Supporting Information

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Nitric oxide inhibitory compounds from Thai medicinal plants *Averrhoa bilimbi* and *Schinus terebinthifolia*

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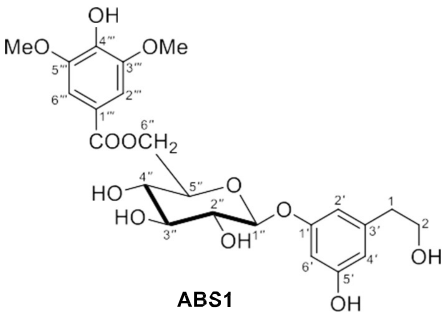
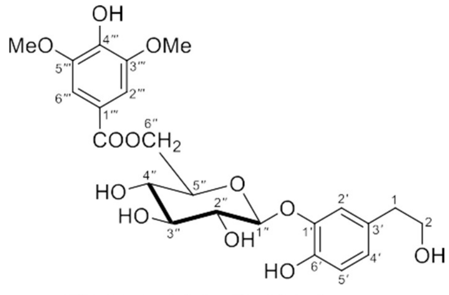
Table S1. ^{1}H NMR and ^{13}C NMR data of **ABS1** and clemomandshuricoside A (δ in ppm, J in Hz)



ABS1



Clemomandshuricoside A

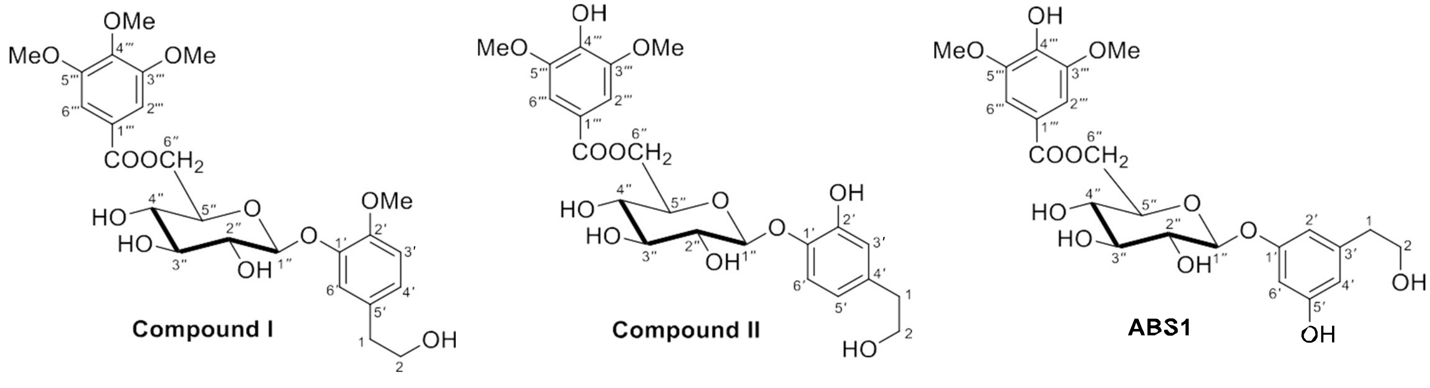
No.	ABS1[a]		Clemomandshuricoside A[b]	
	δ_H	δ_C	δ_H	δ_C
1	2.57 (2H, *m*)	39.4	2.35 (2H, *t*, 7.5)	39.5
2	3.64 (2H, *m*)	62.7	3.47 – 3.49 (2H, *m*)	62.5
1′	-	158.2	-	146.4
2′	6.37 (1H, *t*, 2.0)	109.9	6.85 (1H, *brs*)	119.8
3′	-	141.8	-	132.1
4′	6.41 (1H, *t*, 2.0)	108.4	6.67 (1H, *brs*)	125.5
5′	-	154.5	6.67 (1H, *brs*)	117.0
6′	6.43 (1H, *t*, 2.5)	101.4	-	146.9
1″	4.97 (1H, *d*, 7.5)	100.8	4.80 (1H, *d*, 8.0)	104.4
2″	3.49 (1H, *m*)	73.8	3.45 (1H, *dd*, 8.0, 9.0)	74.9
3″	3.54 (1H, *m*)	76.9	3.64 (1H, *dd*, 9.0, 9.0)	75.8
4″	3.57 (1H, *m*)	70.6	3.41 – 3.44 (1H, *m*)	71.9
5″	3.87 (1H, *m*)	74.2	3.41 – 3.44 (1H, *m*)	77.4
6″	4.72 (1H, *dd*, 11.5, 2.0) 4.40 (1H, *dd*, 11.5, 6.5)	64.0	4.73 (1H, *dd*, 2.4, 12.0) 4.46 (1H, *dd*, 6.9, 12.0)	64.2
1‴	-	121.5	-	119.8
2‴	7.32 (1H, *s*)	107.3	7.28 (1H, *s*)	108.5
3‴	-	147.6	-	149.3
4‴	-	141.8	-	132.1
5‴	-	147.6	-	149.3
6‴	7.32 (1H, *s*)	107.2	7.28 (1H, *s*)	108.5
-COO-	-	165.8	-	168.3
-OCH_3	3.85 (6H, *s*)	55.9	3.82 (6H, *s*)	56.8
2″-OH	4.55 (1H, *d*, 4.0)	-	-	-
3″-OH	4.62 (1H, *d*, 4.0)	-	-	-
4″-OH	4.47 (1H, *d*, 4.0)	-	-	-

[a] 500/125 MHz; Recorded in acetone-d_6

[b] 400/100 MHz; Recorded in DMSO-d_6

S. Shi, D. Jiang, C. Dong, and P. Tu, "New phenolic glycosides from *Clematis mandshurica*", *Helvetica Chimica Acta*, vol. 89, no. 5, pp. 1023–1029, 2006.

Table S2. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of **I**, **II**, and **ABS1** (δ in ppm, J in Hz)



No.	Compound I[a]		Compound II[b]		ABS1[a]	
	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C
1	2.61 (1H, *t*, 7.0)	38.9	2.74 (2H, *m*)	39.2	2.57 (2H, *m*)	39.4
2	3.65 (1H, *t*, 7.0)	63.7	3.51 (2H, *m*)	64.1	3.64 (2H, *m*)	62.7
1′	-	146.1	-	146.3	-	158.2
2′	-	146.1	-	146.8	6.37 (1H, *t*, 2.0)	109.9
3′	6.85 (1H, *d*, 8.0)	116.4	6.91 (1H, *d*, 2.0)	119.9	-	141.8
4′	6.78 (1H, *dd*, 8.0, 2.0)	124.7	-	132.1	6.41 (1H, *t*, 2.0)	108.4
5′	-	131.4	6.74 (1H, *dd*, 8.0, 2.0)	125.5	-	154.5
6′	6.95 (1H, *d*, 2.0)	118.8	6.74 (1H, *d*, 8.0)	117.0	6.43 (1H, *t*, 2.5)	101.4
1″	4.96 (1H, *d*, 8.0)	103.6	4.77 (1H, *d*, 6.1)	104.5	4.97 (1H, *d*, 7.5)	100.8
2″		75.0		75.8	3.49 (1H, *m*)	73.8
3″	3.83 – 3.52 (4H, *m*)	76.7	3.56 – 3.45 (4H, *m*)	77.4	3.54 (1H, *m*)	76.9
4″		70.9		71.9	3.57 (1H, *m*)	70.6
5″		74.1		74.8	3.87 (1H, *m*)	74.2

6″	4.68 (1H, *d*, 12.0) 4.45 (1H, *d*, 12.0)	64.8	4.72 (1H, *dd*, 11.9, 2.1) 4.48 (1H, *dd*, 11.9, 6.7)	65.1	4.72 (1H, *dd*, 11.5, 2.0) 4.40 (1H, *dd*, 11.5, 6.5)	64.0
1‴	-	121.0	-	121.2	-	121.5
2‴	-	109.8	7.34 (1H, *brs*)	108.5	7.32 (1H, *s*)	107.3
3‴	-	145.9	-	148.9	-	147.6
4‴	-	139.1	-	142.2	-	141.8
5‴	-	145.9	-	148.9	-	147.6
6‴	-	109.8	7.34 (1H, *brs*)	108.5	7.32 (1H, *s*)	107.2
-COO-	-	167.1	-	167.9	-	165.8
$-OCH_3$	3.82 (6H, *s*) 3.78 (3H, *s*) 3.76 (3H, *s*)	-	3.86 (6H, *s*)	57.0	3.85 (6H, *s*)	55.9
2″-OH	-	-	-	-	4.55 (1H, *d*, 4.0)	-
3″-OH	-	-	-	-	4.62 (1H, *d*, 4.0)	-
4″-OH	-	-	-	-	4.47 (1H, *d*, 4.0)	-

