Supplementary Information

New Dereplication Method Applied to NMR-Based Metabolomics on Different *Fusarium* Species Isolated from Rhizosphere of *Senna spectabilis*

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Table S1. Gene sequence obtained from the genetic identification of *F. solani* and *F. oxysporum* isolated from *S. spectabilis* rizhosphere

Sample	DNA sequence
F. solani	TCGAACCGTCTTCGGATCTCCGCTTATGAATGTCCTCCGCAGGTTCACCTACGGACGGATCCTCCGCTTATTGATATGTCCTCCGCATGTTCACCTACCGACTGCTCCTCTTATTGTTGATTTCTCCTCCGGATGTTCAACGAACGGCTGCTCCTCTTATTGATGACTCCTCCTCAGGATGGGGGGCCGGCGGCTTGTAGTGATGCTGGAACAGGCATGCCCGCCAGAATACTGGCGGGCGCAATGTGCGTTCAAAGATTCGATGATTCACTGAATTCTGCAATTCACATTACTTATCGCATTTCGCTGCGTTCTTCATCGATGCCAGAGCCAAGAGATCCGTTGTTGAAAGTTTTGATTTATTTGCTTGTTTACTCAGAAAAAACATTATAGAAACAGAGTTAGGGGGTCCTCTGGCGGGGGCGGCCCGTGTTACGGGGCCGTCTGTTCCCGCCGAGGCAACGTTTTAGGTATGTTCACAGGGTTGATGAGTTGTATAACTCGGTAATGATCCCTCCGCAGGTTCACCTACGGA
F. oxysporum	GCCAATGCGGTAAGTTCGTCGTAGGTGACCTGCGGAGGACATATCAATAAGCGGAGGATCCGTCCGCGAGGTGACCTGACGGCCCCCCAGAGGACCCCTAAACTCTGTTTCTATATGTAACTTCTGAGTAAAACCATAAATAAATCAAAACTTTCAACAACGGATCTCTTGGTTCTGGCATCGATGAAGAACGCAGCAAAATGCGATAAGTAATGTGAATTGCAGAATTCAGTGAATCATCGAATCTTTGAACGCACATTGCGCCCGCCAGTATTCTGGCGGGCATGCCTGTTCGAGCGTCATTTCAACCCTCAAGCACAGCTTGGTGTTGGGACTCGCGTTAATTCGCGTTCCTCAAATTGATTGGCGGTCACGTCGAGCTTCCATAGCGTAGTAGTAAAACCCTCGTTACTGGTAATCGTCGCGGCCACGCCGTTAAACCCCAACTTCTGAATGTTGACCTCGGATCAGGTAGGAATACCCGCTGAACTTAAGCATATCAATAAGCGGAGGAA

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Table S2. Data obtained from DNA extraction and sequencing from *F. solani* and *F. oxysporum*

Sample	Concentration / (ng μL^{-1})	Identity / %	Purity (OD260/OD280)	Access number
Fusarium solani	21.8	98	1.8	KC907714.1
Fusarium oxysporum	50.6	99	1.9	LC055797.1

(3*S*,6*R*,9*S*,12*R*,15*S*,18*R*)-3,9,15-Tribenzyl-6,12,18-triisopropyl-4,10,16-trimethyl-1,7,13-trioxa-4,10,16-triazacyclooctadecane-2,5,8,11,14,17-hexone (beauvericin)

UV-Vis λ / nm 204; ^{1}H NMR (600 MHz, MeOD) δ 0.15 (d, 3H, *J* 6.9 Hz, CH$_3$), 0.75 (d, 3H, *J* 6.6 Hz, CH$_3$), 1.7 (m, 1H, CH), 2.94 (dd, 1H, *J* 14.7, 4.6 Hz, CH), 3.05 (s, 3H, CH$_3$), 3.29 (dd, 1H, *J* 14.7, 4.6 Hz, CH), 4.7 (d, 1H, *J* 8.9 Hz, CH), 5.7 (dd, 1H, *J* 12.7, 4.54 Hz, CH), 7.04-7.17 (m, 5H); ^{13}C NMR (150 MHz, MeOH) δ 15.81, 17.61, 34.16, 44.25, 57.54, 127.98; ESI(+)-MS mode for C$_{45}$H$_{57}$N$_3$O$_9$ *m/z* 784.3895 [M + H]$^+$.

