

07H239-A, A New Cytotoxic Eremophilane  
Sesquiterpene from the Marine-Derived Xylariaceous  
Fungus LL-07H239

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Supporting Information

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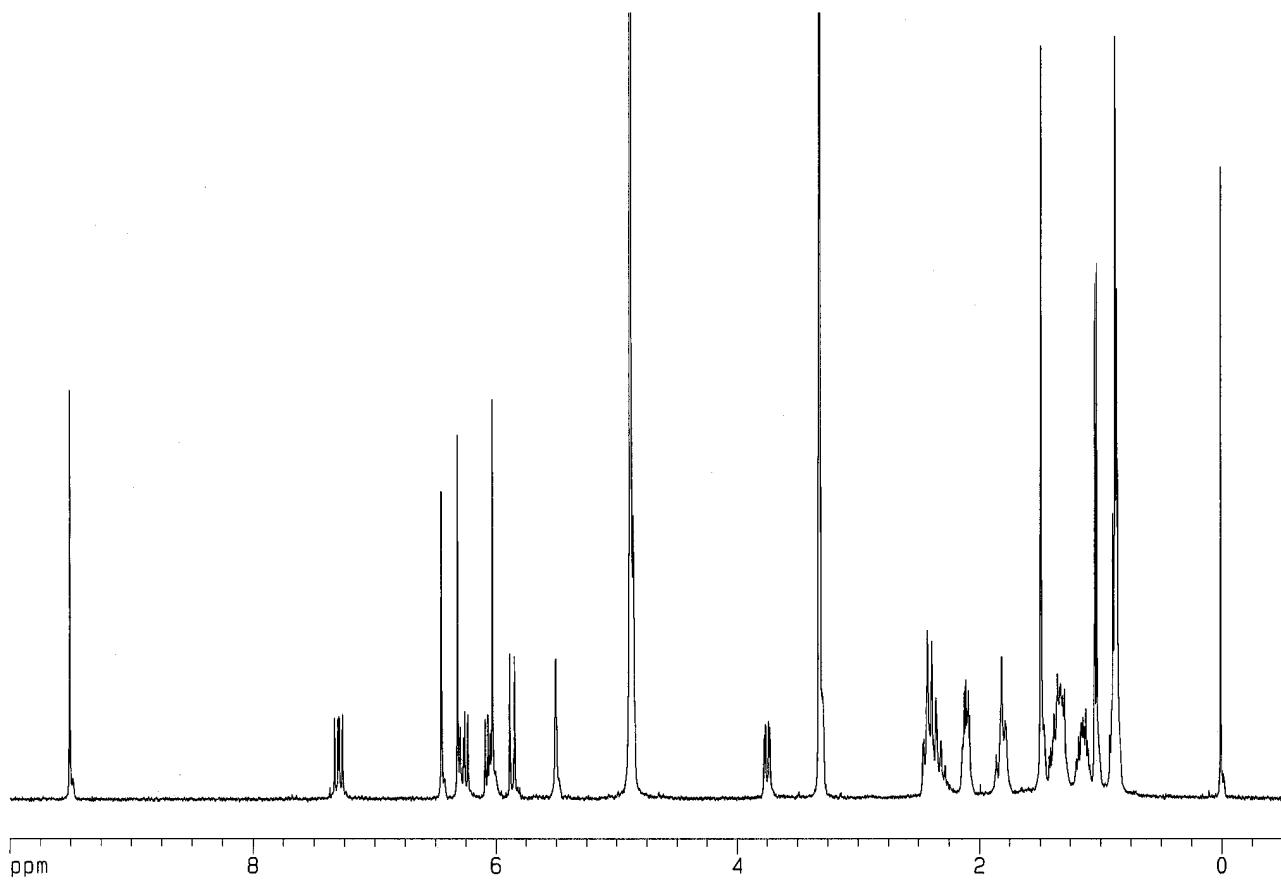
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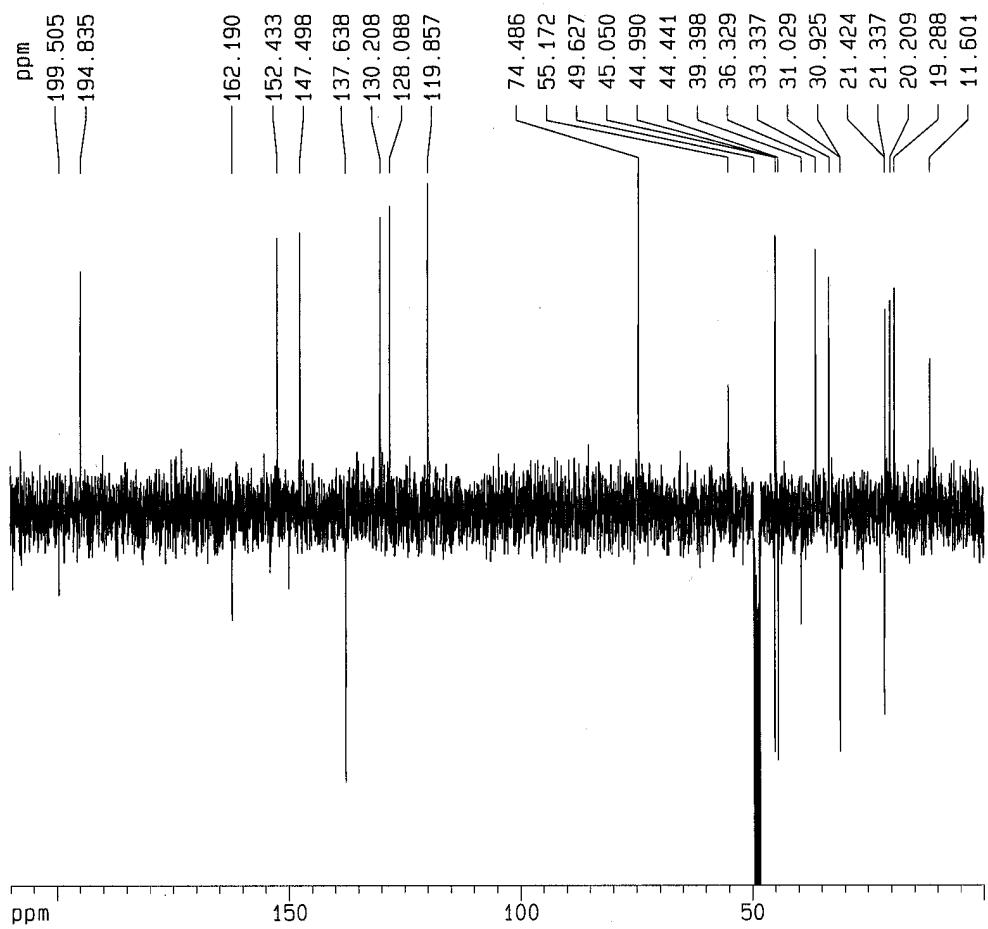
**Table S1.** NMR<sup>a</sup> data with assignments and significant HMBC correlations for 07H239-A (**1**) .