[a] Recorded in acetone-d_6

[b] Recorded in methanol-d_4

Note: Compound **I**: ((2*S*,3*S*,4*S*,5*R*,6*S*)-3,4,5-trihydroxy-6-(5-(2-hydroxyethyl)-2-methoxyphenoxy)tetrahydro-2*H*-pyran-2-yl)methyl-3,4,5-trimethoxybenzoate,

Compound **II**: ((2*S*,3*S*,4*S*,5*R*,6*S*)-3,4,5-trihydroxy-6-(2-hydroxy-4-(2-hydroxyethyl)phenoxy)tetrahydro-2*H*-pyran-2-yl)methy-l,4-hydroxy-3,5-dimethoxybenzoate

Y. Takashi, “Two polyphenol glycosides and tannins from *Rosa cymosa*”, *Phytochemistry*, vol. 32, no. 4, pp. 1033–1036, 1993.
M. Furukawa, “Terpenoids and phenethyl glycosides from *Hyssopus cuspidatus* (Labiate)”, *Phytochemistry*, vol. 72, no. 17, pp. 2244–2252, 2011.

Table S3. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of **ABS2** and syringaresinol (δ in ppm, J in Hz)

No.	**ABS2**[a]		**Syringaresinol**[b]	
	δ_H	δ_C	δ_H	δ_C
1, 1′	-	133.0	-	133.2
2, 2′	6.70 (2H, *s*)	103.5	6.73 (2H, *s*)	104.6
3, 3′	-	147.8	-	149.4
4, 4′	-	136.8	-	136.3
5, 5′	-	147.8	-	149.4
6, 6′	6.70 (2H, *s*)	103.5	6.73 (2H, *s*)	104.6
7, 7′	4.68 (2H, *d*, 4.5)	85.7	4.77 (2H, *d*, 4.5)	87.6
8, 8′	3.11 (2H, *m*)	54.1	3.14 (2H, *m*)	55.5
9, 9′	4.30 (2H, *m*) 3.90 (2H, *dd*, 3.5, 1.0)	71.6	4.30 (2H, *d*, 9.0) 3.93 (2H, *dd*, 3.0, 9.0)	72.7
3, 5-OCH_3 3′, 5′-OCH_3	3.84 (12H, *s*)	56.5	3.89 (12H, *s*)	56.8

[a] Recorded in acetone-d_6
[b] Recorded in methanol-d_4

N. K. Ban, L. H. Truong, T. M. Linh, N. C. Mai, D. T. H. Yen, V. V. Doan, N. X. Nhiem, B. H. Tai, and P. V. Kiem, "Phenolic compounds from *Trigonostemon honbaensis* and their cytotoxic activity", *Vietnam Journal of Chemistry*, vol. 58, no. 6, pp. 759–764, 2020.

Table S4. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of **ABS3** and ciwujiatone in methanol-d_4 (δ in ppm, J in Hz)

No.	ABS3		Ciwujiatone	
	δ_H	δ_C	δ_H	δ_C
1	-	128.7	-	128.7
2	7.32 (1H, *s*)	107.8	7.32 (1H, *s*)	107.8
3	-	149.2	-	149.1
4	-	142.7	-	142.7
5	-	149.2	-	149.1
6	7.32 (1H, *s*)	107.8	7.32 (1H, *s*)	107.8
7	-	200.4	-	200.3
8	4.20 (1H, *m*)	50.2	4.20 (1H, *m*)	50.2
9	4.13 (2H, *m*)	71.6	4.15 (2H, *m*)	71.5
3, 5-OCH_3	3.85 (6H, *s*)	56.9	3.85 (6H, *s*)	56.9
1′	-	132.9	-	132.9
2′	6.65 (1H, *s*)	105.3	6.66 (1H, *s*)	105.4
3′	-	149.2	-	149.2
4′	-	136.3	-	136.4
5′	-	149.2	-	149.2
6′	6.65 (1H, *s*)	105.3	6.66 (1H, *s*)	105.2
7′	4.58 (1H, *d*, 8.0)	85.4	4.58 (1H, *d*, 8.0)	85.4
8′	2.57 (1H, *m*)	55.1	2.59 (1H, *m*)	55.1
9′	3.60 (2H, *m*)	61.4	3.67 (2H, *m*)	61.5
3′, 5′-OCH_3	3.79 (6H, *s*)	56.8	3.79 (6H, *s*)	56.8

P.-F. Tu, D. Chen, Y.-L. Song, C.-X. Nie, and X. Ma, “Chemical constituents from *Aquilaria sinensis* (Lour.) Gilg”, *Journal of Chinese Pharmaceutical Sciences*, vol. 21, no. 1, pp. 88, 2012.

