

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

Jingqiu Dai^a, Analia Sorribas^a, Wesley Y. Yoshida^a, and Philip G. Williams^{a,b,*}

^a *Department of Chemistry, University of Hawaii at Manoa, Honolulu, Hawaii, USA, 96822*

^b *The Cancer Research Center of Hawaii, 651 Ilalo Street, Honolulu, Hawaii, USA, 96813*

*Corresponding author. Tel. +1 808 956 5720; Fax: +1 808 956 5908. *E-Mail address:* philipwi@hawaii.edu (P.G. Williams)

| List of Supporting Information | Page |
|--|-------------|
| Table S1 NMR Spectroscopic Data (500 MHz) in MeOH- <i>d</i> ₄ for Sebestenoid A (1) | 3 |
| Table S2 NMR Spectroscopic Data (500 MHz) in MeOH- <i>d</i> ₄ for Sebestenoid B (2) | 4 |
| Table S3 NMR Spectroscopic Data (500 MHz) in MeOH- <i>d</i> ₄ for Sebestenoid C (3) | 5 |
| Table S4 NMR Spectroscopic Data (500 MHz) in MeOH- <i>d</i> ₄ for Sebestenoid D (4) | 6 |
| Figure S1 ¹ H-NMR spectrum of Sebestenoid A (1) (MeOH- <i>d</i> ₄ , 500 MHz) | 7 |
| Figure S2 ¹³ C-NMR spectrum of Sebestenoid A (1) (MeOH- <i>d</i> ₄ , 125 MHz) | 8 |
| Figure S3 COSY NMR spectrum of Sebestenoid A (1) (MeOH- <i>d</i> ₄ , 500 MHz) | 9 |
| Figure S4 HSQC NMR spectrum of Sebestenoid A (1) (MeOH- <i>d</i> ₄ , 500 MHz) | 10 |
| Figure S5 Expansion of HSQC NMR spectrum of Sebestenoid A (1) (MeOH- <i>d</i> ₄ , 500 MHz) | 11 |
| Figure S6 HMBC NMR spectrum of Sebestenoid A (1) (MeOH- <i>d</i> ₄ , 500 MHz) | 12 |
| Figure S7 ROESY NMR spectrum of Sebestenoid A (1) (MeOH- <i>d</i> ₄ , 500 MHz) | 13 |
| Figure S8 ¹ H-NMR spectrum of Sebestenoid B (2) (MeOH- <i>d</i> ₄ , 500 MHz) | 14 |
| Figure S9 ¹³ C-NMR spectrum of Sebestenoid B (2) (MeOH- <i>d</i> ₄ , 125 MHz) | 15 |
| Figure S10 COSY NMR spectrum of Sebestenoid B (2) (MeOH- <i>d</i> ₄ , 500 MHz) | 16 |
| Figure S11 HSQC NMR spectrum of Sebestenoid B (2) (MeOH- <i>d</i> ₄ , 500 MHz) | 17 |
| Figure S12 HMBC NMR spectrum of Sebestenoid B (2) (MeOH- <i>d</i> ₄ , 500 MHz) | 18 |
| Figure S13 ROESY NMR spectrum of Sebestenoid B (2) (MeOH- <i>d</i> ₄ , 500 MHz) | 19 |
| Figure S14 ¹ H-NMR spectrum of Sebestenoid C (3) (MeOH- <i>d</i> ₄ , 500 MHz) | 20 |
| Figure S15 ¹³ C-NMR spectrum of Sebestenoid C (3) (MeOH- <i>d</i> ₄ , 125 MHz) | 21 |
| Figure S16 COSY NMR spectrum of Sebestenoid C (3) (MeOH- <i>d</i> ₄ , 500 MHz) | 22 |
| Figure S17 HSQC NMR spectrum of Sebestenoid C (3) (MeOH- <i>d</i> ₄ , 500 MHz) | 23 |
| Figure S18 Expansion of HSQC NMR spectrum of Sebestenoid C (3) (MeOH- <i>d</i> ₄ , 500 MHz) | 24 |
| Figure S19 HMBC NMR spectrum of Sebestenoid C (3) (MeOH- <i>d</i> ₄ , 500 MHz) | 25 |
| Figure S20 ROESY NMR spectrum of Sebestenoid C (3) (MeOH- <i>d</i> ₄ , 500 MHz) | 26 |
| Figure S21 ¹ H-NMR spectrum of Sebestenoid D (4) (MeOH- <i>d</i> ₄ , 500 MHz) | 27 |
| Figure S22 ¹³ C-NMR spectrum of Sebestenoid D (4) (MeOH- <i>d</i> ₄ , 125 MHz) | 28 |
| Figure S23 COSY NMR spectrum of Sebestenoid D (4) (MeOH- <i>d</i> ₄ , 500 MHz) | 29 |
| Figure S24 HSQC NMR spectrum of Sebestenoid D (4) (MeOH- <i>d</i> ₄ , 500 MHz) | 30 |
| Figure S25 HMBC NMR spectrum of Sebestenoid D (4) (MeOH- <i>d</i> ₄ , 500 MHz) | 31 |
| Figure S26 ROESY NMR spectrum of Sebestenoid D (4) (MeOH- <i>d</i> ₄ , 500 MHz) | 32 |

Table S1. NMR Spectroscopic Data (500 MHz) in MeOH-*d*₄ for Sebestenoid A (1)

| Position | δ_C , mult. | δ_H (<i>J</i> 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 (<i>J</i> 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 (<i>J</i> 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 (<i>J</i> 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) | H-8''' | | H-2''', H-6''' |
| 8''' | 75.7, CH | 3.02, dd (14.2, 4.0) | | | |
| 9''' | 171.2, qC | 5.19, dd (9.2, 4.0) | H-7''' | | H-2''', H-6''' |
| OCH ₃ | 52.9, CH ₃ | 3.67, s | | H-7''', H-8''', OCH ₃ | |

jd-w-15-6-6a-1h

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

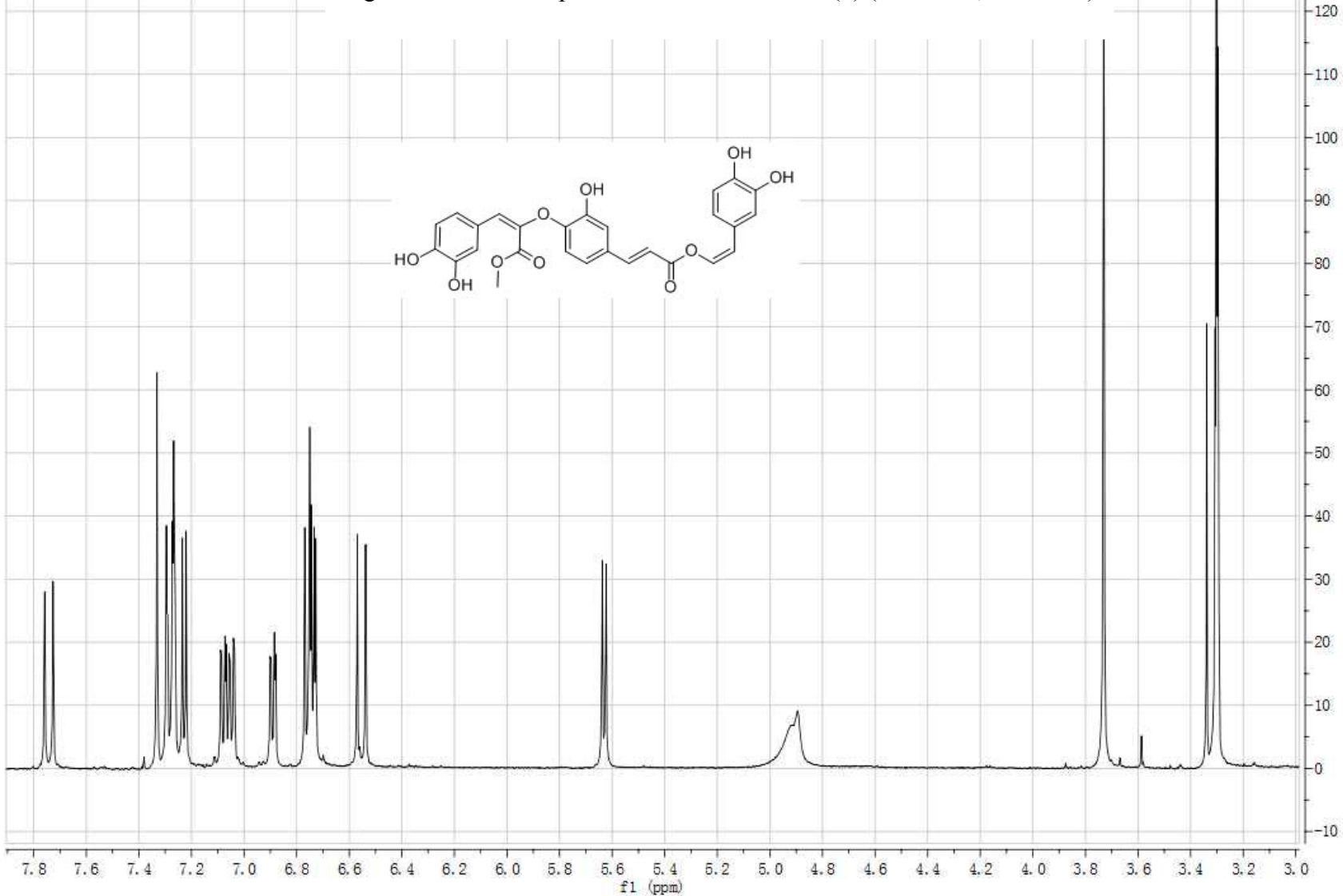


Figure S3 COSY NMR spectrum of Sebestenoid A (**1**) (MeOH-*d*₄, 500 MHz)

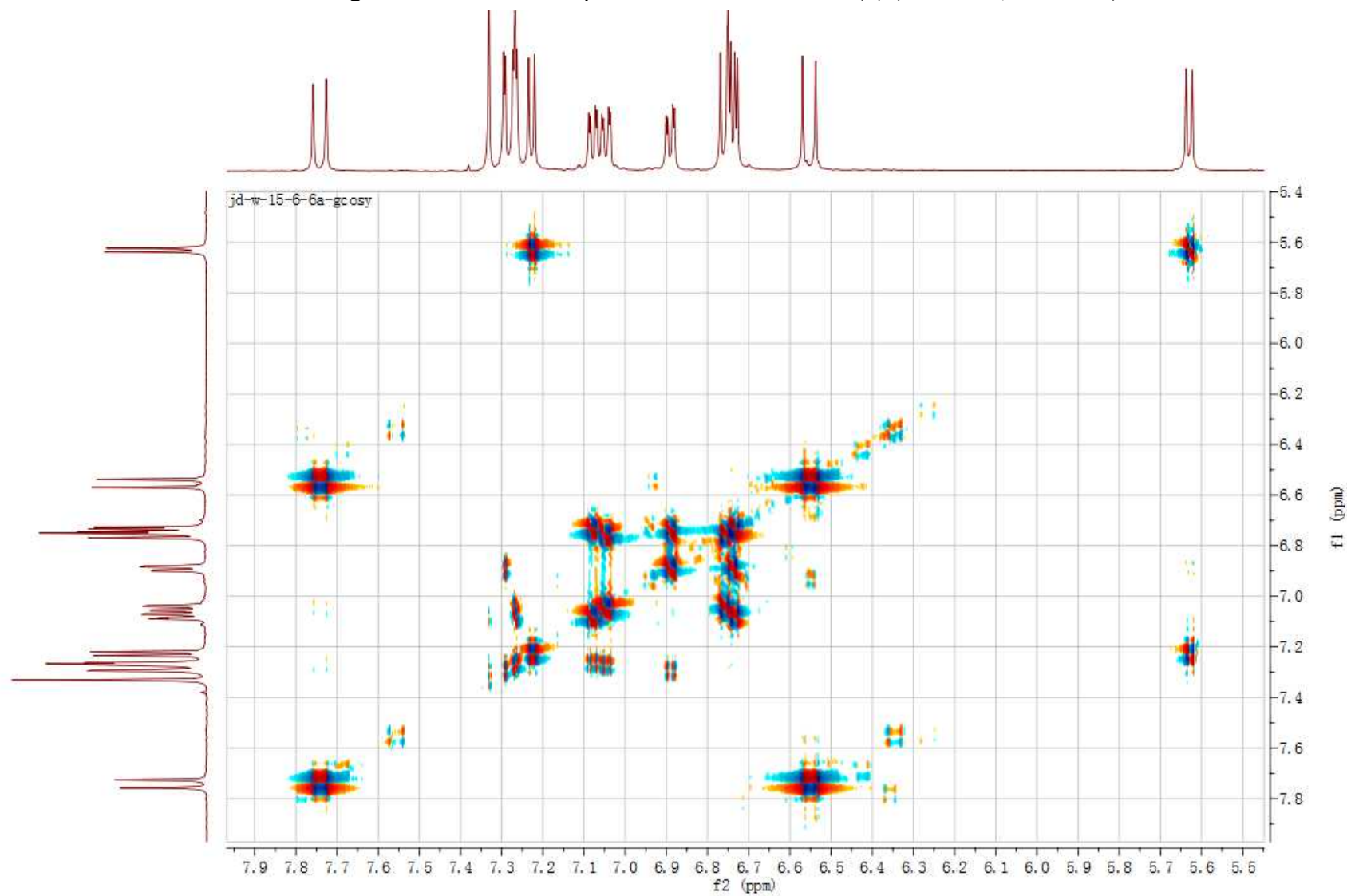


Figure S4 HSQC NMR spectrum of Sebestenoid A (**1**) (MeOH-*d*₄, 500 MHz)

