Supplementary Information

Antimicrobial Screening of Endophytic Fungi Isolated from the Aerial Parts of *Paepalanthus chiquitensis* (Eriocaulaceae) Led to the Isolation of Secondary Metabolites Produced by *Fusarium fujikuroi*

Felipe Hilário,[a] Vanessa M. Chapla,[b] Angela R. Araujo,[b] Paulo T. Sano,[c] Taís M. Bauab[a] and Lourdes C. dos Santos*[b]

[a]*Departamento de Ciências Biológicas, Faculdade de Ciências Farmacêuticas, Universidade Estadual Paulista (UNESP), 14800-903 Araraquara-SP, Brazil*

[b]*Departamento de Química Orgânica, Instituto de Química, Universidade Estadual Paulista (UNESP), 14800-060 Araraquara-SP, Brazil*

[c]*Departamento de Botânica, Instituto de Biociências, Universidade de São Paulo (USP), 05508-090 São Paulo-SP, Brazil*

Fusaric acid (**1**)

λ / nm 210, 228, 271; IR (KBr) ν / cm^{-1} 3415, 2957, 2924, 2853, 1739, 1638, 1558, 1464, 1400, 1380; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.57 (dd, 1H, *J* 7.8, 2.1 Hz, CH), 8.01 (d, 1H, *J* 7.8 Hz, CH), 7.89 (dd, *J* 7.8, 2.1 Hz, CH), 2.68 (t, *J* 7.8 Hz, CH_2), 1.58 (q, *J* 7.2 Hz. CH_2), 1.30 (sext, *J* 7.2 Hz, CH_2), 0.90 (t, *J* 7.2 Hz, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.6, 148.8, 145.6, 142.1, 137.7, 124.1, 32.5, 31.7, 21.7, 0.9. HRMS (ESI QTOF) *m/z*, observed: 180.1919; $C_{14}H_{14}N_3O$ $[M]^-$ requires: 180.1917.

Indol acetic acid (**2**)

λ / nm 225, 278; ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.48 (dd, 1H, *J* 7.2, 2.0 Hz, CH), 7.36 (dd, 1H, *J* 7.1, 0.8 Hz, CH), 7.23 (d, 1H, *J* 2.4 Hz, CH), 7.10 (dt, 1H, *J* 8.1, 7.2, 1.0 Hz, CH), 6.98 (dt, *J* 7.8 Hz, CH), 3.63 (s, 1H, CH), 1.30 (sext, *J* 7.2 Hz, CH_2), 0.90 (t, *J* 7.2 Hz, CH_3); ^{13}C NMR (75 MHz, DMSO-d_6) δ 173.2, 136.1, 127.2, 123.9, 121.0, 118.4, 111.4, 107.7, 31.0. (ESI-QTRAP-MS) *m/z*, observed: 174.0; $C_{14}H_{14}N_3O$ $[M + H]^+$.

2-(4-Butylpicolinamide) acetic acid (**3**)

λ / nm 232, 272; IR (KBr) ν / cm^{-1} 3356, 2953, 2923, 2868, 1545, 1460, 1407, 1362; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.50 (brs, NH), 8.37 (brs, 1H, CH), 8.05 (brs, 1H, CH), 7.60 (brs, 1H, CH), 4.09 (brs, 2H, CH_2), 2.65 (brs, 2H, CH_2), 1.59 (brs, 2H, CH_2), 1.34 (brs, 2H, CH_2), 0.92 (t, 3H, *J* 7.2 Hz, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.5, 165.5, 148.7, 147.0, 141.8, 137.2, 122.3, 41.9, 33.2, 33.1, 22.3, 14.0. HRMS (ESI QTOF) *m/z*, observed: 237.1239; $C_{14}H_{14}N_3O$ $[M]^+$ requires: 237.1237.

*e-mail: loursant@gmail.com

Terpestacin (**4**)

λ / nm 203, 264; ^{1}H NMR (600 MHz, DMSO-d_6) δ 5.26 (m, 1H, CH), 5.23 (m, 1H, CH), 5.10 (m, 1H, CH), 3.81 (dd, 1H, *J* 9.6, 4.6 Hz, CH), 3.60 (m, 1H, CH), 3.48 (m, 1H, CH), 2.78 (m, 1H, CH), 2.62 (m, 1H, CH), 2.32 (m, 1H, CH), 2.24 (m, 1H, CH), 2.23 (m, 1H, CH), 2.16 (m, 1H, CH), 2.06 (s, 1H, CH), 0.98 (s, 1H, CH), 1.97 (s, 1H, CH), 1.69 (s, 1H, CH), 1.62 (1H, CH), 1.58 (s, 1H, CH), 1.58 (s, 3H, CH_3), 1.48 (s, 3H, CH_3), 1.46 (s, 3H, CH_3), 1.16 (d, 3H, *J* 7.2 Hz, CH_3), 0.85 (s, 3H, CH_3); ^{13}C NMR (150 MHz, DMSO-d_6) δ 207.5, 150.6, 147.4, 136.9, 136.2, 132.6, 127.2, 123.5, 122.4, 74.4, 64.0, 48.8, 48.3, 39.2, 40.2, 37.5, 34.7, 30.4, 28.7, 23.5, 16.2, 16.3, 15.8, 14.4, 10.5; (ESI QTRAP-MS) *m/z*, observed: 401.3; $C_{25}H_{38}O_4$ [M – H] $^{-}$.

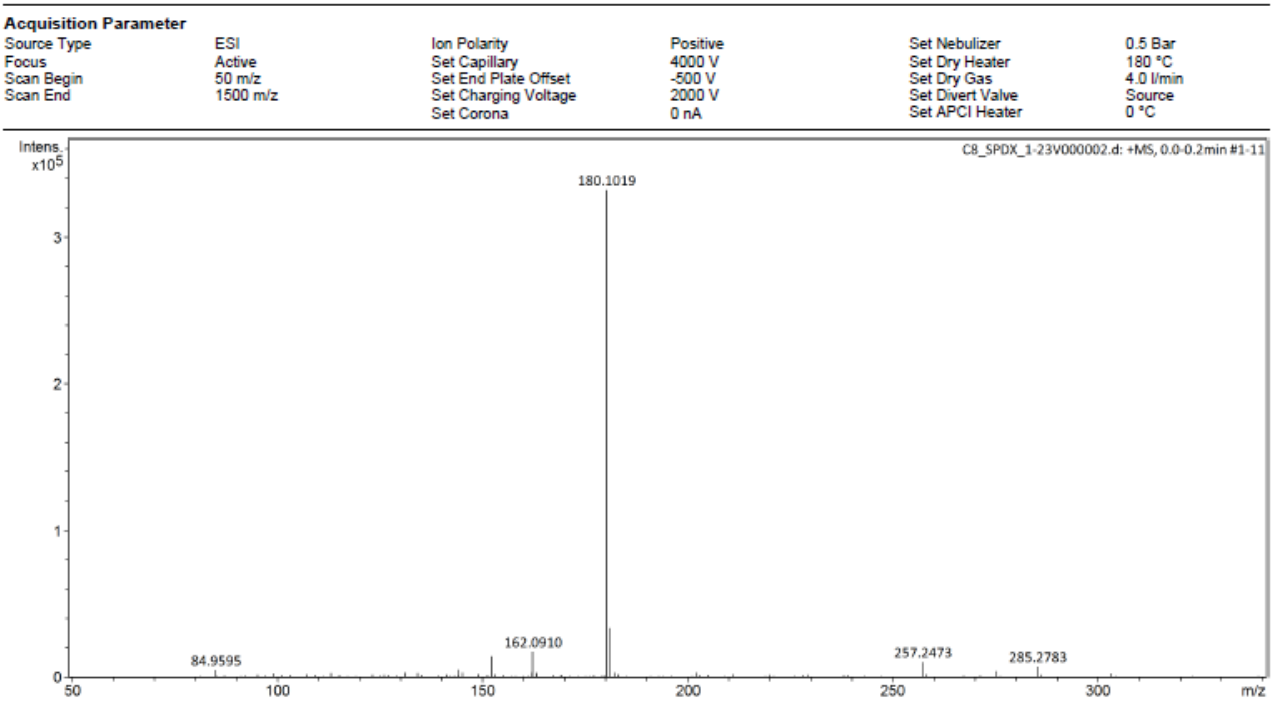


Figure S1. Mass spectrum of compound **1**.

