Sebestenoids A-D, BACE1 inhibitors from *Cordia sebestena*

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Table S1. NMR Spectroscopic Data (500 MHz) in MeOH-d_4 for Sebestenoid A (**1**)

Position	δ_C, mult.	δ_H (J in Hz)	COSY	HMBC	ROESY
1	127.7, qC			H-2, H-5, H-6, H-7, H-8	
2	117.3, CH	7.28, d (2.1)			H-7
3	146.1, qC			H-2, H-5	
4	148.5, qC			H-2, H-5, H-6	
5	116.1, CH	6.73, d (8.2)	H-6		
6	122.7, CH	6.89, dd (8.2, 2.1)	H-5		H-7
7	113.3, CH	5.63, d (7.2)	H-8		H-2, H-6
8	132.8, CH	7.22, d (7.2)	H-7		
1’	130.8, qC			H-2’, H-5’, H-6’, H-7’, H-8’	
2’	116.8, CH	7.27, d (2.0)			H-7’, H-8’
3’	145.5, qC			H-2’, H-5’	
4’	148.4, qC			H-2’, H-5’, H-6’, H-7”	
5’	115.5, CH	6.76, d (8.2)	H-6’		H-7”
6’	122.3, CH	7.04, dd (8.2, 2.0)	H-5’		H-7’, H-8’
7’	148.0, CH	7.75, d (15.8)	H-8’		H-2’, H-6’
8’	115.8, CH	6.55, d (15.8)	H-7’		H-2’, H-6’
9’	165.4, qC			H-7’, H-8’, H-8	
1”	125.4, qC			H-2”, H-5”, H-6”, H-7"	
2”	118.2, CH	7.24, d (2.0)			H-7”
3”	146.1, qC			H-2”, H-5”	
4”	149.2, qC			H-2”, H-5”, H-6”	
5”	116.4, CH	6.73, d (8.4)	H-6”		
6”	125.2, CH	7.08, dd (8.4, 2.0)	H-5”		H-7”
7”	129.8, CH	7.33, s			H-5’, H-2”, H-6”
8”	138.3, qC			H-7”	
9”	165.6, qC			H-7”, OCH_3	
OCH_3	52.8, CH_3	3.72, s			

Table S2. NMR Spectroscopic Data (500 MHz) in MeOH-d_4 for Sebestenoid B (**2**)

Position	δ_C, mult.	δ_H (*J* in Hz)	COSY	HMBC	ROESY
1	127.3, qC			H-2, H-6, H-7, H-8	
2	116.6, CH	6.69, d (1.5)			H-7, H-8
3	146.3, qC			H-2, H-4	
4	113.6, CH	6.83, d (1.5)			
5	146.5, qC			H-4, H-6	
6	119.6, CH	6.70, d (1.5)			H-7, H-8
7	116.8, CH	6.36, d (12.8)	H-8		H-2, H-6
8	135.4, CH	7.78, d (12.8)	H-7		H-2, H-6
1’	130.8, qC			H-2’, H-5’, H-6’, H-7’, H-8’	
2’	116.8, CH	7.23, d (2.0)			H-7’, H-8’
3’	146.6, qC			H-2’, H-5’	
4’	148.8, qC			H-2’, H-5’, H-6’	
5’	115.5, CH	6.74, d (8.4)	H-6’		
6’	122.3, CH	7.00, dd (8.4, 2.0)	H-5’		H-7’, H-8’
7’	147.6, CH	7.69, d (15.8)	H-8’		H-2’, H-6’
8’	115.7, CH	6.42, d (15.8)	H-7’		H-2’, H-6’
9’	165.9, qC			H-8, H-7’, H-8’	
1”	125.4, qC			H-2”, H-5”, H-6”, H-7”	
2”	118.1, CH	7.26, d (2.0)			H-7”
3”	148.0, qC			H-2”, H-5”	
4”	149.2, qC			H-2”, H-5”, H-6”	
5”	116.4, CH	6.72, d (8.4)	H-6”		
6”	125.2, CH	7.07, dd (8.4, 2.0)	H-5”		H-7”
7”	129.8, CH	7.33, s			H-2”, H-6”
8”	138.2, qC			H-7”, H-4	
9”	165.5, qC			H-7”, OCH_3	
OCH_3	52.8, CH_3	3.72, s			

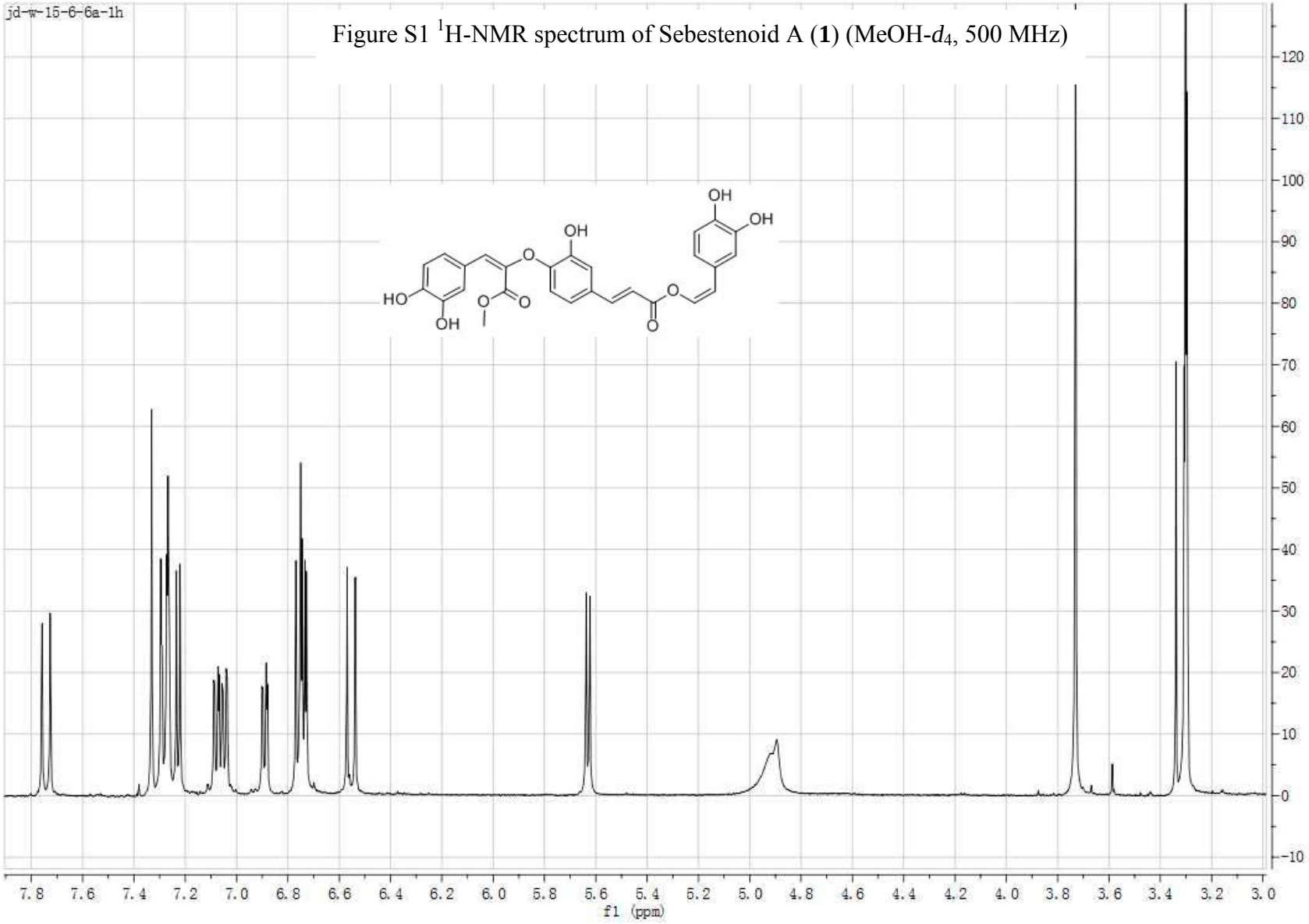
Table S3. NMR Spectroscopic Data (500 MHz) in MeOH-d_4 for Sebestenoid C (**3**)

Position	δ_C, mult.	δ_H (*J* in Hz)	COSY	HMBC	ROESY
1	127.8, qC			H-2, H-5, H-6, H-7, H-8	
2	117.4, CH	7.27, d (2.0)			H-7
3	146.0, qC			H-2, H-5	
4	145.7, qC			H-2, H-5, H-6	
5	116.5, CH	6.75, d (8.2)	H-6		
6	122.8, CH	6.92, dd (8.2, 2.0)	H-5		H-7
7	113.2, CH	5.61, d (7.3)	H-8		H-2, H-6
8	132.9, CH	7.21, d (7.3)	H-7		
1’	124.5, qC			H-5’, H-6’, H-7’, H-8’, H-8”	
2’	126.5, qC			H-6’, H-7’, H-7”, H-8”	
3’	149.1, qC			H-5’, H-7”, H-8”	
4’	145.9, qC			H-5’, H-6’	
5’	118.6, CH	6.87, d (8.3)	H-6’		
6’	122.2, CH	7.30, d (8.3)	H-5’		H-7’, H-8’
7’	144.9, CH	7.80, d (15.9)	H-8’		H-6’, H-8”
8’	115.7, CH	6.44, d (15.9)	H-7’		H-6’
9’	165.5, qC			H-8, H-7’, H-8’	
1”	133.5, qC			H-2”, H-5”, H-6”, H-7", H-8”	
2”	113.3, CH	6.75, d (2.0)			H-7”, H-8”
3”	146.1, qC			H-2”, H-5”	
4”	146.8, qC			H-2”, H-5”, H-6”	
5”	116.3, CH	6.74, d (8.2)	H-6”		
6”	118.3, CH	6.63, dd (8.2, 2.0)	H-5”		H-7”
7”	88.1, CH	5.81, d (4.4)	H-8”		H-2”, H-6”
8”	57.4, CH	4.42, d (4.4)	H-7”		H-2”, H-7’
9”	172.3, qC			H-7”, H-8”, H-8”’	
1”’	128.5, qC			H-2”’, H-5”’, H-6”’, H-7”’, H-8”’	
2”’	117.2, CH	6.56, d (2.0)			H-7”’, H-8”’
3”’	146.6, qC			H-2”’, H-5”’	
4”’	145.2, qC			H-2”’, H-5”’, H-6”’	
5”’	116.5, CH	6.56, d (8.1)	H-6”’		
6”’	121.8, CH	6.36, dd (8.1, 2.0)	H-5”’		H-7”’, H-8”’
7”’	37.4, CH_2	2.84, dd (14.2, 9.2) 2.96, dd (14.2, 4.5)	H-8”’		H-2”’, H-6”’
8”’	75.7, CH	5.16, dd (9.2, 4.5)	H-7”’		H-2”’, H-6”’
9”’	171.2, qC			H-7”’, H-8”’, OCH_3	
OCH_3	52.8, CH_3	3.62, s			

Table S4. NMR Spectroscopic Data (500 MHz) in MeOH-d_4 for Sebestenoid D (**4**)

Position	δ_C, mult.	δ_H (*J* in Hz)	COSY	HMBC	ROESY
1	127.5, qC			H-2, H-6, H-7, H-8	
2	116.5, CH	6.67, d (1.7)			H-7, H-8
3	146.2, qC			H-2, H-4	
4	113.6, CH	6.81, d (1.7)			
5	146.3, qC			H-4, H-6	
6	119.6, CH	6.68, d (1.7)			H-7, H-8
7	116.8, CH	6.35, d (12.8)	H-8		H-2, H-6
8	135.5, CH	7.76, d (12.8)	H-7		H-2, H-6
1’	124.4, qC			H-5’, H-6’, H-7’, H-8’, H-8”	
2’	126.3, qC			H-6’, H-7’, H-7”, H-8”	
3’	149.2, qC			H-5’, H-7”, H-8”	
4’	145.7, qC			H-5’, H-6’	
5’	118.6, CH	6.84, d (8.4)	H-6’		
6’	122.3, CH	7.22, d (8.4)	H-5’		H-7’, H-8’
7’	144.5, CH	7.70, d (15.9)	H-8’		H-6’, H-8”
8’	115.7, CH	6.29, d (15.9)	H-7’		H-6’
9’	165.9, qC			H-8, H-7’, H-8’	
1”	133.5, qC			H-2”, H-5”, H-6”, H-7", H-8”	
2”	113.3, CH	6.73, (2.1)			H-7”, H-8”
3”	146.5, qC			H-2”, H-5”	
4”	146.6, qC			H-2”, H-5”, H-6”	
5”	116.4, CH	6.75, d (8.2)	H-6”		
6”	118.3, CH	6.62, dd (8.2, 2.1)	H-5”		H-7”
7”	88.2, CH	5.80, d (4.6)	H-8”		H-2”, H-6”
8”	57.6, CH	4.38, d (4.6)	H-7”		H-2”, H-7’
9”	172.3, qC			H-7”, H-8”, H-8”’	
1”’	128.5, qC			H-2”’, H-5”’, H-6”’, H-7””, H-8”’	
2”’	117.3, CH	6.59, d (2.0)			H-7””, H-8”’
3”’	146.8, qC			H-2”’, H-5”’	
4”’	145.3, qC			H-2”’, H-5”’, H-6”’	
5”’	116.5, CH	6.62, d (8.1)	H-6”’		
6”’	121.8, CH	6.40, dd (8.1, 2.0)	H-5”’		H-7””, H-8”’
7”’	37.5, CH_2	2.91, dd (14.2, 9.2) 3.02, dd (14.2, 4.0)	H-8”’		H-2””, H-6”’
8”’	75.7, CH	5.19, dd (9.2, 4.0)	H-7”’		H-2””, H-6”’
9”’	171.2, qC			H-7””, H-8”’, OCH_3	
OCH_3	52.9, CH_3	3.67, s			