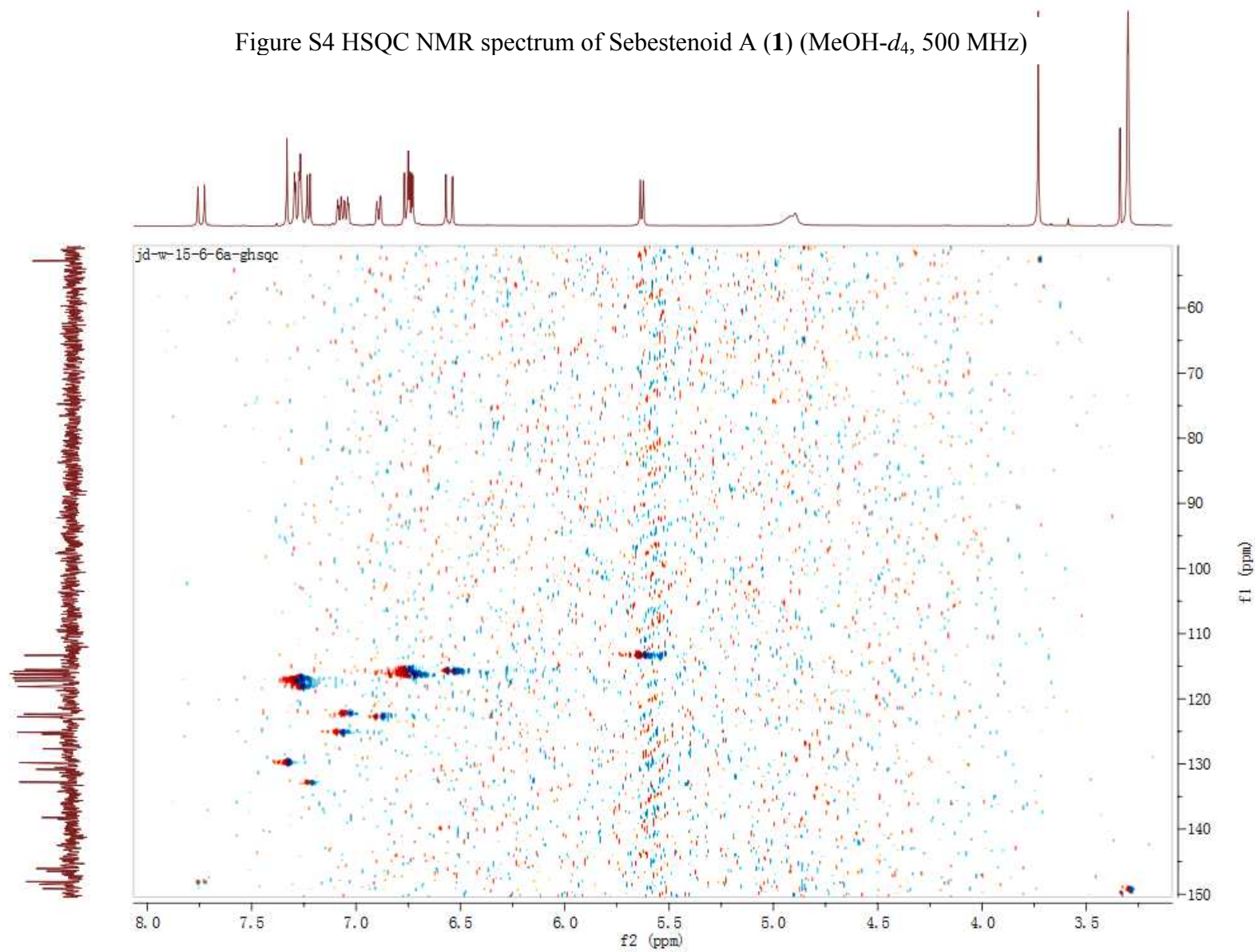


Figure S5 Expansion of HSQC NMR spectrum of Sebestenoid A (1) (MeOH-*d*₄, 500 MHz)

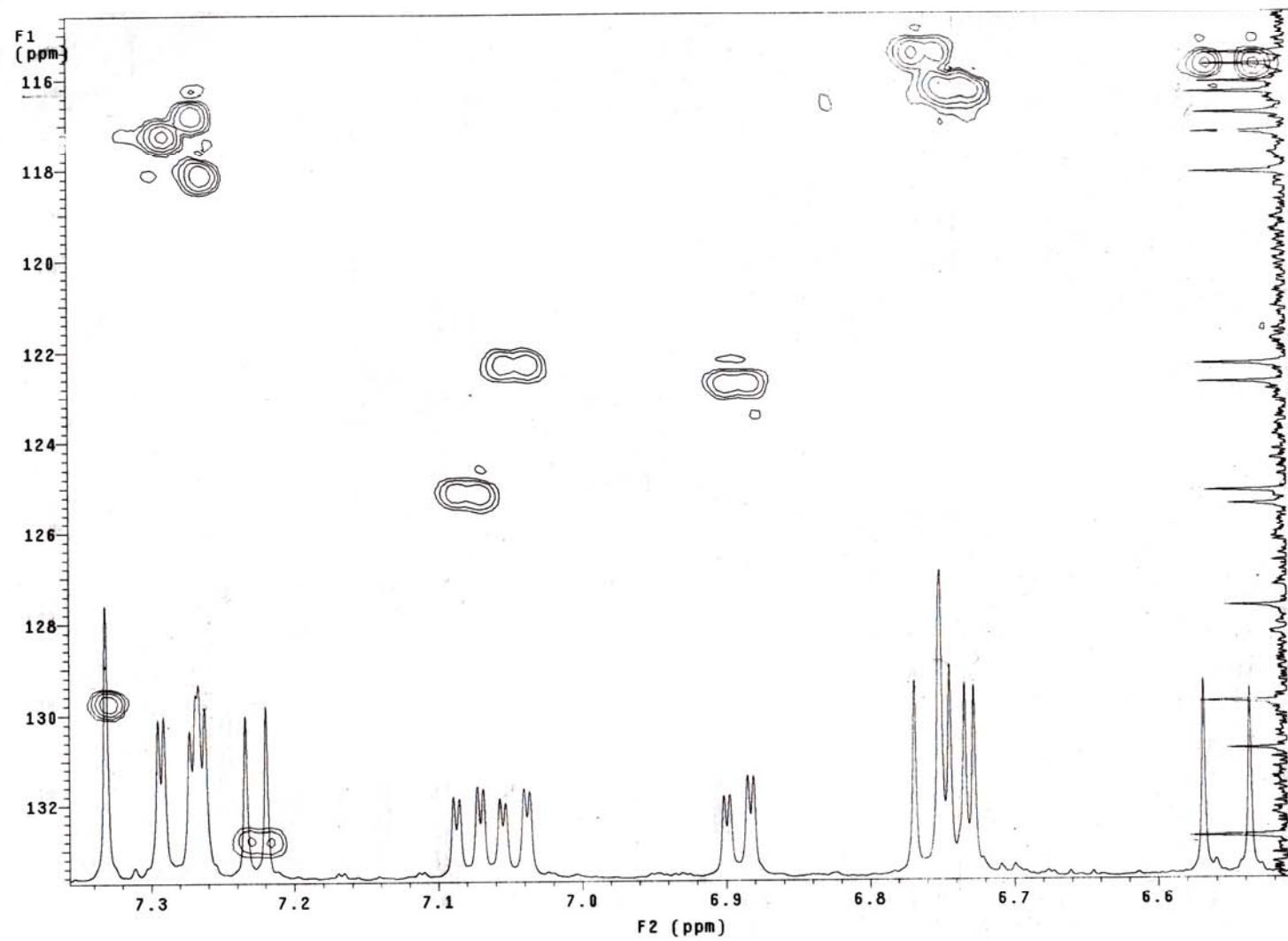


Figure S6 HMBC NMR spectrum of Sebestenoid A (1) (MeOH- d_4 , 500 MHz)

