

A Reassignment of (-) Mycothiazole and the Isolation of a Related Diol

Rachel N. Sonnenschein,[†] Tyler A. Johnson,[†] Karen Tenney,[†] Frederick A. Valeriote,[‡] and Phillip Crews^{†,*}

[†]*Department of Chemistry and Biochemistry & Institute of Marine Sciences, University of California, Santa Cruz, CA 95064*

[‡]*Division of Hematology and Oncology, Josephine Ford Cancer Center, Detroit, MI 48202*

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FOR JNP NOTE

[Supporting Information]

Experimental Procedure.

Figure S1. Original ¹H-NMR of compound **3** in benzene-*d*₆ at 300 MHz.

Figure S2. Simulated versus experimental ¹H-NMR of H-15 for compound **3** in benzene-*d*₆.

Figure S3. ¹H NMR spectrum of **3** in benzene-*d*₆ at 600 MHz.

Figure S4. NOE enhancement of H-13 of **3** in benzene-*d*₆ at 600 MHz.

Figure S5. NOE enhancement of H-16 of **3** in benzene-*d*₆ at 600 MHz.

Figure S6. ¹H NMR spectrum of **3** in CDCl₃ at 500 MHz.

Figure S7. ¹H NMR spectrum of **6** in DMSO-*d*₆ at 500 MHz.

Figure S8. ¹³C NMR spectrum of **6** in DMSO-*d*₆ at 125 MHz.

Figure S9. Isolation scheme.

Figure S10. NCI 60 cell line GI₅₀ mean graph for **3**.

Figure S11. gHMQC spectrum of **6** in DMSO-*d*₆ at 500 MHz.

Figure S12. gHMBC spectrum of **6** in DMSO-*d*₆ at 500 MHz.

Figure S13 Expansion of gHMBC spectrum of **6** in DMSO-*d*₆ at 500 MHz.

Table S1. Comparison of ¹³C-NMR of Synthetic Mycothiazole with Natural Mycothiazole (**3**) and Mycothiazole-4,19-diol (**6**).

*To whom correspondence should be addressed

Tel.: (831) 459-2603. Fax: (831)-459-2935. E-mail: phil@chemistry.ucsc.edu

Figure S1. Original ¹H-NMR of compound 3 in benzene-d₆ at 300 MHz.

3/-02/ALPHA(F 1)/PK1/C6D6
 COSY CAL.

