Electronic Supplementary Material (ESI) for RSC Advances.

Cytotoxic trichothecene-type sesquiterpenes from a sponge-derived fungus *Stachybotrys chartarum* with tyrosine kinase inhibition

Supporting Information

The physical and chemical data of known compounds

Compound **5**, white powder. $[\alpha]_D^{25}$ 14.4 ° (*c* 0.05, MeOH); ^{1}H NMR (400 MHz, DMSO-d_6) δ 5.68 (1H, d, *J* = 12.7 Hz, OH), 3.71 (1H, t, *J* = 5.1 Hz, H-2), 2.44,1.97 (2H, m, H-3), 6.00 (1H, m, H-4), 1.74 (2H, m, H-7), 1.99 (2H, m, H-8), 5.32 (1H, d, *J* = 4.3 Hz, H-10), 3.72 (1H, m, H-11), 3.07, 2.78 (2H, d, *J* = 4.0 Hz ,H-13), 0.75 (3H, s, H-14), 4.03, 4.37 (2H, d, *J* = 12.3 Hz, *J* = 12.3 Hz, H-15), 1.66 (3H, s, H-16), 3.83 (1H, s, H-2''), 2.44 (2H, m, H-4'), 3.88, 3.95 (2H, m, H-5'), 2.92 (2H, m, H-7'), 2.27 (2H, m, H-8'), 6.56 (1H, m, H-9'), 5.81 (1H, d, *J* = 4.3 Hz, H-10'). ^{13}C NMR (DMSO-d_6, 100 MHz) δ78.6 (d, C-2), 34.6 (t, C-3), 73.7 (d, C-4), 49.7 (s, C-5), 43.4 (s, C-6), 19.7 (t, C-7), 27.4 (t, C-8), 138.9 (s, C-9), 119.7 (d, C-10), 66.6 (d, C-11), 65.8 (s, C-12), 47.6 (t, C-13), 8.3 (q, C-14), 63.9 (t, C-15), 23.3 (q, C-16), 167.7 (s, C-1'), 57.9 (s, C-2'), 64.0 (s, C-3'), 23.0 (t, C-4'), 60.3 (t, C-5'), 88.3 (s, C-6'), 22.8 (t, C-7'), 26.2 (t, C-8'), 151.0 (d, C-9'), 120.6 (d, C-10'), 166.4 (s, C-11'). ESI-MS *m*/*z* 545.2$[M+H]^+$.

Compound **6**， white powder. $[\alpha]_D^{25}$ -26.0 °(*c* 0.05, MeOH). ^{1}H NMR (DMSO-d_6, 400 MHz) δ5.46 (1H, d, *J* = 5.72 Hz, OH), 3.71 (1H, m, H-2), 2.43 (2H, m, H-3), 5.97 (1H, m, H-4), 1.72 (2H, m, H-7), 1.94 (2H, m, H-8), 5.33 (1H, d, *J* = 3.7 Hz, H-10), 3.73 (1H, m, H-11), 3.08, 2.79 (2H, d, *J* = 4.0 Hz, H-13), 0.72 (3H, s, H-14), 4.12 (2H, dd, *J* = 12.6 Hz, H-15), 1.66 (3H, s, H-16), 3.61 (1H, s, H-2’), 2.14 (2H, m, H-4'), 3.83 (2H, m, H-5'), 5.78 (1H, d, *J* = 12.6 Hz, H-7'), 6.89 (1H, dd, *J* = 7.9, 16.3 Hz, H-8'), 6.78 (1H, dt, *J* = 7.9, 10.1 Hz, H-9'), 5.89 (1H, d, *J* = 10.1 Hz, H-10') ,4.27 (1H, d, *J* = 5.5 Hz, H-12'), 3.70 (1H, m, H-13'), 1.08 (3H, d, *J* = 6.5 Hz, H-14'). ^{13}C NMR (DMSO-d_6, 100 MHz) δ78.6 (d, C-2), 34.6 (t, C-3), 74.3 (d, C-4), 49.5 (s, C-5), 43.3 (s, C-6), 19.8 (t, C-7), 27.4 (t, C-8), 139.0 (s, C-9), 119.7 (d, C-10), 67.0 (d, C-11), 65.8 (s, C-12), 47.7 (t, C-13), 8.3 (q, C-14), 64.5 (t, C-15), 23.4 (q, C-16), 169.0 (s, C-1'), 54.0 (s, C-2'), 65.4 (s, C-3'), 28.0 (t, C-4'), 60.2 (t, C-5'), 82.6 (s, C-6'), 135.7 (d, C-7'), 128.7 (d, C-8’), 145.1 (d, C-9'), 119.4 (d, C-10'), 166.9 (s, C-11'), 67.1 (d, C-12') , 70.2 (d, C-13'), 17.5 (q, C-14'). ESIMS *m*/*z* 545.2$[M+H]^+$.

Compound **7**, white powder. $[\alpha]_D^{25}$ -8 °(*c* 0.05, MeOH); ^{1}H NMR (DMSO-d_6, 400

MHz) δ3.65 (1H, m, H-2), 2.44, 1.76 (2H, m, H-3), 5.83 (1H, d, *J* = 4.3 Hz, H-4), 1.72 (2H, m, H-7), 1.82, 2.04 (2H, m, H-8), 5.31 (1H, d, *J* = 3.9 Hz, H-10), 3.62 (1H, m, H-11), 2.78, 3.04 (2H, dd, *J* = 3.6, 3.6 Hz, H-13), 0.77 (3H, s, H-14), 3.64, 3.28 (2H, m, d, *J* = 11.5 Hz, H-15), 1.65 (3H, s, H-16), 5.67 (1H, d, *J* = 11.5 Hz, H-2'), 6.76 (1H, t, *J* = 11.5 Hz, H-3'), 7.47 (1H, t, *J* = 15.3 Hz, H-4'), 6.09 (1H, dd, *J* = 7.64, 15.3 Hz, H-5'), 3.71 (1H, t, *J* = 6.37 Hz, H-6'), 3.54 (2H, m, H-7'), 2.68 (2H, m, H-8'), 5.99 (H, s, H-10'), 4.88 (2H, s, H-12'), 3.65 (H, m, H-13'), 0.96 (3H, d, *J* = 5.76 Hz H-14'). ^{13}C NMR (DMSO-d_6, 100 MHz) δ78.3 (d, C-2), 37.1 (t, C-3), 75..8 (d, C-4), 48.8 (s, C-5), 44.4 (s, C-6), 20.7 (t, C-7), 28.1 (t, C-8), 139.4 (s, C-9), 119.6 (d, C-10), 66.9 (d, C-11), 66.0 (s, C-12), 47.6 (t, C-13), 7.3 (q,C-14), 60.7 (t, C-15), 23.4 (q, C-16), 165.7 (s, C-1'), 118.0 (d, C-2'), 144.5 (d, C-3'), 129.4 (d, C-4'), 141.8 (d, C-5'), 84.6 (d, C-6'), 66.5 (d, C-7'), 29.2 (t, C-8'), 157.3 (s, C-9'), 115.5 (d, C-10'), 170.5 (s, C-11'), 73.5 (t,C-12'), 68.3 (d, C-13'), 19.3(q, C-14'). ESIMS *m*/*z* 531.3[M+H]$^+$.

Compound **8**, white powder. [α] $^{25}_{D}$ 51.6 °(*c* 0.05, MeOH). ^{1}H NMR (DMSO-d_6, 400 MHz) δ4.50 (1H, d, *J* = 3.2 Hz, OH), 3.69 (1H, m, H-2), 2.45, 1.95 (2H, m, H-3), 5.89 (1H, m, H-4), 1.78 (2H, m, H-7), 1.97 (2H, m, H-8), 5.34 (1H, s, H-10), 3.72 (1H, m, H-11), 3.06, 2.78 (2H, d, *J* = 4.0 Hz, H-13), 0.71 (3H, s, H-14), 4.43 (2H, d, *J* = 12.7 Hz, H-15), 1.67 (3H, s, H-16), 5.75 (1H, s, H-2'), 3.55 (2H, m, H-4'), 3.48, 3.76 (2H, m, H-5'), 7.26 (1H, dd, *J* = 10.4, 16.7 Hz, H-7'), 6.15 (1H, d, *J* = 16.7 Hz, H-8'), 6.74 (1H, t, *J* = 10.7 Hz, H-9'), 5.89 (1H,d, *J* = 9.8 Hz, H-10'), 3.82 (1H, d, *J* = 4.6 Hz, H-12'), 4.17 (1H, m, H-13'), 0.97 (3H, d, *J* = 6.4 Hz, H-14'). ^{13}C NMR (DMSO-d_6, 100 MHz) δ78.5 (d, C-2), 34.5 (t, C-3), 74.5 (d, C-4), 48.9 (s, C-5), 43.3 (s, C-6), 20.2 (t, C-7), 27.5 (t, C-8), 139.0 (s, C-9), 119.9 (d, C-10), 67.4 (d, C-11), 65.9 (s, C-12), 47.7 (t, C-13), 7.82 (q,C-14), 64.1 (t,C-15), 23.4 (q,C-16), 166.3 (s, C-1'), 117.6 (s, C-2'), 157.3 (s, C-3'), 26.0 (t, C-4'), 59.5 (t, C-5'), 81.5 (s, C-6'), 132.9 (d, C-7'), 135.0 (d, C-8'), 144.1 (d, C-9'), 119.6 (d, C-10'), 167.0 (s, C-11'), 72.6 (d, C-12'), 68.4 (d, C-13'), 17.6 (q, C-14'). ESIMS *m*/*z* 529.2 [M+H]$^+$.

Compound **9**. white powder. [α] $^{25}_{D}$ -20.8 °(*c* 0.05, MeOH). ^{1}H NMR (DMSO-d_6, 400 MHz) δ3.69 (1H, d, *J* = 5.2 Hz, H-2), 2.48, 1.95 (2H, m, H-3), 5.87 (1H, dd, *J* =

3.9, 7.9 Hz, H-4), 1.77 (2H, m, H-7), 1.89 (2H, m, H-8), 5.34 (1H, d, *J* = 4.2 Hz, H-10), 3.75 (1H, m, H-11), 3.0, 2.79 (2H, d, *J* = 4.2Hz, H-13), 0.71 (3H, s, H-14), 4.09, 4.40 (2H, m, H-15), 1.66 (3H, s, H-16), 5.72 (1H, s, H-2'), 2.45 (2H, m, H-4'), 3.70, 4.40 (2H, m, H-5'), 6.21 (1H, d, *J* = 3.9 Hz, H-7'), 7.82 (1H, dd, *J* = 11.6, 15.1 Hz, H-8'), 6.83 (1H, t, *J* = 11.2 Hz, H-9'), 6.24 (1H, s, H-10'), 2.18 (3H, s, H-12'). ^{13}C NMR (DMSO-d_6, 100 MHz) δ78.4 (d, C-2), 34.9 (t, C-3), 75.8 (d, C-4), 49.0 (s, C-5), 43.1 (s, C-6), 20.3 (t, C-7), 27.5 (t, C-8), 139.1 (s, C-9), 119.7 (d, C-10), 66.7 (d, C-11), 65.9 (s, C-12), 47.6 (t, C-13), 7.29 (q, C-14), 63.2 (t, C-15), 23.3 (q, C-16), 165.8 (s, C-1'), 118.0 (s, C-2'), 157.3 (s, C-3'), 39.7 (t, C-4'), 60.9 (t, C-5'), 165.3 (s, C-6'), 128.7 (d, C-7'), 138.6 (d, C-8'), 140.2 (d, C-9'), 125.8 (d, C-10'), 166.0 (s, C-11'), 17.1(q, C-12'). ESIMS *m/z* 485.2 $[M+H]^+$.

Compound **10**. white powder. $[\alpha]_D^{25}$ 5.20 °(*c* 0.05, MeOH). ^{1}H NMR (DMSO-d_6, 400 MHz) δ4.87 (1H, d, *J* = 4.4 Hz, OH), 3.68 (1H, d, *J* = 5.2 Hz, H-2), 2.47, 1.90 (2H, m, H-3), 5.86 (1H, dd, *J* = 4.2, 8.1 Hz, H-4), 1.75 (2H, m, H-7), 1.94 (2H, m, H-8), 5.34 (1H, d, *J* = 4.7 Hz, H-10), 3.77 (1H, m, H-11), 3.04, 2.77 (2H, d, *J* = 4.1 Hz, H-13), 0.69 (3H, s, H-14), 4.34, 3.71 (2H, m, d, *J* = 12.6 Hz, H-15), 1.65 (3H, s, H-16), 5.69 (1H, s, H-2'), 2.37 (2H, m, H-4'), 3.70, 3.45 (2H, m, H-5'), 3.92 (1H, m, H-6'), 6.15, 6.19 (1H, t, *J* = 3.0 Hz, H-7'), 7.19 (1H, dd, *J* = 12.0, 15.2 Hz, H-8'), 6.70 (1H, t, *J* = 11.1 Hz, H-9'), 5.66 (1H, d, *J* = 11.1 Hz, H-10'), 2.18 (3H, s, H-12'), 3.81 (1H, m, H-13'), 0.92 (3H, d, *J* = 11.1 Hz, H-14'). ^{13}C NMR (DMSO-d_6, 100 MHz) δ78.4 (d, C-2), 35.1 (t, C-3), 74.5 (d, C-4), 48.8 (s, C-5), 42.9 (s, C-6), 20.6 (t, C-7), 27.5 (t, C-8), 139.0 (s, C-9), 119.8 (d, C-10), 66.9 (d, C-11), 65.9 (s, C-12), 47.5 (t, C-13), 7.15 (q,C-14), 63.3 (t,C-15), 23.3 (q,C-16), 166.2 (s, C-1'), 116.8 (s, C-2'), 159.3 (s, C-3'), 41.1 (t, C-4'), 68.5 (t, C-5'), 82.5 (d, C-6'), 141.7 (d, C-7'), 125.7 (d, C-8'), 144.9 (d, C-9'), 116.5 (d, C-10'), 166.1 (s, C-11'), 19.4(q, C-12'), 67.5 (d, C-13'), 18.1 (q, C-14'). ESIMS *m/z* 515.2 $[M+H]^+$.

Compound **11**. white powder. $[\alpha]_D^{25}$-118 °(*c* 0.05, MeOH). ^{1}H NMR (DMSO-d_6, 400 MHz) δ4.58 (1H, s, OH), 3.55 (1H, m, H-2), 2.30, 1.67 (2H, m, H-3), 4.35 (1H, s, H-4), 1.72, 1.83 (2H, m, H-7), 1.85 (2H, m, H-8), 5.28 (1H, s, H-10), 3.55 (1H, m, H-

11), 2.93, 2.68 (2H, s, H-13), 0.71 (3H, s, H-14), 3.73, 4.11 (2H, m, dd, *J* = 12.0, 12.7 Hz, H-15), 1.63 (3H, s, H-16), 5.66 (1H, s, H-2'), 2.29 (2H, m, H-4'), 3.55 (2H, m, H-5'), 2.12 (3H, s, H-6'). ^{13}C NMR (DMSO-d_6, 100 MHz) δ 78.7 (d, C-2), 39.2 (t, C-3), 72.4 (d, C-4), 48.7 (s, C-5), 43.0 (s, C-6), 20.8 (t, C-7), 28.0 (t, C-8), 139.4 (s, C-9), 119.6 (d, C-10), 66.5 (d, C-11), 65.8 (s, C-12), 46.6 (t, C-13), 7.6 (q,C-14), 62.8 (t,C-15), 23.4 (q,C-16), 166.1 (s, C-1'), 116.5 (d, C-2'), 158.9 (d, C-3'), 44.0 (d, C-4'), 59.3 (t, C-5'), 18.9 (q, C-6'). ESIMS *m/z* 379.2 $[M+H]^+$.

Compound **12**. white powder. $[\alpha]_D^{25}$ -25.2 °(*c* 0.05, MeOH). ^{1}H NMR (DMSO-d_6, 400 MHz) δ 3.68 (1H, d, *J* = 4.2 Hz, H-2), 2.48, 1.85 (2H, m, H-3), 5.58 (1H, m, H-4), 1.79, 1.38 (2H, m, H-7), 1.92 (2H, m, H-8), 5.30 (1H, d, *J* = 4.0 Hz, H-10), 3.60 (1H, d, *J* = 5.0 Hz, H-11), 2.79, 3.04 (2H, t, *J* = 4.0 Hz, H-13), 0.60 (3H, s, H-14), 0.88 (3H, s, H-15), 1.65 (3H, s, H-16), 5.62 (1H, d, *J* = 11.5 Hz, H-2'), 6.74 (1H, t, *J* = 11.5 Hz, H-3'), 7.44 (1H, dt, *J* = 12.0, 15.5 Hz, H-4'), 6.25 (1H, dd, *J* = 5.0, 14.5 Hz, H-5'), 3.88 (1H, t, *J* = 5.0 Hz, H-6'), 3.51 (1H, t, *J* = 6.0 Hz, H-7'), 1.04 (3H, d, *J* = 6.0 Hz, H-8'). ^{13}C NMR (DMSO-d_6, 100 MHz) δ 78.5 (d, C-2), 36.5 (t, C-3), 74.8 (d, C-4), 49.1 (s, C-5), 40.4 (s, C-6), 24.3 (t, C-7), 27.9 (t, C-8), 138.9 (s, C-9), 119.6 (d, C-10), 70.2 (d, C-11), 65.8 (s, C-12), 47.5 (t, C-13), 6.1 (q,C-14), 16.1 (q,C-15), 23.3 (q,C-16), 165.9 (s, C-1'), 116.4 (d, C-2'), 146.0 (d, C-3'), 126.1 (d, C-4'), 147.0 (d, C-5'), 75.7 (d, C-6'), 70.1 (d, C-7'), 19.8 (q, C-8'). ESIMS *m/z* 405.2 $[M+H]^+$.

