

## Supporting Information

# Monanchosterols A and B, Bioactive Bicyclo[4.3.1]steroids from a Korean Sponge *Monanchora* sp.

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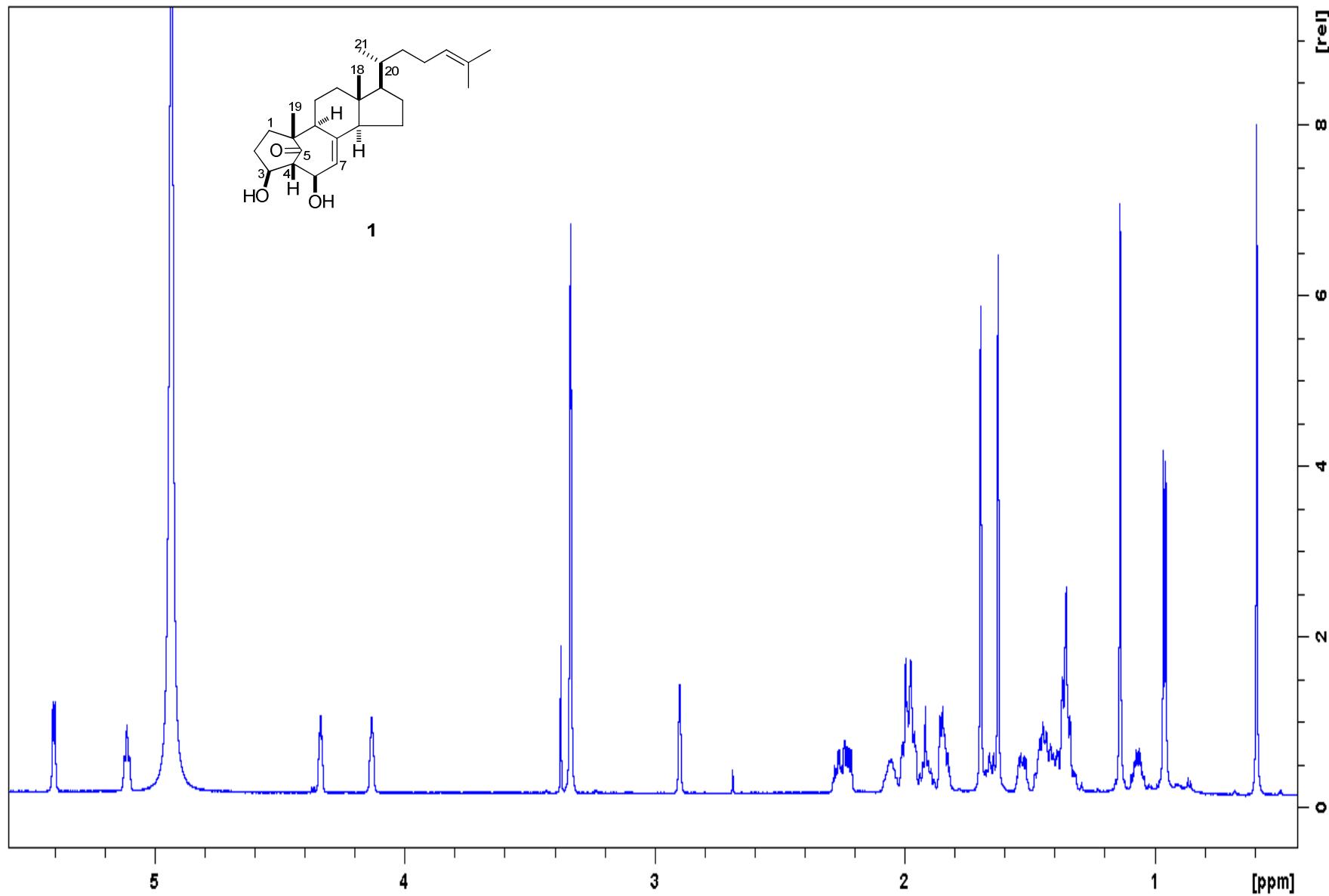
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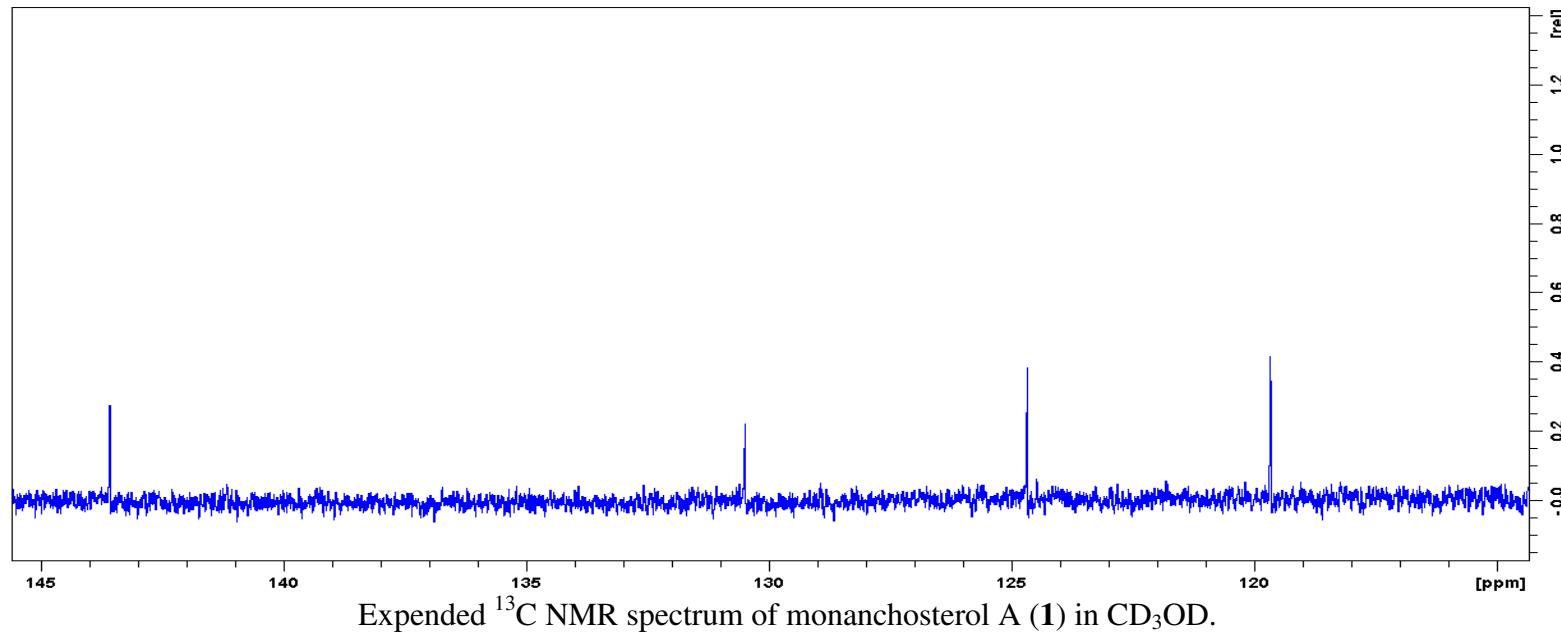
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**Table of Contents:**

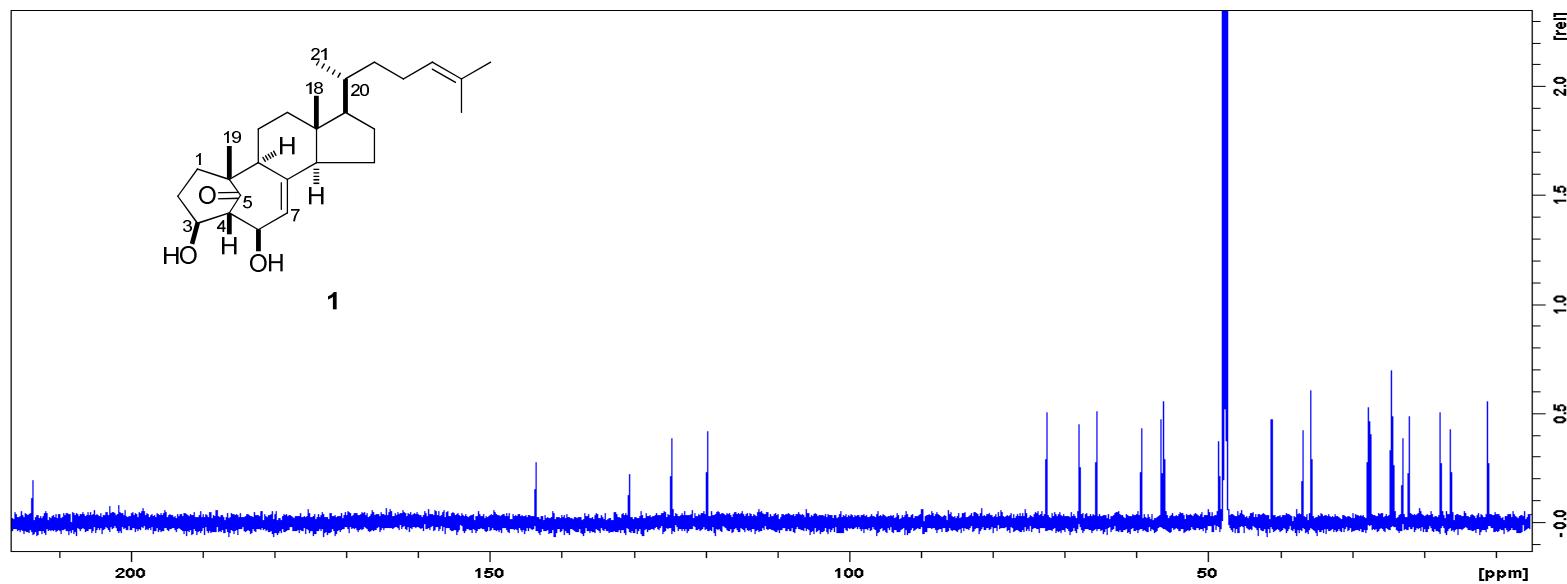
Figure S1. $^1\text{H}$ NMR spectrum of monanchosterol A ( <b>1</b> ) in $\text{CD}_3\text{OD}$ .....	S3
Figure S2. $^{13}\text{C}$ NMR spectrum of monanchosterol A ( <b>1</b> ) in $\text{CD}_3\text{OD}$ .....	S4
Figure S3. COSY spectrum of monanchosterol A ( <b>1</b> ) in $\text{CD}_3\text{OD}$ .....	S5
Figure S4. HSQC spectrum of monanchosterol A ( <b>1</b> ) in $\text{CD}_3\text{OD}$ .....	S6
Figure S5. HMBC spectrum of monanchosterol A ( <b>1</b> ) in $\text{CD}_3\text{OD}$ .....	S7
Figure S6. ROESY spectrum monanchosterol A ( <b>1</b> ) in $\text{CD}_3\text{OD}$ .....	S8
Figure S7. IR spectrum monanchosterol A ( <b>1</b> ) .....	S9
Figure S8 $^1\text{H}$ NMR spectrum of monanchosterol B ( <b>2</b> ) in $\text{CD}_3\text{OD}$ .....	S10
Figure S9 $^{13}\text{C}$ NMR spectrum of monanchosterol B ( <b>2</b> ) in $\text{CD}_3\text{OD}$ .....	S11
Figure S10 COSY spectrum of monanchosterol B ( <b>2</b> ) in $\text{CD}_3\text{OD}$ .....	S12
Figure S11. HSQC spectrum of monanchosterol B ( <b>2</b> ) in $\text{CD}_3\text{OD}$ .....	S13
Figure S12. HMBC spectrum of monanchosterol B ( <b>2</b> ) in $\text{CD}_3\text{OD}$ .....	S14
Figure S13. ROESY spectrum of monanchosterol B ( <b>2</b> ) in $\text{CD}_3\text{OD}$ .....	S15
Figure S14. $^1\text{H}$ NMR spectrum of compound <b>3</b> in $\text{CD}_3\text{OD}$ .....	S16
Figure S15. $^{13}\text{C}$ NMR spectrum of compound <b>3</b> in $\text{CD}_3\text{OD}$ .....	S17
Figure S16 COSY spectrum of compound <b>3</b> in $\text{CD}_3\text{OD}$ .....	S18
Figure S17. HSQC spectrum of compound <b>3</b> in $\text{CD}_3\text{OD}$ .....	S19
Figure S18. HMBC spectrum of compound <b>3</b> in $\text{CD}_3\text{OD}$ .....	S20
Figure S19. ROESY spectrum of compound <b>3</b> in $\text{CD}_3\text{OD}$ .....	S21
Figure S20. IR spectrum of compound <b>3</b> .....	S22
Figure S21. $^1\text{H}$ NMR spectrum of monanchosterol C ( <b>1a</b> ) in $\text{CD}_3\text{OD}$ .....	S23
Figure S22. $^{13}\text{C}$ NMR spectrum of monanchosterol C ( <b>1a</b> ) in $\text{CD}_3\text{OD}$ .....	S24
Figure S23 COSY spectrum of monanchosterol C ( <b>1a</b> ) in $\text{CD}_3\text{OD}$ .....	S25
Figure S24. HSQC spectrum of monanchosterol C ( <b>1a</b> ) in $\text{CD}_3\text{OD}$ .....	S26
Figure S25. HMBC spectrum of monanchosterol C ( <b>1a</b> ) in $\text{CD}_3\text{OD}$ .....	S27
Figure S26. ROESY spectrum of monanchosterol C ( <b>1a</b> ) in $\text{CD}_3\text{OD}$ .....	S28
Figure S27. IR spectrum of monanchosterol C ( <b>1a</b> ).....	S29
Table S1. COSY spectroscopic data for compounds <b>1</b> and <b>1a</b> in $\text{MeOH}-d_4$ .....	S30



