

Supplementary Information

Production of (10S,11S)-(–)-*epi*-Pyriculol and Its HPLC Quantification in Liquid Cultures of *Pyricularia grisea*, a Potential Mycoherbicide for the Control of Buffelgrass (*Cenchrus ciliaris*)

Jesús G. Zorrilla ^{1,2}, Marco Masi ^{1,*}, Suzette Clement ³, Alessio Cimmino ¹ and Susan Meyer ³

¹ Department of Chemical Sciences, University of Naples Federico II, Complesso Universitario Monte S. Angelo, Via Cintia, 80126 Naples, Italy

² Allelopathy Group, Department of Organic Chemistry, Facultad de Ciencias, Institute of Biomolecules (INBIO), University of Cadiz, C/Avenida República Saharaui, s/n, 11510 Puerto Real, Spain

³ Shrub Sciences Laboratory, U.S. Forest Service Rocky Mountain Research Station, 369 N. 100 West Suite 8, Cedar City, UT 84721, USA

* Correspondence: marco.masi@unina.it

S1. ¹ H NMR spectrum and spectroscopic data of (10S,11S)-(–)- <i>epi</i> -pyriculol (CDCl ₃ ; 400 MHz) .	2
S2. ESI MS spectrum of (10S,11S)-(–)- <i>epi</i> -pyriculol recorded in positive mode	3
S3. Graphical representation of the calibration curve of (10S,11S)-(–)- <i>epi</i> -pyriculol standard	3
S4. Chromatograms of the organic extracts obtained at regular pH and pH 2 of isolates 1-12	4

The chemical structure shows a central carbon atom bonded to two 4-hydroxyphenyl groups and a hydroxyl group. The atoms are numbered as follows: 1 for the aldehyde hydrogen, 2 for the central carbon, 3 for the phenyl carbons attached to the central carbon, 4 for the phenyl carbons ortho to the attachment point, 5 for the phenyl carbons meta to the attachment point, 6 for the phenyl carbons para to the attachment point, 7 for the hydroxyl oxygen, 8 for the aldehyde carbon, 9 for the aldehyde oxygen, 10 for the central carbon, 11 for the hydroxyl oxygen, 12 for the phenyl carbons attached to the central carbon, 13 for the phenyl carbons ortho to the attachment point, 14 for the phenyl carbons meta to the attachment point, and 15 for the phenyl carbons para to the attachment point.

11.86 (1H, s, OH-3); 10.30 (1H, s, H-1); 7.45 (1H, t, $J = 8.0$ Hz, H-5); 7.20 (1H, d, $J = 15.5$ Hz, H-8); 6.90 (2H, m, H-4 and H-6); 6.08 (1H, dd, $J = 15.5$ and 5.4 Hz, H-9); 5.86 (1H, dd, $J = 14.7$ and 6.3 Hz, H-13); 5.56 (1H, dd, $J = 14.7$ and 7.1 Hz, H-12); 4.23 (1H, br s, H-10); 4.04 (1H, br s, H-11); 2.57 (1H, s, OH-10/11); 2.10 (1H, s, OH-10/11); 1.76 (3H, d, $J = 6.3$ Hz, H-14).

S2. ESI MS spectrum of (10*S*,11*S*)-(–)-*epi*-pyriculol recorded in positive mode.

