

Supplementary Information

Table S1. NMR data of smenothiazole B (**4**) (700 MHz, CD₃OD).

Pos.	δ_{H} [mult., <i>J</i> (Hz)]	δ_{C} [mult.]	COSY	HMBC
1	7.70 (d, 3.3)	143.1(CH)	2, 4	
2	7.47 (d, 3.3)	120.4 (CH)	1, 4	
3	-	174.4 (C)		
4	5.46 (dd, 8.2, 2.9)	60.5 (CH)	1, 2, 5a, 5b	
5	a 2.35 (m)	33.2 (CH ₂)	4, 5b, 6a, 6b	
	b 2.20 (m)		4, 5a, 6a, 6b	
6	a 2.15 (m).	25.4 (CH ₂)	4a, 5b, 6b, 7a, 7b	
	b 2.11 (m)		4a, 5b, 6a, 7a, 7b	
7	a 4.02 (ddd, 10.1, 8.4, 7.1)	48.9 (CH ₂)	6a, 6b, 7b	
	b 3.88 (ddd, 10.1, 7.8, 4.0)		6a, 6b, 7a	
8	-	173.5 (C)	-	
9	4.55 (d, 7.9)	58.3 (CH)	10	8, 10, 11, 13
10	2.16 (m)	31.9 (CH)	9, 11, 12	8, 9, 11, 12
11	1.01 (d, 6.7)	19.9 (CH ₃)	10	9, 10, 12
12	0.98 (d, 6.7)	18.9 (CH ₃)	10	9, 10, 11
13	-	172.1 (C)	-	
14	-	133.3 (C)	-	
15	1.94 (br. t, 1.5)	13.3 (CH ₃)	16, 17	13, 14, 16
16	6.27 (tq, 7.5, 1.5)	133.6 (CH)	15, 17	15
17	3.14 (br. d, 7.5)	30.3 (CH ₂)	15, 16, 19	14, 16, 18, 19, 20
18	-	141.3 (C)	-	
19	6.04 (br. s)	115.2 (CH)	17, 20	17, 18, 20
20	2.25 (br. t, 7.7)	34.6 (CH ₂)	19, 21	17, 18, 19, 21, 22
21	1.65 (quintet, 7.3)	27.6 (CH ₂)	20, 22	18, 20, 22, 23
22	2.18 (ddd, 7.0, 7.0, 2.8)	18.5 (CH ₂)	21, 24	20, 21, 23, 24
23	-	84.4 (C)	-	
24	2.25 (t, 2.8)	71.0 (CH)	22	

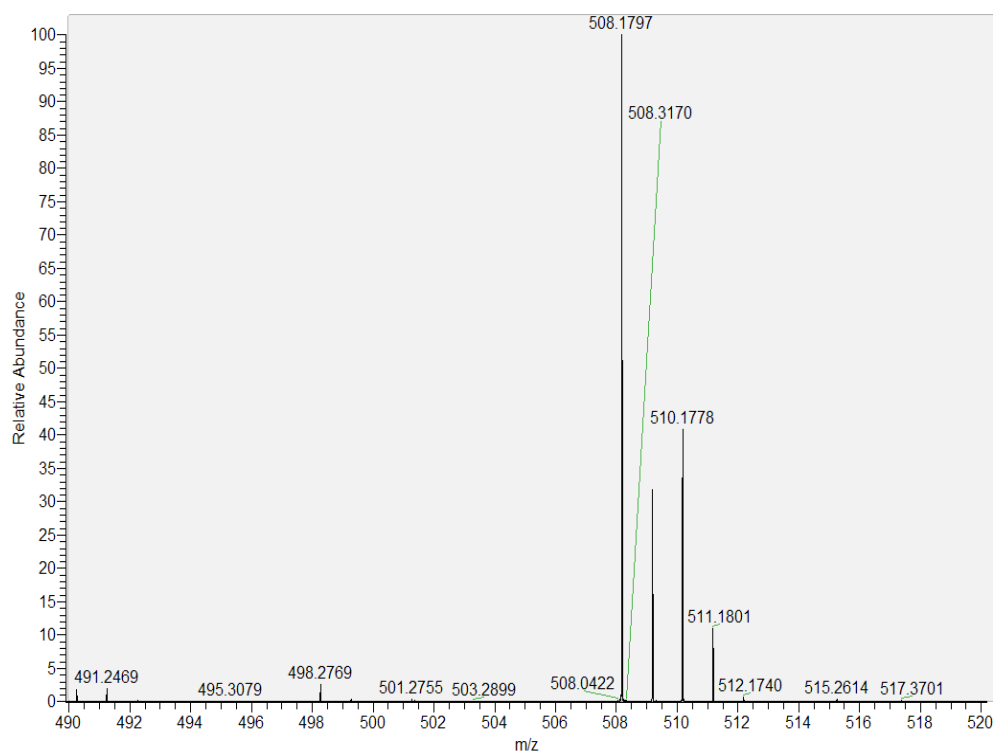


Figure S1. Positive ion mode high-resolution ESI MS spectrum of smenothiazole A (**3**).

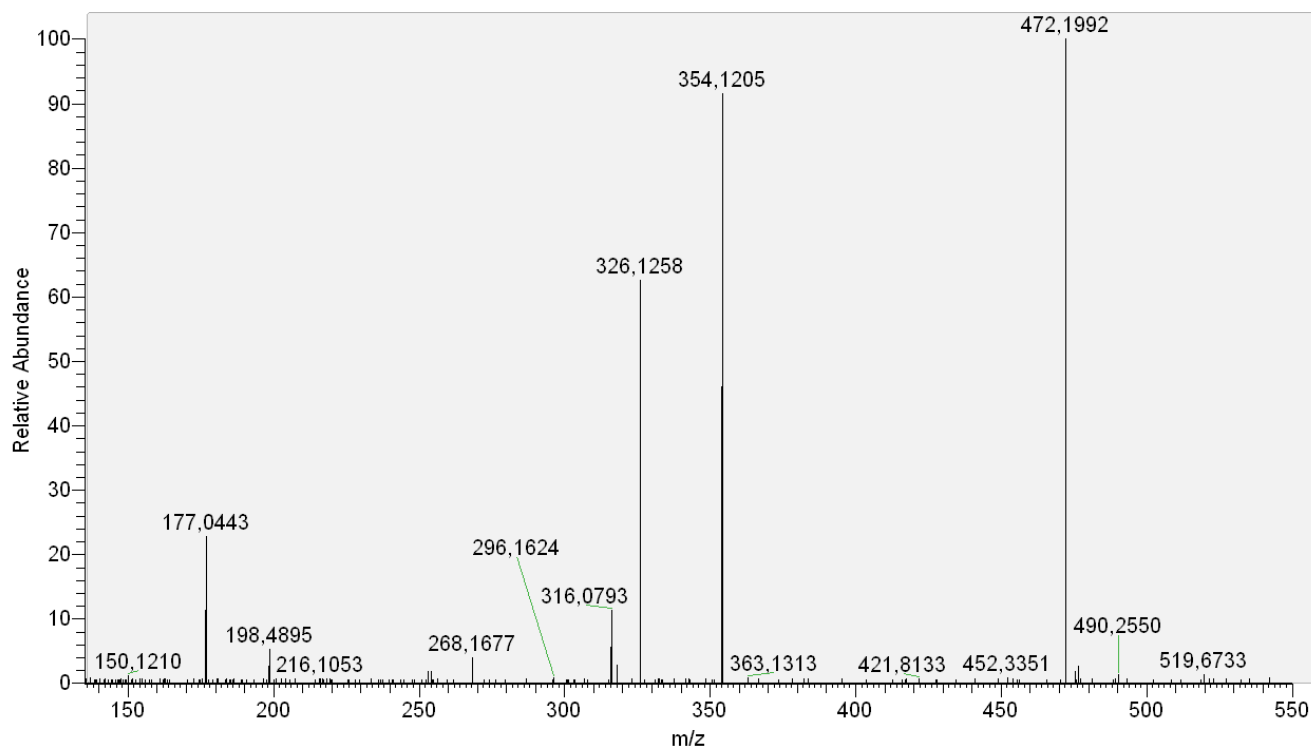


Figure S2. Positive ion mode high-resolution ESI MS/MS spectrum of smenothiazole A (**3**), parent ion at m/z 508.18.