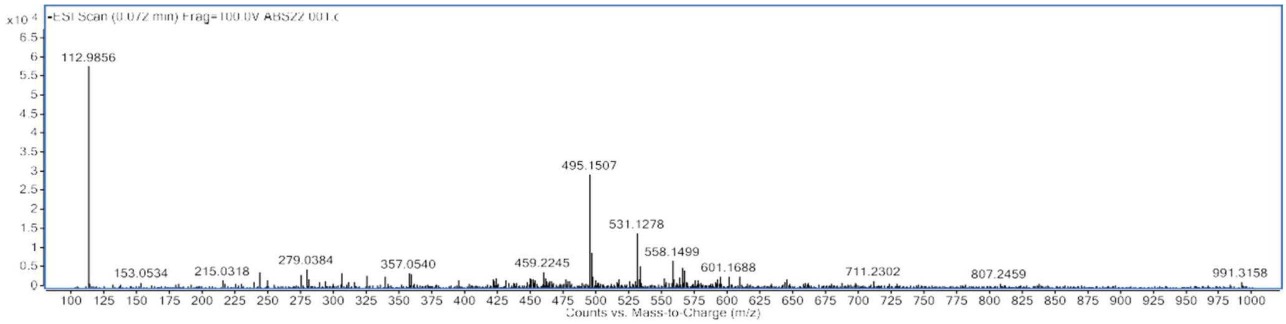


Figure S1. HRESI mass spectrum of **ABS1**

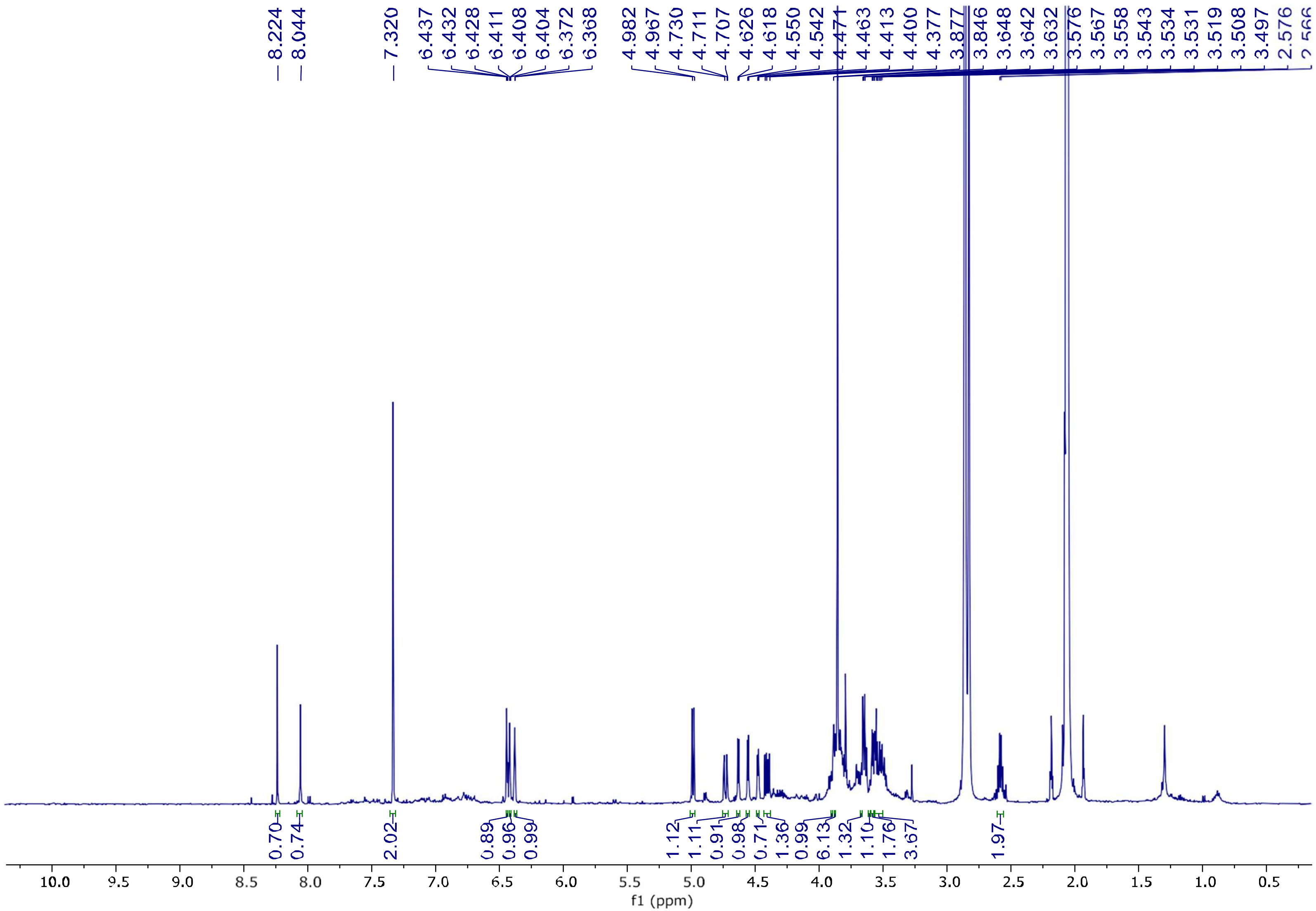


Figure S2A. ^{1}H NMR spectrum of **ABS1** (acetone-d_6)

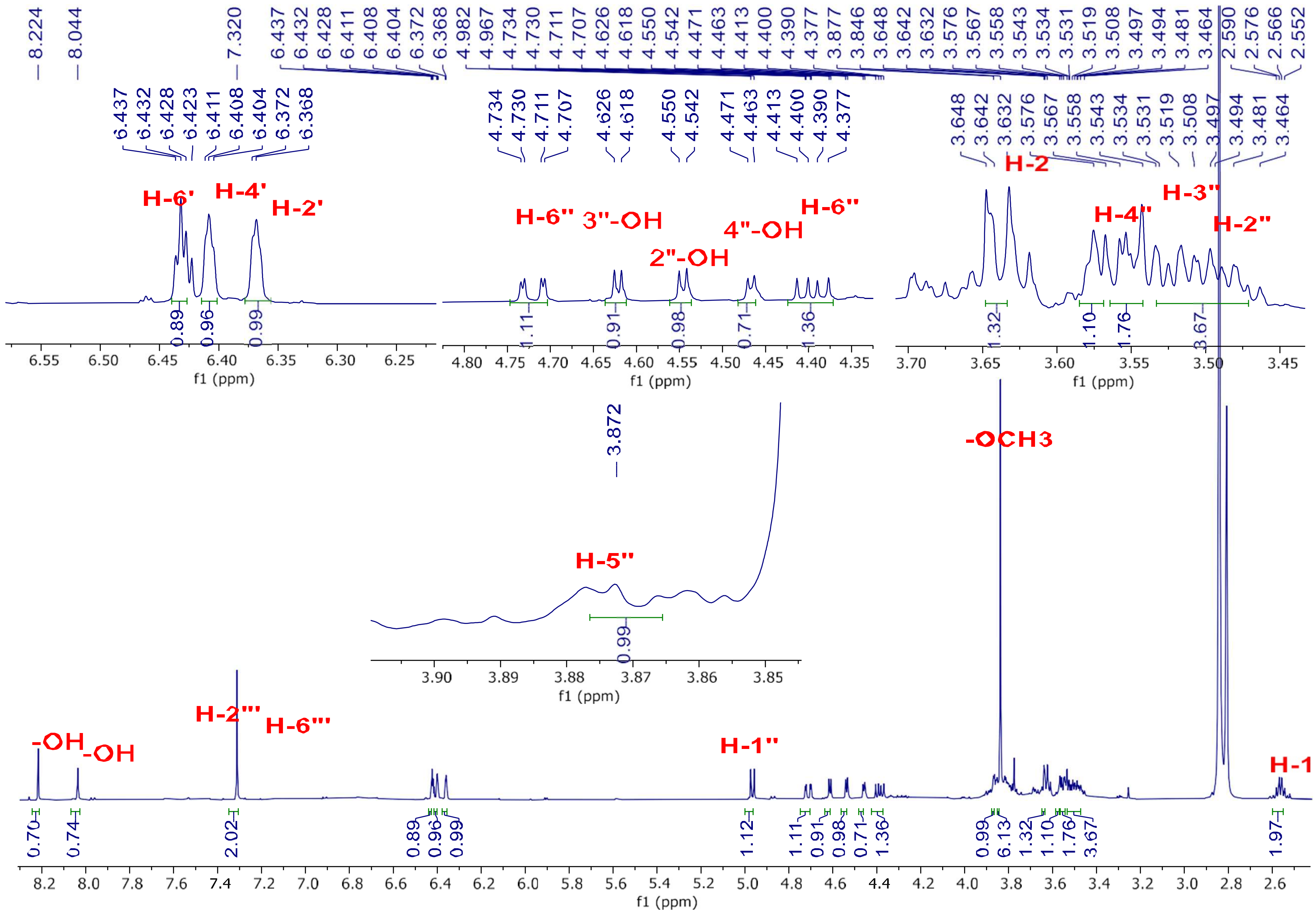


Figure S2B. [1]H NMR spectrum of **ABS1** (acetone-d_6)