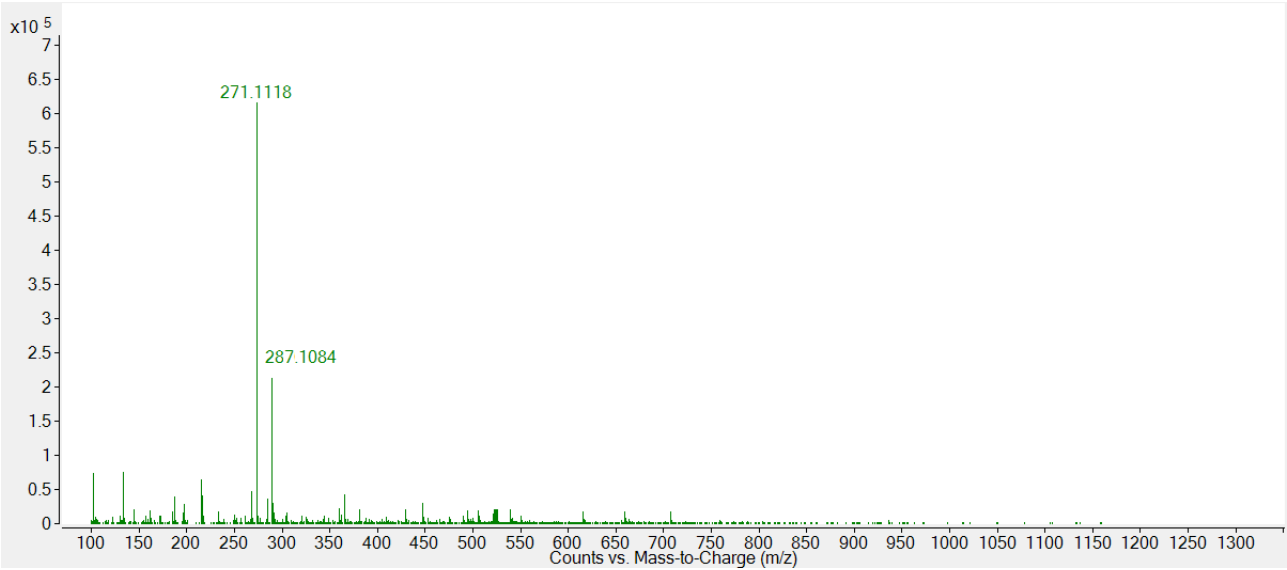


Figure S2. ESI MS spectrum of (10*S*,11*S*)-(–)-*epi*-pyriculol recorded in positive mode.

S3. Graphical representation of the calibration curve of (10*S*,11*S*)-(–)-*epi*-pyriculol standard.

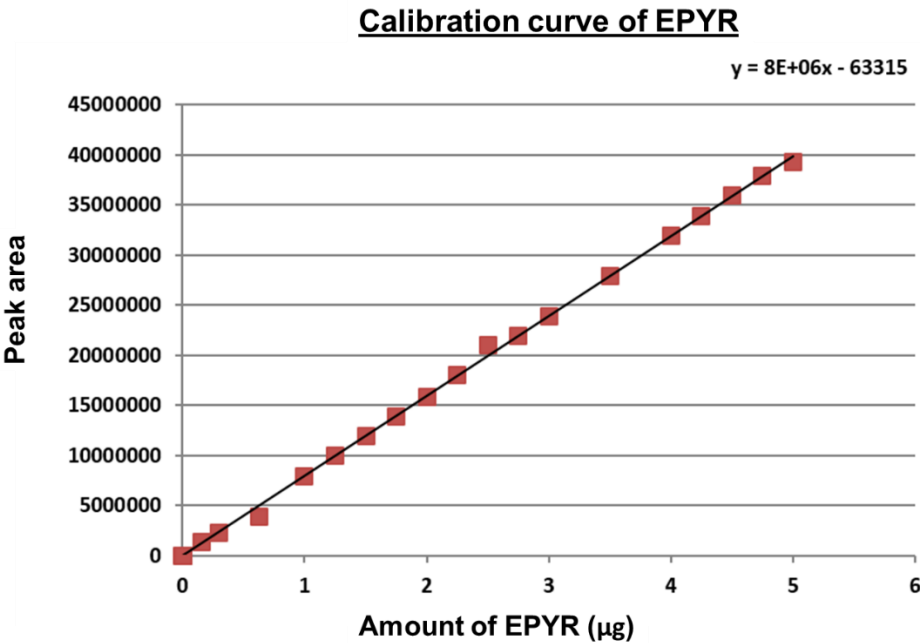


Figure S3. Calibration curve of the (10*S*,11*S*)-(–)-*epi*-pyriculol standard.

S4. Chromatograms of the organic extracts obtained at regular pH and pH 2 of isolates 1-12.