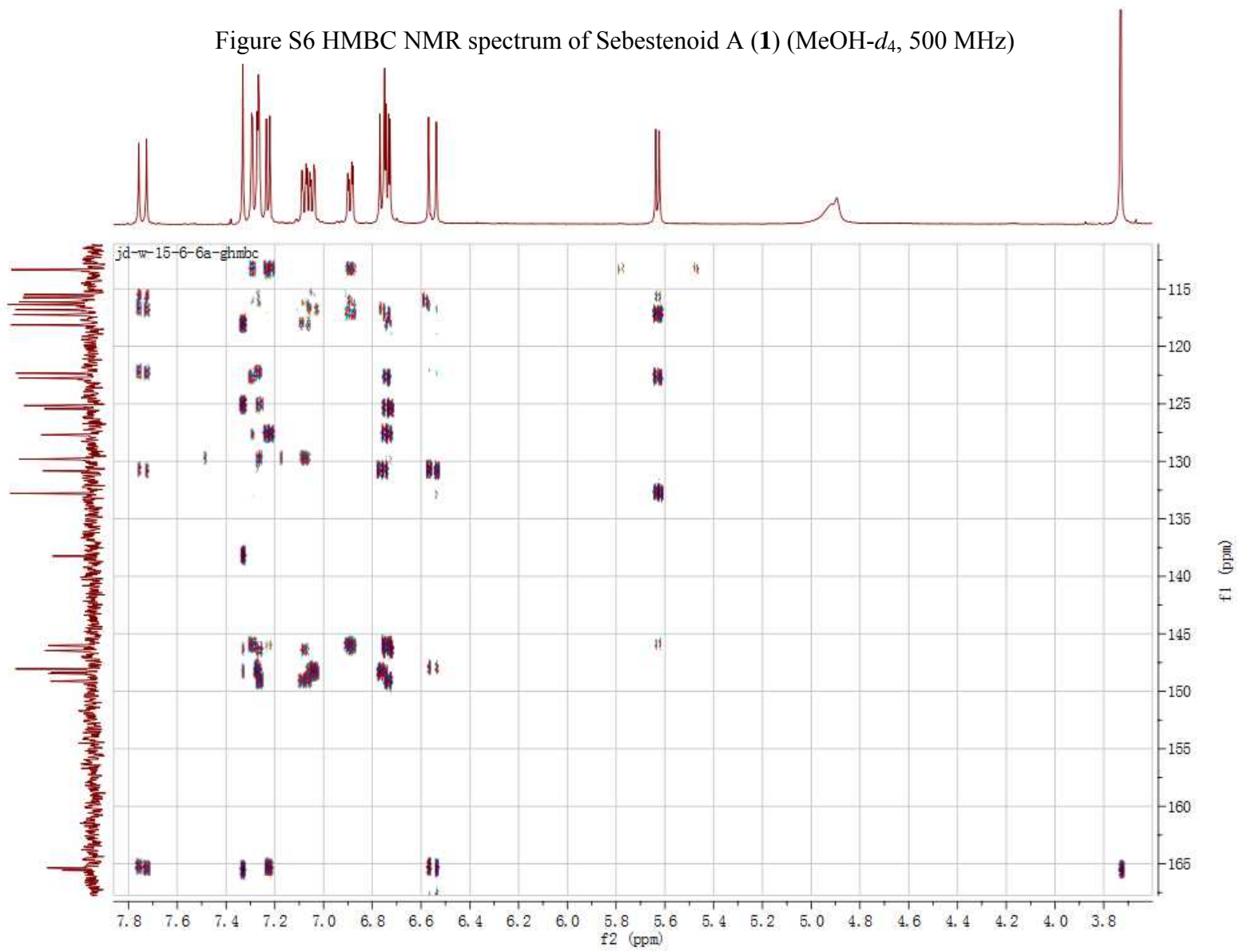
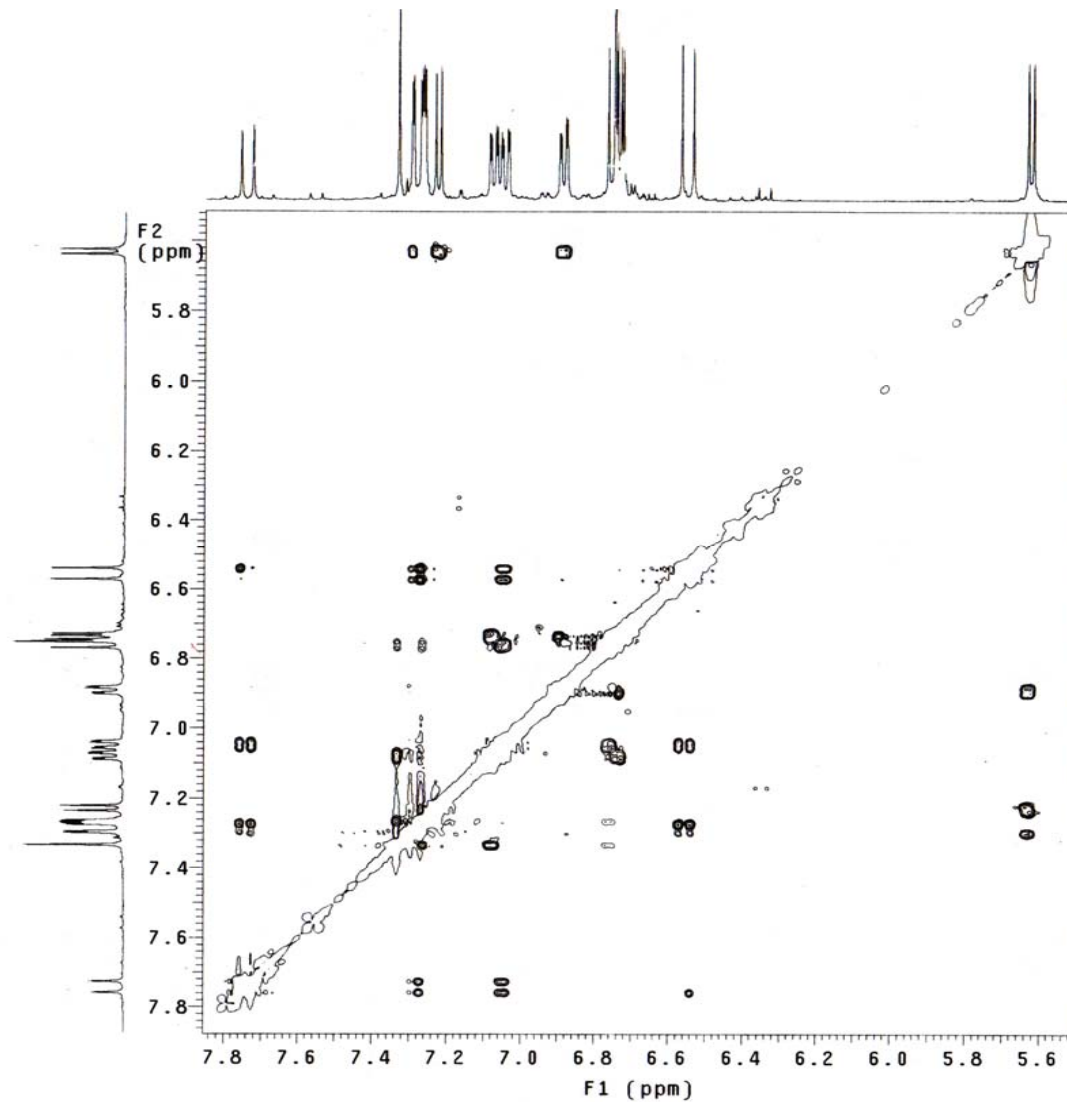


Figure S7 ROESY NMR spectrum of Sebestenoid A (1) (MeOH-*d*₄, 500 MHz)

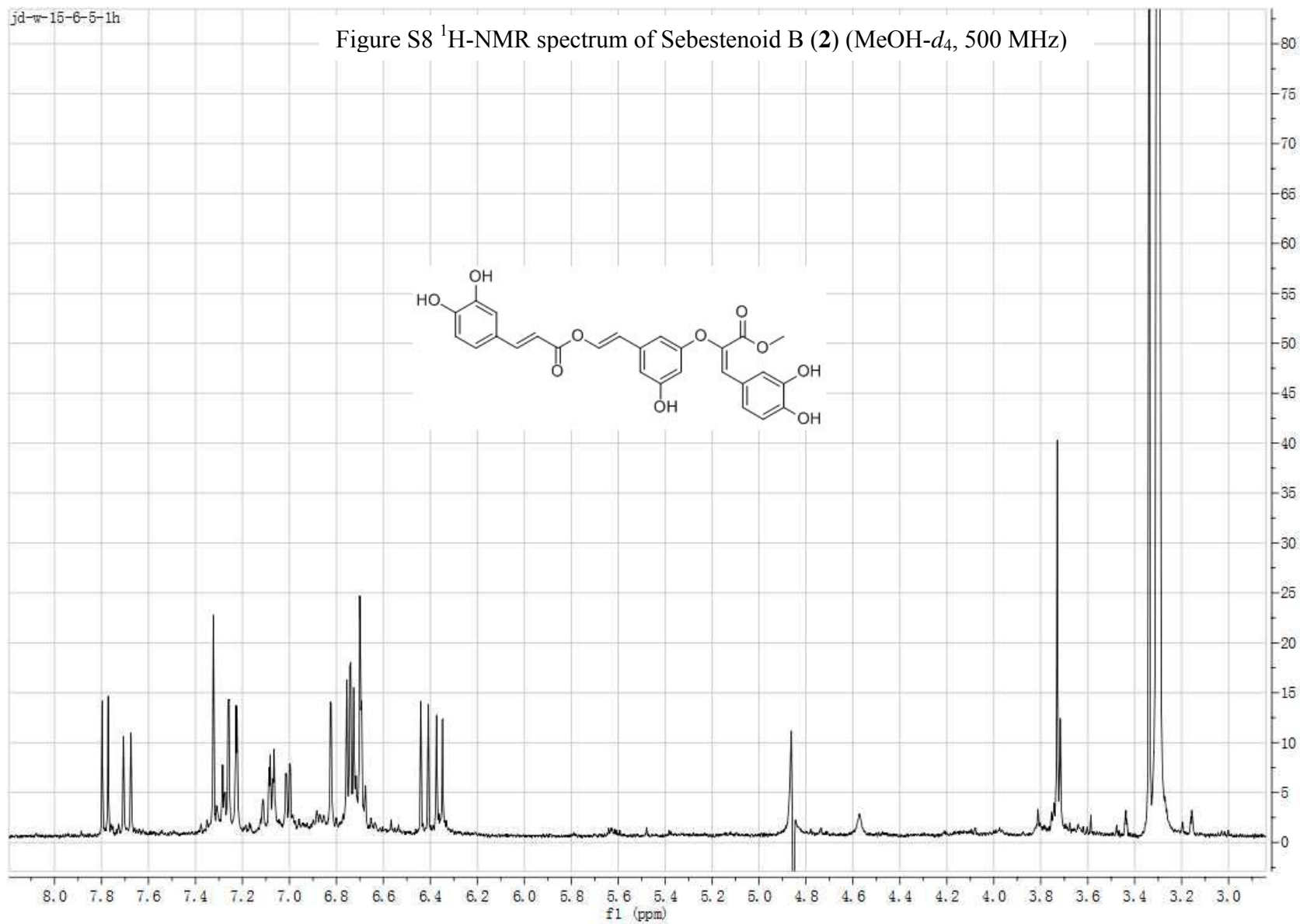
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Width 2514.7 Hz
2D Width 2514.7 Hz
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2 x 256 increments
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DATA PROCESSING
Gauss apodization 0.094 sec
F1 DATA PROCESSING
Gauss apodization 0.094 sec
FT size 2048 x 2048
Total time 2 hr, 21 min, 0 sec



jd-w-15-6-5-1h

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



jd-w-15-6-5a-13c

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

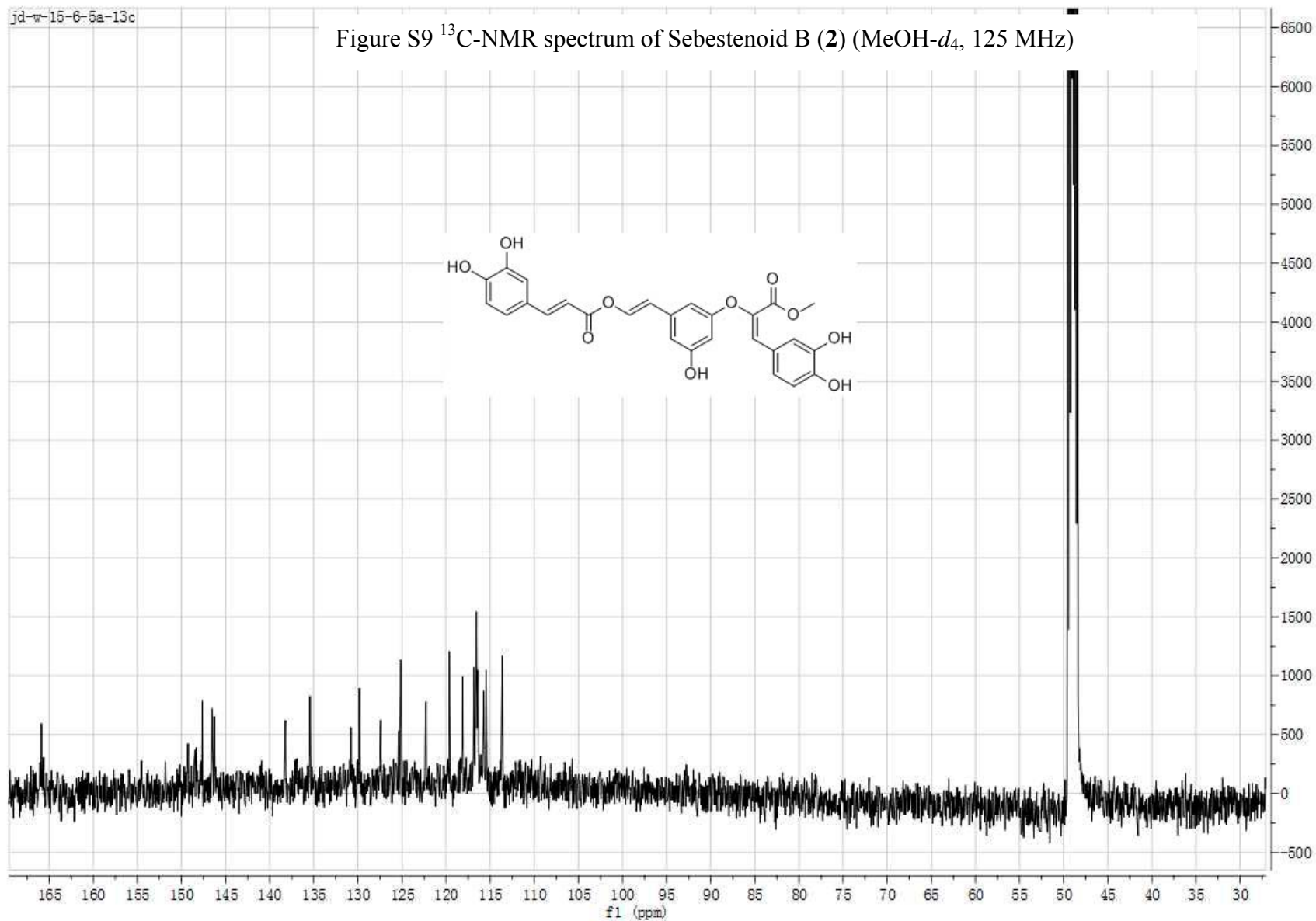


Figure S10 COSY NMR spectrum of Sebestenoid B (**2**) (MeOH-*d*₄, 500 MHz)

