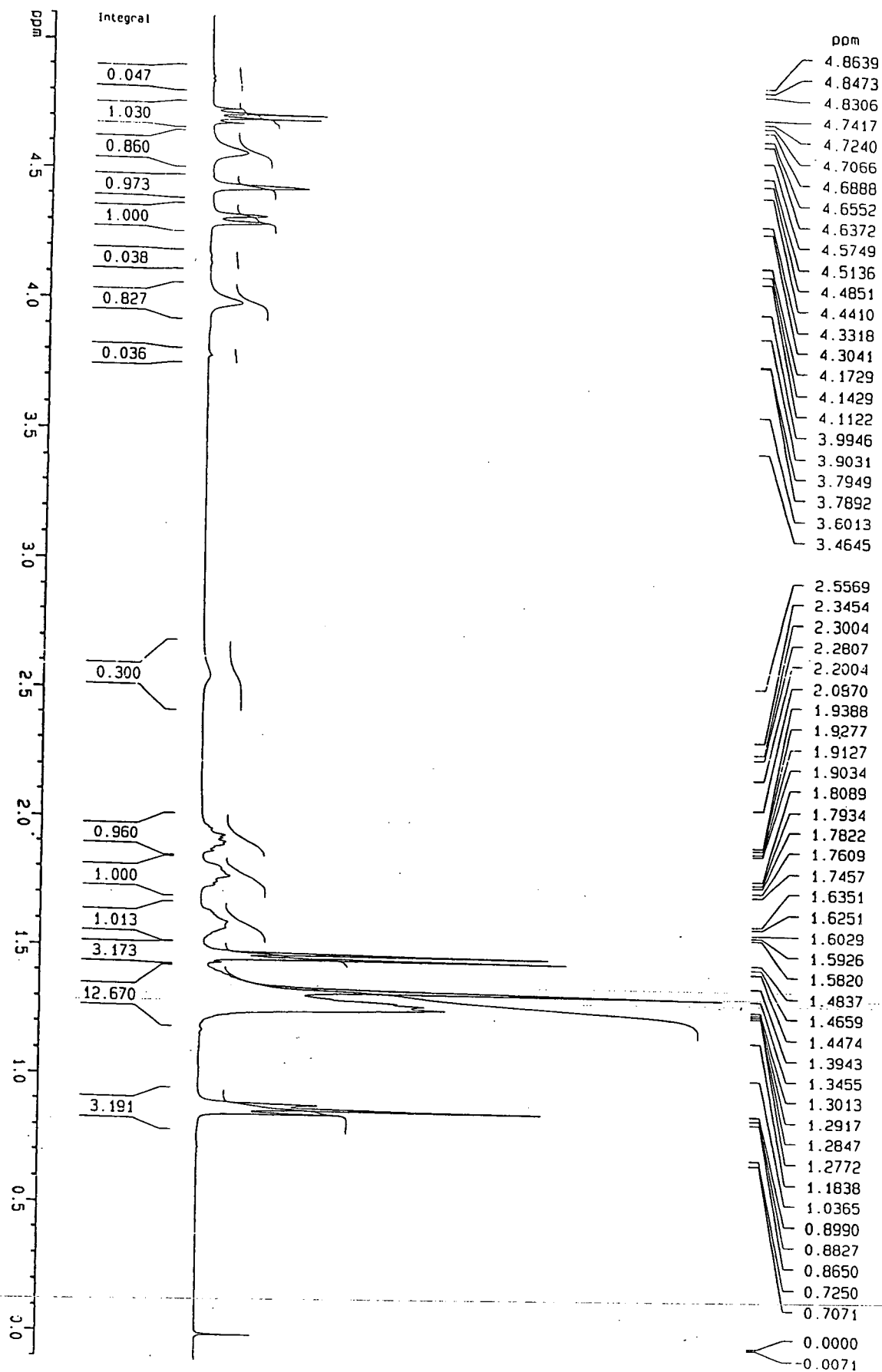


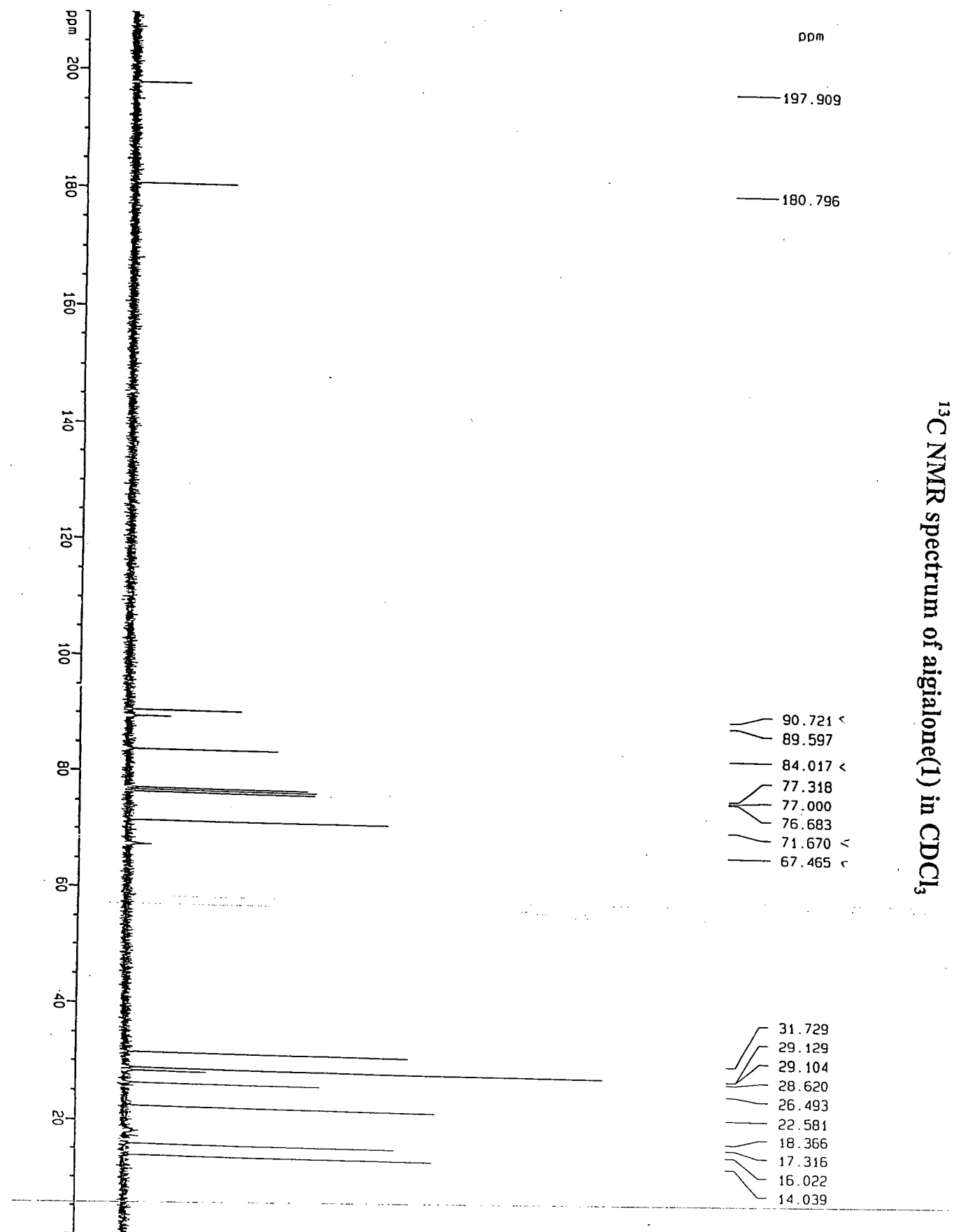
**Ketene Acetal and Spiroacetal