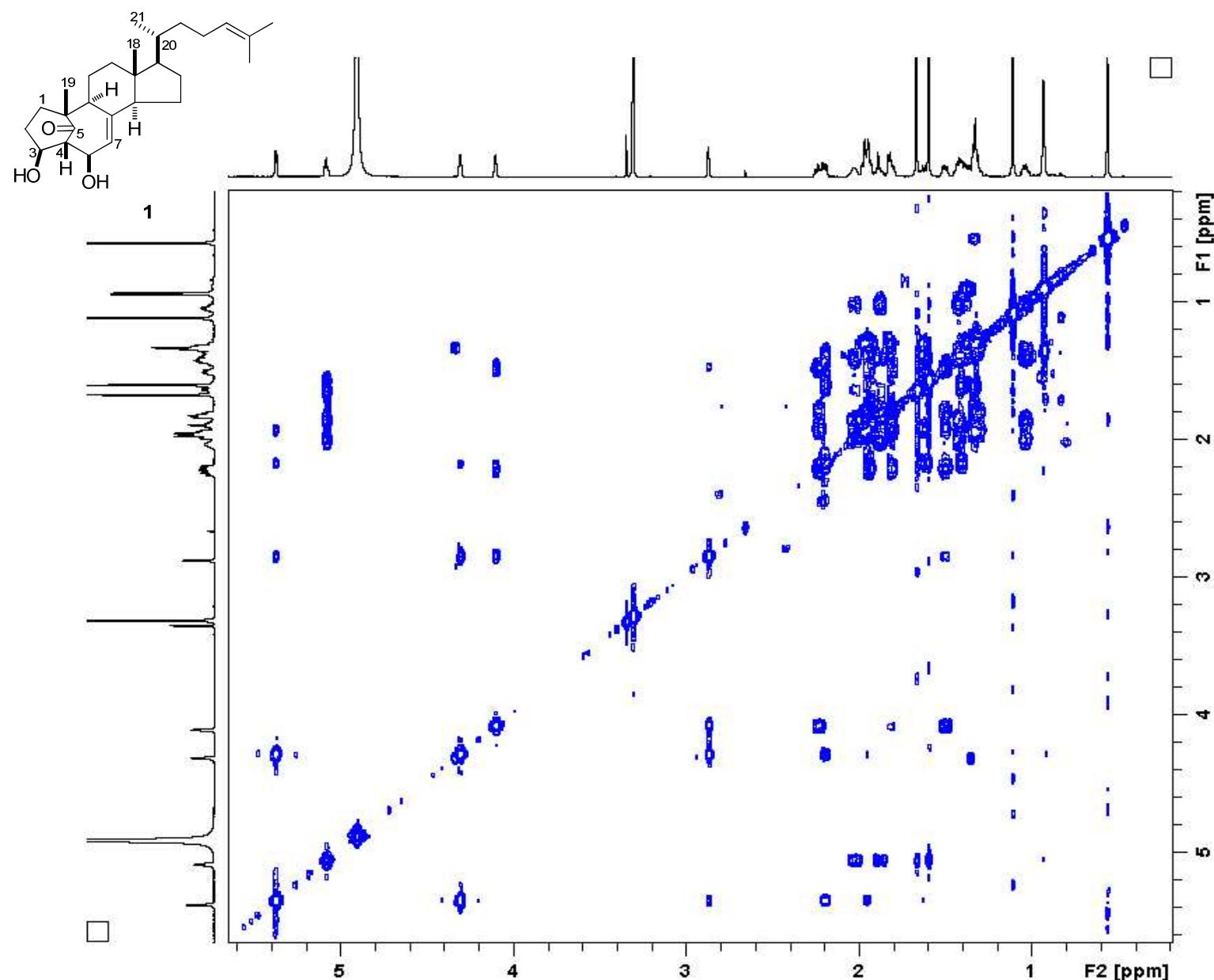
**Figure S1.**  $^1\text{H}$  NMR spectrum of monanchosterol A (**1**) in  $\text{CD}_3\text{OD}$ .



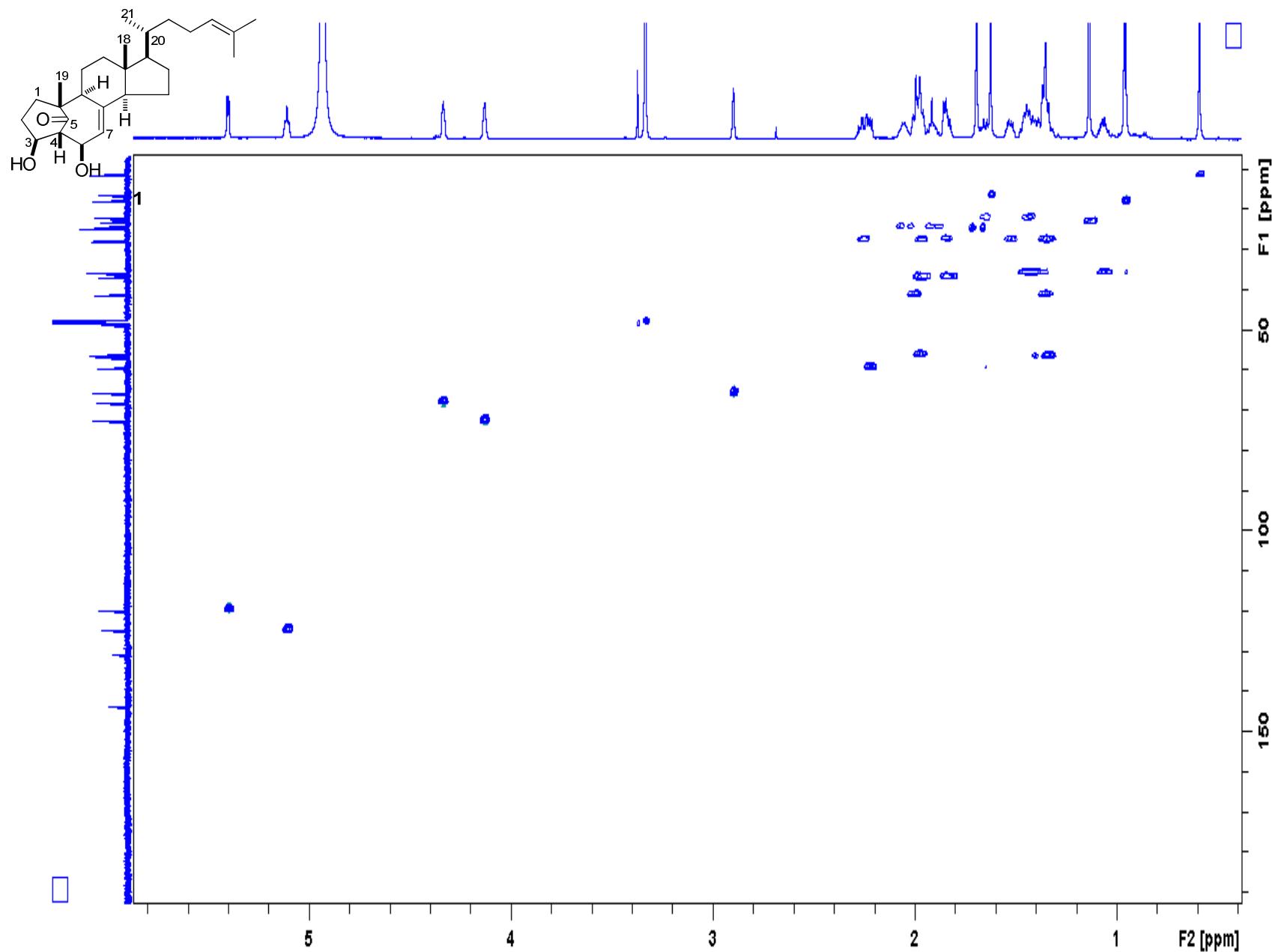
Expended  $^{13}\text{C}$  NMR spectrum of monanchosterol A (**1**) in  $\text{CD}_3\text{OD}$ .



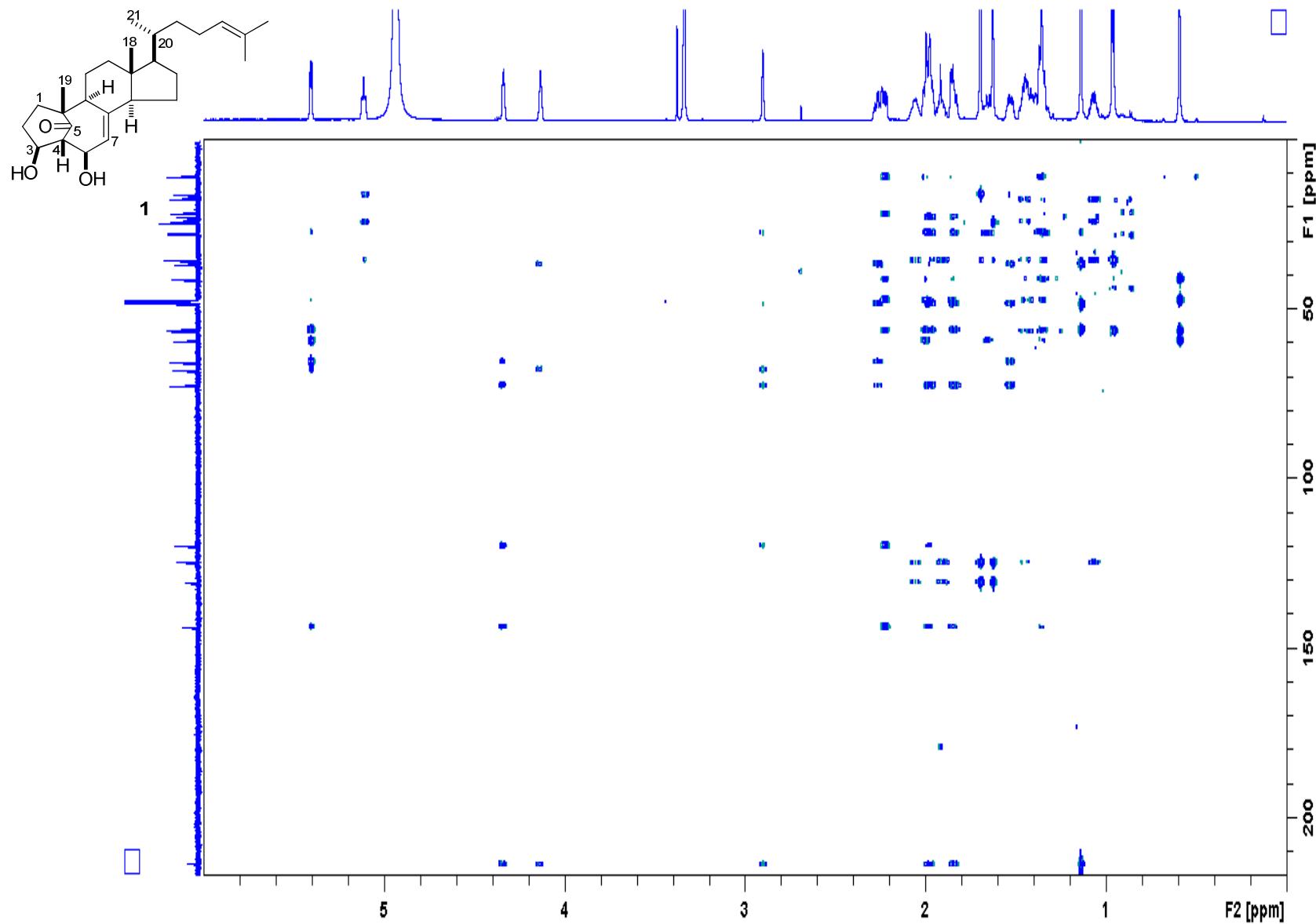
**Figure S2.**  $^{13}\text{C}$  NMR spectrum of monanchosterol A (**1**) in  $\text{CD}_3\text{OD}$ .



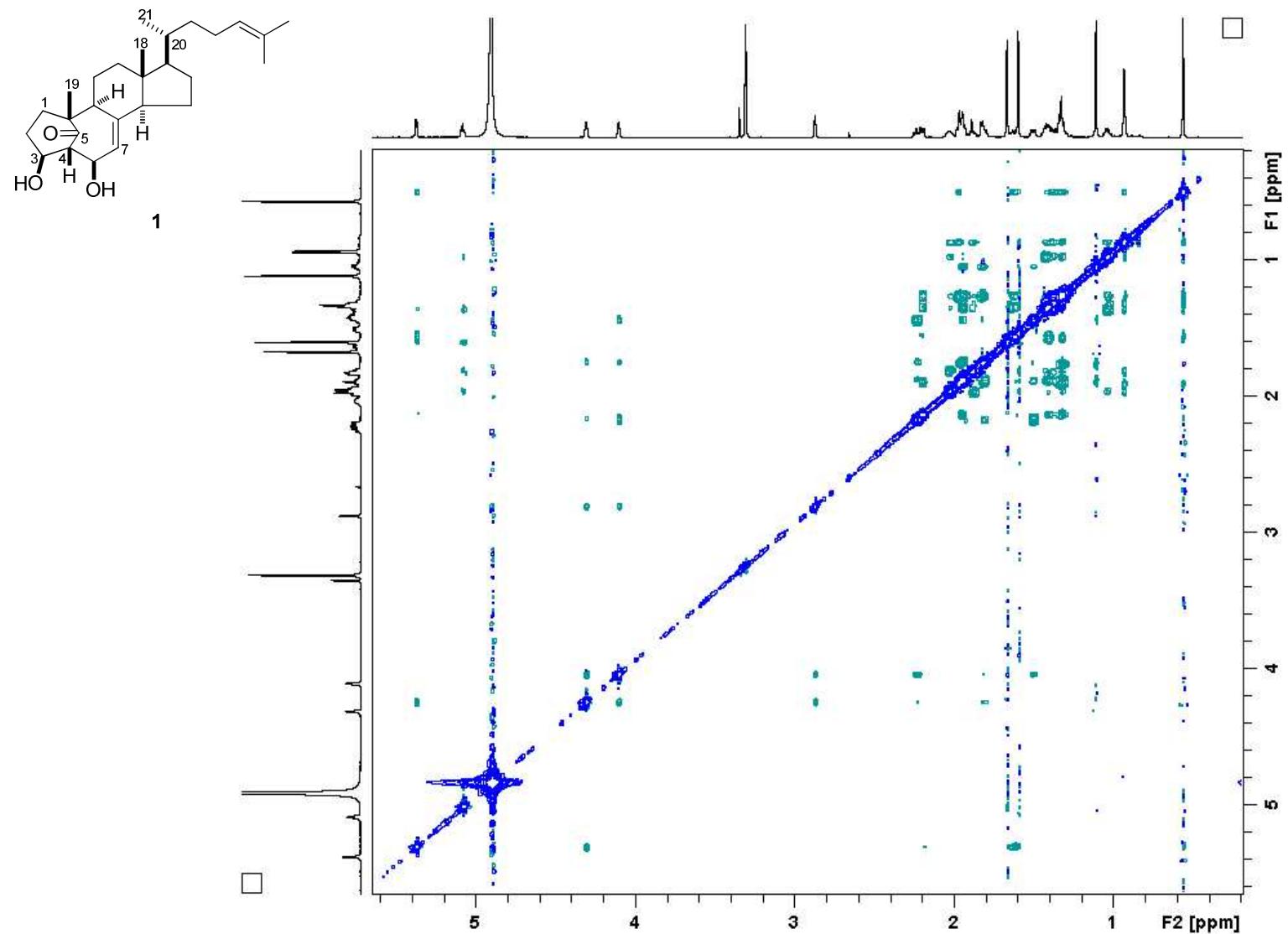
**Figure S3.** COSY spectrum of monanchosterol A (**1**) in  $\text{CD}_3\text{OD}$ .



