

Supplementary materials

Standardized extract of *Atractylodis rhizoma alba* and *Schisandrae fructus* ameliorates coughing and increases expectoration of phlegm

Hee-Sung Chae¹, Sun Young Kim², Pisey Pel¹, Jungmoo Huh¹, Sun-Woo Joo², Yun Young Lim², Shin Jung Park², Jong Lae Lim² and Young-Won Chin^{1,*}

¹ College of Pharmacy and Research Institute of Pharmaceutical Sciences, Seoul National University, 1, Gwanak-ro, Gwanak-gu, Seoul 08826, Republic of Korea; ywchin@snu.ac.kr, chaeheesung83@gmail.com, jmhu112@gmail.com

² Department of Botanical Drug, Chong Kun Dang (CKD) pharm research Institute, Yongin-si, Gyeonggi-do, and Republic of Korea; syk@ckdpharm.com, sunwoo@ckdpharm.com, yylim@ckdpharm.com, parksj@ckdpharm.com, jllim@ckdpharm.com

* Correspondence: ywchin@snu.ac.kr; Tel.: +82-2-880-7859 (Y.W. Chin.)

Figure S1. Chemical structure of all compounds

Figure S2. ^1H -NMR (500 MHz, CDCl_3) spectrum of atractylenolide I

Figure S3. ^{13}C -NMR (125 MHz, CDCl_3) spectrum of atractylenolide I

Figure S4. ^1H -NMR (400 MHz, CDCl_3) spectrum of gomisin N

Figure S5. ^{13}C -NMR (100 MHz, CDCl_3) spectrum of gomisin N

Figure S6. ^1H -NMR (400 MHz, CDCl_3) spectrum of schisandrin

Figure S7. ^{13}C -NMR (100 MHz, CDCl_3) spectrum of schisandrin

Figure S8. ^1H -NMR (400 MHz, CDCl_3) spectrum of gomisin A

Figure S9. ^{13}C -NMR (100 MHz, CDCl_3) spectrum of gomisin A

Figure S10. ^1H -NMR (500 MHz, $\text{DMSO}-d_6$) spectrum of 6(*E*),12(*E*)-tetradecadiene-8,10-diyne-1,3-diol

Figure S11. ^{13}C -NMR (125 MHz, $\text{DMSO}-d_6$) spectrum of 6(*E*),12(*E*)-tetradecadiene-8,10-diyne-1,3-diol

Figure S12. HPLC-UV chromatogram of 6(*E*),12(*E*)-tetradecadiene-8,10-diyne-1,3-diol

Figure S13. HPLC-UV chromatogram of schisandrin

Figure S14. HPLC-UV chromatogram of gomisin A

Figure S15. HPLC-UV chromatogram of atractylenolide I

Figure S16. HPLC-UV chromatogram of schisandrin A

Figure S17. HPLC-UV chromatogram of gomisin N

Figure S18. HPLC-UV chromatogram of γ -schisandrin

Figure S19. HPLC-UV chromatogram of schisandrin C

Figure S20. MS spectrum of atractylenolide I

Figure S21. MS spectrum of gomisin N

Figure S22. MS spectrum of schisandrin

Figure S23. MS spectrum of gomisin A

Figure S24. MS spectrum of spectrum of 6(*E*),12(*E*)-tetradecadiene-8,10-diyne-1,3-diol