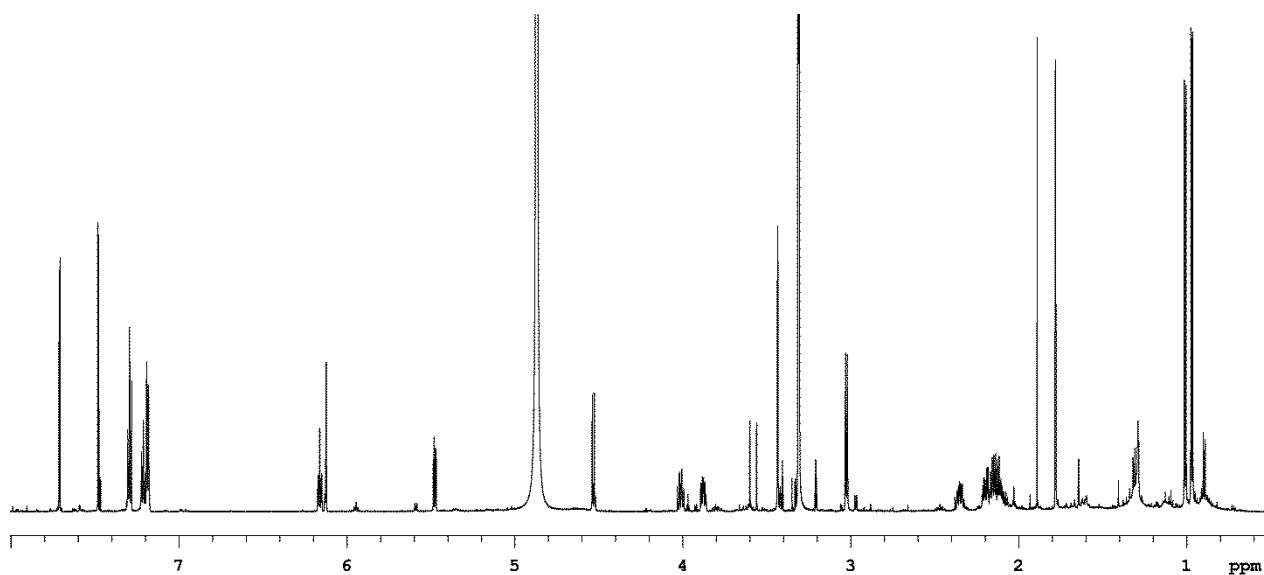


Figure S3. ^1H NMR spectrum of smenothiazole A (**3**) (CD_3OD , 700 MHz).

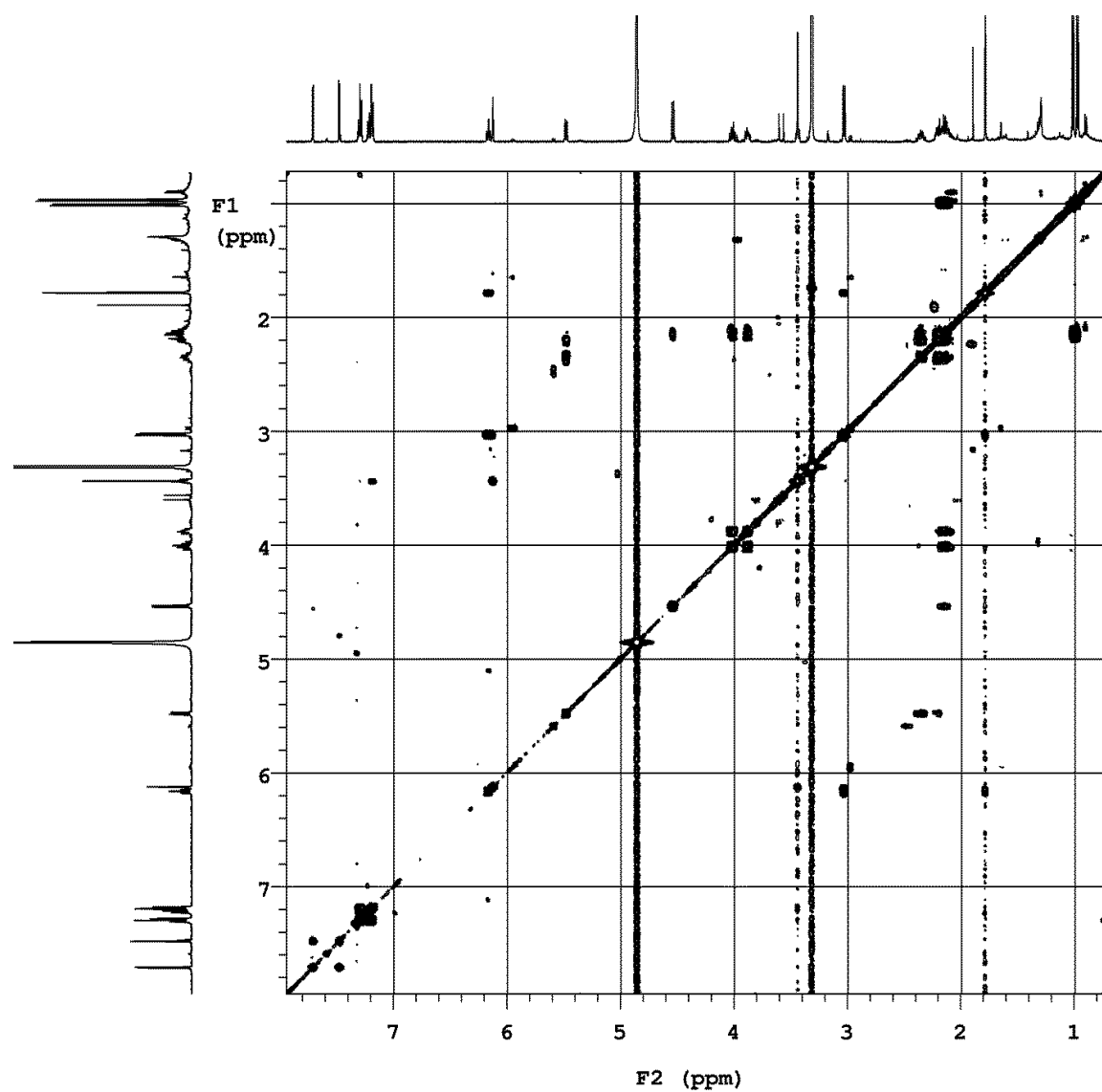


Figure S4. COSY spectrum of smenothiazole A (**3**) (CD_3OD , 700 MHz).