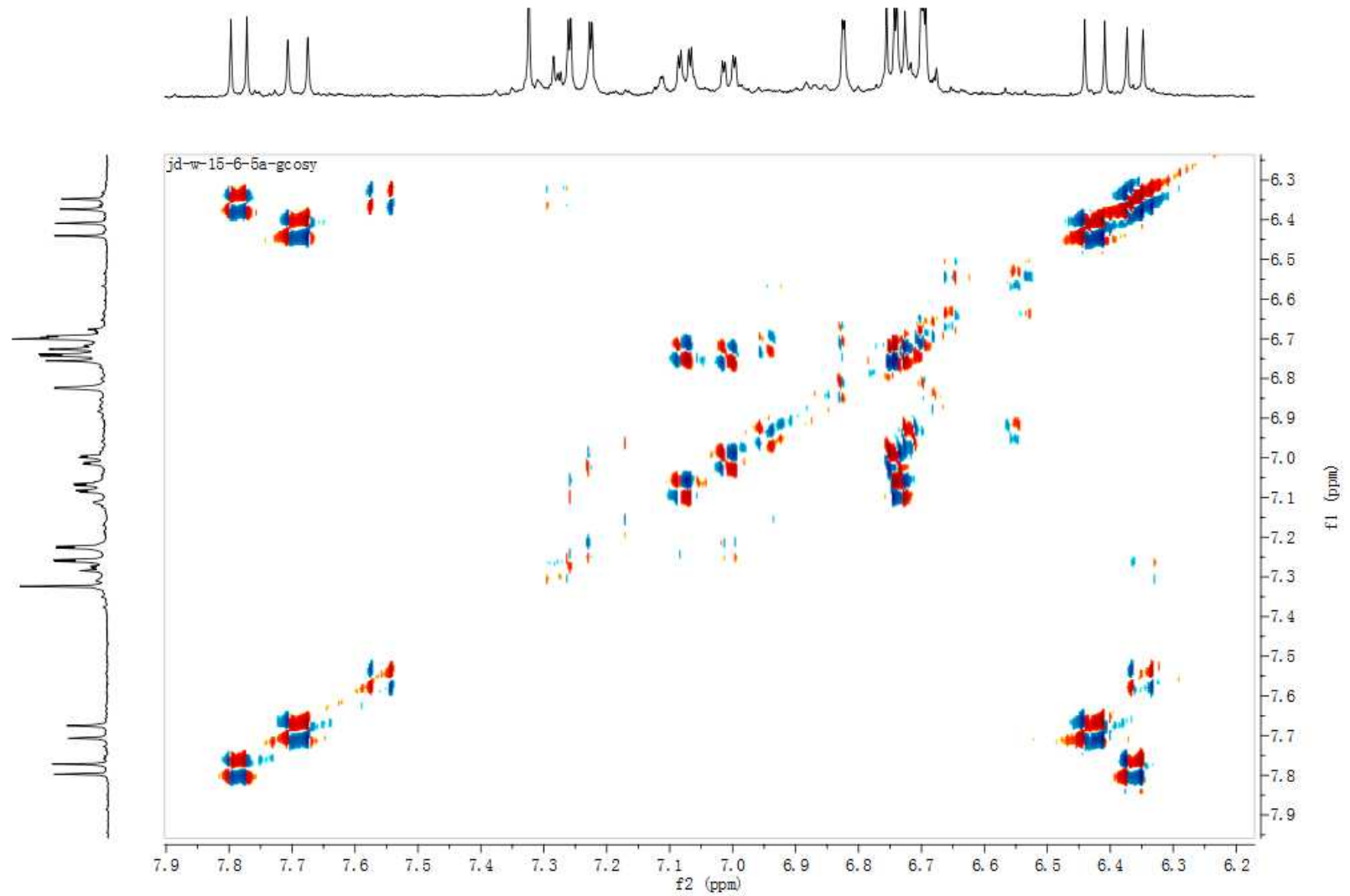


Figure S11 HSQC NMR spectrum of Sebestenoid B (2) (MeOH- d_4 , 500 MHz)

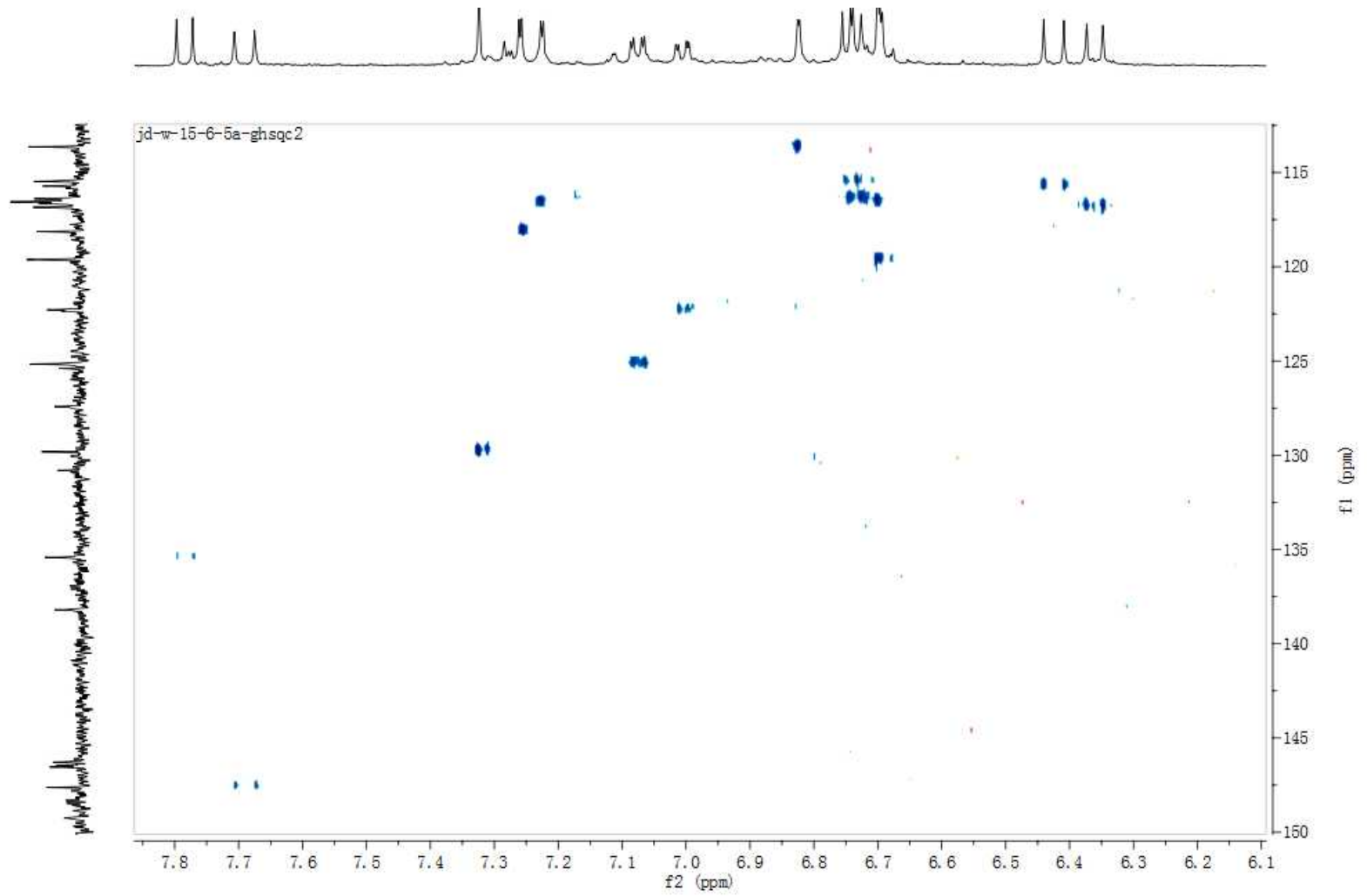


Figure S12 HMBC NMR spectrum of Sebestenoid B (**2**) (MeOH-*d*₄, 500 MHz)

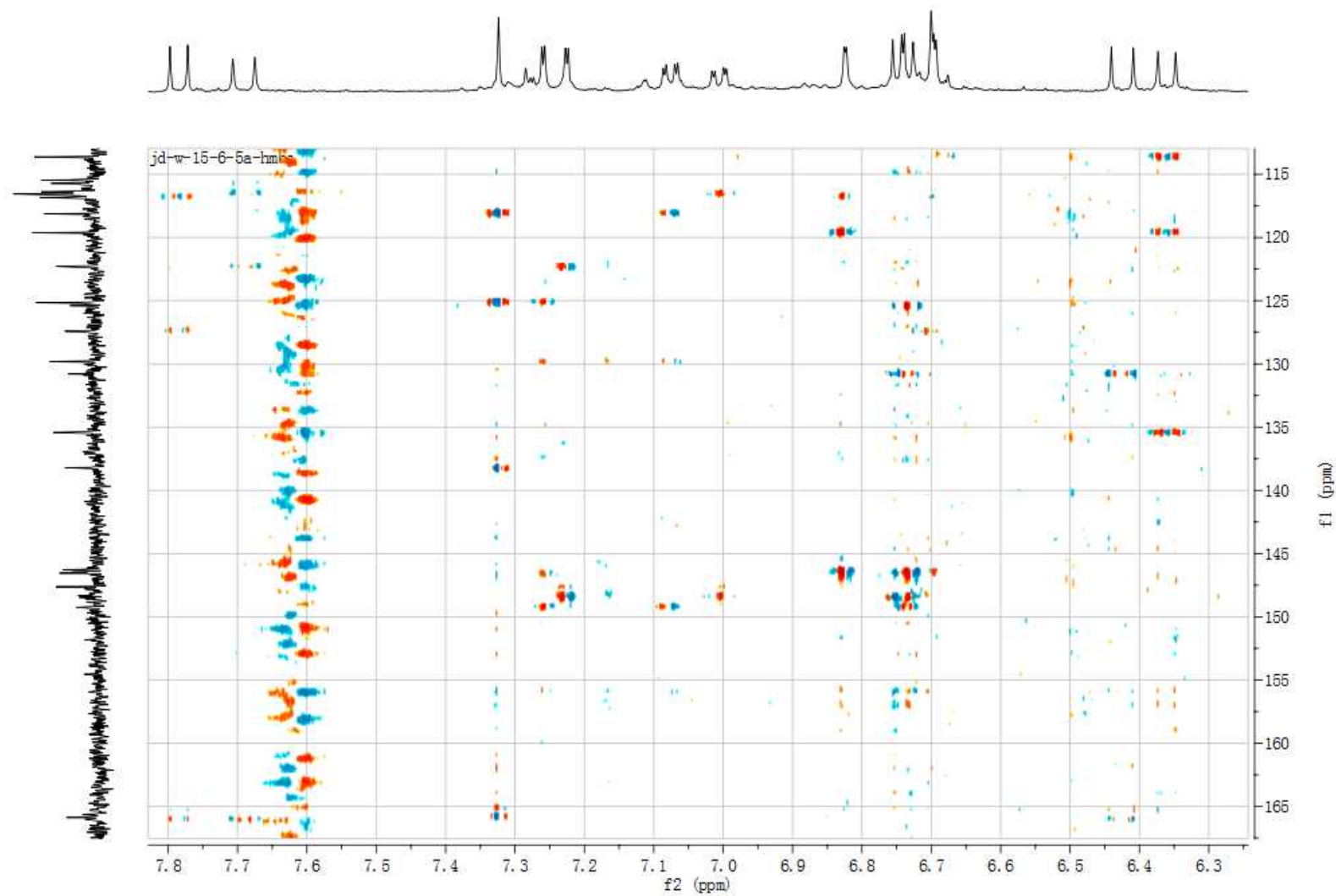
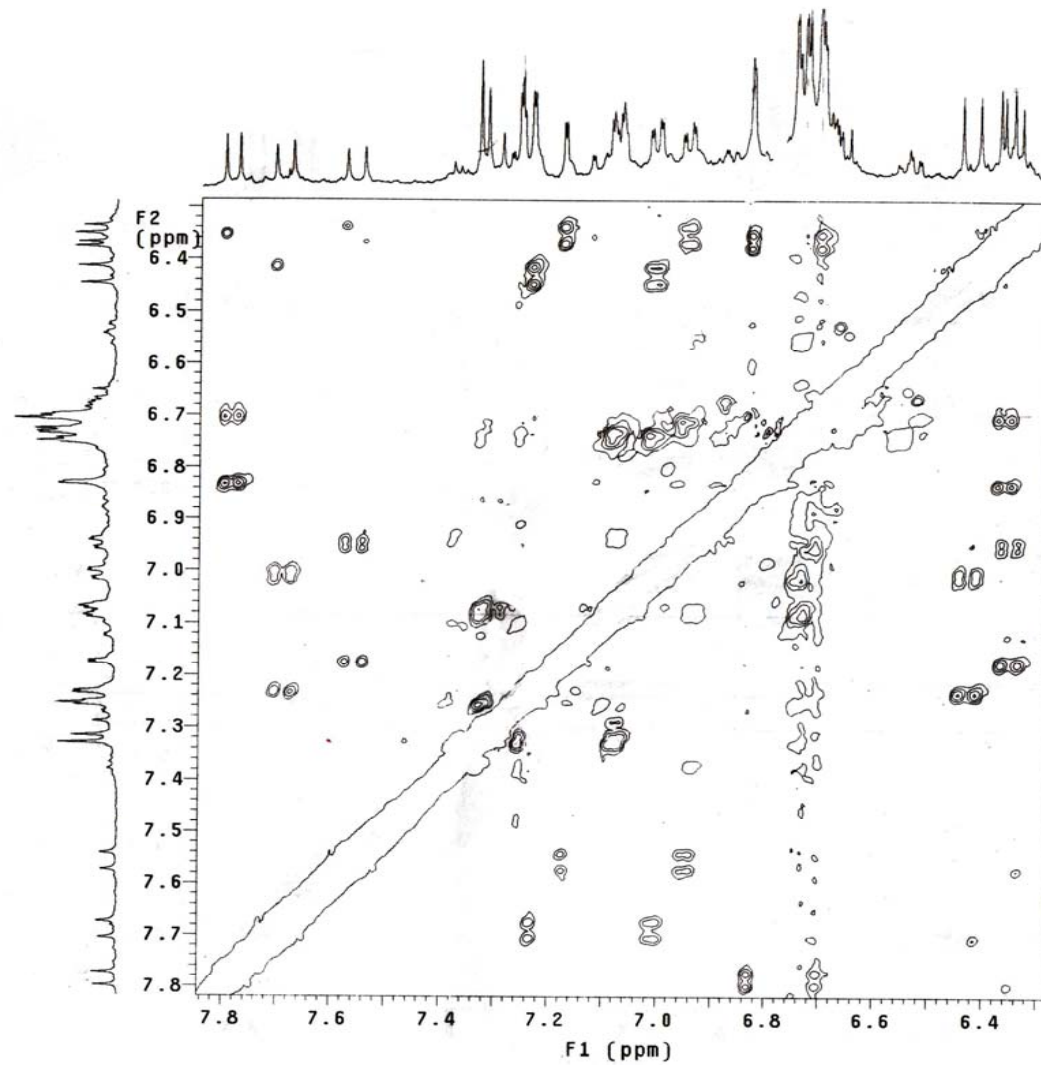