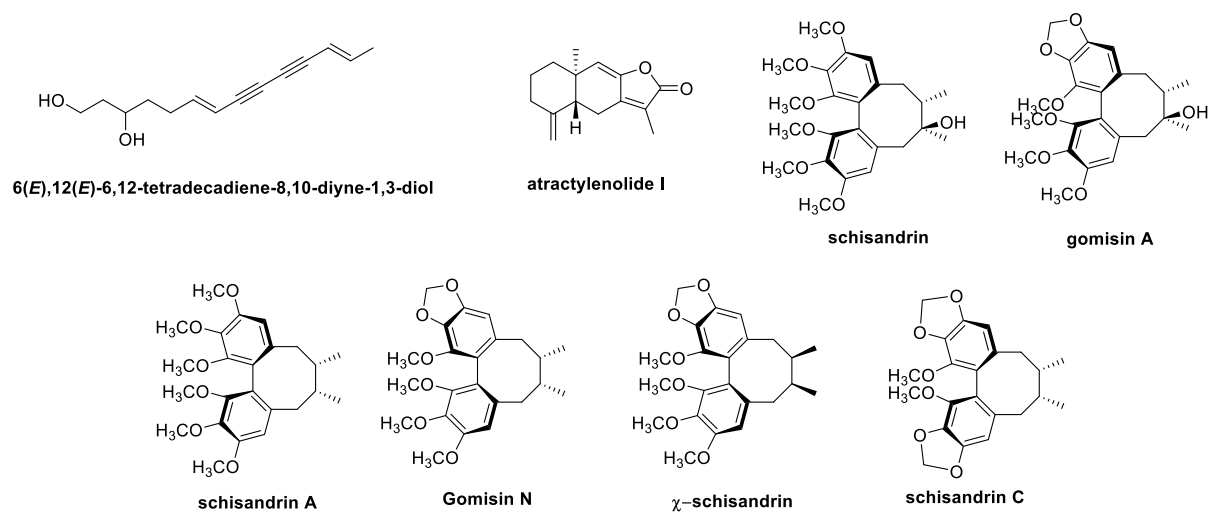


Figure S1. Chemical structures of all compounds

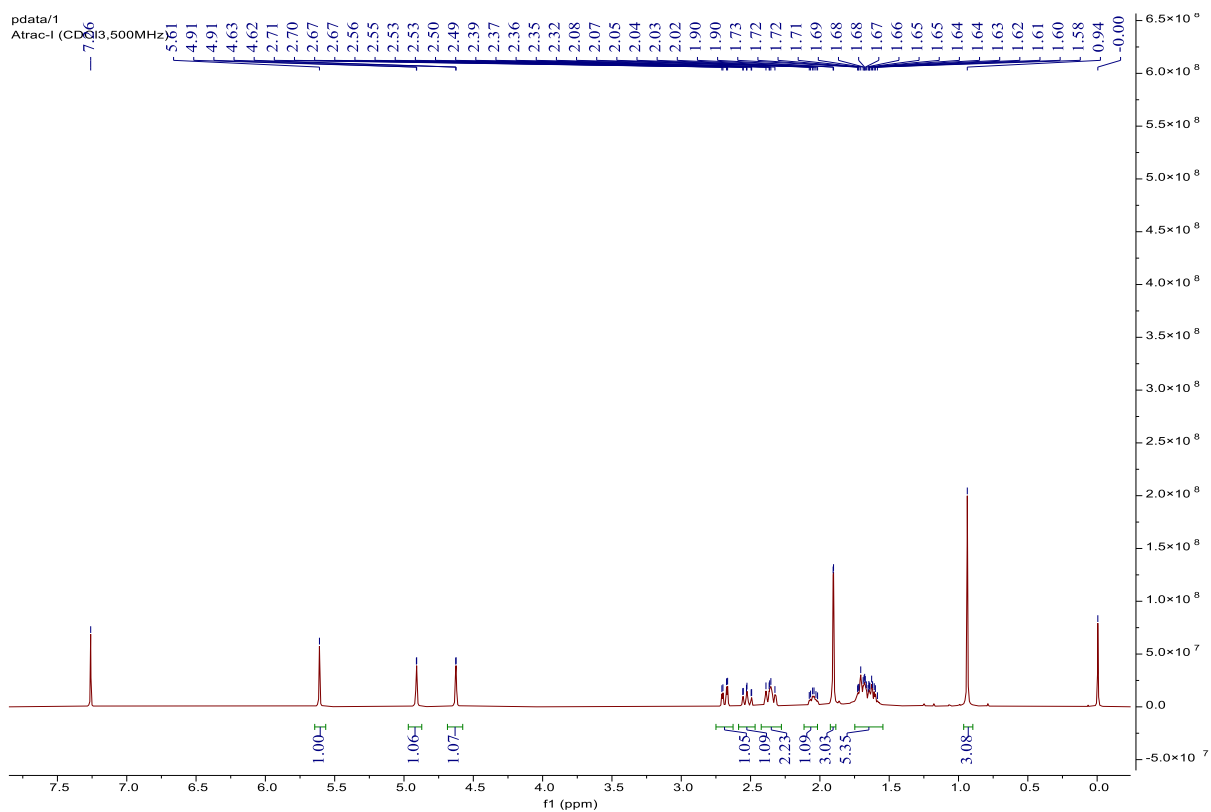


Figure S2. ¹H-NMR (500 MHz, CDCl₃) spectrum of atractylenolide I

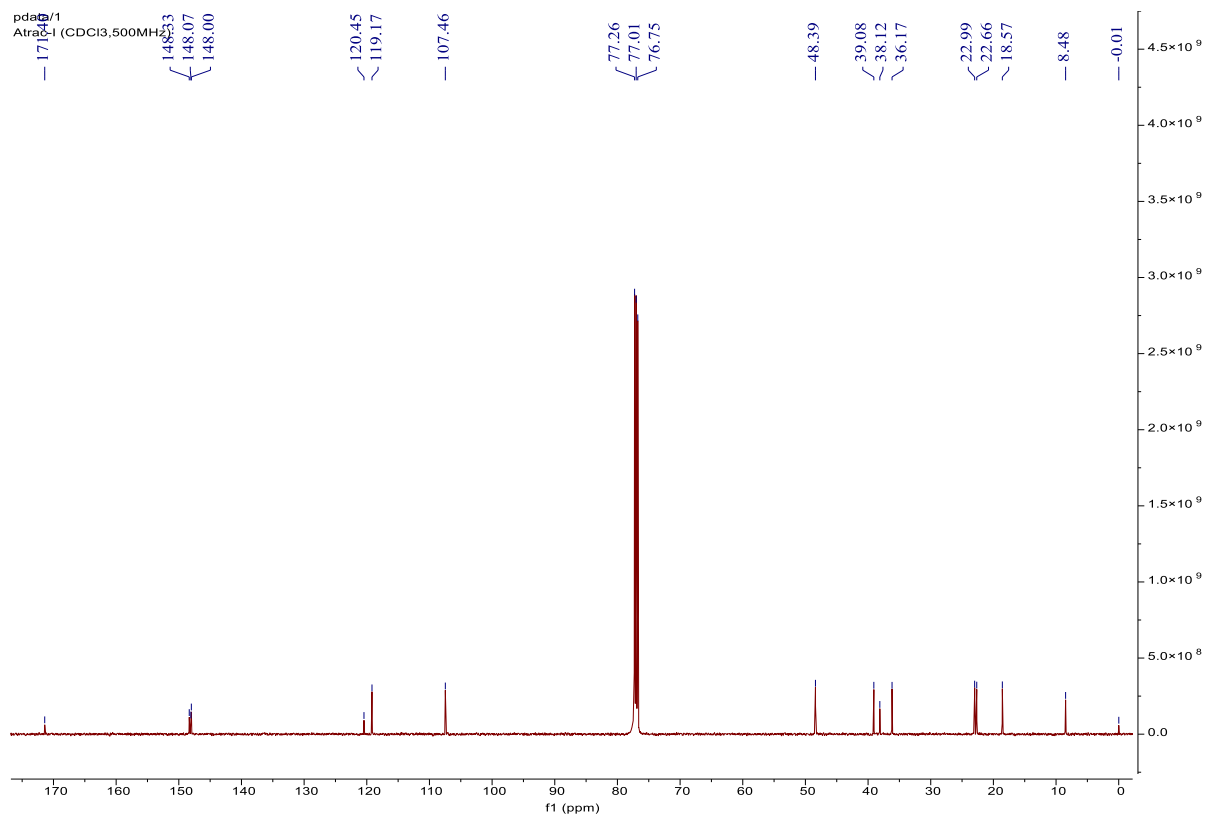


Figure S3. ¹³C-NMR (125 MHz, CDCl₃) spectrum of atractylenolide I

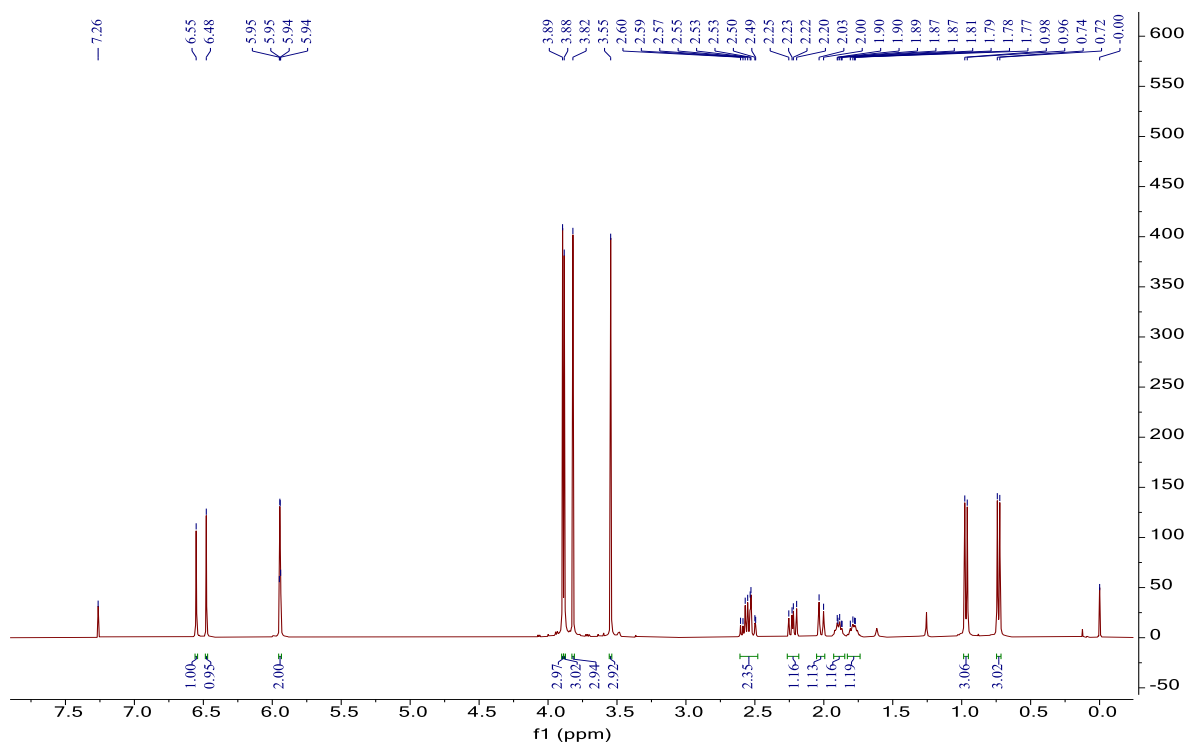


Figure S4. ¹H-NMR (400 MHz, CDCl₃) spectrum of gomisin N