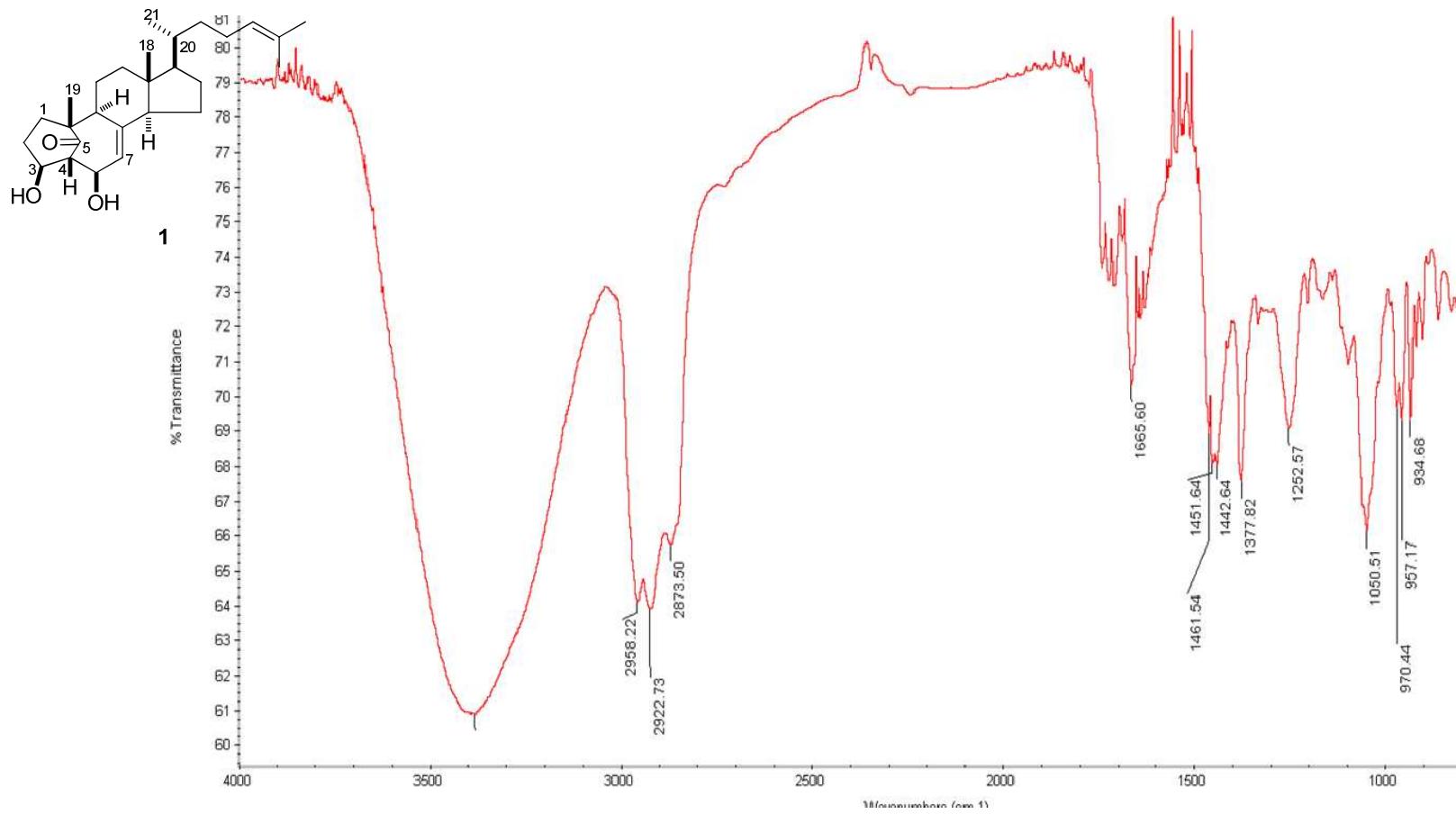
**Figure S4.** HSQC spectrum of monanchosterol A (**1**) in  $\text{CD}_3\text{OD}$ .



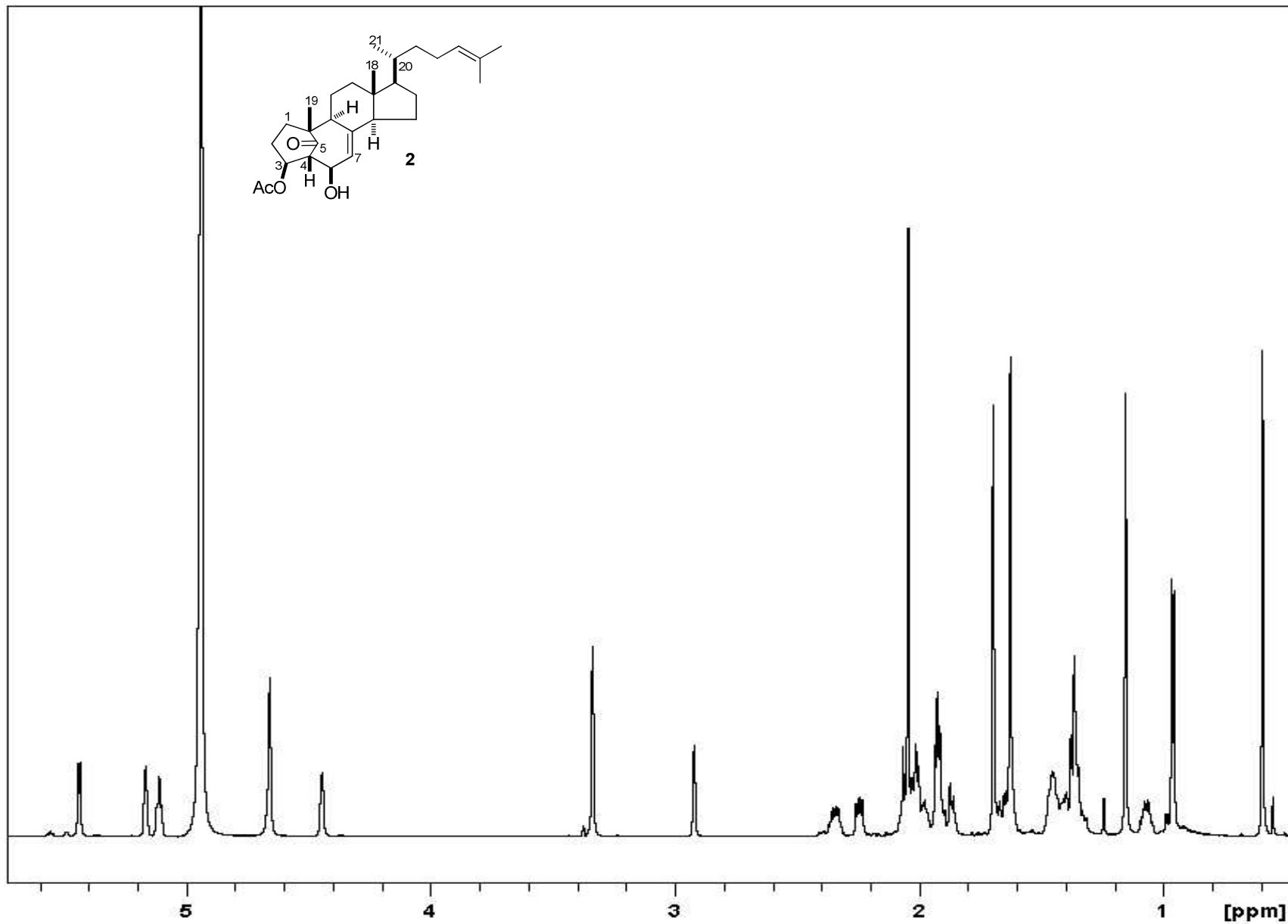
**Figure S5.** HMBC spectrum of monanchosterol A (**1**) in  $\text{CD}_3\text{OD}$ .



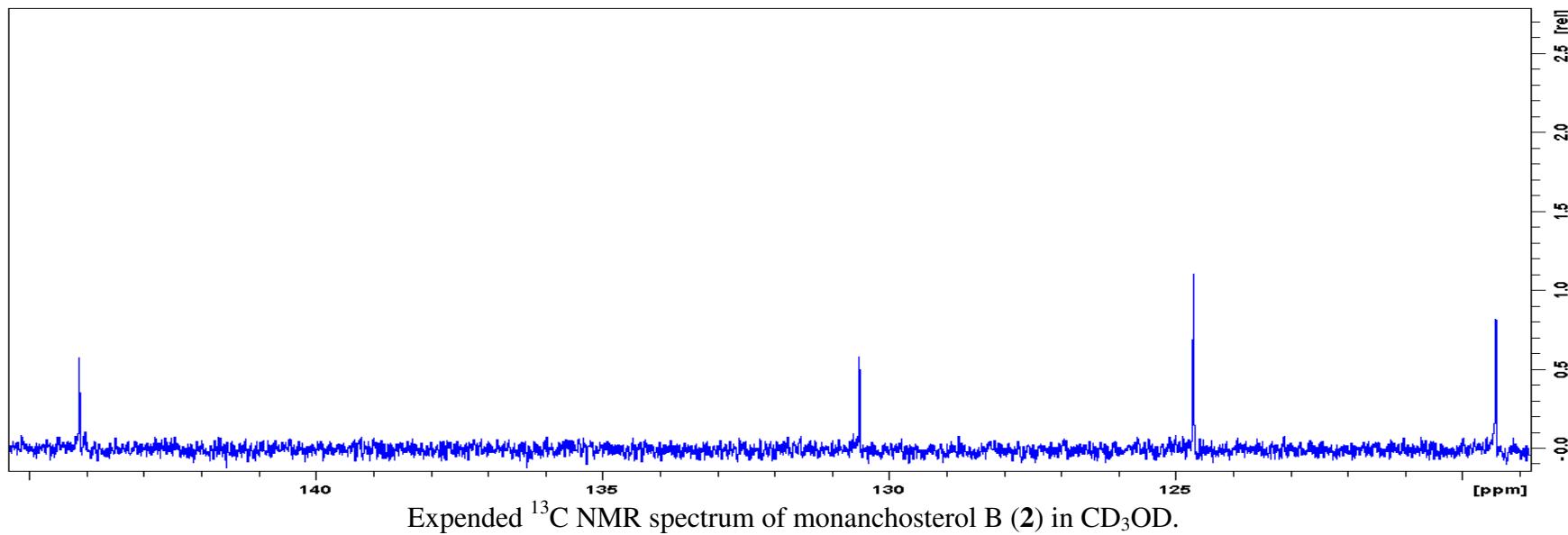
**Figure S6.** ROESY spectrum of monanchosterol A (**1**) in  $\text{CD}_3\text{OD}$ .



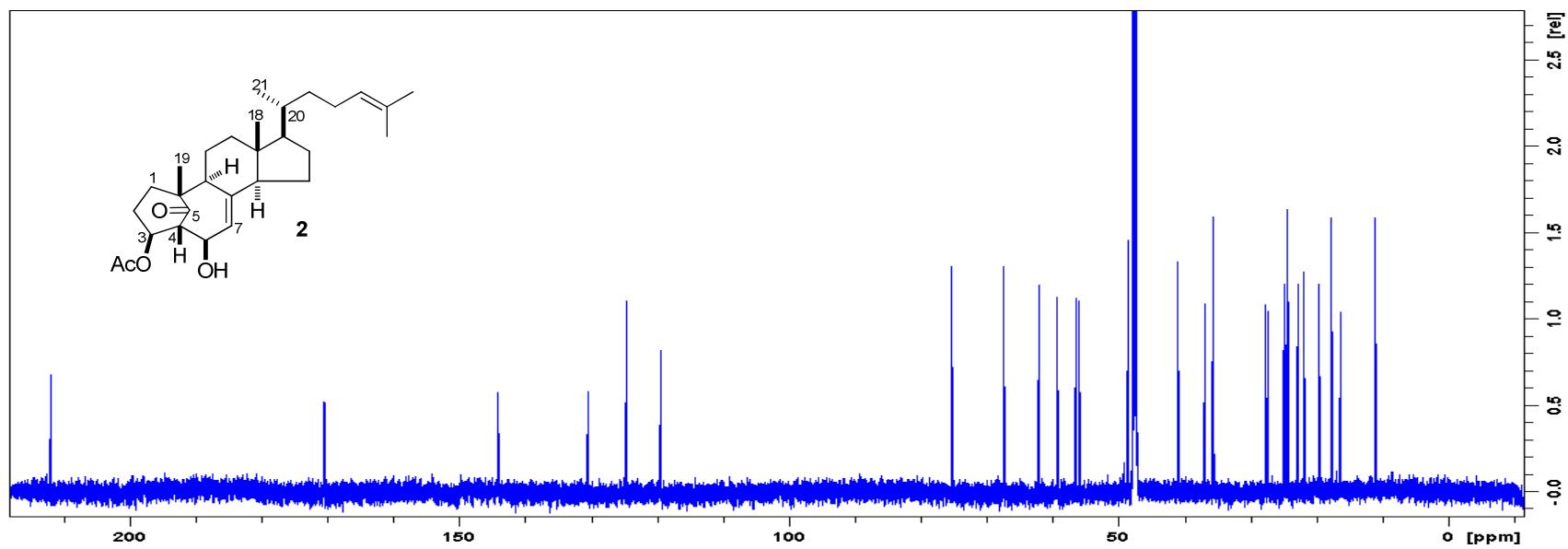
**Figure S7.** IR spectrum of monanchosterol A (**1**).