Compound **13**. white powder. $[\alpha]_D^{25}$ -52.4 °(*c* 0.05, MeOH). ^{1}H NMR (DMSO-d_6, 400 MHz) δ 4.54 (1H, s, OH), 3.64 (1H, d, *J* = 5.0 Hz, H-2), 2.41, 1.77 (2H, m, H-3), 5.82 (1H, d, *J* = 4.7 Hz, H-4), 1.75 (2H, m, H-7), 1.85, 2.04 (2H, m, H-8), 5.30 (1H, d, *J* = 3.9 Hz, H-10), 3.62 (1H, d, *J* = 4.8 Hz, H-11), 2.78, 3.04 (2H, t, *J* = 4.0 Hz, H-13), 0.75 (3H, s, H-14), 3.70, 3.29 (2H, dd, *J* = 9.9, 10.3 Hz, H-15), 1.65 (3H, s, H-16), 5.63 (1H, d, *J* = 11.3 Hz, H-2'), 6.74 (1H, t, *J* = 11.3 Hz, H-3'), 7.46 (1H, t, *J* = 13.2 Hz, H-4'), 6.26 (1H,dd, *J* = 5.7, 15.1 Hz, H-5'), 3.88 (1H, s, H-6'), 3.52 (1H, t, *J* = 5.5 Hz, H-7'), 1.04 (3H, d, *J* = 6.1 Hz, H-8'). ^{13}C NMR (DMSO-d_6, 100 MHz) δ 78.4 (d, C-2), 36.9 (t, C-3), 75..5 (d, C-4), 48.9 (s, C-5), 44.4 (s, C-6), 20.7 (t, C-7), 28.1 (t, C-8), 139.4 (s, C-9), 119.6 (d, C-10), 66.9 (d, C-11), 66.0 (s, C-12), 47.6 (t, C-13), 7.3 (q,C-

14), 60.7 (t,C-15), 23.4 (q,C-16), 165.8 (s, C-1'), 116.6 (d, C-2'), 145.7 (d, C-3'), 126.2 (d, C-4'), 146.8 (d, C-5'), 75.7 (d, C-6'), 70.1 (d, C-7'), 19.7 (q, C-8'). ESIMS *m*/*z* 421.2 $[M+H]^+$.

Compound **14**. $[\alpha]_D^{25}$ 20.4 ° (*c* 0.05, MeOH). IR (KBr) ν_{max} 3386, 2945, 2871,1770,1759, 1375, 1246, 1047, 1605 cm^{-1}. ^1H NMR (400 MHz, DMSO-d_6) δ3.81 (1H, dd, *J* = 5.9 Hz, H-2), 1.55, 1.94 (2H, d, *J* = 11.4 Hz, H-3), 3.91 (1H, m, H-4), 1.81, 1.95 (2H, m, H-7), 1.81, 1.95 (2H, m, H-8), 5.43 (1H, s, H-10), 3.60 (1H, m, H-11), 3.48, 3.56 (2H, m, H-13), 0.89 (3H, s, H-14), 0.77 (3H, s, H-15), 1.65 (3H, s, H-16). ^{13}C NMR (DMSO-d_6, 100MHz) δ76.6 (d, C-2), 40.6 (t, C-3), 69.2 (d, C-4), 57.4 (s, C-5), 42.9 (s, C-6), 25.4 (t, C-7), 28.1 (t, C-8), 139.2 (s, C-9), 119.3 (d, C-10), 76.2 (d, C-11), 90.9 (s, C-12), 63.9 (t, C-13), 9.8 (q, C-14), 14.0 (q, C-15), 23.5 (q, C-16). HRESIMS (*m/z* 269.1751 $[M + H]^+$, calcd 269.1753).

Compound **15**. white powder. $[\alpha]_D^{25}$-161.2 °(*c* 0.05, MeOH). ^1H NMR (DMSO-d_6, 400 MHz) δ4.48 (1H, s, OH), 3.53 (1H, d, *J* = 5.1 Hz, H-2), 2.31,1.70 (2H, m, H-3), 4.26 (1H, s, H-4), 1.78, 1.31 (2H, m, H-7), 1.87 (2H, m, H-8), 5.27 (1H, d, *J* = 4.4 Hz, H-10), 3.45 (1H,d, *J* = 5.0 Hz, H-11), 2.89, 2.66 (2H, t, *J* = 4.2 Hz, H-13), 0.63 (3H, s, H-14), 0.75 (3H, s, H-15), 1.62 (3H, s, H-16). ^{13}C NMR (DMSO-d_6, 100 MHz) δ78.9 (d, C-2), 39.4 (t, C-3), 71.9 (d, C-4), 48.7 (s, C-5), 40.0 (s, C-6), 24.3 (t, C-7), 28.0 (t, C-8), 138.5 (s, C-9), 120.0 (d, C-10), 70.1 (d, C-11), 65.8 (s, C-12), 46.6 (t, C-13), 6.41 (q,C-14), 16.0 (q,C-15), 23.3 (q,C-16). ESIMS *m*/*z* 251.2 $[M+H]^+$.