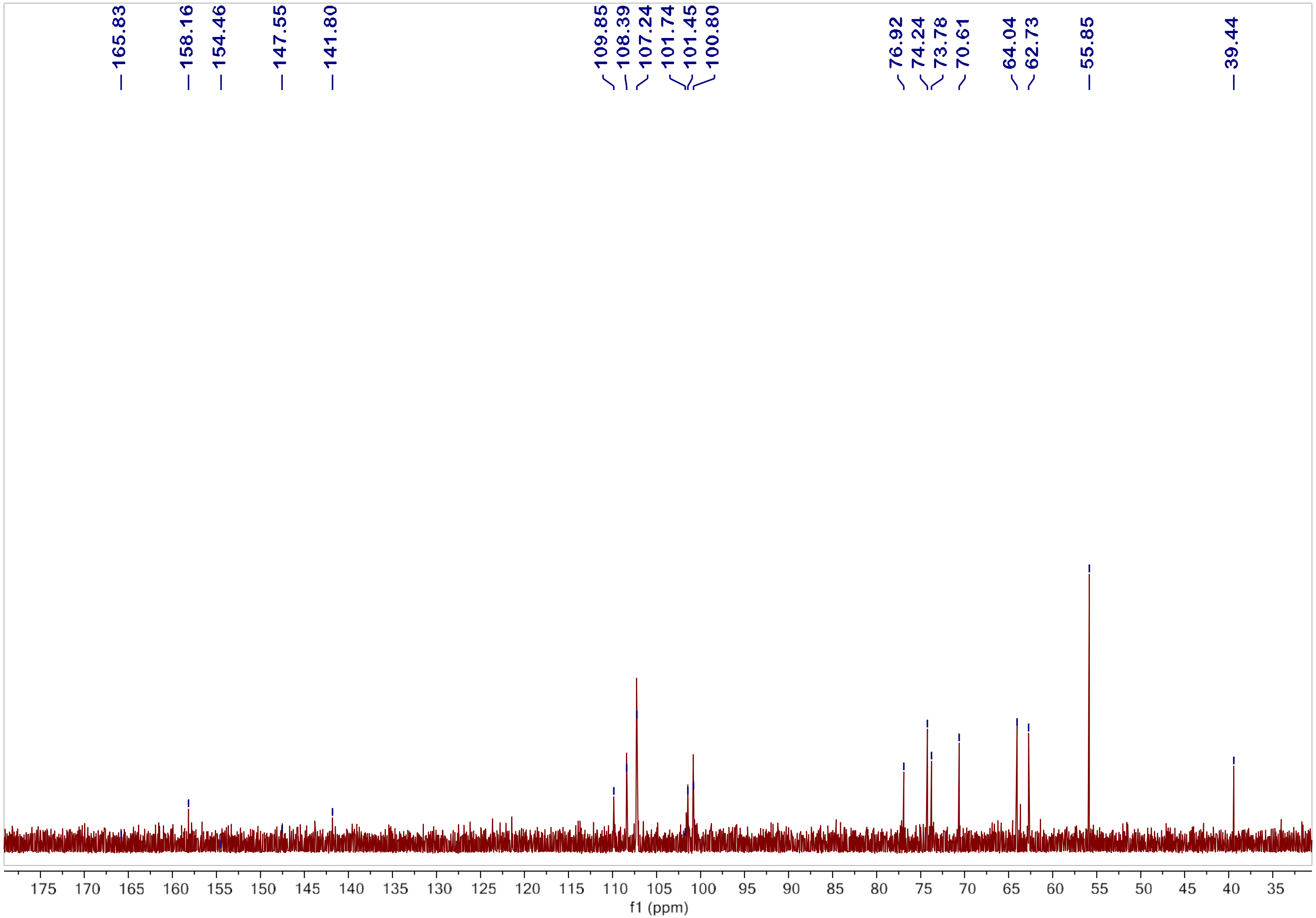


Figure S3A. ^{13}C NMR spectrum of **ABS1** (acetone-d_6)

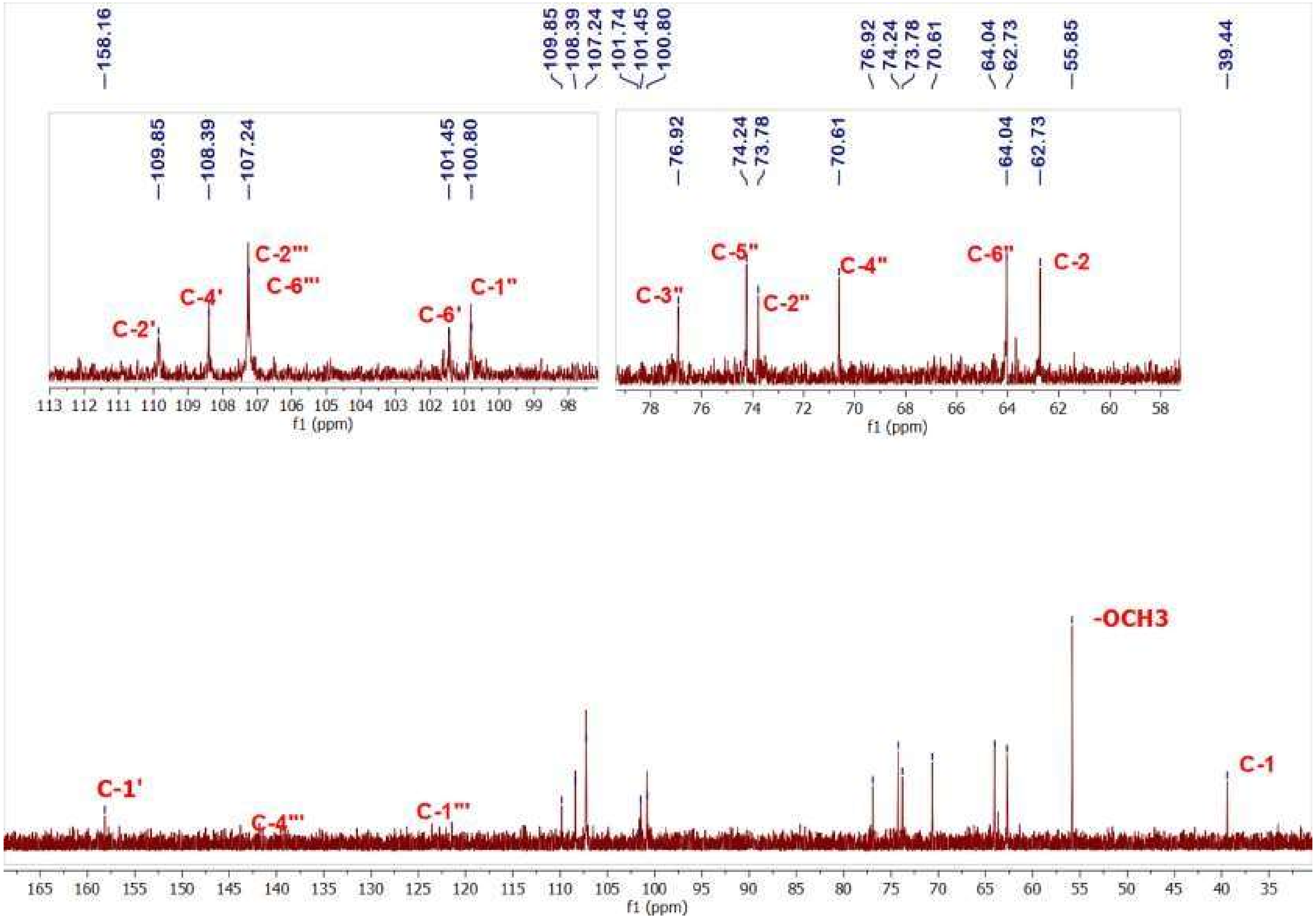


Figure S3B. [13]C NMR spectrum of **ABS1** (acetone-d_6)