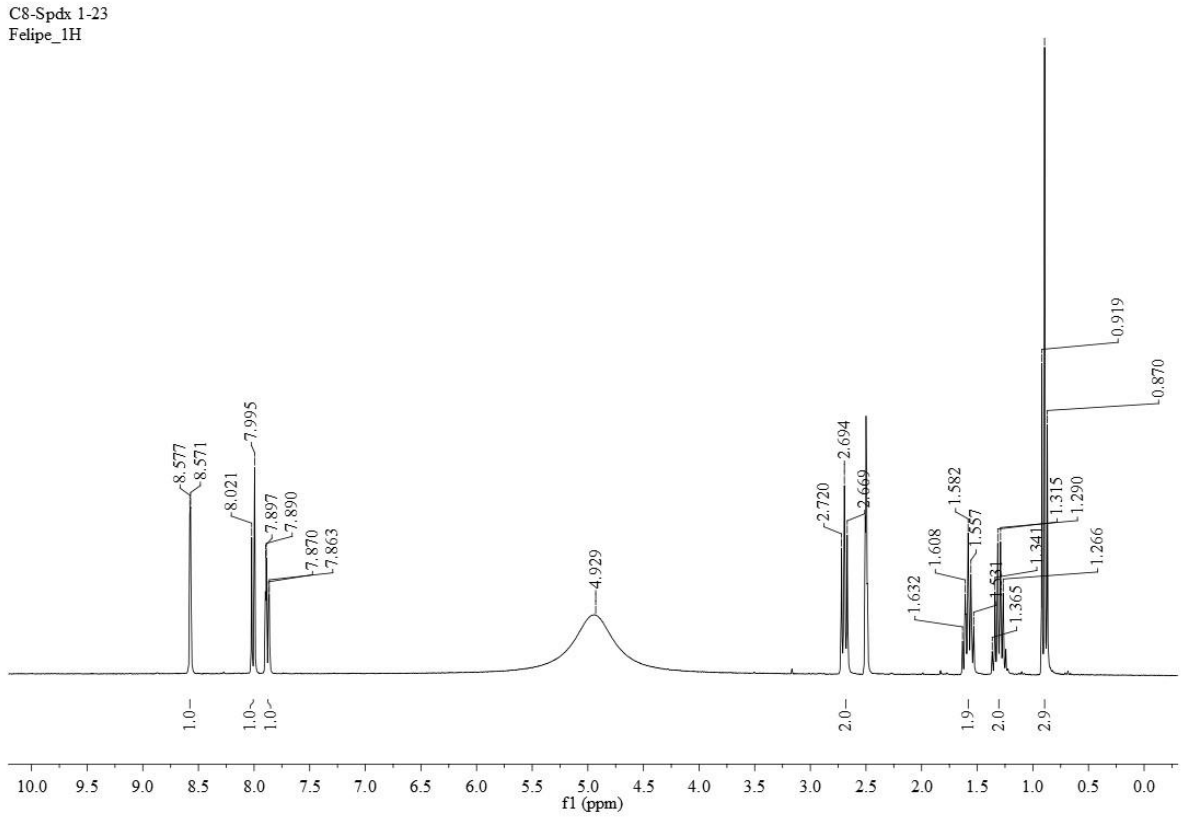


Figure S2. ^{1}H NMR spectrum (300 MHz, DMSO-d_6) of compound **1**.

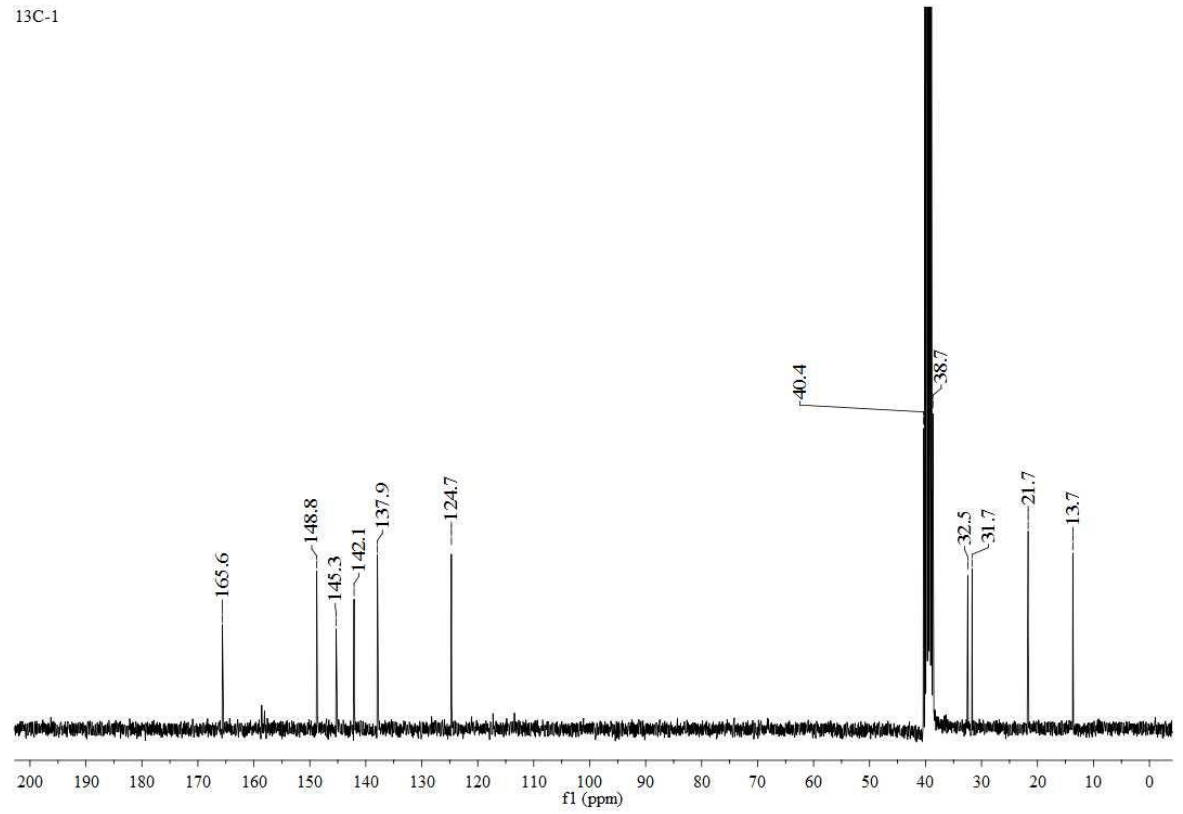


Figure S3. ^{13}C NMR spectrum (75 MHz, DMSO-d_6) of compound **1**.

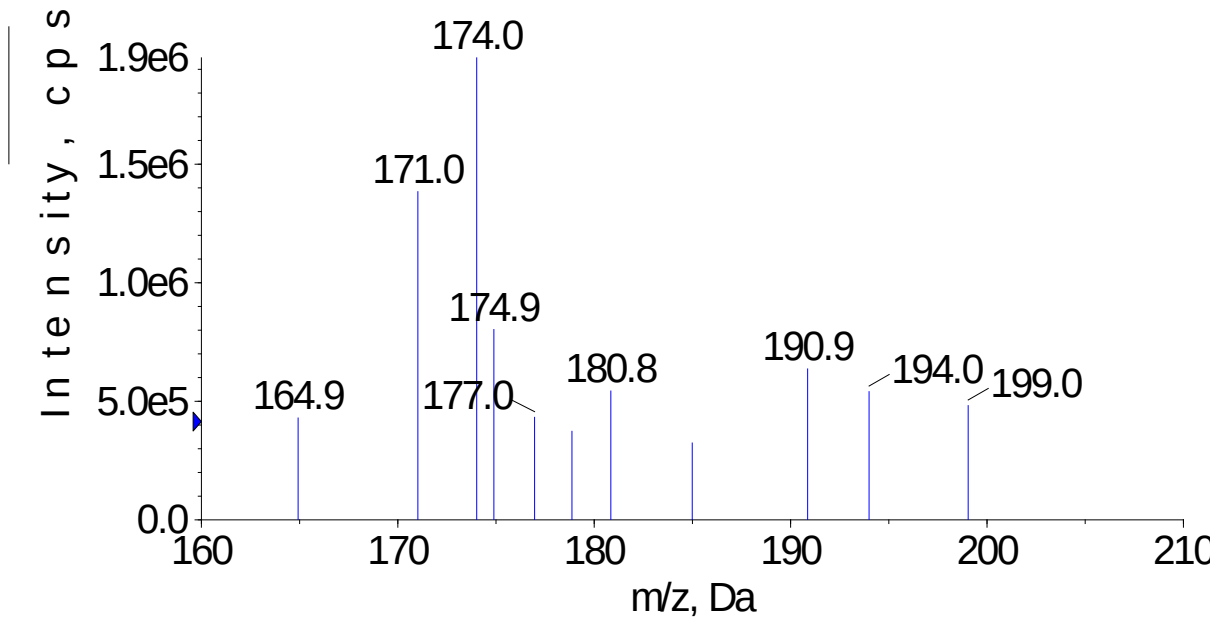


Figure S4. Mass spectrum of compound **2**.

