CHEMISTRY & BIODIVERSITY

Supporting Information

Antifungal Compounds from the Leaves of *Rhynchosia minima*

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Spectroscopic data of compounds

Ayanin (**1**): yellow solid, ^{1}H-NMR (400 MHz, $CDCl_3$): 12.63 (1H, s, OH-5), 7.72 (1H, dd, *J* = 8.6, 2.1 Hz, H-6'), 7.68 (1H, d, *J* = 2.1 Hz, H-2'), 6.96 (1H, d, *J* = 8.6 Hz, H-5'), 6.44 (1H, d, *J* = 2.2 Hz, H-8), 6.34 (1H, d, *J* = 2.2 Hz, H-6), 5.72 (1H, s, OH-3'), 3.98 (3H, s, OCH_3-4'), 3.87 (3H, s, OCH_3-7), 3.86 (3H, s, OCH_3-3). ^{13}C-NMR (100 MHz, $CDCl_3$): 178.9 (C-4, C), 165.5 (C-7, C), 162.0 (C-5, C), 156.8 (C-9, C), 155.7 (C-2, C), 148.8 (C-4', C), 145.6 (C-3', C), 139.2 (C-3, C), 123.7 (C-1', C), 121.7 (C-6', CH), 114.5 (C-2', CH), 110.4 (C-5', CH), 106.1 (C-10, C), 98.0 (C-6, CH), 92.2 (C-8, CH), 60.2 (OCH_3-3, CH_3), 56.1 (OCH_3-4', CH_3), 55.9 (OCH_3-7, CH_3). HR-MS: 345.0983 $[M + H]^+$ (calc for $C_{18}H_{17}O_7$, 345.0974).

Tectorigenin (**2**): colourless solid, ^{1}H-NMR (500 MHz, $CDCl_3$): 13.10 (1H, s, OH-5), 7.86 (1H, s, H-2), 7.40 (2H, d, *J* = 8.5 Hz, H-2', 6'), 6.91 (2H, d, *J* = 8.5 Hz, H-3', 5'), 6.52 (1H, s, H-8), 4.03 (3H, s, OCH_3-6). ^{13}C-NMR (125 MHz, $CDCl_3$): 181.4 (C-4, C), 155.9 (C-4', C), 155.2 (C-7, C), 153.6 (C-9, C), 153.0 (C-5, C), 152.7 (C-2, CH), 130.5 (C-6, C), 130.5 (C-2', 6', CH), 123.3 (C-3, C), 123.1 (C-1', C), 115.7 (C-3', 5', CH), 106.6 (C-10, C), 93.3 (C-8, CH), 61.0 (OCH_3-6, CH_3). HR-MS: 301.0713 $[M + H]^+$ (calc for $C_{16}H_{13}O_6$, 301.0712).

Loliolide (**3**): white amorphous powder, ^{1}H-NMR (400 MHz, $CDCl_3$): 5.68 (1H, s, H-3), 4.32 (1H, quint, *J* = 3.3 Hz, H-6), 2.45 (1H, dt, *J* = 14.0, 2.6 Hz, H-7a), 1.97 (1H, dt, *J* = 14.4, 2.6 Hz, H-5a), 1.77 (1H, dd, *J* = 14.0, 3.9 Hz, H-7b), 1.52 (1H, dd, *J* = 14.4, 3.9 Hz, H-5b), 1.77 (3H, s, H-12), 1.46 (3H, s, H-10), 1.26 (3H, s, H-11). ^{13}C-NMR (75 MHz, $CDCl_3$): 182.7 (C-9, C), 172.1 (C-2, C), 112.9 (C-3, CH), 86.9 (C-8, C), 66.8 (C-6, CH), 47.3 (C-5, CH_2), 45.7 (C-7, CH_2), 36.0 (C-4, C), 30.7 (C-4, CH_3), 27.1 (C-12, CH_3), 26.5 (C-11, CH_3). HR-MS: 197.1182 $[M + H]^+$ (calc for $C_{11}H_{17}O_3$, 197.1178).

Isovitexin (**4**): yellow solid, ^{1}H-NMR (400 MHz, CD_3OD): 7.82 (2H, d, *J* = 8.4 Hz, H-2', 6'), 6.91 (2H, d, *J* = 8.4 Hz, H-3', 5'), 6.58 (1H, s, H-3), 6.49 (1H, s, H-8), 4.91 (1H, overlapped

with water signal, H-1''), 4.17 (1H, t, H-2''), 3.86 – 3.89 (1H, m, *J* = 12.2, 1.9 Hz, H-6''b), 3.74 (1H, dd, *J* = 12.2, 5.1 Hz, H-6''a), 3.45 – 3.49 (2H, m, H-3'', 4''), 3.42 – 3.44 (1H, m, H-5''). ^{13}C-NMR (125 MHz, CD_3OD): 184.0 (C-4, C), 166.1 (C-2, C), 165.0 (C-7, C), 162.8 (C-4', C), 162.0 (C-5, C), 158.7 (C-9, C), 129.4 (C-2', 6', CH), 123.0 (C-1', C), 117.0 (C-3', 5', CH), 109.2 (C-6, CH), 105.1 (C-10, C), 103.8 (C-3, CH), 95.2 (C-8, CH), 82.6 (C-5'', CH), 80.1 (C-3'', CH), 75.2 (C-1'', CH), 72.5 (C-2'', CH), 71.7 (C-4'', CH), 62.8 (C-6'', CH_2). HR-MS: 433.1134 $[M + H]^+$ (calc for $C_{21}H_{21}O_{10}$, 433.1135).

Pinitol (**5**): white powder, ^{1}H-NMR (400 MHz, $(CD_3)_2SO$): 3.60 – 3.64 (2H, m, H-1, 6), 3.47 (3H, s, OCH_3-3), 3.30 – 3.52 (3H, m, H-2, 4, 5), 2.99 (1H, t, *J* = 9.3 Hz, H-3), 4.34 (1H, d, *J* = 5.6 Hz, OH), 4.48 (1H, d, *J* = 6.4 Hz, OH), 4.53 (1H, d, *J* = 4.6 Hz, OH), 4.65 (1H, brs, OH), 4.73 (1H, brs, OH). ^{13}C-NMR (100 MHz, $(CD_3)_2SO$): 83.8 (C-3, CH), 72.6 (C-4, CH), 72.5 (C-1, CH), 72.0 (C-6, CH), 70.9 (C-2, CH), 70.1 (C-5, CH), 59.7 (OCH_3-3, CH_3). HR-MS: 217.0678 $[M + Na]^+$ (calc for $C_7H_{14}O_6Na$, 217.0688).

Vitexin (**6**): yellow amorphous solid, ^{1}H-NMR (400 MHz, $(CD_3)_2SO$): 13.16 (1H, s, OH-5), 8.02 (2H, d, *J* = 8.4 Hz, H-2', 6'), 6.89 (2H, d, *J* = 8.4 Hz, H-3', 5'), 6.77 (1H, s, H-3), 6.26 (1H, s, H-6), 4.68 (1H, d, *J* = 9.8 Hz, H-1''), 3.83 (1H, t, *J* = 9.4 Hz, H-2''), 3.76 (1H, dd, *J* = 12.3, 4.9 Hz, H-6''b), 3.49 – 3.54 (1H, m, H-6''a), 3.37 – 3.40 (1H, m, H-4''), 3.20 – 3.29 (2H, m, H-3'', 5''). ^{13}C-NMR (125 MHz, $(CD_3)_2SO$): 182.0 (C-4, C), 163.9 (C-2, C), 162.6 (C-7, C), 161.1 (C-4', C), 160.3 (C-5, C), 156.0 (C-9, C), 128.9 (C-2', 6', CH), 121.6 (C-1', C), 115.8 (C-3', 5', CH), 104.6 (C-8, C), 104.0 (C-10, C), 102.4 (C-3, CH), 98.1 (C-6, CH), 81.8 (C-5'', CH), 78.6 (C-3'', CH), 73.3 (C-1'', CH), 70.8 (C-2'', CH), 70.5 (C-4'', CH), 61.2 (C-6'', CH_2). HR-MS: 433.1137 $[M + H]^+$ (calc for $C_{21}H_{21}O_{10}$, 433.1135).

Quercetin (**7**): yellow amorphous powder, ^{1}H-NMR (400 MHz, CD_3OD): 7.73 (1H, d, *J* = 2.0 Hz, H-2'), 7.63 (1H, dd, *J* = 8.5, 2.0 Hz, H-6'), 6.88 (1H, d, *J* = 8.5 Hz, H-5'), 6.38 (1H, d, *J* =

1.9 Hz, H-8), 6.18 (1H, d, *J* = 1.9 Hz, H-6). ^{13}C-NMR (125 MHz, CD_3OD): 177.3 (C-4, C), 165.6 (C-7, C), 162.5 (C-5, C), 158.2 (C-9, C), 148.7 (C-4', C), 148.0 (C-2, C), 146.2 (C-3', C), 137.2 (C-3, C), 124.1 (C-1', C), 121.6 (C-6', CH), 116.2 (C-5', CH), 115.9 (C-2', CH), 104.5 (C-10, C), 99.2 (C-6, CH), 94.4 (C-8, CH). HR-MS: 303.0510 $[M + H]^+$ (calc for $C_{15}H_{11}O_7$, 303.0505).

Isoorientin (**8**): light yellow solid, ^{1}H-NMR (500 MHz, CD_3OD): 7.39 (1H, dd, *J* = 8.1, 2.0 Hz, H-6'), 7.37 (1H, s, H-2'), 6.90 (1H, d, *J* = 8.1 Hz, H-5'), 6.55 (1H, s, H-3), 6.49 (1H, s, H-8), 4.89 (1H, overlapped with water signal, H-1"), 4.17 (1H, t, *J* = 9.1 Hz, H-2"), 3.87 (1H, dd, *J* = 12.2, 2.0 Hz, H-6"b), 3.73 (1H, dd, *J* = 11.9, 5.3 Hz, H-6"a), 3.44 – 3.48 (3H, m, H-3", 4", 5"). ^{13}C-NMR (125 MHz, CD_3OD): 183.9 (C-4, C), 166.2 (C-2, C), 162.0 (C-5, C), 161.3 (C-7, C), 158.8 (C-9, C), 151.2 (C-4', C), 147.1 (C-3', C), 123.4 (C-1', C), 120.3 (C-6', CH), 116.8 (C-5', CH), 114.0 (C-2', CH), 109.3 (C-6, C), 105.7 (C-10, C), 103.8 (C-3, CH), 95.3 (C-8, CH), 82.6 (C-5", CH), 80.1 (C-3", CH), 75.3 (C-1", CH), 72.5 (C-2", CH), 71.7 (C-4", CH), 62.8 (C-6", CH_2). HR-MS: 449.1089 $[M + H]^+$ (calc for $C_{21}H_{21}O_{11}$, 449.1084).

Figure 1: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **1**.