Figure S1 ^{1}H NMR spectrum of **1**

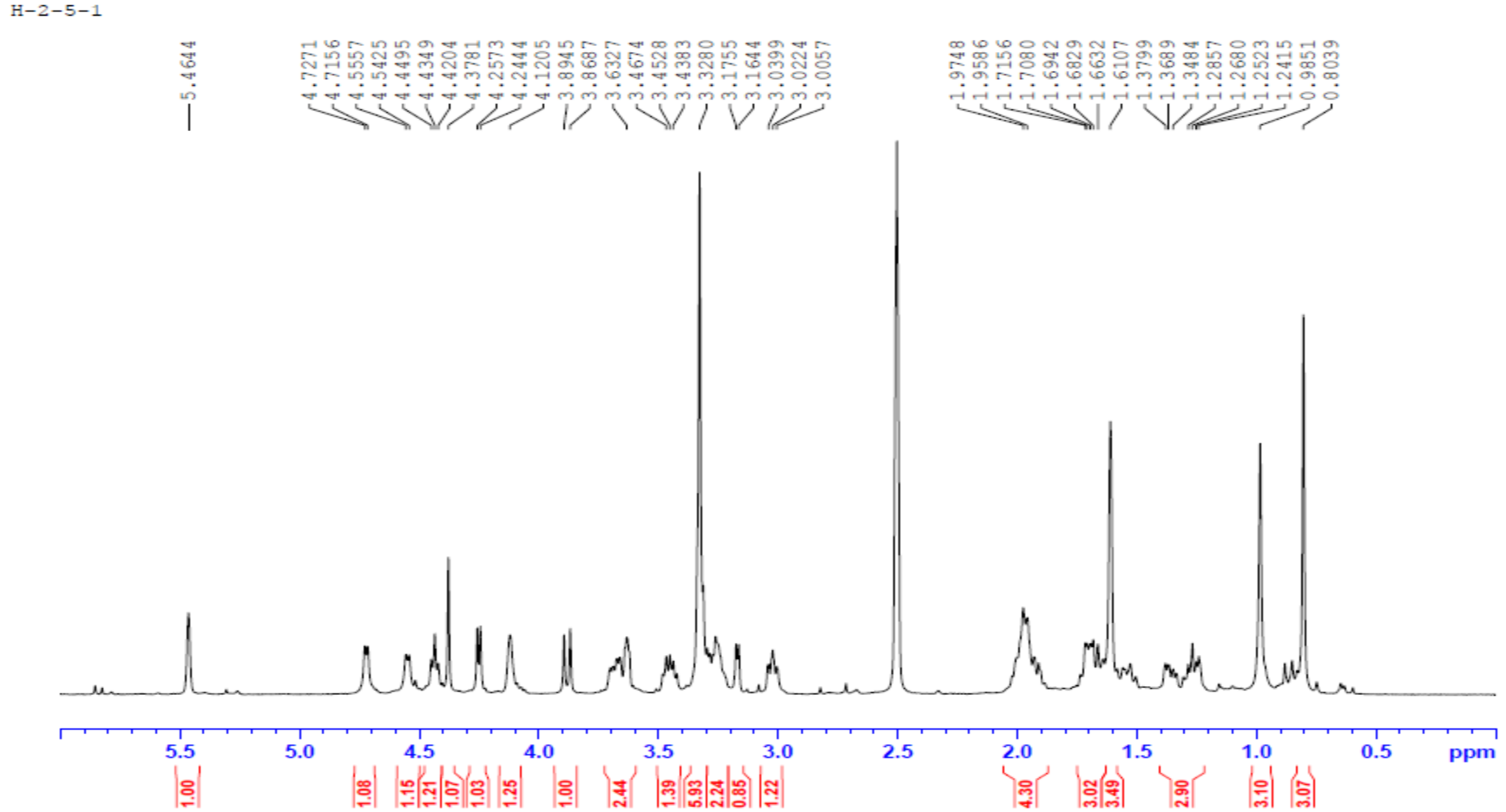

Figure S2 ^{13}C NMR spectrum of **1**

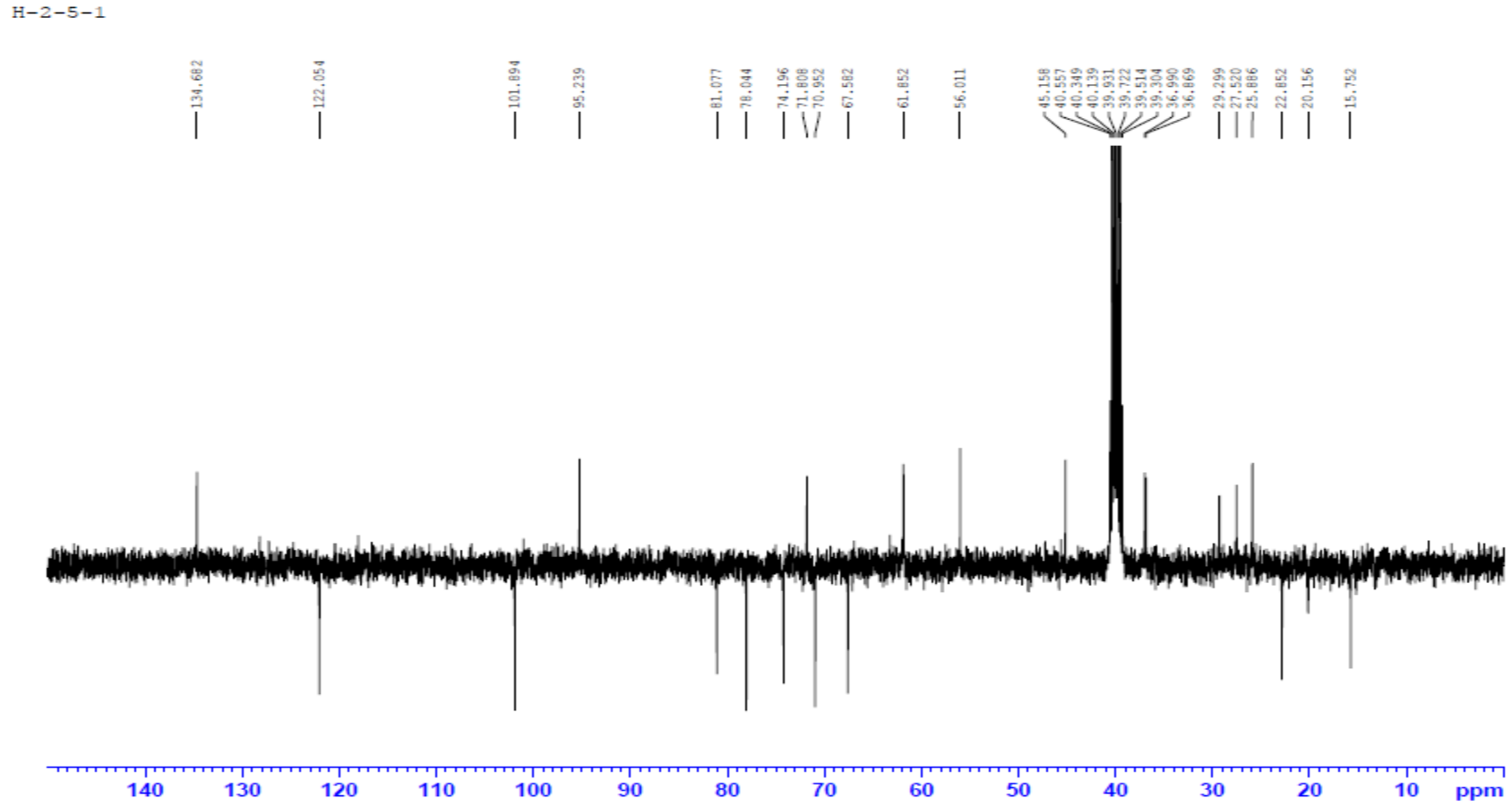

Figure S3 COSY spectrum of **1**

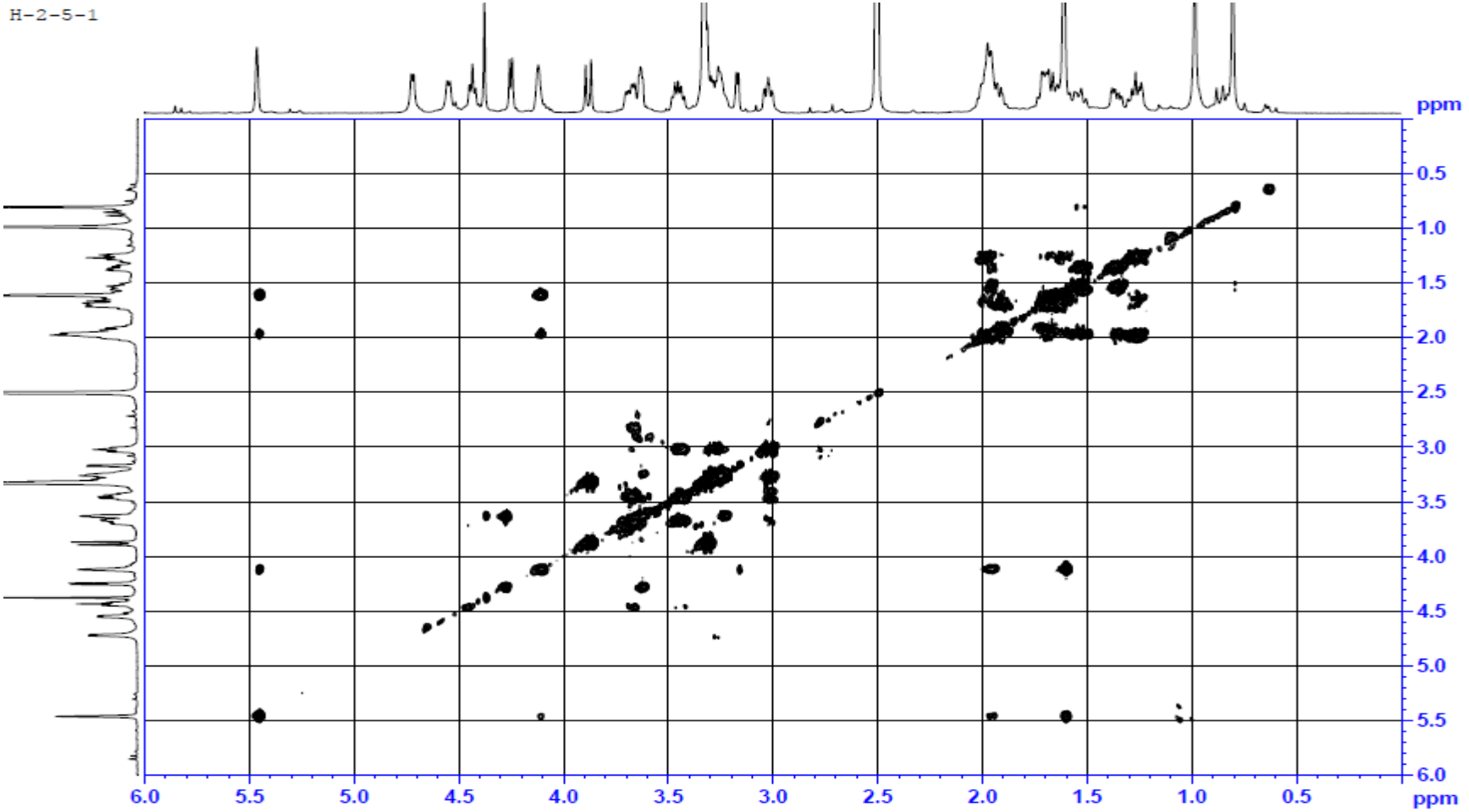

Figure S4 HMQC spectrum of **1**

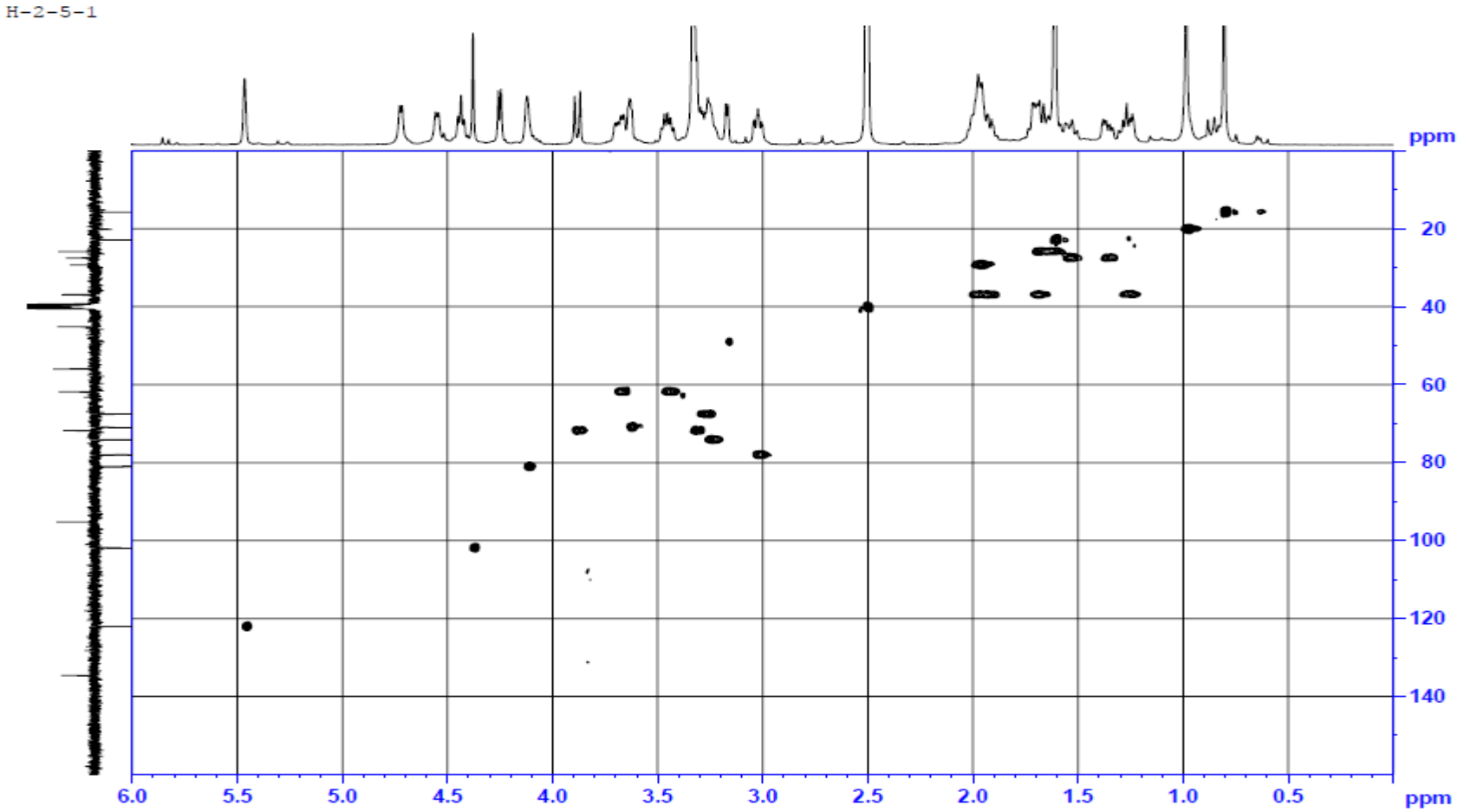

Figure S5 HMBC spectrum of **1**

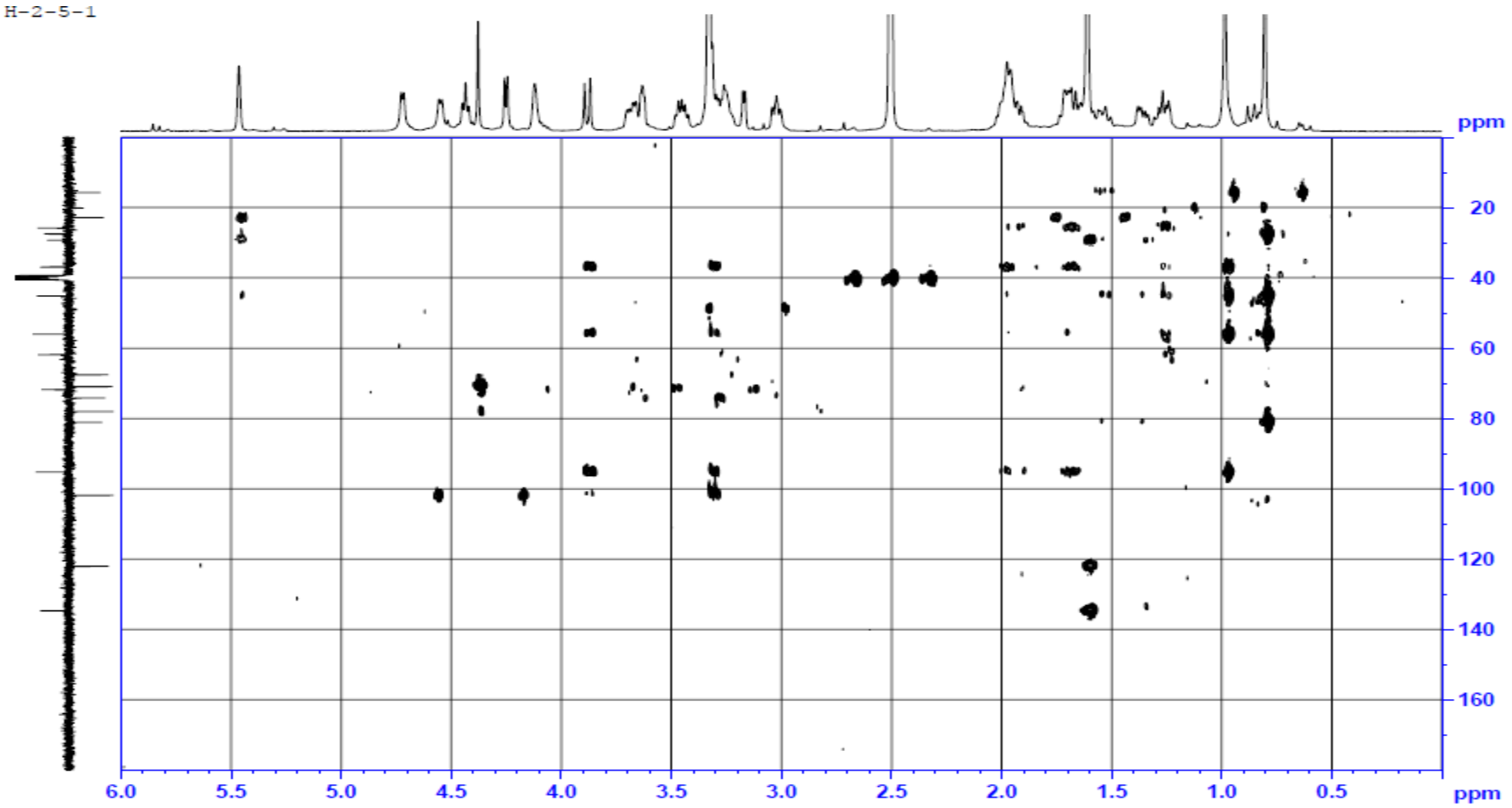

Figure S6 NOESY spectrum of **1**

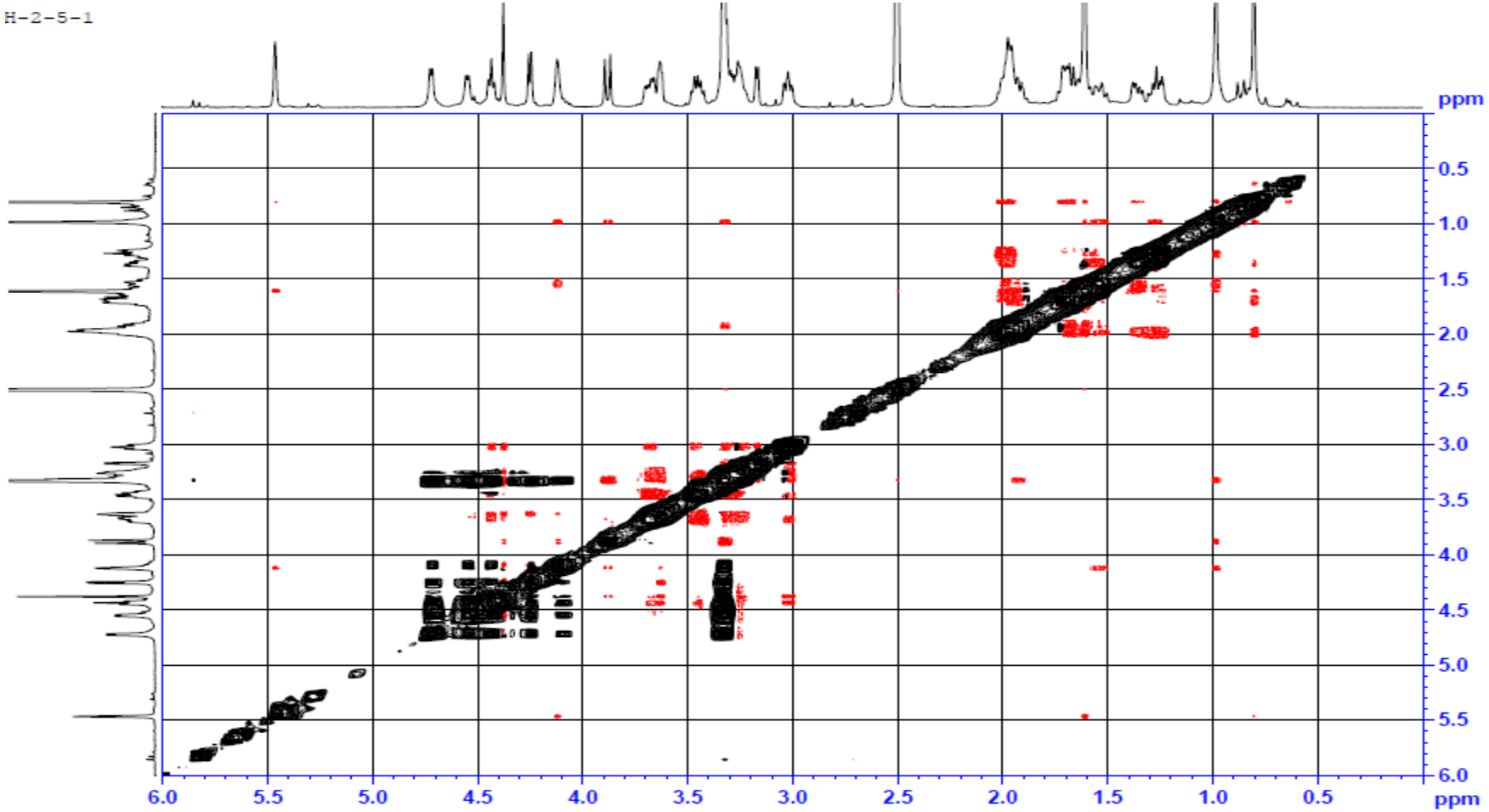