Figure S13 ROESY NMR spectrum of Sebestenoid B (2) (MeOH- d_4 , 500 MHz)

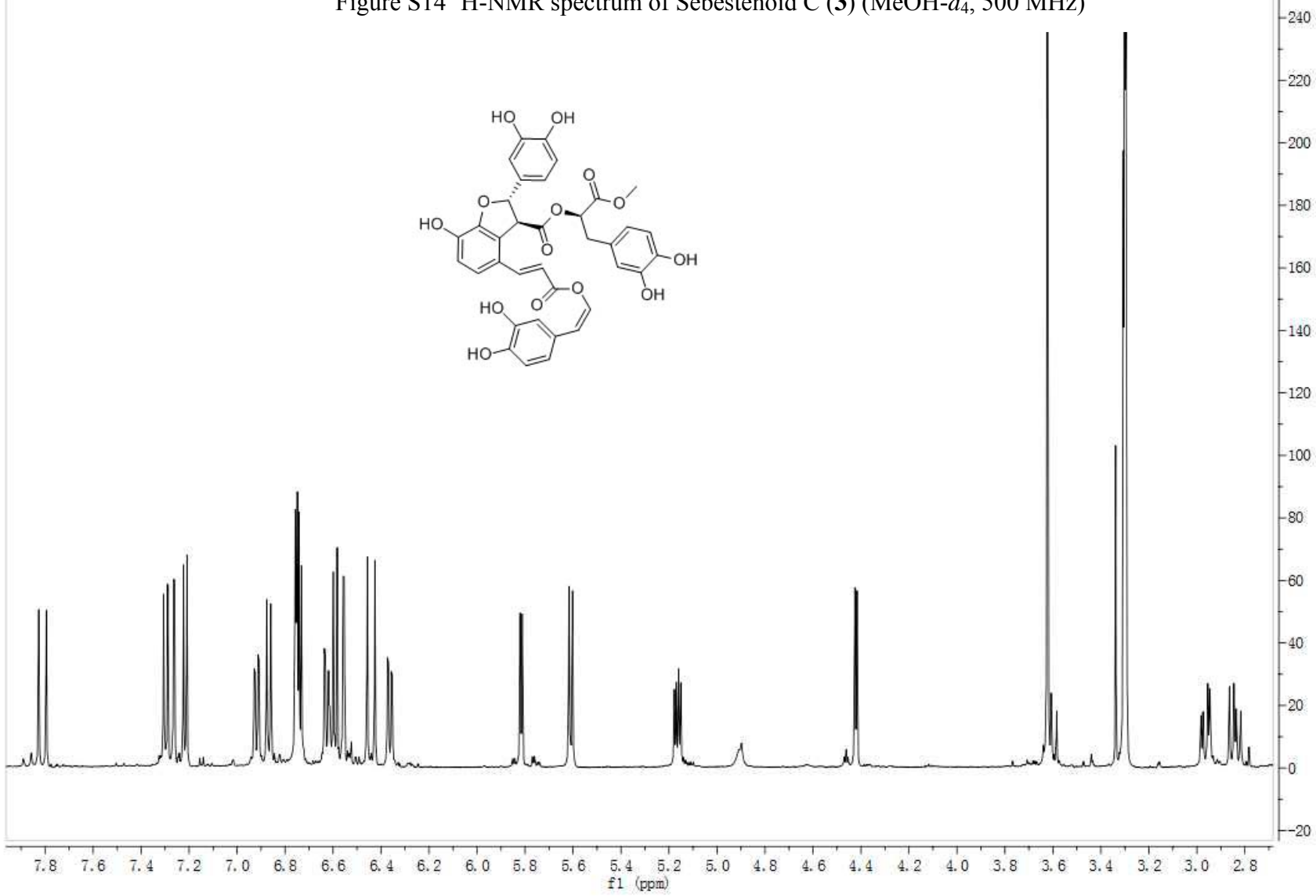
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Temp. 22.0 °C / 295.1 K
Operator: vnmr1
File: jd-w-15-6-5a-roesy
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Acq. time 0.500 sec
Width 2514.7 Hz
2D Width 2514.7 Hz
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2 x 256 increments
OBSERVE H1, 500.1133918 MHz
DATA PROCESSING
Gauss apodization 0.094 sec
F1 DATA PROCESSING
Gauss apodization 0.094 sec
FT size 2048 x 2048
Total time 9 hr, 23 min, 14 sec



jd-w-17-8-4-1h

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



jd-w-17-8-4-13c

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

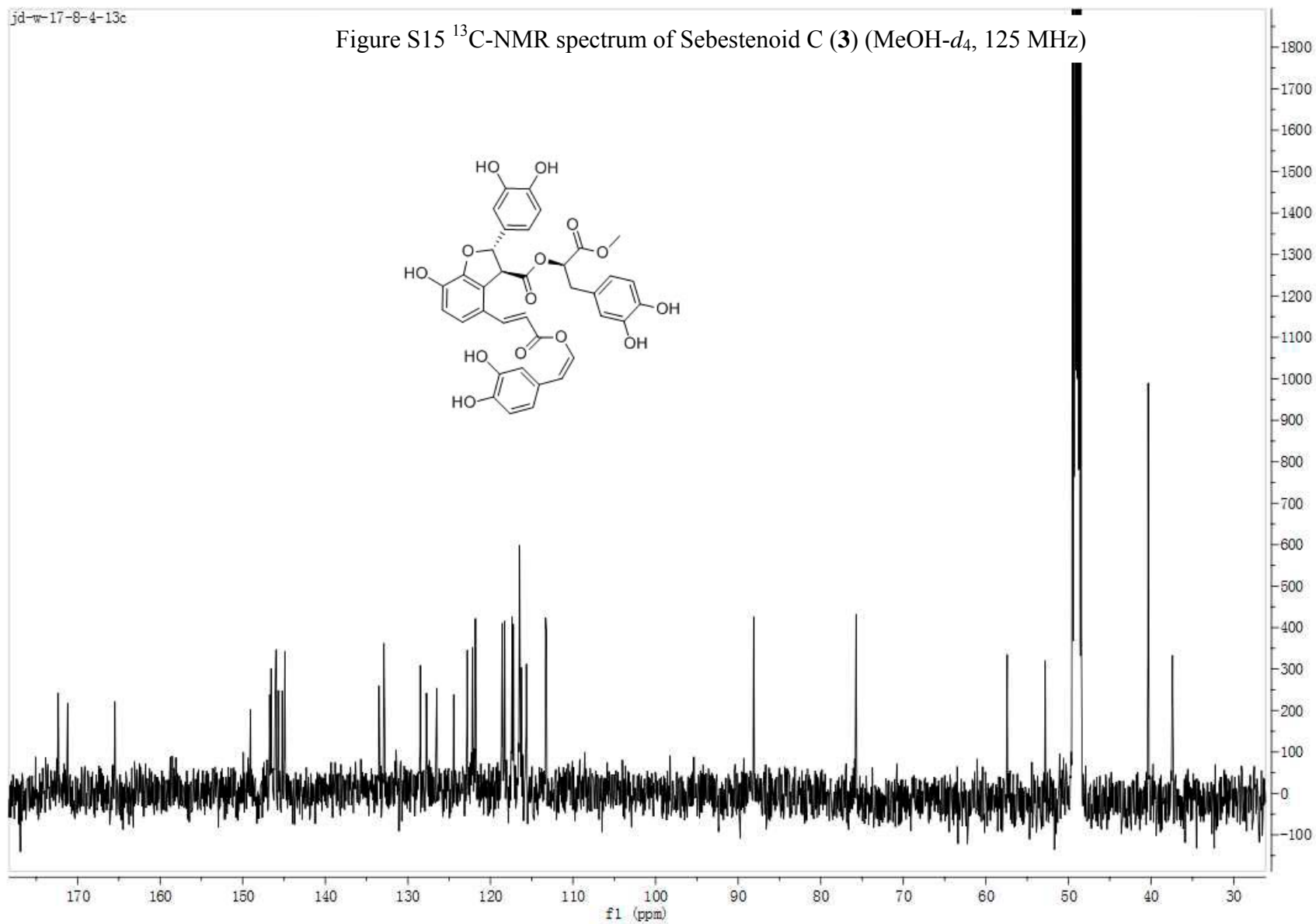


Figure S16 COSY NMR spectrum of Sebestenoid C (**3**) (MeOH-*d*₄, 500 MHz)

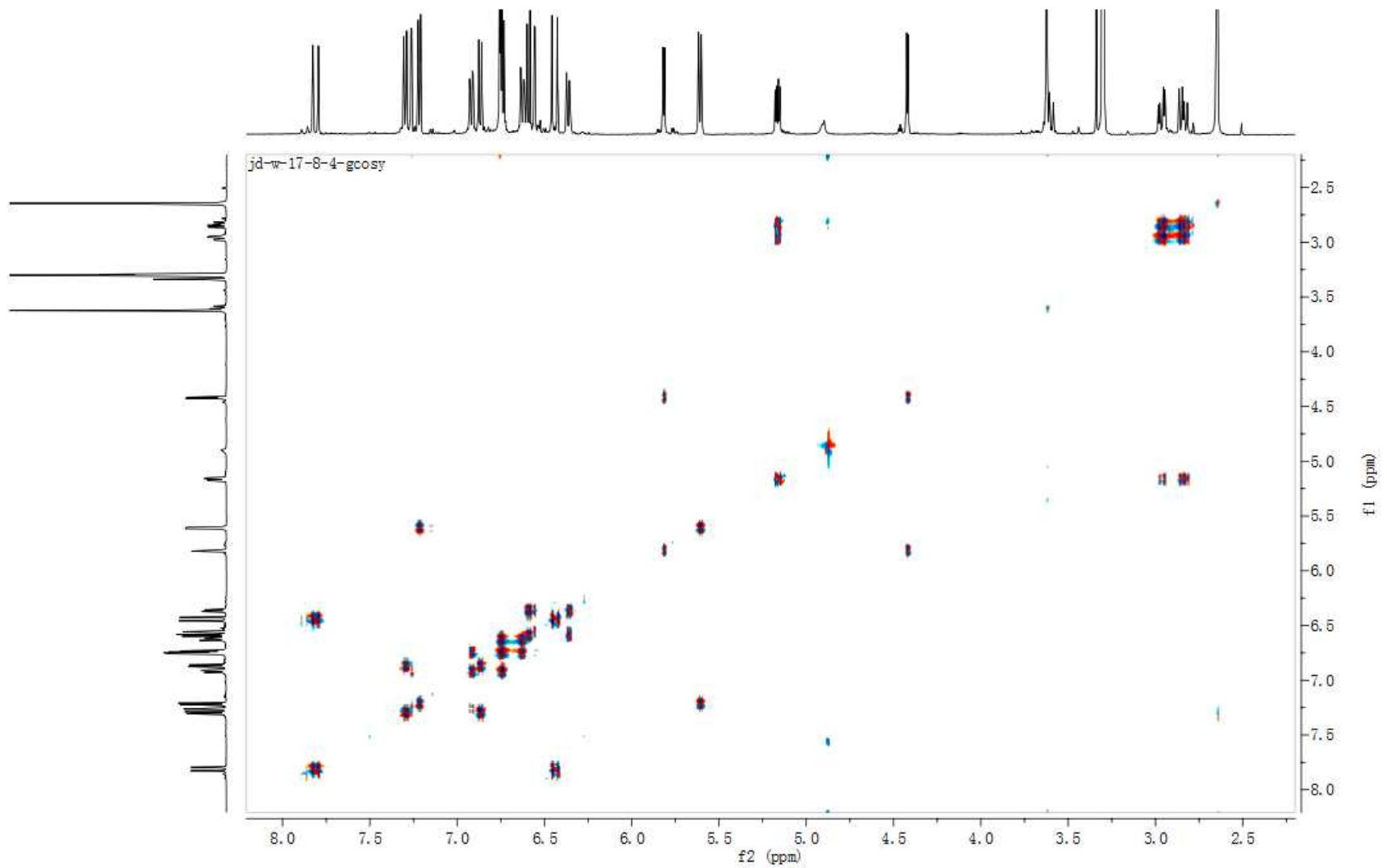


Figure S17 HSQC NMR spectrum of Sebestenoid C (**3**) (MeOH- d_4 , 500 MHz)