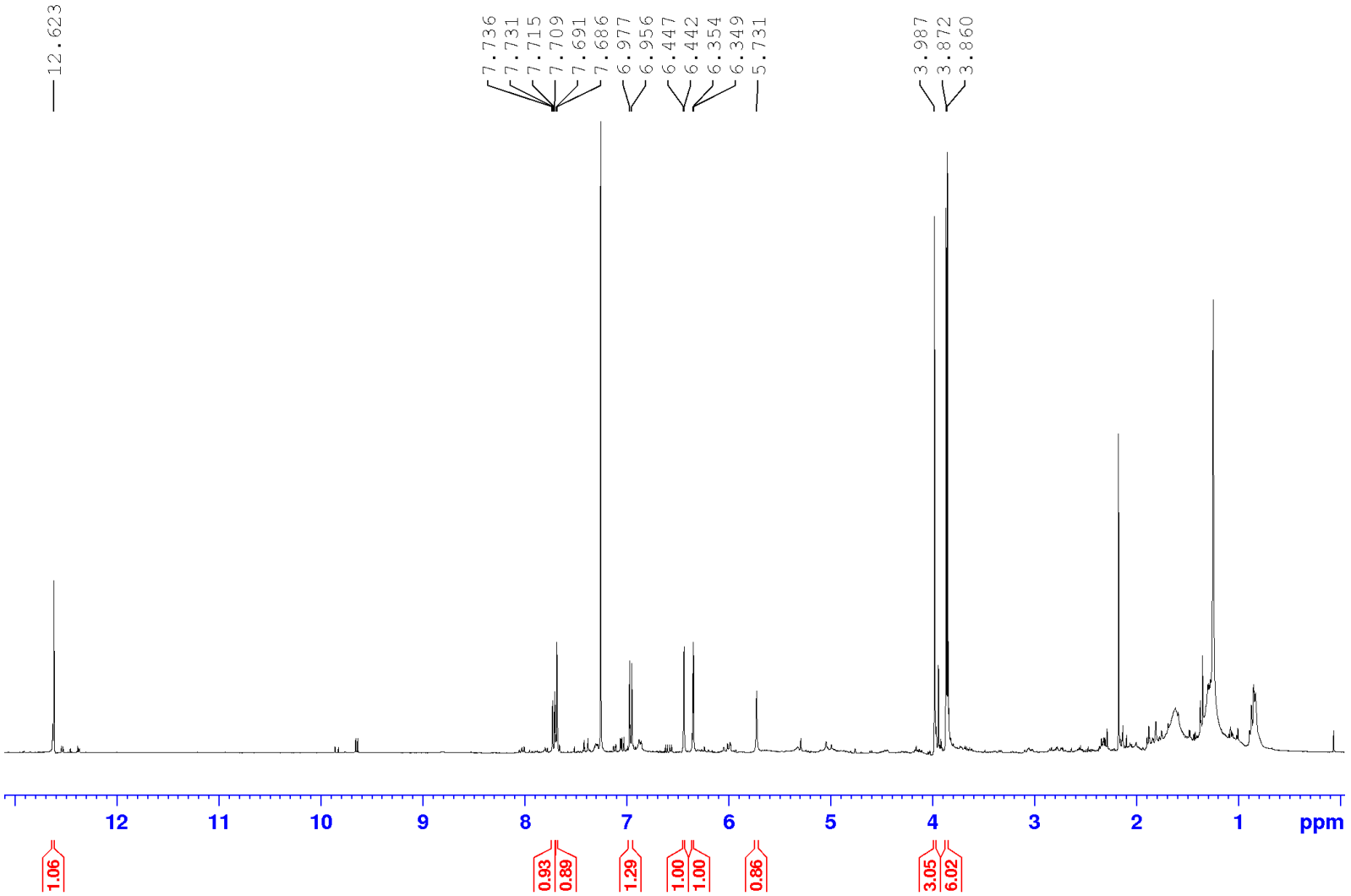

Figure 2: ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **1**.

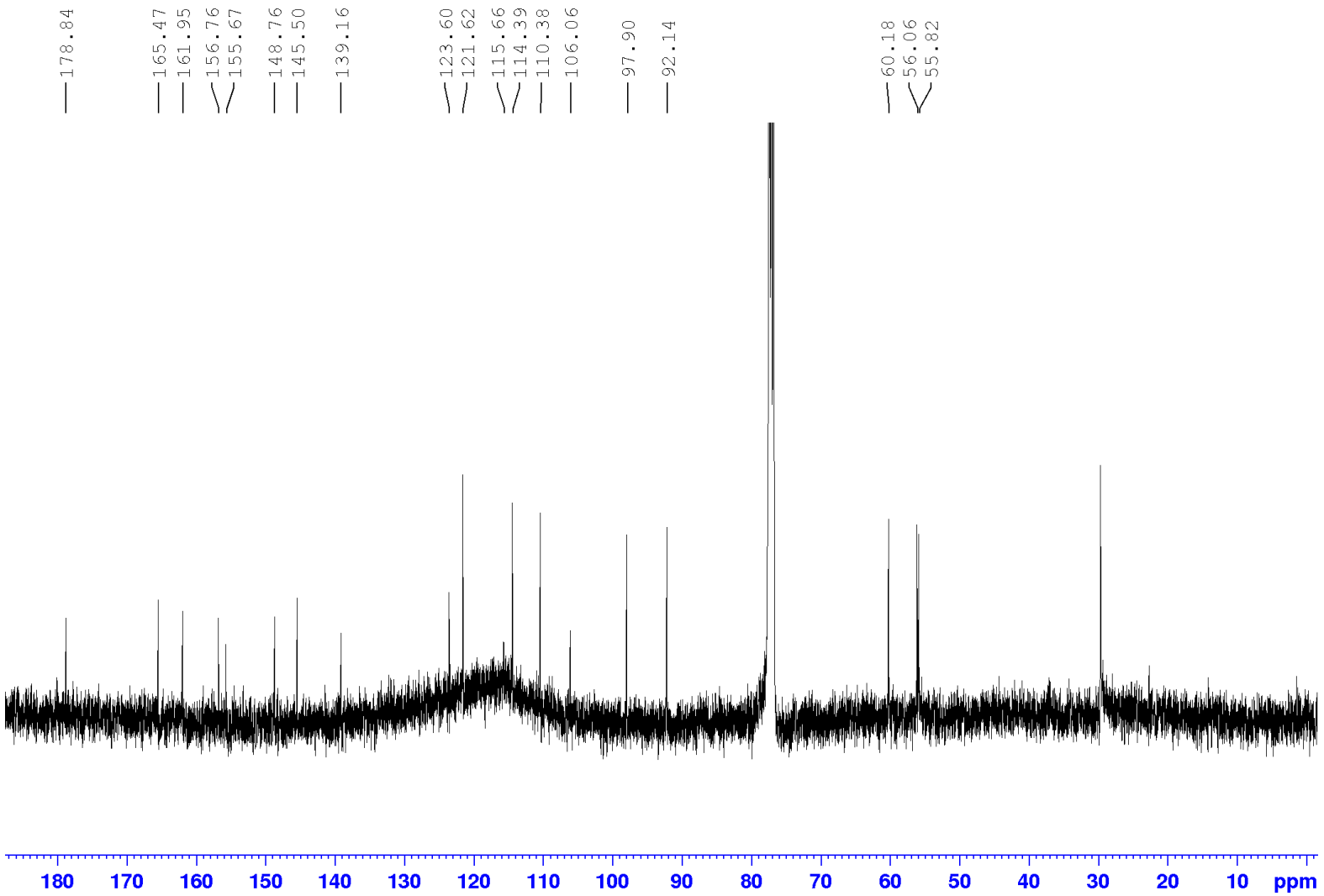

Figure 3: HRESIMS spectrum of compound **1**.

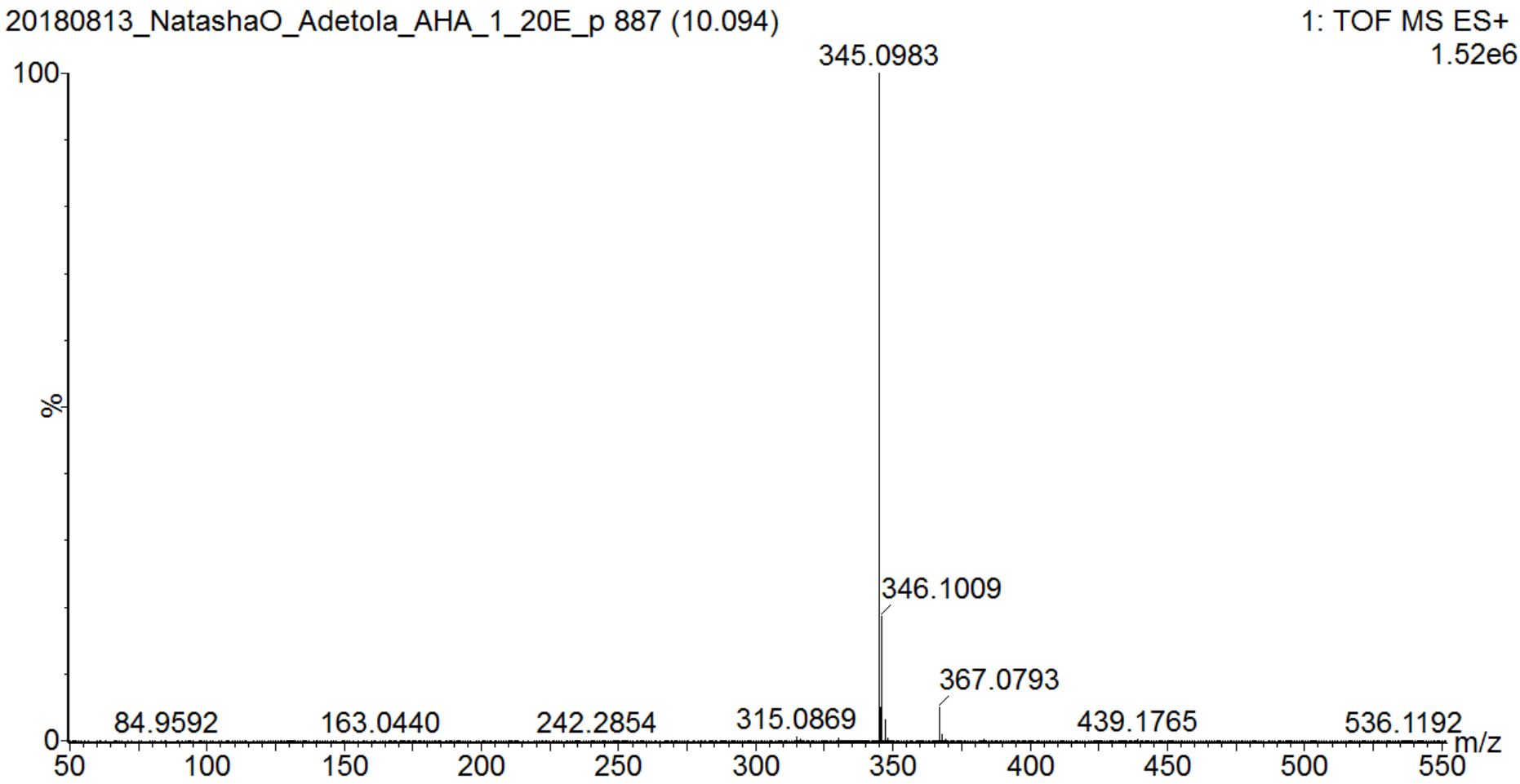

Figure 4: ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **2**.

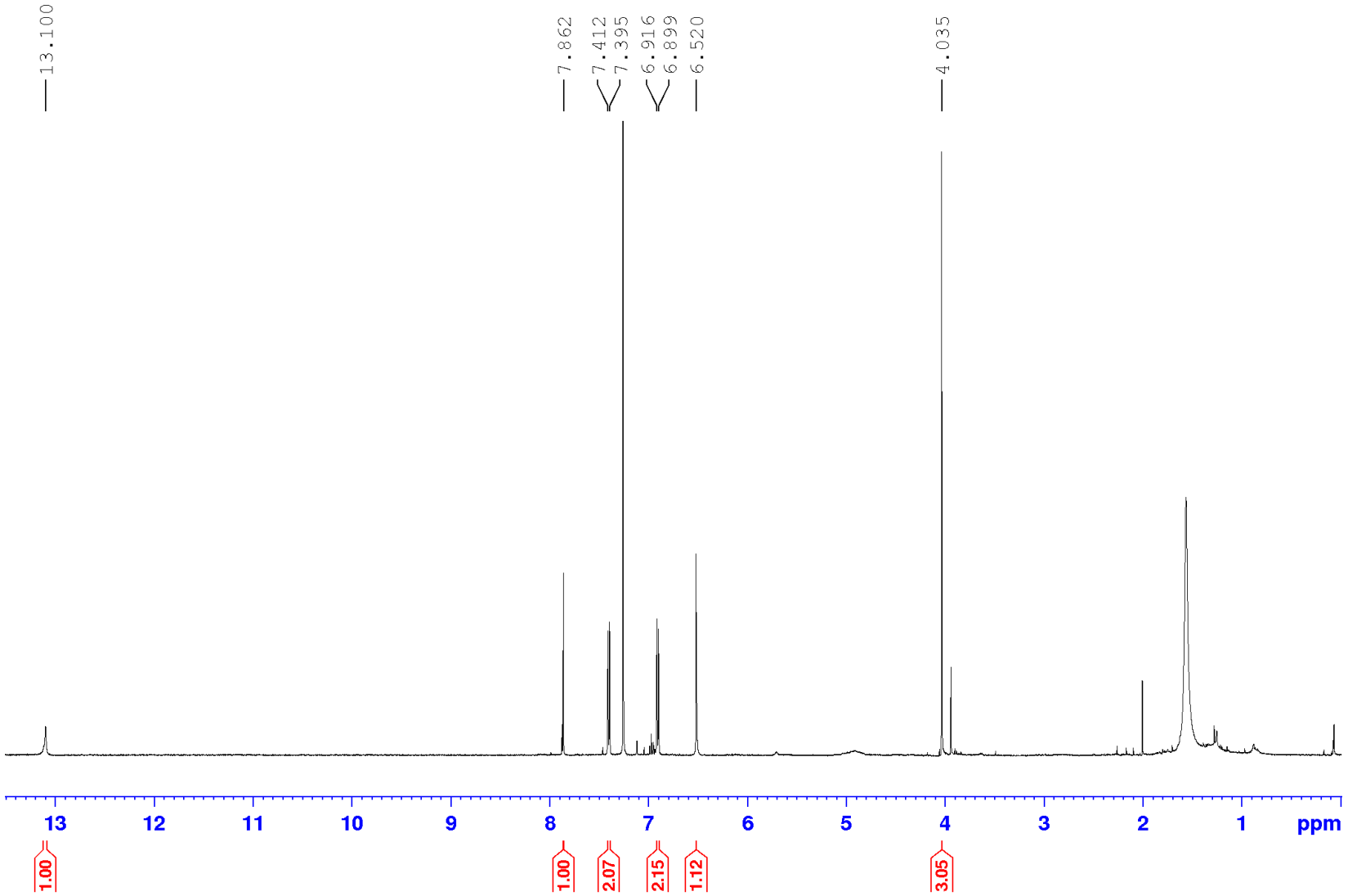

Figure 5: ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **2**.