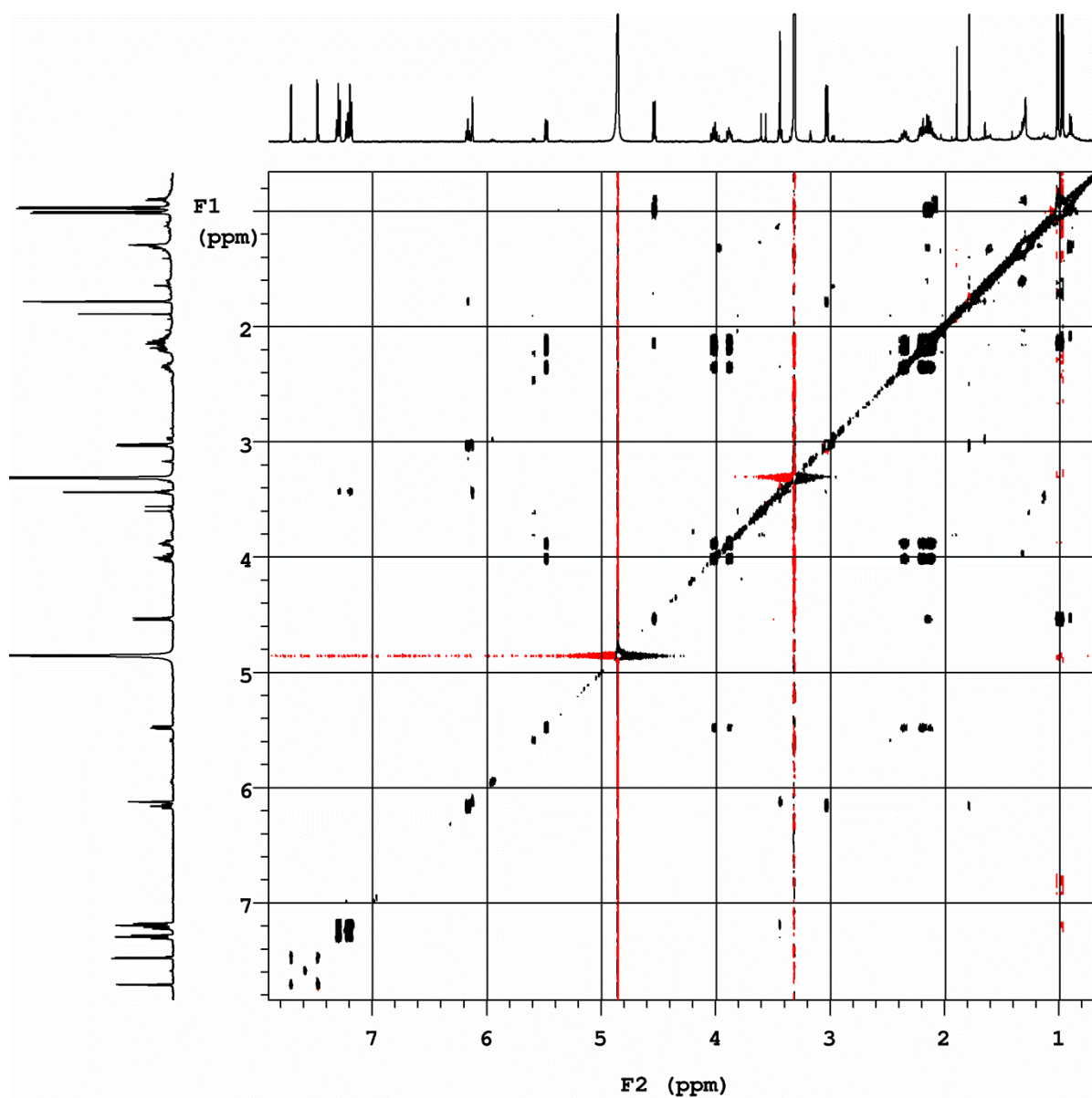


Figure S5. TOCSY spectrum of smenothiazole A (**3**) (CD₃OD, 700 MHz).

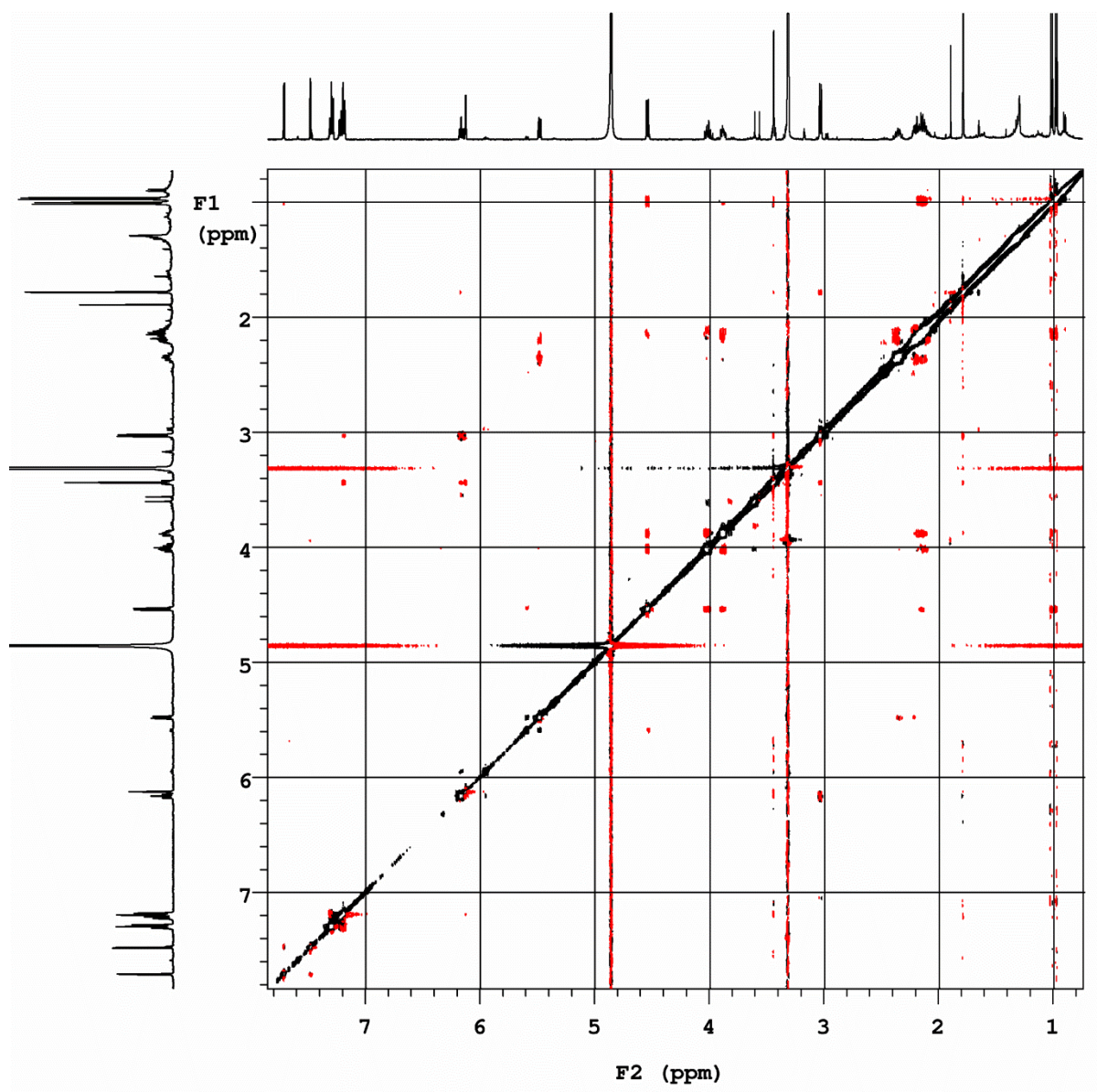


Figure S6. NOESY spectrum of smenothiazole A (**3**) (CD₃OD, 700 MHz).