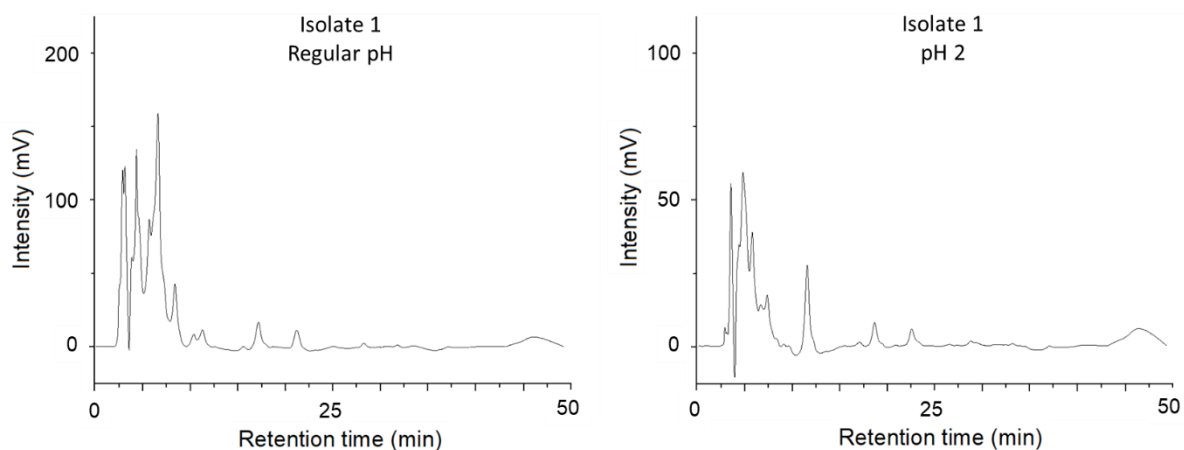


Figure S4. Chromatogram of the organic extract obtained at regular pH (left) and pH 2 (right) of isolate 1 (CB 5B2) analyzed at 2 mg/mL.

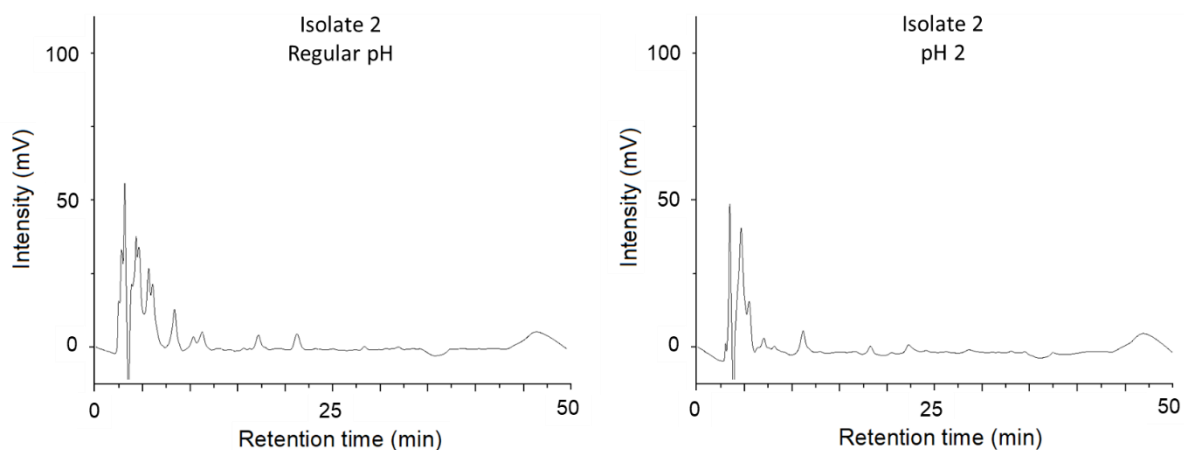


Figure S5. Chromatogram of the organic extract obtained at regular pH (left) and pH 2 (right) of isolate 2 (CB 5C2) analyzed at 2 mg/mL.