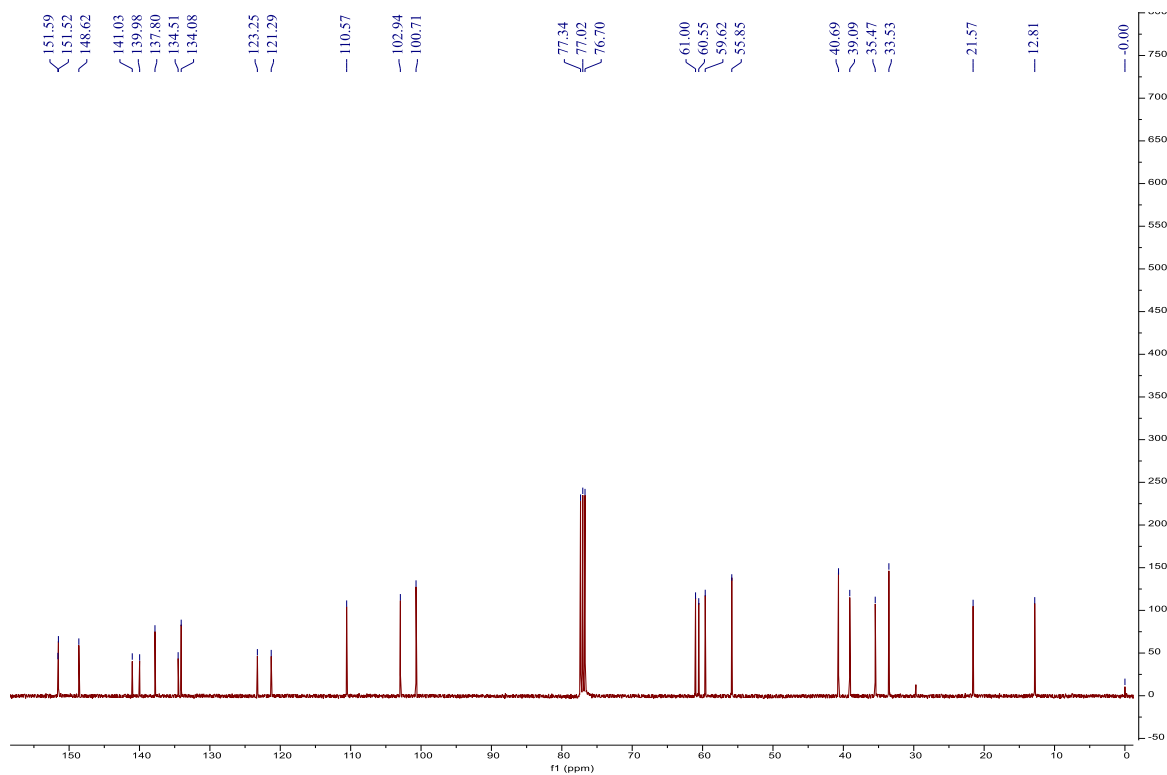


Figure S5. ^{13}C -NMR (100 MHz, CDCl_3) spectrum of gomisin N

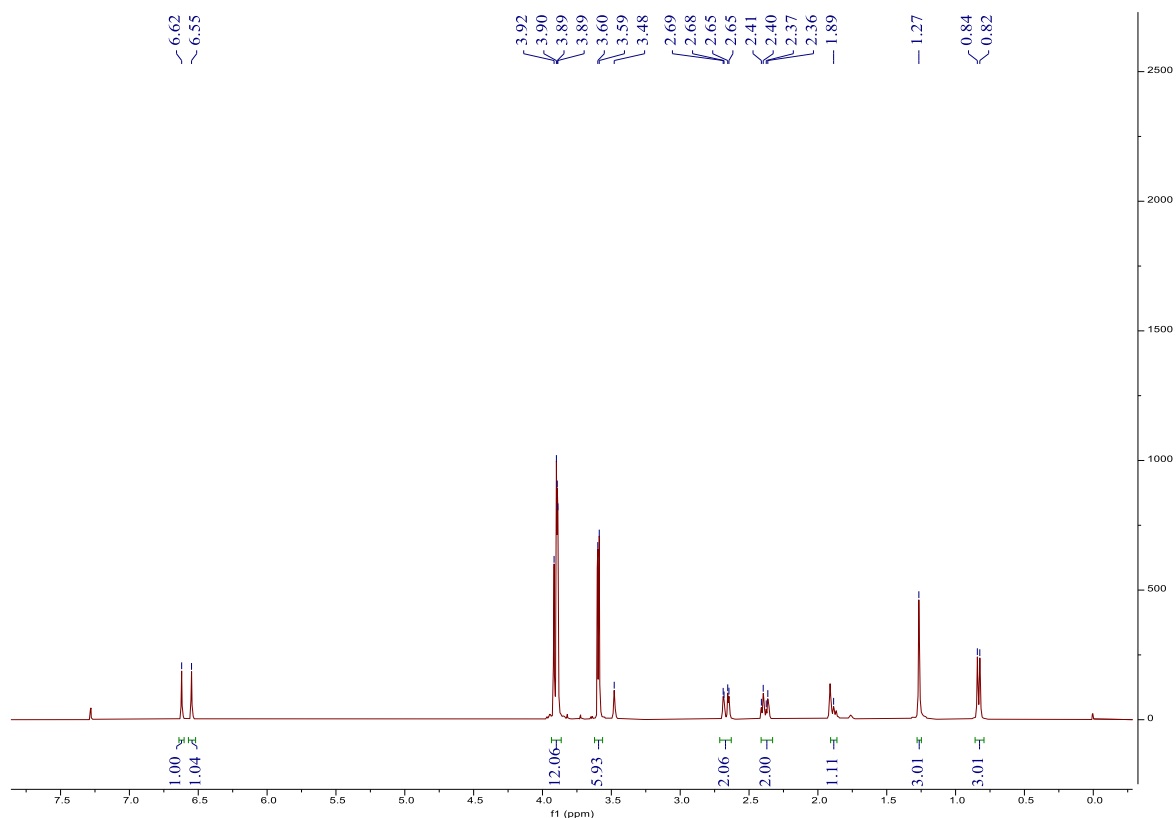


Figure S6. ^1H -NMR (400 MHz, CDCl_3) spectrum of schisandrin

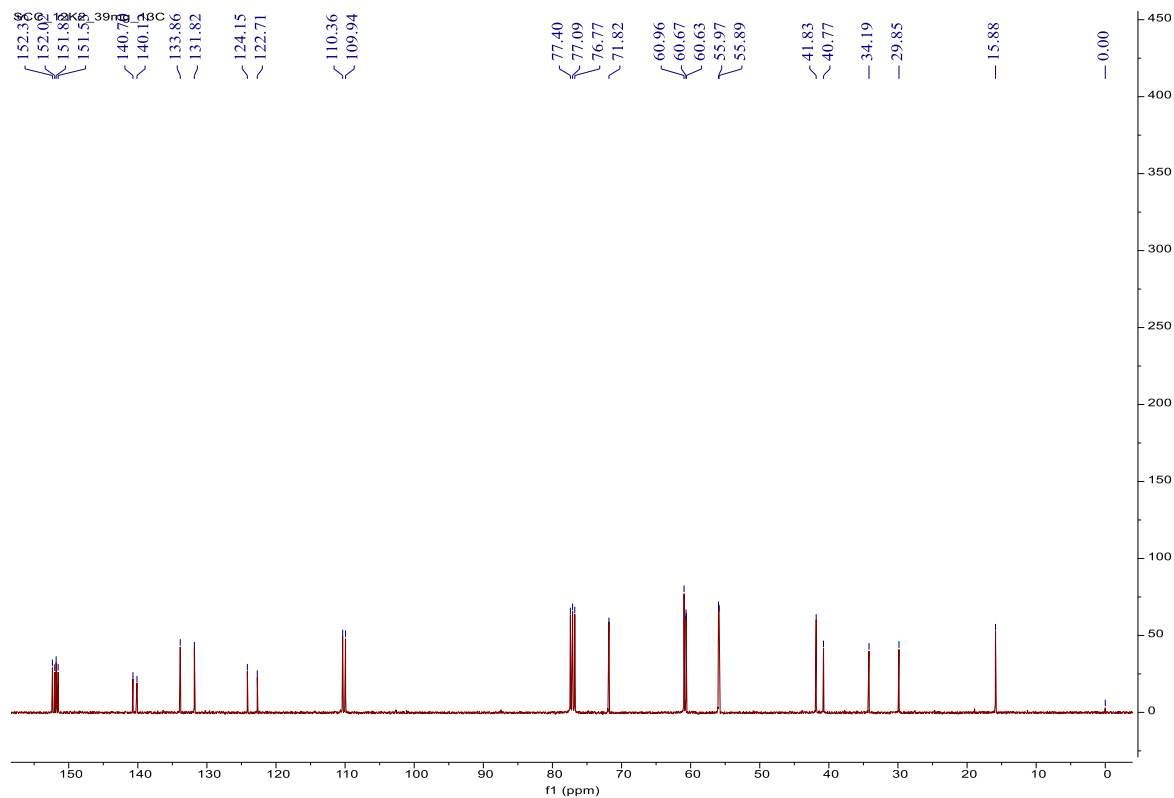


Figure S7. ¹³C-NMR (100 MHz, CDCl₃) spectrum of schisandrin

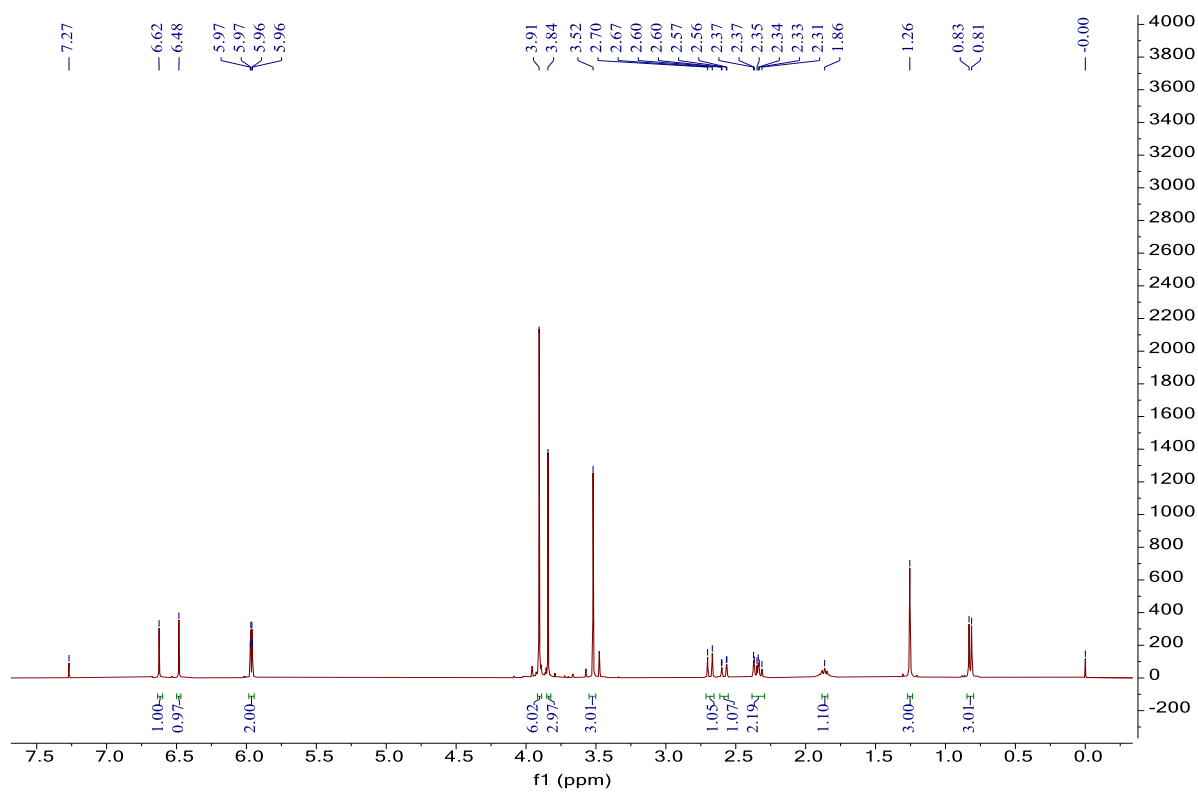


Figure S8. ¹H-NMR (400 MHz, CDCl₃) spectrum of gomisin A