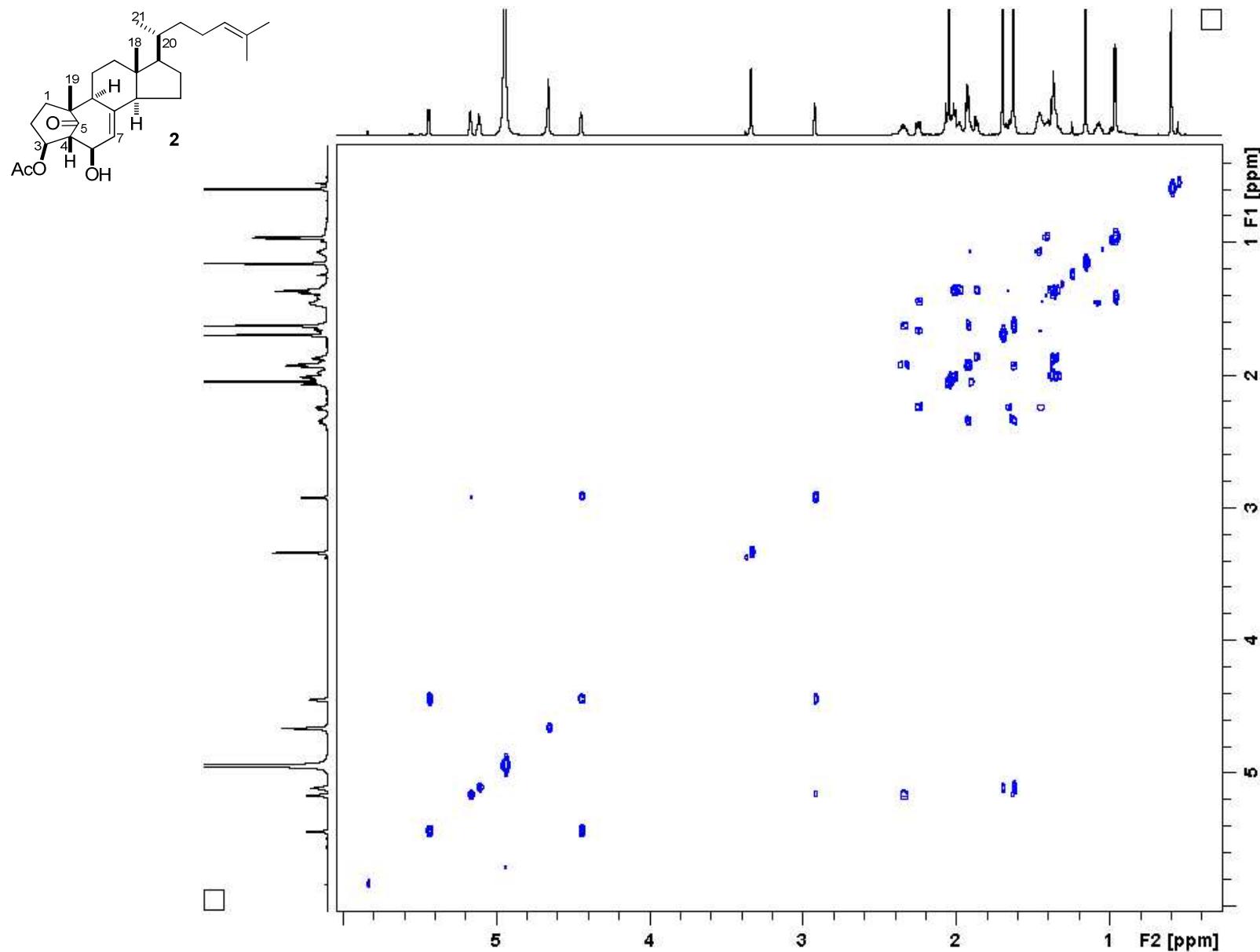
**Figure S8.**  $^1\text{H}$  NMR spectrum of monanchosterol B (**2**) in  $\text{CD}_3\text{OD}$ .



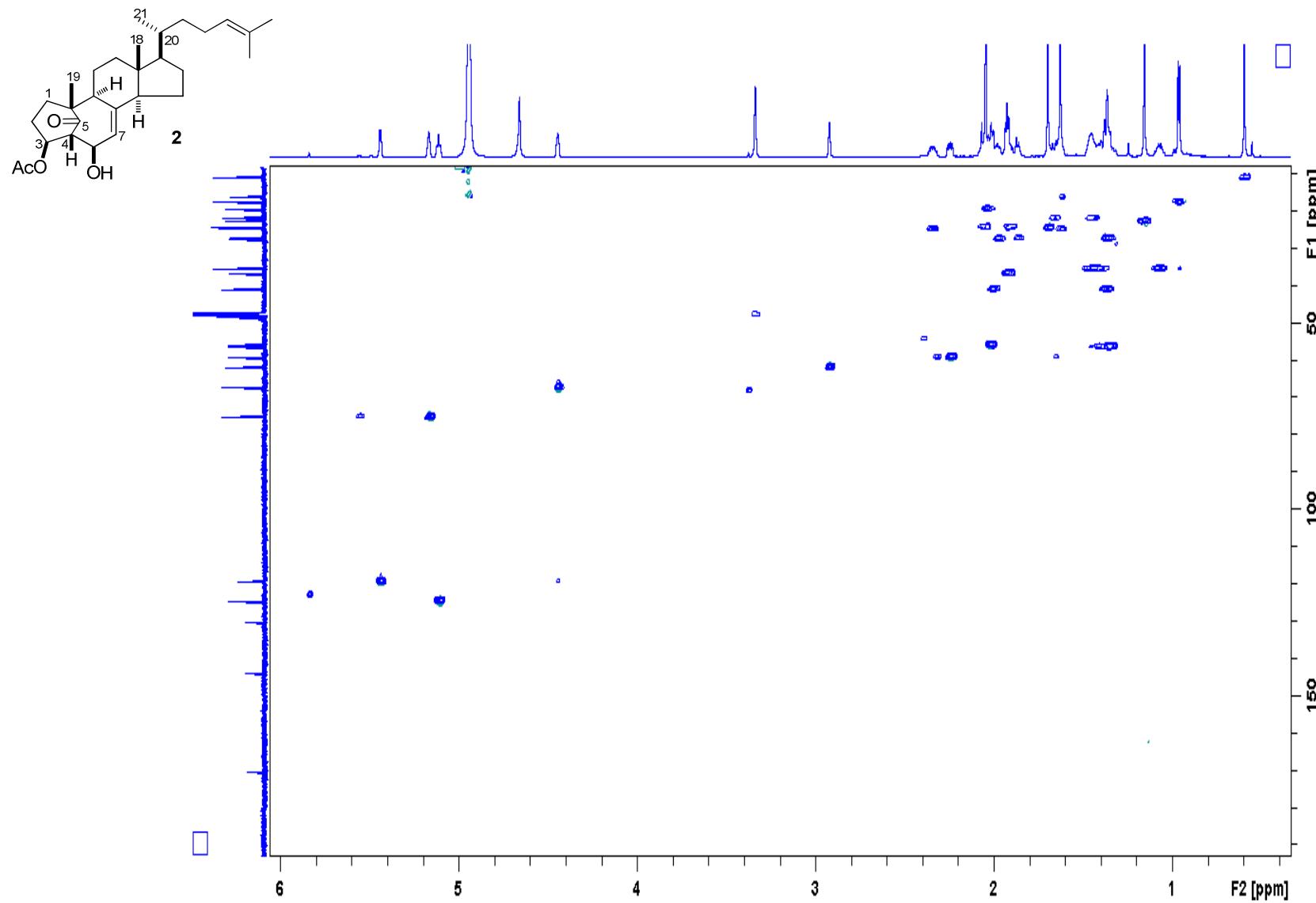
Expended  $^{13}\text{C}$  NMR spectrum of monanchosterol B (2) in  $\text{CD}_3\text{OD}$ .



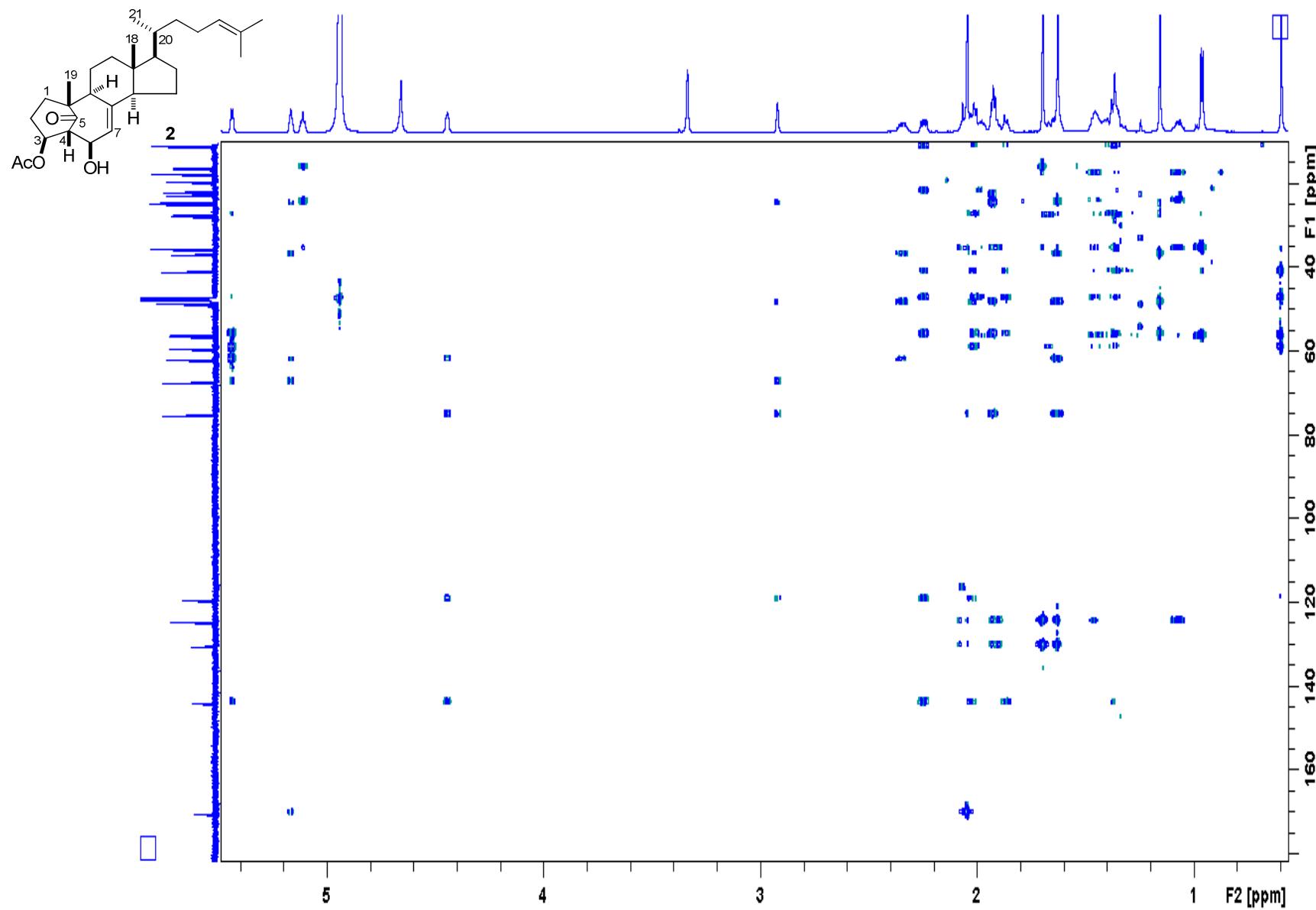
**Figure S9.**  $^{13}\text{C}$  NMR spectrum of monanchosterol B (2) in  $\text{CD}_3\text{OD}$ .



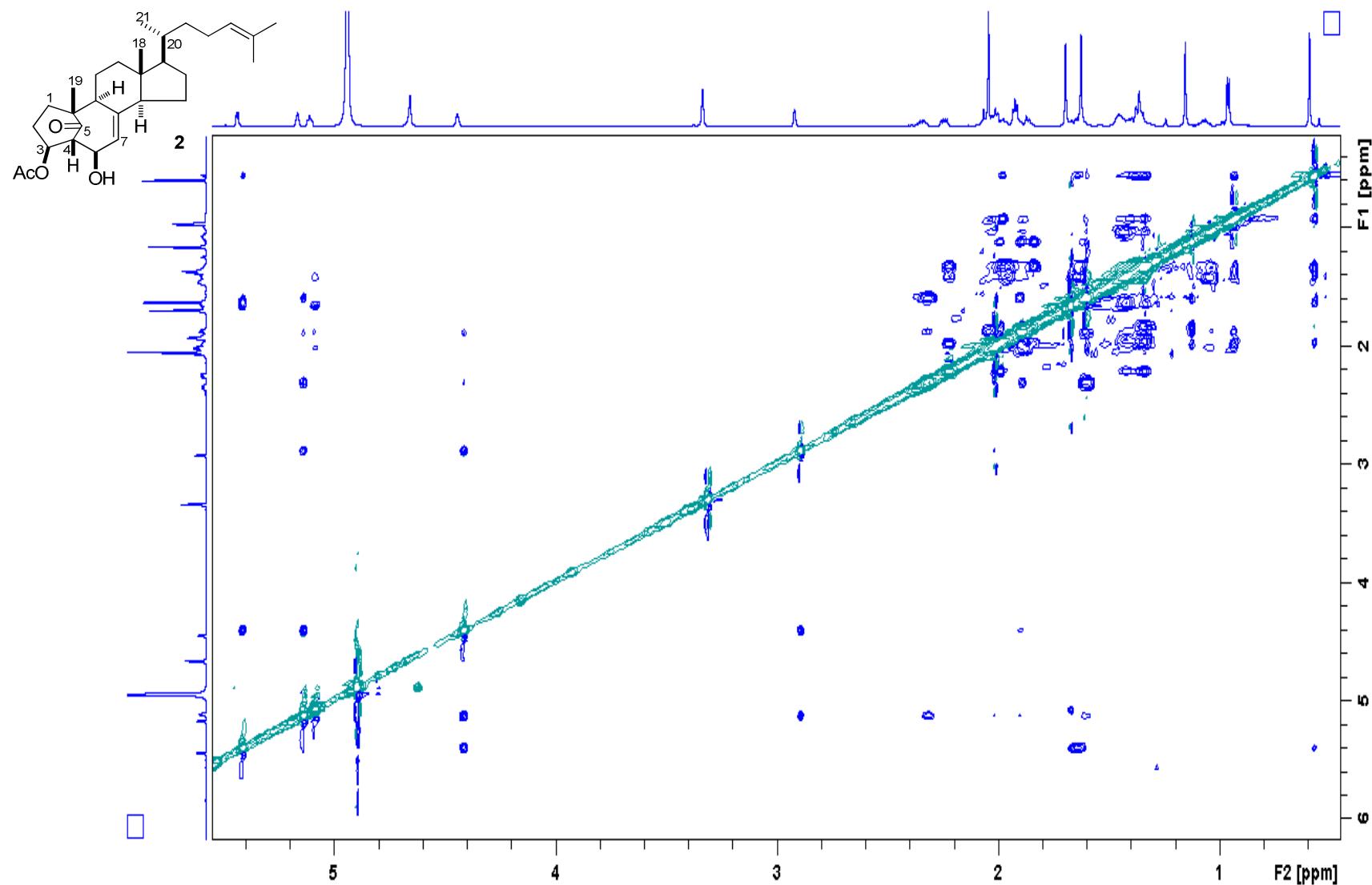
**Figure S10.** COSY spectrum of monanchosterol B (**2**) in  $\text{CD}_3\text{OD}$ .



