Penicillanthone and Penicillidic acids A-C from the Soil-derived Fungus *Penicillium aculeatum* PSU-RSPG105

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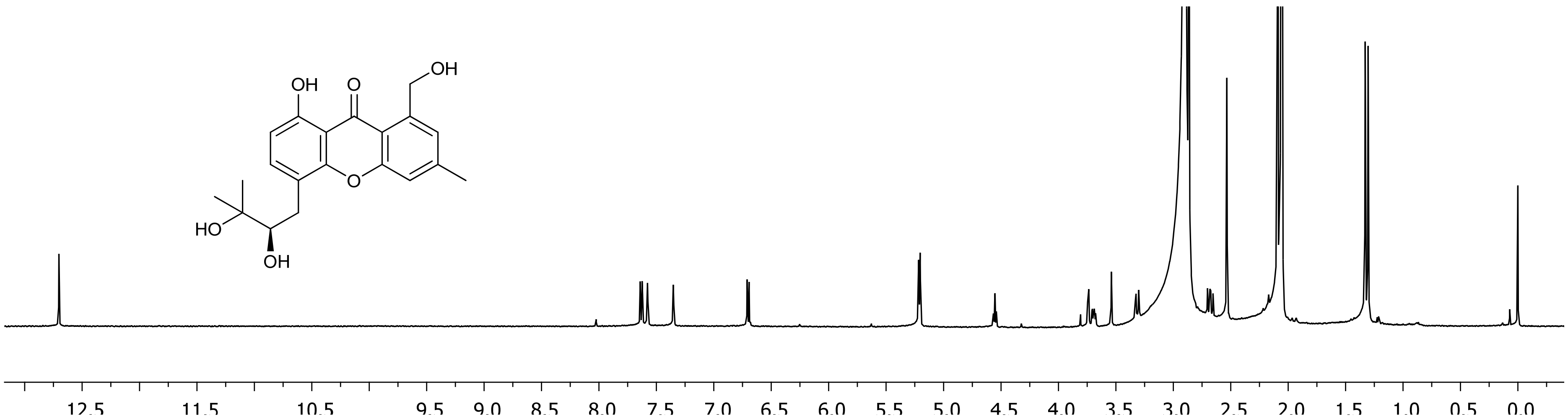

Figure S1. ^{1}H NMR spectrum of penicillanthone (**1**; 300 MHz, Acetone-d_6)

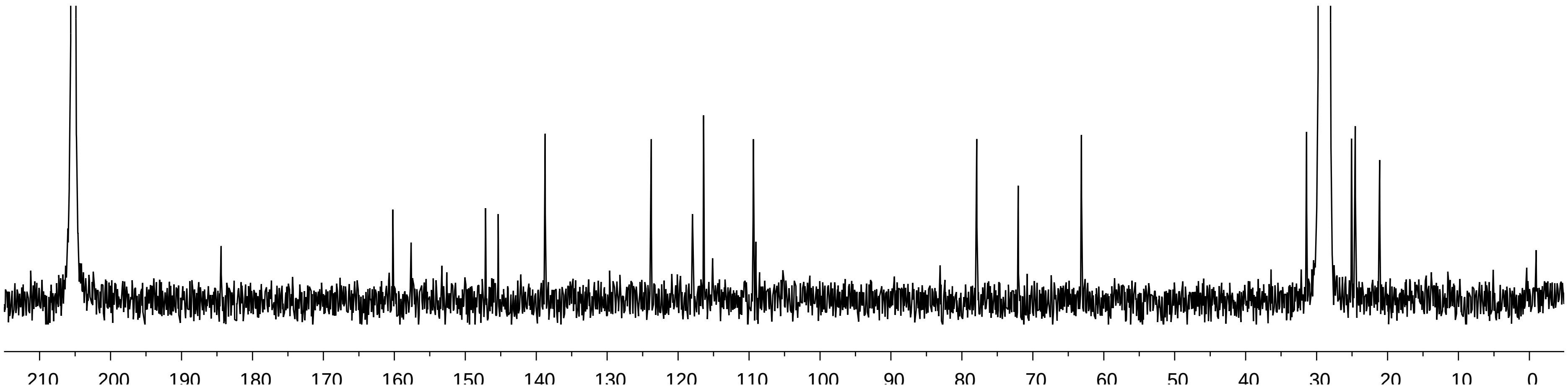

Figure S2. ^{13}C NMR spectrum of penicillanthone (**1**; 75 MHz, Acetone-d_6)