Atom no.	<sup>13</sup> C MeOH-d <sub>4</sub>	<sup>1</sup> H MeOH-d <sub>4</sub>	<sup>13</sup> C Acetone-d <sub>6</sub>	<sup>1</sup> H Acetone-d <sub>6</sub>	HMBC correlations
8	199.4	—	197.1	—	—
12	194.8	9.50, s	193.9	9.55, s	H12- C7, C11
14	176.1	—	174.1	—	—
1'	167.4	—	166.0	—	—
10	162.0	—	160.3	—	—
5'	152.5	6.05, dd, 15.2, 8.4	151.5	6.11, dd, 15.2, 8.4	H5'- C3', C4', C11'
11	149.9	—	149.6	—	—
3'	147.5	7.28, dd, 15.2, 10.8	146.5	7.29, dd, 15.2, 10.8	H3'- C1', 2', C5'
13	137.6	6.43, s 6.30, s	136.8	6.43, s 6.31, s	H13a- C7, C11, C12 H13b- C7, C11, C12
9	130.3	6.03, s	130.0	5.99, s	H9- C1, C5, C7
4'	128.1	6.25, dd, 15.2, 10.8	127.7	6.30, dd, 15.2, 10.8	H4'- C2', C3', C5', C6'
2'	119.9	5.85, d, 15.2	120.0	5.90, d, 15.2	H2'- C1', C4'
1	74.5	5.50, bs	73.7	5.50, bs	H1- C1', C5
4	54.7	2.41, obs <sup>b</sup>	53.9	2.49, obs	H4- C5, C14
7'	45.1	1.37, obs 1.11, obs	44.6	1.39, obs 1.10, obs	H7'a- C6' H7'b- C5', C6', C8', C11', C12'
7	45.0	3.72, dd, 14.4, 4.5	44.5	3.77, dd, 14.4, 4.3	H7- C6, C8, C11, C12, C13
6	44.5	2.39, obs 2.09, obs	43.9	2.40, obs 2.11, obs	H6ax- C4, C5, C7, C8, C11, C15 H6eq- C5, C7, C8, C10, C11, C15
5	39.4	—	38.9	—	—
6'	36.3	2.40, obs	35.7	2.43, obs	—
8'	33.4	1.34, obs	32.8	1.33, obs	—
9'	31.0	1.34, obs 1.15, obs	30.4	1.31, obs 1.13, obs	H9'a- C8' H9'b- C7', C8', C10'
2	30.9	2.12, obs 1.79, obs	30.4	2.11, obs 1.85, obs	— H2ax- C4
3	21.4	2.32, obs 1.83, obs	21.1	2.31, obs 1.83, obs	— H3ax- C4
11'	21.3	1.03, d, 6.6	21.3	1.02, d, 6.6	H11'- C5', C6', C7'
15	20.2	1.48, s	20.0	1.51, s	H15- C4, C5, C6, C10
12'	19.3	0.85, obs	19.2	0.85, obs	H12'- C7', C8', C9'
10'	11.6	0.87, obs	11.5	0.85, obs	H10'- C8', C9'

