Supporting Information

for

Analogs of the carotane antibiotic fulvoferruginin from submerged cultures of a Thai *Marasmius* sp.

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HRESIMS profiles and copies of NMR spectra for compounds 1–6 in CD$_3$OD, and for metabolite 3 also in CDCl$_3$; minimum inhibitory concentrations (MIC) of 1–6 for bacteria, yeasts and fungi as well as half inhibitory concentrations (IC$_{50}$) for different cell lines
Table S1. NMR chemical shifts ($^1$H 700 MHz, $^{13}$C 176 MHz) of Fulvoferruginin C (3) in chloroform-$d$. ................................................................. S4

Table S2. Minimum inhibitory concentration (MIC) for bacteria, yeasts and fungi and half-inhibitory concentration ($IC_{50}$) for cell lines, in µg/ml. ................................................................. S5

Table S3. NMR chemical shifts ($^1$H 500 MHz, $^{13}$C 125 MHz) of Fulvoferruginin (A) (1) in methanol-$d_4$. .............................................................................................................. S6

Figure S1. ECD spectra of Fulvoferruginin (1), Fulvoferruginin C (3) and D (4) in methanol. .......................................................................................... S7

HRESIMS of Fulvoferruginin A (1).................................................................................................................. S8

$^1$H NMR spectrum (500 MHz, methanol-$d_4$) of Fulvoferruginin A (1). .................................................. S9

$^{13}$C NMR spectrum (125 MHz, methanol-$d_4$) of Fulvoferruginin A (1). .................................................. S10

HSQC-dept NMR spectrum (500 MHz, methanol-$d_4$) of Fulvoferruginin A (1). .................................. S11

HMBC NMR spectrum (500 MHz, methanol-$d_4$) of Fulvoferruginin A (1). .......................................... S12

COSY NMR spectrum (500 MHz, methanol-$d_4$) of Fulvoferruginin A (1). ........................................... S13

ROESY NMR spectrum (500 MHz, methanol-$d_4$) of Fulvoferruginin A (1). ......................................... S14

HRESIMS of Fulvoferruginin B (2).................................................................................................................. S15

$^1$H NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin B (2). ........................................... S16

$^{13}$C NMR spectrum (176 MHz, methanol-$d_4$) of Fulvoferruginin B (2). ........................................... S17

HSQC-dept NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin B (2). .............................. S18

HMBC NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin B (2). ................................... S19

COSY NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin B (2). ........................................ S20

ROESY NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin B (2). ........................................... S21

HRESIMS of Fulvoferruginin C (3).............................................................................................................. S22

$^1$H NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin C (3). ........................................... S23

$^{13}$C NMR spectrum (176 MHz, methanol-$d_4$) of Fulvoferruginin C (3). ........................................... S24

HSQC-dept NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin C (3). .............................. S25

HMBC NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin C (3). ...................................... S26

COSY NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin C (3). ....................................... S27

ROESY NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin C (3). .................................... S28

$^1$H NMR spectrum (700 MHz, chloroform-$d$) of Fulvoferruginin C (3). ........................................ S29

$^{13}$C NMR spectrum (176 MHz, chloroform-$d$) of Fulvoferruginin C (3). ........................................ S30

HSQC-dept NMR spectrum (700 MHz, chloroform-$d$) of Fulvoferruginin C (3). ............................ S31

HMBC NMR spectrum (700 MHz, chloroform-$d$) of Fulvoferruginin C (3). ................................... S32

COSY NMR spectrum (700 MHz, chloroform-$d$) of Fulvoferruginin C (3). ...................................... S33

ROESY NMR spectrum (700 MHz, chloroform-$d$) of Fulvoferruginin C (3). .................................... S34
HRESIMS of Fulvoferruginin D (4) ................................................................. S35
$^1$H NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin D (4) .......... S36
$^{13}$C NMR spectrum (176 MHz, methanol-$d_4$) of Fulvoferruginin D (4) .......... S37
HSQC-dept NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin D (4) ... S38
HMBC NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin D (4) .......... S39
COSY NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin D (4) .......... S40
ROESY NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin D (4) .......... S41
HRESIMS of Fulvoferruginin E (5) .................................................................. S42
$^1$H NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin E (5) .......... S43
$^{13}$C NMR spectrum (176 MHz, methanol-$d_4$) of Fulvoferruginin E (5) .......... S44
HSQC-dept NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin E (5) ... S45
HMBC NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin E (5) .......... S46
COSY NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin E (5) .......... S47
ROESY NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin E (5) .......... S48
HRESIMS of Fulvoferruginin F (6) .................................................................. S49
$^1$H NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin F (6) .......... S50
$^{13}$C NMR spectrum (176 MHz, methanol-$d_4$) of Fulvoferruginin F (6) .......... S51
HSQC-dept NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin F (6) ... S52
HMBC NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin F (6) .......... S53
COSY NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin F (6) .......... S54
ROESY NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin F (6) .......... S55
Table S1. NMR chemical shifts (\(^1\text{H} 700 \text{ MHz}, \ ^{13}\text{C} 176 \text{ MHz})\) of Fulvoferruginin C (3) in chloroform-\(d\).