Figure S1 ^{1}H-NMR spectrum of Sebestenoid A (**1**) (MeOH-d_4, 500 MHz)



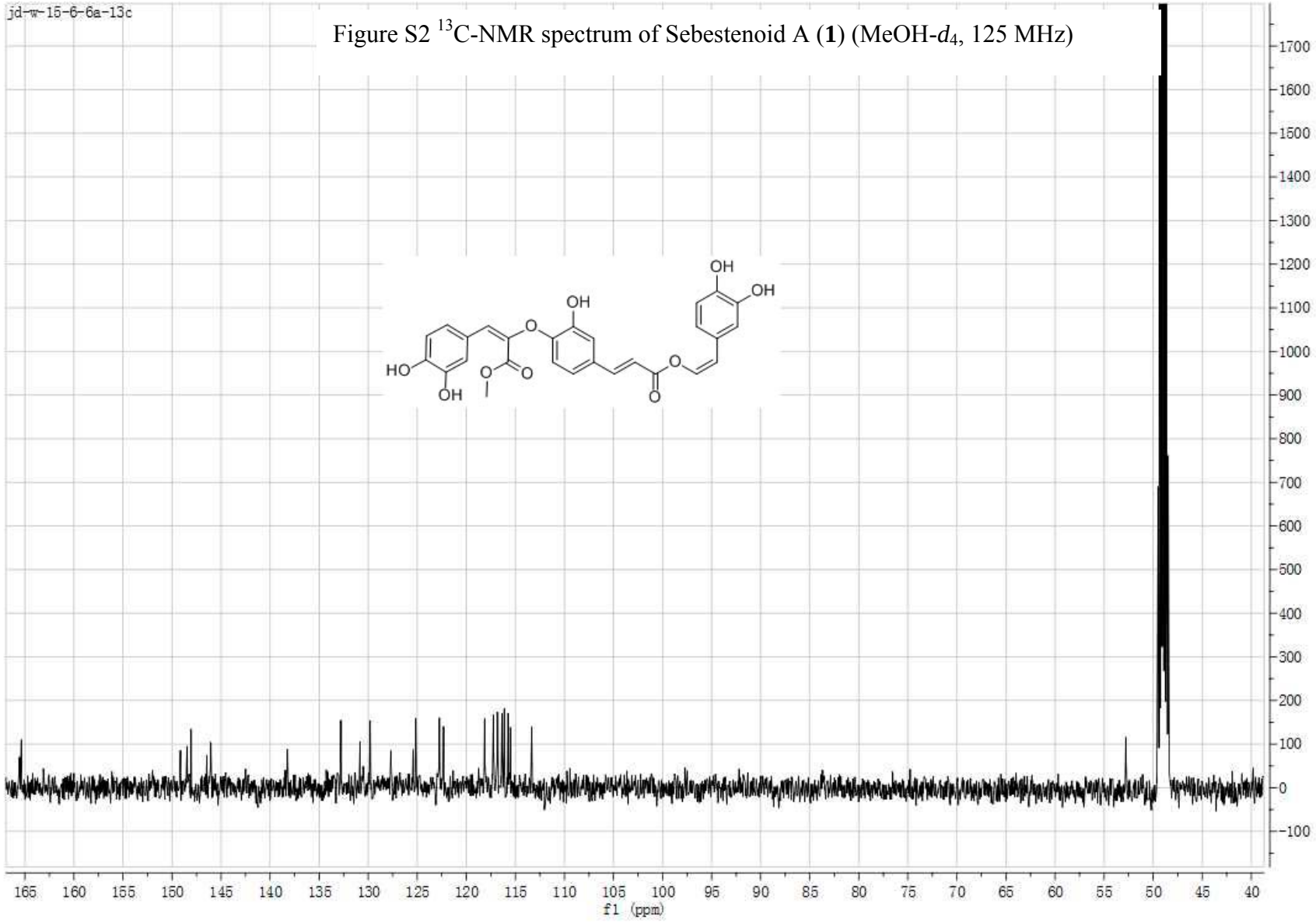


Figure S2 ^{13}C-NMR spectrum of Sebestenoid A (**1**) (MeOH-d_4, 125 MHz)

Figure S3 COSY NMR spectrum of Sebestenoid A (**1**) (MeOH-d_4, 500 MHz)

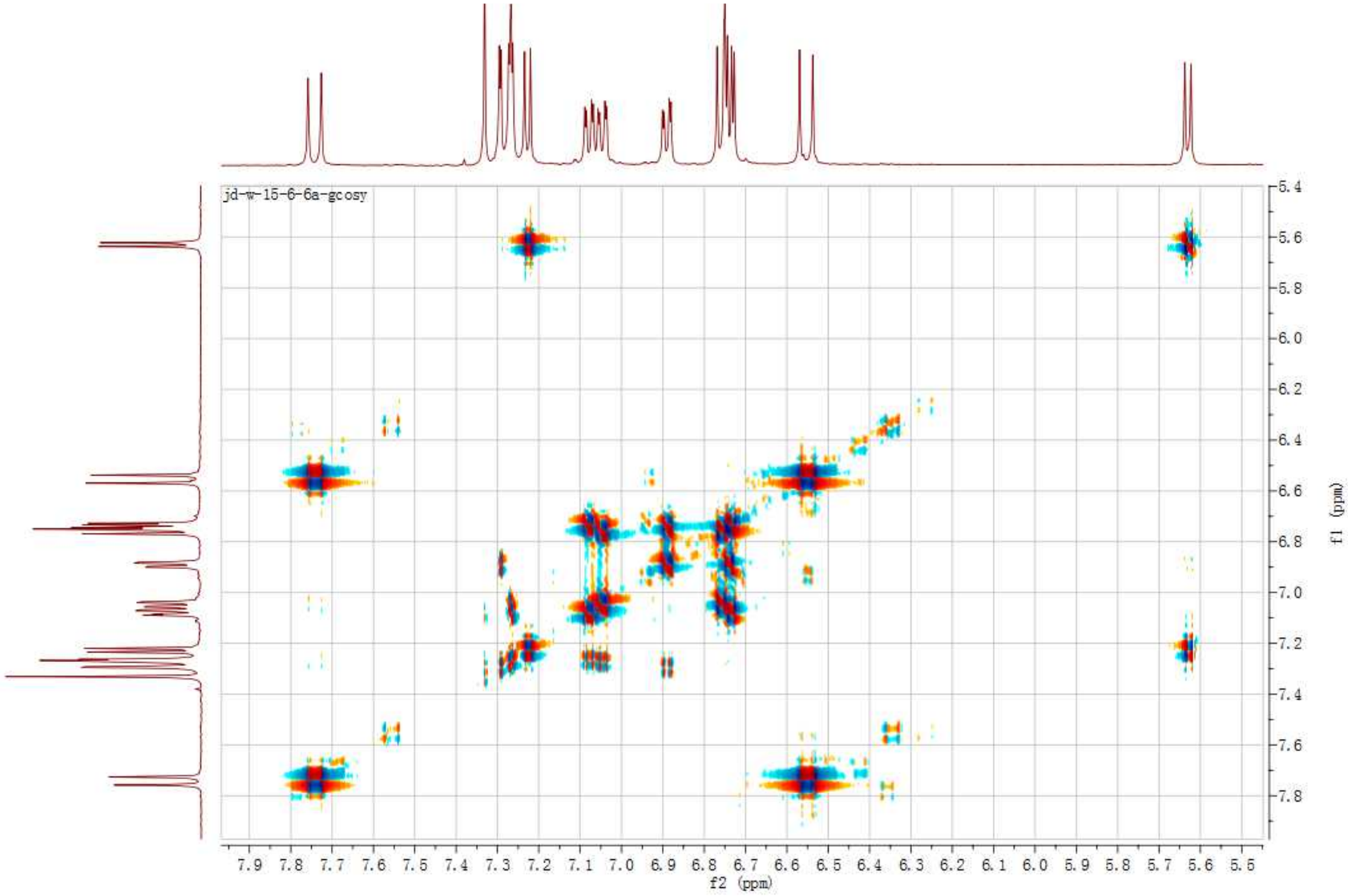


Figure S4 HSQC NMR spectrum of Sebestenoid A (**1**) (MeOH-d_4, 500 MHz)

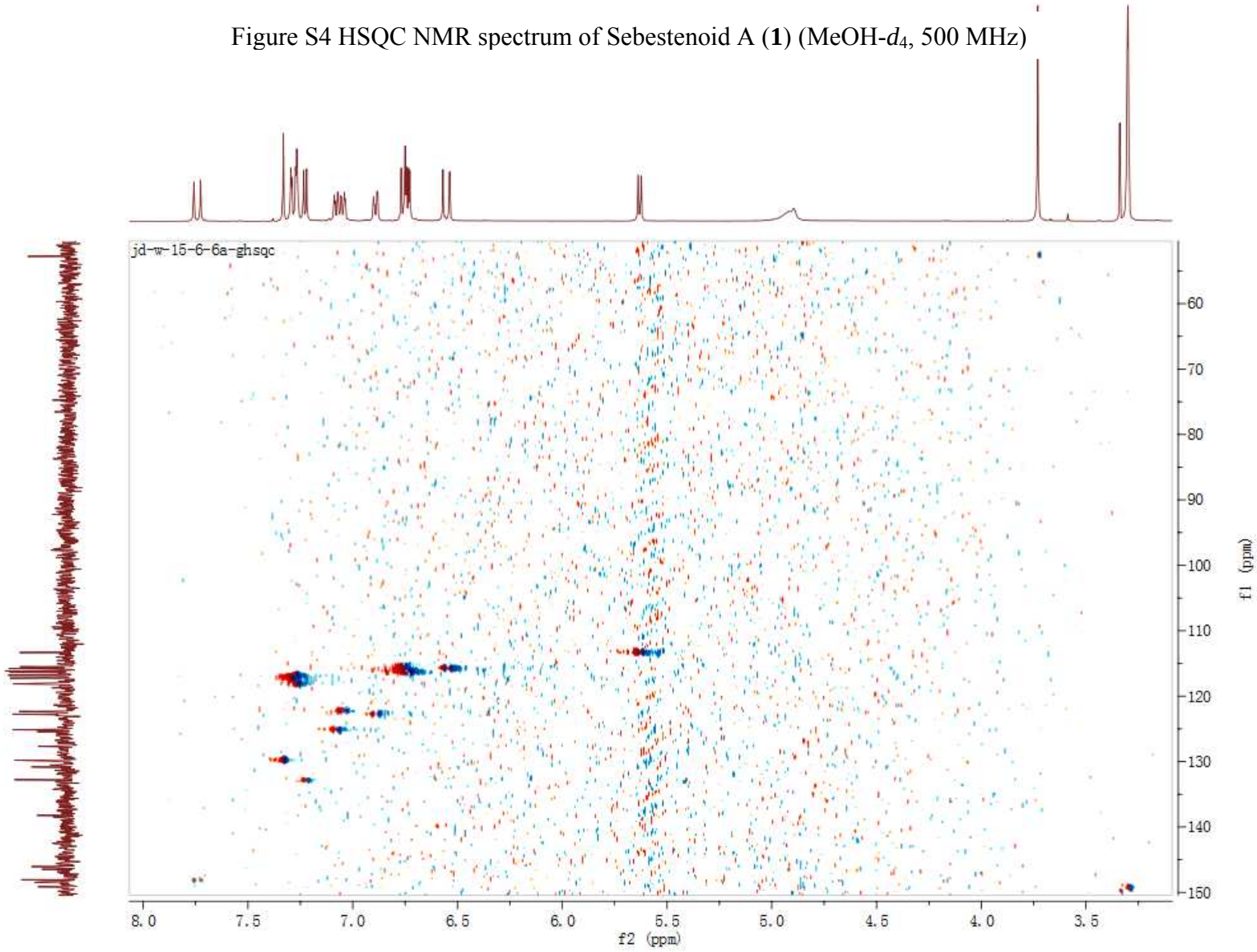


Figure S5 Expansion of HSQC NMR spectrum of Sebestenoid A (**1**) (MeOH-d_4, 500 MHz)