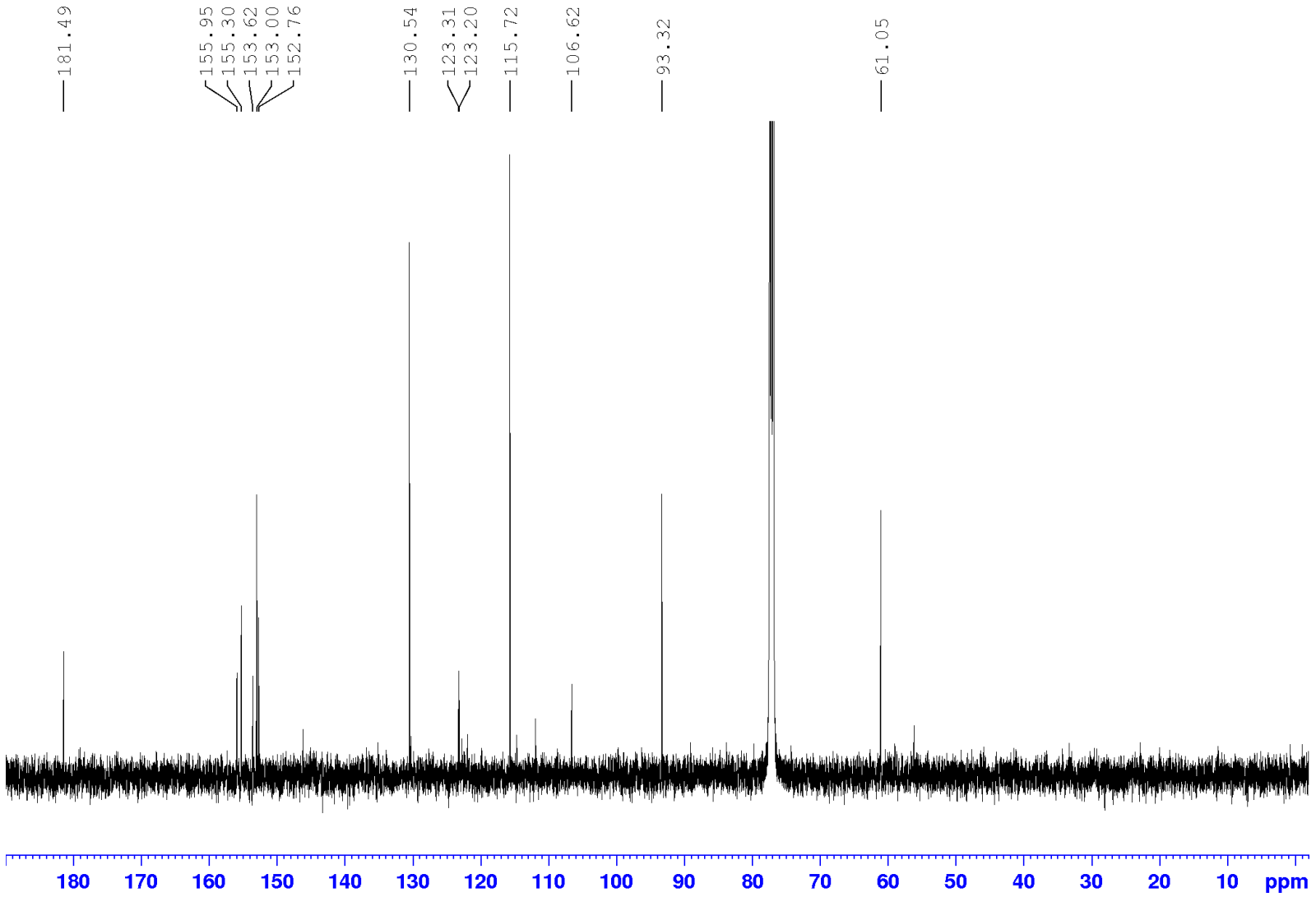

Figure 6: HRESIMS spectrum of compound **2**.

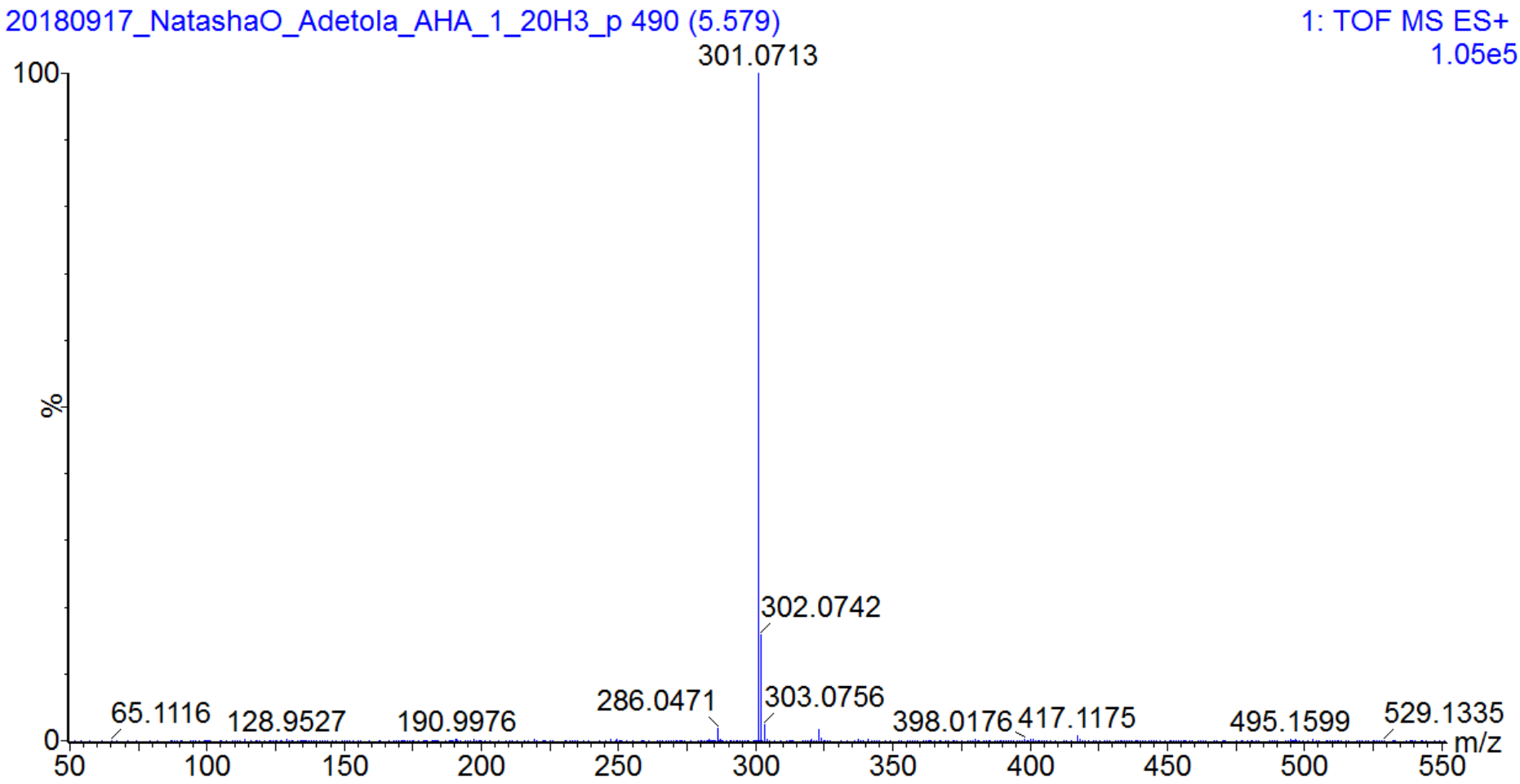

Figure 7: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **3**.

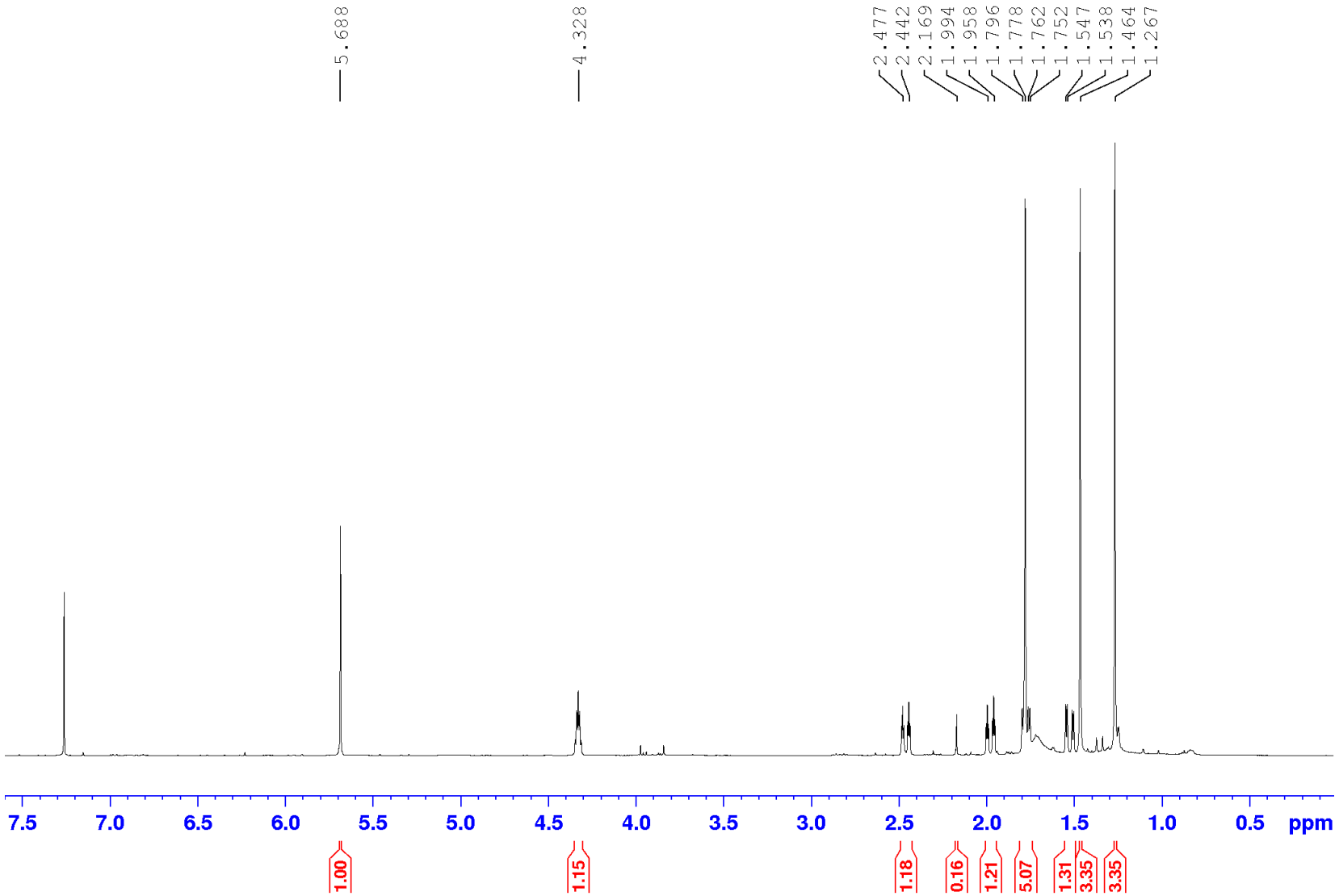

Figure 8: ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **3**.