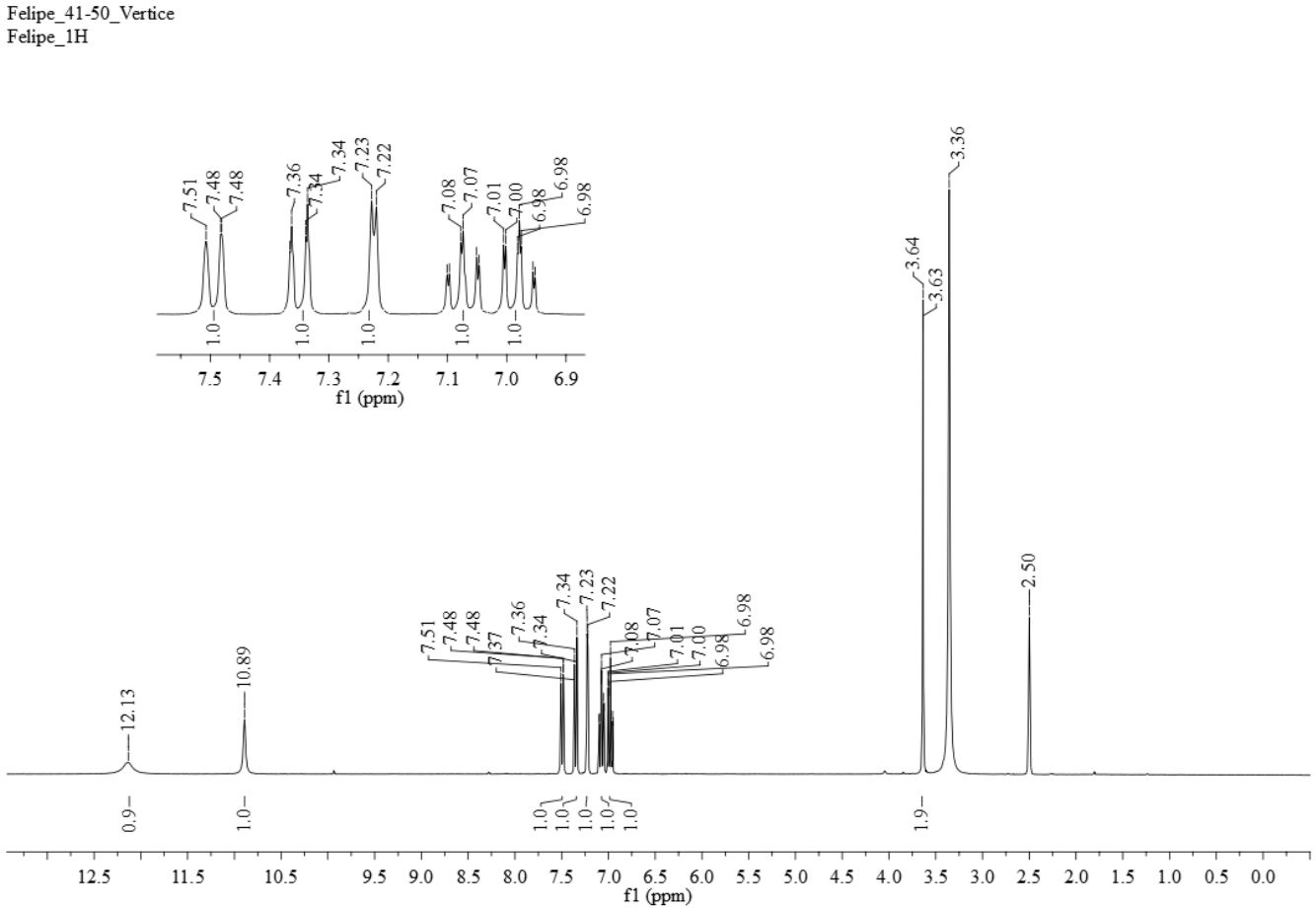


Figure S5. ^{1}H NMR spectrum (300 MHz, DMSO-d_6) of compound **2**.

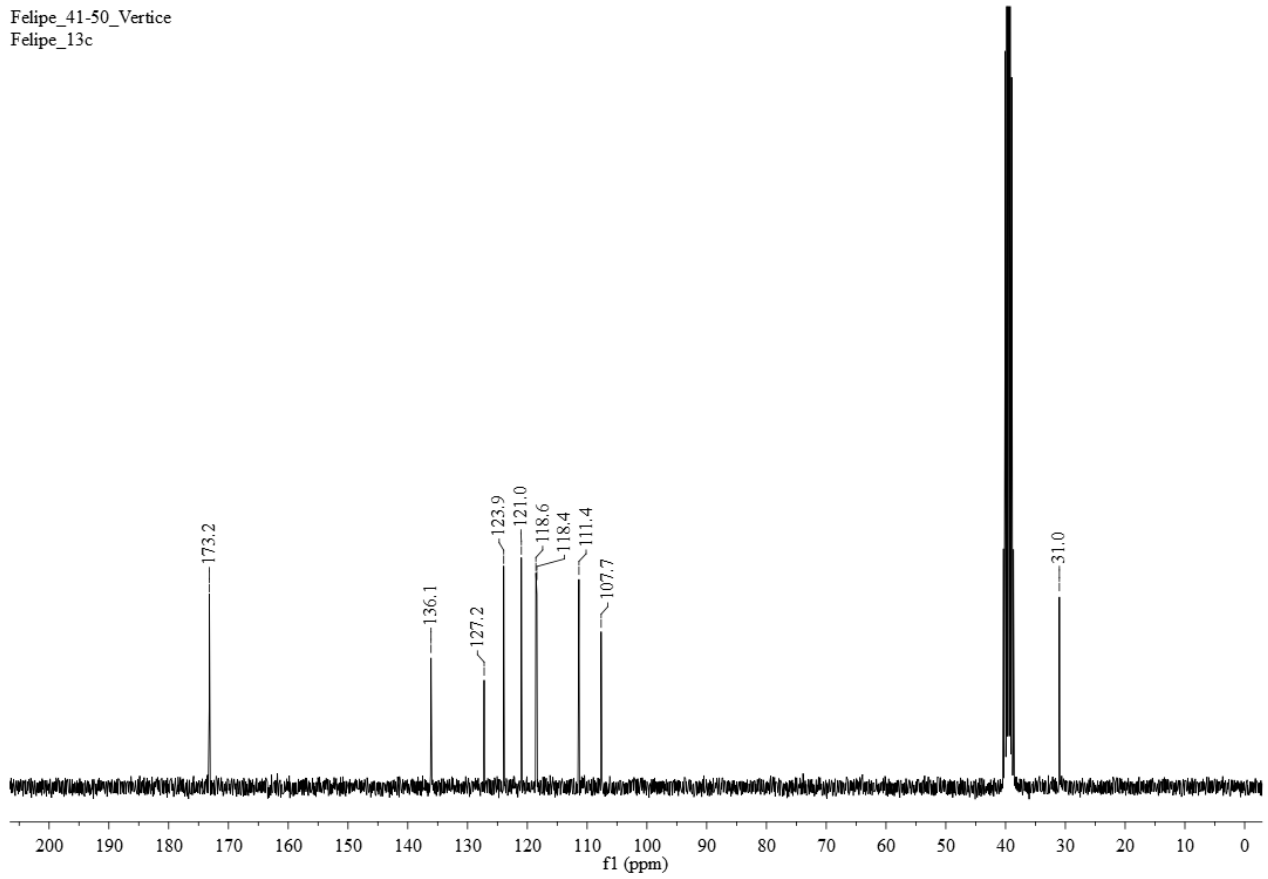


Figure S6. ^{13}C NMR spectrum (75 MHz, DMSO-d_6) of compound **2**.

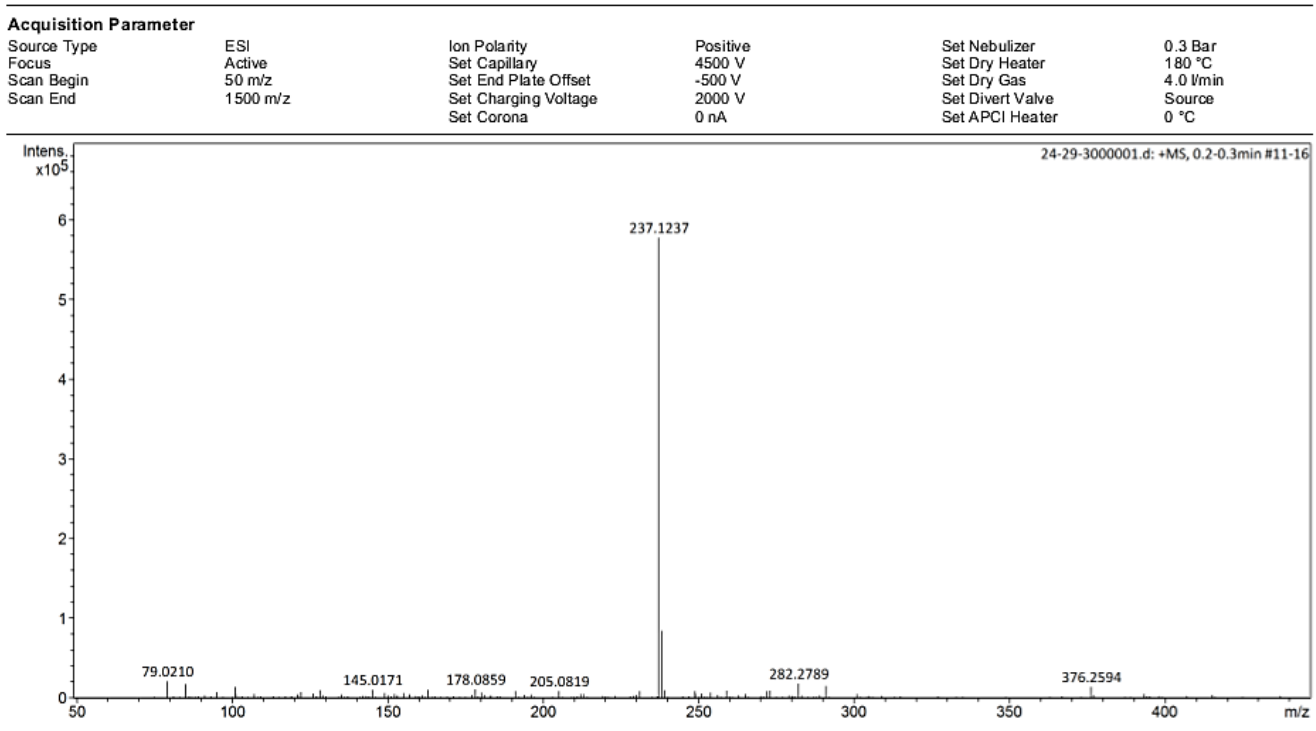


Figure S7. High resolution mass spectrum of compound **3**.

