In vivo Determination of Analgesic and Anti-inflammatory Activities of Isolated Compounds from *Cleome amblyocarpa* and Molecular Modelling for the Top Active Investigated Compounds.

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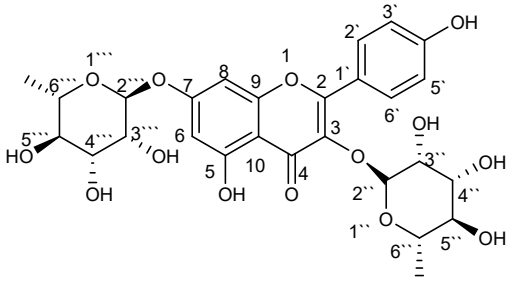
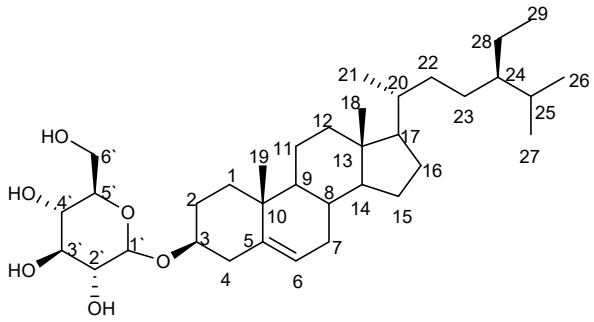
Table 1: ^{1}H-NMR (300 MHz) and ^{13}C-NMR (75 MHz) in DMSO-*d*6 spectra data of compound (1)



Position	δ_H ppm (No. of H, *m*, *J* Hz)	δ_C (ppm)
2	-	156.2
3	-	134.6
4	-	178.0
5	-	161.0
6	6.44 (1H, *d*, *J*= 2.3 Hz)	98.5
7	-	161.8
8	6.76 (1H, *d*, *J*= 2.2Hz)	94.7
9	-	157.9
10	-	105.9
1`	-	120.4
2`,6`	7.78 (2H, *d*, *J*= 8.7 Hz)	130.8
3`,5`	6.93 (2H, *d*, *J*= 8.7 Hz)	115.6
4`	-	160.3
1``	5.29 (1H, *d*, *J*= 1.2 Hz)	102.0
2``	3.15: 5.13 (8H, *m*)	70.4
3``		70.8
4``		71.7
5``		70.2
6``	0.81 (3H, *d*, *J*= 6Hz)	18.0
1```	5.54 (1H, *d*, *J*= 1.2 Hz)	99.6
2```	3.15: 5.13 (8H, *m*)	70.3
3```		70.4
4```		71.2
5```		69.9
6```	1.13 (3H, *d*, *J*= 6 Hz)	17.6

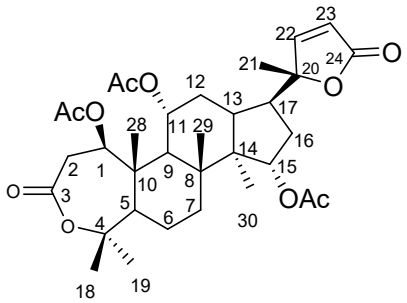
Table 2: ^{1}H-NMR (400 MHz) and ^{13}C-NMR (75 MHz) in DMSO-*d6* spectra data of compound (2)



Position	δ_H ppm (No. of H, *m*, *J* Hz)	δ_C (ppm)	Position	δ_H ppm (No. of H, *m*, *J* Hz)	δ_C (ppm)
1		36.7	19	1.02 (3H, *s*)	19.6
2		29.7	20		36.0
3	3.50 (1H, *m)*	77.2	21	0.96 (3H, *d*, *J*=6.3 Hz)	19.1
4		38.8	22		33.8
5		140.9	23		25.9
6	5.38 (1H, *m*)	121.6	24		45.6
7		31.9	25		29.2
8		31.8	26	0.90 (3H, *d*, *J*=6.6 Hz*)*	20.2
9		50.1	27	0.86 (3H, *d*, *J*=6.6 Hz)	19.4
10		36.7	28		23.1
11		21.1	29	0.86 (3H, *t, J*=7 Hz)	12.2
12		37.3	1`	4.28 (1H, *d*, *J*=7.8)	101.3
13		42.3	2`	3.13 -3.48 (4H, *m*)	73.9
14		56.7	3`		77.4

15		24.3	4`		70.5
16		28.3	5`		77.2
17		55.9	6`	3.63 (1Ha, *dd*, *J*=10.4, 5.2Hz*)* 3.18 (1Hb, *m*),	61.5
18	0.71 (3H, *s*)	12.1			

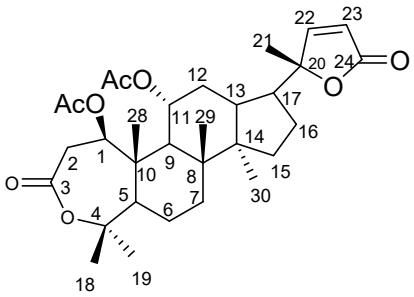
Table 3: ^{1}H-NMR (300 MHz) and ^{13}C-NMR (75 MHz) in $CDCl_3$-CD_3OD spectra data of compound (3)



Position	δ_H ppm (No. of H, *m*, *J* Hz)		δ_C (ppm)
1	5.17 (1H, *br d*, *J*=5 Hz)		80.4
2	2 a	3.21 (1H, *m*)	37.9
	2 b	3.09 (1H, *m*)	
3			174.9
4	-		86.6
5	1.97 (1H, *m*)		53.9
6	6 a	1.76 (1H, *m*)	24.4
	6 b	1.41 (1H, *m*)	
7	7 a	1.25 (1H, *m*)	35.7
	7 b	1.66 (1H, *m*)	
8	-		51.8
9	1.94 (1H, *m*)		52.1
10	-		45.0
11	5.10 (1H, *m*)		73.6
12 overlaps	12 a	1.48 (1H, *m*)	34.7
	12 b	1.90 (1H, *m*)	
13	1.77 (1H, *m*)		40.9
14	-		43.2
15	4.93 (1H, *m*)		74.8
16	16 a	1.70 (1H, *m*)	33.4
	16 b	2.06(1H, *m*)	

17	2.18 (1H, *m*)	45.5
18	1.36 (3H, *s*)	27.3
19	1.43 (3H, *s*)	30.9
20	-	92.8
21	1.40 (3H, *s*)	24.4
22	7.71 (1H, *d*, *J* = 6 Hz)	161.1
23	6.14 (1H, *d*, *J* = 6 Hz)	122.5
24	-	174.2
25	-	-
26	-	-
27	-	-
28	1.18 (3H, *s*)	15.5
29	1.17 (3H, *s*)	18.0
30	1.16 (3H, *s*)	11.2
COCH3 1	-	172.0
COCH3 1[a]	1.97 (3H, *s*)	21.9
COCH3 11	-	172.3
COCH3 11[a]	1.93 (3H, *s*)	22.2
COCH3 15	-	172.4
COCH3 15[a]	2.00 (3H, *s*)	22.3

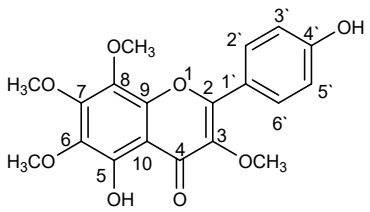
Table 4: ^{1}H-NMR (300 MHz) and ^{13}C-NMR (75 MHz) in $CDCl_3$ spectra data of compound (4)



Position	δ_H ppm (No. of H, *m*, *J* Hz)		δ_C (ppm)
1	5.17 (1H, *d*, *J*=5.9 Hz)		72.6
2	2 a	3.18 (1H, *dd*, *J* = 15.6, 5.4 Hz)	36.9
	2 b	2.91 (1H, *br d*, *J* = 15.9 Hz)	
3	-		172.1
4	-		84.5
5			41.8
6			23.4

7		30.4
8	-	41.4
9		46.4
10	-	43.8
11	5.16 (1H, *m*)	78.7
12		34.3
13		51.0
14	-	50.0
15		34.7
16		28.9
17		53.4
18	0.92 (3H, *s*)	14.3
19	1.11 (3H, *s*)	15.6
20	-	91.1
21	1.21 (3H, *s*)	17.0
22	7.34 (1H, *d*, *J* = 5.6 Hz)	159.4
23	6.05 (1H, *d*, *J* = 5.6 Hz)	121.0
24	-	172.2
25	-	-
26	-	-
27	-	-
28	1.46 (3H, *s*)	30.2
29	1.41 (3H, *s*)	26.5
30	1.43 (3H, *s*)	23.1
COCH3 1	-	170.6
COCH3 1[a]	2.00 (3H, *s*)	21.6
COCH3 11	-	170.4
COCH3 11[a]	1.94 (3H, *s*)	21.5

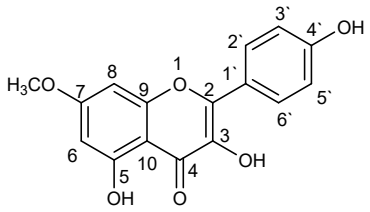
Table 5: Table: ^{1}H-NMR (300 MHz) and ^{13}C-NMR (75 MHz) in $CDCl_3$-CD_3OD spectra data of compound (5)



Position	δ_H ppm (No. of H, *m*, *J* Hz)	δ_C (ppm)
2	-	156.8
3	3.80(3H, *s*)	137.7

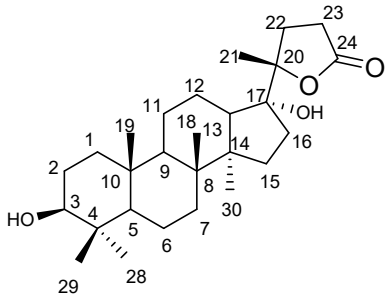
4	-	178.8
5	-	148.1
6	3.90 (3H, *s*)	135.4
7	4.08 (3H, *s*)	152.3
8	3.94 (3H, *s*)	132.5
9	-	144.6
10	-	106.8
1`	-	120.7
2`,6`	8.05 (2H, *d*, *J*= 9 Hz)	129.9
3`,5`	6.94 (2H, *d*, *J*= 9 Hz)	115.2
4`	-	159.9
(7-OCH_3)	-	61.5
(8- OCH_3)	-	61.0
(6- OCH_3)	-	60.5
(3- OCH_3)	-	59.3

Table 6: ^{1}H-NMR (300 MHz) and ^{13}C-NMR (75 MHz) in CD_3OD spectra data of compound (6)



Position	δ_H ppm (No. of H, *m*, *J* Hz)
2	-
3	3.77(3H, *s*)
4	-
5	-
6	6.21(1H , *d* ,J= 2.1 Hz)
7	
8	6.42(1H, *d* ,J= 1.8 Hz)
9	-
10	-
1`	-
2`,6`	7.97(2H , *d* ,J= 9 Hz)
3`,5`	6.94(2H, *d*, J= 9 Hz)
4`	-

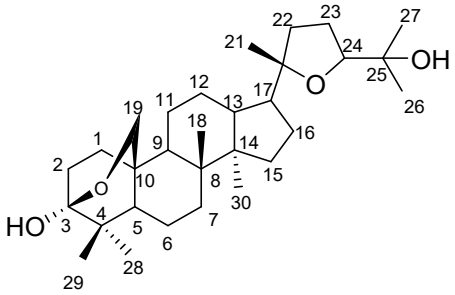
Table 7: ^{1}H-NMR (300 MHz) and ^{13}C-NMR (75 MHz) in $CDCl_3$ spectra data of compound (7)



Position	δ_H ppm (No. of H, *m*, *J* Hz)	δ_C (ppm)
1	-	33.6
2	-	25.3
3	3.40 (1H, *b t*, *J*=2.9Hz)	76.2
4	-	37.2
5	-	49.4
6	-	18.2
7	-	34.5
8	-	41.1
9	-	50.4
10	-	37.6
11	-	21.3
12	-	22.8
13	-	45.9
14	-	49.9
15	-	32.5
16	-	36.2
17	-	83.4
18	0.85 (3H, s)	16.1
19	0.87 (3H, s)	15.7
20	-	92.9
21	1.44 (3H, *s*)	22.9
22	-	29.2
23	2.54-2.72 (2H, *m*)	29.2
24	-	176.7
25	-	-
26	-	-
27	-	-

28	0.97 (3H, *s*)	28.3
29	1.17 (3H, *s*)	22.1
30	0.95 (3H, *s*)	17.0

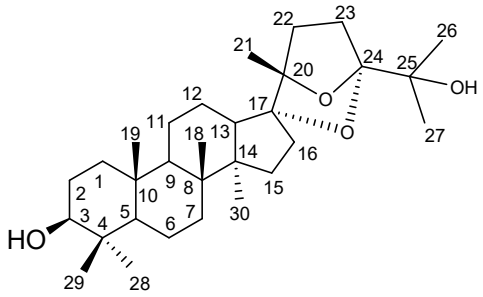
Table 8: ^{1}H-NMR (300 MHz) and ^{13}C-NMR (75 MHz) in CDCl3 spectra data of compound (8)



Position	δ_H ppm (No. of H, *m*, *J* Hz)		δ_C (ppm)
1			36.0
2			29.4
3			98.2
4			40.4
5			49.4
6			19.7
7			33.3
8			39.2
9			45.2
10			35.4
11			22.6
12			27.3
13			43.1
14			49.5
15			31.3
16			25.5
17			49.9
18	0.83 (3H, *s*)		15.1
19	19a	4.22 (1H, *dd*, J=8.8 Hz)	68.0
	19b	3.71 (1H, *br d*, J = 8.1 Hz)	
20			86.3
21	1.19 (3H, *s*)		23.2
22			35.5
23			26.2
24	3.70 (1H, *m*)		83.2
25			71.5

26	1.11 (6H, *s*)	26.7
27	Overlapped	24.3
28	1.01 (3H, *s*)	27.3
29	0.97 (3H, *s*)	18.4
30	0.87 (3H, *s*)	15.9

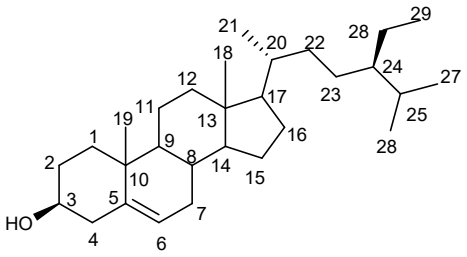
Table 9: ^{1}H-NMR (300 MHz) and ^{13}C-NMR (75 MHz) in $CDCl_3$ spectra data of compound (9)



Position	δ_H ppm (No. of H, *m*, *J* Hz)		δ_C (ppm)
1	1a	1.87 (1H, *m*)	33.6
	1b	1.32 (1H, *m*)	
2	2a	1.92 (1H, *m*)	25.3
	2b	1.89 (1H, *m*)	
3	3.48 (1H, *br s)*		76.2
4	-		37.2
5	1.85 (1H, *m*)		49.5
6	1.67-1.42 (2H, *m*)		18.2
7	7a	1.24 (1H, *m*)	34.6
	7b	1.22 (1H, *m*)	
8	-		40.6
9	1.70 (1H, *m*)		50.8
10	-		37.6
11	11a	1.72 (1H, *m*)	21.5
	11b	1.26 (1H, *m*)	
12	1.67-1.42 (2H, *m*)		23.7
13	1.36 (1H, *m*)		44.3
14	-		49.6
15	15a	1.20 (1H, *m*)	31.8
	15b	1.11 (1H, *m*)	
16	16a	2.04 (1H, *m*)	37.7
	16b	1.70 (1H, *m*)	
17	-		89.3
18	0.95 (3H, *s*)		15.5
19	0.88 (3H, *s*)		16.2
20	-		91.3
21	1.27 (3H, *s*)		16.2
22	22a	1.97 (1H, *m*)	32.1

	22b	1.35 (1H, *m*)	
23	23a	2.14 (1H, *m*)	31.9
	23b	1.90 (1H, *m*)	
24	-		112.6
25	-		70.3
26	1.41 (3H, *s*)		25.5
27	1.29 (3H, *s*)		24.0
28	1.03 (3H, *s*)		28.3
29	0.85 (3H, *s*)		22.0
30	0.95 (3H, *s*)		18.1

Table 10: ^{1}H-NMR (300 MHz) and ^{13}C-NMR (75 MHz) in $CDCl_3$ spectra data of compound (10)



Position	*δH* ppm (No. of H, *m*, *J* Hz)	*δC* (ppm)
1	-	37.2
2	-	29.7
3	3.51 (1H, *m*)	71.8
4	-	42.3
5	-	140.7
6	5.35 (1H, *m*)	121.7
7		31.9
8		31.6
9		50.1
10		36.5
11		21.1
12		39.7
13		42.3
14		56.7
15		24.3
16		28.2
17		56.0
18	0.69 (3H, *s*)	12.0
19	1.02 (3H, *s*)	19.4
20		36.1

21	0.92 (3H, d, *J*=6.6 Hz)	18.8
22		33.9
23		26.0
24		45.8
25		29.1
26	0.83 (3H, *d*, *J*=6.9 Hz)	19.8
27	0.81 (3H, *d*, *J*=6.1 Hz)	19.0
28		23.0
29	0.86 (3H, *m*)	11.8

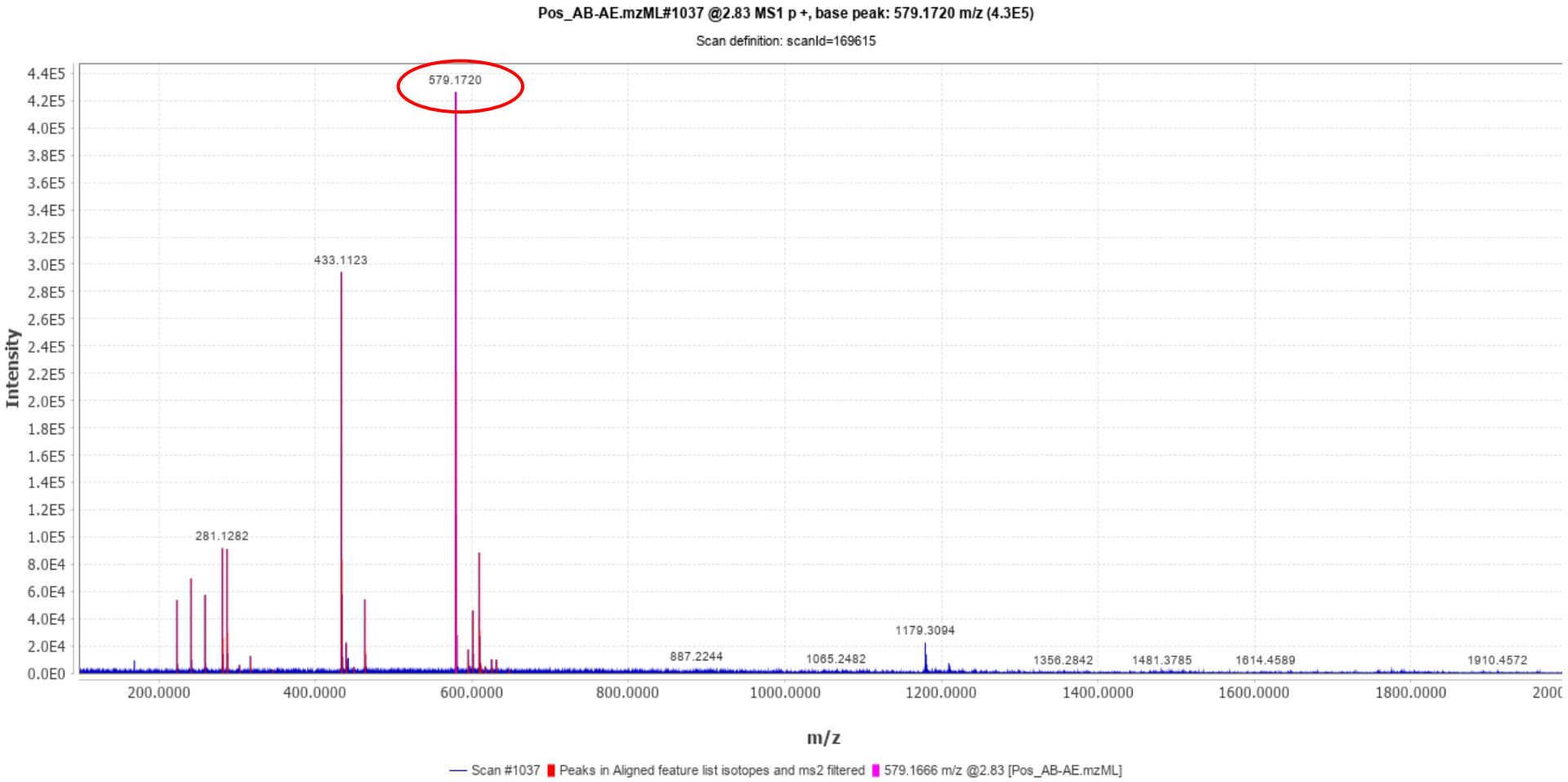


Figure 1: LC-MS/MS of compound 1

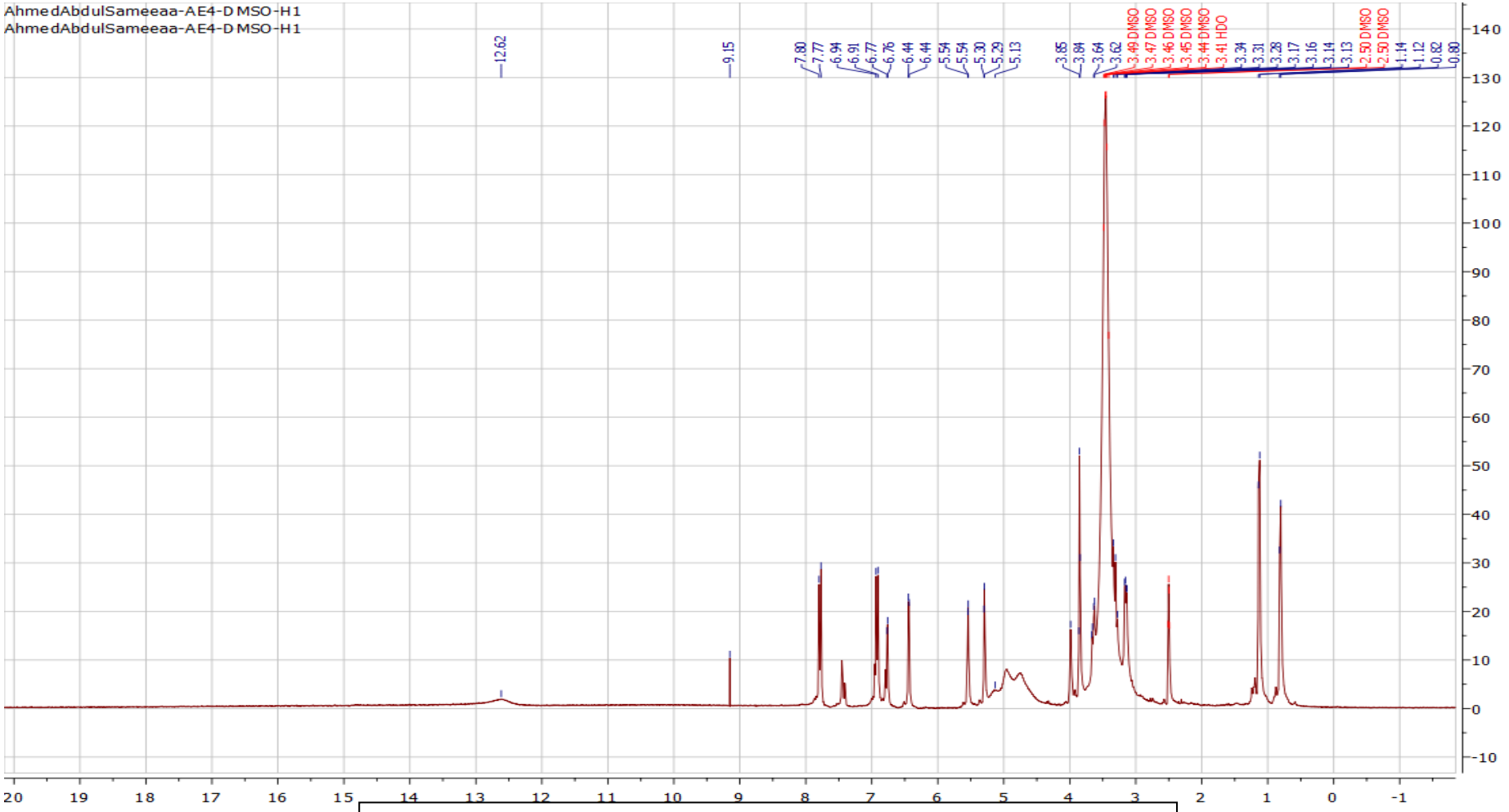


Figure 2: ^{1}H-NMR spectrum of compound 1 (300 MHz, DMSO-*d6*)

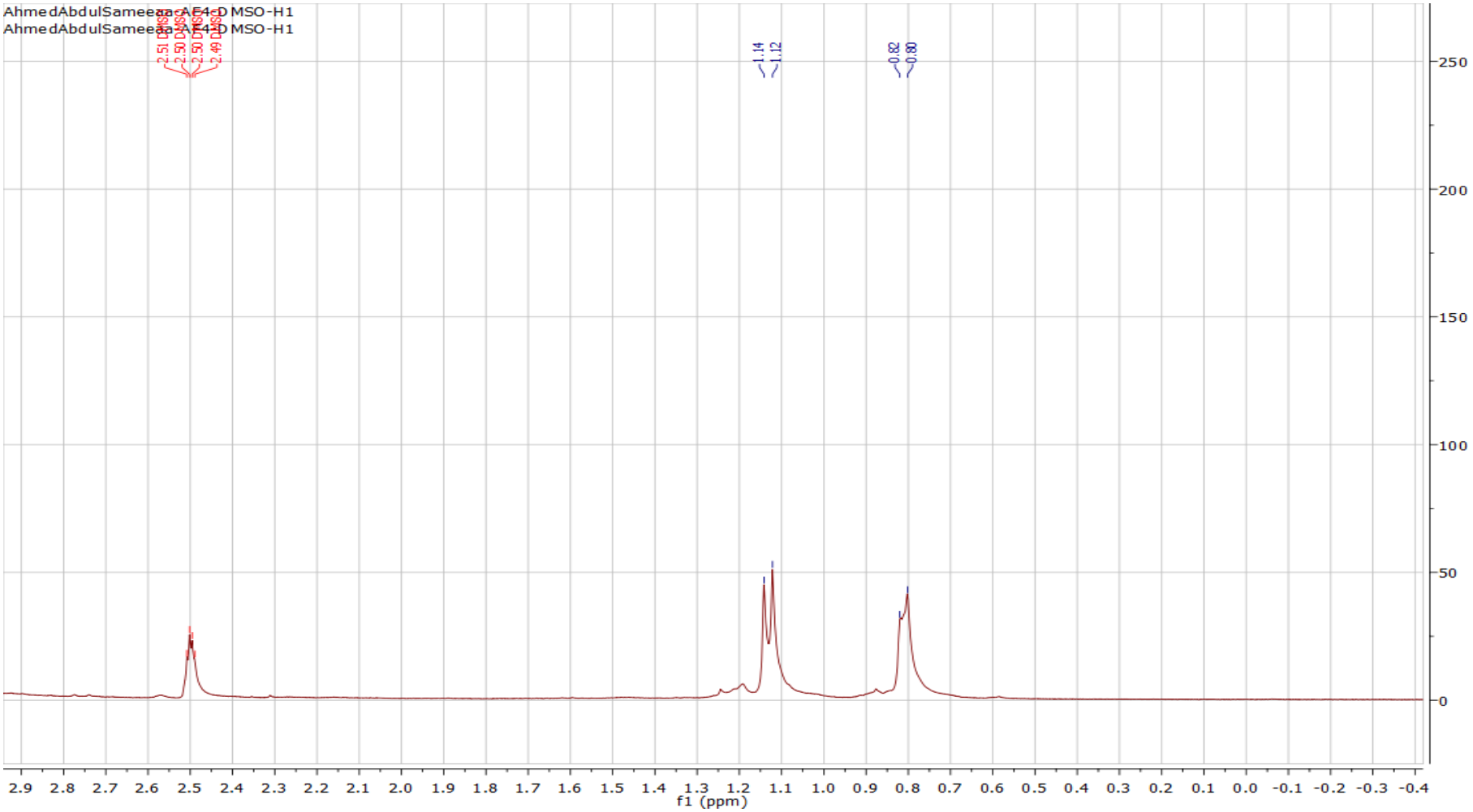


Figure 3: Partial expansion of ^{1}H-NMR spectrum of compound 1 (300 MHz, DMSO-*d6*).

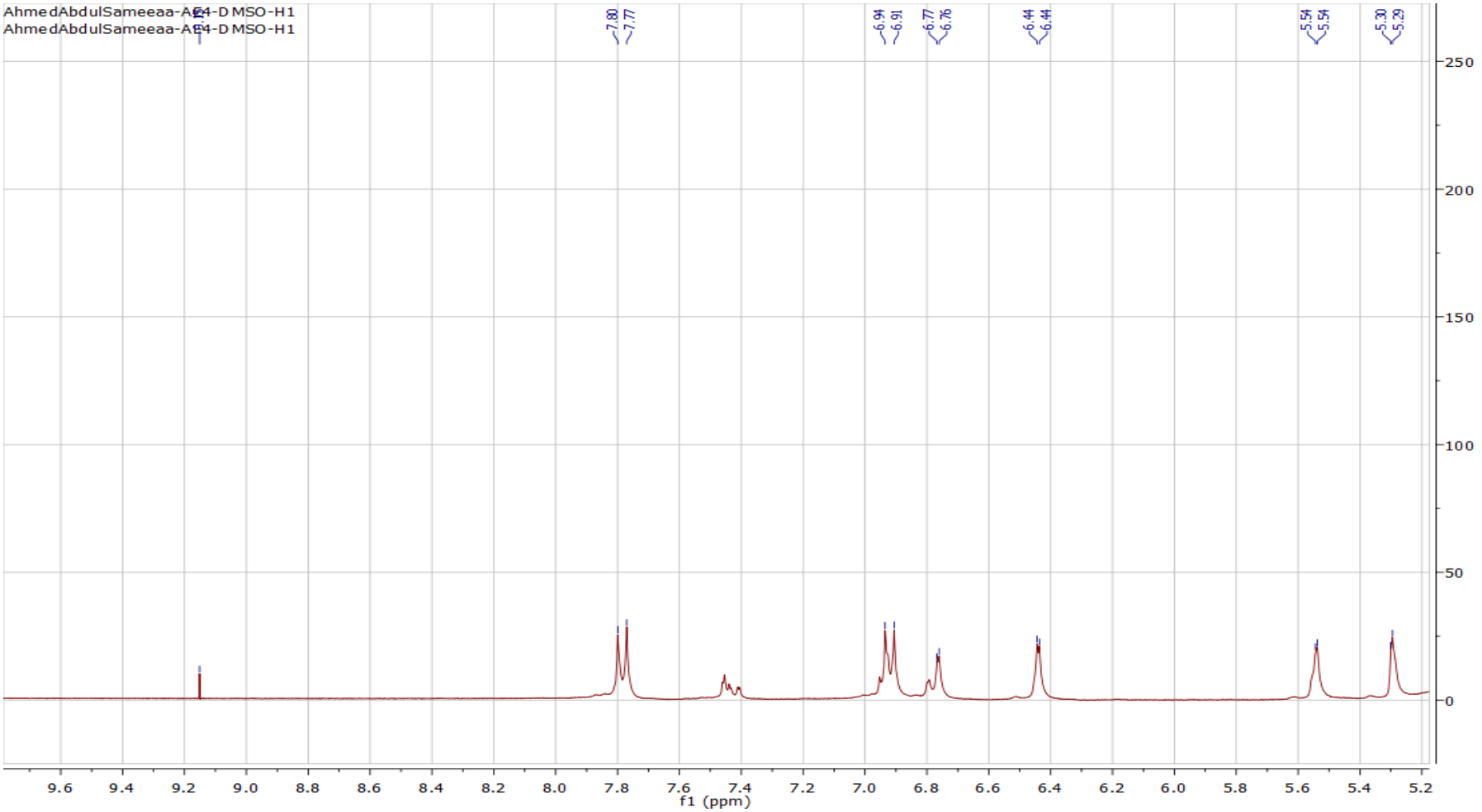


Figure 4: Partial expansion of ^{1}H-NMR spectrum of compound 1 (300 MHz, DMSO-*d6*).