Figure S7 IR spectrum of **1**

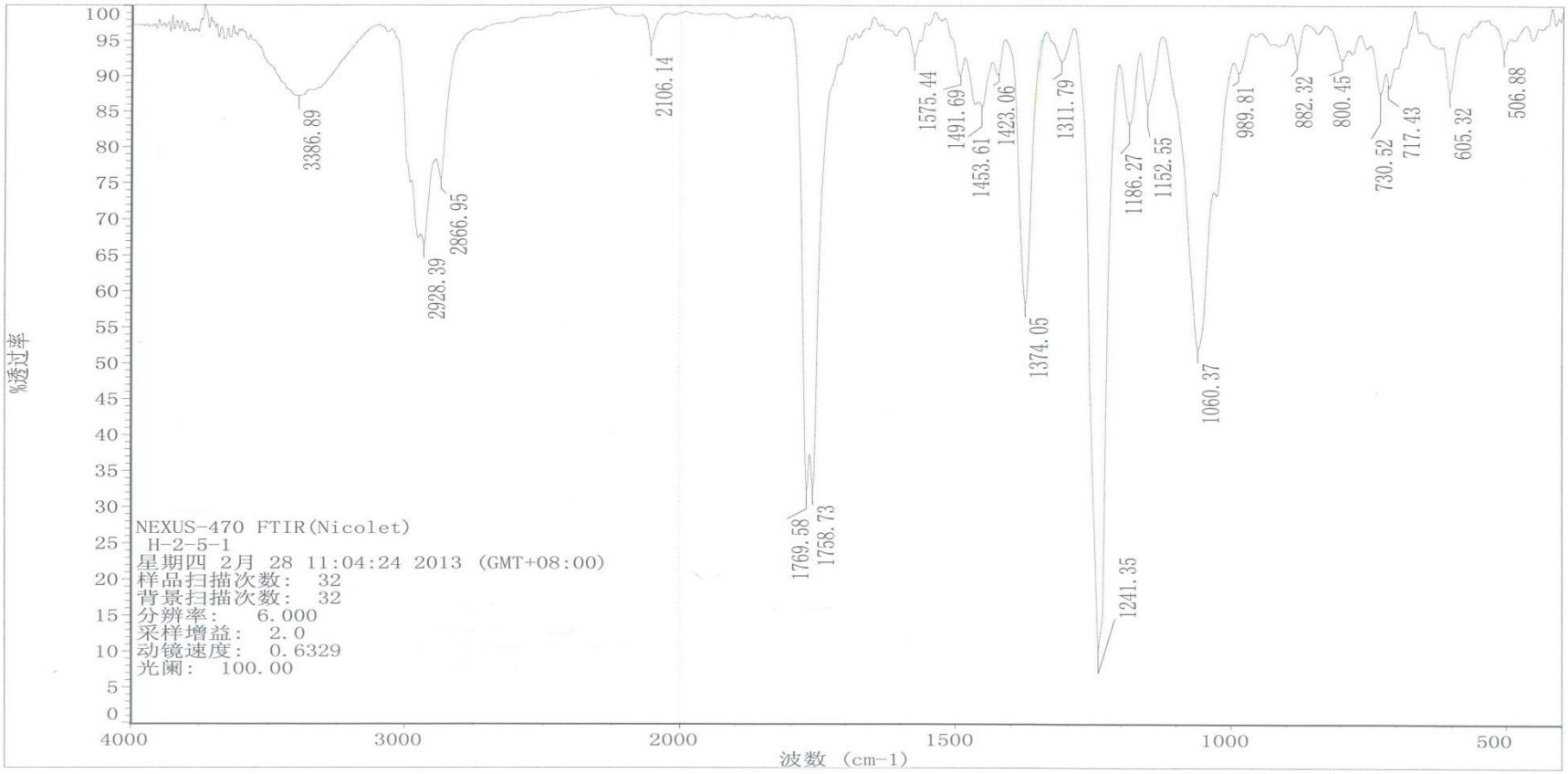

Figure S8 HRESIMS spectrum of **1**

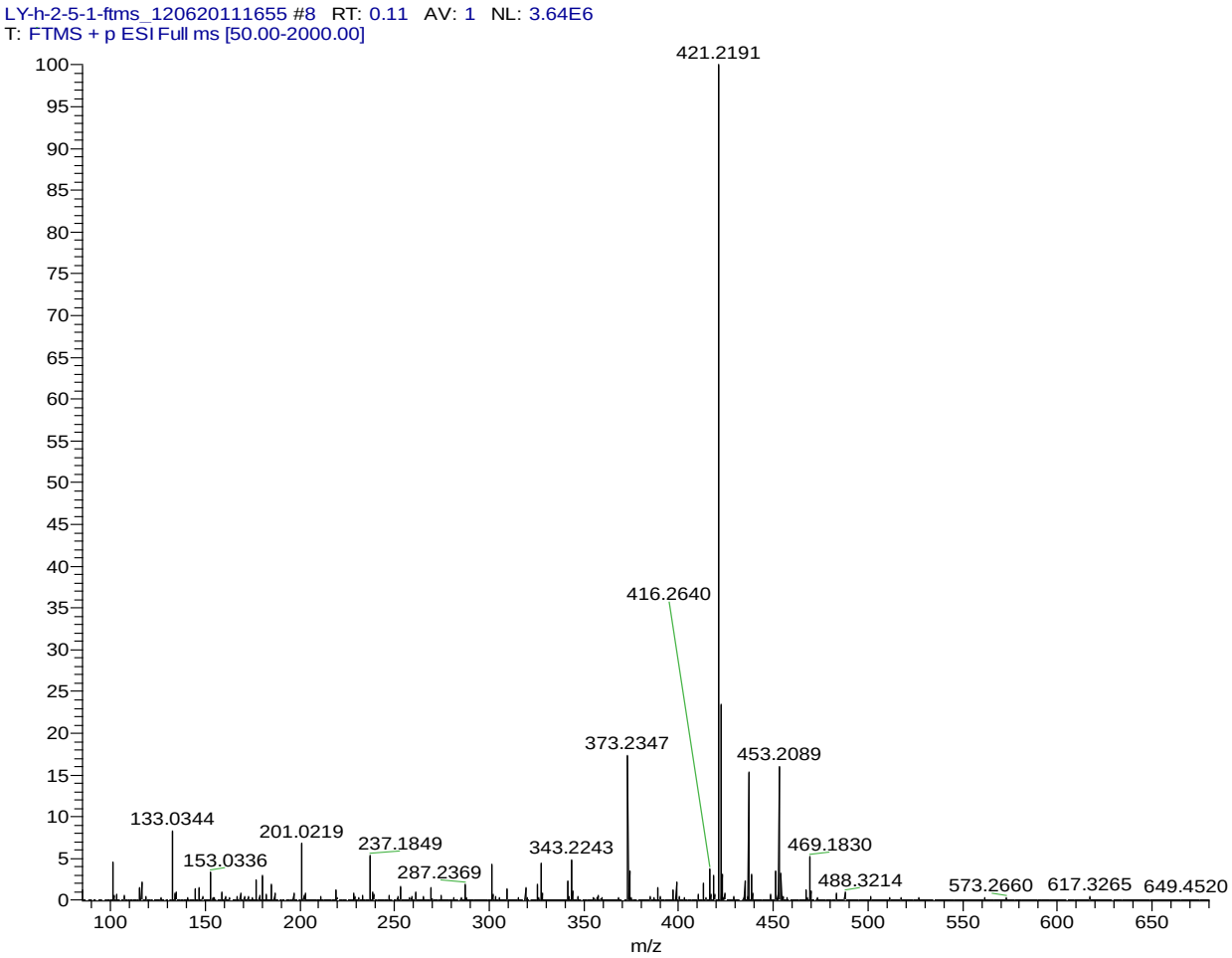

Figure S9 UV spectrum and HPLC purity of **1**

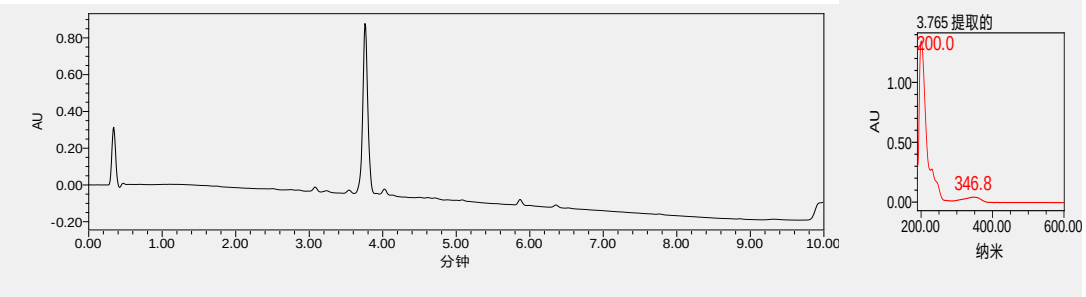

Figure S10 ^{1}H NMR spectrum of **2**

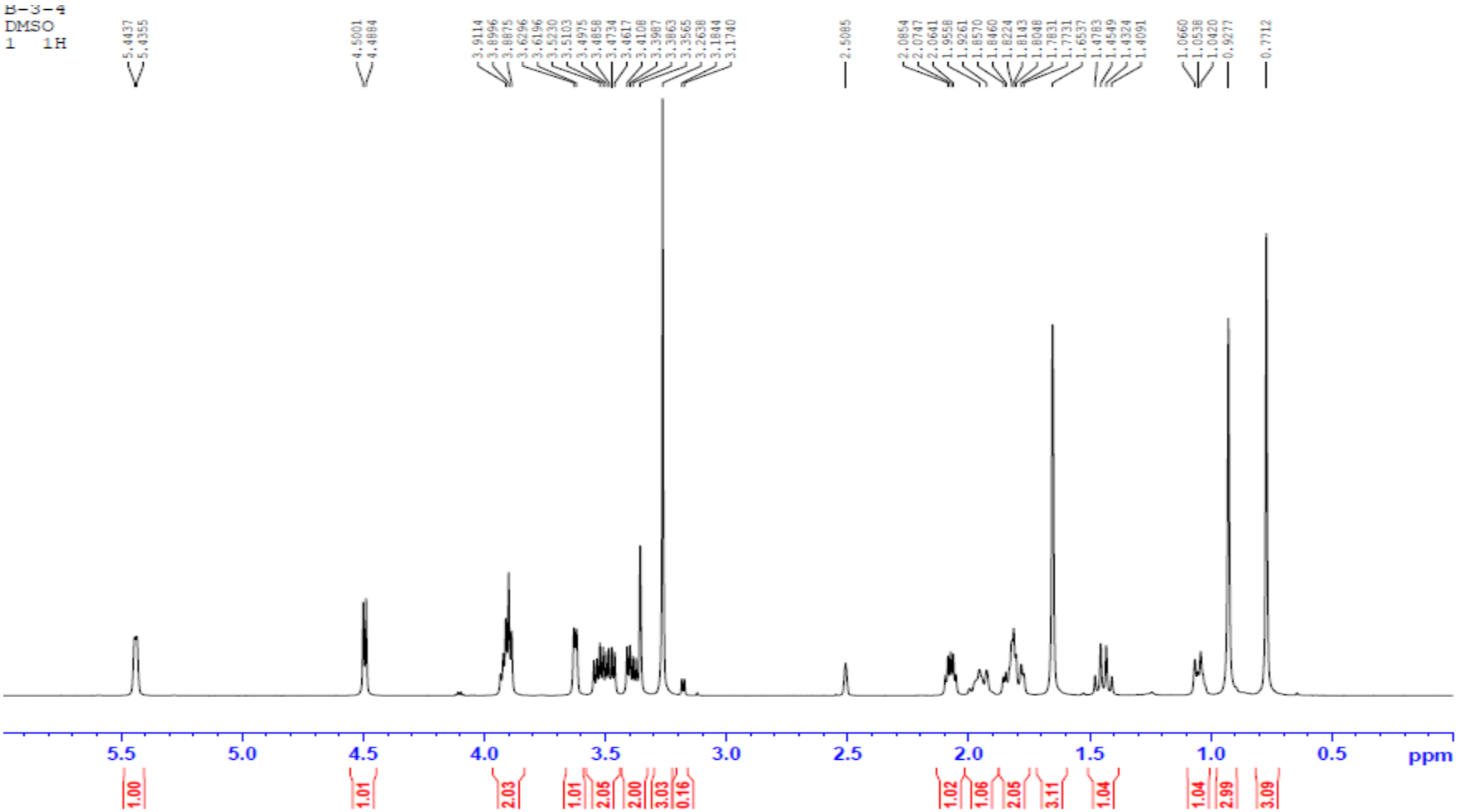

Figure S11 ^{13}C NMR spectrum of **2**

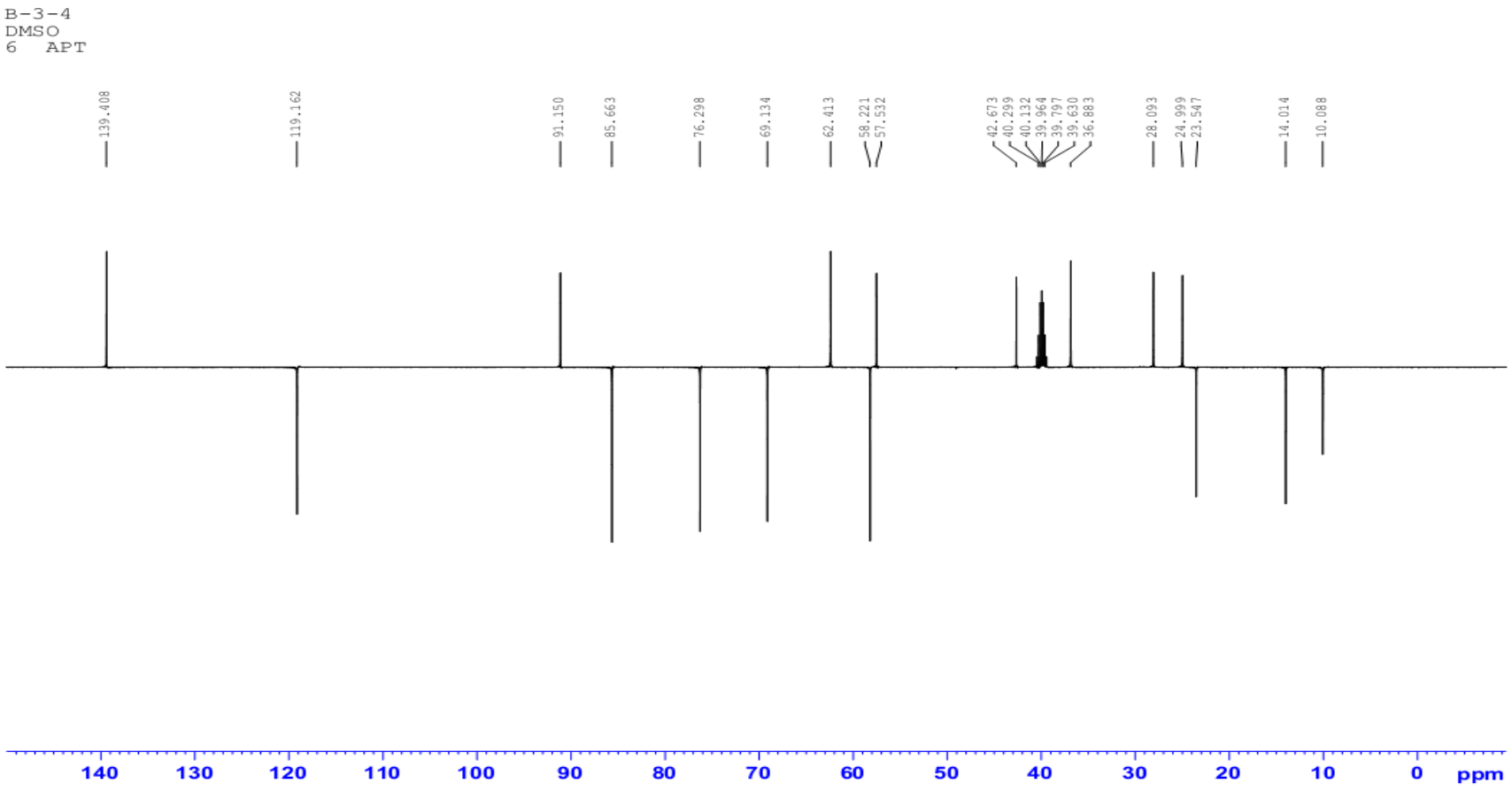

Figure S12 COSY spectrum of **2**

