Supporting Information

Synthesis and Anti-cancer activity of Acetals of Arjunolic acid

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Isolation and separation of arjunolic acid and asiatic acid from the heartwood of *Terminalia arjuna*

Briefly, coarsely powdered dried heartwood of *Terminalia arjuna* (1kg) was exhaustively extracted by refluxing with ethyl acetate. The extract was filtered and concentrated. The crude extract was purified by chromatography. The complete procedure to isolate and separate arjunolic acid and asiatic acid has been patented. (Indian patent Application No: 202441015549 Published on 22/03/2023).

Characterization:

Arjunolic acid (**AA)**: Yield 1.15 %, m.p. 334.1- 335.4 °C

FTIR (KBr) cm^{-1}: 3041-3581 (broad, O-H stretch), 2937 (C-H stretch), 1699 (s, C=O stretch), 1457 (C-H bend), 1045 (C-O stretch); **^{1}H NMR (400 MHz, DMSO) δ**: 12(1H, s, COOH), 5.17 (1H, t (J=3.6Hz), H12), 4.4 (1H,m, 23OH), 4.23 (1H, d, 2OH/3OH), 4.16 (1H,d, 2OH/3OH), 3.45 (1H, m(J=4Hz, H2), 3.14 (1H, d (J=7.9Hz), H3), 3.16 (1H, d (J= 12Hz), H_a-23), 2.73 (1H, d (J= 12Hz), H_b-23), 2.34-0.8 (terpenoid protons), 0.87 (6H, H29&H30), 1.01 (3H, s, H-27), 0.53 (3H, s, H24), 0.70 (3H, s, H26), 0.98(3H, s, H25); **^{13}C NMR (100 MHz, MeOD) δ:** C1(45.81), C2(68.26), C3(76.77), C4(42.7), C5(46.76), C6(17.69), C7(32.40), C8(39.15), C9(46.47), C10(37.60), C11(22.63), C12(122.03), C13(143.97), C14(41.62), C15(27.38), C16(22.57), C17(46.21), C18(41.37), C19(47.54), C20(30.20), C21(32.15), C22(31.90), C23(64.88), C24(12.46), C25(16.36), C26(16.12), C27(25.06), C28(180.42), C29(33.48), C30(23.21); **Mass (*m/z*)**: 511.3404 $[M+Na]^+$

General procedure for the synthesis of various acetals of arjunolic acid (AA-1 – AA-19)

Arjunolic acid 100 mg (0.20 mmol) was dissolved in 2 mL of DMSO in a 10 mL round bottom flask. To this benzaldehyde(substituted) and a catalytic amount of PPTs were added. The reaction contents were heated at 70°C till the reaction was completed. Completion of the reaction was monitored by TLC. The reaction mixture was cooled to room temperature and neutralized using saturated aqueous sodium bicarbonate solution. The mixture was extracted using DCM (10 mL × 2). The organic layers were pooled, dried over anhydrous sodium sulphate and concentrated under reduced pressure to give a crude product. The crude product was purified using column chromatography (hexane: ethyl acetate; 60:40).

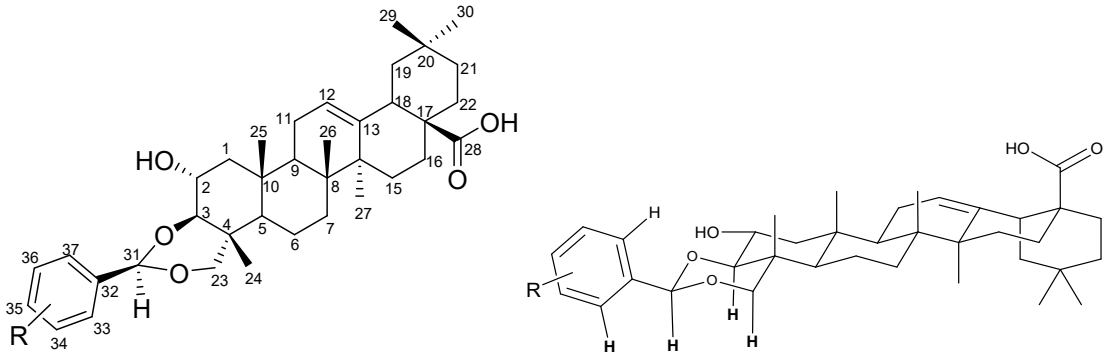


Fig. S1 Structure of substituted 2,23- benzylidene acetals of arjunolic acid.

Characterization

3,23-benzylidene arjunolic acid (AA-1): Yield 80%, m.p. 276-277 °C

UV (λ_{max}, nm): 244 & 280**; FTIR(KBr)cm^{-1}**: 3217-3535 (Broad, O-H stretch), 2924 (C-H stretch), 1694 (s, C=O stretch), 1456 (C-H bending), 1075(C-O stretch), 697 (C-H aromatic out of plane bending); **^{1}H NMR (400 MHz, DMSO) δ:**12.03 (1H, s, COOH), 7.48-7.46(2H, m, aromatic protons), 7.39-7.32(3H, m, aromatic protons), 5.50(1H, s, H31), 5.17 (1H, t, (J= 3.5Hz), H12), 4.59 (1H, d, (J= 4.72Hz), -OH), 3.68 (1H, m, H2), 3.25 (1H, d, (J= 9.7Hz), H3), 3.79 (1H, d (J= 12Hz), H_a-23), 3.47 (1H, d (J= 12Hz) H_b-23), 2.34-0.8 (Terpenoid protons), 1.13 (3H, s, H24), 0.98 (3H, H25), 0.71 (3H, , H26), 1.09 (3H, s, H27), 0.87 (6H, s, H29&H30); **^{13}C NMR (100 MHz, DMSO) δ**: C1(45.88), C2(63.90), C3(90.06), C4(38.12), C5(48.47), C6(17.78), C7(33.30), C8(39.23), C9(50.77), C10(37.12), C11(23.04), C12(121.72), C13(144.37), C14(41.83), C15(26.18), C16(23.31), C17(46.15), C18(41.83), C19(47.48), C20(30.87), C21(32.55), C22(33.77), C23(78.02), C24(14.77), C25(17.51), C26(17.21), C27(27.65), C28(179.03), C29(23.84), C30(32.22), C31(102.19), C32(139.32), C33(128.41), C34(126.84), C35(129.11), C36(126.14), C37(128.41); **Mass (*m/z*)** 575.3146 $[M-H]^+$

3,23-(2-Fluorobenzylidene) arjunolic acid (AA-2): Yield 80%, m.p. 260.1 – 261.9 °C

UV (λ_{max}, nm): 242, 280; **FTIR(KBr)cm^{-1}**: 3180-3538(Broad, O-H stretch), 2942(C-H stretch), 1692(C=O stretch), 1234 (C-F stretch), 1014(C-O stretch), 774(aromatic C-H out of plane bending); **^{1}H NMR (400 MHz, $CDCl_3$) δ**: 7.67(1H, m (J=8.44Hz, J=1.3Hz), H35), 7.34(1H, dd (J= 7.8Hz, J=5.7Hz, J=1.7Hz), H37), 7.18(1H, t (J=7.5Hz), H36), 7.05(1H, t (J=9.6Hz), H34), 5.86(1H, s, H31), 5.17(1H, t, (J=3.1Hz) H12), 3.90(1H, m, H2), 3.34(1H, d (J=9.7Hz), H3), 3.90(1H, d (J= 10.4Hz), H_a-23) 3.51(1H, d (J= 10.4Hz), H_b-23), 2.34-0.8(Terpenoid protons), 0.92(6H, s, H29&H30), 0.74(3H, s, H27), 1.25(3H, s, H24), 1.06(3H, s, H26), 1.15(3H, s, H25); **^{13}C NMR (100 MHz, $CDCl_3$) δ**: C1(45.77), C2(65.12), C3(90.49), C4(38.12), C5(47.64), C6(17.76), C7(33.05), C8(39.34), C9(51.34), C10(36.96), C11(22.77), C12(122.28), C13(143.48), C14(41.56), C15(25.96), C16(23.51), C17(46.31), C18(40.88), C19(46.45), C20(30.67), C21(32.40), C22(33.75), C23(78.50),

C24(14.34), C25(17.62), C26(17.06), C27(27.60), C28(183.85), C29(23.55), C30(31.99), C31(97.31, d, J=3.3Hz), C32(125.64, d, J= 12Hz), C33(160.02, d, J= 247.6Hz), C34(115.51, d, J= 21.1Hz), C35(130.74, d, J=8.6Hz), C36(127.91, d, J=3.3Hz), C37(124.21, d, J=3.34Hz); **Mass (*m/z*)**: 595.3820 $[M+H]^+$

3,23-(3-Fluorobenzylidene) arjunolic acid (AA-3): Yield 80%, m.p. 299.8 – 300.5 °C
UV (λ_{max}, nm): 245, 287; **FTIR(KBr)cm^{-1}**: 3190-3492 (Broad, O-H stretch), 2918 (C-H stretch), 1692 (s, C=O stretch), 1145 (C-F stretch), 1014,1074 (C-O stretch), 774 (aromatic C-H, out of plane bending); **^{1}H NMR (400 MHz, $CDCl_3$) δ**: 7.33(1H, m (J_{H-H}= 7.9Hz, J_{F-H}= 5.7Hz, H36), 7.05(1H, t (J=8.4Hz), H35), 7.27(1H, d, (7.92), H33), 7.24(1H, d, (8.2Hz), H36) 5.52 (1H, s, H31), 5.29 (1H, t, (J= 3.5Hz) C12), 3.90 (1H, m, H2), 3.31 (1H, d (J=9.7Hz), H3), 3.90(2H, d (J= 10.4Hz), H_a-23), 3.47 (1H, d (J= 10.4Hz), H_b-23), 2.34-0.8 (Terpenoid protons), 0.92 (6H, s, H29&H30), 1.17 (3H, s, H27), 0.74 (3H, s, H24),1.03 (3H, s, H25),1.15 (3H, s, H26); **^{13}C NMR (100 MHz, $CDCl_3$) δ**: C1(45.78), C2(65.14), C3(90.36), C4(38.14), C5(46.39), C6(17.06), C7(33.05), C8(39.35), C9(51.36), C10(36.94), C11(23.55), C12(122.34), C13(143.49), C14(41.58), C15(25.95), C16(22.77), C17(46.46), C18(40.92), C19(47.65), C20(30.68), C21(32.41), C22(33.76), C23(78.75), C24(14.37), C25(17.73), C26(17.72), C27(27.61), C28(183.76), C29(23.25), C30(31.92), C31(101.73), C32(140.51,d, J=7.4Hz), C33(115.97, d, J= 20.9Hz), C34(162.75, d, J=244.3Hz), C35(113.45, d, J= 22.4Hz), C36(129.92, d, J= 8.0Hz), C37(122.05, d, J=2.6Hz); **Mass (*m/z*)**: 593.3021 $[M-H]^+$

3,23-(4-fluorobenzylidene) arjunolic acid (AA-4): Yield 80%, m.p. 320.3 – 321.8 °C
UV (λ_{max}, nm): 258 & 294; **FTIR(KBr)cm^{-1}**: 3145-3498 (Broad, O-H stretch), 2922 (C-H stretch), 1695 (s, C=O stretch), 1457 (C-H bending), 1171 (C-F stretch), 1078 (C-O stretch), 857 (aromatic C-H out of plane bending); **^{1}H NMR (400 MHz, $CDCl_3$) δ**: 7.49(2H, dd (J_{H-H}= 8.6Hz, J_{F-H}= 5.5Hz), H33&H37), 7.06(2H, t, (J=8.7Hz) H34&H36), 5.49(1H, s, H31), 5.29(1H, t, H12), 3.64 (1H, m, H2), 3.49 (1H, d (J=11Hz), H3), 3.89(1H, d (J= 11.8Hz), H_a-23), 3.33 (1H, d (J= 11.8Hz), H_b-23), 2.34-0.8 (Terpenoid protons), 0.92 (6H, s, H29&H30), 1.17 (3H, s, H24), 0.74 (3H, s, H27), 1.04 (3H, s, H25),1.15 (3H, s, H26); **^{13}C NMR (100 MHz, $CDCl_3$) δ**: C1(45.78), C2(65.16), C3(90.37), C4(38.14), C5(47.66), C6(17.75), C7(33.05), C8(39.34), C9(51.34), C10(36.95), C11(22.81), C12(122.26), C13(143.50), C14(41.60), C15(25.96), C16(23.24), C17(46.43), C18(40.96), C19(46.43), C20(30.68), C21(33.75), C22(32.38), C23(78.73), C24(14.35), C25(17.63), C26(17.02), C27(27.60), C28(182.87), C29(23.54), C30(31.96), C31(100.87), C32(134.17, d, J=3.0Hz), C33&C37(128.25, 2C, d, J=8.2Hz), C34&C36(115.25, 2C, d, J=21.6Hz), C35(163.12, d, J=245.8Hz) **Mass (*m/z*)**: 595.3806 $[M+H]^+$

3,23-(3,5-difluorobenzylidene) arjunolic acid (AA-5): Yield 80%, m.p. 326.7 – 327.8 °C

UV (λ_{max}, nm): 247, 294; **FTIR(KBr)cm^{-1}**: 3214-3506 (Broad, O-H stretch), 2919 (C-H stretch), 1692(s, C=O stretch), 1457 (C-H bending), 1224 (C-F stretch),1078 (C-O stretch), 833 (aromatic C-H out of plane bending); **^{1}H NMR (400 MHz, $CDCl_3$) δ**: 7.05(2H, d (J=5.6Hz), H33&H37), 6.79(1H, t (J= 8.8Hz), H35), 5.52(1H, s, H31), 5.28(1H, br s, H12), 3.90 (1H, m, H2), 3.30 (1H, d (J=9.7Hz), H3), 3.89(2H, d (J= 10.4Hz), H_a-23), 3.47 (1H, d (J= 10.4Hz), H_b-23), 2.34-0.8 (Terpenoid protons), 0.92 (6H, s, H29&H30), 1.06 (3H, s, H27), 1.03 (3H, s, H24), 1.18 (3H, s, H25),0.74 (3H, s, H26); **^{13}C NMR (100 MHz, DMSO) δ**: C1(45.87), C2(63.83), C3(90.05), C4(38.02), C5(48.18), C6(17.78), C7(33.75), C8(39.34), C9(50.62), C10(37.12), C11(23.83), C12(121.70), C13(144.35), C14(41.81), C15(26.18), C16(23.01), C17(46.13), C18(41.13), C19(47.45), C20(30.86), C21(32.18), C22(33.29), C23(78.02), C24(14.70), C25(17.50), C26(17.19), C27(27.64), C28(179.05), C29(23.29), C30(32.18), C31(99.95), C32(143.33), C33&C37(110.01, 2C, dd J= 25.7Hz, J= 6.8Hz), C34&C36(162.63, 2C, dd, J=257.3Hz, J= 13.0Hz), C35(104.46, t, J=26.3Hz); **Mass (*m/z*)**: 612.1804 $[M]^+$

3,23-(2-Chlorobenzylidene) arjunolic acid (AA-6): Yield 80%, m.p. 285.6-287 °C

UV (λ_{max}, nm): 264; **FTIR(KBr)cm^{-1}**: 3203-3497(Broad, O-H stretch), 2922(C-H stretch), 1694(s, C=O stretch), 1457(C-H bending), 1086(C-Cl stretch), 1006(C-O stretch), 755(aromatic C-H out of plane bending); **^{1}H NMR (400 MHz, DMSO) δ**: 12.03 (1H, s, COOH), 7.68(1H, aromatic proton), 7.45-7.38(3H, m, aromatic protons), 5.32 (1H, s, H31), 5.29 (1H, br s, H12), 3.90 (1H, m, H2), 3.31 (1H, d (J=9.7Hz), H3), 3.90(1H, d (J=10.4Hz), H_a-23), 3.48 (1H, d (J=10.4Hz), H_b-23), 2.34-0.8 (Terpenoid protons), 0.92 (6H, s, H29&H30), 1.17 (3H, s, H27), 0.74 (3H, s, H24), 1.03 (3H, s, H25), 1.15 (3H, s, H26); **^{13}C NMR(100MHz,DMSO) δ**: C1(45.89), C2(63.85), C3(90.40), C4(38.10), C5(48.49), C6(17.77), C7(33.30), C8(39.22), C9(50.59), C10(37.17), C11(23.03), C12(121.70), C13(144.39), C14(41.83), C15(26.16), C16(23.31), C17(46.14), c18(41.26), C19(47.44), C20(30.88), C21(32.21), C22(33.78), C23(78.29), C24(14.82), C25(17.50), C26(17.21), C27(27.65), C28(179.03), C29(23.84), C30(32.54), C31(99.29), C32(136.29), C33(132.26), C34(129.59), (130.97) ,C36(129.01), C37(127.66); **Mass (*m/z*)**: 633.3346 $[M+Na]^+$, 635.3305[M+Na+2]

3,23-(3-chlorobenzylidene) arjunolic acid (AA-7): Yield 80%, m.p. 286.7-287.4 °C

UV (λ_{max}, nm): 243, 274; **FTIR(KBr)cm^{-1}**: 3242-3518 (Broad, O-H stretch), 2932 (C-H stretch), 1694 (s, C=O stretch), 1457 (C-H bending), 1077 (C-Cl stretch), 1011 (C-O stretch), 786 (aromatic C-H, out of plane bending); **^{1}H NMR (400 MHz, DMSO) δ**: 12.03 (1H, s, COOH), 7.53(1H, broad s, H33), 7.39-7.29(3H, m, aromatic protons), 5.52 (1H, s, H31), 5.17 (1H, t, (J= 3.3Hz) H12), 4.65 (1H,d(J= 4.4 Hz),-OH), 3.69 (1H, m, H2), 3.25 (1H, d (J=9.8Hz), H3), 3.90(1H, d (J= 10.4Hz), H_a-23), 3.47 (1H, d (J= 10.4Hz), H_b-23), 2.34-0.80 (Terpenoid protons), 0.88 (6H,

s, H29&H30), 0.71 (3H, s, H27), 1.09 (3H, s, H24), 1.12 (3H, s, H25), 0.98 (3H, s, H26); **^{13}C NMR(100MHz,DMSO) δ**: C1(45.88), C2(63.85), C3(90.06), C4(38.10), C5(48.35), C6(17.77), C7(33.76), C8(40.89), C9(50.71), C10(37.13), C11(23.02), C12(121.71), C13(144.36), C14(41.82), C15(26.18), C16(23.83), C17(46.10), C18(41.24), C19(47.46), C20(30.89), C21(32.20), C22(33.30), C23(78.03), C24(14.47), C25(17.30), C26(17.50), C27(27.64), C28(179.04), C29(23.30), C30(32.54), C31(100.88), C32(141.51), C33(126.71), C34(133.21), C35(129.00), C36(130.50), C37(125.58); **Mass (*m/z*)**: 610.1850 $[M]^+$, 612.1833 [M+2]

3,23-(4-chlorobenzylidene) arjunolic acid (AA-8): Yield 80%, m.p. 298.2-300 °C
UV (λ_{max}, nm): 249; **FTIR(KBr)cm^{-1}**: 3178-3540 (Broad, O-H stretch), 2927 (C-H stretch), 1705 (s, C=O stretch), 1457 (C-H bending), 1080(C-Cl stretch), 1015 (C-O stretch), 818 (aromatic C-H out of plane bending); **^{1}H NMR (400 MHz, DMSO) δ**: 12.03 (1H, s, COOH), 7.50 (2H, d, (J= 8.6Hz) H33&H37), 7.44 (2H, d, (J= 8.5Hz), H34&H36), 5.51 (1H, s, H31), 5.17 (1H, t, (J= 3.6Hz), H12), 3.68 (1H, m, H2), 3.25 (1H, d (J=9.8Hz), H3), 3.79(1H, d (J= 10.4Hz), H_a-23), 3.47 (1H, d (J= 10.4Hz), H_b-23), 2.34-0.8 (Terpenoid protons), 0.88 (6H, s, H29&H30), 0.71(3H, s, H27), 1.12(3H, s, H24), 1.07(3H, s, H25), 0.98 (3H, s, H26);
^{13}C NMR(100 MHz, DMSO) δ: C1(45.88), C2(63.87), C3(90.04), C4(38.11), C5(48.43), C6(17.77), C7(33.29), C8(39.11), C9(50.74), C10(37.77), C11(23.03), C12(121.71), C13(144.37), C14(41.25), C15(26.18), C16(23.30), C17(46.04), C18(41.83), C19(47.47), C20(30.88), C21(32.41), C22(33.77), C23(78.02), C24(14.74), C25(17.50), C26(17.27), C27(27.63), C28(179.03), C29(23.83), C30(32.54), C31(101.23), C32(138.23), C33(128.84), C34(128.50), C35(133.64), C36(128.50), C37(128.84); **Mass (*m/z*)**: 610.1868 $[M]^+$, 612.1843 $[M+2]^+$, 633.1525 $[M+Na]^+$.

3,23-(2-bromobenzylidene) arjunolic acid (AA-9): Yield 85%, m.p. 266.5 – 268.00 °C
UV (λ_{max}, nm): 240; **FTIR (KBr) cm^{-1}**: 3162-3560 (Broad, O-H stretch), 2919 (C-H bending), 1689 (s, C=O stretch), 1457 (C-H bending), 1266 (C-O stretch),1080 (C-Br stretch), 755 (aromatic C-H out of plane bending); **^{1}H NMR (400MHz, $CDCl_3$) δ**: 7.74(1H, d, (J= 7.8Hz), H37), 7.55 (1H, d, (J= 8Hz), H34), 7.36(1H, t, (J= 7.5Hz), H36), 7.22(1H, dt, (J= 7.8Hz, J= 1.2Hz), H35), 5.81 (1H, s, H31), 5.29 (1H, t, (J=3.5Hz), H12), 3.94 (1H, m, H2), 3.38 (1H, d (J=9.7Hz), H3), 3.93(1H, d (J= 10.4Hz), H_a-23), 3.55 (1H, d (J= 10.4Hz), H_b-23), 2.34-0.8 (Terpenoid protons), 0.93 (6H, s, H29&H30), 0.74 (3H, s, H27), 1.19 (3H, s, H24), 1.06 (3H, s, H25), 0.94 (3H, s, H26);
^{13}C NMR (100 MHz, $CDCl_3$) δ: C1(45.77), C2(65.13), C3(90.50), C4(38.14), C5(47.63), C6(17.75), C7(33.05), C8(39.35), C9(51.34), C10(36.89), C11(22.77), C12(122.30), C13(143.48), C14(41.56), C15(25.96), C16(23.26), C17(46.22), C18(40.88), C19(46.45), C20(30.67), C21(31.99), C22(33.75), C23(78.93), C24(14.42), C25(17.65), C26(17.08), C27(27.60), C28(183.72), C29(23.55), C30(32.39), C31(101.54), C32(136.89), C33(122.01), C34(132.60), C35(130.51), C36(127.56), C37(128.48); **Mass (*m/z*)**: 655.2920 $[M]^+$, 657.2927 $[M+2]^+$

3,23-(3-bromobenzylidene) arjunolic acid (AA-10): Yield 80%, m.p. 294.5 – 296.2 °C
UV (λ_{max}, nm): 244; **FTIR(KBr)cm^{-1}**: 3142-3510 (Broad, O-H stretch), 2921 (C-H stretch), 1695 (s, C=O stretch), 1107 (C-O stretch), 1078 (C-Br stretch), 782 (aromatic C-H out of plane bending);**^{1}H NMR (400 MHz, CDCl$_3$) δ**: 7.67 (1H, s, H33), 7.49 (1H, d, (J= 8Hz), H37), 7.43 (1H, d, (J= 7.8),H35), 5.50 (1H, s, H31), 5.29 (1H, t, (J=3.3Hz), H12), 3.94 (1H, m, H2), 3.30 (1H, d (J=9.7Hz), H3), 3.90(1H, d (J= 10.4Hz), H_a-23), 3.47 (1H, d J= 10.4Hz, H_b-23), 2.34-0.8 (Terpenoid protons), 0.93 (6H, s, H29&H30), 0.74 (3H, s, H27), 1.18 (3H, s, H24), 1.15 (3H, s, H25), 1.06 (3H, s, H26); **^{13}C NMR (100 MHz, CDCl$_3$) δ**: C1(45.81), C2(65.19), C3(90.40), C4(38.16), C5(47.68), C6(17.79), C7(33.06), C8(39.36), C9(51.37), C10(36.94), C11(22.77), C12(123.29), C13(143.50), C14(41.61), C15(25.99), C16(23.27), C17(46.37), C18(40.94), C19(46.45), C20(30.69), C21(32.40), C22(33.77), C23(78.78), C24(14.41), C25(17.65), C26(17.03), C27(27.63), C28(183.26), C29(23.56), C30(32.02), C31(101.68), C32(140.23), C33(140.06), C34(122.45), C35(129.94), C36(129.53), C37(125.07); **Mass (*m/z*)**: 655.2988 $[M]^+$, 657.2983 $[M+2]^+$

