SUPPLEMENTARY MATERIAL

Anti-neuroinflammatory constituents from the Fungus

*Penicillium purpurogenum* MHZ 111

Jing Sun\textsuperscript{ab}, Zhi-Xiang Zhu\textsuperscript{a}, Yue-Lin Song\textsuperscript{a}, Yi Ren\textsuperscript{ab}, Dan Dong\textsuperscript{c}, Jiao Zheng\textsuperscript{a}, Ting Liu\textsuperscript{c}, Yun-Fang Zhao\textsuperscript{a}, Peng-Fei Tu\textsuperscript{a} and Jun Li\textsuperscript{a}

\textsuperscript{a}Modern Research Center for Traditional Chinese Medicine, Beijing University of Chinese Medicine, Beijing 100029, People’s Republic of China; \textsuperscript{b}School of Chinese Materia Medica, Beijing University of Chinese Medicine, Beijing 100102, People’s Republic of China; \textsuperscript{c}Institute of Plant and Environment Protection, Beijing Academy of Agriculture and Forestry Sciences, Beijing 100097, People’s Republic of China

CONTACT

Jun Li, drlj666@163.com; Peng-Fei Tu, pengfeitu@163.com.
ABSTRACT

A new dihydroisocoumarin (1) and a new coumarin (2), along with eight known metabolites (3–10), were isolated from the solid substrate fermentation cultures of the fungus *Penicillium purpurogenum* MHZ 111. Their structures were elucidated by extensive spectroscopic analysis and comparison of their spectroscopic and physicochemical data with the literature values. Compounds 2 and 8 showed inhibition of nitric oxide production in lipopolysaccharide-activated BV-2 microglial cells with IC$_{50}$ values of 26.5 and 52.7 μM, respectively.

KEYWORDS

*Penicillium purpurogenum*; dihydroisocoumarin; coumarin; anti-neuroinflammatory activity
The list of contents

| NO. | Content                                      |
|-----|----------------------------------------------|
| S1  | The 18S rDNA sequences data of *Penicillium purpurogenum* MHZ 111. |
| S12 | The ITS rDNA sequences data of *Penicillium purpurogenum* MHZ 111. |
| Figure S1 | $^1$H NMR spectrum of compound 1 |
| Figure S2 | $^{13}$C NMR spectrum of compound 1 |
| Figure S3 | gHSQC spectrum of compound 1 |
| Figure S4 | gHMBC spectrum of compound 1 |
| Figure S5 | $^1$H-$^1$H COSY spectrum of compound 1 |
| Figure S6 | Selected HMBC correlations of 1 and 2 |
| Figure S7 | ECD spectrum of compound 1 |
| Figure S8 | $^1$H NMR spectrum of compound 2 |
| Figure S9 | $^{13}$C NMR spectrum of compound 2 |
| Figure S10 | gHSQC spectrum of compound 2 |
| Figure S11 | gHMBC spectrum of compound 2 |
Figure S1 $^1$H NMR spectrum of compound 1 (500 MHz, methanol-$d_4$)

Figure S2 $^{13}$C NMR spectrum of compound 1 (125 MHz, methanol-$d_4$)
Figure S3 gHSQC spectrum of compound 1 (500 MHz, methanol-d$_4$)

Figure S4 gHMBC spectrum of compound 1 (500 MHz, methanol-d$_4$)
Figure S5 $^1$H-$^1$H COSY spectrum of compound 1 (500 MHz, methanol-$d_4$)

Figure S6 Selected HMBC correlations of 1 and 2.