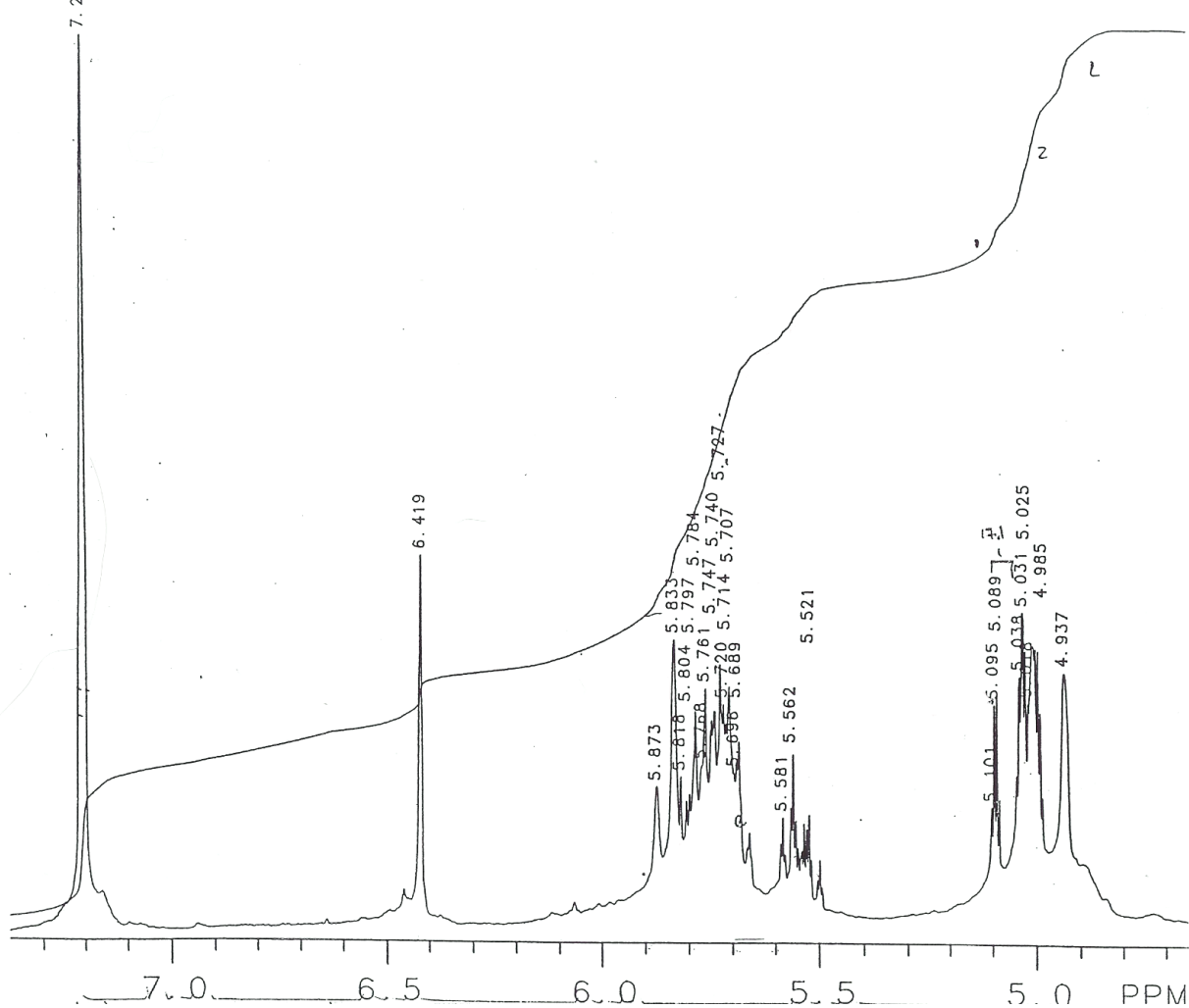


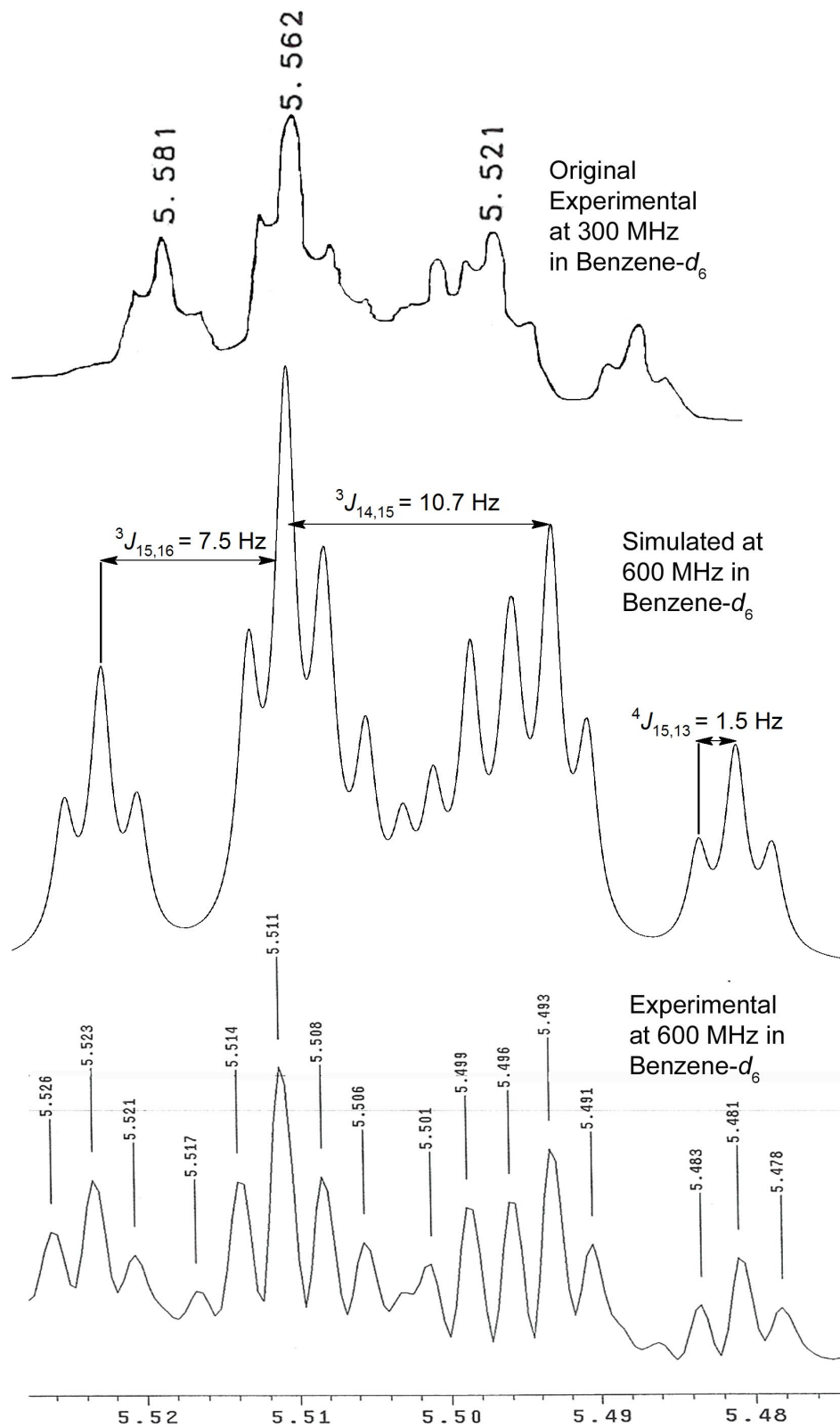
Figure S2. Simulated versus experimental $^1\text{H-NMR}$ of H-15 for compound **3** in benzene- d_6 .

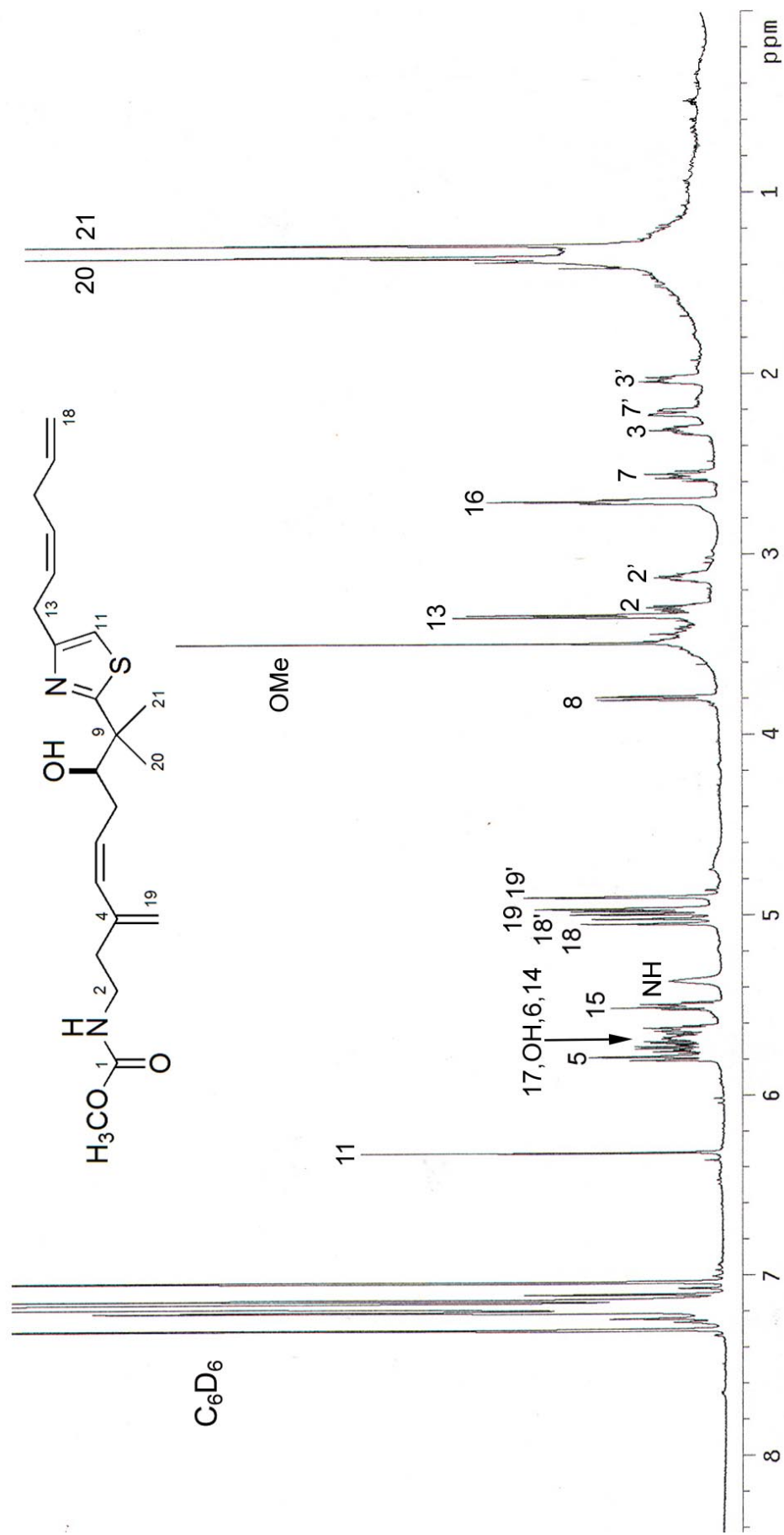
Figure S3. ¹H NMR spectrum of **3** in benzene-*d*₆ at 600 MHz.

