NMR data for compounds 2–9

NO.	2^a δ_c	3^a δ_c	4^a δ_c	5^b δ_c	6^b δ_c	7^c δ_c	8^b δ_c	9^b δ_c
1	36.7	62.0	89.2	56.1	57.1	30.1	45.8	50.1
2	39.4	117.9	30.3	24.2	26.1	27.6	124.8	22.7
3	24.8	143.5	38.5	41.3	34.6	24.9	134.5	31.0
4	37.4	40.1	83.1	80.5	36.4	39.0	31.3	135.0
5	28.0	25.3	76.5	47.3	39.7	153.6	21.8	122.2
6	32.8	36.9	27.7	29.7	28.4	53.6	26.6	39.9
7	24.5	33.0	35.6	26.9	26.8	26.2	44.3	46.8
8	37.3	37.6	135.3	19.2	20.2	41.9	37.0	22.0
9	32.7	25.0	125.4	42.8	44.6	81.1	18.7	42.2
10	37.4	37.6	24.8	71.9	75.3	54.5	72.5	72.4
11	25.1	32.9	34.9	20.9	19.3	20.4	35.5	26.0
12	39.9	37.5	133.2	28.7	15.8	28.8	23.7	21.5
13	140.4	24.7	121.0	16.5	28.6	16.5	15.5	15.1
14	123.1	39.6	32.0	25.0	20.2	106.4	21.8	20.8
15	59.5	28.2	33.4	30.6	16.0		28.1	23.8
16	22.7	22.9	18.1					
17	22.6	22.9	16.0					
18	19.8	19.9	22.0					
19	19.7	20.0	18.0					
20	16.2	16.6	17.7					
1'		172.3	171.2					
2'		32.2	21.3					
3'		19.6						
4'		140.1						
5'		139.9						
6'		171.5						
7'		8.9						
8'		171.3						

^a ¹³C NMR Data in CDCl₃ at 150 MHz, ^b ¹³C NMR Data in CDCl₃ at 125 MHz, ^c ¹³C NMR Data in CDCl₃ at 100 MHz.

Table S2. ¹H NMR data for compounds 2–9

NO.	2^a	3^a	4^a	5^b	6^b	7^c	8^b	9^b
	δ_{H}	δ_{H}	δ_{H}	δ_{H}	δ_{H}	δ_{H}	δ_{H}	δ_{H}
1		4.60 d (7.1)		1.25 m	1.21 s	2.09 s	2.04 m	1.27 s
2	1.14 m	5.31 t (7.2)	1.87 m	1.62 m	1.42 m	1.31 m	5.25 s	1.32 m
3	1.38 m		1.88 m	1.63 m	1.43 m	1.36 m		1.75 m
4	1.26 m	1.98 m			1.52 m		2.18 m	
5	1.54 m	1.41 m	4.87d (10.3)	1.21 s	1.21 m	1.25 s	1.31 m	5.37 s
6	1.06 m	1.28 m	1.68 m	1.22 m	1.25 m	1.15 m	1.75 m	1.92 m
7	1.21 m	1.42 m	2.01 m	1.23 m	1.27m	1.15 m	1.18 m	1.30 m
8	1.38 m	1.29 m		1.42 m	1.42 m	1.31 m	1.42 m	1.31 m
9	1.39 m	1.30 m	5.16 m	1.45 m	1.72 m	2.04 m	1.31 m	1.48 m
10	1.26 m	1.29 m	2.01 m					
11	1.38 m	1.42 m	2.01 m				1.41 m	1.45 m
12	2.01 m	1.28 m		1.03 s	1.03 s	1.04 s	1.69 s	0.81 d (6.9)
13		1.30 m	5.16 m	1.06 s	1.05 s	1.05 s	0.81 d (6.9)	0.96 d (6.9)
14	5.38 t (7.6)	1.15 m	2.18 m	1.32 s	0.94 d (7.1)	1.28 s	0.96 d (6.9)	1.21 s
15	4.70 t (7.1)	1.52 m		1.36 s	1.13 s	4.68 d (10.4)	1.13 s	1.78 s
16	0.88 s	0.87 d (6.7)	1.12 s					
17	0.85 s	0.86 d (6.7)	1.66 s					
18	0.86 d (6.5)	0.84 d (6.7)	1.66 s					
19	0.87 d (6.5)	0.85 d (6.7)	0.90 d (6.8)					
20	1.69 s	1.68 s	0.89 d (6.8)					
2'		2.63 t (6.9)	2.06 s					
3'		2.70 t (6.9)						
7'		2.00 s						

^a ¹H NMR Data in CDCl₃ at 600 MHz, ^b ¹H NMR Data in CDCl₃ at 500 MHz, ^c ¹H NMR Data in CDCl₃ at 400 MHz.