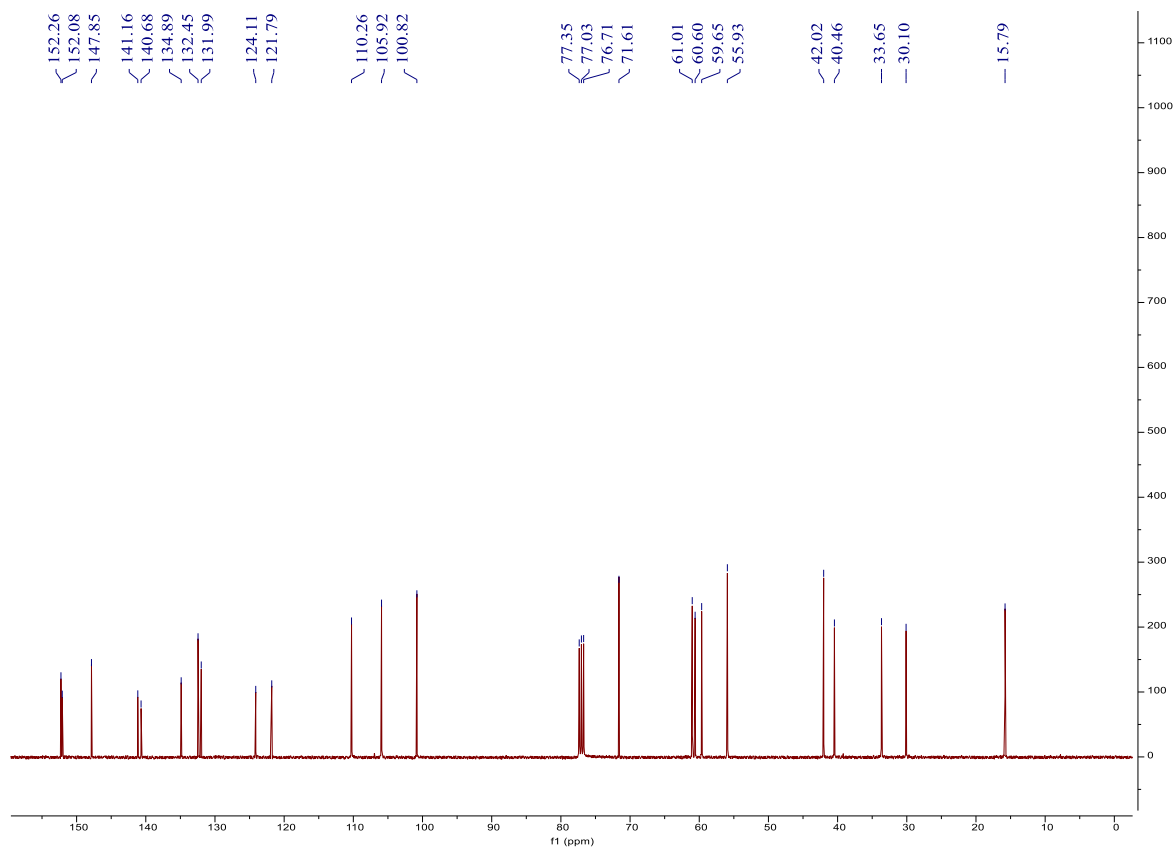


Figure S9. ¹³C-NMR (100 MHz, CDCl₃) spectrum of gomisin A

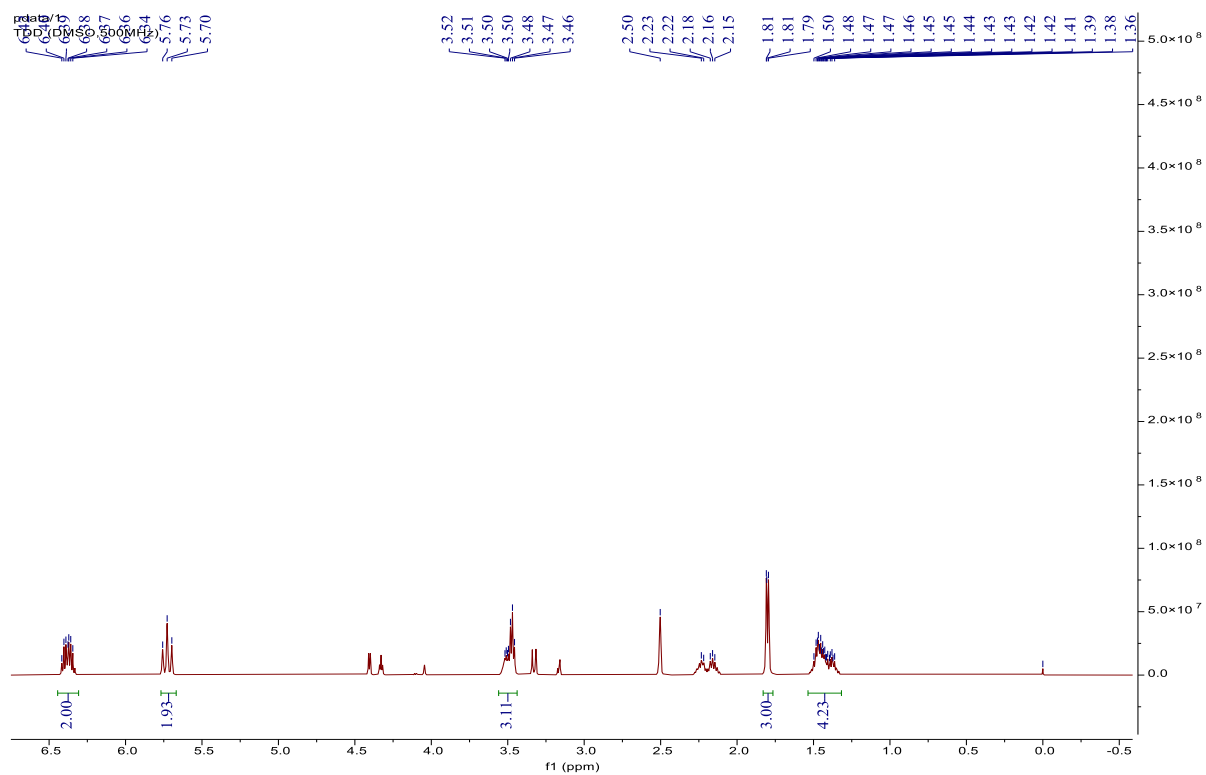


Figure S10. ¹H-NMR (500 MHz, DMSO-*d*₆) spectrum of 6(*E*),12(*E*)-tetradecadiene-8,10-diyne-1,3-diol

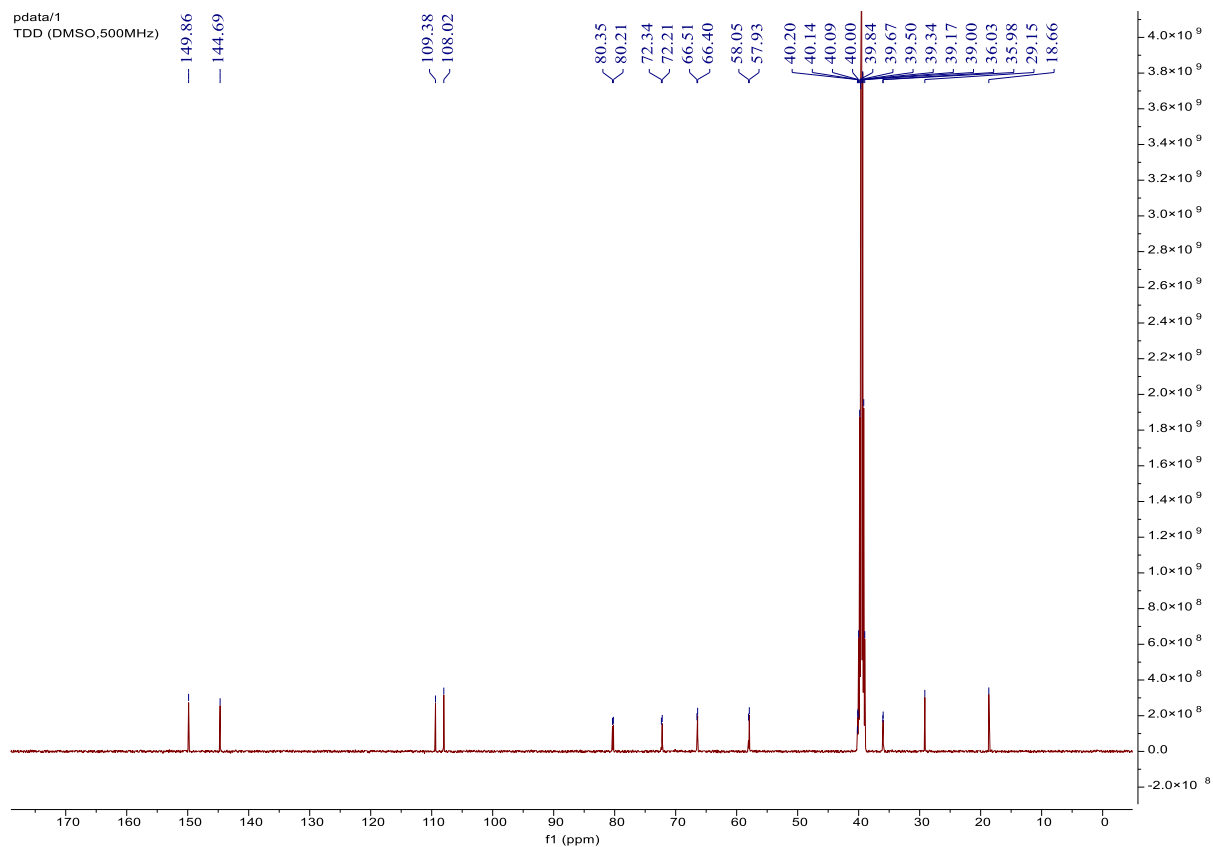


Figure S11. ^{13}C -NMR (125 MHz, $\text{DMSO}-d_6$) spectrum of 6(*E*),12(*E*)-tetradecadiene-8,10-diyne-1,3-diol