Constituents of the Marine Fungus,  
*Aigialus parvus* BCC 5311**

Pornrapee Vongvilai,<sup>†</sup> Masahiko Isaka,<sup>\*,‡</sup> Prasat Kittakoop,<sup>‡</sup> Prasert Srikitikulchai,<sup>‡</sup>  
Palangpon Kongsaree,<sup>†</sup> and Yodhathai Thebtaranonth<sup>†,‡</sup>

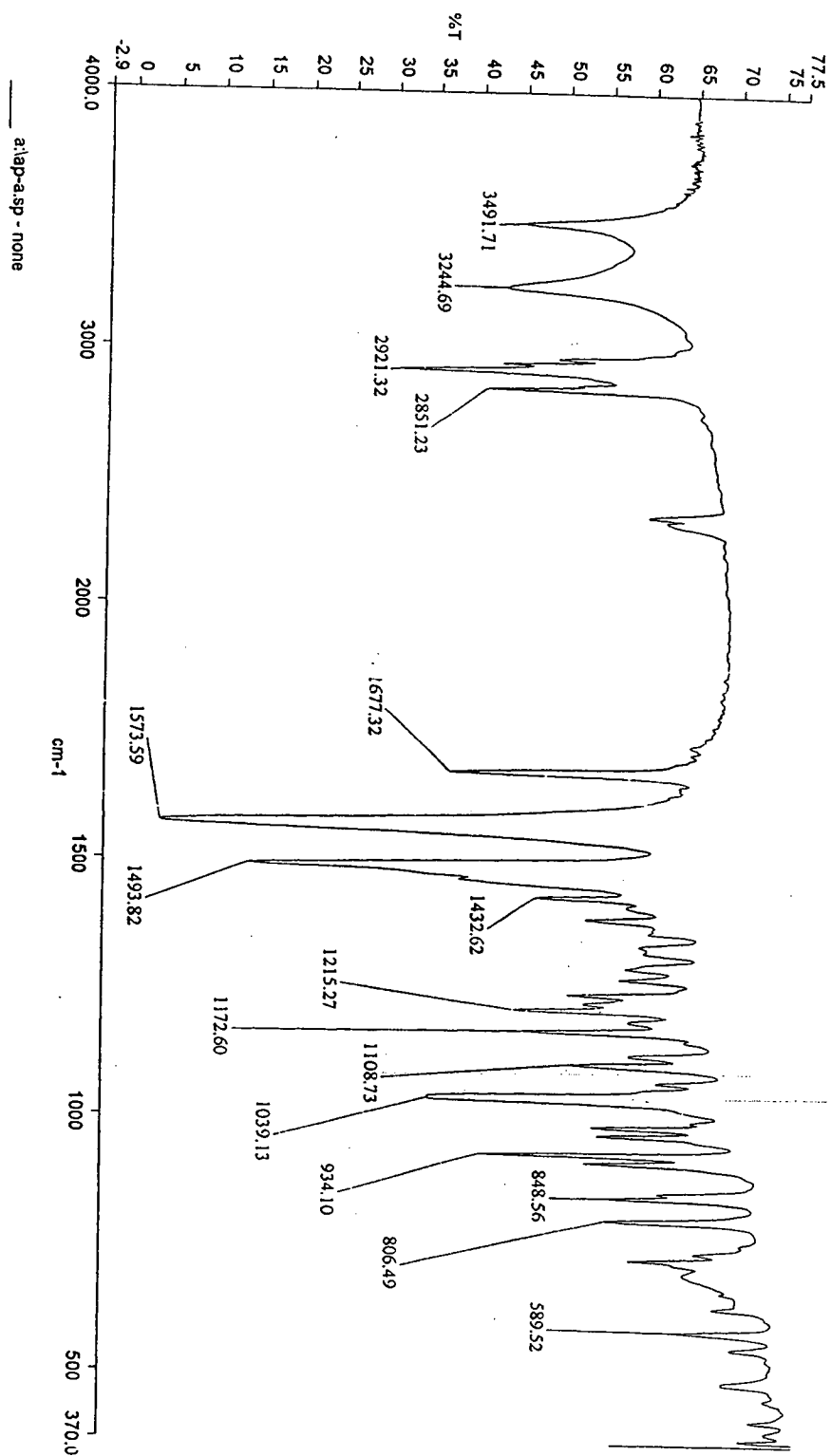
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