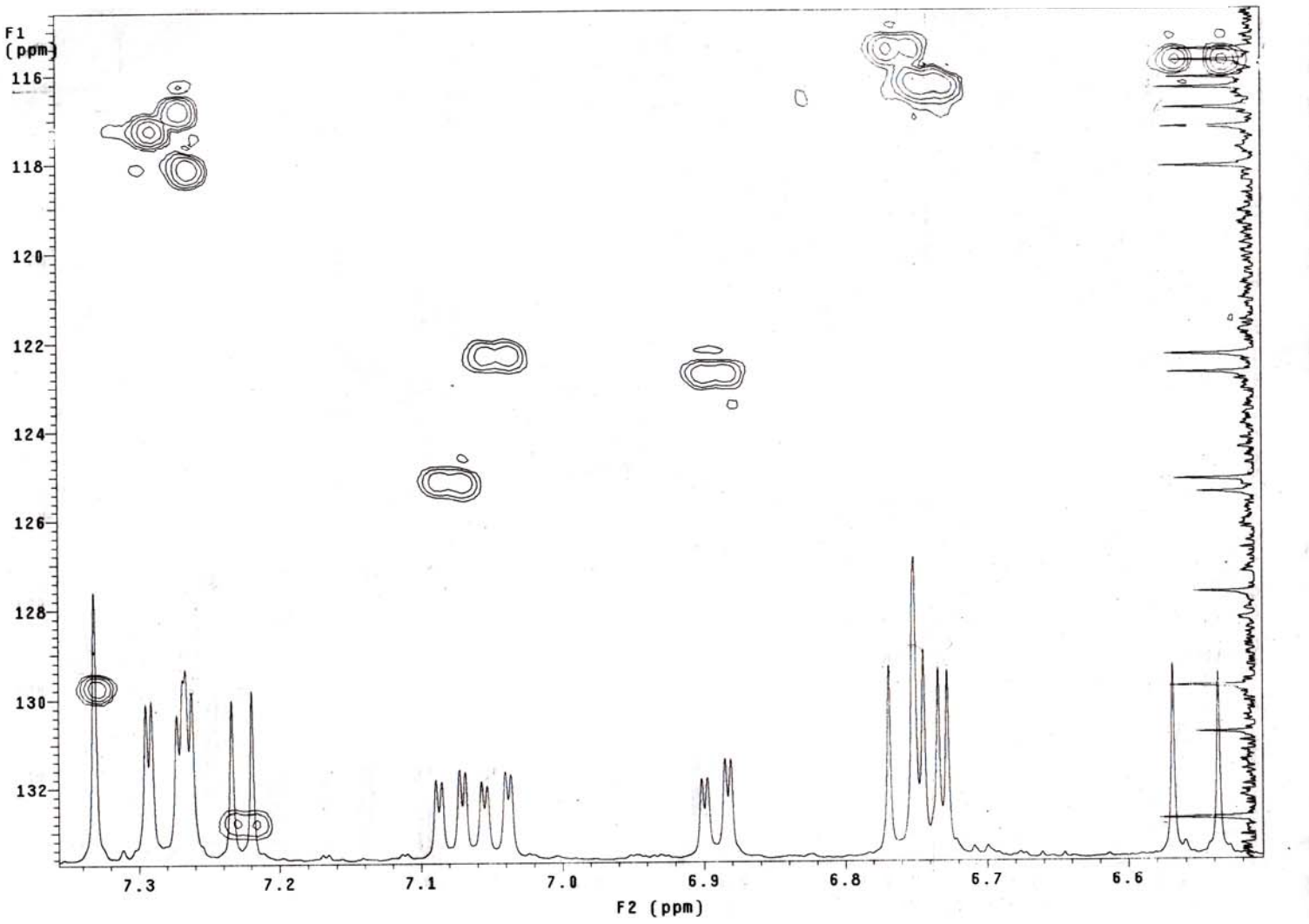


Figure S6 HMBC NMR spectrum of Sebestenoid A (**1**) (MeOH-d_4, 500 MHz)

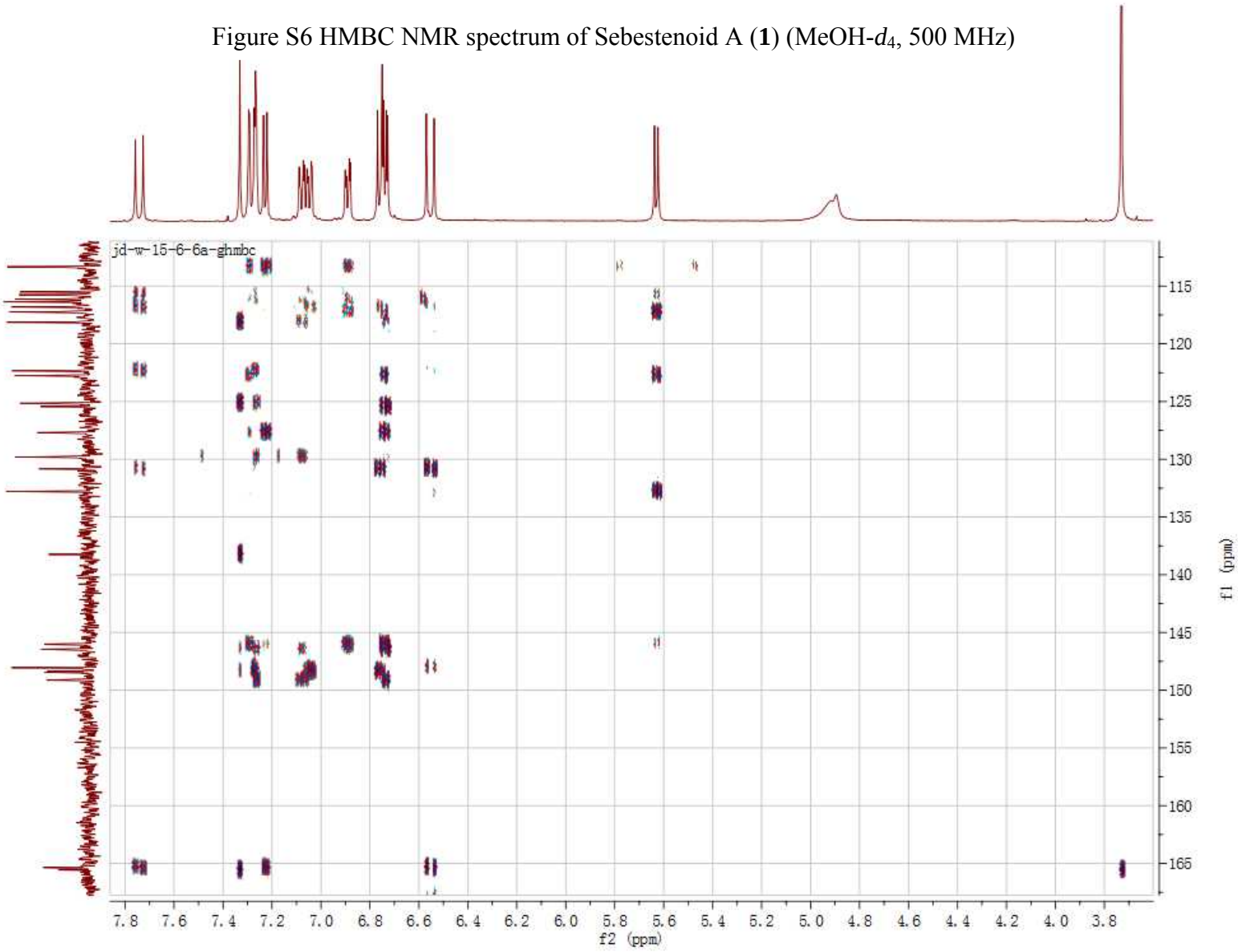
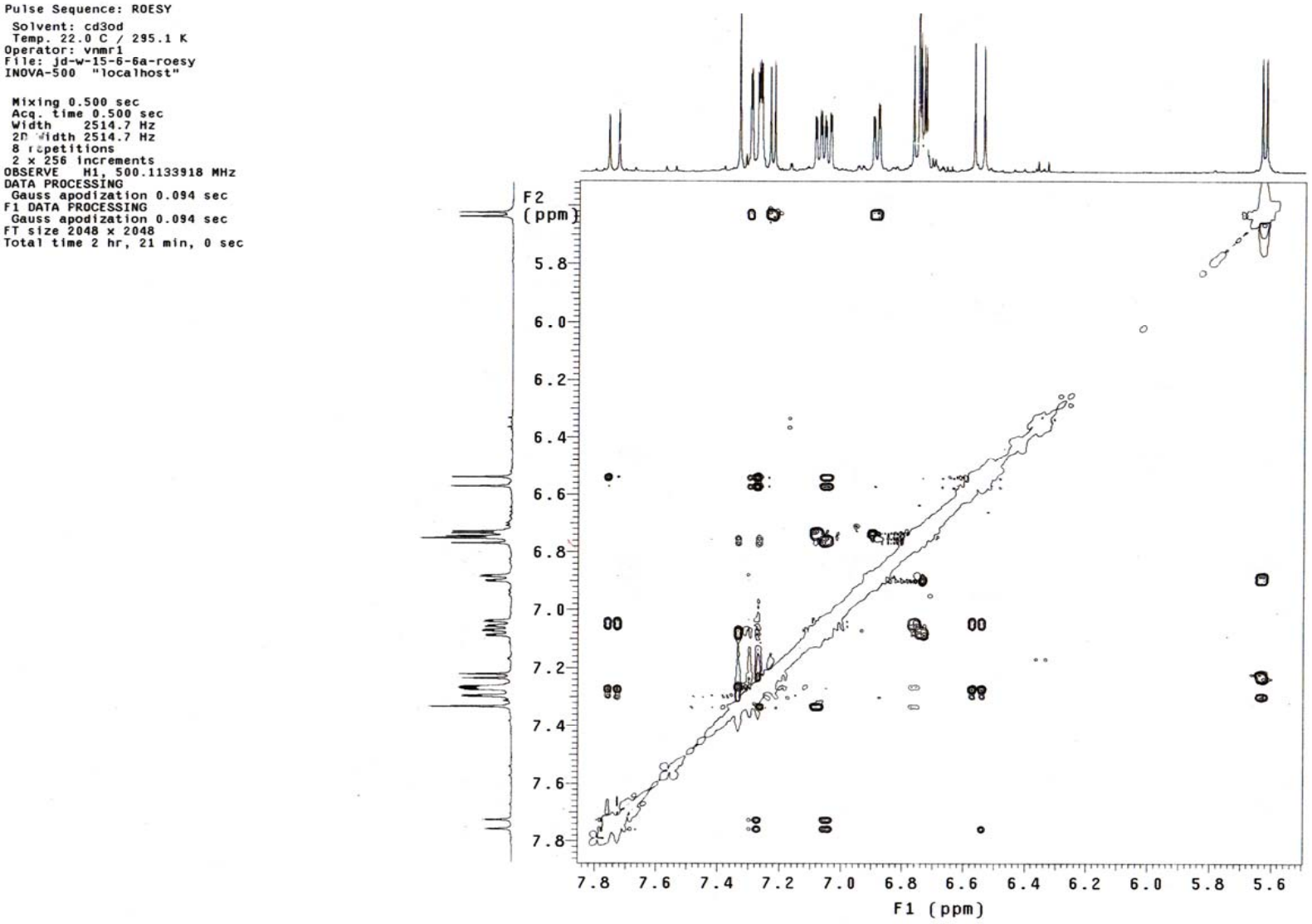


Figure S7 ROESY NMR spectrum of Sebestenoid A (**1**) (MeOH-d_4, 500 MHz)



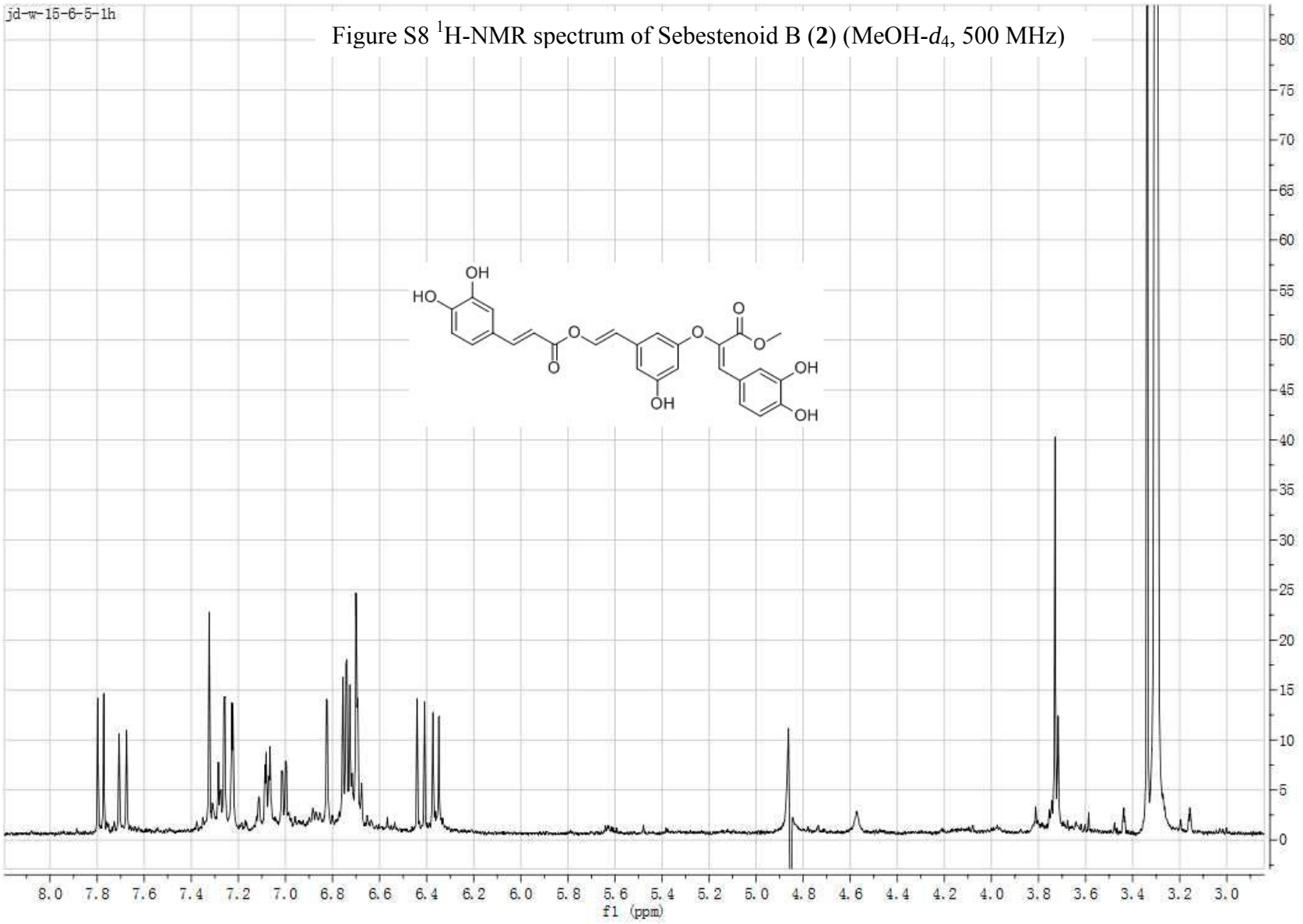


Figure S8 ^{1}H-NMR spectrum of Sebestenoid B (**2**) (MeOH-d_4, 500 MHz)