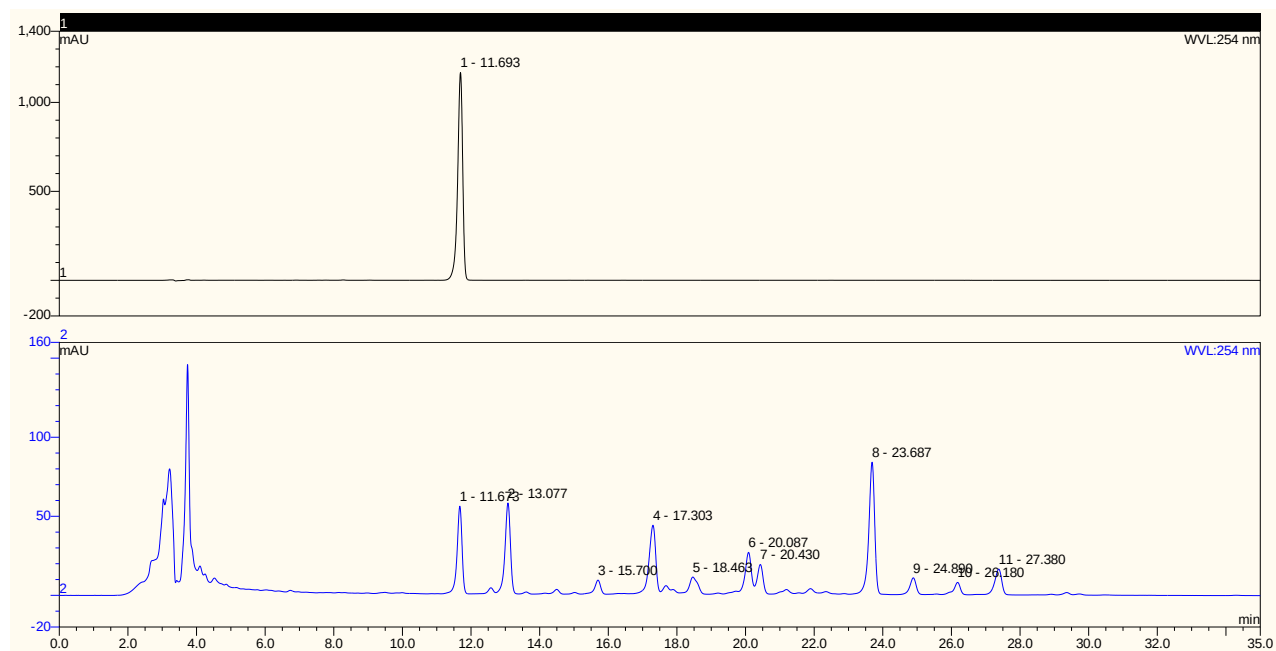


Figure S12. HPLC-UV chromatogram of 6(*E*),12(*E*)-tetradecadiene-8,10-diyne-1,3-diol

