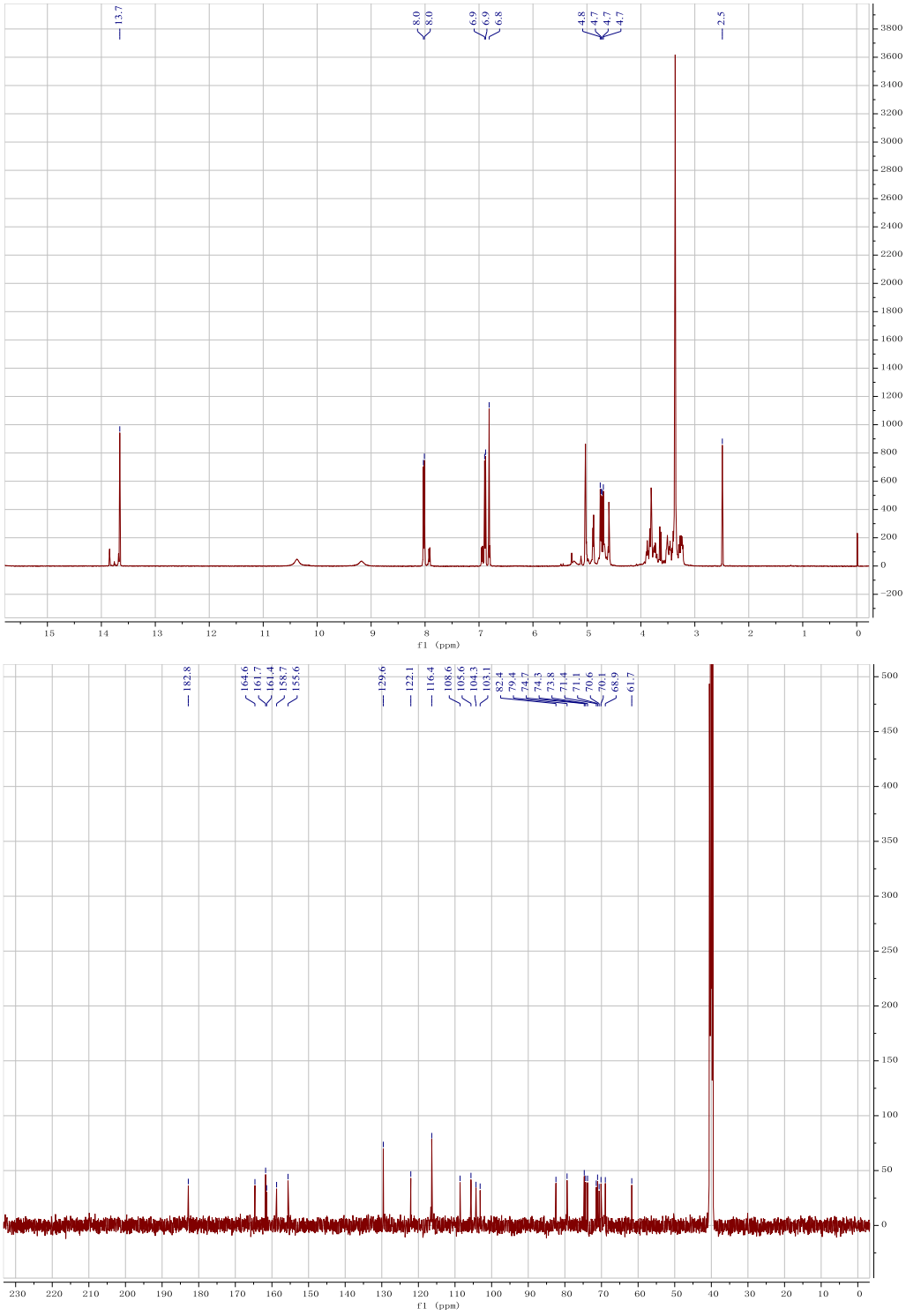

Figure S1. ^{1}H-NMR and ^{13}C-NMR spectra of Isoschaftoside. ^{1}H-NMR (500 MHz, DMSO-d6) δ: 13.67 (1H, s, 5-OH), 8.03(2H, d, J = 8.8 Hz, H-2',6'), 6.90 (2H, d, J = 8.8Hz, H-3',5'), 6.81 (1H, s, H-3), 4.74 (1H, d, J = 9.9 Hz, H-1'''), 4.70 (1H, d, J = 9.6 Hz, H-1''),. ^{13}C-NMR (126 MHz, DMSO-d6) δ: 182.85 (C-4), 164.64 (C-2), 161.73 (C-4'), 161.44 (C-5), 158.72 (C-7), 155.61 (C-9), 129.59 (C-2'), 122.08 (C-1'), 116.36 (C-5'), 108.63 (C-6), 105.64 (C-8), 104.27 (C-10), 103.14 (C-3), 82.44 (C-5'''), 79.40 (C-3'''), 74.70 (C-3''), 68.95 (C-2''), 61.73 (C-6''').