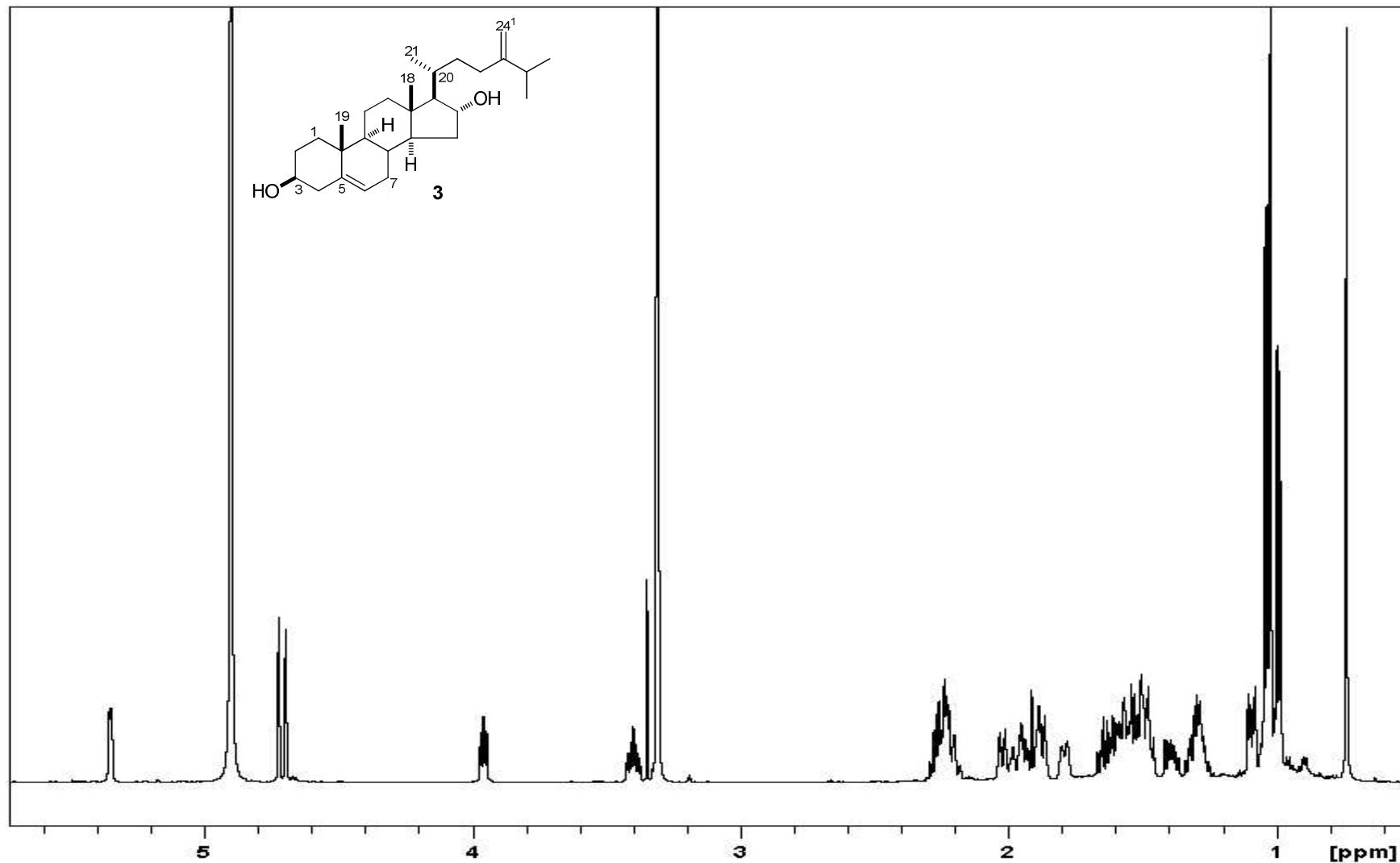
**Figure S11.** HSQC spectrum of monanchosterol B (**2**) in  $CD_3OD$ .



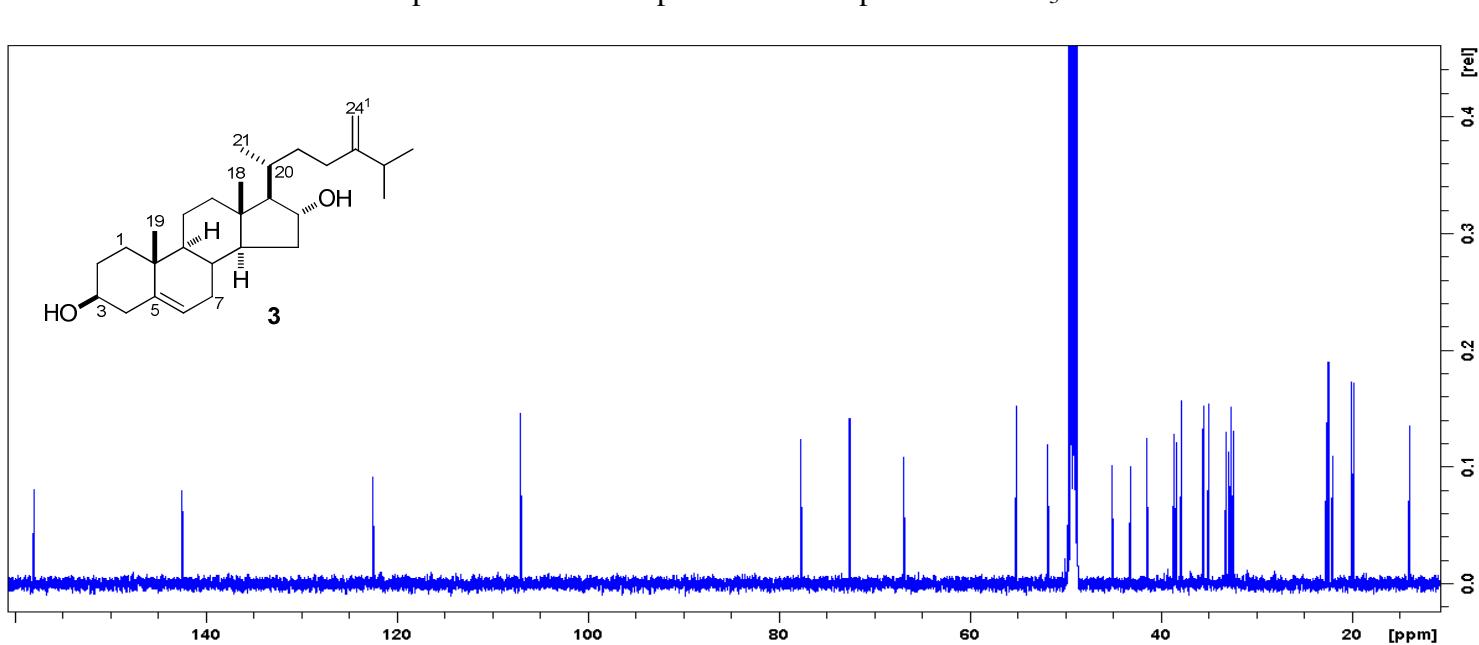
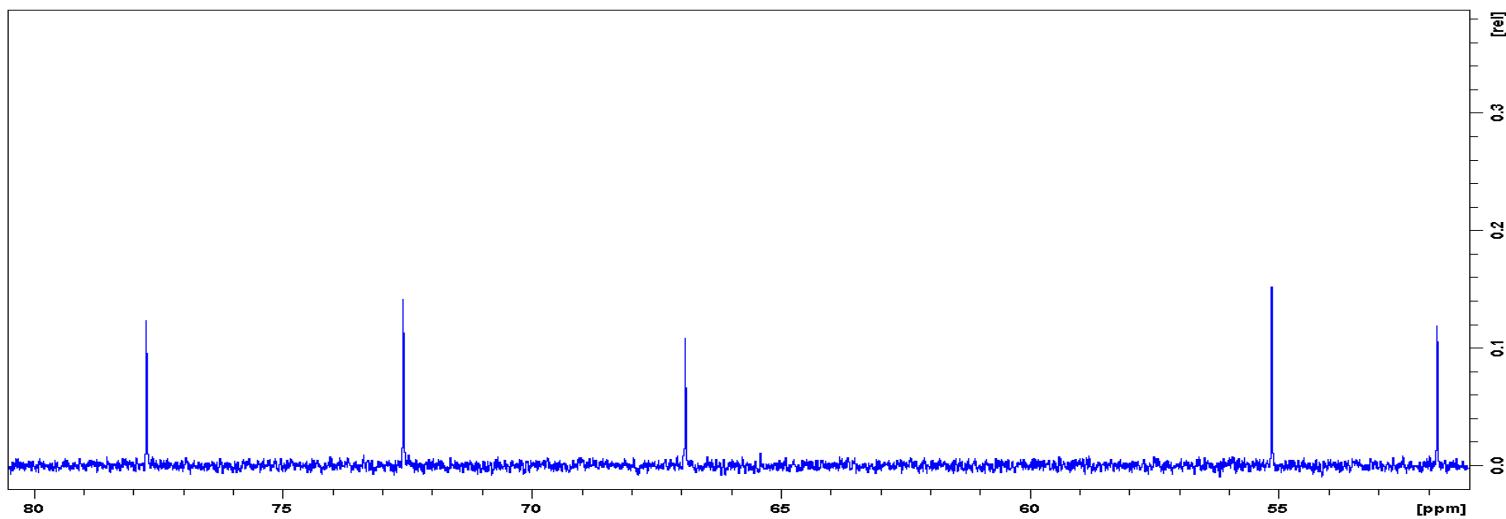
**Figure S12.** HMBC spectrum of monanchosterol B (**2**) in  $\text{CD}_3\text{OD}$ .



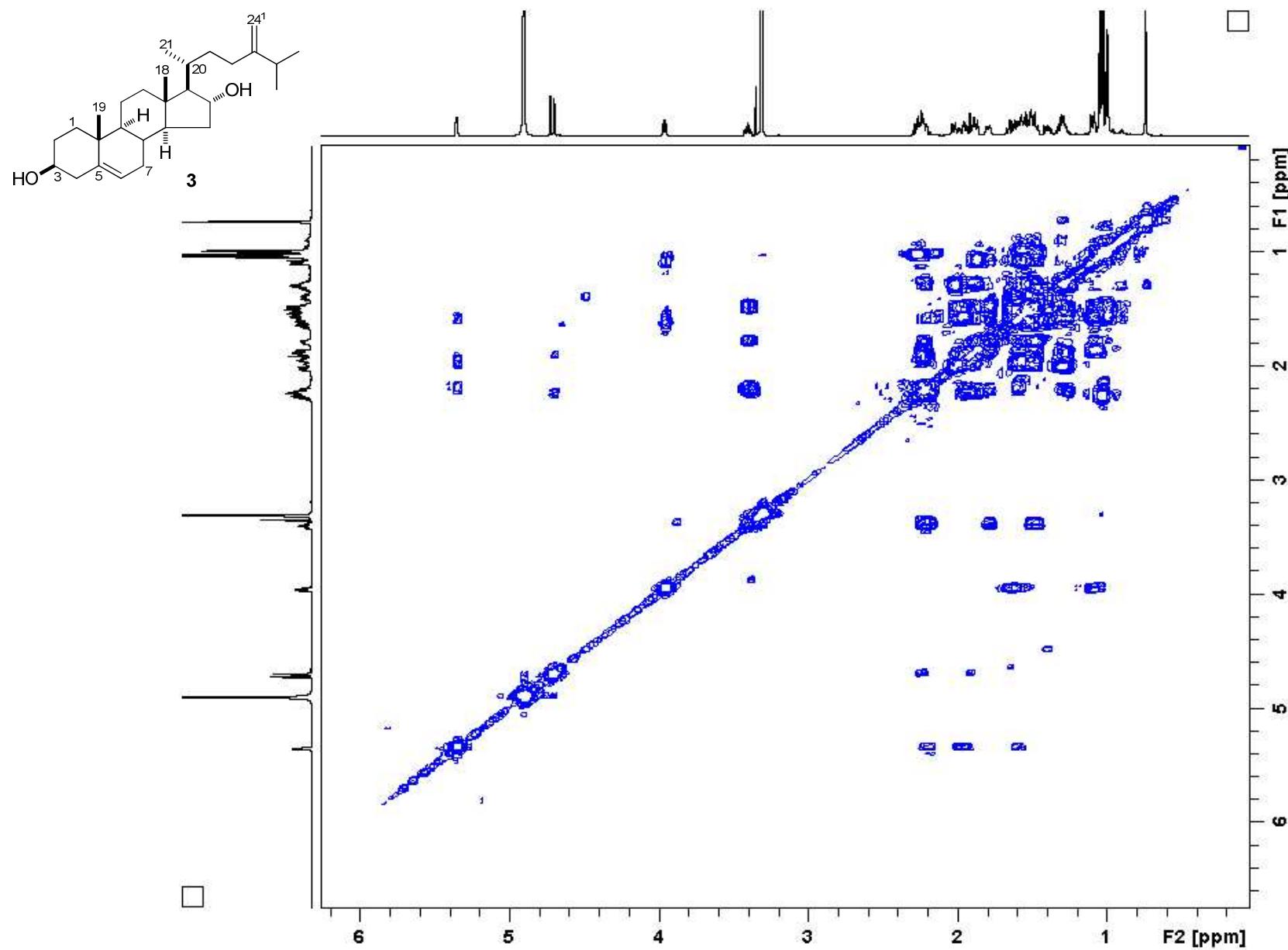
**Figure S13.** ROESY spectrum of monanchosterol B (**2**) in  $\text{CD}_3\text{OD}$ .