Figure S4. NOE enhancement of H-13 of **3** in benzene-*d*₆ at 600 MHz.

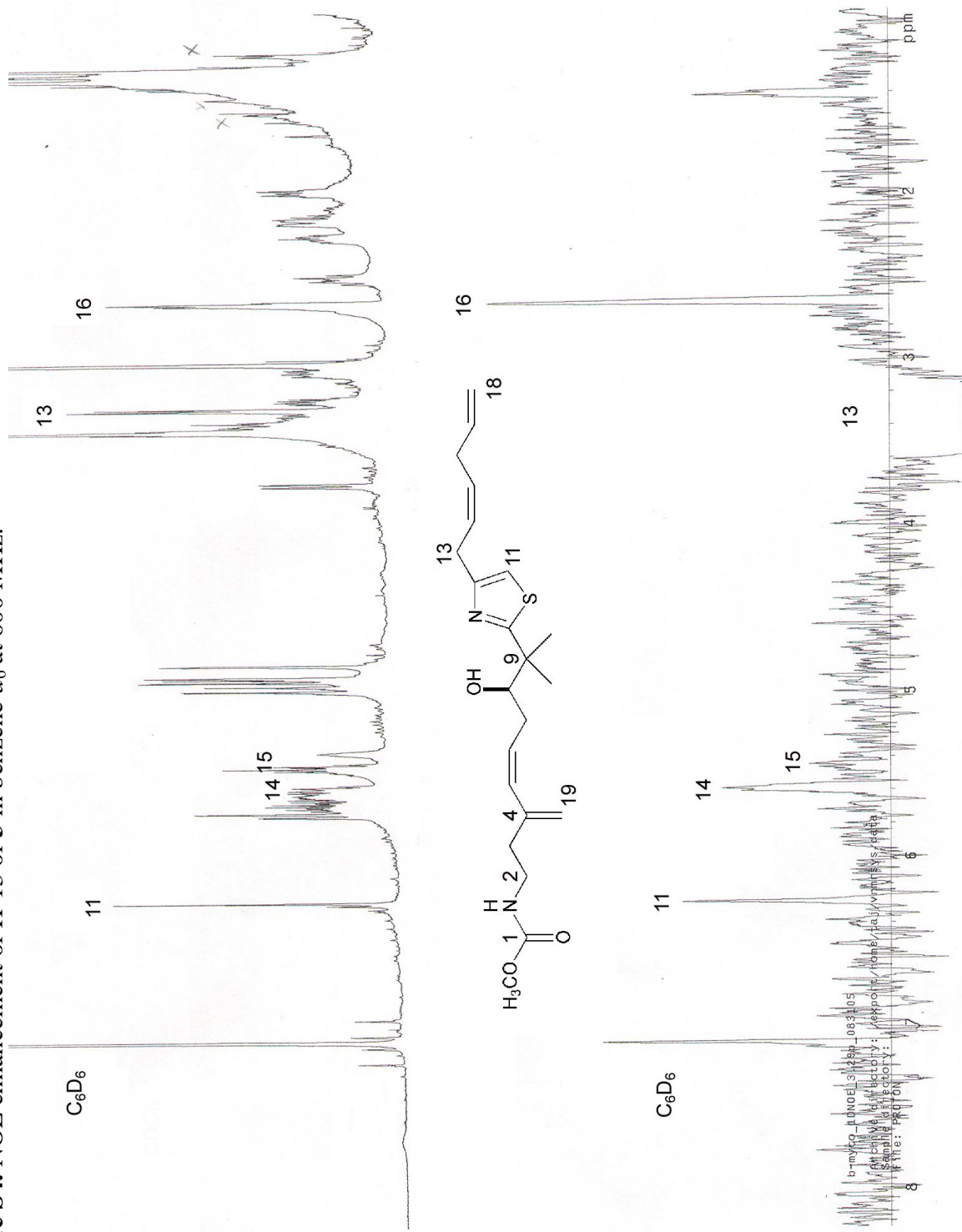


Figure S5. NOE enhancement of H-16 of **3** in benzene- d_6 at 600 MHz.