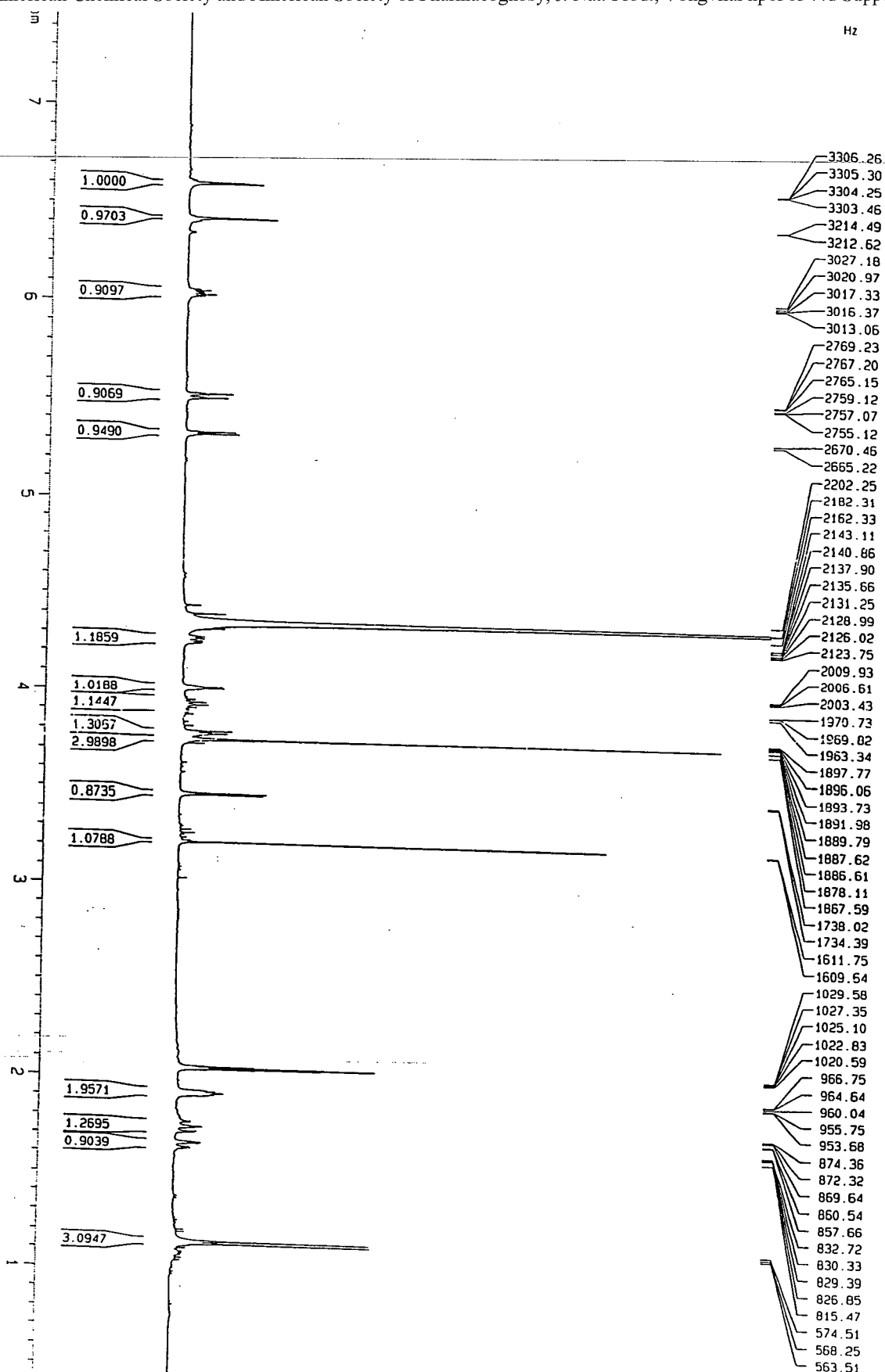




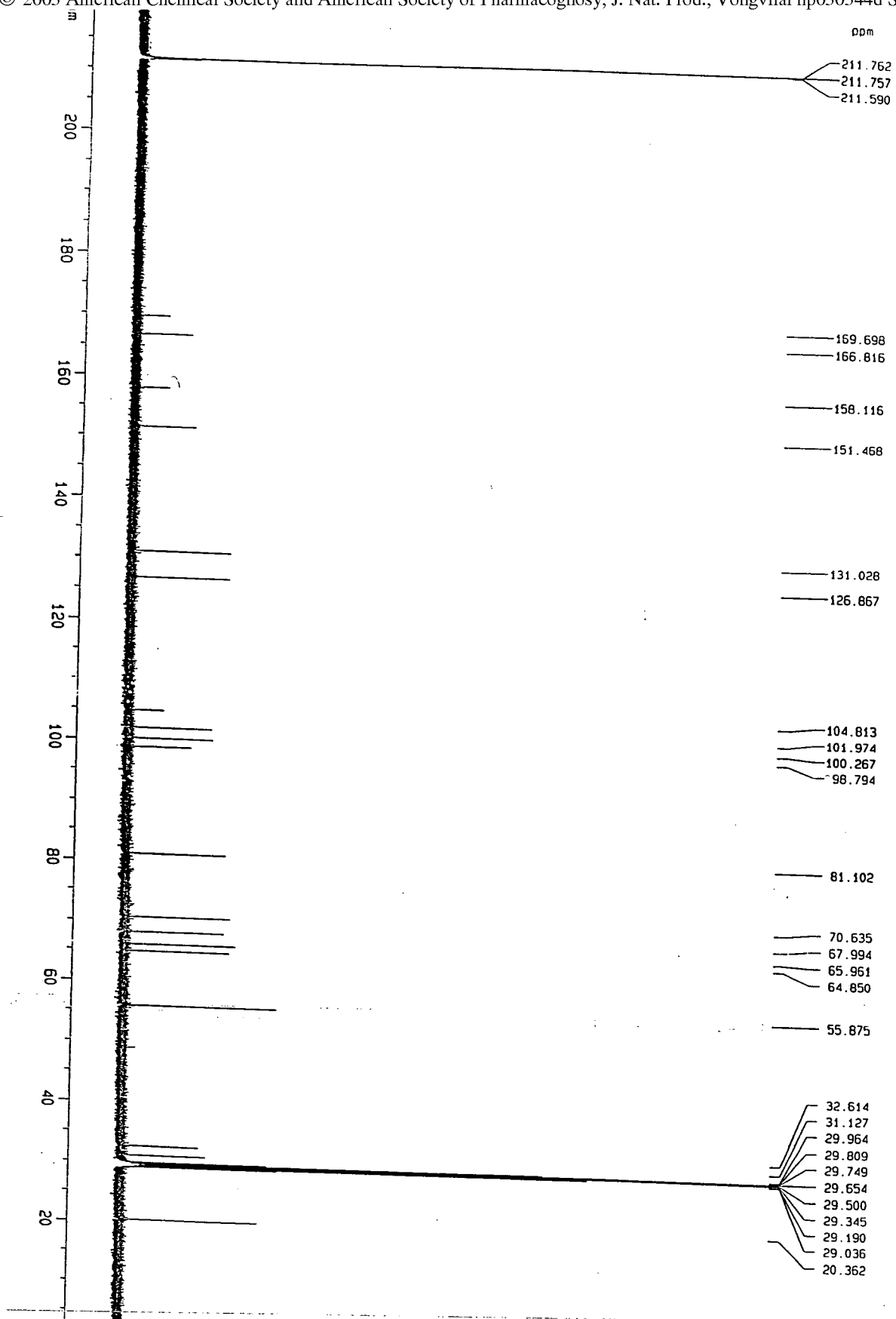