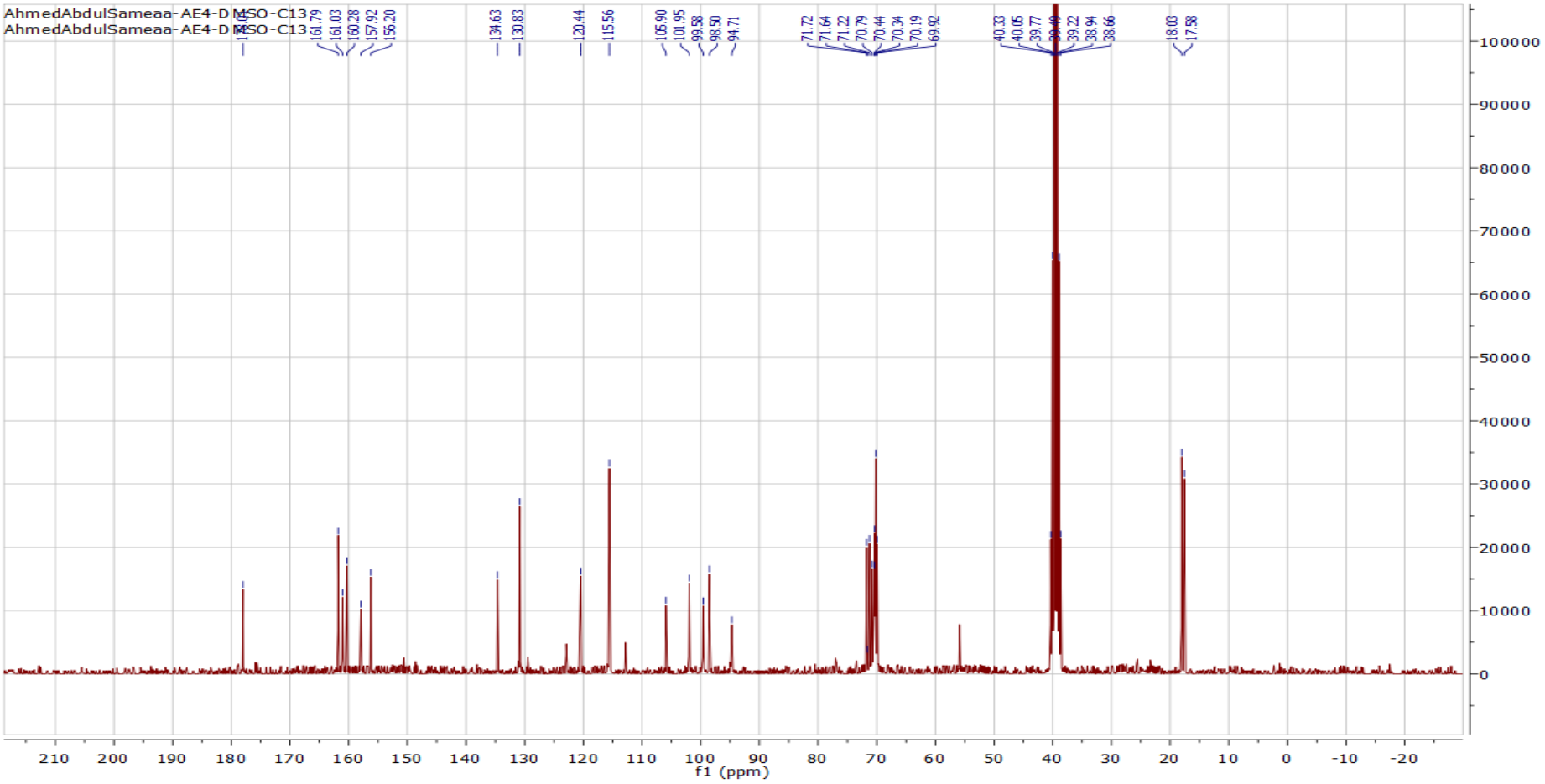


Figure 5: ^{13}C-NMR spectrum of compound 1 (75 MHz, DMSO-*d6*)

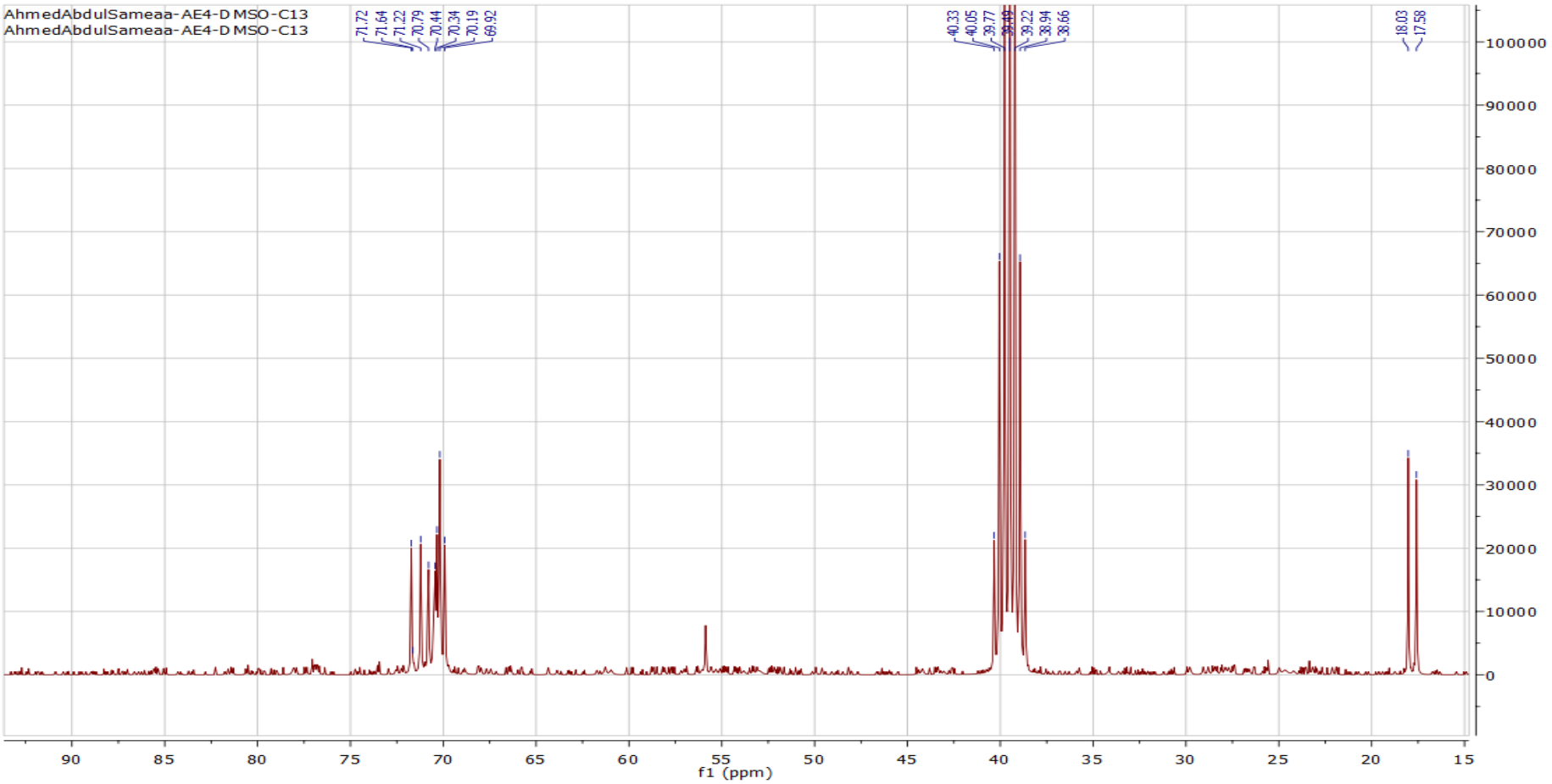


Figure 6: Partial expansion of ^{13}C-NMR spectrum of compound 1 (75 MHz, DMSO-*d6*)

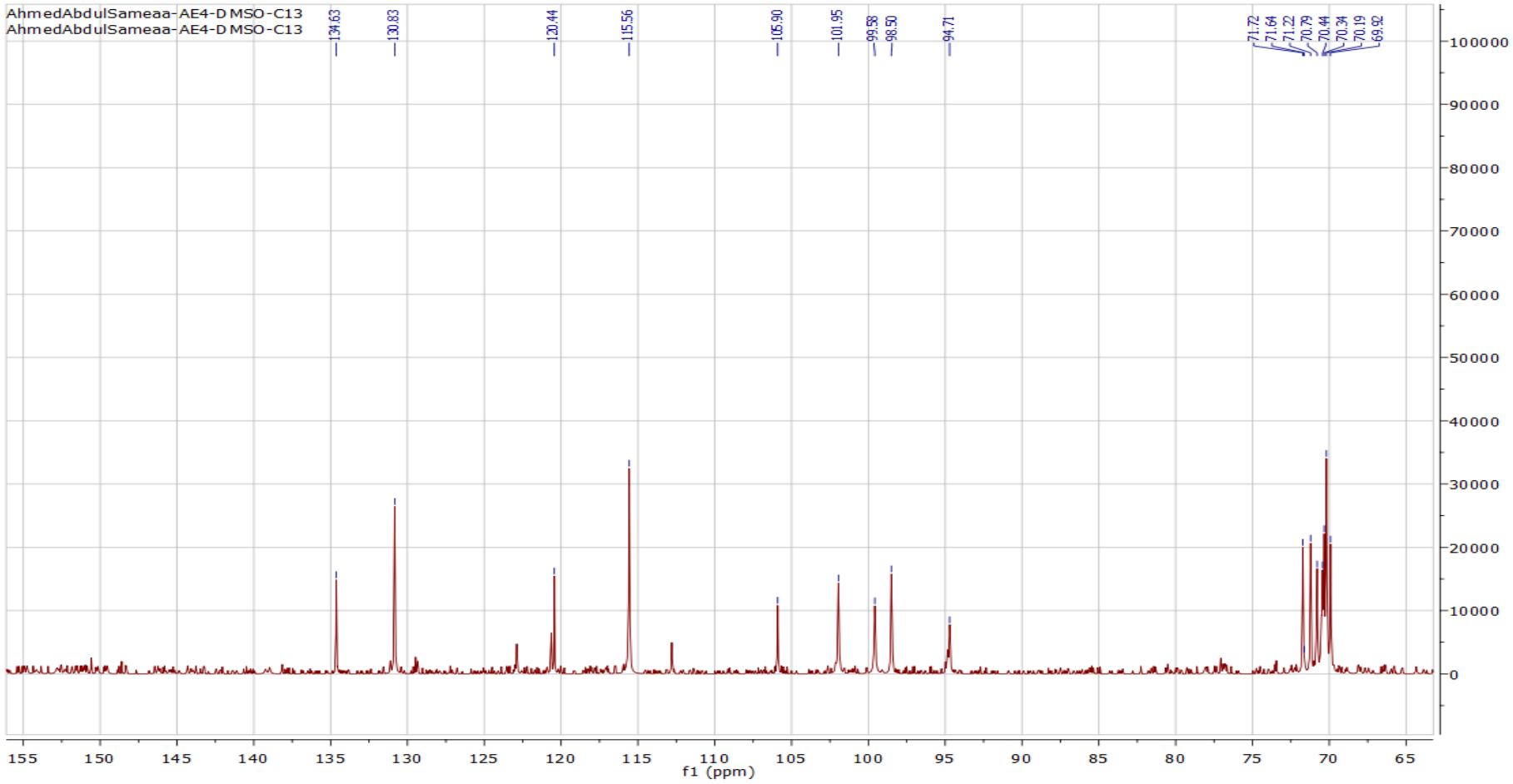


Figure 7: Partial expansion of ^{13}C-NMR spectrum of compound 1 (75 MHz, DMSO-*d6*)

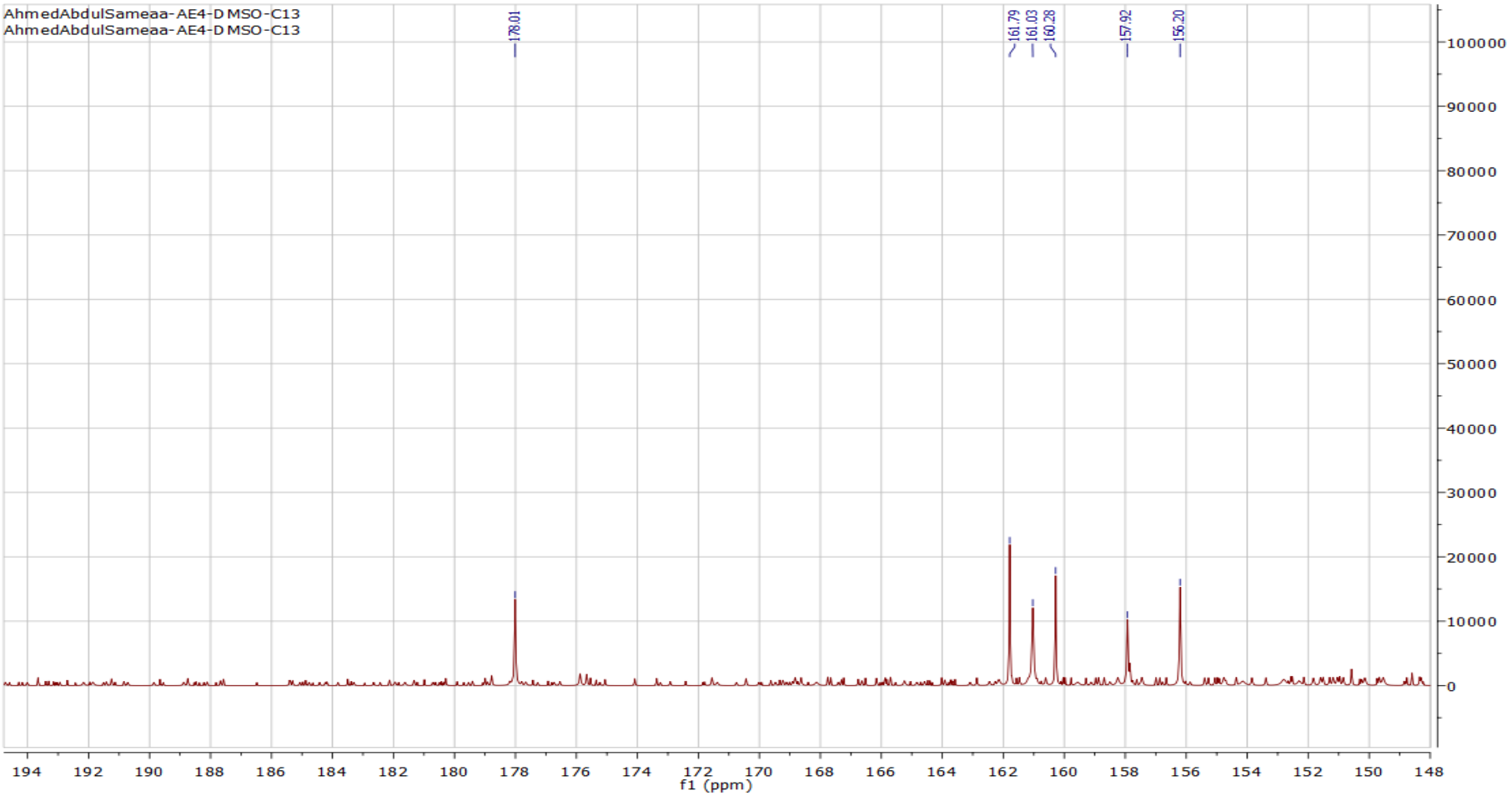


Figure 8: Partial expansion of ^{13}C-NMR spectrum of compound 1 (75 MHz, DMSO-*d6*)

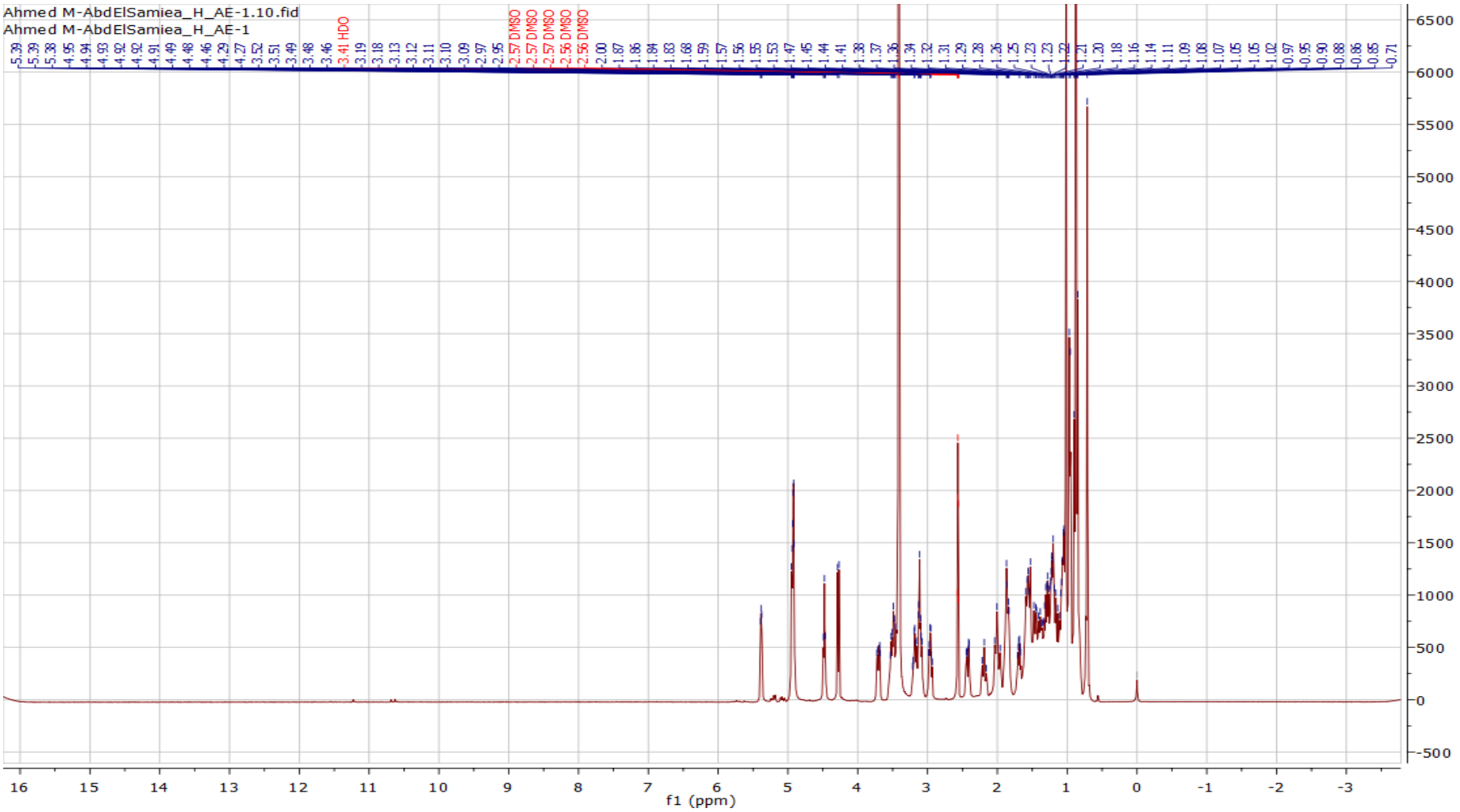


Figure 9: ^{1}H-NMR spectrum of compound 2 (300 MHz, DMSO-*d6*)

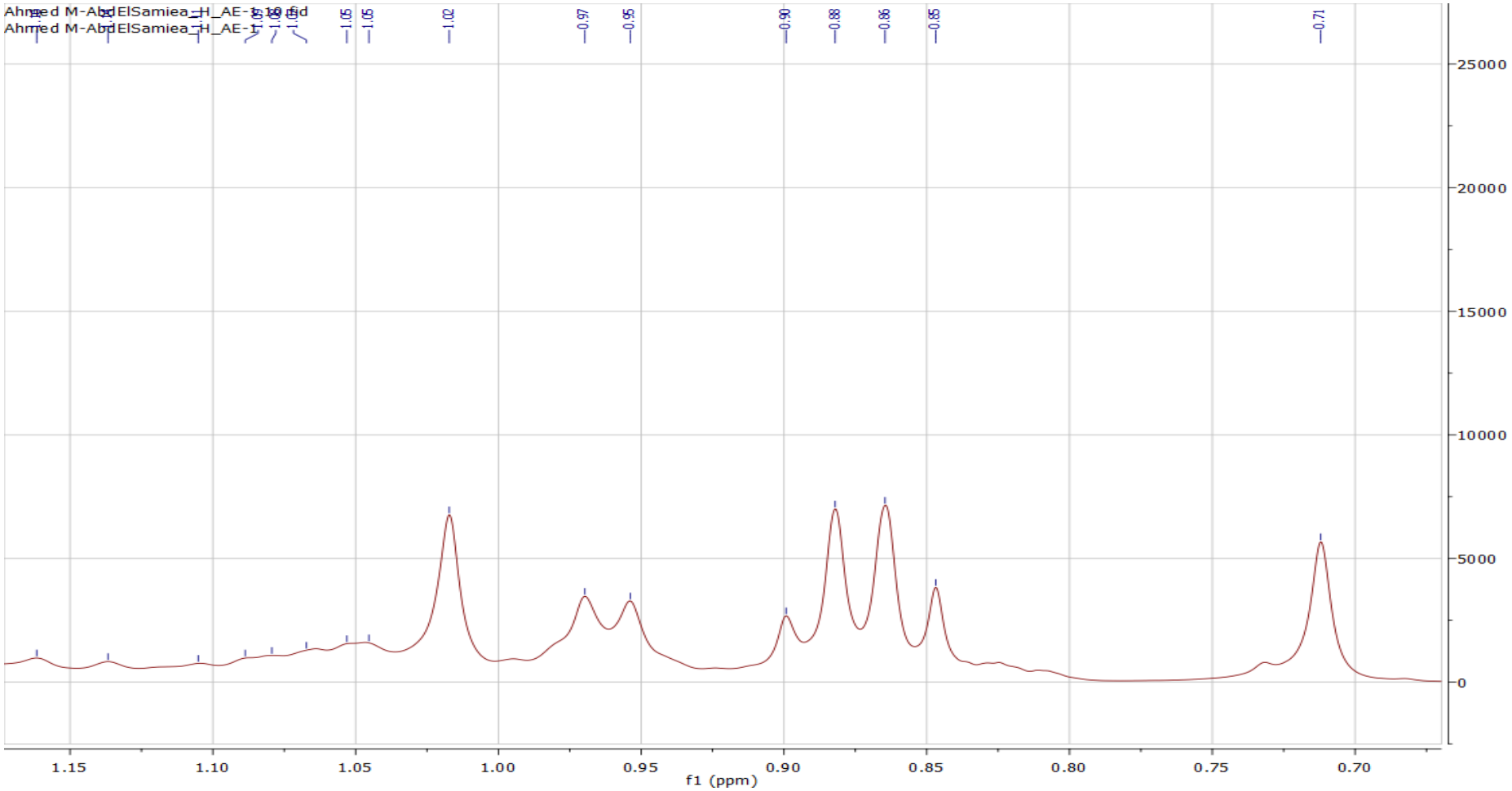


Figure 10: Partial expansion of ^{1}H-NMR spectrum of compound 2 (400 MHz, DMSO-*d6*).

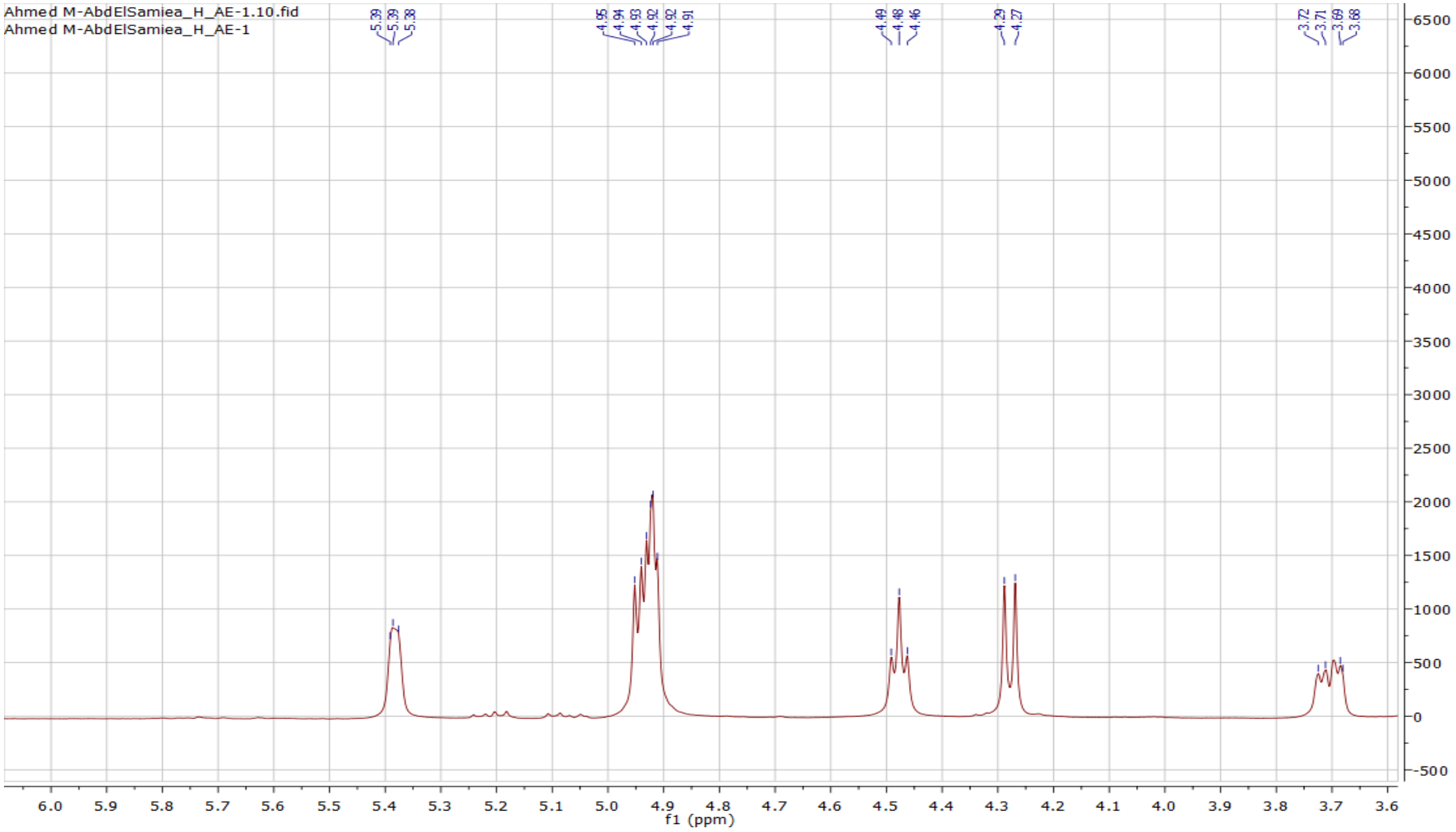


Figure 11: Partial expansion of ^{1}H-NMR spectrum of compound 2 (400 MHz, DMSO-*d6*).