| Pos. | \(\delta_{\text{C}}\) | mult | \(\delta_{\text{H}}\) | mult (\(J\), Hz) |
|------|-----------------|------|-----------------|-----------------|
| 1    | 142.2           | CH   | 6.04            | d (11.2)        |
| 2    | 125.9           | CH   | 5.57            | d (11.2)        |
| 3    | 132.8           | C    |                 |                 |
| 4    | 123.7           | CH   | 5.72            | d (0.6)         |
| 5    | 78.1            | CH   | 4.89            | br d (12.1)     |
| 6    | 45.1            | CH   | 2.57            | t (12.1)        |
| 7    | 43.9            | C    |                 |                 |
| 8    | 39.8            | CH\(_2\) | 1.77 | m           |
| 9    | 30.4            | CH\(_2\) | 1.66 | m           |
|      |                 |       | 2.19            | m               |
| 10   | 37.7            | CH   | 2.75            | m               |
| 11   | 51.6            | CH   | 3.38            | d (13.3)        |
| 12   | 27.7            | CH\(_3\) | 1.91 | m (1.7)    |
| 13   | 20.9            | CH\(_3\) | 1.01 | s          |
| 14   | 172.1           | C    |                 |                 |
| 15   | 170.5           | C    |                 |                 |
Table S2. Minimum inhibitory concentration (MIC) for bacteria, yeasts and fungi and half-inhibitory concentration (IC\textsubscript{50}) for cell lines, in µg/ml.

A total of 2 µL and 20 µL of a 1 mg/mL stock solution (6.7 and 67 µg/mL) of 1–6 were tested. MeOH (20 µL) served as negative control and showed no inhibitory effects. Oxytetracycline served as a reference antimicrobial for bacteria; Nystatin for yeasts and filamentous fungi; Epothilon B was used as positive control for cell lines.

| Organism               | MIC (µg/ml) | 1  | 2  | 3  | 4  | 5  | 6  | Ref. |
|------------------------|-------------|----|----|----|----|----|----|------|
| *Schizos. pombe* DSM70572 |             | 66.7 | -  | -  | -  | -  | -  | 16.7 |
| *Mucor hiemalis* DSM2656 |             | 16.7 | -  | -  | -  | -  | -  | 16.7 |
| *Candida albicans* DSM1665 |             | 8.3  | -  | -  | -  | -  | -  | 16.7 |
| *Rhodoturula glutinis* DSM10134 |             | 33.3 | -  | -  | -  | -  | -  | 16.7 |
| *Micrococcus luteus* DSM1790 |             | -   | -  | -  | -  | -  | -  | 0.5  |
| *Staph.aureus* DSM346 |             | -   | -  | -  | -  | -  | -  | 8.3  |
| *Bacillus subtilis* DSM10 |             | -   | -  | -  | -  | -  | -  | 8.3  |
| *Escherichia coli* DSM1116 |             | -   | -  | -  | -  | -  | -  | 4.2  |
| *Pichia anomala* DSM6766 |             | 33.3 | -  | -  | -  | -  | -  | 16.7 |

| Cell line | IC\textsubscript{50} (µg/ml) | 1 | 2 | 3 | 4 | 5 | 6 | Ref. |
|-----------|------------------------------|----|----|----|----|----|----|------|
| L929      |                              | 0.6 | * | * | 9.5 | * | * | 0.00062 |
| KB3.1     |                              | 0.7 | 23 | * | 20 | * | 32 | 0.000003 |
| A549      |                              | 0.5 | n.t. | n.t. | n.t. | n.t. | n.t. | 0.000016 |
| A431      |                              | 0.06 | n.t. | n.t. | n.t. | n.t. | n.t. | 0.000048 |
| SKOV-3    |                              | 0.7 | n.t. | n.t. | n.t. | n.t. | n.t. | 0.00013 |
| MCF-7     |                              | 0.3 | n.t. | n.t. | n.t. | n.t. | n.t. | 0.000072 |
| PC-3      |                              | 0.1 | n.t. | n.t. | n.t. | n.t. | n.t. | n.t. |

