SUPPLEMENTARY MATERIAL

A new pyrone derivative from an endophytic *Aspergillus tubingensis* of *Lycium ruthenicum*

Yang-min Ma*, Ting Li Cong-cong Ma

Key Laboratory of Auxiliary Chemistry & Technology for Chemical Industry, Ministry of Education, Shaanxi University of Science & Technology, Xi'an, 710021, P. R. China

Abstract: A new pyrone named 6-isovaleryl-4-methoxy-pyran-2-one (**1**), along with three known pyrone compounds, rubrofusarin B (**2**), asperpyrones A (**3**), and campyrone A (**4**) were isolated from fermentation of *Aspergillus tubingensis* in *Lycium ruthenicum*. Their structures were confirmed by spectroscopic techniques, such as IR, NMR and HRESI-MS. Compound **2** indicated strong inhibitory activity against *Escherichia coli*, with MIC value of 1.95 µg/mL.

Key words: pyrone; 6-isovaleryl-4-methoxy-pyran-2-one; *Aspergillus tubingensis*; endophytic fungi; *Lycium ruthenicum*

* Corresponding author. E-mail: mym63@sina.com(Ma. Y. M) Tel.:029-86168312.

Supplementary material 1: The NMR of compound 1
 All the NMR data were given by Bruker Avance III-400

The structure and main correlations in the HMBC of compound 1

Table S1 NMR data of compound 1

Position	$\delta_{\text{H}}(\text{DMSO}-d_6)$	$\delta_{\text{C}}(\text{DMSO}-d_6)$	$^1\text{H}-^1\text{H}\text{COSY}$
2	-	161.2	-
3	5.97(d, $J = 2.2$)	93.5	-
4	-	169.5	-
4-OCH ₃	3.87(s)	56.9	-
5	6.94(d, $J = 2.2$ Hz)	104.8	-
6	-	153.9	-
7	-	192.6	-
8	2.76(d, $J = 6.7$ Hz)	45.6	H-9
9	2.14-2.04(m)	23.8	H-10, H-11
10,11	0.91(6H, d, $J = 6.64$ Hz)	22.2

^1H -NMR of compound 1

^{13}C NMR of compound **1**

The ^1H - ^1H COSY of compound **1**

The DEPT-135 of compound **1**

The HMBC of compound **1**

The HMBC fragment of compound **1**

The HMBC fragment of compound **1**

The HSQC of compound **1**

Supplementary material 2: The IR and HR-ESI-MS of compound **1**

E:\MYM1\20140310-5.0

20140310-5

S

2014-3-10

The (+)-HR-ESI-MS of compound **1**

Supplementary material 3: The NMR of compounds 2-4

2

¹H-NMR of compound 2

¹³C NMR of compound 2

4

¹H-NMR of compound 4

¹³C-NMR of compound 4

Supplementary material 4: Strain identification of R43

The microscopic features of endophytic fungi R43

The nucleotide sequence of R43 (without primer sequences)

```
CAACCTCCCATCCGTGTCTATTATACCCTGTTGCTTCGGCGGGCCCCGCCGC
TTGTCGGCCGCGGGGGGGCGCCTTTGCCCCCGGGCCCGTGCCCGCCGG
AGACCCCAACACGAACACTGTCTGAAAGCGTGCAGTCTGAGTTGATTGAA
TGCAATCAGTTAAACTTTCAACAATGGATCTCTTGGTTCCGGCATCGATG
AAGAACGCAGCGAAATGCGATAACTAATGTGAATTGCAGAATTCAGTGA
ATCATCGAGTCTTTGAACGCACATTGCGCCCCCTGGTATTCCGGGGGGGCAT
GCCTGTCCGAGCGTCATTGCTGCCCTCAAGCCCGGCTTGTGTGTTGGGTCG
CCGTCCCCCTCTCCGGGGGGGACGGGCCCCGAAAGGCAGCGGCGGCACCGC
GTCCGATCCTCGAGCGTATGGGGCTTTGTACATGCTCTGTAGGATTGGCC
GGCGCCTGCCGACGTTTTCCAACCATTTTTTCCAGGTTGACCTCGGATCAG
GTAGGGATACCCGCTGAACTTAAGCATATCAATAAGGCGAAGGAA
```

System phylogenetic tree of strain R43 based 18S rDNA-ITS sequence