5-Butylpyridine-2-carboxylic acid (fusaric acid)

UV-Vis (water) λ / nm 269; ^{1}H NMR (600 MHz, CDCl$_3$) δ 0.86 (t, 3H, *J* 7.0 Hz, CH$_3$), 1.29 (m, 2H, CH$_2$), 1.56 (m, 2H, CH$_2$), 2.66 (t, *J* 8.0 Hz, 2H, CH$_2$), 7.80 (d, 1H, *J* 8.3 Hz, CH), 8.01 (d, 1H, *J* 8.3 Hz, CH), 8.41 (s, 1H, CH). ^{13}C NMR (150 MHz, MeOH) δ12.92, 21.62, 32.76, 77.38, 124.54, 138.61; ESI(+)-MS mode for C$_{10}$H$_{13}$NO$_2$ *m/z* 180.0959 [M + H]$^+$.
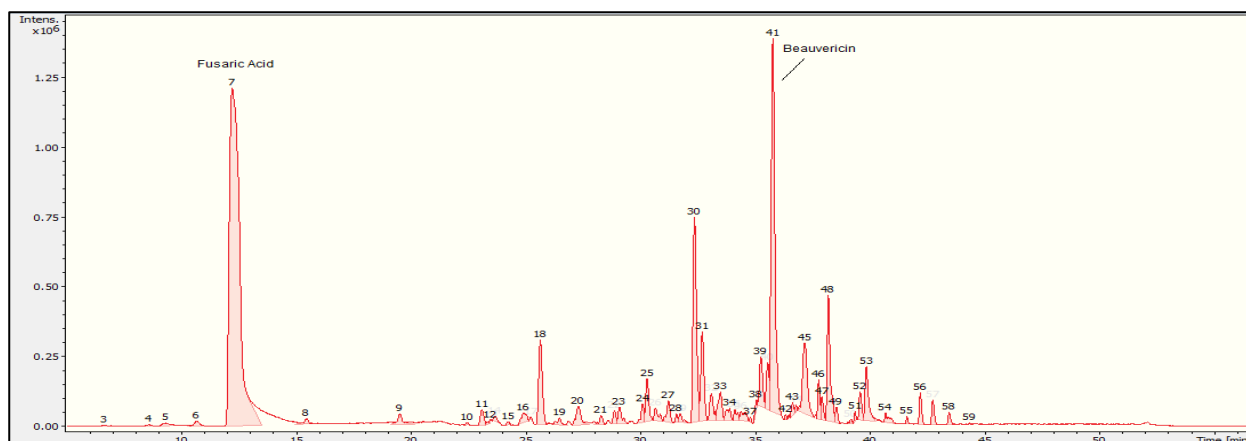