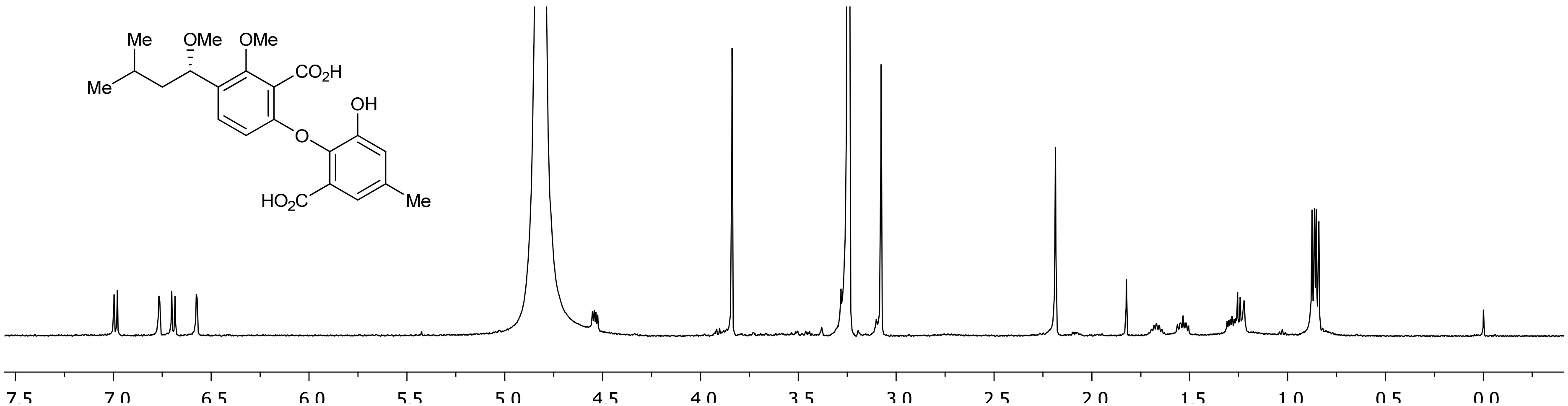

Figure S3. ^{1}H NMR spectrum of penicillidic acid A (**2**; 500 MHz, CD_3OD)

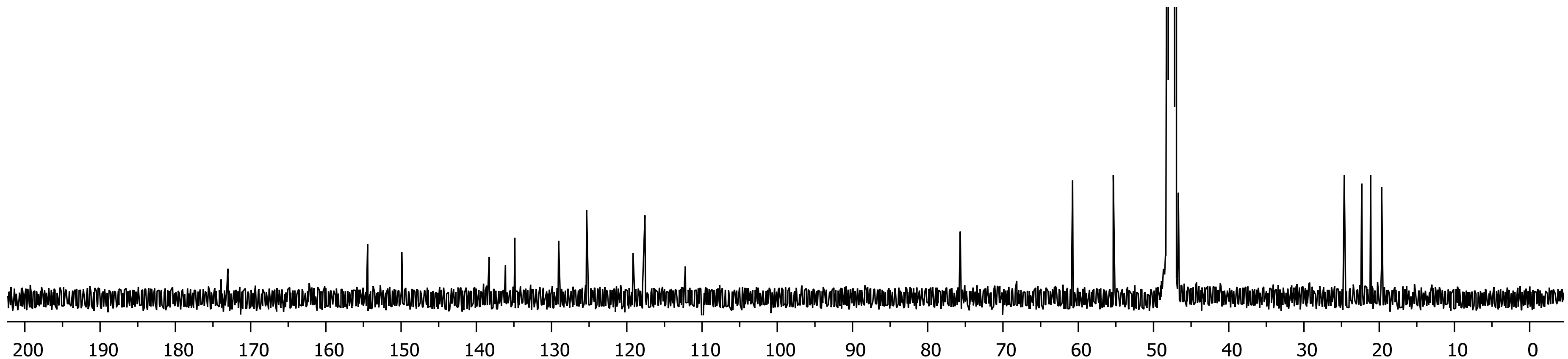

Figure S4. ^{13}C NMR spectrum of penicillidic acid A (**2**; 125 MHz, CD_3OD)