3,23-(4-bromobenzylidene) arjunolic acid (AA-11): Yield 80%, m.p. 303.7 – 305.2 °C
UV (λ_{max}, nm): 235, 290; **FTIR(KBr)cm^{-1}**: 3150-3576 (Broad, O-H stretch), 2921 (C-H stretch), 1698(C=O stretch), 1011 (C-O stretch), 1077 (C-Br stretch), 810 (aromatic C-H out of plane bending);**^{1}H NMR (400MHz, CDCl$_3$) δ**: 7.51(1H, d, (J= 8.9Hz), H34&H36), 7.39(1H, d, (J= 8.4Hz), H34&H37), 5.50 (1H, s, H31), 5.28 (1H, t, (J= 3.4Hz), H12), 3.90 (1H, m, H2), 3.30 (1H, d (J=9.7Hz), H3), 3.90(1H, d (J= 10.5Hz), H_a-23), 3.47 (1H, d (J= 10.5Hz), H_b-23), 2.34-0.8 (Terpenoid protons), 0.93 (6H, s, C29&C30), 0.74 (3H, s, H27), 1.05 (3H, s, H24), 1.15(3H, s, H25), 1.17 (3H, s, H26); **^{13}C NMR(100MHz,CDCl$_3$) δ**: C1(45.78), C2(65.17), C3(90.33), C4(38.14), C5(47.65), C6(17.76), C7(33.05), C8(39.34), C9(51.35), C10(36.89), C11(22.78), C12(123.17), C13(143.48), C14(41.60), C15(25.97), C16(23.26), C17(46.34), C18(40.90), C19(46.44), C20(30.67), C21(31.99), C22(33.75), C23(78.72), C24(14.36), C25(17.62), C26(17.06), C27(27.61), C28(183.52), C29(23.55), C30(32.39), C31(101.97), C32(137.13), C33(128.09), C34(131.48), C35(122.77), C36(131.48), C37(128.09); **Mass (*m/z*)**: 655.3028 $[M]^+$, 657.2983 $[M+2]^+$

3,23-(2-Nitrobenzylidene) arjunolic acid (AA-12): Yield 80%, m.p. 309.8-310.2 °C

UV (λ_{max}, nm): 260; **FTIR(KBr)cm^{-1}**: 3244-3498 (Broad, O-H stretch), 2938 (C-H stretch), 1707 (C=O stretch), 1535 (N=O stretch), 1457 (C-H bending), 1362 (N=O stretch), 1071 (C-O stretch), 742 (aromatic C-H out of plane bending); **^{1}H NMR (400 MHz, DMSO) δ**: 7.93(1H, d, (J= 7.6Hz) H37), 7.85(1H, d, (J= 8Hz) H33), 7.63(1H, t, (J= 5.2Hz) H34), 7.50(1H, t, (J= 7.9), H36) 6.12 (1H, s, C31), 5.20 (1H, t, (J=3.2Hz) H12), 3.91 (1H, m, H2), 3.37 (1H, d (J=9.7Hz), H3), 3.89(1H, d (J= 10.4Hz), H_a-23), 3.59 (1H, d (J= 10.4Hz), H_b-23), 2.34-0.8 (Terpenoid protons), 0.93 (6H, s, H29&H30), 0.73 (3H, s, H27), 1.14 (3H, s,

H24), 1.04 (3H, s, H25), 1.13 (3H, s, H26); **^{13}C NMR (100 MHz, DMSO) δ**: C1(45.76), C2(65.18), C3(90.64), C4(38.14), C5(47.61), C6(17.76), C7(33.12), C8(39.34), C9(51.21), C10(37.03), C11(22.78), C12(123.12), C13(143.49), C14(41.56), C15(25.96), C16(23.25), C17(46.41), C18(40.89), C19(46.44); C20(30.67); C21(31.96); C22(33.75); C23(78.97), C24(14.41), C25(17.63), C26(17.06), C27(27.60), C28(183.51), C29(23.55), C30(33.05), C31(97.90), C32(132.79), C33(148.34), C34(123.97), C35(127.76), C36(132.04), C37(129.63); **Mass (*m/z*)**: 622.3730 $[M+H]^+$

3,23-(3-nitrobenzylidene)-arjunolic acid (AA-13): Yield 80%, m.p. 323.9-324.3 °C
UV (λ_{max}, nm): 262; **FTIR(KBr)cm^{-1}**: 3101-3404 (Broad, O-H stretch), 2943 (C-H stretch), 1714 (C=O stretch), 1533 (N=O stretch), 1457 (C-H bending), 1349 (N=O stretch), 1096 (C-O stretch), 732 (aromatic C-H out of plane bending); **^{1}H NMR (400 MHz, DMSO) δ**: 12.03 (1H, s, COOH), 8.30(1H, s, H32), 8.24(1H, d, (J= 8.2Hz), H34), 7.94(1H, d, (J= 7.8Hz), H36), 7.70(1H, t, (8Hz), H37), 5.68 (1H, s, H31), 5.18 (1H, t, (J=3.5Hz), H12), 4.70 (1H, d (J=4.5Hz), OH), 3.72 (1H, m, H2), 3.31(1H, overlapping with moisture signal in DMSO,H3), 3.84(1H, d (J= 10.4Hz), H_a-23), 3.54(1H, d (J= 10.4Hz), H_b-23), 2.34-0.8 (Terpenoid protons), 0.88 (6H, s, H29&H30), 0.78 (3H, s, H27), 1.13 (3H, s, H24), 1.08 (3H, s, H25), 0.99 (3H, s, H26); **^{13}C NMR (100MHz, DMSO) δ**: C1(45.88), C2(63.48), C3(90.13), C4(38.12), C5(48.42), C6(17.77), C7(33.30), C8(39.23), C9(50.70), C10(37.18), C11(23.03), C12(121.70), C13(144.37), C14(41.25), C15(26.18), C16(23.30), C17(46.25), C18(41.83), C19(47.47), C20(30.88), C21(32.20), C22(33.77), C23(78.11), C24(14.74), C25(17.52), C26(17.21), C27(27.65), C28(182.03), C29(23.84), C30(32.54), C31(100.30), C32(141.11), C33(124.09), C34(148.02), C35(121.43), C36(130.32), C37(133.59); **Mass (*m/z*)**: 620.2929 $[M-H]^+$

3,23-(4-Nitrobenzylidene) arjunolic acid (AA-14): Yield 80%, m.p. 326.3 – 327.8 °C
UV (λ_{max}, nm): 263; **FTIR(KBr)cm^{-1}**: 3062-3317 (Broad, O-H stretch), 2947 (C-H stretch), 1710 (C=O stretch), 1531 (N=O stretch), 1457 (C-H bending), 1352 (N=O stretch), 1080 (C-O stretch), 853 (aromatic C-H out of plane bending); **^{1}H NMR (400 MHz, DMSO) δ**: 12.04 (1H, s, COOH), 8.25(2H, d, (J= 8.7Hz), H33&H37), 7.77(2H, d, (J= 8.7Hz), H34&H36), 5.66 (1H, s, H31), 5.18 (1H, t, (J=2.9Hz), H12), 4.67 (1H, d (J=4.2 Hz), -OH), 3.70 (1H, m, H2), 3.83(1H, d (J=10.4Hz), H_a-23), 3.53(1H, d (J=10.4Hz), H_b-23), 3.30 (1H, overlapping with moisture signal in DMSO,H3), 2.340.8 (Terpenoid protons), 0.88 (6H, s, H29&H30), 0.71 (3H, s, H27), 1.13 (3H, s, H24), 1.08 (3H, s H25), 0.99 (3H, s, H26); **^{13}C NMR (100 MHz, DMSO) δ**: C1(45.88), C2(63.85), C3(90.00), C4(38.12), C5(48.40), C6(17.77), C7(33.30), C8(39.11), C9(50.10), C10(37.21), C11(23.03), C12(121.71), C13(144.37), C14(41.25), C15(26.18), C16(23.29), C17(46.15), C18(41.25), C19(47.48), C20(30.88), C21(32.26), C22(33.30), C23(78.10), C24(14.73), C25(17.75), C26(17.21),

C27(27.64), C28(179.03), C29(23.84), C30(32.54), C31(100.00), C32(145.78), C33(128.27), C34(123.80), C35(148.12), C36 (123.80), C37(128.27); **Mass (*m/z*)**: 620.2937 $[M-H]^+$

3,23-(4-Methoxybenzylidene) arjunolic acid (AA-15): Yield 80%, m.p. 294-295 °C
UV (λ_{max}, nm): 269; **FTIR(KBr)cm^{-1}**: 3020-3476 (Broad, O-H stretch), 2944 (C-H stretch), 1715 (C=O stretch), 1456 (C-H bending), 1251,1077 (C-O stretch), 832 (aromatic C-H out of plane bending); **^{1}H NMR (400 MHz, $CDCl_3$) δ**: 7.44(2H, d, (J=8.6Hz), H33&H37), 6.90(2H, d, (J=8.6Hz), H34&H36), 5.49 (1H, s, H31), 3.80 (3H, s, H38 -OCH_3), 5.28 (1H, t, (J=3.8Hz), H12), 3.90 (1H, m, H2), 3.29 (1H, d (J=9.7Hz), H3), 3.89 (1H, d (J= 10.3Hz), H_a-23), 3.46(1H, d (J= 10.3Hz), H_b-23), 2.34-0.8 (Terpenoid protons), 0.93 (3H, s, H29), 0.91 (3H, s, H30), 1.19 (3H, s, H27), 1.15 (3H, s, H24), 0.74 (3H, H26),0.95 (3H, H25); **^{13}C NMR(100 MHz, $CDCl_3$) δ**: C1(45.78), C2(65.18), C3(90.00), C4(38.14), C5(47.65), C6(17.76), C7(33.05), C8(39.35), C9(51.38), C10(36.82), C11(22.77), C12(122.31), C13(143.48), C14(41.56), C15(25.98), C16(23.26), C17(46.45), C18(40.89), C19(46.45), C20(30.67), C21(32.01) ,C22(33.75), C23(78.74), C24(14.38), C25(17.63), C26(17.08), C27(27.61), C28(183.72), C29(23.55), C30(32.40), C31(102.69), C32(130.71), C33(127.73), C34(113.73), C35(160.16), C36(113.73), C37(127.73),C38(55.32); **Mass (*m/z*)**: 607.3599 $[M+H]^+$

3,23-(2-Hydroxybenzylidene) arjunolic acid (AA-16): Yield 80%, m.p. 254.4-255 °C
UV (λ_{max}, nm): 247, 311; **FTIR(KBr)cm^{-1}**: 3058-3540 (Broad, O-H stretch), 2921 (C-H stretch), 1699 (C=O stretch), 1457 (C-H bending), 1074 (C-O stretch),754 (aromatic C-H out of plane bending). **^{1}H NMR (400 MHz, DMSO) δ**: 12.03 (1H, s, COOH), 7.41(1H, m, aromatic proton), 7.14(1H, m, aromatic proton), 6.81-6.77(2H, m, aromatic protons), 5.50 (1H, s, H31), 5.17 (1H, t, (3.4Hz), H12), 4.52 (1H, d, (4.9Hz), H2, -OH), 3.65 (1H, m, H2), 3.75 (1H, d (J=9.7Hz), H3), 3.75(1H, d (J= 12Hz), H_a-23), 3.41(1H, d (J= 12Hz), H_b-23), 2.34-0.8 (Terpenoid protons), 0.87 (6H, s, H29&H30), 1.09 (3H, s, H27), 1.13 (3H, s, H24), 0.70 (3H, H26),0.98(3H, H25); **^{13}C NMR(100 MHz, DMSO) δ**: C1(45.2), C2(63.69), C3(90.32), C4(37.15), C5(48.51), C6(17.79), C7(33.30), C8(38.54), C9(50.69), C10(38.11), C11(23.03), C12(121.72), C13(144.10), C14(41.81), C15(28.31), C16(27.66), C17(46.14), C18(41.28), C19(47.44), C20(30.88), C21(31.16), C22(33.77), C23(78.18), C24(14.28), C25(17.50), C26(17.21), C27(26.19), C28(179.05), C29(23.81), C30(32.21), C31(97.82), C32(130.00), C33(154.7), C34(115.81), C35(125.51), C36(121.2), C37(128.2); **Mass (*m/z*)**: 591.3062 $[M-H]^+$

3,23-(2-Pyrilidene) arjunolic acid (AA-17): Yield 80%, m.p. 340.2 – 341.5 °C
UV (λ_{max}, nm): 252; **FTIR(KBr)cm^{-1}**: 3067-3538(Broad, O-H stretch), 2921(C-H stretch), 1717(C=O), 1457(C-H bending), 1079(C-O stretch), 1007(C-N stretch), 775(aromatic C-H out of plane bending); **^{1}H NMR (400MHz, DMSO) δ**: 12.03(1H, s, COOH), 8.52(1H, d, (J= 2.2Hz),

H33), 7.85(1H, t, (J=7.3Hz), H34), 7.59(1H, d, (J=7.8Hz), H36), 7.39(1H, t, (J= 5.6Hz), H35), 5.49(1H, s, H31), 5.17(1H, br s, H12), 3.68(1H, m, H2), 4.56(1H, d (J=9.7Hz), H3), 3.79(1H, d (J= 10.4Hz), H_a-23), 3.50(1H, d (J=10.4Hz), H_b-23), 2.34-0.8(Terpenoid protons), 0.88(6H, s, H29&H30), 0.71(3H,H27), 1.13(3H, s, H24), 0.13(3H, H26), 0.99(3H, H25); **^{13}C NMR (100 MHz, DMSO) δ**: C1(45.88), C2(63.88), C3(90.00), C4(38.12), C5(48.51), C6(17.77), C7(33.30), C8(39.12), C9(50.66), C10(37.25), C11(23.03), C12(121.71), C13(144.38), C14(41.83), C15(26.19), C16(23.30), C17(46.14), C18(41.25), C19(47.46), C20(30.89), C21(32.19), C22(33.77), C23(77.94), C24(14.80), C25(17.49), C26(17.21), C27(27.64), C28(179.03), C29(23.84), C30(32.55), C31(103.31), C32(157.48),C33(148.77),C34(121.63),C35(137.63),C36(124.66); **Mass (*m/z*)**: 578.3874 $[M+H]^+$, 600.3683 $[M+23]^+$

3,23-(2-Furfurylidene) arjunolic acid (AA-18): Yield 80%. m.p. 266-268 °C
UV (λ_{max}, nm): 246; **FTIR(KBr)cm^{-1}**: 3047-3478 (broad, O-H stretch), 2922 (C-H stretch), 1718 (C=O stretch), 1457 (C-H bending)1083,1005 (C-O stretch), 739 (aromatic C-H out of plane bending). **^{1}H NMR (400 MHz, $CDCl_3$) δ**: 7.41(1H, d, H35), 6.48(1H, d, (J= 3.2Hz), H33), 6.38(1H, dd, (J= 3.1Hz, J= 1.8Hz), H34), 5.62 (1H, s, H31), 5.28 (1H, t, (J=3.2Hz) H12), 5.33 (1H, s, -OH), 3.98 (1H, m, H2), 3.26 (1H, d (J=9.7Hz), H3), 3.88 (1H, d (J= 10.5Hz), H_a-23), 3.45(1H, d (J= 10.5Hz), H_b-23), 2.34-0.8 (Terpenoid protons), 0.91 (3H, s, H29), 0.93 (3H, s, H30),1.14 (3H, s, H27), 1.18 (3H, s, H24), 0.73 (3H, H26),0.05 (3H, H25); **^{13}C NMR (100MHz, $CDCl_3$) δ**: C1(45.77), C2(65.30), C3(90.33), C4(38.11), C5(47.64), C6(17.76), C7(33.05), C8(39.33), C9(51.32), C10(39.06), C11(22.77), C12(122.26), C13(143.48), C14(41.56), C15(25.97), C16(23.24), C17(46.30), C18(40.88), C19(46.44), C20(30.67), C21(31.99), C22(33.75), C23(78.73), C24(14.22), C25(17.61), C26(17.01), C27(27.60), C28(183.71), C29(23.54), C30(32.39), C31(96.85), C32(150.67), C33(107.85), C35(110.22), C36(142.64); **Mass (*m/z*)**: 567.3694 $[M+H]^+$

3,23-(2-Thiophenylidene) arjunolic acid (AA-19): Yield 80%, m.p. 115.7-117.2 °C
UV (λ_{max}, nm): 247, 296; **FTIR(KBr)cm^{-1}**: 3142-3540 (Broad, O-H stretch), 2921 (C-H stretch), 1690 (C=O stretch), 1457 (C-H bending), 1073 (C-O stretch), 1004, 699 (C-s stretch); **^{1}H NMR (400 MHz, DMSO) δ**: 12.03 (1H, s, COOH), 5.80 (1H, s, H31), 7.35 (1H, d, (J=4.9Hz), H33), 7.0 (1H, dd, (J= 4.9Hz, J= 3.7Hz), H34), 7.30 (1H, d, (J= 3.1Hz), H35), 5.29 (1H, t, (3.5Hz), H12), 3.90 (1H, m, H2), 3.29 (1H, d (J=9.7Hz), H3), 3.91(1H, d (J= 10.5Hz), H_a-23), 3.47 (1H, d (J= 10Hz), H_b-23), 2.34-0.8 (Terpenoid protons), 0.92 (6H, s, H29&H30), 0.74 (3H, s, H27), 1.18 (3H, s, H24), 1.04 (3H, H26),1.15 (3H, H25); **^{13}C NMR (100 MHz, DMSO) δ**: C1(45.78), C2(65.09), C3(90.29), C4(38.12), C5(47.65), C6(17.74), C7(33.05), C8(39.34), C9(51.31), C10(36.87), C11(22.79), C12(122.28), C13(143.47), C14(41.59), C15(25.97), C16(23.25), C17(46.29), C18(40.29), C19(46.44), C20(30.67), C21(33.75), C22(32.39), C23(78.79), C24(14.29), C25(17.03),

C26(17.01), C27(27.60), C28(180.13), C29(23.54), C30(30.94), C31(99.05), C32(141.03), C33(125.43), C34(125.92), C35(126.42); **Mass (*m/z*)**: 583.3457 $[M+H]^+$, 605.3265 $[M+23]^+$

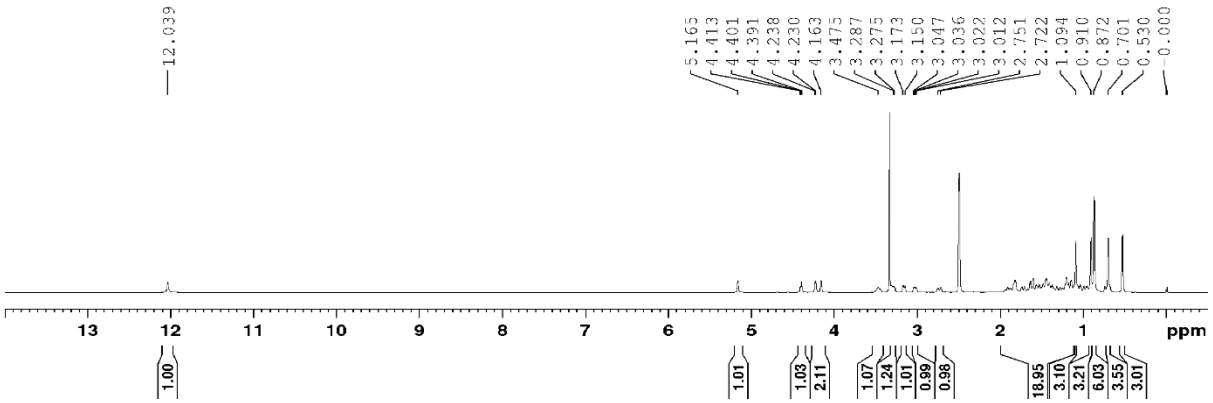


Fig. S2 ^{1}H NMR spectrum of Arjunolic acid

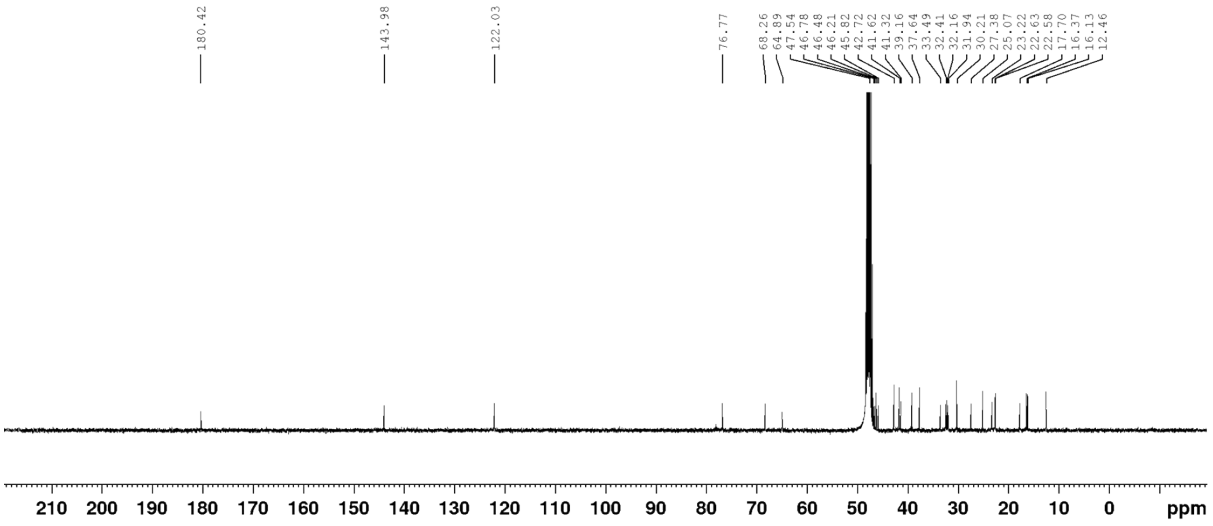


Fig. S3 ^{13}C NMR spectrum of Arjunolic acid

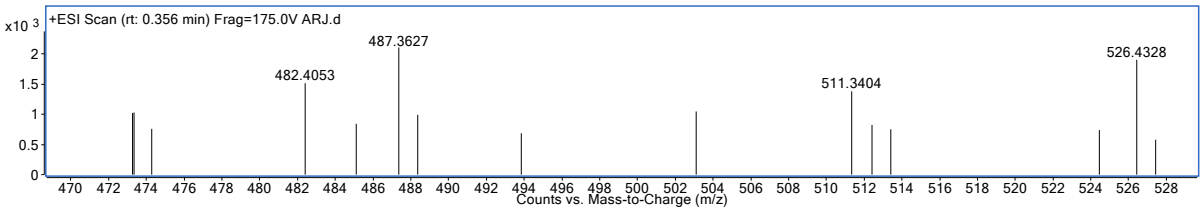


Fig. S4 Mass spectrum of Arjunolic acid

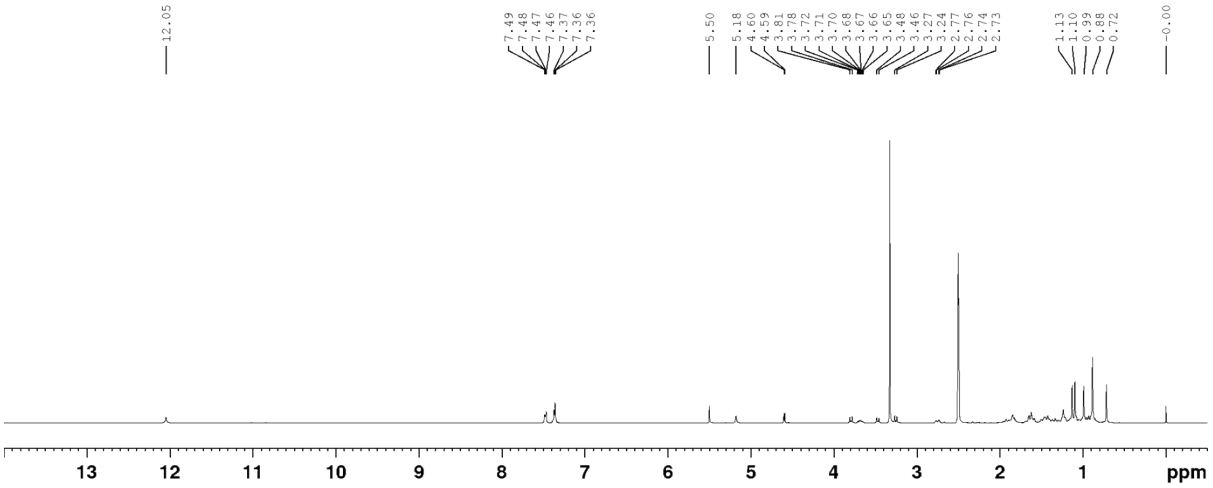


Fig. S5 ^{1}H NMR spectrum of 3,23-benzylidene arjunolic acid (AA-1)