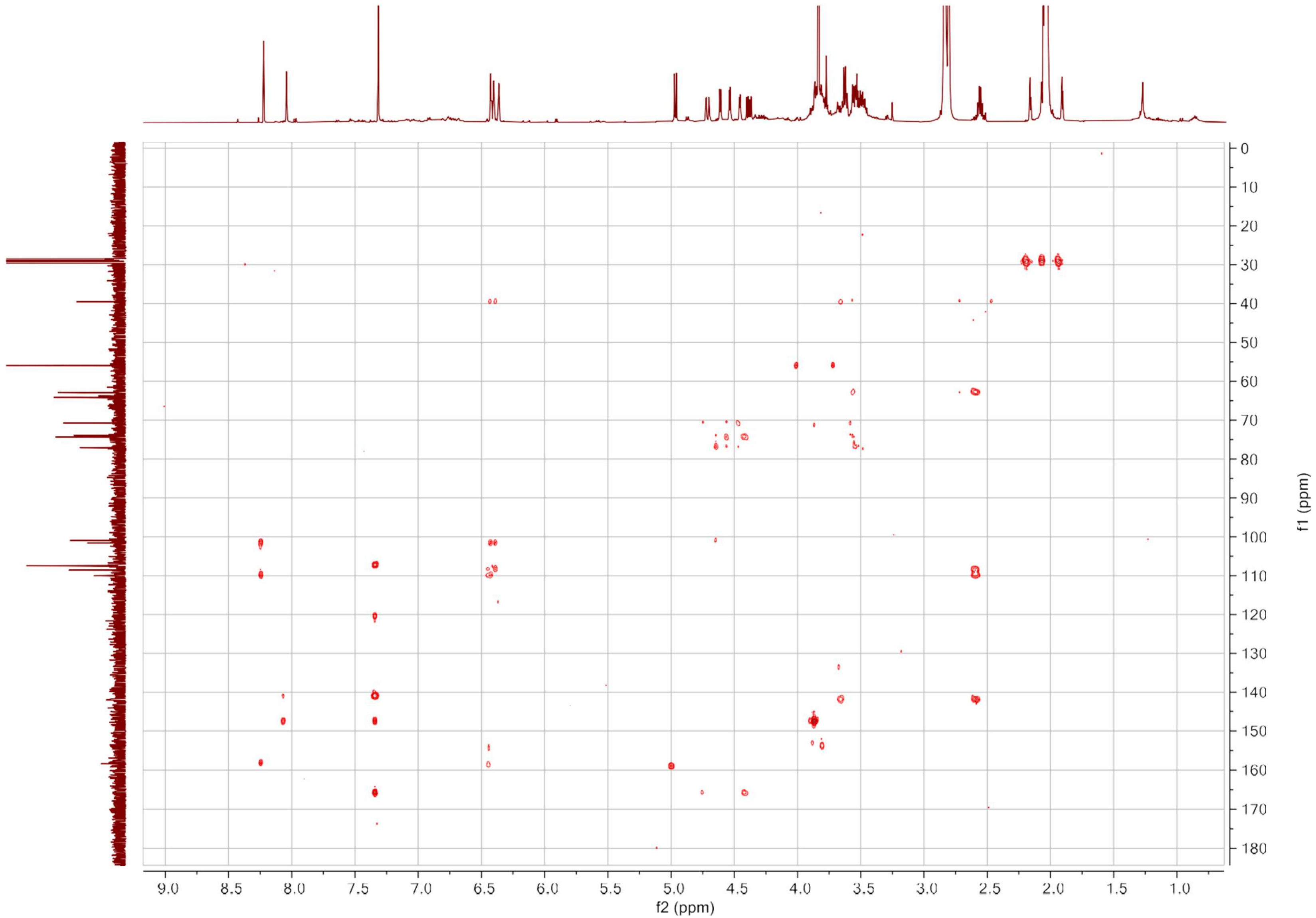
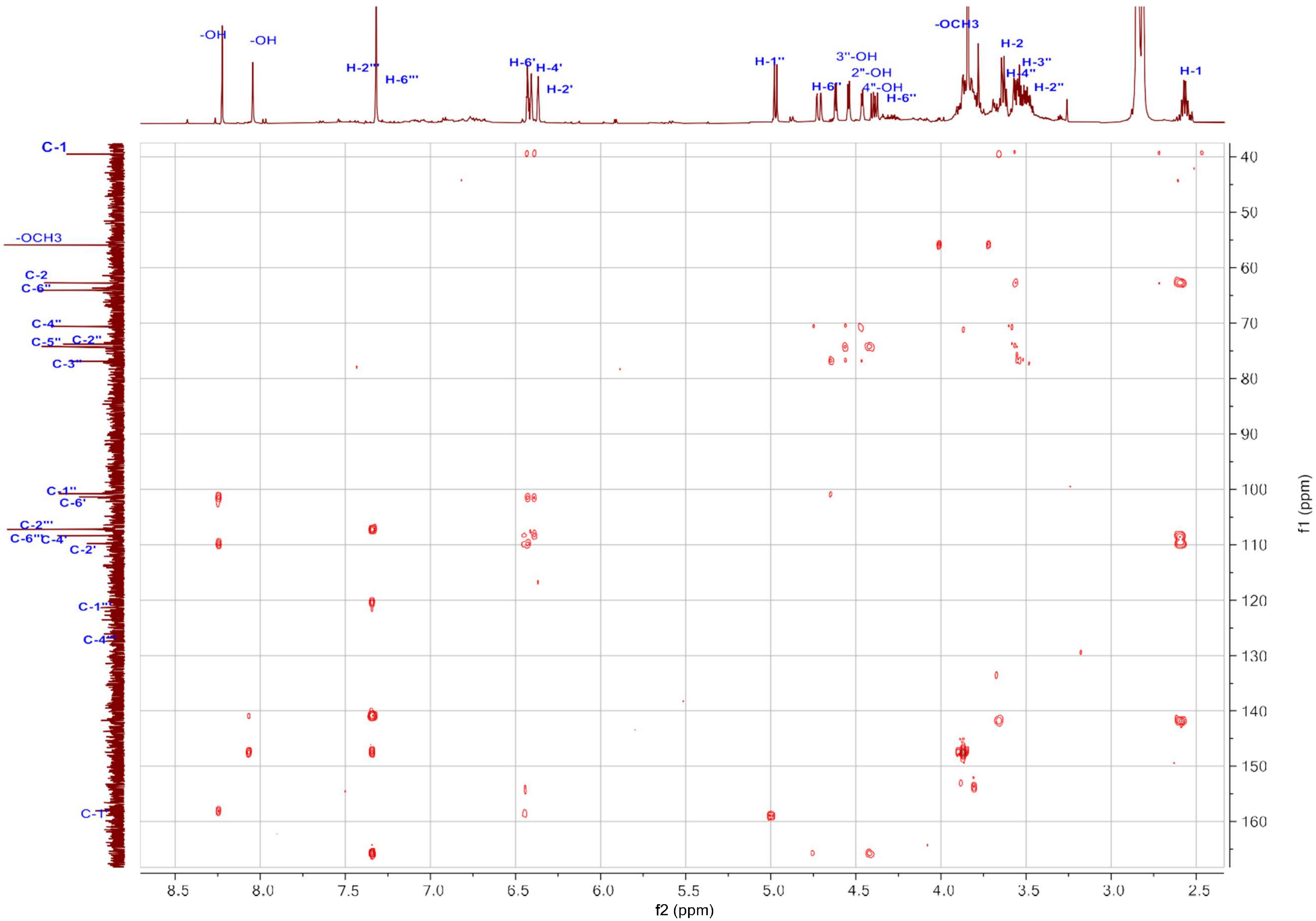


Figure S4A. HMBC spectrum of **ABS1** (acetone-d_6)



-OH
-OH
H-2'''
H-6'''
H-6'
H-4'
H-2'
H-1''
H-6''
3''-OH
2''-OH
4''-OH
H-6''
-OCH3
H-2
H-4''
H-3''
H-2''
H-1
C-1
-OCH3
C-2
C-6''
C-4''
C-5''
C-2''
C-3''
C-1''
C-6'
C-2'''
C-6''
C-4'
C-2'
C-1'''
C-4'''
C-1'
f2 (ppm)
f1 (ppm)

Figure S4B. HMBC spectrum of **ABS1** (acetone-d_6)

f2 (ppm)

