Supplementary Information (SI) for RSC Advances.

In vitro and *in silico* studies of SARS-CoV-2 main protease inhibition and antioxidant activities of isolated compounds from *Marrubium alysson* L.

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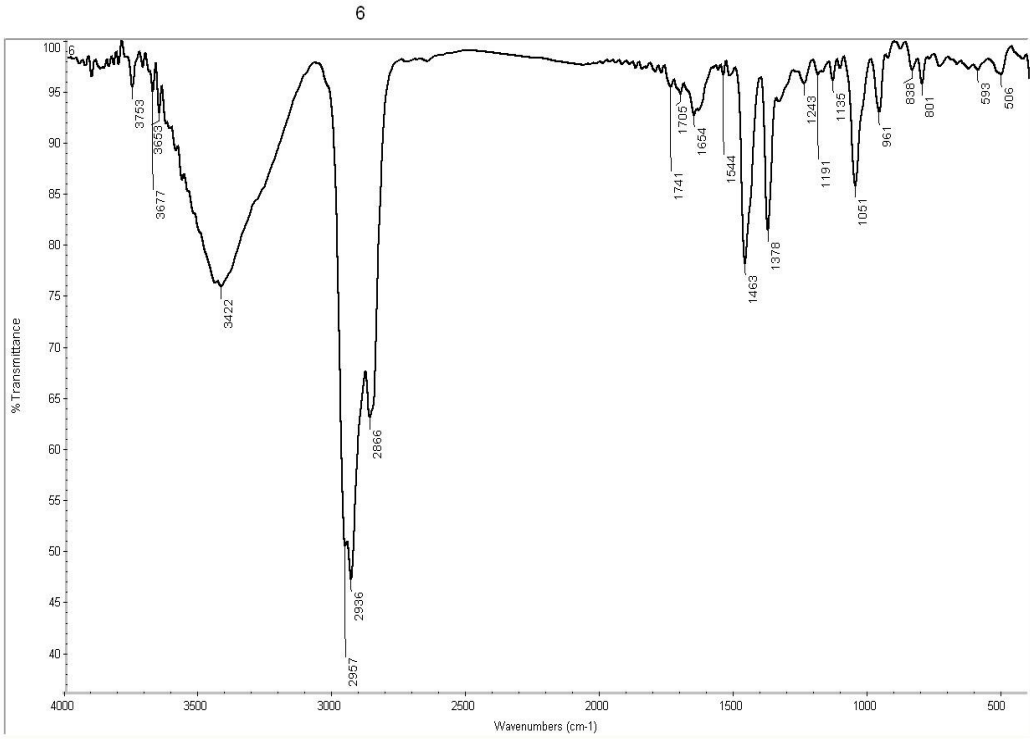

Figure (1). IR spectrum (KBr, U_{max} cm^{-1}) of compound 1

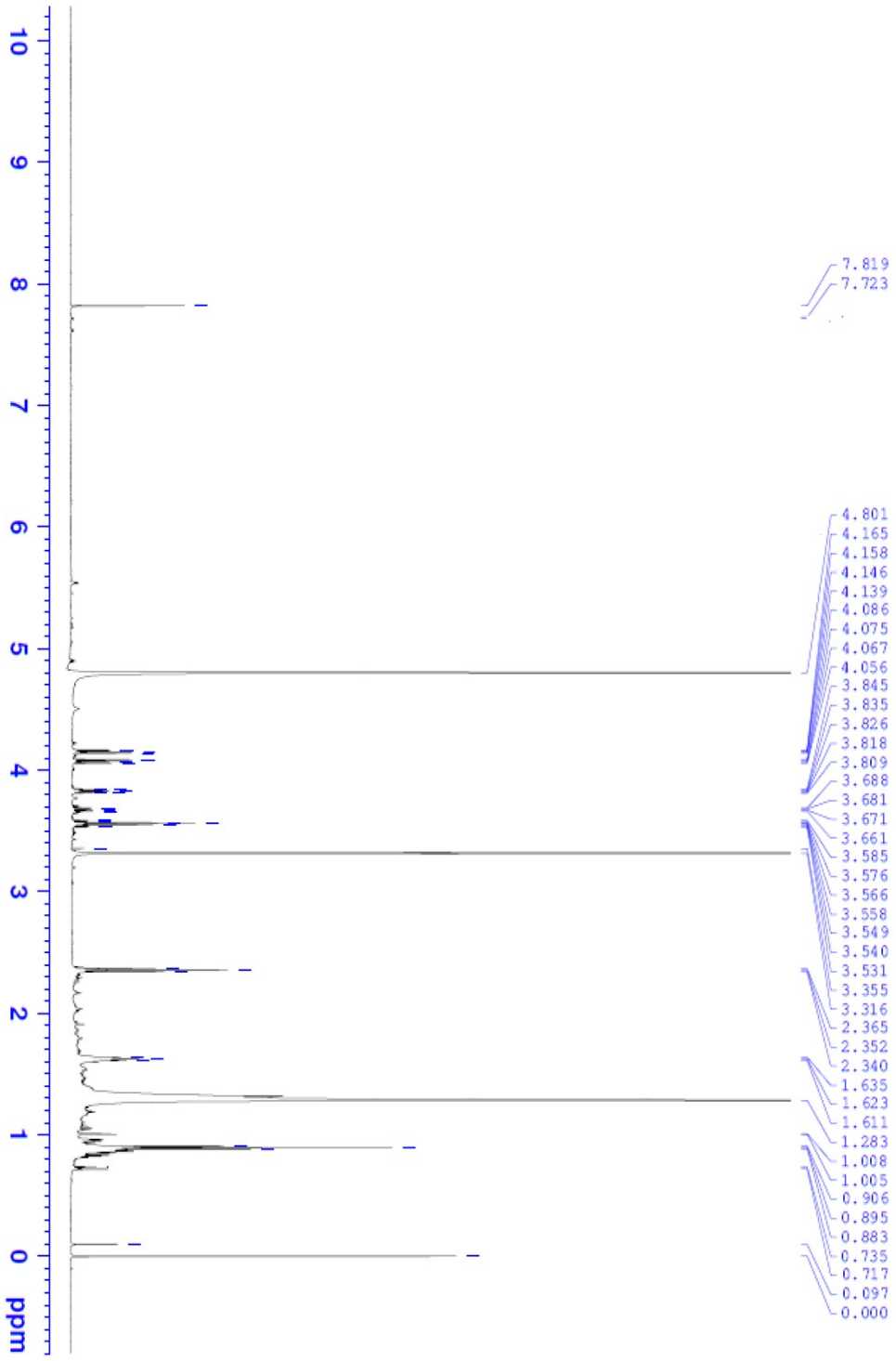

Figure (2): ^{1}H-NMR spectrum of compound 2 in ($CDCl_3$, CD_3OD mix) at 600 MHz

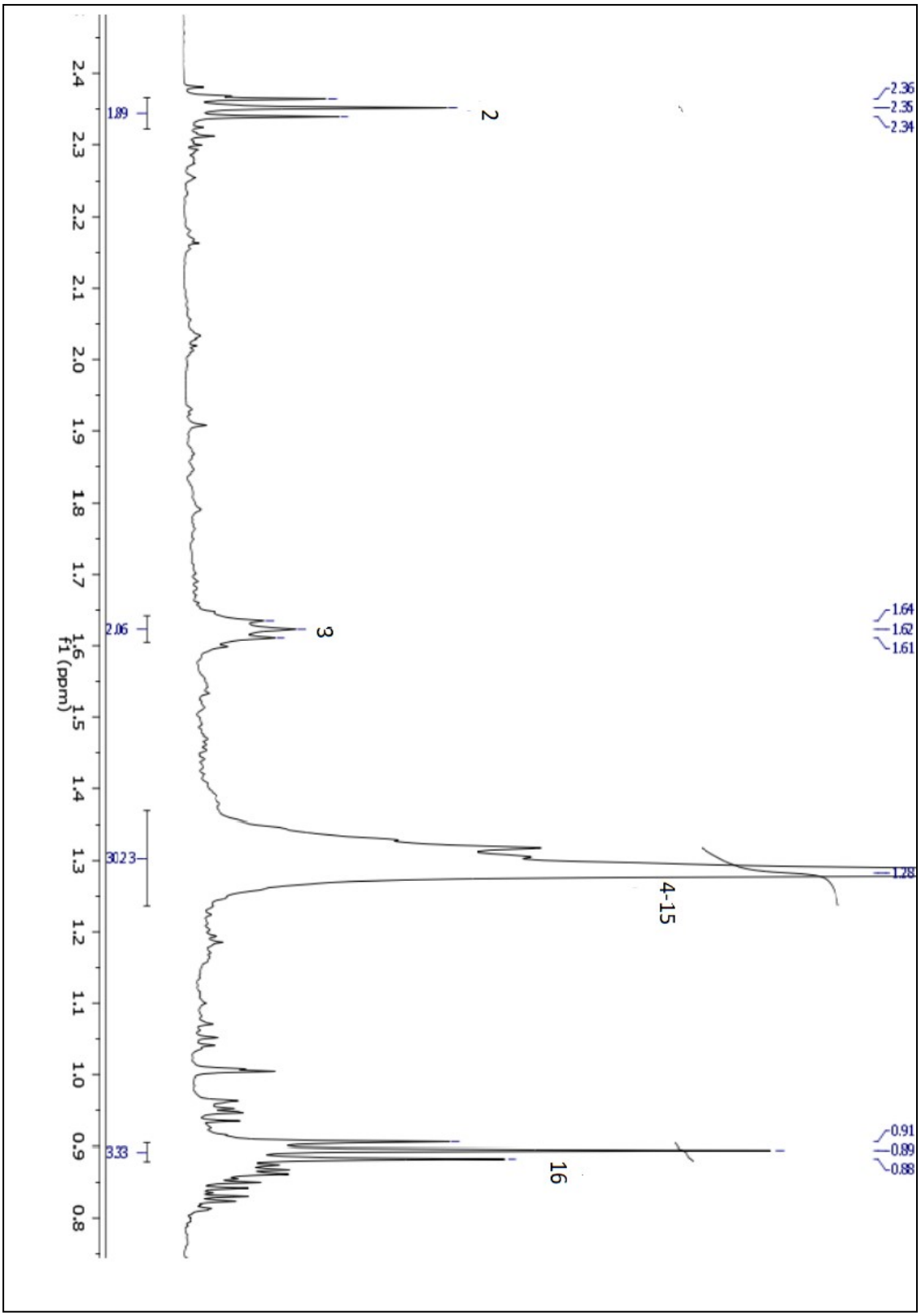

Figure (2.a): Expansion of ^{1}H-NMR spectrum of compound 2 in ($CDCl_3$, CD_3OD mix,) at δ_H: (0.8-2.4) ppm.

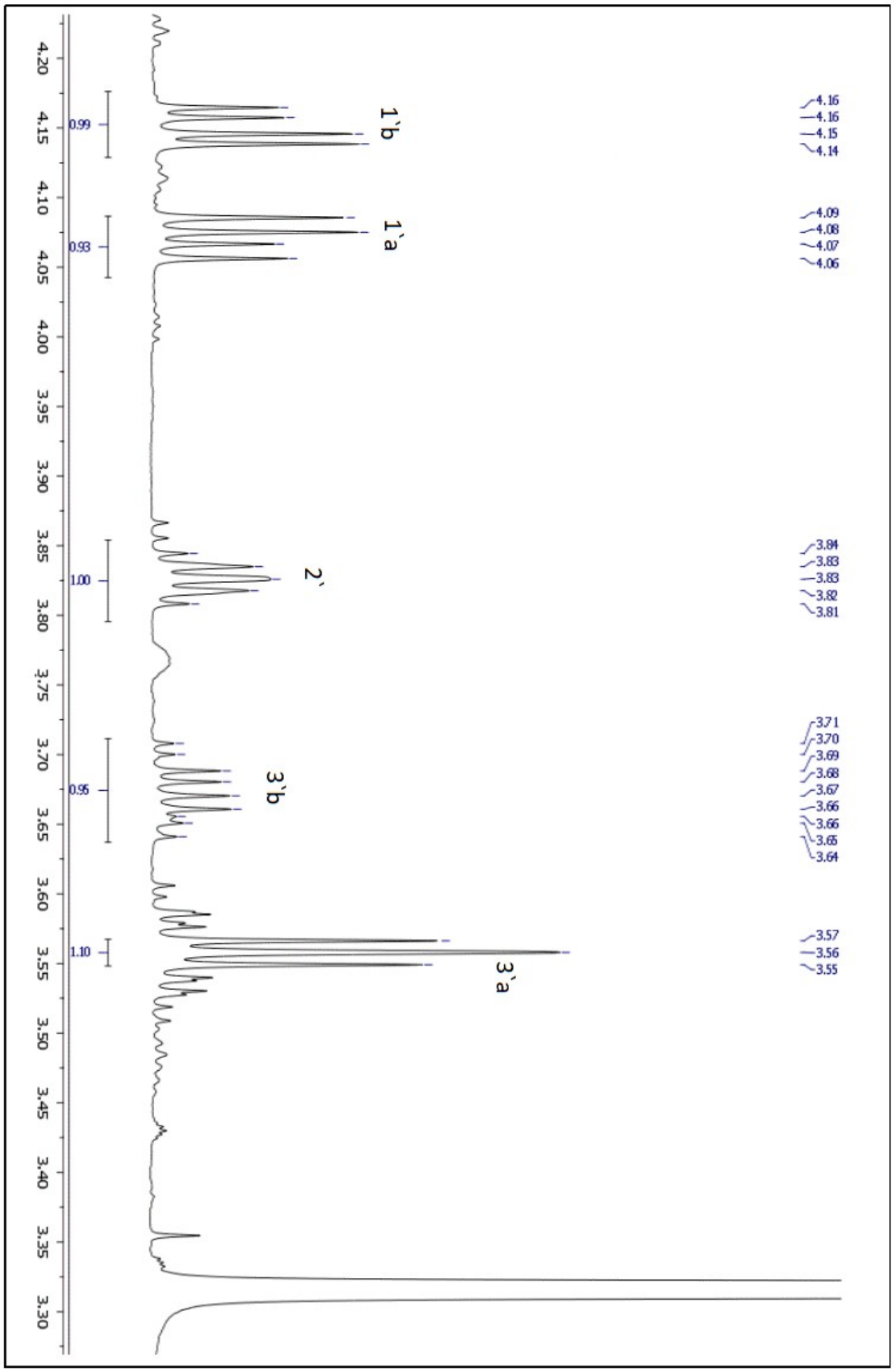

Figure (2.b): Eexpansion of ^{1}H-NMR spectrum of compound 2 in ($CDCl_3$, CD_3OD mix,) at δ_H: (3.3-4.2) ppm.

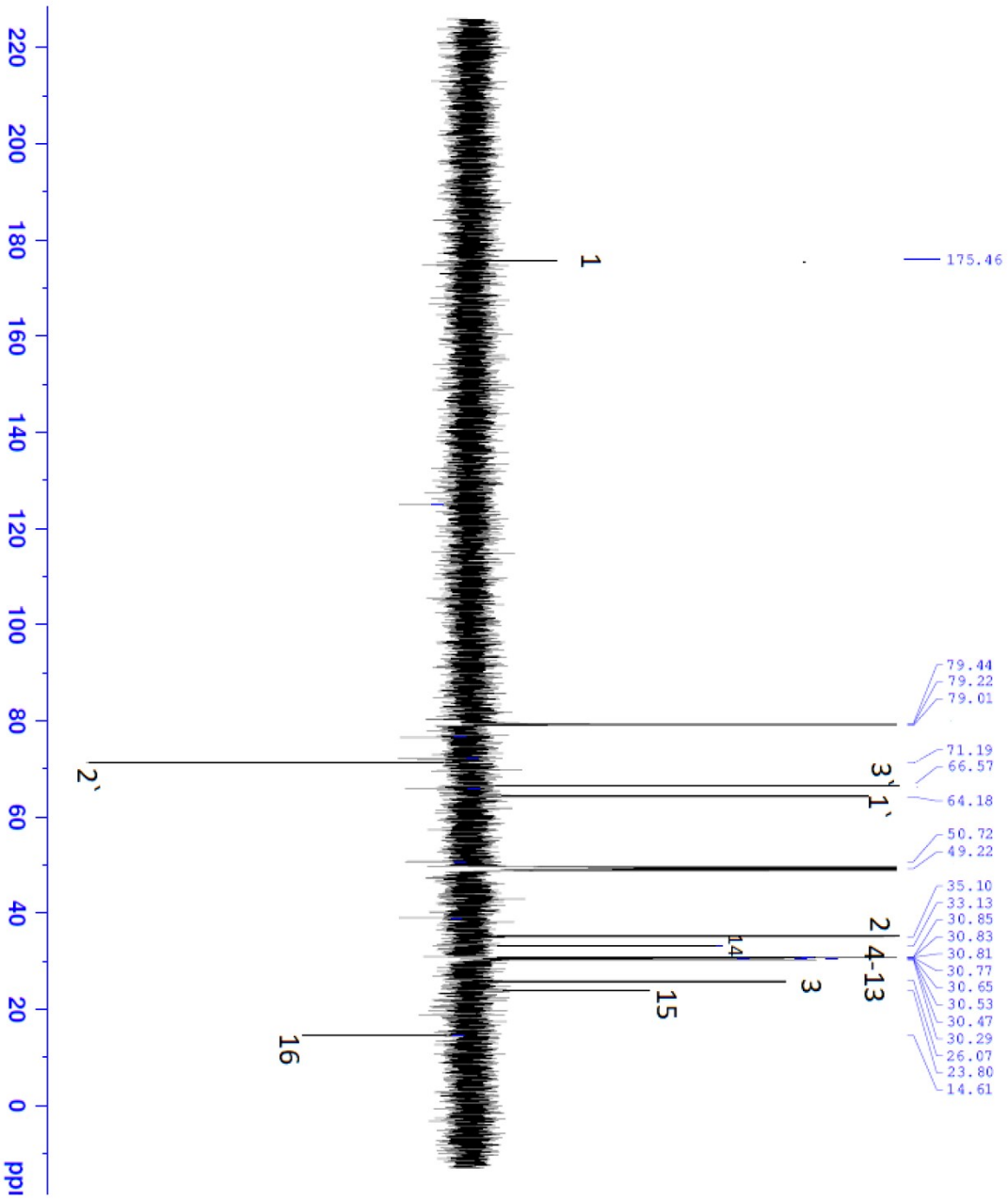

Figure (3): APT spectrum of compound 2 in ($CDCl_3$, CD_3OD mix) at 150 MHz

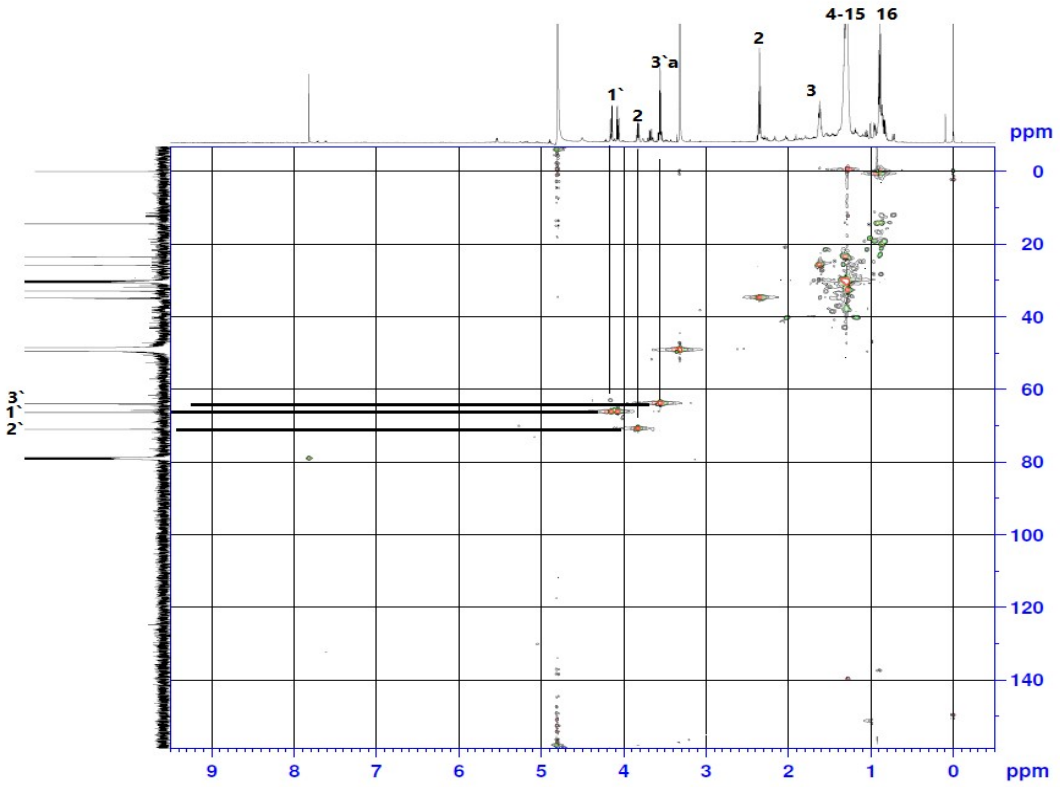

Figure (4): HSQC of compound 2 in ($CDCl_3$:CD_3OD mix)

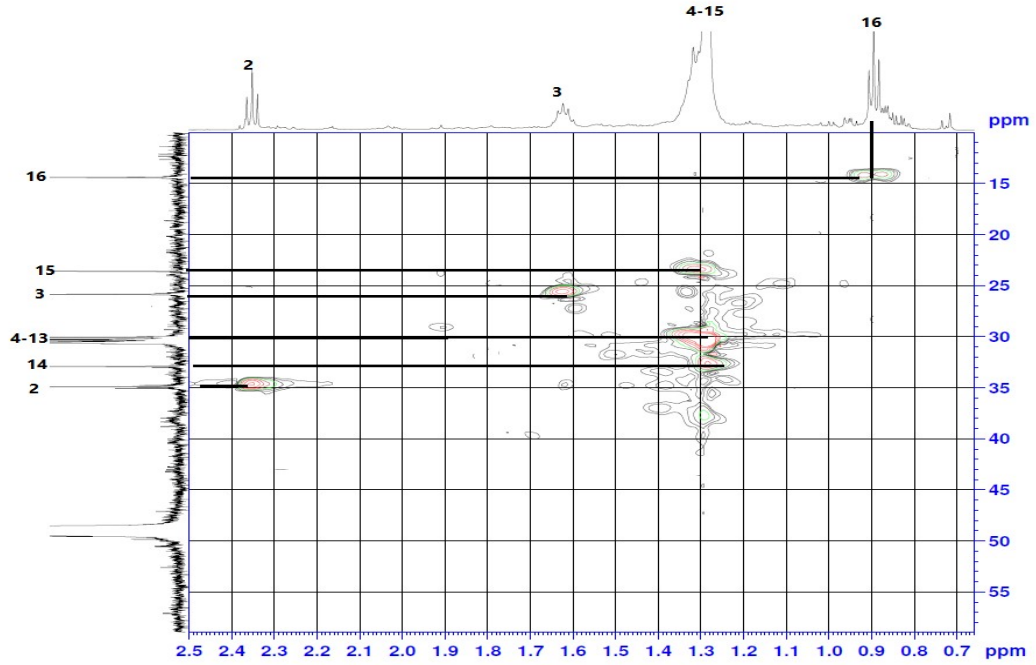

Figure (4.a): Expansion of HSQC spectrum of compound 2 at δ_H: 0.7-2.5 ppm and δ_c: 10-60 ppm.