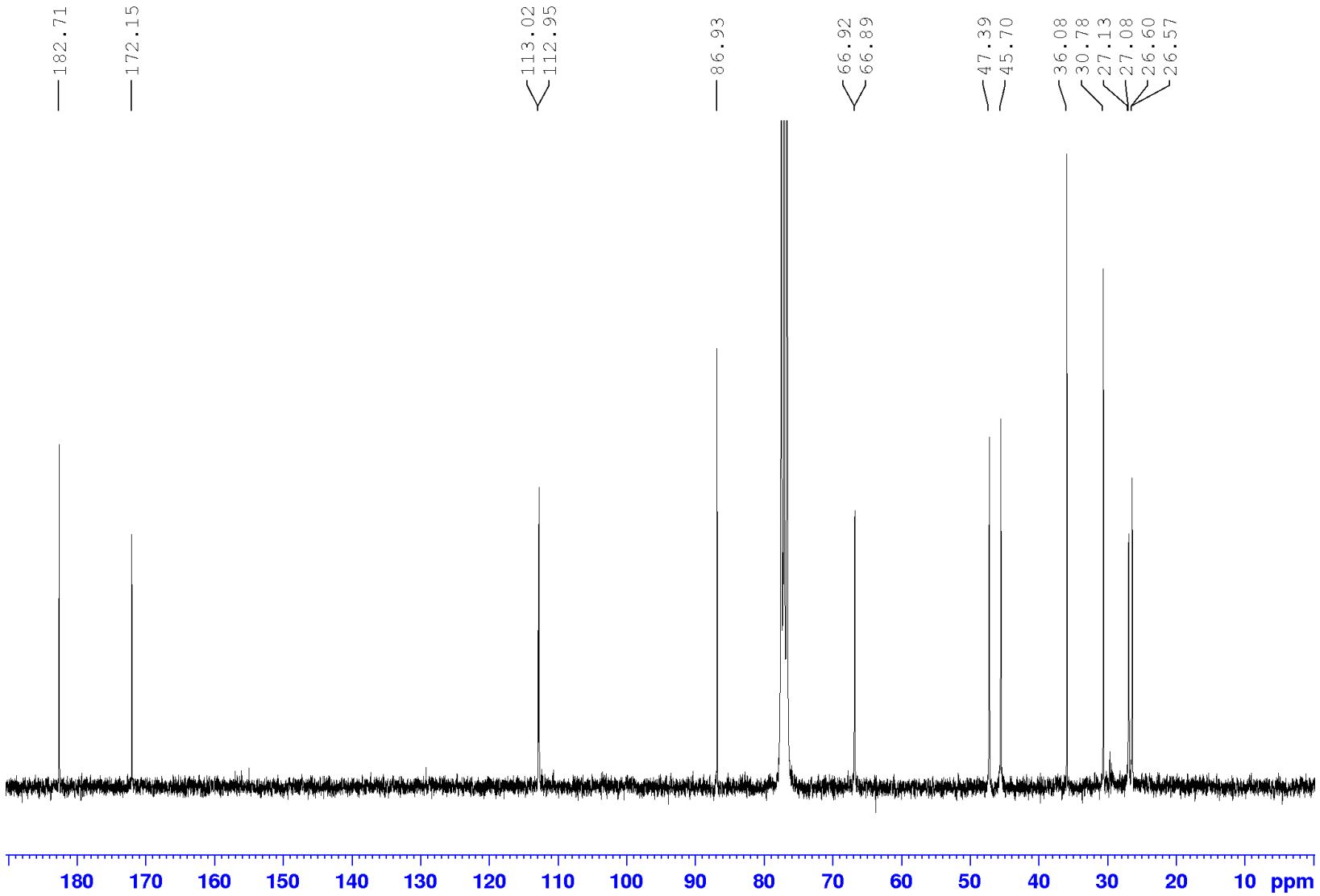

Figure 9: HRESIMS spectrum of compound **3**.

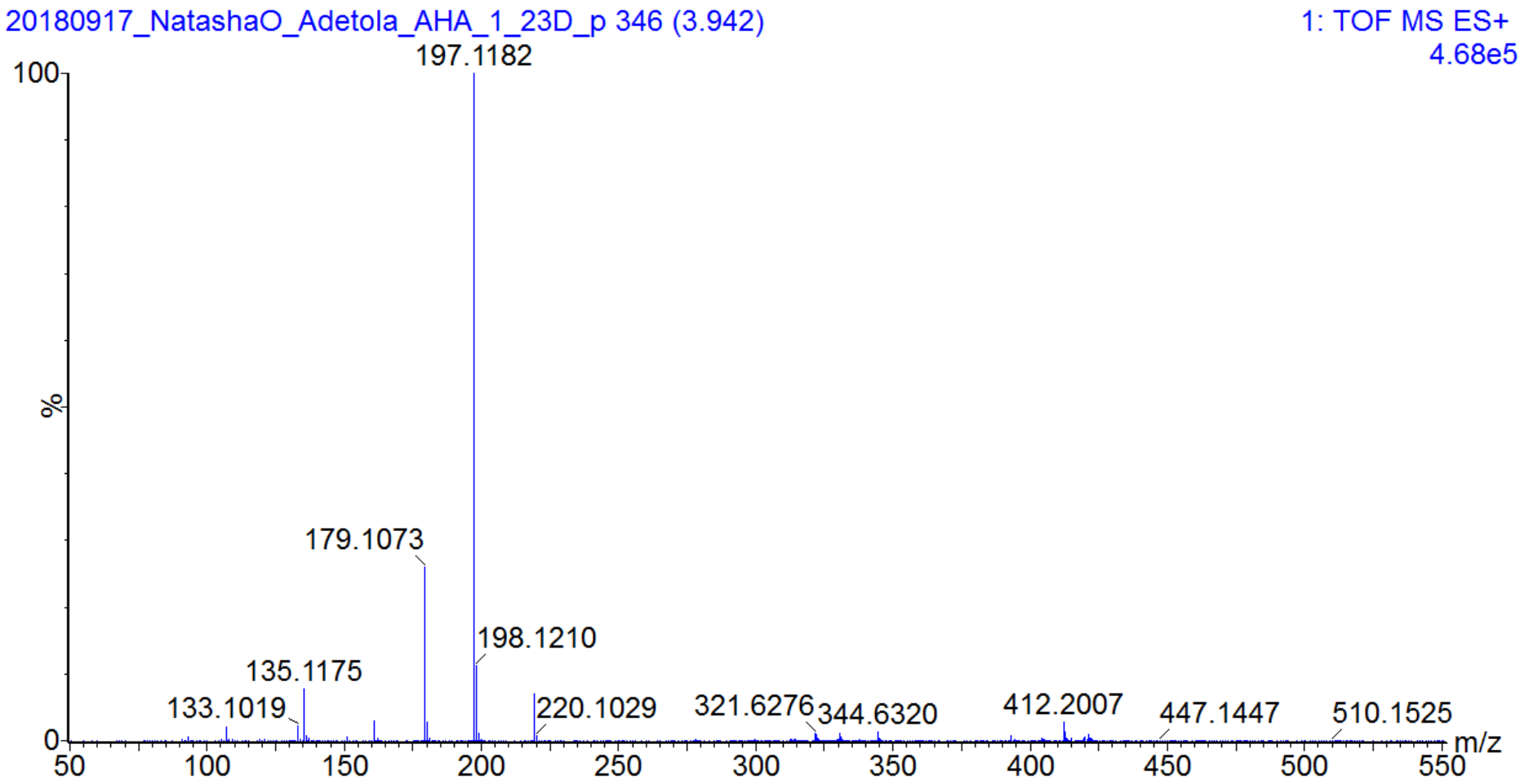

Figure 10: ^{1}H NMR (400 MHz, CD_3OD) spectrum of compound **4**.

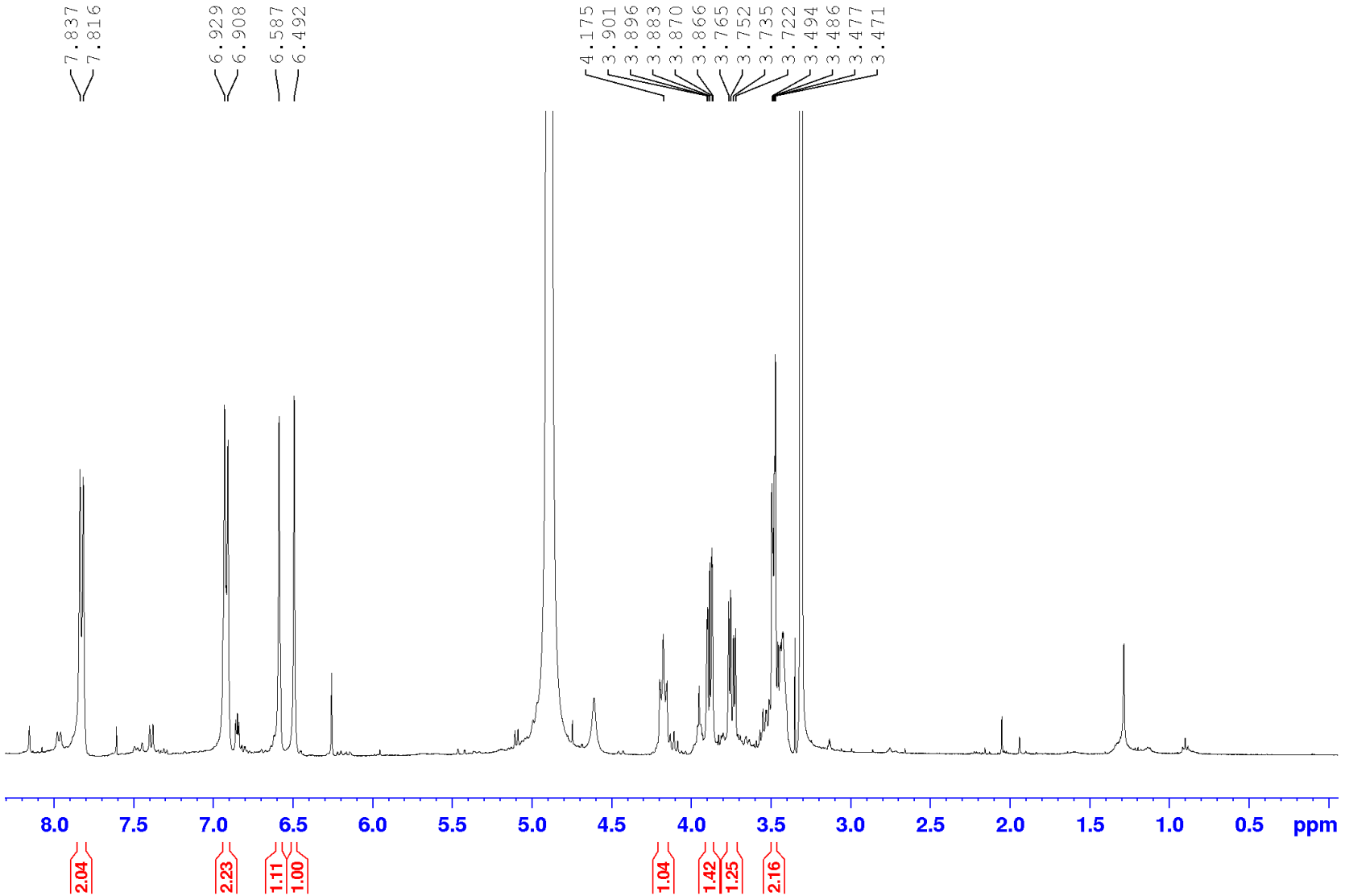

Figure 11: ^{13}C NMR (125 MHz, CD_3OD) spectrum of compound **4**.