# IR spectrum of aigialone (1) (KBr)



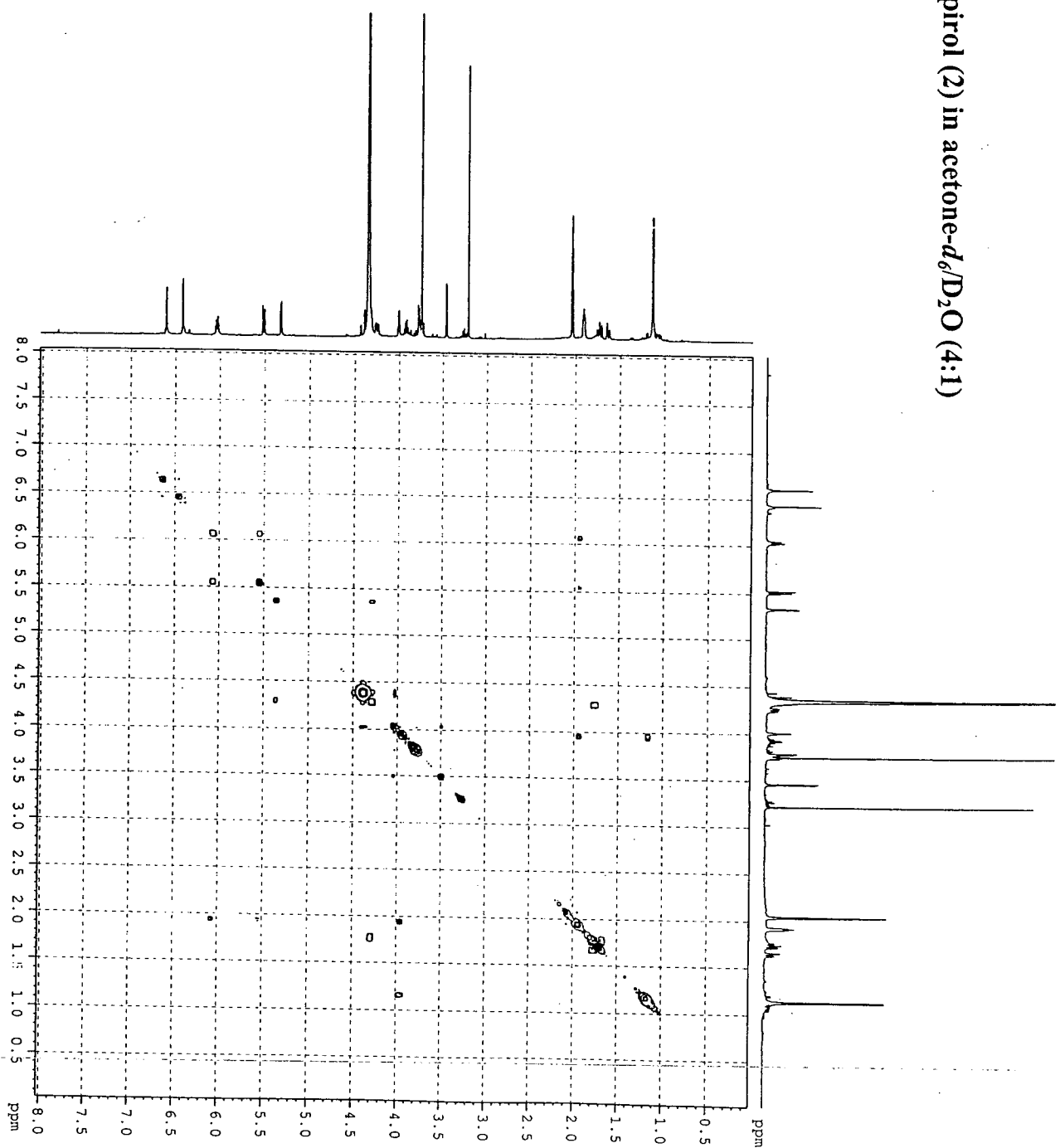
45

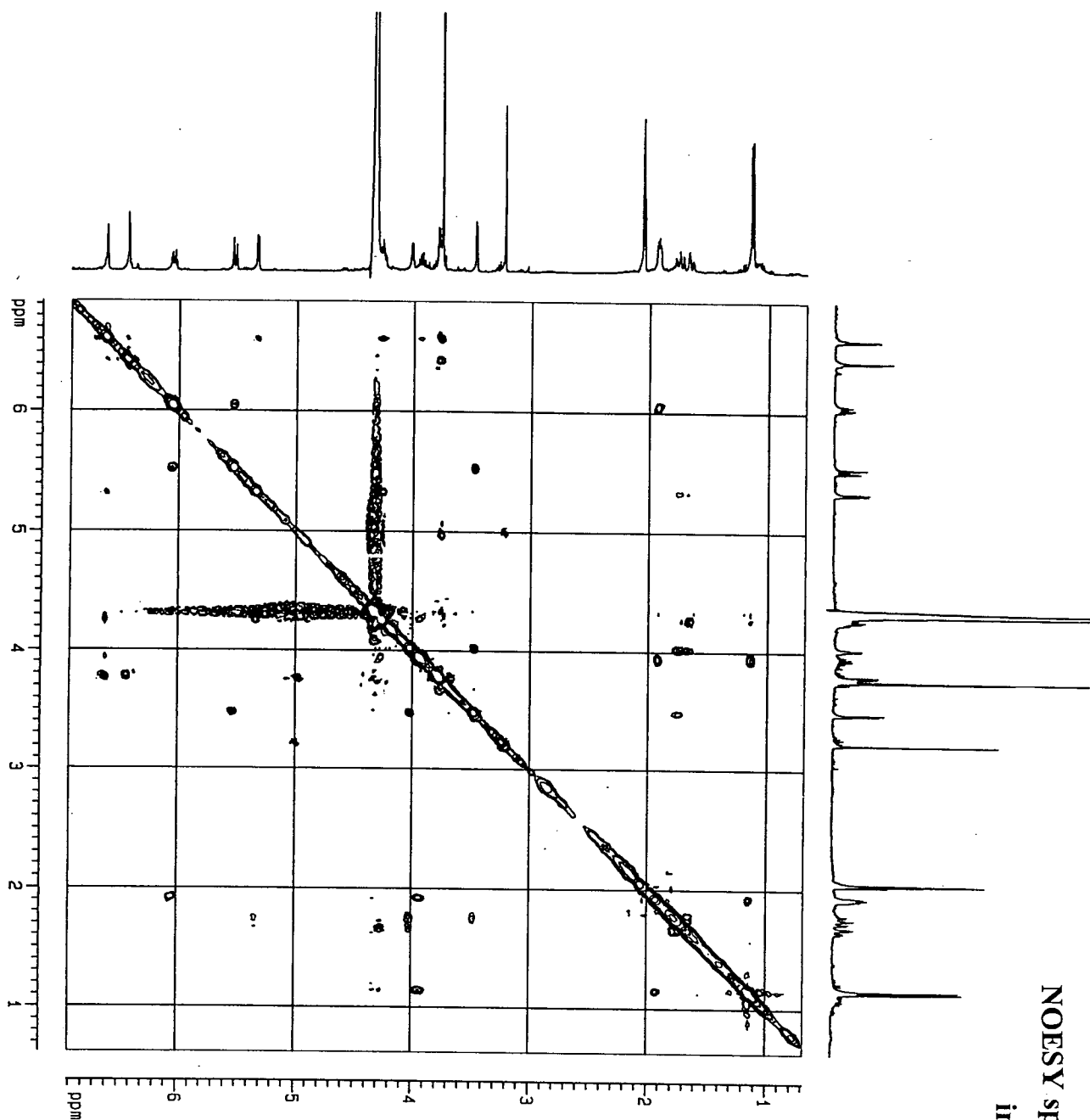