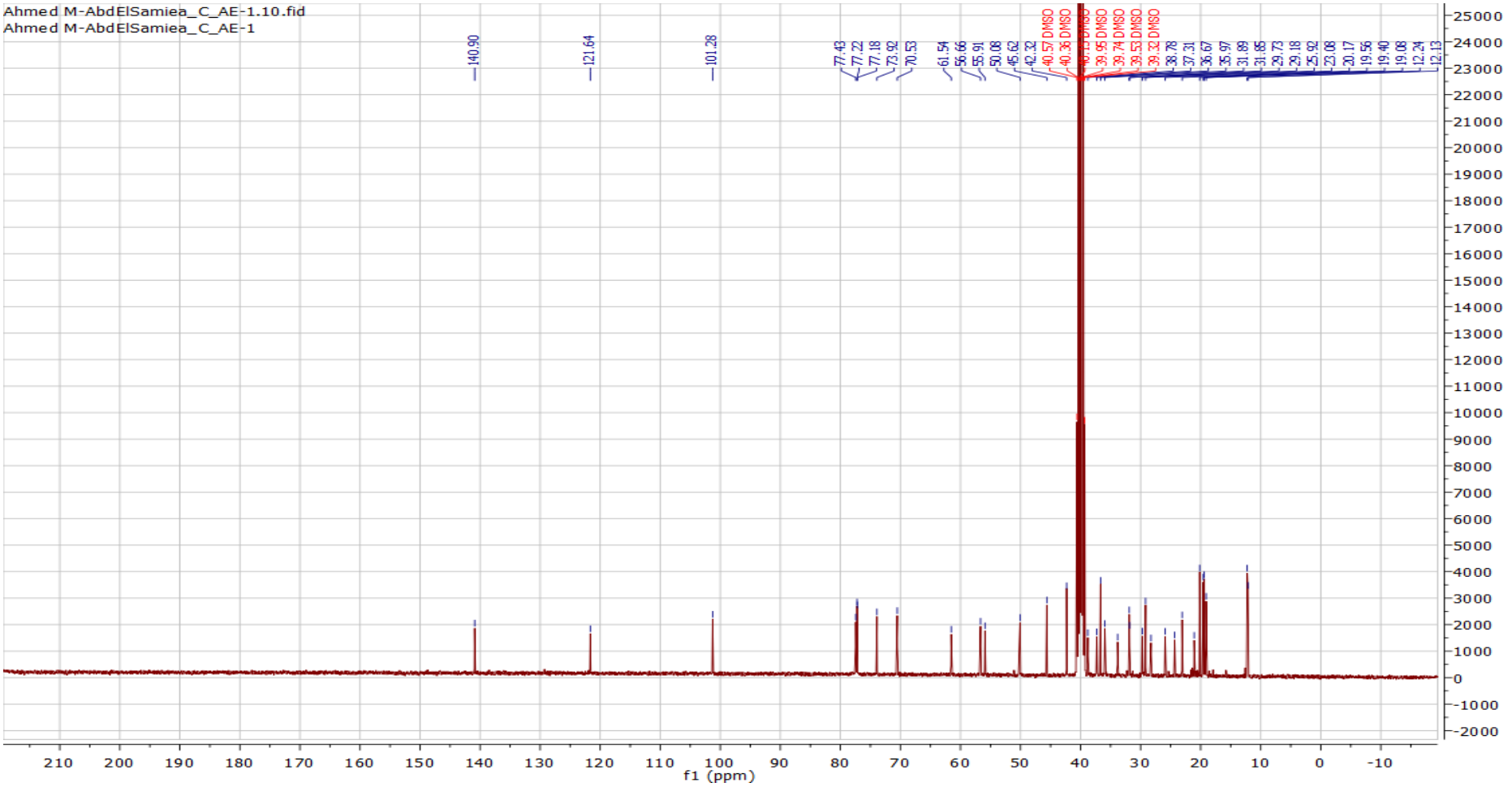


Figure 12: ^{13}C-NMR spectrum of compound 2 (100 MHz, DMSO-*d6*)

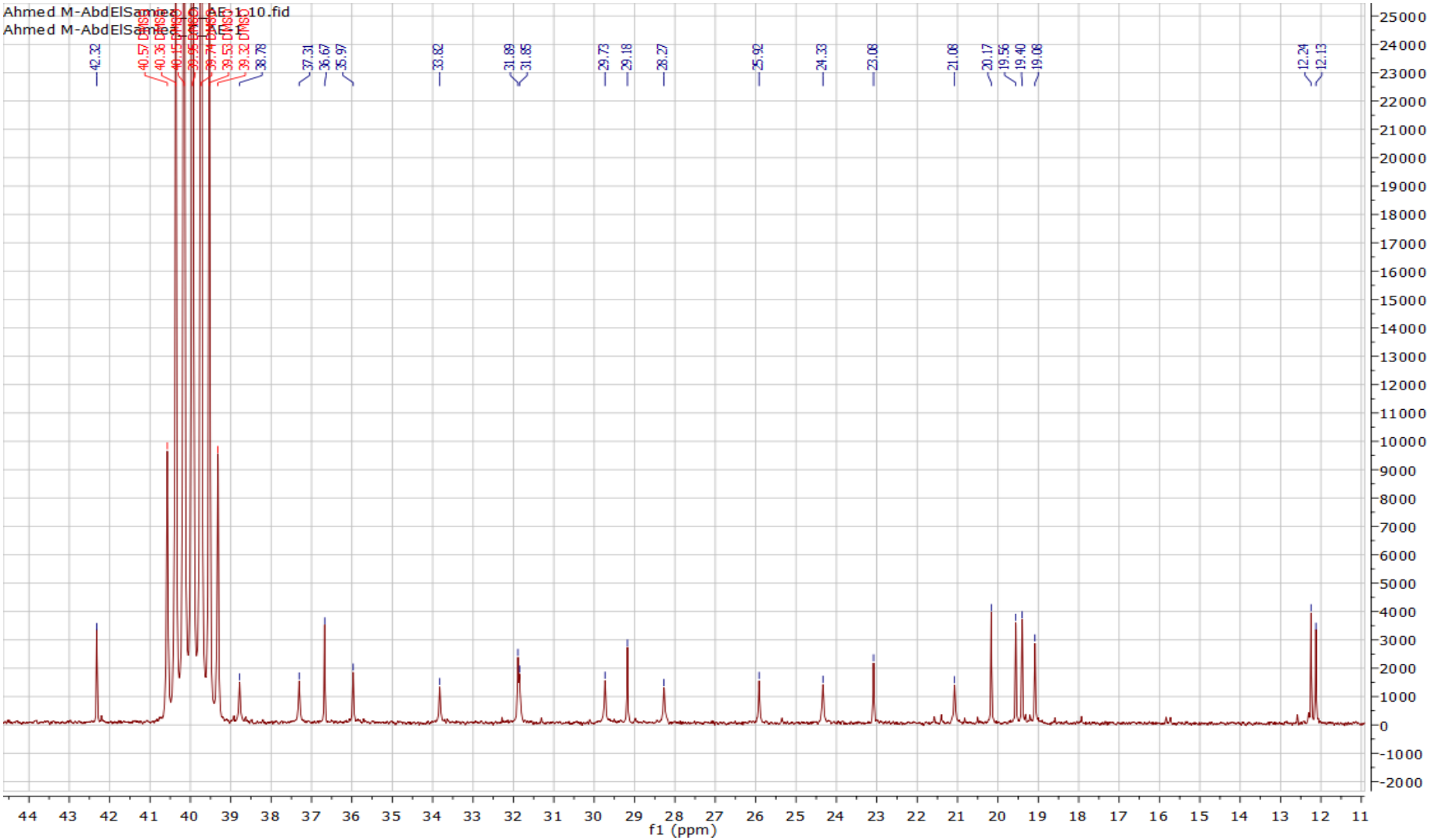


Figure 13: Partial expansion of ^{13}C-NMR spectrum of compound 2 (100 MHz, DMSO-*d6*)

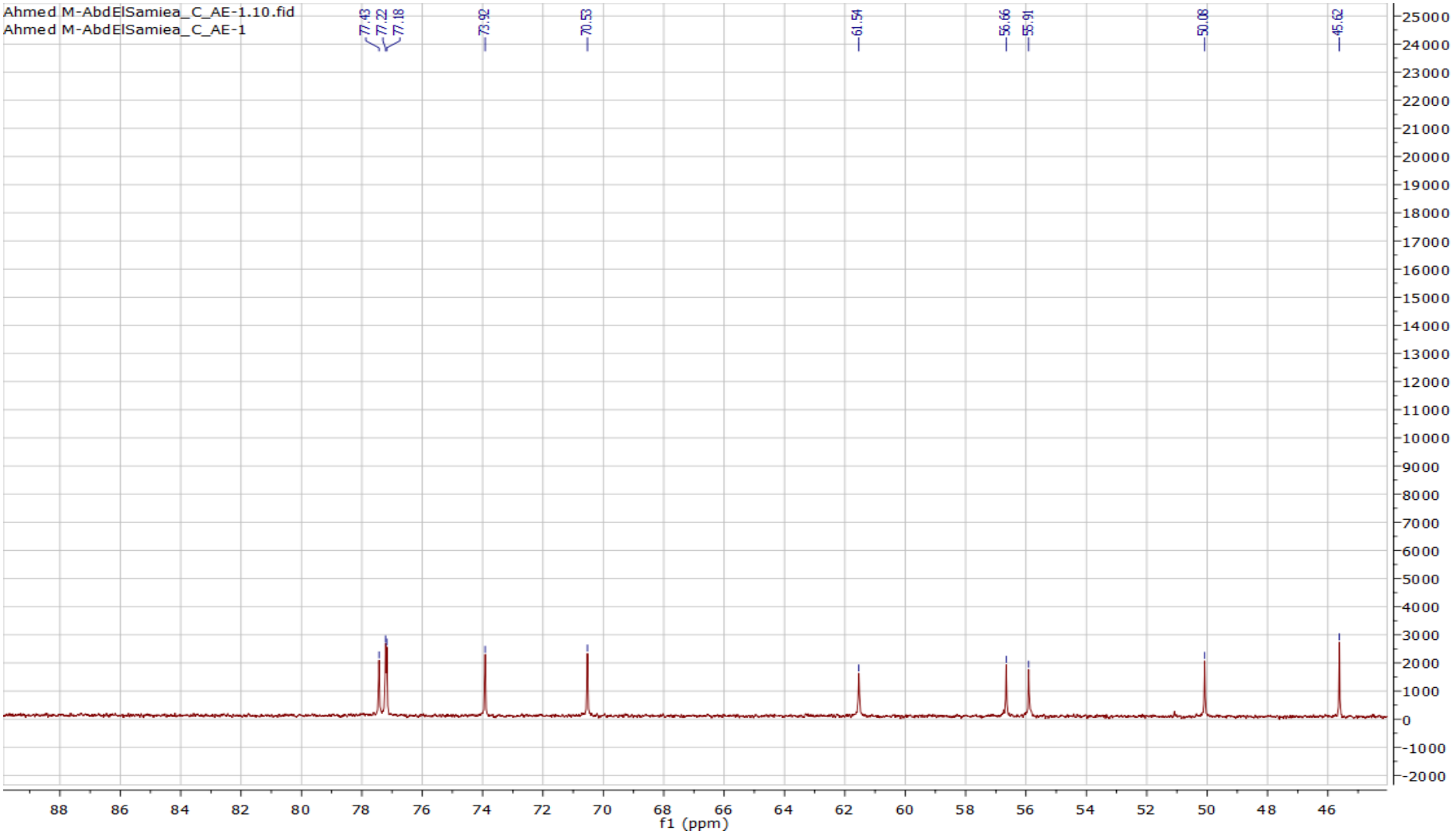


Figure 14: Partial expansion of ^{13}C-NMR spectrum of compound 2 (100 MHz, DMSO-*d6*)

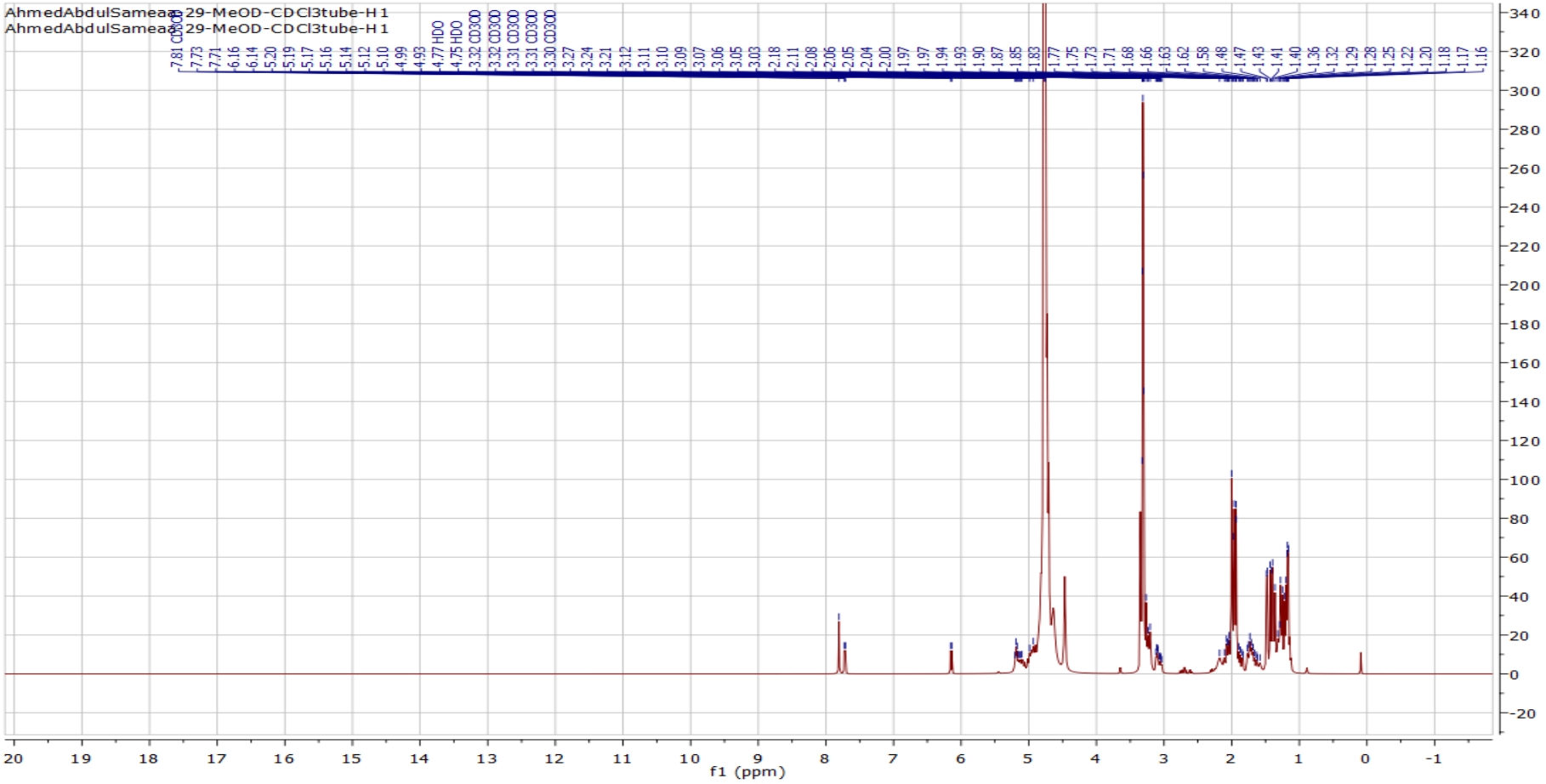


Figure 15: ^{1}H-NMR spectrum of compound 3 (300 MHz, $CDCl_3$-CD_3OD)

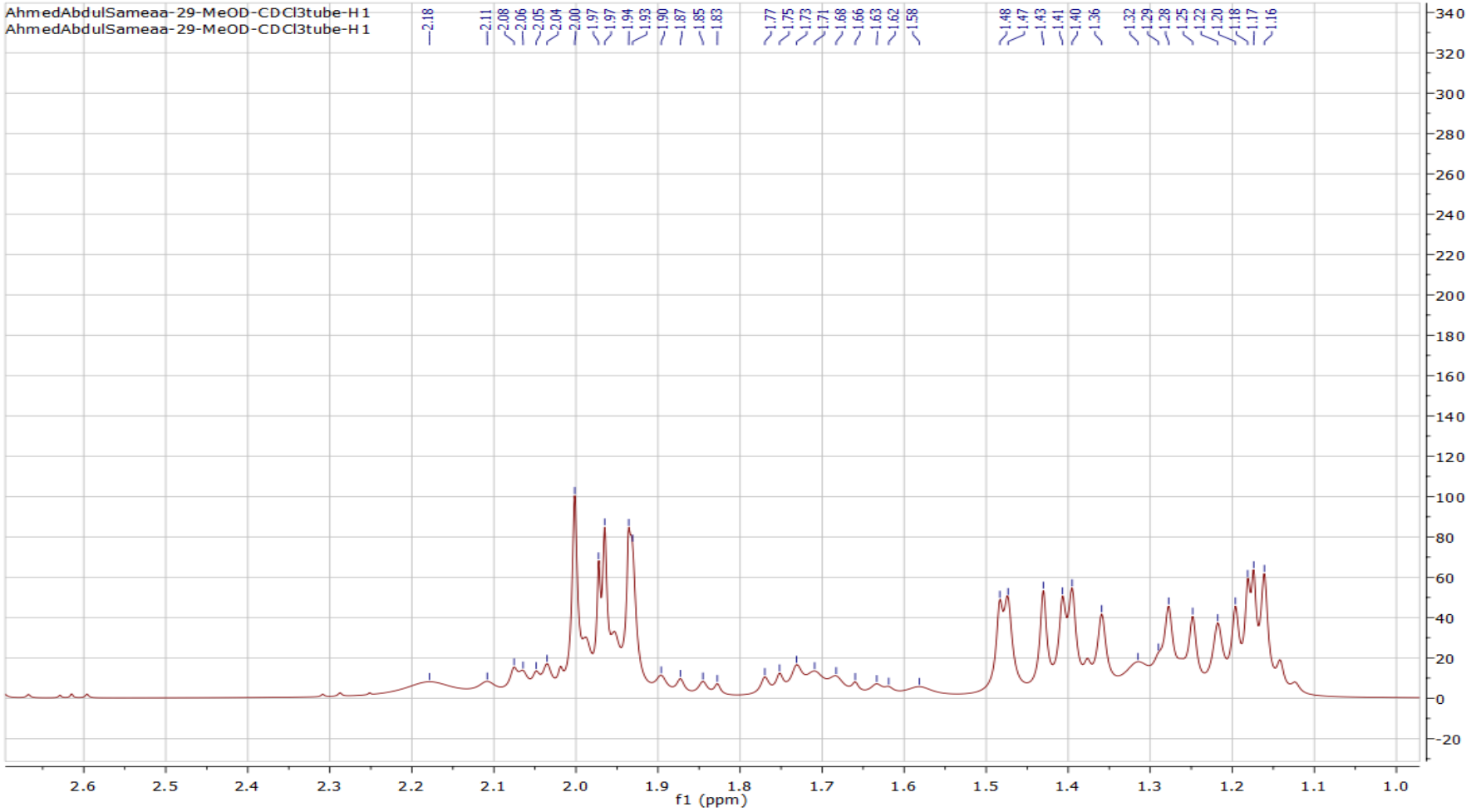


Figure 16: Partial expansion of ^{1}H-NMR spectrum of compound 3 (300 MHz, $CDCl_3$-CD_3OD)

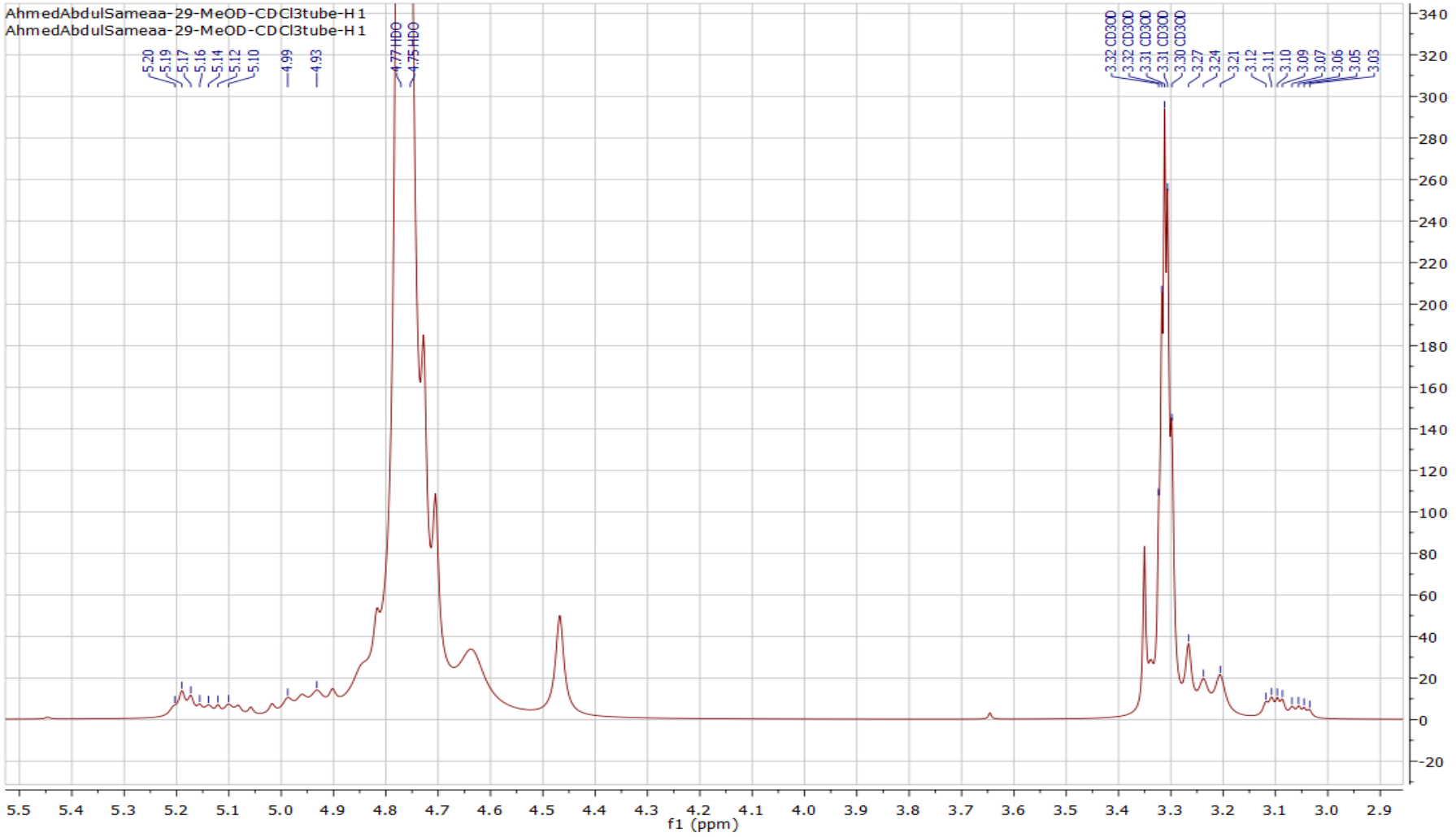


Figure 17: Partial expansion of ^{1}H-NMR spectrum of compound 3 (300 MHz, $CDCl_3$-CD_3OD)

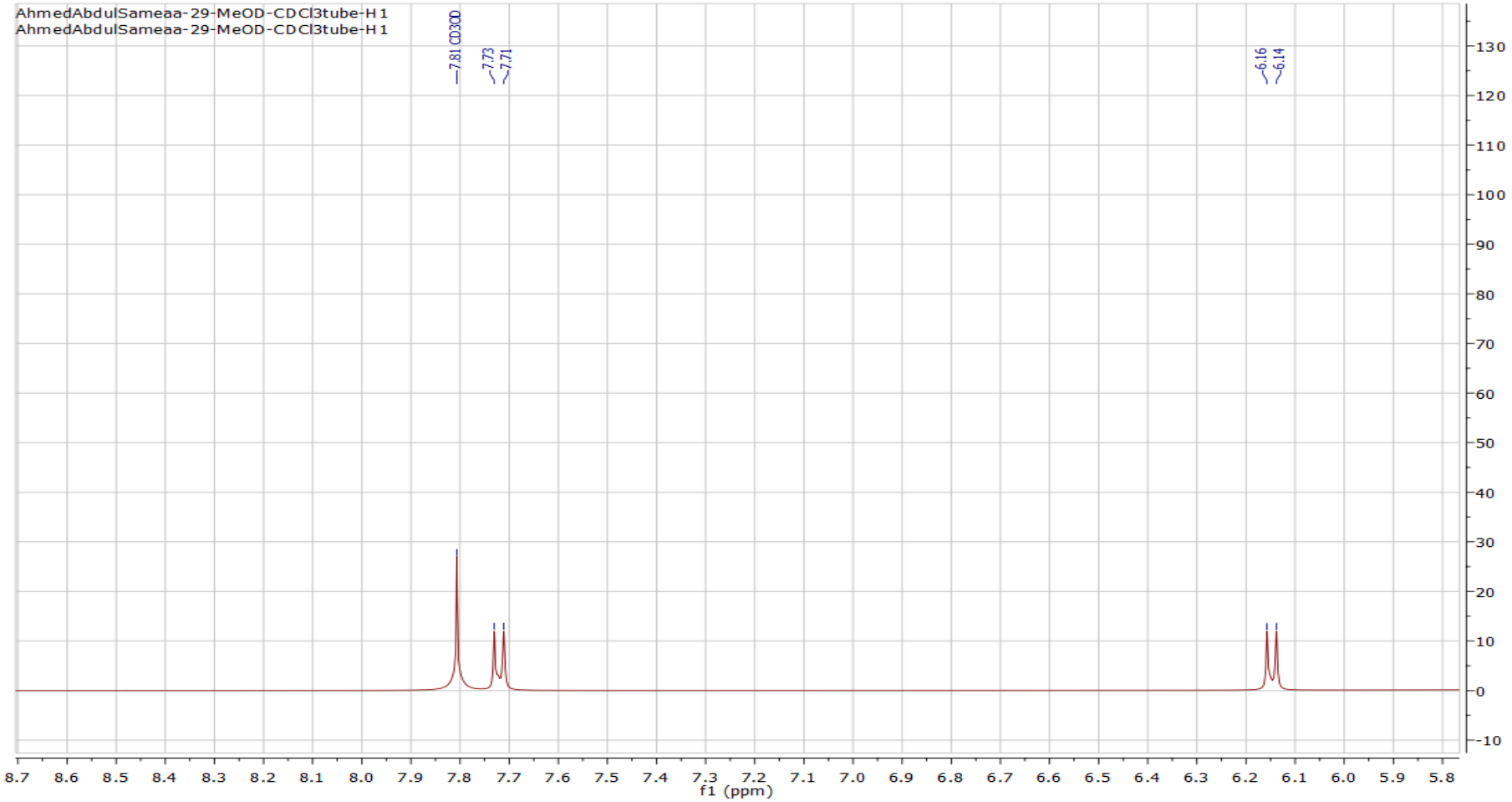


Figure 18: Partial expansion of ^{1}H-NMR spectrum of compound 3 (300 MHz, $CDCl_3$-CD_3OD)

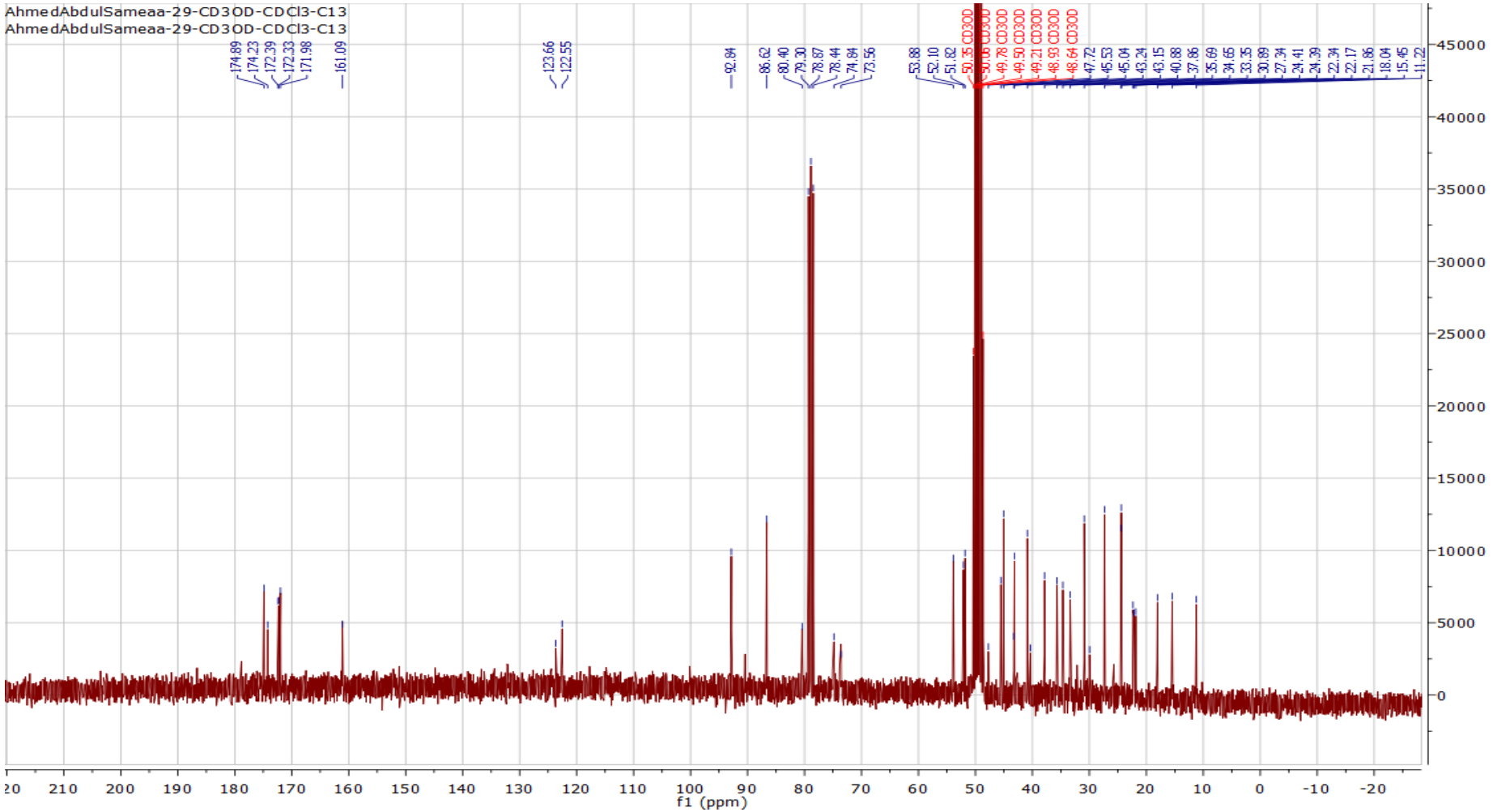


Figure 19: ^{13}C-NMR spectrum of compound 3 (75 MHz, $CDCl_3$-CD_3OD)

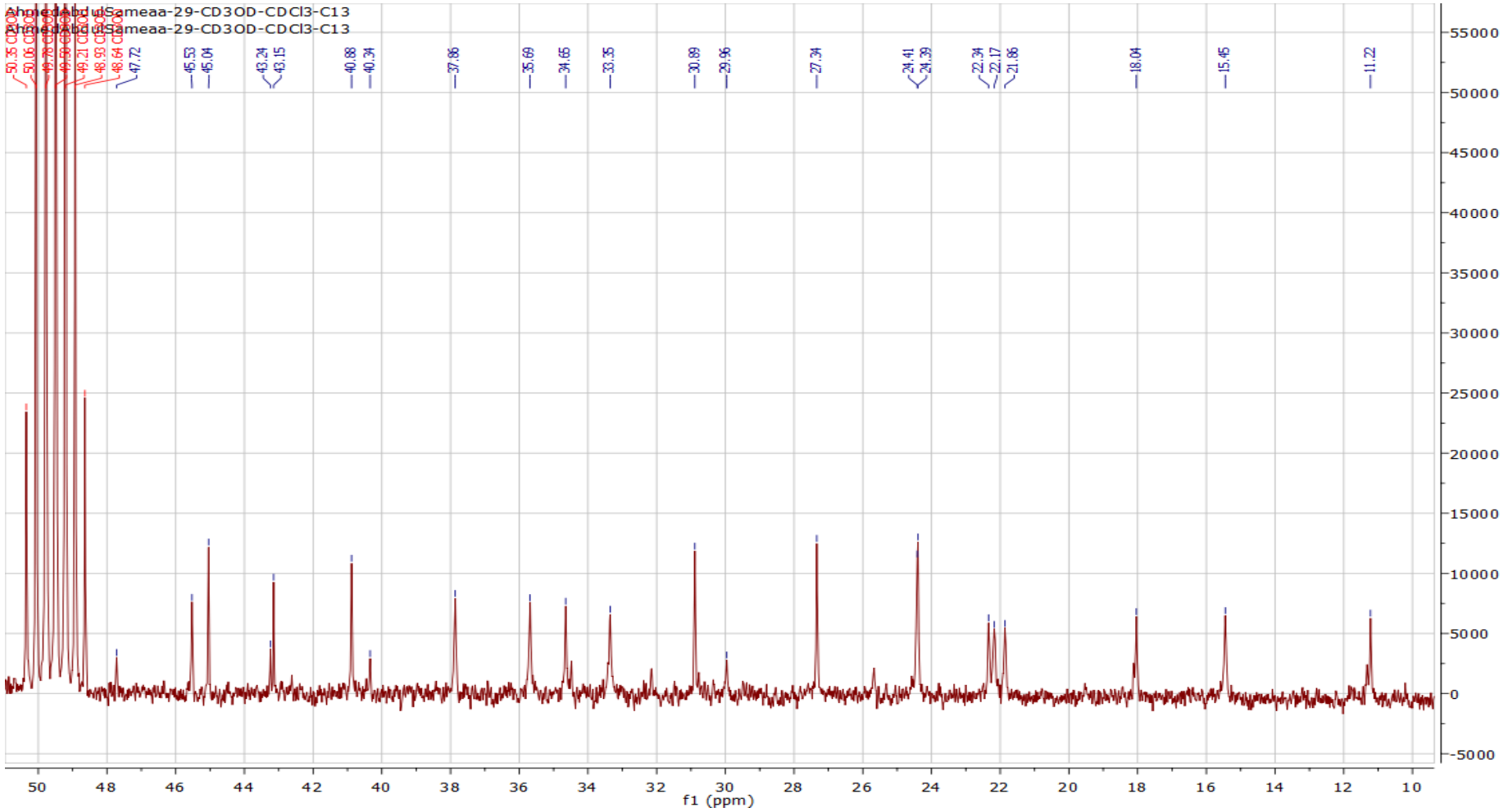


Figure 20: Partial expansion of ^{13}C-NMR spectrum of compound 3 (75 MHz, $CDCl_3$-CD_3OD)