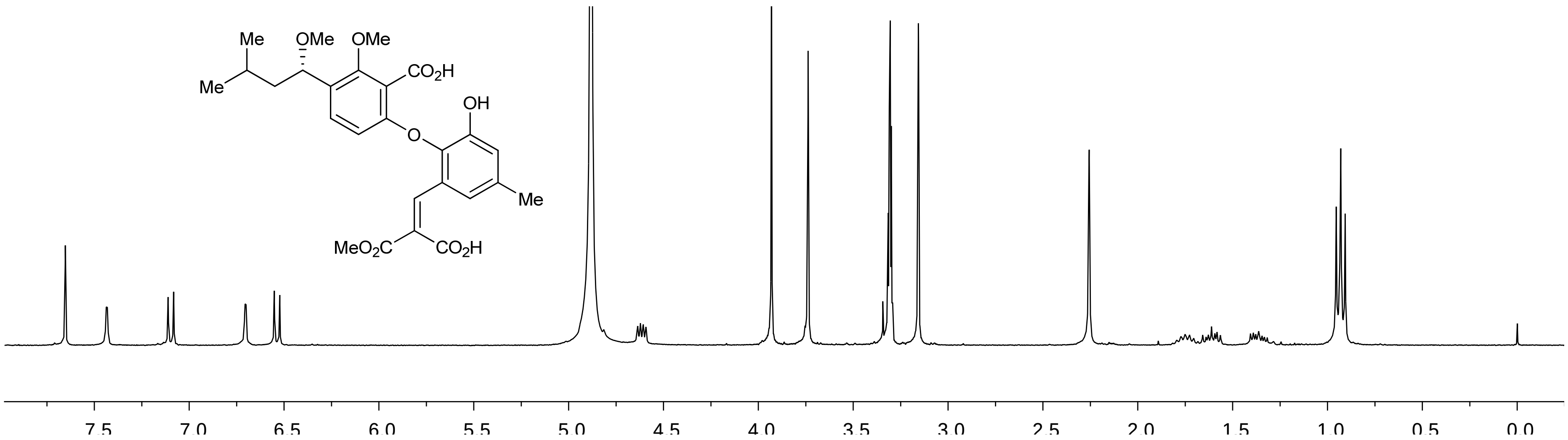

Figure S5. ^{1}H NMR spectrum of penicillidic acid B (**3**; 300 MHz CD_3OD)

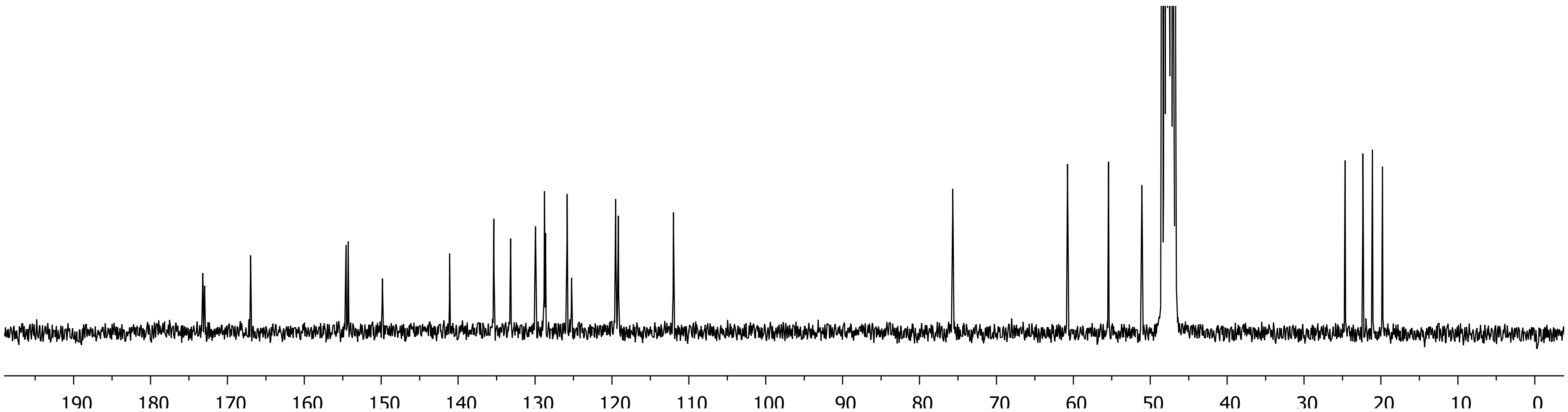

Figure S6. ^{13}C NMR spectrum of penicillidic acid B (**3**; 75 MHz, CD_3OD)