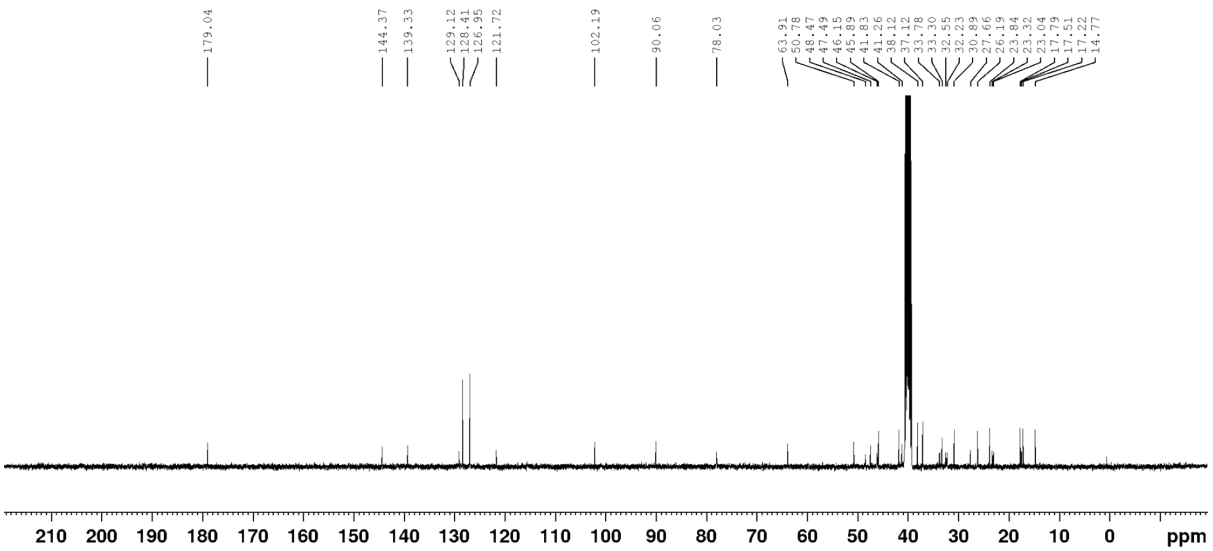


Fig. S6 ^{13}C NMR spectrum of 3,23-benzylidene arjunolic acid (AA-1)

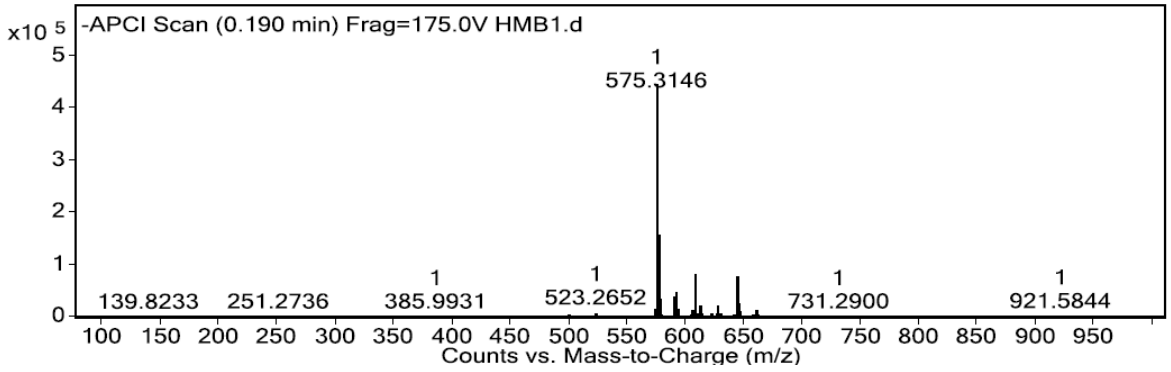


Fig. S7 Mass spectrum of 3,23-benzylidene arjunolic acid (AA-1)

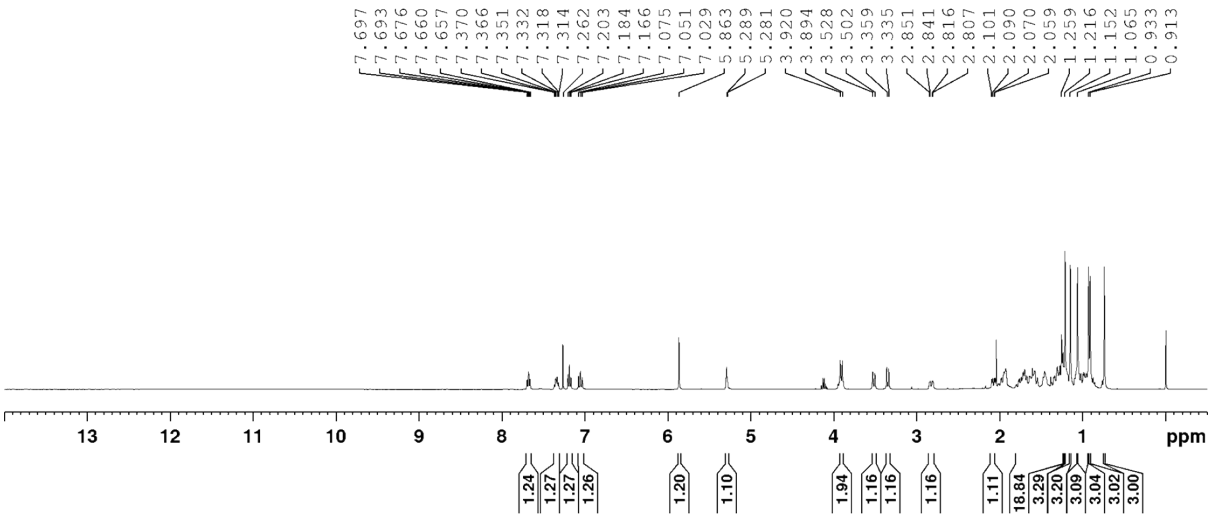


Fig. S8 ^{1}H NMR of spectrum of 3,23-(2-fluorobenzylidene) arjunolic acid (AA-2)

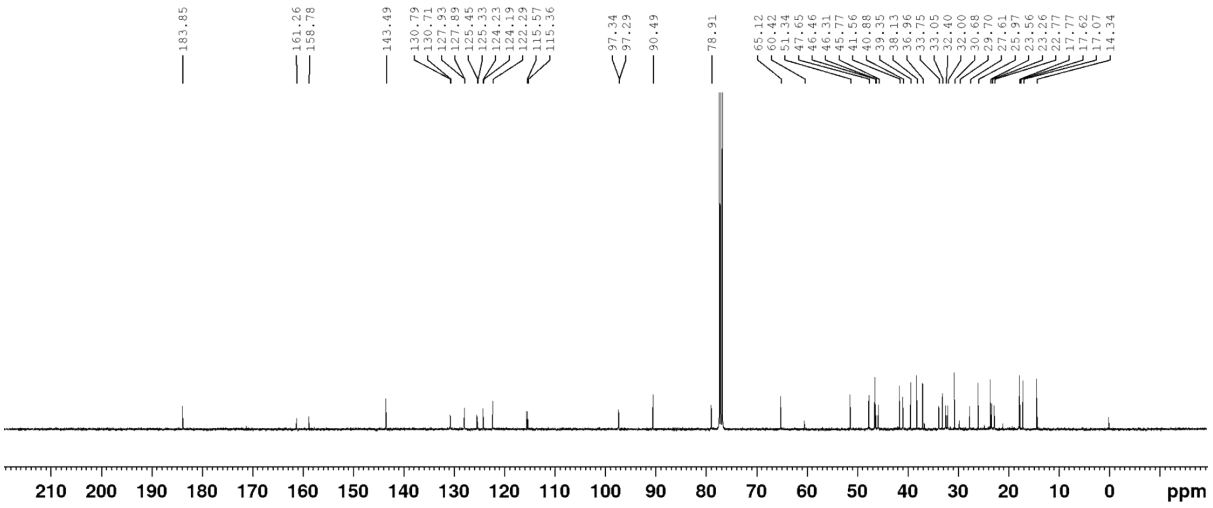


Fig. S9 ^{13}C NMR spectrum of 3,23-(2-fluorobenzylidene) arjunolic acid (AA-2)

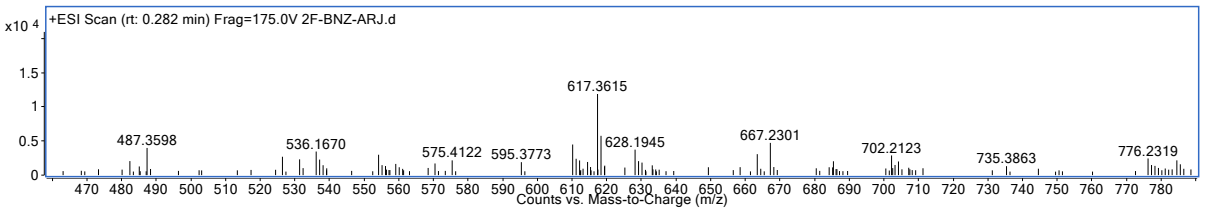


Fig. S10 Mass spectrum of 3,23-(2-fluorobenzylidene) arjunolic acid (AA-2)

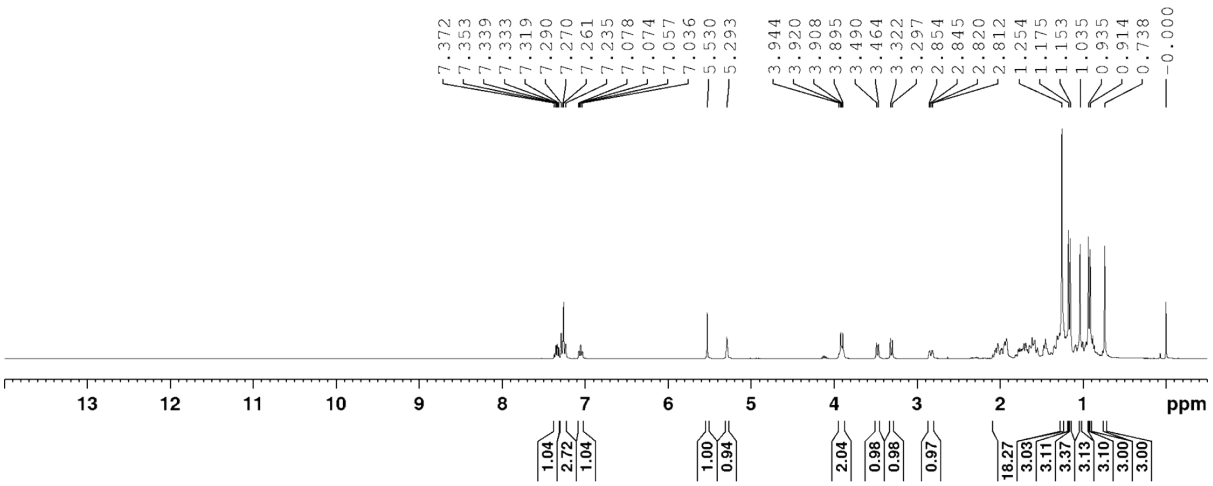


Fig. S11 ^{1}H NMR spectrum of 3,23-(3-fluorobenzylidene) arjunolic acid (AA-3)

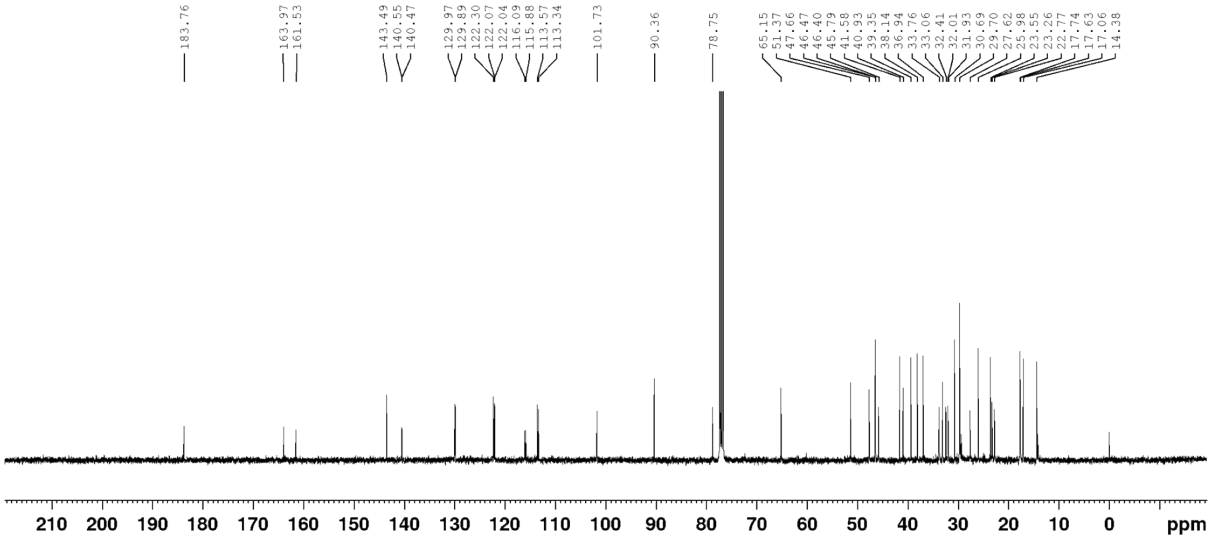


Fig. S12 ^{13}C NMR spectrum of 3,23-(3-fluorobenzylidene) arjunolic acid (AA-3)

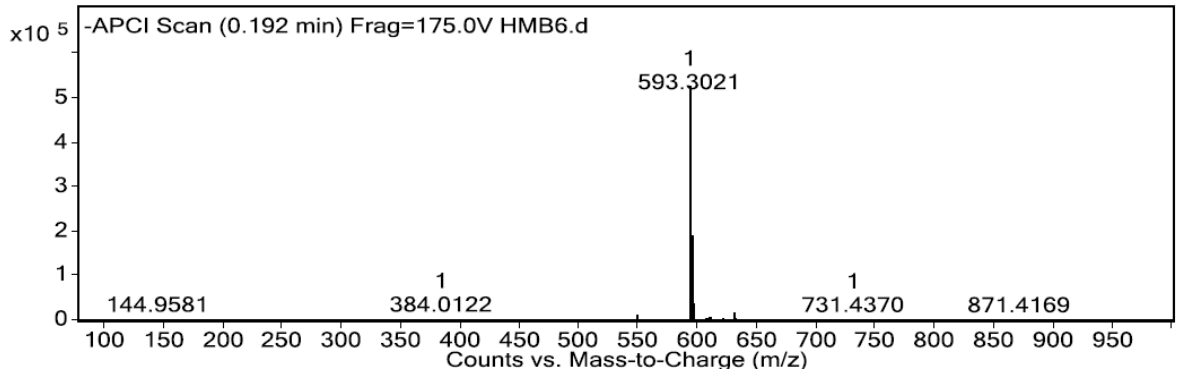


Fig. S13 Mass spectrum of 3,23-(3fluorobenzylidene) arjunolic acid (AA-3)

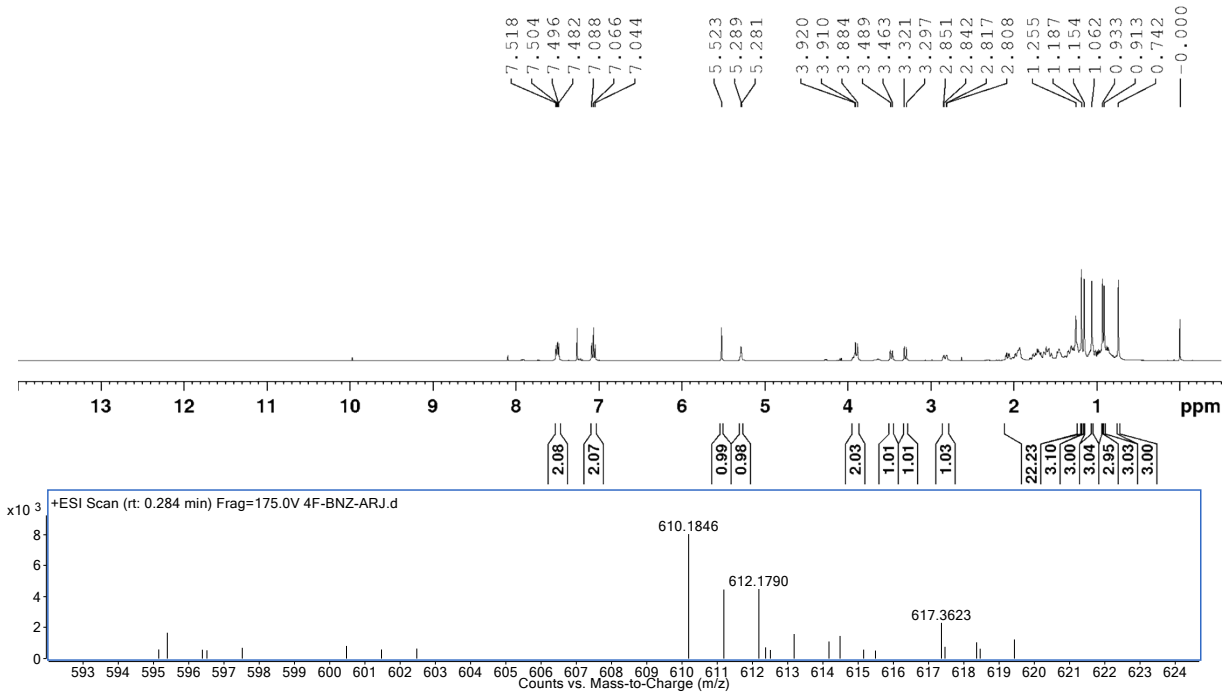


Fig. S14 ^{1}H NMR spectrum of 3,23-(4-fluorobenzylidene) arjunolic acid (AA-4)

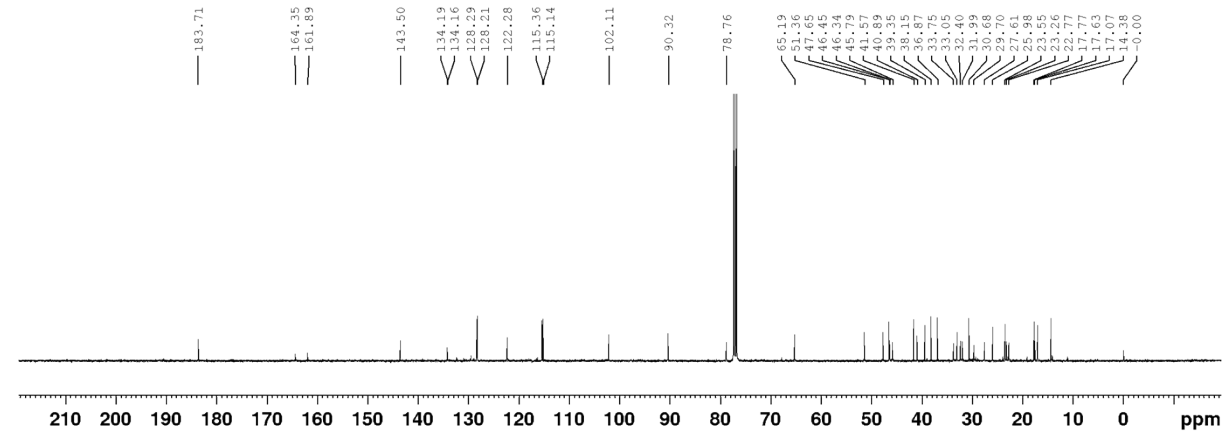


Fig. S15 ^{13}C NMR of 3,23-(4-fluorobenzylidene) arjunolic acid (AA-4)

Fig. S6 Mass spectrum of 3,23-(4-fluorobenzylidene) arjunolic acid (AA-4)

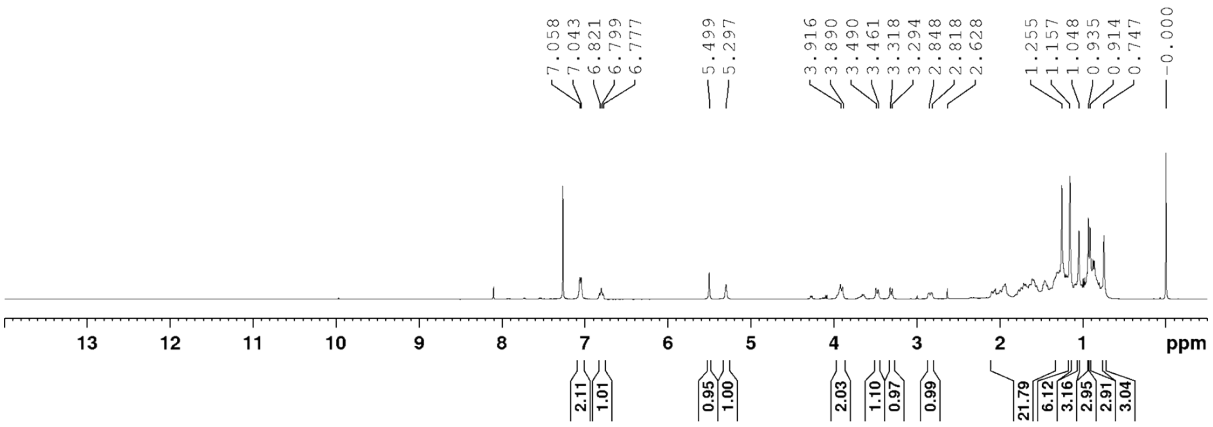


Fig. S17 ^{1}H NMR spectrum of 3,23-(3,5-di-fluorobenzylidene) arjunolic acid (AA-5)

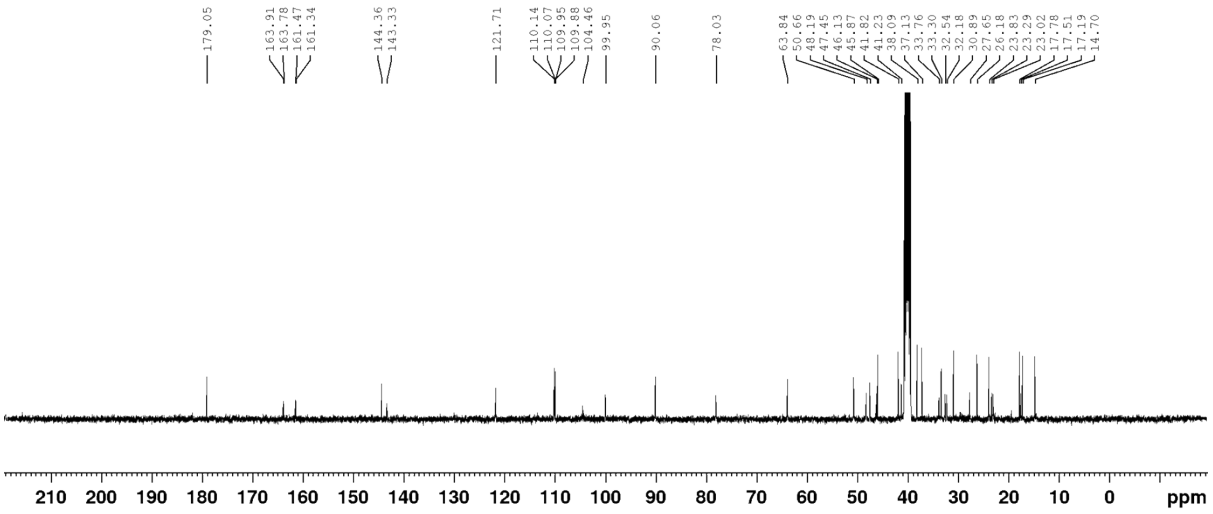


Fig. S18 ^{13}C NMR of 3,23-(3,5-di-fluorobenzylidene) arjunolic acid (AA-5)

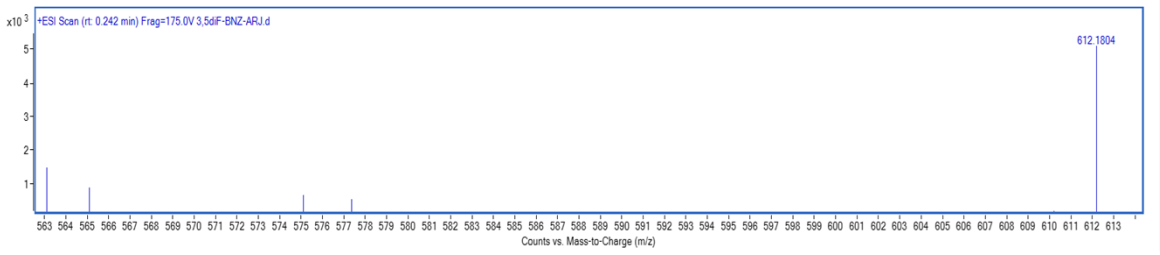


Fig. S19 Mass spectrum of 3,23-(3,5-di-fluorobenzylidene) arjunolic acid (AA-5)