Figure S9 ^{13}C-NMR spectrum of Sebestenoid B (**2**) (MeOH-d_4, 125 MHz)

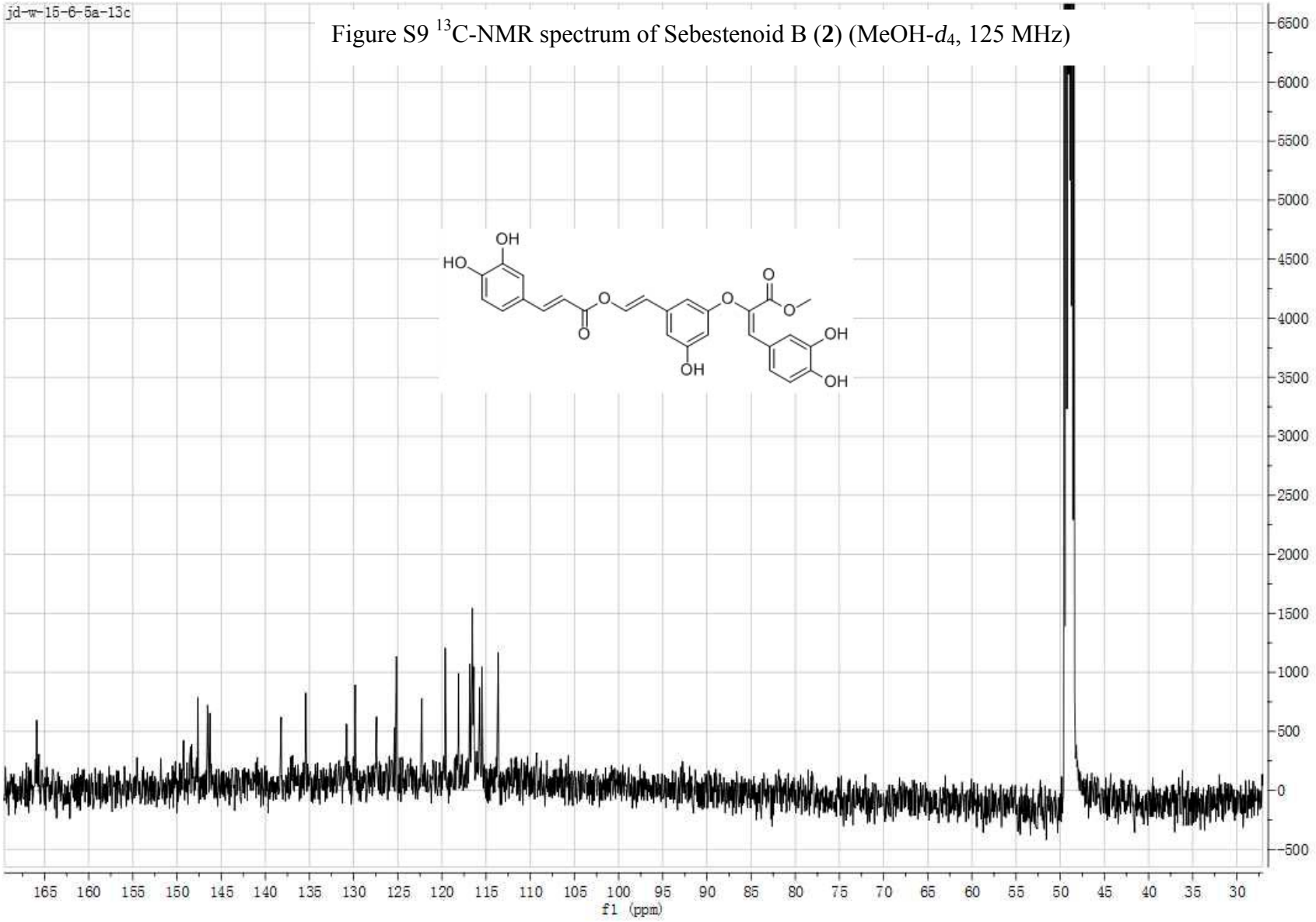


Figure S10 COSY NMR spectrum of Sebestenoid B (**2**) (MeOH-d_4, 500 MHz)

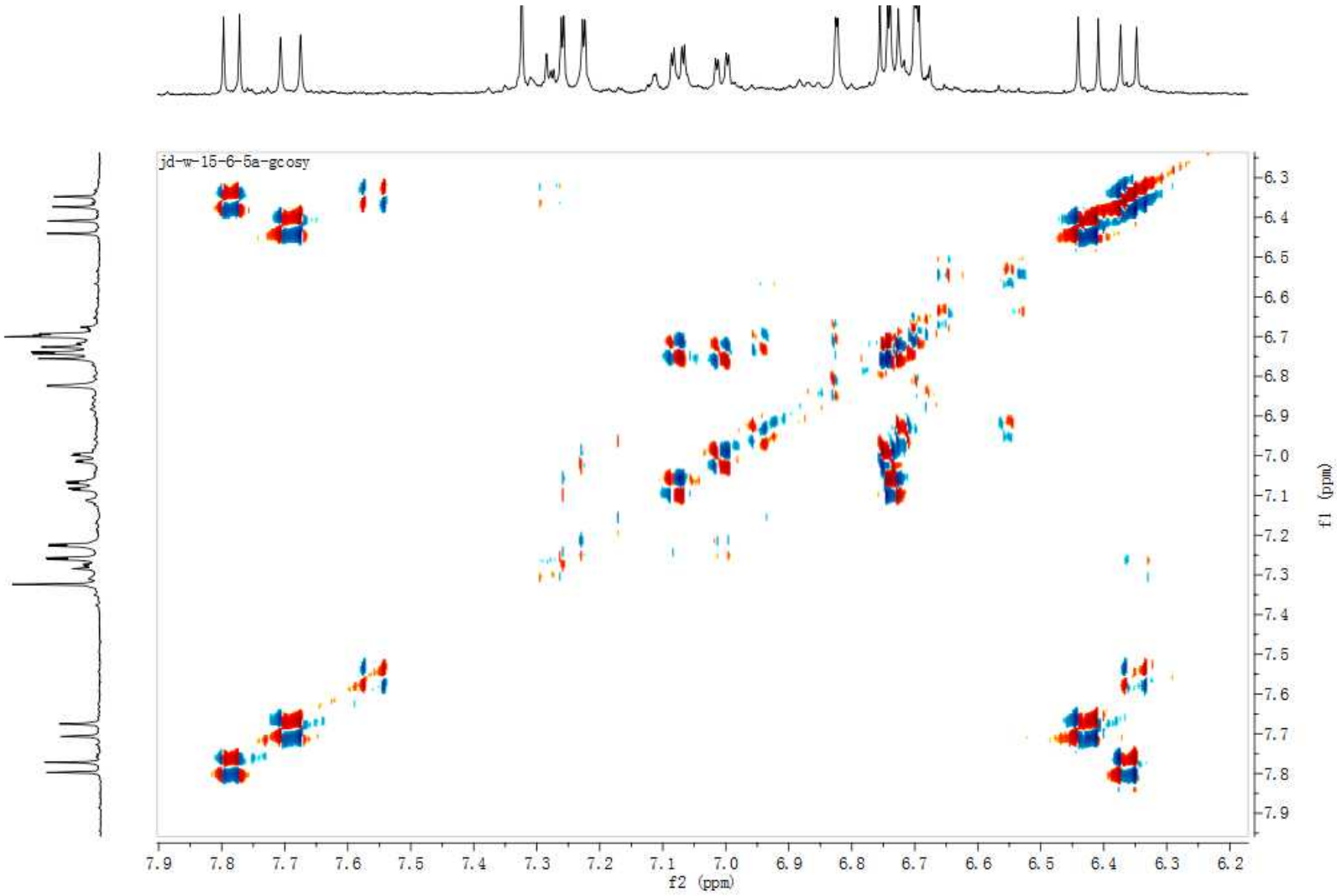


Figure S11 HSQC NMR spectrum of Sebestenoid B (**2**) (MeOH-d_4, 500 MHz)

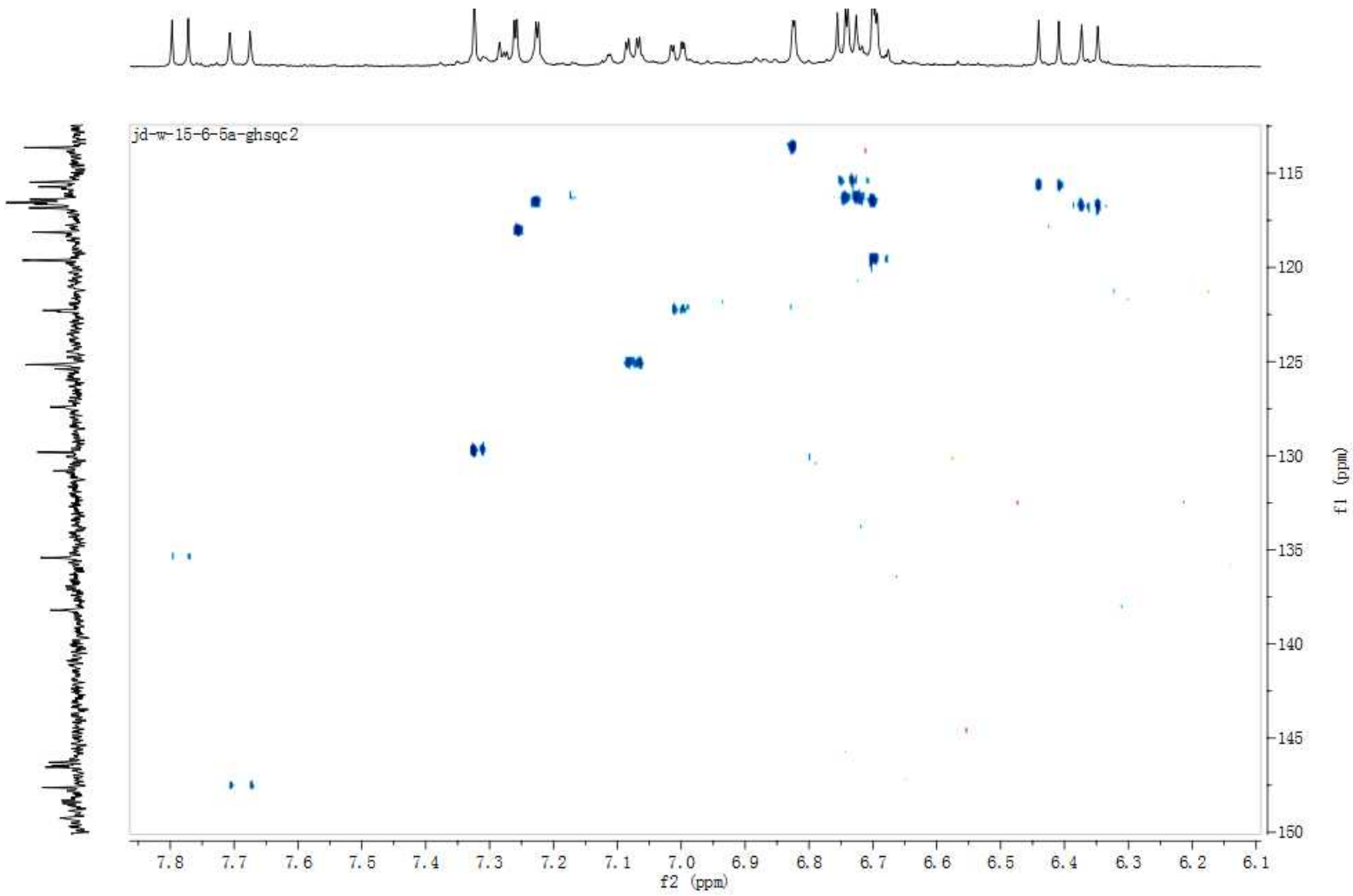


Figure S12 HMBC NMR spectrum of Sebestenoid B (**2**) (MeOH-d_4, 500 MHz)