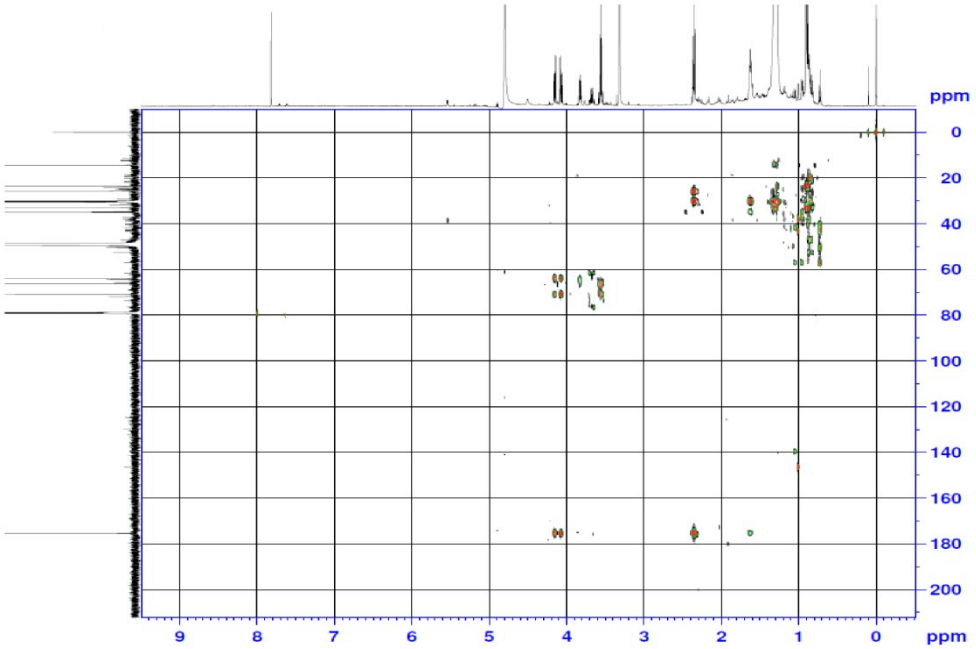

Figure (5): HMBC of compound 2 in ($CDCl_3$, CD_3OD mix)

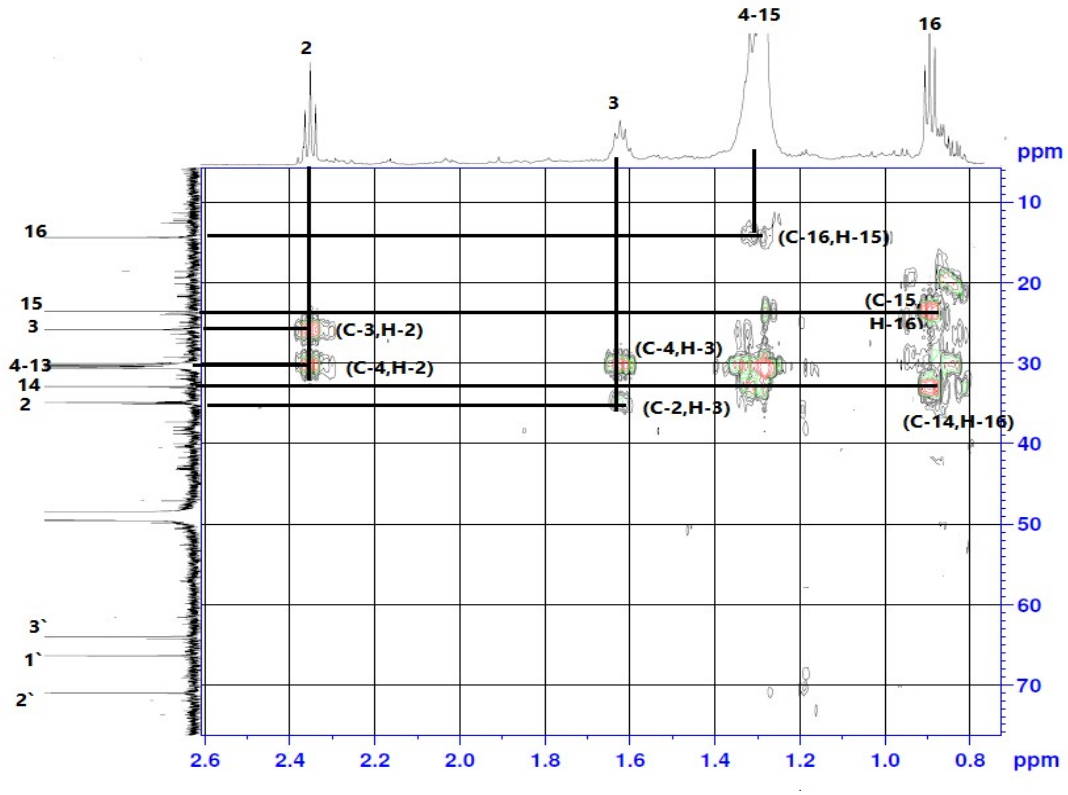

Figure (5.a): Expansion of HMBC spectrum of compound M2 at δ_H: 0.8-2.6 ppm and δ_c: 5-75 ppm.

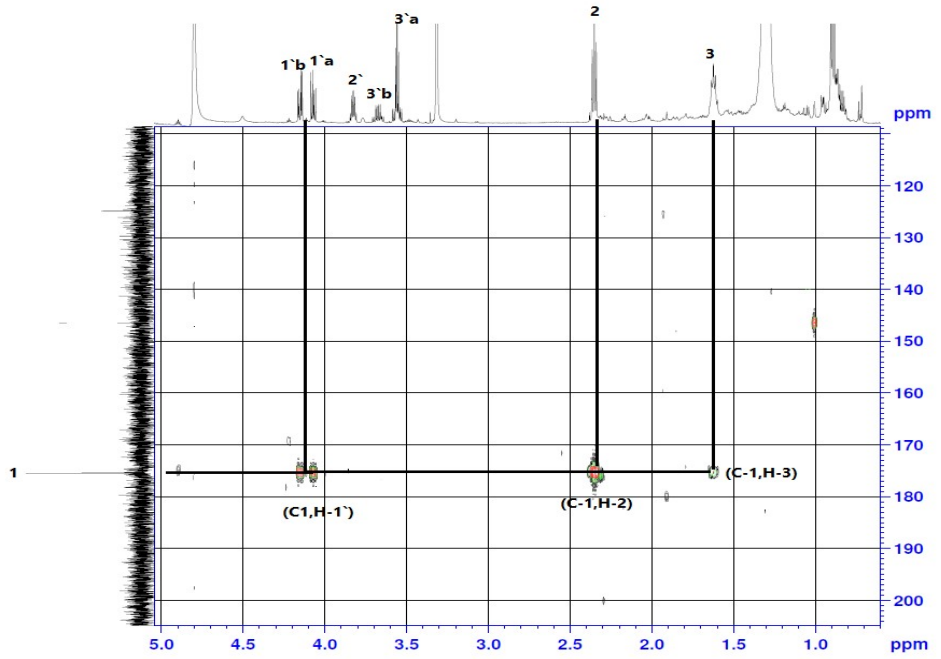

Figure (5.b): Expansion of HMBC spectrum of compound 2 at δ_H: 0-5.0 ppm and δ_c: 110-200 ppm.

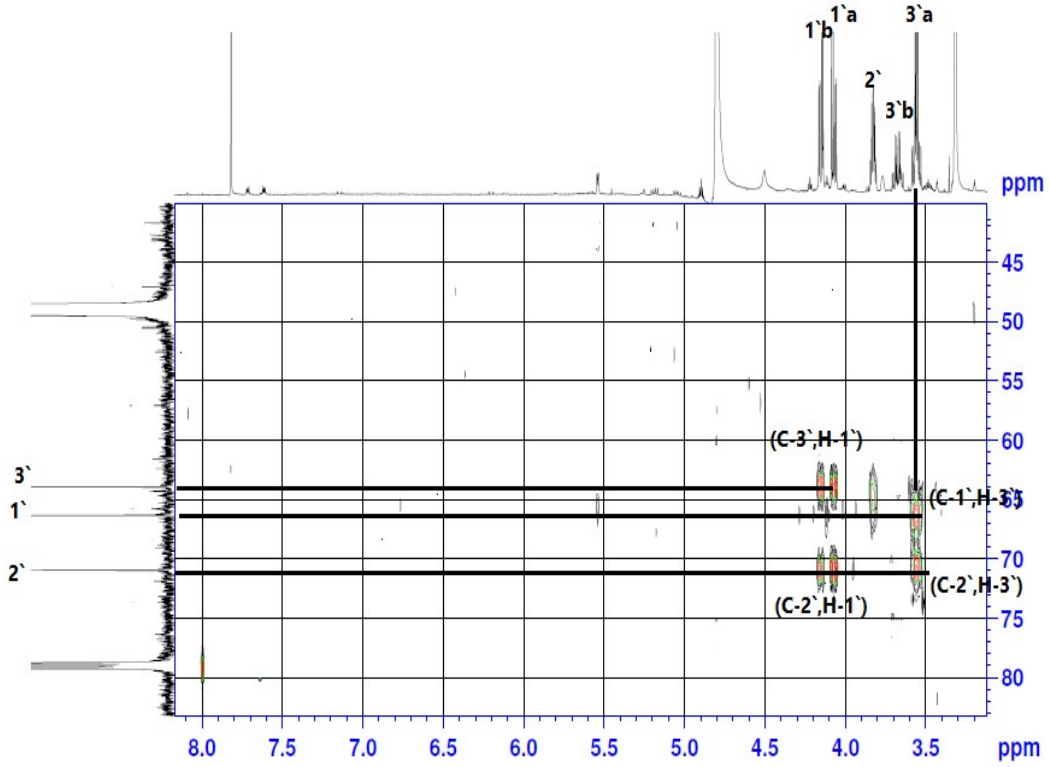

Figure (5.c): Expansion of HMBC spectrum of compound 2 at δ_H: 3.0-8.0 ppm and δ_c: 40-80 ppm.

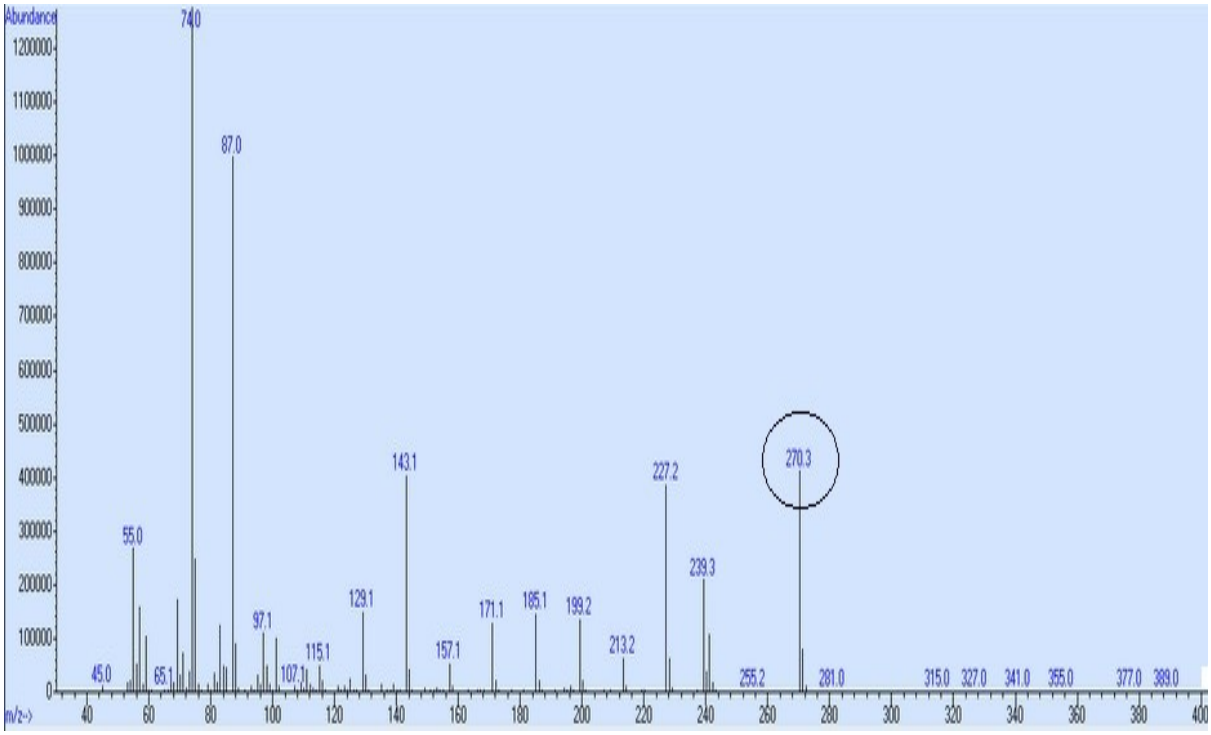

Figure (6): GC-MS of fatty acid methyl ester of compound 2 after hydrolysis.

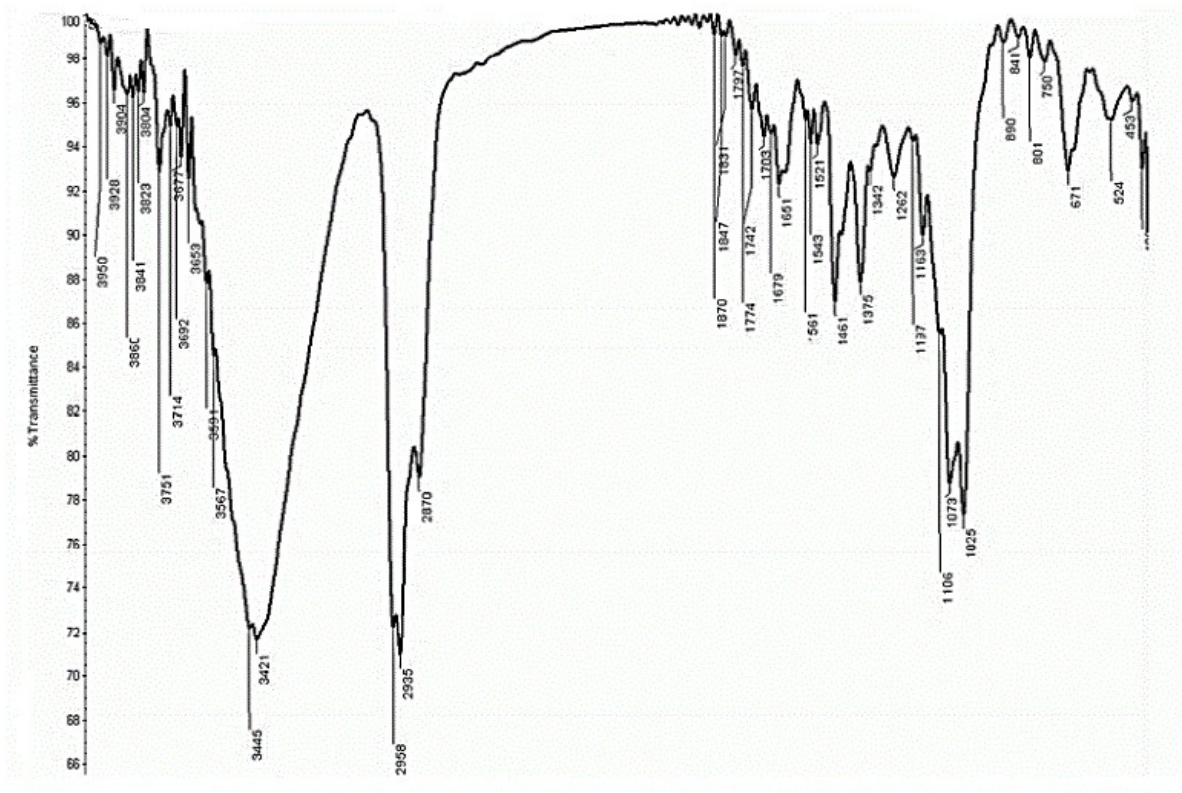

Figure (7): IR spectrum of compound 3 (KBr, U_{max} cm^{-1})

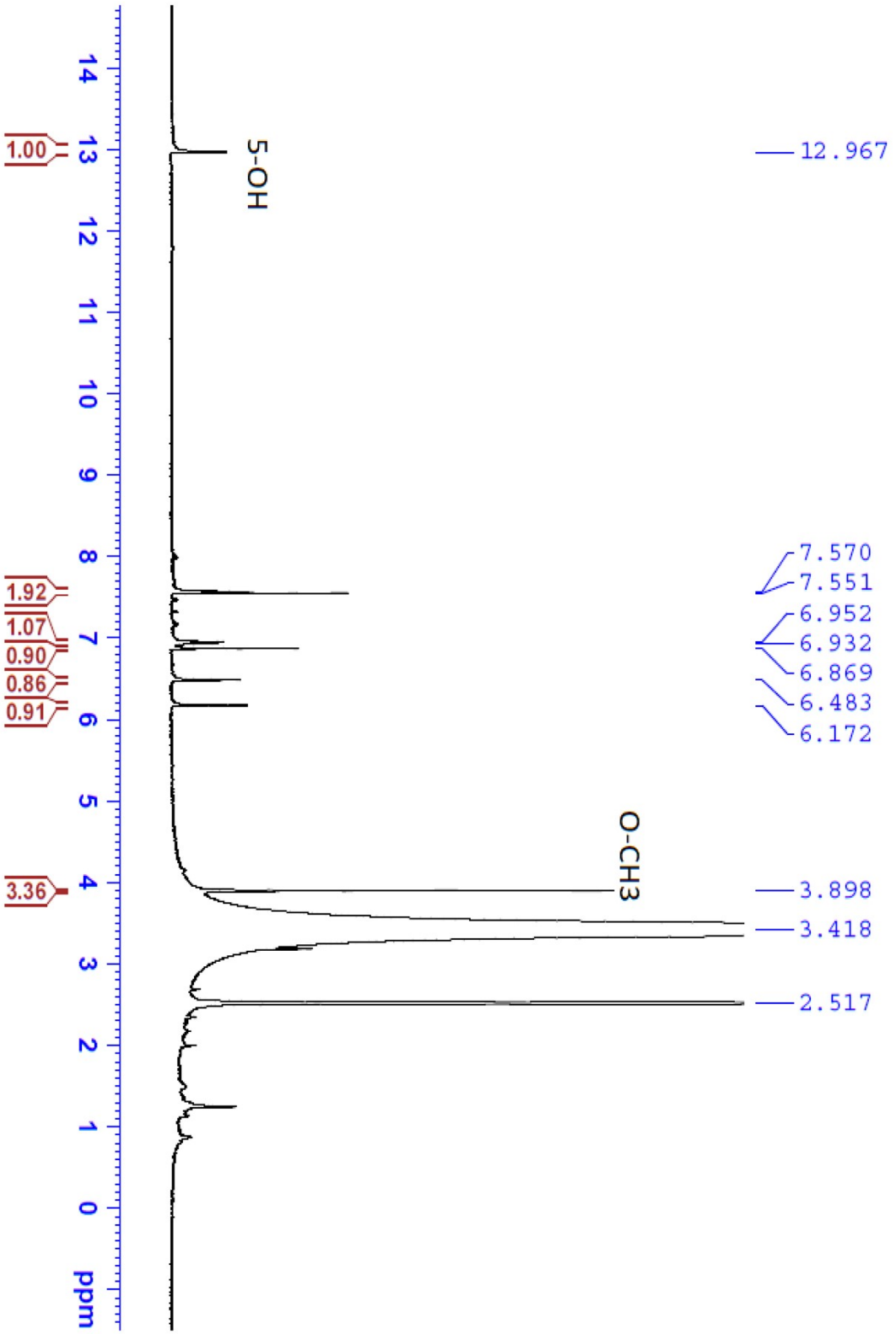

Fig. (8): ^{1}H-NMR spectrum of compound 4 in DMSO-d_6 at 400 MHz

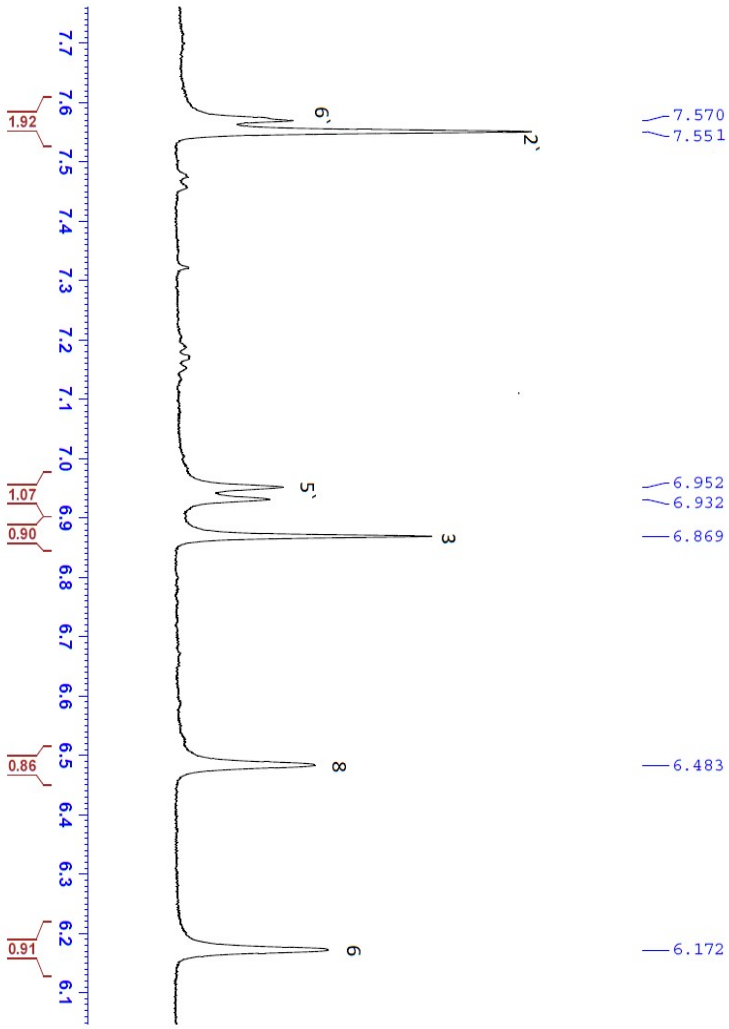

Fig. (8.a): Expansion of ^{1}H-NMR spectrum of compound 4 in DMSO-d_6 at δ_H: 6.1-7.7 ppm