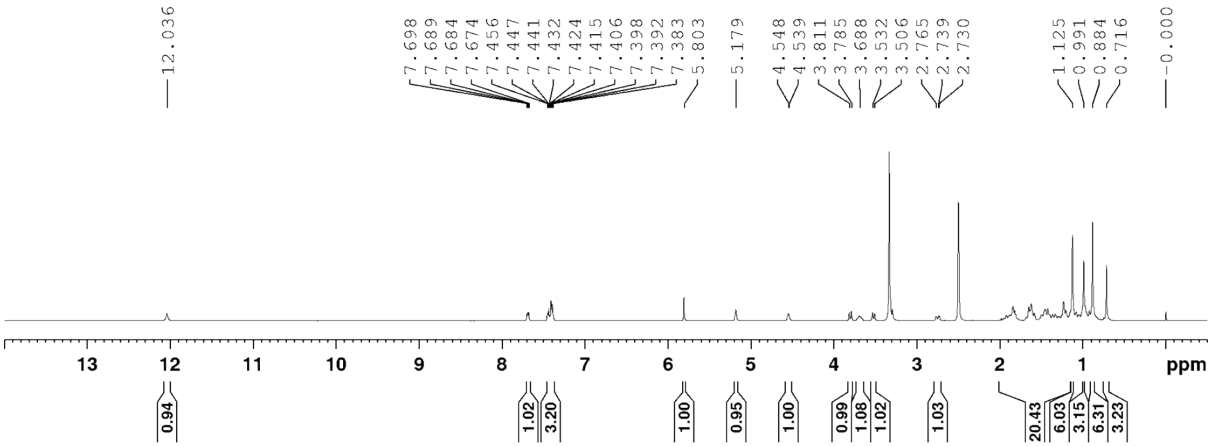


Fig. S20 ^{1}H NMR spectrum of 3,23-(2-chlorobenzylidene) arjunolic acid (AA-6)

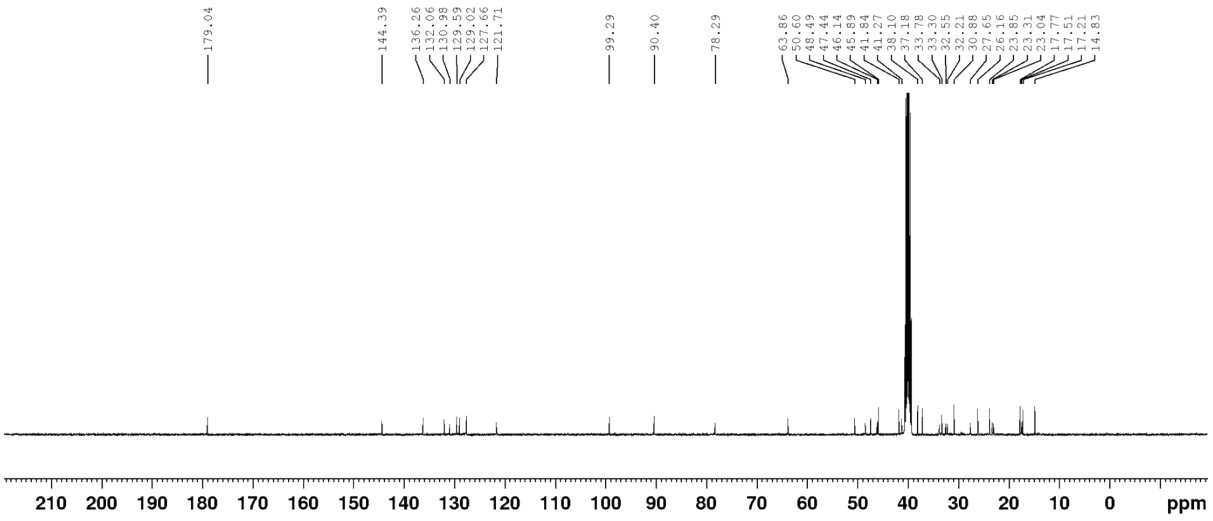


Fig. S21 ^{13}C NMR of 3,23-(2-chlorobenzylidene) arjunolic acid (AA-6)

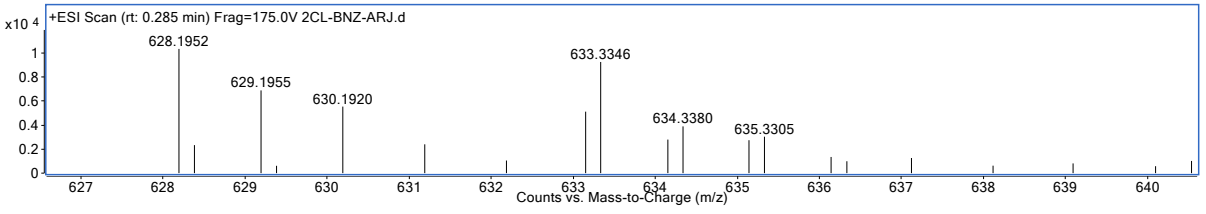


Fig. S22 Mass spectrum of 3,23-(2-chlorobenzylidene) arjunolic acid (AA-6)

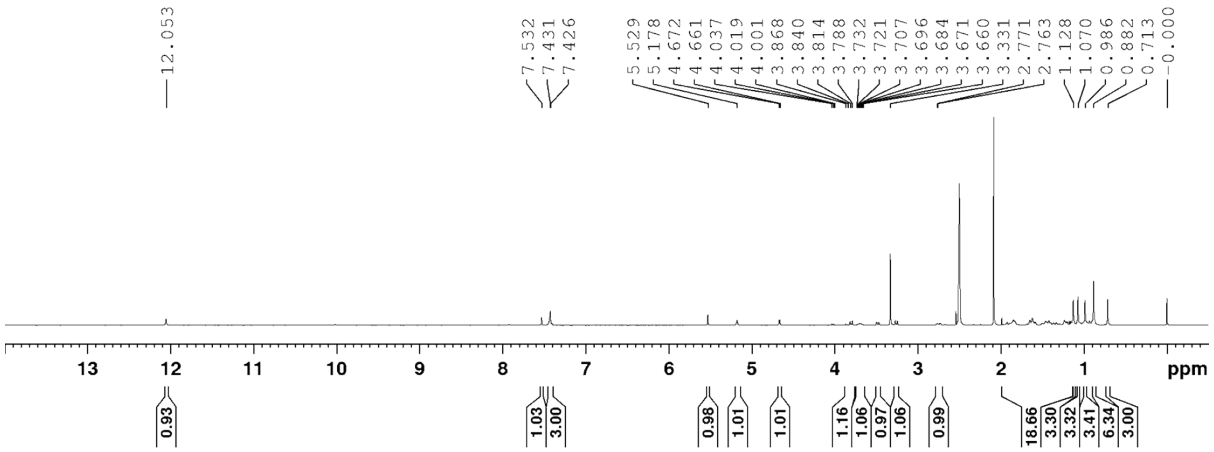


Fig. S23 ^{1}H NMR of 3,23-(3-chlorobenzylidene) arjunolic acid (AA-7)

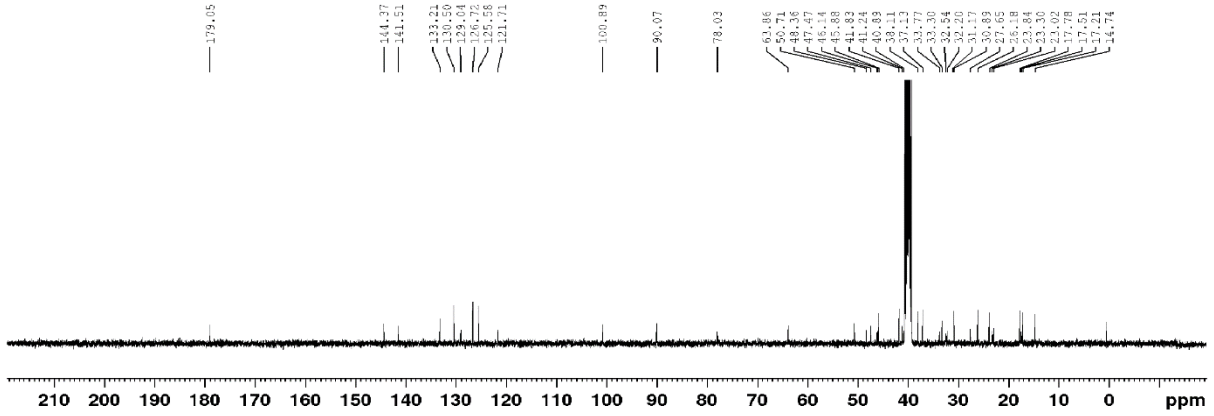


Fig. S24 ^{13}C NMR of 3,23-(3-chlorobenzylidene) arjunolic acid (AA-7)

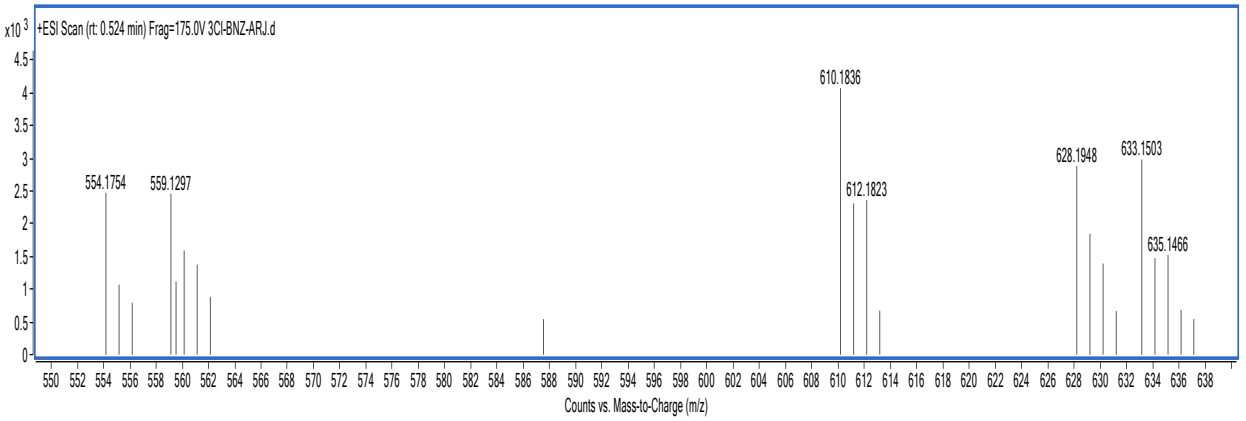


Fig. S25 Mass spectrum of 3,23-(3-chlorobenzylidene) arjunolic acid (AA-7)

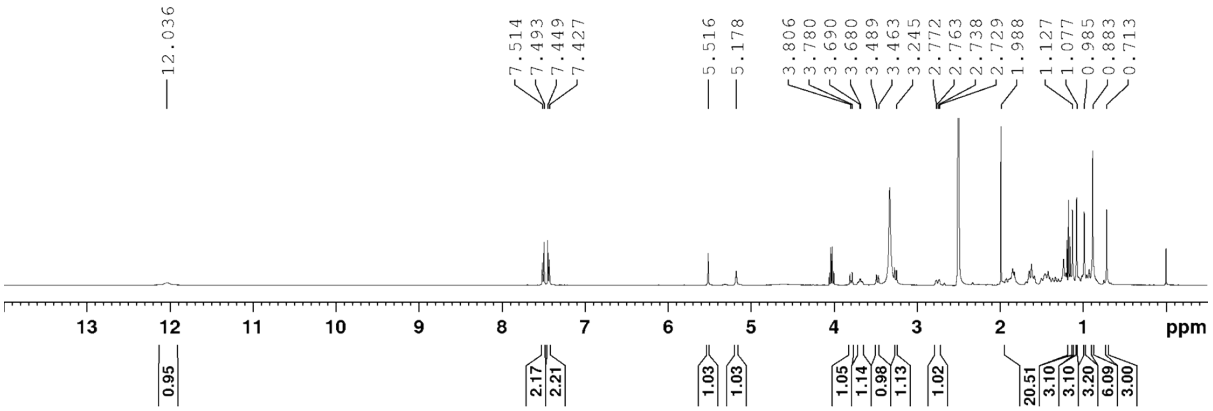


Fig. S26 ^{1}H NMR spectrum of 3,23-(4-chlorobenzylidene) arjunolic acid (AA-8)

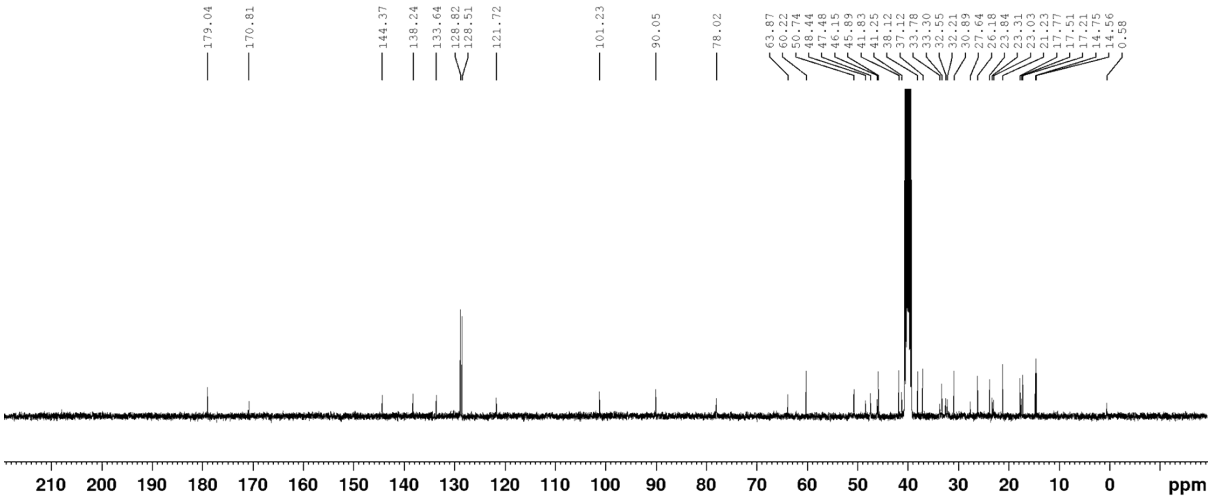


Fig. S27 ^{13}C NMR of 3,23-(4-chlorobenzylidene) arjunolic acid (AA-8)

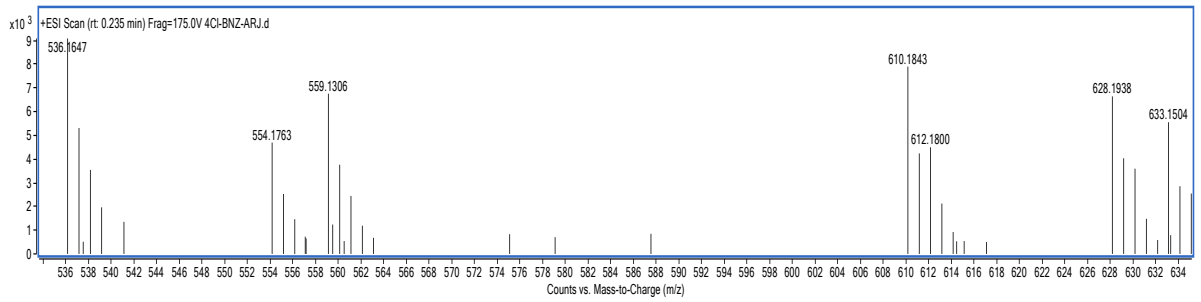


Fig. S28 Mass spectrum of 3,23-(4-chlorobenzylidene) arjunolic acid (AA-8)

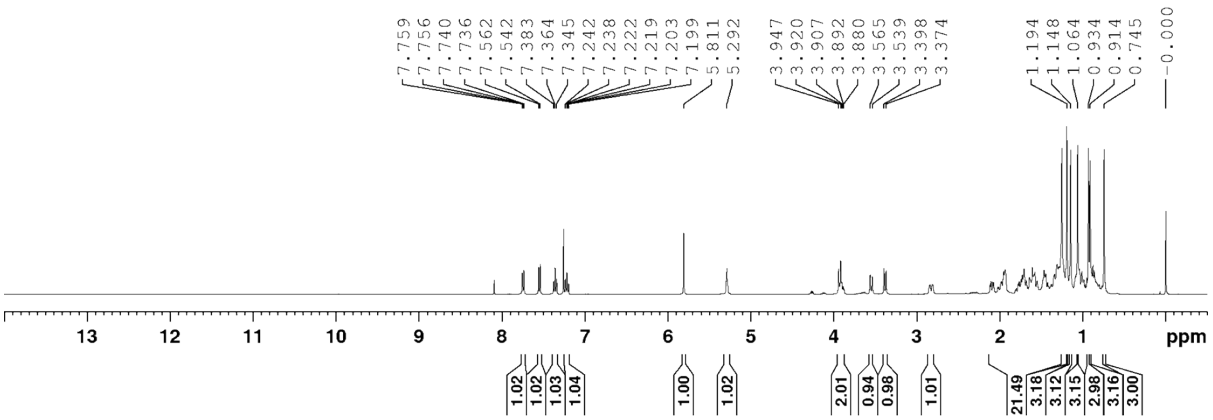


Fig. S29 ^{1}H NMR of 3,23-(2-bromobenzylidene) arjunolic acid (AA-9)

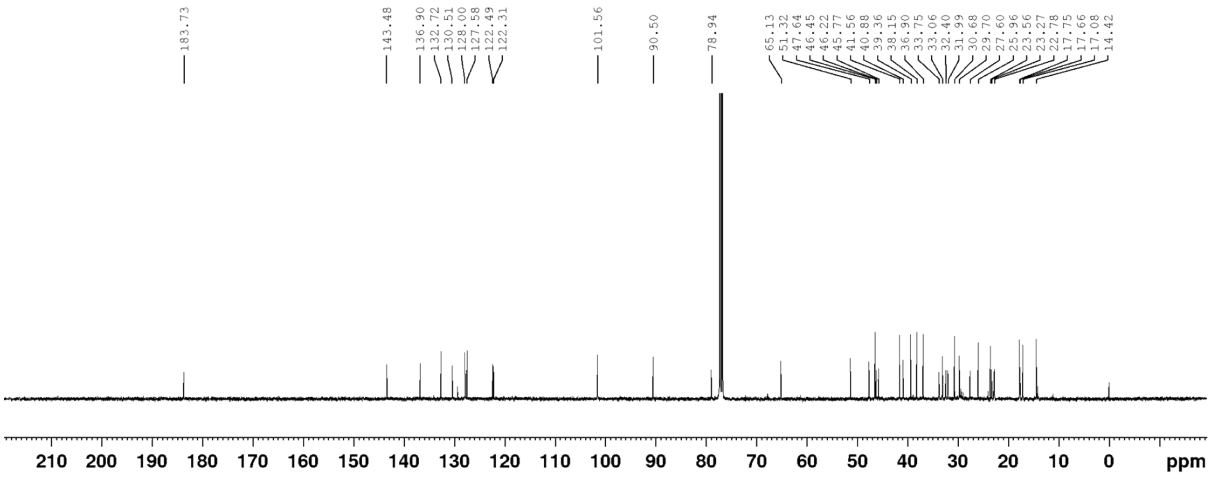


Fig. S30 ^{13}C NMR spectrum of 3,23-(2-bromobenzylidene) arjunolic acid (AA-9)

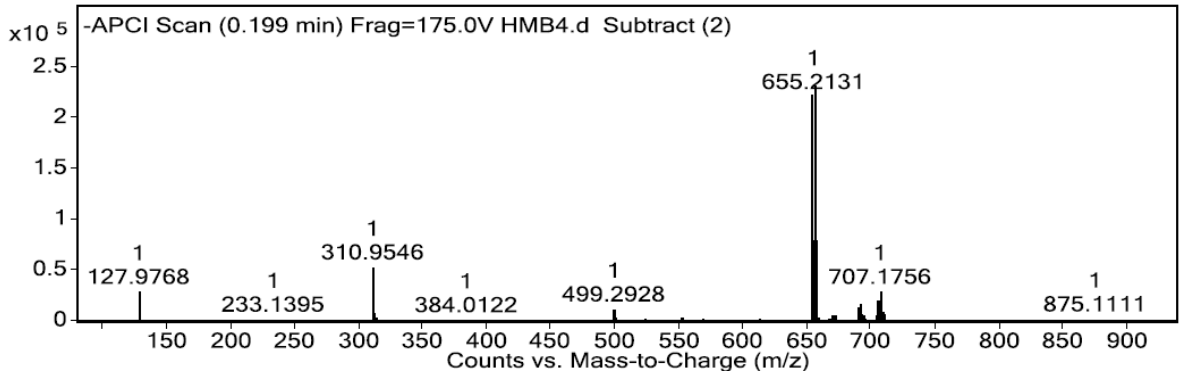


Fig. S31 Mass spectrum of 3,23-(2-bromobenzylidene) arjunolic acid (AA-9)

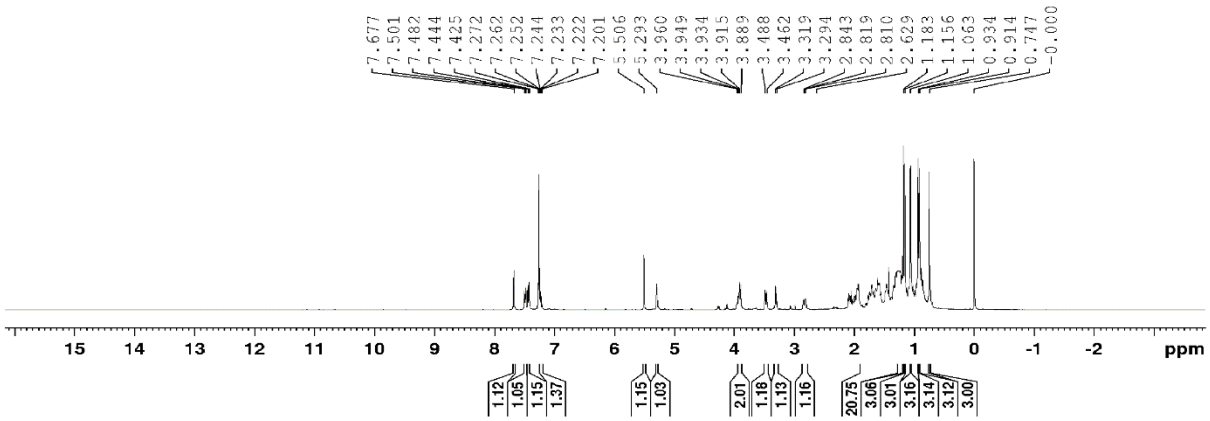


Fig. S32 ^{1}H NMR spectrum of 3,23-(3-bromobenzylidene) arjunolic acid (AA-10)

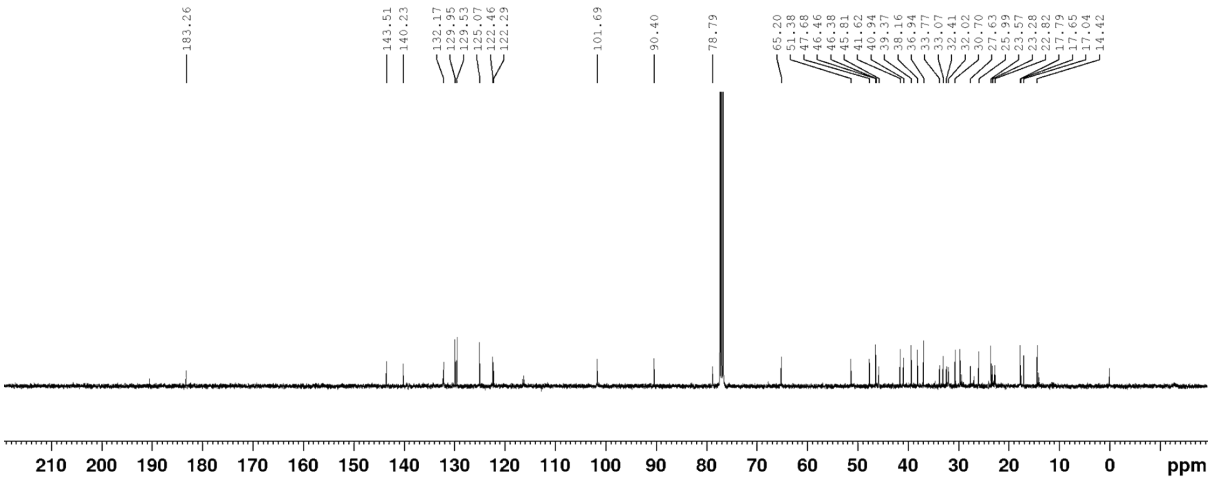


Fig. S33 ^{13}C NMR spectrum of 3,23-(3-bromobenzylidene) arjunolic acid (AA-10)