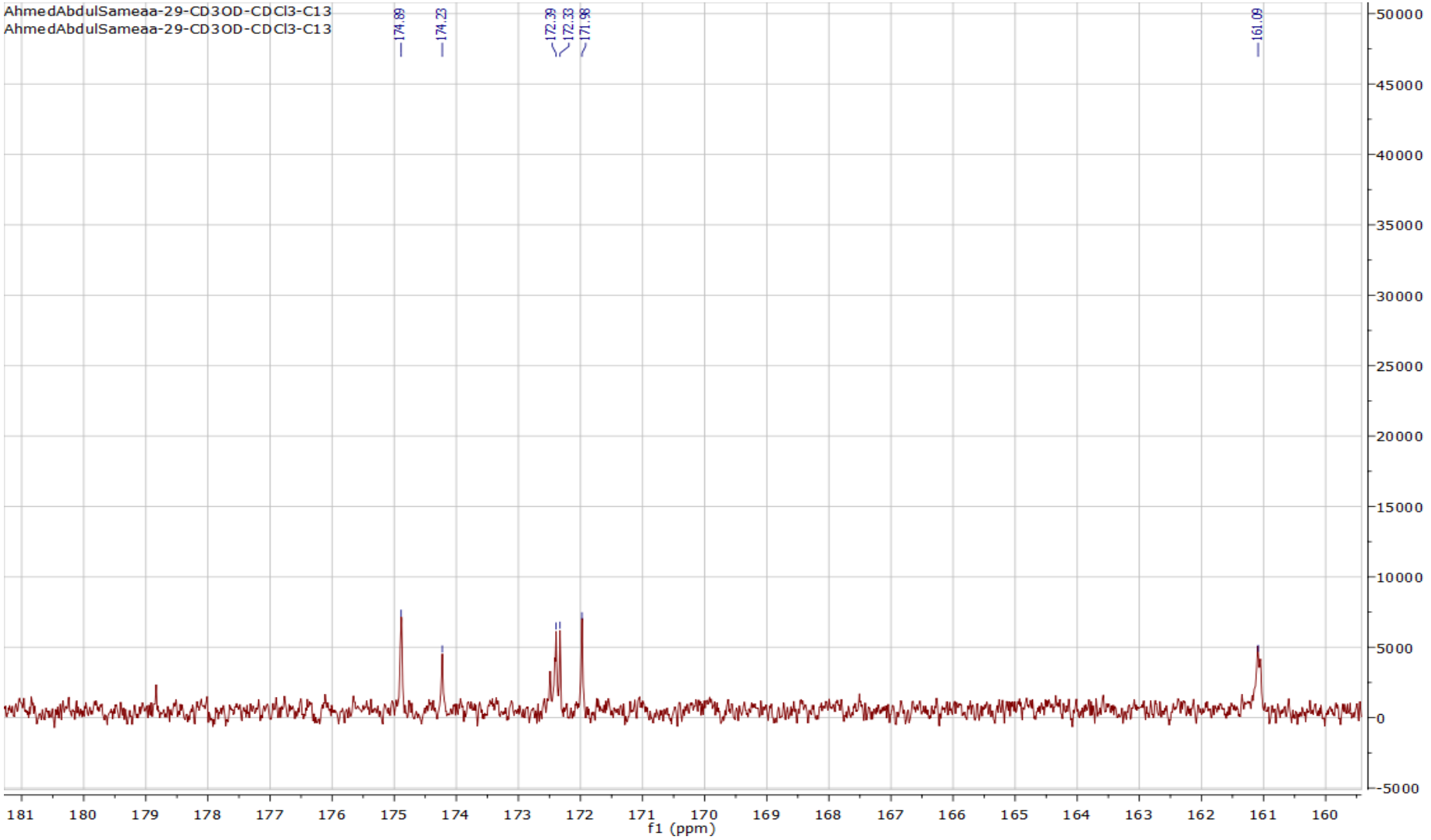


Figure 21: Partial expansion of ^{13}C-NMR spectrum of compound 3 (75 MHz, $CDCl_3$-CD_3OD)

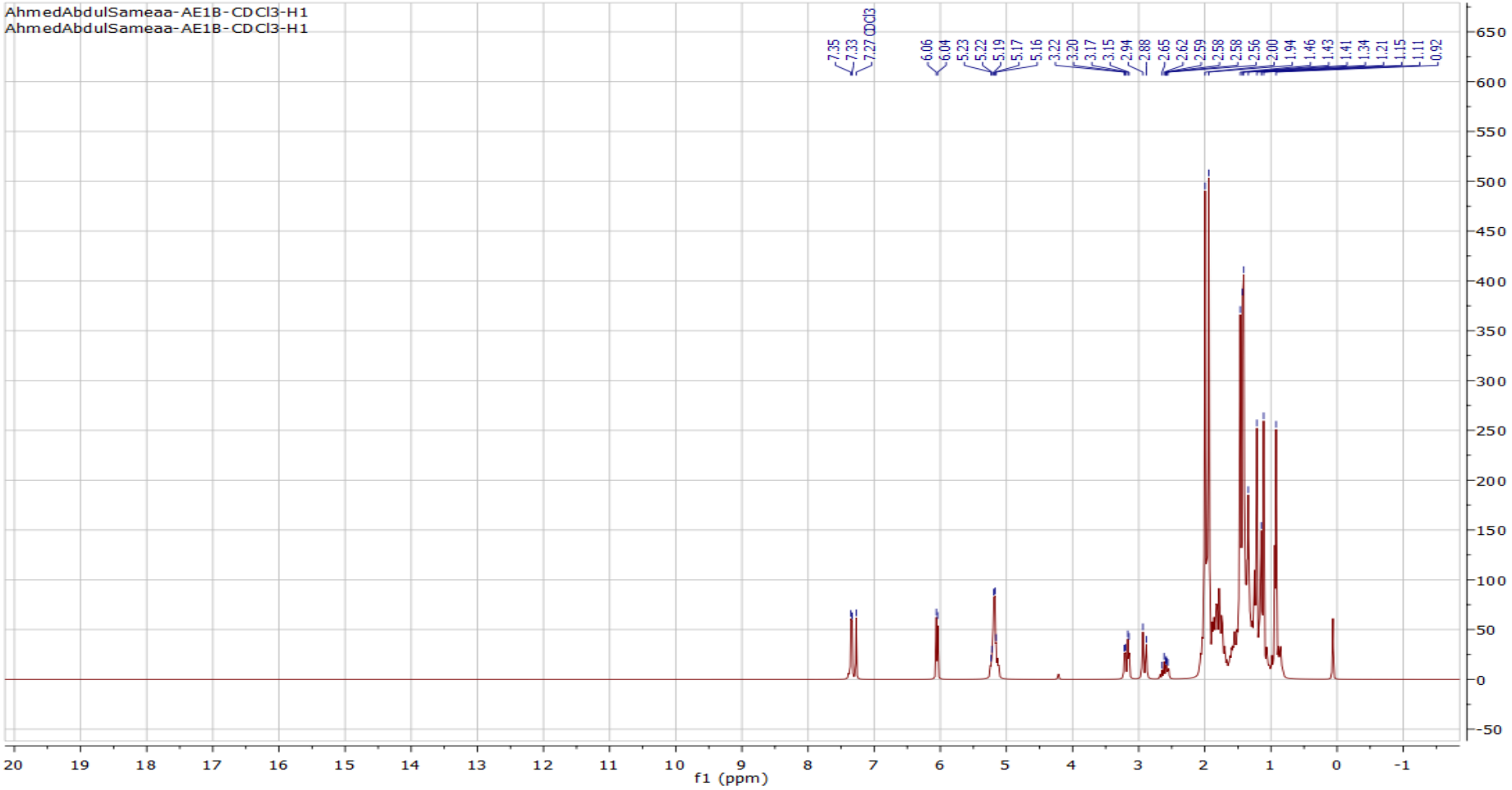


Figure 22: ^{1}H -NMR spectrum of compound 4 (300 MHz, $CDCl_3$)

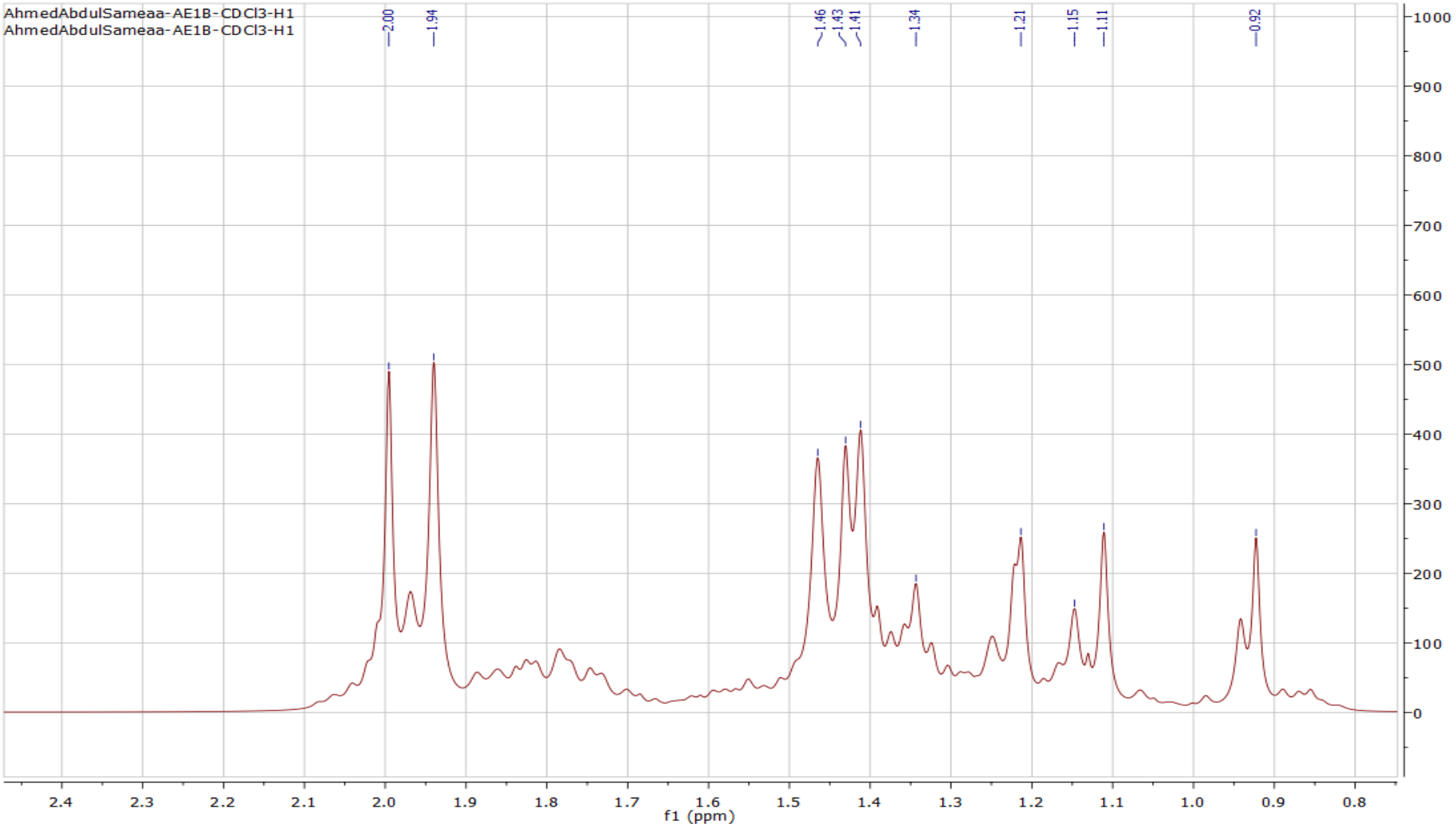


Figure 23: Partial expansion of ^{1}H -NMR spectrum of compound 4 (300 MHz, $CDCl_3$)

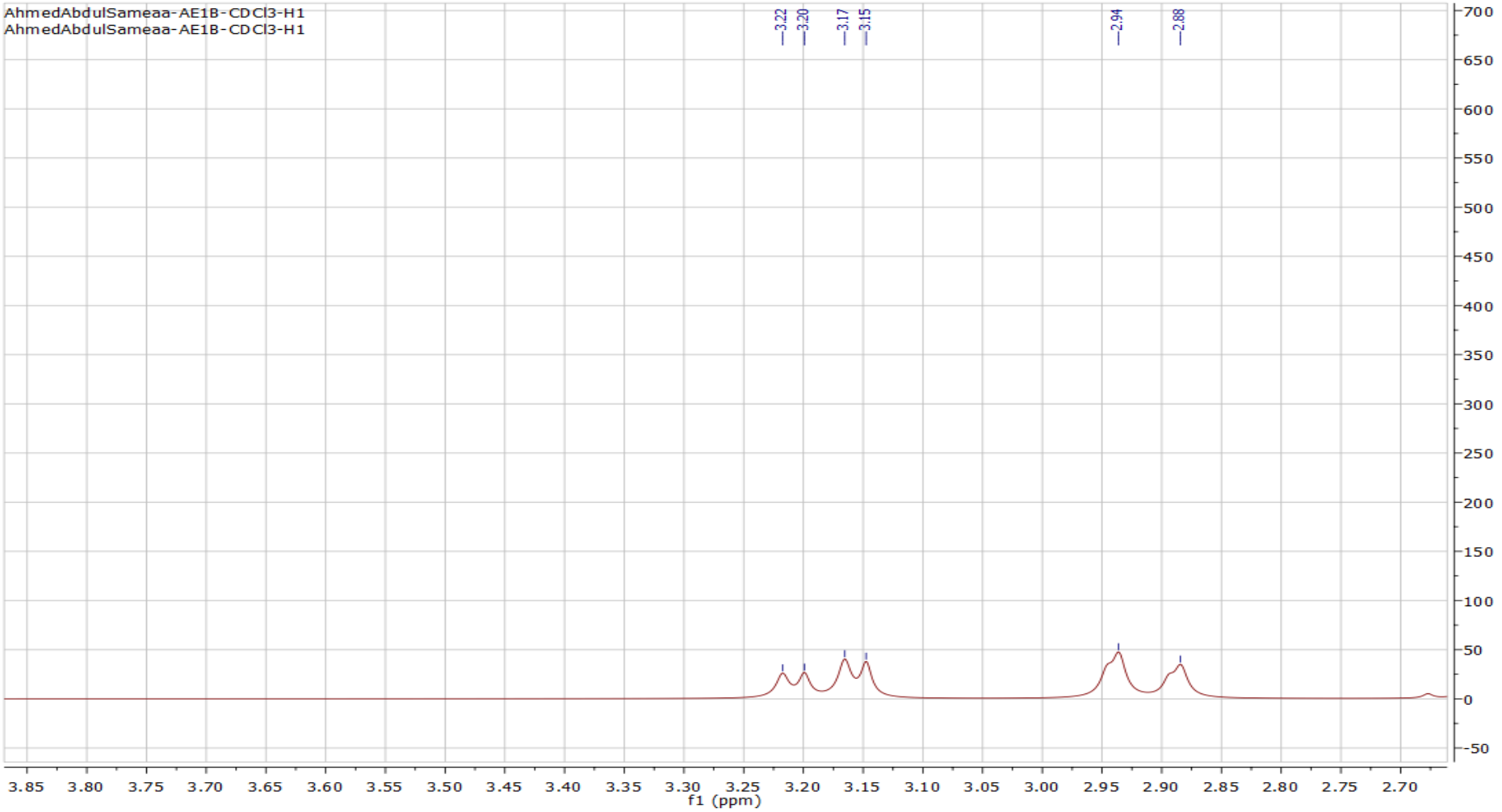


Figure 24: Partial expansion of ^{1}H -NMR spectrum of compound 4 (300 MHz, $CDCl_3$)

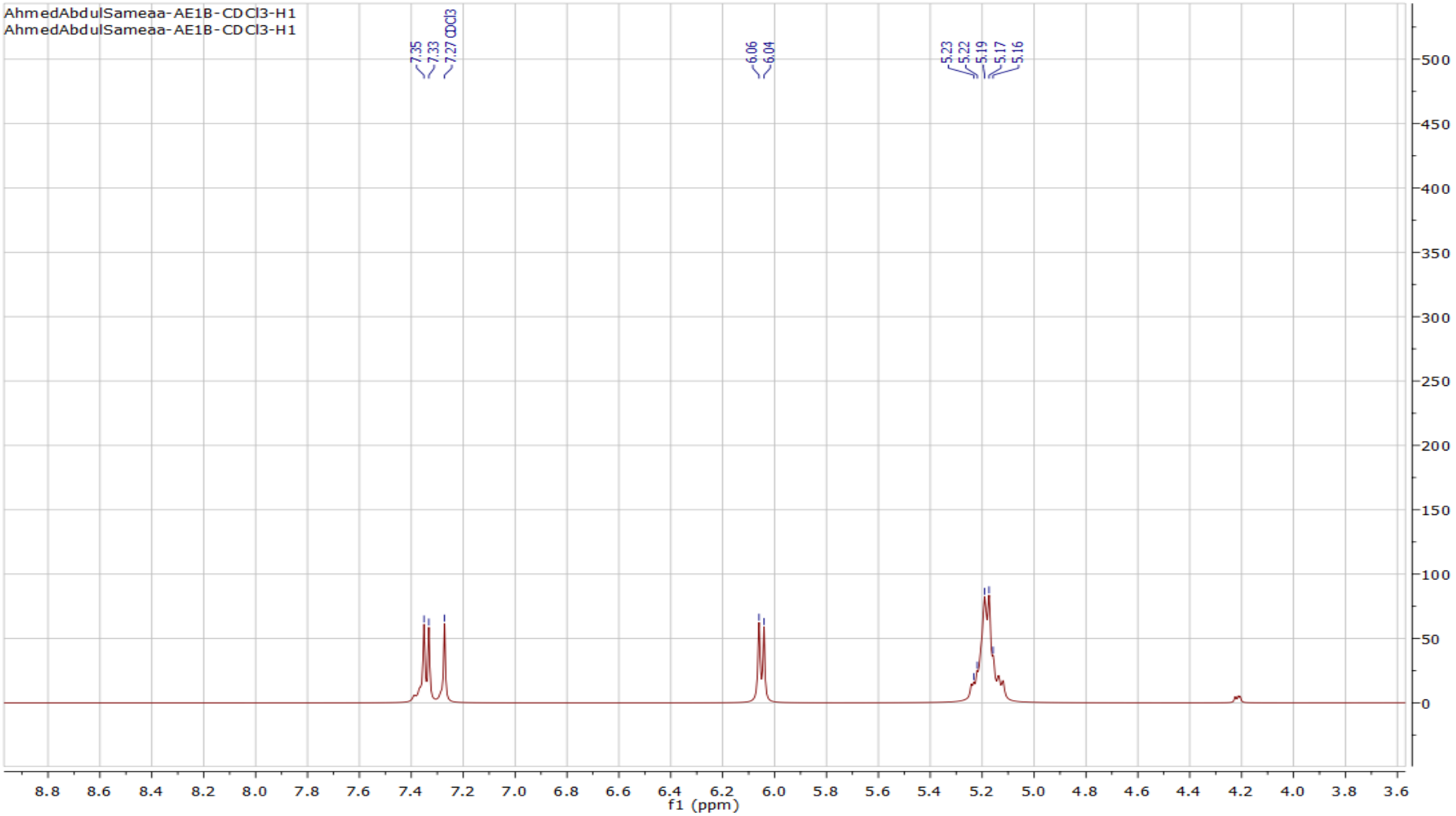


Figure 25: Partial expansion of ^{1}H -NMR spectrum of compound 4 (300 MHz, $CDCl_3$)

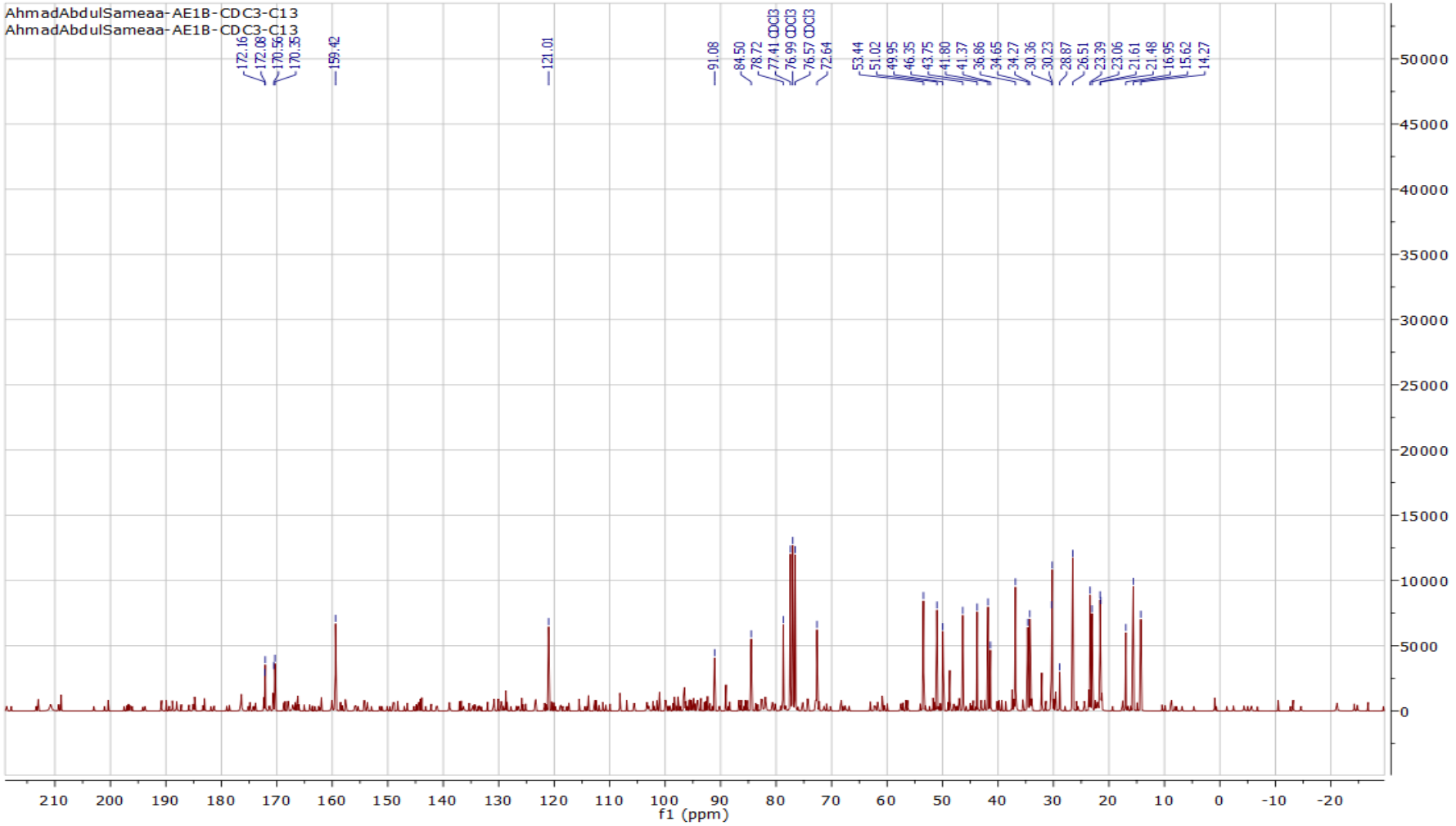


Figure 26: ^{13}C-NMR spectrum of compound 4 (75 MHz, $CDCl_3$)

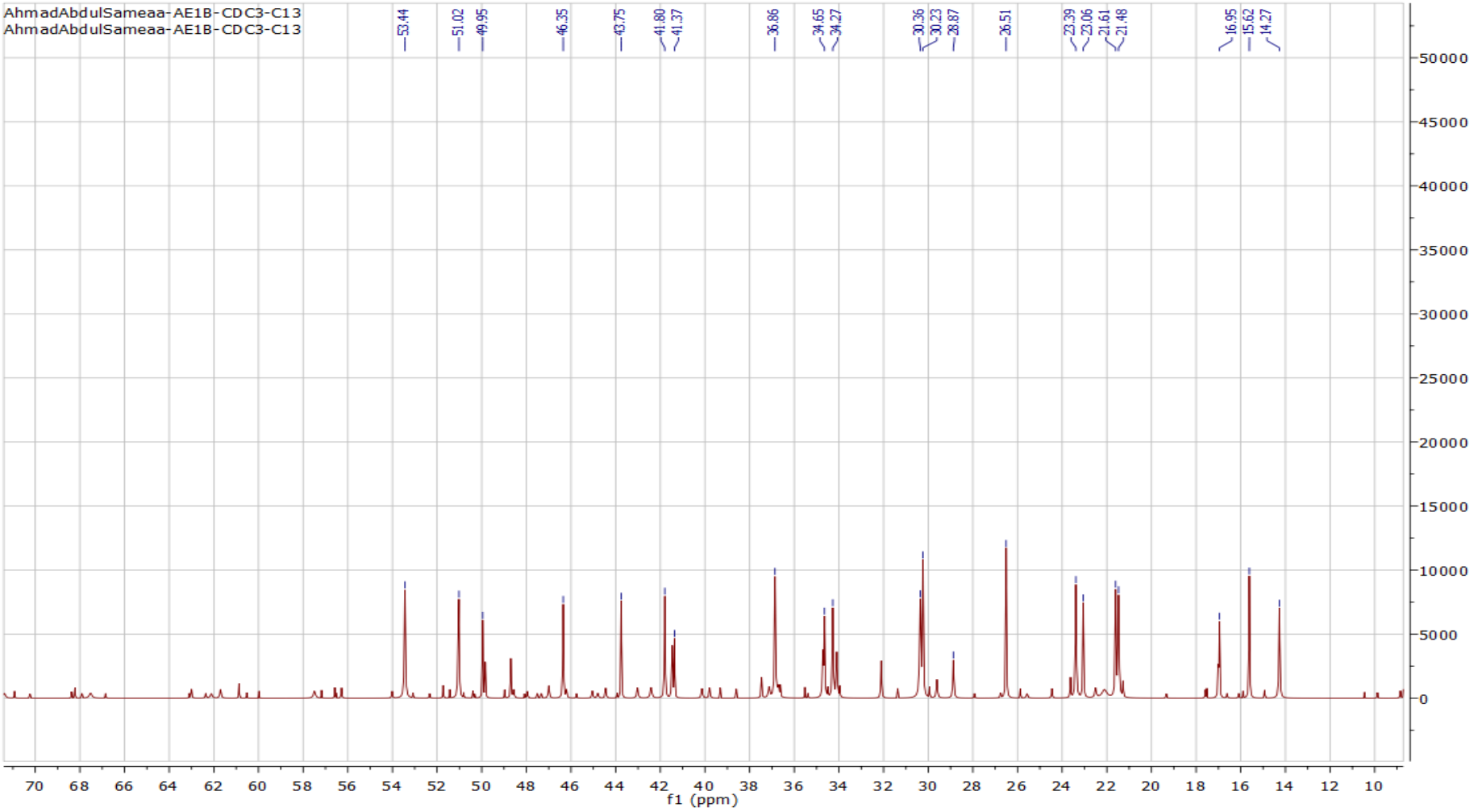


Figure 27: Partial expansion of ^{13}C -NMR spectrum of compound 4 (75 MHz, $CDCl_3$)

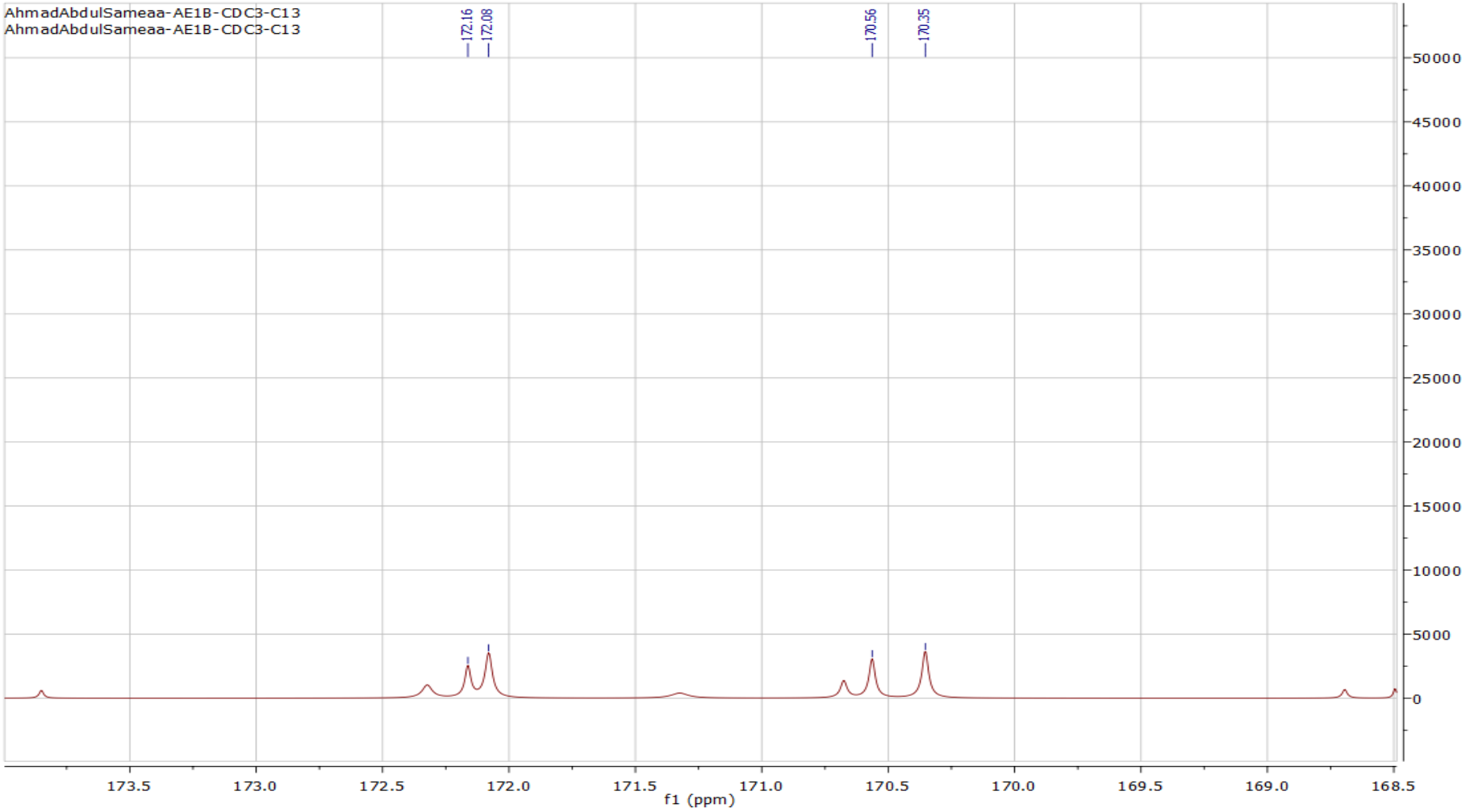


Figure 28: Partial expansion of ^{13}C -NMR spectrum of compound 4 (75 MHz, $CDCl_3$)