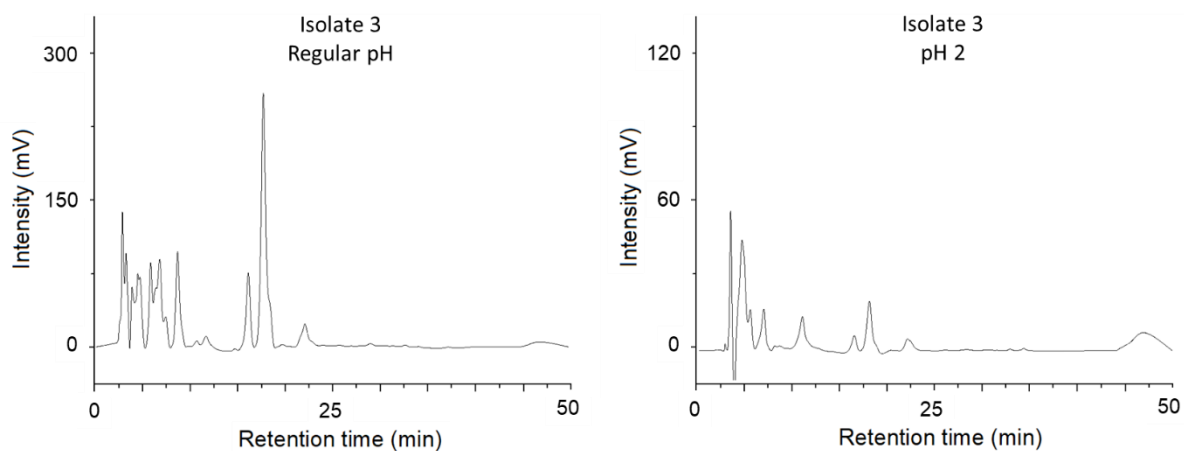


Figure S6. Chromatogram of the organic extract obtained at regular pH (left) and pH 2 (right) of isolate 3 (MR 4D1) analyzed at 2 mg/mL.

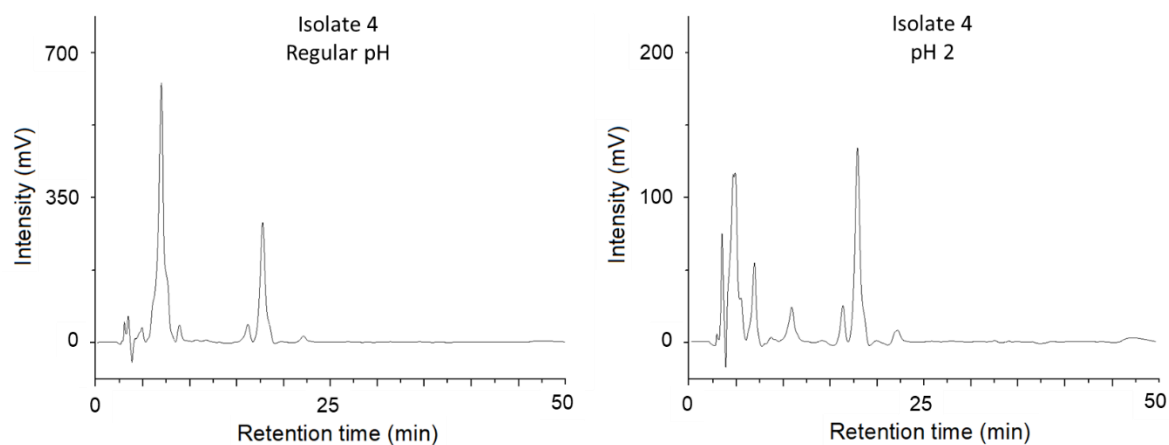


Figure S7. Chromatogram of the organic extract obtained at regular pH (left) and pH 2 (right) of isolate 4 (SNM 2-1A3) analyzed at 2 mg/mL.