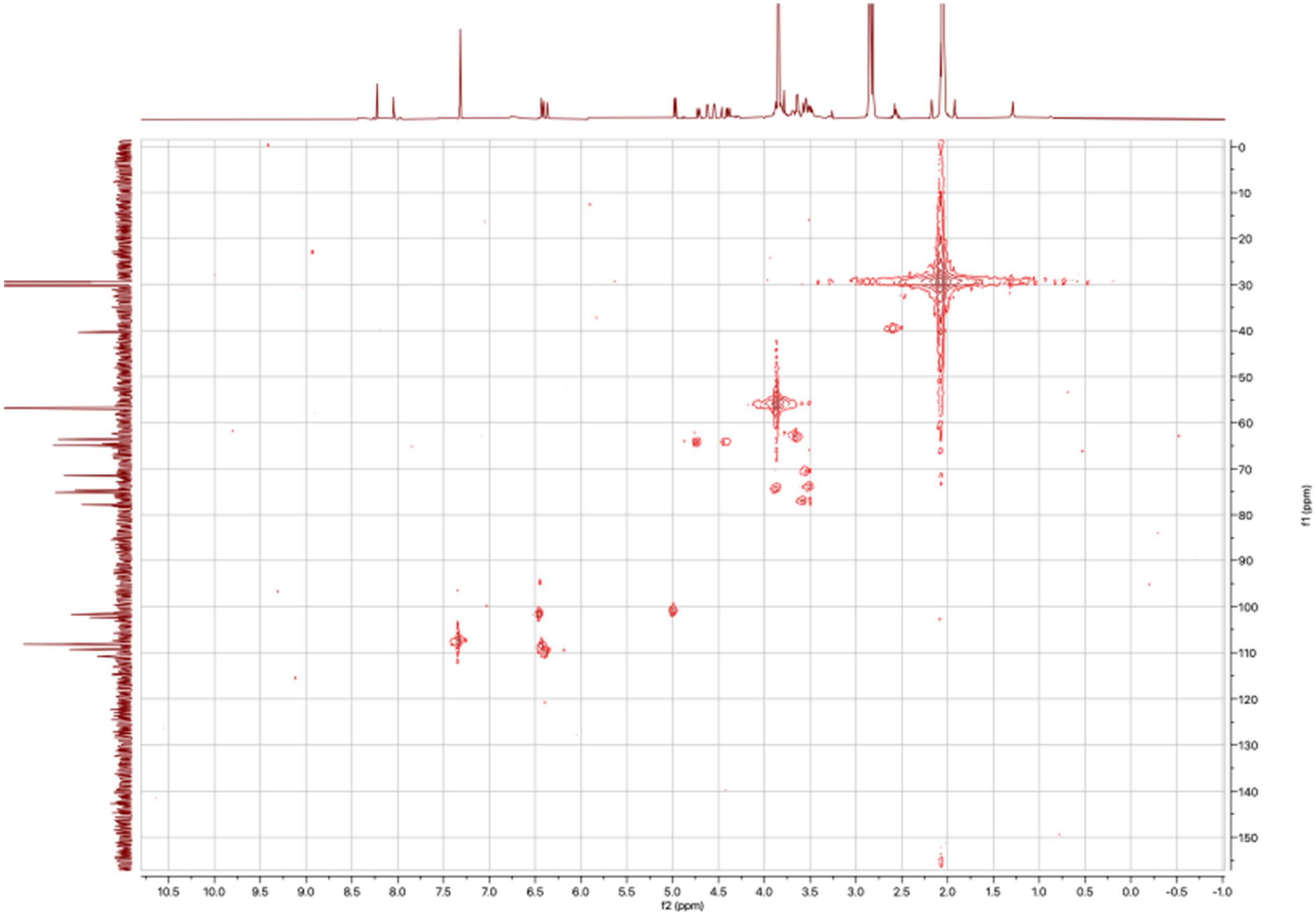


Figure S5. HMQC spectrum of **ABS1** (acetone-d_6)

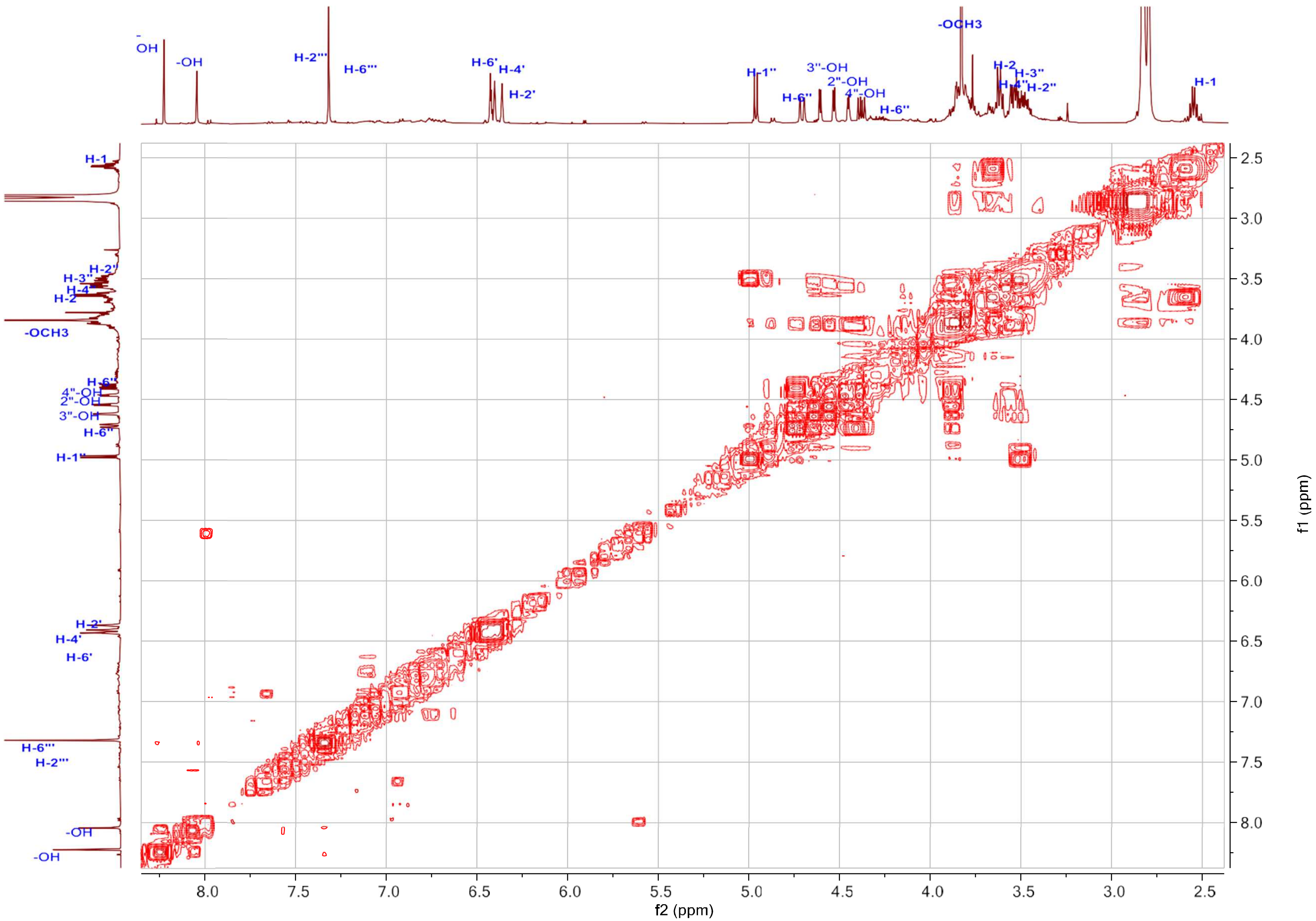
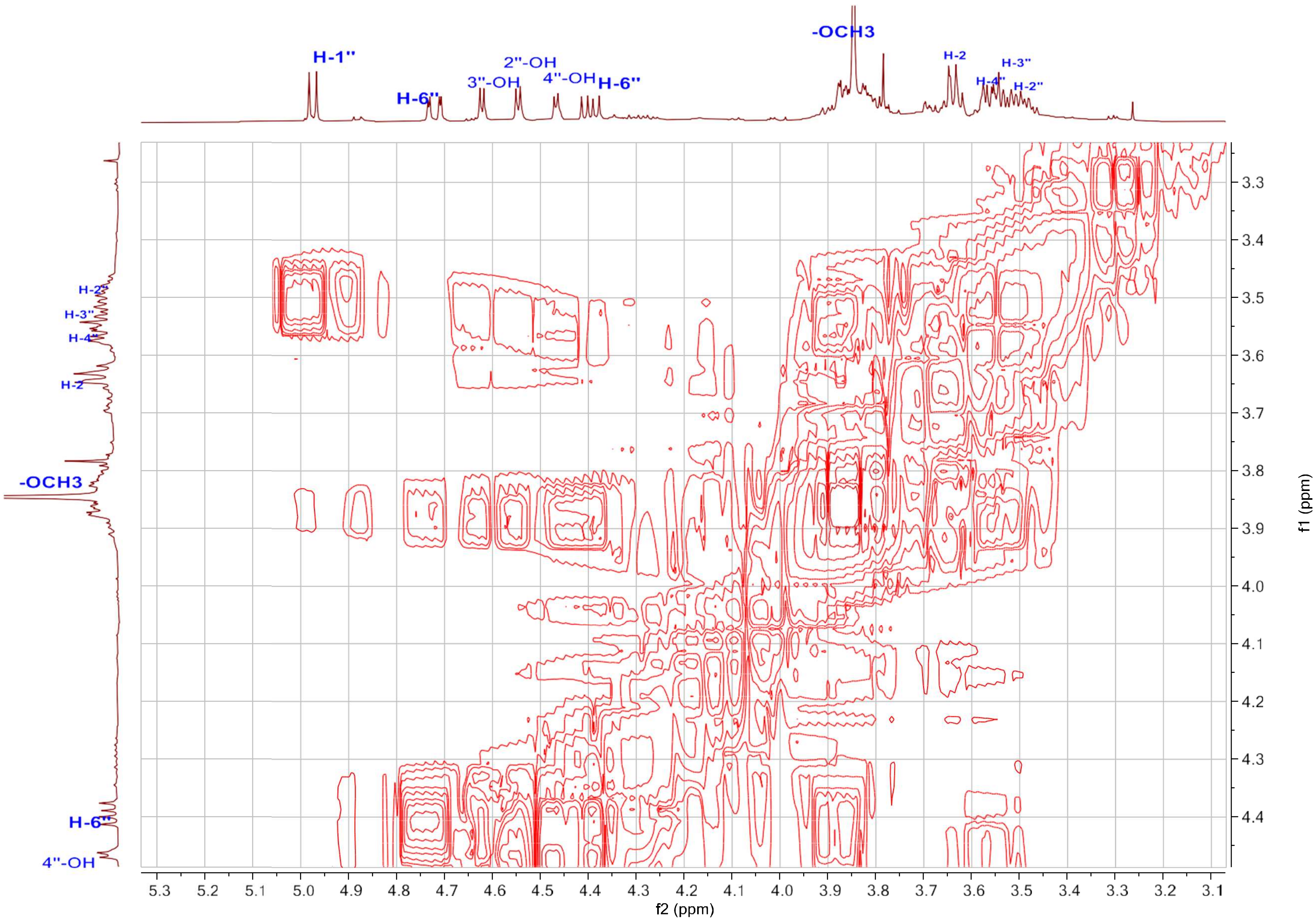