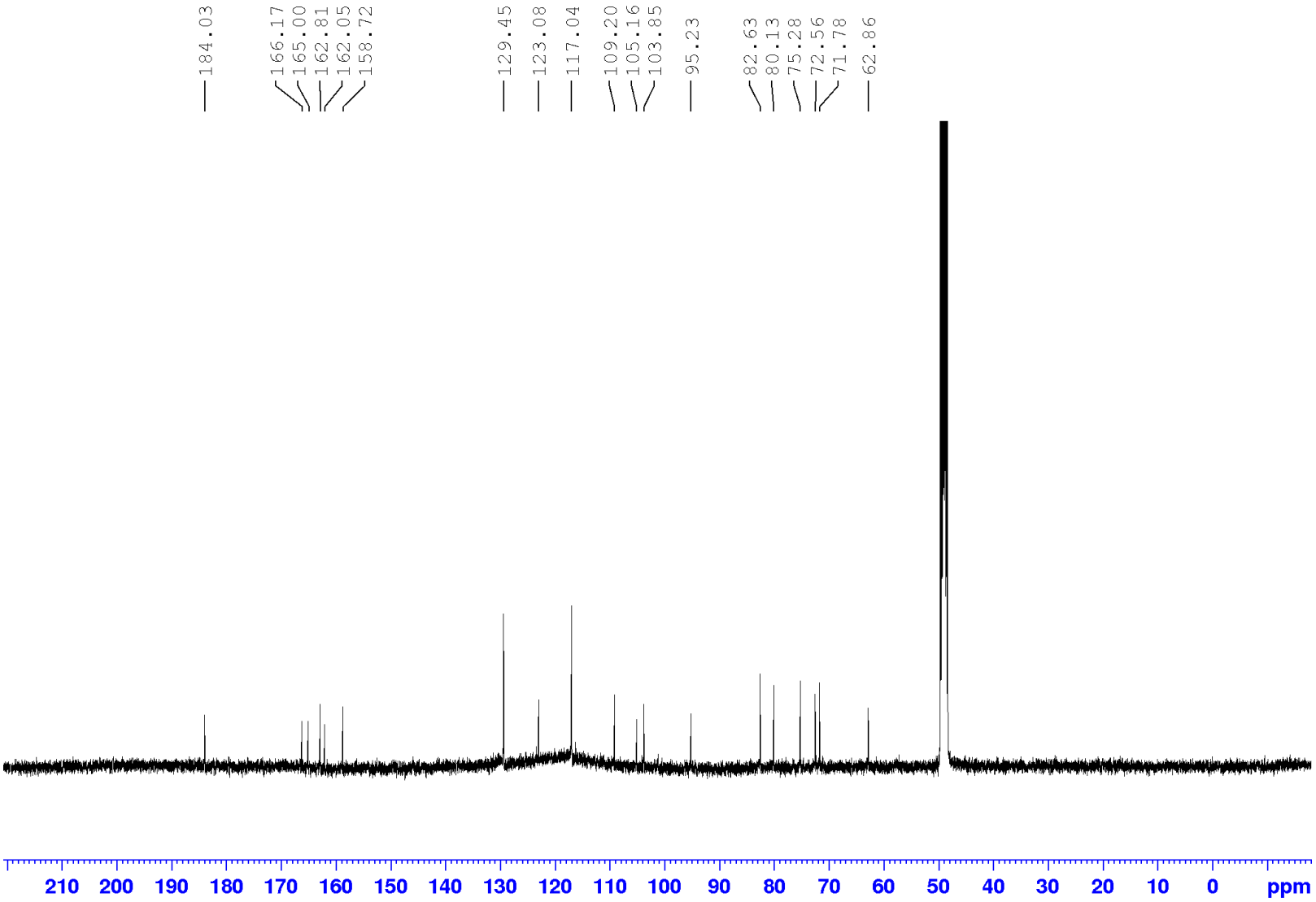

Figure 12: HRESIMS spectrum of compound **4**.

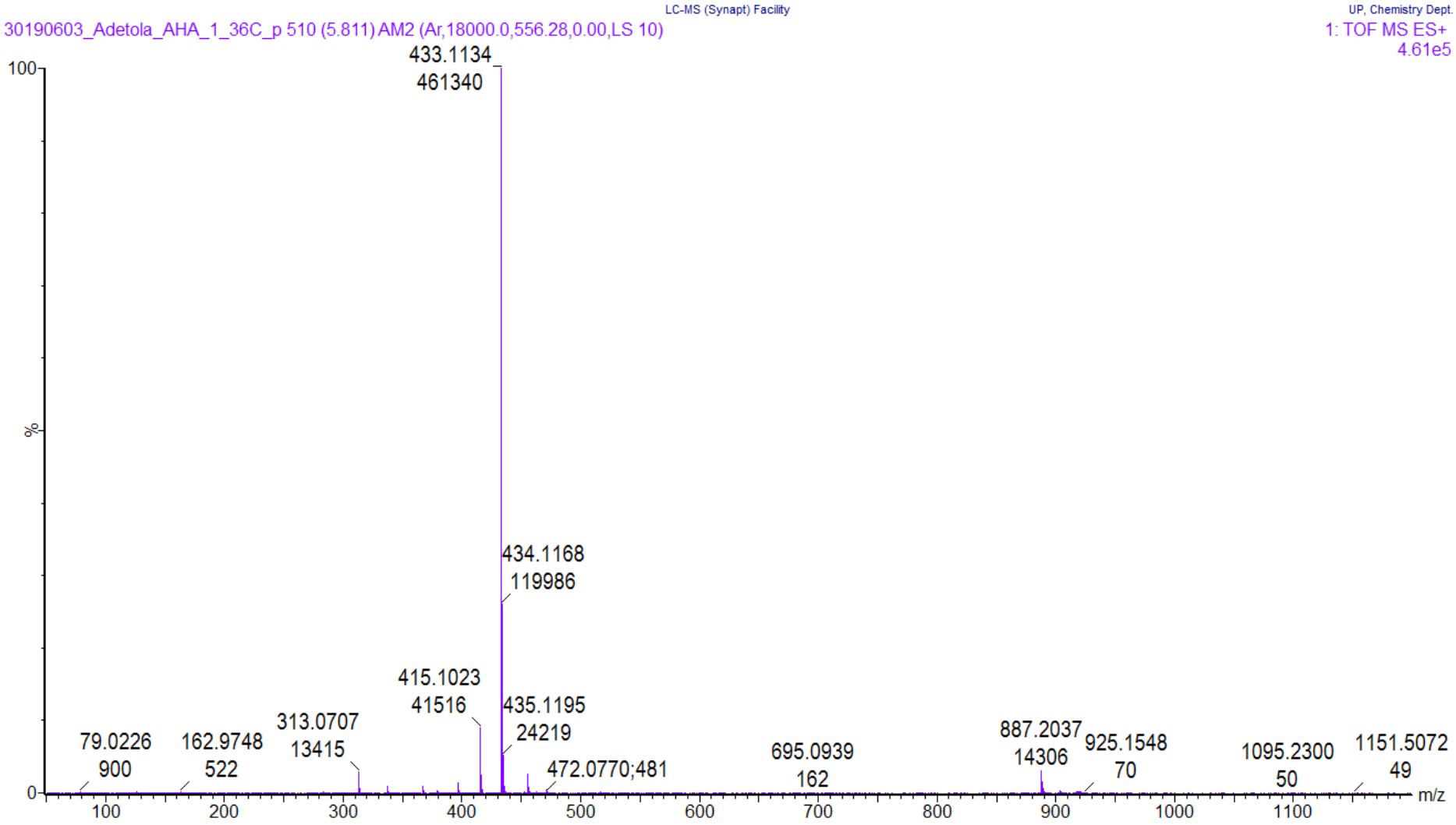

Figure 13: ^{1}H NMR [400 MHz, $(CD_3)_2SO$] spectrum of compound **5**.

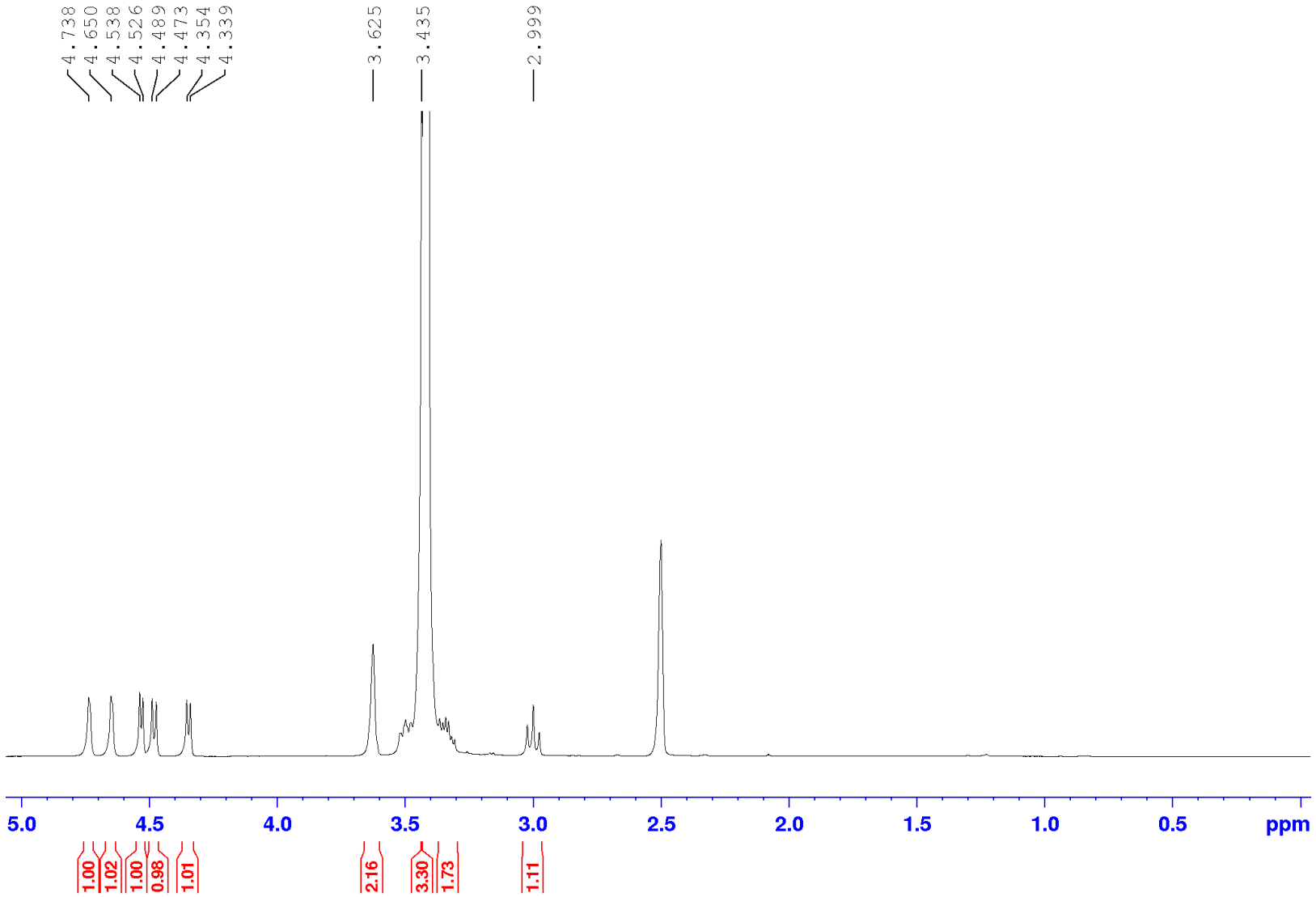

Figure 14: ^{13}C NMR [100 MHz, $(CD_3)_2SO$] spectrum of compound **5**.