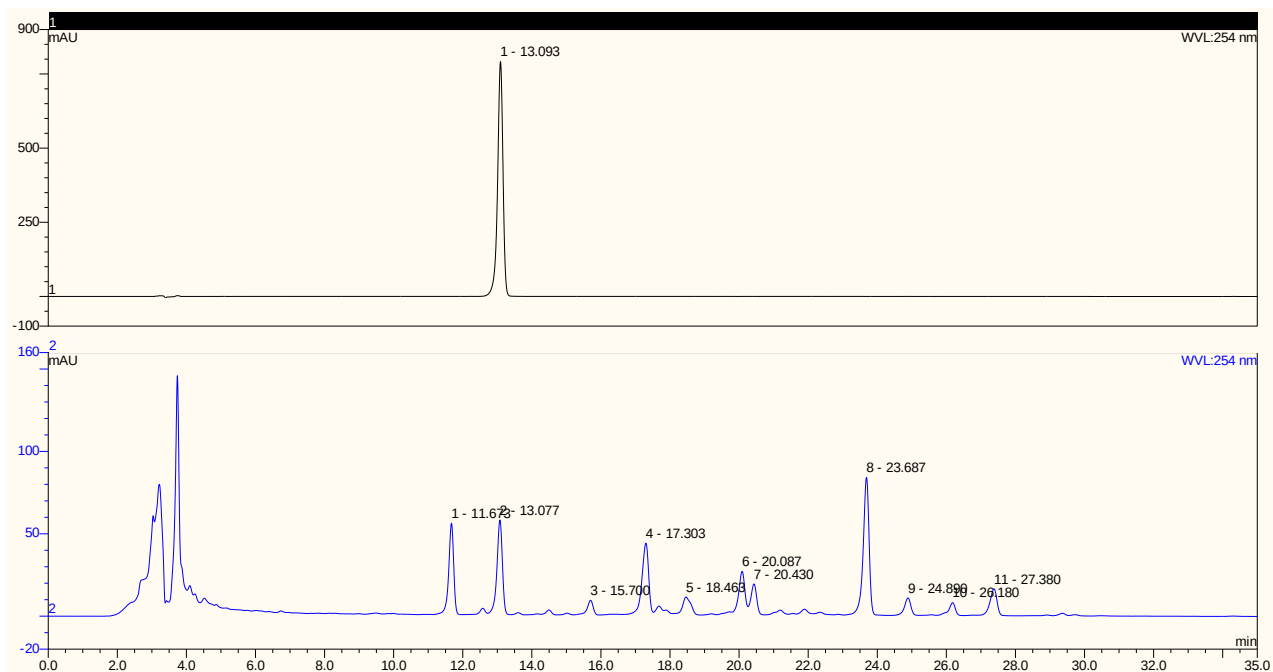


Figure S13. HPLC-UV chromatogram of schisandrin

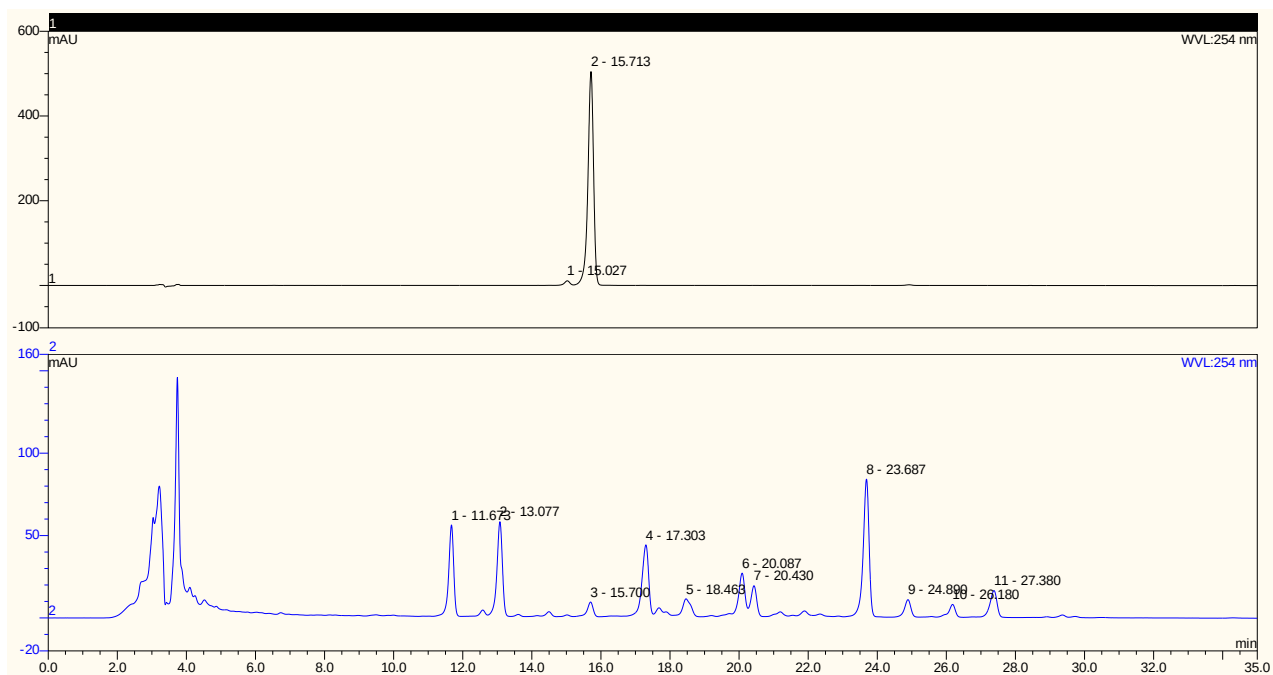


Figure S14. HPLC-UV chromatogram of gomisin A

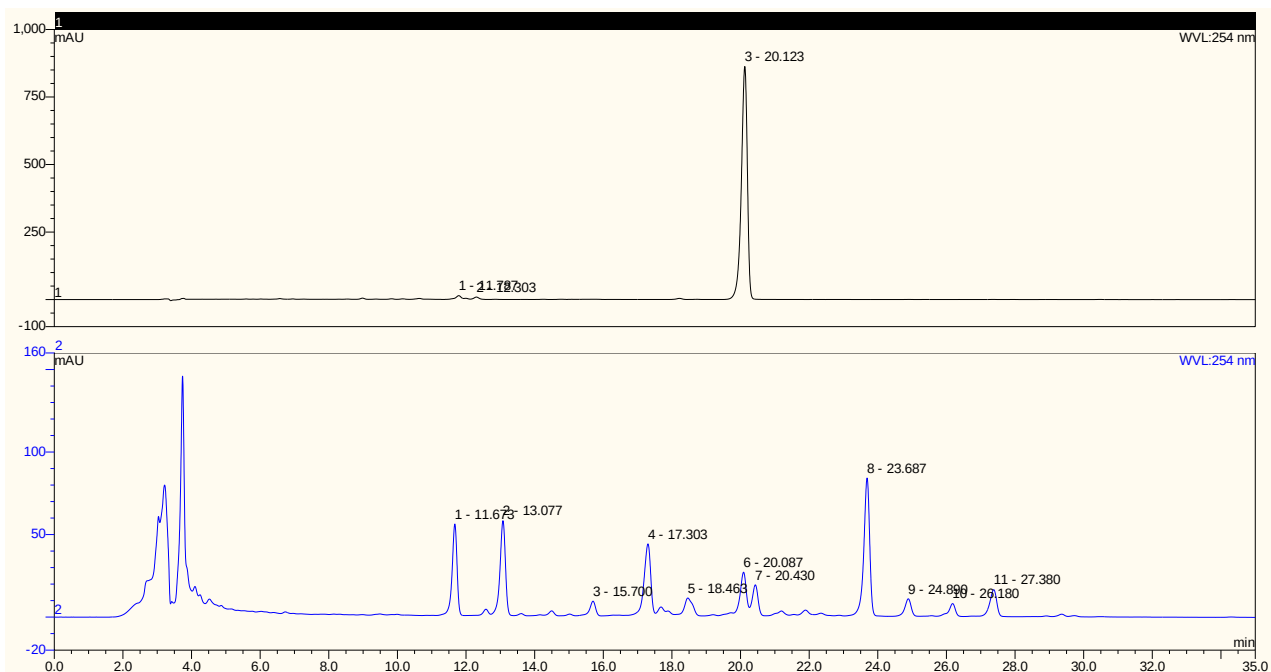


Figure S15. HPLC-UV chromatogram of atractylenolide I

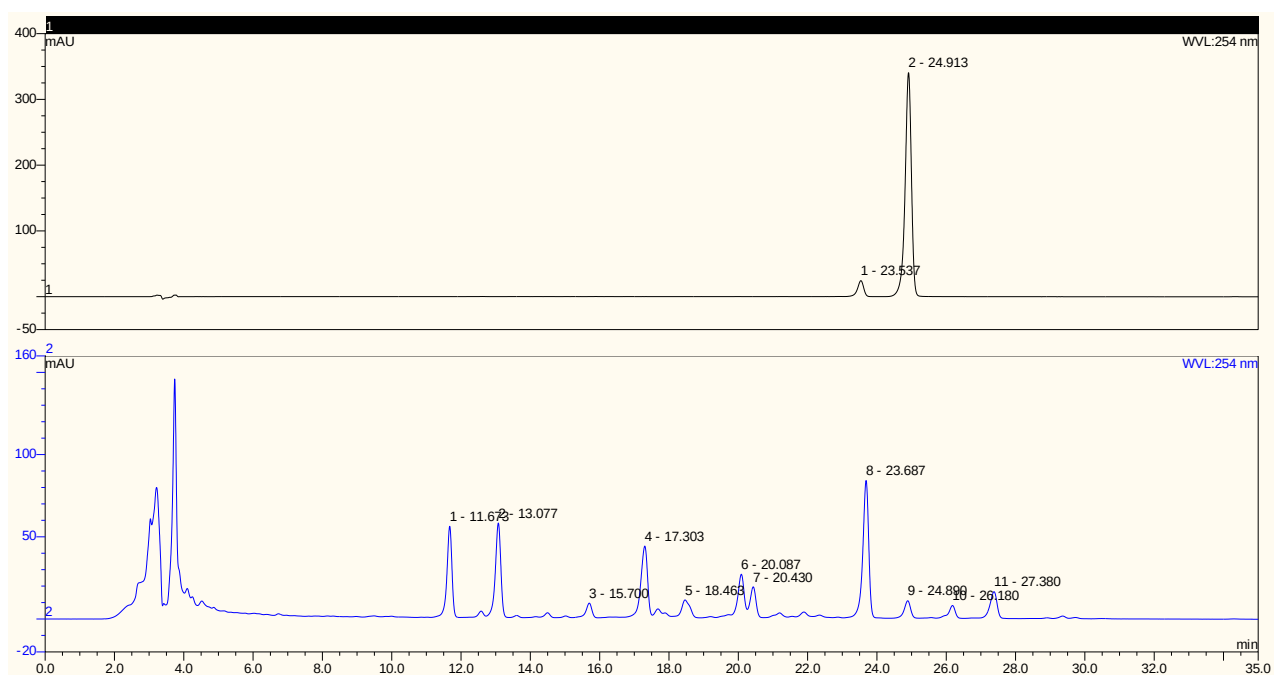


Figure S16. HPLC-UV chromatogram of schisandrin A