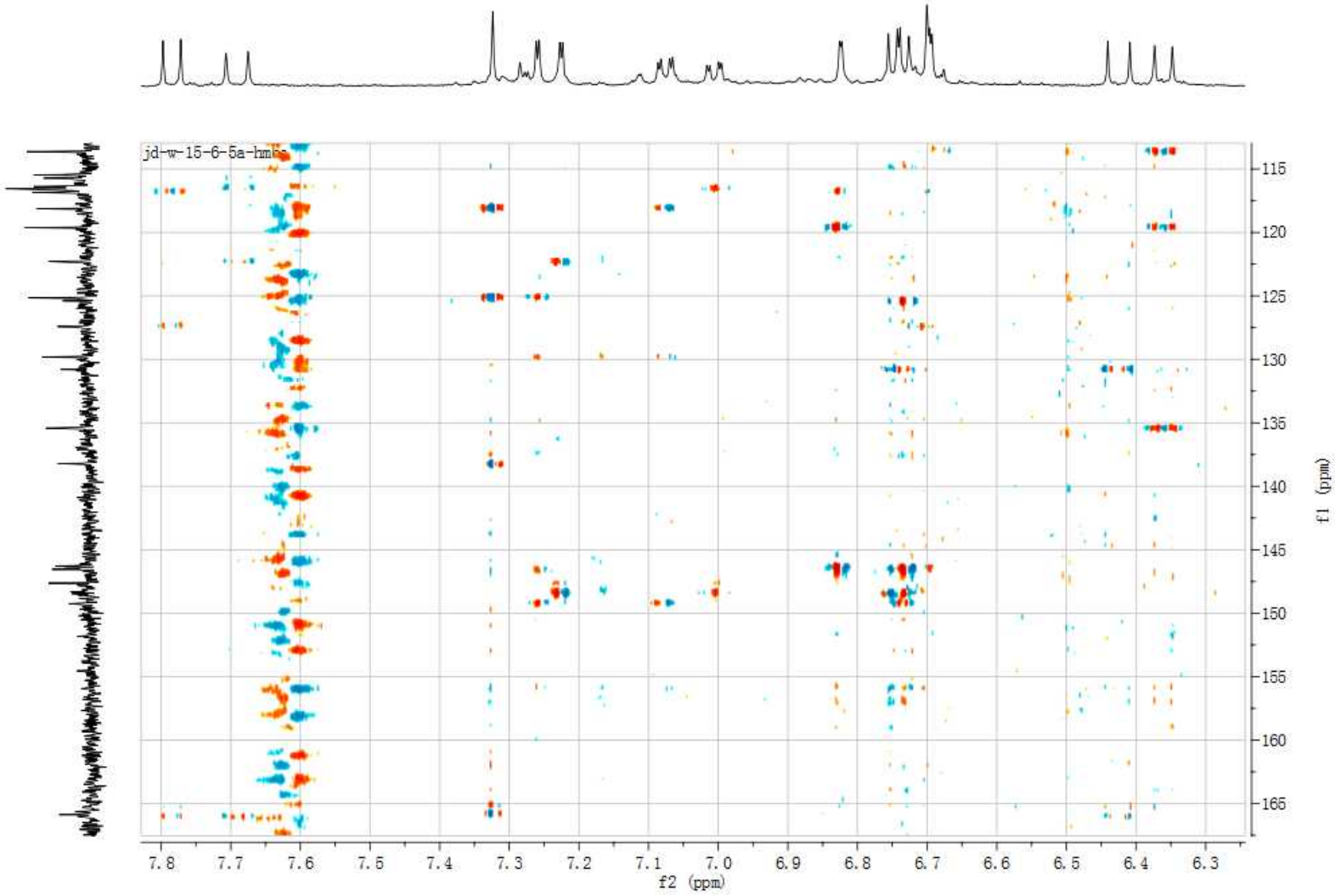


Figure S13 ROESY NMR spectrum of Sebestenoid B (**2**) (MeOH-d_4, 500 MHz)

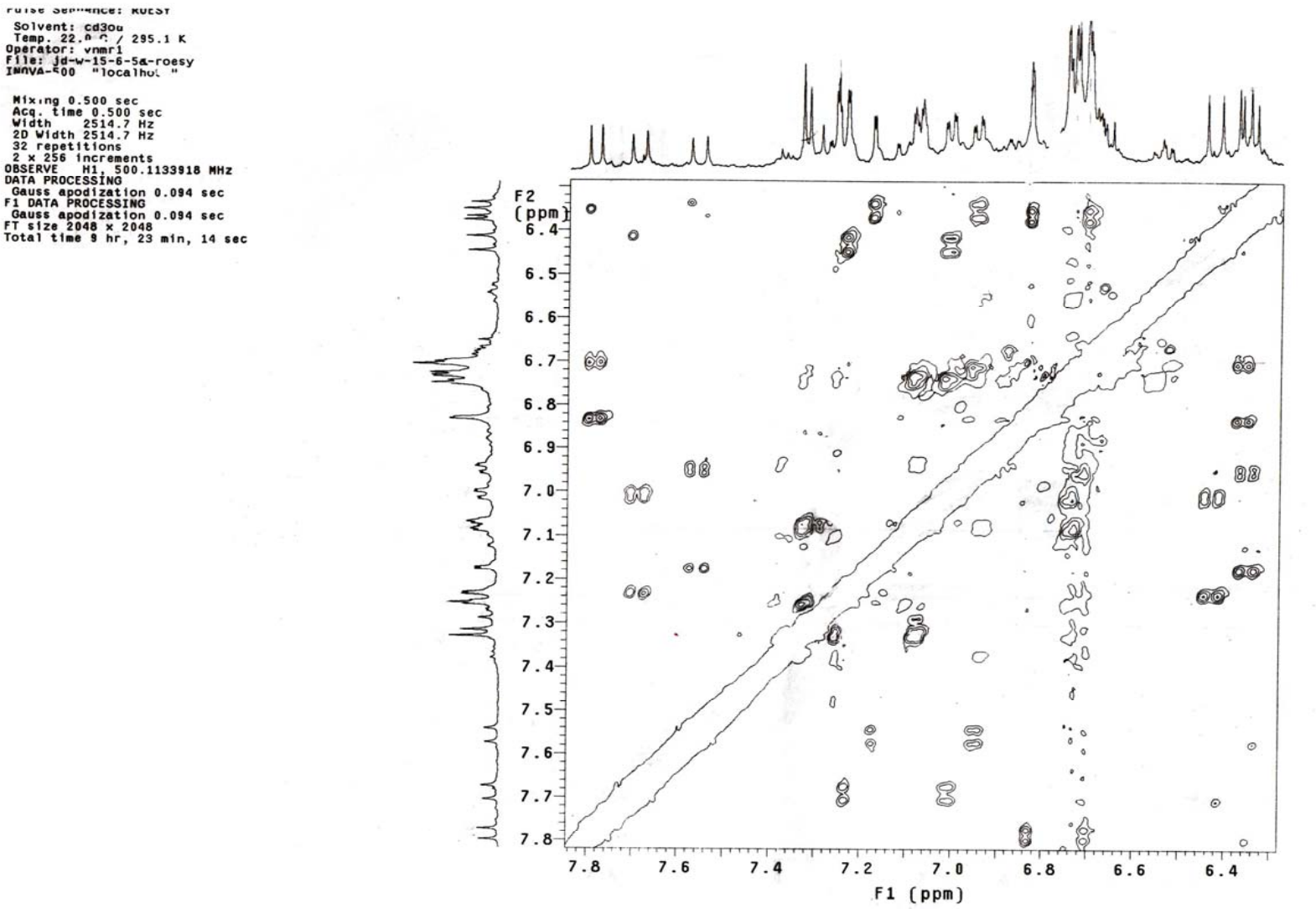


Figure S14 ^{1}H-NMR spectrum of Sebestenoid C (**3**) (MeOH-d_4, 500 MHz)

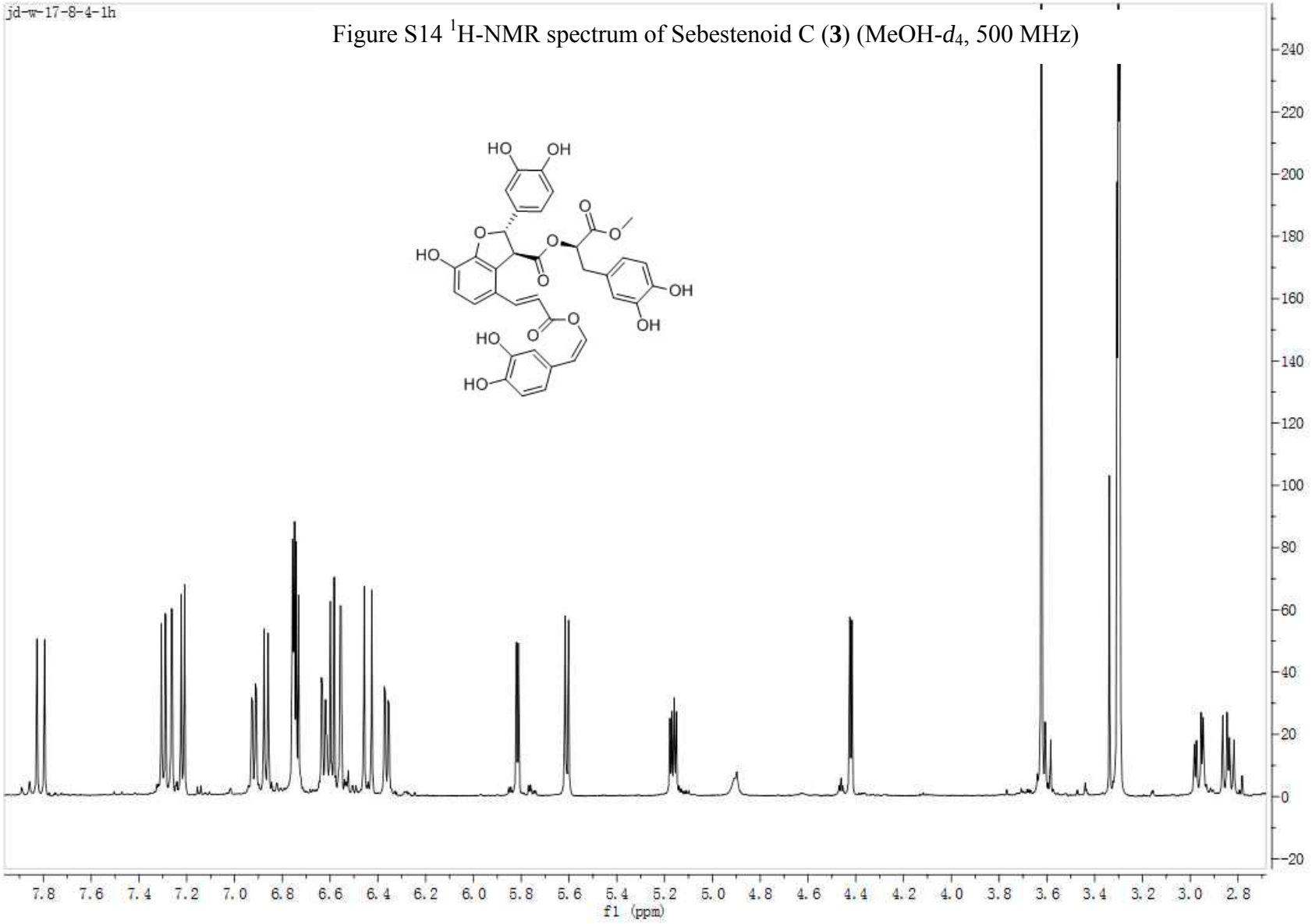


Figure S15 ^{13}C-NMR spectrum of Sebestenoid C (**3**) (MeOH-d_4, 125 MHz)

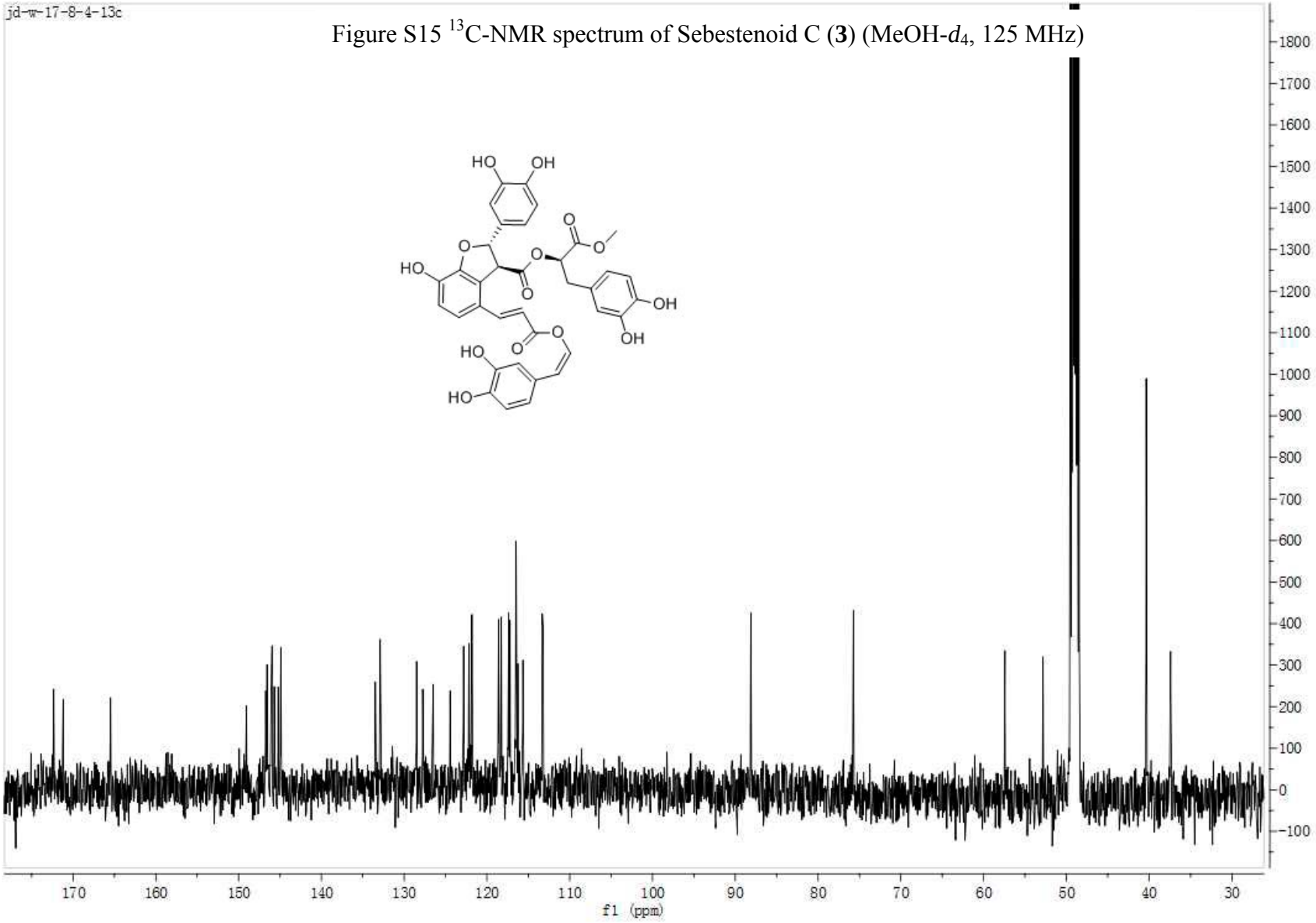


Figure S16 COSY NMR spectrum of Sebestenoid C (**3**) (MeOH-d_4, 500 MHz)

