





## Mollicellins O-R, Four New Depsidones Isolated from the Endophytic Fungus *Chaetomium* sp. Eef-10

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Received: 15 November 2018; Accepted: 4 December 2018; Published: 5 December 2018

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**Figure S1.1** UV spectrum of mollicellin O (1)



Figure S1.2 IR spectrum of mollicellin O (1)



Figure S1.3 <sup>1</sup>H NMR spectrum of mollicellin O (1) (Acetone-d<sub>6</sub>, 600MHz)



Figure S1.4 <sup>13</sup>C NMR spectrum of mollicellin O (1) (Acetone-d<sub>6</sub>, 150 MHz)



Figure S1.5 HSQC spectrum of mollicellin O (1) (Acetone-d<sub>6</sub>)



Figure S1.6 HMBC spectrum of mollicellin O (1) (Acetone-d<sub>6</sub>)



Figure S1.7 NOESY spectrum of mollicellin O (1) (Acetone-*d*<sub>6</sub>)



Figure S1.8 HR-ESI-MS spectrum of mollicellin O (1)



Figure S1.9 HMBC correlation of H-2' with C-4a and C-3 in mollicellin O (1)



Figure S2.1 UV spectrum of mollicellin P (2)



Figure S2.2 IR spectrum of mollicellin P (2)



Figure S2.3 <sup>1</sup>H NMR spectrum of mollicellin P (2) (Acetone-d<sub>6</sub>, 600MHz)



Figure S2.4 <sup>13</sup>C NMR spectrum of mollicellin P (2) (Acetone-d<sub>6</sub>, 150 MHz)



Figure S2.5 HSQC spectrum of mollicellin P (2) (Acetone-d<sub>6</sub>)



Figure S2.6 HMBC spectrum of mollicellin P (2) (Acetone-d<sub>6</sub>)



Figure S2.7 NOESY spectrum of mollicellin P (2) (Acetone-*d*<sub>6</sub>)



Figure S2.8 HR-ESI-MS spectrum of mollicellin P (2)



Figure S2.9 HMBC correlation of H-2' with C-4a and C-3 in mollicellin P (2)



Figure S3.1 UV spectrum of mollicellin Q (3)



Figure S3.2 IR spectrum of mollicellin Q (3)





Figure S3.3 <sup>1</sup>H NMR spectrum of mollicellin Q (3) (Acetone-d<sub>6</sub>, 600MHz)



Figure S3.4 <sup>13</sup>C NMR spectrum of mollicellin Q (3) (Acetone-*d*<sub>6</sub>, 150 MHz)



Figure S3.5 HSQC spectrum of mollicellin Q (3) (Acetone-d<sub>6</sub>)



Figure S3.6 HMBC spectrum of mollicellin Q (3) (Acetone-*d*<sub>6</sub>)



Figure S3.7 NOESY spectrum of mollicellin Q (3) (Acetone-*d*<sub>6</sub>)

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Figure S3.8 HR-ESI-MS spectrum of mollicellin Q (3)



Figure S3.9 HMBC correlation of H-2' with C-4a and C-3 in mollicellin Q (3)



Figure S4.1 UV spectrum of mollicellin R (4)



Figure S4.2 IR spectrum of mollicellin R (4)



Figure S4.3 <sup>1</sup>H NMR spectrum of mollicellin R (4) (Acetone-d<sub>6</sub>, 600MHz)

-194.92





Figure S4.4 <sup>13</sup>C NMR spectrum of mollicellin R (4) (Acetone-d<sub>6</sub>, 150 MHz)



Figure S4.5 HSQC spectrum of mollicellin R (4) (Acetone-d<sub>6</sub>)



Figure S4.6 HMBC spectrum of mollicellin R (4) (Acetone-d<sub>6</sub>)



Figure S4.7 NOESY spectrum of mollicellin R (4) (Acetone-d<sub>6</sub>)



Figure S4.8 HR-ESI-MS spectrum of mollicellin R (4)



Figure S4.9 HMBC correlation of H-2' with C-4a and C-3 in mollicellin R (4)



Figure S5.1 UV spectrum of mollicellin G (5)



Figure S5.2 IR spectrum of mollicellin G (5)



Figure S5.3 <sup>1</sup>H NMR spectrum of mollicellin G (5) (Acetone-d<sub>6</sub>, 600MHz)



Figure S5.4 <sup>13</sup>C NMR spectrum of mollicellin G (5) (Acetone-*d*<sub>6</sub>, 600MHz)

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391.1 759.2	151 1 403 1	C21H20NaO6 C42H40NaO12	100.00	391.1152 759.2412	0.2	0.1 0.9	77.9 15.8	11.5 22.5	even	ok ok					

Figure S5.5 HR-ESI-MS spectrum of mollicellin G (5)



Figure S6.1 UV spectrum of mollicellin H (6)



Figure S6.2 IR spectrum of mollicellin H (6)



Figure S6.3 <sup>1</sup>H NMR spectrum of mollicellin H (6) (DMSO-d<sub>6</sub>, 600MHz)



Figure S6.4 <sup>13</sup>C NMR spectrum of mollicellin H (6) (DMSO-d<sub>6</sub>, 150 MHz)



Figure S6.5 HSQC spectrum of mollicellin H (6) (DMSO-d<sub>6</sub>)





Figure S6.6 HMBC spectrum of mollicellin H (6) (DMSO-d<sub>6</sub>)



Figure S6.7 NOESY spectrum of mollicellin H (6) (DMSO-d<sub>6</sub>)



Mass Spectrum SmartFormula Report

## 1+ 370.1375 0.2 1+ 371.1400 374.9056 0.0+ 362 364 366 368 370 372 374 376 378 m/z err [mDa] 0.2 e<sup>C</sup> Conf N-Rule Ion Formula mSigma Meas, m/z rdb # Score m/z err [ppm] 369.134420 C22H17N4O2 100.00 369.134602 0.5 1.3 16.5 1 ok even -1.2 -3.2 0.5 2 C21H21O6 66.00 369.133265 -3.1 12.8 11.5 even ok 737.259253 737.261928 22.5 32.5 23.08 -4.3 0.7 19.3 40.2 737.262442 1 C42H41012 even ok 100.00 2 C44H33N8O4 ok even

## Figure S6.8 HR-ESI-MS spectrum of mollicellin H (6)





Figure S7.1 <sup>1</sup>H NMR spectrum of mollicellin I (7) (Acetone-*d*<sub>6</sub>, 600MHz)



Figure S7.2 <sup>13</sup>C NMR spectrum of mollicellin I (7) (Acetone-d<sub>6</sub>, 600MHz)



Figure S7.3 HR-ESI-MS spectrum of mollicellin I (7)



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