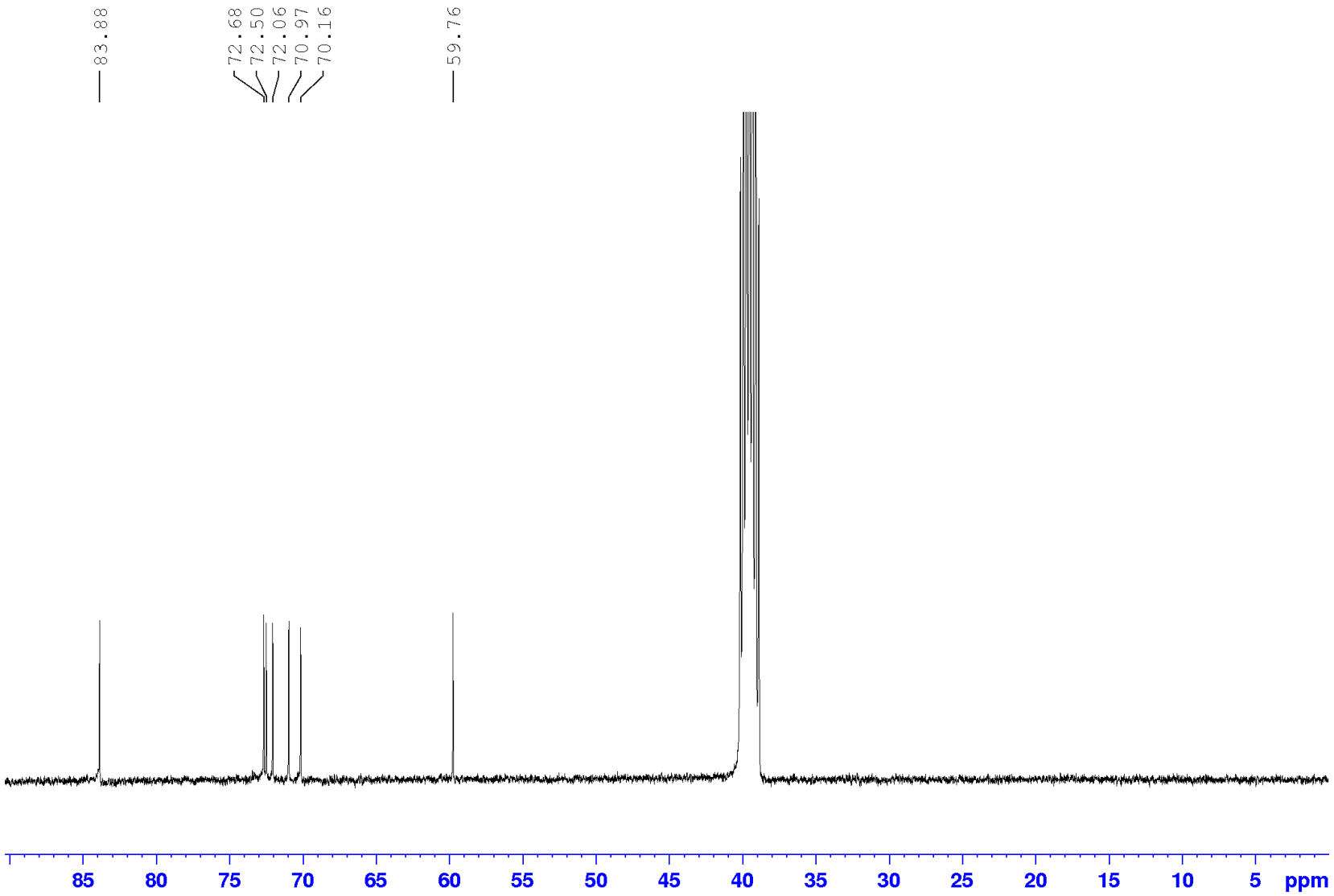

Figure 15: HRESIMS spectrum of compound **5**.

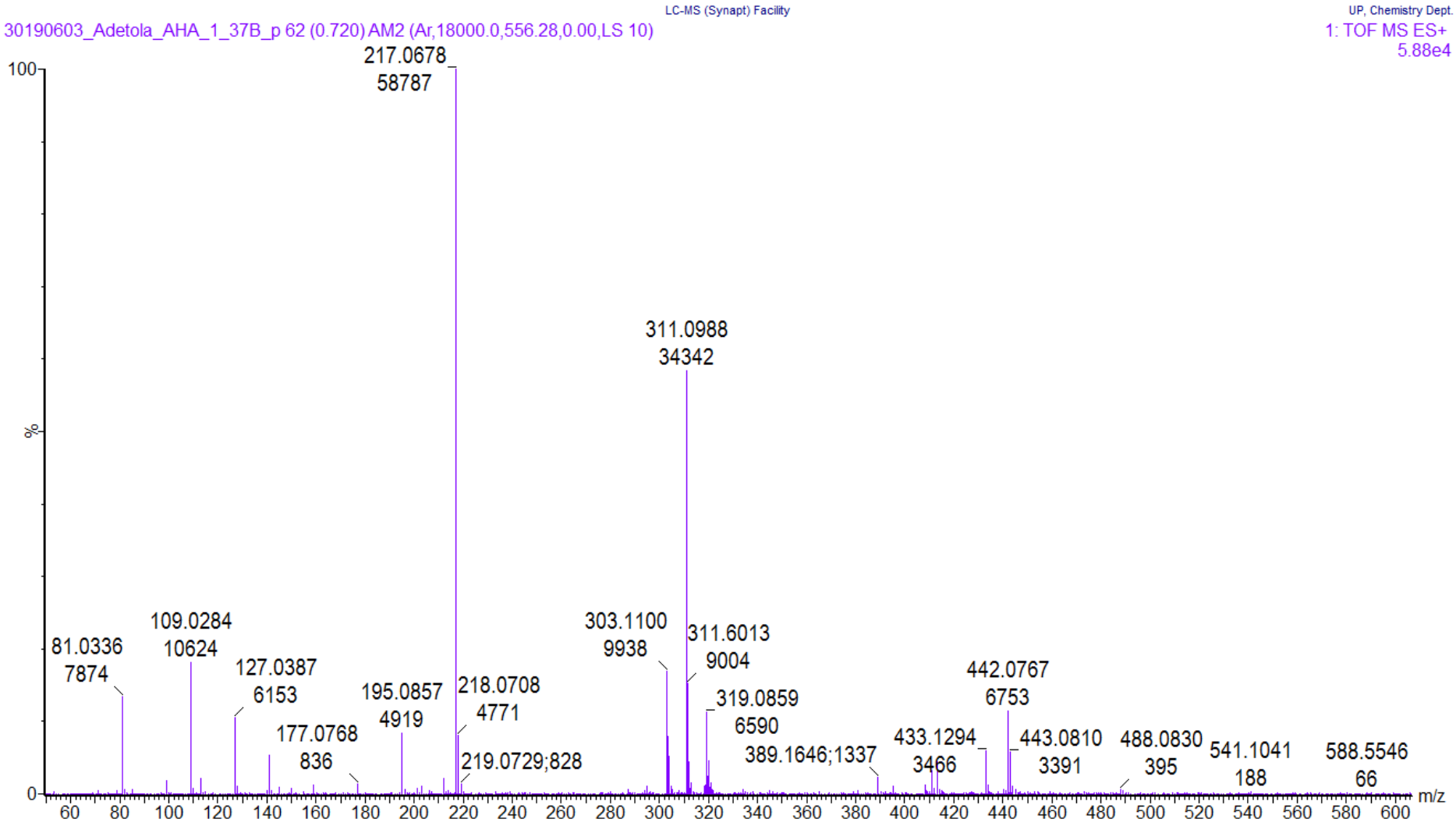

Figure 16: ^{1}H NMR [400 MHz, $(CD_3)_2SO$] spectrum of compound **6**.

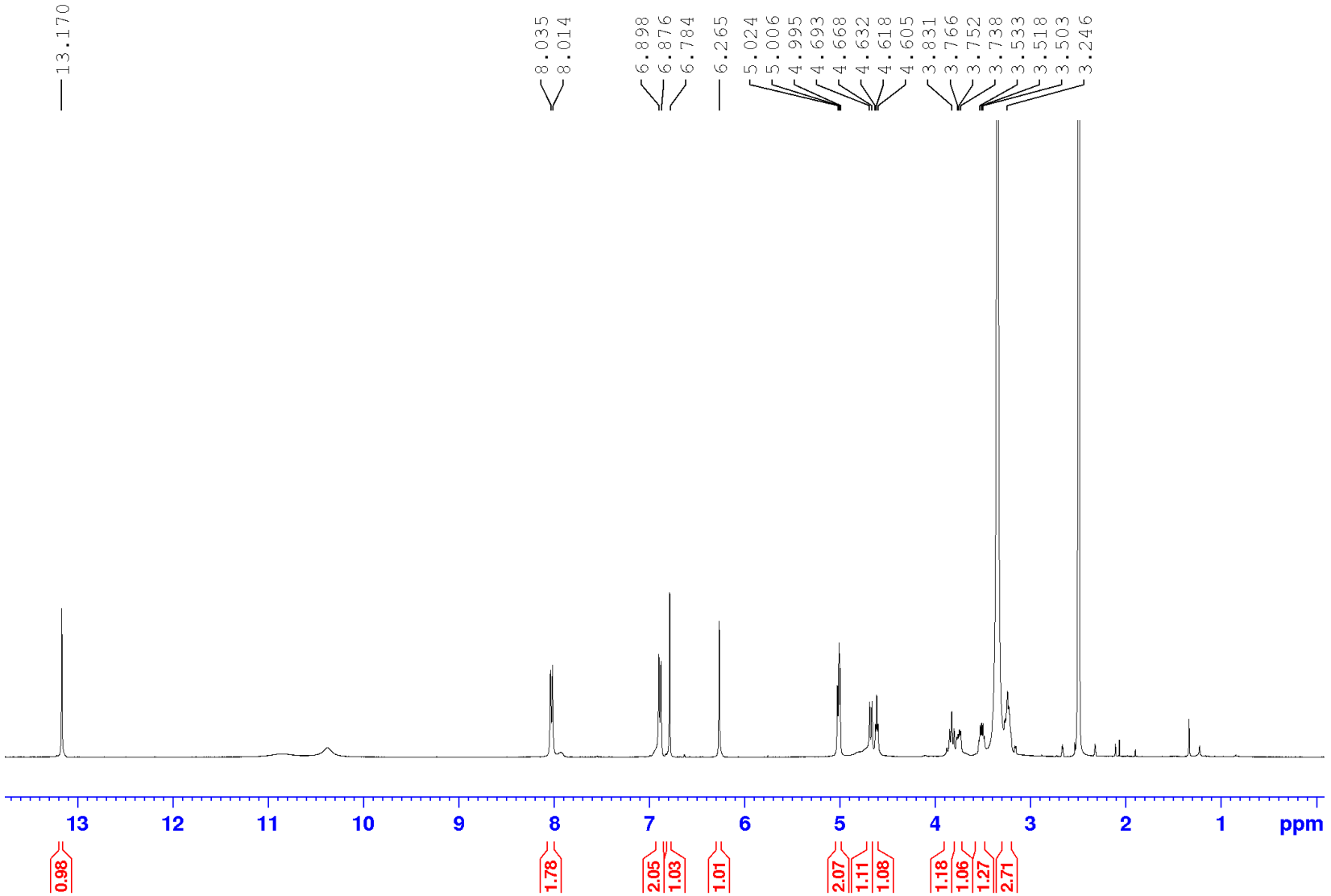

Figure 17: ^{13}C NMR [125 MHz, $(CD_3)_2SO$] spectrum of compound **6**.

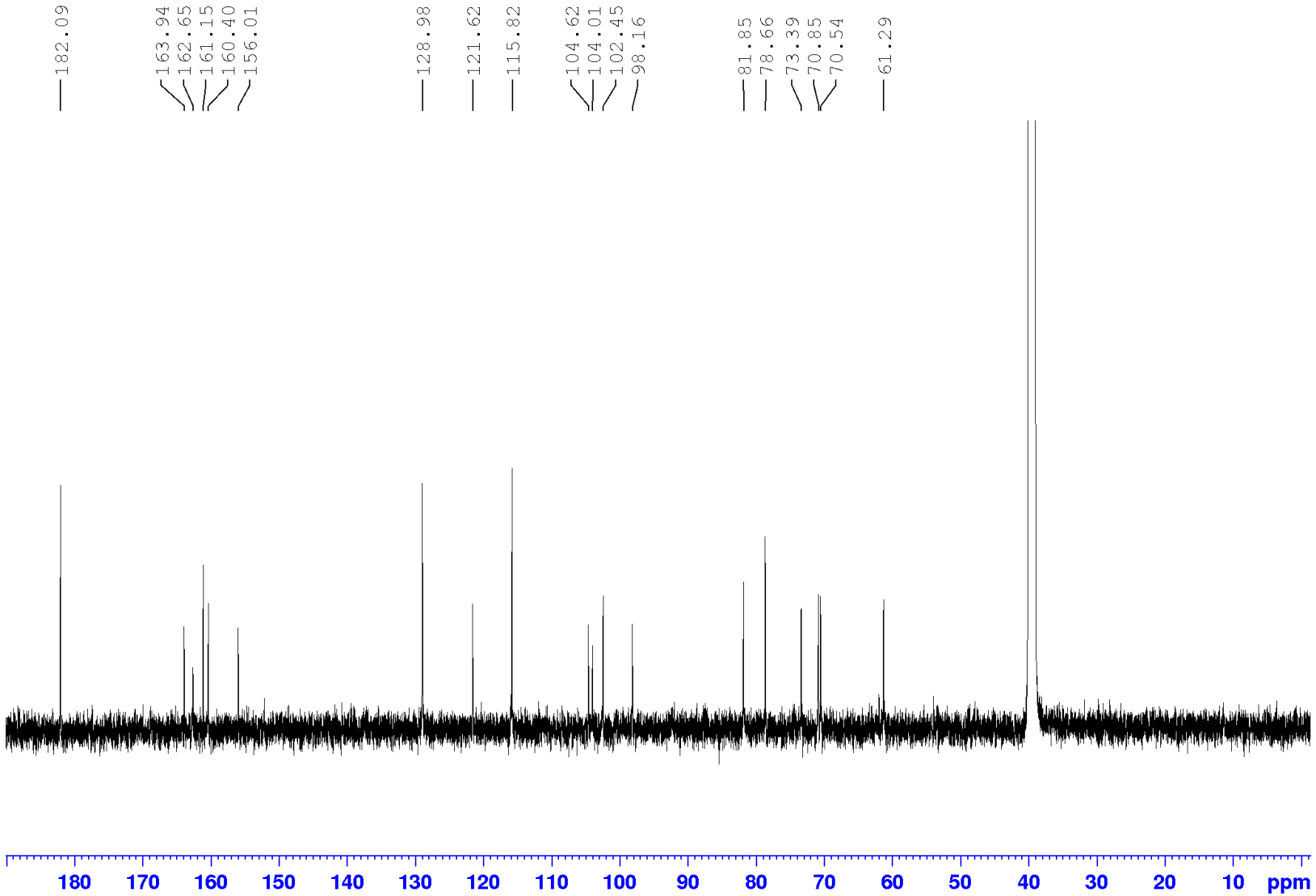

Figure 18: HRESIMS spectrum of compound **6**.