Figure S1. Total ion chromatogram (TIC) of *F. oxysporum* extract (50-minute gradient).
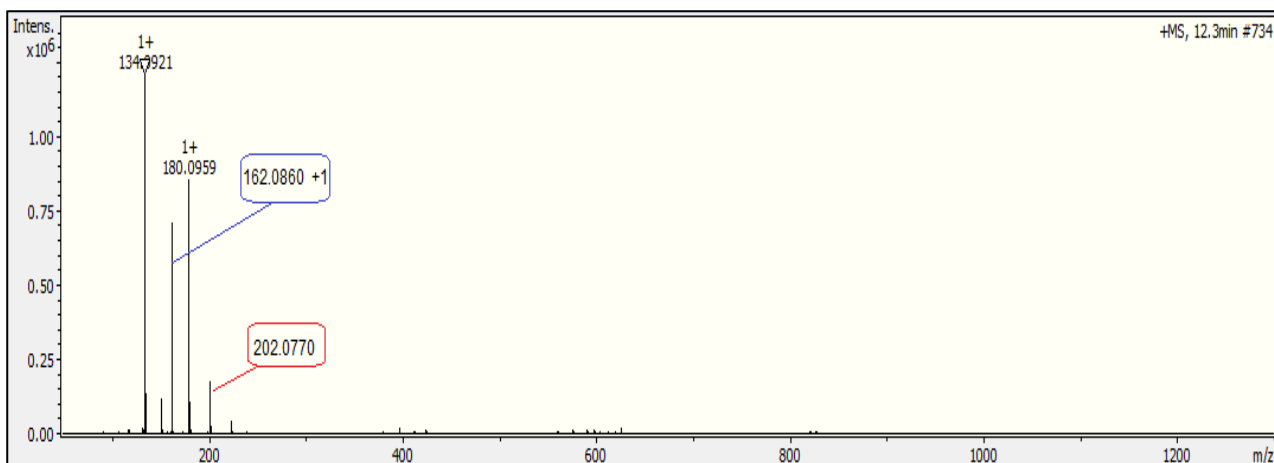
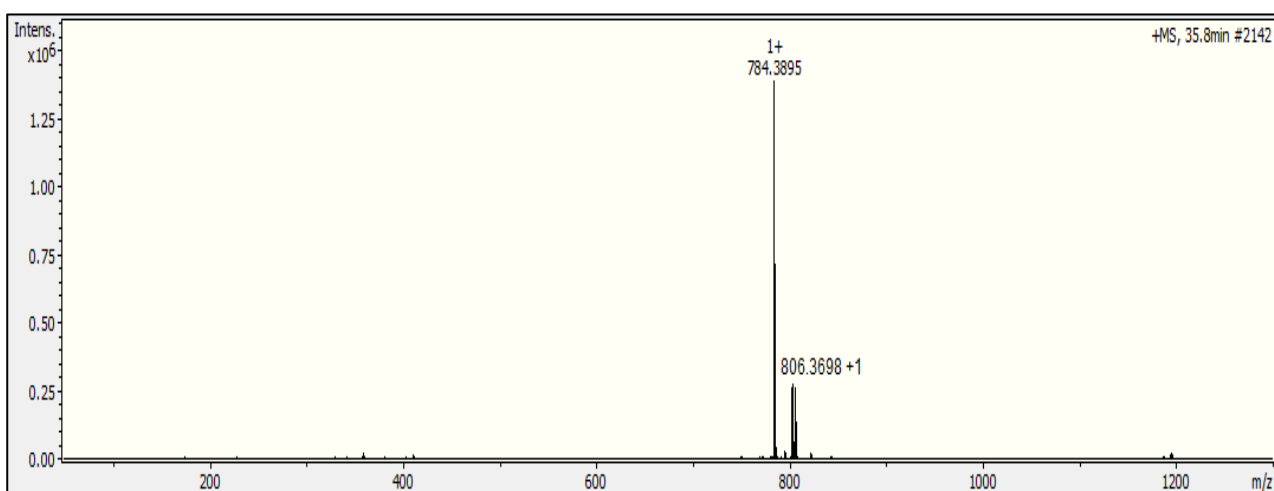**Figure S2.** Mass spectra of fusaric acid. LC-HRMS-ESI at 12.3 minutes on a 50-minute gradient.