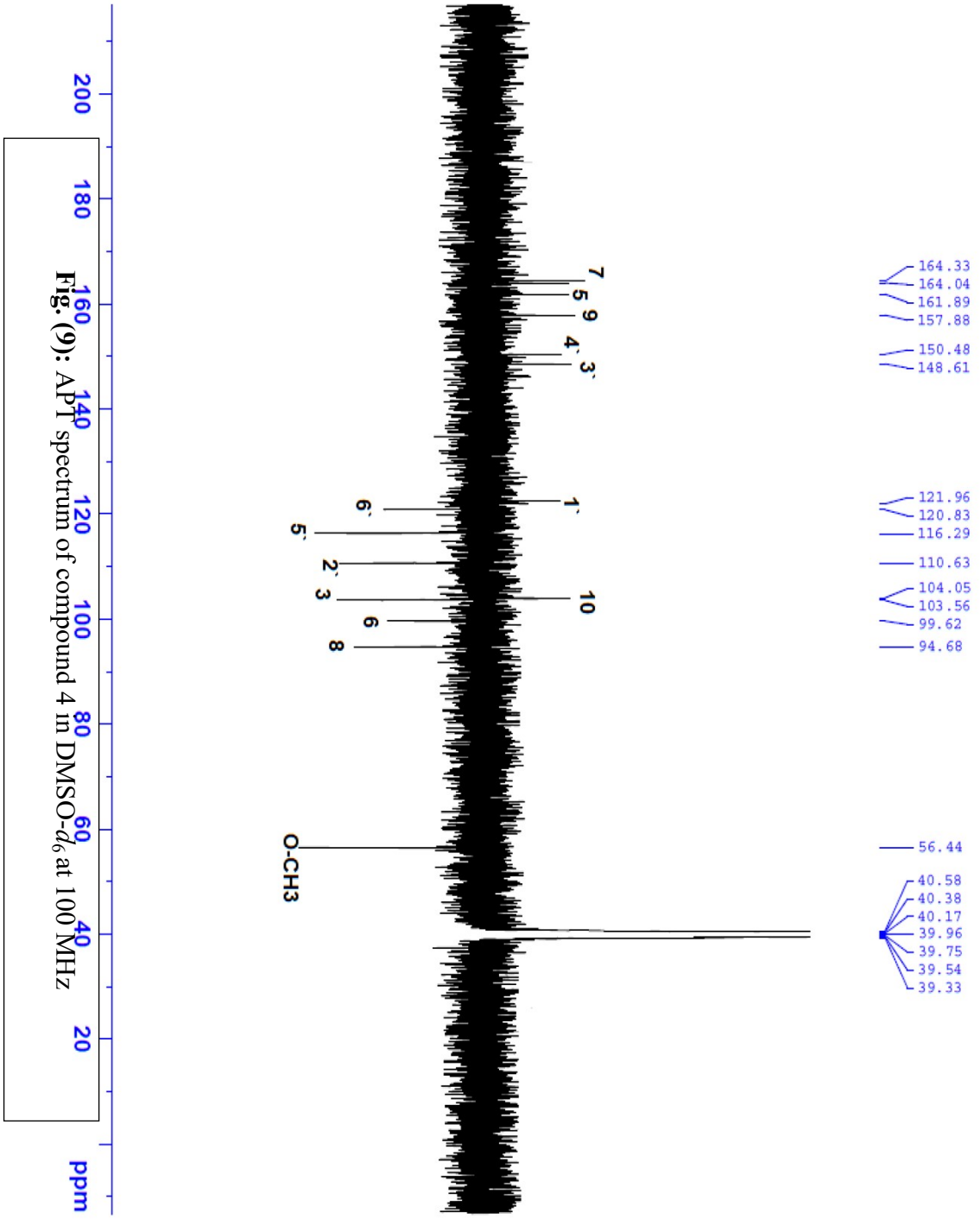

Fig. (9): APT spectrum of compound 4 in DMSO-d_6 at 100 MHz

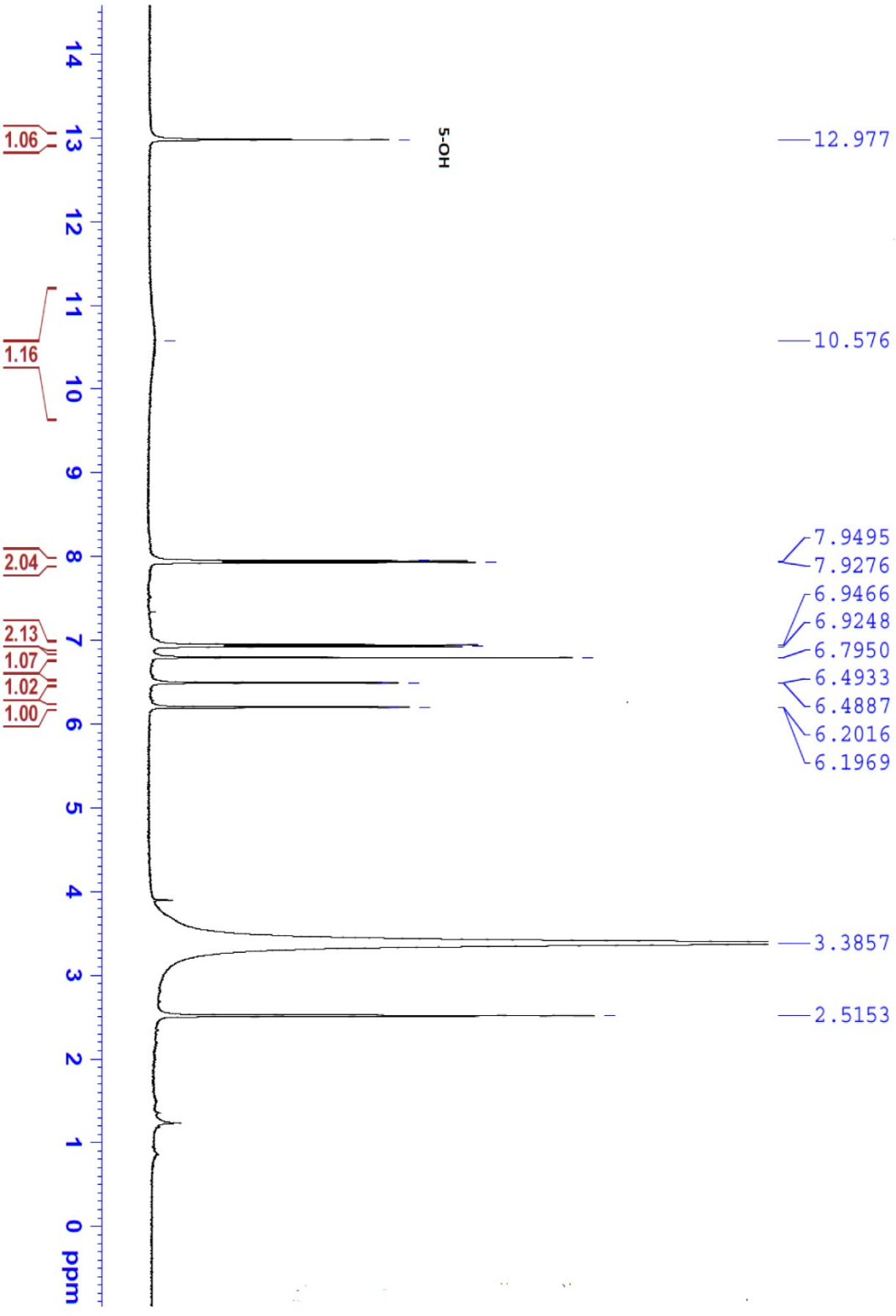

Fig. (10): ^{1}H-NMR spectrum of compound 5 in DMSO-d_6 at 400 MHz

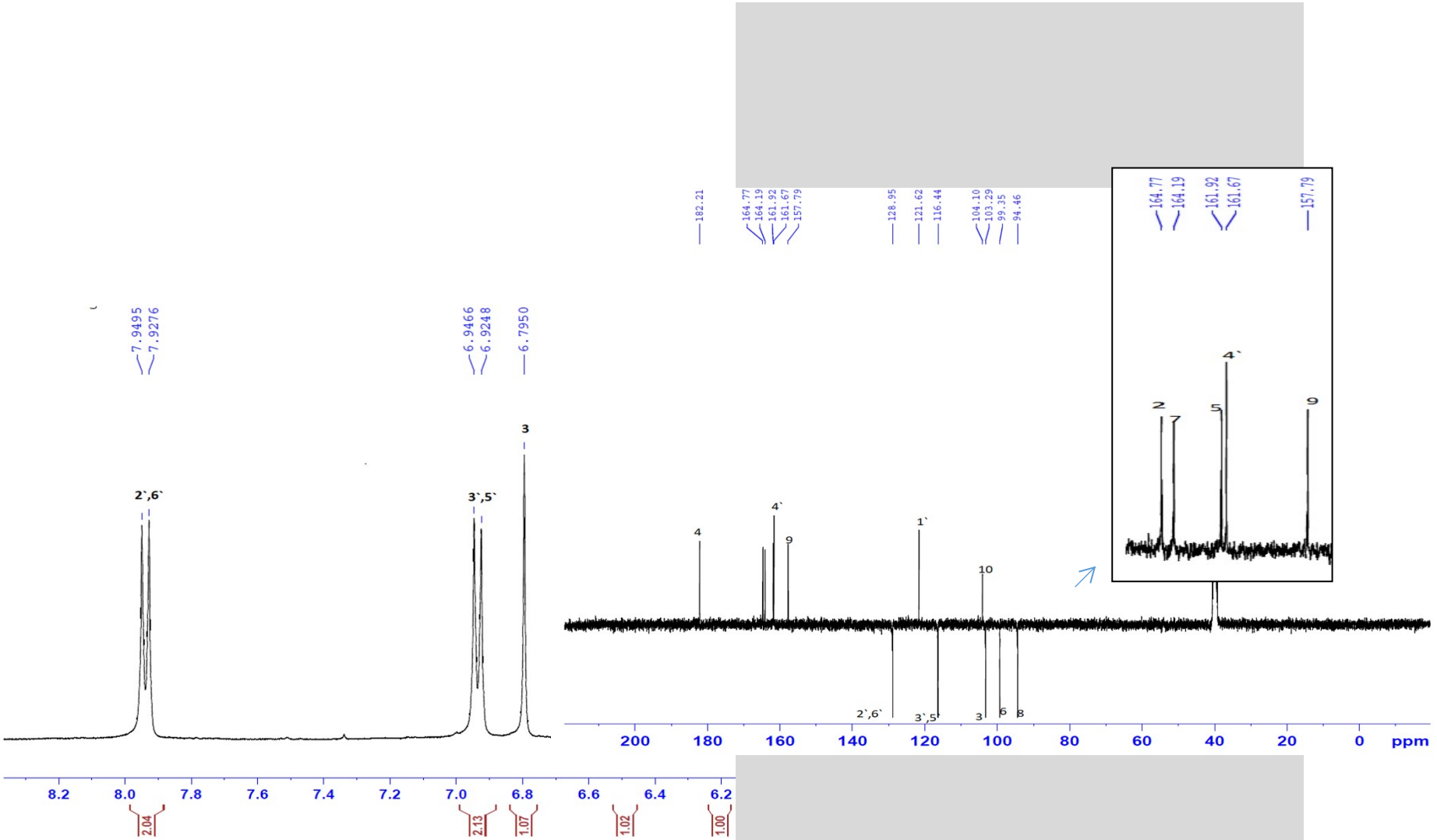

Fig. (11): APT spectrum of compound 5 in DMSO-d_6 at 100 MHz

Fig. (10.a): Expansion of ^{1}H-NMR spectrum of compound 5 in DMSO-d_6 at the range (6.0-8.2) ppm.

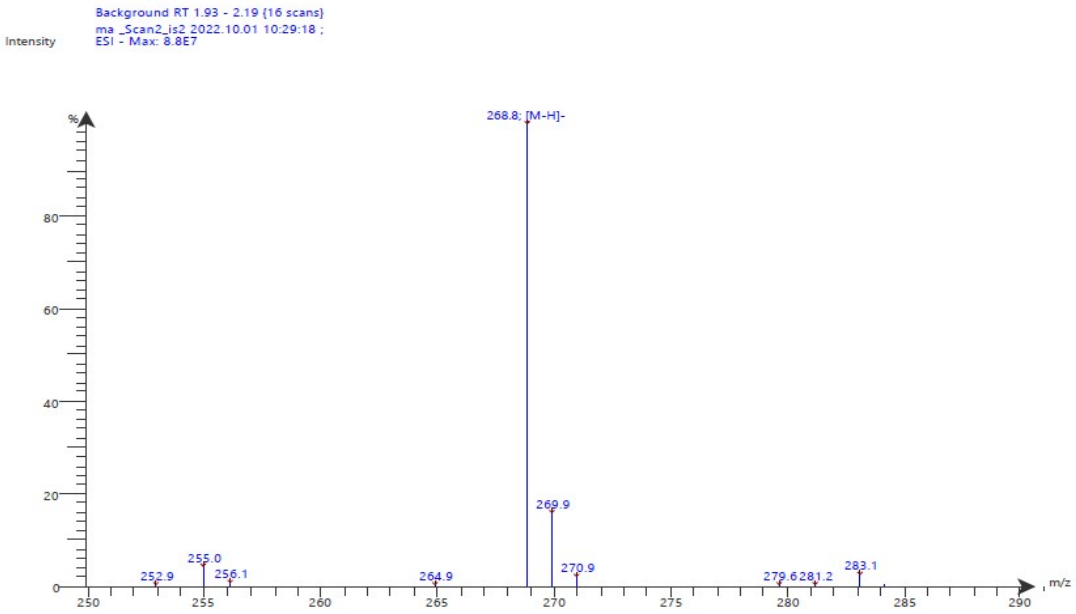

Fig. (12): Negative ESI -MS spectrum of compound 5.

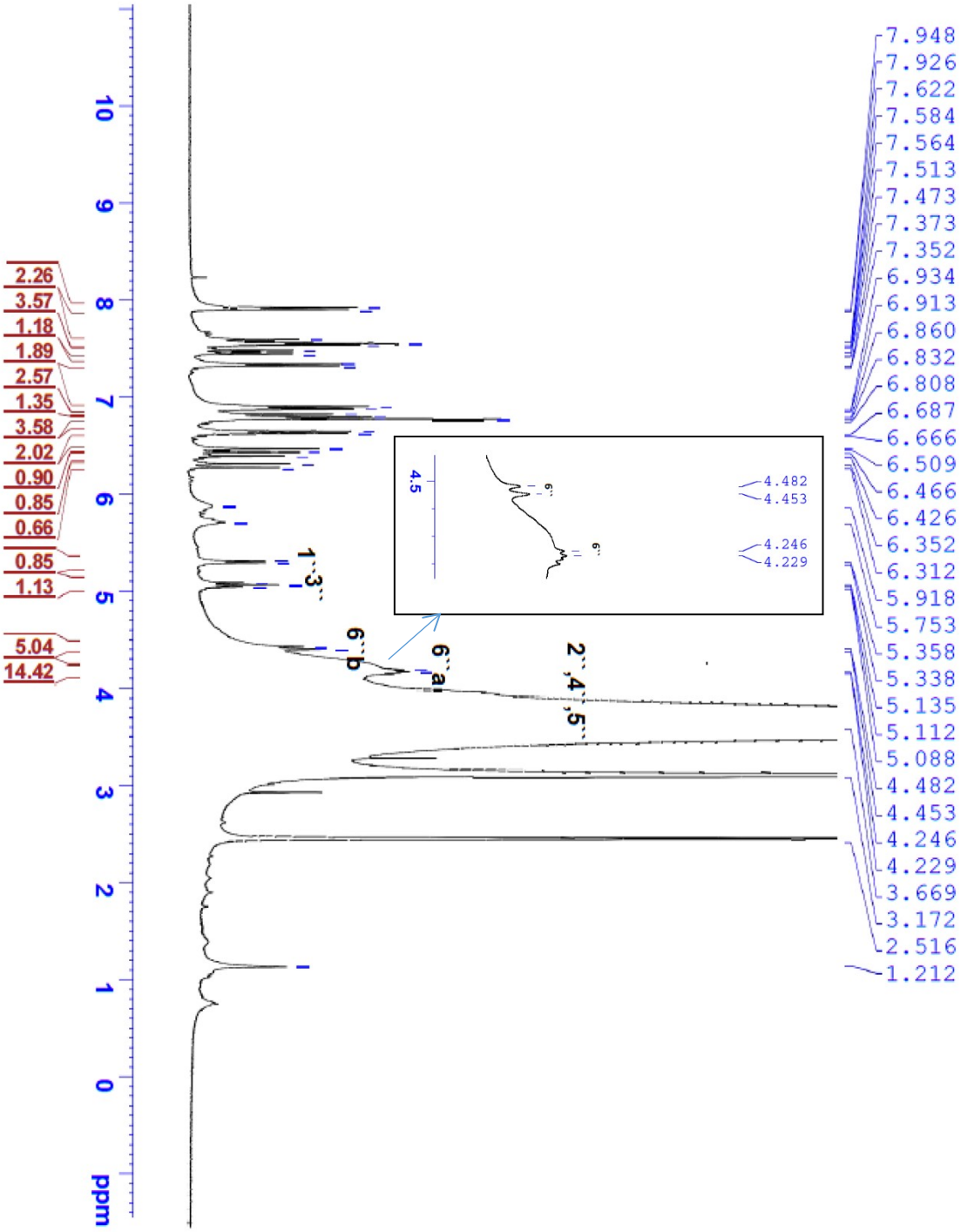

Fig. (13): ^{1}H-NMR spectrum of compound 6 in DMSO-d_6 at 400 MHz

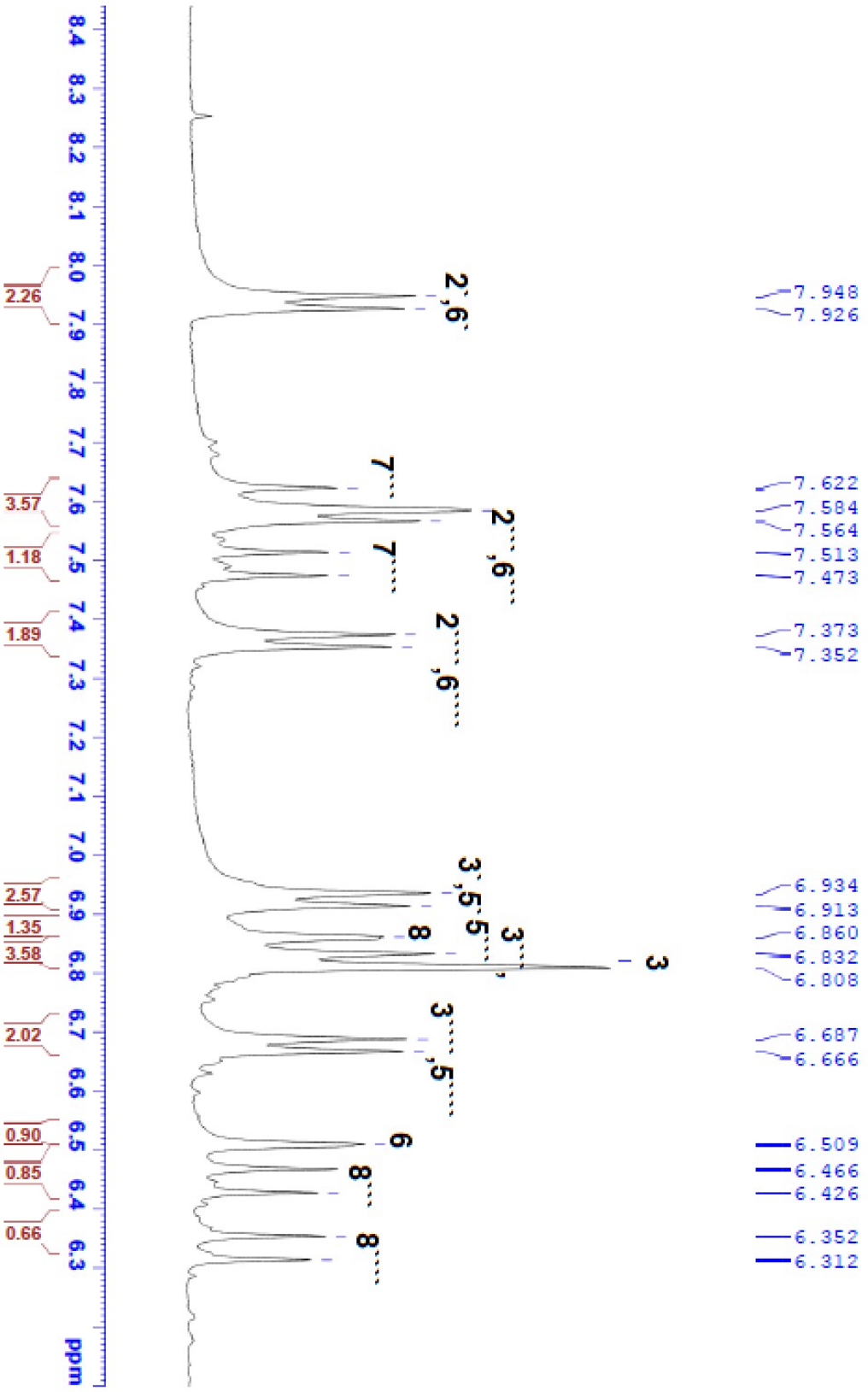

Fig. (13.a): Expansion of ^{1}H-NMR spectrum of compound 6 in DMSO-d_6 at the range (6.2-8) ppm.