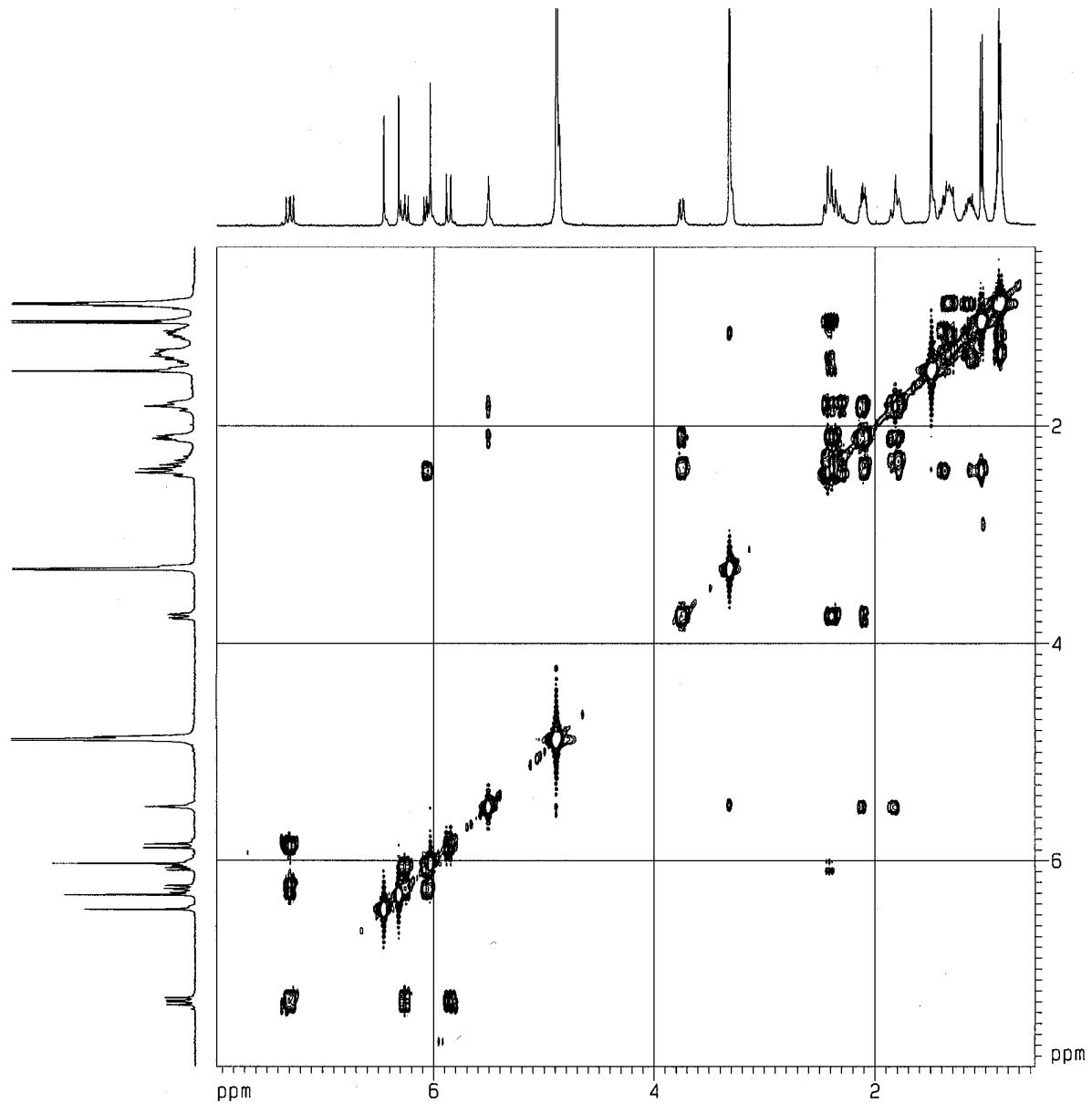
<sup>a</sup> NMR data acquired at 300 (or 400) MHz for proton and 75 (or 100) MHz for carbon.<sup>b</sup> obs = multiplicity obscured. HMBC correlations derived from multiple data sets.



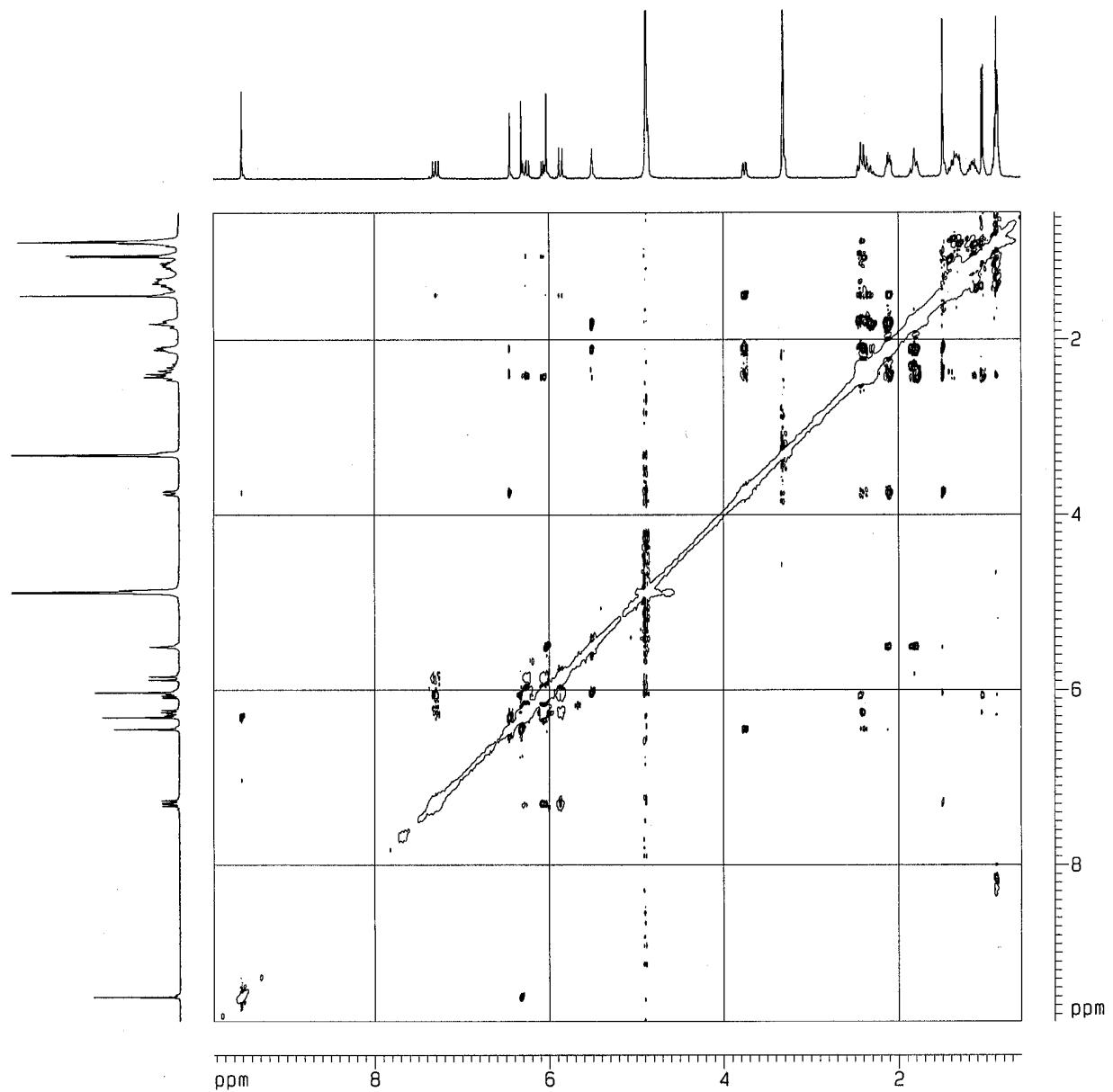
**Figure S1.** <sup>1</sup>H NMR (MeOH, 400 MHz) spectrum of 07H239-A (**1**).