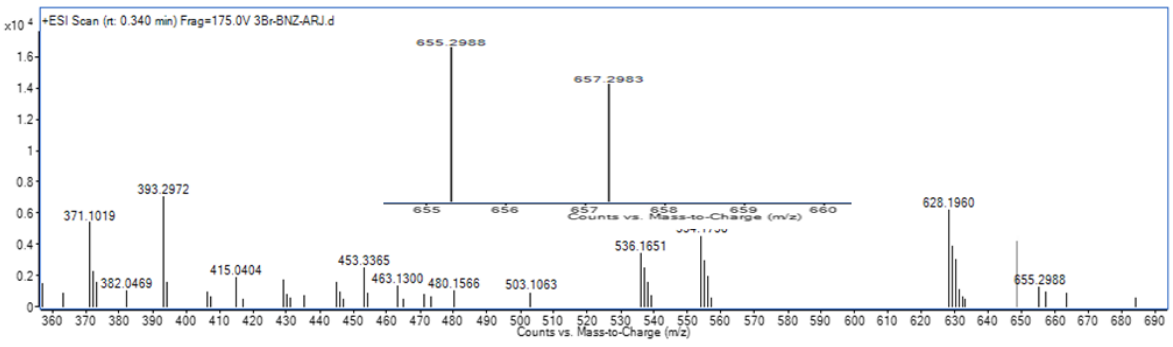


Fig. S34 Mass spectrum of 3,23-(3-bromobenzylidene) arjunolic acid (AA-10)

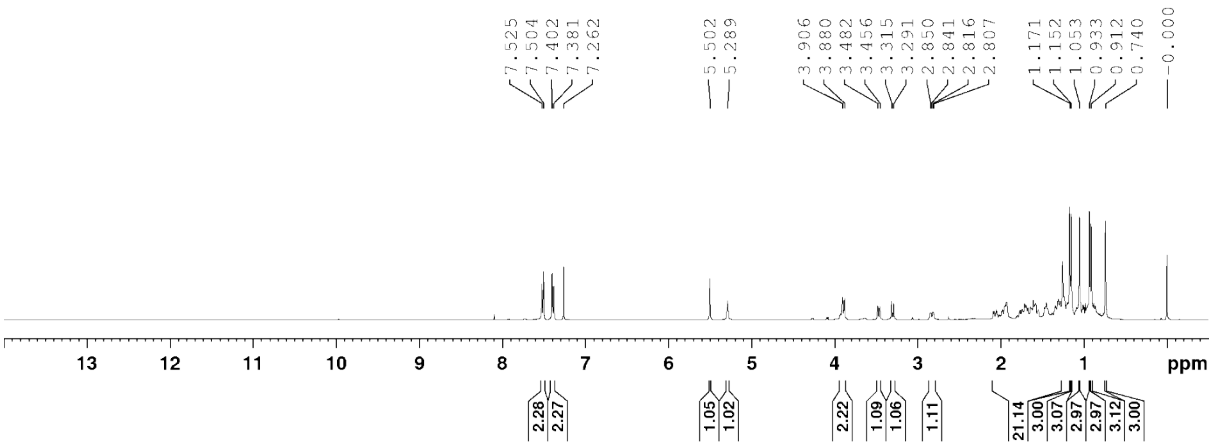


Fig. S35 ^{1}H NMR spectrum of 3,23-(4-bromobenzylidene) arjunolic acid (AA-11)

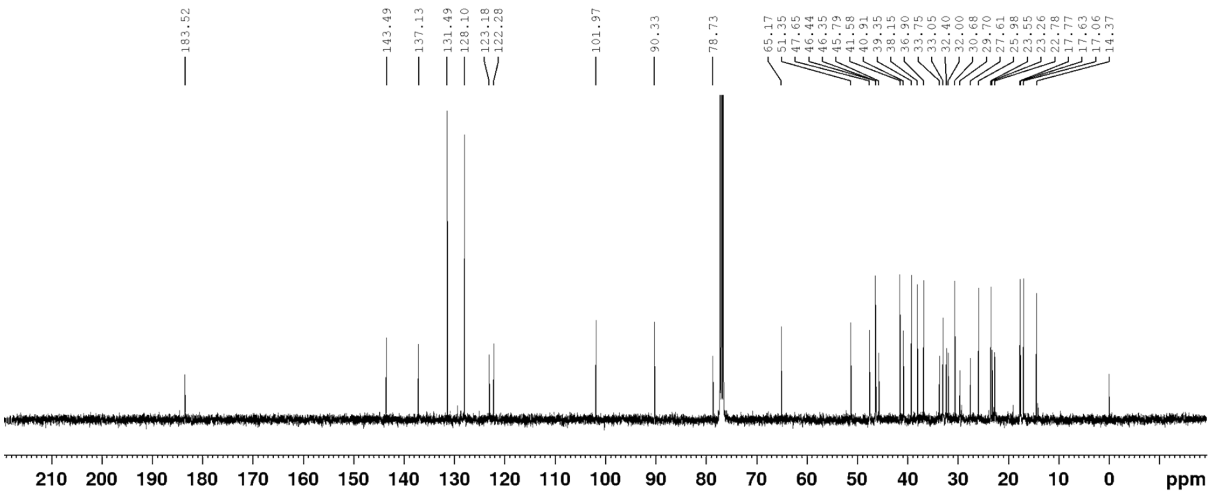


Fig. S36 ^{13}C NMR of 3,23-(4-bromobenzylidene) arjunolic acid (AA-11)

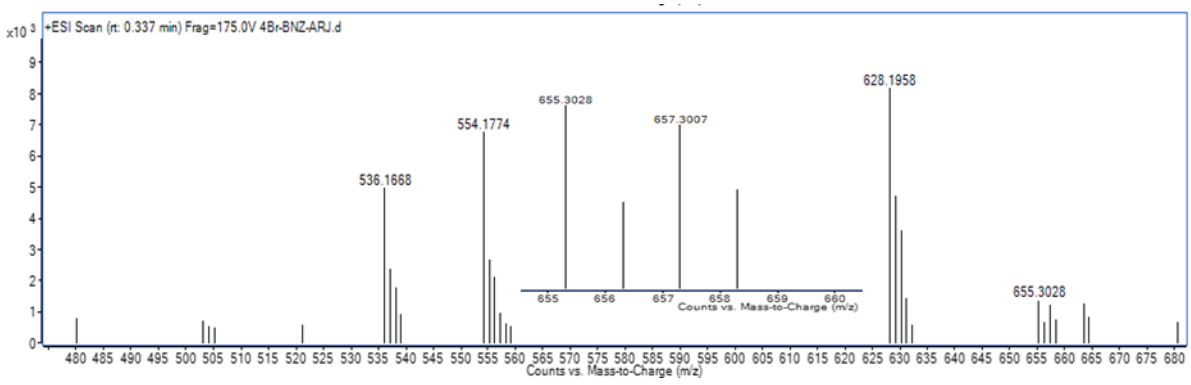


Fig. S37 Mass spectrum of 3,23-(4-bromobenzylidene) arjunolic acid (AA-11)

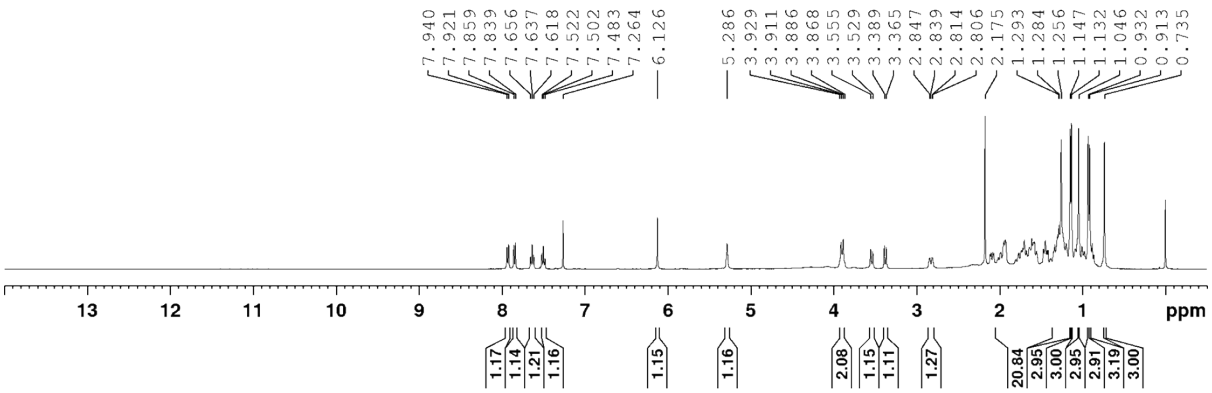


Fig. S38 ^{1}H NMR spectrum of 3,23-(2-nitrobenzylidene) arjunolic acid (AA-12)

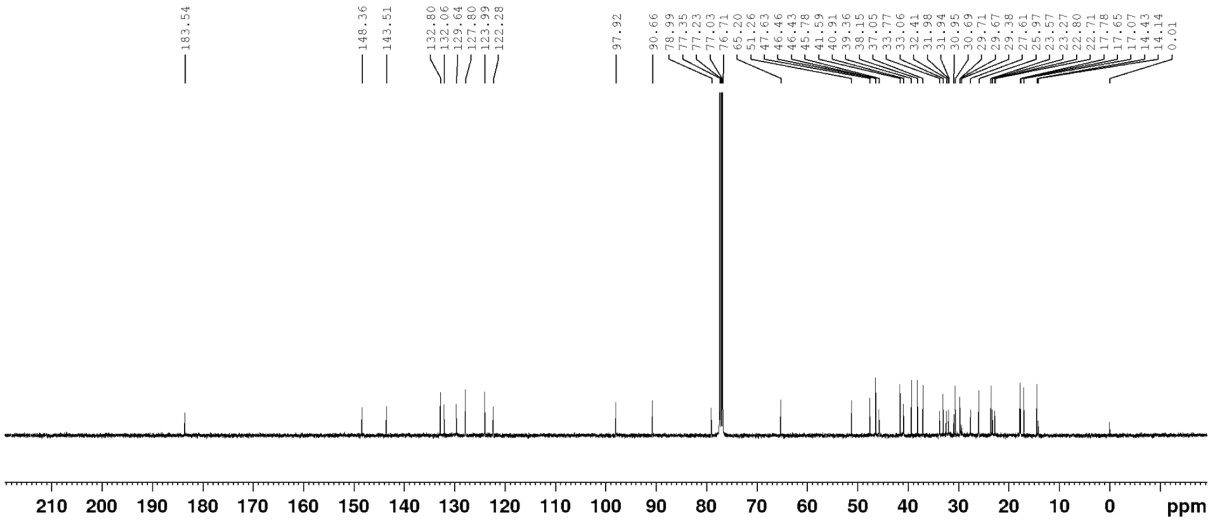


Fig. S39 ^{13}C NMR spectrum of 3,23-(2-nitrobenzylidene) arjunolic acid (AA-12)

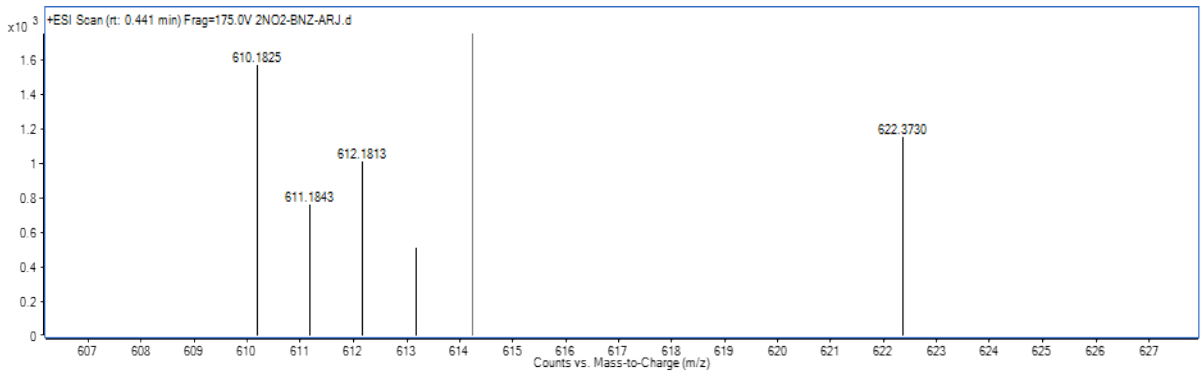


Fig. S40 Mass spectrum of 3,23-(2-nitrobenzylidene) arjunolic acid (AA-12)

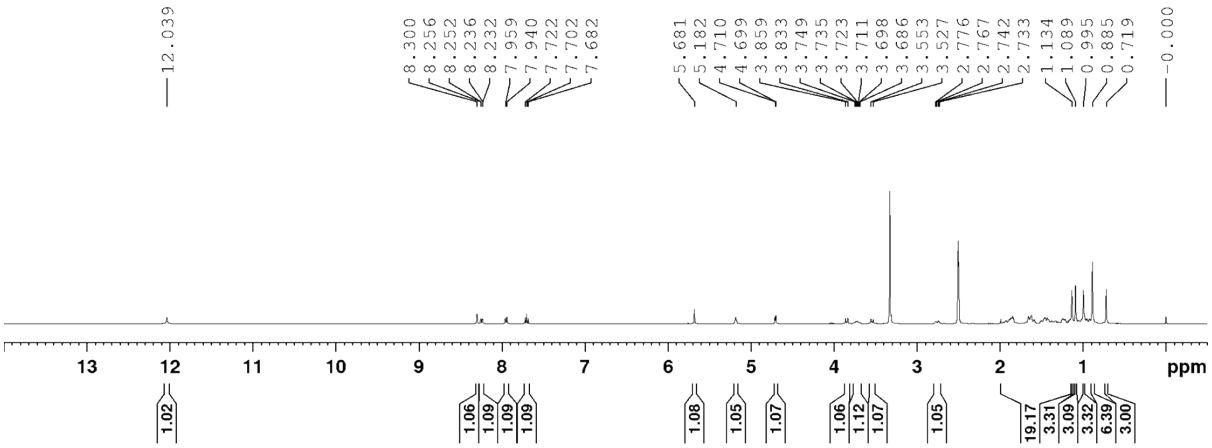


Fig. S41 ^{1}H NMR of 3,23-(3-nitrobenzylidene) arjunolic acid (AA-13)

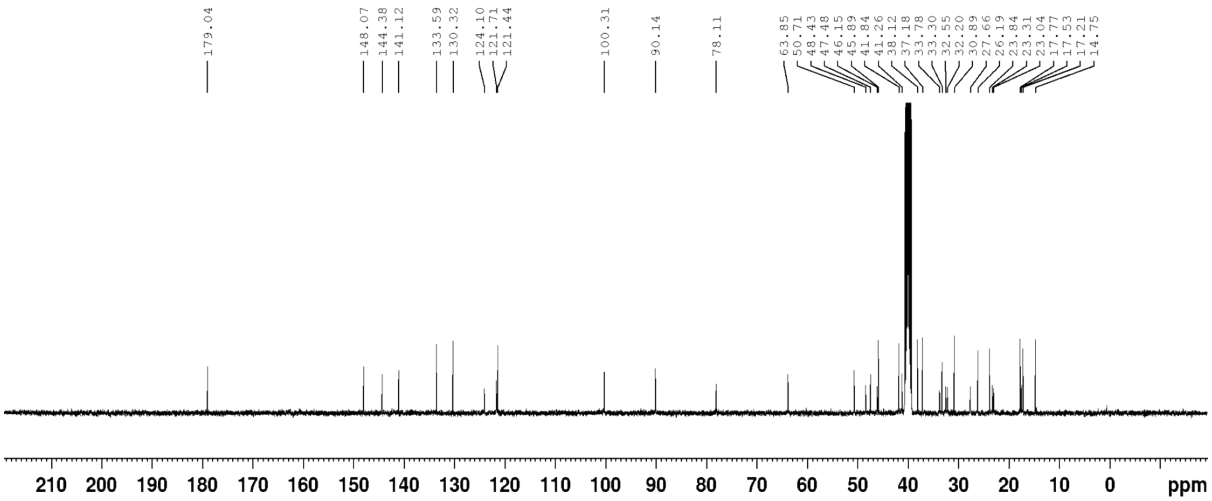


Fig. S42 ^{13}C NMR of 3,23-(3-nitrobenzylidene) arjunolic acid (AA-13)

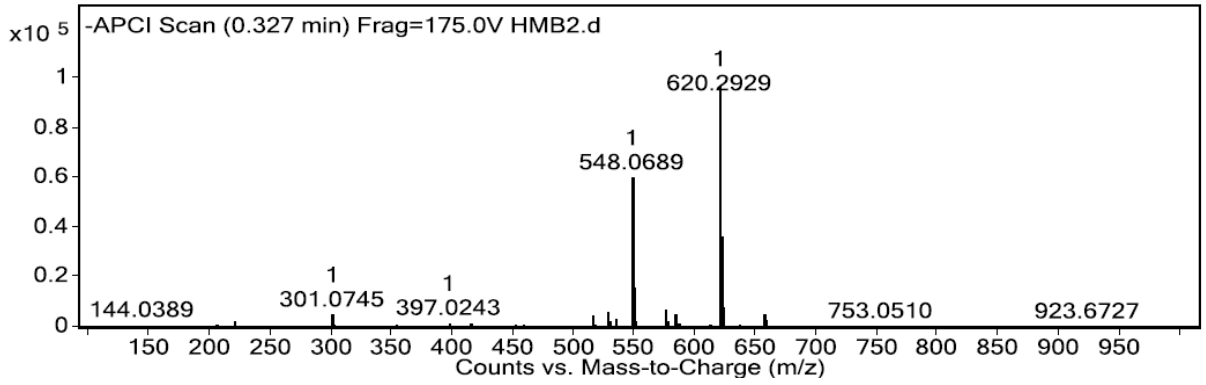


Fig. S43 Mass spectrum of 3,23-(3-nitrobenzylidene) arjunolic acid (AA-13)

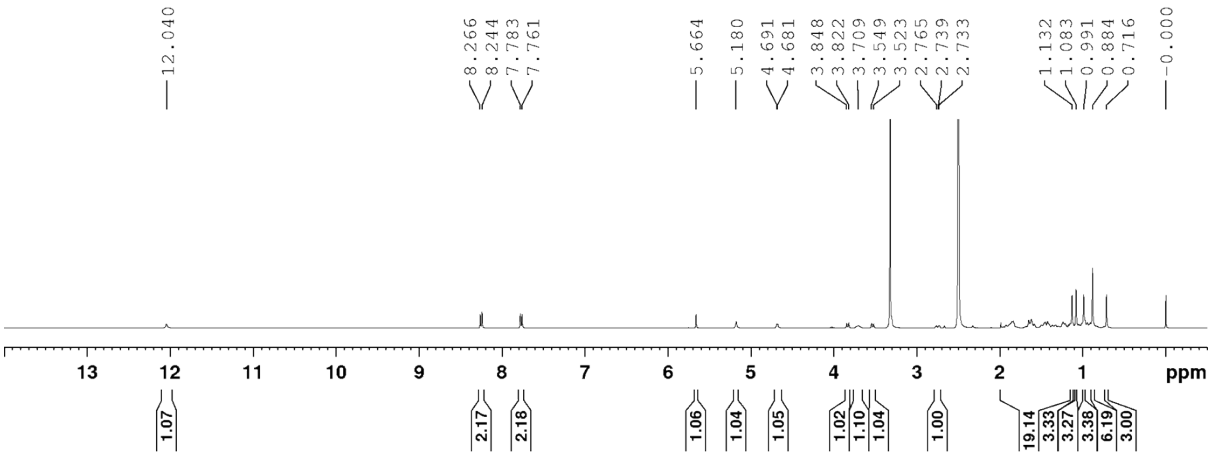


Fig. S44 ^{1}H NMR spectrum of 3,23-(4-nitrobenzylidene) arjunolic acid (AA-14)

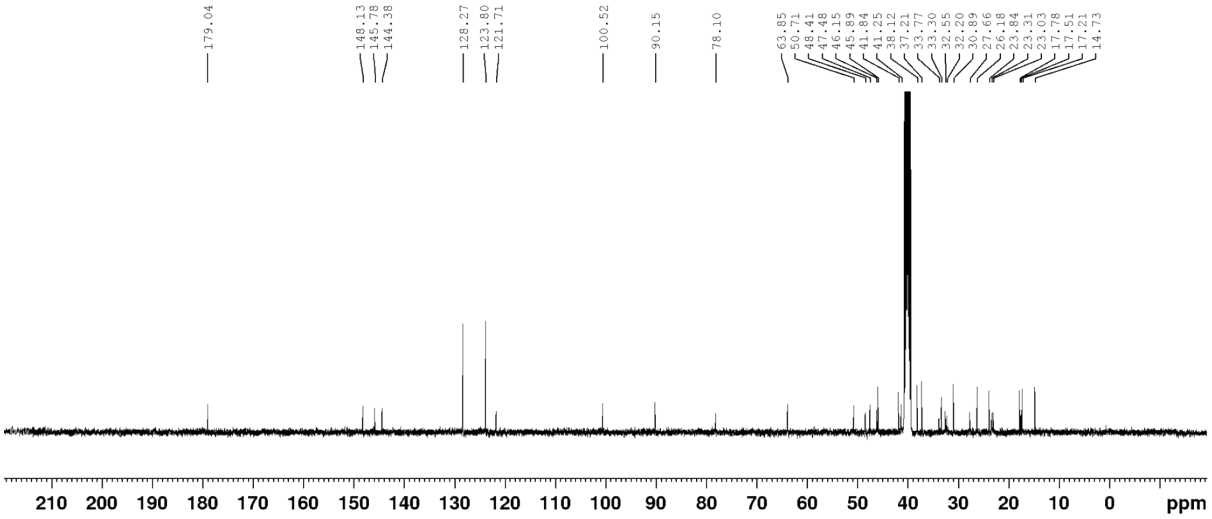


Fig. S45 ^{13}C NMR spectrum of 3,23-(4-nitrobenzylidene) arjunolic acid (AA-14)

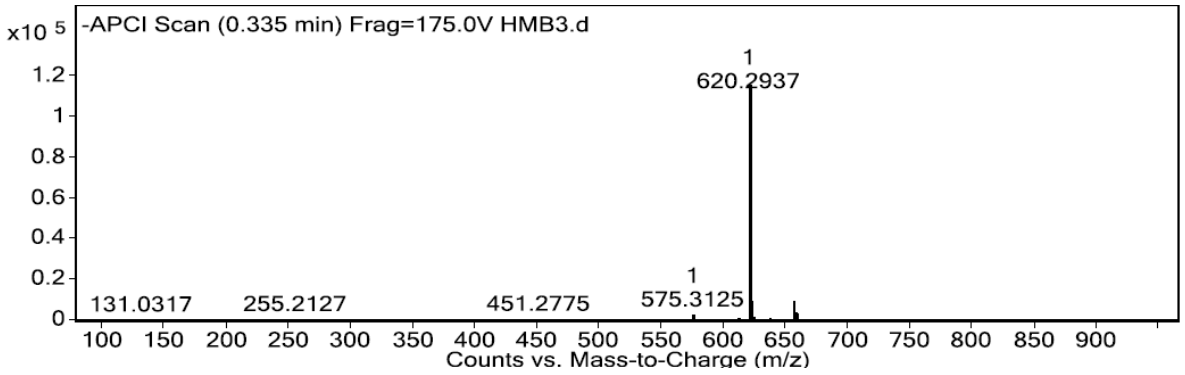


Fig. S46 Mass spectrum of 3,23-(4-nitrobenzylidene) arjunolic acid (AA-14)

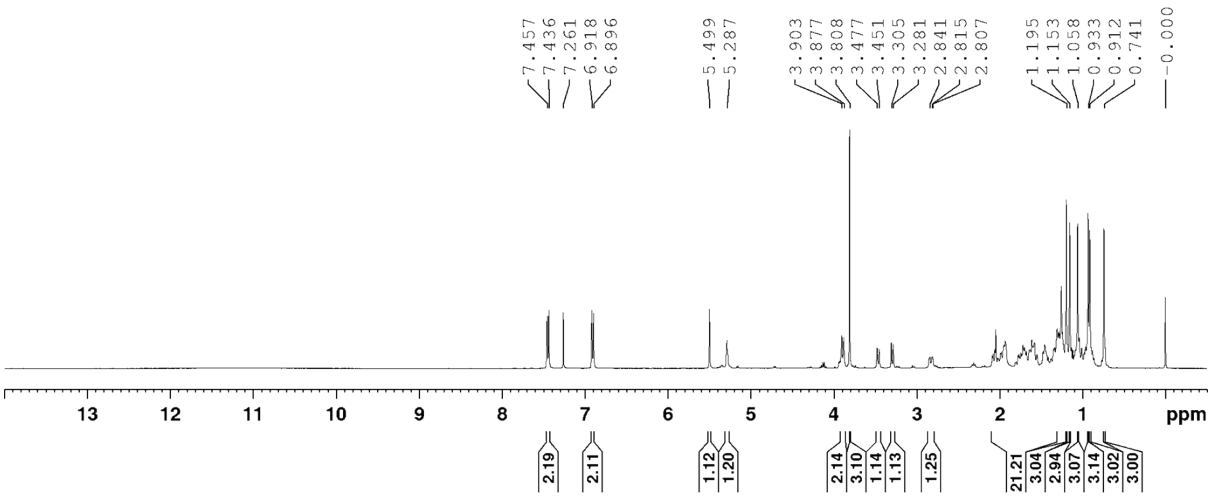


Fig. S47 ^{1}H NMR of 3,23-(4-methoxybenzylidene) arjunolic acid (AA-15)