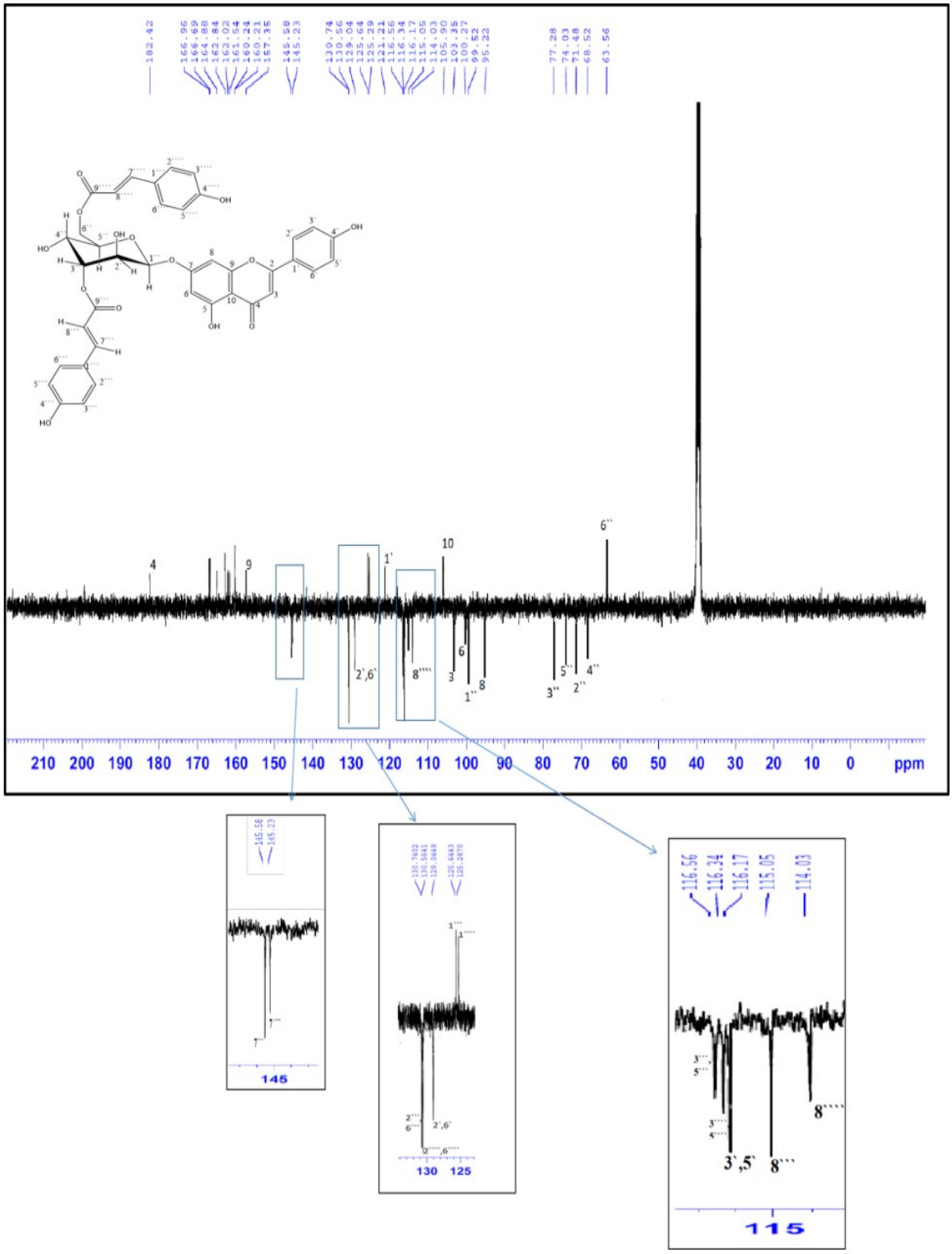

Fig. (14): APT spectrum of compound 6 in DMSO-d_6 with its expansions at 100 MHz

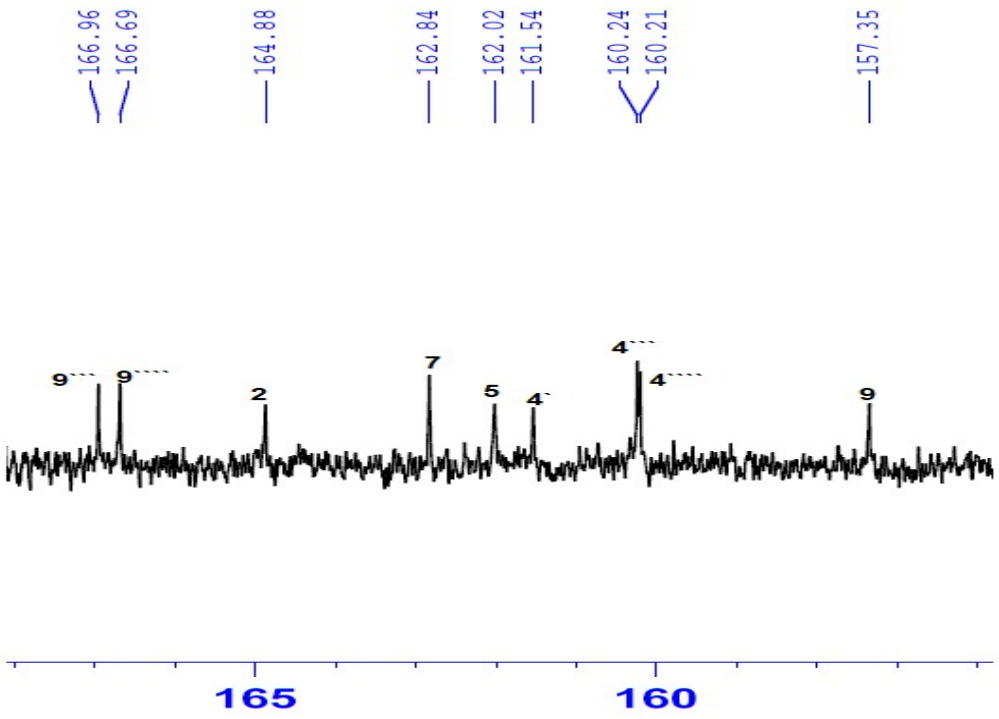

Fig. (14.a): Expansion of APT spectrum of compound 6 in DMSO-d_6 at δ_C: 156-168 ppm.

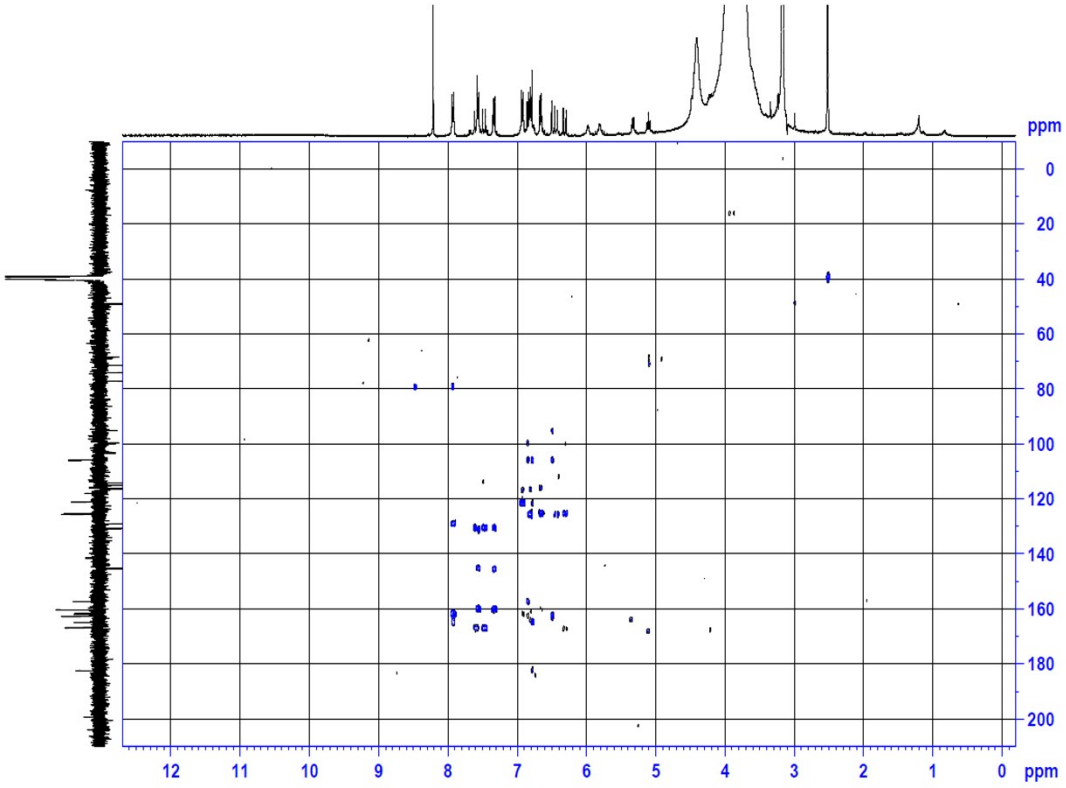

Figure (15): HMBC of compound 6 in DMSO-d_6.

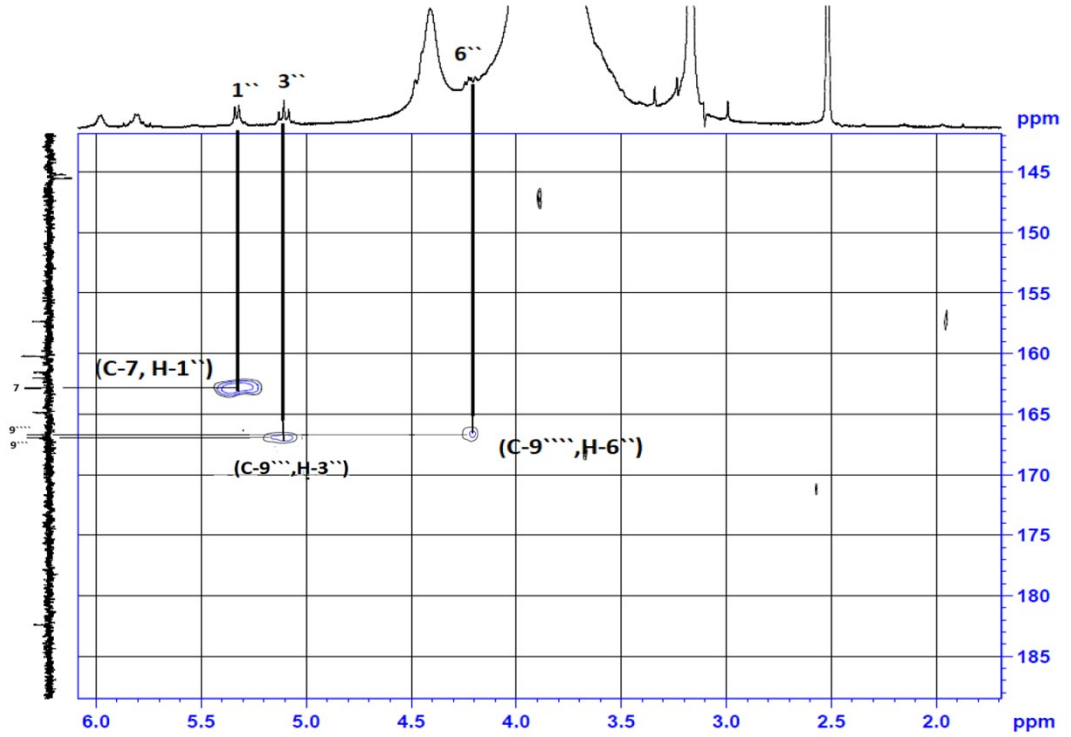

Figure (15.a): Expansion of HMBC spectrum of compound 6 at δ_H: 1.7-6.0 ppm and at δ_C: 142-187 ppm

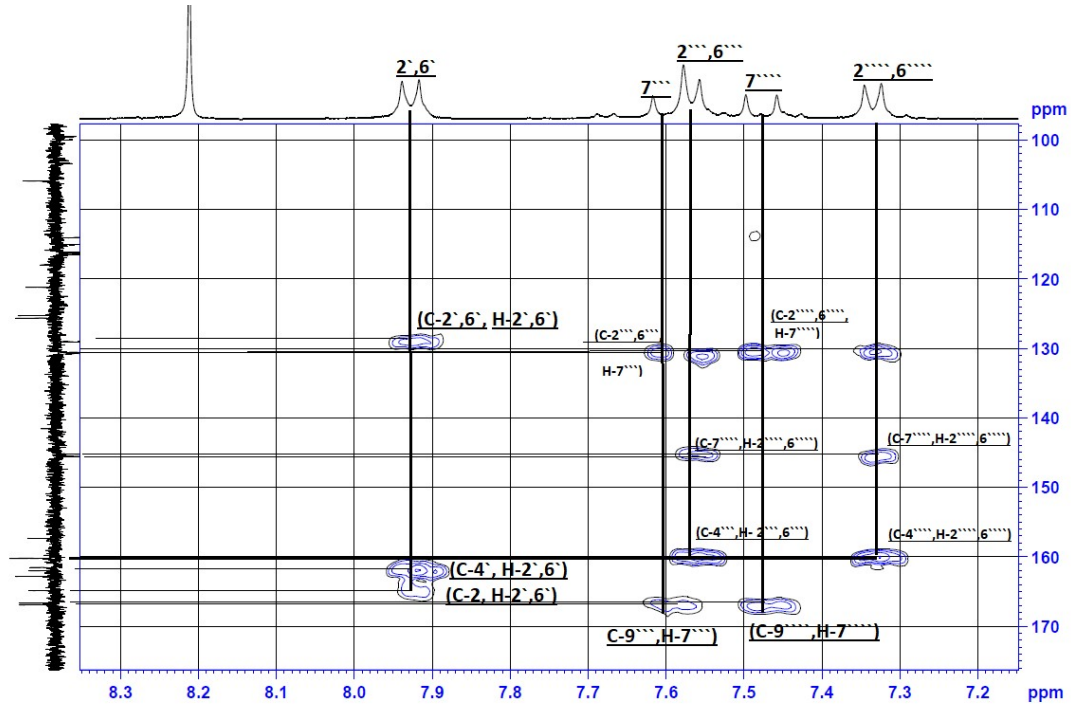

Figure (15.b): Expansion of HMBC spectrum of compound 6 at δ_H: 7.2-8.3 ppm and at δ_C: 100-175 ppm

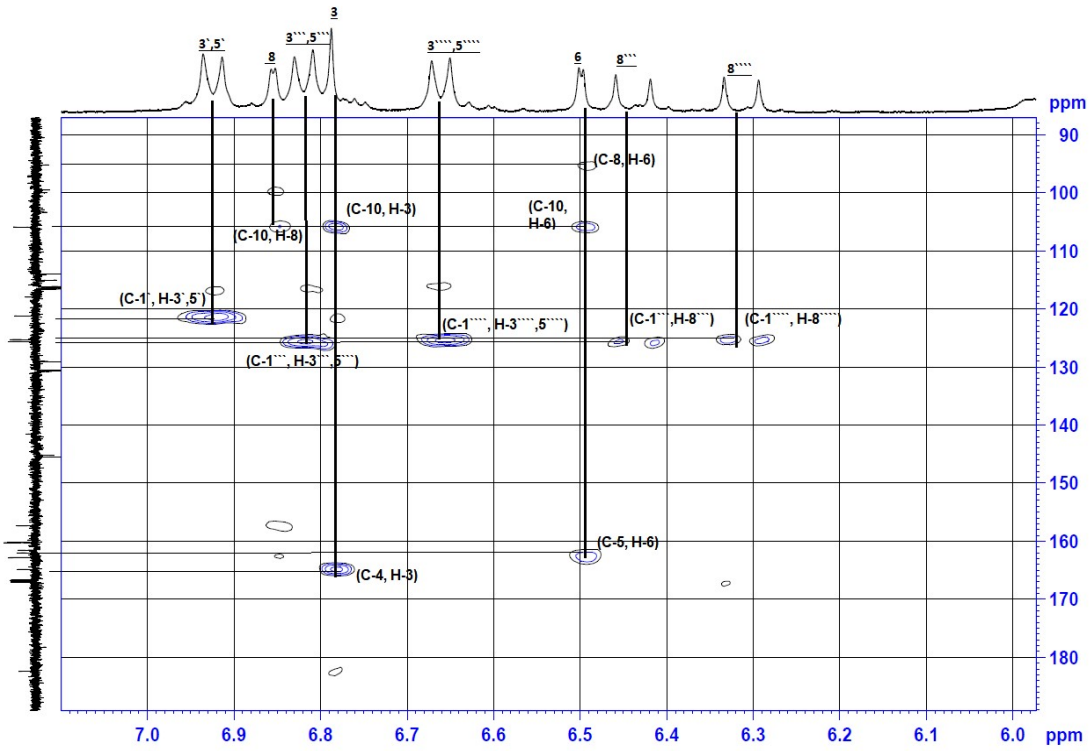

Figure (15.c): Expansion of HMBC spectrum of compound 6 at δ_H: 7.2-8.3 ppm and at δ_C: 90-190 ppm

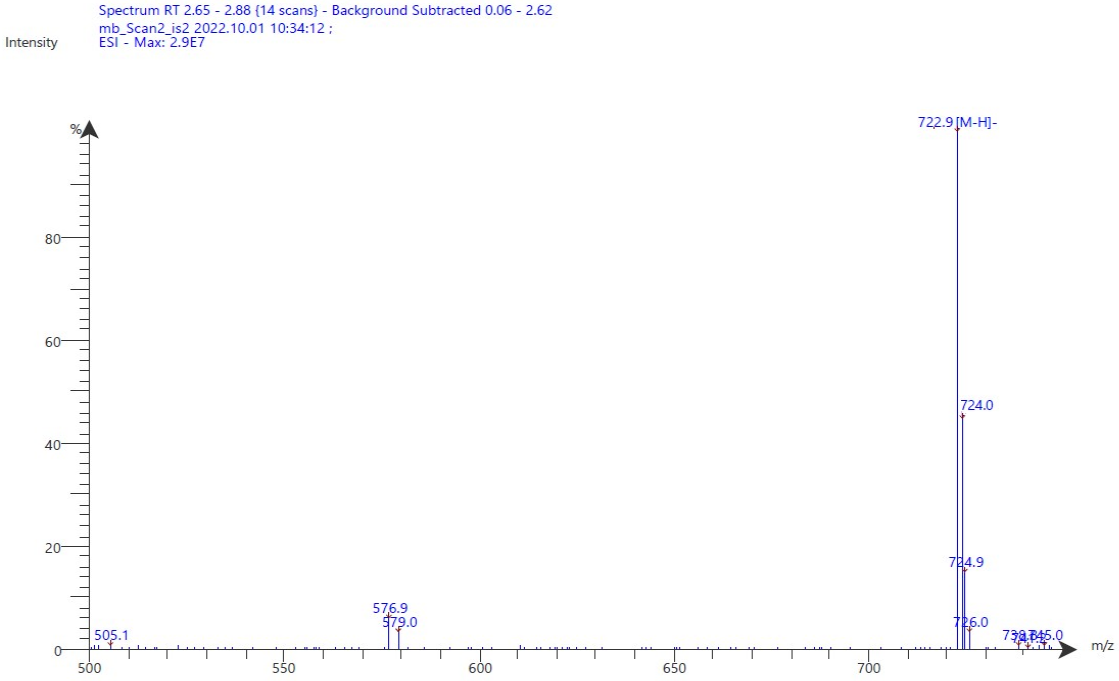

Fig. (16): Negative ESI -MS spectrum of 6.