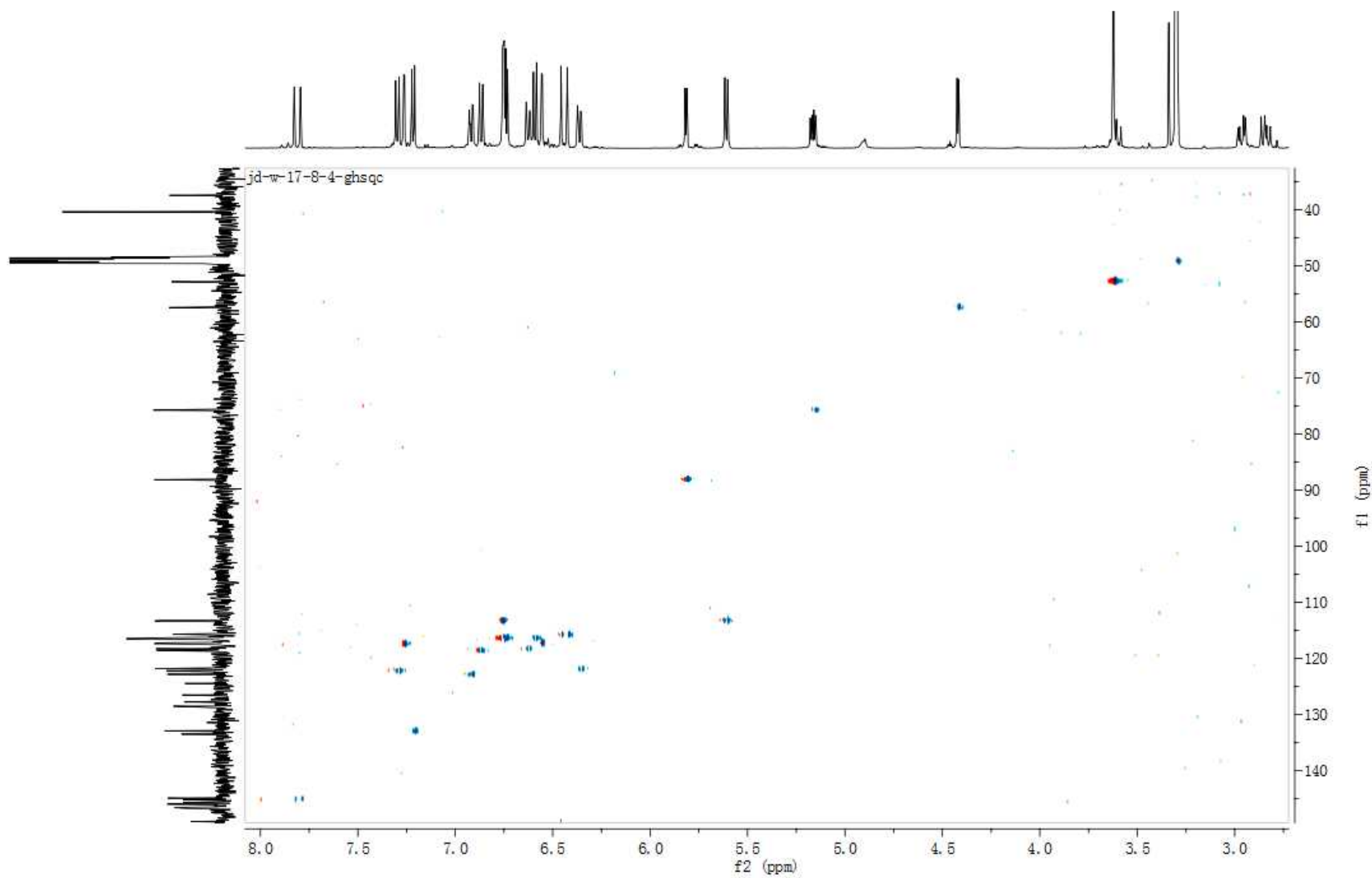


Figure S18 Expansion of HSQC NMR spectrum of Sebestenoid C (**3**) (MeOH-*d*₄, 500 MHz)

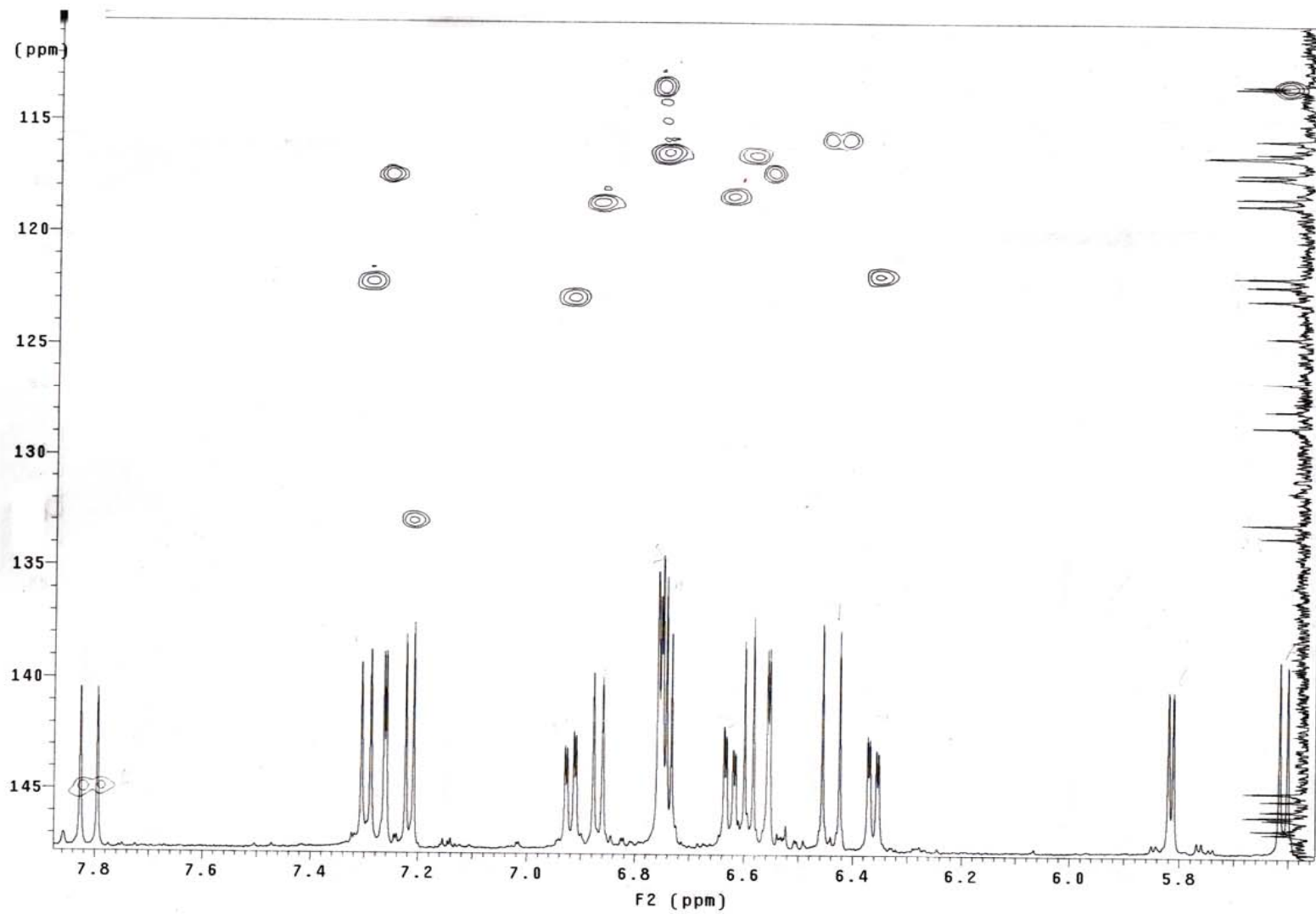


Figure S19 HMBC NMR spectrum of Sebestenoid C (**3**) (MeOH-*d*₄, 500 MHz)