* showed cytotoxic effects, but no IC\textsubscript{50} determinable in conducted assays
n.t. not tested, – no inhibitory effects observed up to 67 µg/mL.
Table S3. NMR chemical shifts (\(^1\)H 500 MHz, \(^{13}\)C 125 MHz) of Fulvoferruginin (A) (1) in methanol-\(d_4\).

| Pos. | \(\delta_{C}\) | mult | \(\delta_{H}\) | mult (\(J, \)Hz) |
|------|----------------|------|----------------|------------------|
| 1    | 143.6          | CH   | 6.11           | d (11.2)         |
| 2    | 126.6          | CH   | 5.61           | d (11.2)         |
| 3    | 133.9          | C    |                |                  |
| 4    | 125.3          | CH   | 5.70           | dd (2.2, 1.14)   |
| 5    | 78.6           | CH   | 4.63           | dt (12.6, 2.2)   |
| 6    | 57.6           | CH   | 2.40           | d (12.6)         |
| 7    | 45.3           | C    |                |                  |
| 8    | 38.4           | CH\(_2\) | 2.10   | td (13.6, 12.0, 6.5) |
| 9    | 36.2           | CH\(_2\) | 2.40   | dt (13.6, 6.6)    |
| 9    |                |      | 1.95           | dd (13.6, 6.6)   |
| 10   | 80.7           | C    |                |                  |
| 11   | 144.9          | C    |                |                  |
| 12   | 27.9           | CH\(_3\) | 1.91   | t (1.9)          |
| 13   | 19.8           | CH\(_3\) | 0.89   | s                |
| 14   | 121.7          | CH\(_2\) | 5.96   | s                |
| 15   | 171.8          | C    |                |                  |
Figure S1. ECD spectra of Fulvoferuginin (1), Fulvoferuginin C (3) and D (4) in methanol ($\Delta \varepsilon$ [cm$^2$/mmol], c 1.0). $\lambda_{\text{max}}$ ($\Delta \varepsilon$) for 1: 216 (-30.4), 249 (23.2); for 3: 218 (-13.7), 248 (24.8); for 4: 216 (-32.3), 247 (52.0).
HRESIMS of Fulvoferuginin A (1).
$^1$H NMR spectrum (500 MHz, methanol-$d_4$) of Fulvoferruginin (A) (1).
$^{13}$C NMR spectrum (125 MHz, methanol-$d_4$) of Fulvoferruginin A (1).
HSQC-dept NMR spectrum (500 MHz, methanol-$d_4$) of Fulvoferruginin A (1).

F2 Chemical Shift (ppm)

- 5.5
- 5.0
- 4.5
- 4.0
- 3.5
- 3.0
- 2.5
- 2.0
- 1.5
- 1.0
- 0.5
- 0.0

0 20 40 60 80 100 120 140

1.15 1.07 1.15 0.76 1.11 1.15 0.62 1.10 1.08 1.03 0.57 1.00 0.51

5.95, 121.73 (14, 14)

4.63, 78.59 (5, 5)

2.40, 57.57 (6, 6)

1.74, 38.42 (8, 8)

0.89, 19.78 (13, 13)

1.91, 27.89 (12, 12)

2.10, 38.45 (8, 8)
HMBC NMR spectrum (500 MHz, methanol-$d_4$) of Fulvoferruginin A (1).
COSY NMR spectrum (500 MHz, methanol-\textit{d}_4) of Fulvoferruginin A (1).
ROESY NMR spectrum (500 MHz, methanol-$d_4$) of Fulvoferruginin A (1).
HRESIMS of Fulvo ferruginin B (2).
$^{1}H$ NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin B (2).
$^{13}$C NMR spectrum (176 MHz, methanol-$d_4$) of Fulvoferruginin B (2).
HSQC-dept NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin B (2).
HMBC NMR spectrum (700 MHz, methanol-\(d_4\)) of Fulvoferruginin B (2).
COSY NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferuginin B (2).
ROESY NMR spectrum (700 MHz, methanol-d$_4$) of Fulvoferruginin B (2).
HRESIMS of Fulvoferuginin C (3).
\(^1\)H NMR spectrum (700 MHz, methanol-\(d_4\)) of Fulvoferruginin C (3).
$^{13}$C NMR spectrum (176 MHz, methanol-$d_4$) of Fulvoferruginin C (3).
HSQC-dept NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin C (3).
HMBC NMR spectrum (700 MHz, methanol-\textit{d}_4) of Fulvoferruginin C (3).
COSY NMR spectrum (700 MHz, methanol-d$_4$) of Fulvoferuginin C (3).
ROESY NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin C (3).
$^1$H NMR spectrum (700 MHz, chloroform-$d$) of Fulvoferruginin C (3).
$^{13}$C NMR spectrum (176 MHz, chloroform-$d$) of Fulvoferruginin C (3).
HSQC-dept NMR spectrum (700 MHz, chloroform-d) of Fulvoferruginin C (3).
HMBC NMR spectrum (700 MHz, chloroform-d) of Fulvoferruginin C (3).
COSY NMR spectrum (700 MHz, chloroform-\textit{d}) of Fulvoferruginin C (3).
ROESY NMR spectrum (700 MHz, chloroform-\(d\)) of Fulvoferruginin C (3).