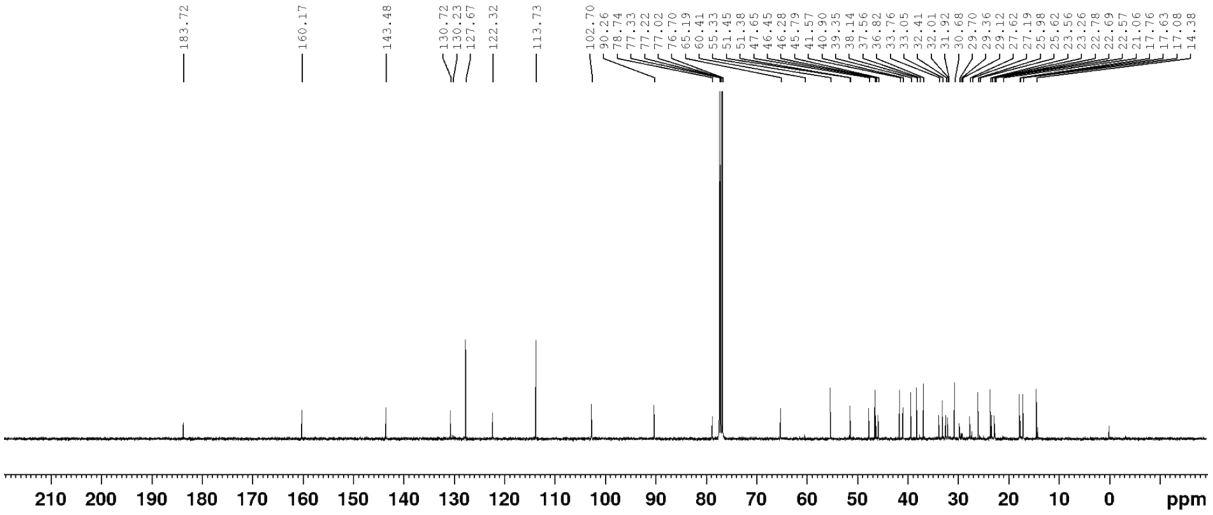


Fig. S48 ^{13}C NMR spectrum of 3,23-(4-methoxy benzylidene) arjunolic acid (AA-15)

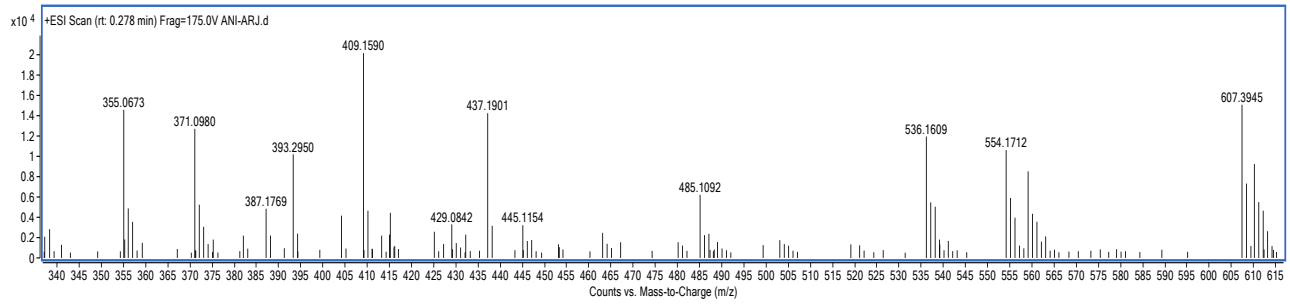


Fig. S49 Mass spectrum of 3,23-(4-methoxybenzylidene) arjunolic acid (AA-15)

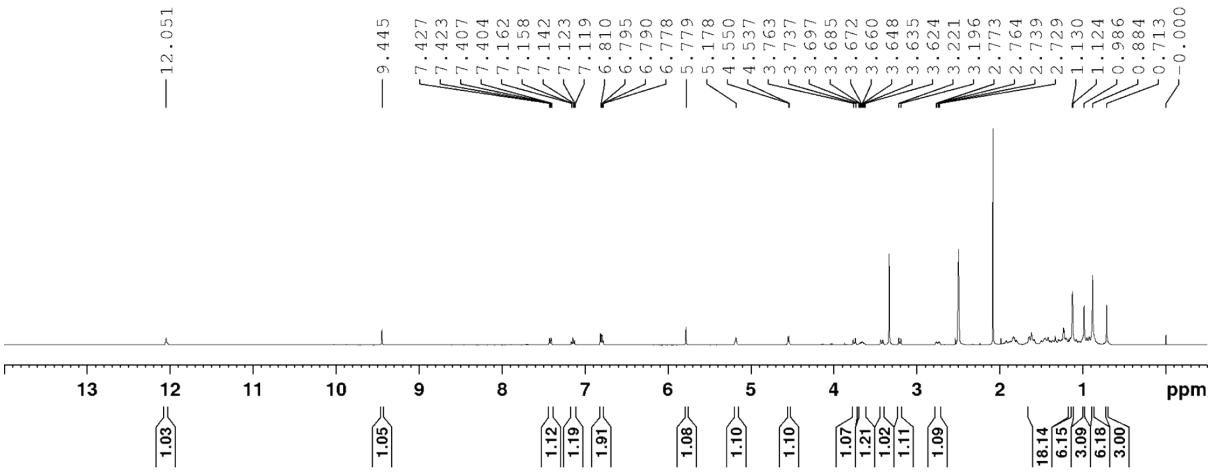


Fig. S50 ^{1}H NMR spectrum of 3,23-(2-hydroxybenzylidene) arjunolic acid (AA-16)

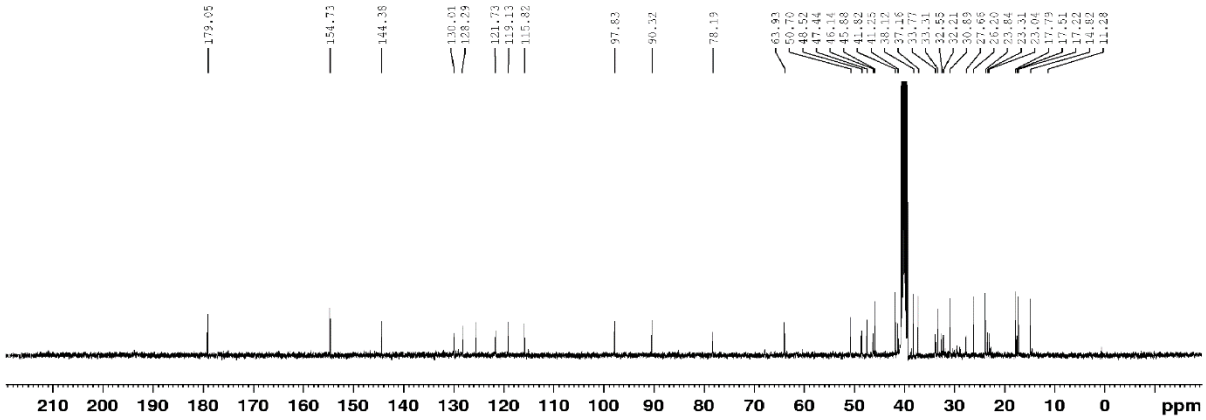


Fig. S51 ^{13}C NMR spectrum of 3,23-(2-hydroxybenzylidene) arjunolic acid (AA-16)

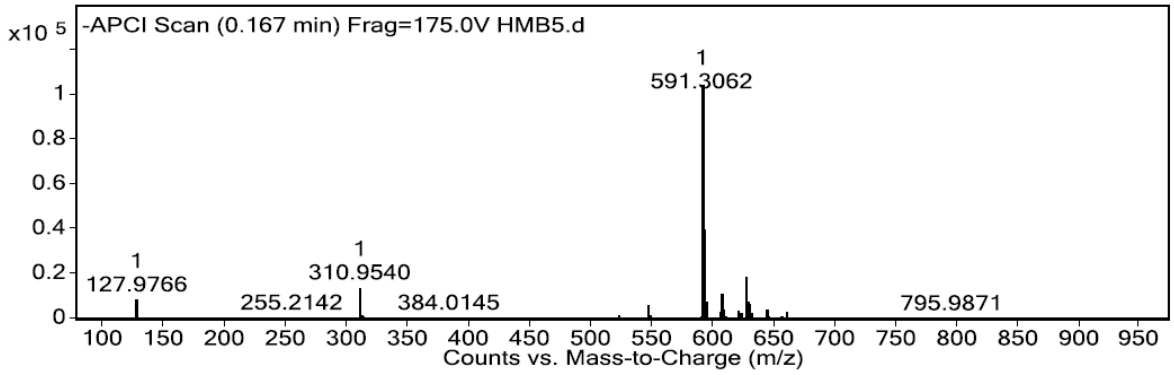


Fig. S52 Mass spectrum of 3,23-(2-hydroxybenzylidene) arjunolic acid (AA-16)

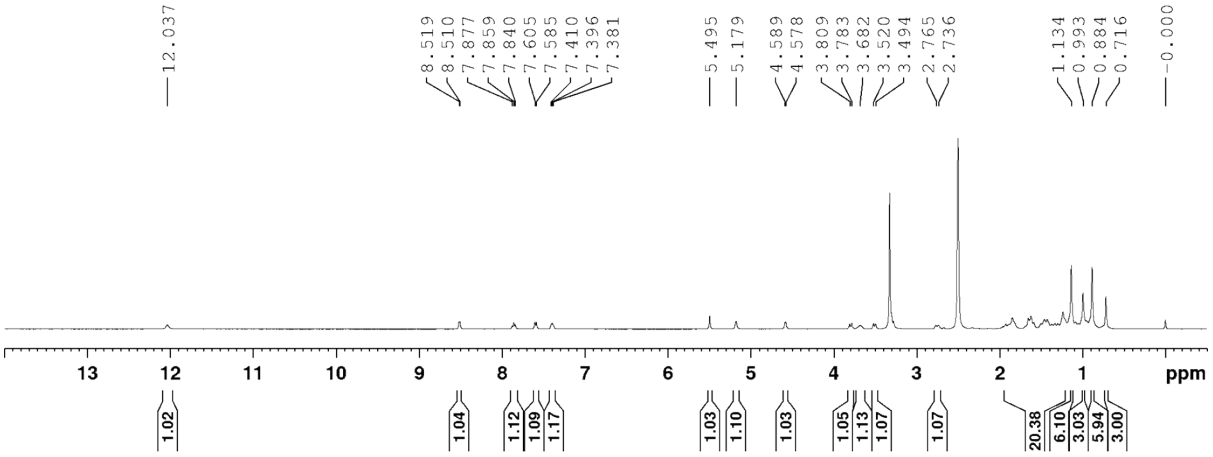


Fig. S53 ^{1}H NMR spectrum of 3,23-(2-pyrilidene) arjunolic acid (AA-17)

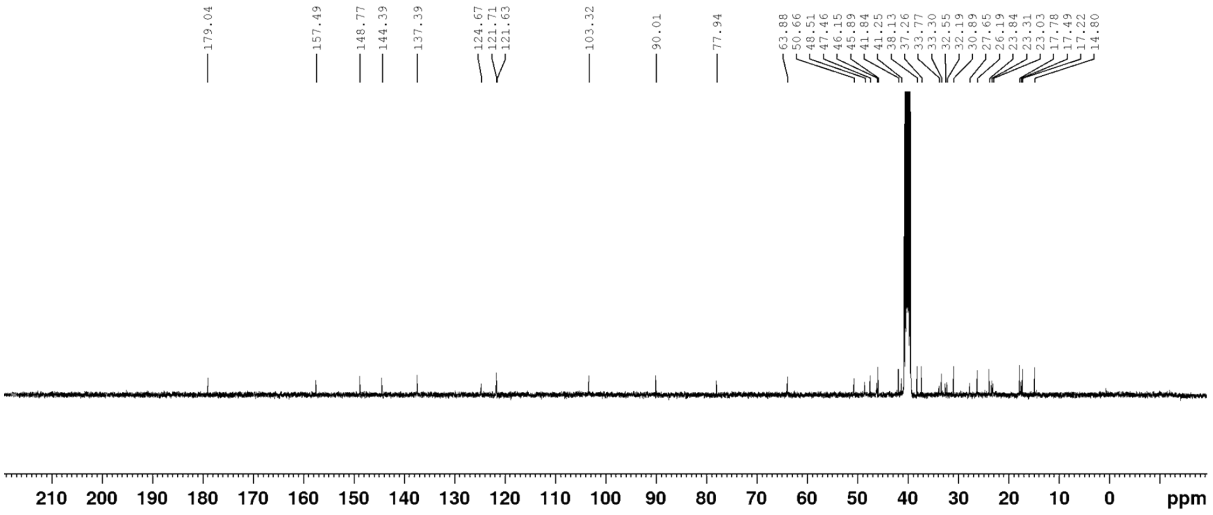


Fig. S54 ^{13}C NMR of 3,23-(2-pyrilidene) arjunolic acid (AA-17)

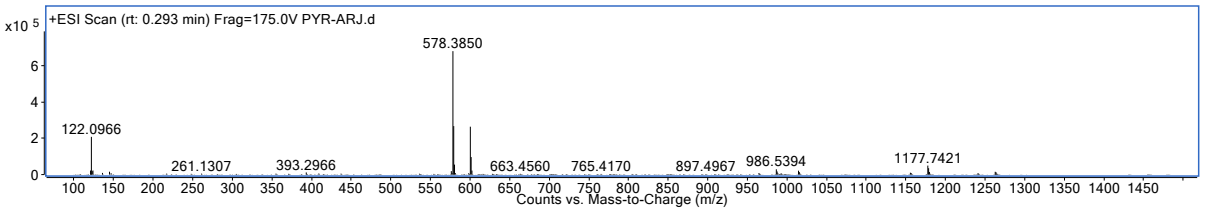


Fig. S55 Mass spectrum of 3,23-(2-pyrilidene) arjunolic acid (AA-17)

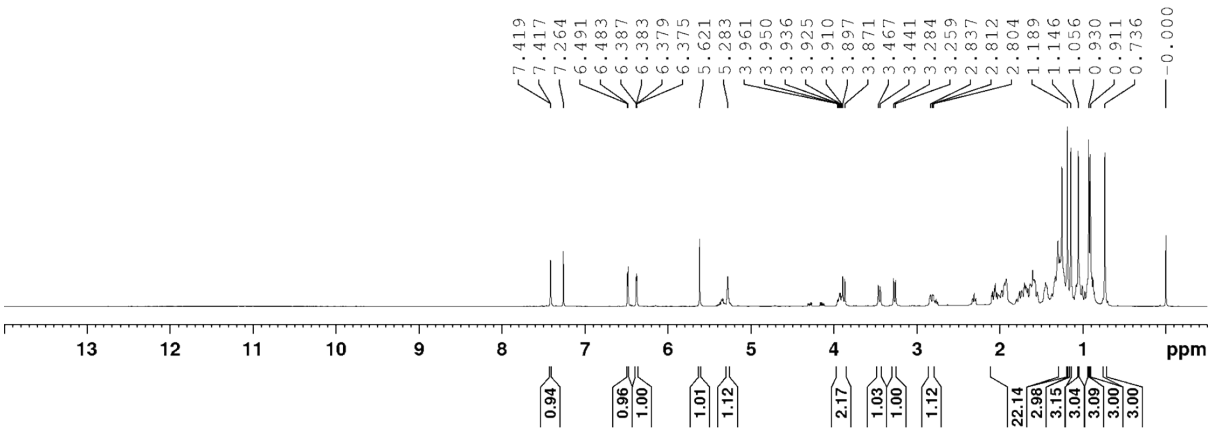


Fig. S56 ^{1}H NMR spectrum of 3,23-(2-furfuryldene) arjunolic acid (AA-18)

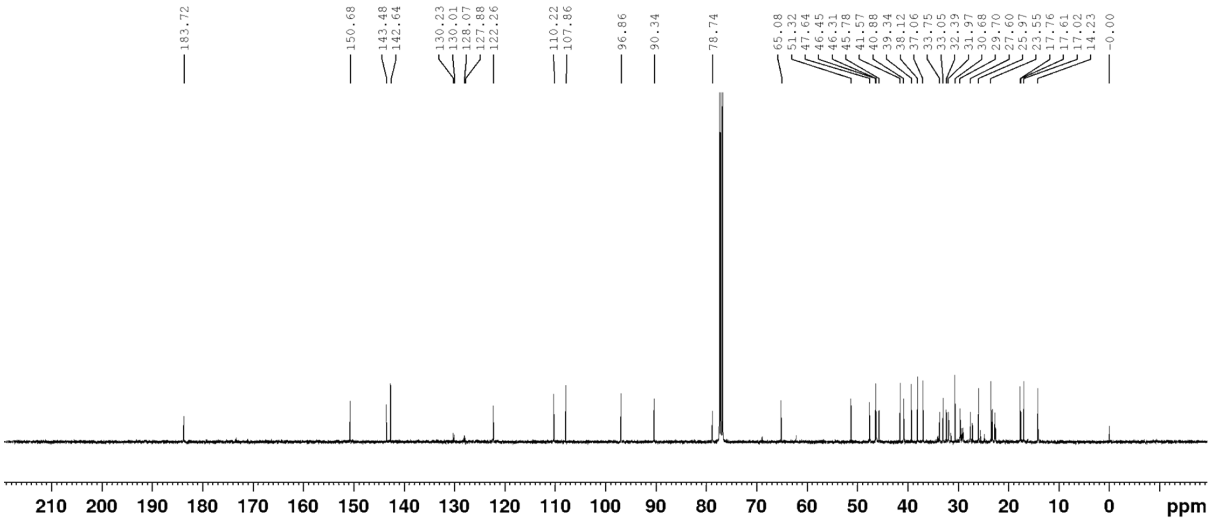


Fig. S57 ^{13}C NMR of 3,23-(2-furfuryldene) arjunolic acid (AA-18)

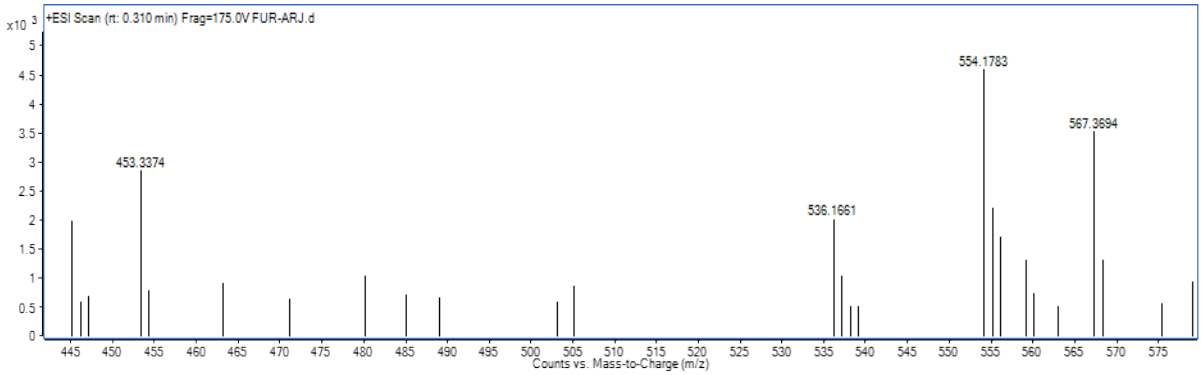


Fig. S58 Mass spectrum of 3,23-(2-furfuryldene) arjunolic acid (AA-18)

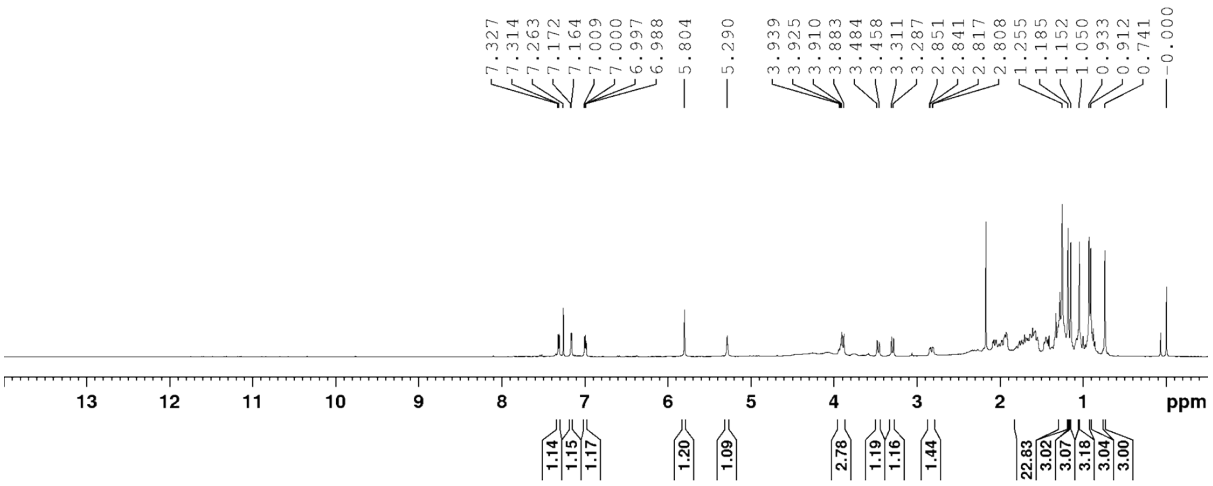


Fig. S59 ^{1}H NMR spectrum of 3,23-(2-thiophenylidene) arjunolic acid (AA-19)

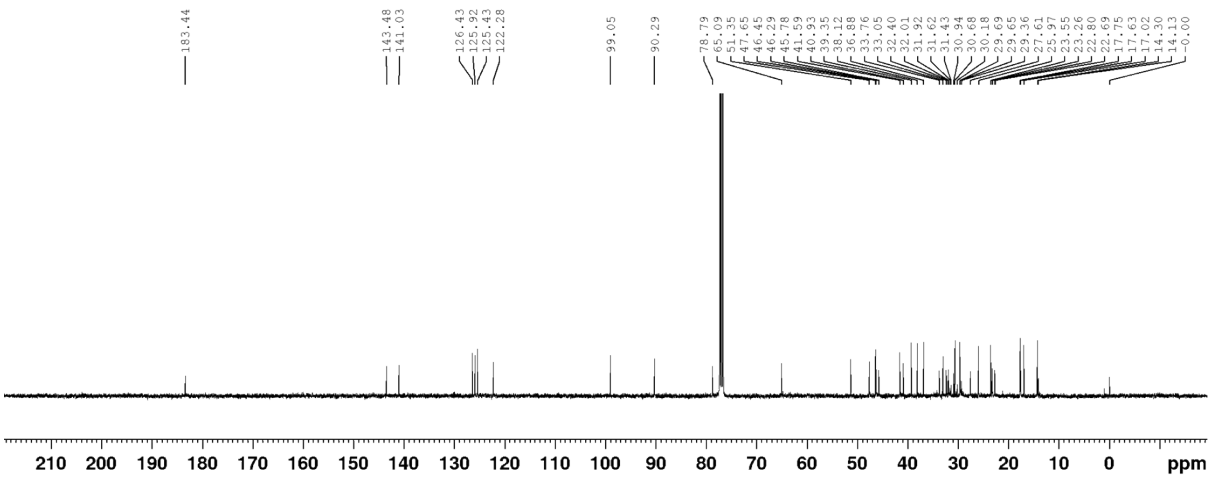


Fig. S60 ^{13}C NMR spectrum of 3,23-(2-thiophenylidene) arjunolic acid (AA-19)

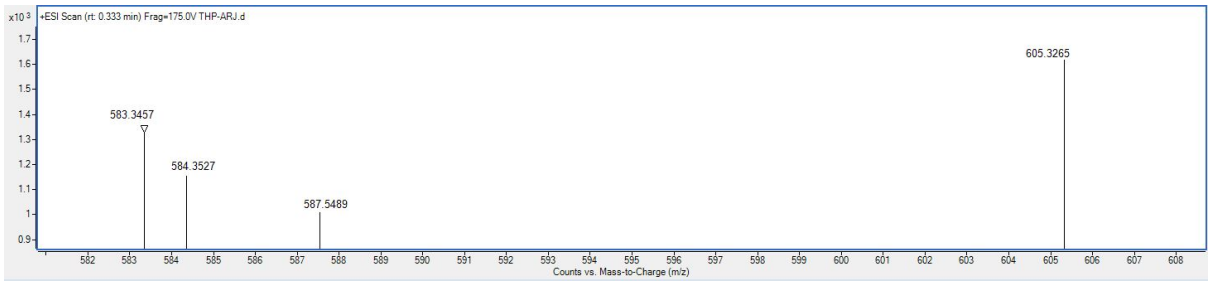


Fig. S61 Mass spectrum of 3,23-(2-thiophenylidene) arjunolic acid (AA-19)

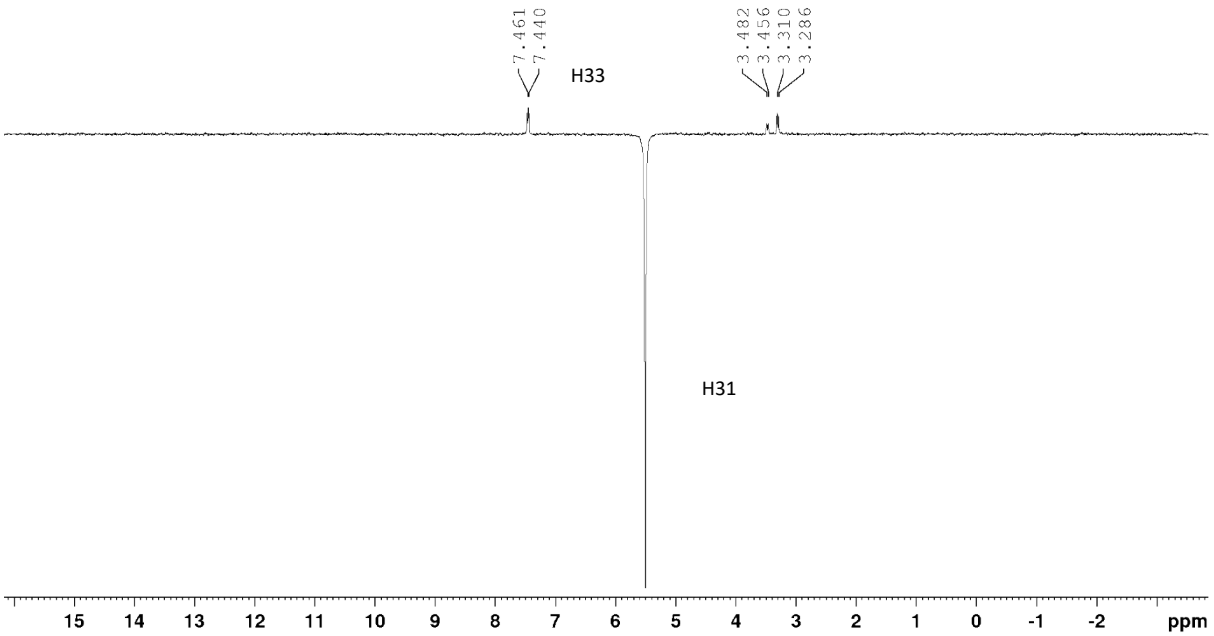


Fig. S62: NOE difference spectrum of 3,23-(4-methoxy benzylidene) arjunolic acid (AA-15) H31 irradiated.

