

Supplementary Materials

In vitro* analysis of the antagonistic biological and chemical interactions between the endophyte *Sordaria tomento-alba* and the phytopathogen *Botrytis cinerea

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Table S1. NMR Spectroscopic data of *trans*-sordariol (1) (¹H at 500 MHz, ¹³C at 125 MHz, CD₃OD).

| Position | Proton | δ _H (Hz) | δ ¹³ C | HMBC |
|----------|--------|--|-------------------|--------------------|
| 1 | H-1 | - | 125.2 | |
| 2 | H-2 | - | 157.3 | |
| 3 | H-3 | 6.7 (1H, dd, <i>J</i> = 8.0, 1.2 Hz) | 115.4 | C1, C2, C5 |
| 4 | H-4 | 7.06 (1H, t, <i>J</i> = 8.0 Hz) | 129.7 | C2, C6 |
| 5 | H-5 | 7.0 (1H, dd, <i>J</i> = 8.0, 1.2 Hz) | 118.7 | C1, C3, C4, C6 |
| 6 | H-6 | - | 139.7 | |
| 7 | H-7 | 4.8 (1H, s) | 56.6 | C1, C2, C6 |
| 1' | H-1' | 6.98 (1H, d, <i>J</i> = 15.7, 1.0 Hz) | 130.6 | C1, C3', C5, C6 |
| 2' | H-2' | 6.17 (1H, dd, <i>J</i> = 15.7, 6.6 Hz) | 132.6 | C3', C4', C6 |
| 3' | H-3' | 4.1 (1H, ddd, <i>J</i> = 6.6, 4.9, 1.3 Hz) | 78.0 | C1', C2', C4', C5' |
| 4' | H-4' | 3.8 (1H, qd, <i>J</i> = 6.4, 4.9 Hz) | 71.7 | C2', C3', C5' |
| 5' | H-5' | 1.2 (3H, d, <i>J</i> = 6.4 Hz) | 18.9 | C3', C4' |

Table S2. NMR Spectroscopic data of *trans*-sordarial (2) (¹H at 500 MHz, ¹³C at 125 MHz, CDCl₃).

| Position | Proton | δ_{H} (Hz) | $\delta^{13}\text{C}$ | HMBC |
|----------|--------|---------------------------------------|-----------------------|----------------------|
| 1 | H-1 | - | 117.3 | |
| 2 | H-2 | - | 162.8 | |
| 3 | H-3 | 6.9 (1H, dt, $J = 8.4, 0.9$ Hz) | 117.3 | C1, C2, C5 |
| 4 | H-4 | 7.46 (1H, dd $J = 8.4, 7.7$ Hz) | 137.2 | C2, C6 |
| 5 | H-5 | 6.94 (1H, dt, $J = 7.7, 0.9$ Hz) | 118.9 | C1, C3, C4, C1' |
| 6 | H-6 | - | 142.1 | |
| 7 | H-7 | 10.3 (1H, s) | 195.2 | C1, C2 |
| 1' | H-1' | 7.2 (1H, dt, $J = 15.7, 1.0$ Hz) | 126.9 | C1, C2', C3', C5, C6 |
| 2' | H-2' | 6.2 (1H, dd, $J = 15.7, 6.1$ Hz) | 134.8 | C1', C3', C4', C6 |
| 3' | H-3' | 4.3 (1H, ddd, $J = 6.1, 3.5, 1.5$ Hz) | 75.8 | C1', C2', C4' |
| 4' | H-4' | 4.0 (1H, qd, $J = 6.5, 3.5$ Hz) | 70.2 | C2' |
| 5' | H-5' | 1.2 (3H, d, $J = 6.5$ Hz) | 17.7 | C3', C4' |

Table S3. NMR Spectroscopic data of 3'-episordariol (3) (¹H at 500 MHz, ¹³C at 125 MHz, (CDCl₃)).