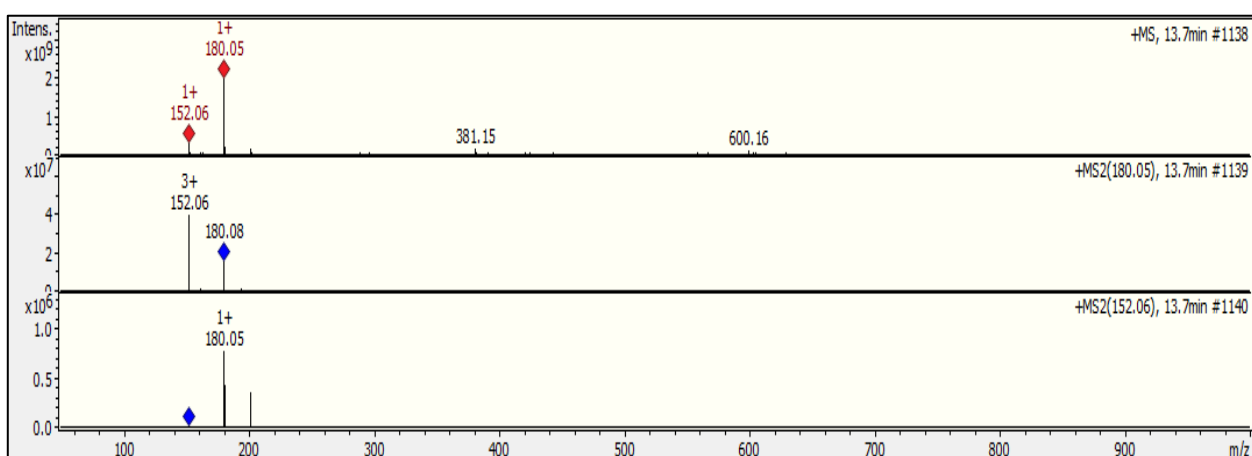**Figure S3.** Mass spectra of beauvericin. LC-HRMS-ESI at 35.8 minutes on a 50-minute gradient.

Figure S4. Mass spectra of fusaric acid. (MS 13.7 min) LC-MS-ESI; (MS2 m/z 180.05) tandem MS of m/z 180.05 [M + H]$^+$; (MS2 m/z 152.06) tandem MS of m/z 152.06 (frag.).
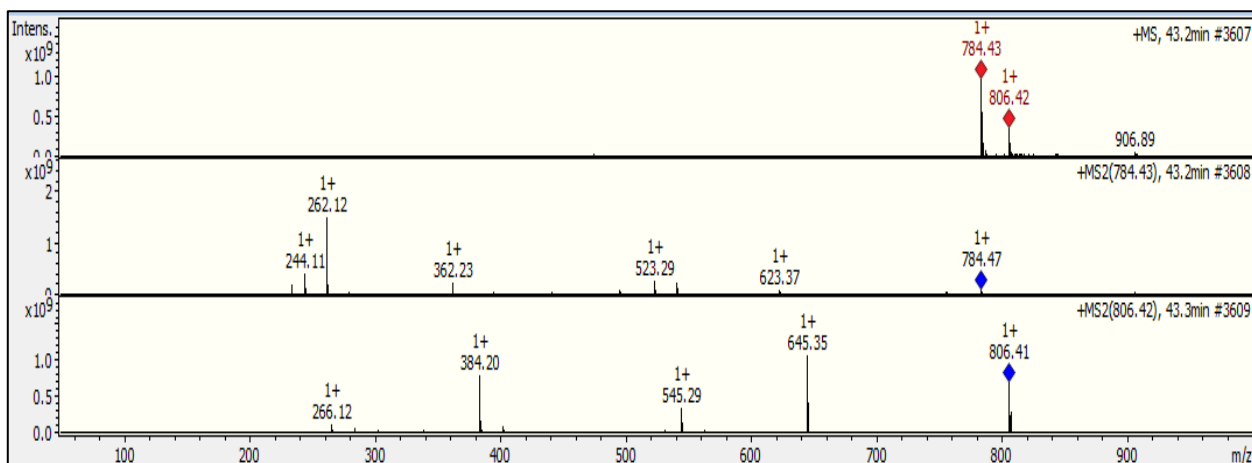
Figure S5. Mass spectra of beauvericin. (MS 43.2 min) LC-MS-ESI; (MS2 *m/z* 784.43) tandem MS of *m/z* 784.43 [M + H]⁺; (MS2 *m/z* 806.42) tandem MS of *m/z* 806.42 [M + Na]⁺.
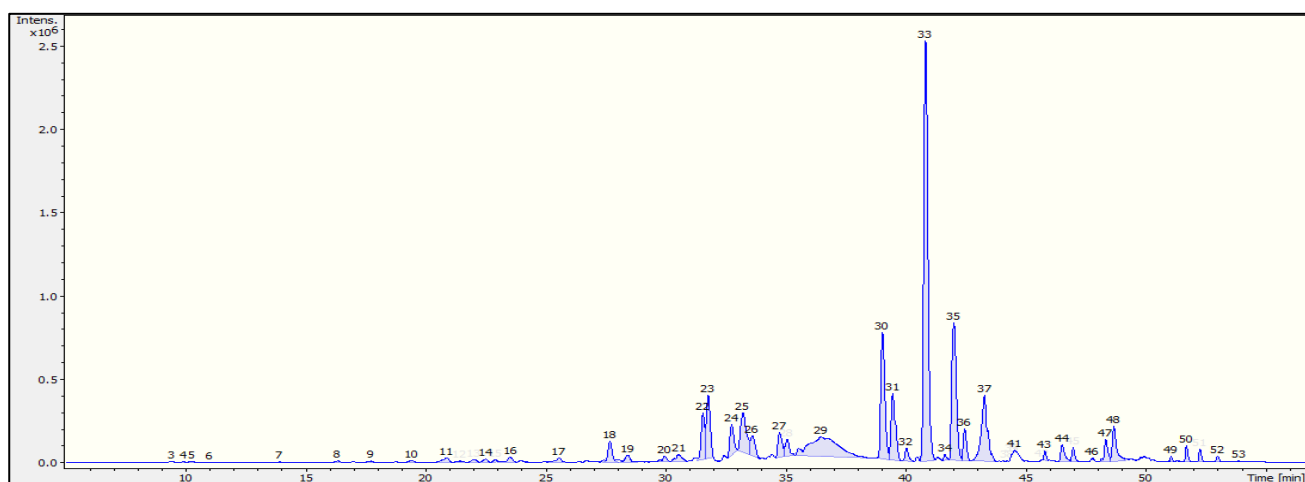