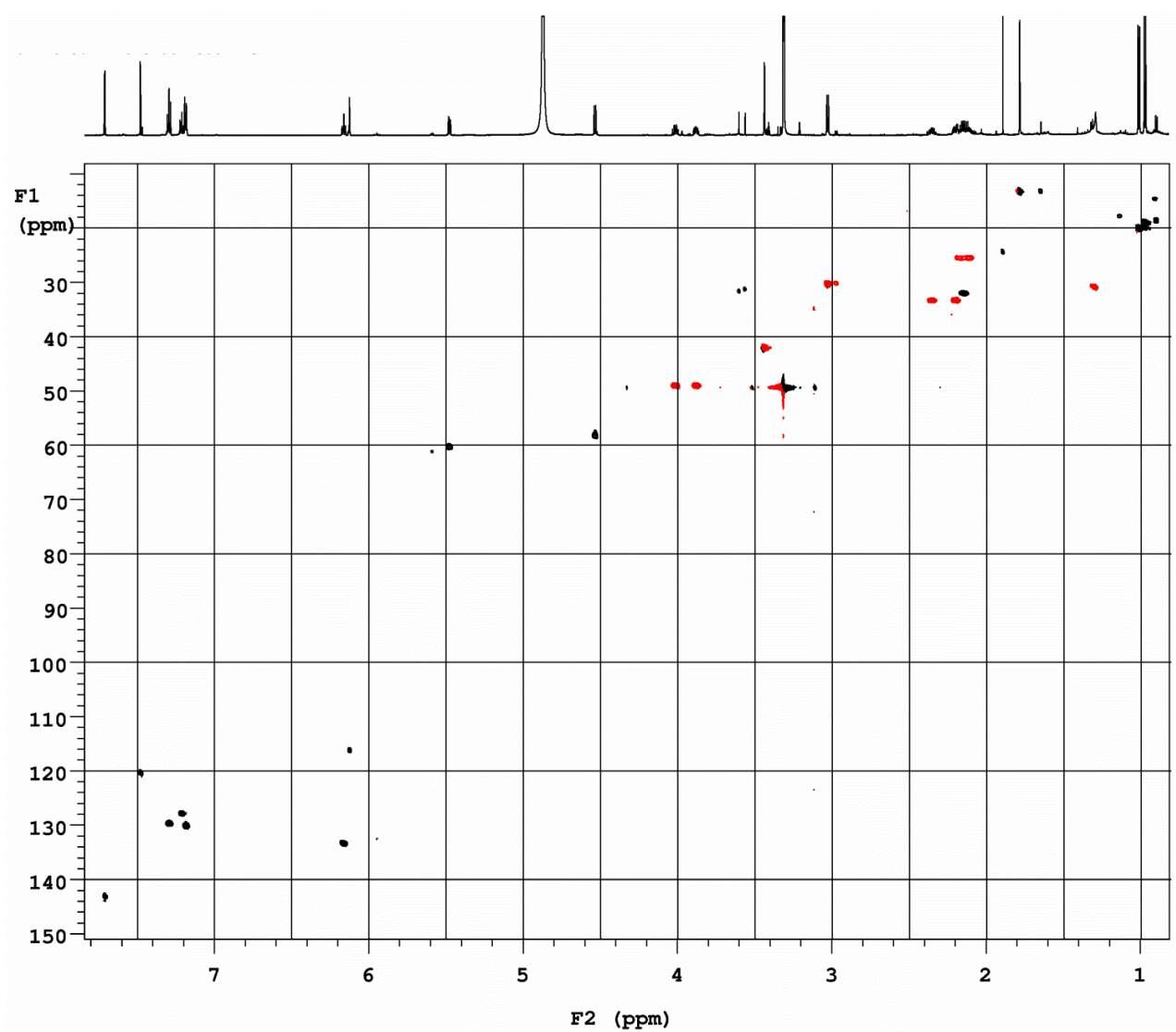


Figure S7. HSQC spectrum of smenothiazole A (**3**) (CD_3OD , 700 MHz).

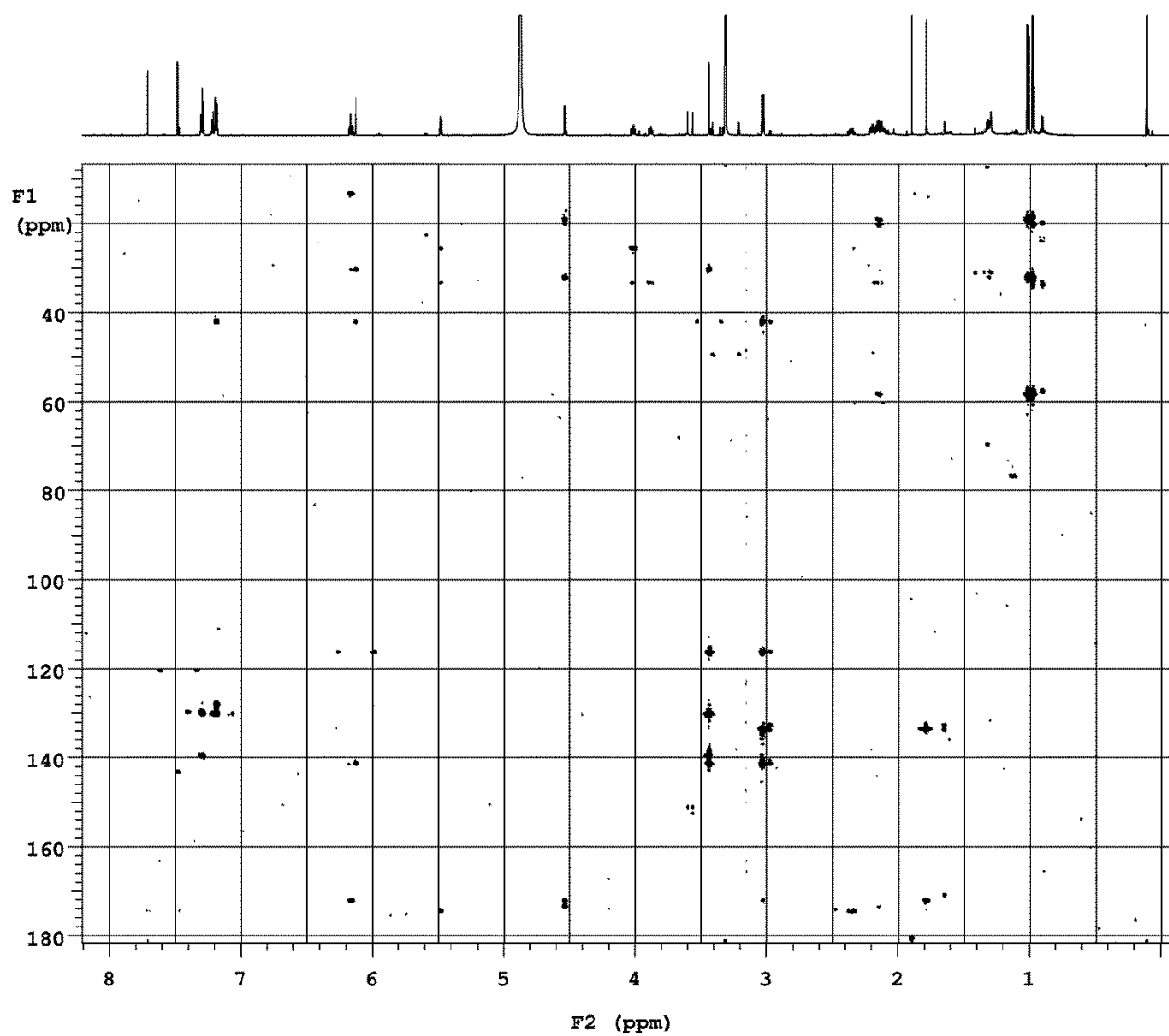


Figure S8. HMBC spectrum of smenothiazole A (3) (CD₃OD, 700 MHz).