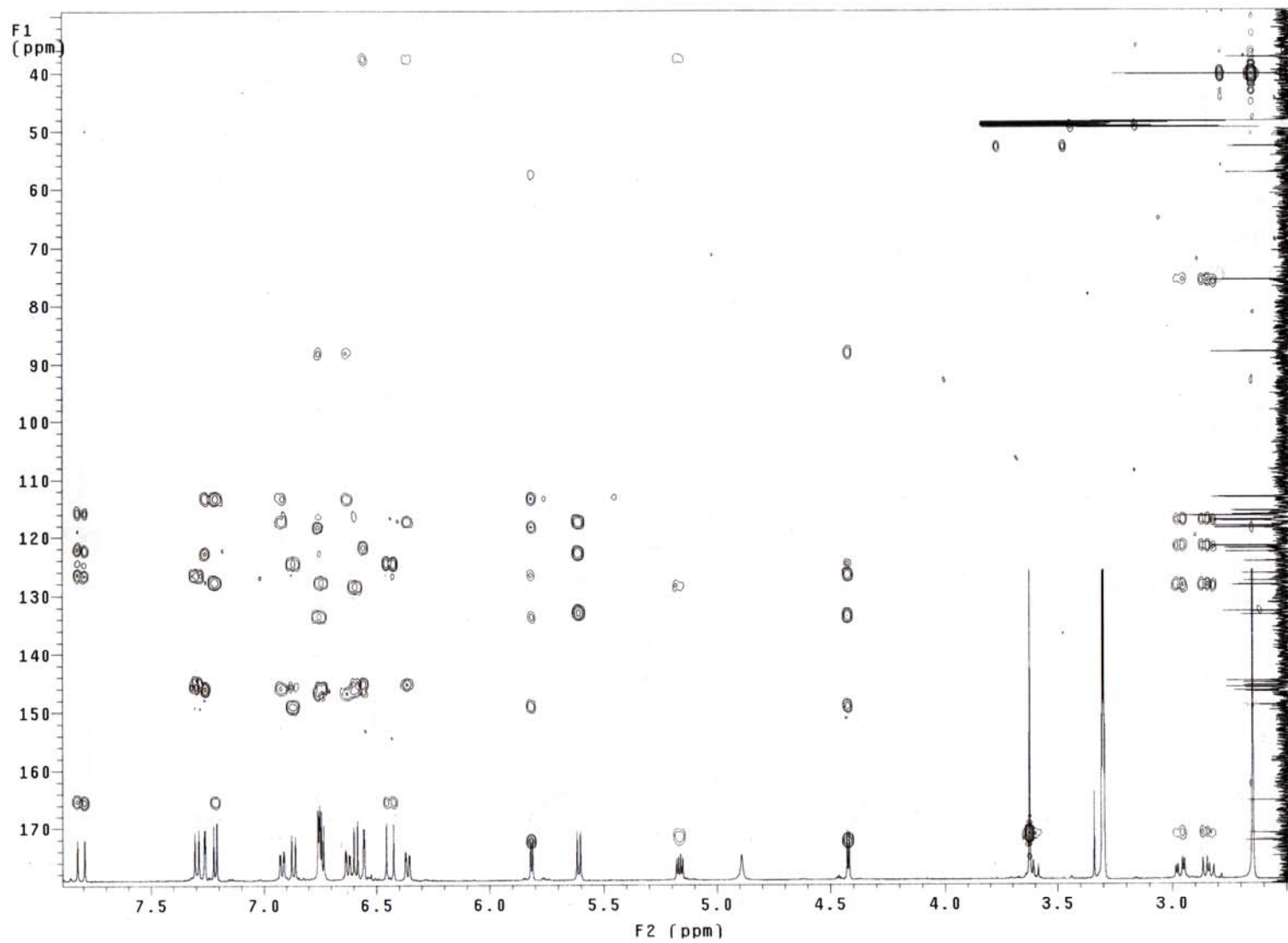
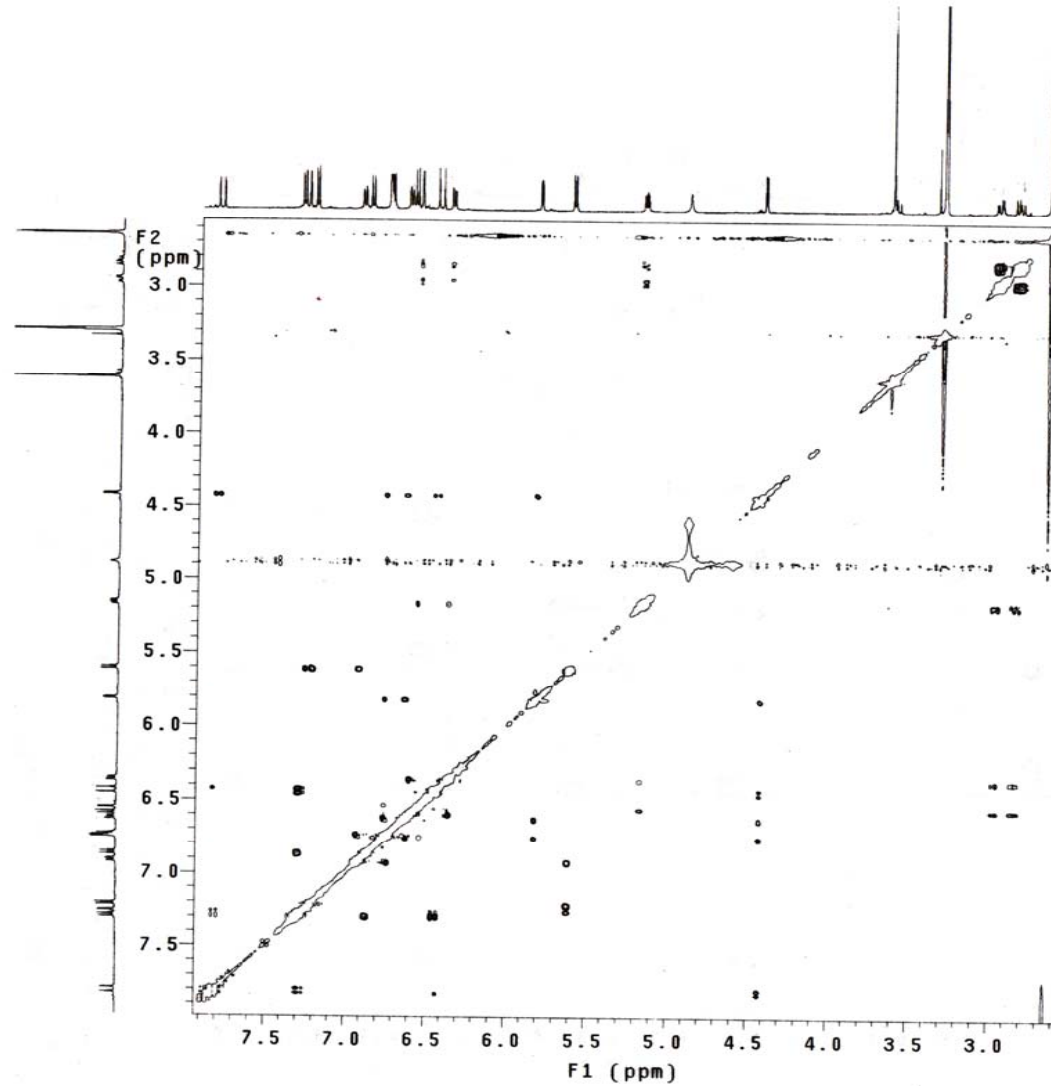


Figure S20 ROESY NMR spectrum of Sebestenoid C (**3**) (MeOH-*d*₄, 500 MHz)

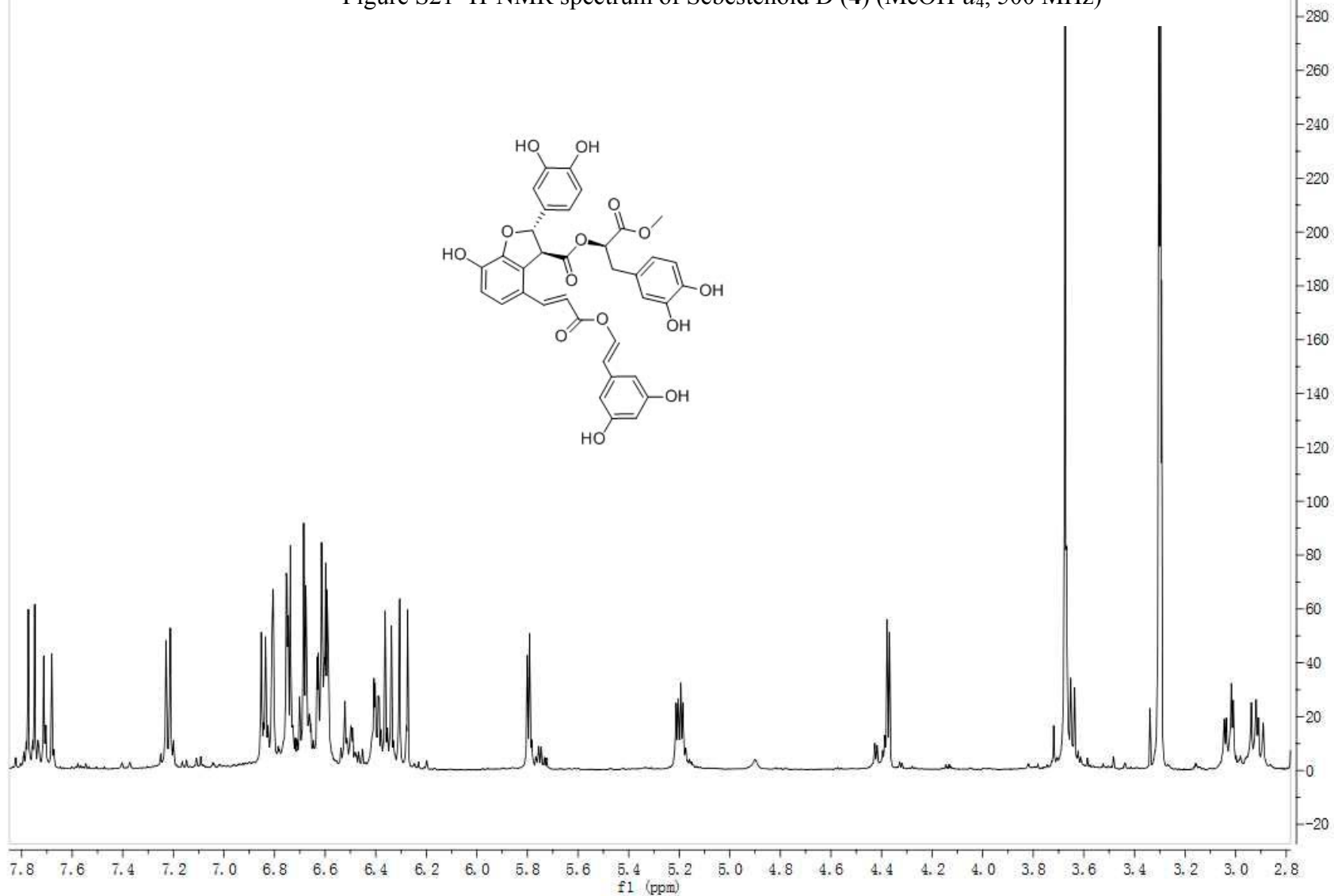
Pulse Sequence: ROESY
Solvent: cd3od
Temp. 22.0 C / 295.1 K
Operator: vnmr1
File: jd-w-17-8-4-roesy
INOVA-500 "localhost"

Mixing 0.500 sec
Acq. time 0.500 sec
Width 3004.7 Hz
2D Width 3004.7 Hz
16 repetitions
2 x 256 increments
OBSERVE H1, 500.1133918 MHz
DATA PROCESSING
Gauss apodization 0.079 sec
F1 DATA PROCESSING
Gauss apodization 0.079 sec
FT size 2048 x 2048
Total time 4 hr, 40 min, 37 sec



jd-w-17-8-3-1h

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



jd-w-17-8-3-13c

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

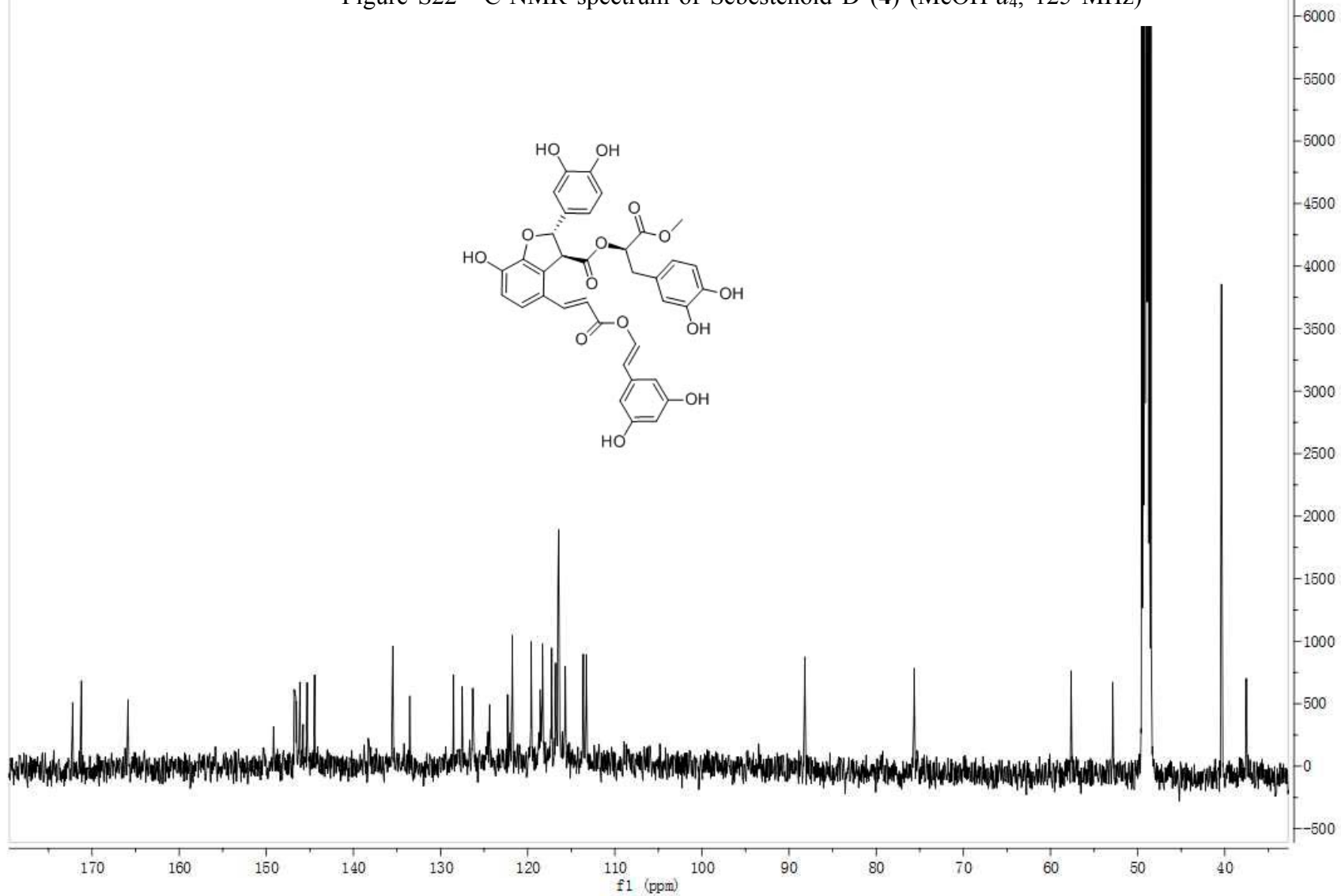


Figure S23 COSY NMR spectrum of Sebestenoid D (4) (MeOH-*d*₄, 500 MHz)