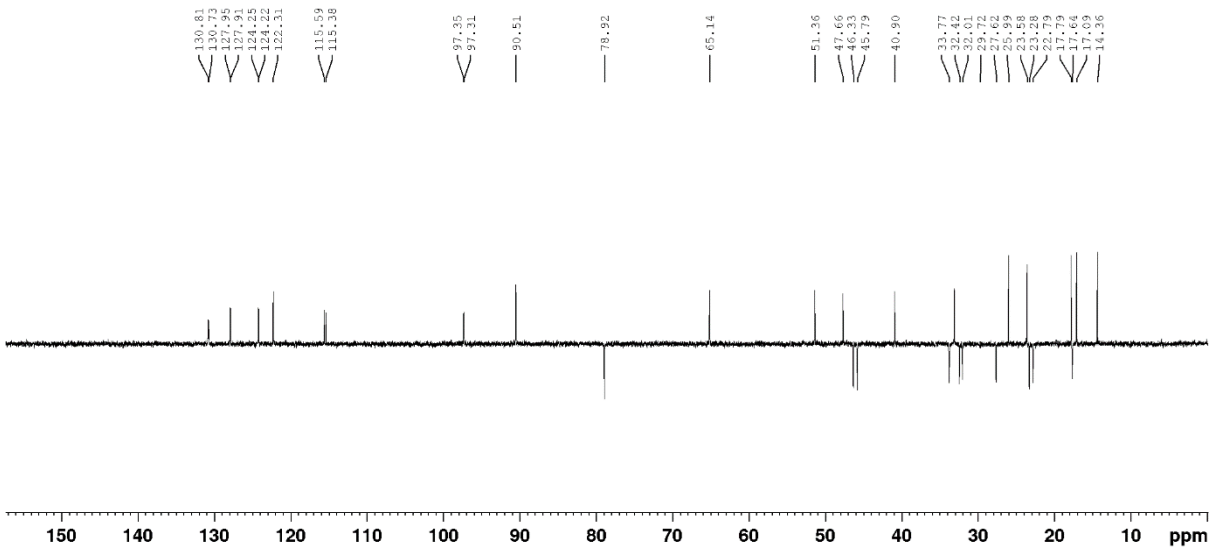


Fig. S63: DEPT 135 spectrum of 3,23-(2-fluorobenzylidene) arjunolic acid (AA-2)

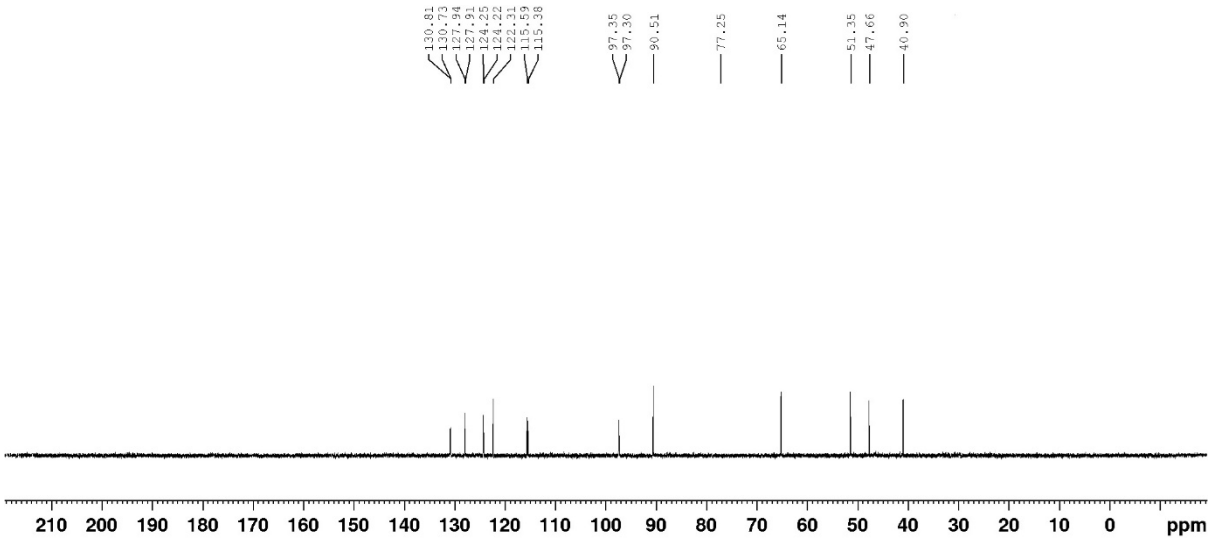


Fig: S64. DEPT 90 spectrum of 3,23-(2-fluorobenzylidene) arjunolic acid (AA-2)

FTIR Data:

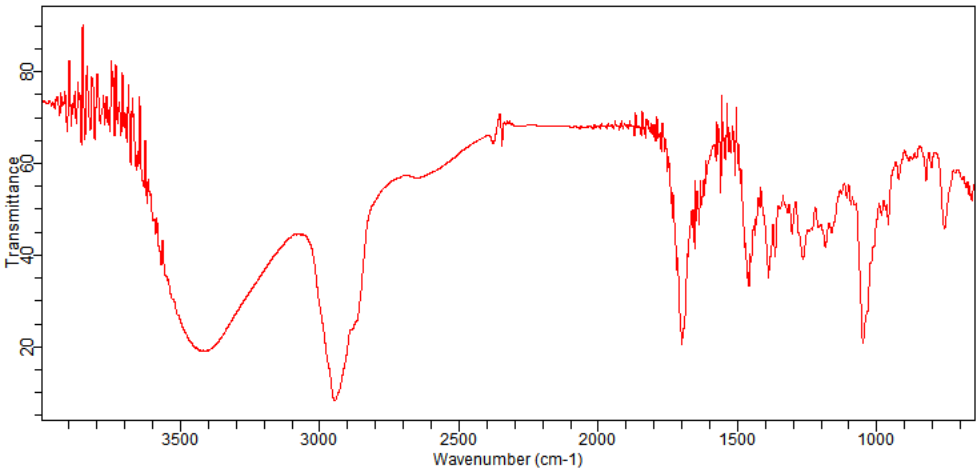


Fig. S65: FTIR spectrum of arjunolic acid.

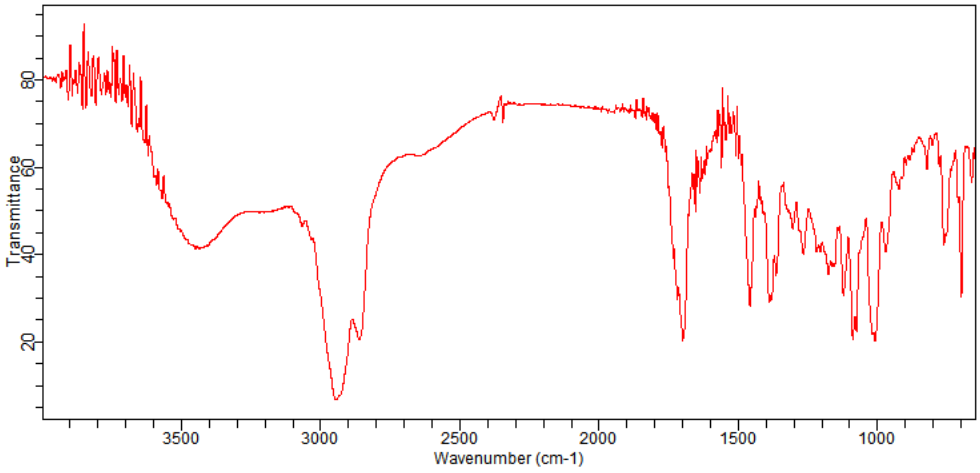


Fig. S66: FTIR spectrum of 3,23-benzylidene arjunolic acid (AA-1)

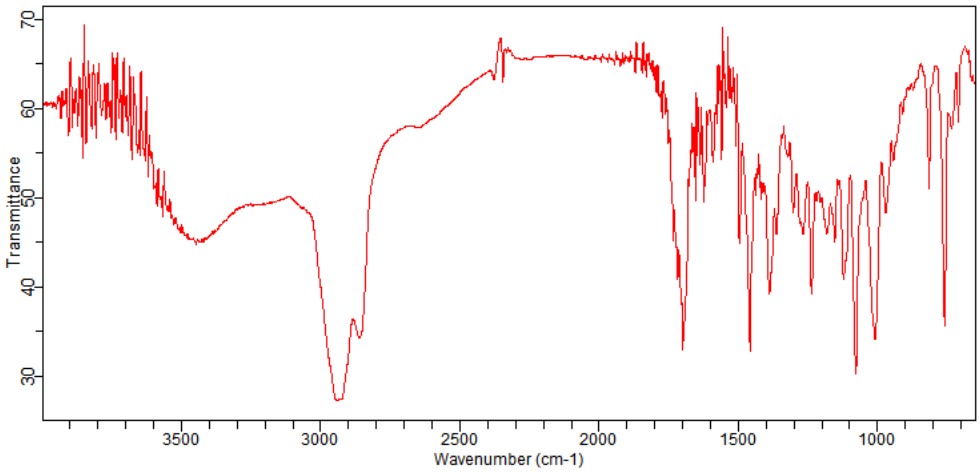


Fig. S67: FTIR spectrum of 3,23-(2-florobenzylidene) arjunolic acid (AA-2)

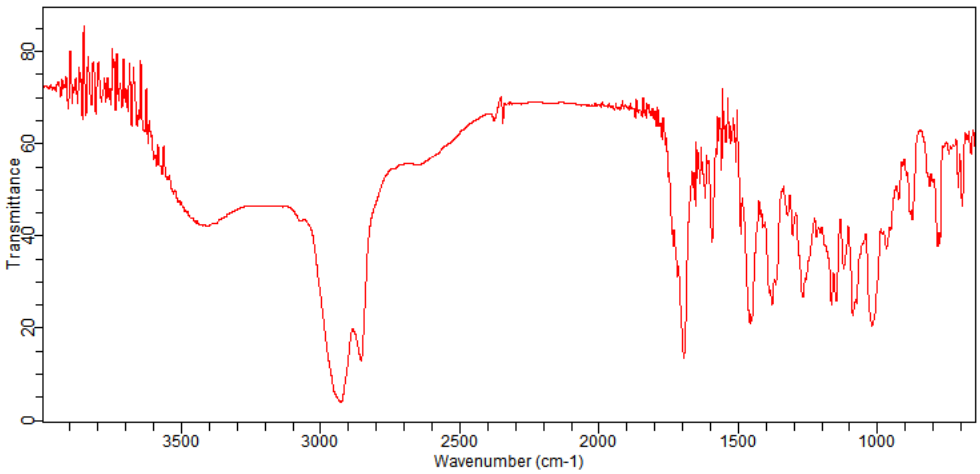


Fig. S68: FTIR spectrum of 3,23-(3-florobenzylidene) arjunolic acid (AA-3)

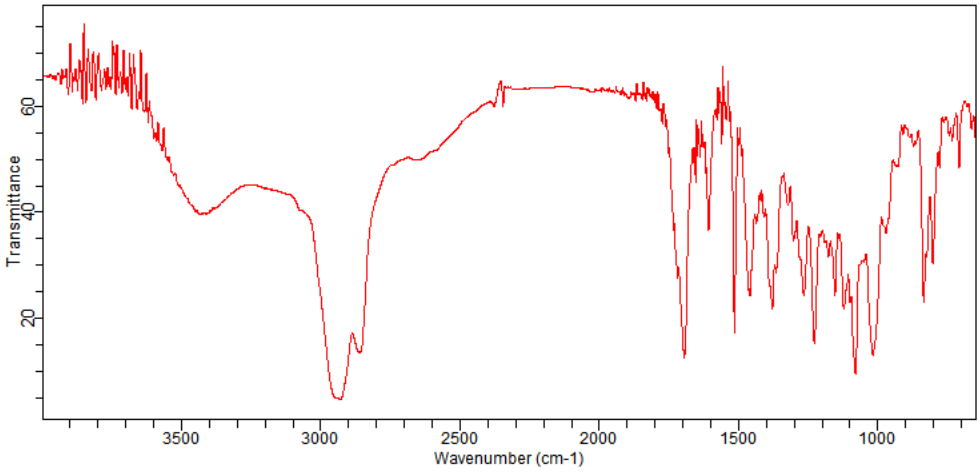


Fig. S69: FTIR spectrum of 3,23-(4-florobenzylidene) arjunolic acid (AA-4)

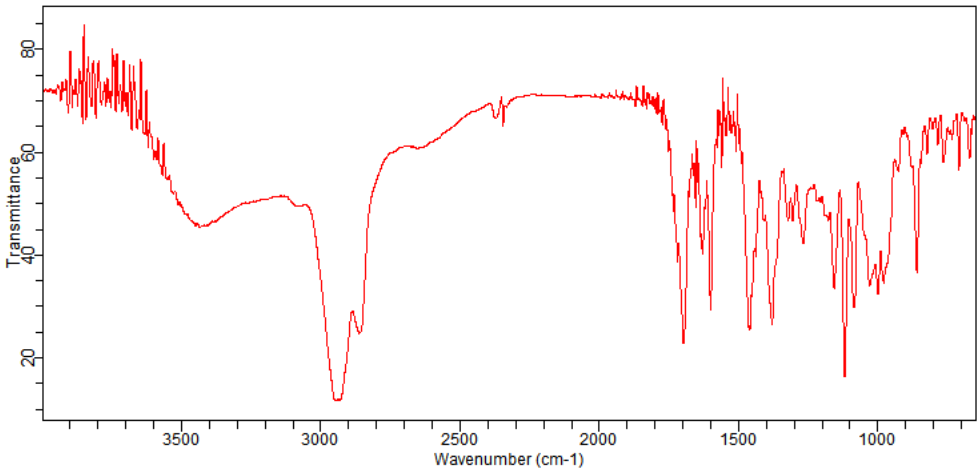


Fig. S70: FTIR spectrum of 3,23-(3,5-florobenzylidene) arjunolic acid (AA-5)

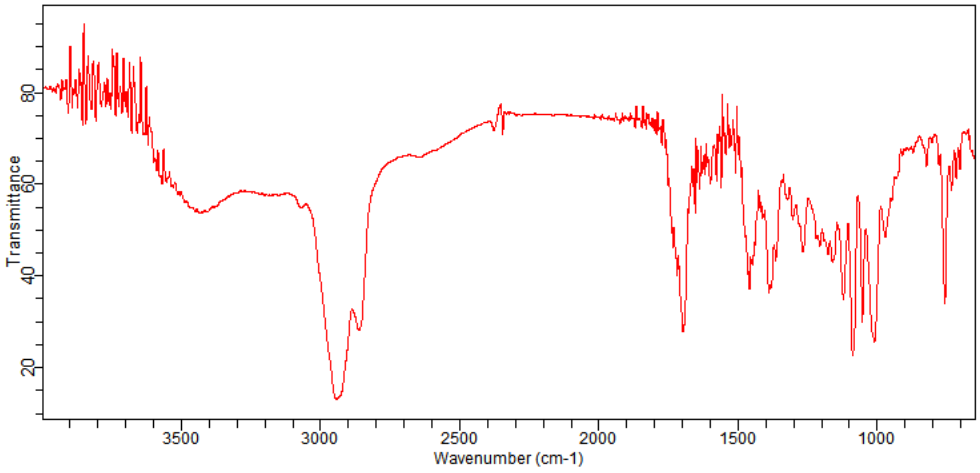


Fig. S71: FTIR spectrum of 3,23-(2-chlorobenzylidene) arjunolic acid (AA-6)

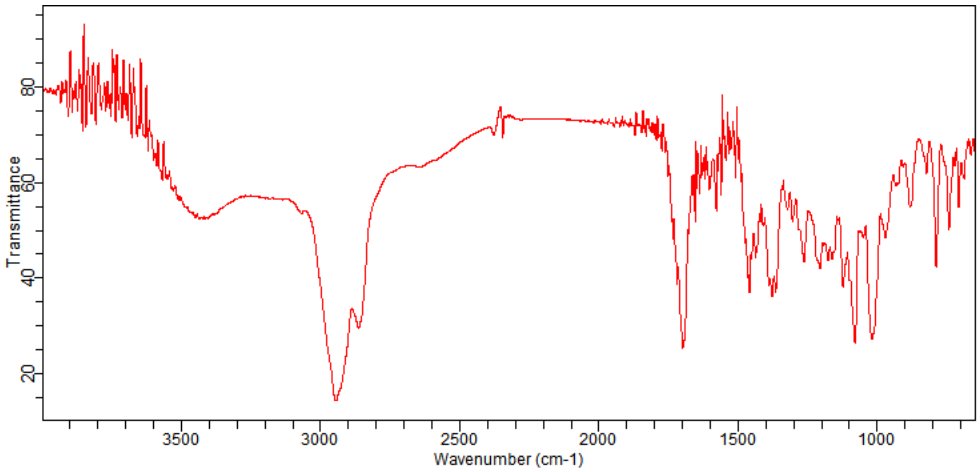


Fig. S72: FTIR spectrum of 3,23-(3-chlorobenzylidene) arjunolic acid (AA-7)

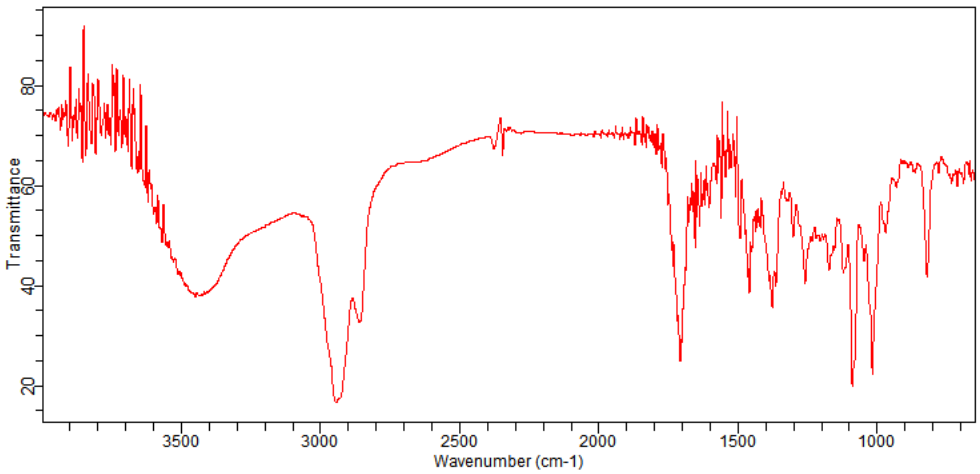


Fig. S73: FTIR spectrum of 3,23-(4-chlorobenzylidene) arjunolic acid (AA-8)

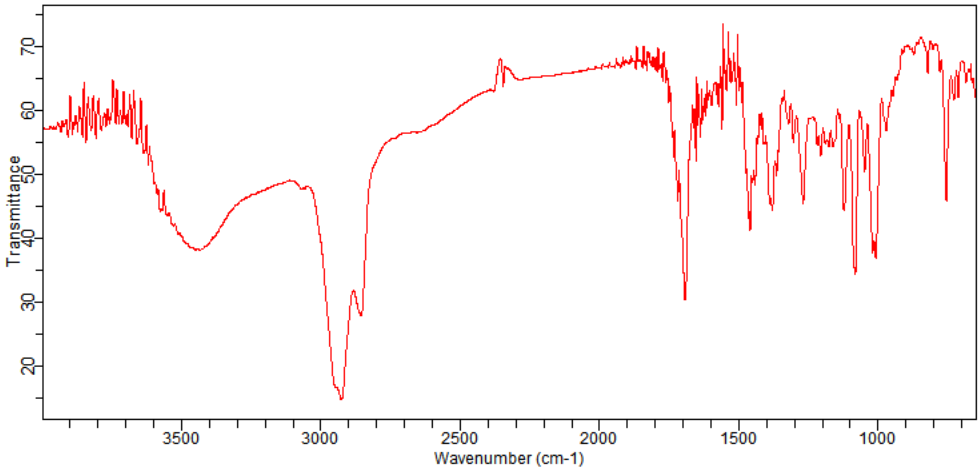


Fig. S74: FTIR spectrum of 3,23-(2-bromobenzylidene) arjunolic acid (AA-9)

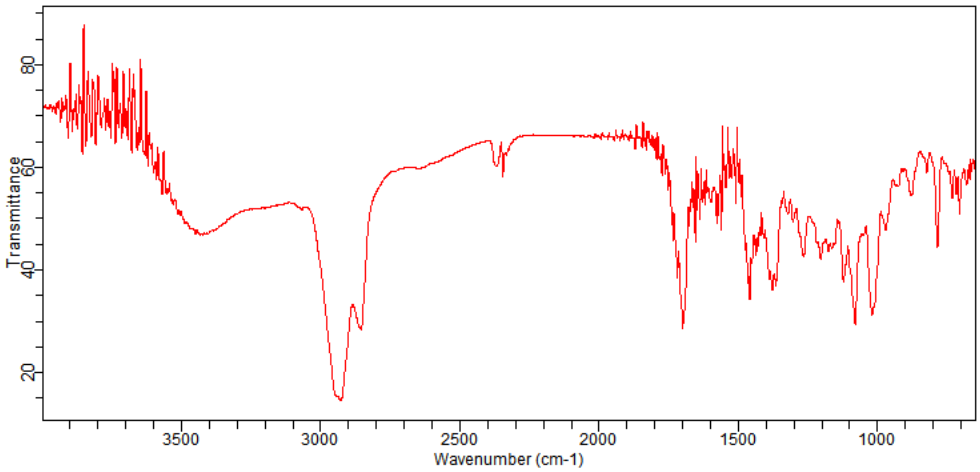


Fig. S75: FTIR spectrum of 3,23-(3-bromobenzylidene) arjunolic acid (AA-10)