| Position | Proton | δ _H (Hz) | δ ¹³ C | HMBC |
|----------|--------|---|-------------------|------------|
| 1 | H-1 | - | 121.8 | |
| 2 | H-2 | - | 156.5 | |
| 3 | H-3 | 6.83 (1H, d(superimposed), <i>J</i> = 7.9 Hz) | 116.2 | C2, C5 |
| 4 | H-4 | 7.16 (1H, t, <i>J</i> = 7.8 Hz) | 129.1 | C2, C6 |
| 5 | H-5 | 6.94 (1H, dd, <i>J</i> = 7.8, 1.1 Hz) | 118.9 | C1, C3, C4 |
| 6 | H-6 | - | 136.2 | |
| 7 | H-7 | 5.0 (1H, s) | 60.2 | |
| 1' | H-1' | 6.85 (1H, d, <i>J</i> = 15.7 Hz) | 129.6 | C3', C5 |
| 2' | H-2' | 6.1 (1H, dd, <i>J</i> = 15.7, 6.6 Hz) | 131.0 | C-6 |
| 3' | H-3' | 4.3 (1H, s(br)) | 76.2 | |
| 4' | H-4' | 4.0 (1H, dd(br), <i>J</i> = 6.4, 3.6 Hz) | 70.3 | C2' |
| 5' | H-5' | 1.2 (3H, d, <i>J</i> = 6.5 Hz) | 17.7 | C3', C4' |
| | | | | |

Table S4. NMR Spectroscopic data of heptacyclosordariolone (4) (¹H at 500 MHz, ¹³C at 125 MHz, Cl₃CD).

| Position | Proton | δ _H (Hz) | δ ¹³ C | HMBC |
|----------|--------|--------------------------------------|-------------------|------------------|
| 1 | H-1 | - | 126.7 | |
| 2 | H-2 | - | 151.8 | |
| 3 | H-3 | 6.7 (1H, dd, <i>J</i> = 7.7, 0.8 Hz) | 131.0 | C5 |
| 4 | H-4 | 7.13 (1H, t, <i>J</i> = 7.7 Hz) | 127.9 | C2, C6 |
| 5 | H-5 | 6.9 (1H, dd, <i>J</i> = 7.7, 0.8 Hz) | 123.4 | C1, C3, C4, C1' |
| 6 | H-6 | - | 137.1 | |
| 7 | H-7a | 4.64 (1H, d, <i>J</i> = 14 Hz) | 56.7 | C1, C2, C6, C3' |
| | H-7b | 5.1 (1H, d, <i>J</i> = 14 Hz) | | C1, C2, C6, C3' |
| 1' | H-1' | 6.7 (1H, d, <i>J</i> = 12.5 Hz) | 114.6 | C1, C2', C3', C5 |
| 2' | H-2' | 5.97 (1H, d, <i>J</i> = 12.5 Hz) | 130.9 | C3', C6 |
| 3' | H-3' | - | 104.0 | |
| 4' | H-4' | 4.15 (1H, q, <i>J</i> = 6.5 Hz) | 66.9 | C5', C3', C2' |
| 5' | H-5' | 1.1 (3H, d, <i>J</i> = 6.5 Hz) | 16.1 | C3', C4' |
| C2-OH | | | | C1, C2 |

Table S5. NMR Spectroscopic data of cyclosordariolone (5) (¹H at 400 MHz, ¹³C at 100 MHz, CD₃OD).

| Position | Proton | δ _H (Hz) | δ ¹³ C | HMBC |
|----------|--------|----------------------------------|-------------------|--------------|
| 1 | H-1 | - | 126.3 | |
| 2 | H-2 | - | 156.6 | |
| 3 | H-3 | 6.91 (1H, d, <i>J</i> =8.5 Hz) | 118.3 | C1, C5 |
| 4 | H-4 | 7.47 (1H, d, <i>J</i> =8.5 Hz) | 127.3 | C2, C6, C4' |
| 5 | H-5 | - | 139.0 | |
| 6 | H-6 | - | 129.9 | |
| 7 | H-7a | 4.9 (1H, d, <i>J</i> = 11.8 Hz) | 55.0 | C1, C2, C6 |
| | H-7b | 4.84 (1H, d, <i>J</i> = 11.8 Hz) | | |
| 1' | H-1' | 7.97 (1H, d, <i>J</i> = 10.3 Hz) | 143.3 | C1, C5, C3' |
| 2' | H-2' | 6.14 (1H, d, <i>J</i> = 10.3 Hz) | 124.3 | C4', C6 |
| 3' | H-3' | - | 206.8 | |
| 4' | H-4' | | 77.5 | |
| 5' | H-5' | 1.45 (3H, s) | 32.2 | C3', C4', C5 |