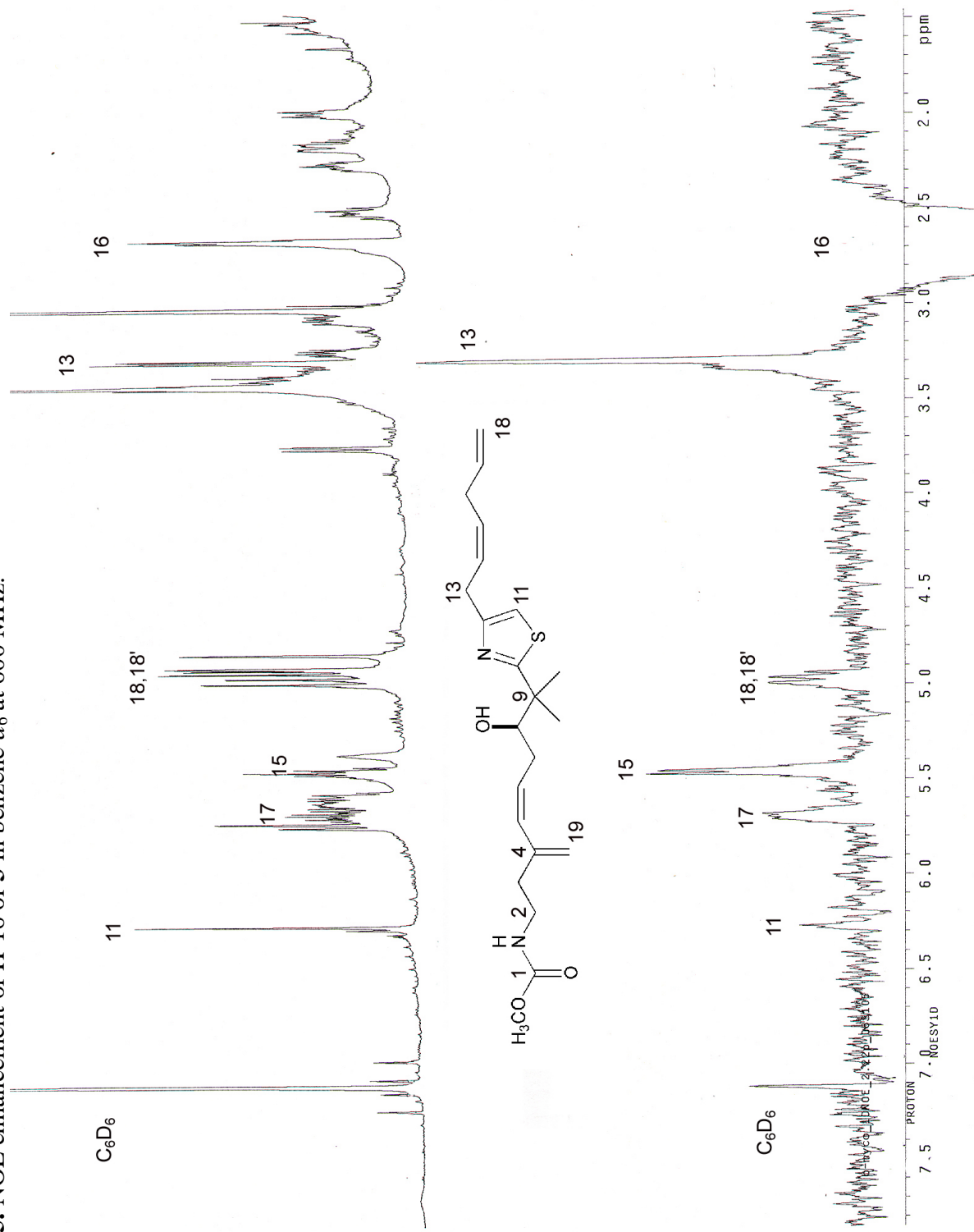


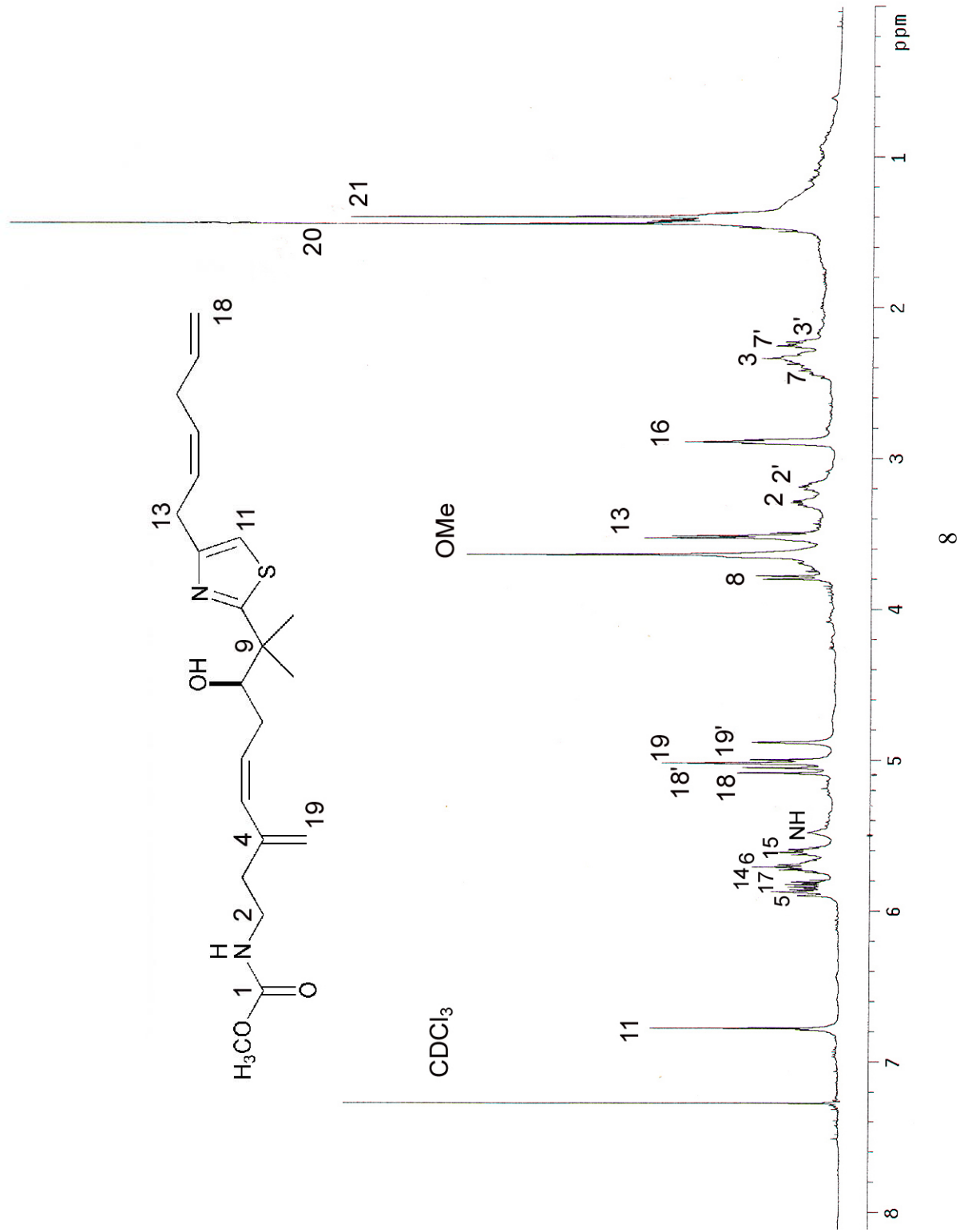
Figure S6. ^1H NMR spectrum of **3** in CDCl_3 at 500 MHz.

Figure S7. ¹H NMR spectrum of **6** in DMSO-*d*₆ at 500 MHz.