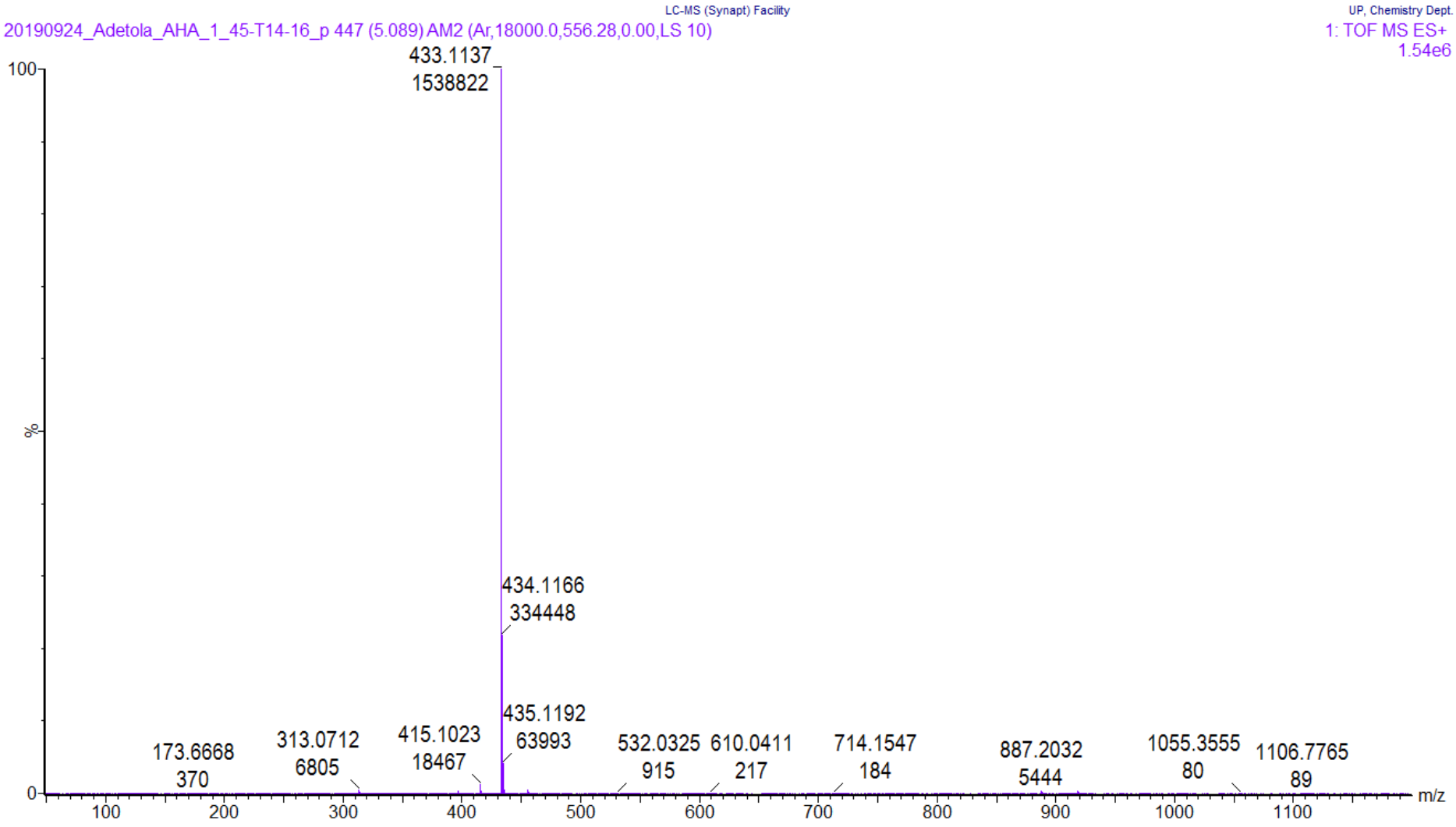

Figure 19: ^{1}H NMR (400 MHz, CD_3OD) spectrum of compound **7**.

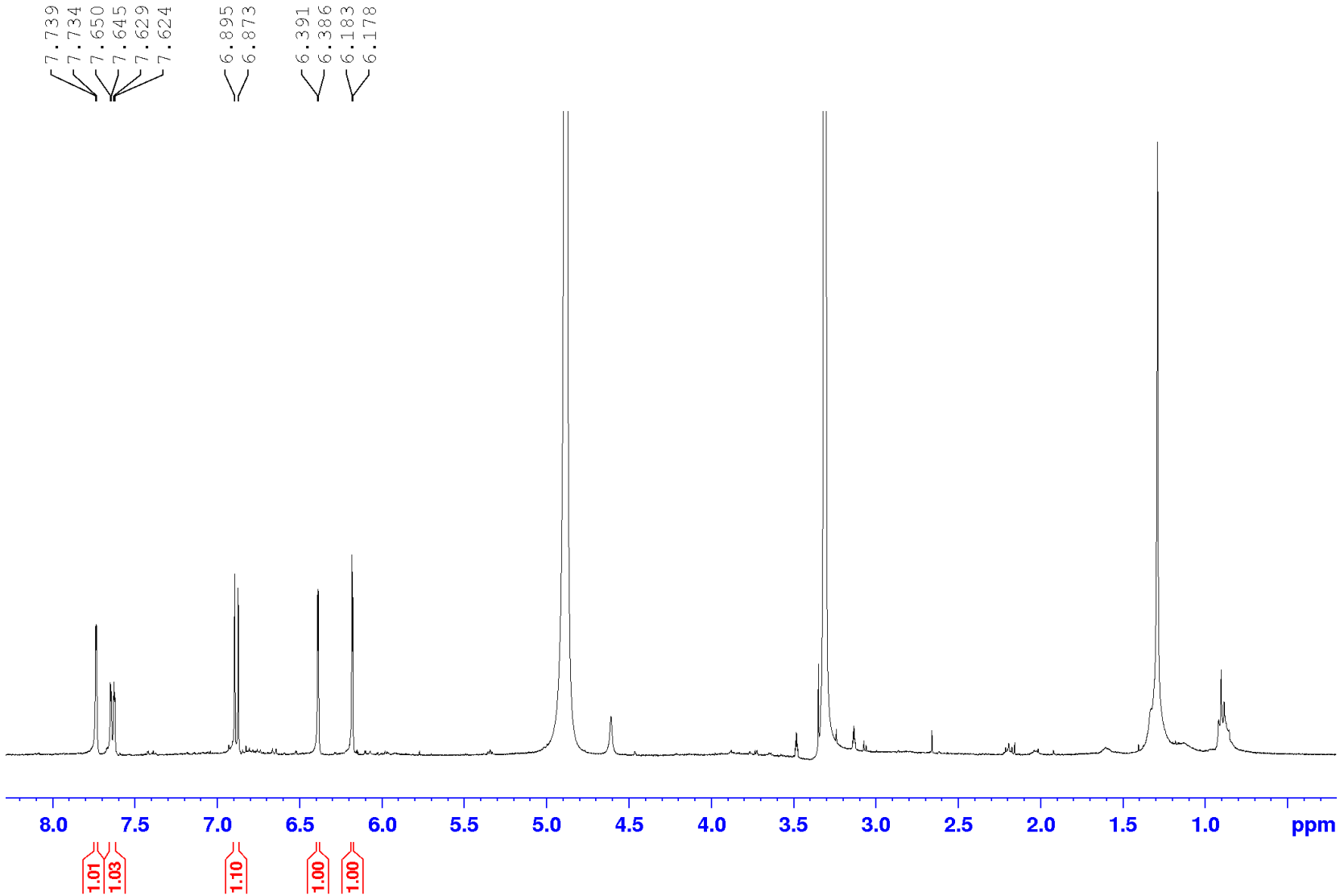

Figure 20: ^{13}C NMR (125 MHz, CD_3OD) spectrum of compound **7**.

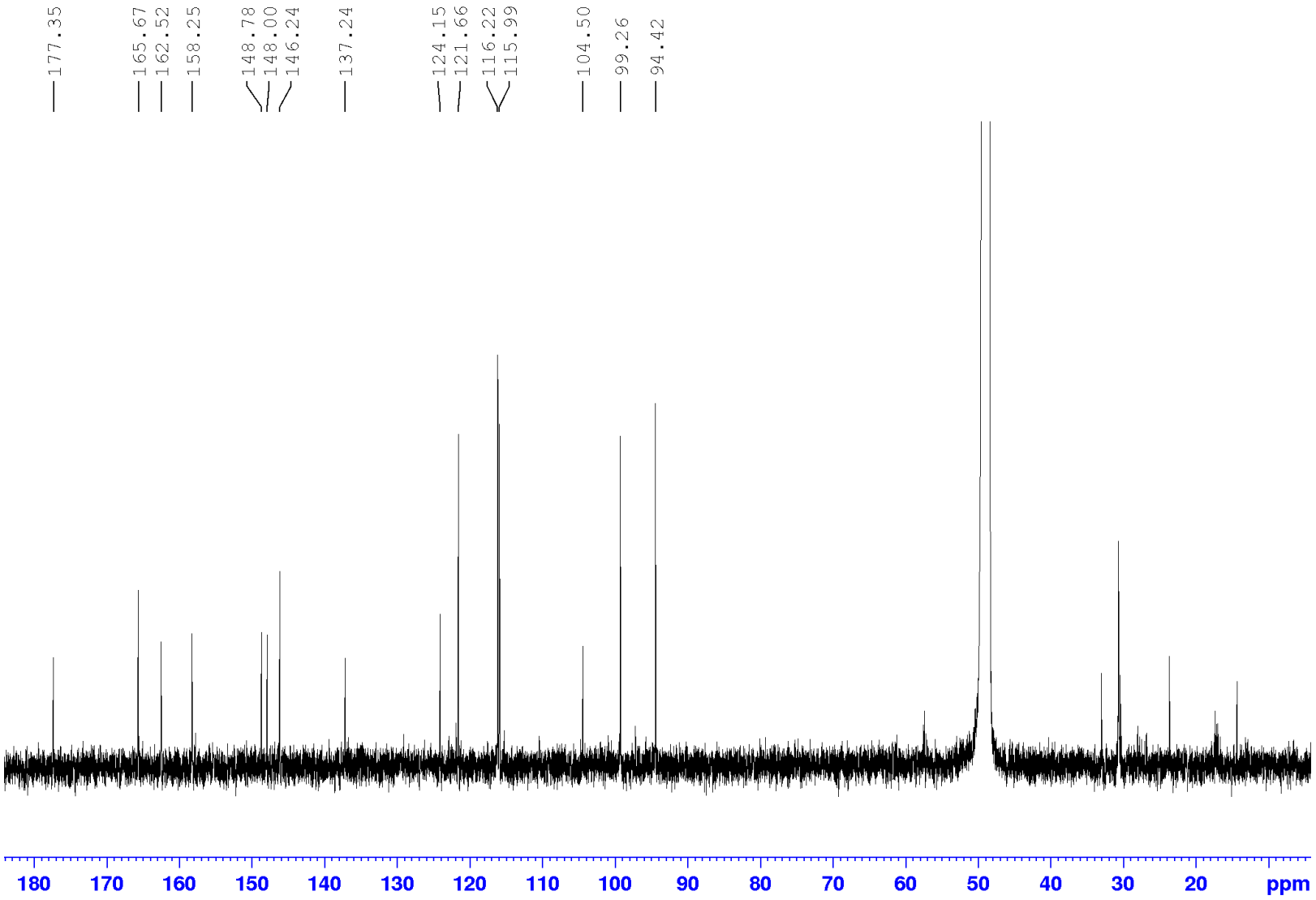

Figure 21: HRESIMS spectrum of compound **7**.