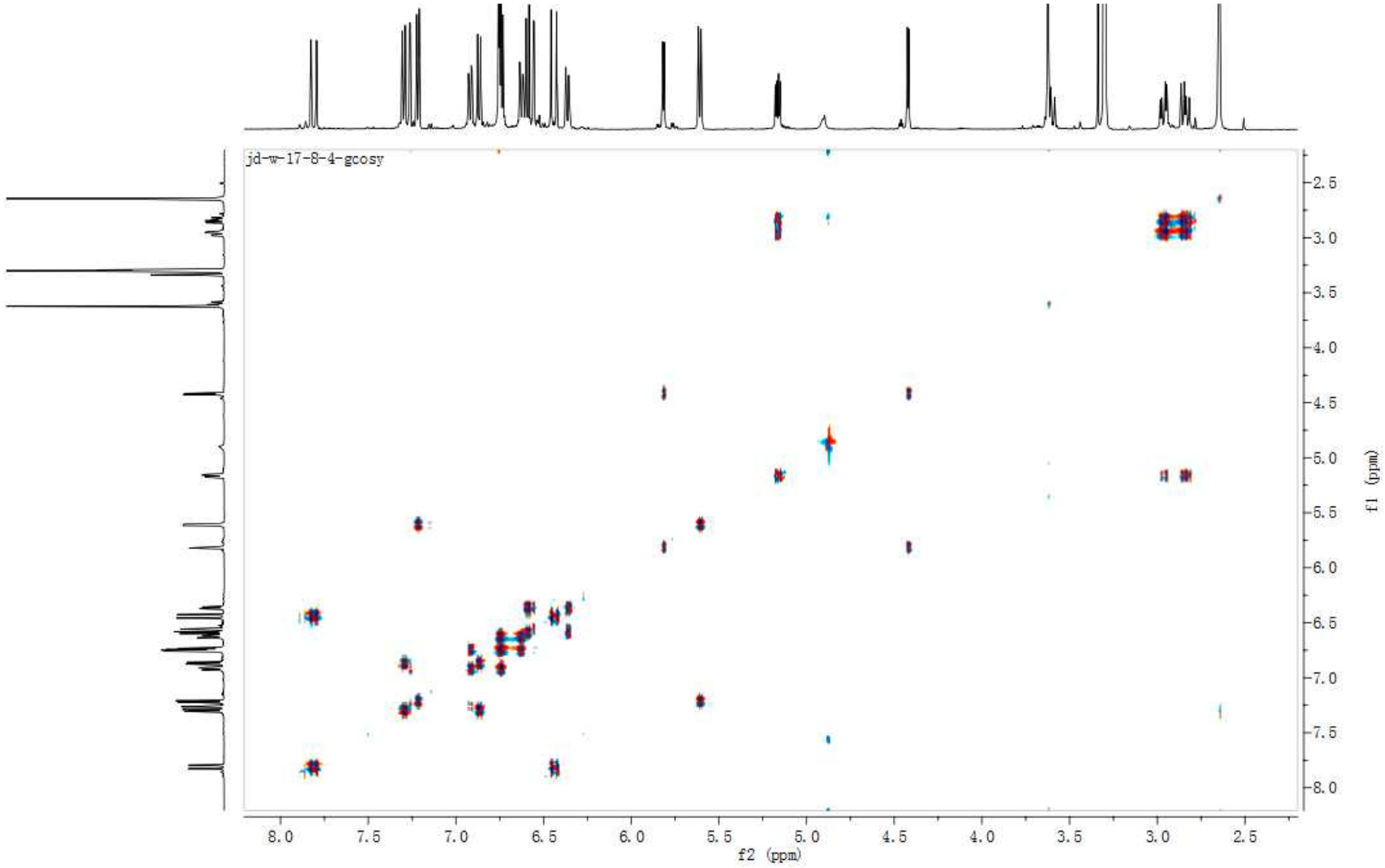


Figure S17 HSQC NMR spectrum of Sebestenoid C (**3**) (MeOH-d_4, 500 MHz)

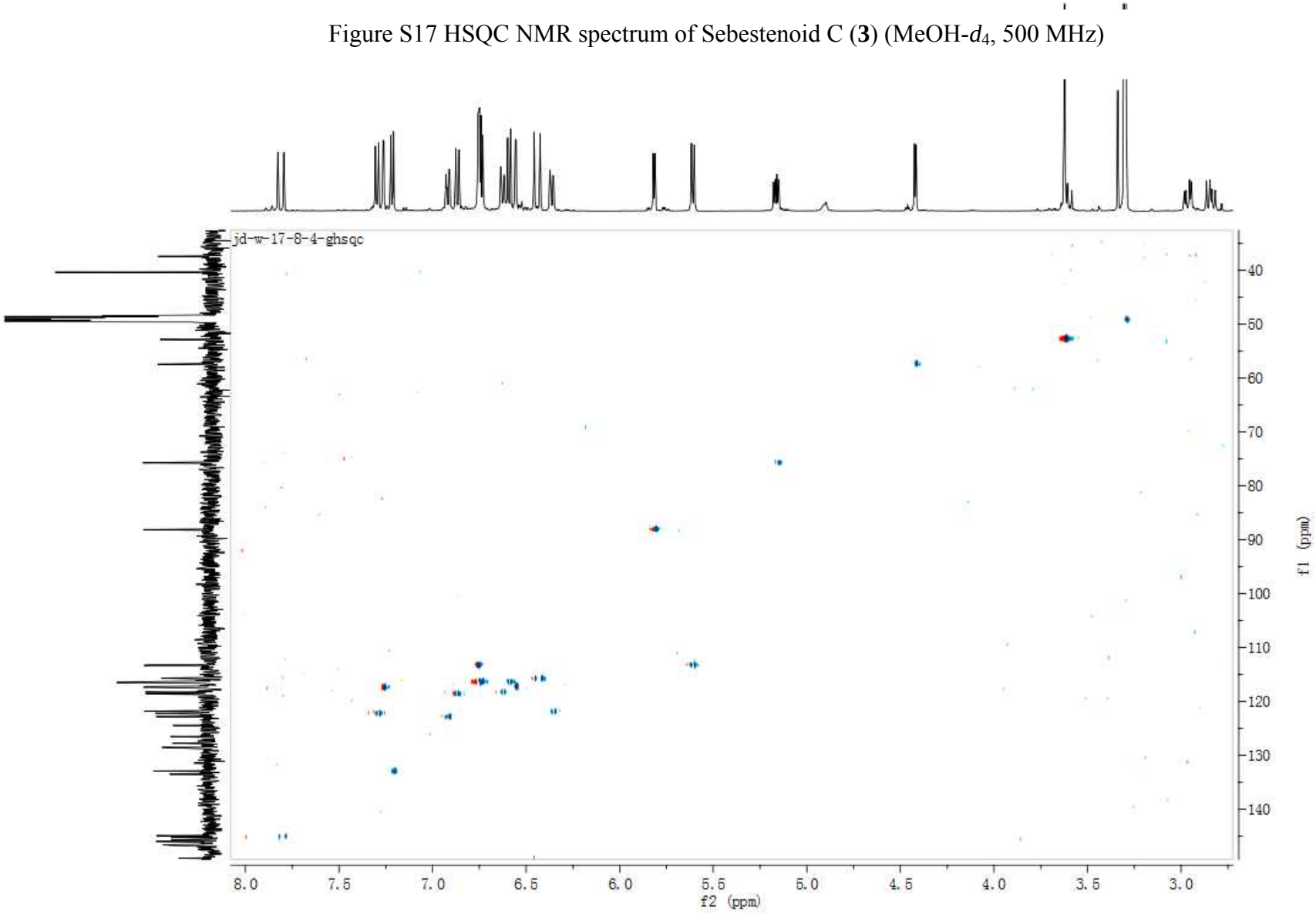


Figure S18 Expansion of HSQC NMR spectrum of Sebestenoid C (**3**) (MeOH-d_4, 500 MHz)

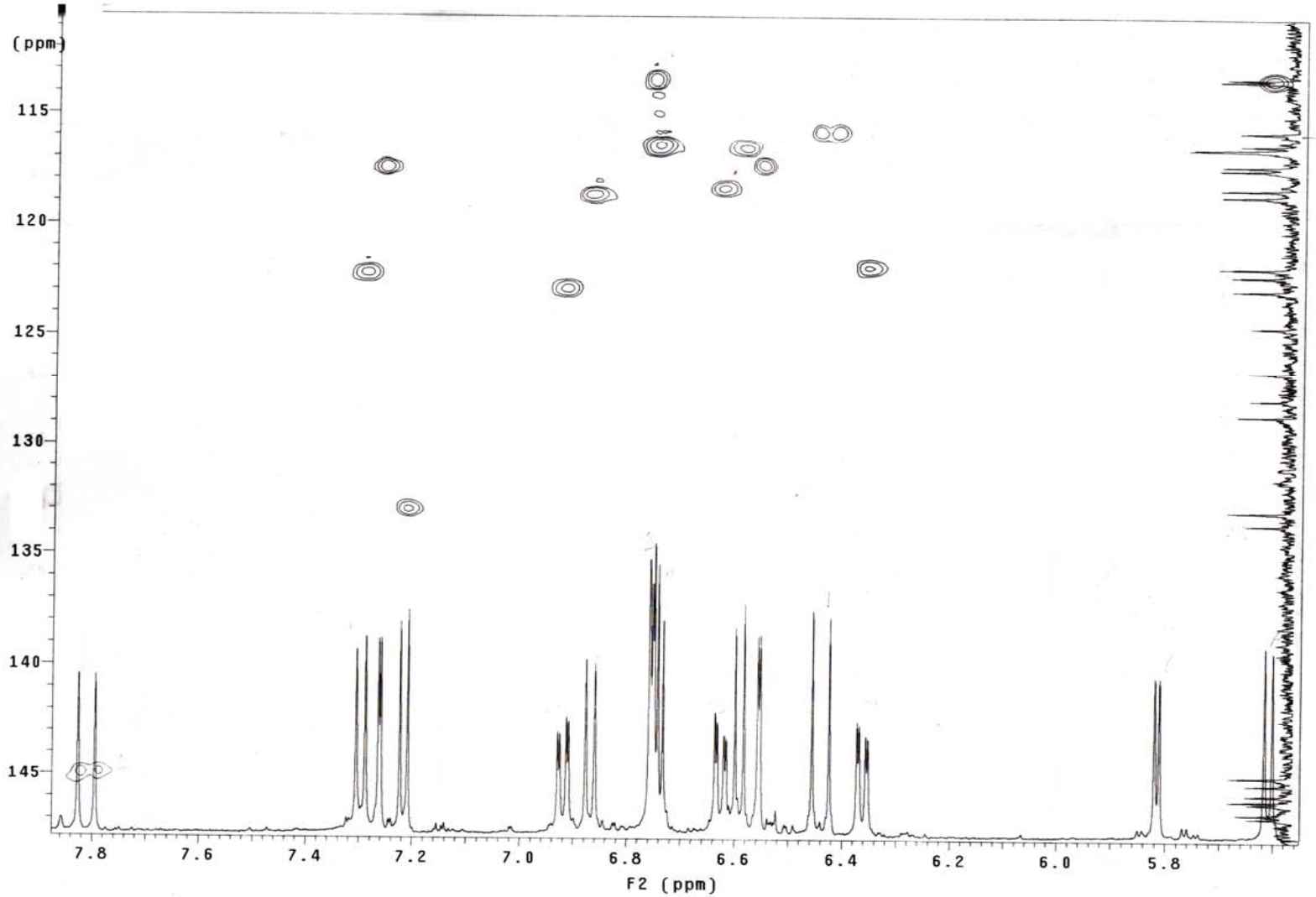


Figure S19 HMBC NMR spectrum of Sebestenoid C (**3**) (MeOH-d_4, 500 MHz)