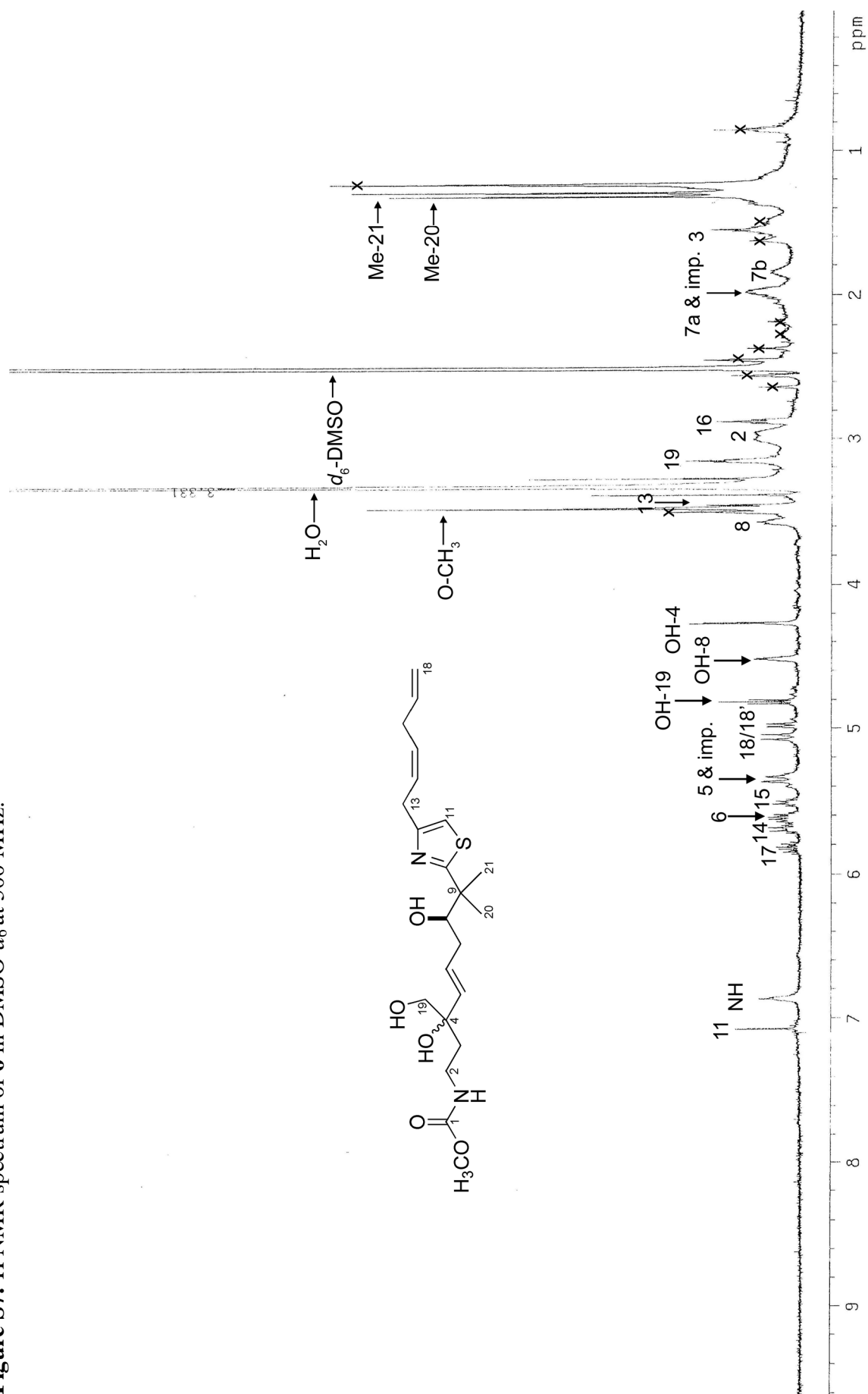


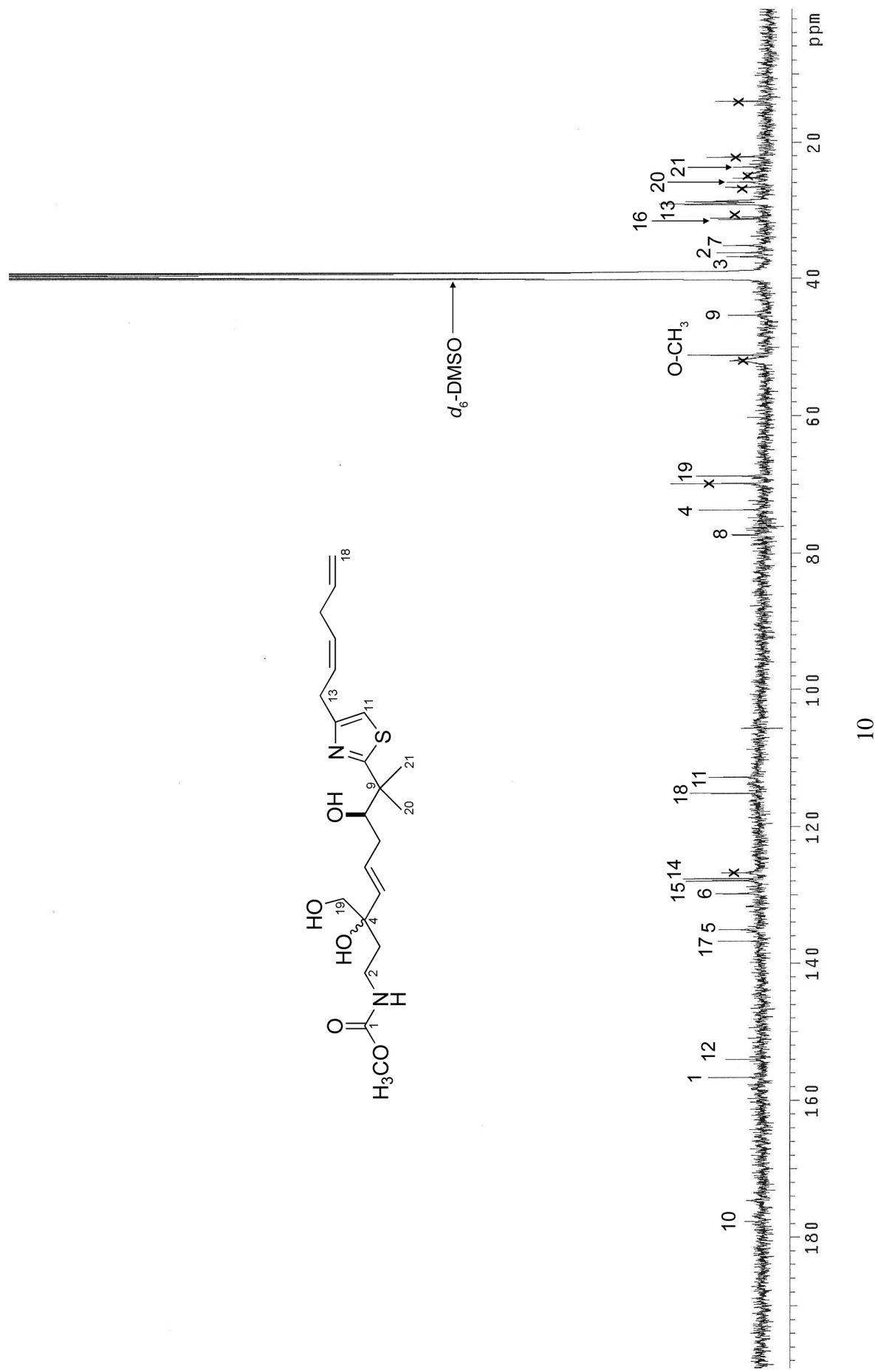
Figure S8. ^{13}C NMR spectrum of **6** in $\text{DMSO-}d_6$ at 125 MHz.

Figure S9. Isolation scheme.