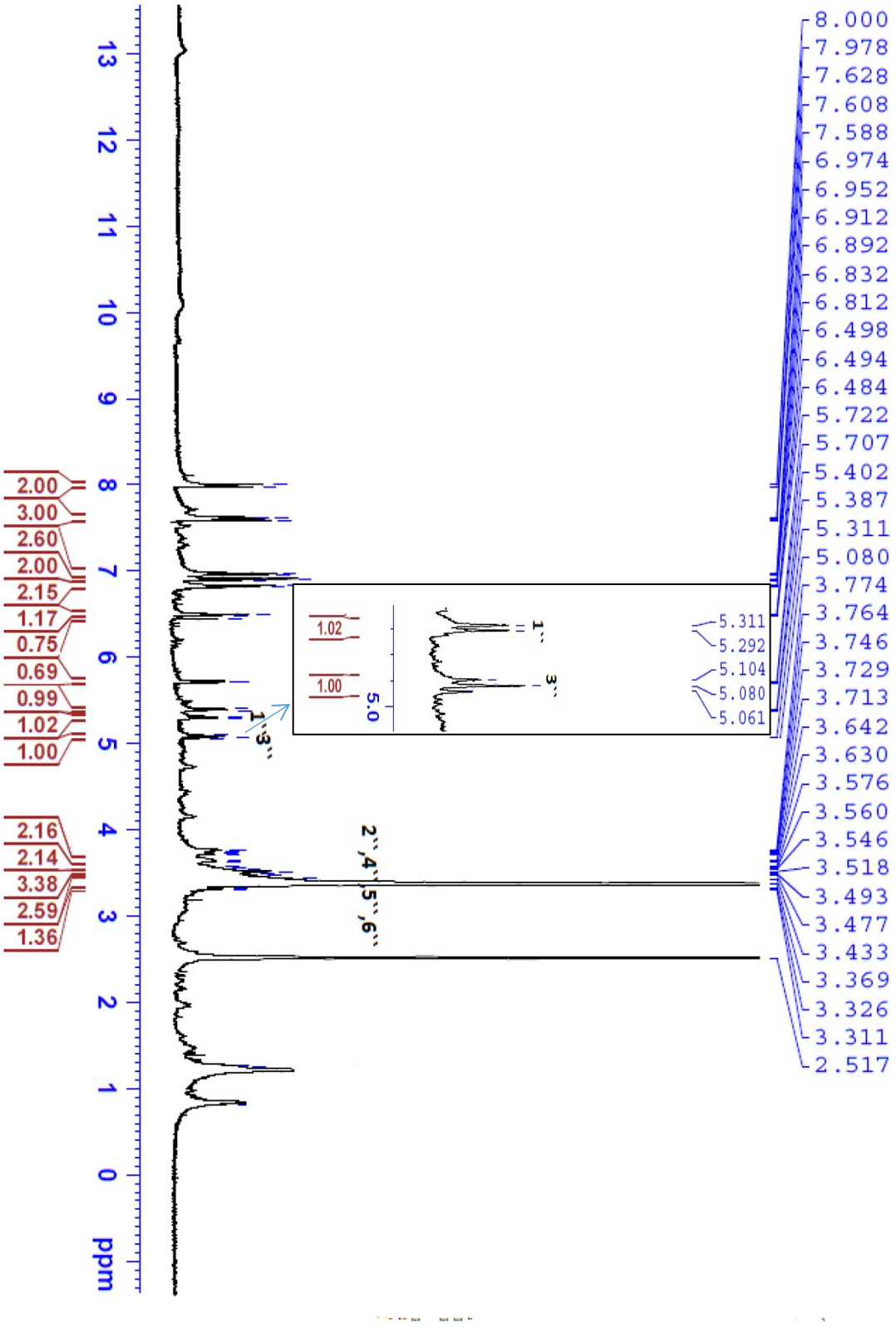

Fig. (17): ^{1}H-NMR spectrum of compound 7 in DMSO-d_6 at 400 MHz

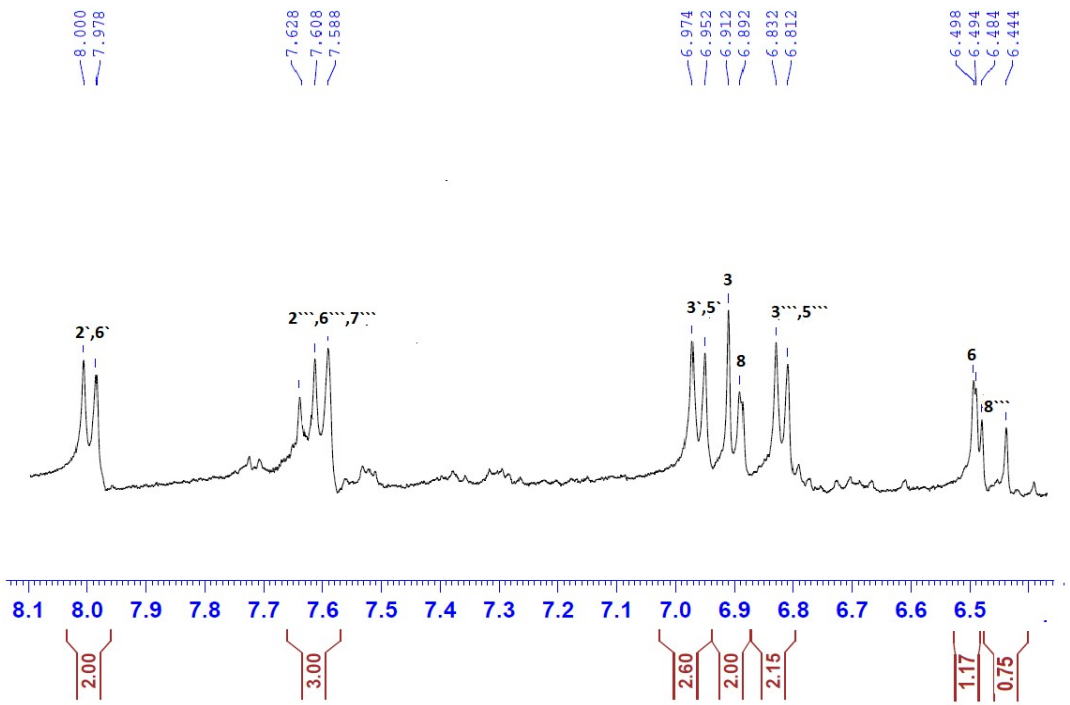

Fig. (17.a): expansion of ^{1}H-NMR spectrum of compound 7 in DMSO-d_6 at the range (6.4-8.1) ppm.

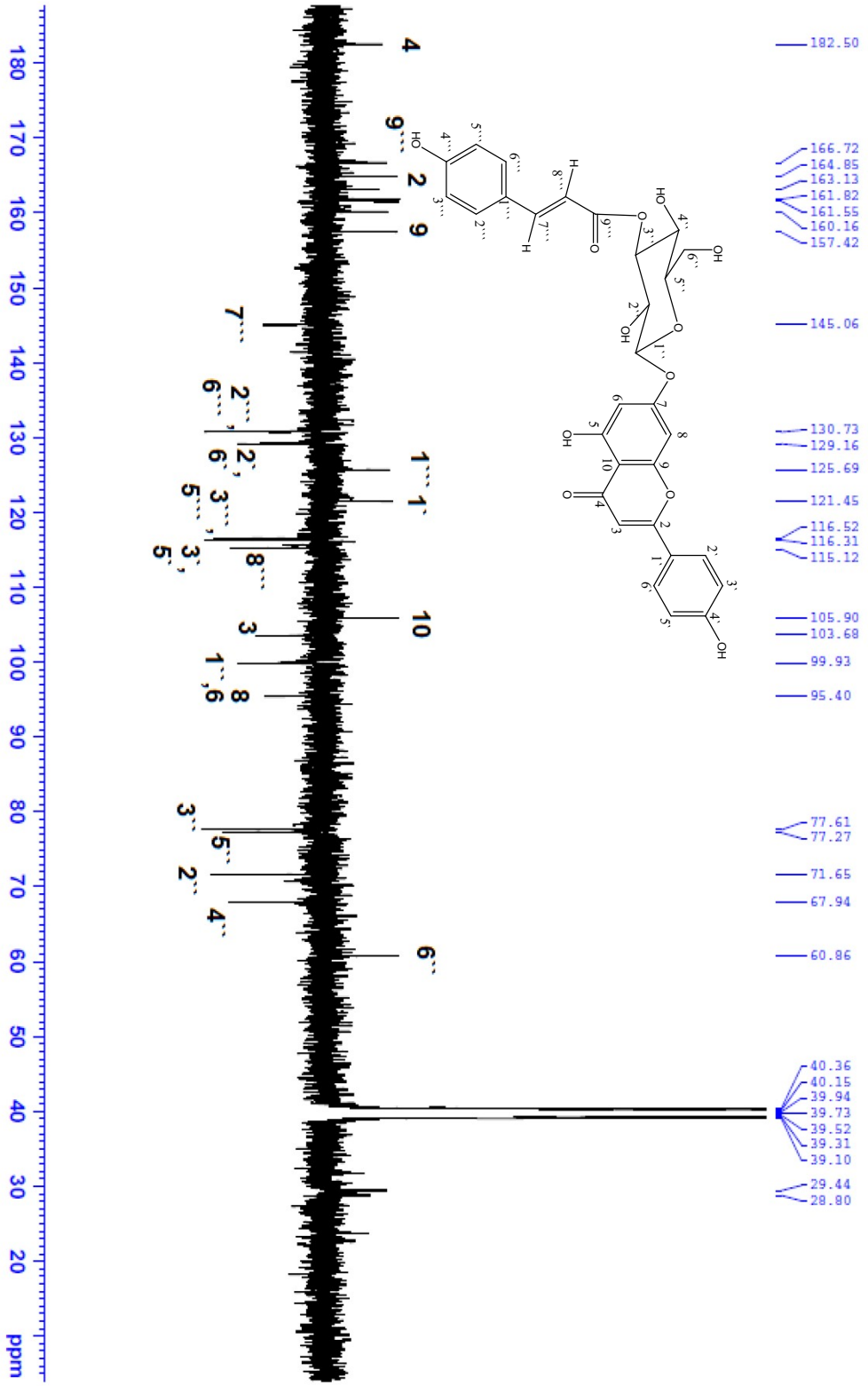

Fig. (18): APT spectrum of compound 7 in DMSO-d_6 at 100 MHz

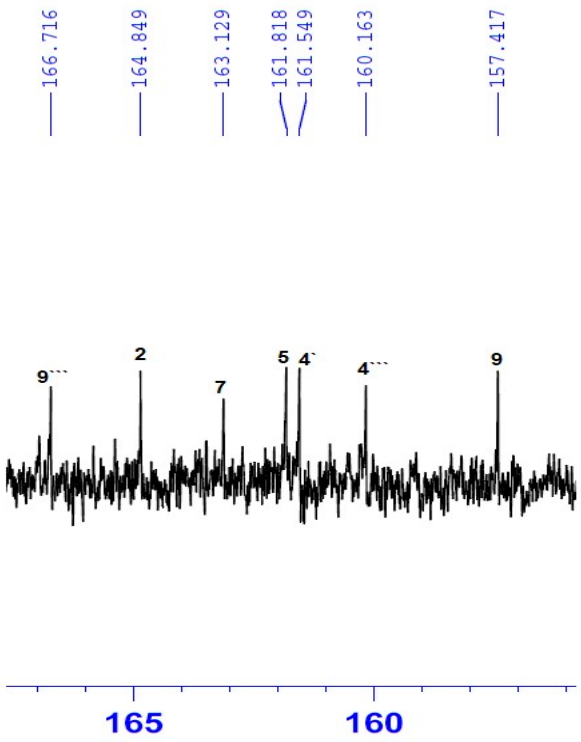

Fig. (18.a): Expansion of APT spectrum of compound 7 in DMSO-d_6 at the range 155-168 ppm.

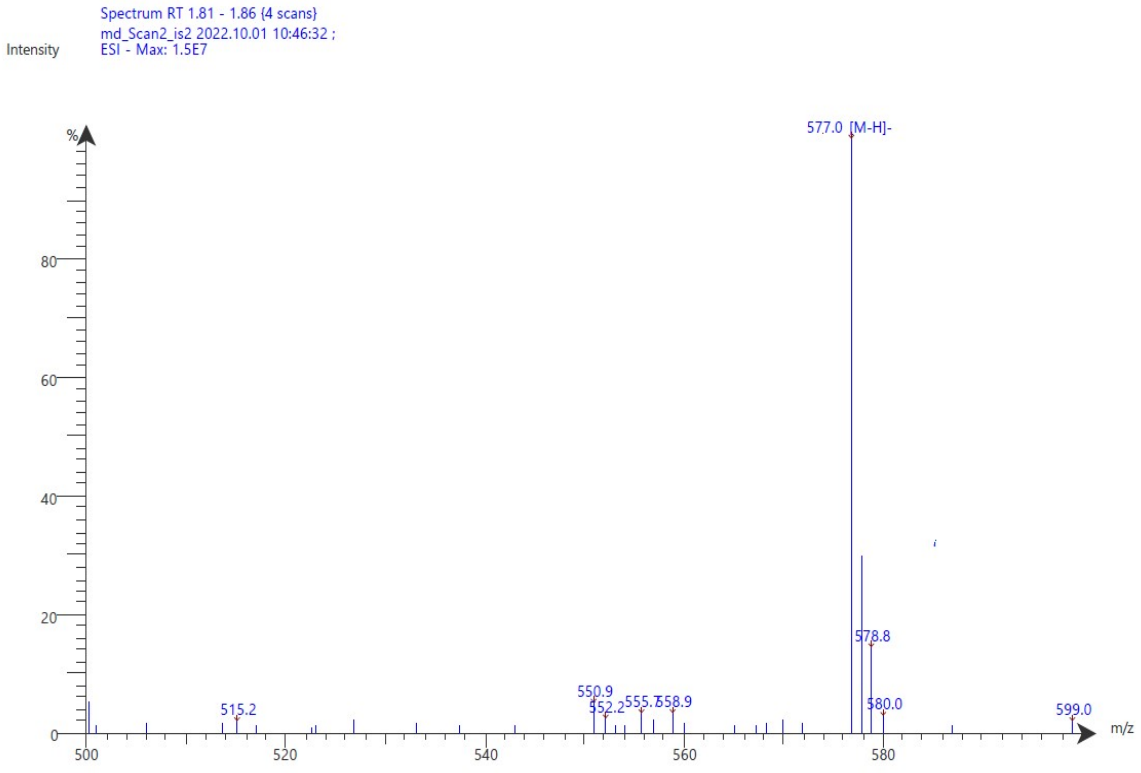

Fig. (19): Negative ESI -MS spectrum of compound 7.

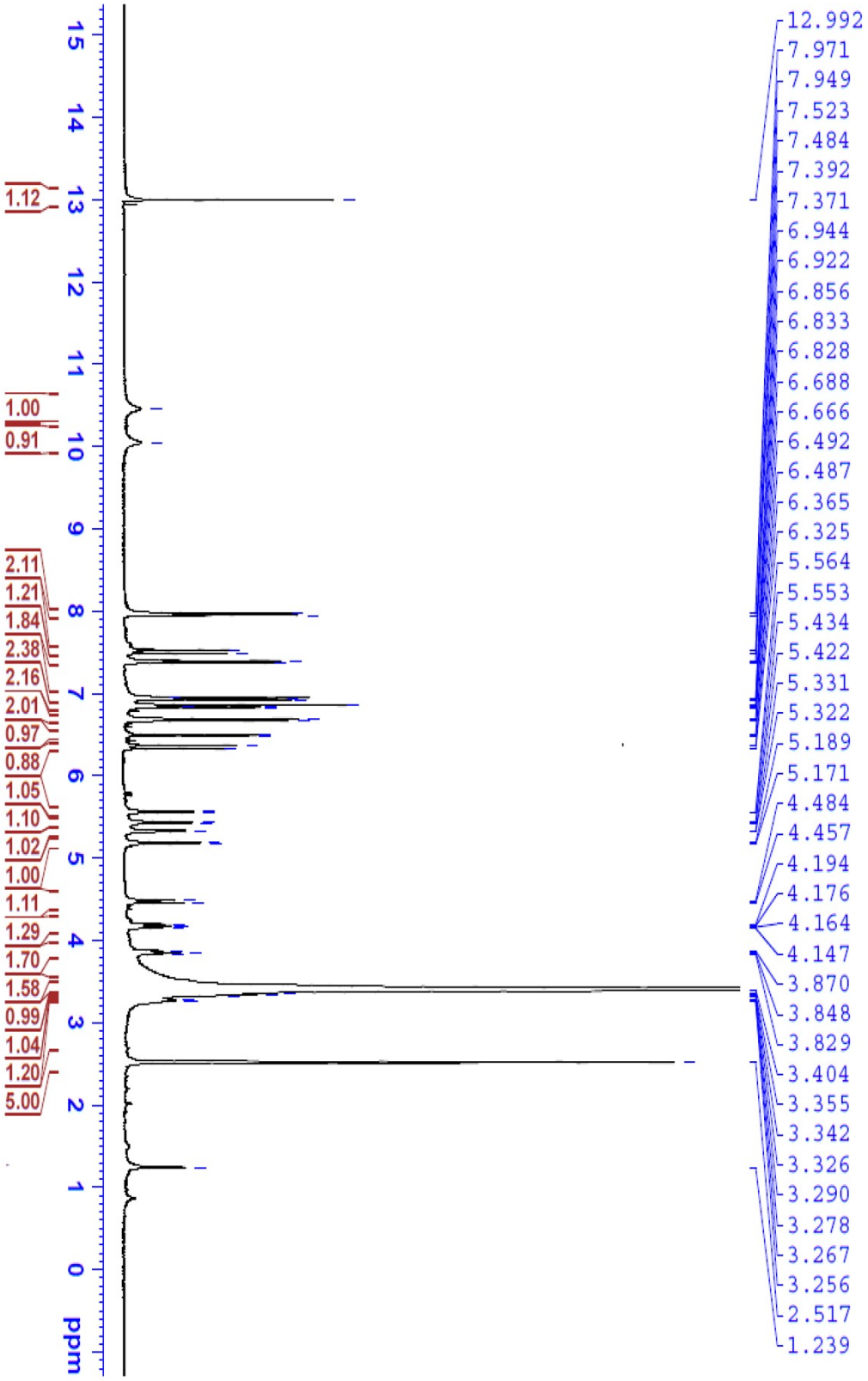

Fig. (20): ^{1}H-NMR spectrum of compound 8 in DMSO-d_6 at 400 MHz

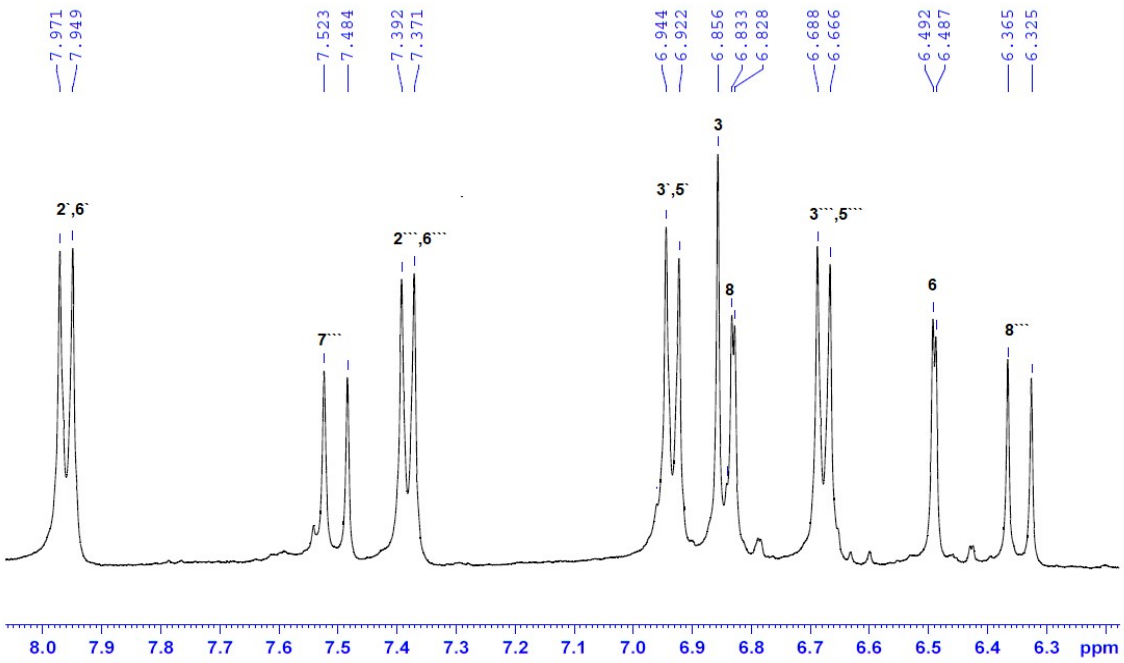

Fig. (20.a): Expansion of ^{1}H-NMR spectrum of compound 8 in DMSO-d_6 at the range 6.3-8 ppm**.**

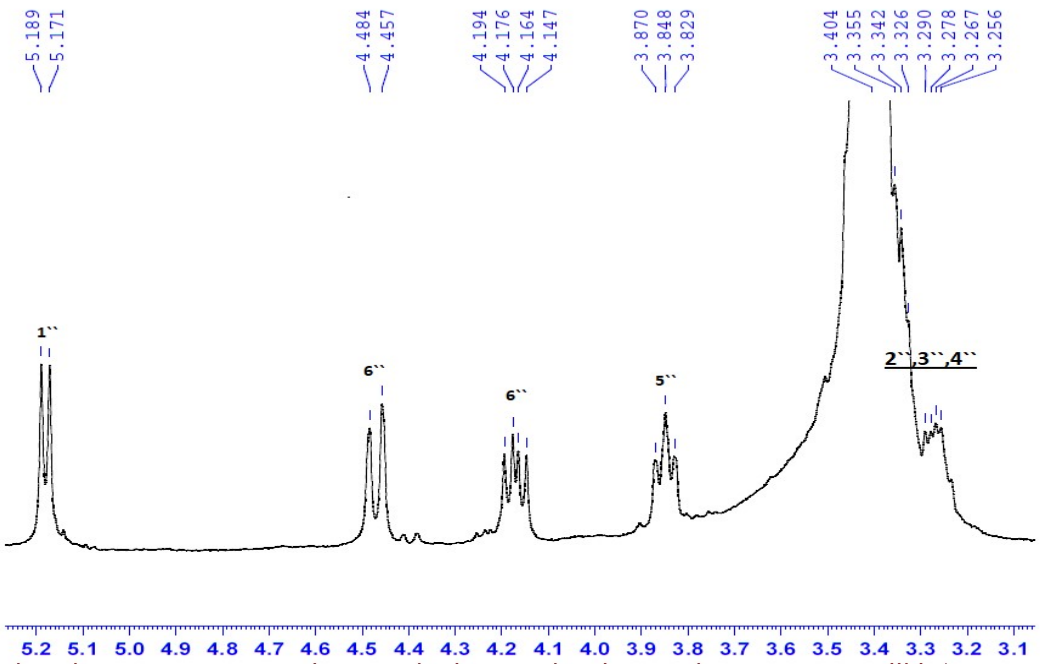

Fig. (20.b): Expansion of ^{1}H-NMR spectrum of compound 8 in DMSO-d_6 at the range 3.1-5.2 ppm.