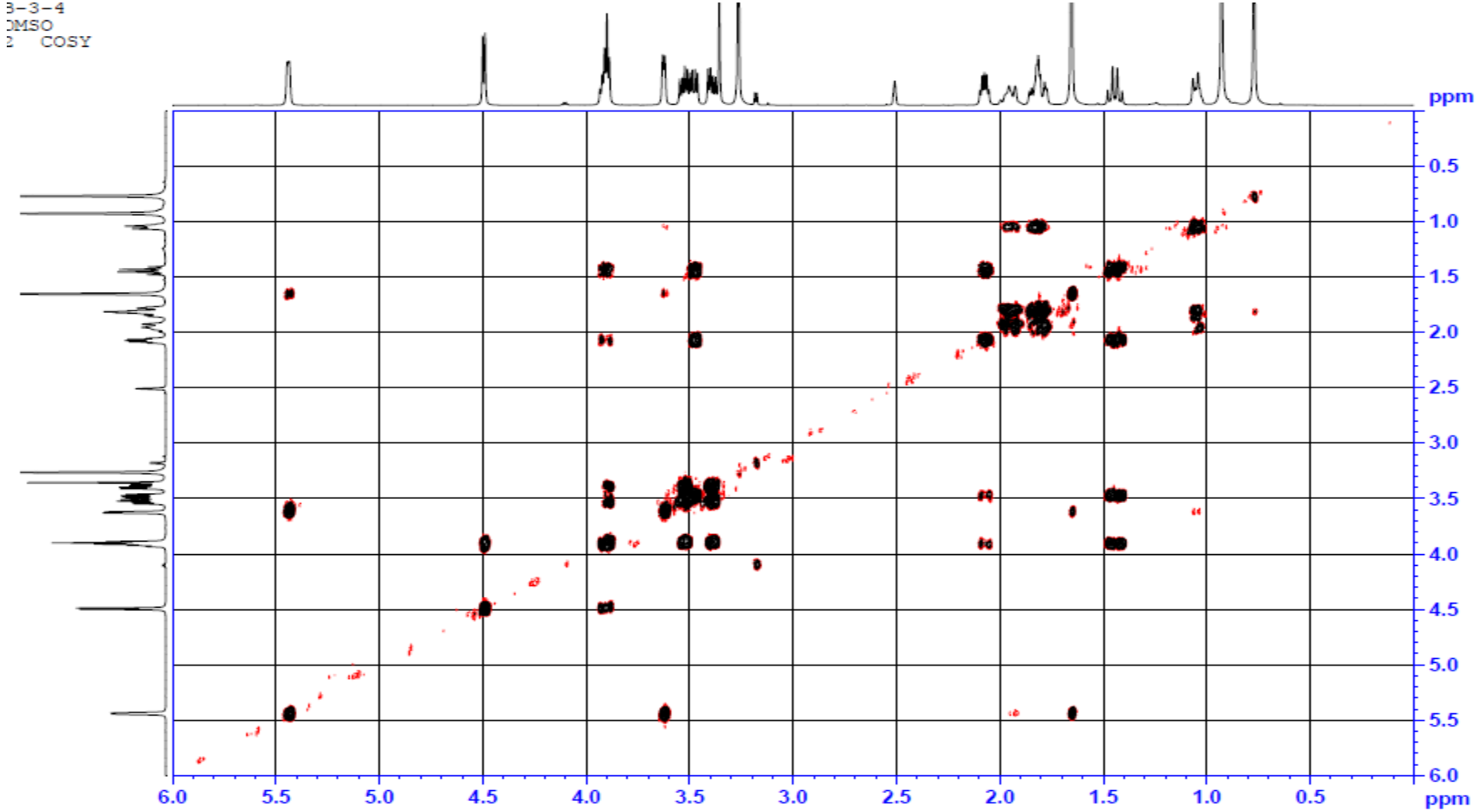

Figure S13 HMQC spectrum of **2**

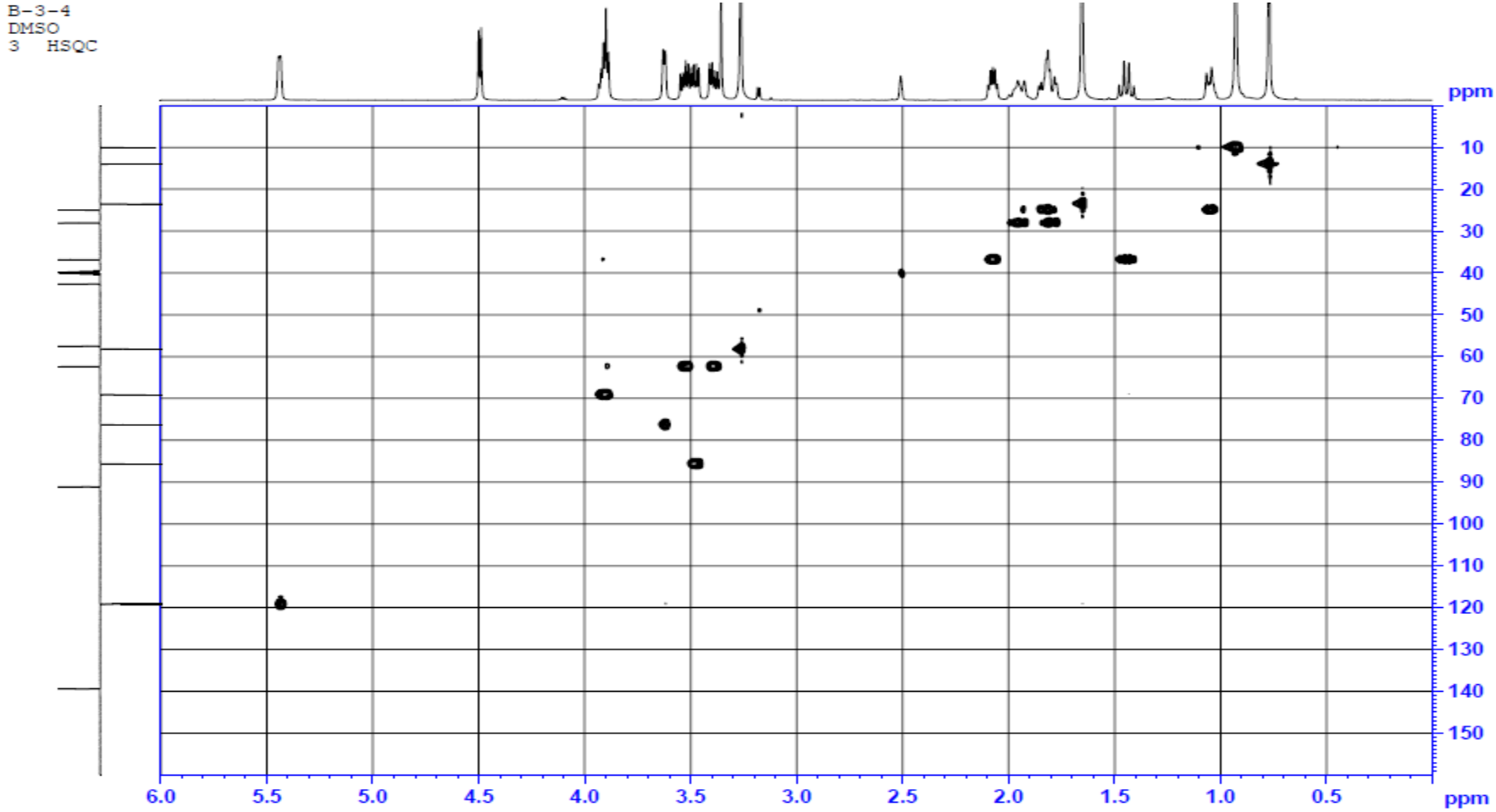

Figure S14 HMBC spectrum of **2**

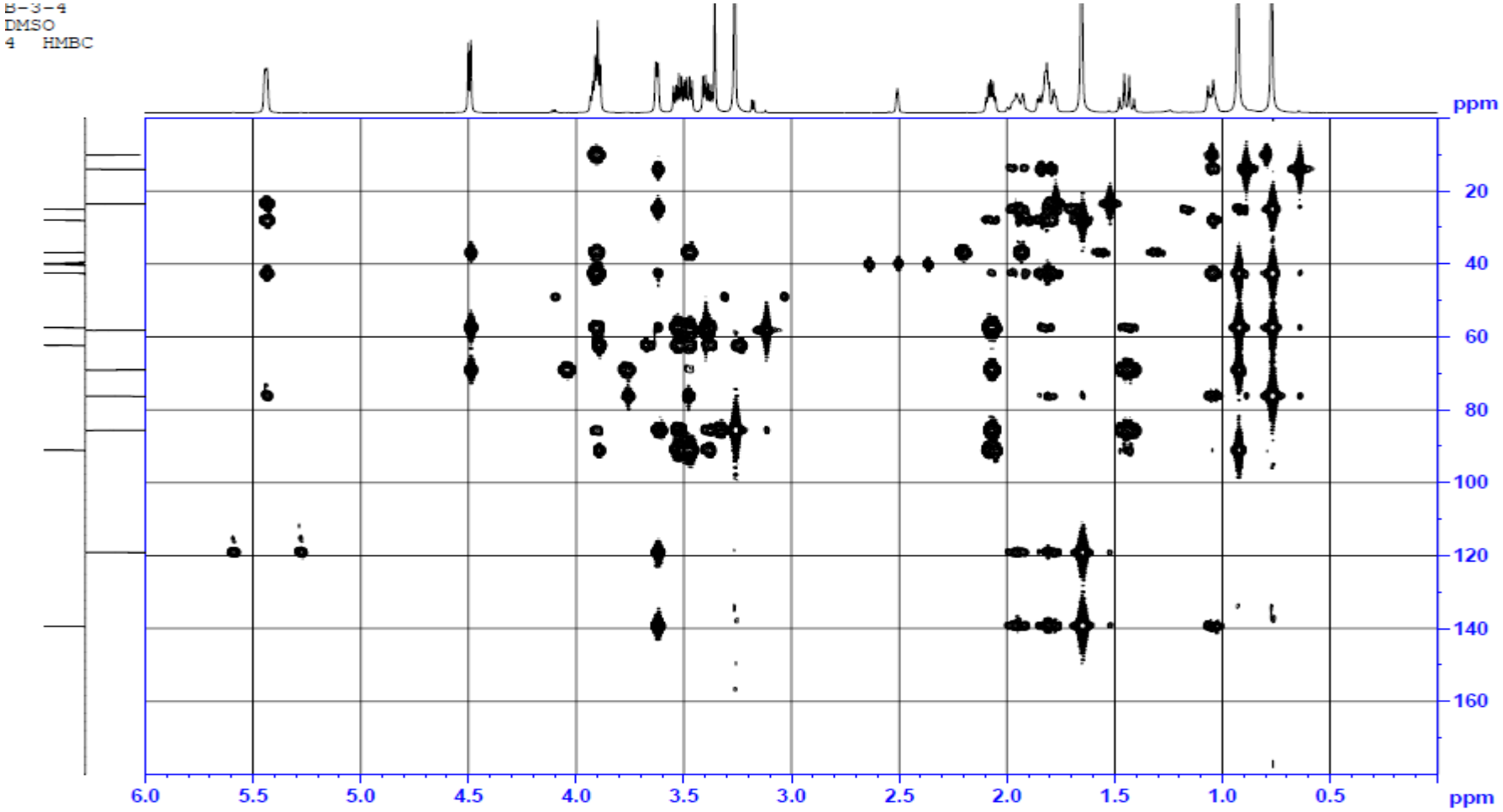

Figure S15 NOESY spectrum of **2**

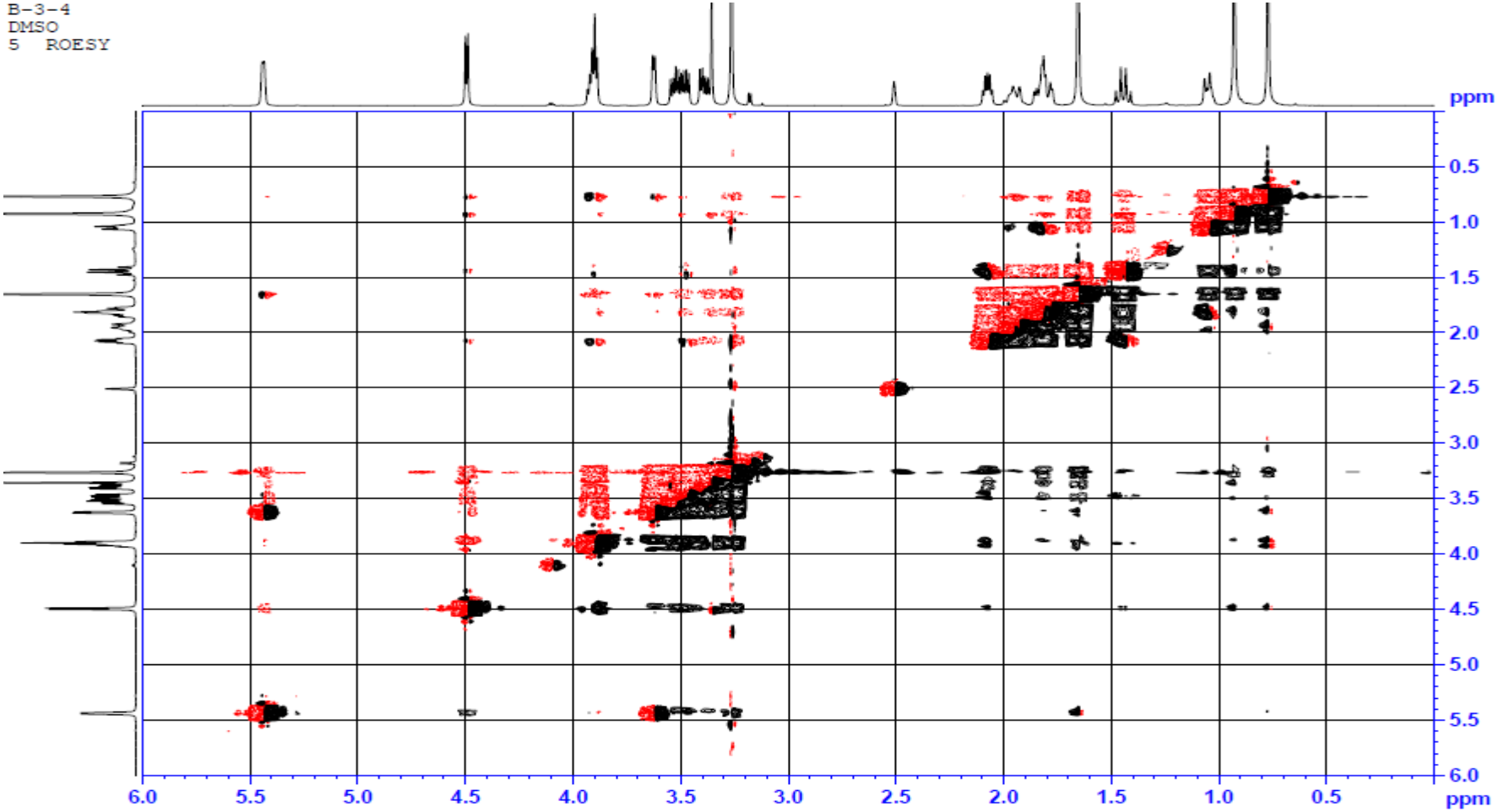

Figure S16 IR spectrum of **2**

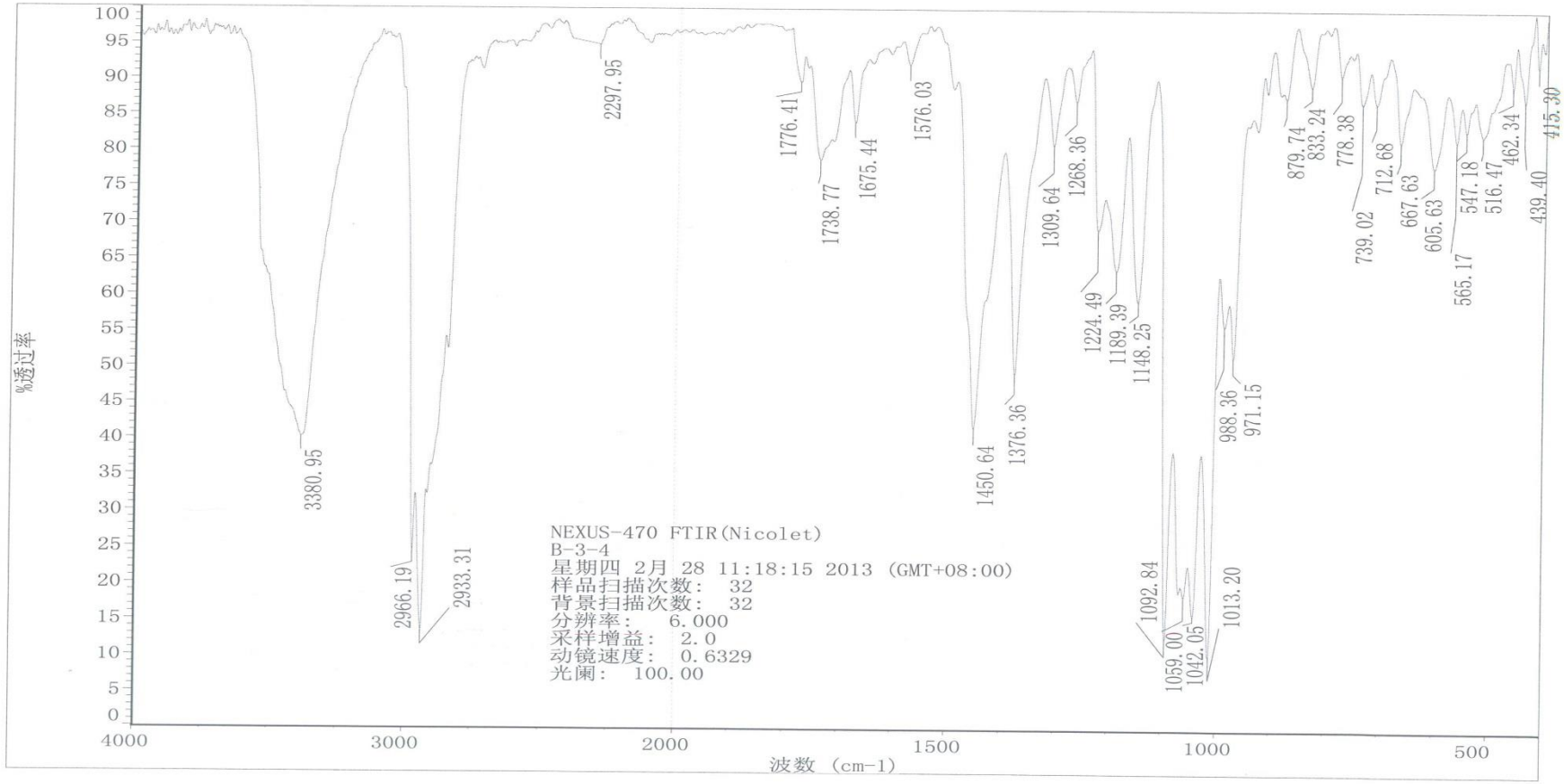

Figure S17 HRESIMS spectrum of **2**

Figure S18 UV spectrum and HPLC purity of **2**

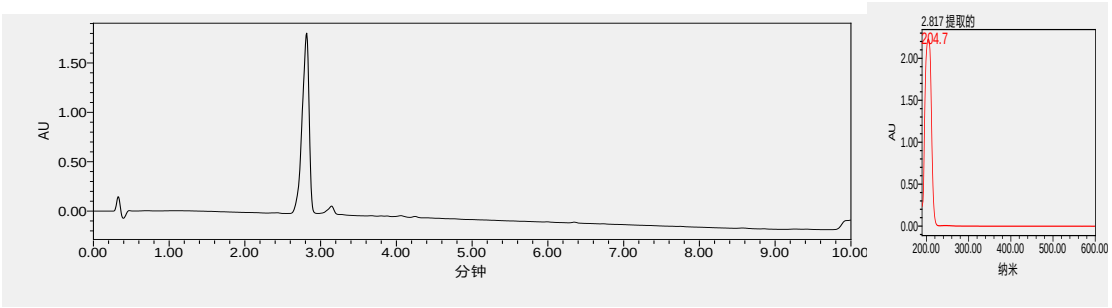