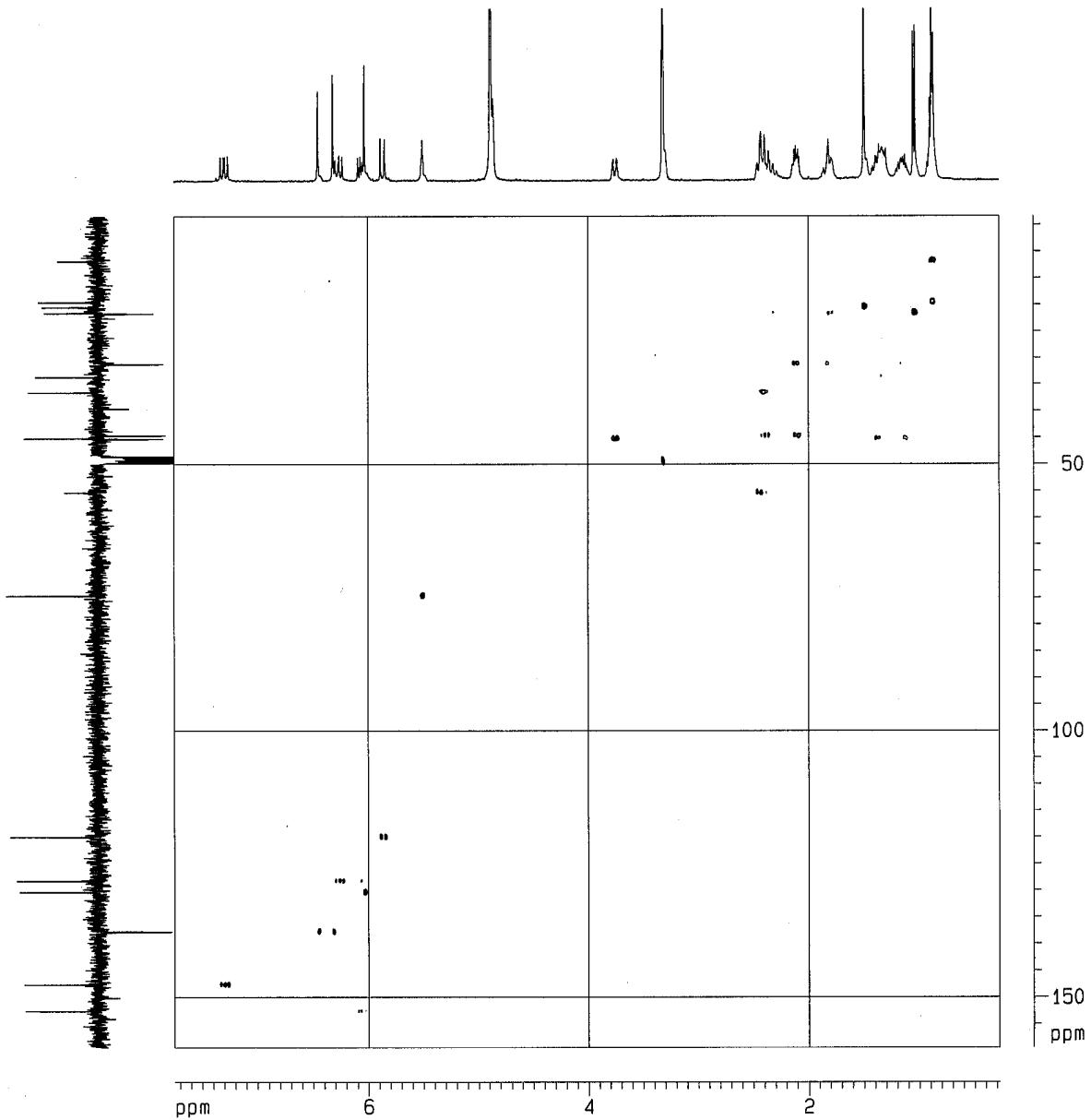
**Figure S2.** <sup>13</sup>C APT (*MeOH*, 100 MHz) spectrum of 07H239-A (**1**).