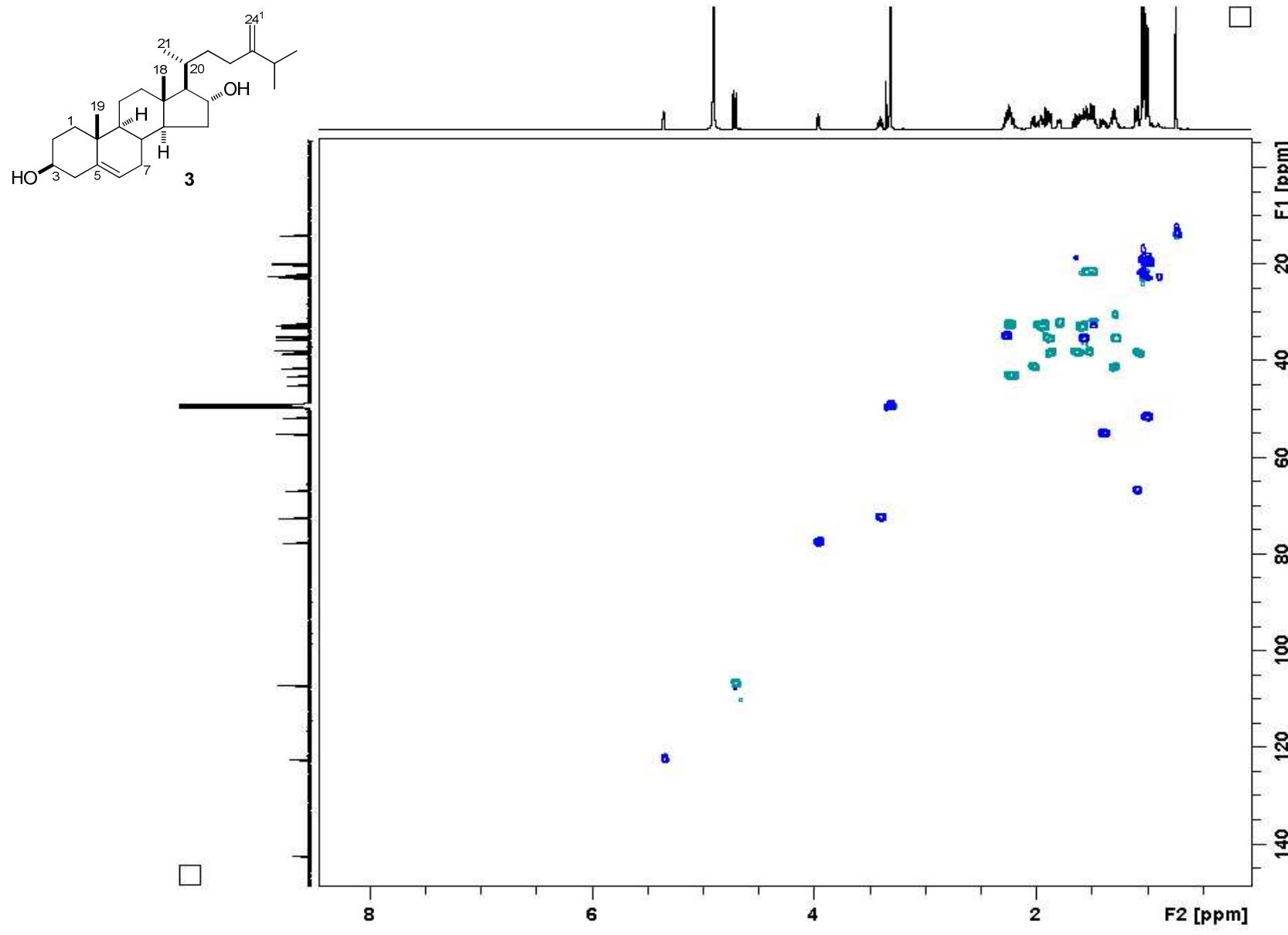
**Figure S14.**  $^1\text{H}$  NMR spectrum of compound **3** in  $\text{CD}_3\text{OD}$ .



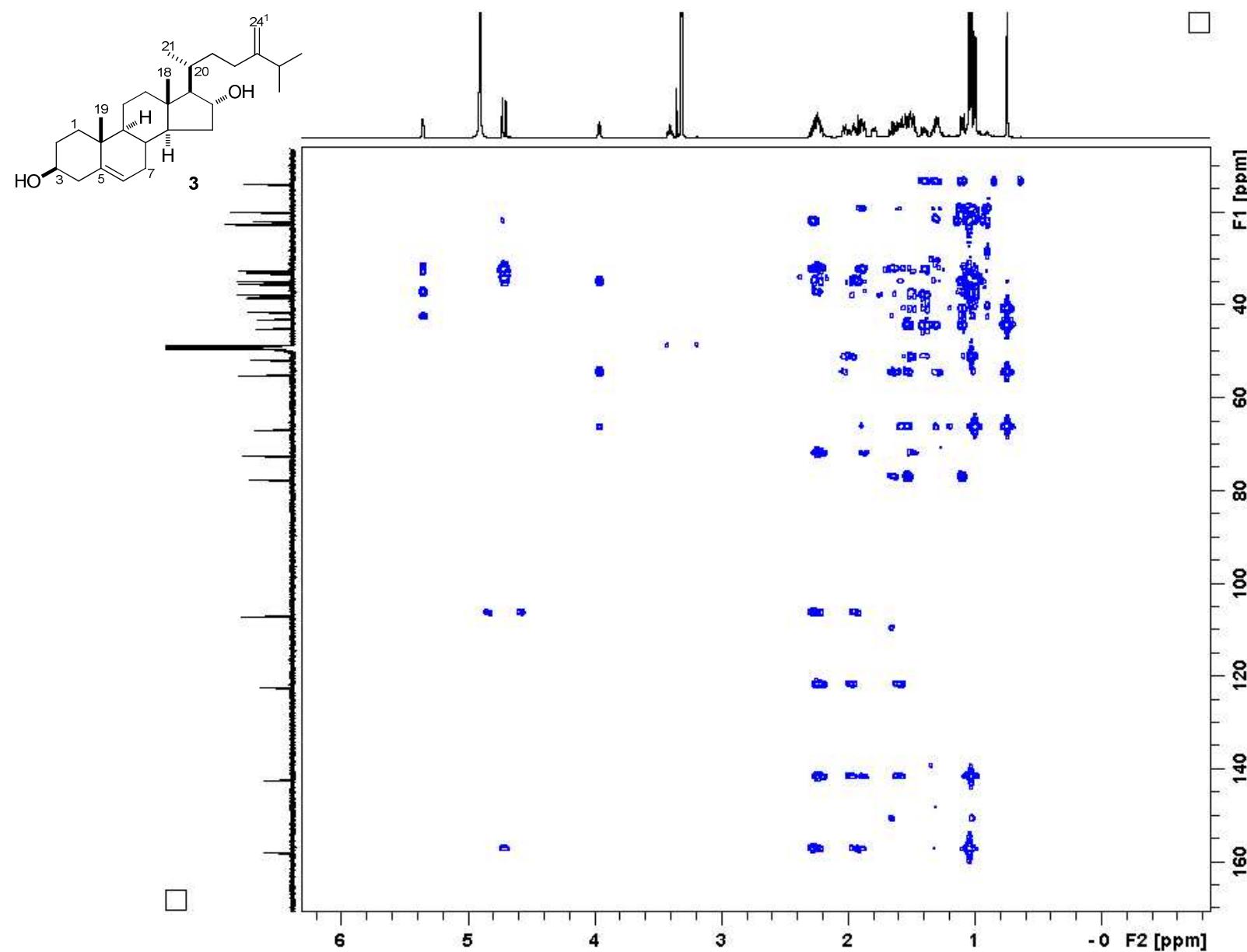
**Figure S15.**  $^{13}\text{C}$  NMR spectrum of compound 3 in  $\text{CD}_3\text{OD}$ .



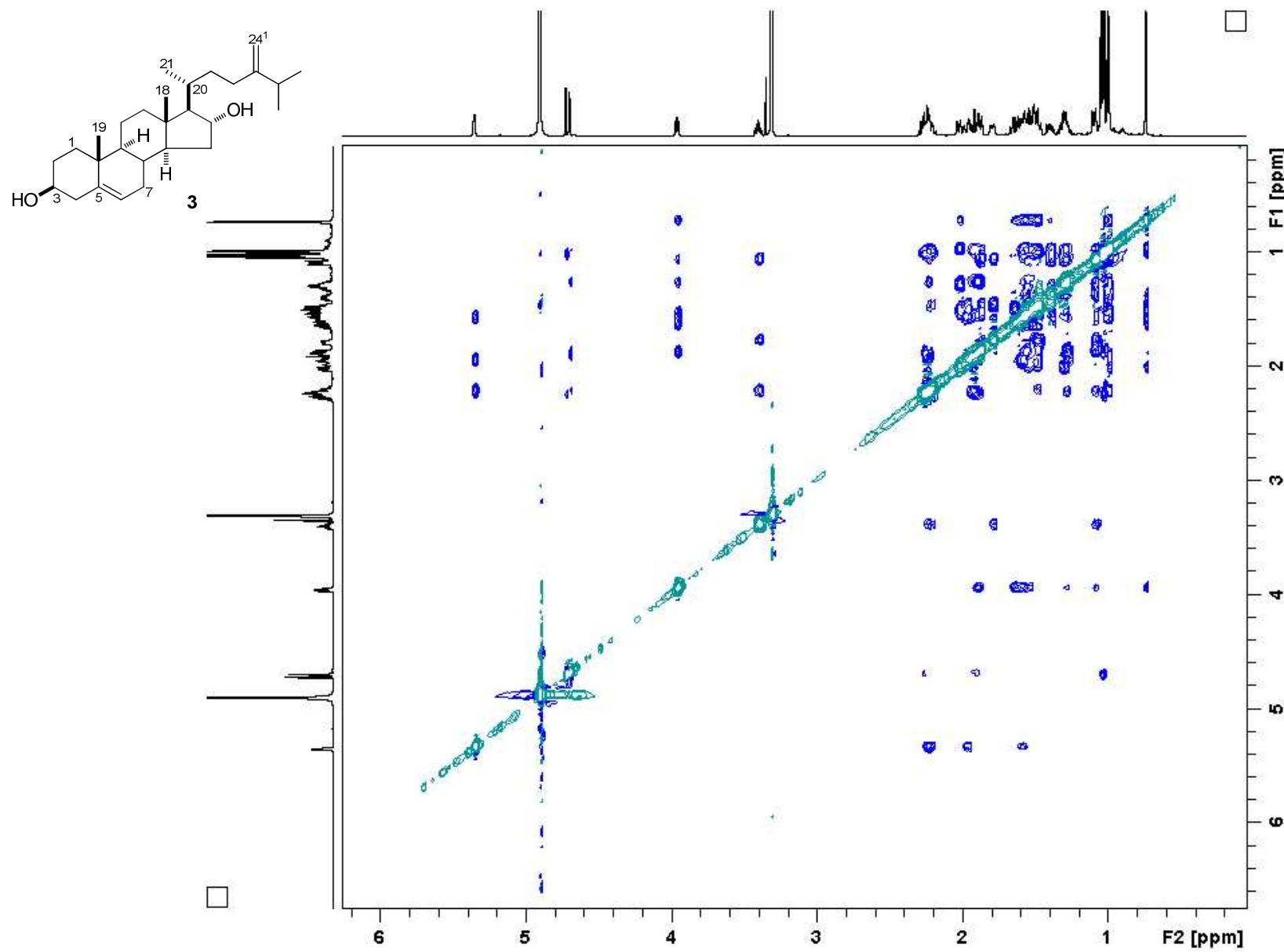
**Figure S16.** COSY spectrum of compound 3 in  $CD_3OD$ .



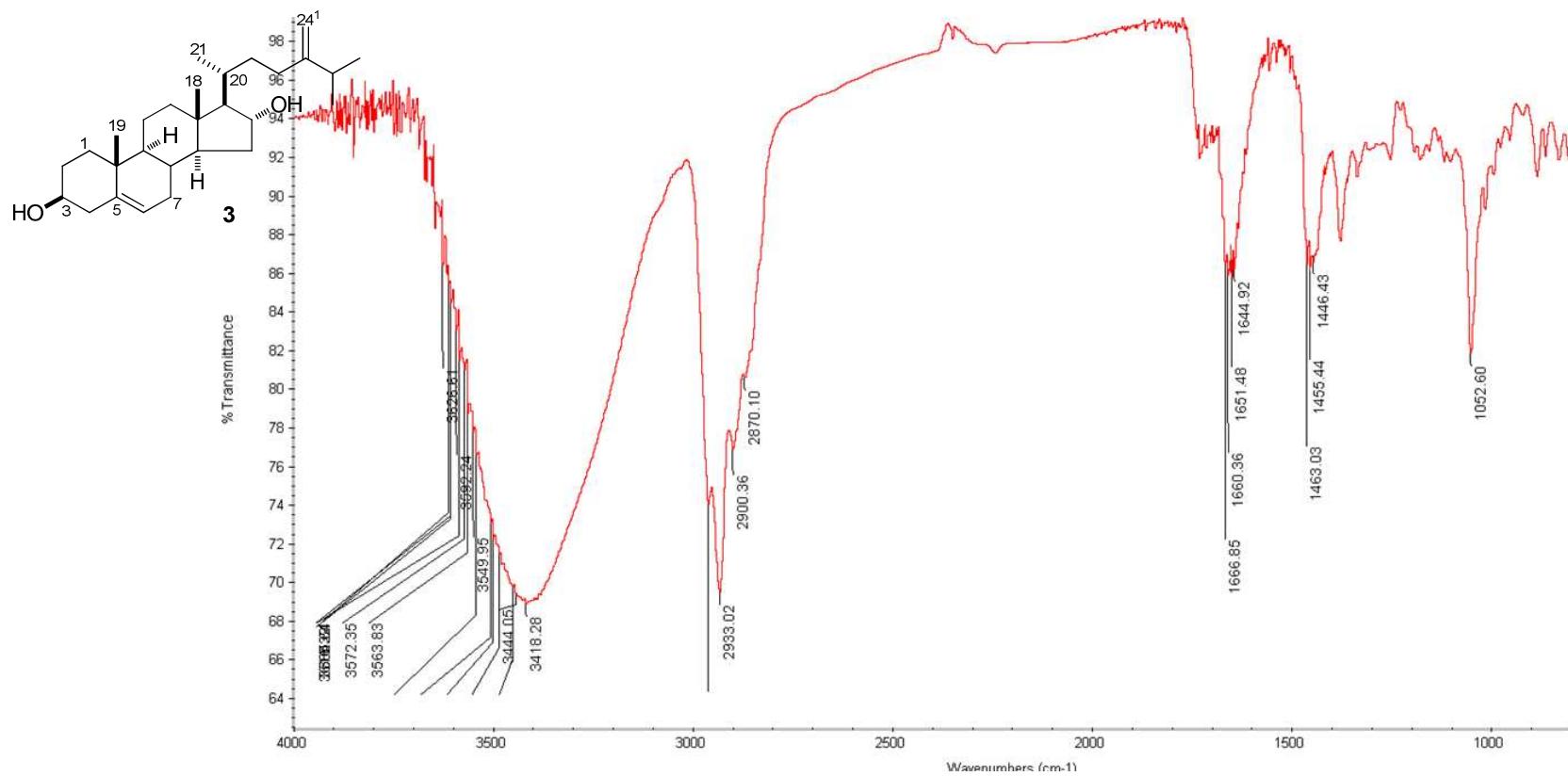
**Figure S17.** Edited HSQC spectrum of compound **3** in  $\text{CD}_3\text{OD}$ .