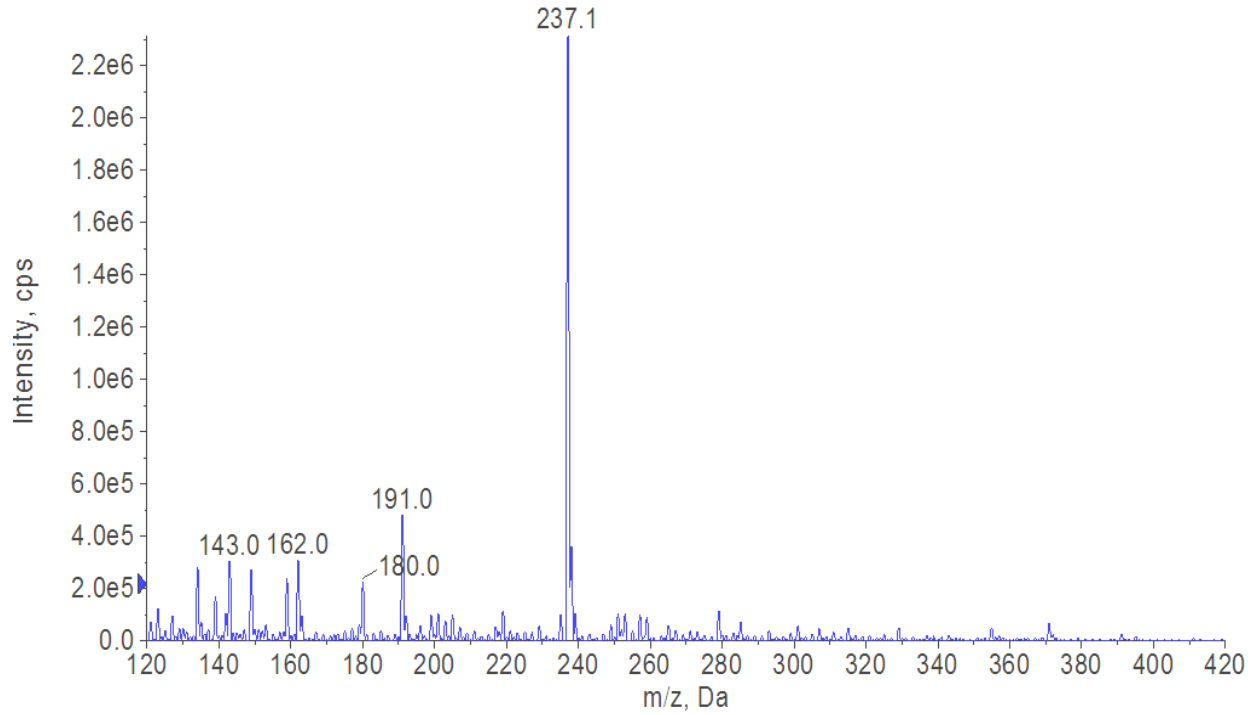


Figure S8. ESI-QTrap-MS spectrum of compound **3** (positive mode).

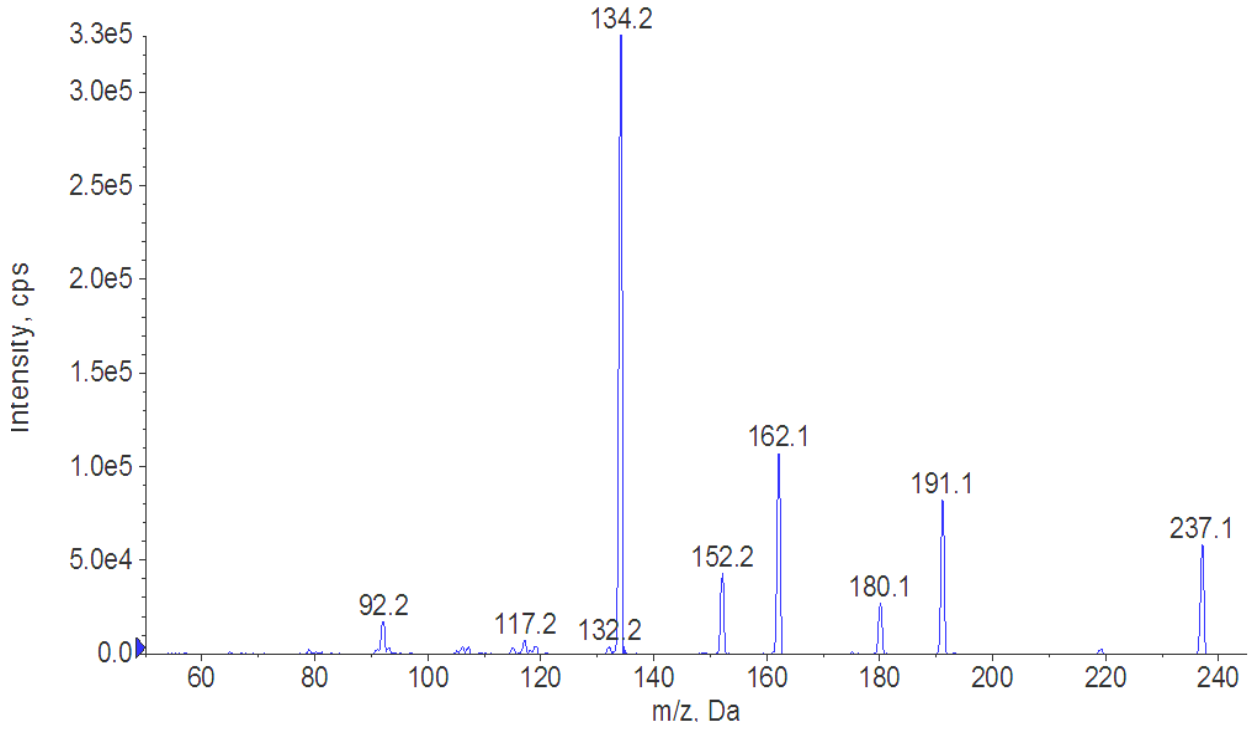


Figure S9. ESI-QTrap-MS/MS spectrum of compound **3** (positive mode).

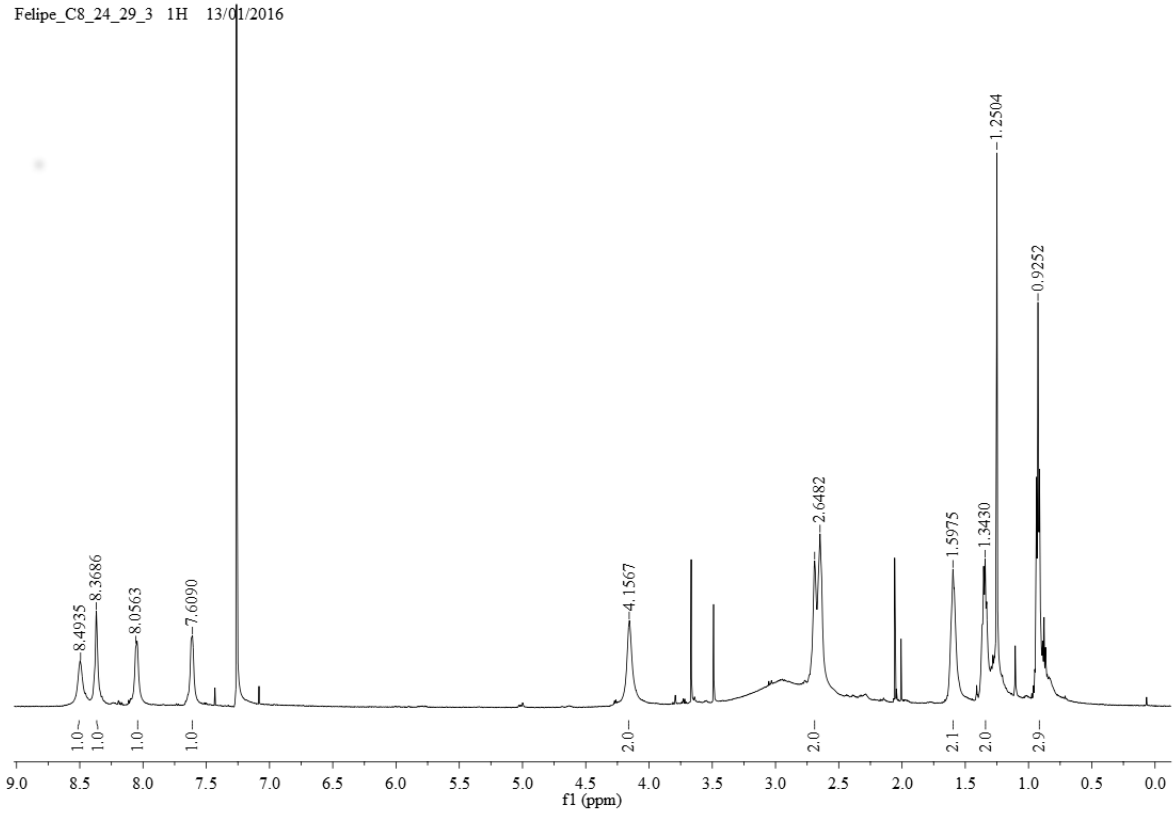


Figure S10. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **3**.