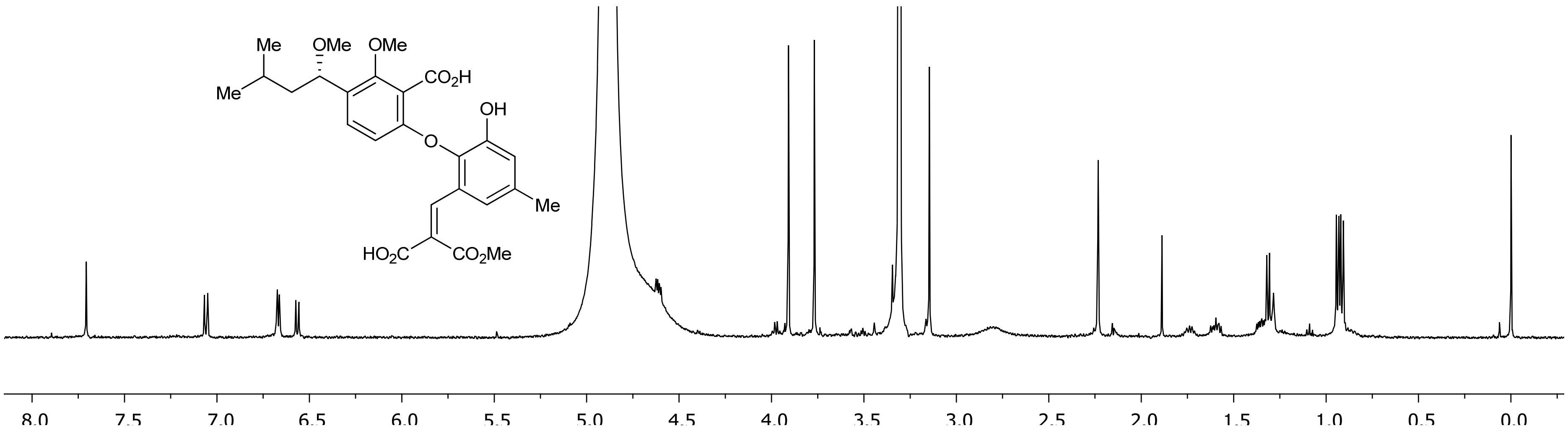

Figure S7. ^{1}H NMR spectrum of penicillidic acid C (**4**; 500 MHz, CD_3OD)

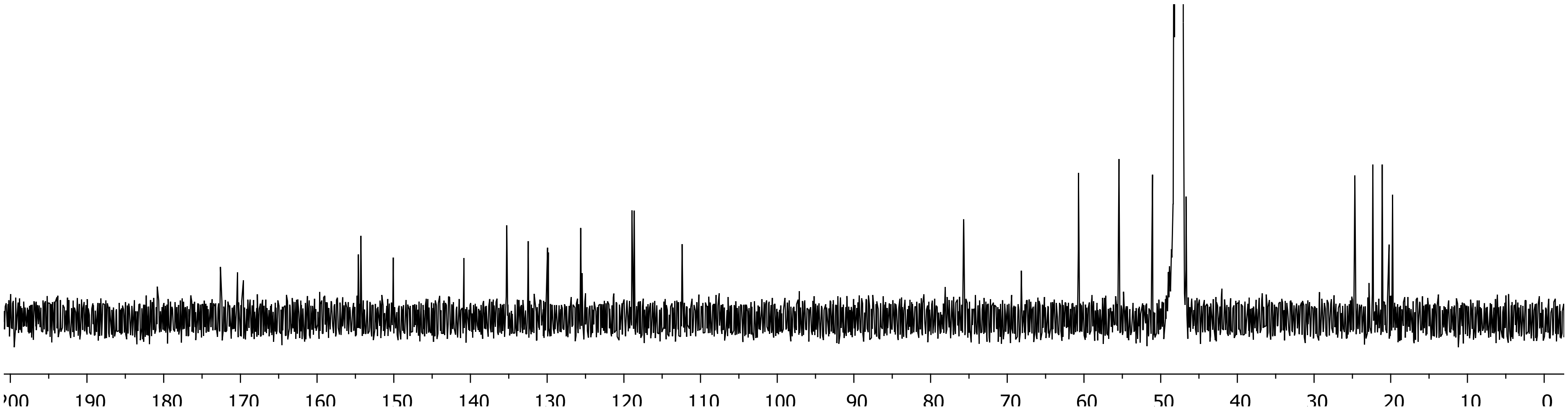

Figure S8. ^{13}C NMR spectrum of penicillidic acid C (**4**; 125 MHz, CD_3OD)