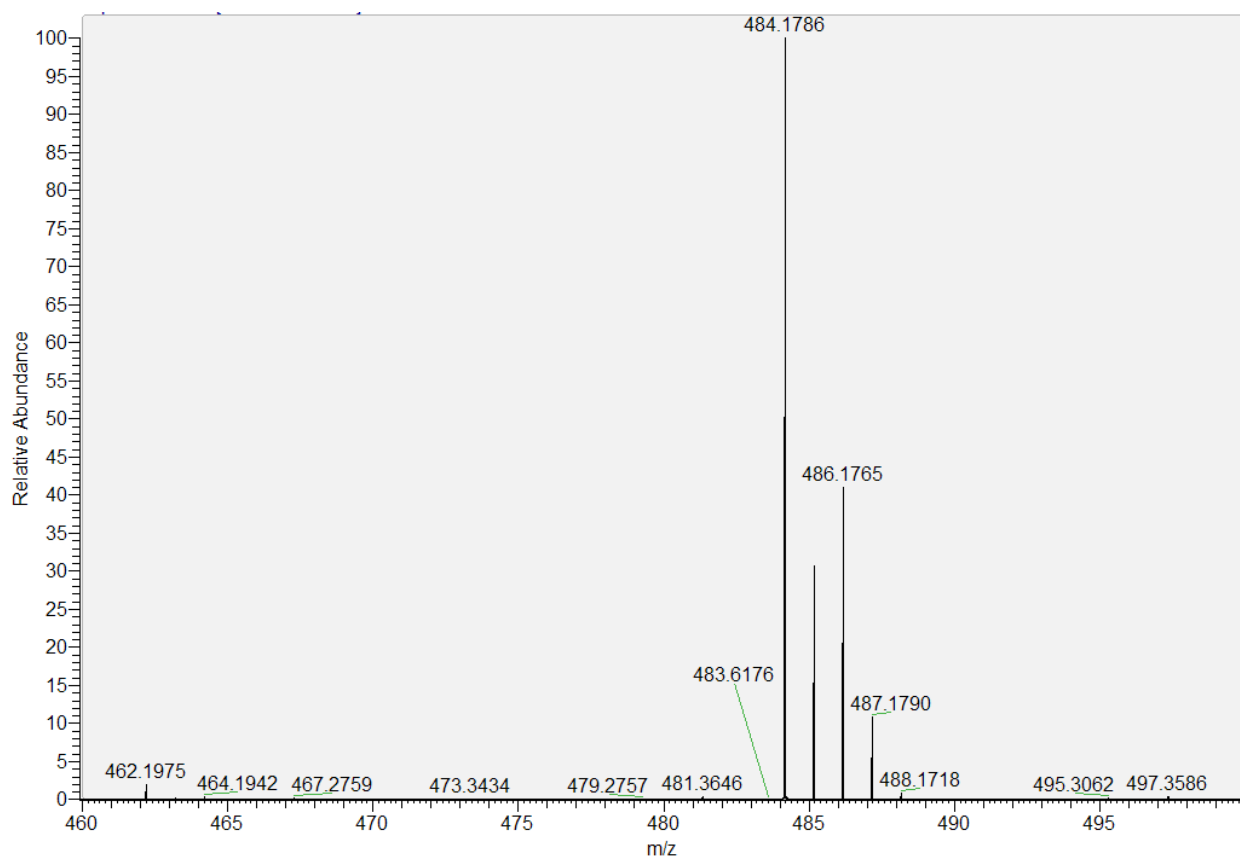


Figure S9. Positive ion mode high-resolution ESI MS spectrum of smenothiazole B (**4**).

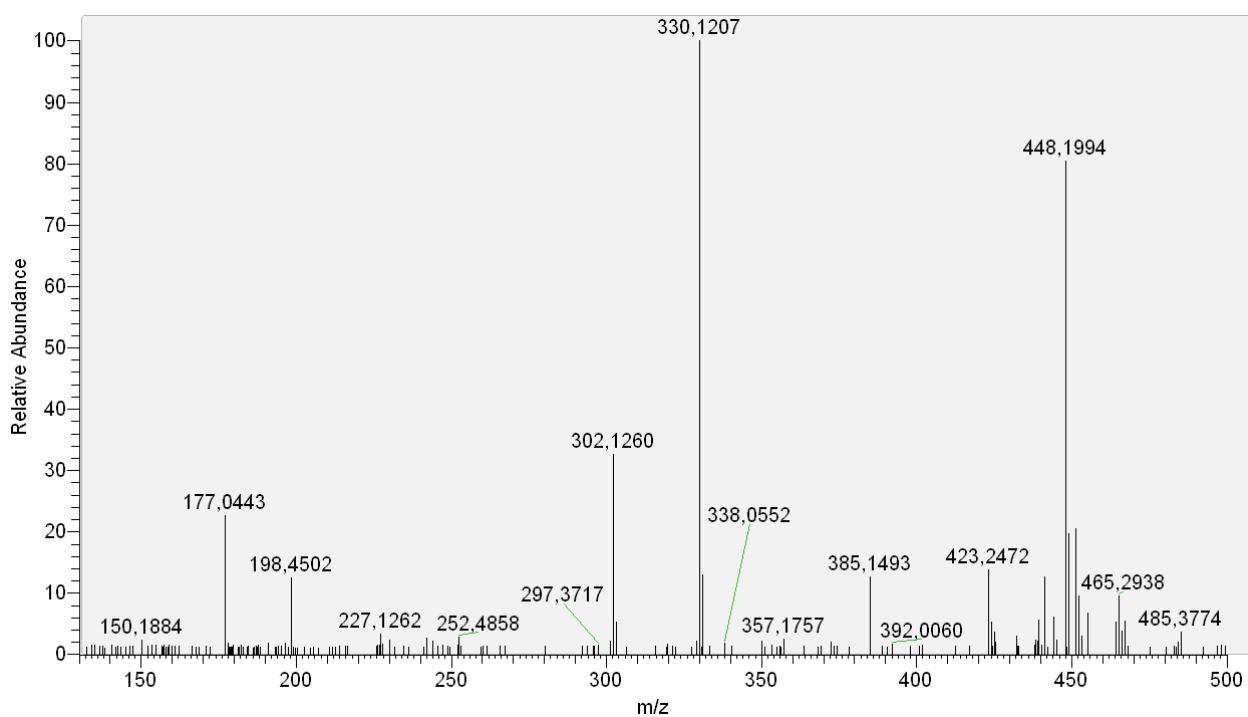


Figure S10. Positive-ion high-resolution ESI MS/MS spectrum of smenothiazole B (**4**), parent ion at m/z 484.18.

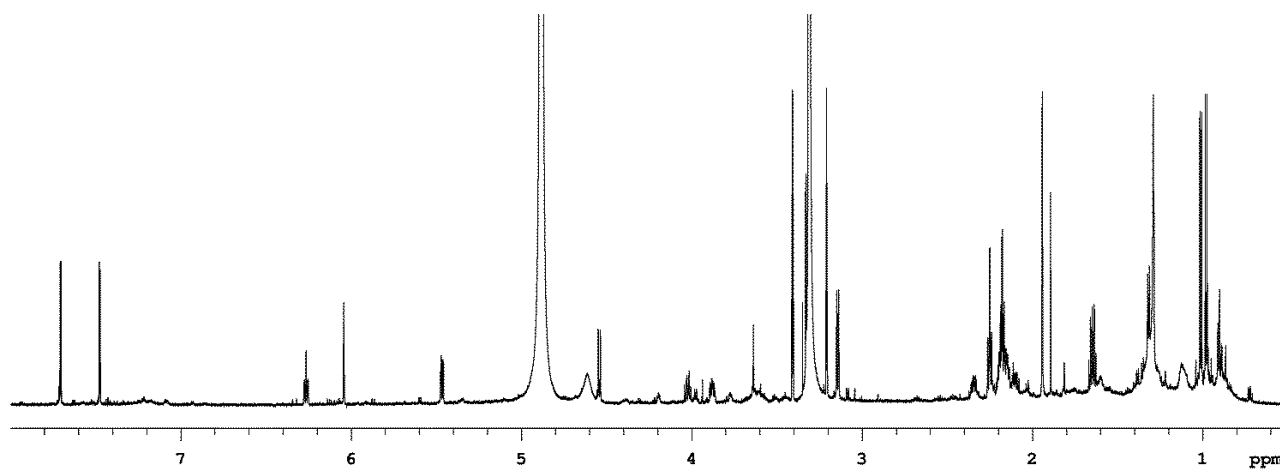


Figure S11. ^1H NMR spectrum of smenothiazole B (**4**) (CD_3OD , 700 MHz).