Figure S6. Total ion chromatogram (TIC) of *F. solani* extract (50-minute gradient).
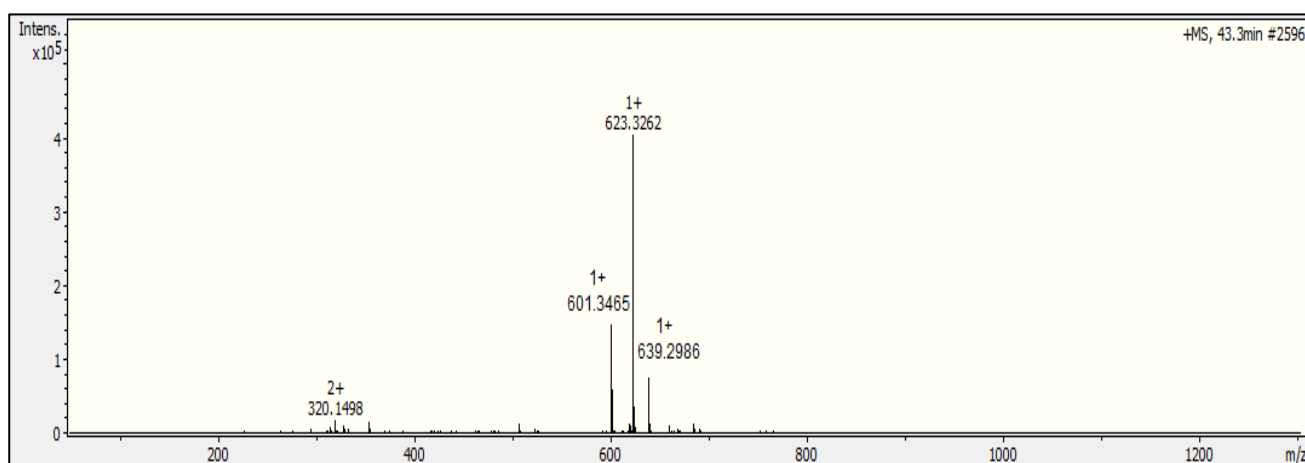

Figure S7. Mass spectra of HA 23. LC-HRMS-ESI at 12.3 minutes on a 50-minute gradient.