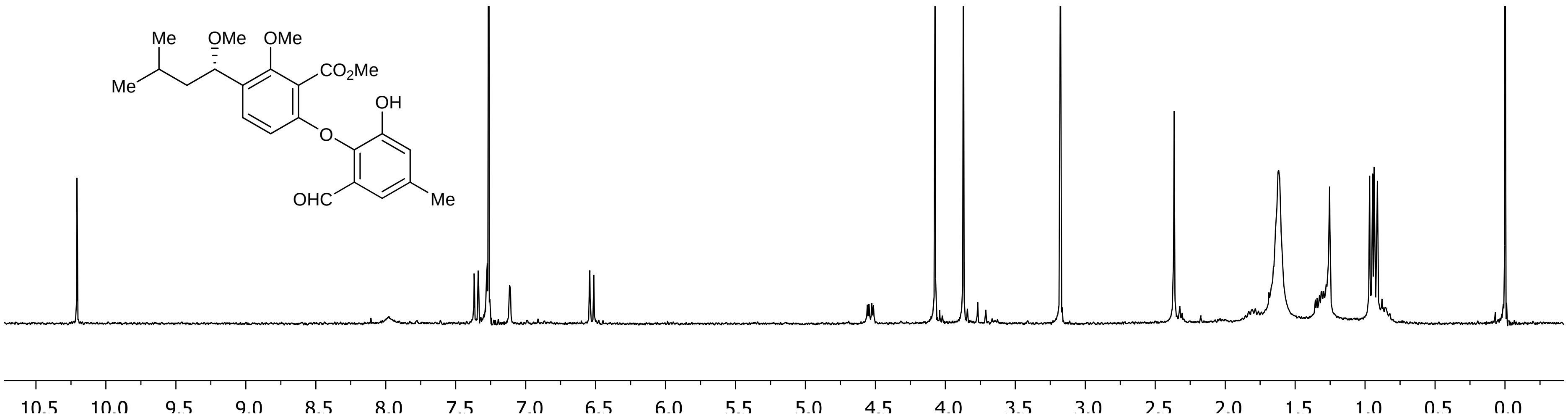

Figure S9. [1]H NMR spectrum of tenellic acid A methyl ester (**14**; 300 MHz, $CDCl_3$)

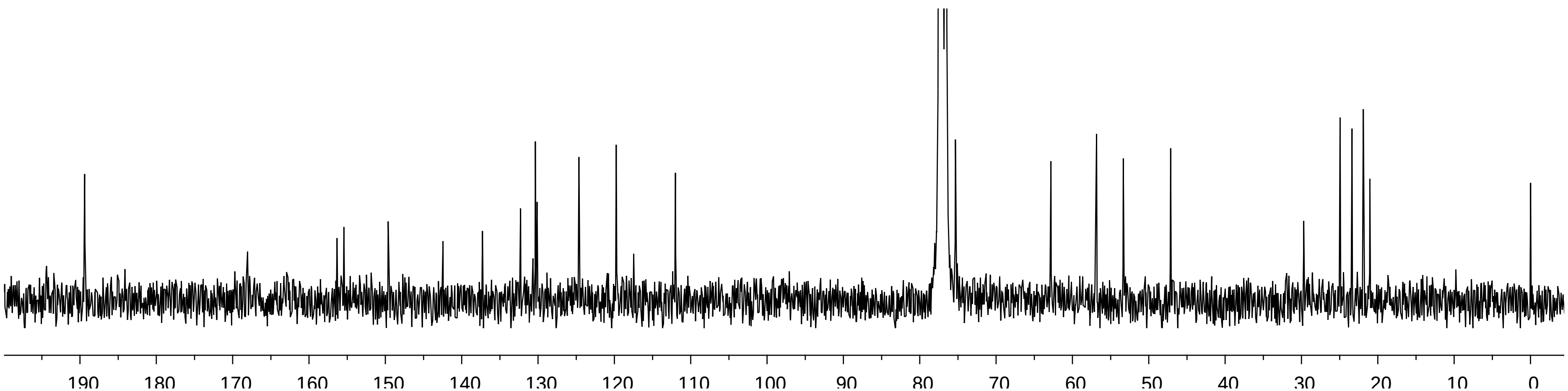

Figure S10. [13]C NMR spectrum of tenellic acid A methyl ester (**14**; 75 MHz, $CDCl_3$)