Table S6. NMR Spectroscopic data of sordamentone A (6) (¹H at 500 MHz, ¹³C at 125 MHz, Cl₃CD).

| Position | Proton | δ _H (Hz) | δ ¹³ C | HMBC |
|----------|--------|--|-------------------|------------------|
| 1 | H-1 | - | 125.3 | |
| 2 | H-2 | - | 150.1 | |
| 3 | H-3 | 6.68 (1H, dt, <i>J</i> =8.1, 0.7 Hz) | 114.4 | C1, C2, C5 |
| 4 | H-4 | 7.16 (1H, dd, <i>J</i> =8.1, 7.4 Hz) | 129.5 | C2, C6 |
| 5 | H-5 | 6.73 (1H, dt, <i>J</i> = 7.4, 0.7 Hz) | 113.4 | C1, C3, C6 |
| 6 | H-6 | - | 143.1 | |
| 7 | H-7a | 5.15 (1H, dd, <i>J</i> = 12.3, 2.8 Hz) | 70.8 | C1, C2, C6, C1', |
| | H-7b | 5.07 (1H, dt, <i>J</i> = 12.3, 1.8 Hz) | | C1,C2, C6 C1', |
| 1' | H-1' | 5.72 (1H, q, <i>J</i> = 3.6, 2.8 Hz) | 80.5 | C6 |
| 2' | H-2a' | 3.06 (1H, dd, <i>J</i> = 16, 7.8 Hz) | 44.5 | C1', C3', C6 |
| | H-2b' | 2.86 (1H, dd. <i>J</i> = 16, 4.7 Hz) | | C1', C3', C6 |
| 3' | H-3' | - | 210.5 | |
| 4' | H-4' | 4.27 (1H, q, <i>J</i> = 7.2 Hz) | 73.4 | C3', C5' |
| 5' | H-5' | 1.41 (3H, d, <i>J</i> = 7.2 Hz) | 19.3 | C3', C4' |
| C2-OH | | 4.94 (1H, s(br)) | | |
| C4'-OH | | 3.6 (1H, s(br)) | | |

Table S7. NMR Spectroscopic data of sordamentone B (7) (¹H at 500 MHz, ¹³C at 125 MHz, Cl₃CD).

| Position | Proton | δ _H (Hz) | δ ¹³ C | HMBC |
|----------|--------|--|-------------------|------------------|
| 1 | H-1 | - | 125.3 | |
| 2 | H-2 | - | 150.1 | |
| 3 | H-3 | 6.69 (1H, d(br), <i>J</i> =8.0 Hz) | 114.4 | C1, C2, C5 |
| 4 | H-4 | 7.17 (1H, dd, <i>J</i> =8.0, 7.5 Hz) | 129.5 | C2, C6 |
| 5 | H-5 | 6.75 (1H, d(br), <i>J</i> = 7.5 Hz) | 113.4 | C1, C3, C6 |
| 6 | H-6 | - | 143.1 | |
| 7 | H-7a | 5,15 (1H, ddd, <i>J</i> = 12.3, 2.6, 1.1 Hz) | 70.8 | C1, C2, C6, C1', |
| | H-7b | 5.07 (1H, dt, <i>J</i> = 12.3, 2.6 Hz) | | C1,C2, C6 C1', |
| 1' | H-1' | 5.72 (1H, m) | 80.5 | C6 |
| 2' | H-2a' | 2.96 (1H, dd, <i>J</i> = 16, 8 Hz) | 44.5 | C1', C3', C6 |
| | H-2b' | 2.91 (1H, dd. <i>J</i> = 16, 4.4 Hz) | | C1', C3', C6 |
| 3' | H-3' | - | 210.5 | |
| 4' | H-4' | 4.30 (1H, q, <i>J</i> = 7.1 Hz) | 73.4 | C3', C5' |
| 5' | H-5' | 1.38 (3H, d, <i>J</i> = 7.1 Hz) | 19.3 | C3', C4' |
| C2-OH | | 5.05 (1H, s(br)) | | |
| C4'-OH | | 3.6 (1H, s(br)) | | |