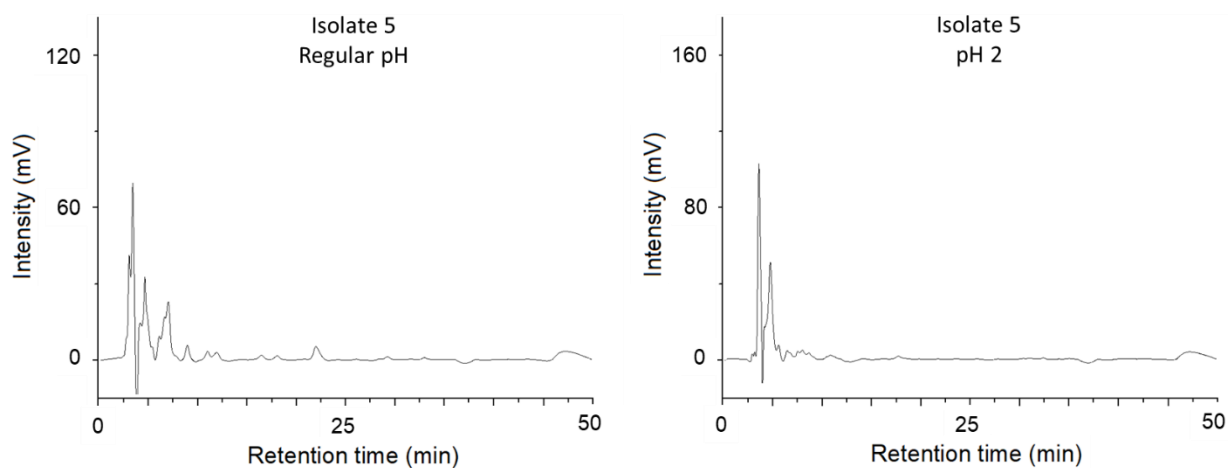


Figure S8. Chromatogram of the organic extract obtained at regular pH (left) and pH 2 (right) of isolate 5 (SNM 2-2A1) analyzed at 2 mg/mL.

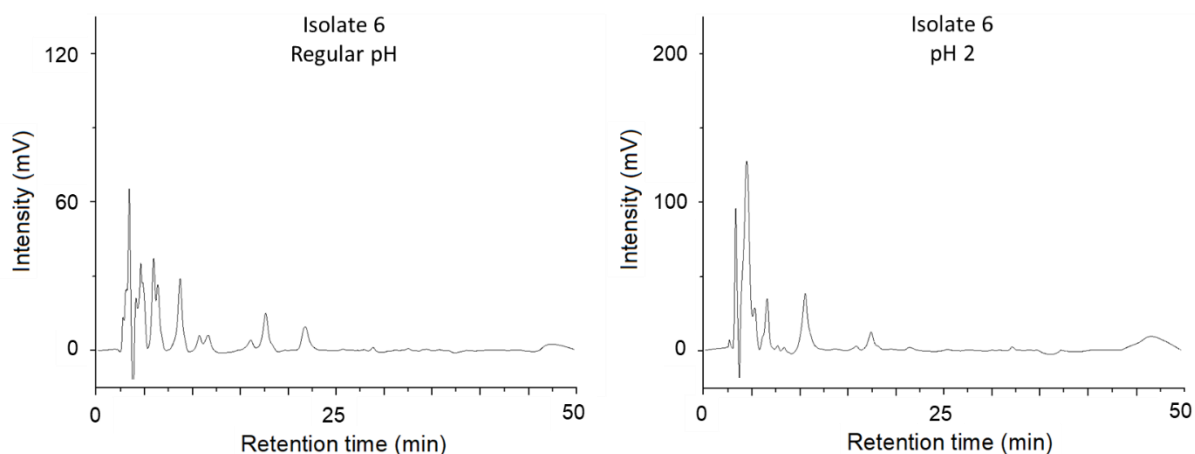


Figure S9. Chromatogram of the organic extract obtained at regular pH (left) and pH 2 (right) of isolate 6 (SNM 2-2A2) analyzed at 2 mg/mL.