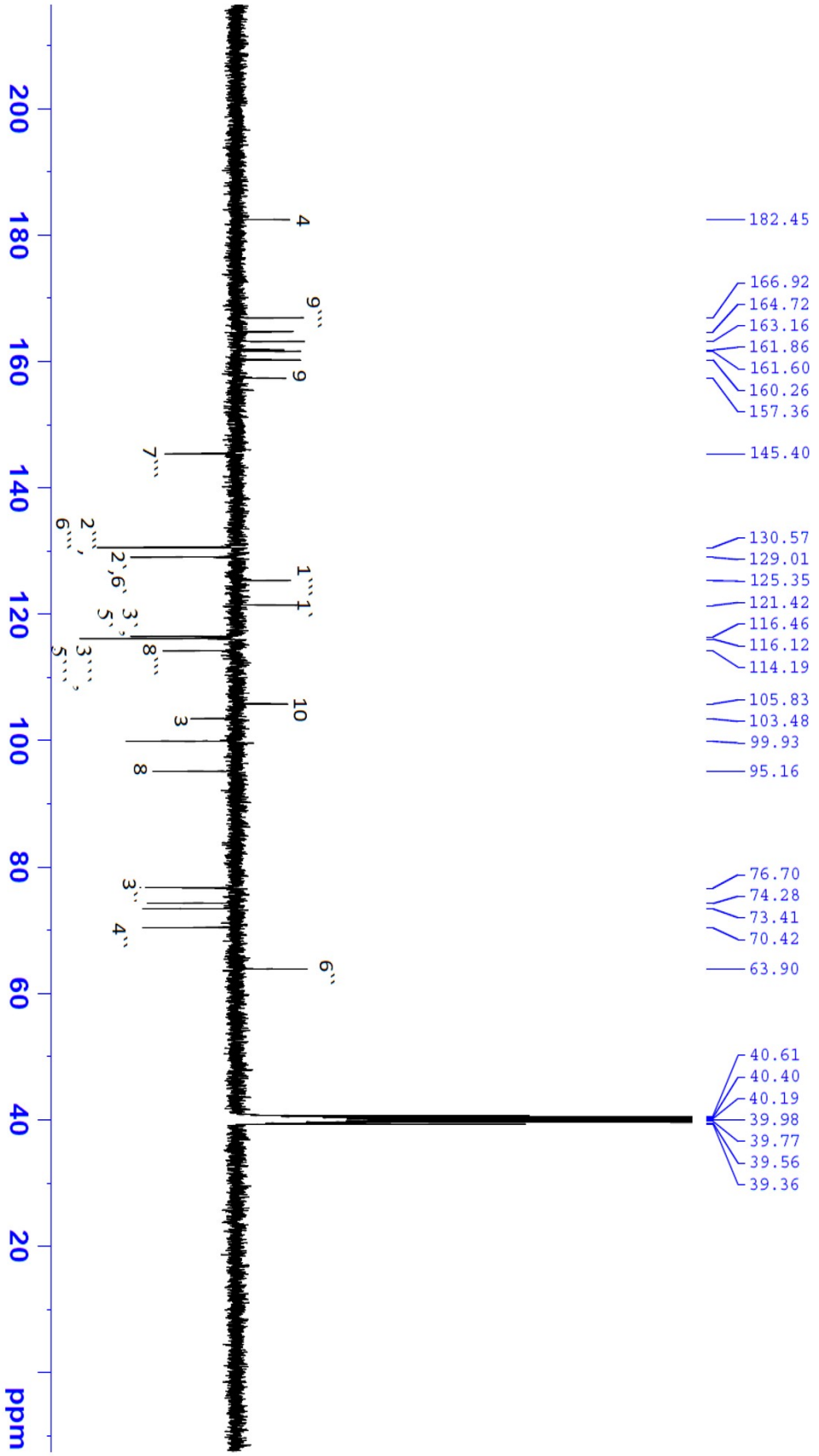

Fig. (21): APT spectrum of compound 8 in DMSO-d_6 at 100 MHz

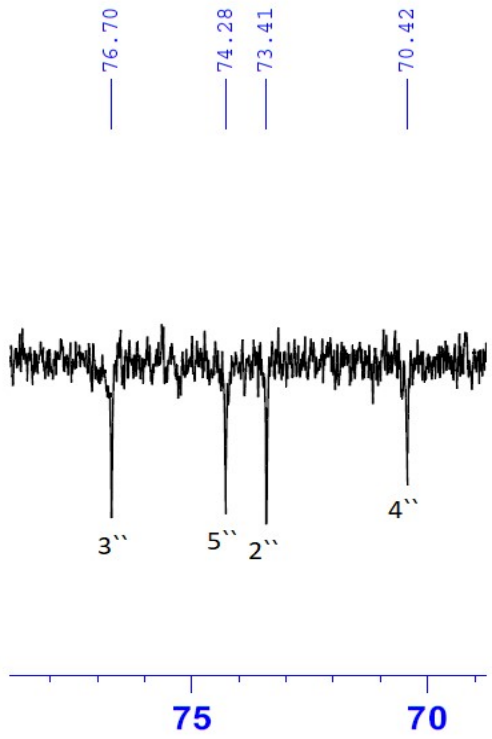

Fig. (21.a): Expansion of APT spectrum of compound 8 in DMSO-d_6 at the range 70-77 ppm.

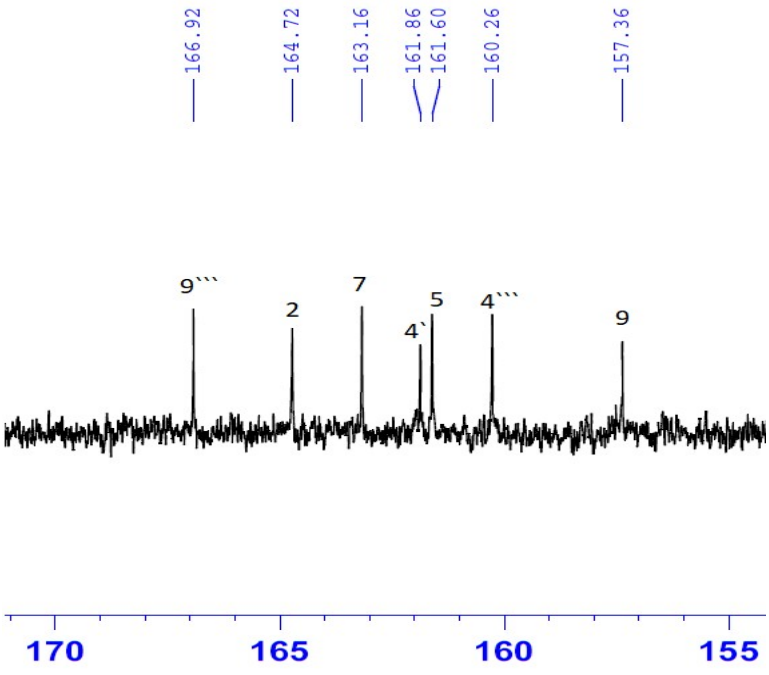

Fig. (21.b): Expansion of APT spectrum of compound 8 in DMSO-d_6 at the range 155-170 ppm.

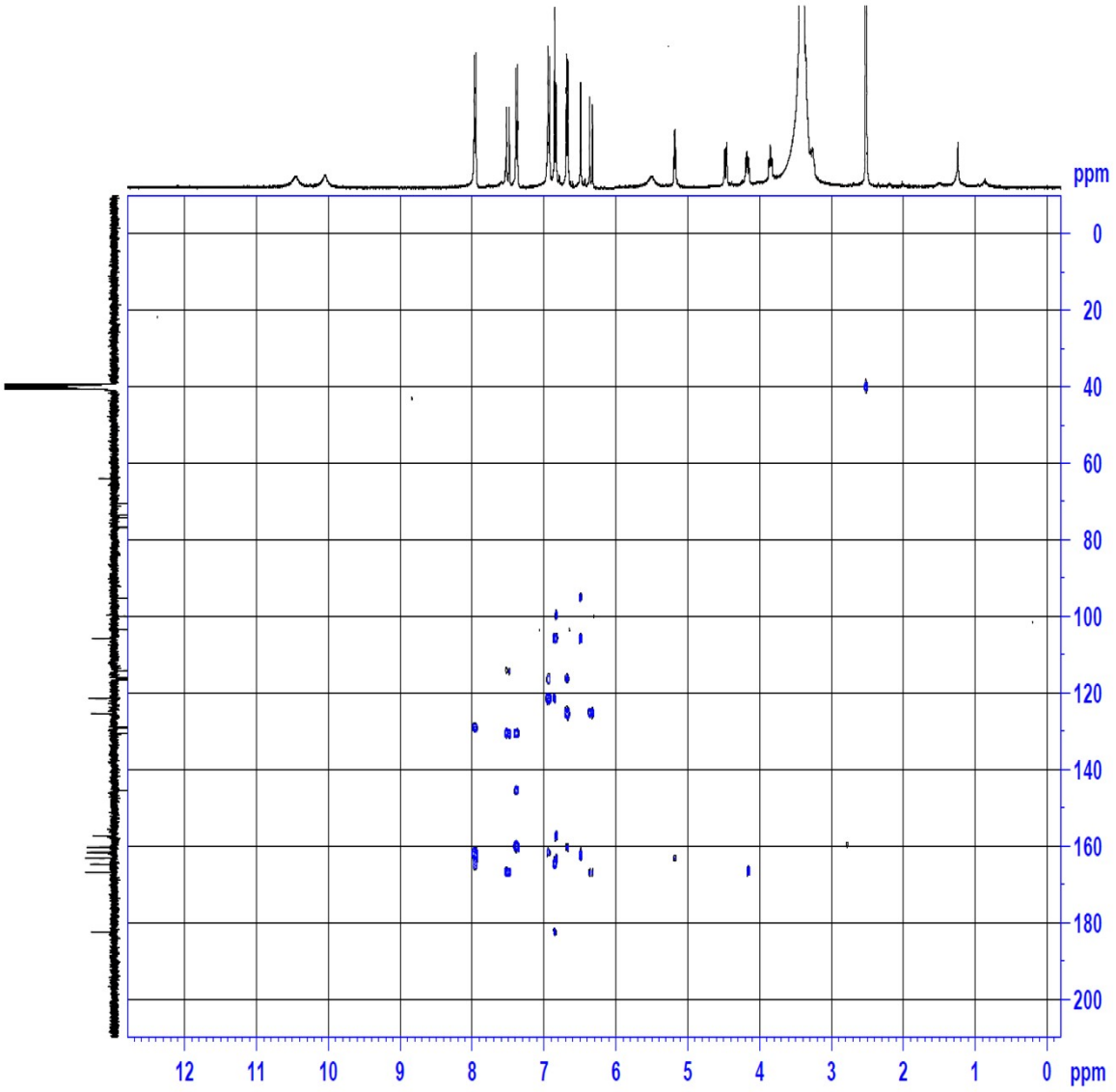

Figure (22): HMBC of compound 8 in DMSO-d_6.

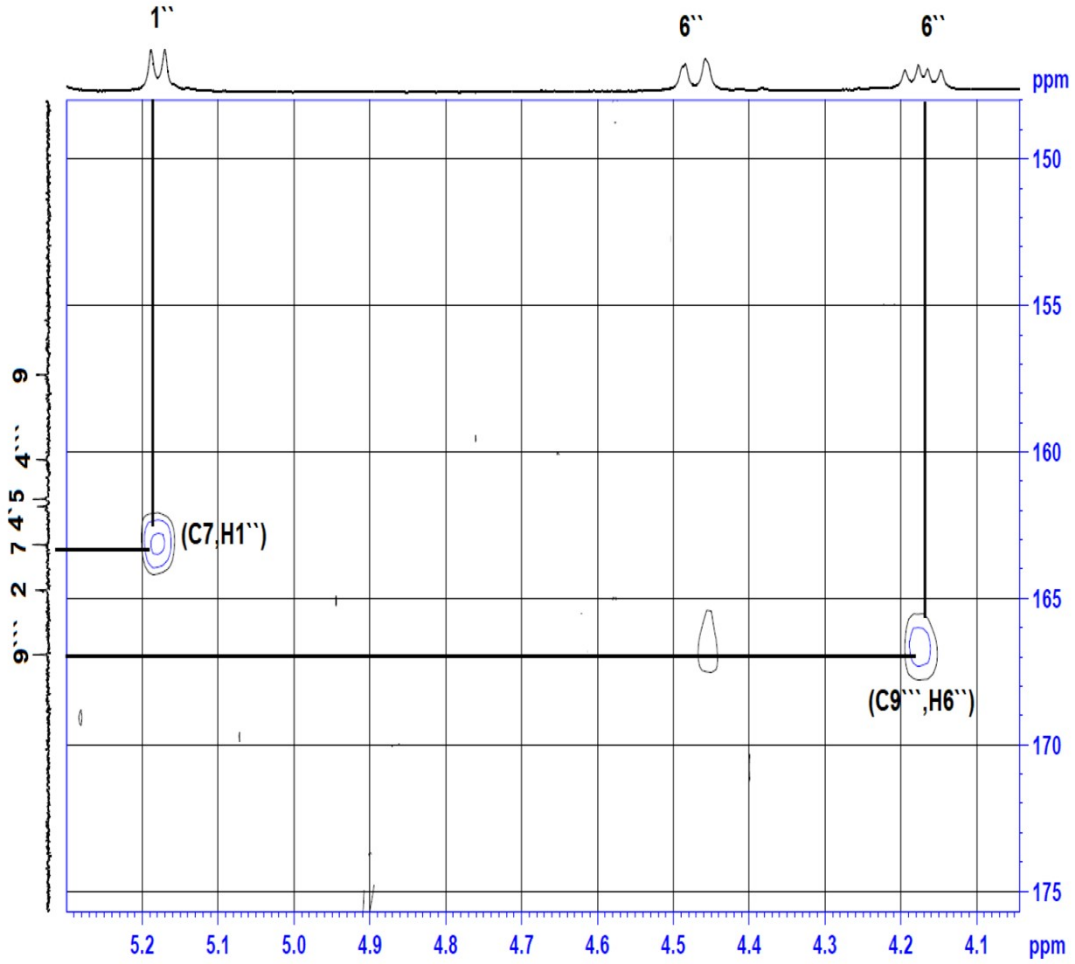

Figure (22.a): Expansion of HMBC spectrum of compound 8 at δ_H: 4-5.3 ppm and δ_C: 148-175 ppm.

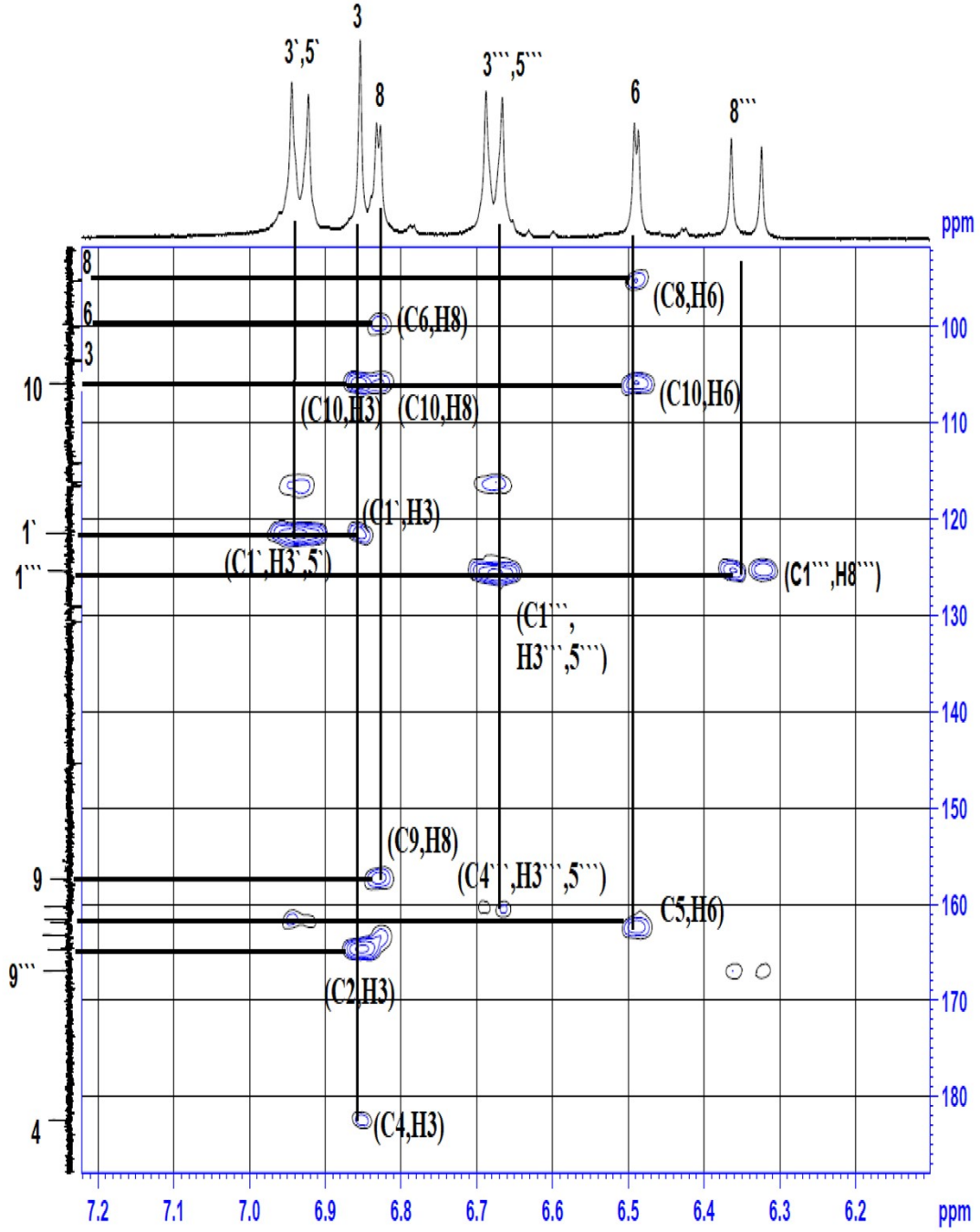

Figure (22.b): Expansion of HMBC spectrum of compound 8 at δ_H: 6.1-7.2 ppm and δ_C: 90-170 ppm