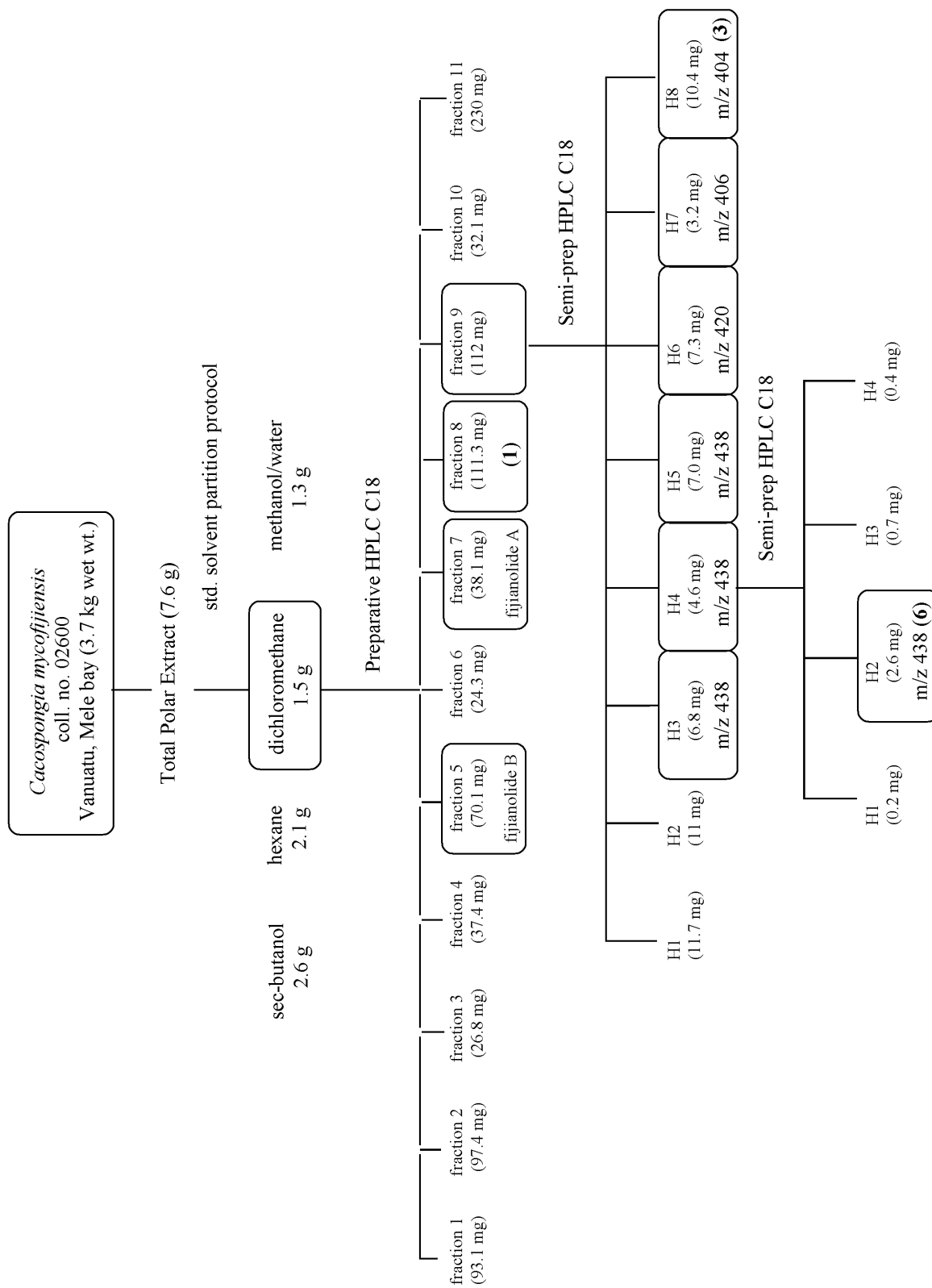


Figure S10. NCI 60 cell line GI₅₀ mean graph for 3.

GI₅₀ Mean Graph for Compound 647640

NCI Cancer Screen Current Data, August 2004
 Average GI₅₀ over all cell lines is 2.84E-5