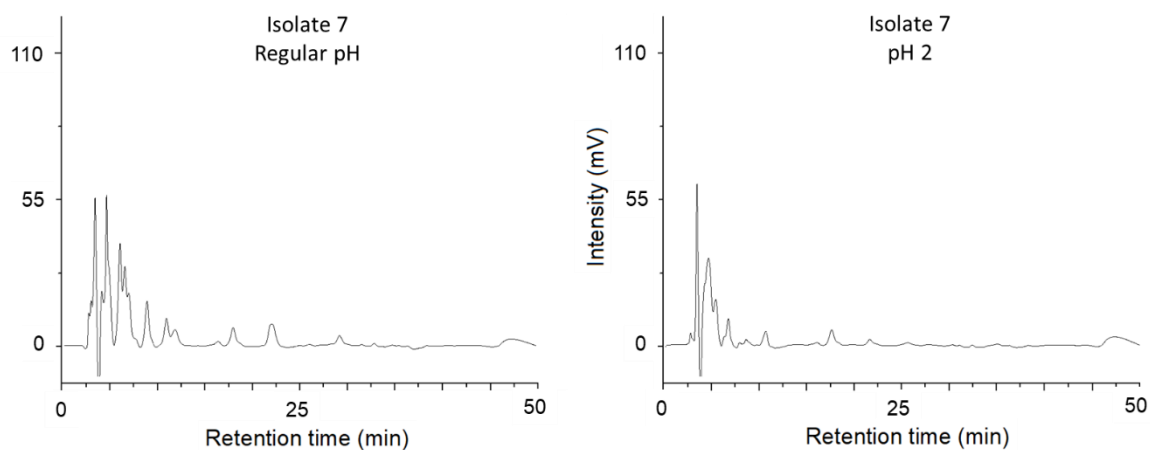


Figure S10. Chromatogram of the organic extract obtained at regular pH (left) and pH 2 (right) of isolate 7 (SNM 3B2) analyzed at 2 mg/mL.

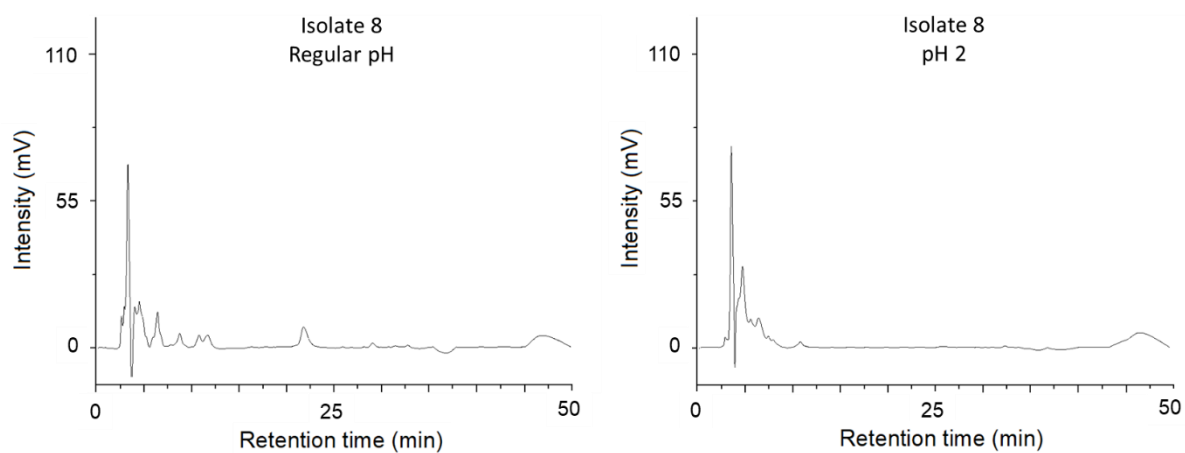


Figure S11. Chromatogram of the organic extract obtained at regular pH (left) and pH 2 (right) of isolate 8 (SNM 3E2A) analyzed at 2 mg/mL.