Figure S19 ^{1}H NMR spectrum of **3**

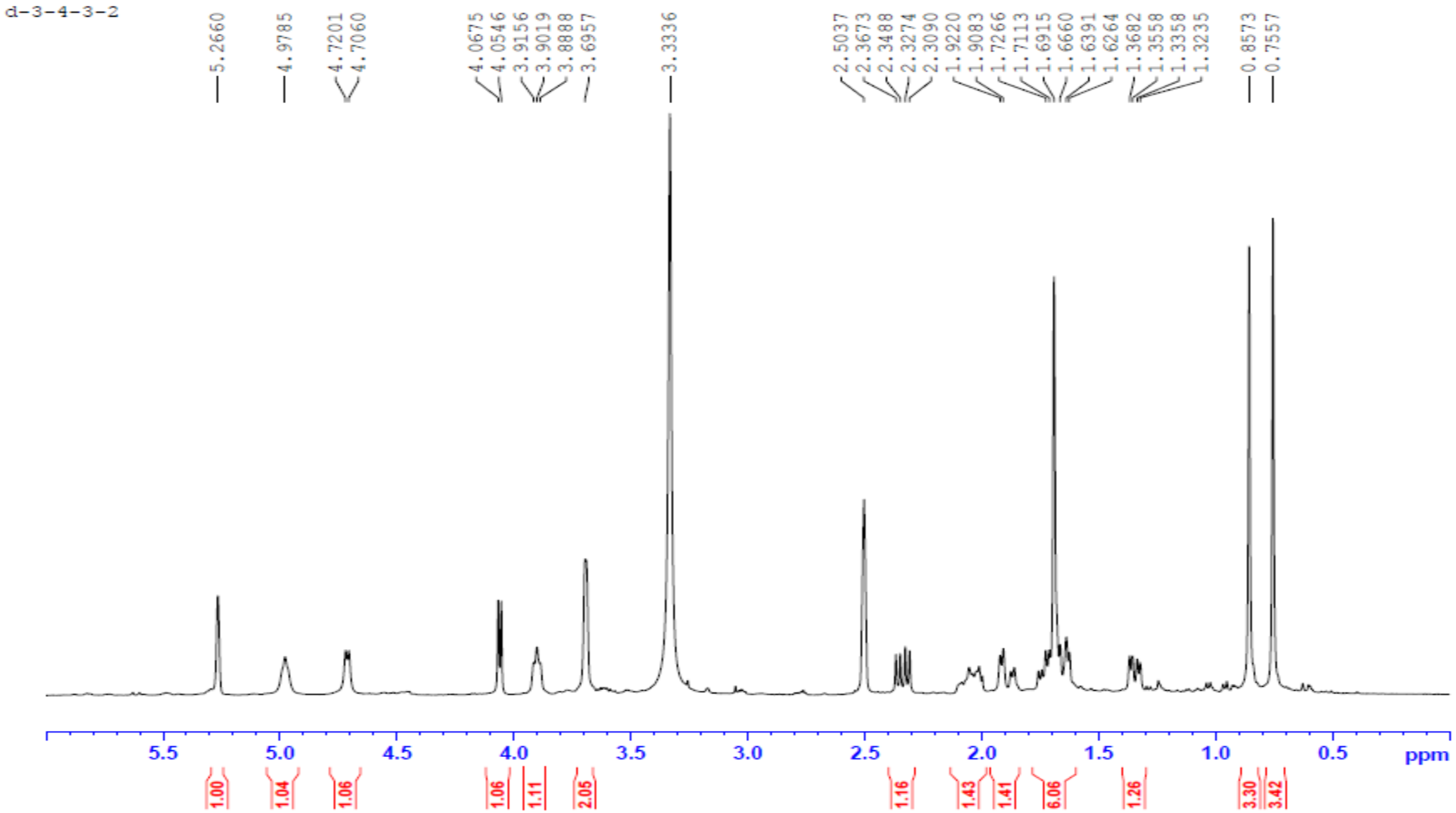

Figure S20 ^{13}C NMR spectrum of **3**

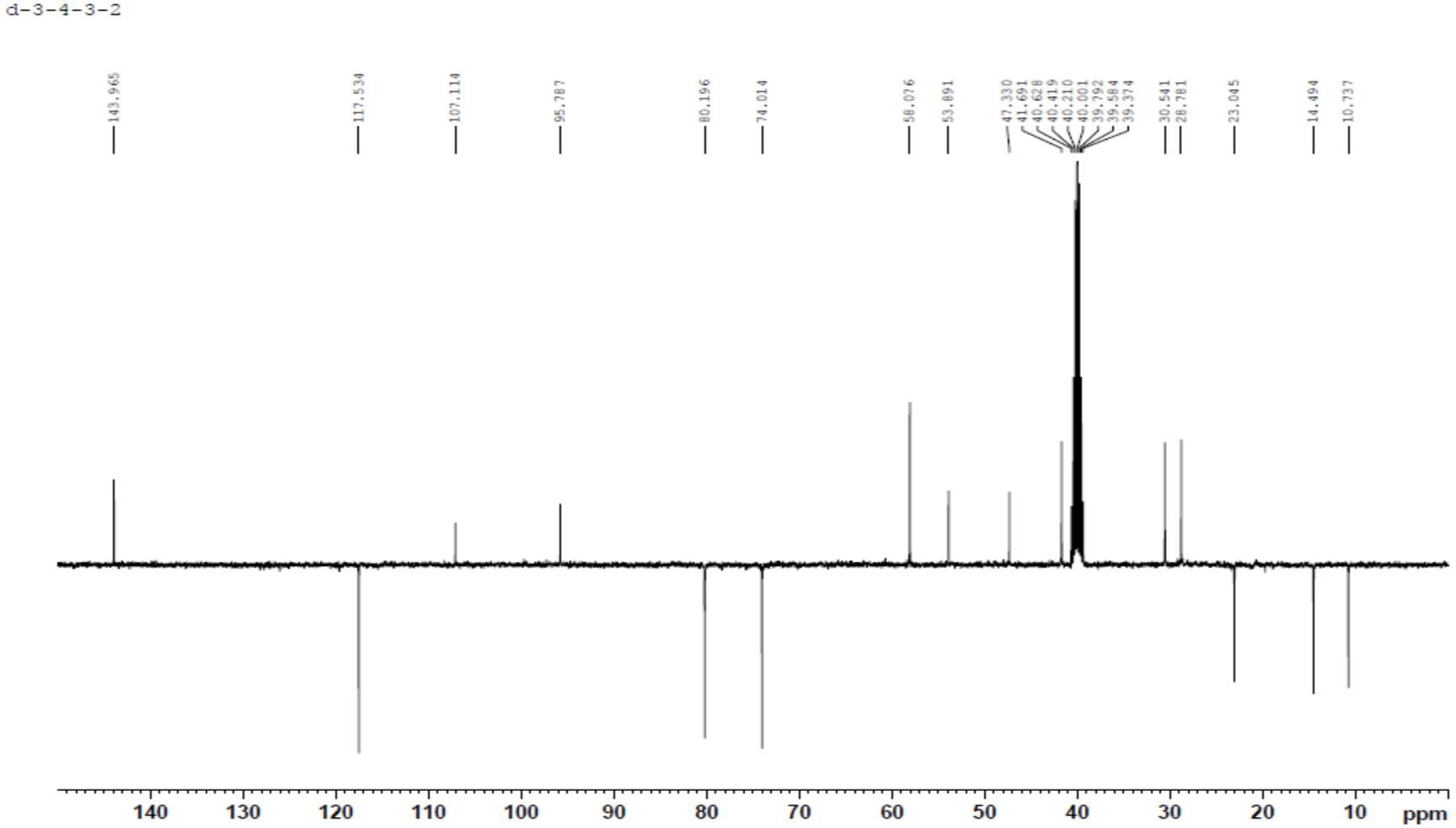

Figure S21 COSY spectrum of **3**

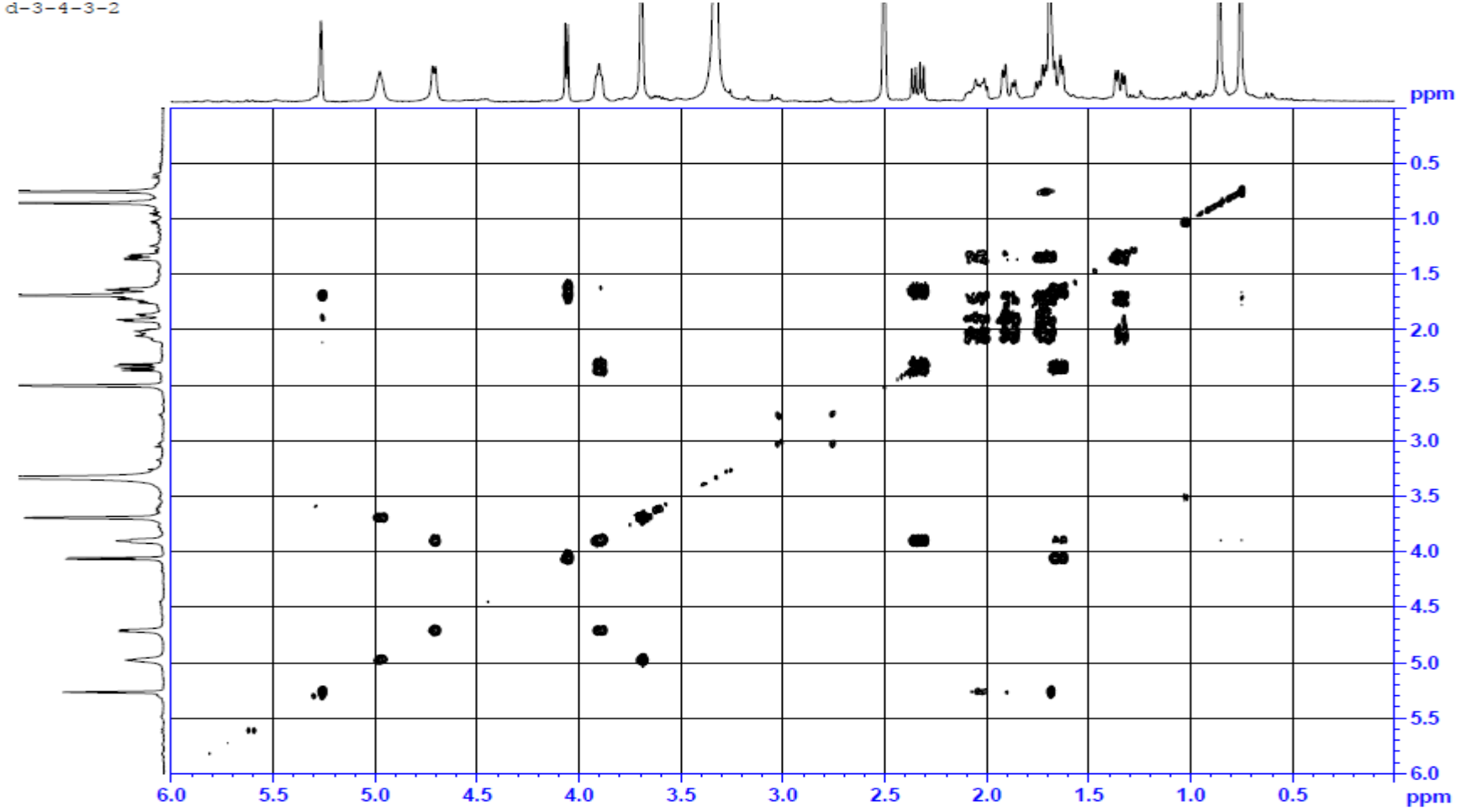

Figure S22 HMQC spectrum of **3**

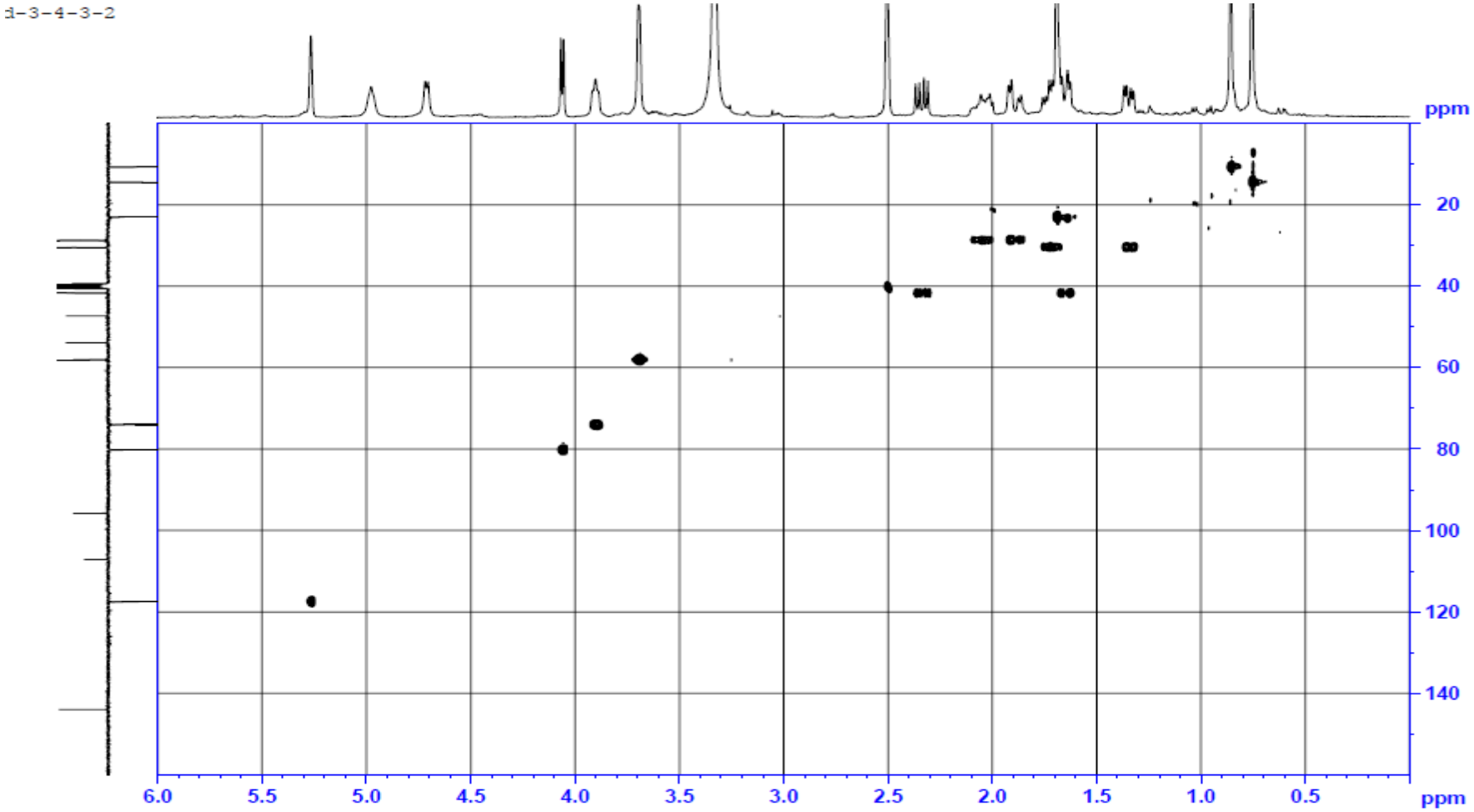

Figure S23 HMBC spectrum of **3**

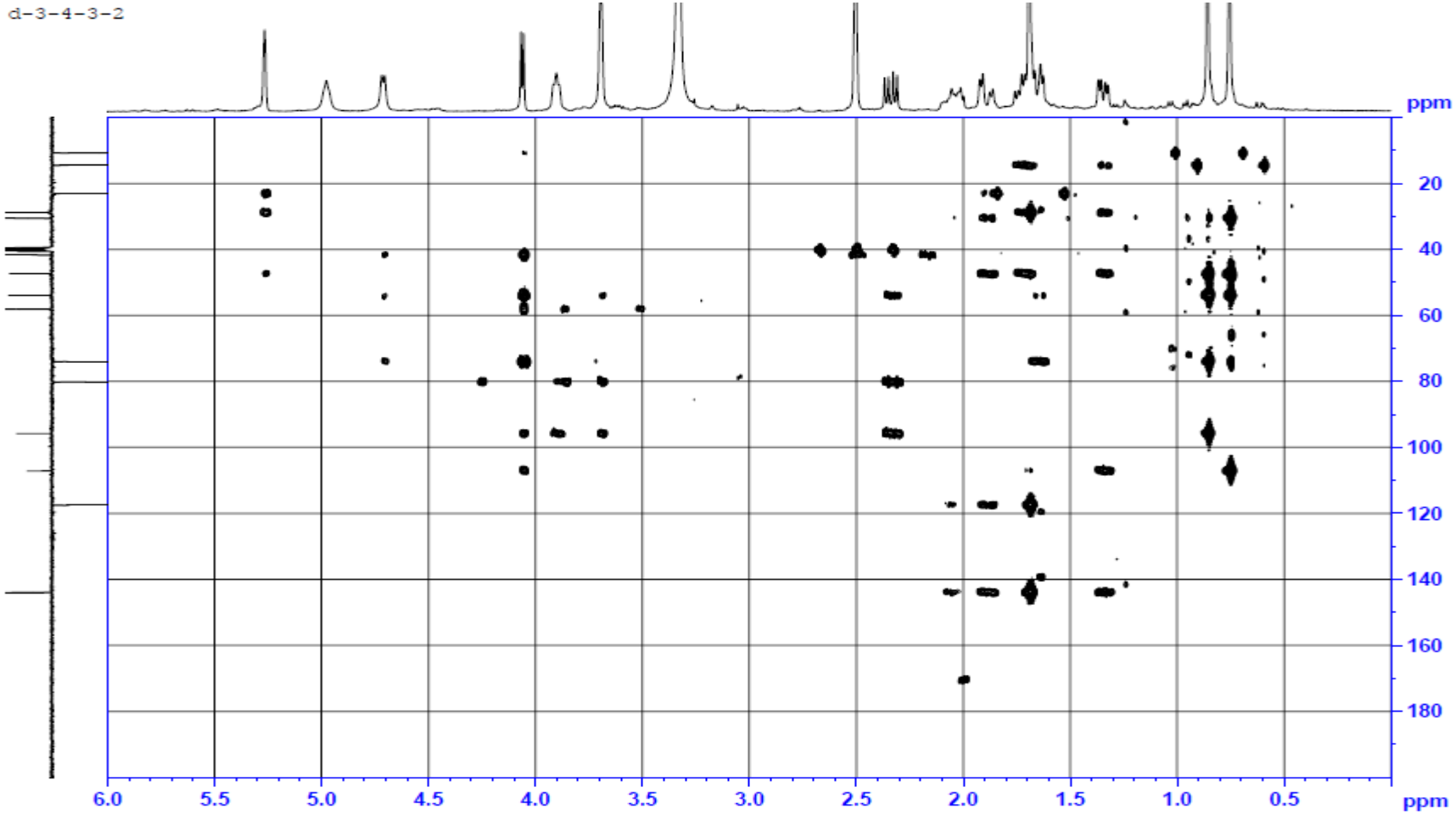

Figure S24 NOESY spectrum of **3**

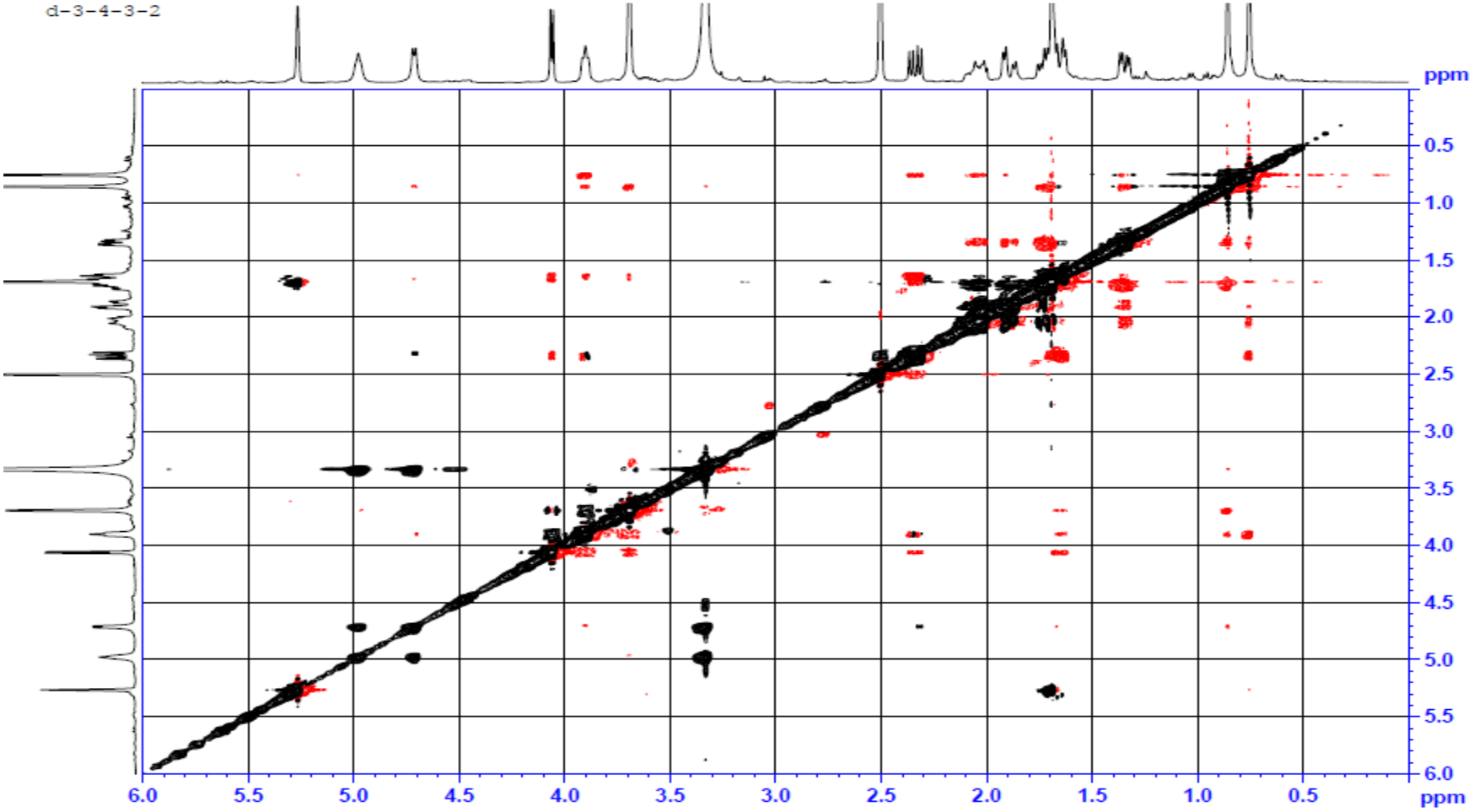