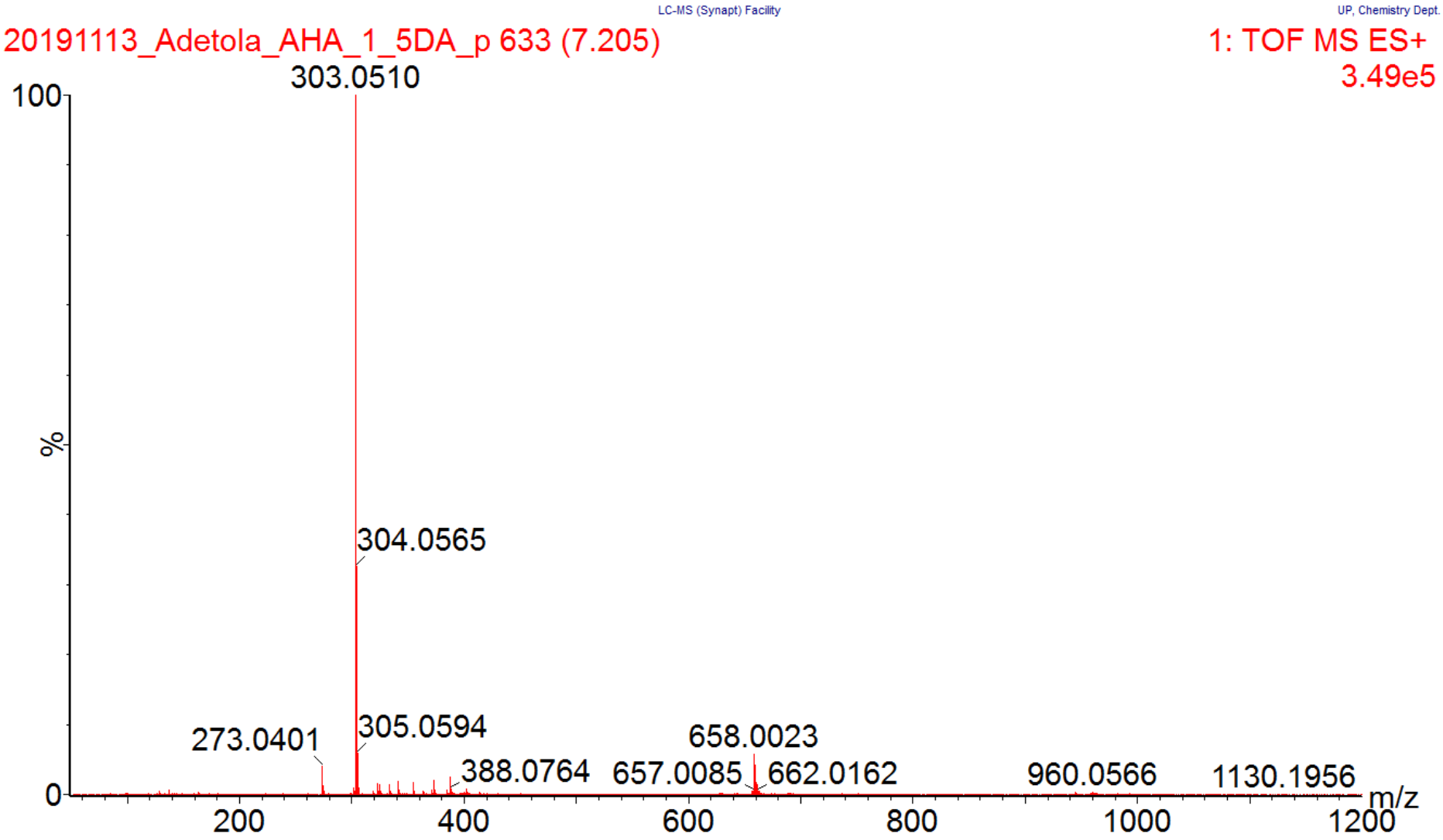

Figure 22: ^{1}H NMR (500 MHz, CD_3OD) spectrum of compound **8**.

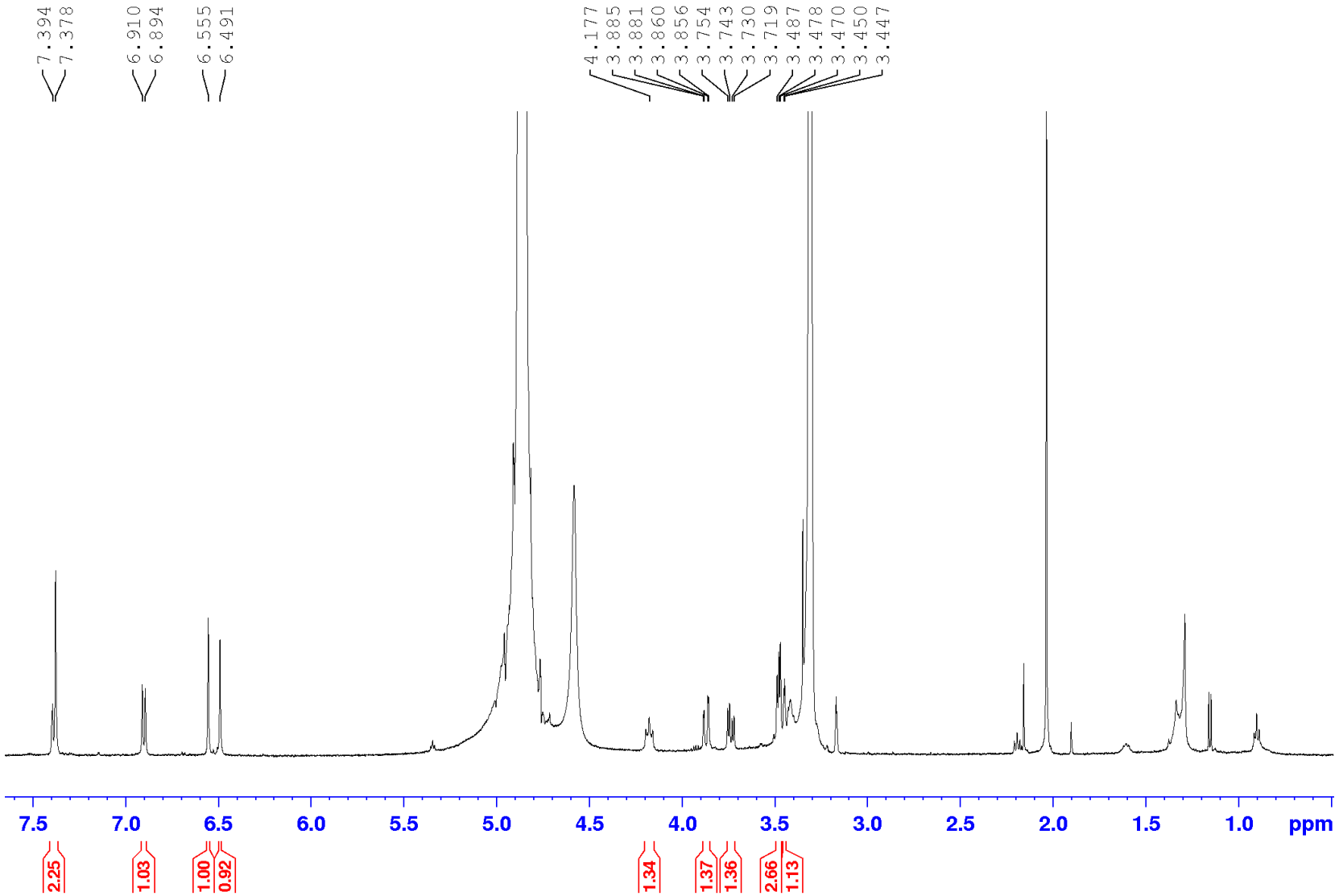

Figure 23: ^{13}C NMR (125 MHz, CD_3OD) spectrum of compound **8**.

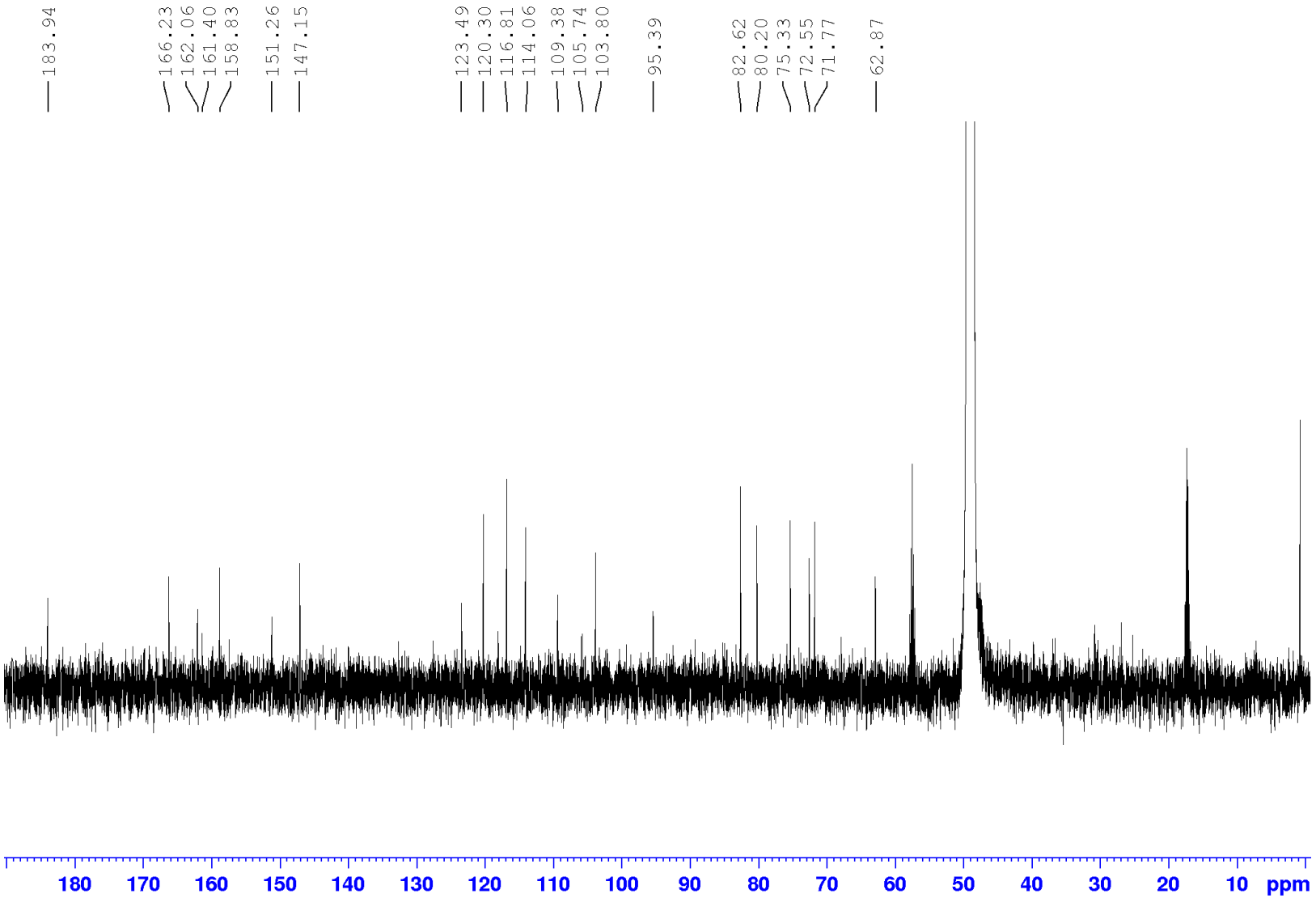

Figure 24: HRESIMS spectrum of compound **8**.