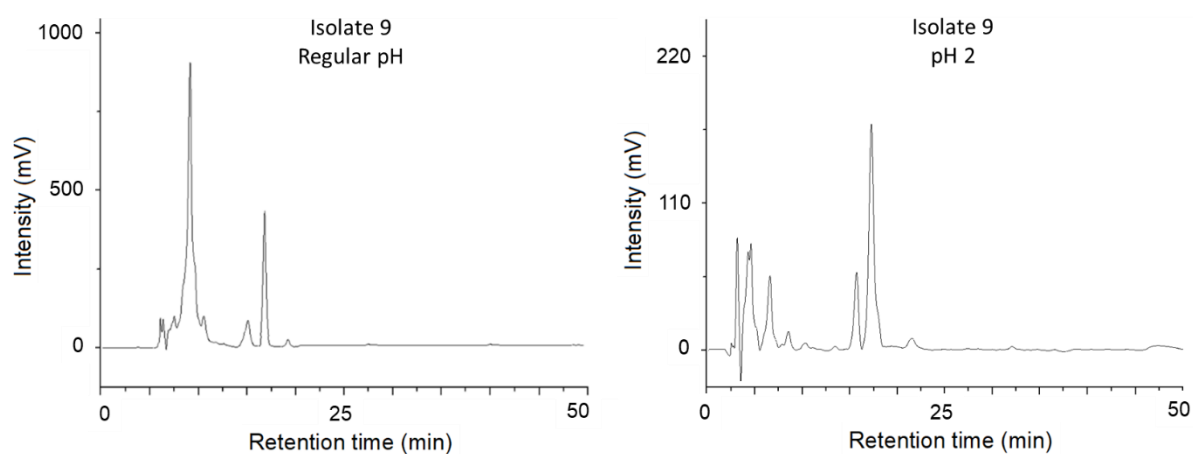


Figure S12. Chromatogram of the organic extract obtained at regular pH (left) and pH 2 (right) of isolate 9 (SNM 5A2) analyzed at 2 mg/mL.

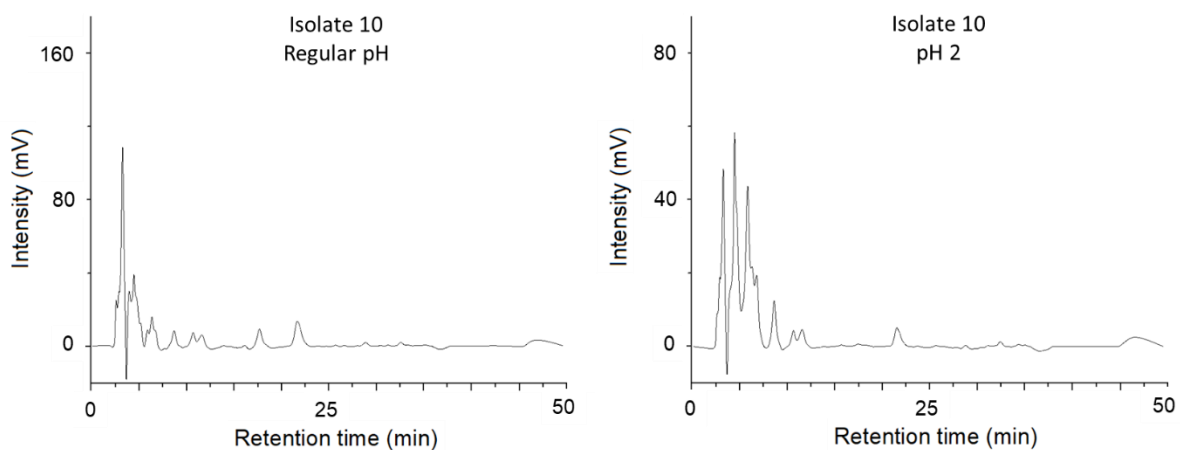


Figure S13. Chromatogram of the organic extract obtained at regular pH (left) and pH 2 (right) of isolate 10 (SNM 5B1) analyzed at 2 mg/mL.