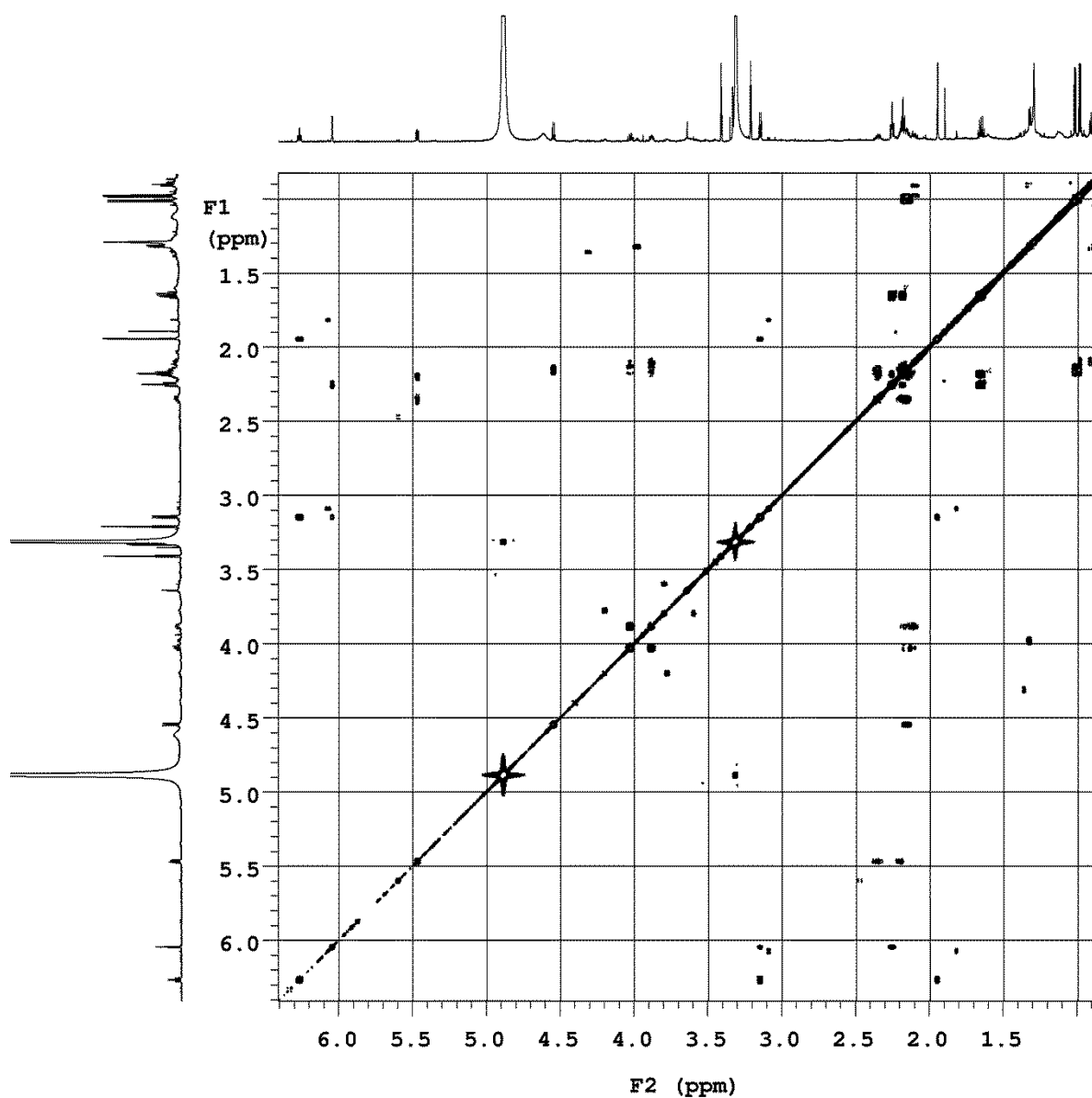


Figure S12. COSY spectrum of smenothiazole B (**4**) (CD_3OD , 700 MHz).

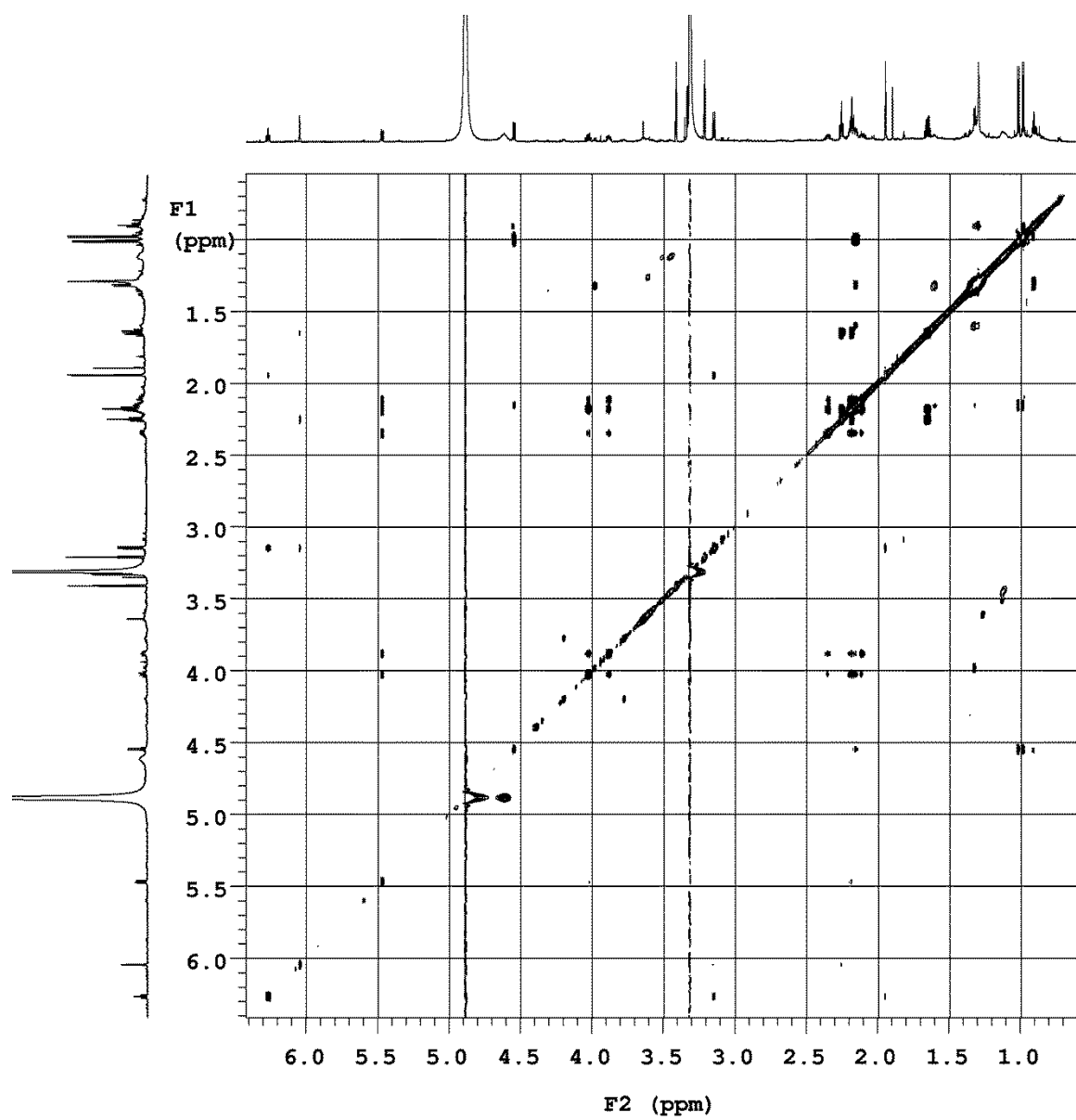


Figure S13. TOCSY spectrum of smenothiazole B (4) (CD₃OD, 700 MHz).