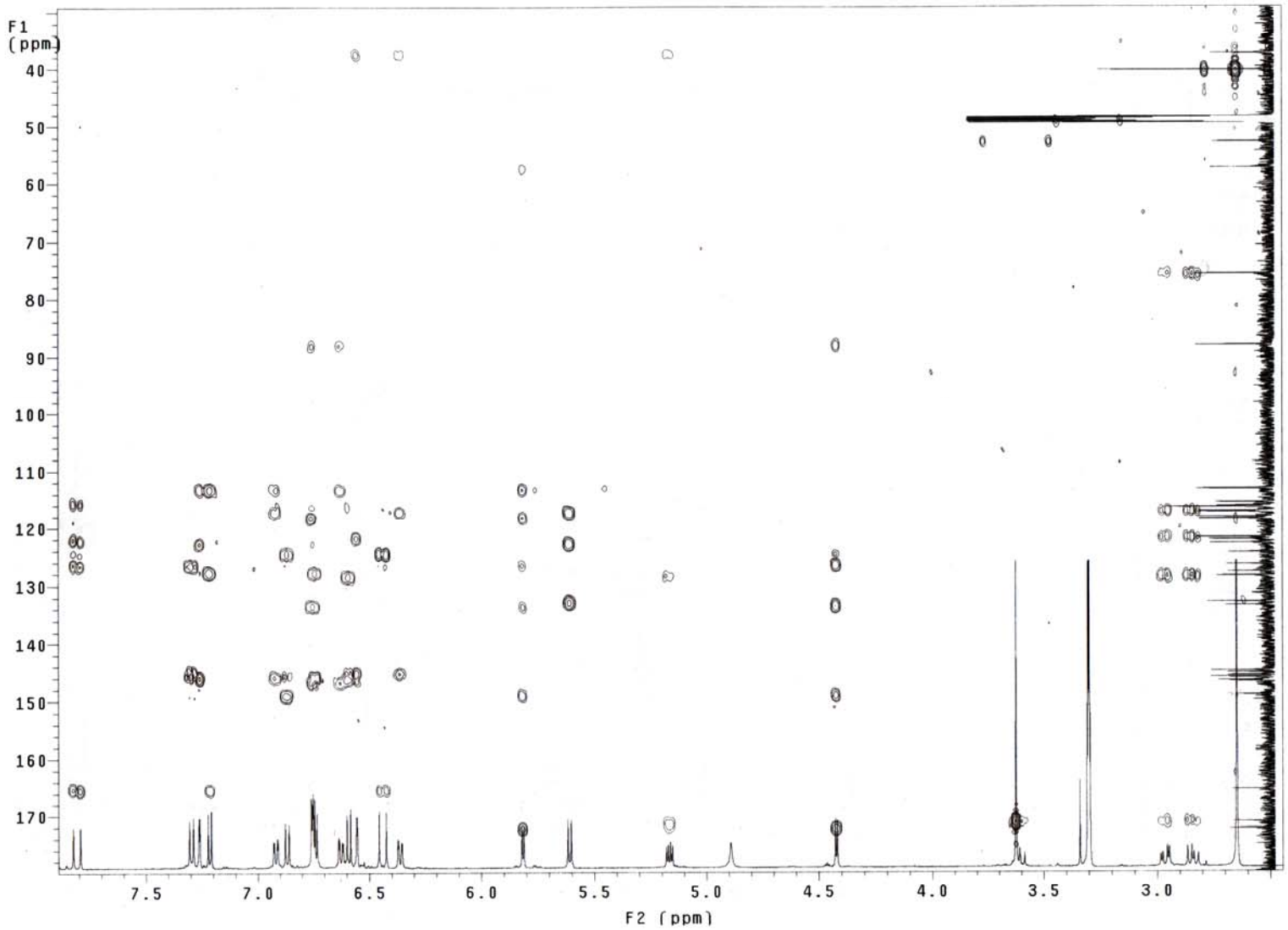


Figure S20 ROESY NMR spectrum of Sebestenoid C (**3**) (MeOH-d_4, 500 MHz)

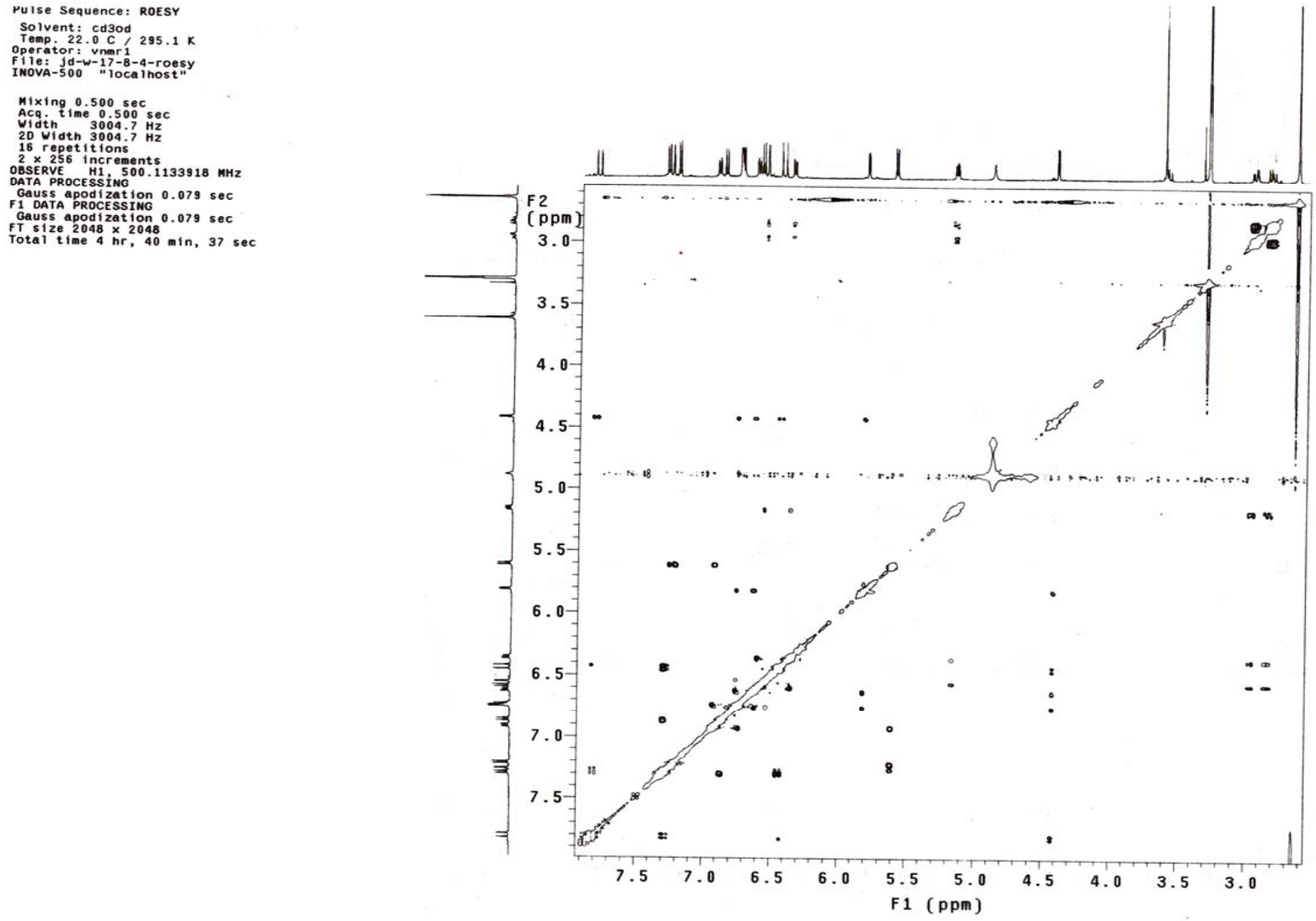


Figure S21 ^{1}H-NMR spectrum of Sebestenoid D (**4**) (MeOH-d_4, 500 MHz)

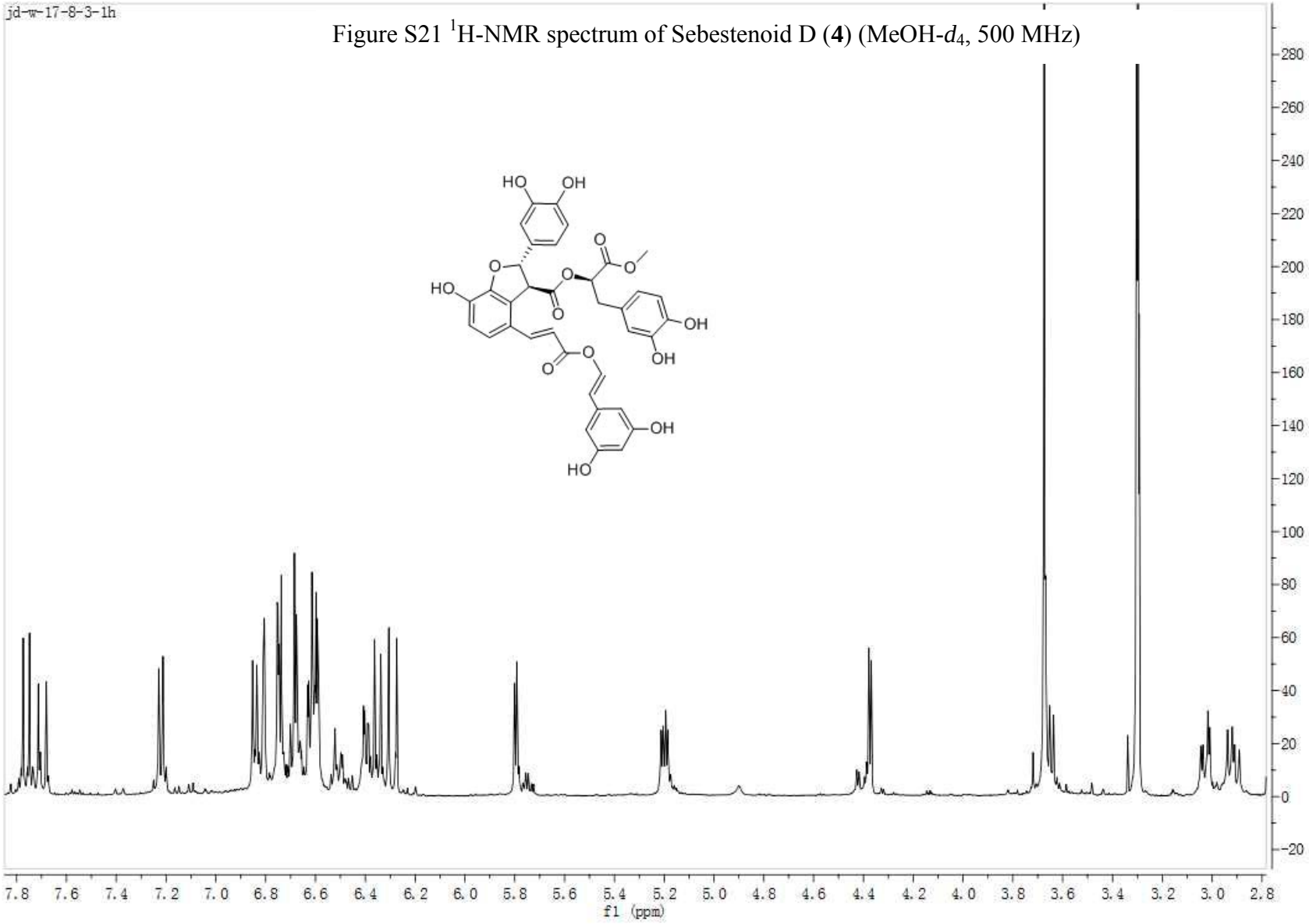


Figure S22 ^{13}C-NMR spectrum of Sebestenoid D (**4**) (MeOH-d_4, 125 MHz)

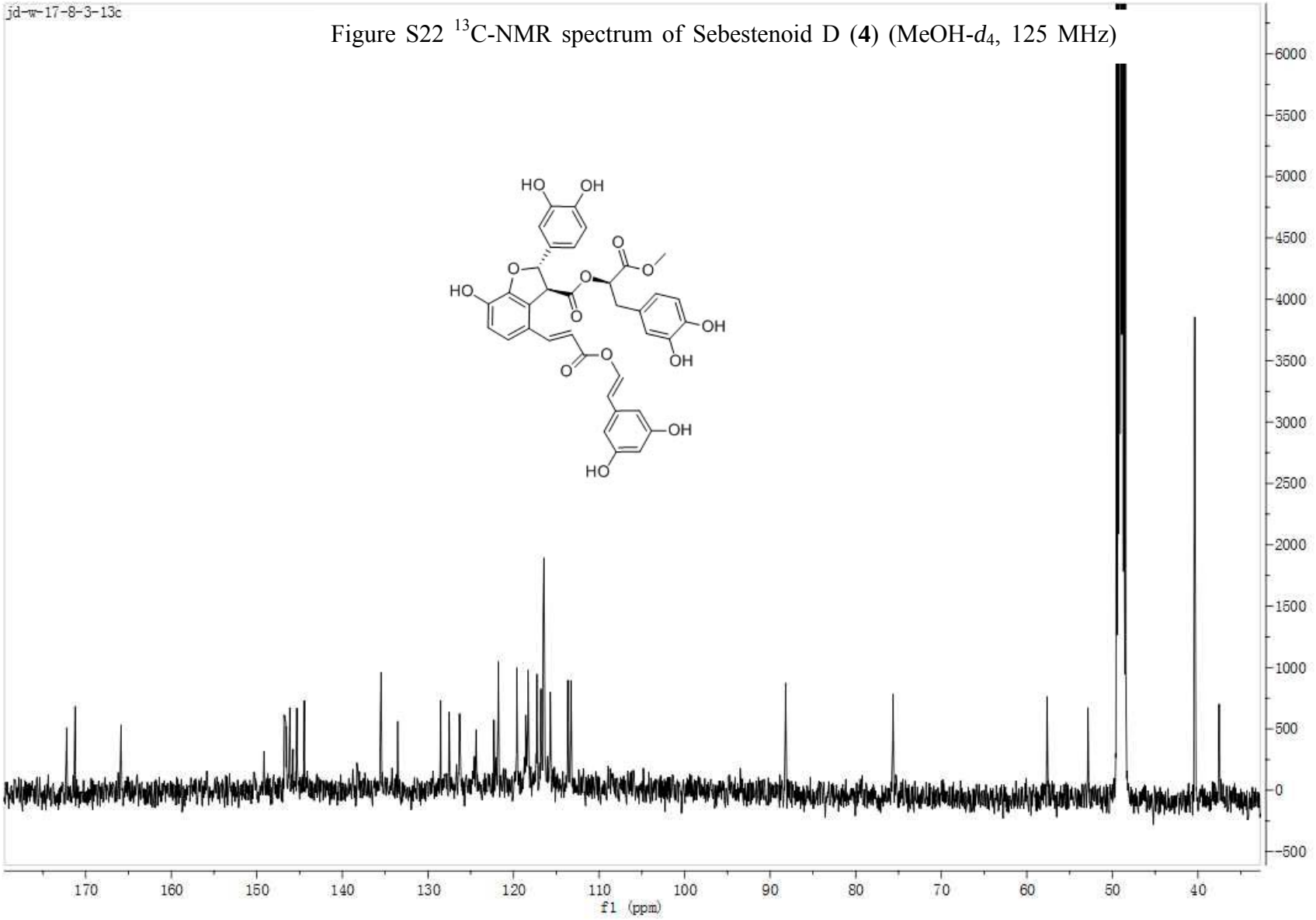


Figure S23 COSY NMR spectrum of Sebestenoid D (**4**) (MeOH-d_4, 500 MHz)