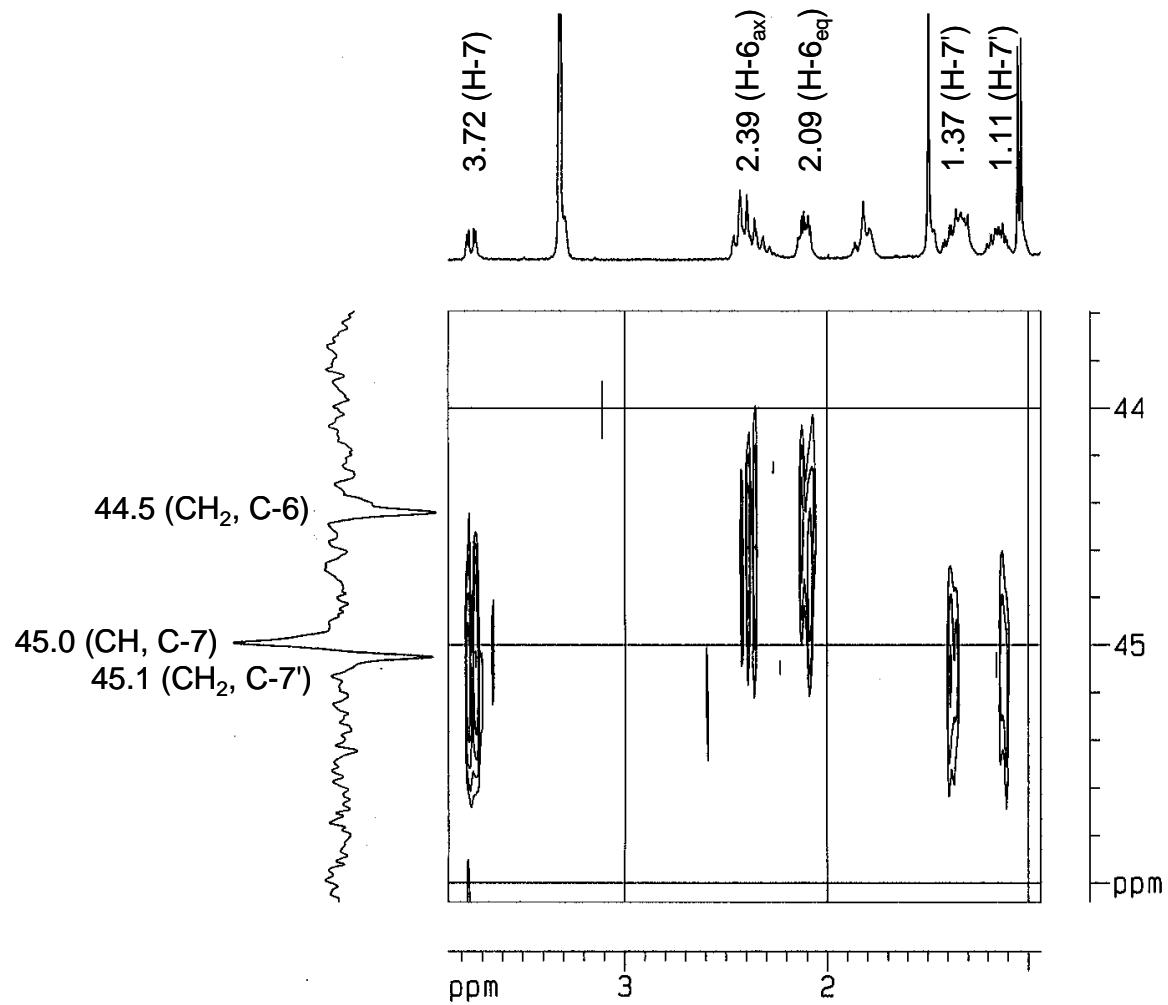
**Figure S3.** Section of  $^1\text{H}$ - $^1\text{H}$  COSY NMR (MeOH, 400 MHz) spectrum of 07H239-A (**1**).