Figure S25 IR spectrum of **3**

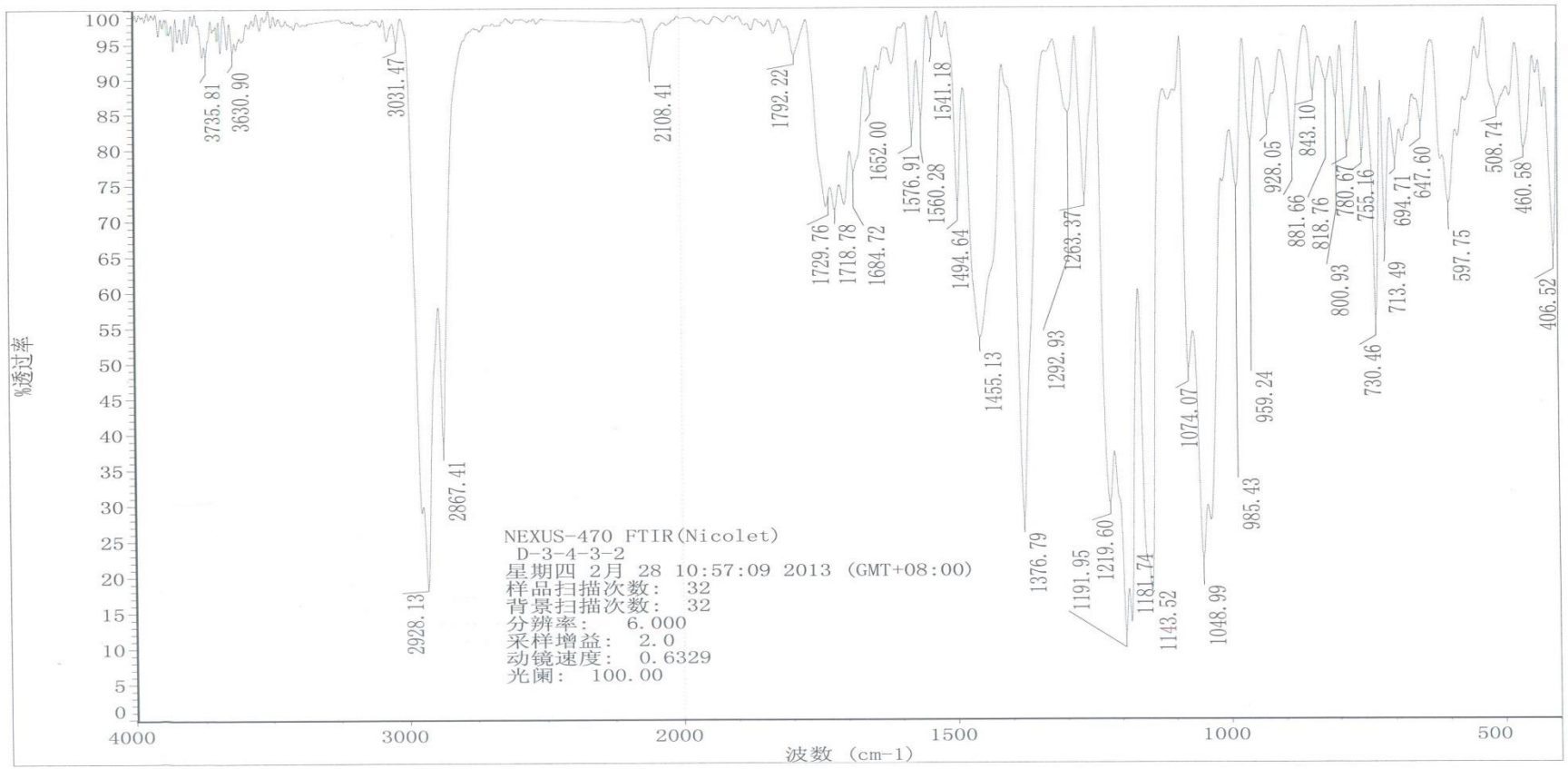

Figure S26 HRESIMS spectrum of **3**

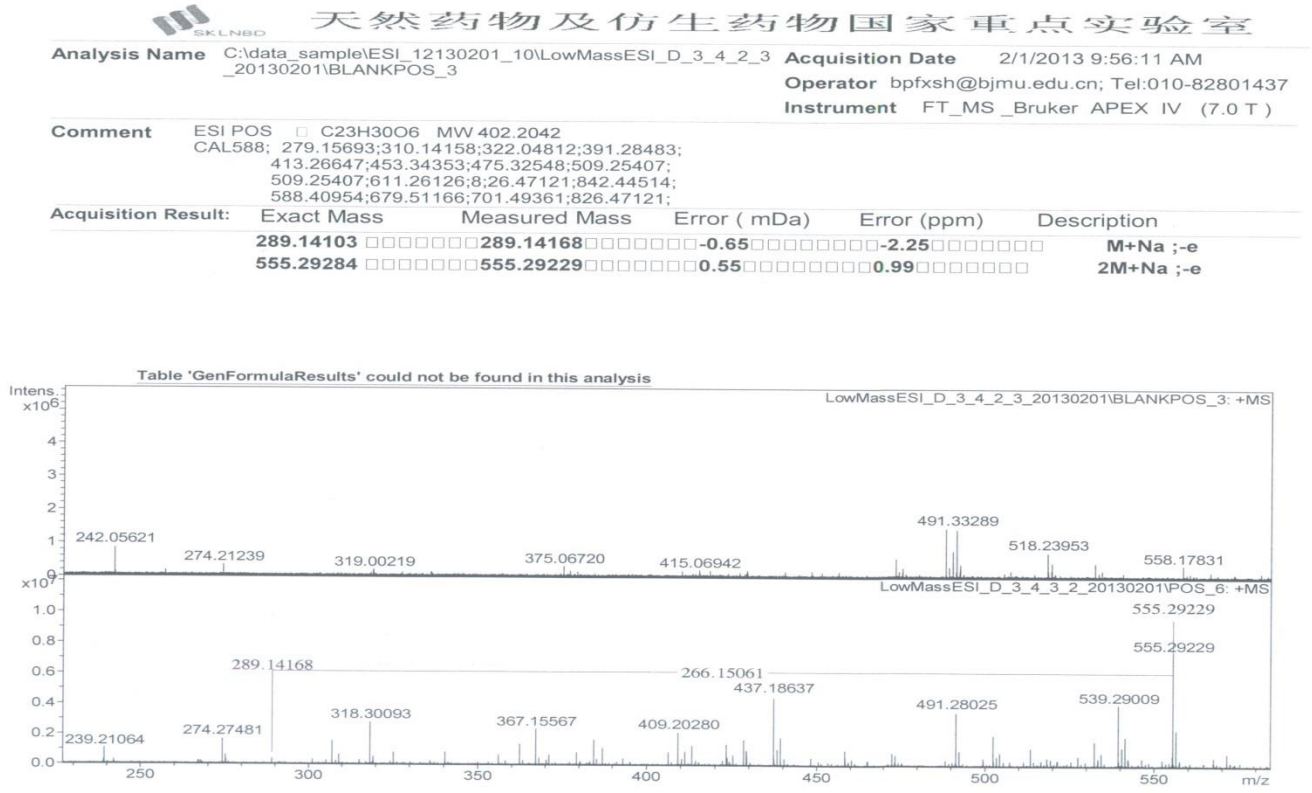

Figure S27 UV spectrum HPLC purity of **3**

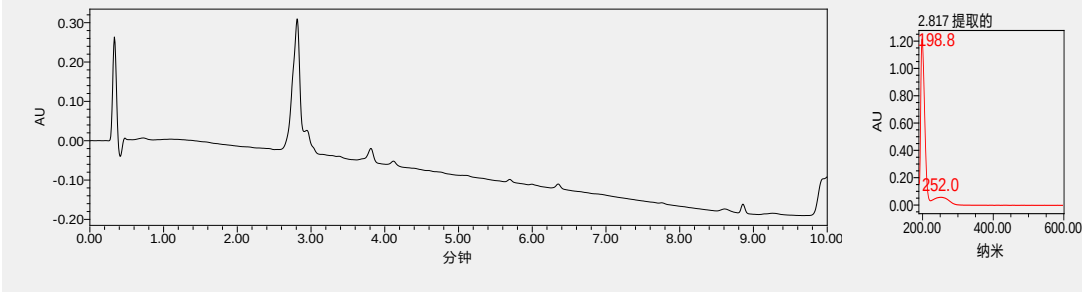

Figure S28 ^{1}H NMR spectrum of **4**

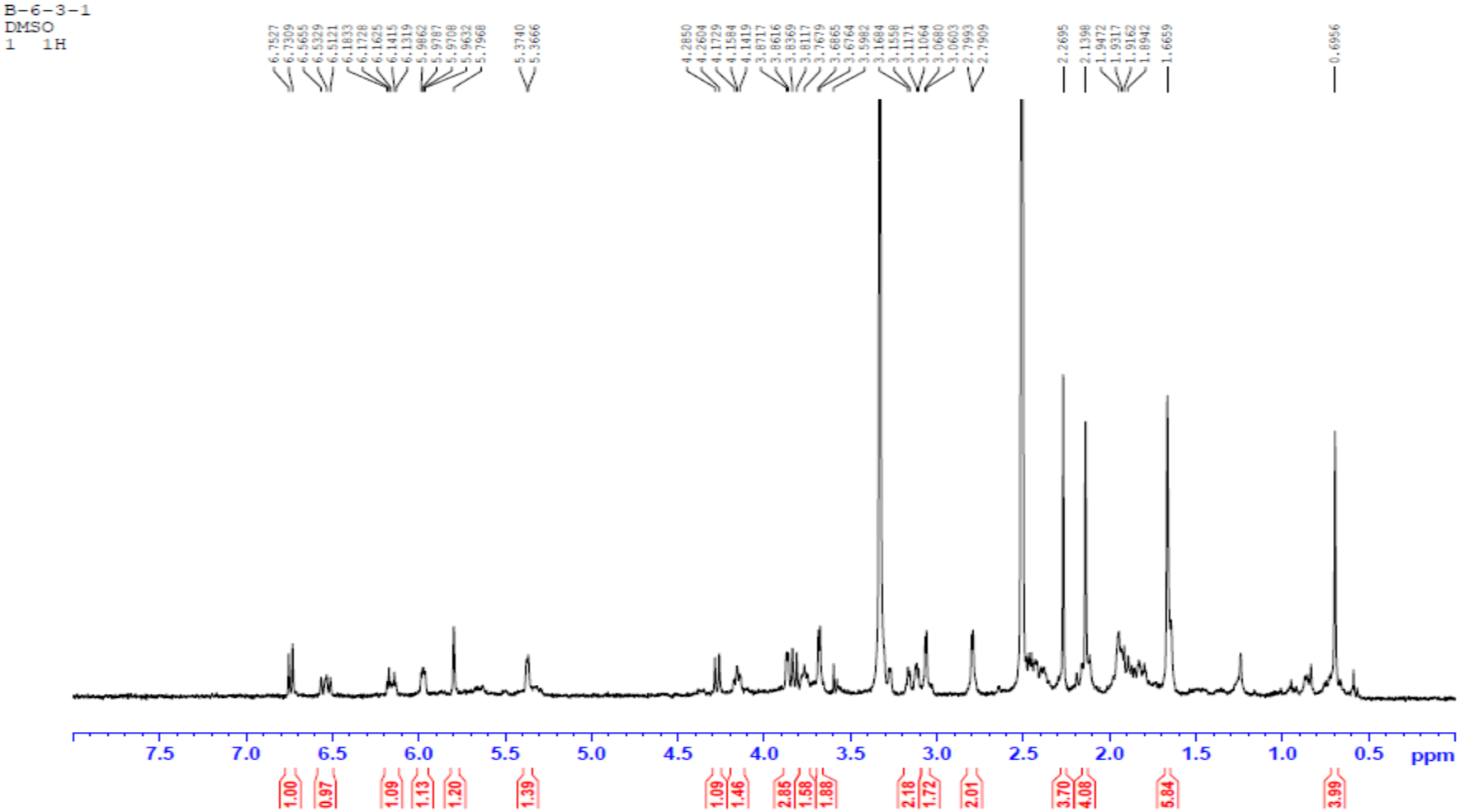

Figure S29 ^{13}C NMR spectrum of **4**

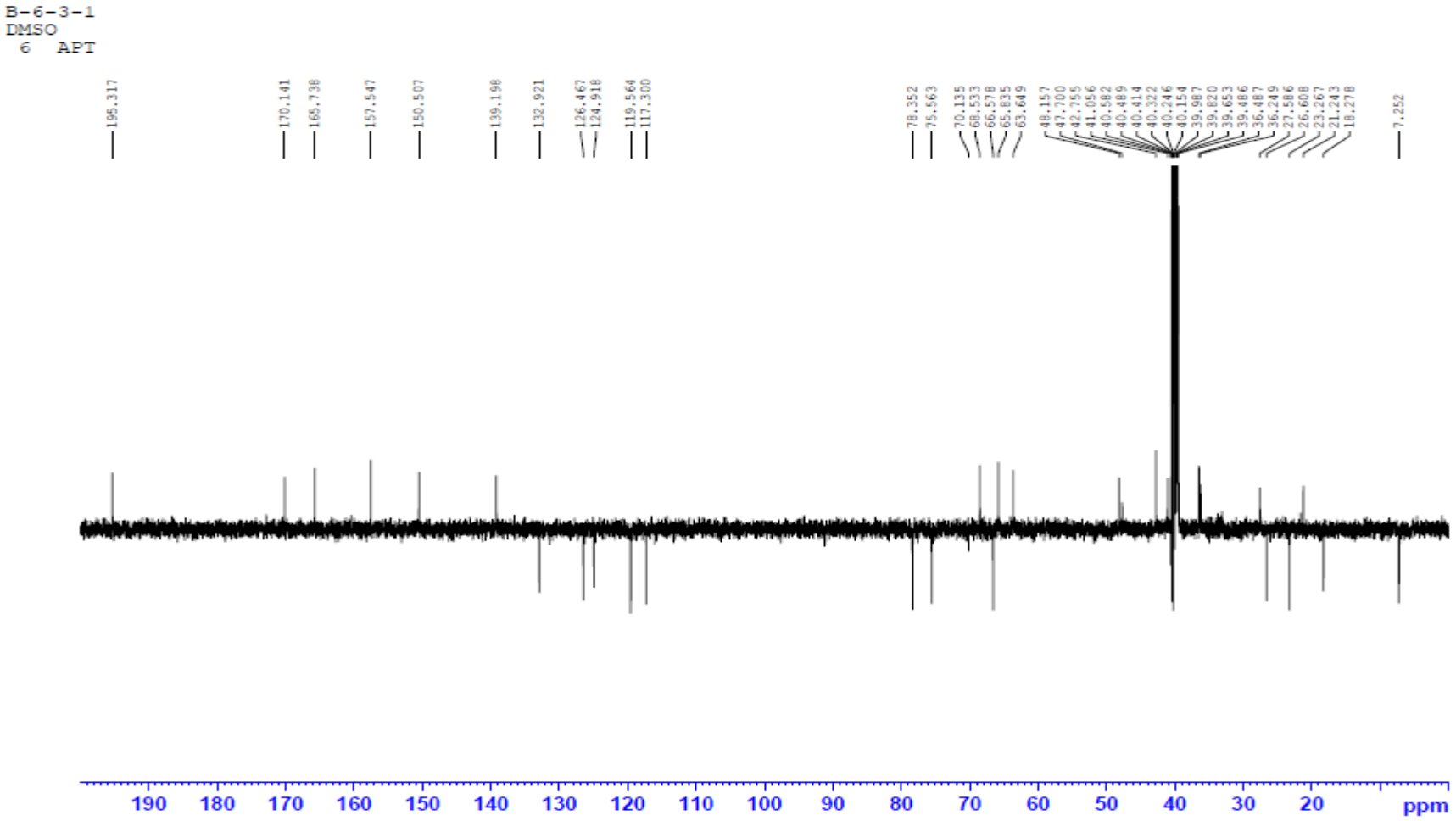

Figure S30 COSY spectrum of **4**