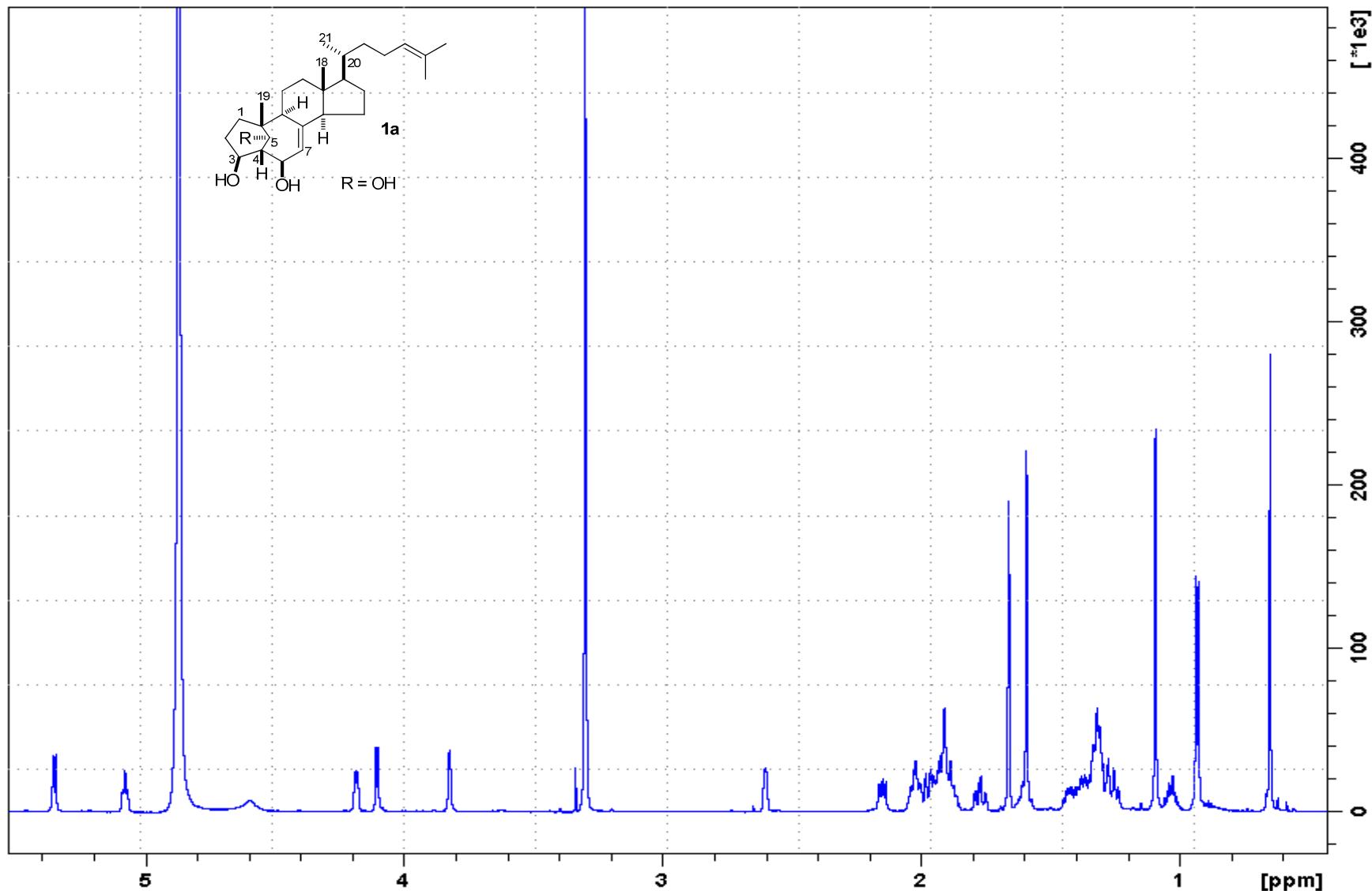
**Figure S18.** HMBC spectrum of compound **3** in  $\text{CD}_3\text{OD}$ .



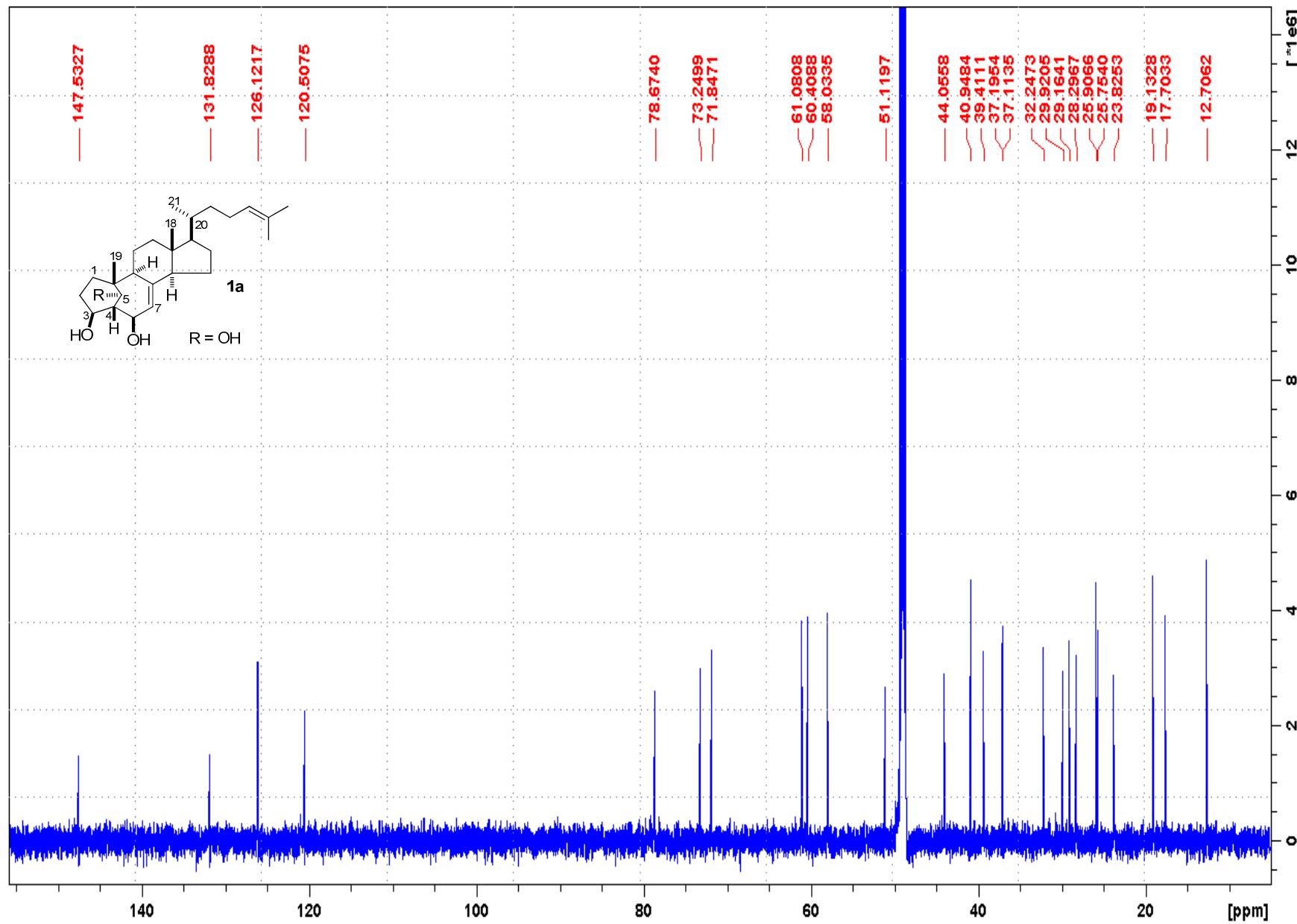
**Figure S19.** ROESY spectrum of compound **3** in  $\text{CD}_3\text{OD}$ .



**Figure S20.** IR spectrum of compound **3**.



**Figure S21.**  $^1\text{H}$  NMR spectrum of monanchosterol C (**1a**) in  $\text{CD}_3\text{OD}$ .



**Figure S22.**  $^{13}\text{C}$  NMR spectrum of monanchosterol C (**1a**) in  $\text{CD}_3\text{OD}$ .

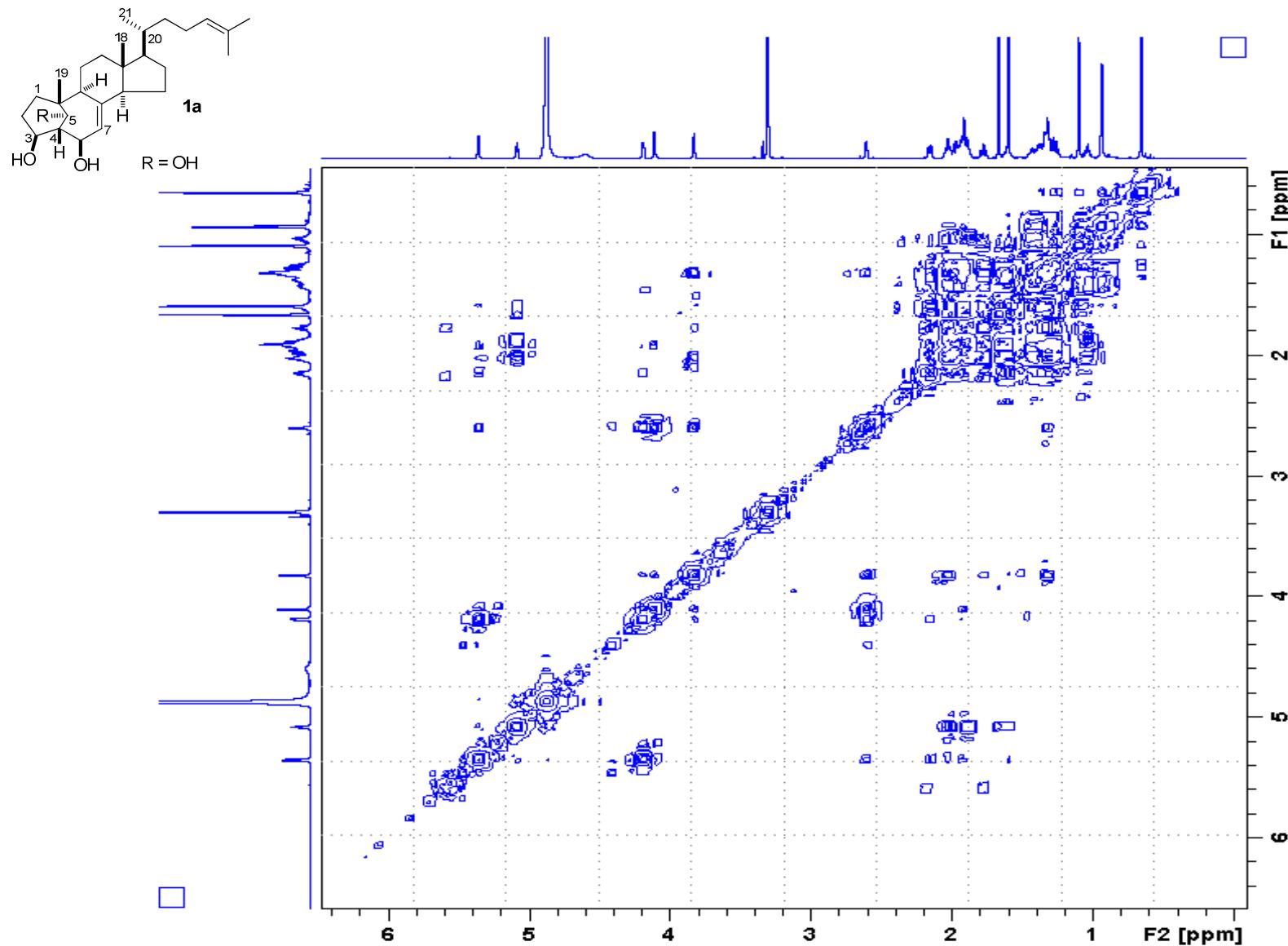
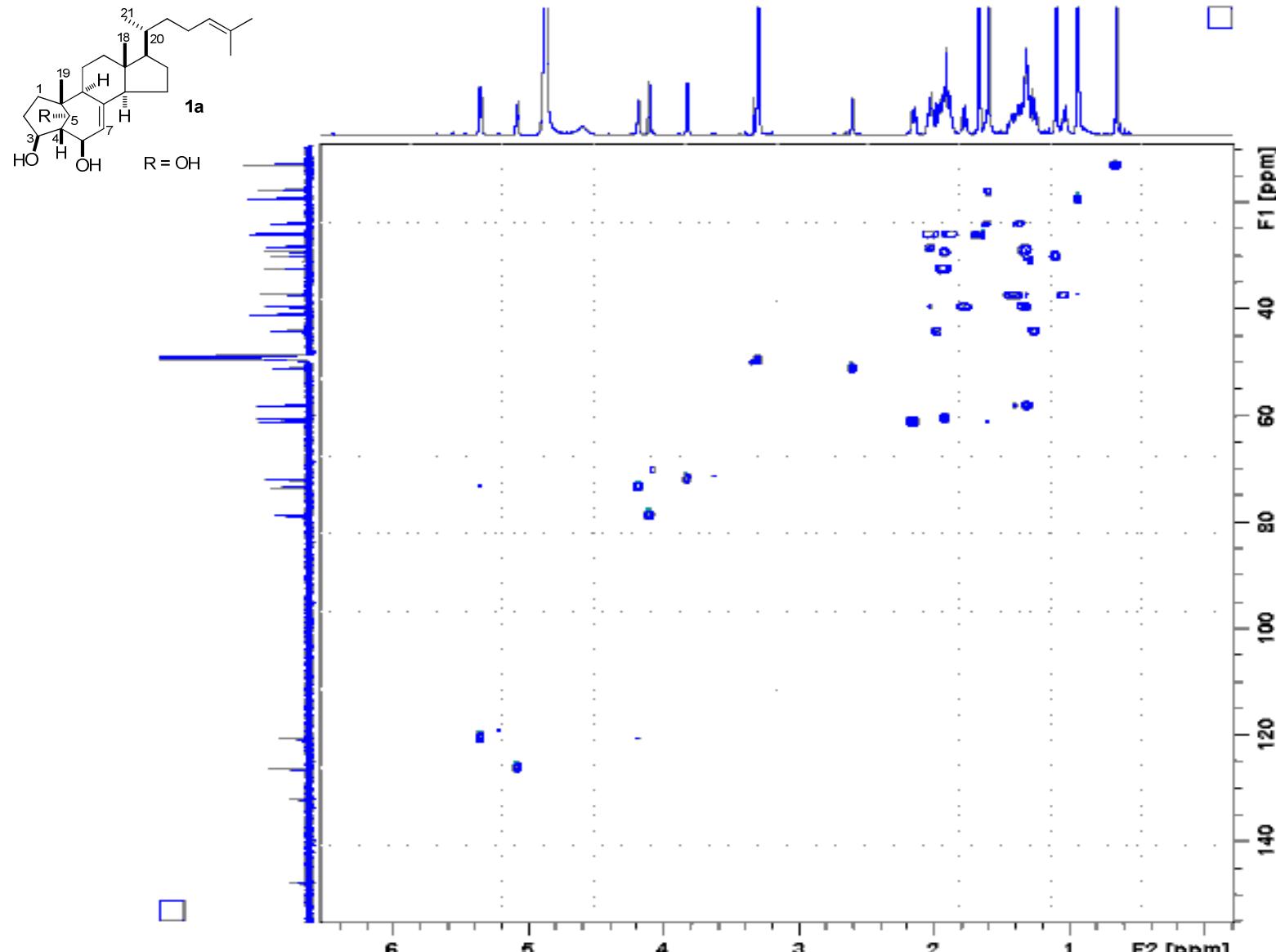
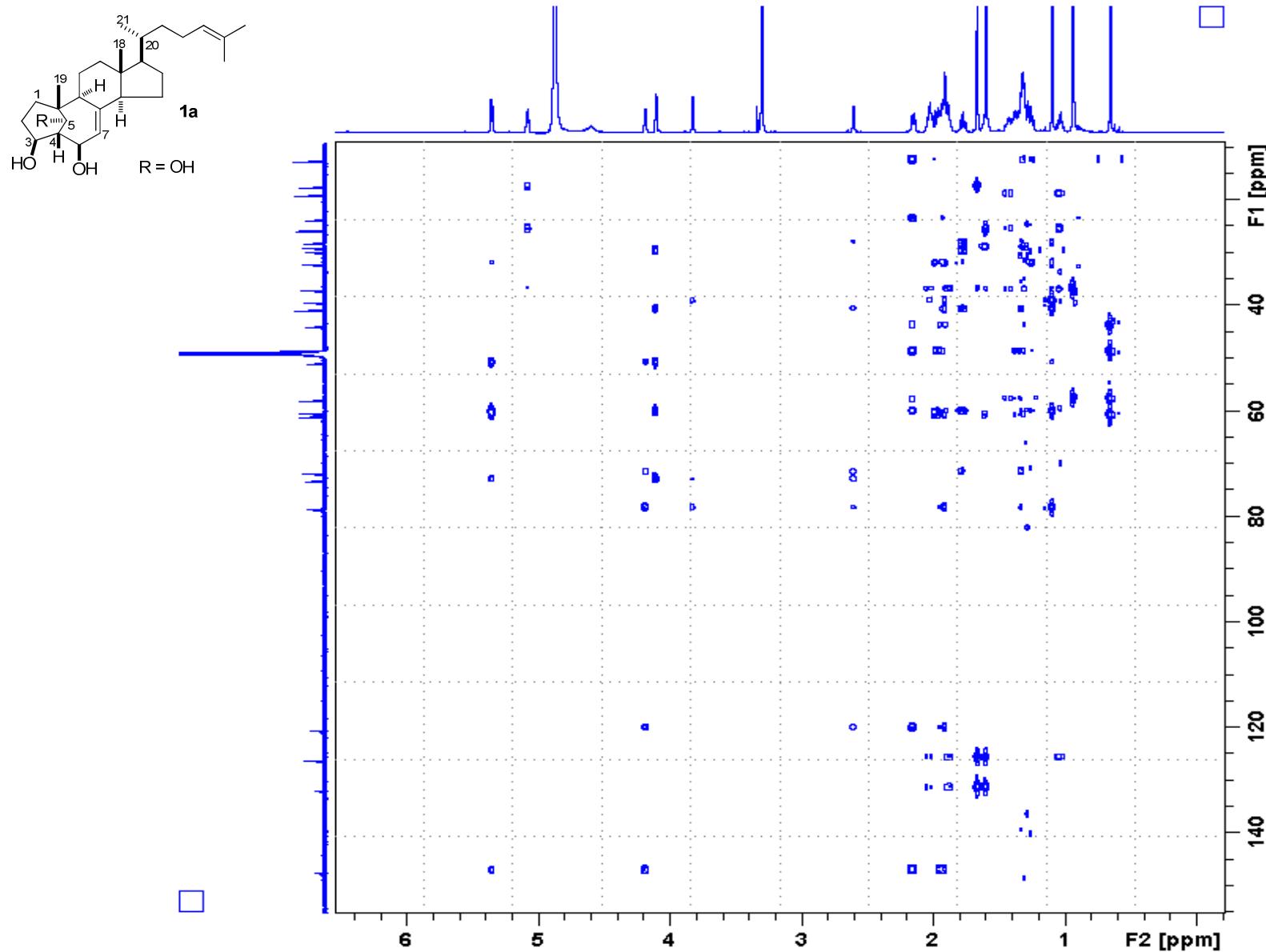