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

Relax. delay 1.000 sec
Acq. time 0.500 sec
Width 2901.5 Hz
2D Width 2901.5 Hz
8 repetitions
2 x 128 increments
OBSERVE H1, 500.1133918 MHz
DATA PROCESSING
Sq. sine bell 0.132 sec
Shifted by -0.088 sec
F1 DATA PROCESSING
Sq. sine bell 0.037 sec
Shifted by -0.025 sec
FT size 2048 x 2048
Total time 52 min, 39 sec

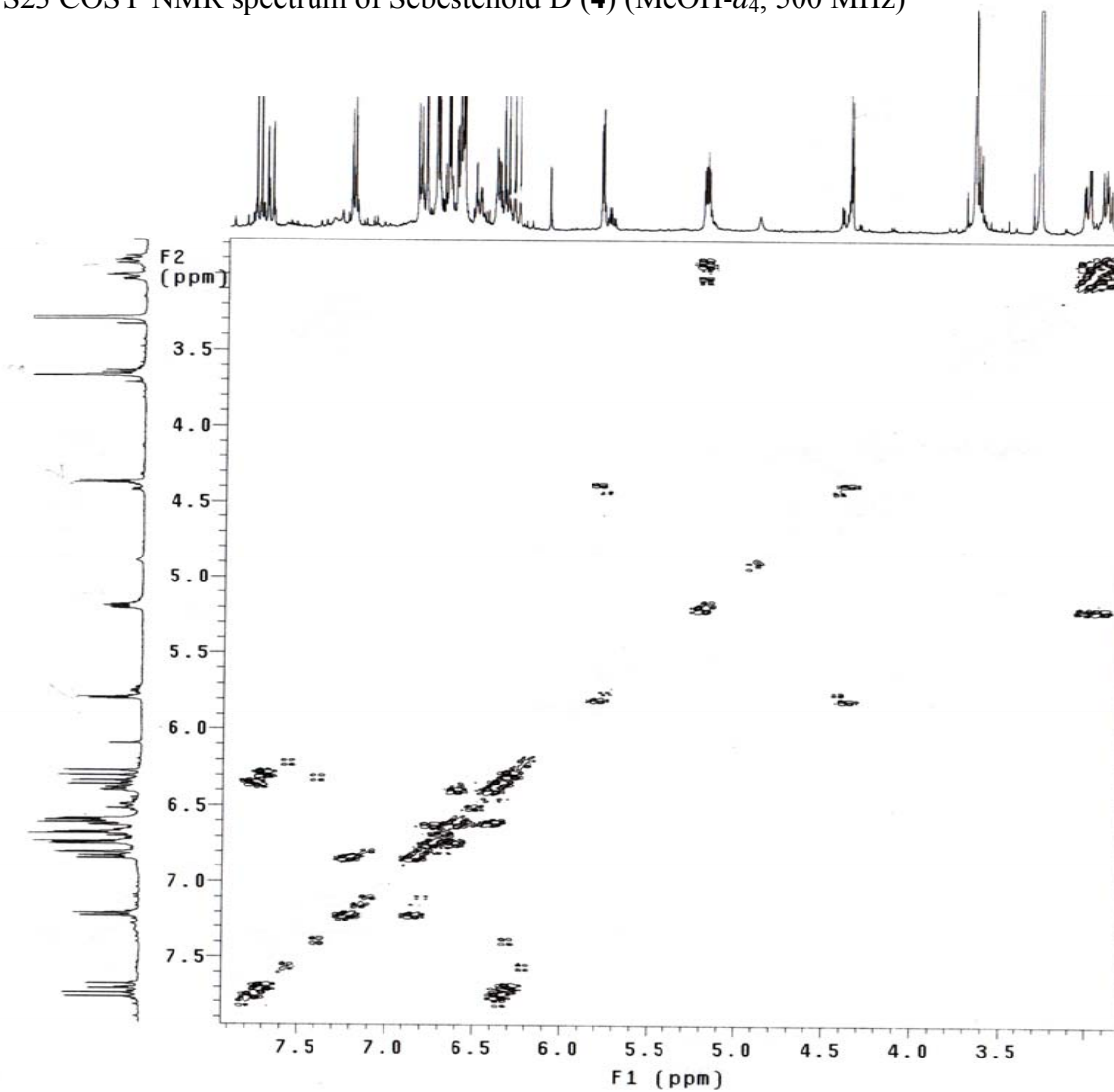


Figure S24 HSQC NMR spectrum of Sebestenoid D (**4**) (MeOH-*d*₄, 500 MHz)

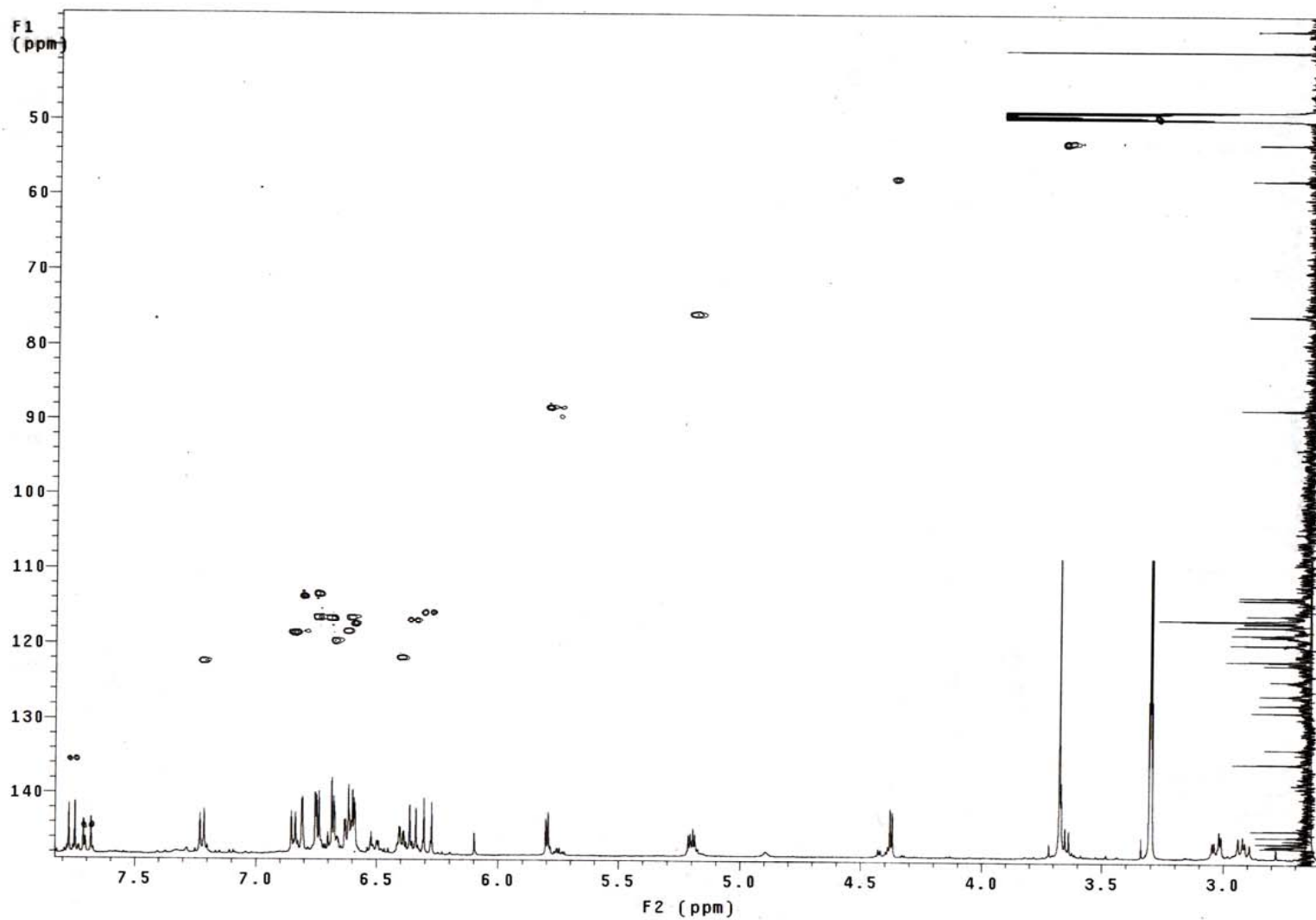


Figure S25 HMBC NMR spectrum of Sebestenoid D (4) (MeOH-*d*₄, 500 MHz)

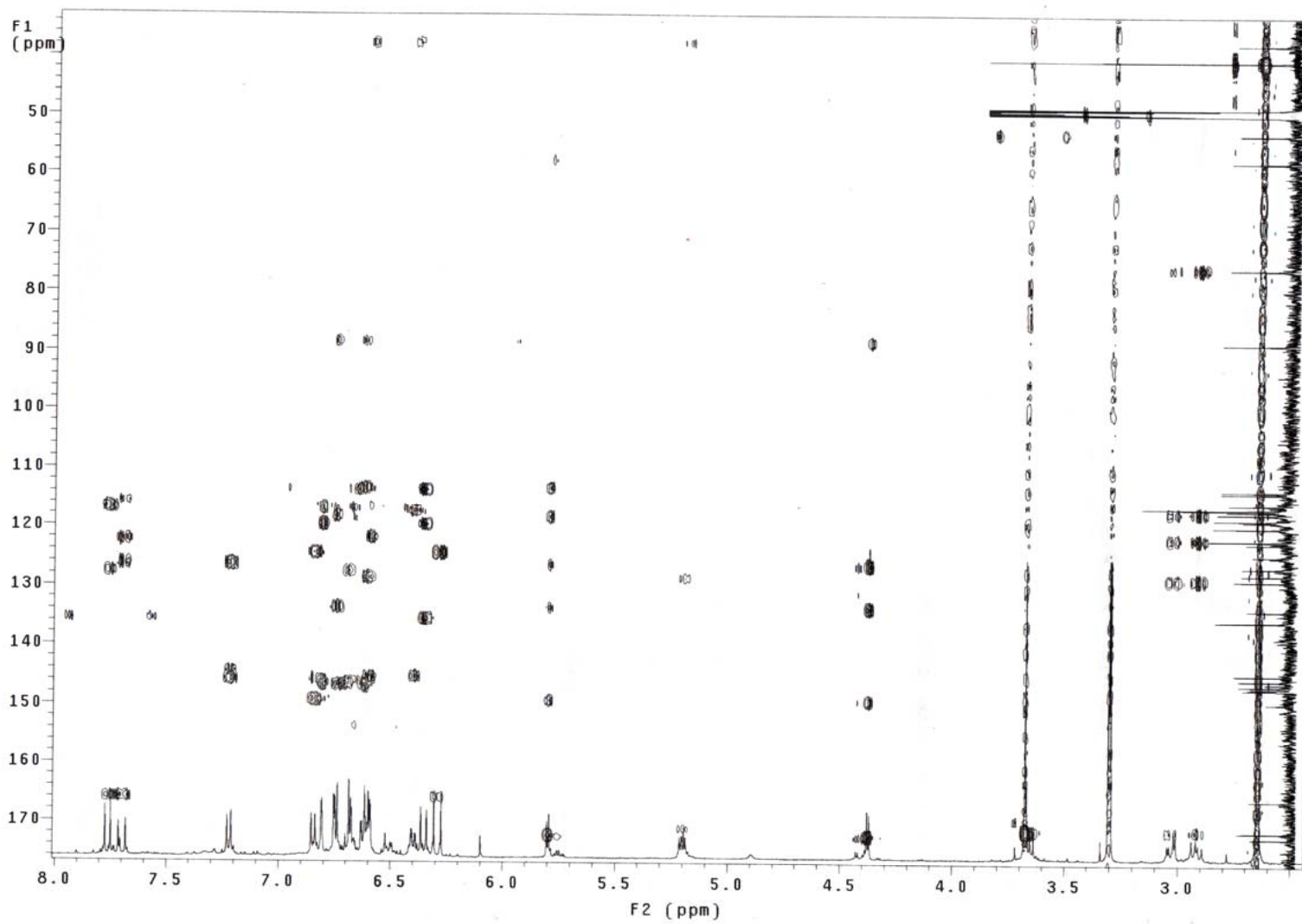


Figure S26 ROESY NMR spectrum of Sebestenoid D (4) (MeOH- d_4 , 500 MHz)

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