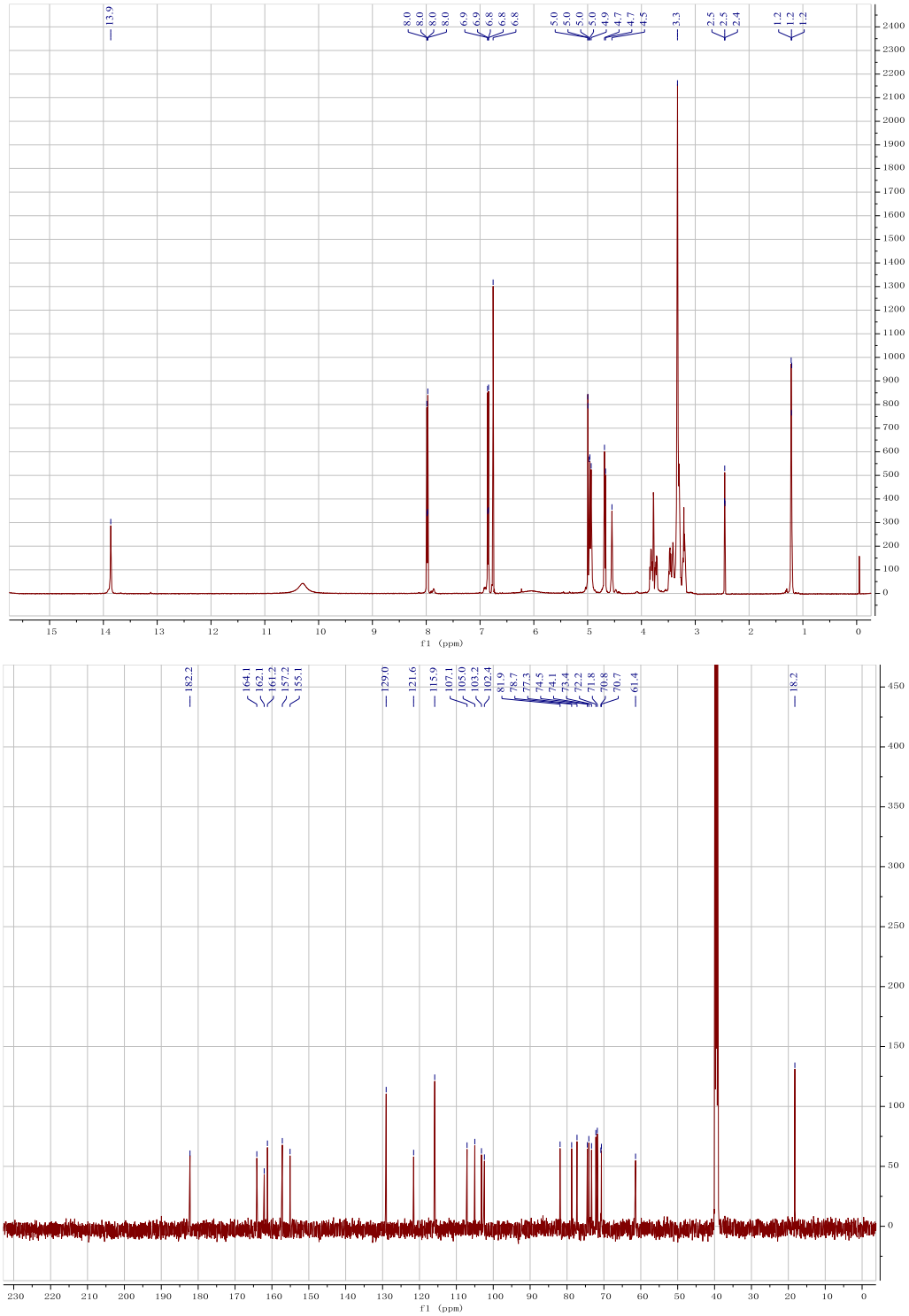

Figure S2 [1]H-NMR and [13]C-NMR spectra of Isoviolanthin.[1]H-NMR (500 MHz, DMSO-d6) δ: 8.04-7.99 (2H, d, H-2', 6'), 6.89 (2H, d, J = 8.8 Hz, H-3',5'), 6.79 (1H, s, H-3), 5.04 (2H, d, J = 1.1 Hz), 5.02-4.97 (8H, m), 4.74-4.72 (4H, m), 4.60 (2H, t, J = 5.7 Hz), 1.29-1.21 (6H, m). [13]C-NMR (126 MHz, DMSO-d6) δ: 182.21 (C-4), 164.10 (C-2), 162.10 (C-4'), 161.22 (C-7), 157.18 (C-5), 155.08 (C-9), 129.03 (C-2',6'), 121.59 (C-1'), 115.87(C-3',5'), 107.10 (C-6), 105.00 (C-8), 103.20 (C-10), 