SUPPLEMENTARY MATERIAL

Cytotoxic tremulanes and 5,6-secotremulanes, four new sesquiterpenoids from a plant-associated fungus X1-2

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Abstract: Two new tremulanes and two new 5,6-secotremulanes, davotremulanes A-D 1-4, along with four known compounds 5-8, were isolated from the culture extract of X1-2, an unidentified plant-associated fungus, which was isolated from the endangered plant, Davidia involucrate Baill. in Shennongjia District. The structures of new compounds 1-4 were established on the basis of extensive spectroscopic analysis. Compounds 1-8 were evaluated for cytotoxic activity to four cancer cell lines, and compounds 1, 2 and 5 displayed selectively moderate activities to A549 cell line with IC_{50} at 15.3, 25.2, 35.2 μg/mL.

Keywords: Tremulanes; 5,6-secotremulanes; Plant-associated fungus; Secondary metabolites; Cytotoxic activity.
Figure S1. The NMR spectrums of Davotremulanes A
Figure S2. The NMR spectrums of Davotremulanes B
Figure S3. The NMR spectrums of Davotremulanes C and D
Figure S4. The HR-MS spectra of Davotremulanes A.
Figure S5. the HR-MS spectrums of Davotremulanes B

Figure S6. the HR-MS spectrums of Davotremulanes C and D
Figure S7. The CD spectrums of Davotremulanes A and B

the CD and the configuration analysis of Davotremulanes A

the CD and the configuration analysis of Davotremulanes B

Figure S8 the key HMBC correlations of compounds 1-4

Figure S9 the key NOESY correlations of compounds 1-4
Table S1: The NMR data of compounds 1-2 (400MHz for $^1$H NMR and 100MHz for $^{13}$C in CDCl$_3$)

| NO | $^{13}$C | $^1$H($J$ in Hz) | $^{13}$C | $^1$H($J$ in Hz) |
|----|---------|-----------------|---------|-----------------|
| 1  | 139.0(s) | -               | 37.7(d)  | 2.89 (dd, 10.0, 14.7, 1H) |
| 2  | 125.2(s) | -               | 164.7(s) | -               |
| 3  | 37.4(d)  | 3.64(m,1H)      | 123.3(s) | -               |
| 4  | 30.1(t)  | 1.82(d,14.3,1H) | 27.9(t)  | 2.75(dd,5.0,14.0,1H) |
|    |          | 2.06(m,1H)      |          | 2.54(dd,2.4,13.6,1H) |
| 5  | 72.4(d)  | 4.06(t,4.0,1H)  | 71.6(d)  | 3.91(s, 1H)     |
| 6  | 38.3(d)  | 1.91(m,1H)      | 39.1(d)  | 2.17 (br s, 1H) |
| 7  | 39.7(d)  | 3.37(m,1H)      | 40.8(d)  | 2.57 (m,1H)     |
| 8  | 39.2(t)  | 1.39(dd,11.0,13.0,1H) | 39.5(t)  | 1.34 (t,8.0,1H) |
|    |          | 1.78(dd,8.0,11.0,1H) |          | 1.69(t,5.0,8.0,1H) |
| 9  | 43.8(s)  | -               | 41.8(s)  | -               |
| 10 | 41.4(t)  | 2.13(d,12.5,1H) | 38.8(t)  | 1.63 (d,7.5,2H) |
|    |          | 1.85(m,1H)      |          |                  |
| 11 | 69.5(t)  | 4.74(dd,10.0,13.0,2H) | 70.6(t)  | 4.71 (d,14.4,1H) |
|    |          |                  |          | 4.58 (d,14.8,1H) |
| 12 | 180.1(s) | -               | 175.7(s) | -               |
| 13 | 11.5(q)  | 0.87(d,7.0,3H)  | 11.2(q)  | 1.01(d,7.0,1H)  |
| 14 | 23.5(q)  | 1.12(s,3H)      | 26.1(q)  | 1.05 (s,3H)     |
| 15 | 68.5(t)  | 3.28(dd,10.8,14.6,2H) | 71.4(t)  | 3.41(s,2H)     |

Table S2. The NMR data of compounds 3-4 (400MHz for $^1$H NMR and 100MHz for $^{13}$C in CDCl$_3$)
| NO |  $^{13}$C  | $^1$H($J$ in Hz) |  $^{13}$C  | $^1$H($J$ in Hz) |
|----|------------|-----------------|------------|-----------------|
| 1  | 147.3(s)   | -               | 142.1(s)   | -               |
| 2  | 129.6(s)   | -               | 124.1(s)   | -               |
| 3  | 37.3(d)    | 3.81(m,1H)     | 35.6(d)    | 3.37(m,1H)     |
| 4  | 32.9(t)    | 2.57 (dd,1.2,9.4,1H) | 32.1(t)    | 2.76(dd,4.4,16.0,1H) |
|    |            | 2.57(dd,4.2,16.0,1H) |            | 2.57(dd,4.2,16.0,1H) |
| 5  | 177.5(s)   | -               | 173.1(s)   | -               |
| 6  | 141.7(d)   | 5.72 (dd,8.1,10.0,1H) | 139.6(d)   | 5.64(m,1H)     |
| 7  | 45.3(d)    | 3.42 (m, 1H)   | 45.7(d)    | 3.49(s,1H)     |
| 8  | 42.7(t)    | 1.74 (m,1H)    | 43.0(t)    | 1.74(m,1H)     |
|    |            | 1.53 (m,1H)    |            | 1.53(m,1H)     |
| 9  | 43.2 (C)   | -               | 43.2(s)    | -               |
| 10 | 41.0(t)    | 2.26 (dd,1.6,14.0,1H) | 41.1(t)    | 2.32(d,7.6,1H), |
|    |            | 2.37 (d,14.0,1H) |            | 2.08(d, 7.8,1H) |
| 11 | 60.3(t)    | 4.19 (d,12.01H) | 69.2(t)    | 4.82(d,14.0,1H), |
|    |            | 4.27 (d,12.0,1H) |            | 4.72 (d,14.01H) |
| 12 | 71.2(t)    | 4.26 (t,8.8,1H) | 63.5(t)    | 3.68(d,8.0,1H) |
|    |            | 4.37 (t,8.8,1H) |            | 3.59(d,8.01H)  |
| 13 | 114.0(t)   | 5.01(t,3.8,6.2,1H) | 114.9(t)   | 5.05(d,12.0,1H) |
|    |            | 5.04 (m, 1H)   |            | 5.11(d,12.4, 1H) |
| 14 | 22.7(q)    | 0.96 (s,3H)    | 22.8(q)    | 0.97(s,3H)     |
| 15 | 70.6(t)    | 3.49 (s,2H)    | 70.5(t)    | 3.50(s,2H)     |