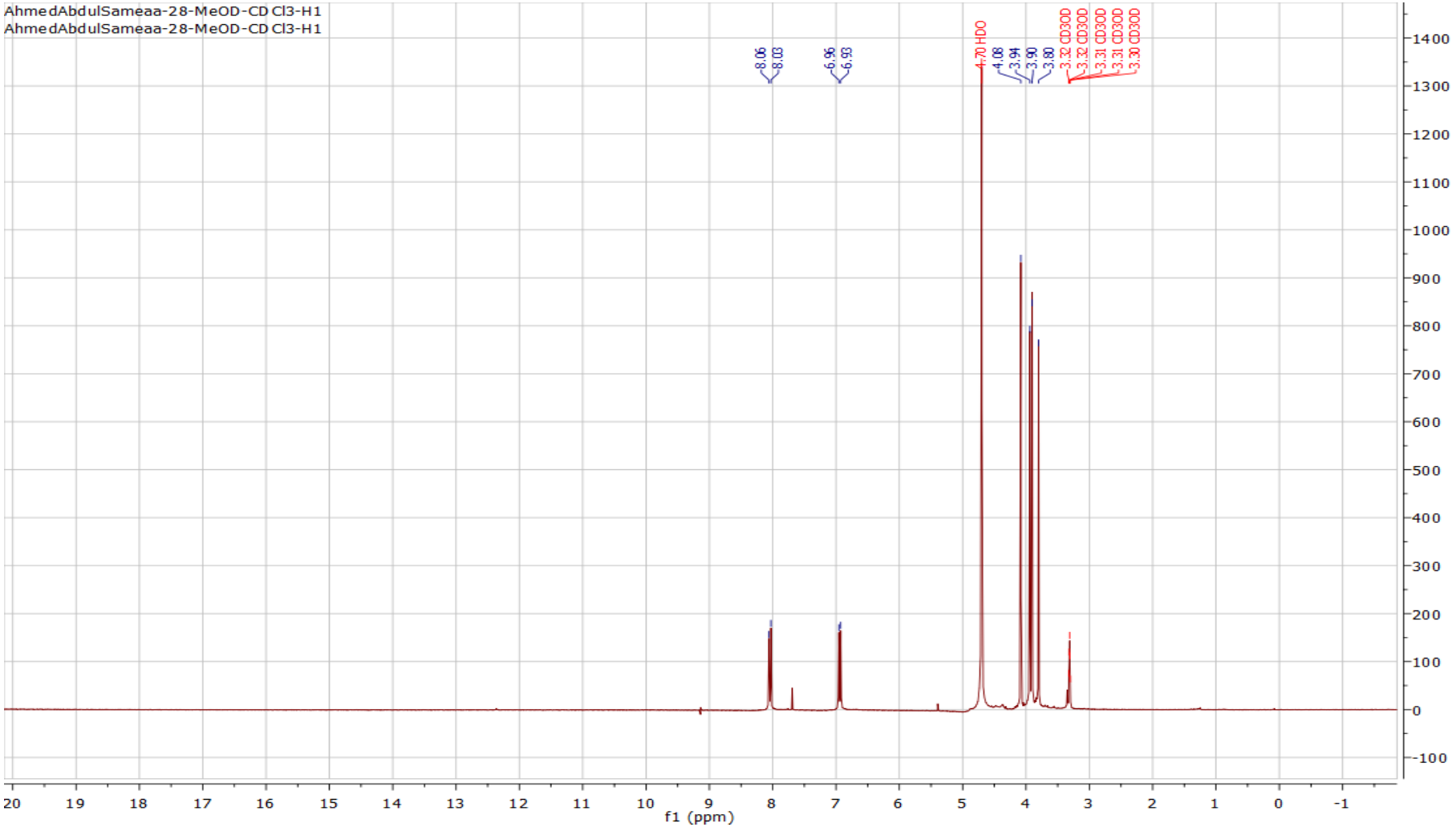


Figure 29: ^{1}H-NMR spectrum of compound 5 (300 MHz, $CDCl_3$-CD_3OD)

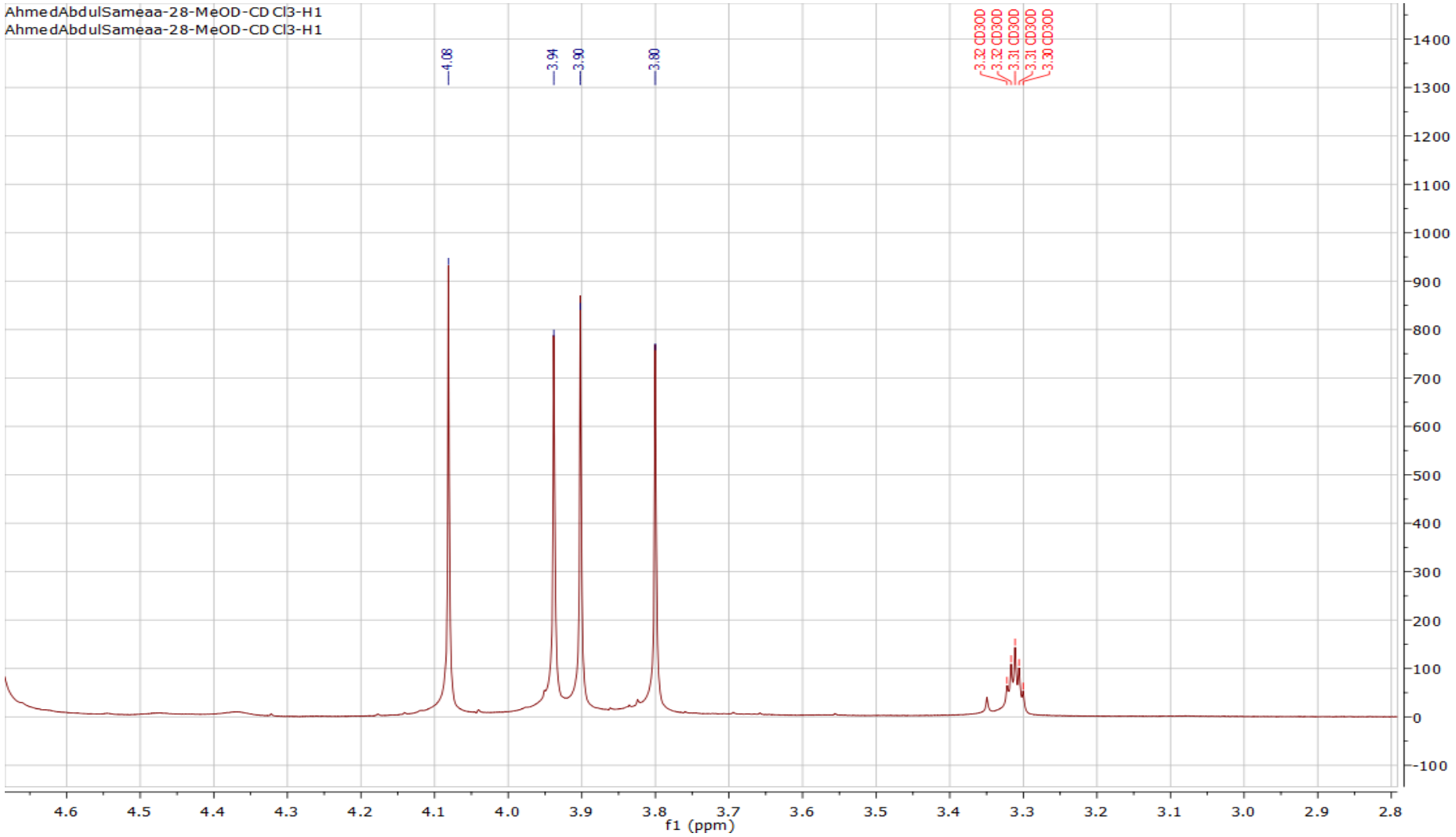


Figure 30: Partial expansion of ^{1}H-NMR spectrum of compound 5 (300 MHz, $CDCl_3$-CD_3OD)

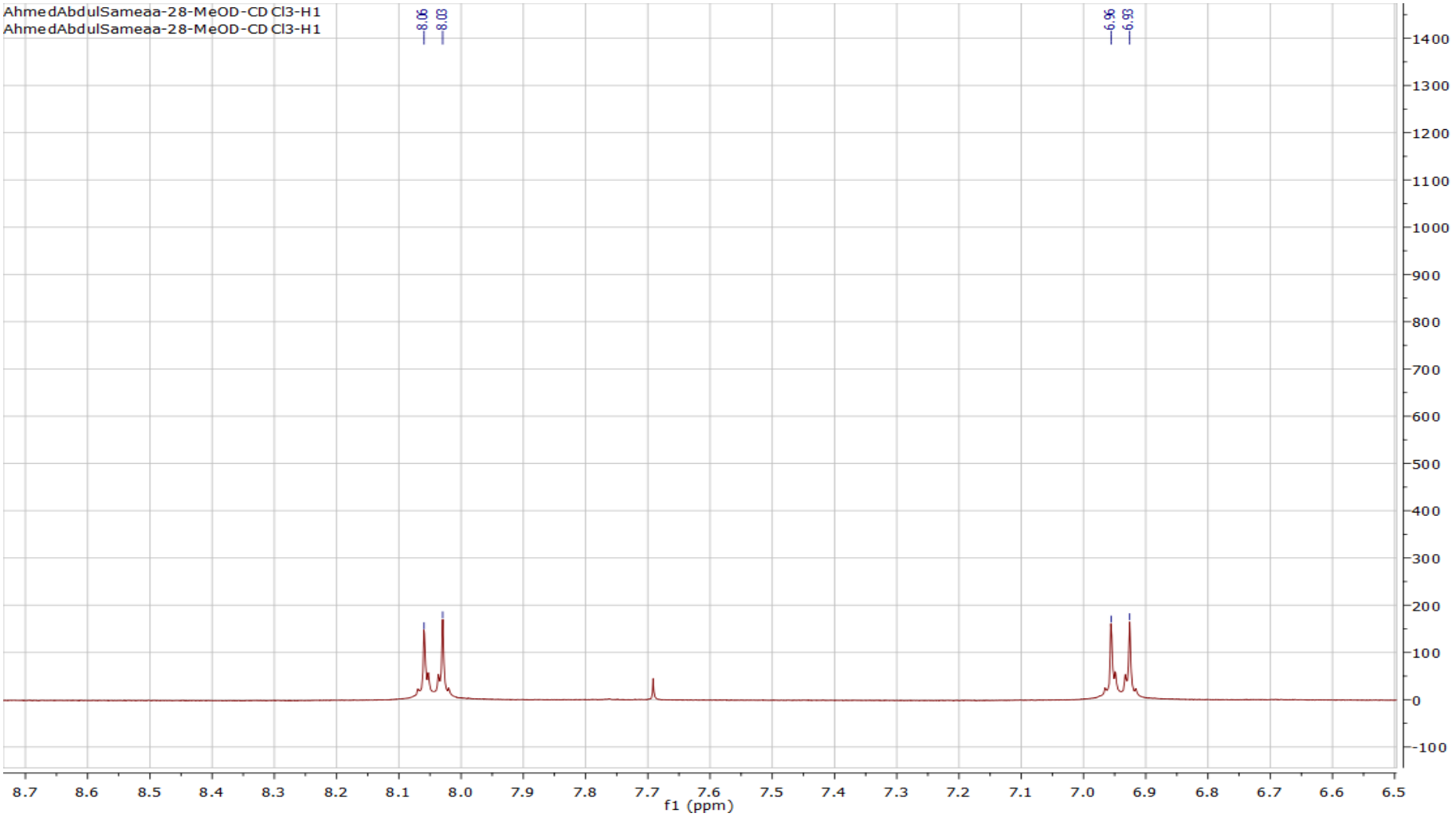


Figure 31: Partial expansion of ^{1}H-NMR spectrum of compound 5 (300 MHz, $CDCl_3$-CD_3OD)

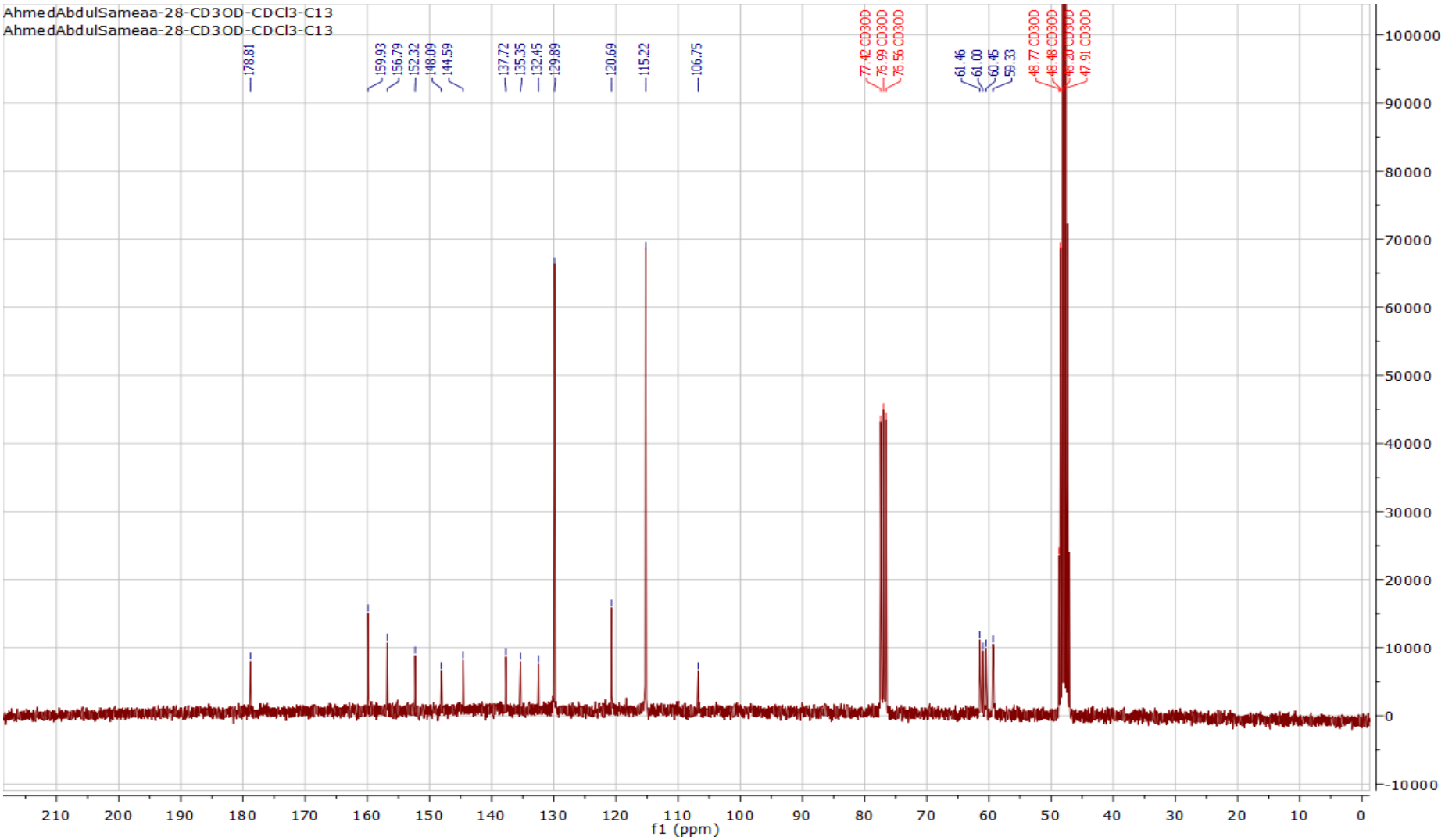


Figure 32: ^{13}C-NMR spectrum of compound 5 (75 MHz, $CDCl_3$-CD_3OD)

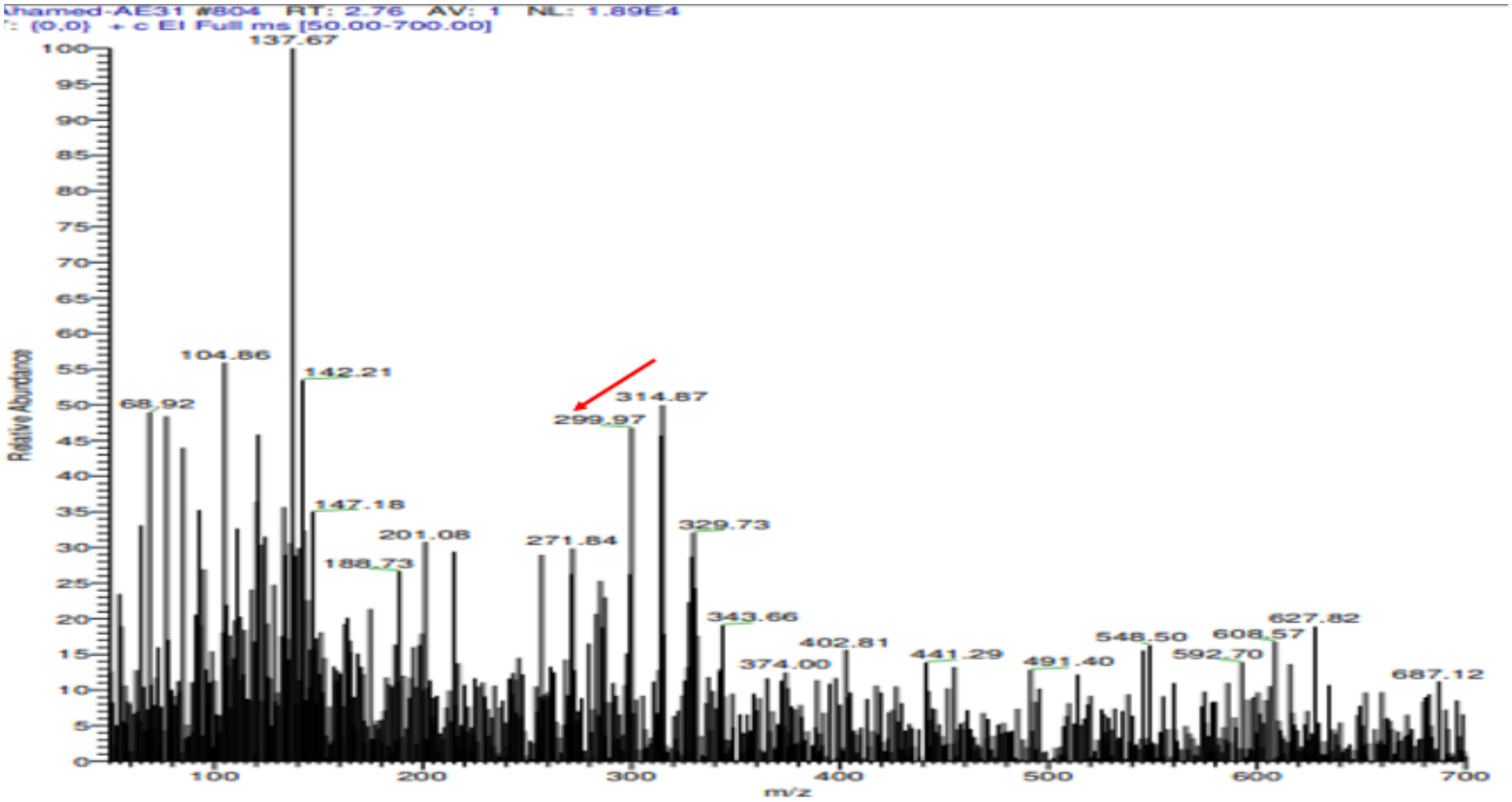


Figure 33: EI-MS of Compound 6

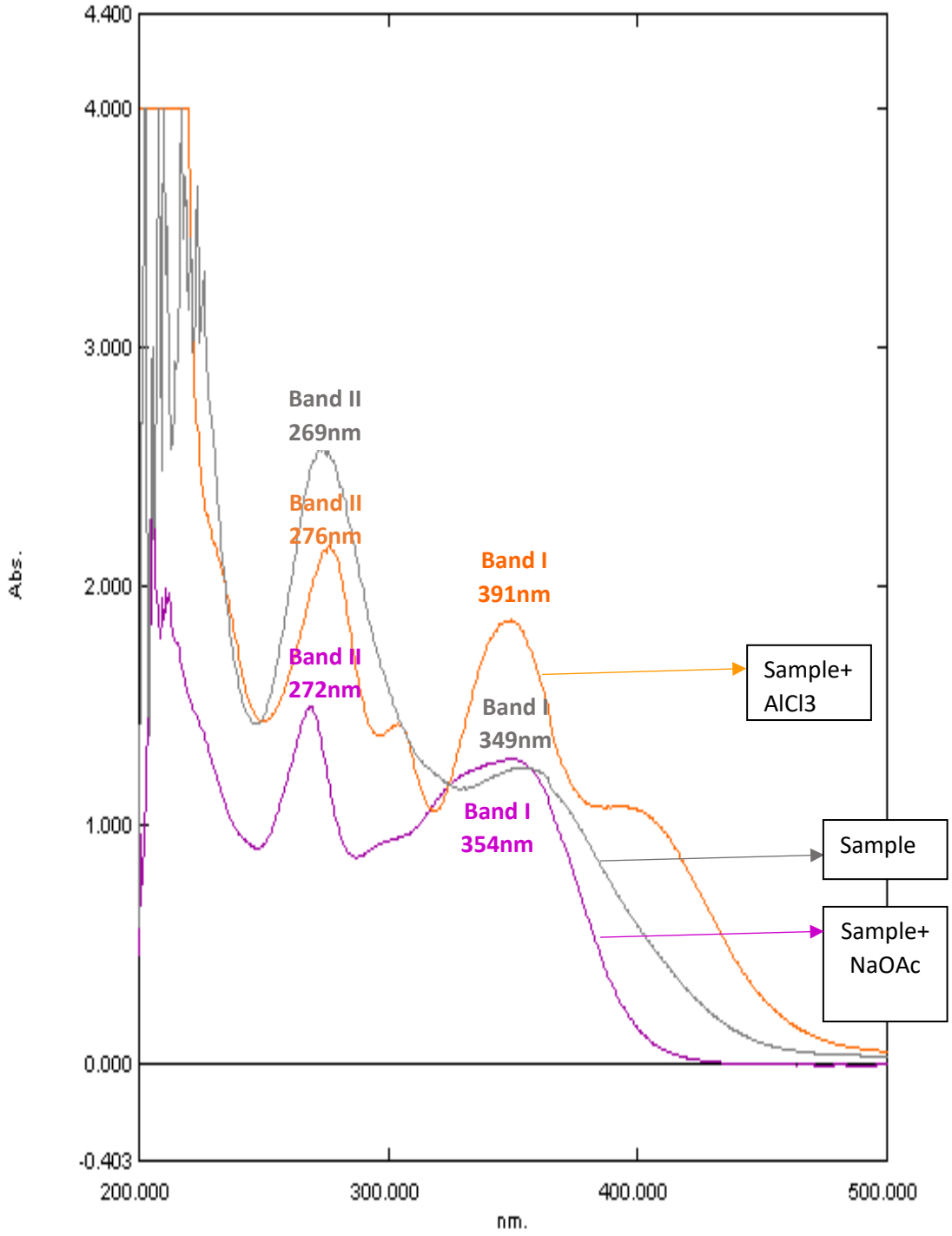


Figure 34: UV-Vis spectrum analysis of Compound 6

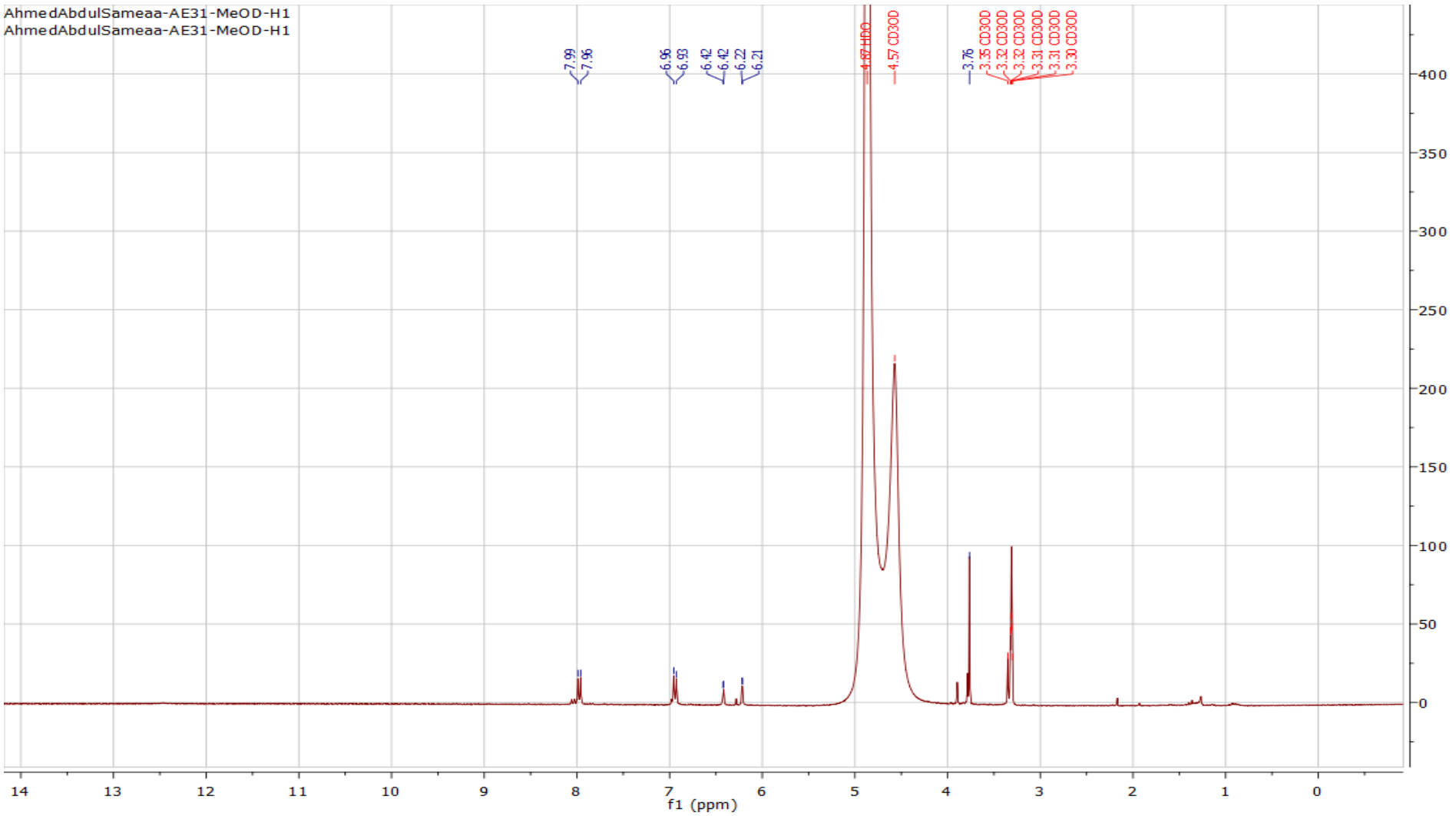


Figure 35: ^{1}H-NMR spectrum of compound 6 (300 MHz, CD_3OD)

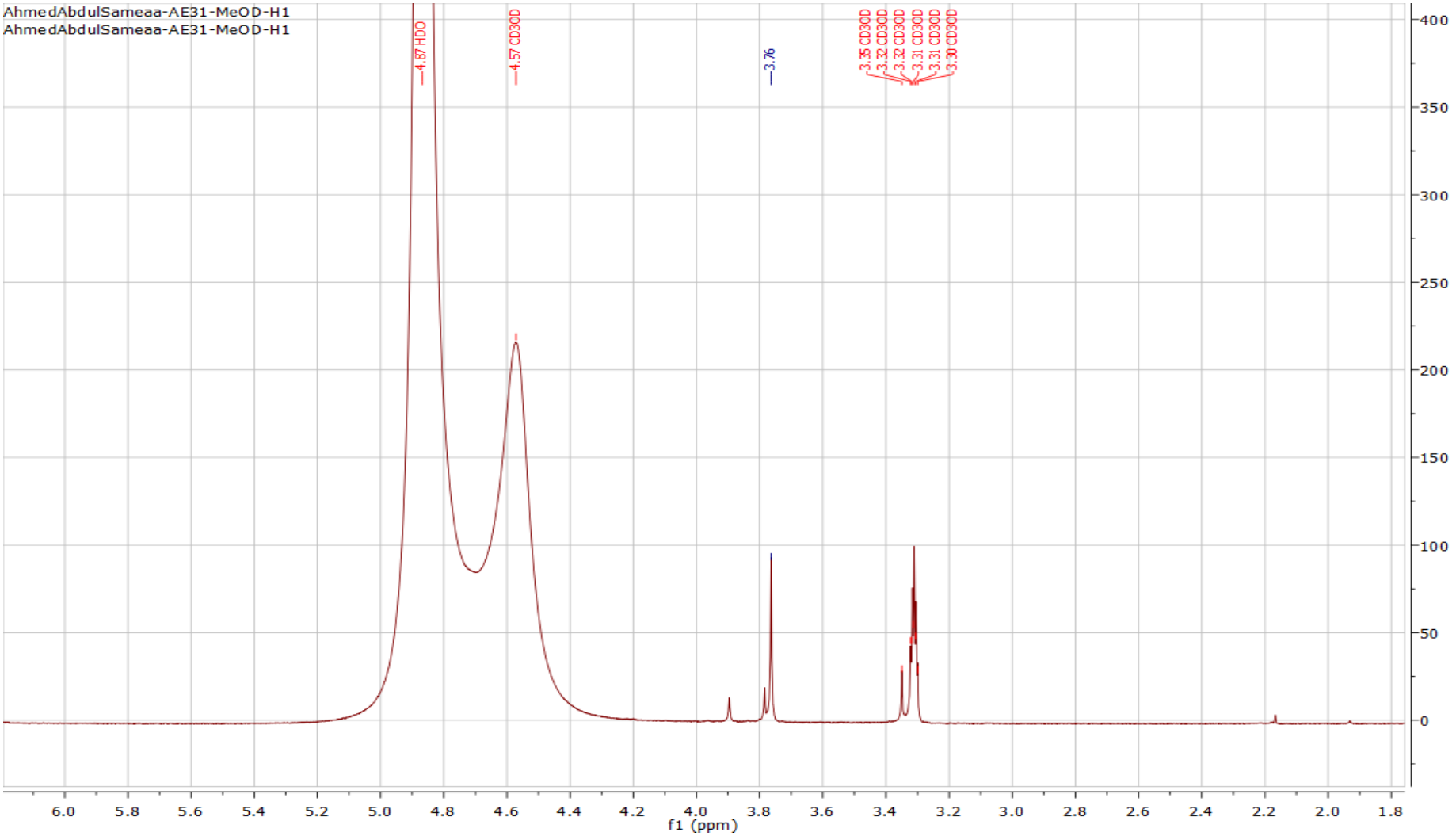


Figure 36: Partial expansion of ^{1}H-NMR spectrum of compound 6 (300 MHz, CD_3OD)