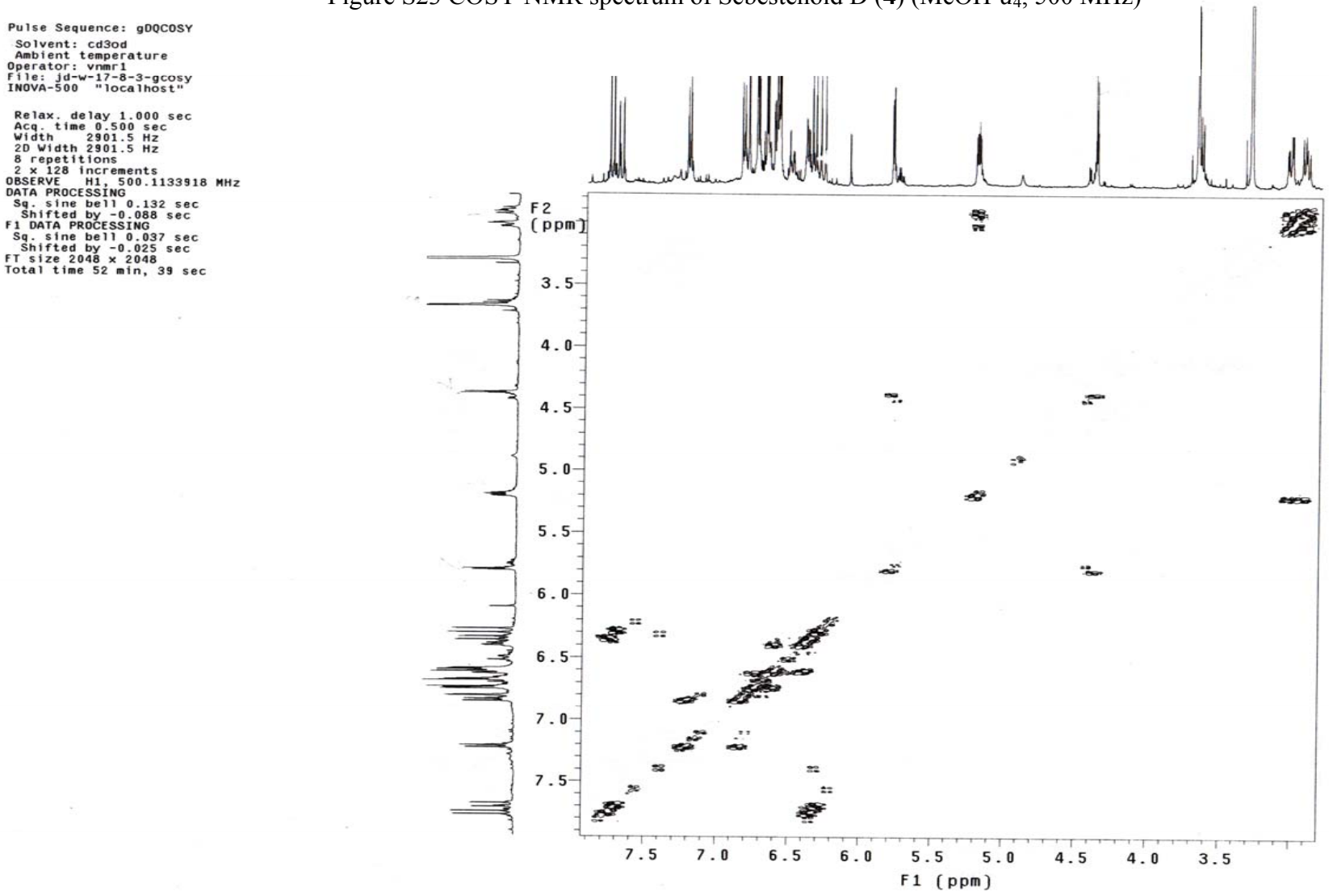


Figure S24 HSQC NMR spectrum of Sebestenoid D (**4**) (MeOH-d_4, 500 MHz)

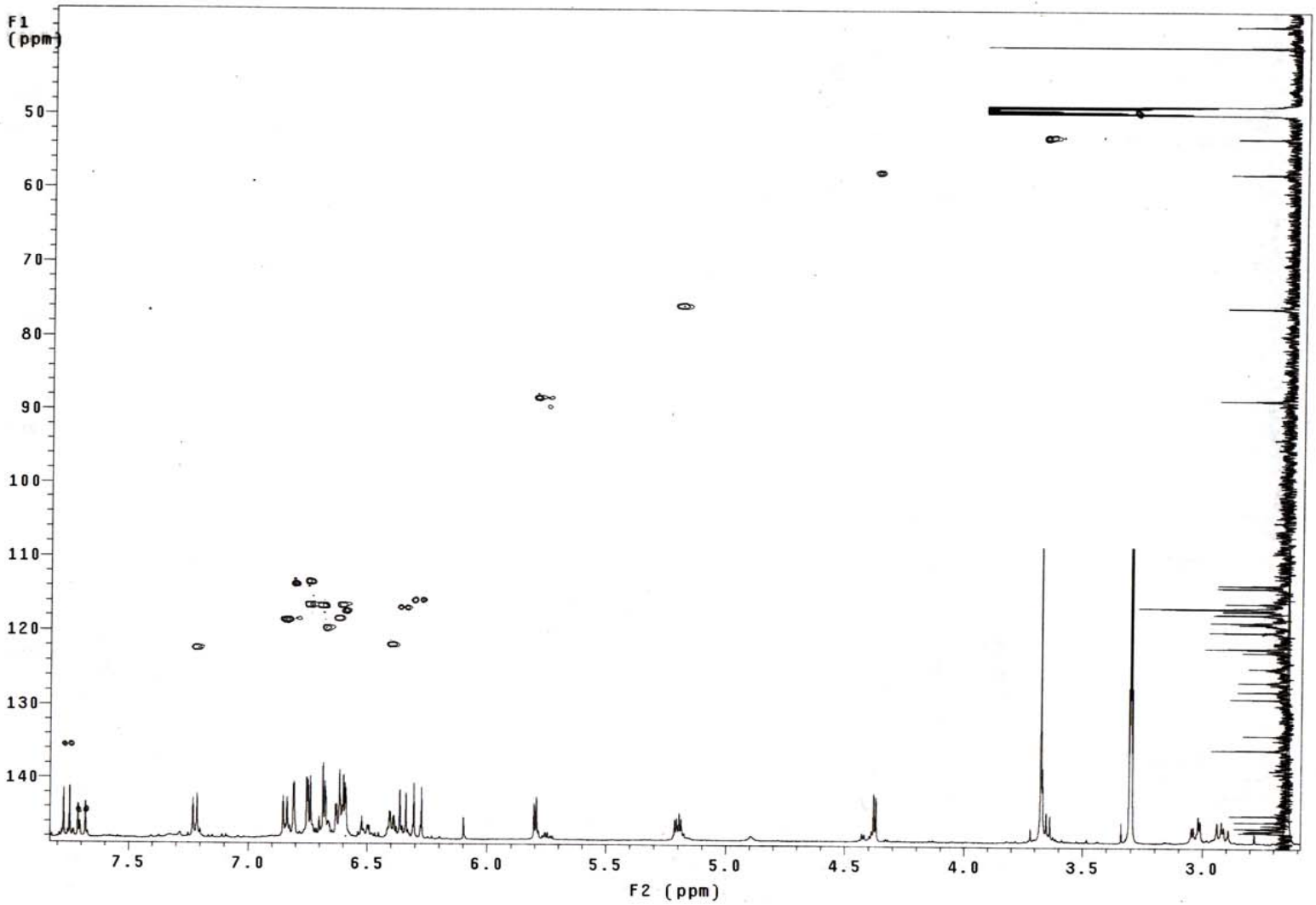


Figure S25 HMBC NMR spectrum of Sebestenoid D (**4**) (MeOH-d_4, 500 MHz)

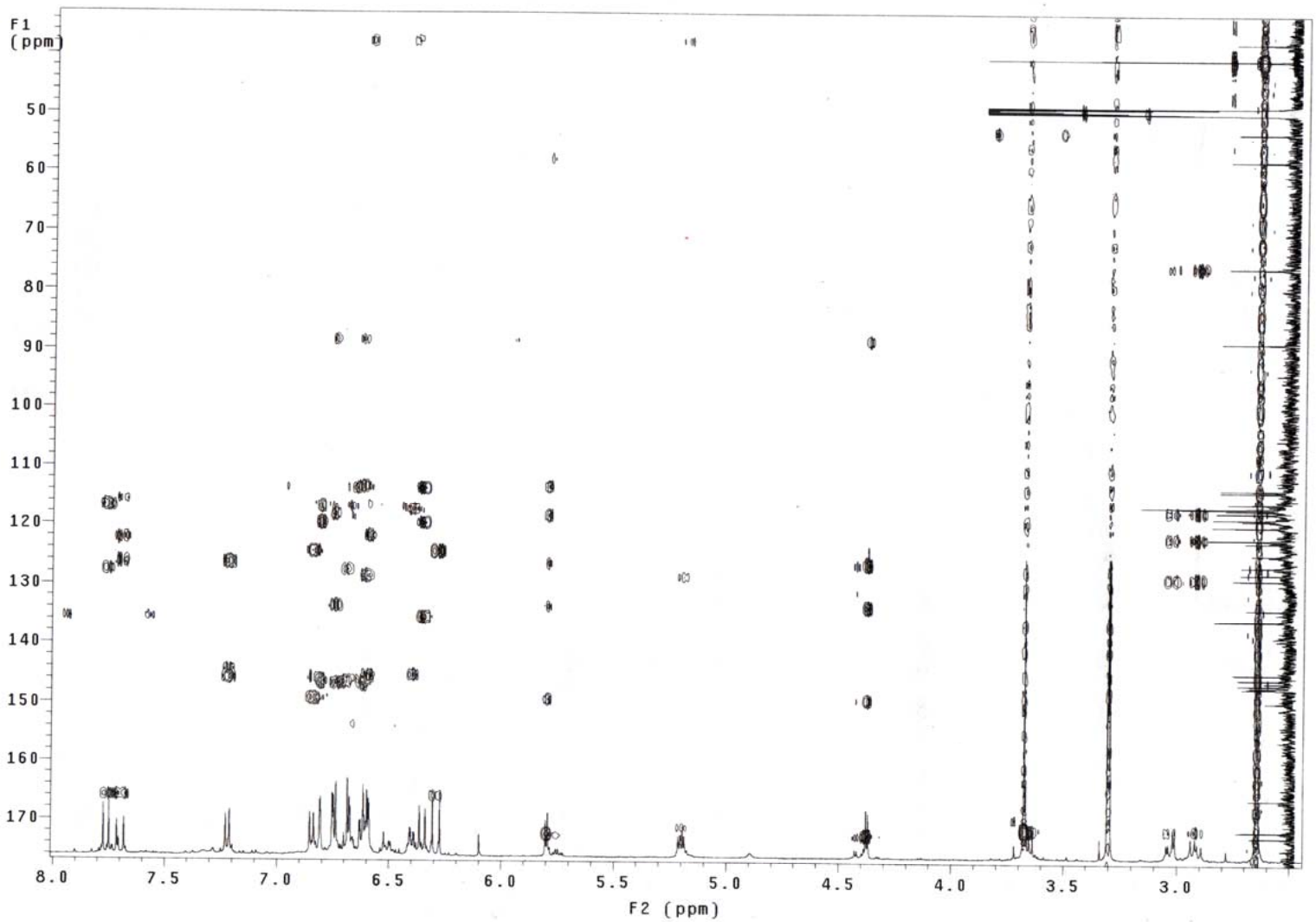


Figure S26 ROESY NMR spectrum of Sebestenoid D (**4**) (MeOH-d_4, 500 MHz)

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Pulse Sequence: ROESY
 Solvent: cd3od
 Ambient temperature
Operator: vnmr1
File: jd-w-17-8-3-roesy
INOVA-500  "localhost"

 Mixing 0.500 sec
 Acq. time 0.500 sec
 Width    2901.5 Hz
 2D Width 2901.5 Hz
 16 repetitions
 2 x 256 increments
OBSERVE   H1, 500.1133918 MHz
DATA PROCESSING
 Gauss apodization 0.082 sec
F1 DATA PROCESSING
 Gauss apodization 0.081 sec
FT size 2048 x 2048
Total time 4 hr, 40 min, 51 sec
```