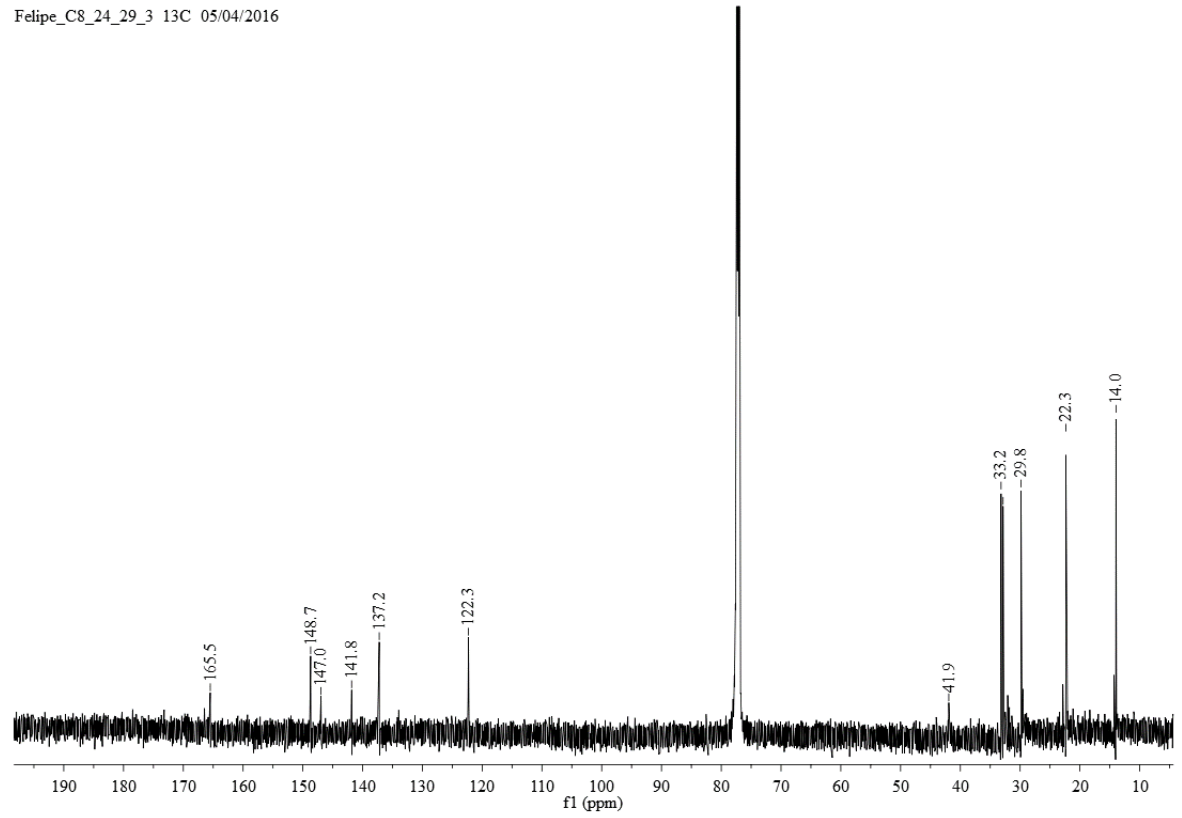


Figure S11. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound **3**.

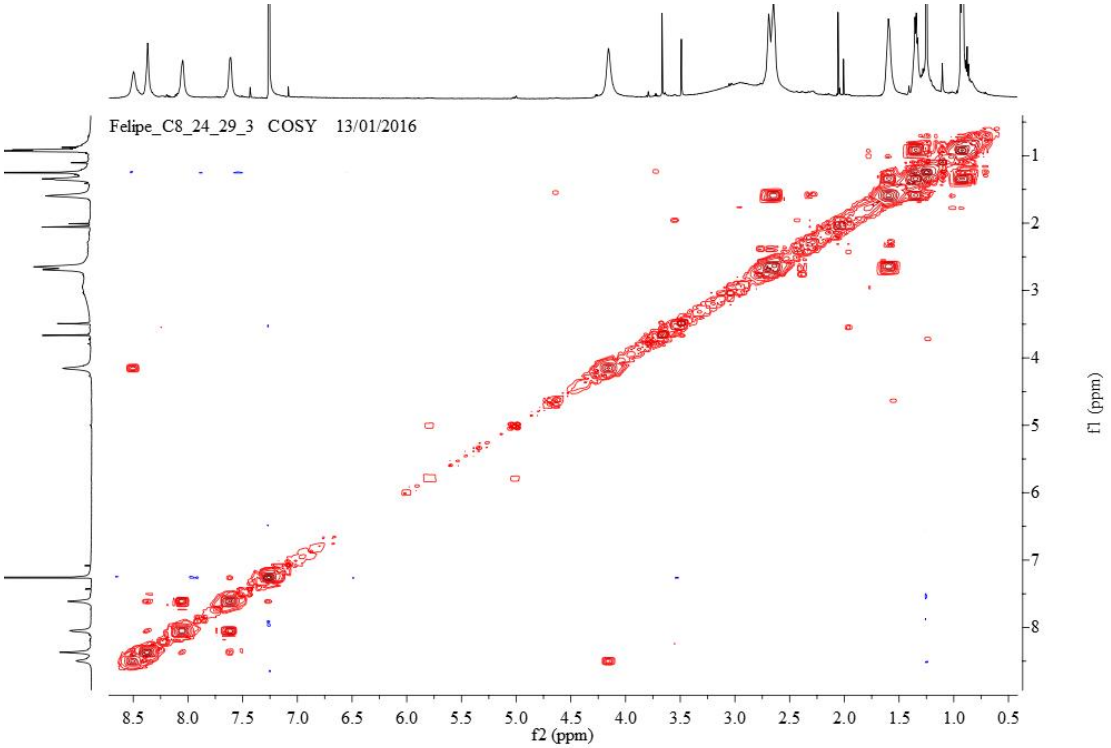


Figure S12. COSY spectrum of compound **3**.

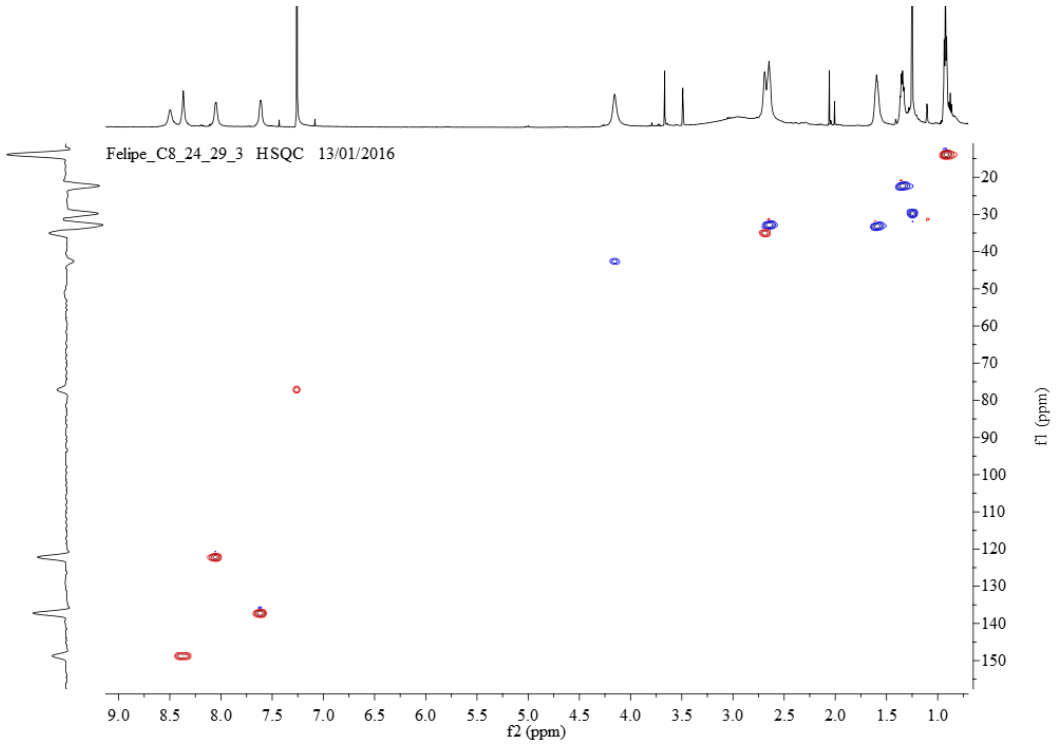


Figure S13. HSQC spectrum of compound **3**.