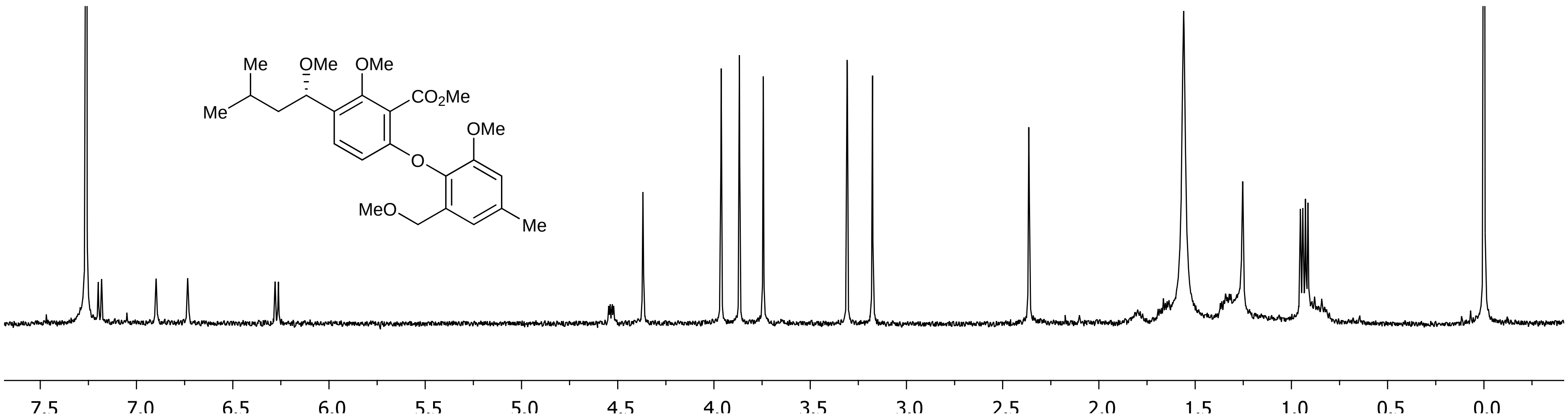

Figure S11. [1]H NMR spectrum of penicillide methyl ester A (**6b**; 500 MHz, $CDCl_3$)

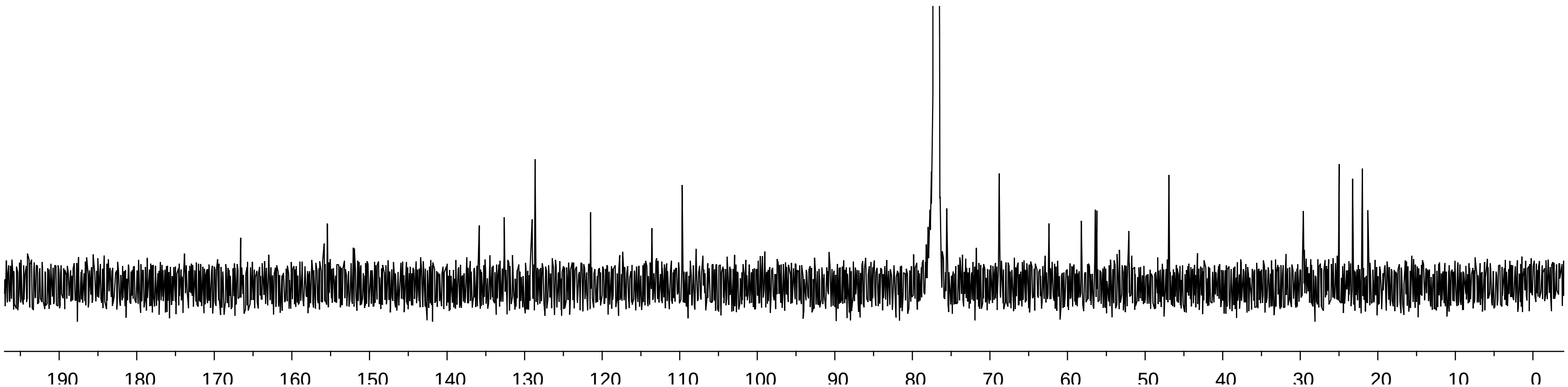

Figure S12. [13]C NMR spectrum of penicillide methyl ester A (**6b**; 125 MHz, $CDCl_3$)

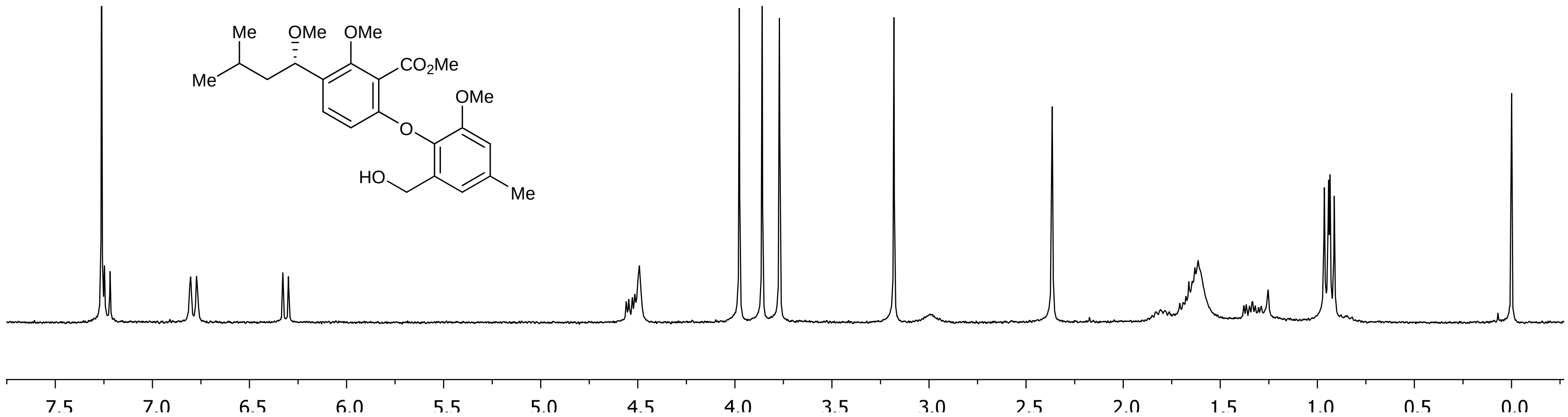

Figure S13. [1]H NMR spectrum of penicillide methyl ester B (**9a**; 300 MHz, $CDCl_3$)