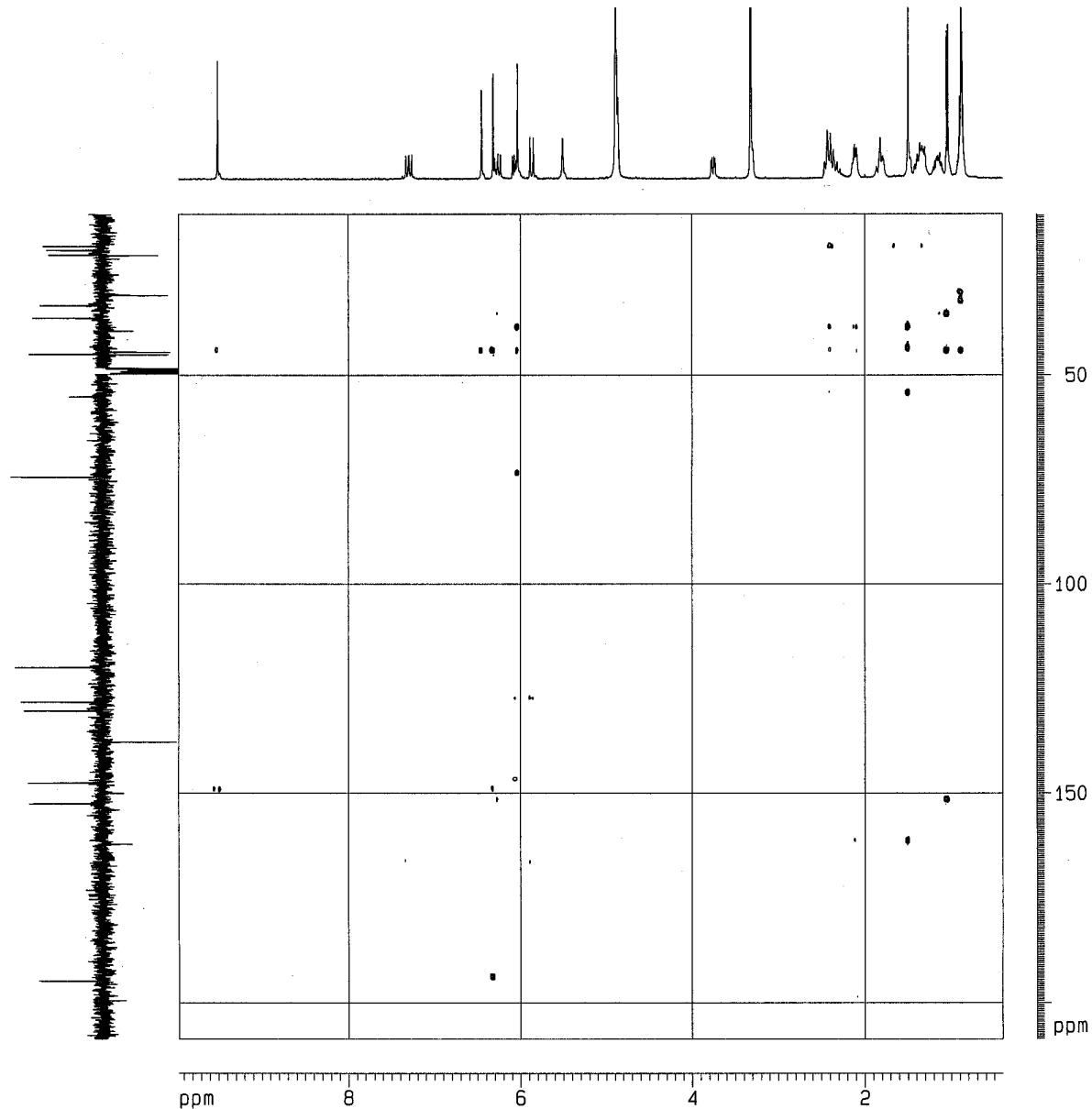
**Figure S4.** ROESY NMR ( $\text{MeOH}$ , 400 MHz, spin lock = 250 ms) spectrum of 07H239-A (**1**).



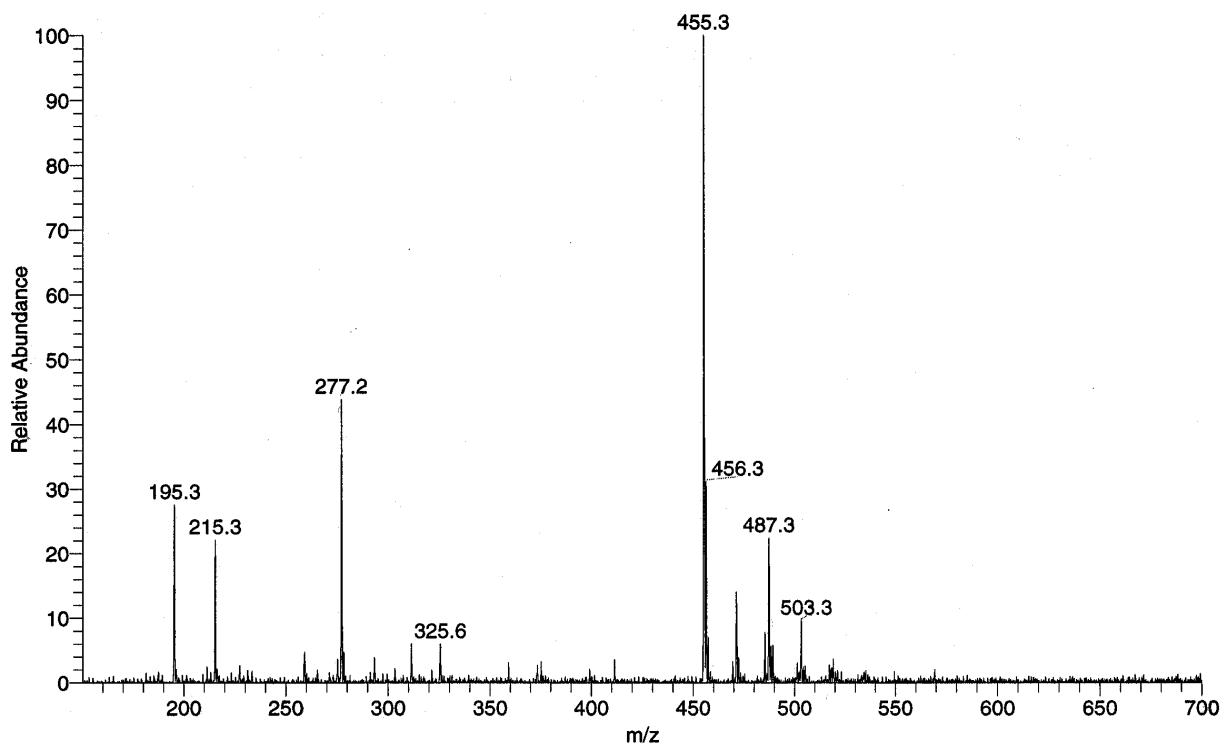
**Figure S5.**  $^1\text{H}$ - $^{13}\text{C}$  HMQC NMR (MeOH, 400 MHz) spectrum of 07H239-A (**1**).