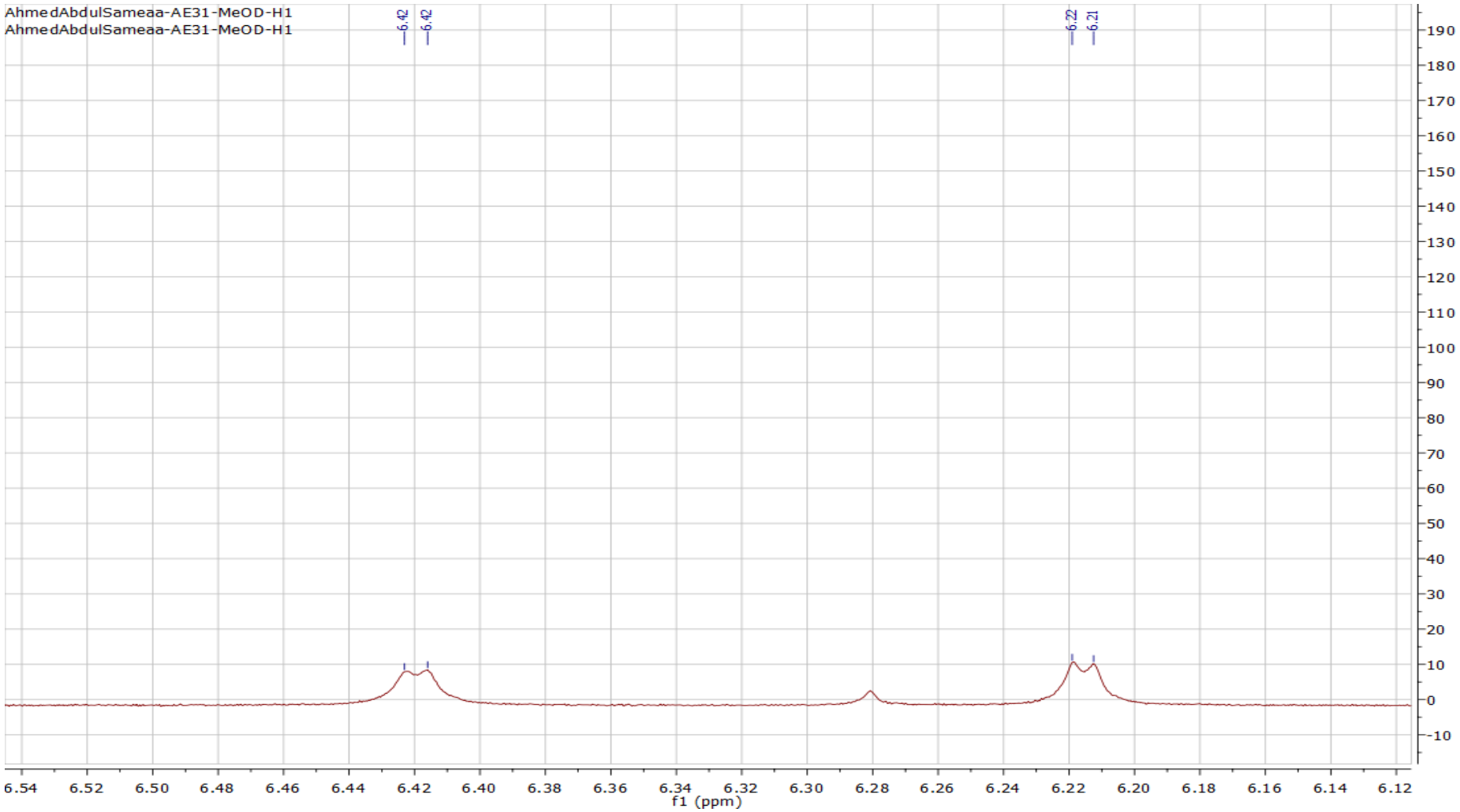


Figure 37: Partial expansion of ^{1}H-NMR spectrum of compound 6 (300 MHz, CD_3OD)

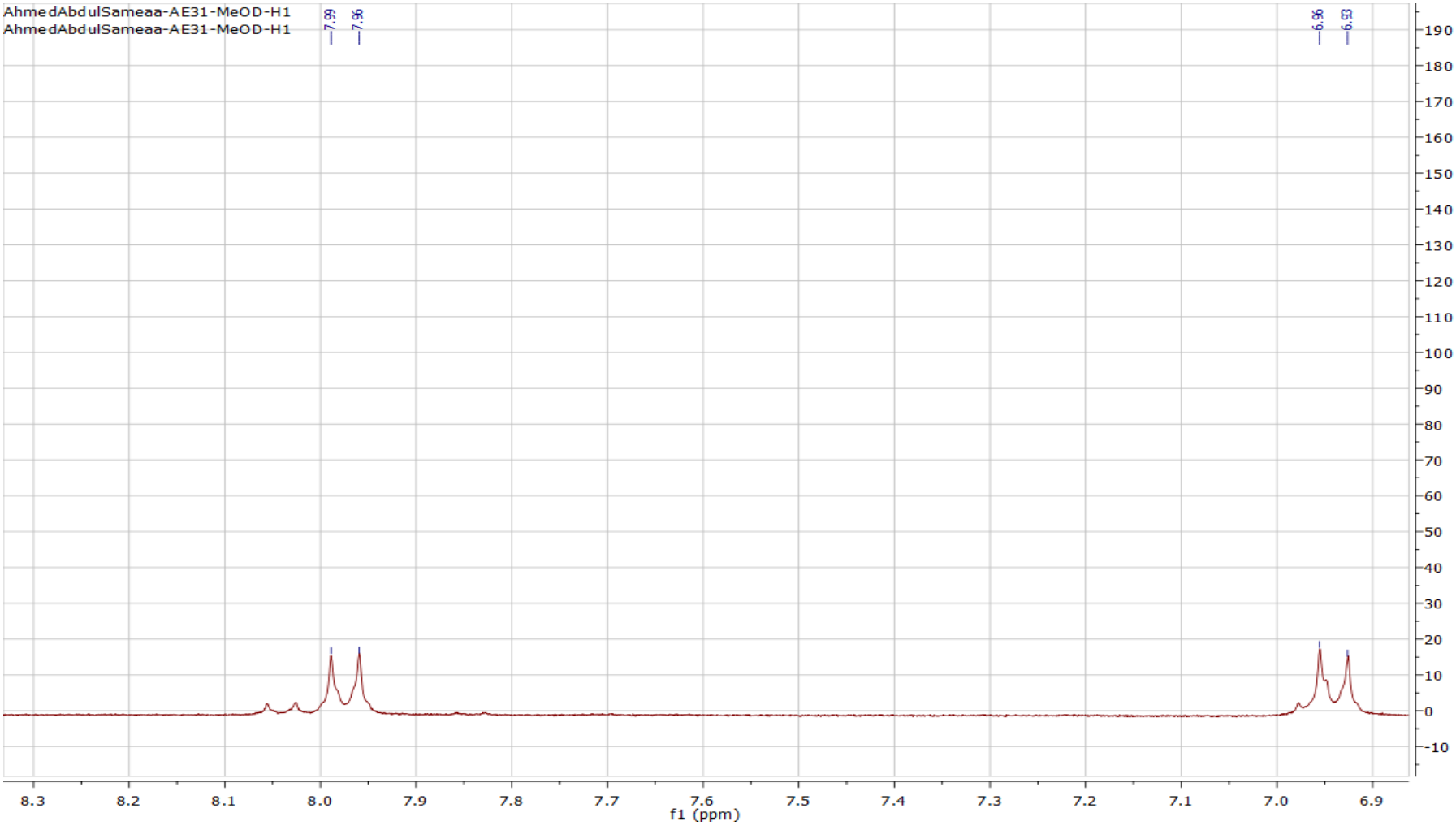


Figure 38: Partial expansion of ^{1}H-NMR spectrum of compound 6 (300 MHz, CD_3OD)

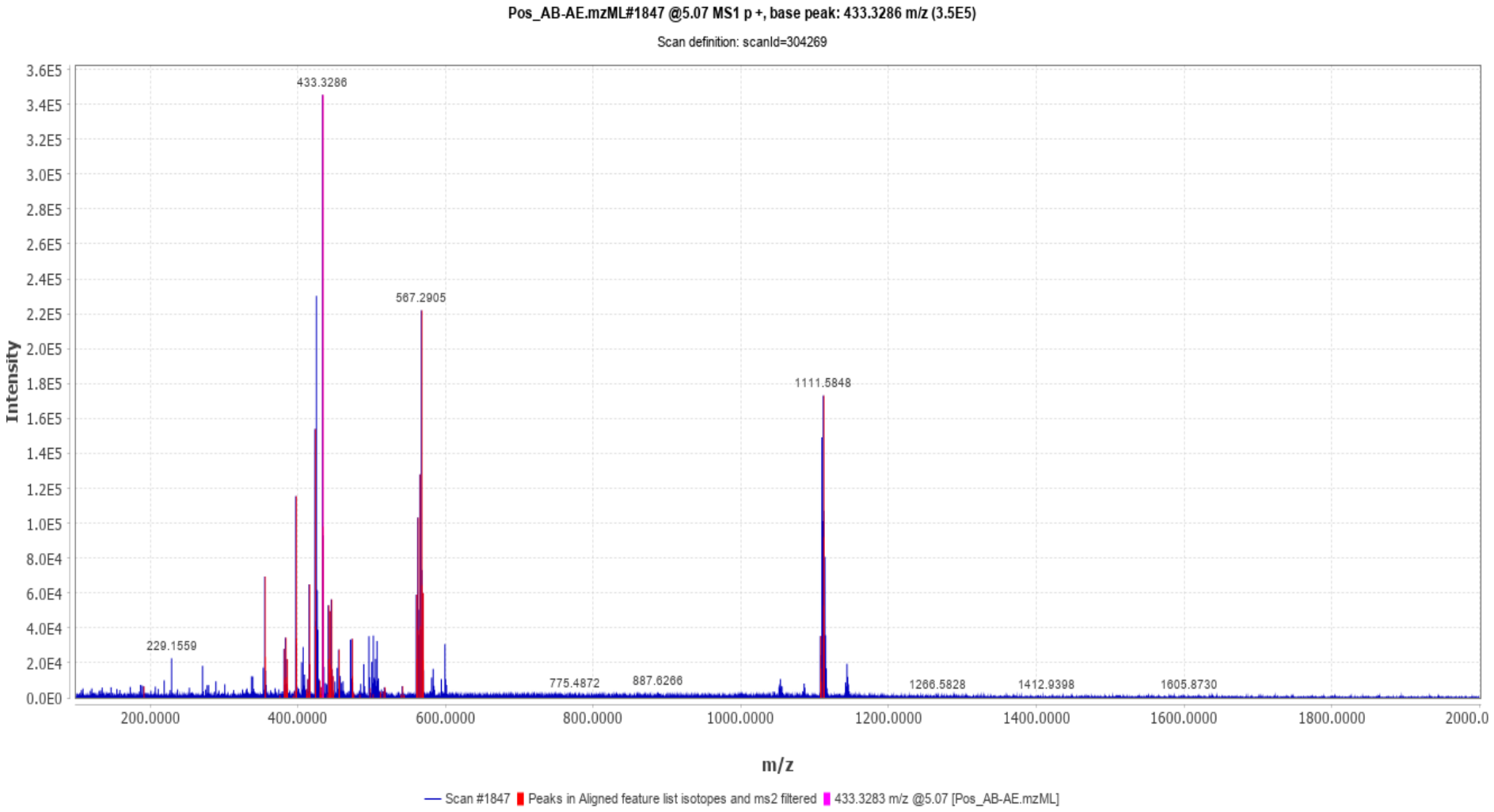


Figure 39: LC-MS/MS of compound 7

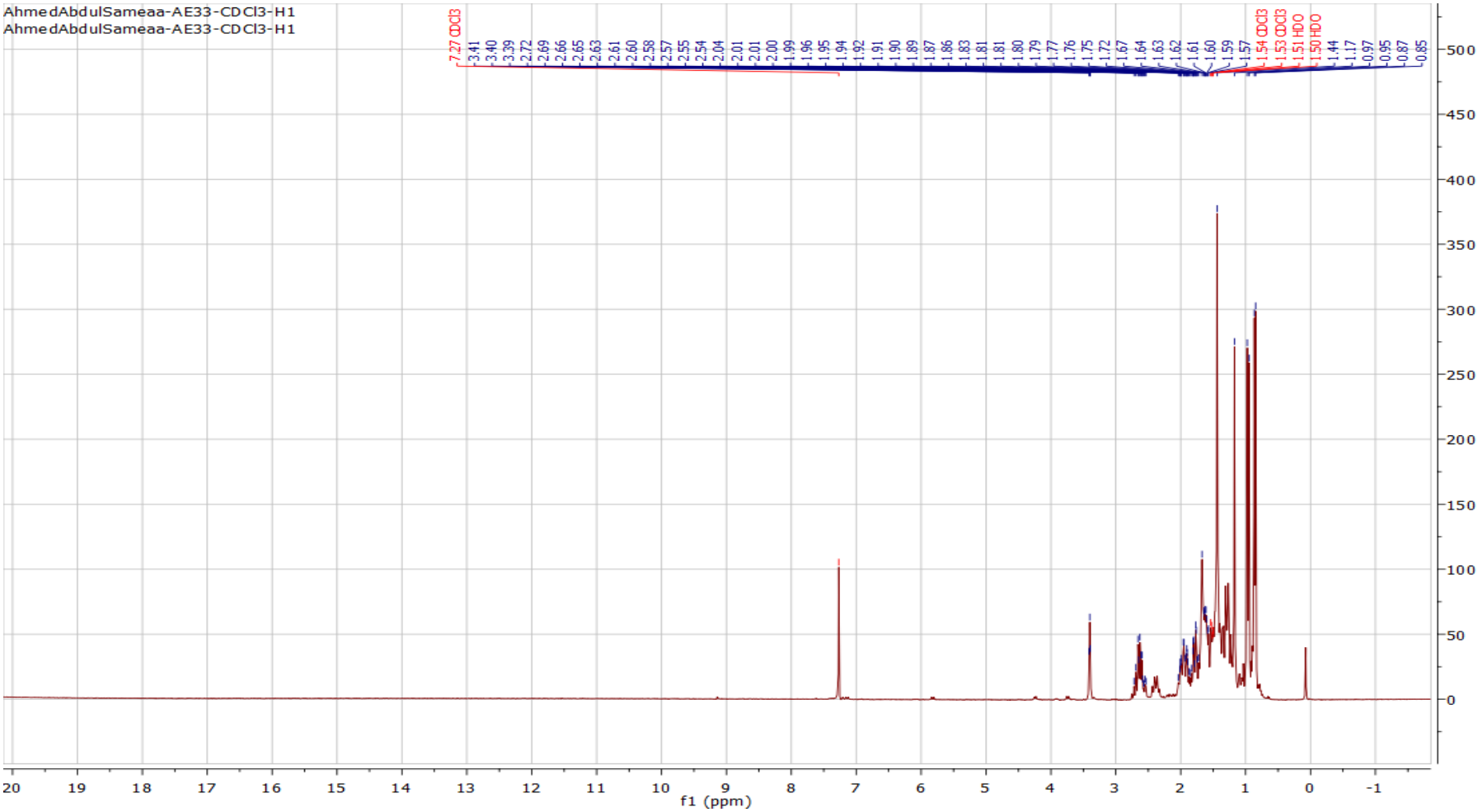


Figure 40: ^{1}H-NMR spectrum of compound 7 (300 MHz, $CDCl_3$)

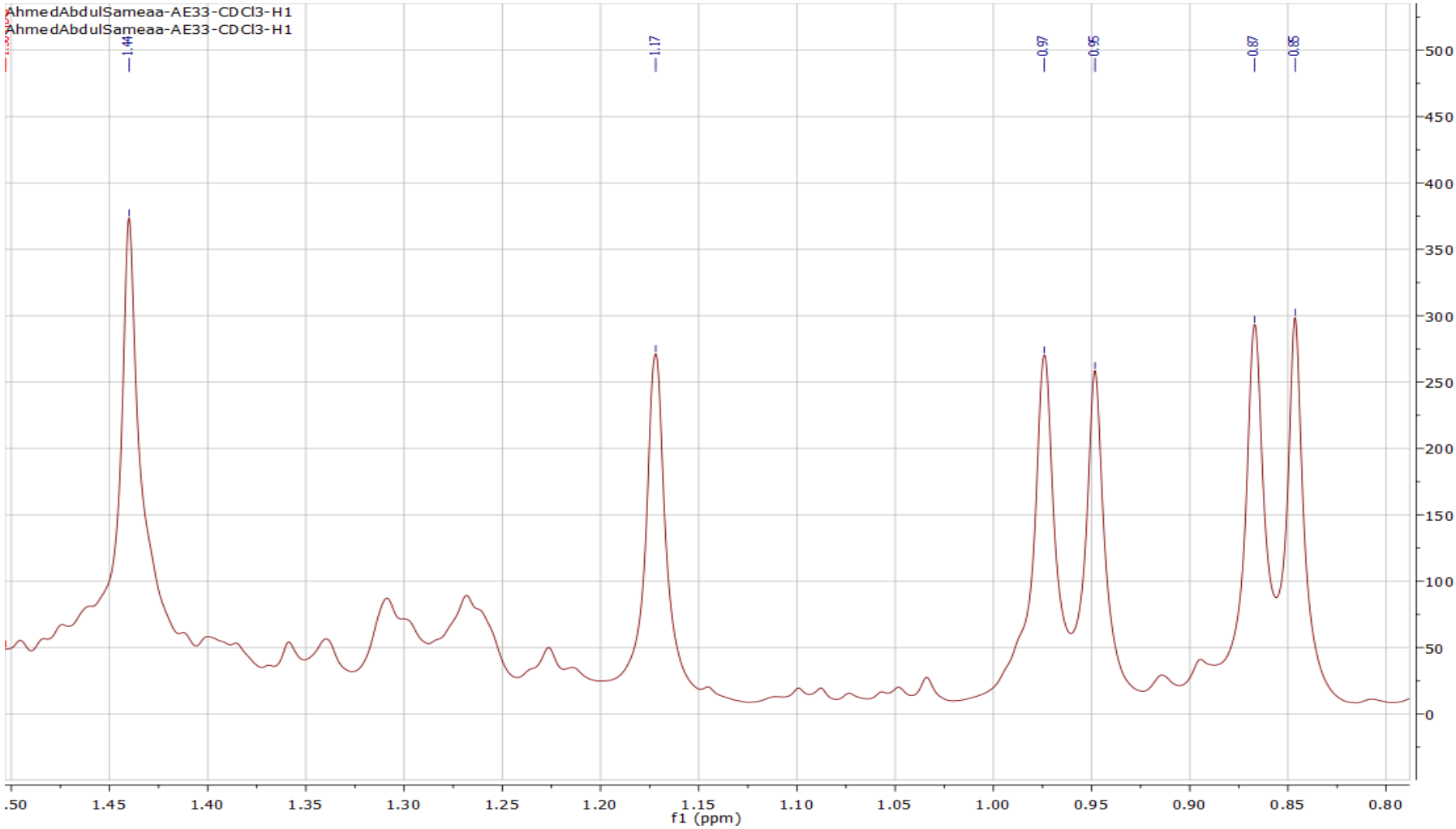


Figure 41: Partial expansion of ^{1}H-NMR spectrum of compound 7 (300 MHz, $CDCl_3$)

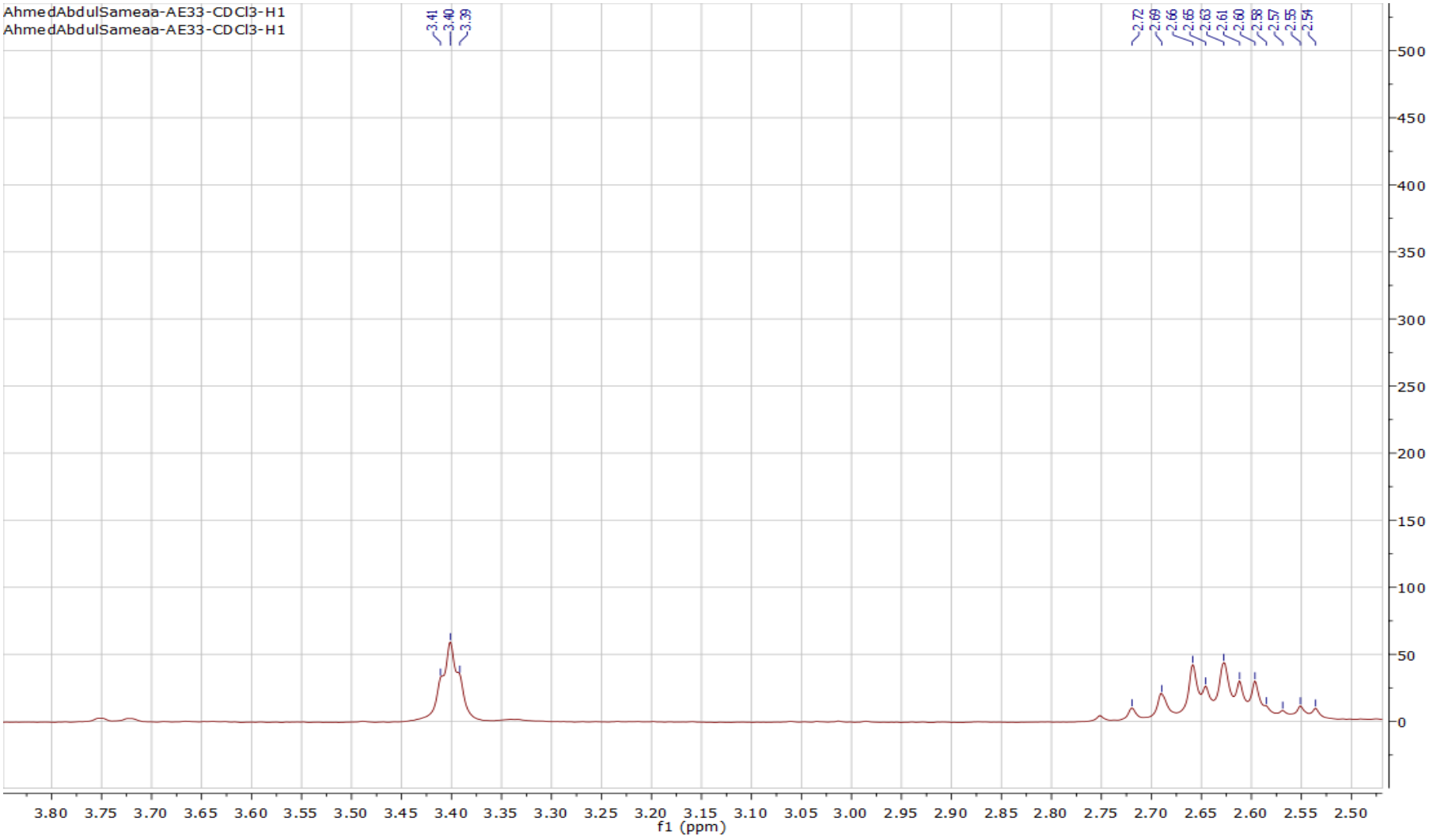


Figure 42: Partial expansion of ^{1}H-NMR spectrum of compound 7 (300 MHz, $CDCl_3$)

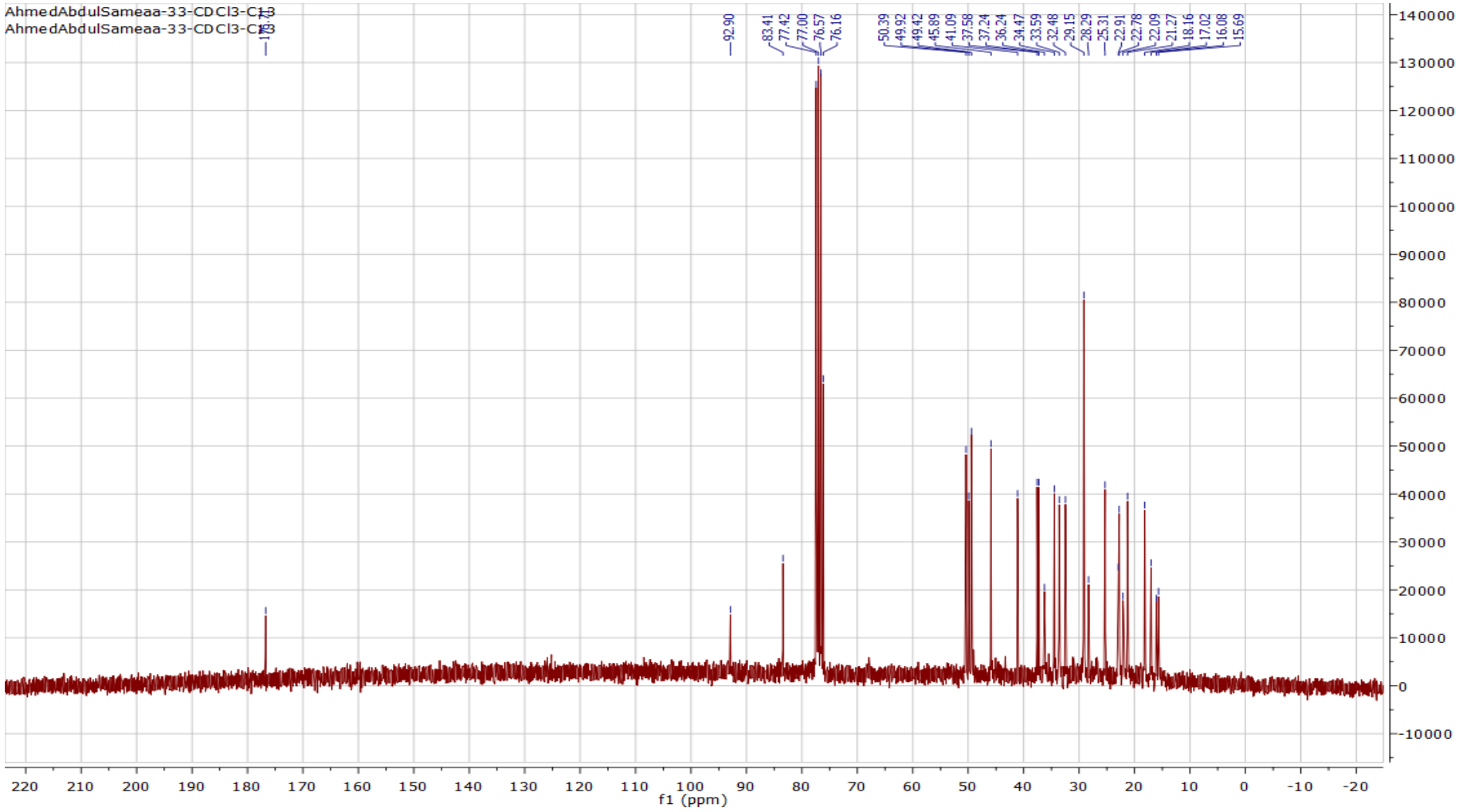


Figure 43: ^{13}C-NMR spectrum of compound 7 (75 MHz, $CDCl_3$)

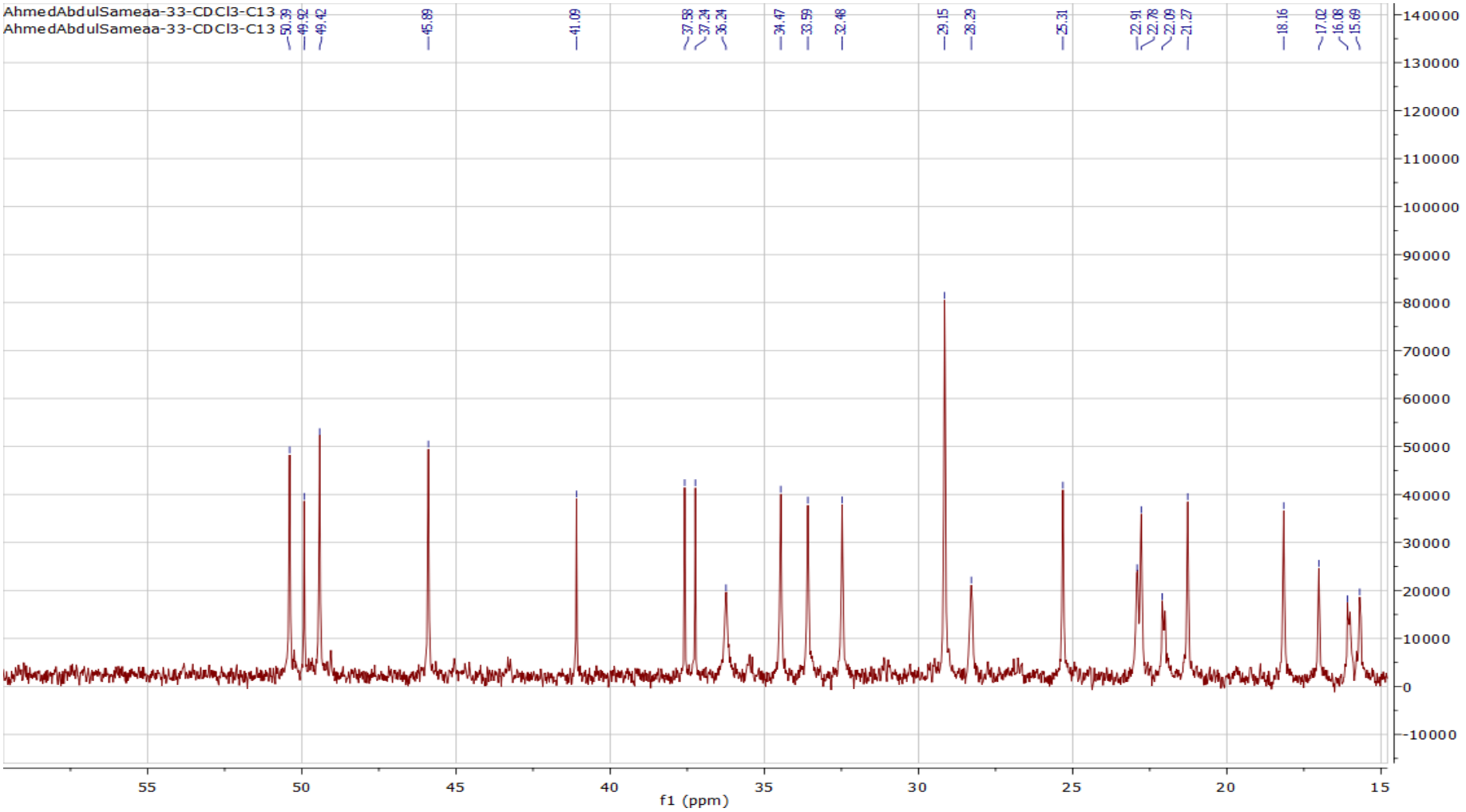


Figure 44: Partial expansion of ^{13}C-NMR spectrum of compound 7 (75 MHz, $CDCl_3$)

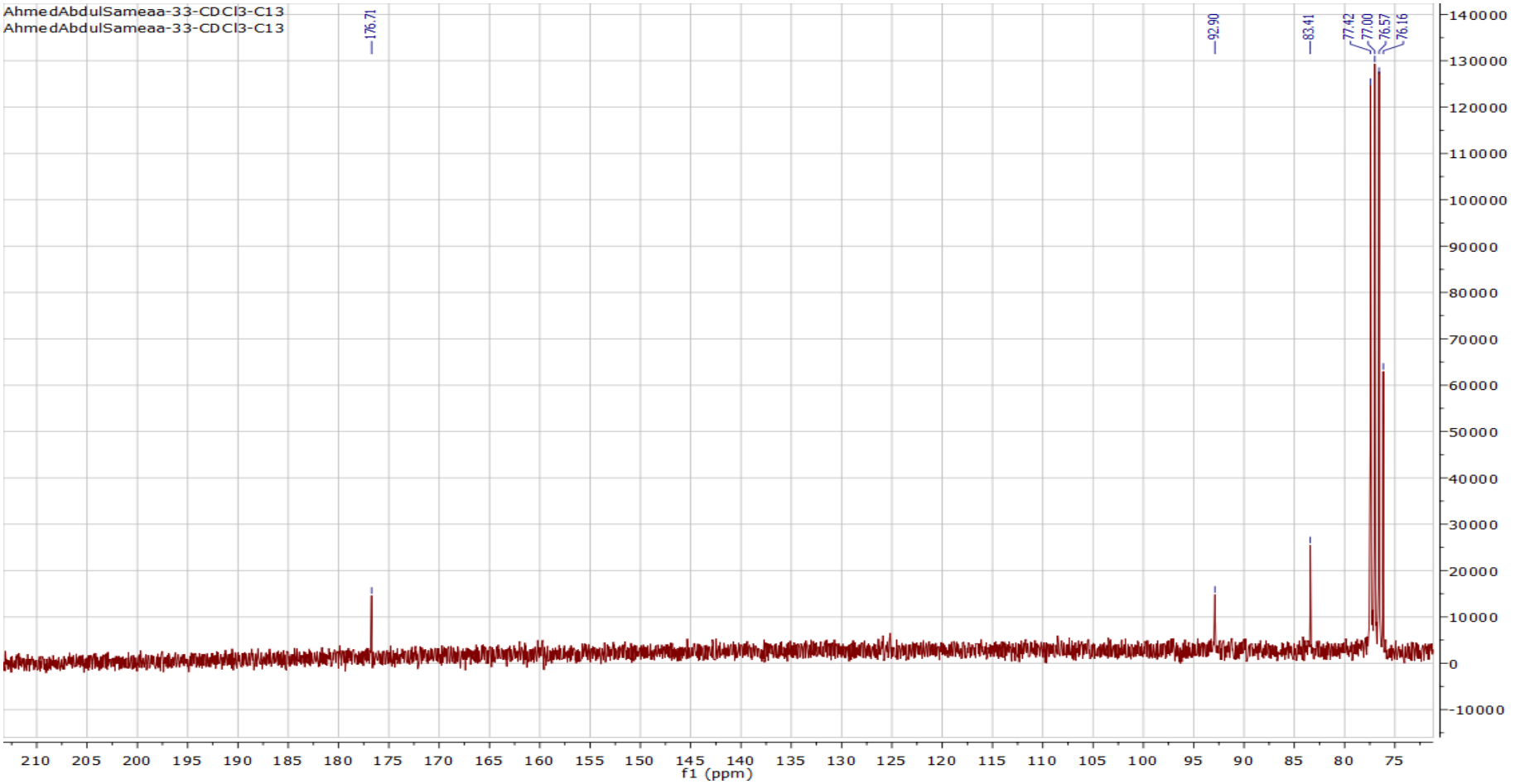


Figure 45: Partial expansion of ^{13}C-NMR spectrum of compound 7 (75 MHz, $CDCl_3$)