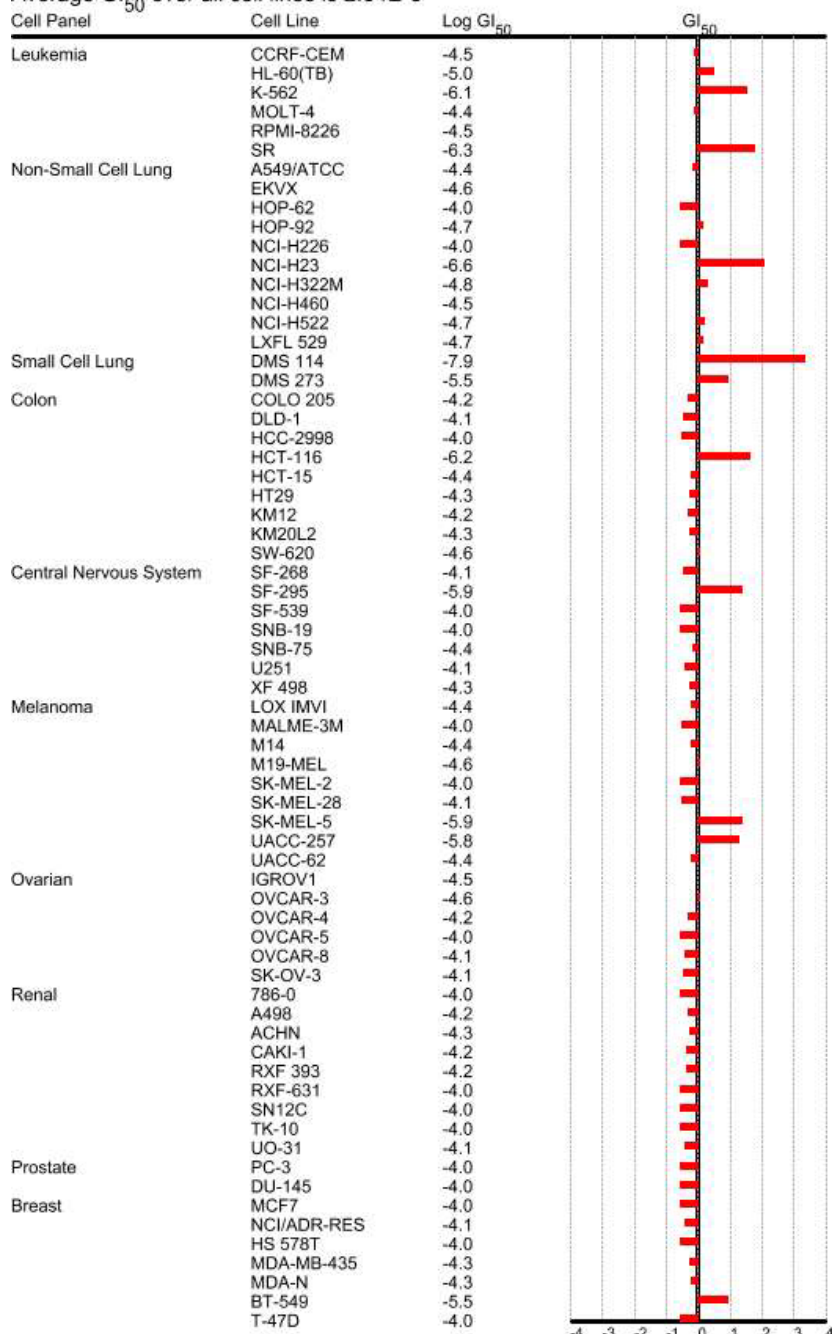


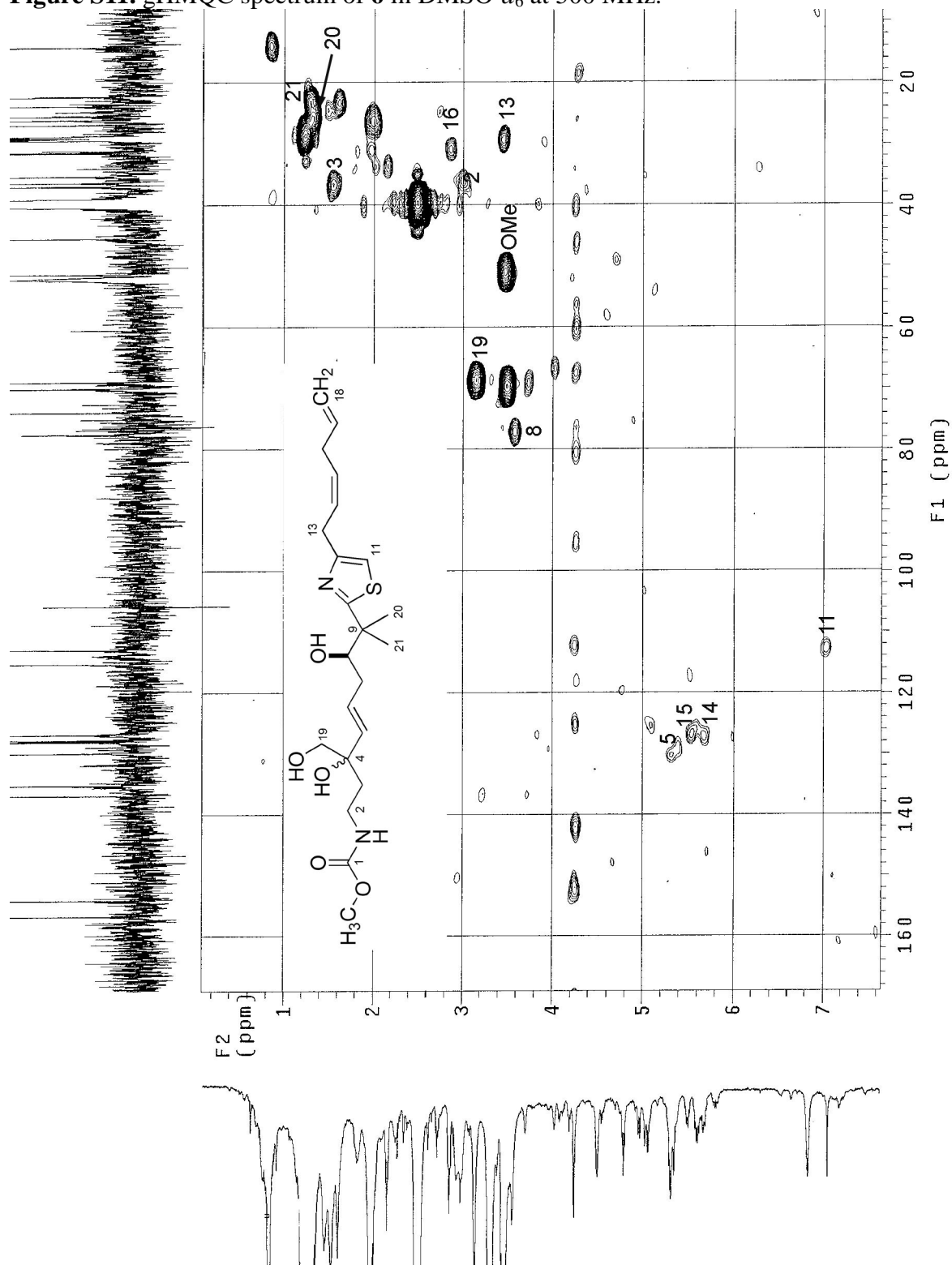
Figure S11. gHMBC spectrum of **6** in DMSO-*d*₆ at 500 MHz.

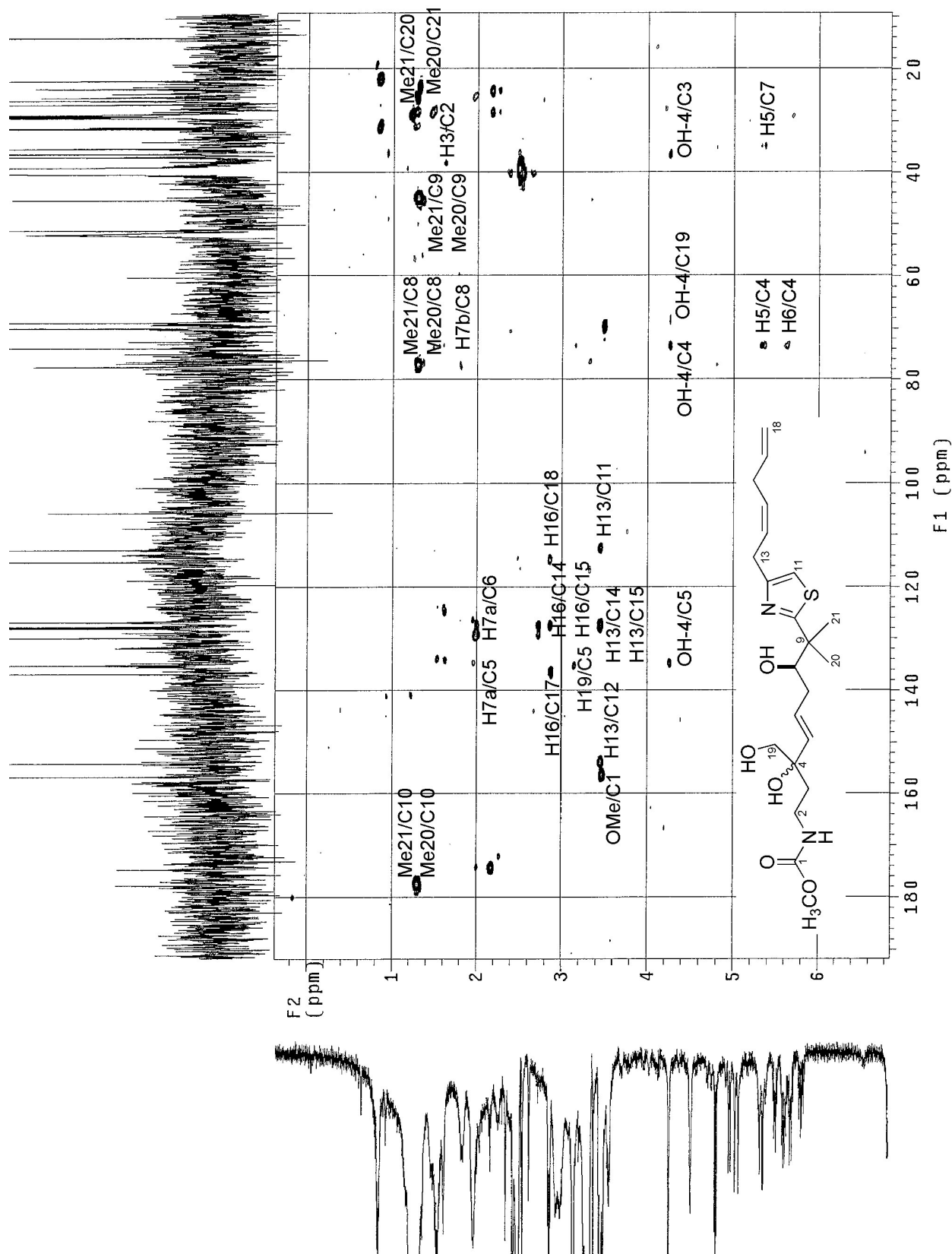
Figure S12. gHMBC spectrum of **6** in DMSO-*d*₆ at 500 MHz.