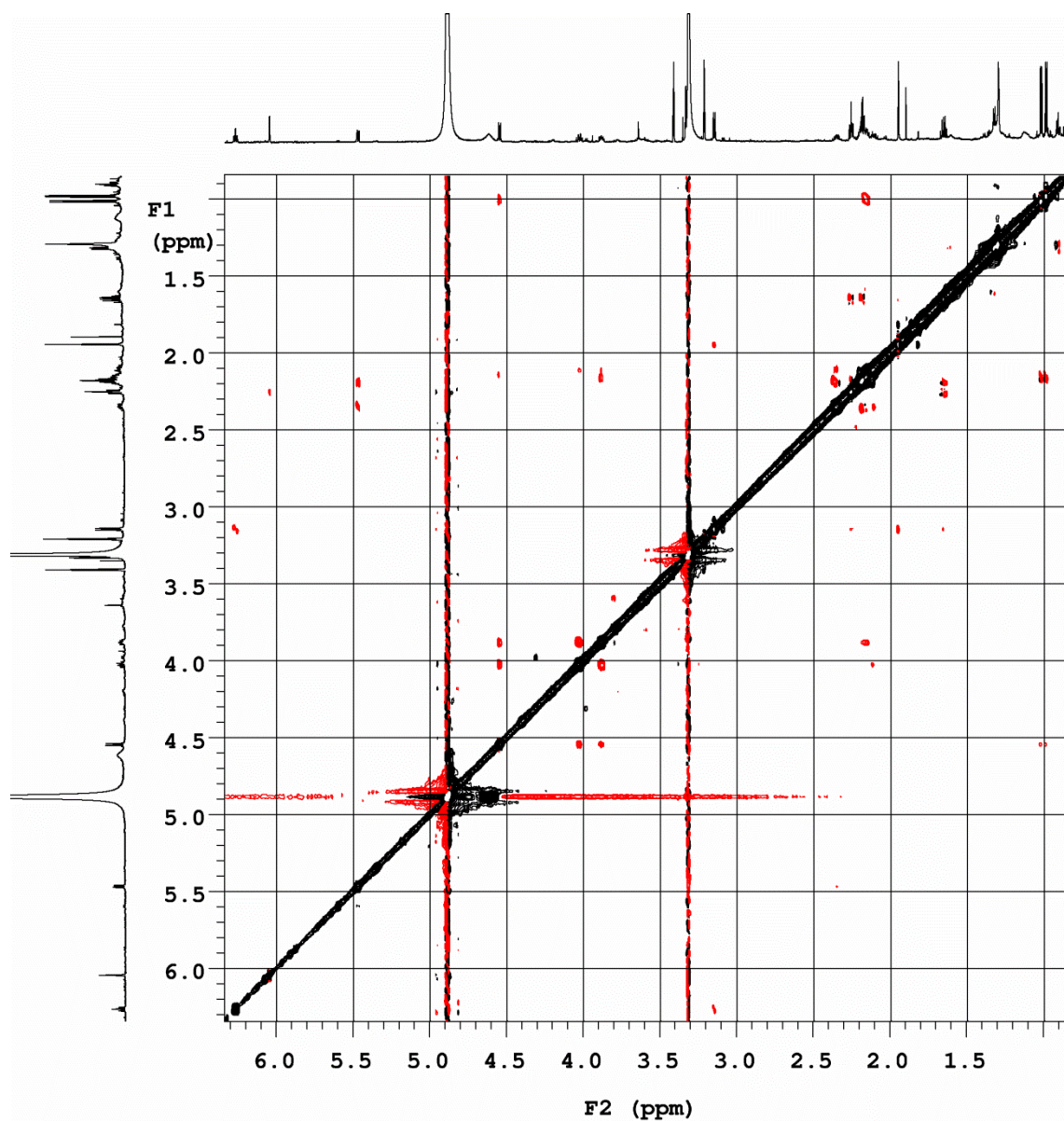


Figure S14. ROESY spectrum of smenothiazole B (**4**) (CD₃OD, 700 MHz).

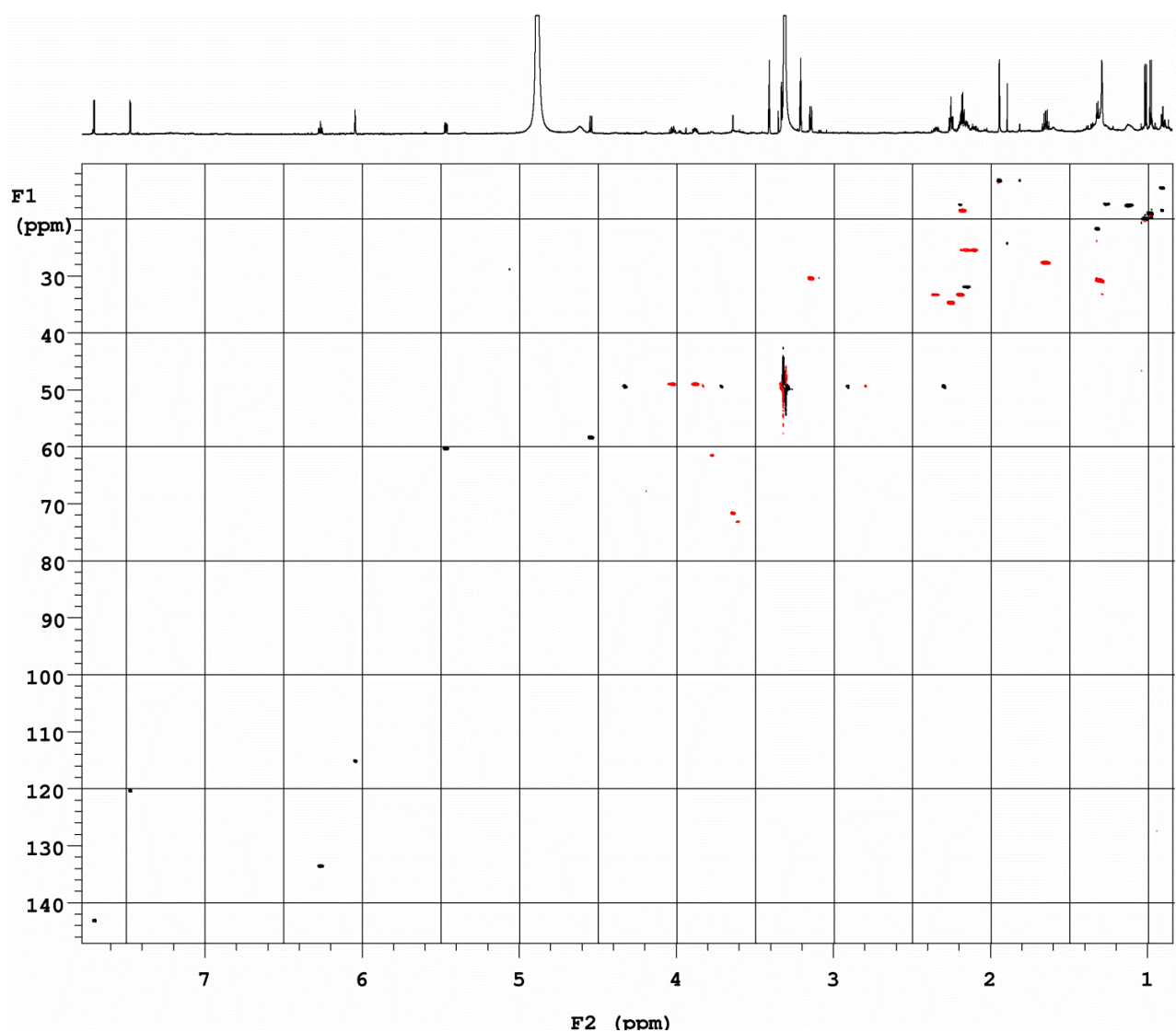


Figure S15. HSQC spectrum of smenothiazole B (4) optimized for $^1J_{\text{CH}} = 150$ Hz (CD₃OD, 700 MHz).