Figure S6A. COSY spectrum of **ABS1** (acetone-d_6)



H-1''
H-6''
3''-OH
2''-OH
4''-OH
H-6''
-OCH3
H-2
H-3''
H-4''
H-2''
f2 (ppm)
f1 (ppm)

Figure S6B. COSY spectrum of **ABS1** (acetone-d_6)

f2 (ppm)

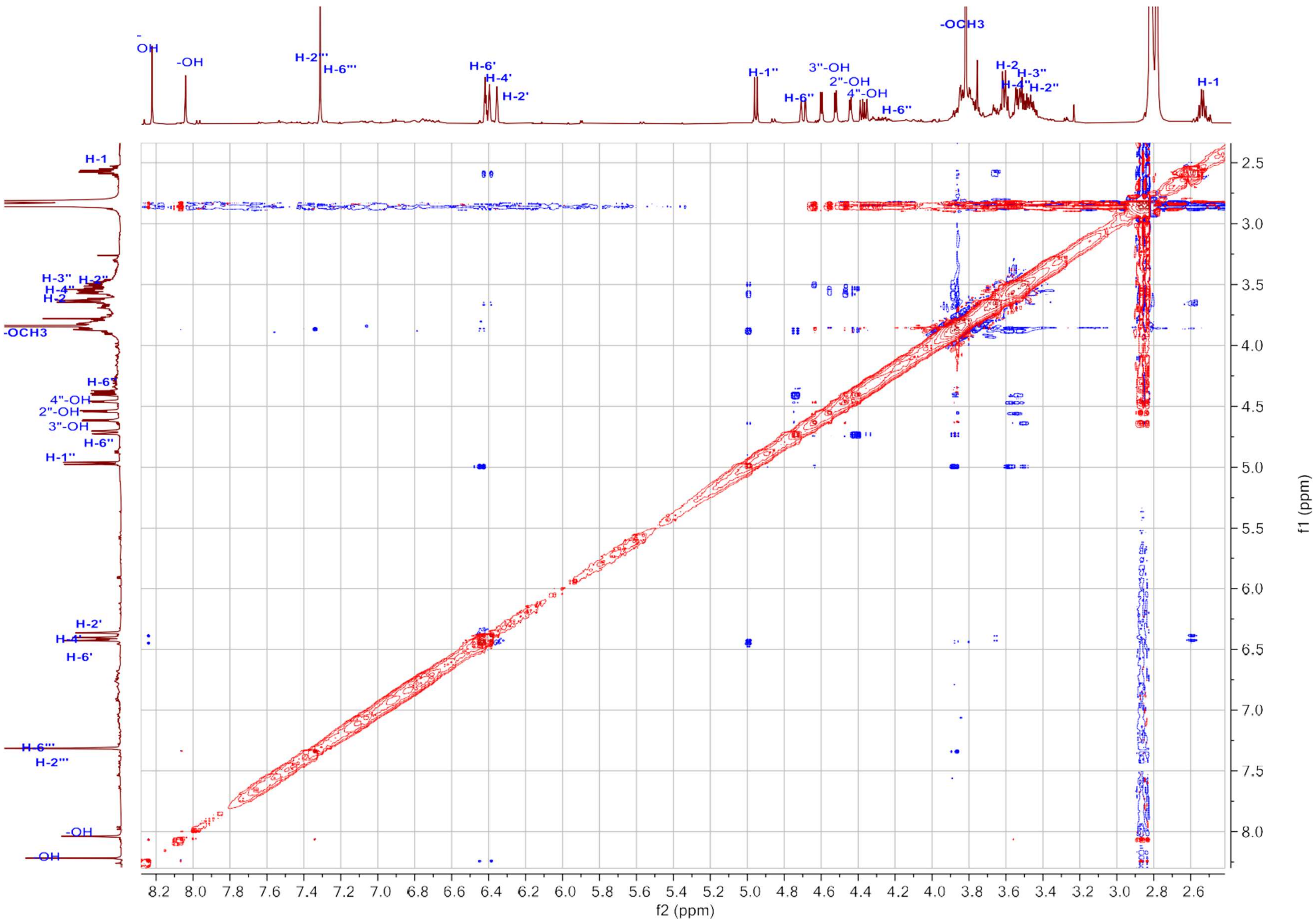


Figure S7A. NOESY spectrum of **ABS1** (acetone-d_6)

