SUPPLEMENTARY MATERIAL

Identification of a New Antifungal Oligoacetal Derivative Produced by *Streptomyces toxytricini* Against *Candida albicans*

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Abstract

Thirty actinomycete isolates were isolated from soil and tested against *Candida albicans* in-vitro. The active isolate was identified by 16s-rRNA gene sequencing method as *Streptomyces toxytricini*. The antifungal compound was extracted with ethyl acetate followed by di-ethyl ether. Both HPLC and GC-MS analysis confirmed presence of one pure compound in the diethyl ether extract. The compound is a yellow liquid has a maximum absorbance at 240nm. in methanol. The chemical structure was elucidated by 1D and 2D-NMR and IR analysis. The elucidated molecular formula was C₃₆H₅₄O₁₄. The compound is a polyacetal tricyclononane derivative, composed of a tricyclononane ring attached from the carbon atom number four with an oligo-acetal chain (six acetal groups in chain) and from the carbon atom number seven with a methoxy carbonyl benzene-1,3-dicarboxylic acid. The purposed name is: 4- {[tricycle(3.2.1.1^{1,3})non-8-yl] methoxy carbonyl benzene-1,3-dicarboxylic acid} (2,4,5,6,7, 8, 9 heptaoxa, 3-ethoxy, 5,6,7,9-tetramethyl undecane).

Keywords: Antifungal, *Streptomyces toxytricini*, *Candida albicans*, tricyclononane.

Table S1. The chemical shift values for H^1 , C^{13} , COSY and HMBC NMR data analysis:

C No.	σC	σH	Assignment	COSY	HMBC $\sigma H \rightarrow \sigma C$
1	18.5	1.28 (t,7)	CH_3	3.59, 3.89	64.6
2	64.6	3.59 (m) 3.89 (m)	CH_2	1.28	18.5, 105.05
3	105.05	4.95 (q, 5.5)	CH	1.28	64.6
4	105.05	5.07 (d)	CH	1.31	18.38, 105.05, 105.18
5	105.18	5.38 (q, 5.4)	CH	1.33	105.05
6	103	5.23(q, 5.4)	CH	1.33	--
7	105.05	5.14 (q, 5.5)	CH	1.28	--
8	30	1.24 (m)	CH_2	5.33	104.4, 105.05
9	104.4	5.33	CH	1.24	--
10	64.6	3.59 (m) 3.89 (m)	CH_2	1.18	15.57, 104.4
11, 13	15.57	1.18 (t, 7)	CH_3	3.59, 3.89, 3.48	64.6, 66.8
12	66.8	3.48 (q,7)	CH_2	1.15	15.4, 104.4
14, 17	18.5	1.28 (d, 5.9)	CH_3	4.95, 5.14	105.05, 15.4
15, 16	18.5	1.33 (d, 5.7)	CH_3	5.23, 5.38	103, 105.18
1'	30.6	-	C quaternary	-	-
2'	30	1.33	CH_2	0.83	23.9
3'	14.38	0.83(m)	CH	1.31, 1.33	23.9, 30
4'	18.38	1.31 (m)	CH	0.83, 0.91, 5.07	14.38, 23.9, 30, 31.5, 105.05
5'	11.38	0.91 (m)	CH	1.37, 1.42	24.8, 40
6'	24.8	1.42 (m)	CH_2	0.91	11.38, 18.38, 31.5, 40.
7'	31.5	1.37 (m)	CH_2	0.91, 1.68	18.38
8'	40	1.68 (p, 6.1)	CH	1.37, 4.21	11.38, 24.8, 30.6, 31.5
9'	23.9	1.33(d, 5.7)	CH_2	0.83	14.38, 30
10'	69	4.21(m)	CH_2	1.68	30.6, 31.5, 40,169
1'', 2'', 6''	133.4	-	C quaternary	-	--
3'', 5''	132.3	7.6 (m)	=CH (aromatic)	129.7	129.7, 169
4''	129.7	7.7 (m)	=CH (aromatic)	132.3	132.3, 133.4
7'', 8'', 9''	169.1	-	C=O	-	
OH		11.5			
OH		11.44

Fig. S1. The HPLC chromatograms of the diethyl ether extract. The analysis was performed on ODS column with methanol as a mobile phase and detection at 240nm.

Fig. S2: The GC/MS chromatogram for the pure antifungal compound produced by *S. toxytrici*.

Fig.S3: The mass spectrum of the antifungal compound produced by *S. toxytrici*.

Spectral Parameters

Acquisition Parameters

Acquire Date: 2014-03-11T19:20:00
 Spect Frequency: 699.81 MHz
 Nucleus: ^1H
 Pulse Program: s2pul
 Number of Points: 50223
 Acquisition Time: 4.5 s
 Number of Scans: 16
 Relaxation Delay: 1s
 Sweep Width: 11160.7 Hz
 Temperature: 25 °C
 Solvent: cd3od_insert

Processing Parameters

Line Broadening: 1 Hz

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 11:21:17 -0400

Fig. S4: ^1H -NMR spectrum of the antifungal compound produced by *S. toxytrici*

Spectral Parameters

Acquisition Parameters

Acquire Date: 2014-03-11T14:29:31
 Spect Frequency: 125.65 MHz
 Nucleus: ^{13}C
 Pulse Program: s2pul
 Number of Points: 60976
 Acquisition Time: 2 s
 Number of Scans: 256
 Relaxation Delay: 0.2s
 Sweep Width: 30487.8 Hz
 Temperature: 25 °C
 Solvent: cd3od

Processing Parameters

Line Broadening: 0.49999580002 Hz

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Fig. S5: C^{13} spectrum of the antifungal compound produced by *S. toxytrici*

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Spectral Parameters

Acquisition Parameters

Acquire Date: 2014-03-12T19:30:44
Spect Frequency: 125.65 MHz
Nucleus: ^{13}C
Pulse Program: CRAPT
Number of Points: 60976
Acquisition Time: 2 s
Number of Scans: 256
Relaxation Delay: 1s
Sweep Width: 30487.8 Hz
Temperature: 25 °C
Solvent: cd3od

Processing Parameters

Line Broadening: 2 Hz

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Fig. S6: APT spectrum of the antifungal compound produced by *S. toxytrici*

Fig. S7: HSQC spectrum of the antifungal compound produced by *S. toxytrici*

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Fig. S8: COSY spectrum of the antifungal compound produced by *S. toxytrici*

Fig. S9: HMBC spectrum of the antifungal compound produced by *S. toxytrici*

Fig. S10. The HMBC data interpretation of the antifungal compound produced by *S. toxytricini*.