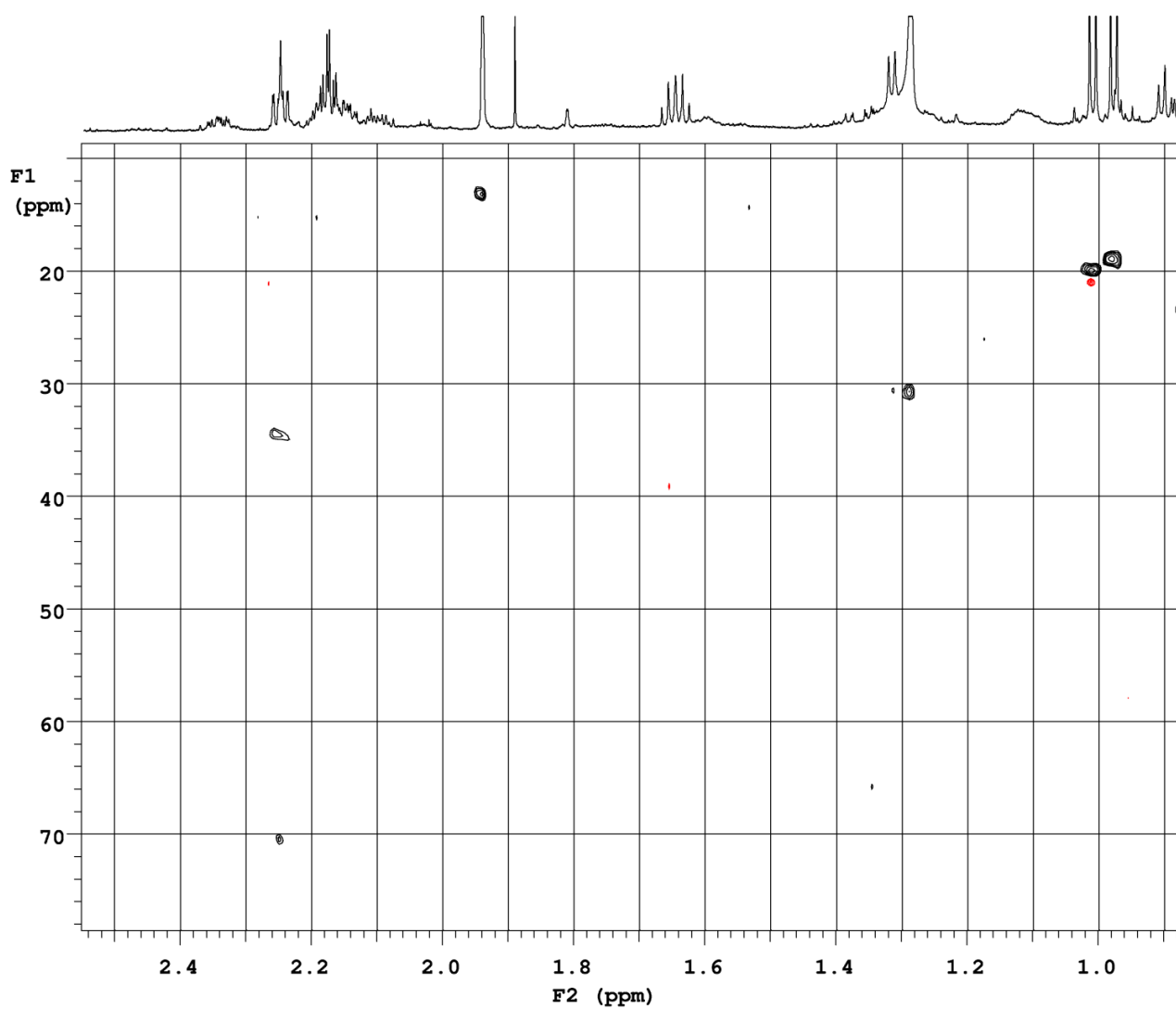


Figure S16. HSQC spectrum of smenothiazole B (**4**) optimized for $^1J_{\text{CH}} = 250$ Hz (CD_3OD , 700 MHz).

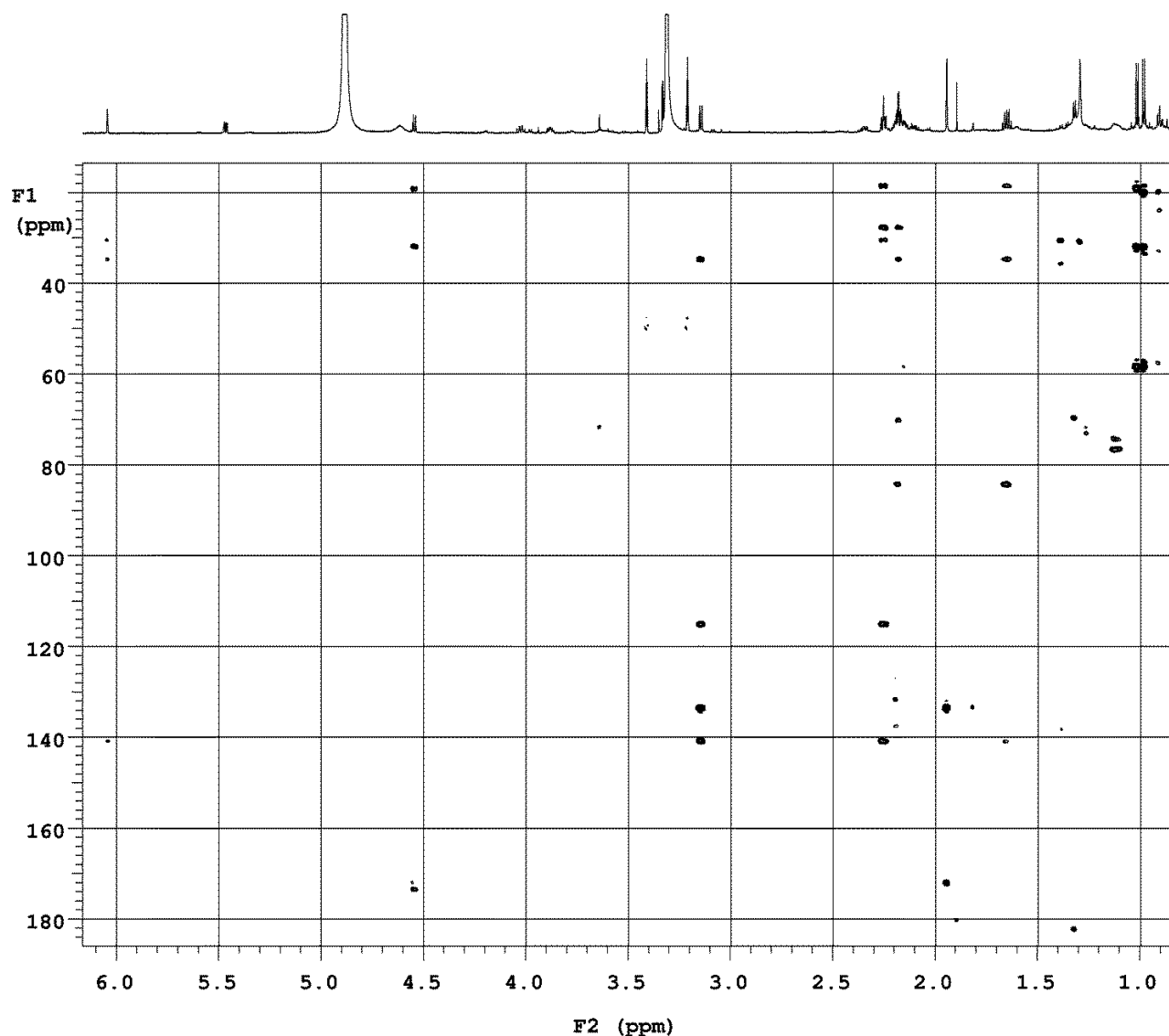


Figure S17. HMBC spectrum of smenothiazole B (**4**) (CD₃OD, 700 MHz).

© 2015 by the authors; licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution license (<http://creativecommons.org/licenses/by/4.0/>).