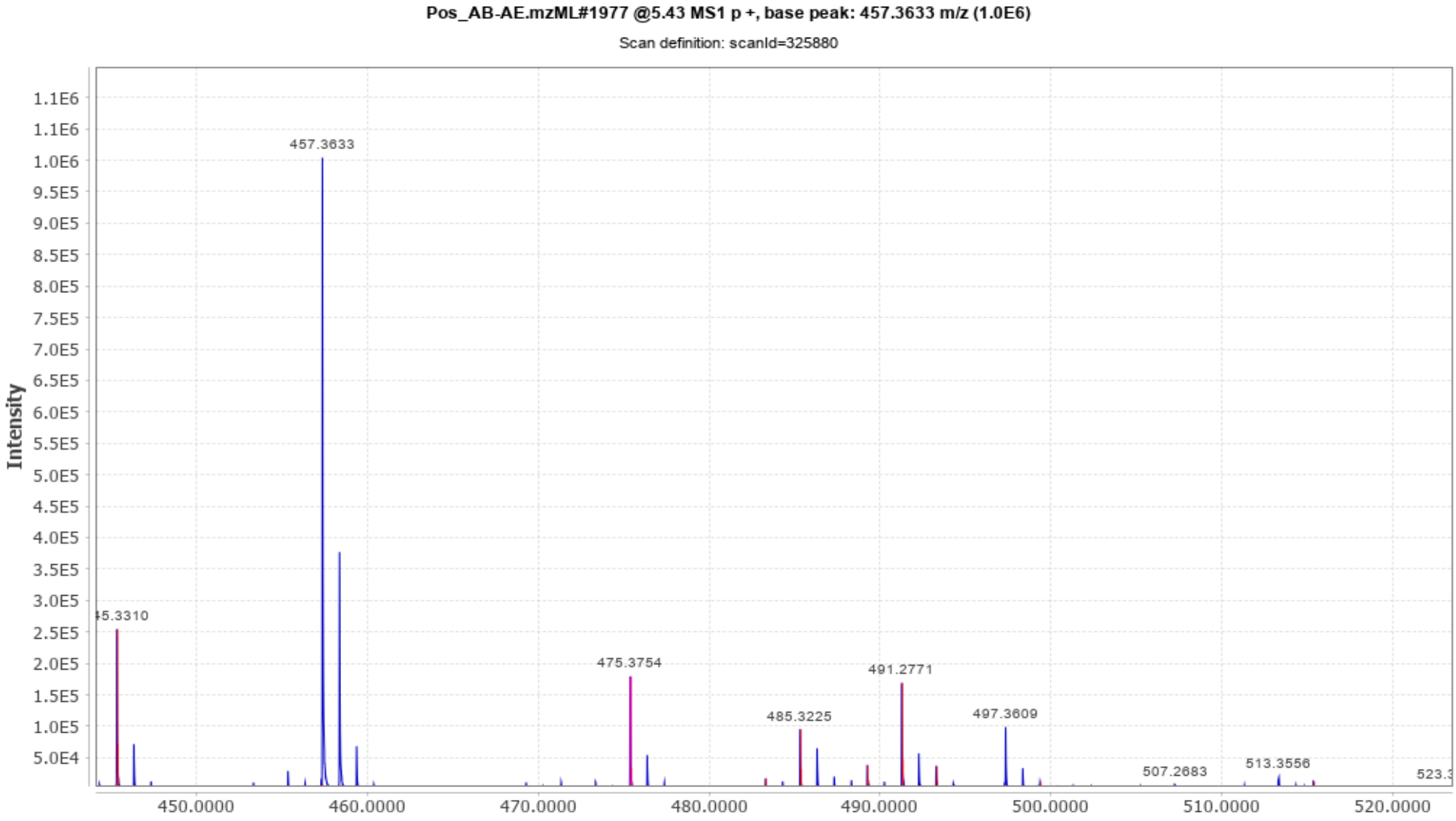


Figure 46: LC-MS/MS of compound 8

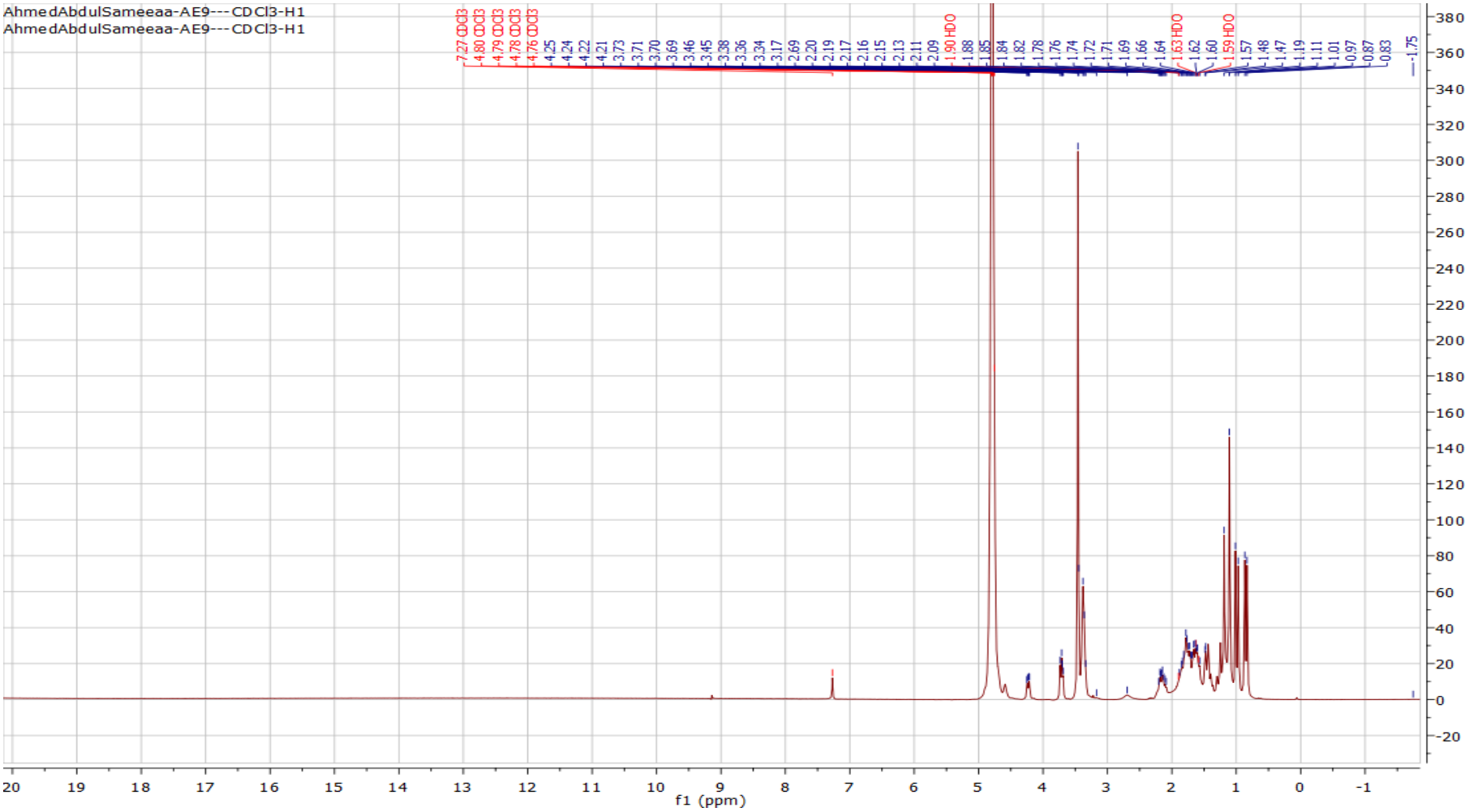


Figure 47: ^{1}H-NMR spectrum of compound 8 (300 MHz, $CDCl_3$)

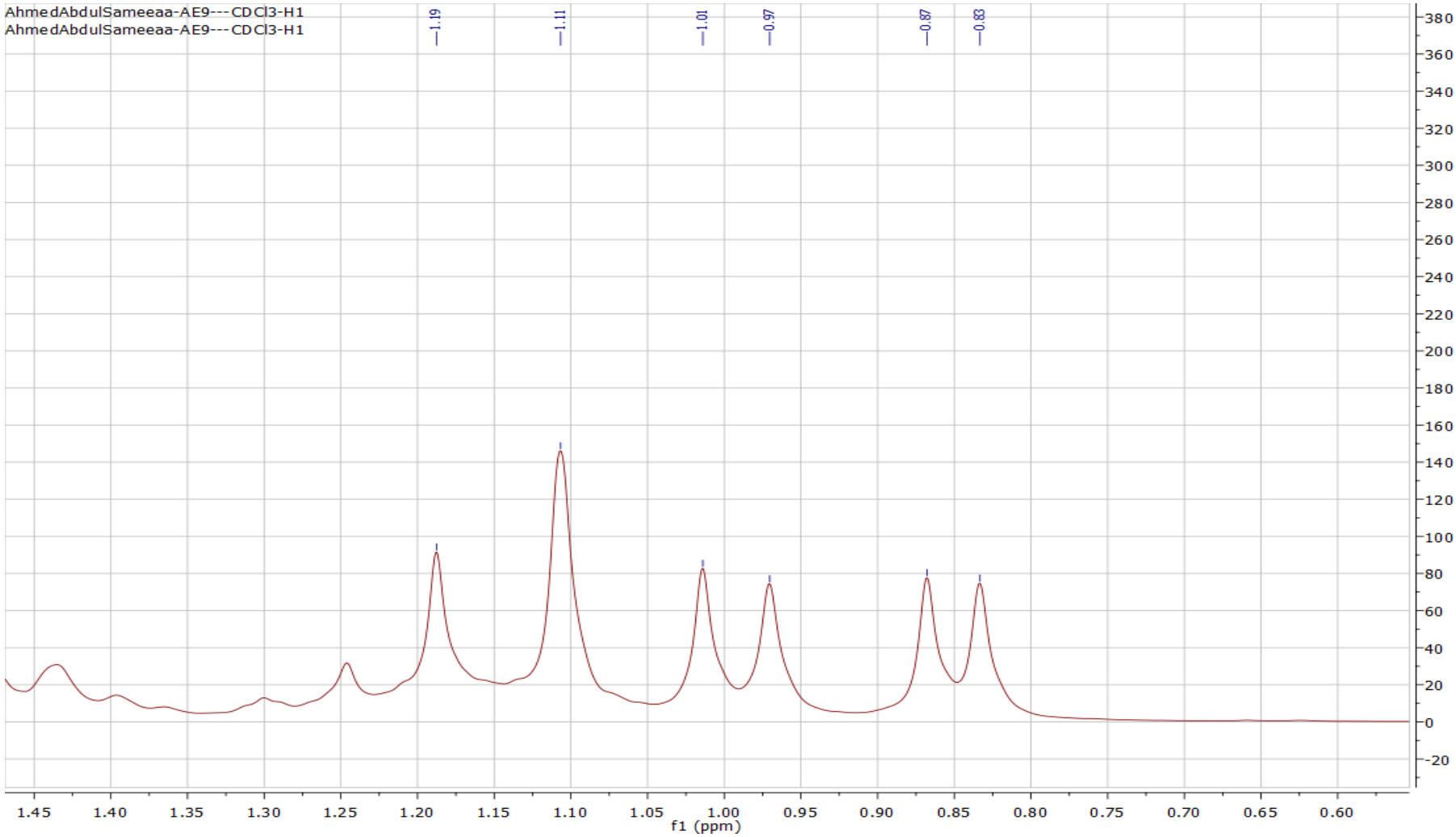


Figure 48: Partial expansion of ^{1}H-NMR spectrum of compound 8 (300 MHz, $CDCl_3$)

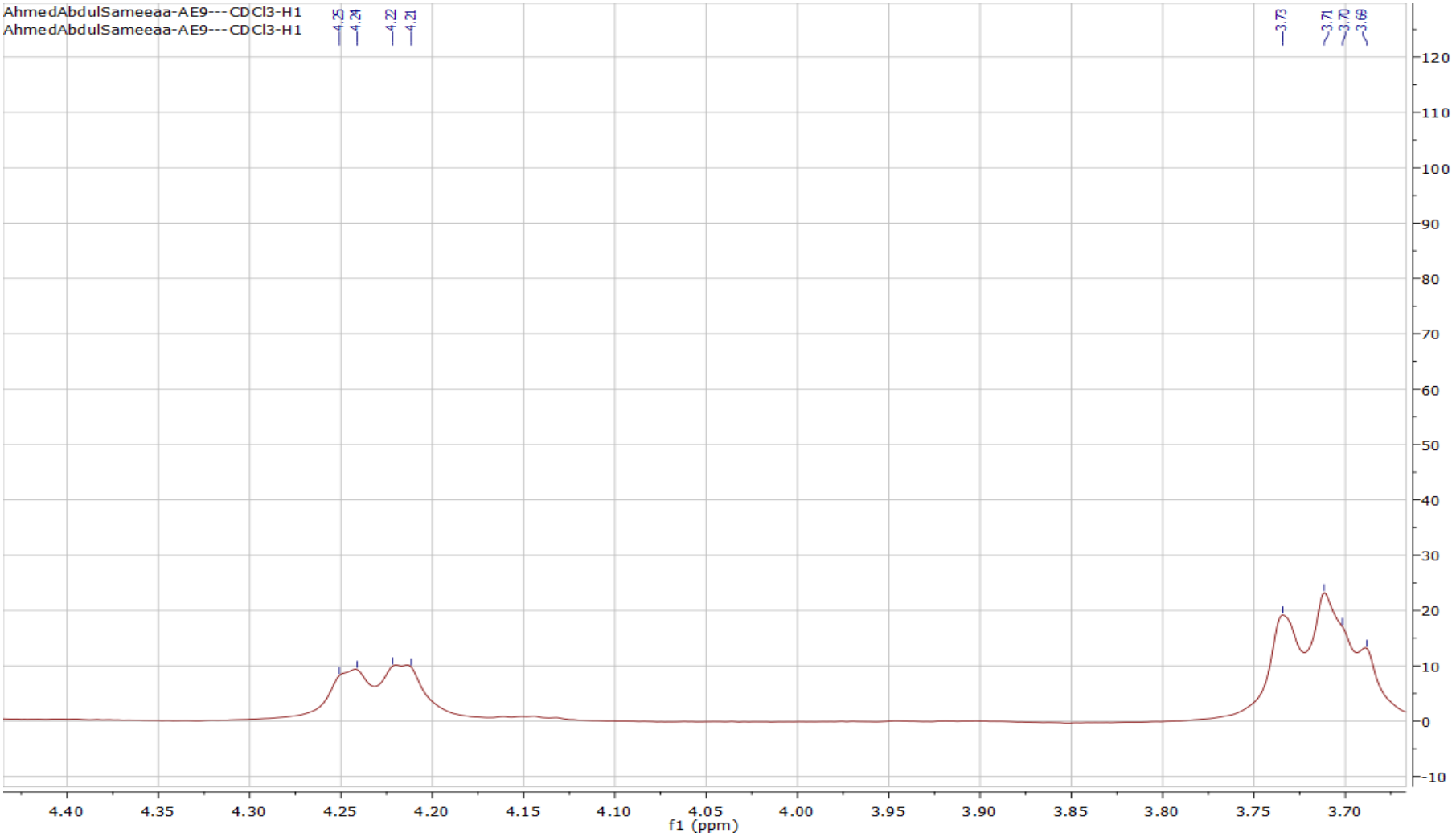


Figure 49: Partial expansion of 1H-NMR spectrum of compound 8 (300 MHz, $CDCl_3$)

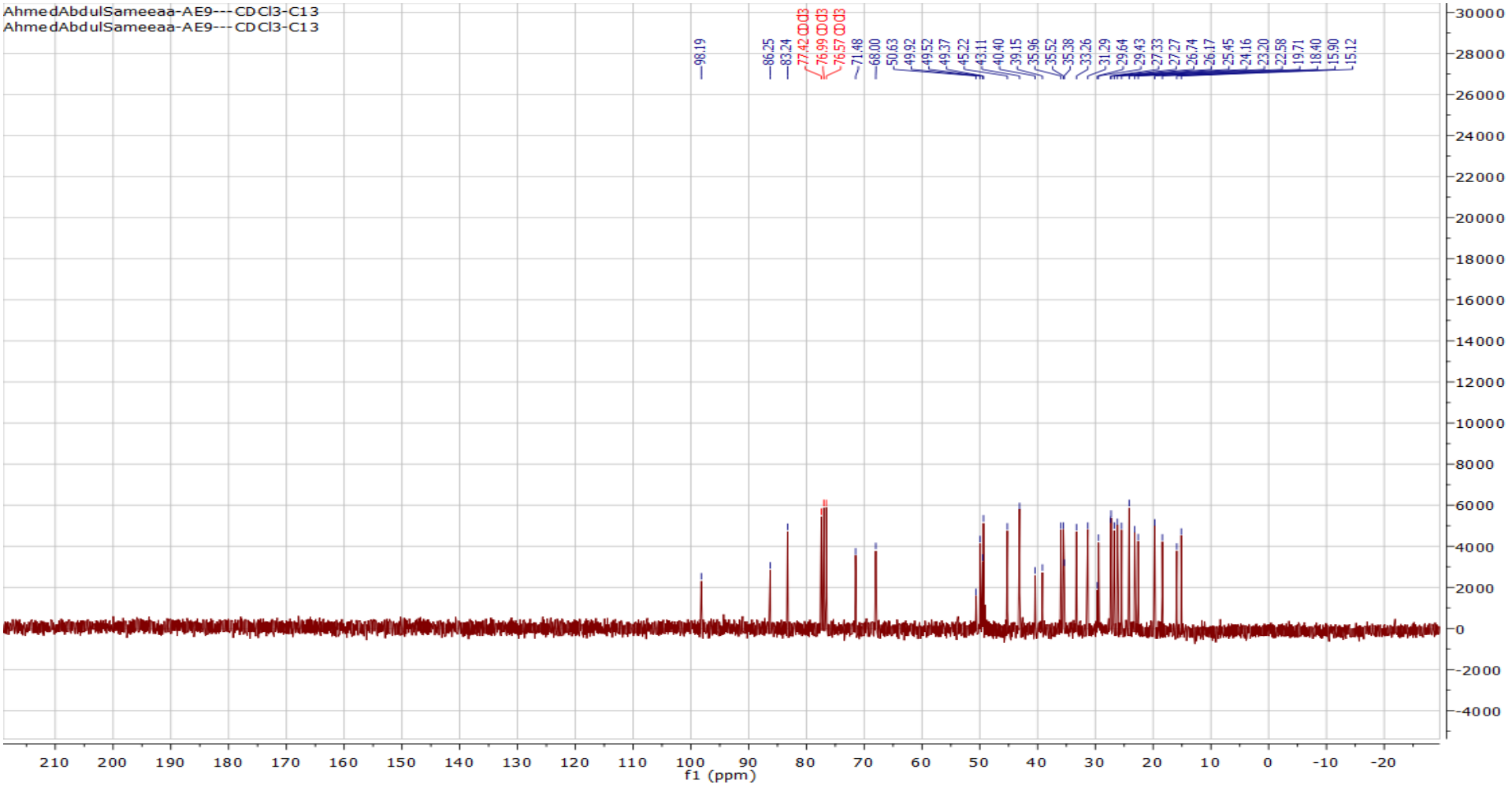


Figure 50: ^{13}C-NMR spectrum of compound 8 (75 MHz, $CDCl_3$)

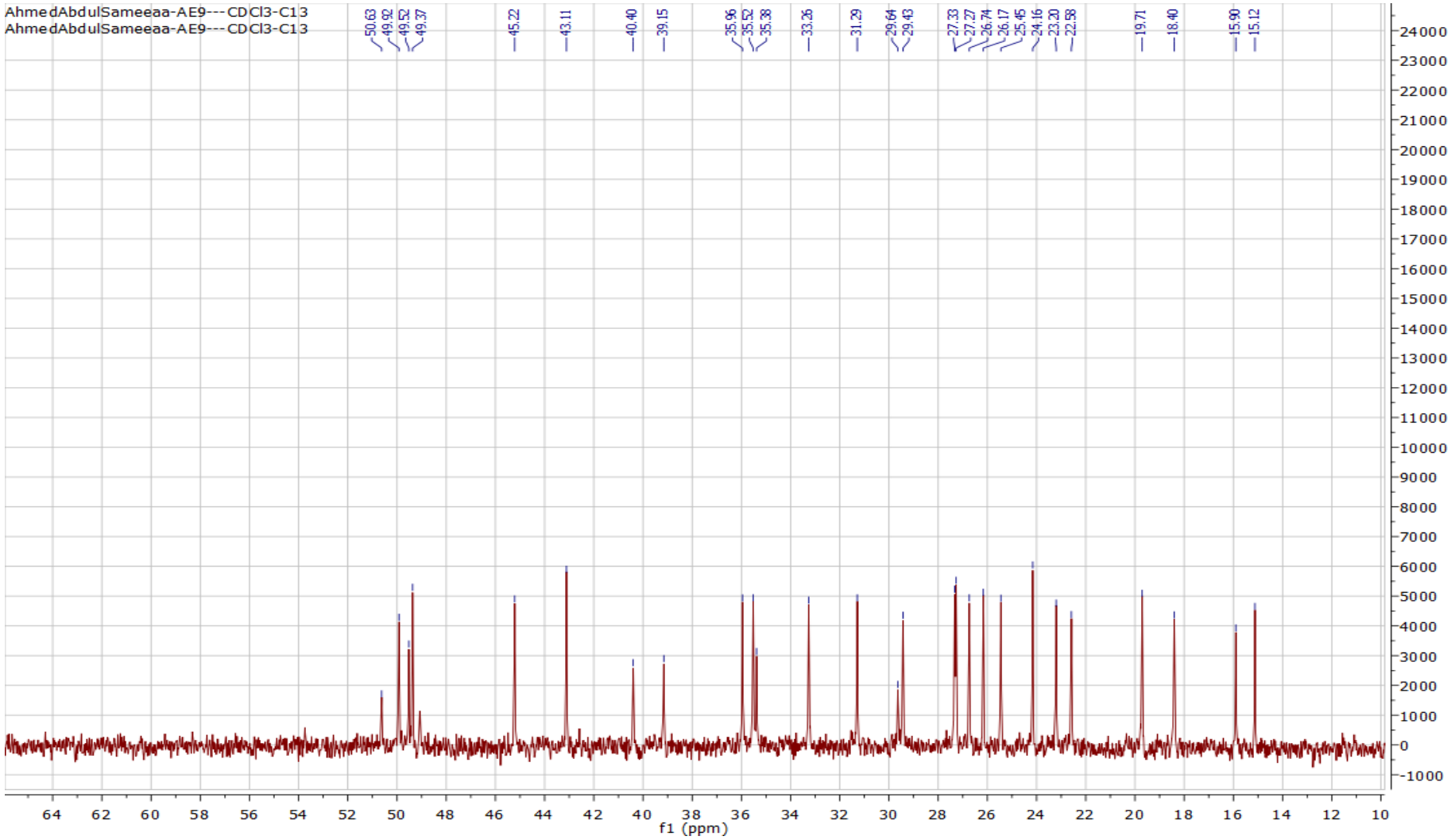


Figure 51: Partial expansion of ^{13}C-NMR spectrum of compound 8 (75 MHz, $CDCl_3$)

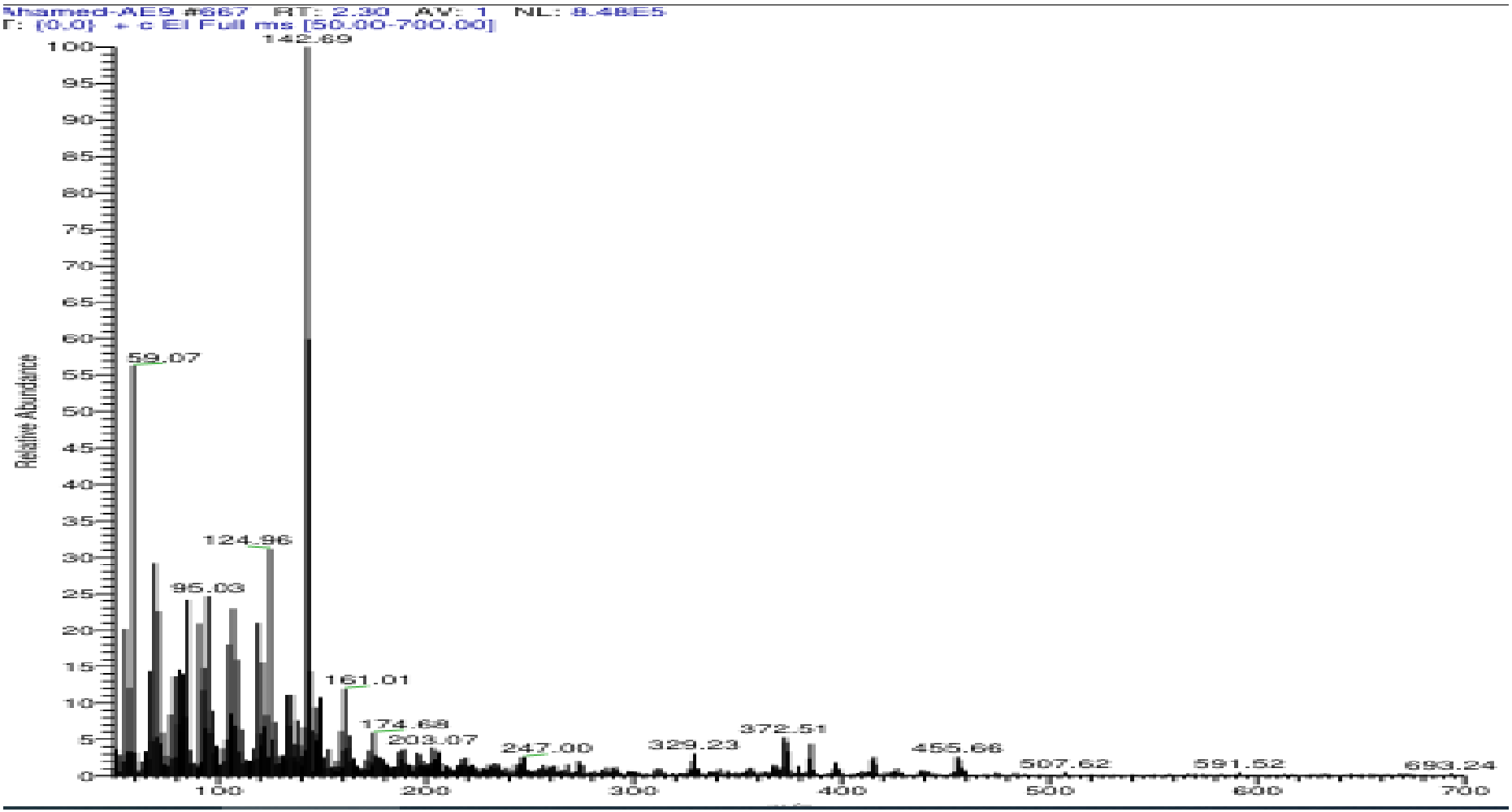


Figure 52: EI-MS of Compound 9

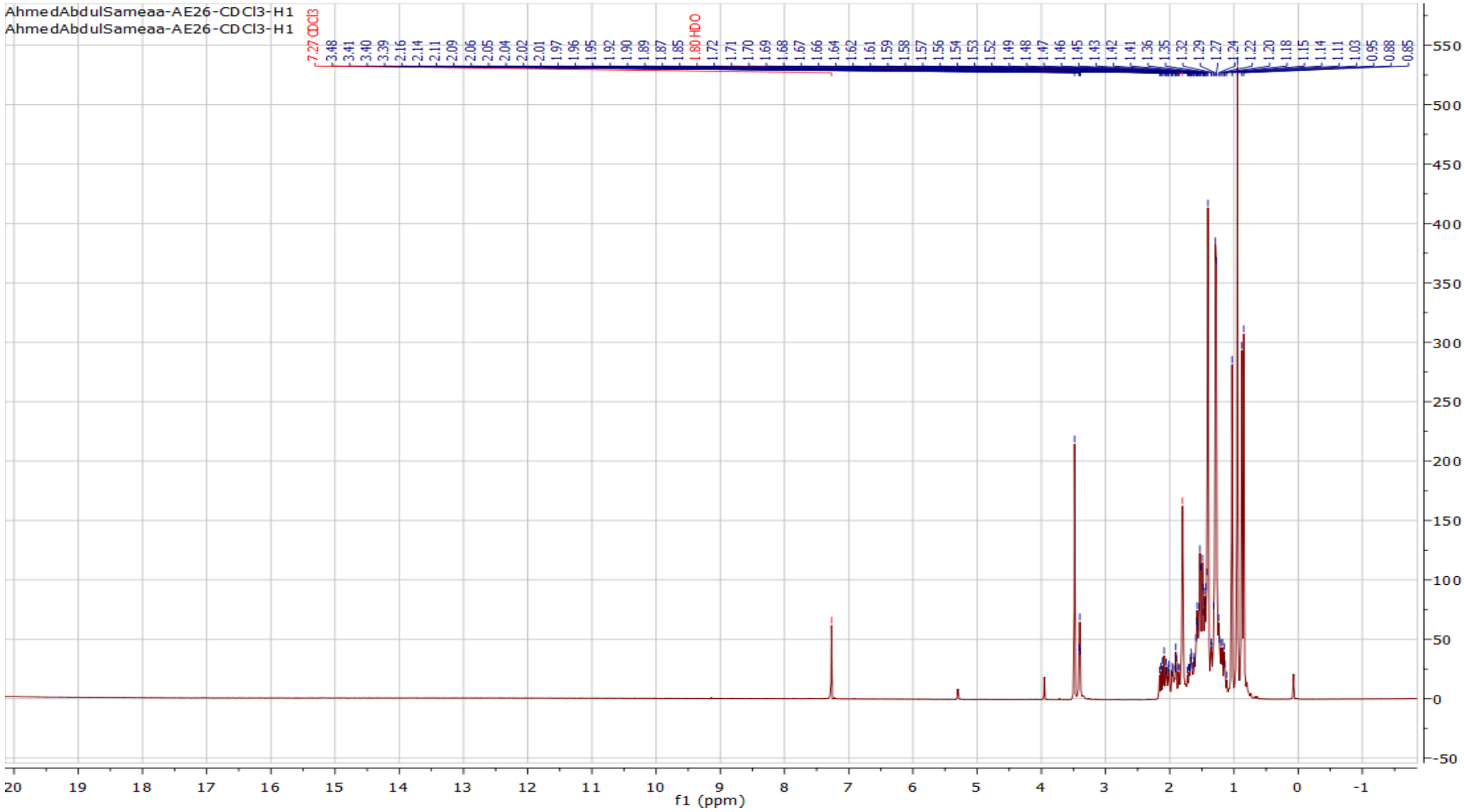


Figure 53: ^{1}H-NMR spectrum of compound 9 (300 MHz, $CDCl_3$)

