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

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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
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 | δ_H(DMSO-d_6) | δ_C(DMSO-d_6) | H-H 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          |           |
The $^1$H-$^1$HCOSY of compound 1
The DEPT-135 of compound 1

The HMBC 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
The (+)-HR-ESI-MS of compound 1
Supplementary material 3: The NMR of compounds 2-4

![NMR spectra of compound 2](image)

$^1$H-NMR of compound 2

$^{13}$C NMR of compound 2
$^1$H-NMR of compound 3

$^{13}$C-NMR of compound 3
\[ \text{H-NMR of compound 4} \]

\[ \text{C-NMR of compound 4} \]
Supplementary material 4: Strain identification of R43

The microscopic features of endophytic fungi R43

The nucleotide sequence of R43 (without primer sequences)

CAACCTCCCATCCGTGCTATATTATACCCCTGTTGCTTCCGGCGGGCCCGCCGC
TTGTCGGCGGCCGGGGGGGGGCCTTTGCCCCCGCGGCCGGGCCTGCGCCGG
AGACCCCAACACGACACTGTCTGAAAGCGTGCAGTCTGAGTTGATTGAA
TGCAATCAGTTAAACTTTCAACATGGATCTCTTGGTTCCGGCATCGATG
AAGAACGCAGCGAAATGCGATAACTATGTGAATTGCAGAATTCAGTGA
ATCATTGAGTCTTTTGAACGCACATTCGCGCCCCCTGTATTCCCGGGGCG
GCCTGTCCGAGCGTATTTGCTGCTCCTCAAGCCCGCTTCATTCGCGGCTG
CCGGCCCTCTCGGGGACGGGCGGCCCCGAAAGGCACGCACGCCACC
GTCCAGATCGCAGCGATGGGGCTTTGTCACATGCTCTGTAGGATTGCC
GGCGCCTCCGACGTTCTTTTCAACATTCTTTTCCAGTTGACCTCGGATCAG
GTAGGGATACCCCGCTGAACCTAAGCAATATCAATAAGCCGAAAG

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