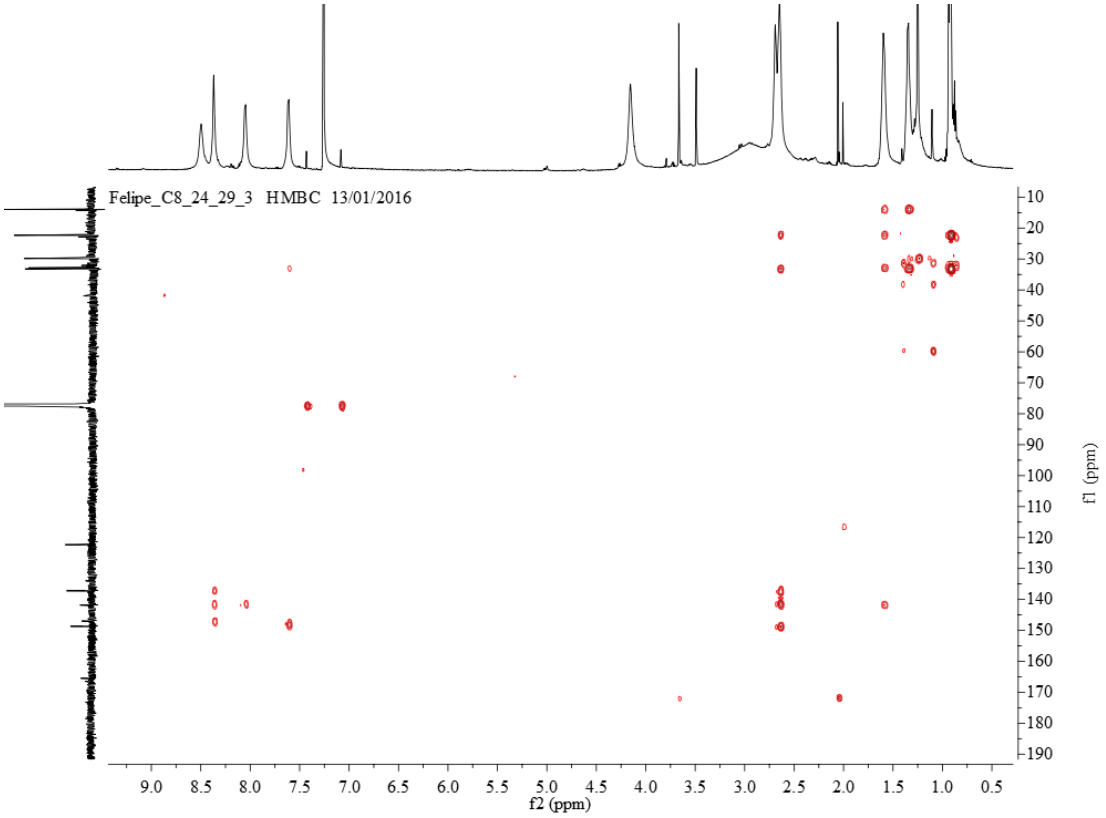


Figure S14. HMBC spectrum of compound **3**.

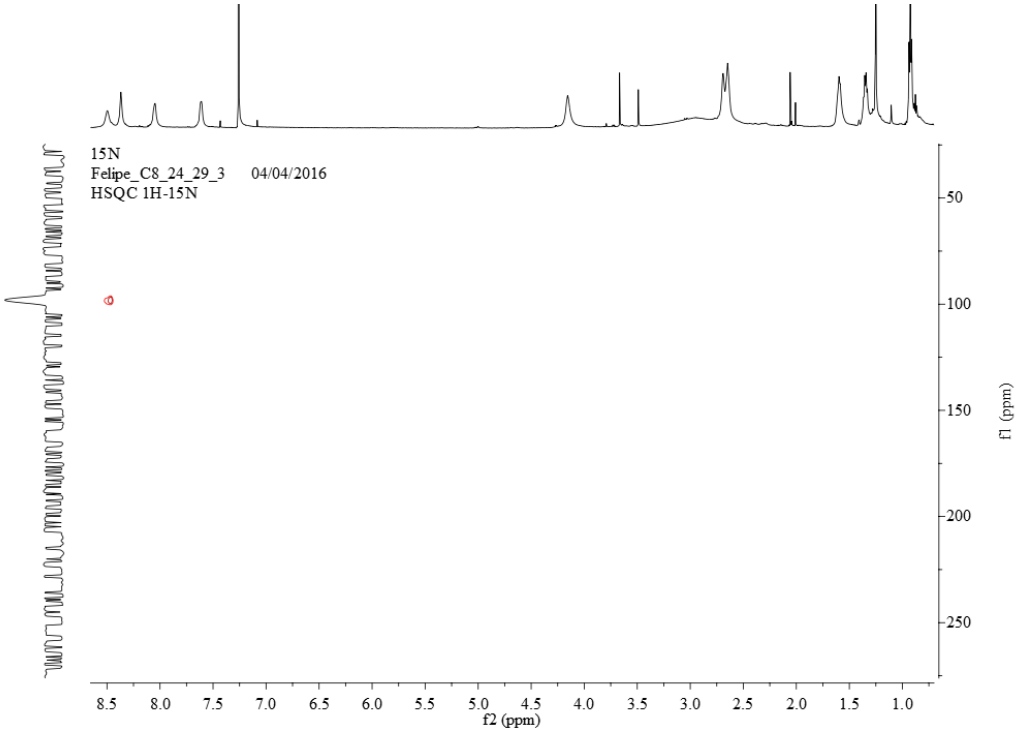


Figure S15. HSQC ^{15}N spectrum of compound **3**.

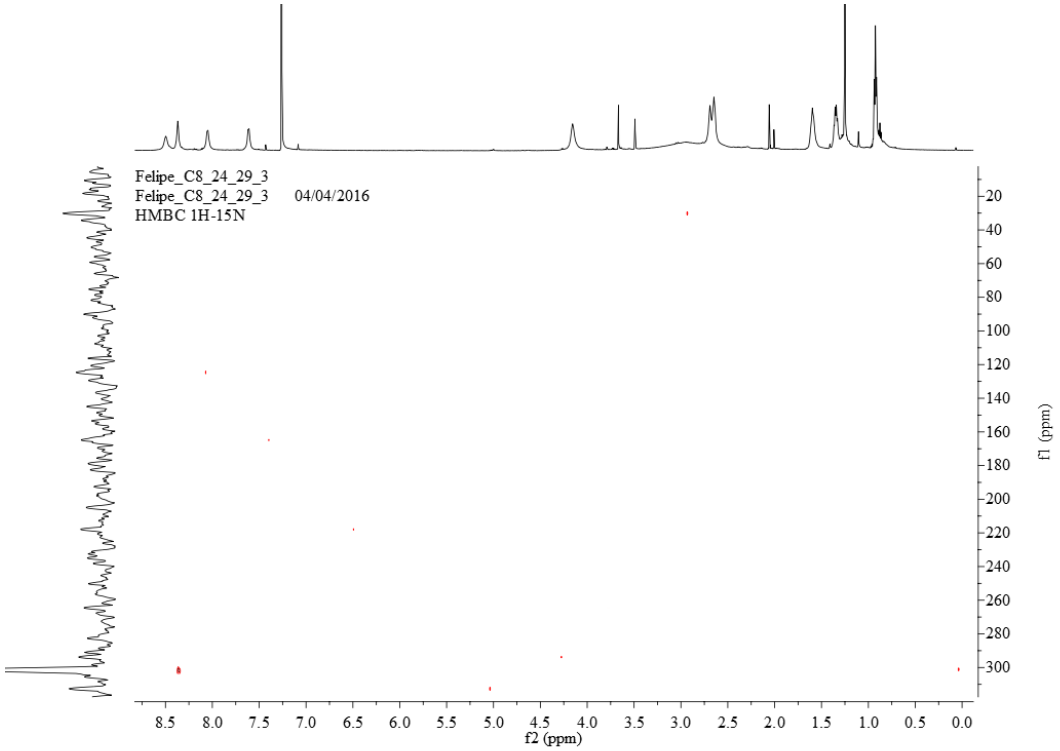


Figure S16. HMBC ^{1}H-^{15}N spectrum of compound **3**.

