Polyketide derivatives from the sponge associated fungus *Aspergillus europaeus* with antioxidant and NO inhibitory activities

Supporting Information
Spectra of compound 1

UV spectrum

IR spectrum

\(^1\)H-NMR spectrum (400 MHz, DMSO-d\(_6\))
$^1$C-NMR spectrum (100 MHz, DMSO-$d_6$)

HSQC spectrum

$^1$H-$^1$H COSY spectrum
HMBC spectrum

ECD spectrum
Elemental Composition Report
Single Mass Analysis
Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
733 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-100  H: 0-200  N: 0-10  O: 0-15
Minimum:  -1.5
Maximum:   5   3   50
Mass  Calc. Mass  mDa  PPM  DBE  i-FIT  Norm  Conf(%)  Formula
421.0779  421.0771  0.8  1.9  11.5  89.2  0.158  85.39  C19 H17 O11

HRESIMS spectrum
Spectra of compound 2

UV spectrum

IR spectrum
$^1$H-NMR spectrum (400 MHz, DMSO-$d_6$)

$^{13}$C-NMR spectrum (100 MHz, DMSO-$d_6$)

HSQC spectrum
$^1$H-$^1$H COSY spectrum

HMBC spectrum

ECD spectrum
Elemental Composition Report
Single Mass Analysis
Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
765 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-100   H: 0-200   N: 0-10   O: 0-15
Minimum: -1.5
Maximum: 5   3   50
<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Norm</th>
<th>Conf(%)</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>435.0924</td>
<td>435.0927</td>
<td>-0.3</td>
<td>-0.7</td>
<td>11.5</td>
<td>127.6</td>
<td>0.81</td>
<td>44.5</td>
<td>C20 H19 O11</td>
</tr>
</tbody>
</table>

HRESIMS spectrum
Spectra of compound 3

UV spectrum

IR spectrum
$^1$H-NMR spectrum (400 MHz, DMSO-$d_6$)

$^1$C-NMR spectrum (100 MHz, DMSO-$d_6$)

HSQC spectrum
$^1$H-$^1$H COSY spectrum

HMBC spectrum
Elemental Composition Report
Single Mass Analysis
Tolerance = 5.0 PPM   /   DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
57 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:
C: 0-100    H: 0-200    O: 0-20

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Norm</th>
<th>Conf(%)</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>303.0507</td>
<td>303.0505</td>
<td>0.2</td>
<td>0.7</td>
<td>10.5</td>
<td>91.5</td>
<td>n/a</td>
<td>n/a</td>
<td>C15 H11 O7</td>
</tr>
</tbody>
</table>

HRESIMS spectrum
Spectra of compound 4

UV spectrum

IR spectrum
$^{1}$H-NMR spectrum (400 MHz, DMSO-$d_6$)

$^{13}$C-NMR spectrum (100 MHz, DMSO-$d_6$)

HSQC spectrum
Elemental Composition Report
Single Mass Analysis
Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
722 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-100    H: 0-200    N: 0-10    O: 0-15
Minimum:        -1.5
Maximum:        5        3        50

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Norm</th>
<th>Conf(%)</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>417.0828</td>
<td>417.0822</td>
<td>0.6</td>
<td>1.4</td>
<td>12.5</td>
<td>95.2</td>
<td>1.346</td>
<td>26.02</td>
<td>C20 H17 O10</td>
</tr>
</tbody>
</table>

HRESIMS spectrum
Spectra of compound 5

UV spectrum

IR spectrum
$^1$H-NMR spectrum (400 MHz, DMSO-$d_6$)

$^{13}$C-NMR spectrum (100 MHz, DMSO-$d_6$)

HSQC spectrum
## Elemental Composition Report

**Single Mass Analysis**

- **Tolerance**: 3.0 PPM
- **DBE**: min = -1.5, max = 50.0
- **Element prediction**: Off
- **Number of isotope peaks used for i-FIT**: 3
- **Monoisotopic Mass, Even Electron Ions**: 696 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass)

**Elements Used:**
- C: 0-100
- H: 0-200
- N: 0-10
- O: 0-15

**Minimum:** -1.5

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Norm</th>
<th>Conf(%)</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>403.0656</td>
<td>403.0665</td>
<td>-0.9</td>
<td>-2.2</td>
<td>12.5</td>
<td>157.1</td>
<td>0</td>
<td>99.99</td>
<td>C19 H15 O10</td>
</tr>
</tbody>
</table>

**HRESIMS spectrum**
Spectra of compound 6

\[ \text{UV spectrum} \]

\[ \text{1H-NMR spectrum (400 MHz, DMSO-}d_6) \]
$^{13}$C-NMR spectrum (100 MHz, DMSO-$d_6$)

ESIMS spectrum
Spectra of compound 7

UV spectrum

IR spectrum
$^1\text{H-NMR}$ spectrum (400 MHz, DMSO-$d_6$)

$^{13}\text{C-NMR}$ spectrum (100 MHz, DMSO-$d_6$)

HSQC spectrum
\[ ^1H-^1H \text{ COSY spectrum} \]

\[ \text{HMBC spectrum} \]
Elemental Composition Report
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
58 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-100    H: 0-200    O: 0-20
Minimum:  -1.5
Maximum:  5    5    50

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Norm</th>
<th>Conf(%)</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>317.066</td>
<td>317.0661</td>
<td>-0.2</td>
<td>-0.6</td>
<td>10.5</td>
<td>160.9</td>
<td>n/a</td>
<td>n/a</td>
<td>C16 H13 O7</td>
</tr>
</tbody>
</table>

HRESIMS spectrum