\[
\begin{align*}
5.72, 1.91 \ (4, 12) \\
1.91, 5.72 \ (12, 4) \\
2.19, 1.66 \ (9, 9) \\
1.01, 4.89 \ (13, 5) \\
1.66, 2.19 \ (9, 9) \\
1.01, 1.66 \ (13, 9) \\
2.57, 2.75 \ (6, 10) \\
2.19, 1.77 \ (9, 8) \\
1.91, 5.56 \ (12, 2) \\
5.56, 6.04 \ (2, 1) \\
4.89, 5.72 \ (5, 4) \\
1.91, 5.72 \ (12, 4) \\
1.91, 5.56 \ (11, 13) \\
4.89, 3.38 \ (11, 5) \\
3.38, 4.89 \ (11, 5) \\
6.04, 5.56 \ (1, 2) \\
5.56, 6.04 \ (2, 1) \\
5.56, 1.91 \ (2, 12) \\
5.72, 1.91 \ (4, 12) \\
5.72, 4.89 \ (4, 5) \\
3.38, 1.66 \ (11, 9) \\
2.19, 1.66 \ (9, 9) \\
2.19, 1.77 \ (9, 8) \\
1.91, 1.66 \ (13, 9) \\
1.66, 2.19 \ (9, 9) \\
\end{align*}
\]
HRESIMS of Fulvo ferruginin D (4).
$^1$H NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin D (4).
$^{13}$C NMR spectrum (176 MHz, methanol-d$_4$) of Fulvoferruginin D (4).
HSQC-dept NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin D (4).
HMBC NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin D (4).
COSY NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin D (4).
ROESY NMR spectrum (700 MHz, methanol-\textit{d}_4) of Fulvoferruginin D (4).
HRESIMS of Fulvoferruginin E (5).
$^1$H NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin E (5).
$^{13}$C NMR spectrum (176 MHz, methanol-$d_4$) of Fulvoferruginin E (5).
HSQC-dept NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin E (5).
HMBC NMR spectrum (700 MHz, methanol-d$_4$) of Fulvoferruginin E (5).

**Diagram Description**

- **Chemical Shifts**
  - F2 Chemical Shift (ppm)
  - Various chemical shifts are marked with corresponding assignments.
  - For example, 5.66, 29.01 (4, 12) is noted for a set of peaks.

- **Assignments**
  - Assignments are provided for each peak, indicating the proton and carbon assignments.
  - For example, 1.84, 17.83 (8, 13).

- **Structure**
  - The molecular structure of Fulvoferruginin E is shown with labeled peaks and assignments.

- **Legend**
  - The legend indicates the chemical shifts and assignments for each peak.

- **Peptide**
  - The structure includes hydrogen bonds and other chemical interactions.

- **Additional Information**
  - Key chemical shifts are highlighted for clarity.
  - The spectrum shows the correlation between the carbon and proton signals.

- **Context**
  - This NMR spectrum is crucial for understanding the molecular structure and interactions within Fulvoferruginin E.
COSY NMR spectrum (700 MHz, methanol-d₄) of Fulvoferruginin E (5).
ROESY NMR spectrum (700 MHz, methanol-d4) of Fulvoferruginin E (5).
HRESIMS of Fulfoderruginin F (6).
$^1$H NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin F (6).
$^{13}$C NMR spectrum (176 MHz, methanol-$d_4$) of Fulvoferruginin F (6).
HSQC-dept NMR spectrum (700 MHz, methanol-$d_4$) of Fulvoferruginin F (6).
HMBC NMR spectrum (700 MHz, methanol-\textit{d}_4) of Fulvoferruginin F (6).
COSY NMR spectrum (700 MHz, methanol-\textit{d}_4) of Fulvoferruginin F (6).
ROESY NMR spectrum (700 MHz, methanol-\(d_4\)) of Fulvoferruginin F (6).