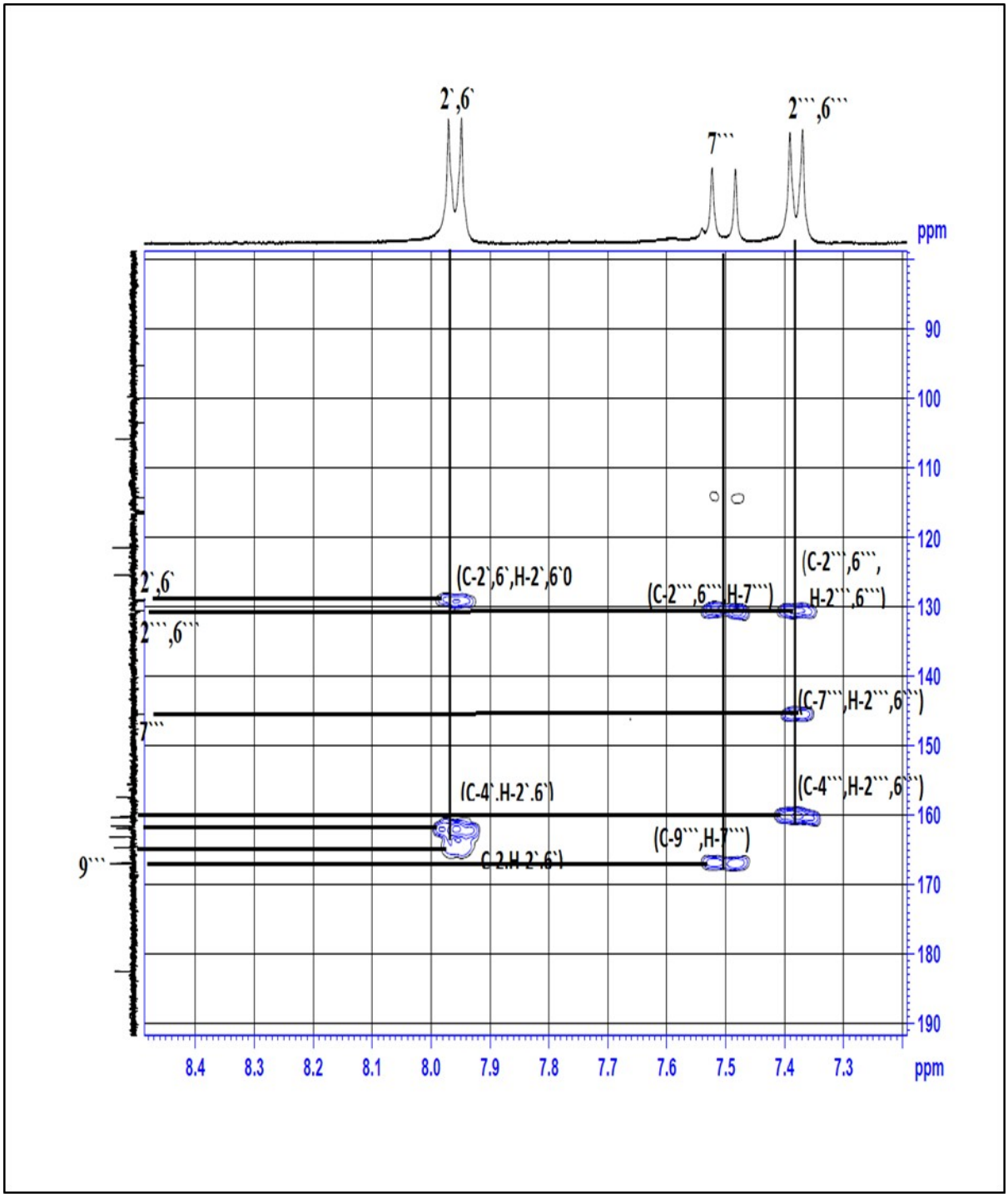

Figure (22.c): Expansion of HMBC spectrum of compound 8 at δ_H: 7.2-8.4 ppm and δ_C: 80-190 ppm.

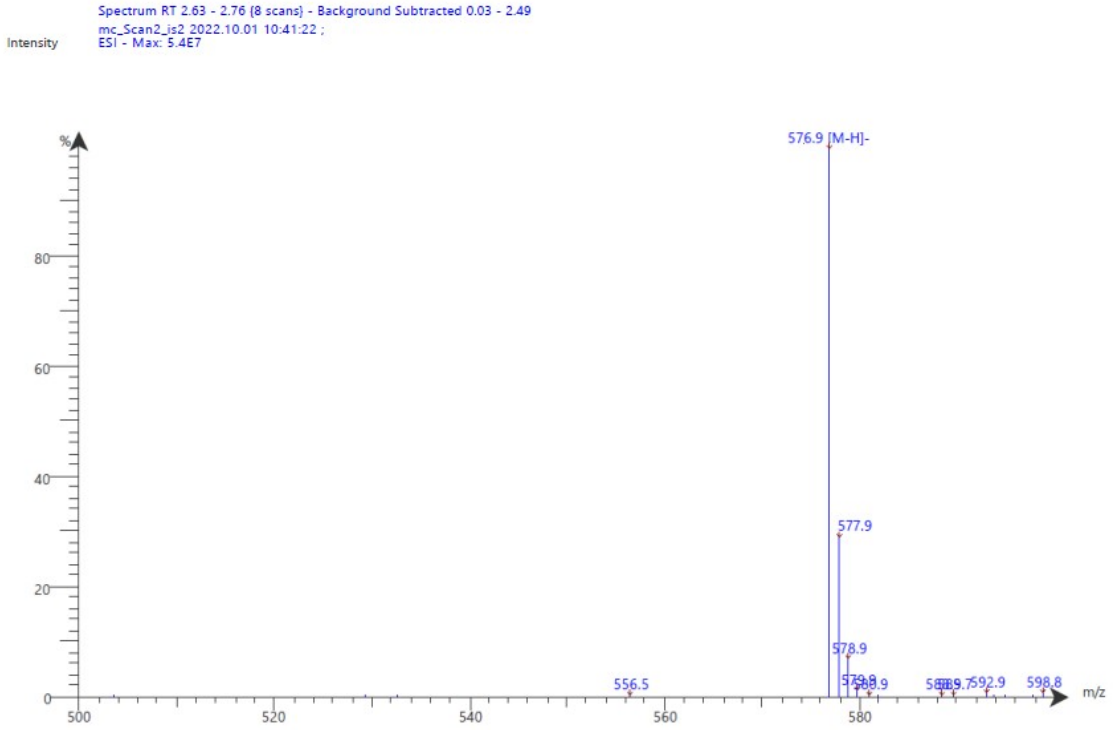

Fig. (23): Negative ESI -MS spectrum of compound 8

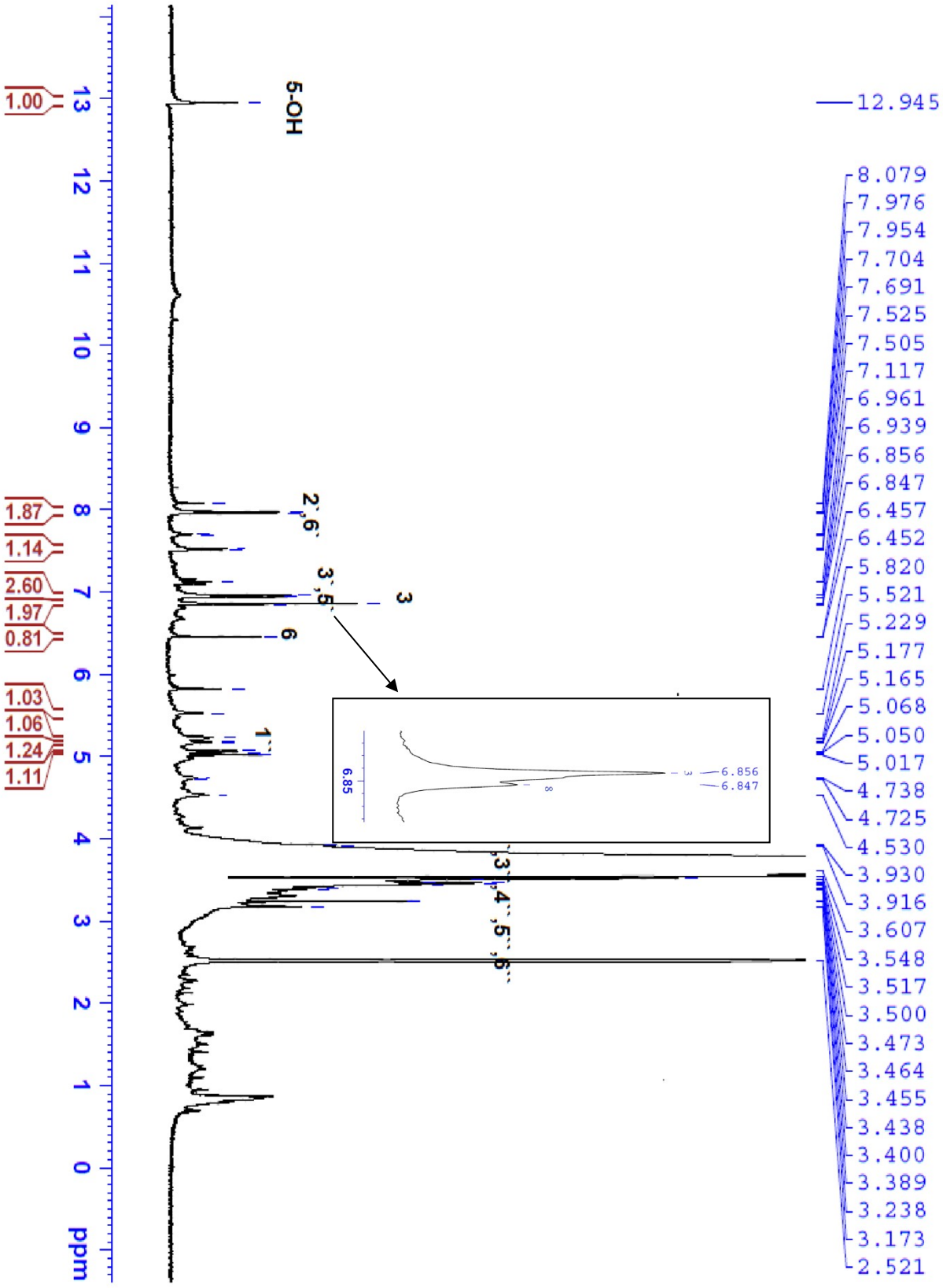

Fig. (24): ^{1}H-NMR spectrum of compound 9 in DMSO-d_6 at 400 MHz

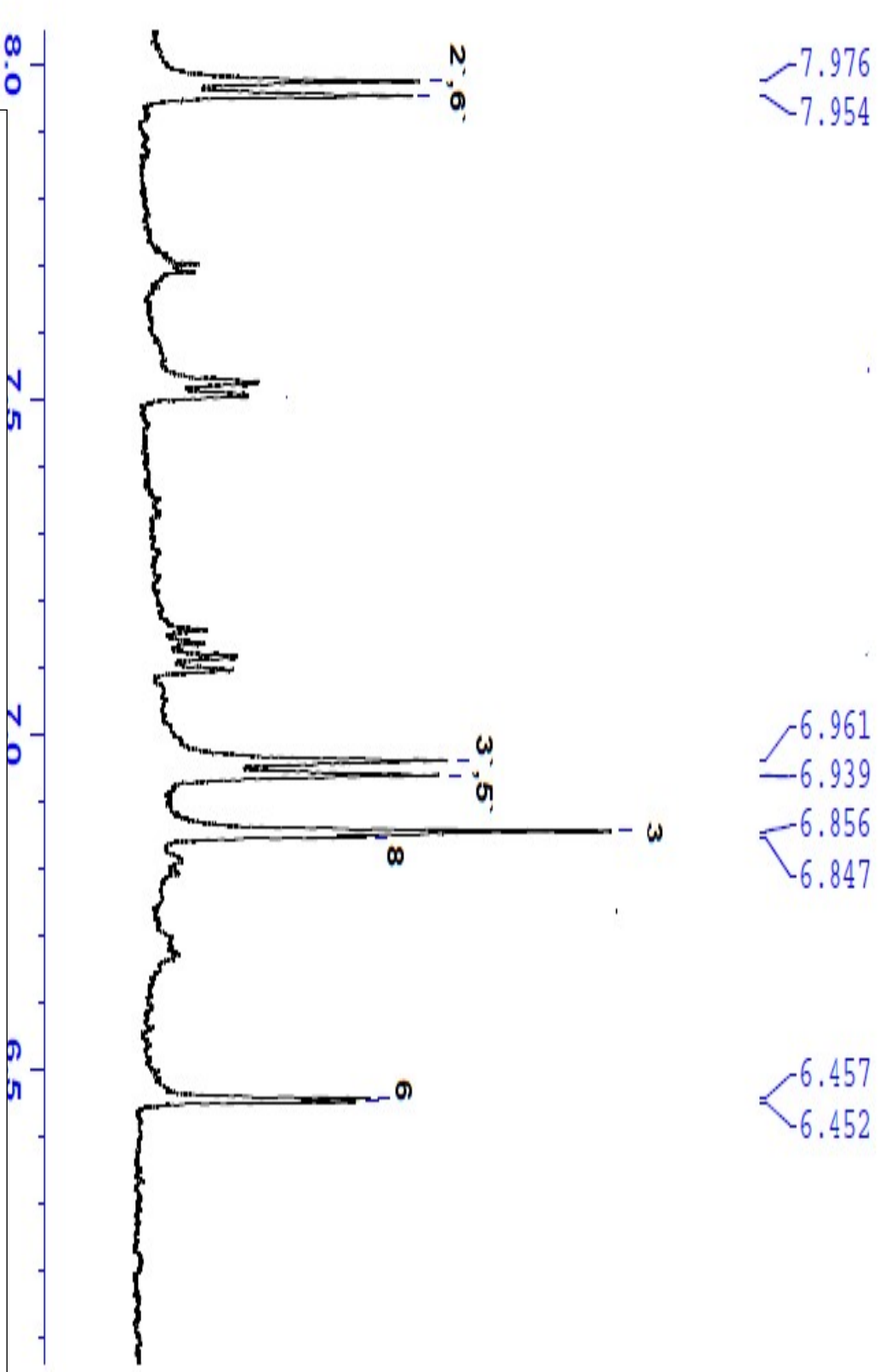

Fig. (24.a): Expansion of ^{1}H-NMR spectrum of compound 9 in DMSO-d_6 at the range (6.4-8) ppm.