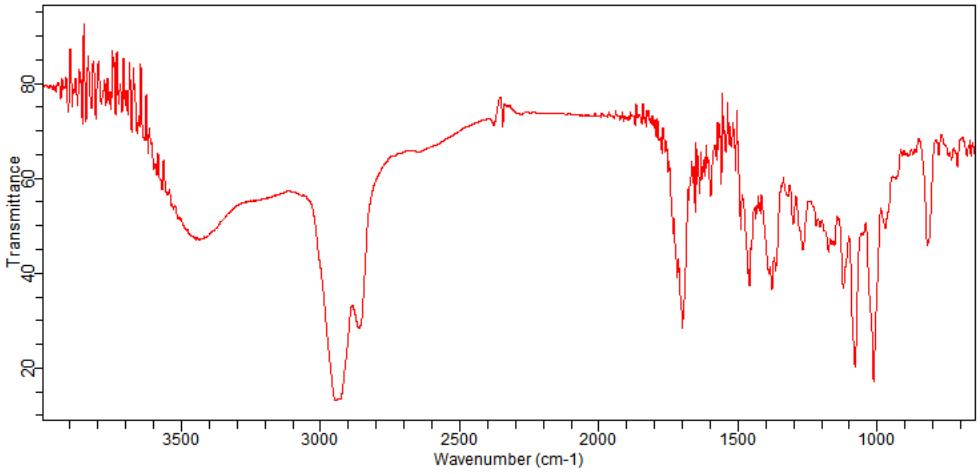


Fig. S76: FTIR spectrum of 3,23-(4-bromobenzylidene) arjunolic acid (AA-11)

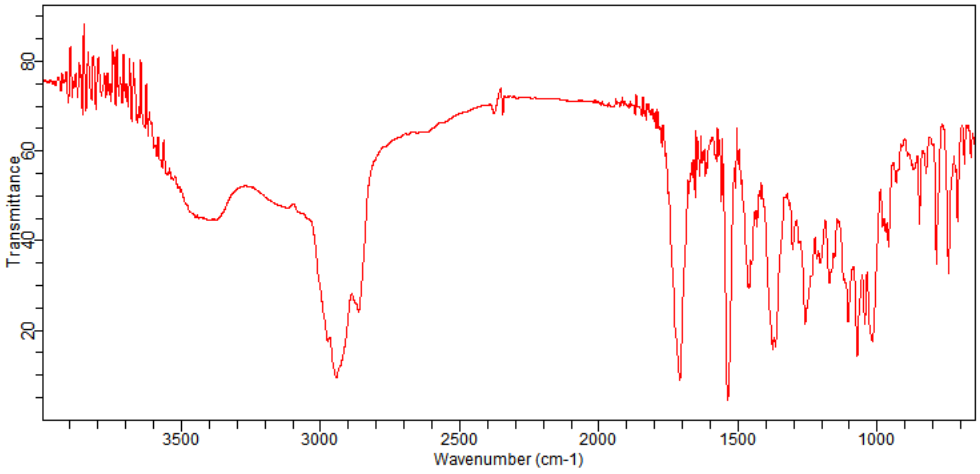


Fig. S77: FTIR spectrum of 3,23-(2-nitrobenzylidene) arjunolic acid (AA-12)

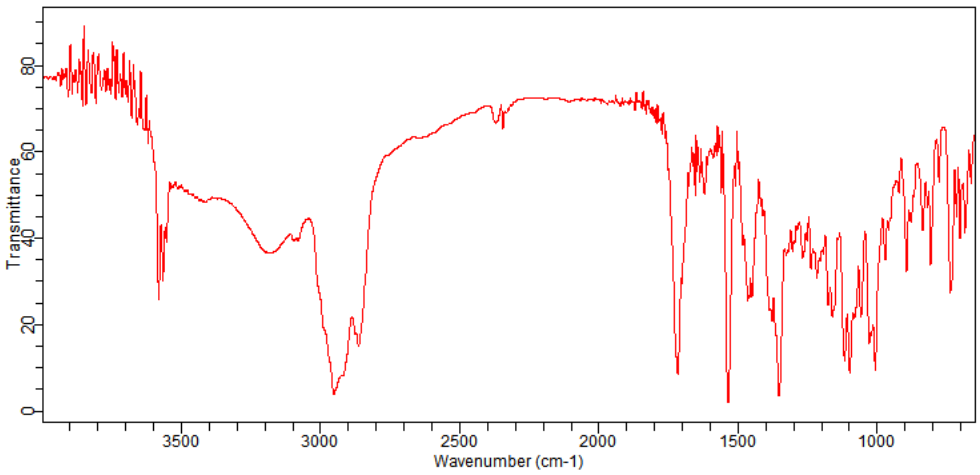


Fig. S77: FTIR spectrum of 3,23-(3-nitrobenzylidene) arjunolic acid (AA-13)

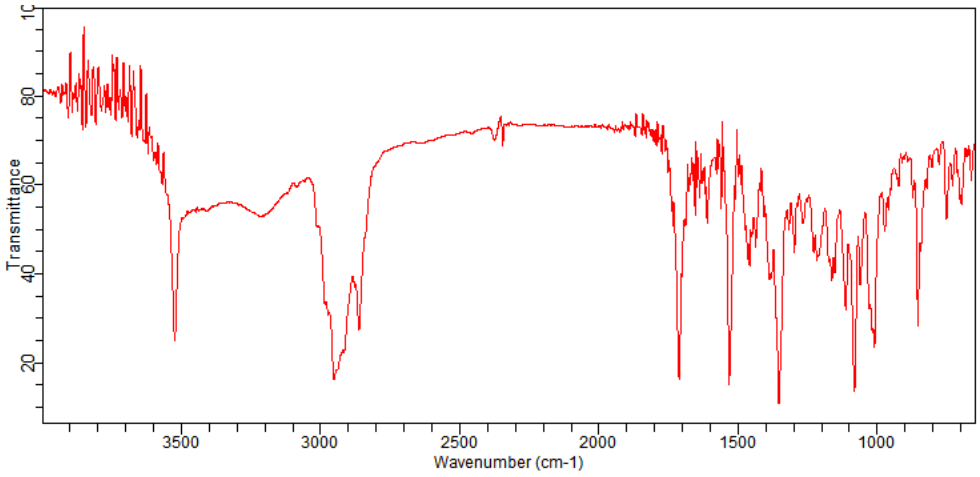


Fig. S78: FTIR spectrum of 3,23-(4-nitrobenzylidene) arjunolic acid (AA-14)

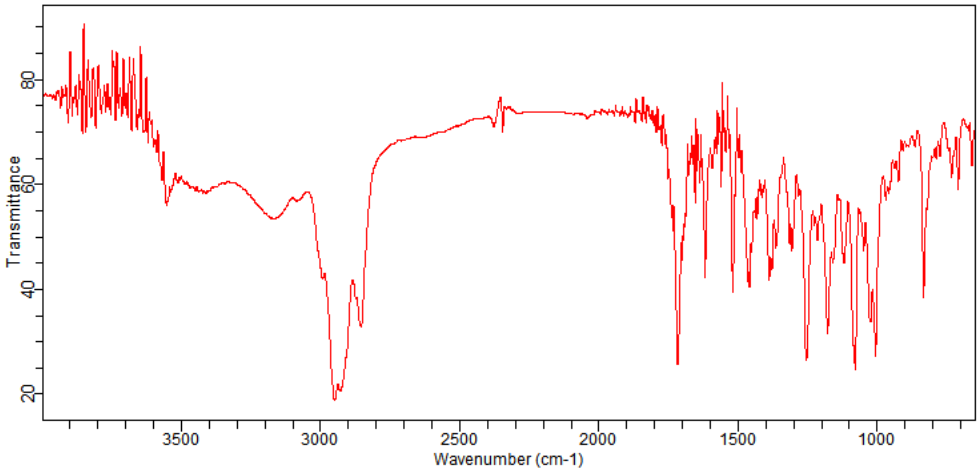


Fig. S79: FTIR spectrum of 3,23-(4-methoxybenzylidene) arjunolic acid (AA-15)

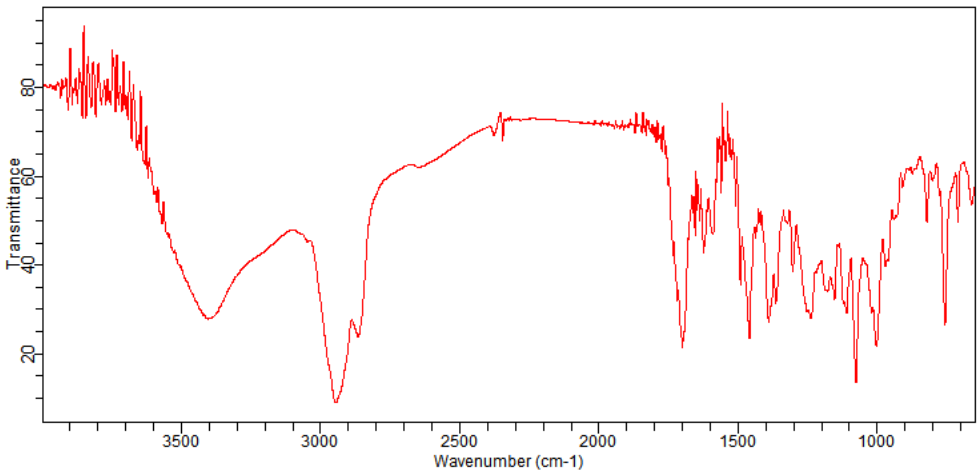


Fig. S80: FTIR spectrum of 3,23-(2-hydroxybenzylidene) arjunolic acid (AA-16)

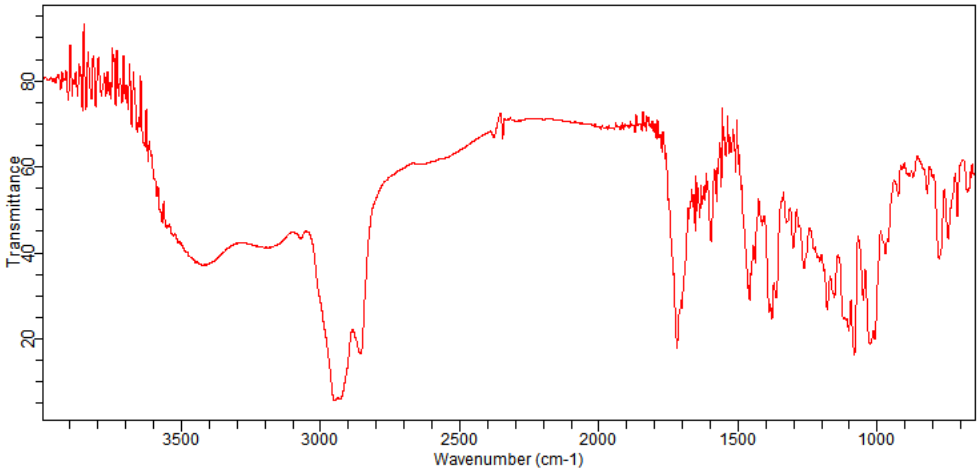


Fig. S81: FTIR spectrum of 3,23-(2-pyridine) arjunolic acid (AA-17)

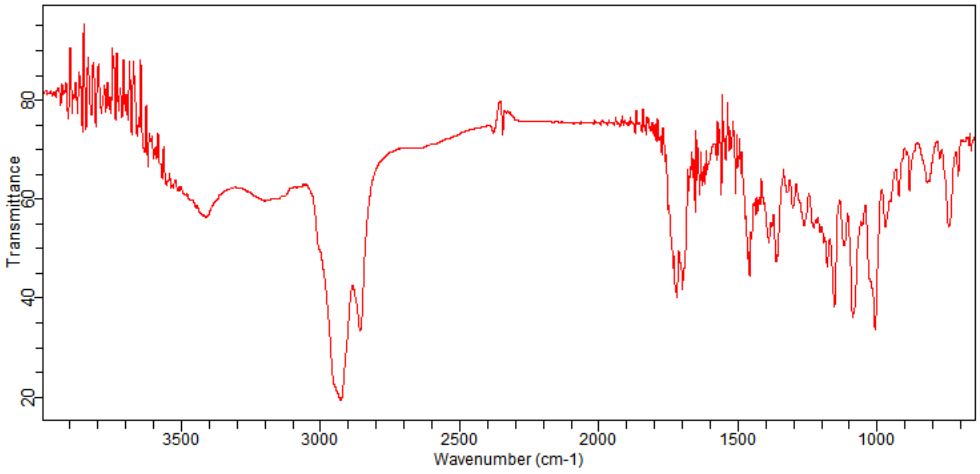


Fig. S82: FTIR spectrum of 3,23-(2-furfuryldene) arjunolic acid (AA-18)

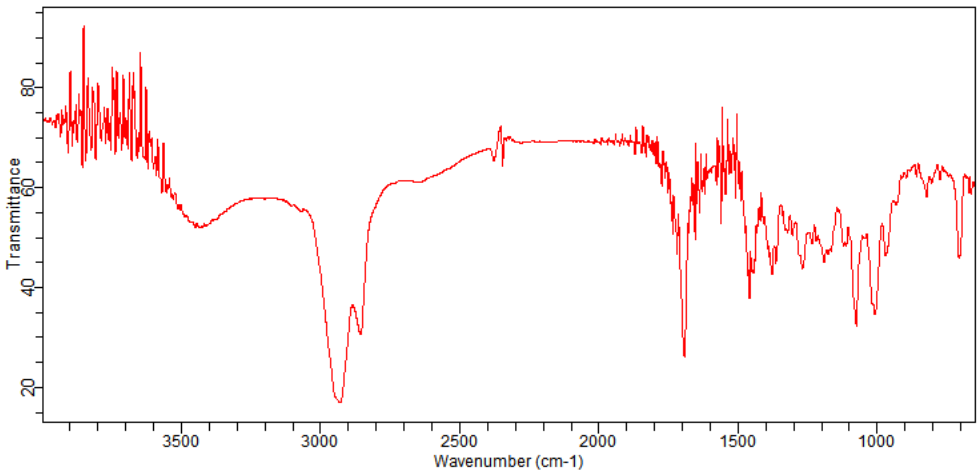
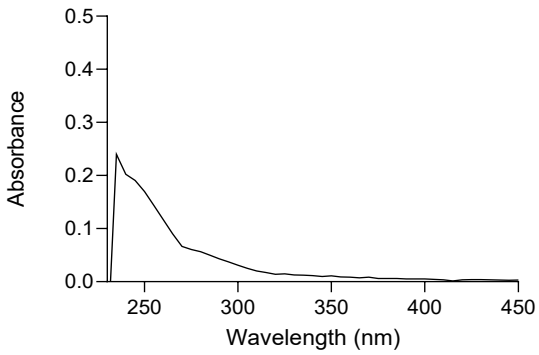
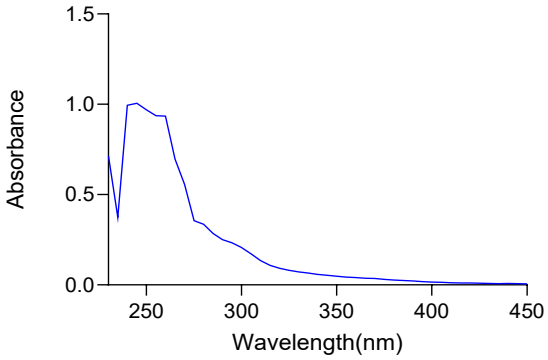


Fig. S73: FTIR spectrum of 3,23-(2-thiophenyldene) arjunolic acid (AA-19)

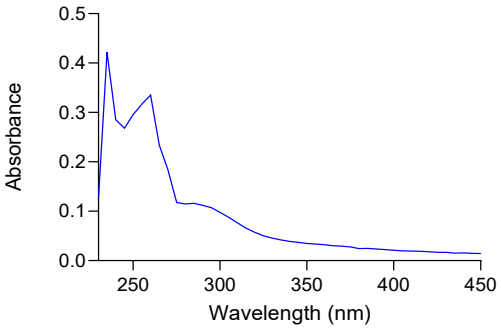
UV spectra of acetals of arjunolic acid



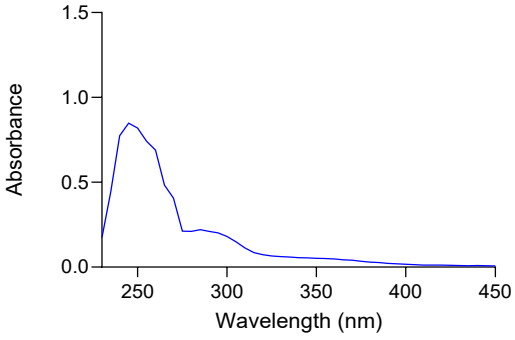
AA-1



AA-2



AA-3



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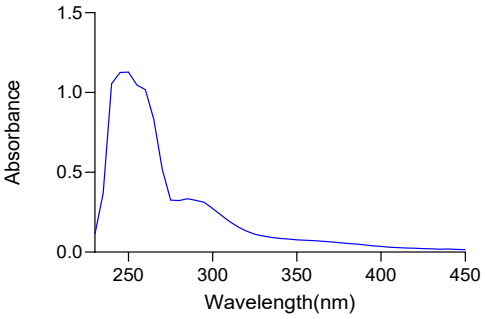
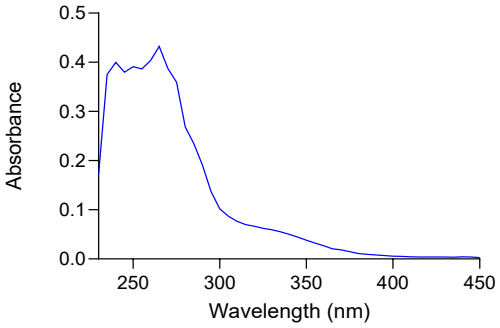
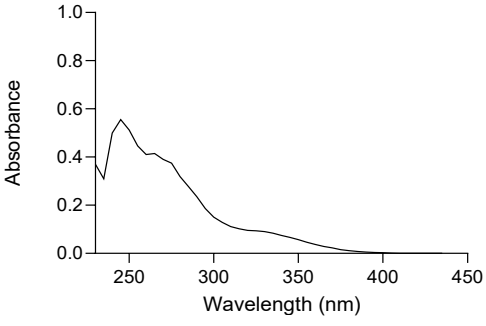


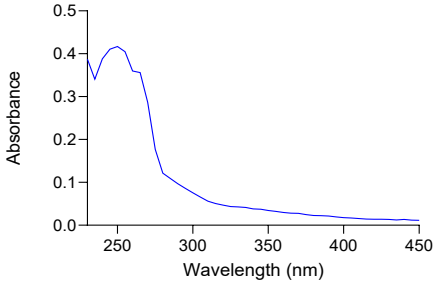
AA-5



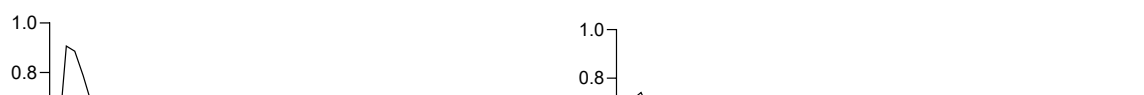
AA-6



AA-7



AA-8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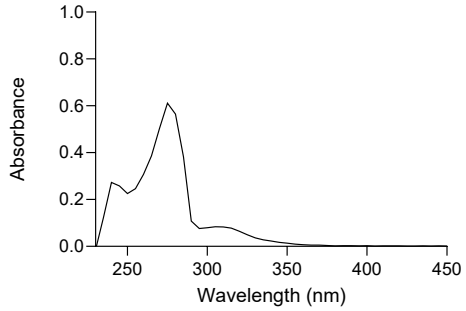
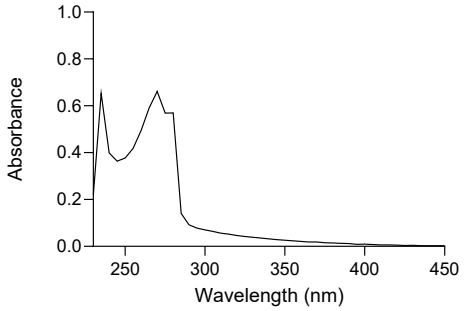
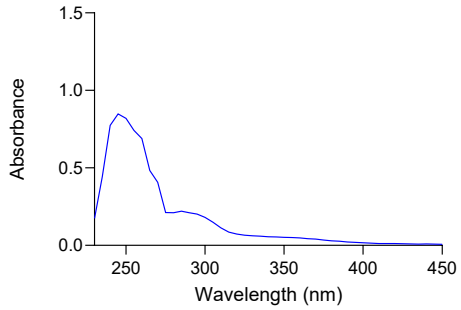


AA-17



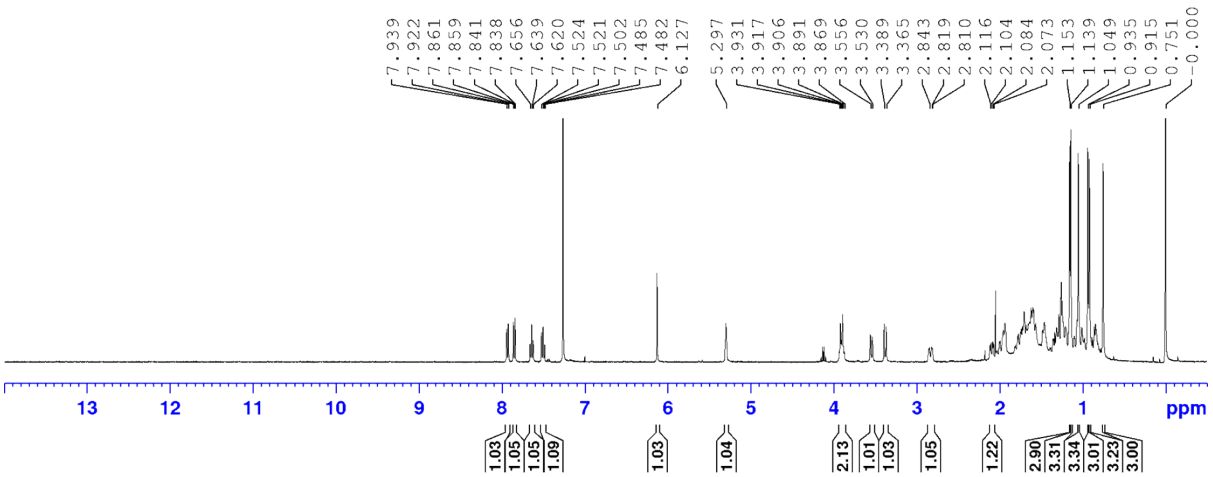
AA-18



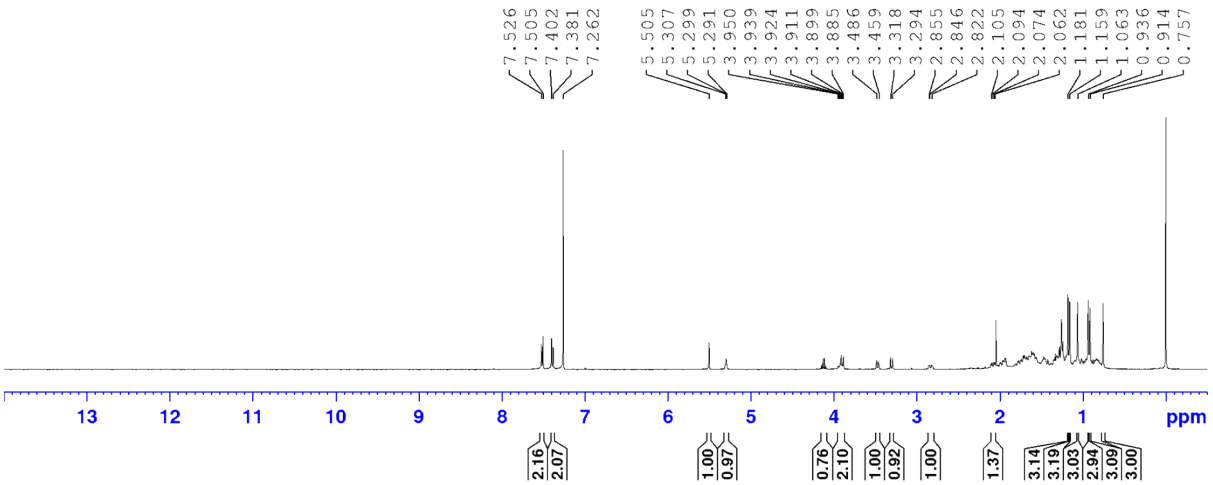
AA-19

Stability studies of 3,23 (2-chlorobenzilidene) arjunolic acid and 3,23 (4-bromobenzilidene) arjunolic acid using ^{1}H NMR

The compounds (AA-7 and AA-11) were added to the culture media (RPMI-1640) separately and were kept in this media for 14 days at room temperature. During these 14 days status of compounds was monitored by TLC. No change was observed in the Rf value of the compounds from the media with respect to the pure compound. After 14 days, the compounds were extracted with EtOAc, dried over anhydrous sodium sulphate and the solvent evaporated. The compounds were dried in a vacuum oven overnight. Then ^{1}H NMR spectra were recorded for these compounds using $CDCl_3$ as solvent.



^{1}H NMR spectrum of 3,23 (2-chlorobenzilidene) arjunolic acid



^{1}H NMR spectrum of 3,23 (4-bromobenzilidene) arjunolic acid.