102.39 (C-3), 81.88 (C-5''), 78.74 (C-3''), 77.29 (C-5'''), 74.50 (C-1'''), 74.09 (C-3'''),73.35 (C-1''), 72.18 (C-2'''), 71.78 (C-4'''), 70.83 (C-2''), 70.68 (C-4''), 61.42 (C-6''), 18.23 (C-6''').

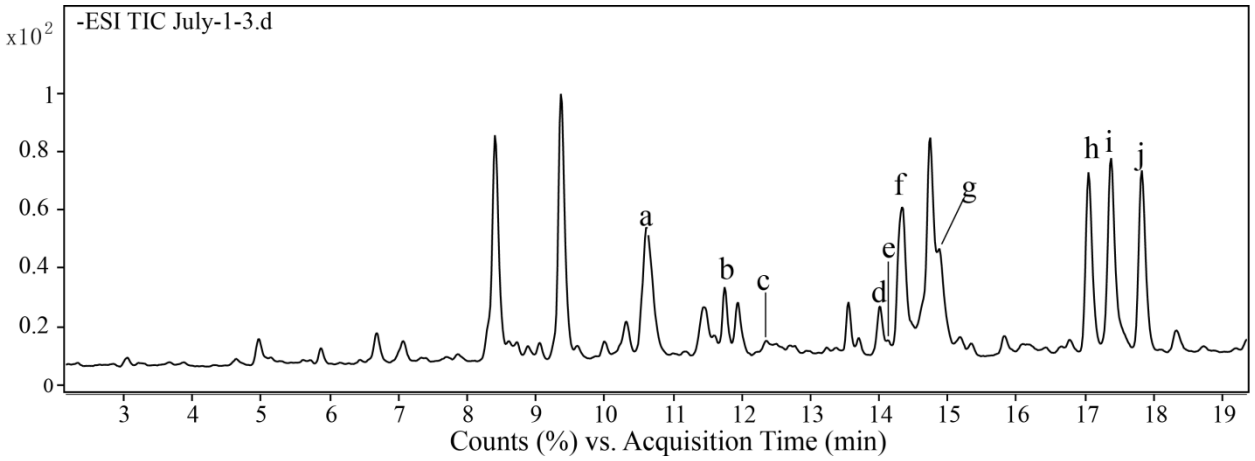

Figure S3. The UPLC-ESI(-)-qTOF-MS total ion current (TIC) of the methanol extract of Microctis Folium. vicenin-2 (a), isoschaftoside (b), schaftoside (c), vitexin (d), 2''-O-rhamnosylvitexin (e), isovitexin (f), isoviolanthin (g), nicotiflorin (h), astragalin (i) and narcissoside (j).