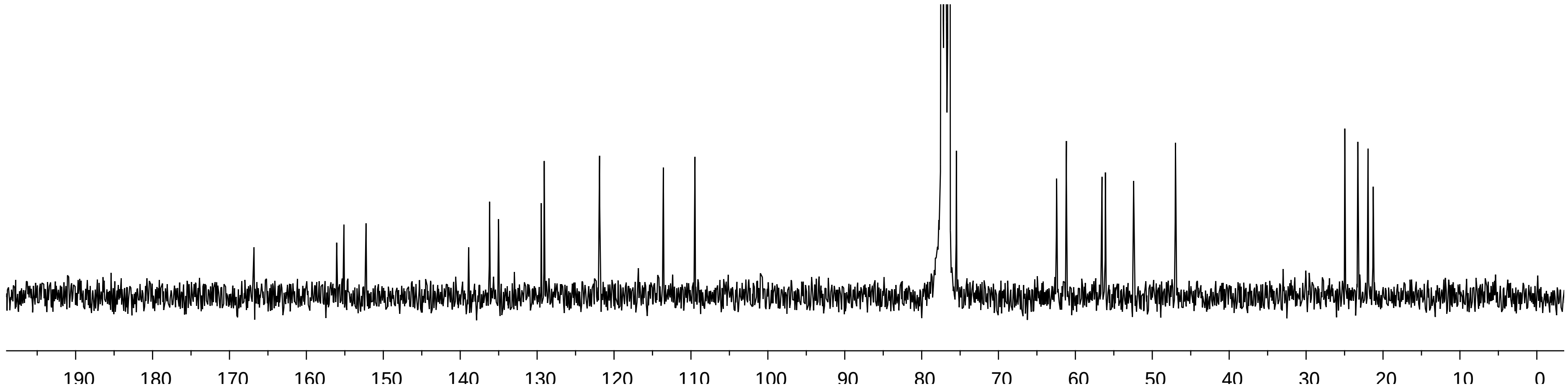

Figure S14. [13]C NMR spectrum of penicillide methyl ester B (**9a**; 75 MHz, $CDCl_3$)

Table S1 Optical rotations of compounds **5**, **6-9**, **11** and **13-18**.

Compounds	Observed optical rotation	Lit. optical rotation[ref]
5	$[\alpha]_D^{24}$ +25.2° (*c* 0.13, CH_3OH)	$[\alpha]_D^{20}$ +33.3° (*c* 1.14, CH_3OH)[6]
6	$[\alpha]_D^{24}$ +4.1° (*c* 0.82, CH_3OH)	$[\alpha]_D^{24}$ +4.9° (*c* 0.82, CH_3OH)[8]
6a	$[\alpha]_D^{24}$ +3.7° (*c* 0.82, CH_3OH)	$[\alpha]_D^{24}$ +3.8° (*c* 0.82, CH_3OH)[8]
6b	$[\alpha]_D^{24}$ -10.0° (*c* 0.18, CH_3OH)	-
7	$[\alpha]_D^{24}$ -55.8° (*c* 0.62, CH_3OH)	$[\alpha]_D$ -57.6° (*c* 0.62, CH_3OH)[7]
8*	$[\alpha]_D^{24}$ -4.8° (*c* 0.18 CH_3OH)	$[\alpha]_D^{24}$ -6.1° (*c* 0.18, CH_3OH)[9]
9	$[\alpha]_D^{24}$ +5.3° (*c* 0.64, CH_3OH)	$[\alpha]_D^{25}$ +3.1° (*c* 0.64, CH_3OH)[10]
9a	$[\alpha]_D^{24}$ -9.3° (*c* 0.18, CH_3OH)	-
11	$[\alpha]_D^{24}$ +5.8° (*c* 0.098, $CH_3OH:CHCl_3$)	$[\alpha]_D^{28}$ +8.21° (*c* 0.098, $CH_3OH:CHCl_3$)[12]
13*	$[\alpha]_D^{27}$ +5.5° (*c* 0.53, CH_3OH)	Hydroxytenellic acid B : $[\alpha]_D^{25}$ +5.0 (*c* 0.53, CH_3OH)[10]
14*	$[\alpha]_D^{27}$ -10.6° (*c* 0.18, CH_3OH)	-
15	$[\alpha]_D^{24}$ -35.7° (*c* 0.20, $CHCl_3$)	$[\alpha]_D^{29}$ -50.0° (*c* 0.20, $CHCl_3$)[7]
16*	$[\alpha]_D^{24}$ -40.2° (*c* 0.20, CH_3OH)	-
17*	$[\alpha]_D^{24}$ -54.6° (*c* 0.62, CH_3OH)	-
18	$[\alpha]_D^{24}$ -253.7° (*c* 0.11, $CHCl_3$)	$[\alpha]_D^{20}$ -298° (*c* 0.11, $CHCl_3$)[16]

* = The absolute configuration has not been reported.