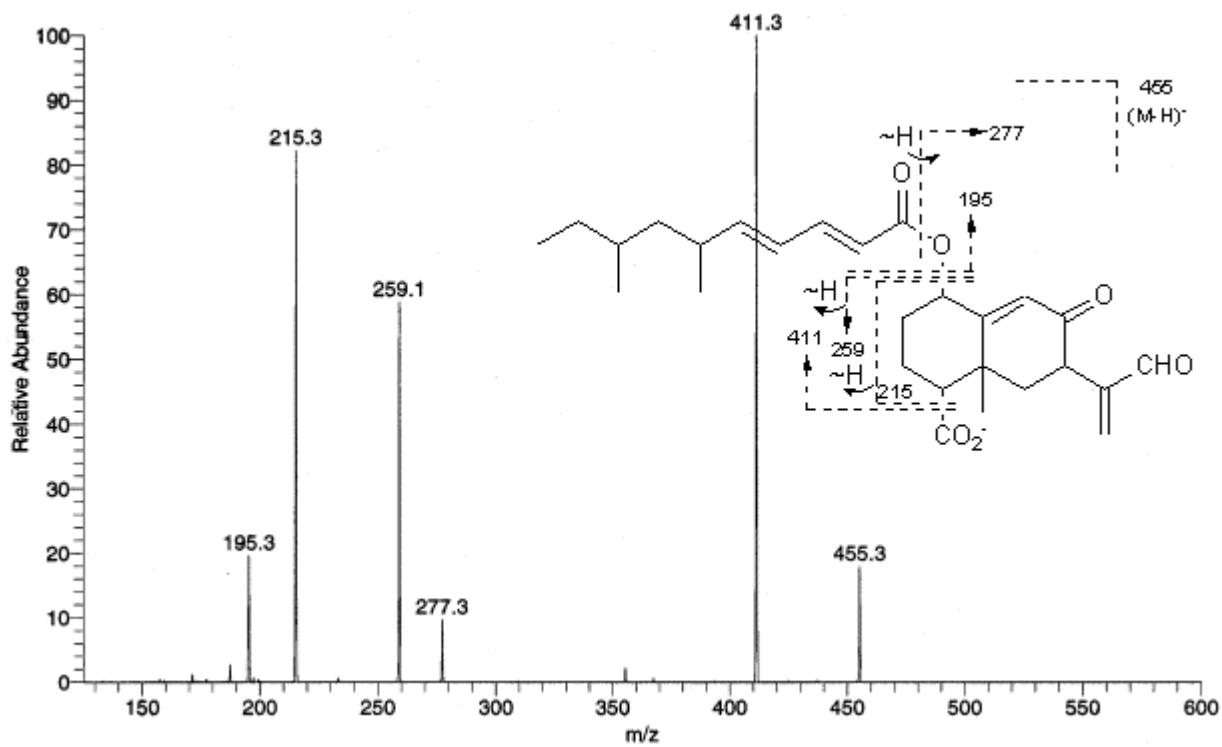
**Figure S6.** Region of  $^1\text{H}$ - $^{13}\text{C}$  HMQC NMR (MeOH, 400 MHz) spectrum of 07H239-A (**1**).



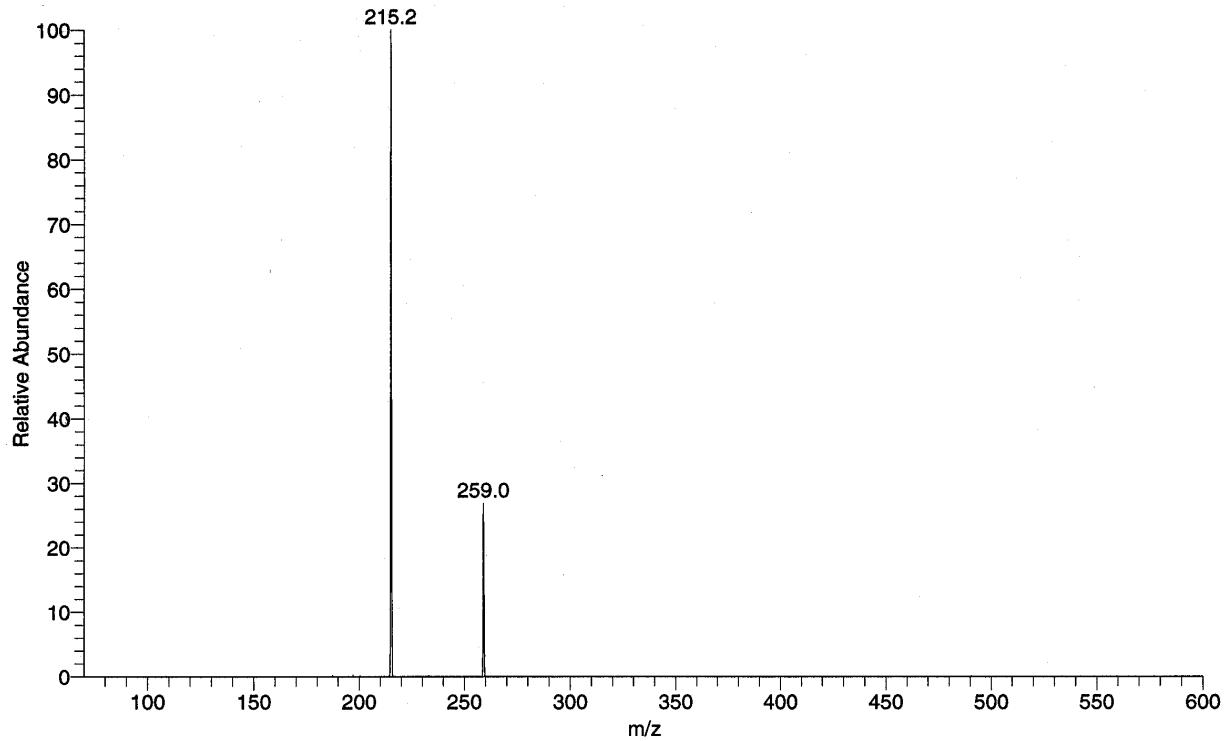
**Figure S7.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC NMR (MeOH, 400 MHz) spectrum of 07H239-A (**1**).