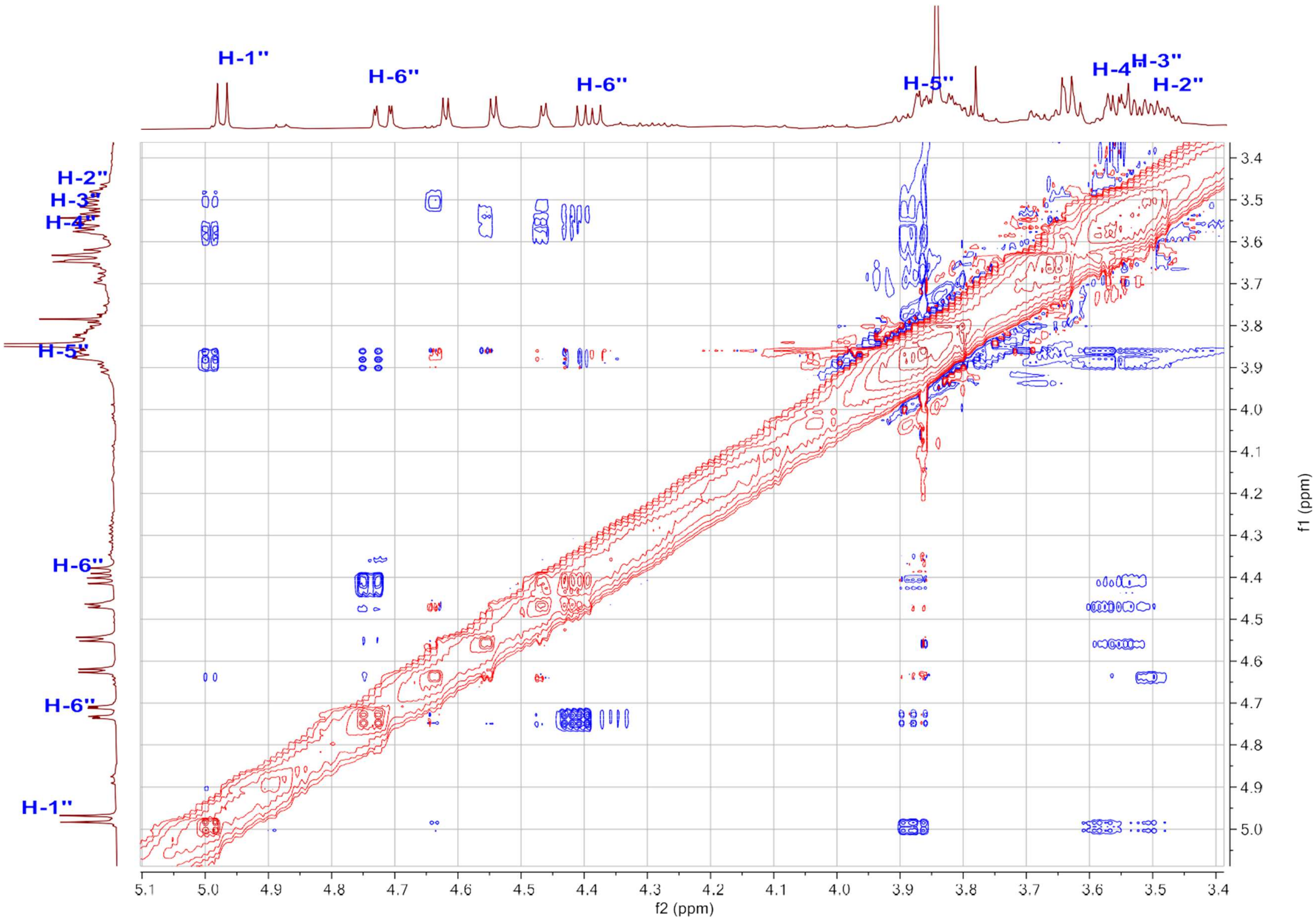


Figure S7B. NOESY spectrum of **ABS1** (acetone-d_6)

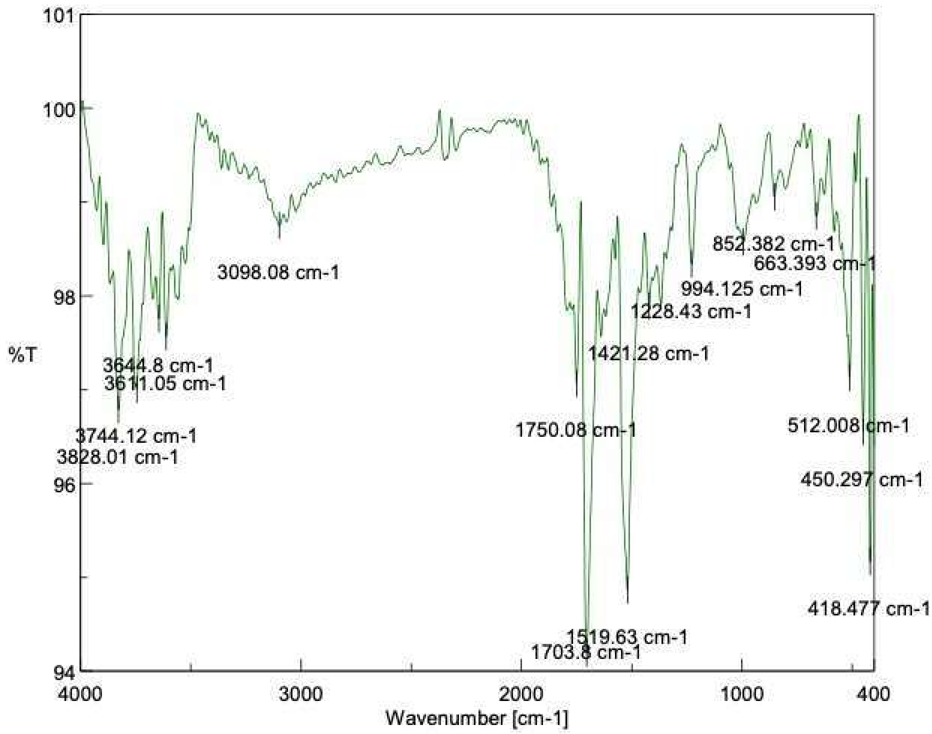
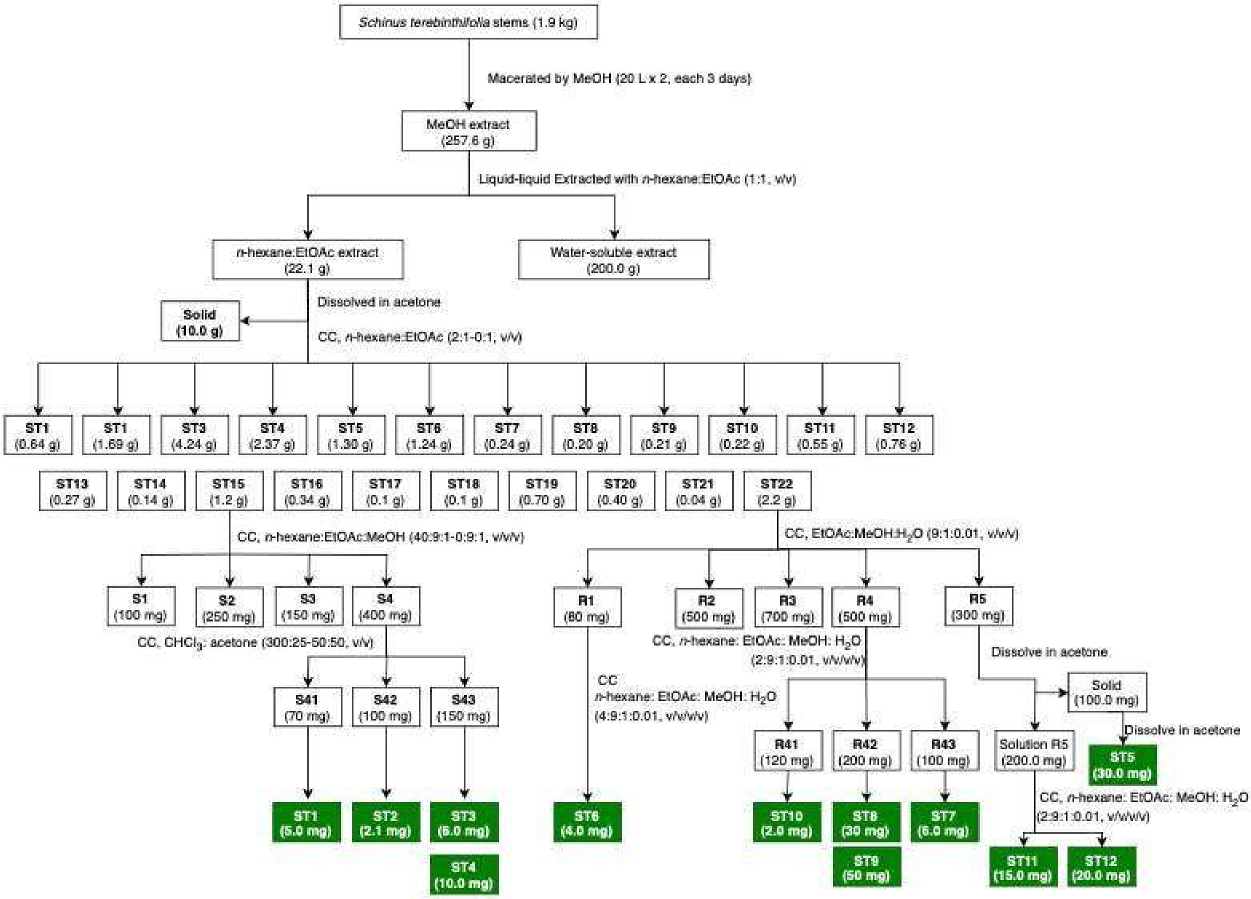


Figure S8. IR spectrum of **ABS1** (acetone-d_6)



Scheme S1. Isolation procedure of the *Schinus terebinthifolia* stems