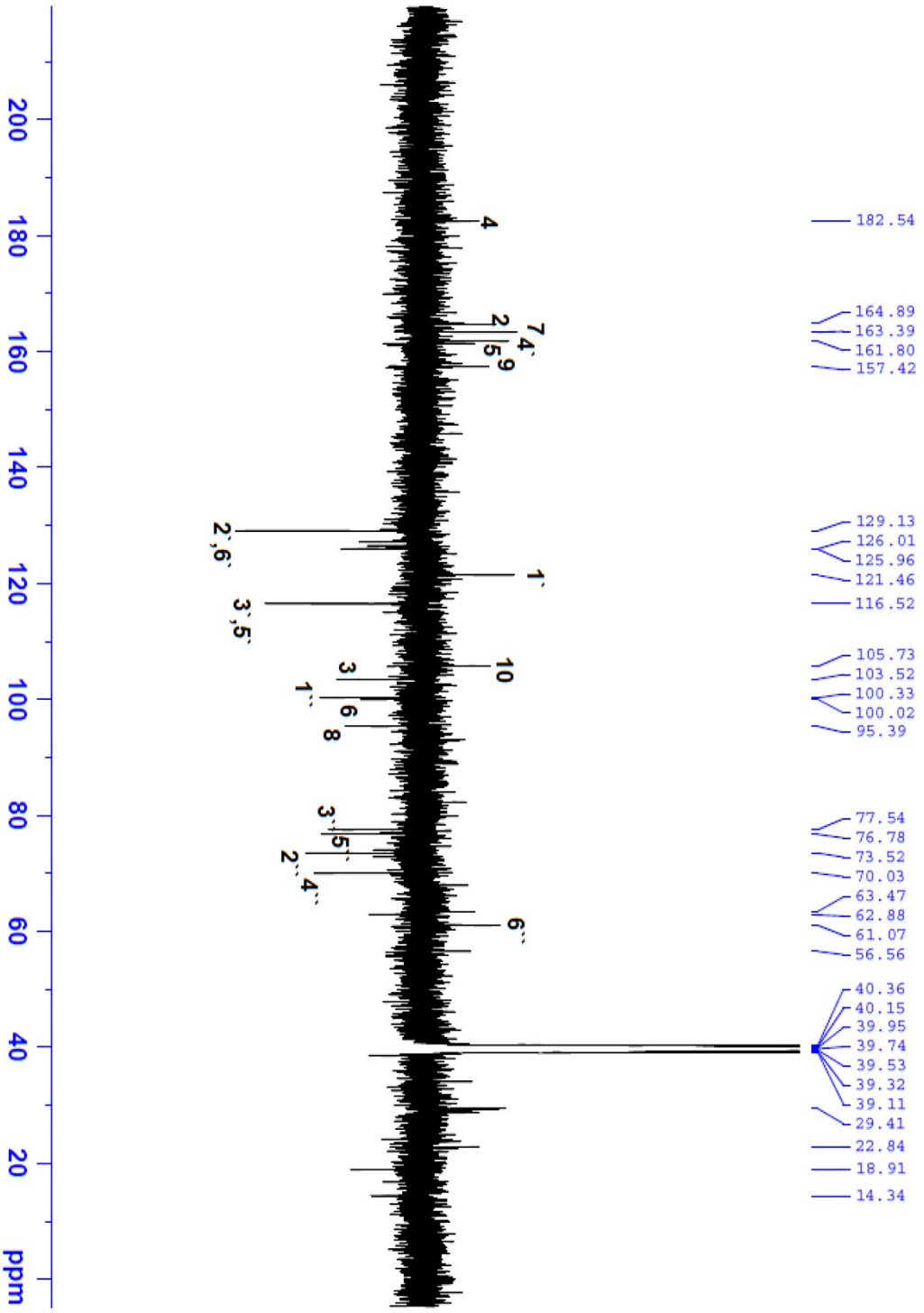

Fig. (25): APT spectrum of compound 9 in DMSO-d_6 at 100 MHz

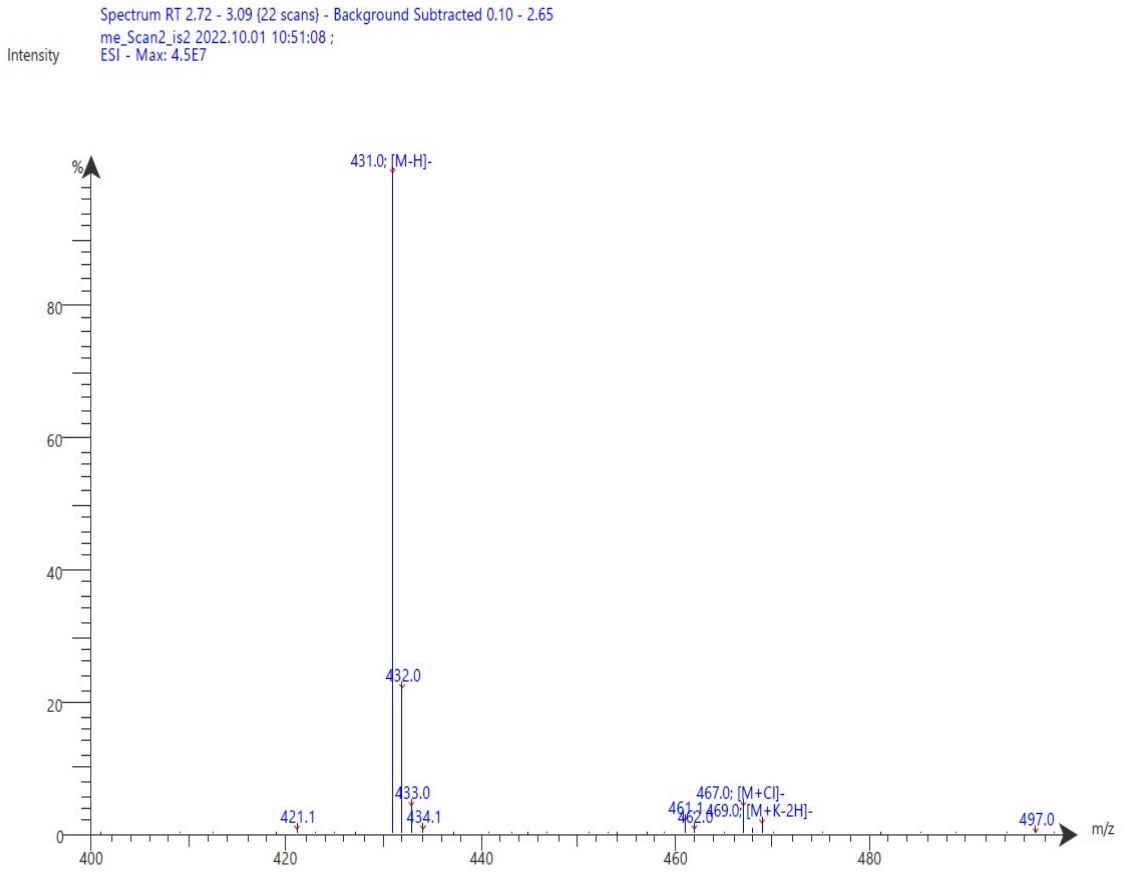

Fig. (26): Negative ESI -MS spectrum of 9

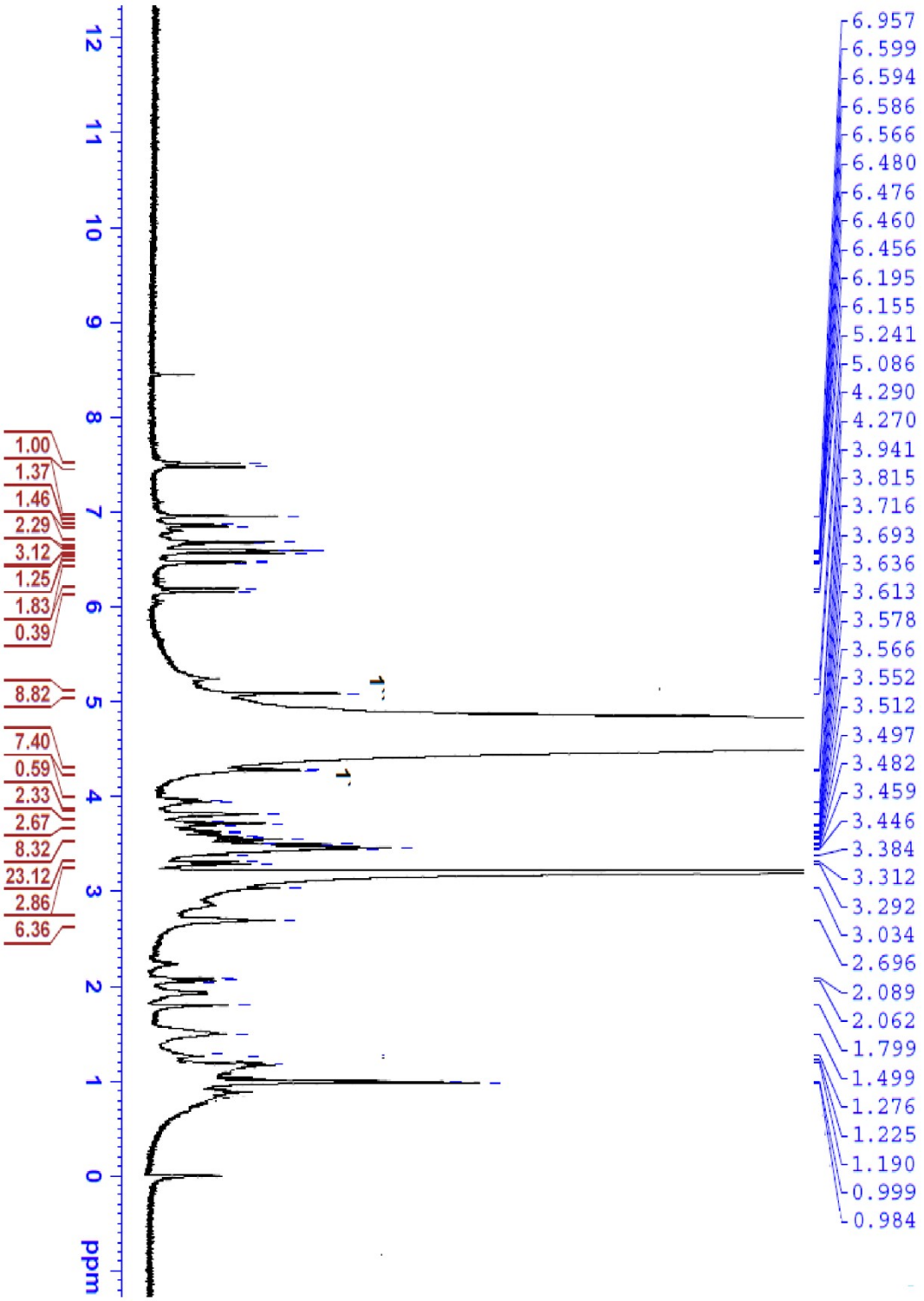

Fig. (27): ^{1}H-NMR spectrum of compound 10 in CD_3OD

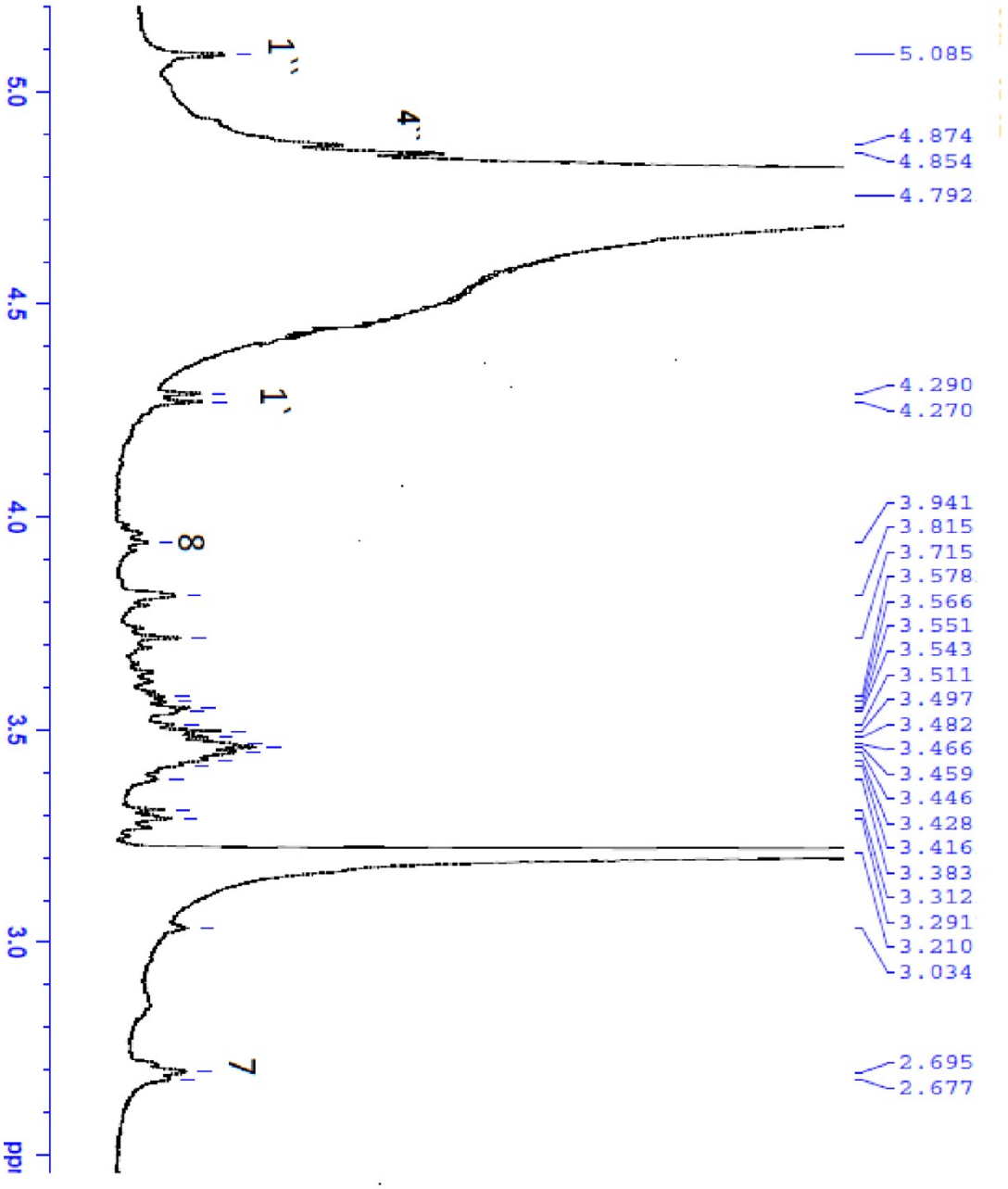

Fig. (27.a): Expansion of ^{1}H-NMR spectrum of compound 10 in CD_3OD at the range (2.5- 5.2) ppm.

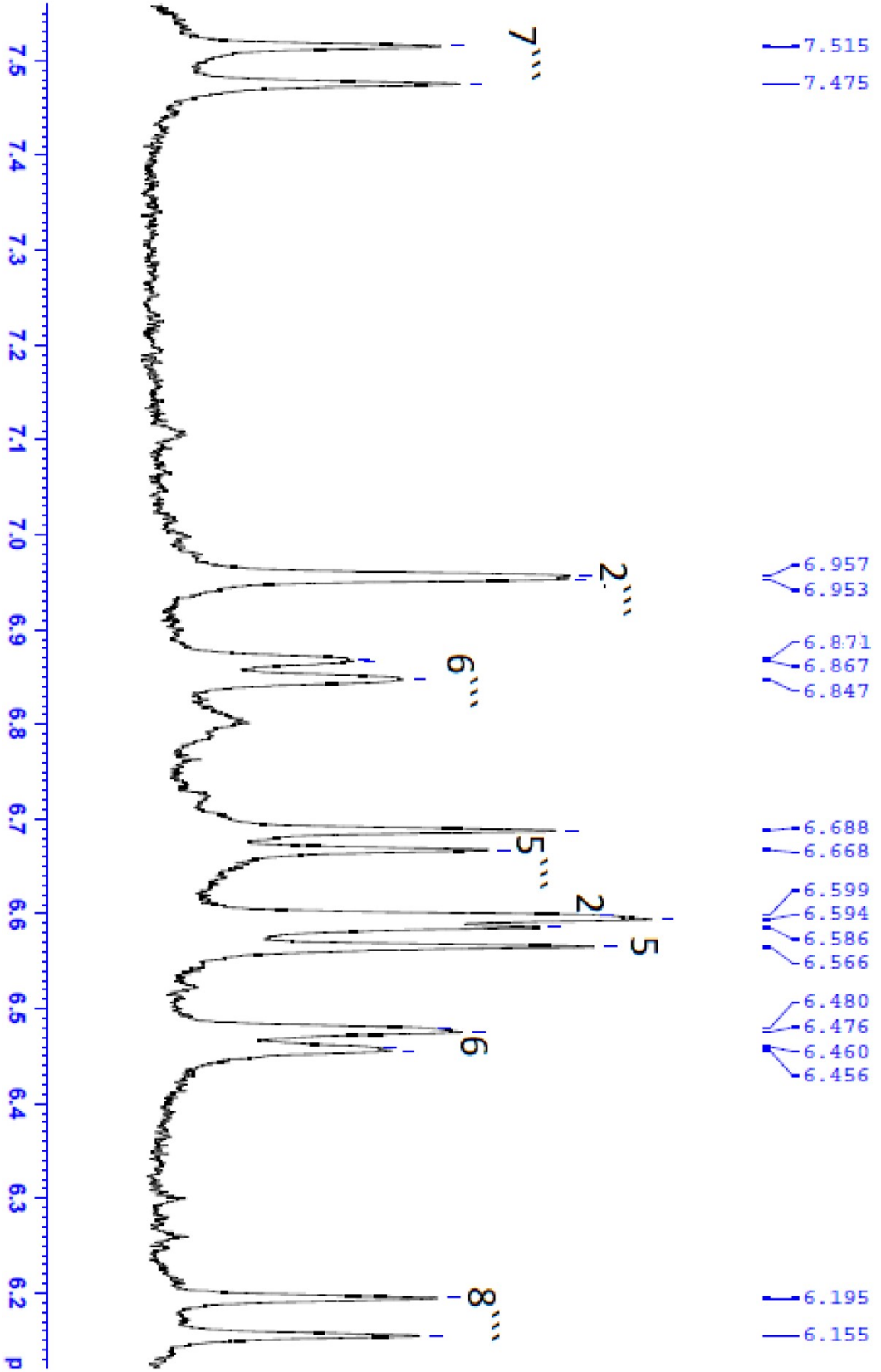

Fig. (27.b): Expansion of ^{1}H-NMR spectrum of compound 10 in CD_3OD at the range (6-7.6) ppm.

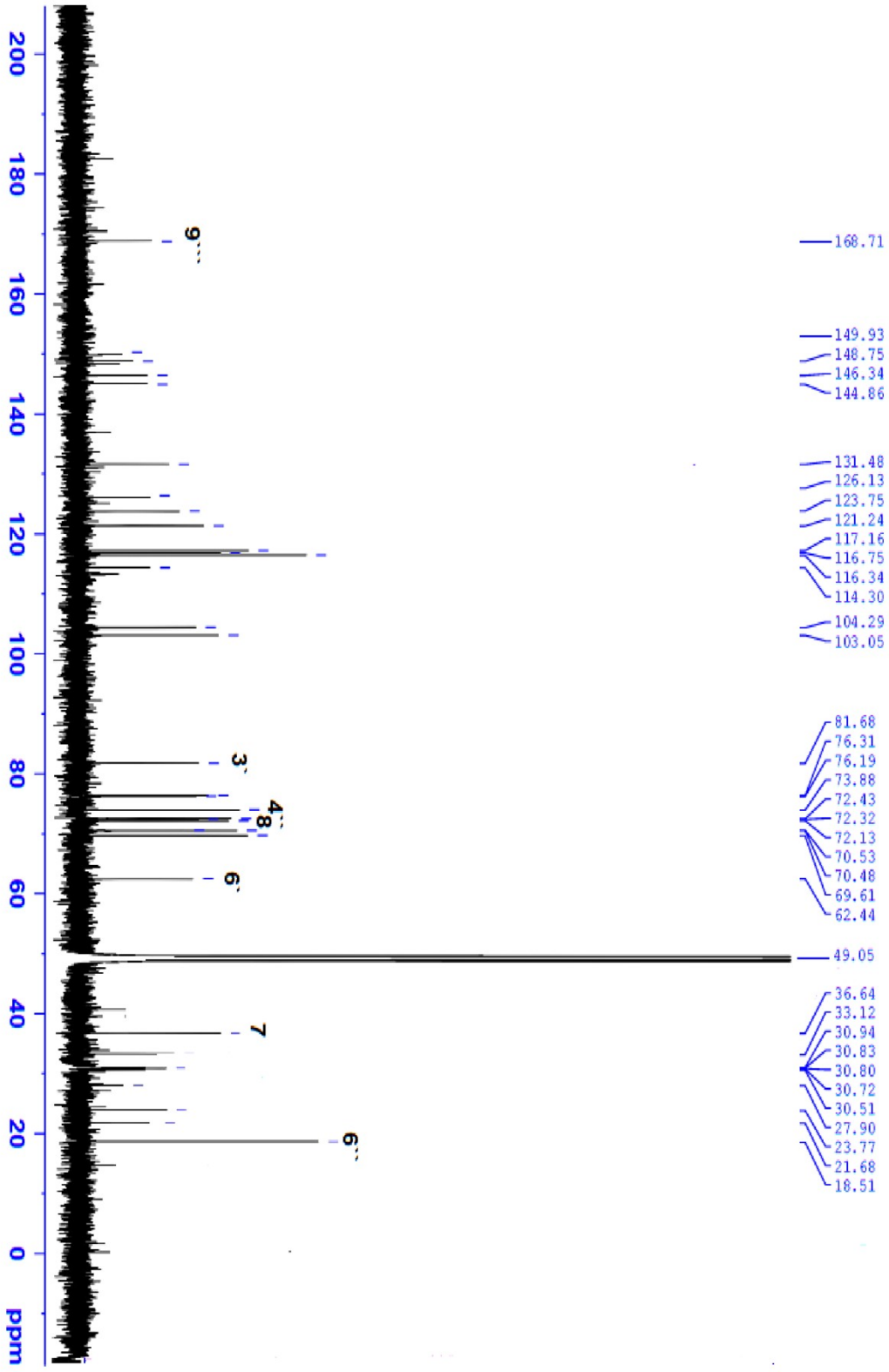

Fig. (28): ^{13}C-NMR spectrum of compound 10 in CD_3OD

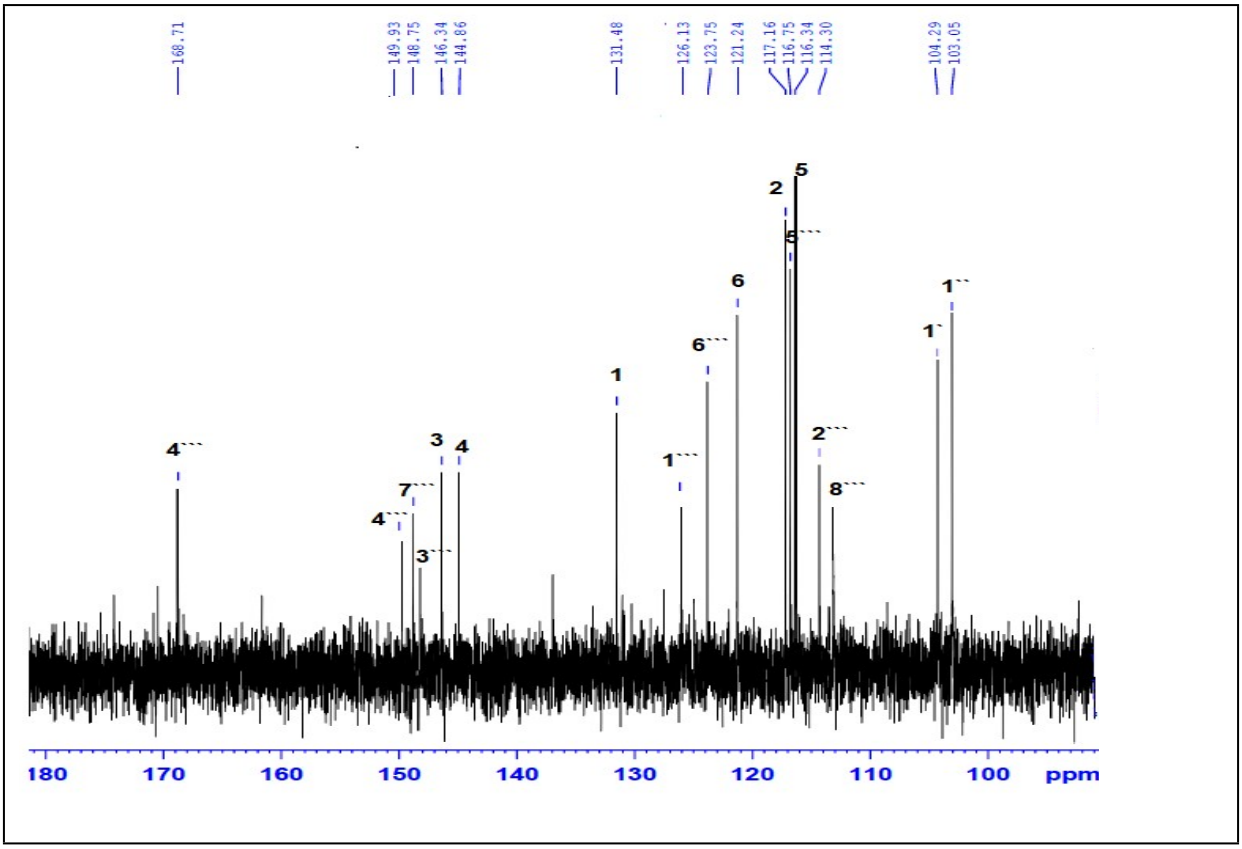

Fig. (28.a): Expansion of ^{13}C-NMR spectrum of compound 10 in CD_3OD at the range 90-180 ppm.

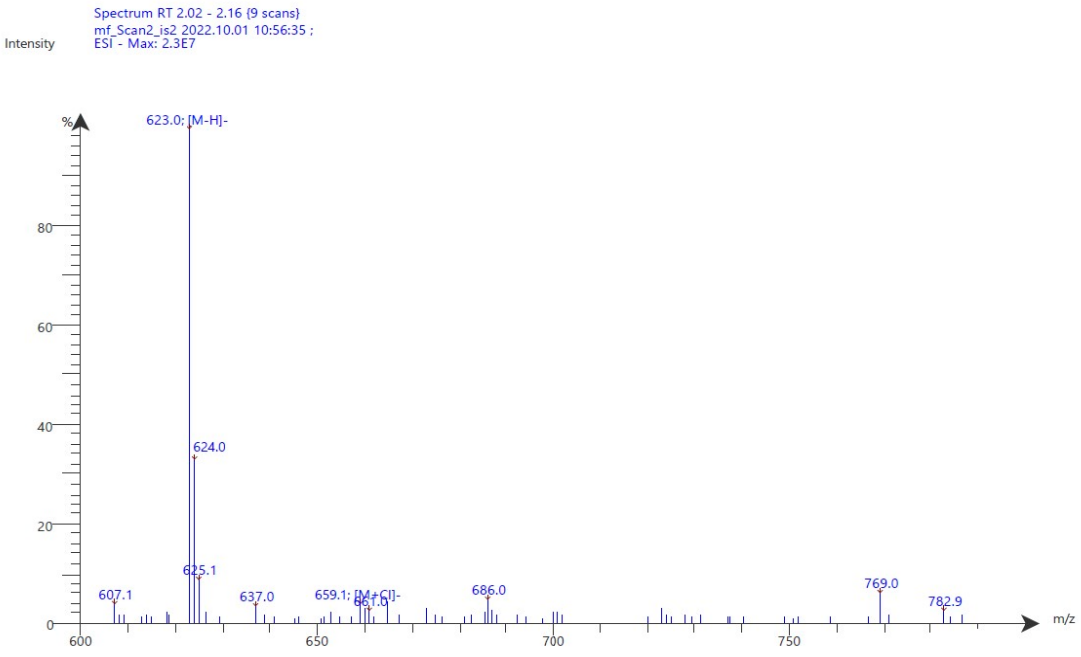

Fig. (29): Negative ESI -MS spectrum of 10.