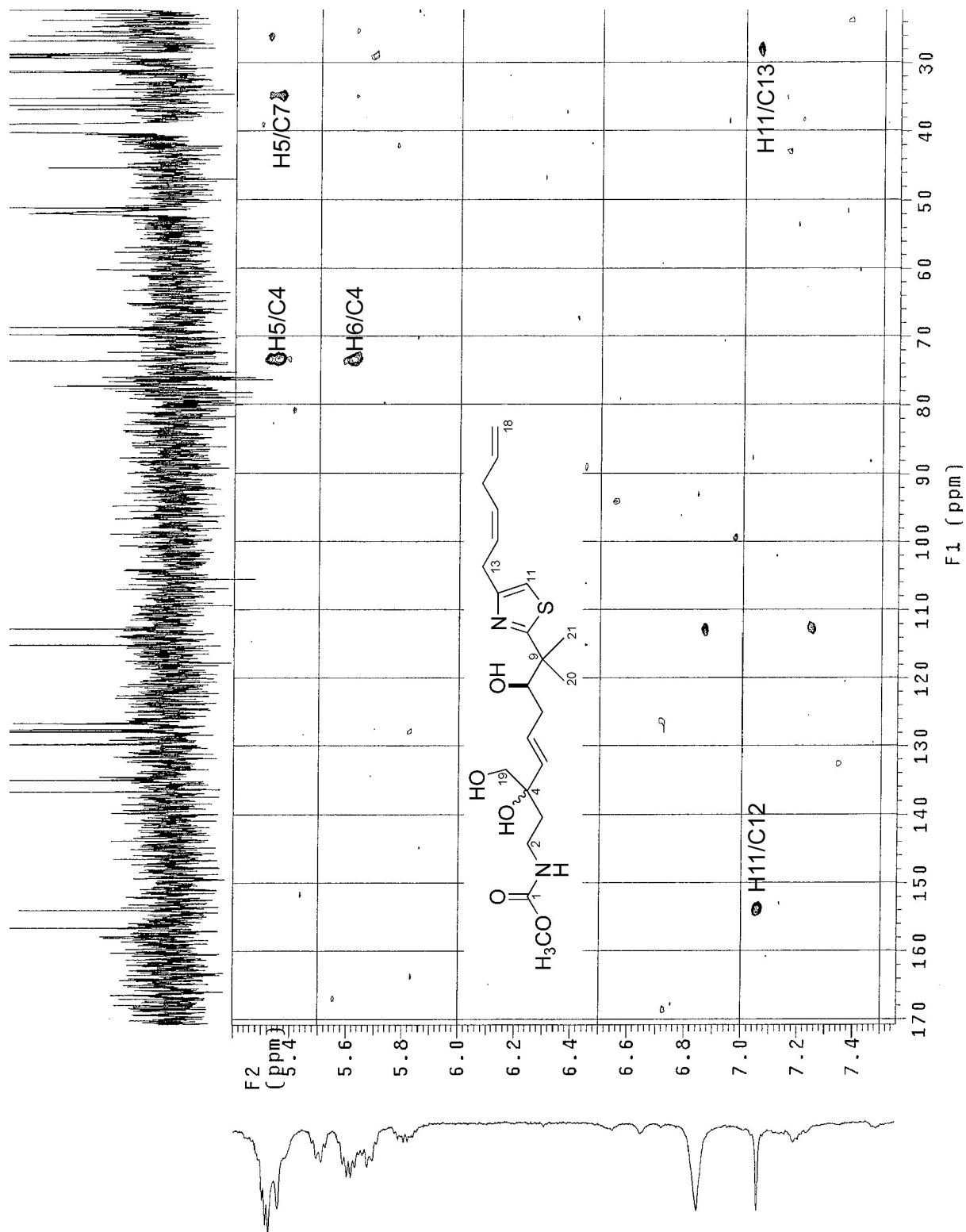
Figure S13 Expansion of gHMBC spectrum of **6** in DMSO-*d*₆ at 500 MHz.

Table S1. Comparison of ^{13}C -NMR of Synthetic Mycothiazole with Natural Mycothiazole (**3**) and Mycothiazole-4,19-diol (**6**).

Position	synthetic (-)-mycothiazole ^a		synthetic (-)-mycothiazole ^b		natural mycothiazole (3) ^c		mycothiazole-4,19-diol (6) ^d	
	δ_{C}	δ_{C}	δ_{C}	δ_{C}	δ_{C}	δ_{C}	δ_{C}	δ_{C}
1	157.2	157.1	157.1	157.1	157.1	156.6	156.6	156.6
2	39.4	39.4	39.4	39.4	39.4	36.1	36.1	36.1
3	37.1	37.1	37.1	37.1	37.1	36.7	36.7	36.7
4	*	142.5	142.5	142.5	142.4	73.7	73.7	73.7
5	130.9	130.9	130.9	130.9	130.8	135.0	135.0	135.0
6	130.6	130.6	130.6	130.6	130.8	129.8	129.8	129.8
7	30.6	30.6	30.6	30.6	30.6	35.2	35.2	35.2
8	78.1	78.1	78.1	78.1	78.1	77.3	77.3	77.3
9	44.6	44.5	44.5	44.5	44.5	45.3	45.3	45.3
10	*	179.4	179.4	179.4	179.4	177.7	177.7	177.7
11	112.0	112	112	112	111.8	112.8	112.8	112.8
12	155.4	155.4	155.4	155.4	154.9	154.0	154.0	154.0
13	34.7	34.7	34.7	34.7	29.4	29.2	29.2	29.2
14	127.6	127.6	127.6	127.6	126.7	127.6	127.6	127.6
15	130.5	130.4	130.4	130.4	128.8	127.9	127.9	127.9
16	36.6	36.6	36.6	36.6	31.5	31.3	31.3	31.3
17	136.8	136.8	136.8	136.8	136.4	136.7	136.7	136.7
18	115.2	115.2	115.2	115.2	115	115.1	115.1	115.1
19	115.9	115.8	115.8	115.8	115.8	68.8	68.8	68.8
20	26.7	26.7	26.7	26.7	26.6	25.9	25.9	25.9
21	23.9	23.9	23.9	23.9	23.9	23.6	23.6	23.6
O-Me	51.8	51.8	51.8	51.8	51.8	51.1	51.1	51.1

^a Data from Le Flohic *et. al*
Org. Lett. **2005**, 7, 339-342.

^b Data from Sugiyama *et. al*
Tetrahedron **2003**, 59, 6579-6593

^c Data from Crews *et. al*
J.A.C.S. **1988**, 110, 4365-4368.

^d Obtained in DMSO-d₆

* The corresponding signals could not be assigned