Table S2 Cotton effects in CD spectrum of compounds **7**, **15-17**.

Compounds	*Δ*ε (nm)	Lit. *Δ*ε (nm)[ref]
7	-0.1 (202), +0.3 (243), +0.2 (269), -0.2 (291)	-7.0 (202), +1.0 (243), +0.5 (269), -0.8 (291)[19]
15	-7.6 (213), +1.9 (250), -1.6 (283)	-6.2 (213), +0.4 (250), -0.6 (283)[7]
16	-2.7 (213), +0.2 (250), -0.4 (283)	-
17	-13.6 (202), +1.2 (243), +0.8 (269), -0.8 (291)	-

Table S3. ^{1}H NMR data of compounds **6b**, **9a** and **14** (J in Hz)

Position	**14**[a]	**6b**[b]	**9a**[a]
1	6.53, d (8.7)	6.27, d (8.5)	6.31, d (8.7)
2	7.35, d (8.7)	7.19, d (8.5)	7.23, d (8.7)
4-OMe	3.87, s	3.87, s	3.86, s
5-OMe	4.08, s	3.96, s	3.98, s
7	10.21, s	4.37, s	4.94, s
7-OMe		3.31, s	
8	7.28, brd (1.5)	6.90, brs	6.80, brs
9-Me	2.37, s	2.36, s	2.37, s
10	7.11, brd (1.5)	6.73, brs	6.77, brs
11-OMe		3.74, s	3.77, s
1′	4.54, dd (3.9, 9.3)	4.53, dd (4.0, 9.5)	4.54, dd (3.9, 9.3)
2′a	1.64, m	1.67, m	1.66, ddd (5.1, 9.3, 14.1)
2′b	1.32, ddd (3.9,	1.36, m	1.34, ddd (3.9, 8.7, 14.1)
3′	1.80, m	1.78, m	1.80, m
4′	0.92, d (6.6)	0.92, d (6.5)	0.92, d (6.6)
5′	0.96, d (6.9)	0.95, d (6.5)	0.95, d (6.6)
6′	3.18, s	3.18, s	3.18, s

[a]Recorded in $CDCl_3$ (300 MHz). [b]Recorded in $CDCl_3$ (500 MHz).

Table S4. ^{13}C NMR data of compounds **6b**, **9a** and **14** (δ_C, type)

Position	**14**[a]	**6b**[b]	**9a**[a]
1	112.0, CH	109.7, CH	109.5, CH
2	130.4, CH	128.6, CH	129.1, CH
3	132.3, C	132.6, C	129.5, C
4	156.3, C	155.8, C	156.1, C
4-OMe	62.8, CH_3	62.4, CH_3	62.5, CH_3
4a	117.5, C	117.4, C	116.8, C
5	168.1, C	166.7, C	166.8, C
5-OMe	53.4, CH_3	52.1, CH_3	52.4, CH_3
7	189.4, CH	68.8, CH_2	61.2, CH_2
7-OMe		52.2, CH_3	
7a	130.1, C	132.6, C	135.0, C
8	119.8, CH	121.5, CH	121.9, CH
9	137.3, C	135.9, C	136.2, C
9-Me	21.0, CH_3	21.3, CH_3	21.3, CH_3
10	124.7, CH	113.6, CH	113.6, CH
11	149.6, C	152.0, C	152.3, C
11-OMe		56.2, CH_3	56.1, CH_3
11a	142. 5, C	139.4, C	138.9, C
12a	155.4, C	155.4, C	155.1, C
1′	75.3, CH	75.6, CH	75.5, CH
2′	47.1, CH_2	46.9, CH_2	47.0, CH_2
3′	25.0, CH	25.0, CH	25.0, CH
4′	23.4, CH_3	23.3, CH_3	23.3, CH_3
5′	21.9, CH_3	22.0, CH_3	22.0, CH_3
6′	56.9, CH_3	56.4, CH_3	56.6, CH_3

[a]Recorded in $CDCl_3$ (75 MHz). [b]Recorded in $CDCl_3$ (125 MHz).