Figure S7 ECD spectrum of compound 1
Figure S8 $^1$H NMR spectrum of compound 2 (500 MHz, CDCl$_3$)

Figure S9 $^{13}$C NMR spectrum of compound 2 (125 MHz, CDCl$_3$)
**Figure S10** gHSQC spectrum of compound 2 (500 MHz, CDCl$_3$)

**Figure S11** gHMBC spectrum of compound 2 (500 MHz, CDCl$_3$)
The 18S rDNA sequences data of *Penicillium purpureogenum* MHZ 111.

```
S12

CCAGTAGTCATATGCTTGTCTCAAAAGATTAAGCCCATGCACTGTCTAAGTATAA
GCACTCTTTTACTGTGAAACTGCGAATGGCTCATTAAATCAGTATTATCGTTTA
TTTGATAGTACCCTACTACATGGGATACCTGTGGTAATTCTAGAGCTAATACAT
GCGCAAAAACCCGACTTCGGGAAGGGGTGTATTATTTATTAGATAAAAAACCAAT
GCCCTTCGGGCTCCTTGGGTGATTCATAATAACTTCACGAATTCGATGGCCT
TGCCGCCGGCAGTGTTCCATTCAAAATTTCTGCCCTATCAACTTCTCGATGGTAG
GATAGTGGCCTACCATGGTGGCAACGGGAATTAGGGTTTCGATT
CCGGAGAGGGAGCTGGAAACATCTCCCTTCCACATCAAAGGAAGGCAGCAG
GCGCGCAAATTACCAATCCCGATACGGGGAGGTAGTGACAATAAATACTG
ATACAGGGCTCTTTTGTCTGTAATTGGAATGAAACTCCTAAATCCCT
CCAGCTCCATAGGATATTAAAGTGTGGTGCAAGTTAAAAGGCTCGTAGTTG
AACCTTGGGCCCGTCTCGCCGGTCCCTCACCAGCTCCAGCGTACTGGTGCTCGGAT
GGGCTTTTCTTTCTGGGGAATCCCATCGCCTTTCCACTGGCTGTGCGGGGAA
CCAGGAACCTTTACTGTGAAAAAATTAGAGTGTTCAAAGCAGGCCTTGCTCC
GGATACATTAGCATGGAATAATAGGAGCAGTGCGGTTCTATTTTGTTGG
TTTCTAGGACCAGCGTAATGATTAAATAGGAGTAGTGCGGTGGGGGGGAA
GGGAAACTCCAGGTCCAGACAAAATAAGGATTGACAGATTGAGAGCTCTTTCTTGATCTTTTGGATGGTGCGATGGCCGTTCTTAGTTGGTGGA
GTGATTTTGTCTGTTAATTGCGATAACGAACGAGACCTCGGCCCTTAAATAG
CCCGGGGAACCTACAGCGGCAGTGCCAGCAAAATAAGGAGTAGTGACAGATGGAGA
GCTCTTTCTTGATTTTGGATGTTGCGATGCGCCGTTCTTAGTTGGTGGA
GTGATTTTGTCTGTTAATTGCGATAACGAAGACGACCTCGGCCCTTTAAATAG
CCCGGGGCGTTGCGGGGCGGCTGCTTCTAGGGGACTATCGGCTCAA
GCCGATGGAAGTGACGTGGCAATAACAGGTCTGTGATGCCCTTAGATGTTCT
GGGCCGCACCGCGCTACACTGACAGGGCCAGCGGAGTGACATCACCTTTGGC
```
CGAGAGGTTCTGGGTAAATCTTGTTAAACCTGTCGTGCTGGGATAGAGCAT
TGCAATATTATGCTCTTTCAACGAGGAATGCCTAGTAGGACAGGTCACAGC
TCGTGCCGATTACGTCCCTGCCCCTTTGTACACACCAGGCTTCGCTACTACCG
ATTGAATGGGCT

**S13** The ITS rDNA sequences data of *Penicillium purpurogenum* MHZ 111.

TCCGTAGGTGAACCTGCAGGAAGGATCATTACCAGTGCAGGCGGCTCGTGCC
CCAACCTCCACCCTTTGCTCTCTATACACCTGTGGCTTTGGGGCCACCG
GGGCCACCTCCGCCGGGCCGGACATCTGTCCCCGGCCGCGCCGCCGA
AGCGCTCTGTGAACCCCTGATGAAGATGGGCTGTCTGAGTACTATGAAAATT
GTCAAAAACCTTTCAACATGGATCTCTTGTTCCGAGCATCGATGAGAACGC
AGCA