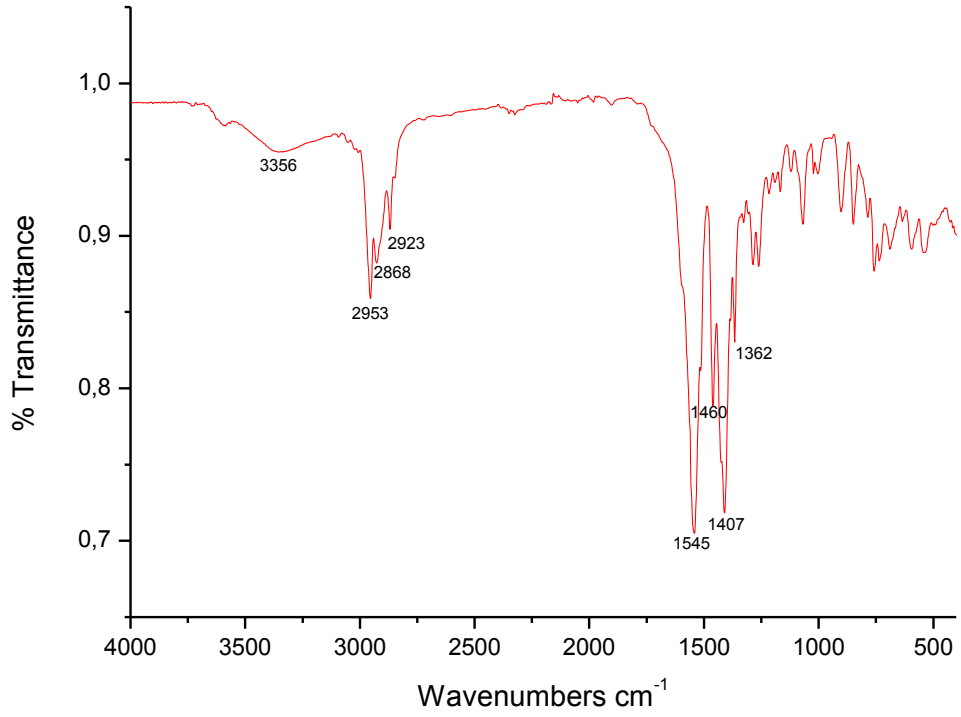


Figure S17. FTIR spectrum of compound **3**.

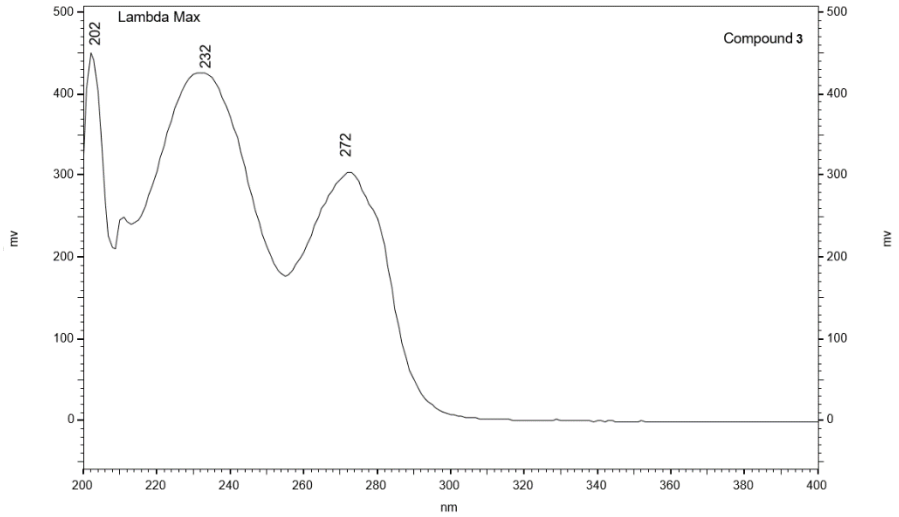


Figure S18. UV spectrum of compound **3**.

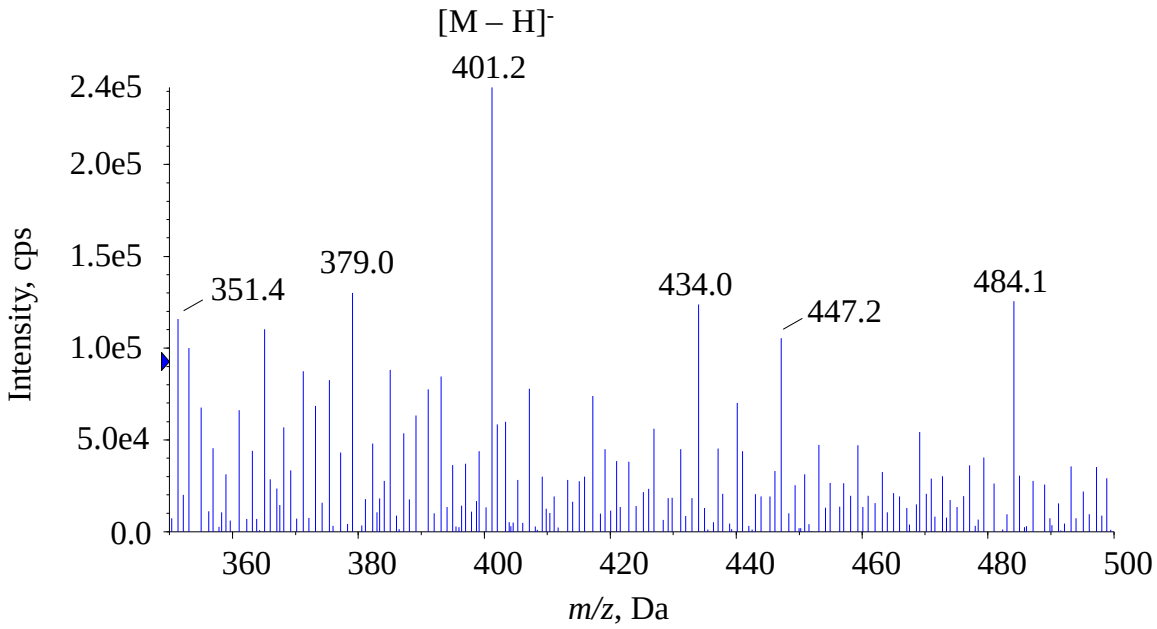


Figure S19. Mass spectrum of compound **4**.

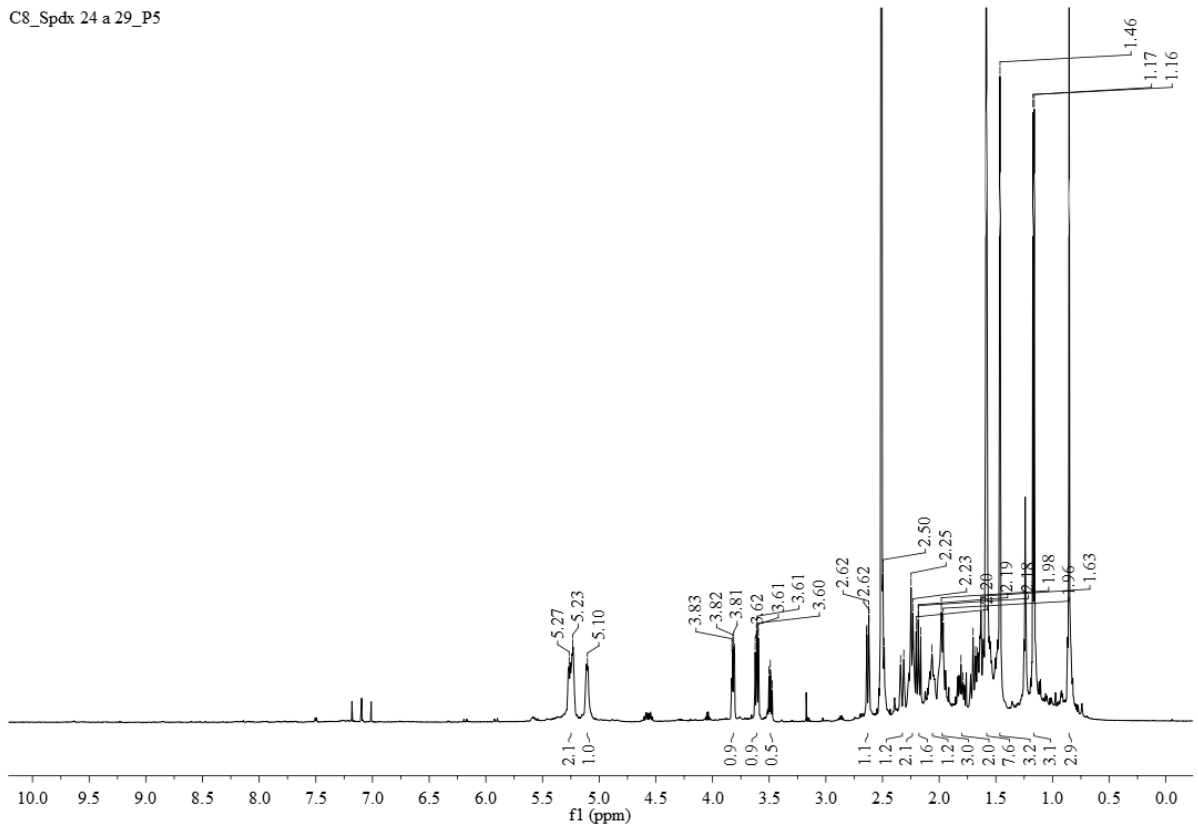


Figure S20. ^{1}H NMR spectrum (600 MHz, DMSO-d_6) of compound **4**.