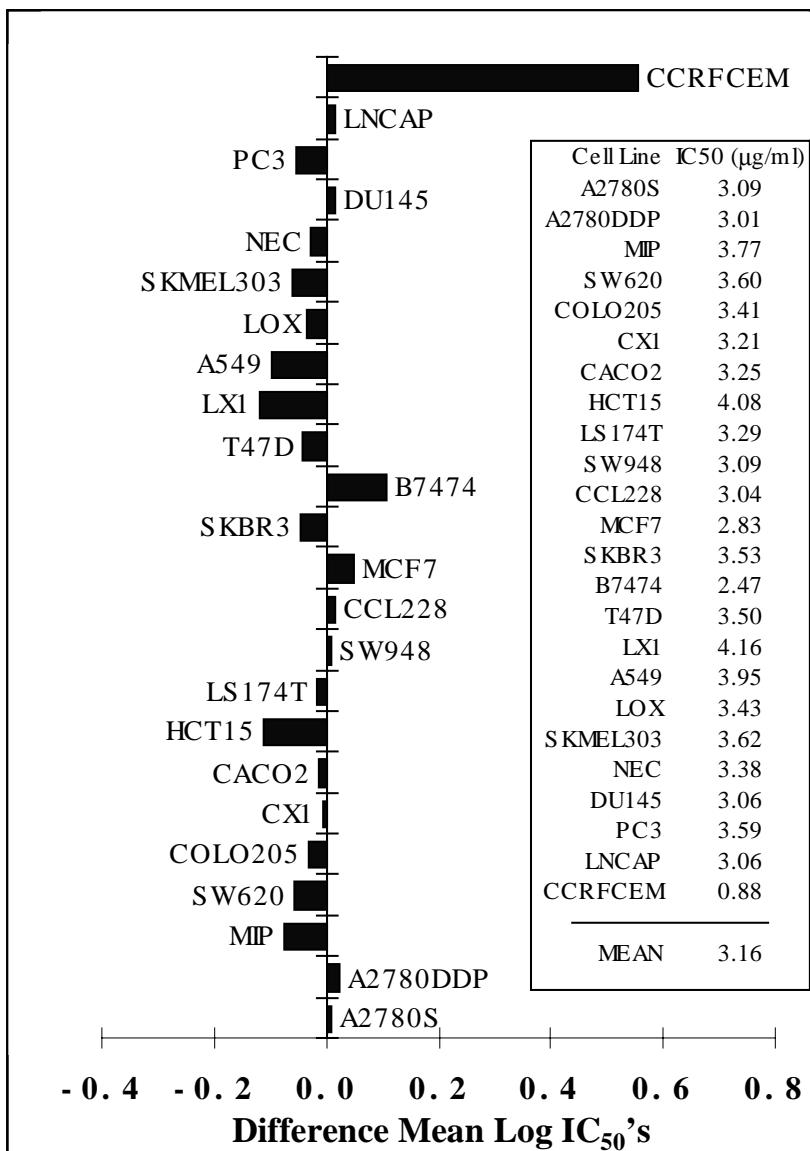
**Figure S8.** Negative ion electrospray MS (Full scan) spectrum of 07H239-A (**1**).



**Figure S9.** Negative ion electrospray MS<sup>2</sup> (*m/z* 455) spectrum of 07H239-A (**1**).

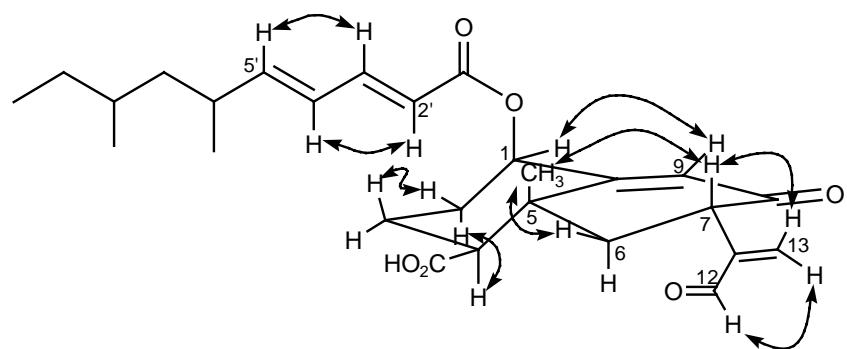


**Figure S10.** Negative ion electrospray  $\text{MS}^3$  ( $m/z$  455= $\gt$ 259) spectrum of 07H239-A (**1**).



**Figure S11.** Mean bar graph for 07H239-A (**1**) showing activity against a diverse panel of cancer cell lines. Bars to the right of the mean = cell line more sensitive to compound **1**.

**Scheme S1.** Significant ROESY correlations for 07H239-A (1).



**Scheme S2.** Proposed positive ion MS fragmentation for 07H239-A (**1**).