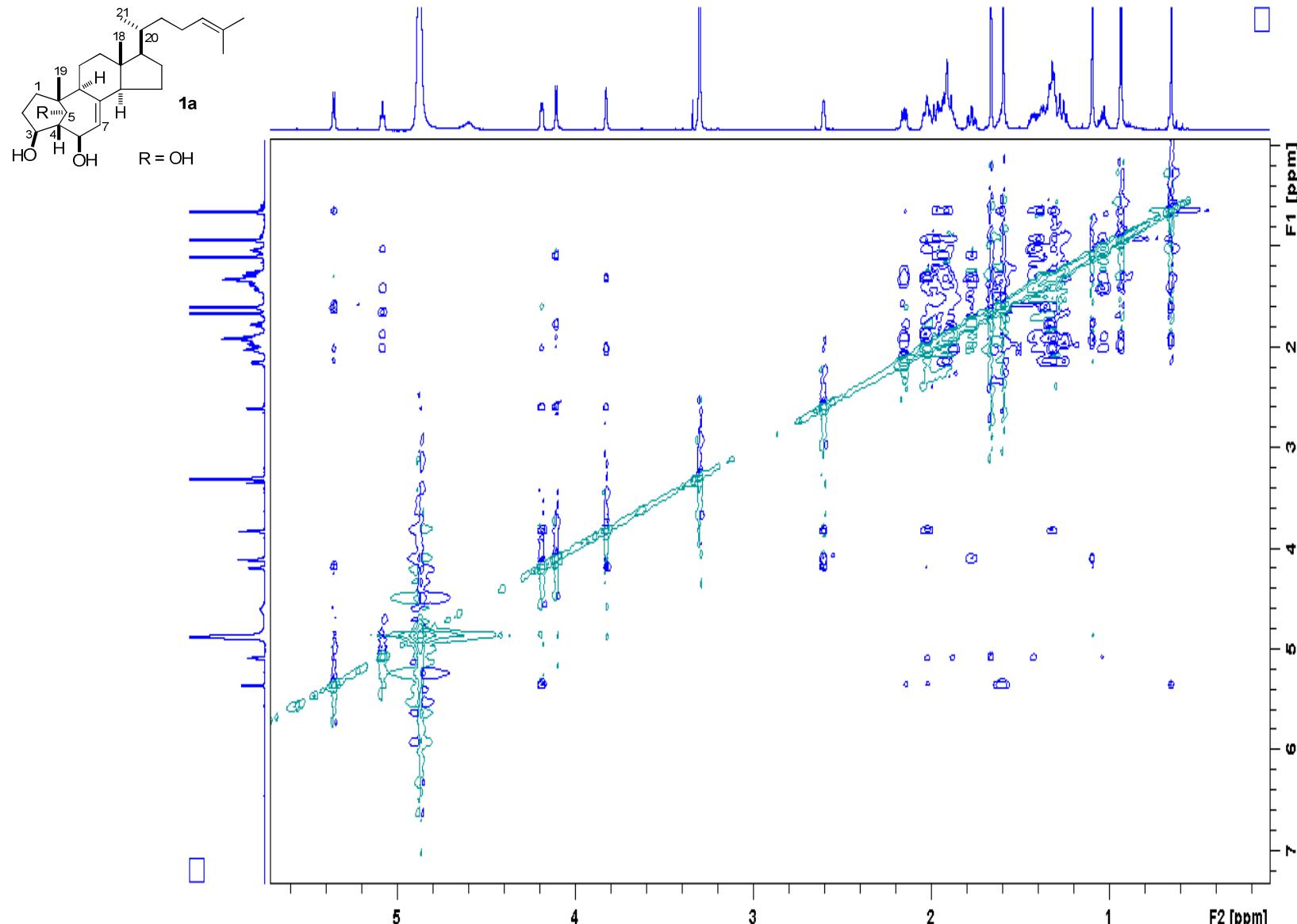
Figure S23. COSY spectrum of monanchosterol C (**1a**) in  $\text{CD}_3\text{OD}$ .



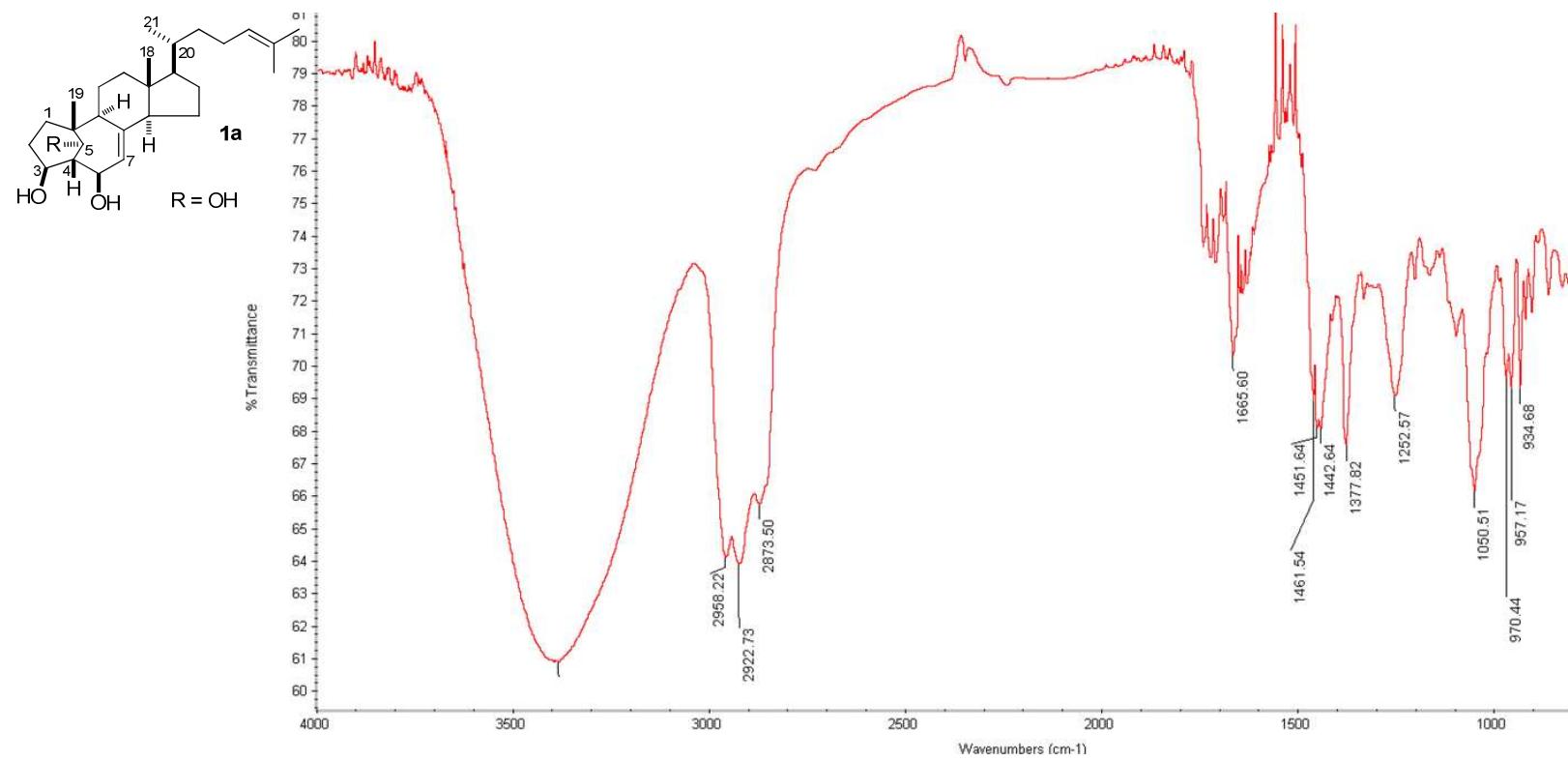
**Figure S24.** HSQC spectrum of monanchosterol C (**1a**) in  $\text{CD}_3\text{OD}$ .



**Figure S25.** HMBC spectrum of monanchosterol C (**1a**) in  $\text{CD}_3\text{OD}$ .



**Figure S26.** ROESY spectrum of monanchosterol C (**1a**) in  $\text{CD}_3\text{OD}$ .



**Figure S27.** IR spectrum of monanchosterol C (**1a**).

**Table S1.** COSY Spectroscopic Data for Compounds **1** and **1a** in MeOH-*d*<sub>4</sub>

position	<b>1</b>		<b>1a</b>	
	$\delta_{\text{H}}$ ( <i>J</i> in Hz)	COSY	$\delta_{\text{H}}$ ( <i>J</i> in Hz)	COSY
1a	1.93, m	2a, 2b, 1b	1.78, td (14.1, 4.6)	2a, 2b, 1b
1b	1.81, m	2a, 2b, 1a	1.33, m	2a, 2b, 1a
2a	2.23, m	1a, 1b, 2b, 3	2.02, m	1a, 1b, 2b, 3
2b	1.50, m	1a, 1b, 2a, 3	1.32, m	1a, 1b, 2a, 3
3	4.10, br dd (6.5, 4.2)	2a, 2b, 4	3.82, br d (1.9)	2a, 2b, 4
4	2.87, br s	3, 6	2.60 br s,	3, 5, 6
5			4.10, d (5.7)	4
6	4.31, dd (5.0, 4.3)	4, 7	4.18, dd (7.0, 2.7)	4, 7
7	5.38, d (5.0)	6, 9, 14	5.35, d (7.0)	6, 9, 14
8				
9	1.94, m	7, 11a, 11b	1.92, m	7, 11a, 11b
10				
11a	1.82, m	9, 12a	1.95, m	9
11b	1.32, m	9, 12a	1.92, m	9
12a	1.97, m	11a, 11b, 12b	1.98, m	12b
12b	1.32, m	12a	1.25, m	12a
13				
14	2.18, dd (12.5, 6.3)	7, 15a, 15b	2.15, dd (12.7, 6.4)	7, 15a, 15b
15a	1.62, m	14, 16a	1.61 m	14, 16a
15b	1.39, m	14	1.37 m	14
16a	1.94, m	15a, 16b	1.92, m	15a, 16b
16b	1.32, m	16a	1.32, m	16a
17	1.32, m		1.31, m	
18	0.57, s		0.65, s	
19	1.11, s		1.09, s	
20	1.37, m	21	1.39, m	21
21	0.93, d (6.4)	20	0.93, d (6.5)	20
22a	1.42, m	22b	1.43, m	22b
22b	1.03, m	22a, 23a, 23b	1.04, m	22a, 23a, 23b
23a	2.02, m	22b, 24	2.02, m	22b, 24
23b	1.87, m	22b, 24	1.88, m	22b, 24
24	5.08, t (7.1)	26, 27, 23a, 23b	5.08, t (7.1)	26, 27, 23a, 23b
25				
26	1.60, s	24	1.59, s	24
27	1.67, s	24	1.66, s	24