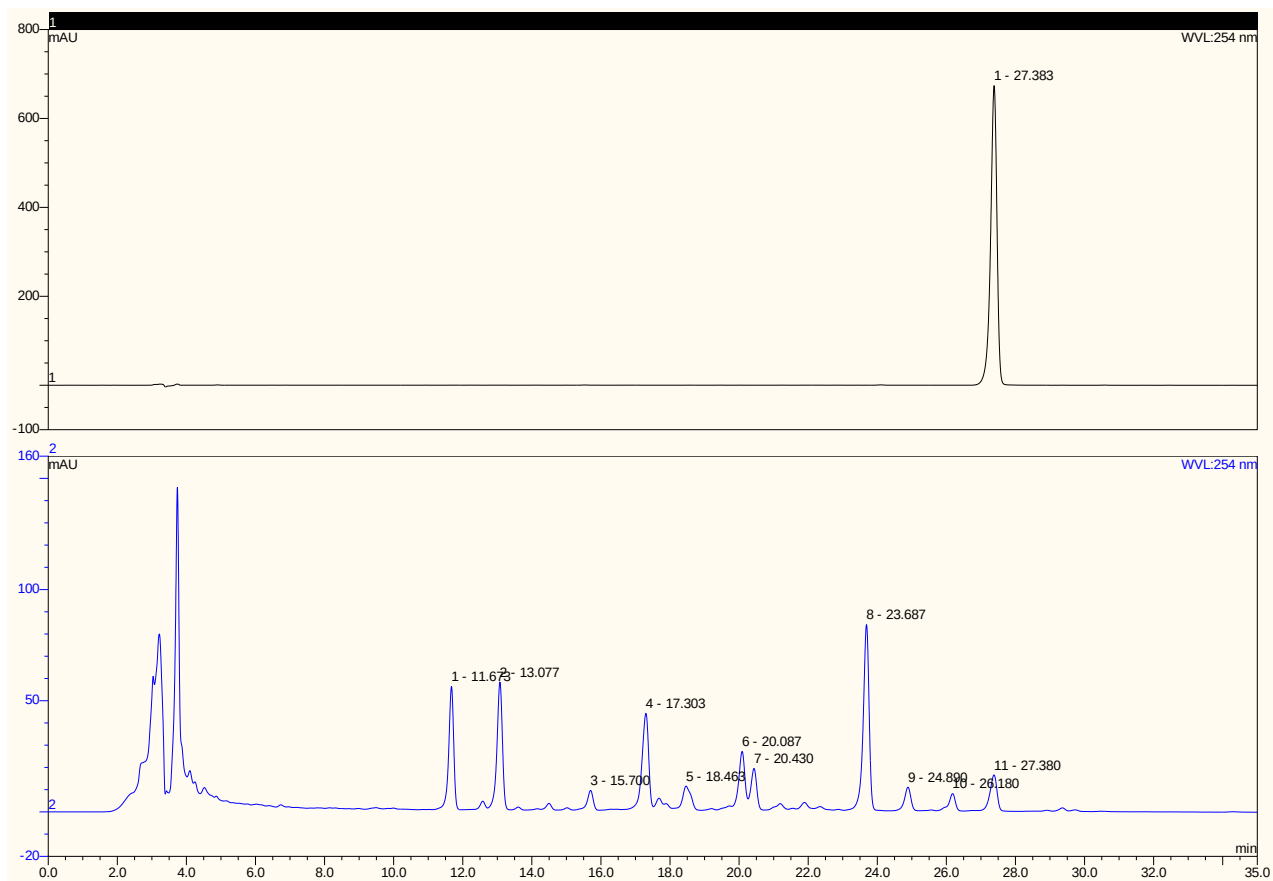


Figure S17. HPLC-UV chromatogram of gomisin N

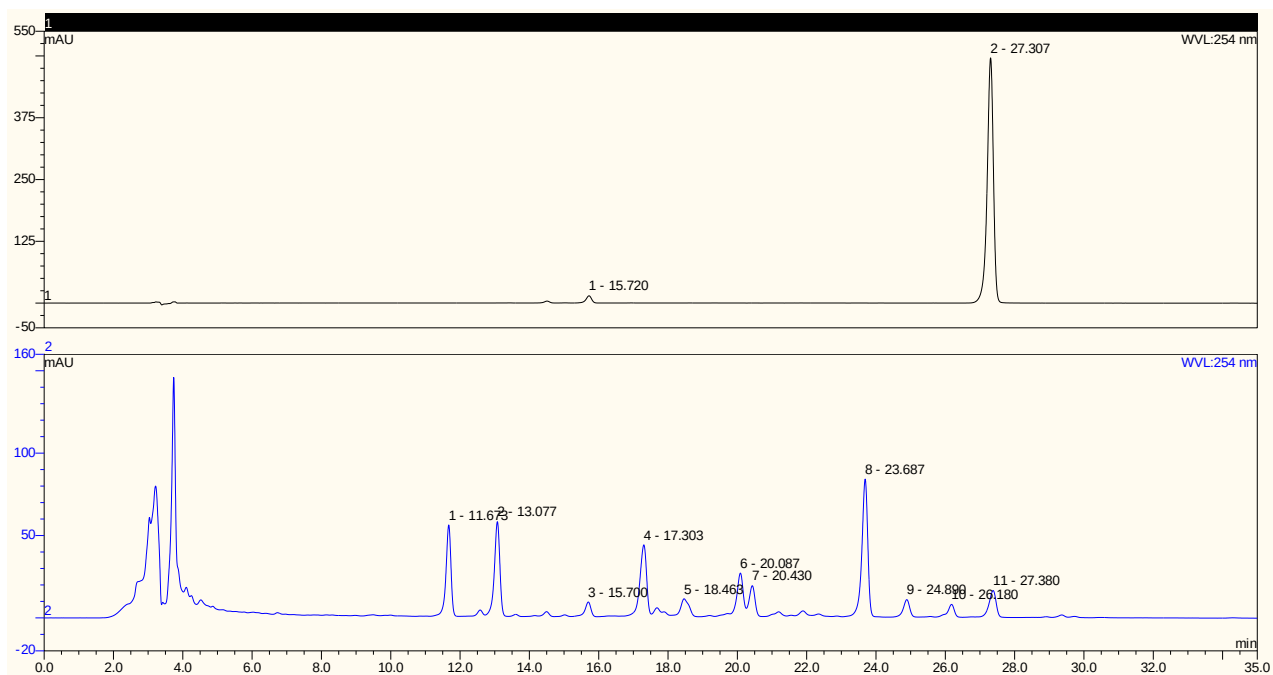


Figure S18. HPLC-UV chromatogram of γ -schisandrin

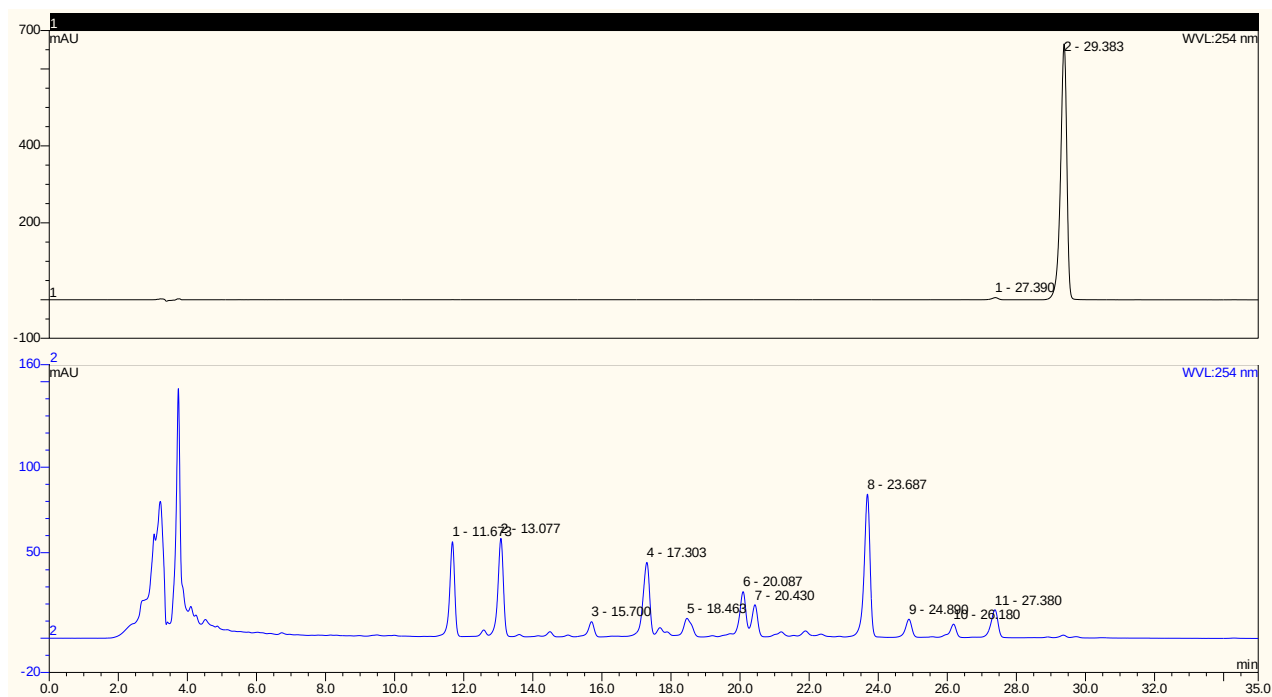


Figure S19. HPLC-UV chromatogram of schisandrin C

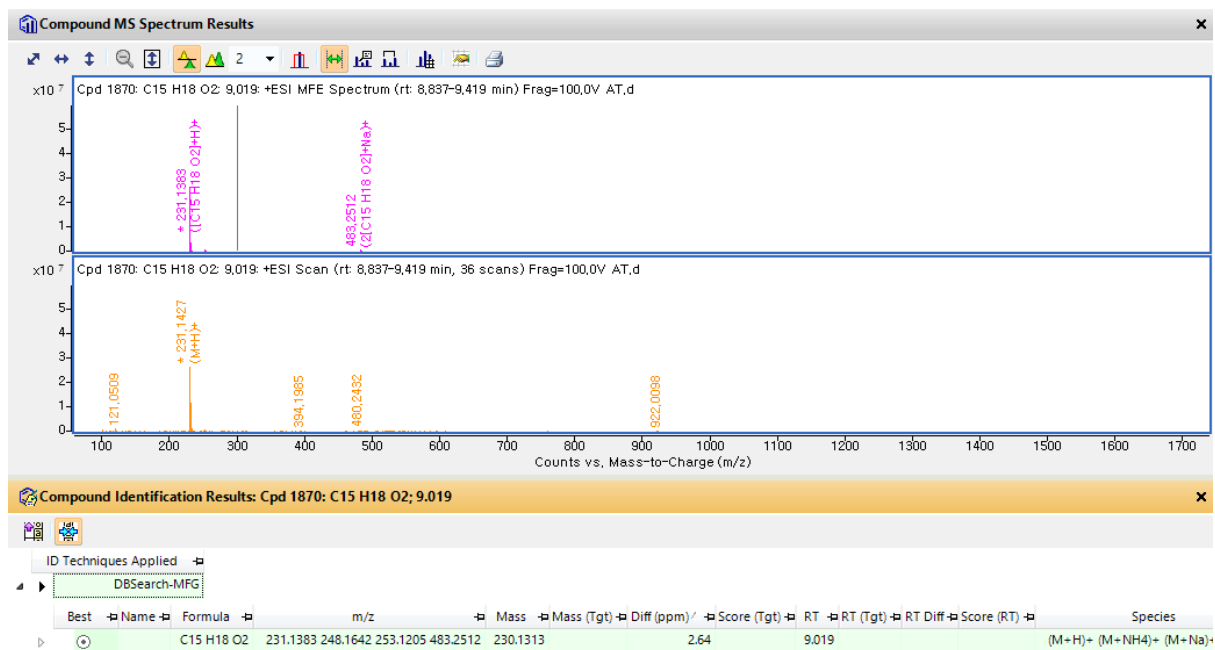


Figure S20. MS spectrum of atractylenolide I