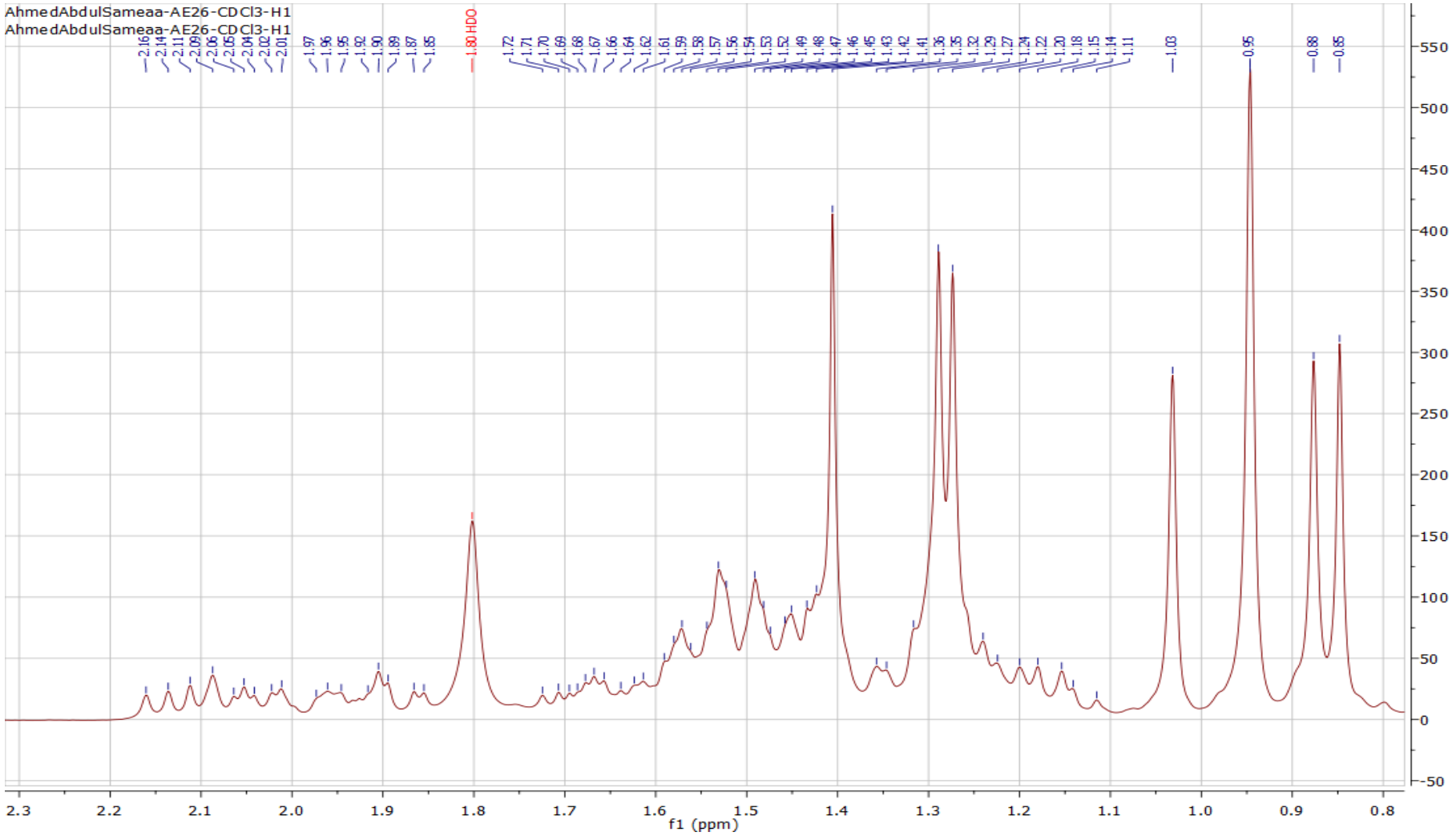


Figure 54: Partial expansion of ^{1}H-NMR spectrum of compound 9 (300 MHz, $CDCl_3$)

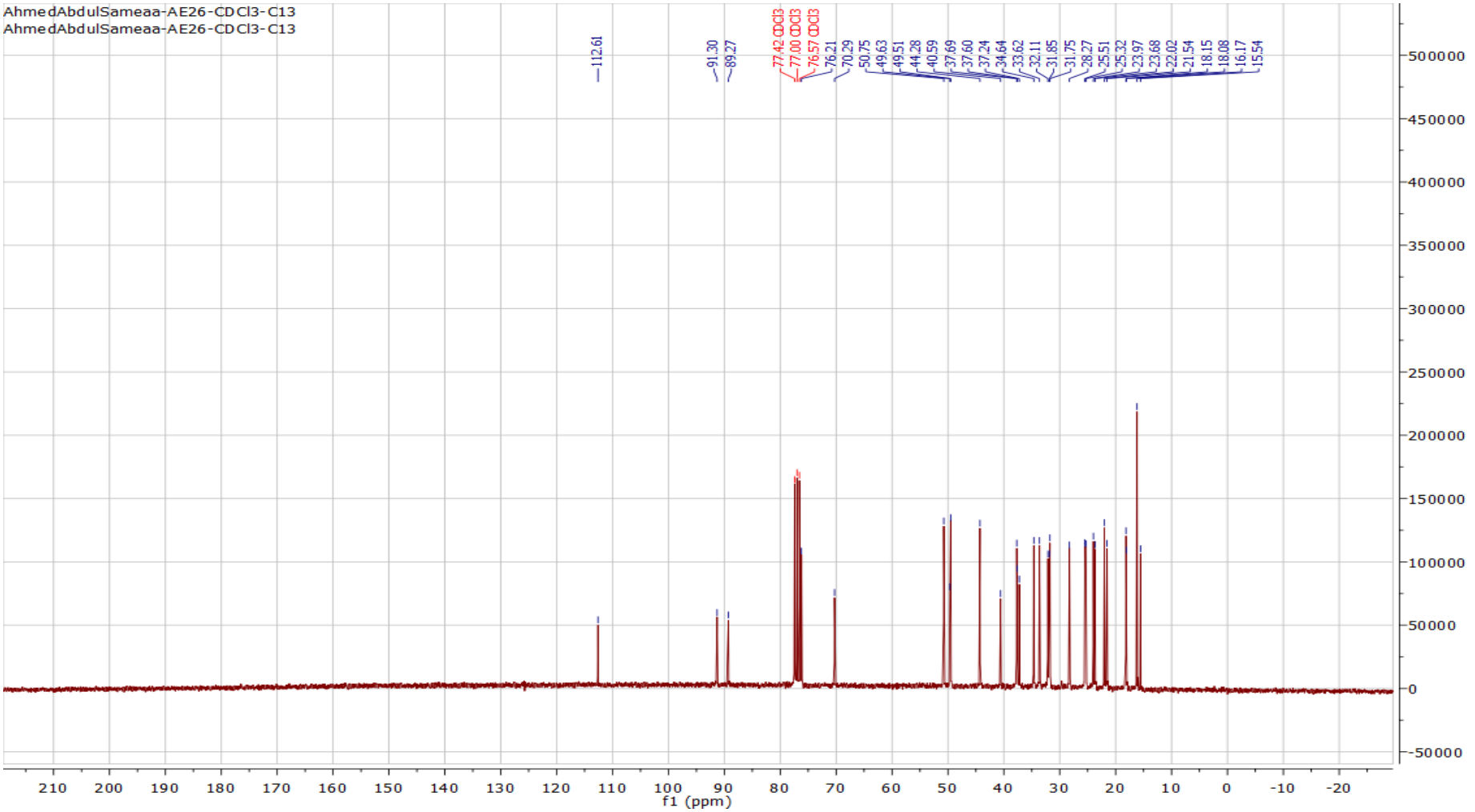


Figure 55: ^{13}C-NMR spectrum of compound 9 (75 MHz, $CDCl_3$)

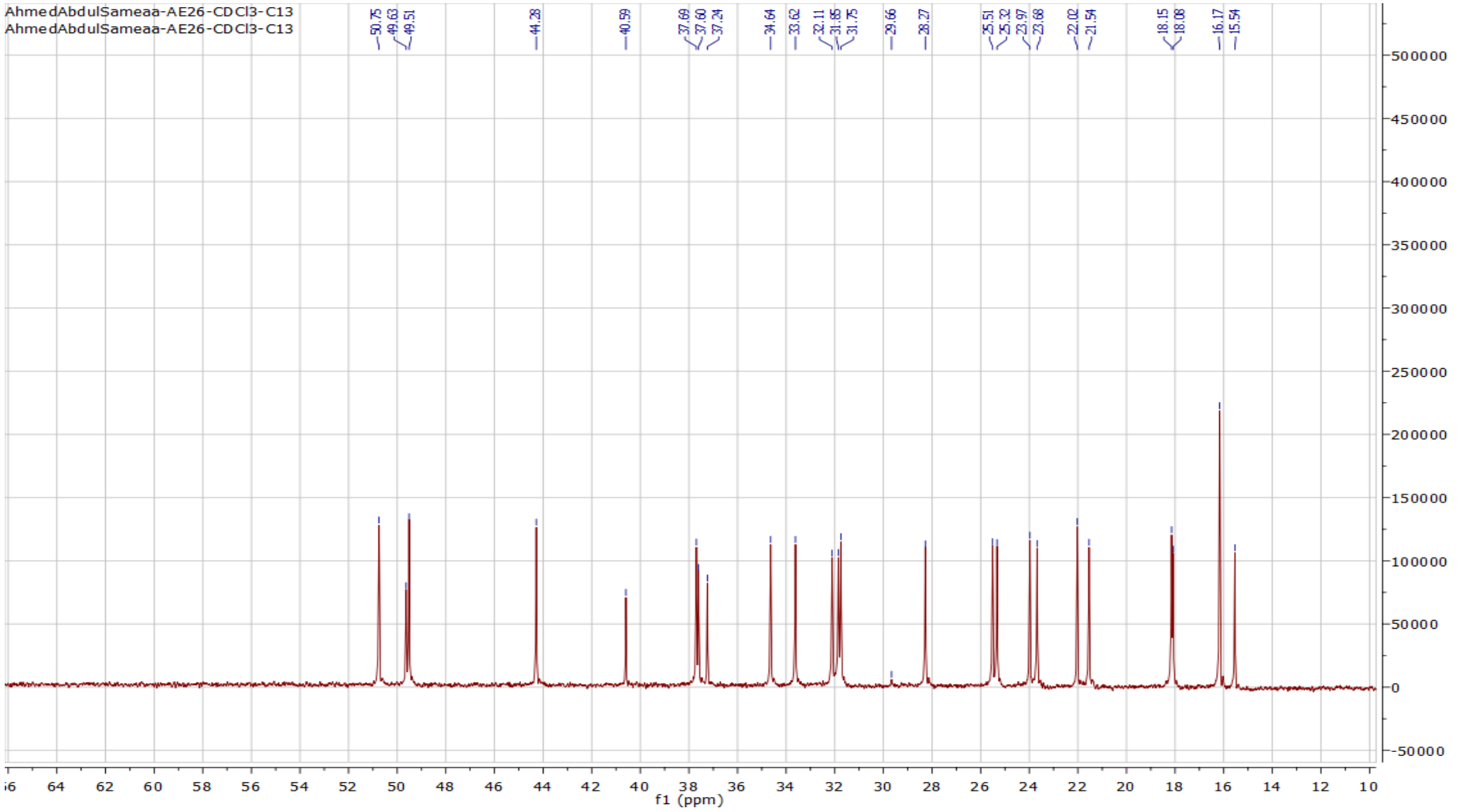


Figure 56: Partial expansion of ^{13}C-NMR spectrum of compound 9 (75 MHz, $CDCl_3$)

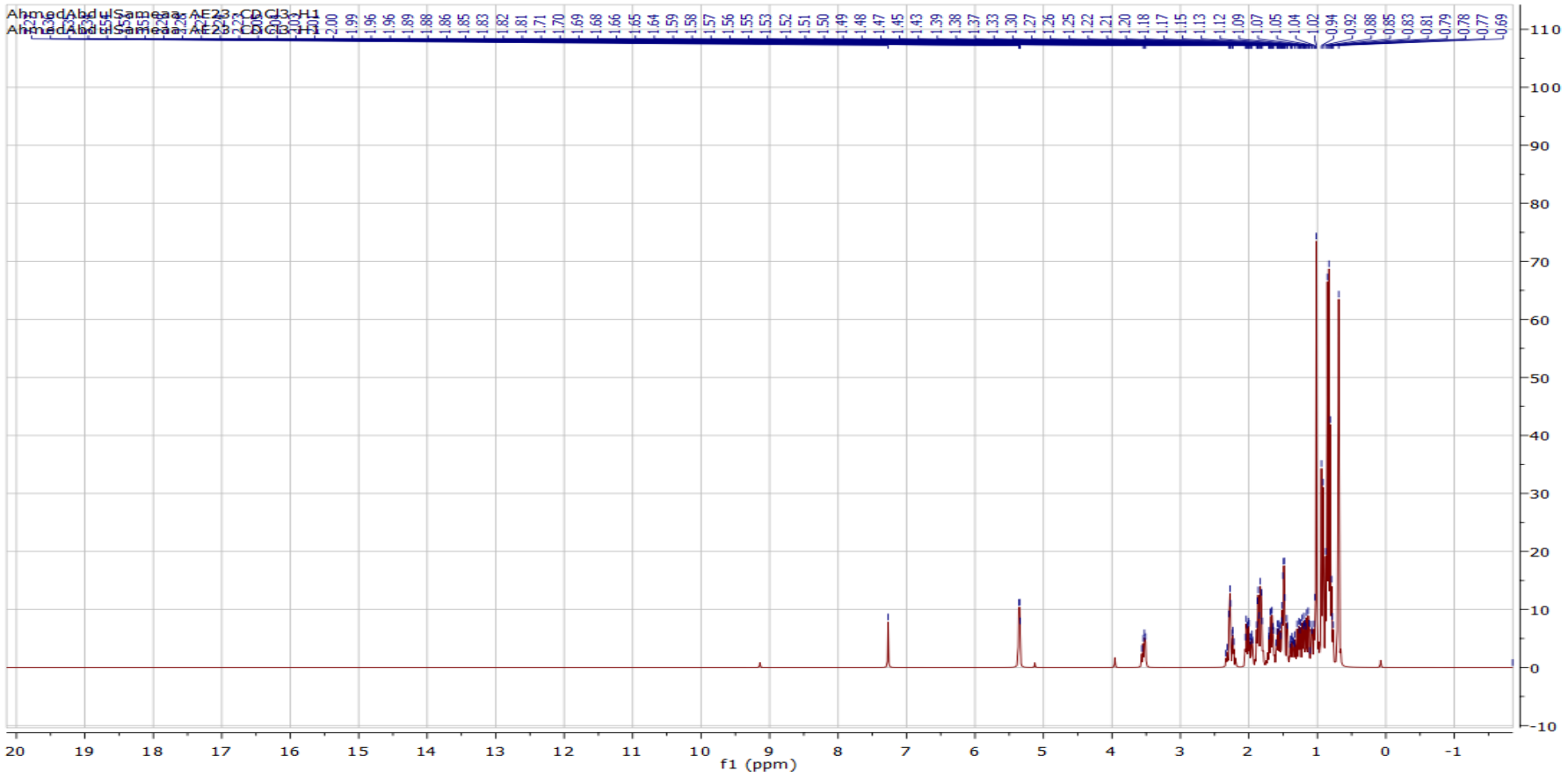


Figure 57: ^{1}H-NMR spectrum of compound 10 (300 MHz, $CDCl_3$)

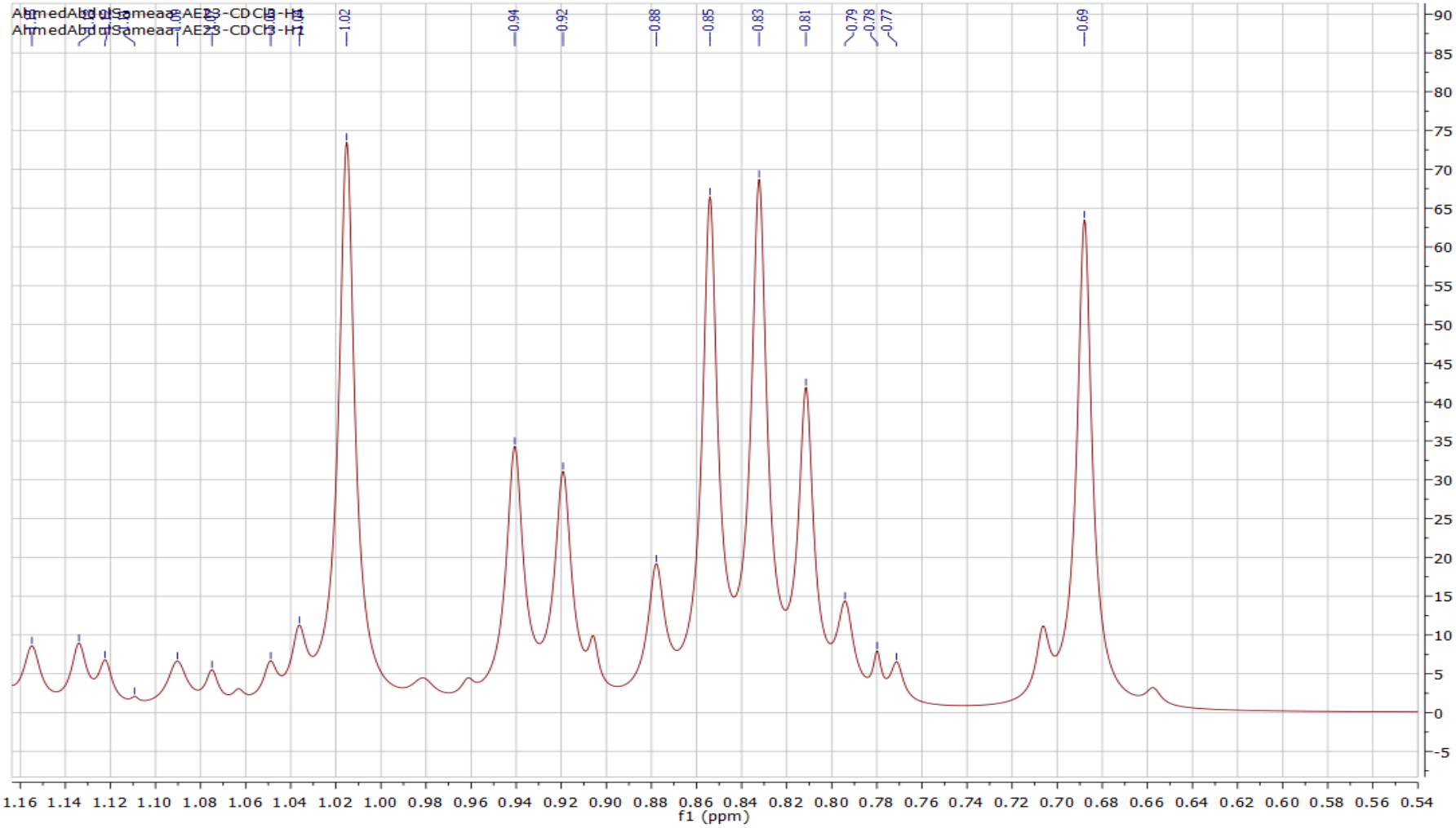


Figure 58: Partial expansion of ^{1}H-NMR spectrum of compound 10 (300 MHz, $CDCl_3$)

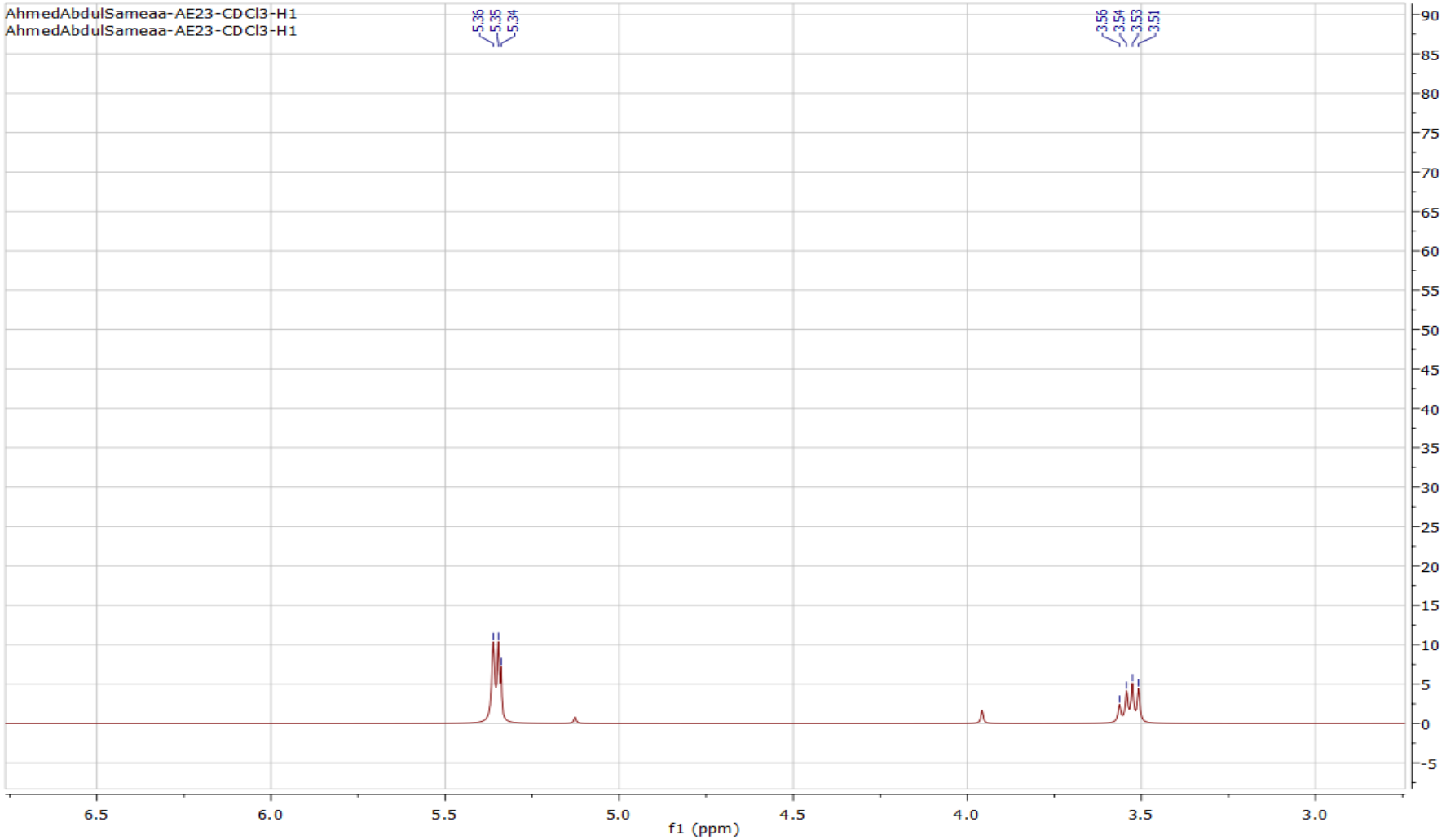


Figure 59: Partial expansion of ^{1}H-NMR spectrum of compound 10 (300 MHz, $CDCl_3$)

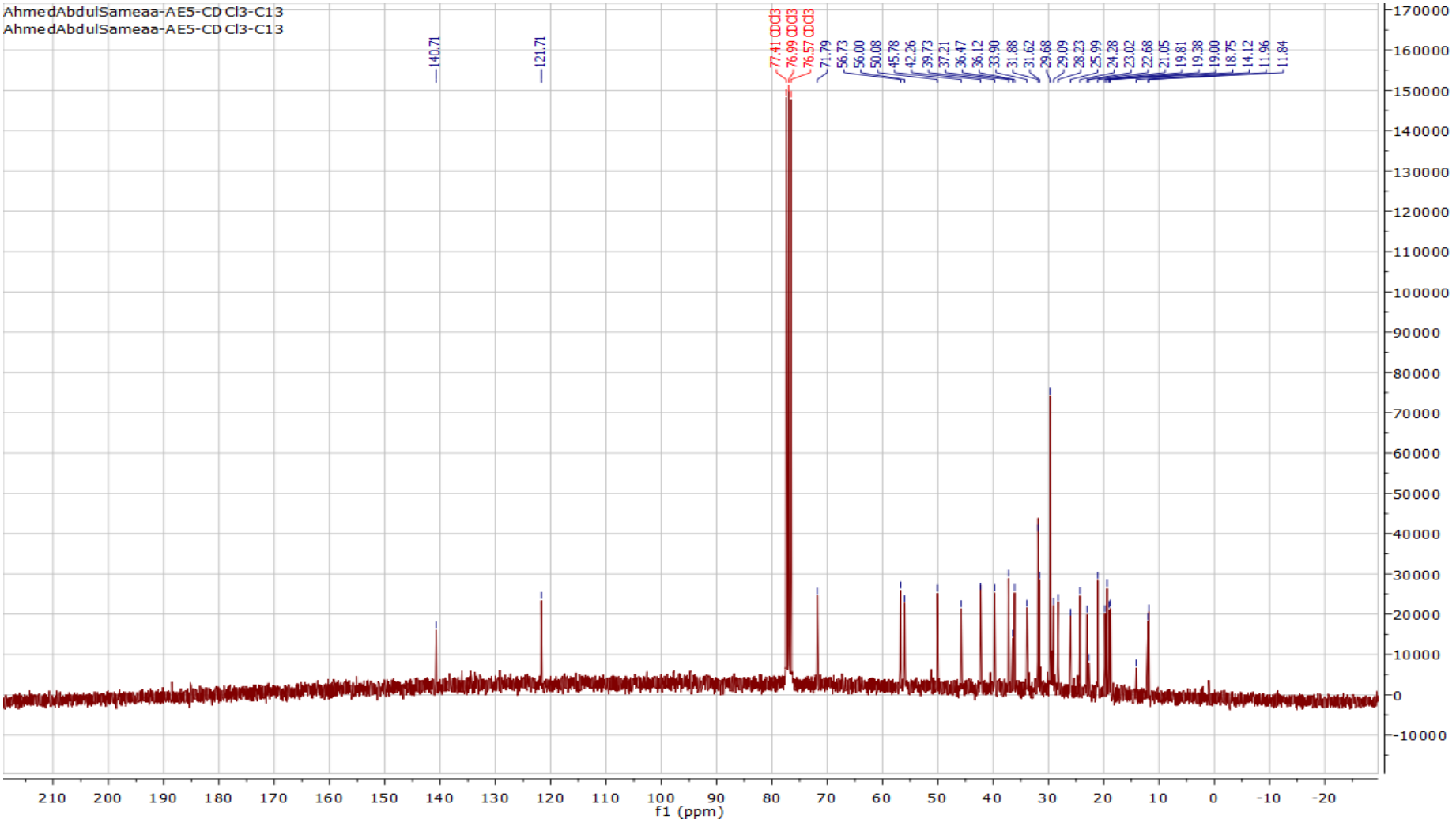


Figure 60: ^{13}C-NMR spectrum of compound 10 (75 MHz, $CDCl_3$)

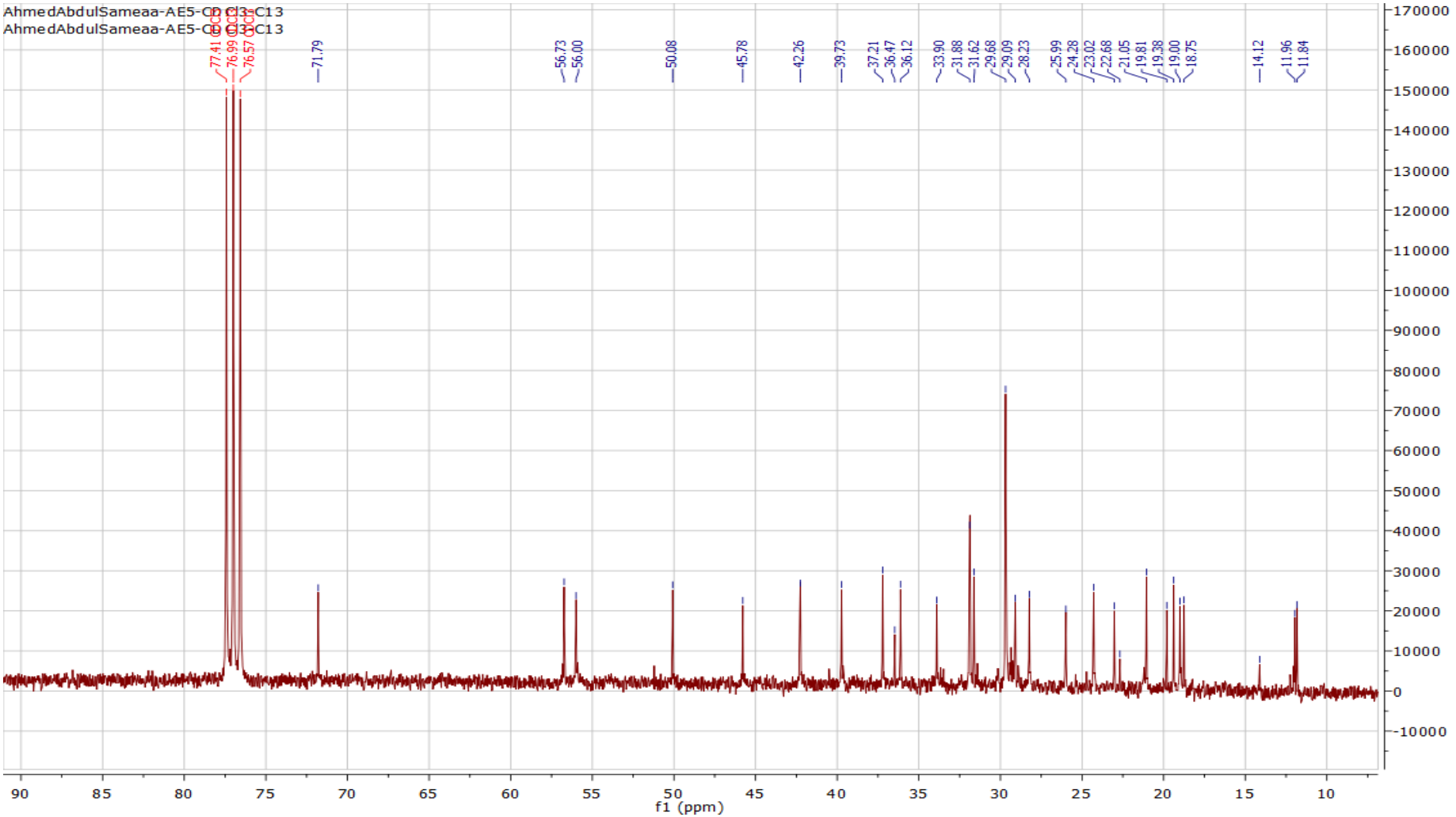


Figure 61: Partial expansion of ^{13}C-NMR spectrum of compound 10 (75 MHz, $CDCl_3$)