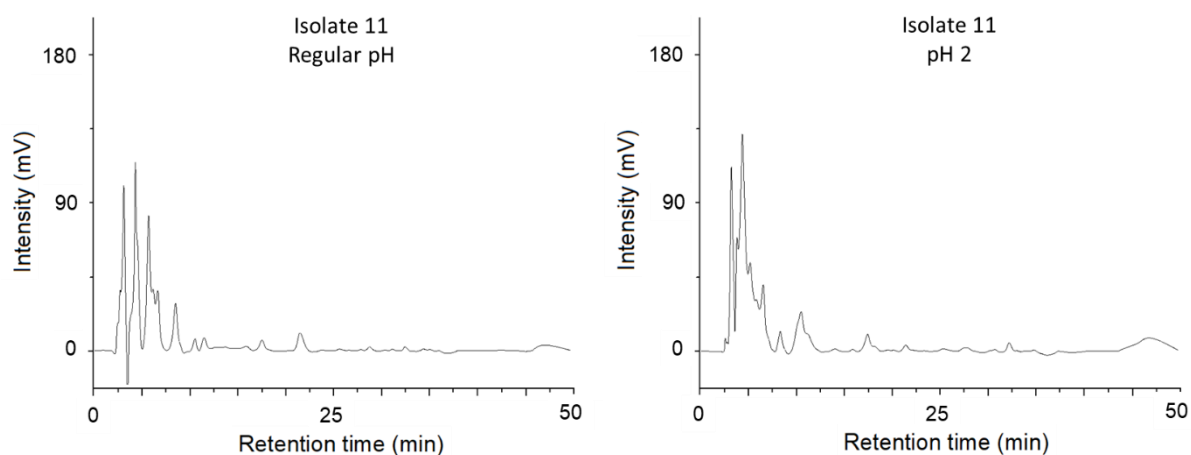


Figure S14. Chromatogram of the organic extract obtained at regular pH (left) and pH 2 (right) of isolate 11 (SNM 5B2) analyzed at 2 mg/mL.

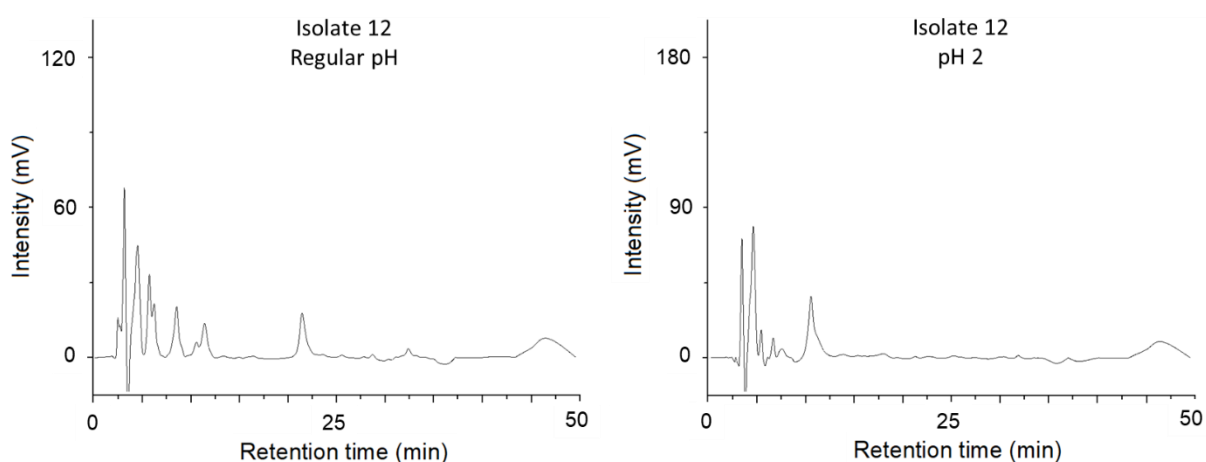


Figure S15. Chromatogram of the organic extract obtained at regular pH (left) and pH 2 (right) of isolate 12 (SNM 5D1) analyzed at 2 mg/mL.