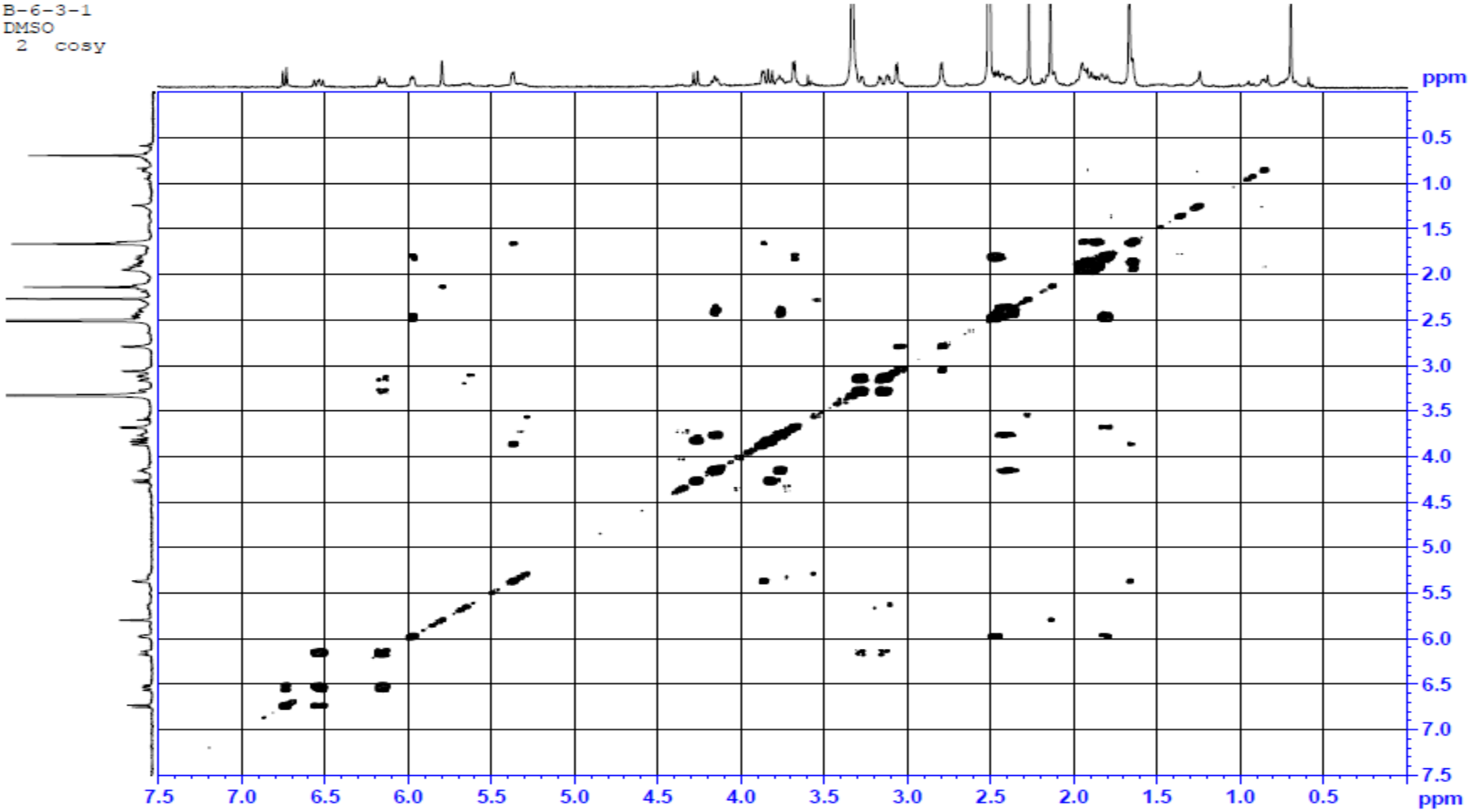

Figure S31 HMQC spectrum of **4**

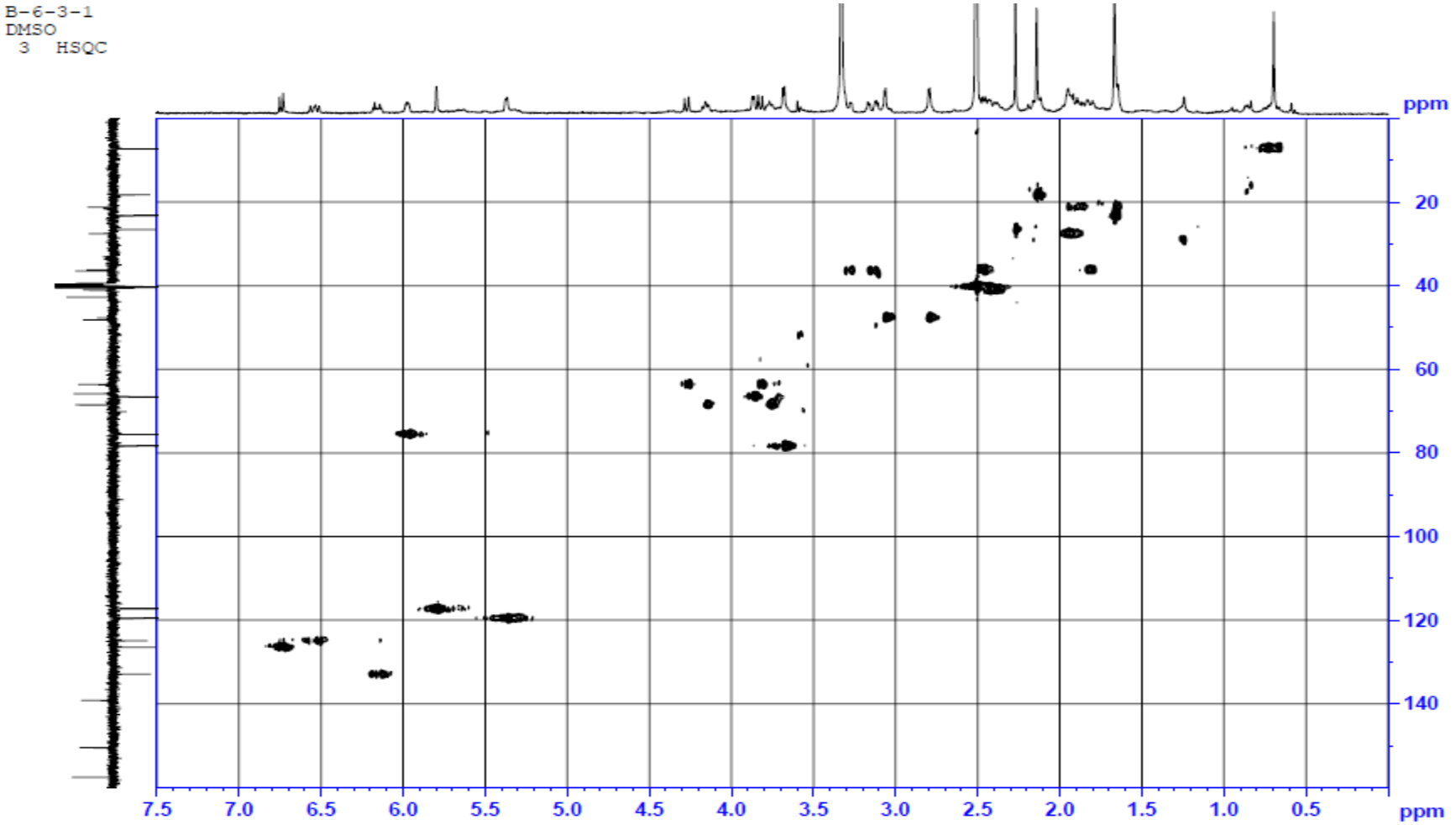

Figure S32 HMBC spectrum of **4**

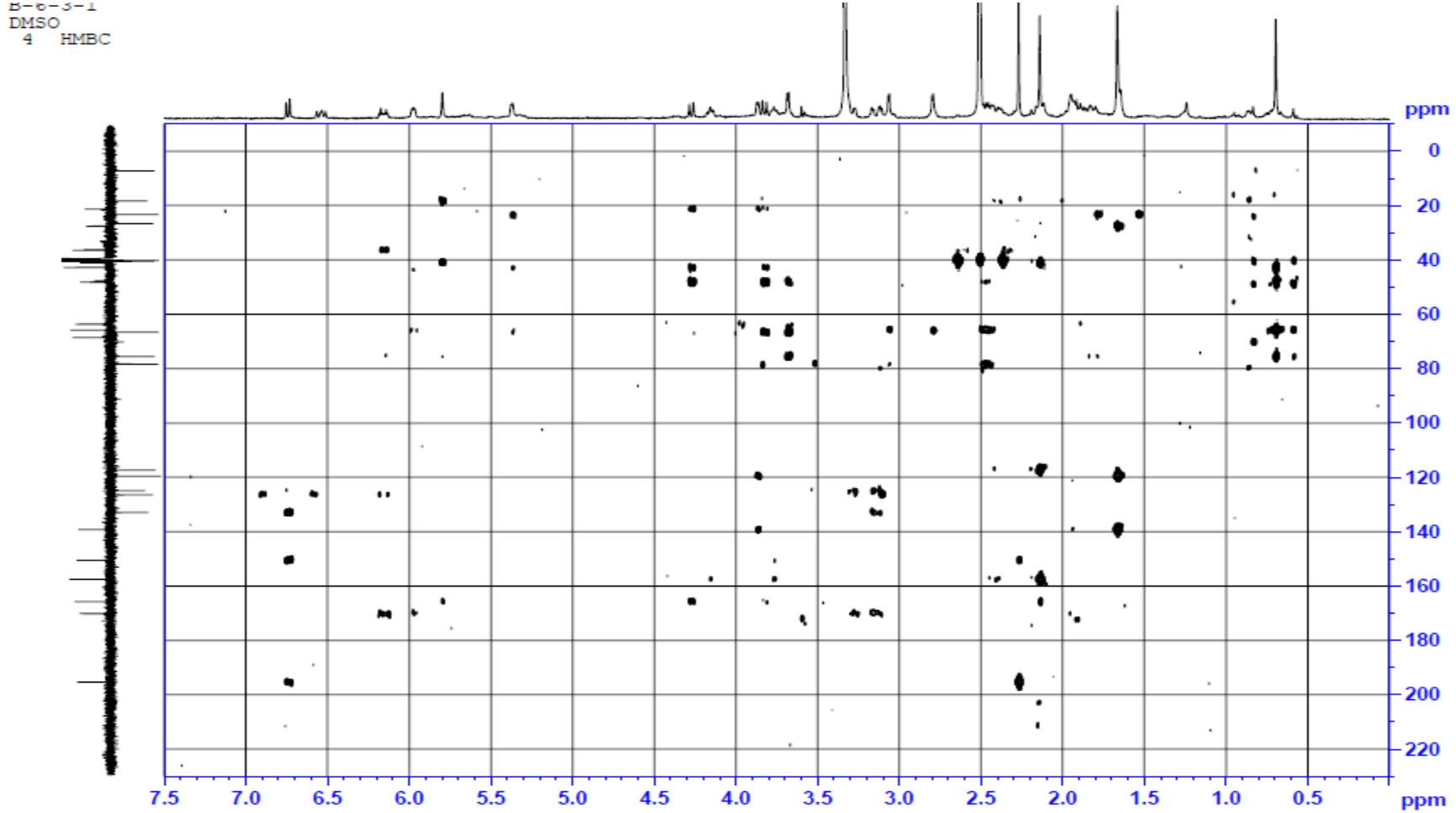

Figure S33 NOESY spectrum of **4**

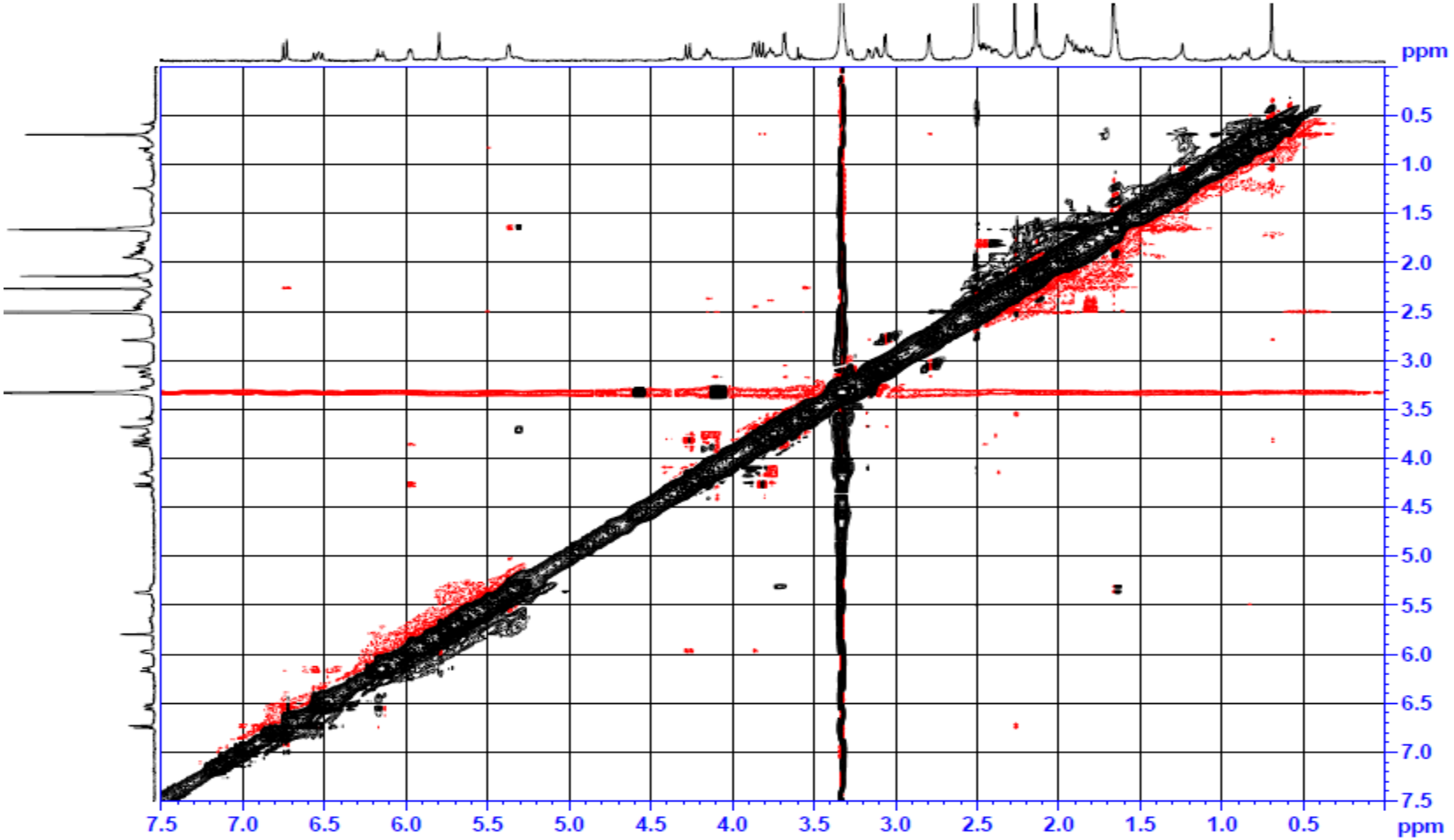

Figure S34 IR spectrum of **4**

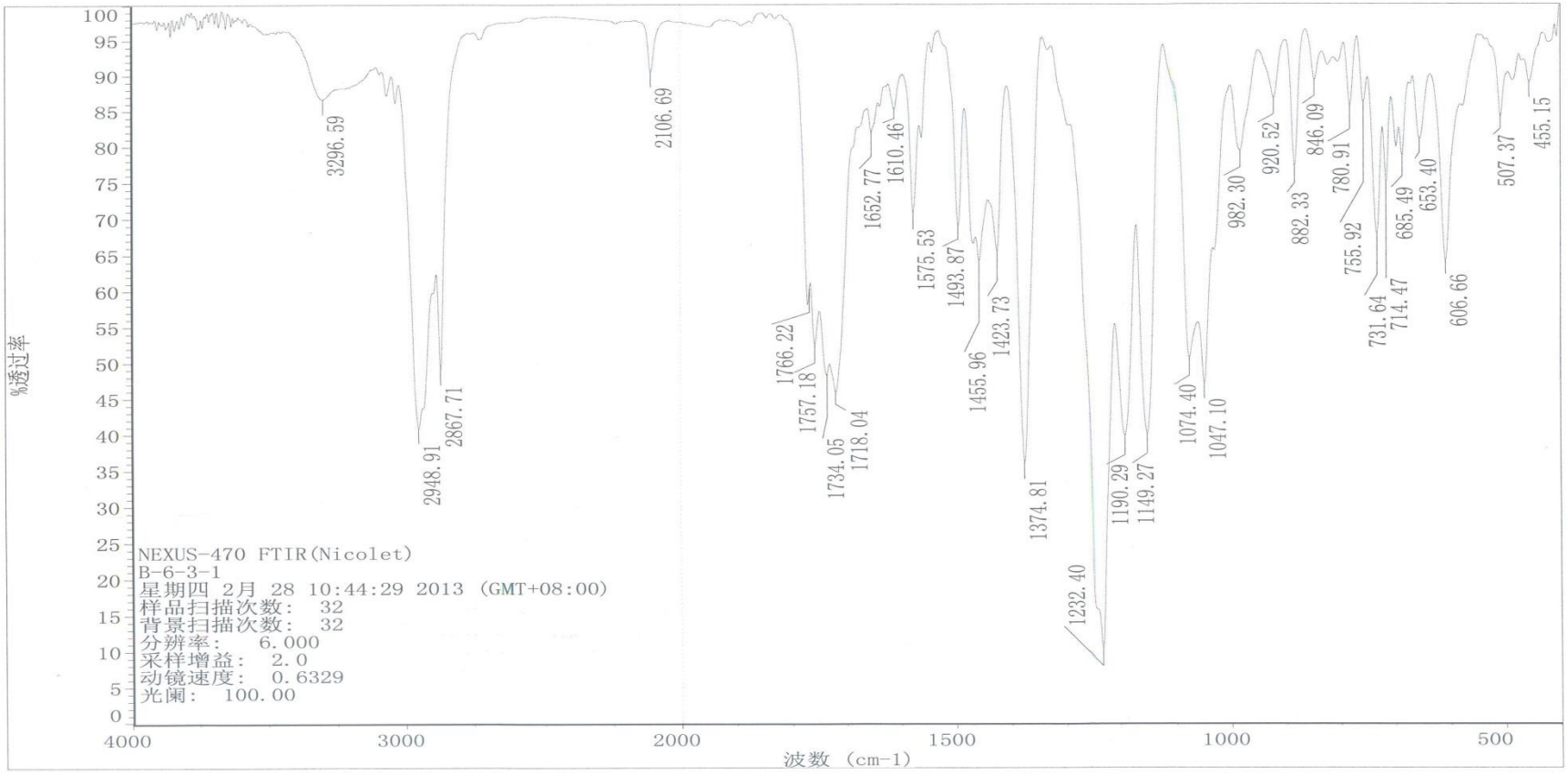

Figure S35 HRESIMS spectrum of **4**

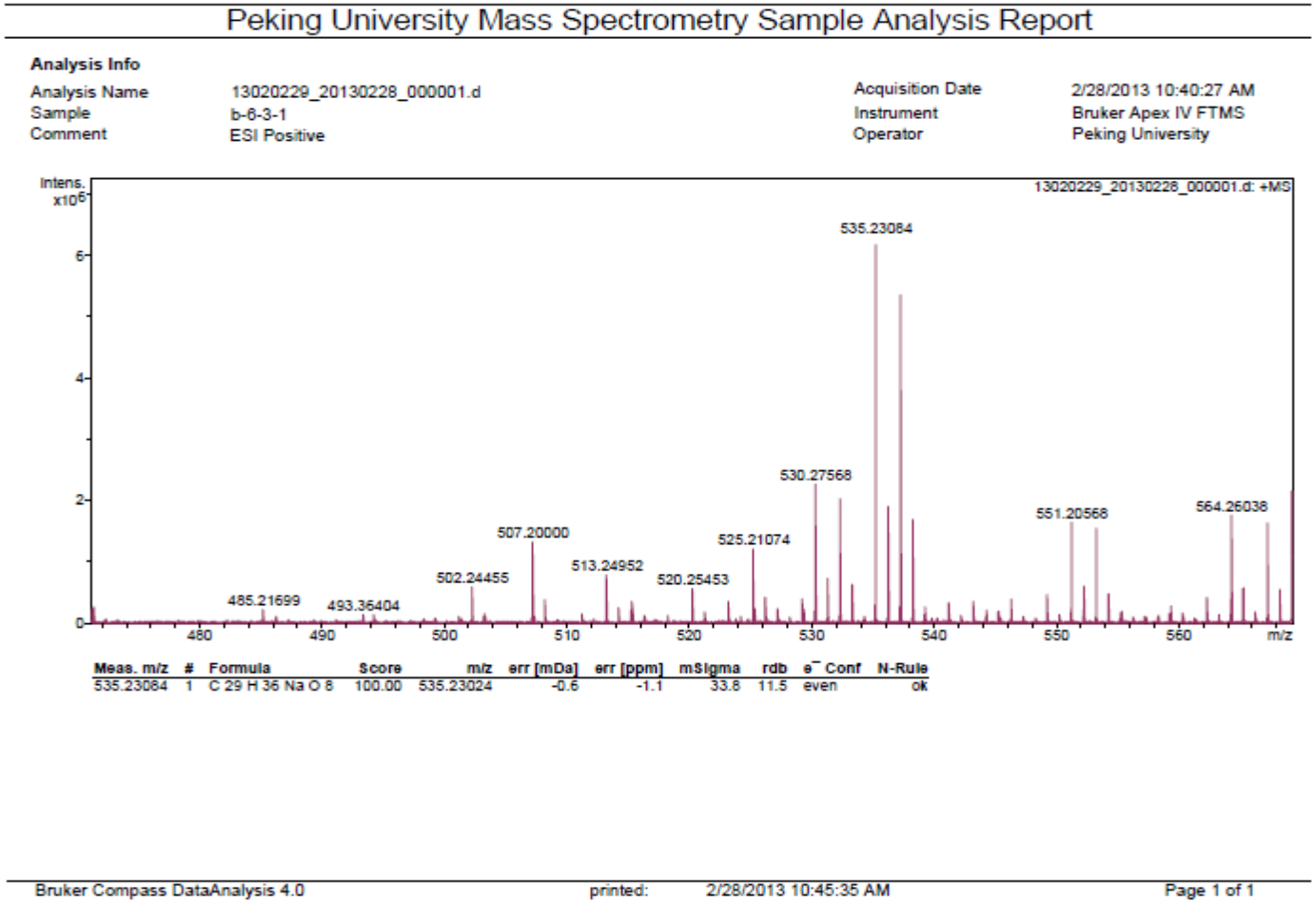

Figure S36 UV spectrum and HPLC purity of **4**