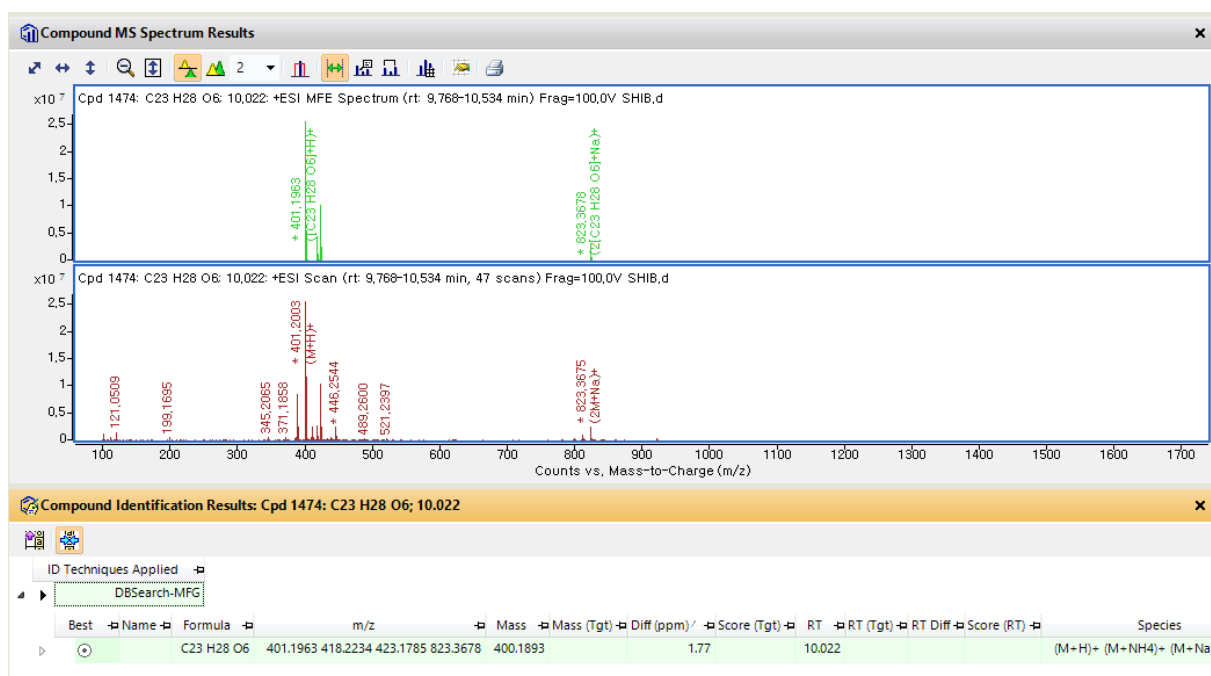


Figure S21. MS spectrum of gomisin N

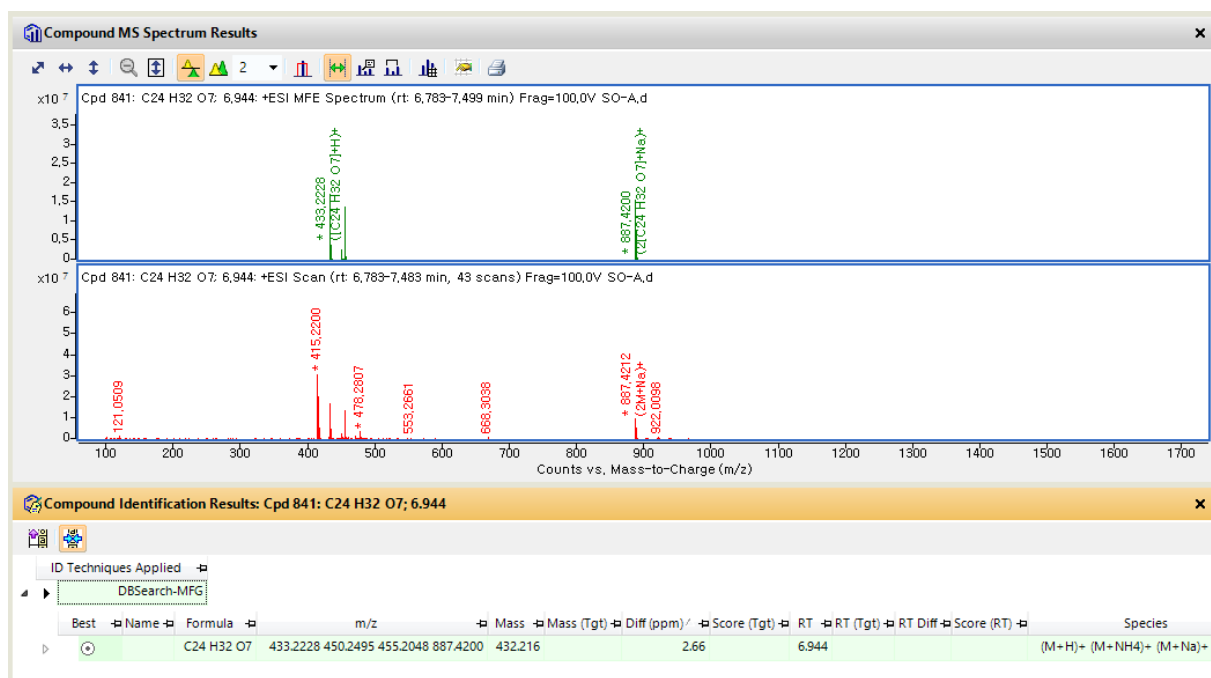


Figure S22. MS spectrum of schisandrin

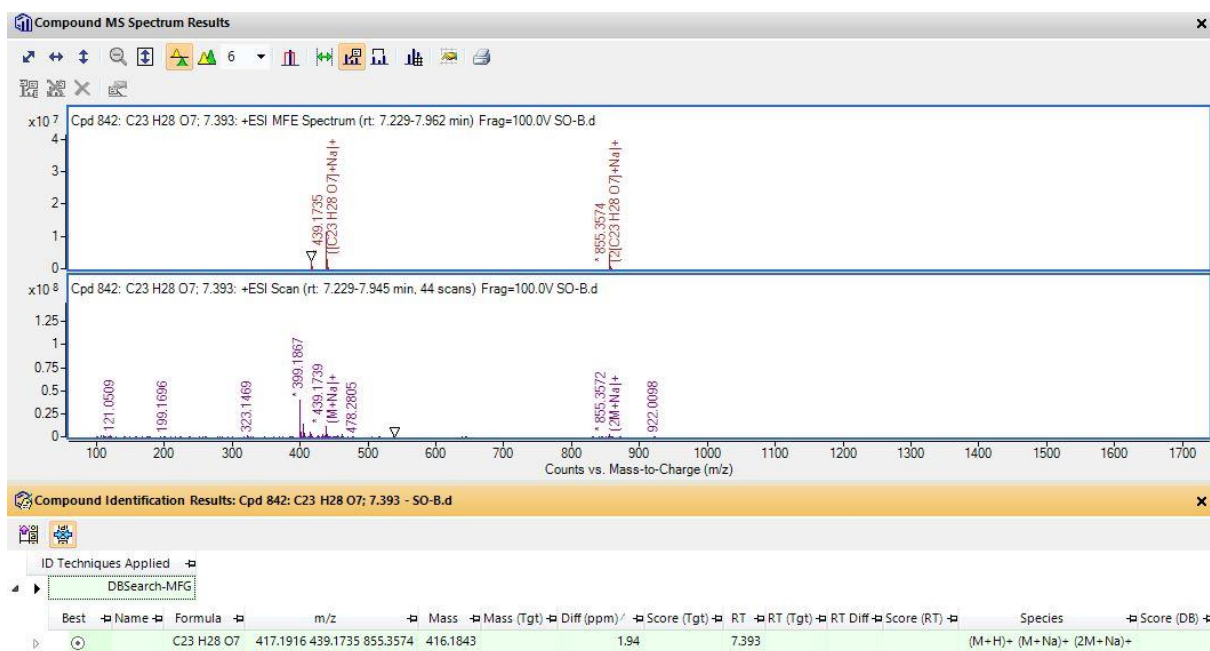


Figure S23. MS spectrum of gomisin A

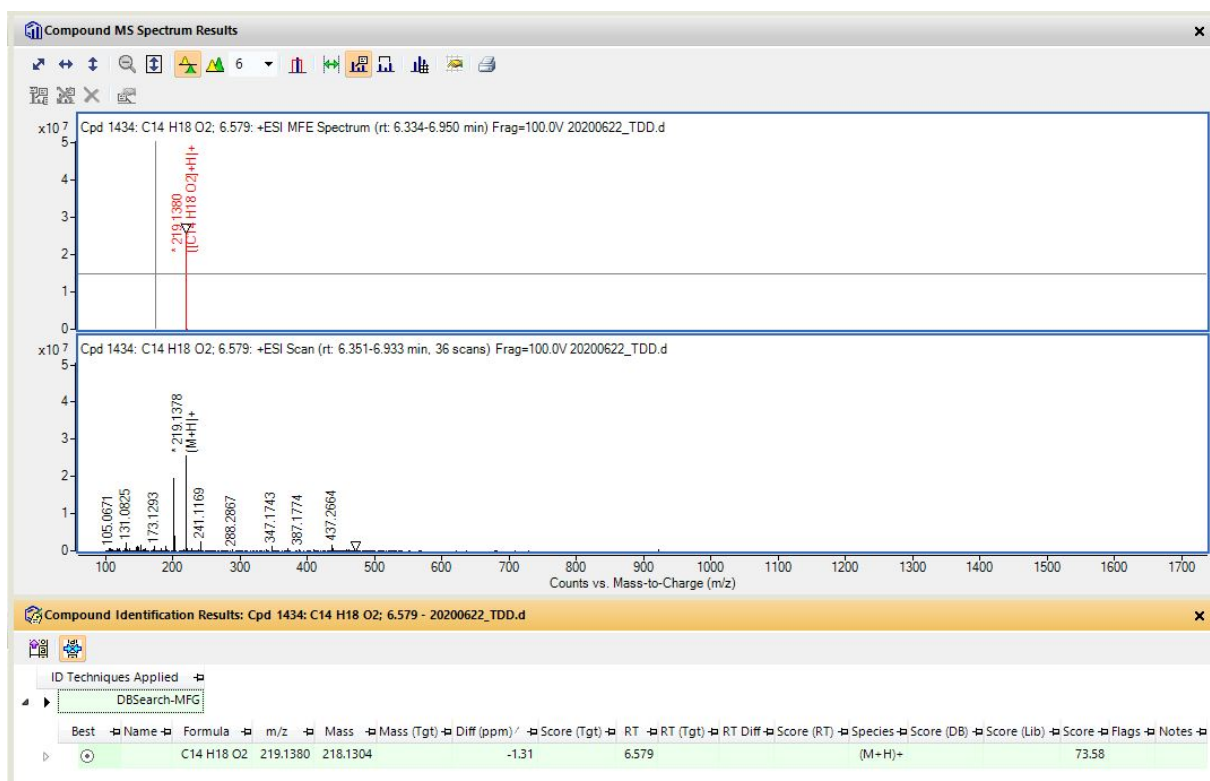


Figure S24. MS spectrum of spectrum of 6(E),12(E)-tetradecadiene-8,10-diyne-1,3-diol