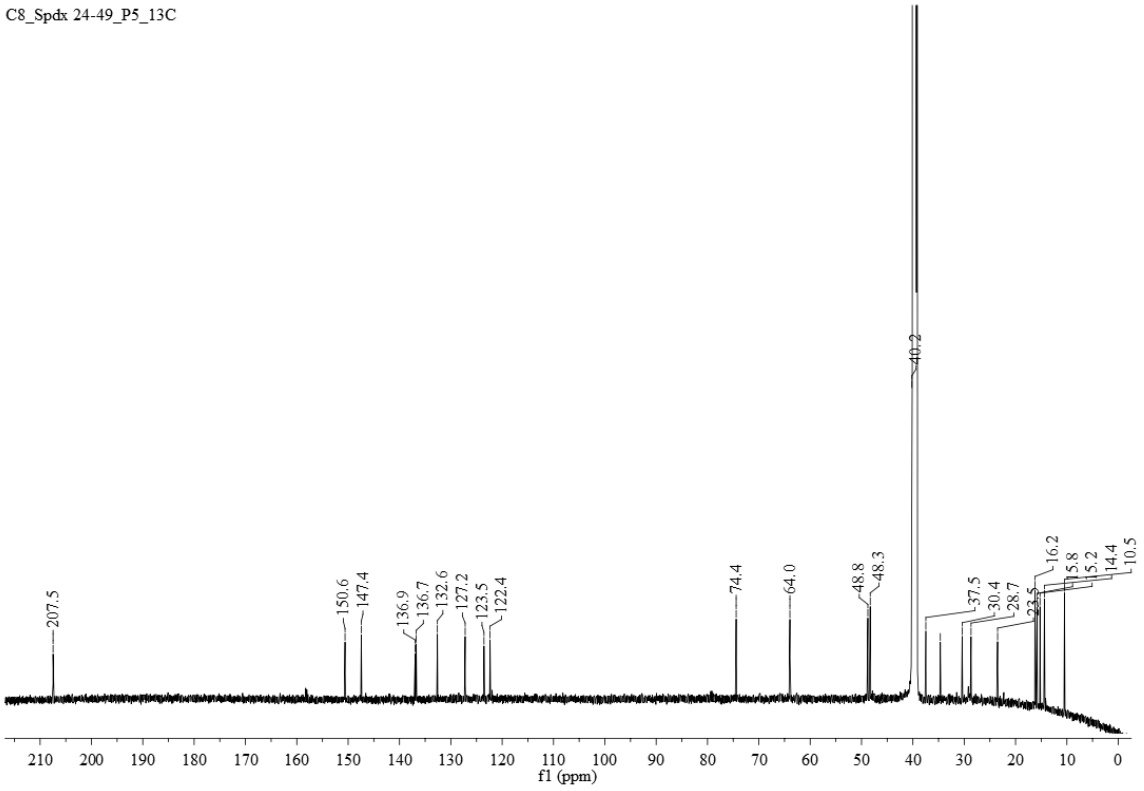


Figure S21. ^{13}C NMR spectrum (150 MHz, DMSO-d_6) of compound **4**.

Fungal identification

Fusarium fujikuroi isolate FZ04 18S ribosomal RNA gene, partial sequence; internal transcribed spacer 1, 5.8S ribosomal RNA gene, and internal transcribed spacer 2, complete sequence; and 28S ribosomal RNA gene, partial sequence

CCTTCCGTAGGGGTGACCTGCGGAGGGATCATTACCGAGTTTACAACTCCCAAACCCCTGTGAACATACC
AATTGTTGCCTCGGCGGATCAGCCCGCTCCCGGTAAAACGGGACGGCCCGCCAGAGGACCCCTAAACTCT
GTTTCTATATGTAACTTCTGAGTAAAACCATAAATAAATCAAAACTTTCAACAACGGATCTCTTGGTTCTG
GCATCGATGAAGAACGCAGCAAAATGCGATAAGTAATGTGAATTGCAGAATTCAGTGAATCATCGAATCT
TTGAACGCACATTGCGCCCGCCAGTATTCTGGCGGGCATGCCTGTTCGAGCGTCATTTCAACCCTCAAGCC
CAGCTTGGTGTTGGGACTCGCGAGTCAAATCGCGTTCCCCAAATTGATTGGCGGTCACGTCGAGCTTCCAT
AGCGTAGTAGTAAAACCCTCGTTACTGGTAATCGTCGCGGCCACGCCGTTAAACCCCAACTTCTGAATGTT
GACCTCGGATCAGGTAGGAATACCCGCTGAACTTAAGCATATCAATAAGGCGGAGGAA

LOCUS KJ000432 552 bp DNA linear PLN 29-MAR-2014
DEFINITION Fusarium fujikuroi isolate FZ04 18S ribosomal RNA gene, partial sequence; internal transcribed spacer 1, 5.8S ribosomal RNA gene, and internal transcribed spacer 2, complete sequence; and 28S ribosomal RNA gene, partial sequence.
ACCESSION KJ000432
VERSION KJ000432.1 GI:5915089870
KEYWORDS .
SOURCE *Fusarium fujikuroi* (*Gibberella fujikuroi*)
ORGANISM *Fusarium fujikuroi*
Eukaryota; Fungi; Dikarya; Ascomycota; Pezizomycotina; Sordariomycetes; Hypocreomycetidae; Hypocreales; Nectriaceae; *Fusarium*; *Fusarium fujikuroi* species complex.
REFERENCE 1 (bases 1 to 552)
AUTHORS Lin,Z., Que,Y. and Zhang,M.
TITLE Race specific quantitative TaqMan real-time PCR for detection and identification of *Fusarium* moniliforme, pathogen of sugarcane Pokkah boeng
JOURNAL Unpublished
REFERENCE 2 (bases 1 to 552)
AUTHORS Lin,Z., Que,Y. and Zhang,M.
TITLE Direct Submission
JOURNAL Submitted (26-DEC-2013) National Sugarcane Industry Research Center, Sugarcane Research Institute of Fujian Agriculture and Forestry University, Cangshan, Fuzhou, Fujian 3200000, China

> Sequencia Consenso_(MC-002)

ttccgtaggggtgacctgcggagggatcattaccgagtttacaactcccaaaccccctgtg

aacataccaattgttgcctcggcggatcagcccgctcccggtaaaacggGAcggcccgcc

agaggacccctaaactctgtttctatatgtaacttctgagtaaaaccataaataaatcaa

aactttcaacaacggatctcttggttctggcatcgatgaagaacgcagcaaaatgcgata

agtaatgtgaattgcagaattcagtgaatcatcgaatctttgaacgcacattgcgcccgc

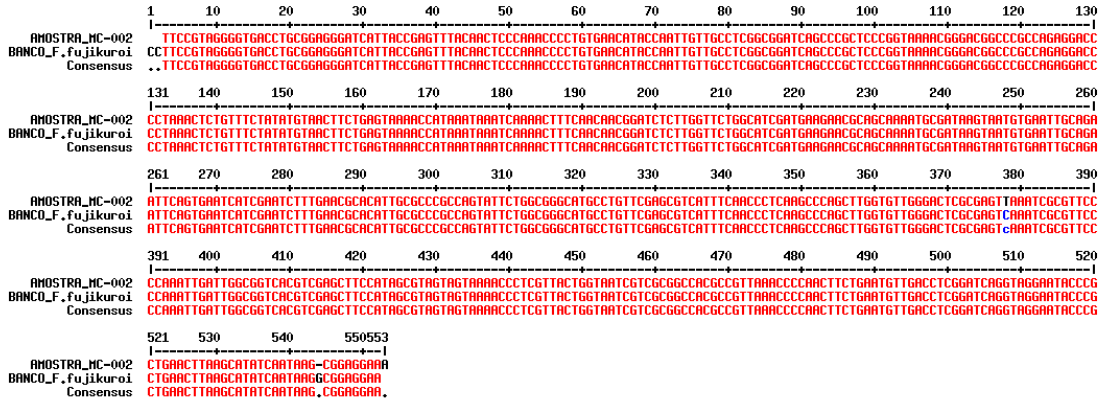
cagtattctggcgggcatgcctgttcgagcgtcatttcaaccctcaagcccagcttggtg

ttgggactcgcgagttaaatcgcgttccccaaattgattggcggtcacgtcgagcttcca

tagcgtaGtagtaaaaccctcgttactggtaatcgtcgcggccacgccgttaaaccccaa

cttctgaatgttgacctcggatcaggtaggaatacccgctgaacttaagcatatcaataa

gcggaggaaa



Informações adicionais amostras

Max score: 1003

Query cover: 99%

E value: 0,0

Identidade: 99%

Acession: KJ000432