<sup>1</sup>H NMR spectrum of aigialospirol (2) in acetone-*d*<sub>6</sub>/D<sub>2</sub>O (4:1)



COSY spectrum of aigialospirol (2) in acetone- $d_6$ /D<sub>2</sub>O (4:1)

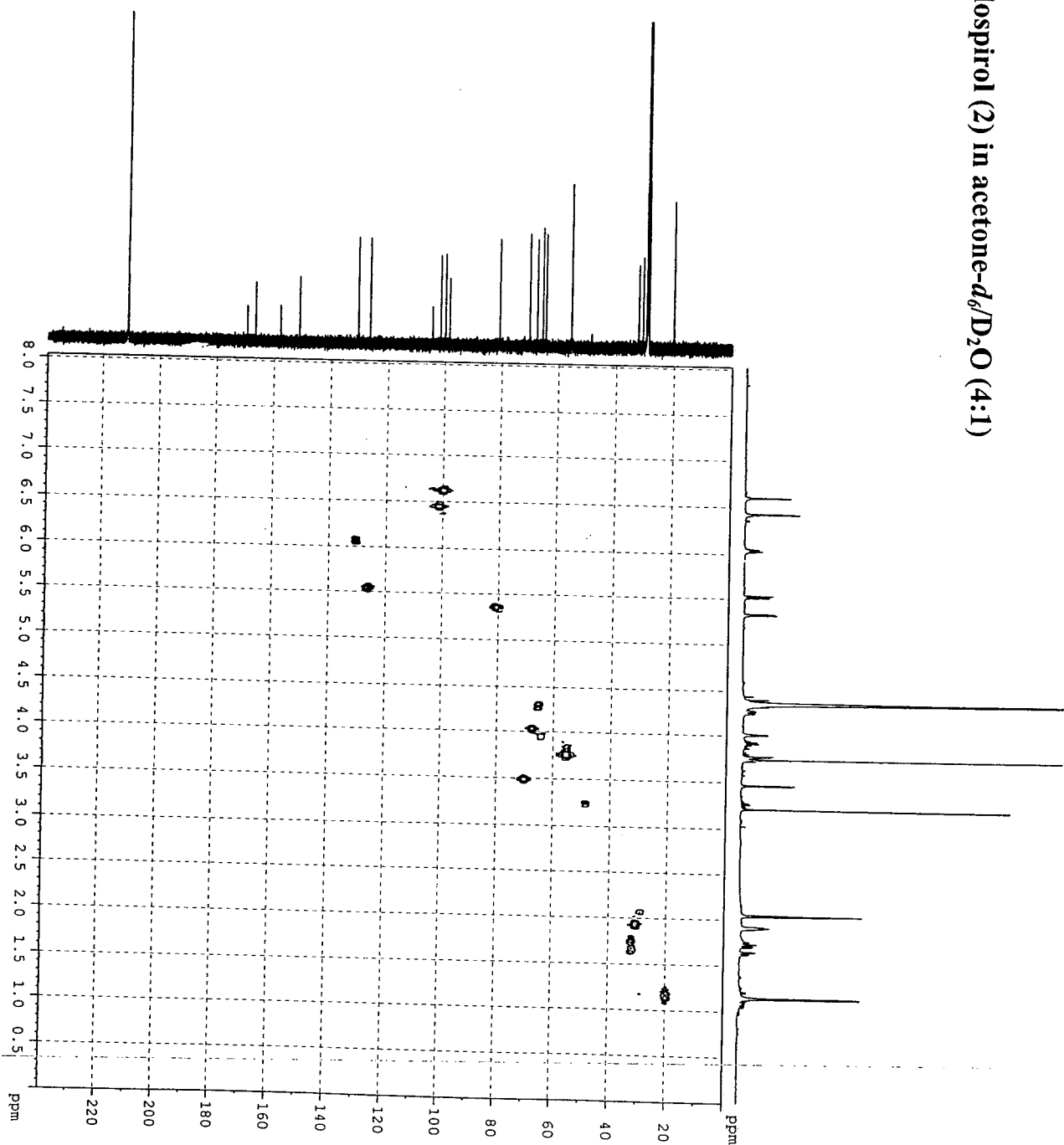




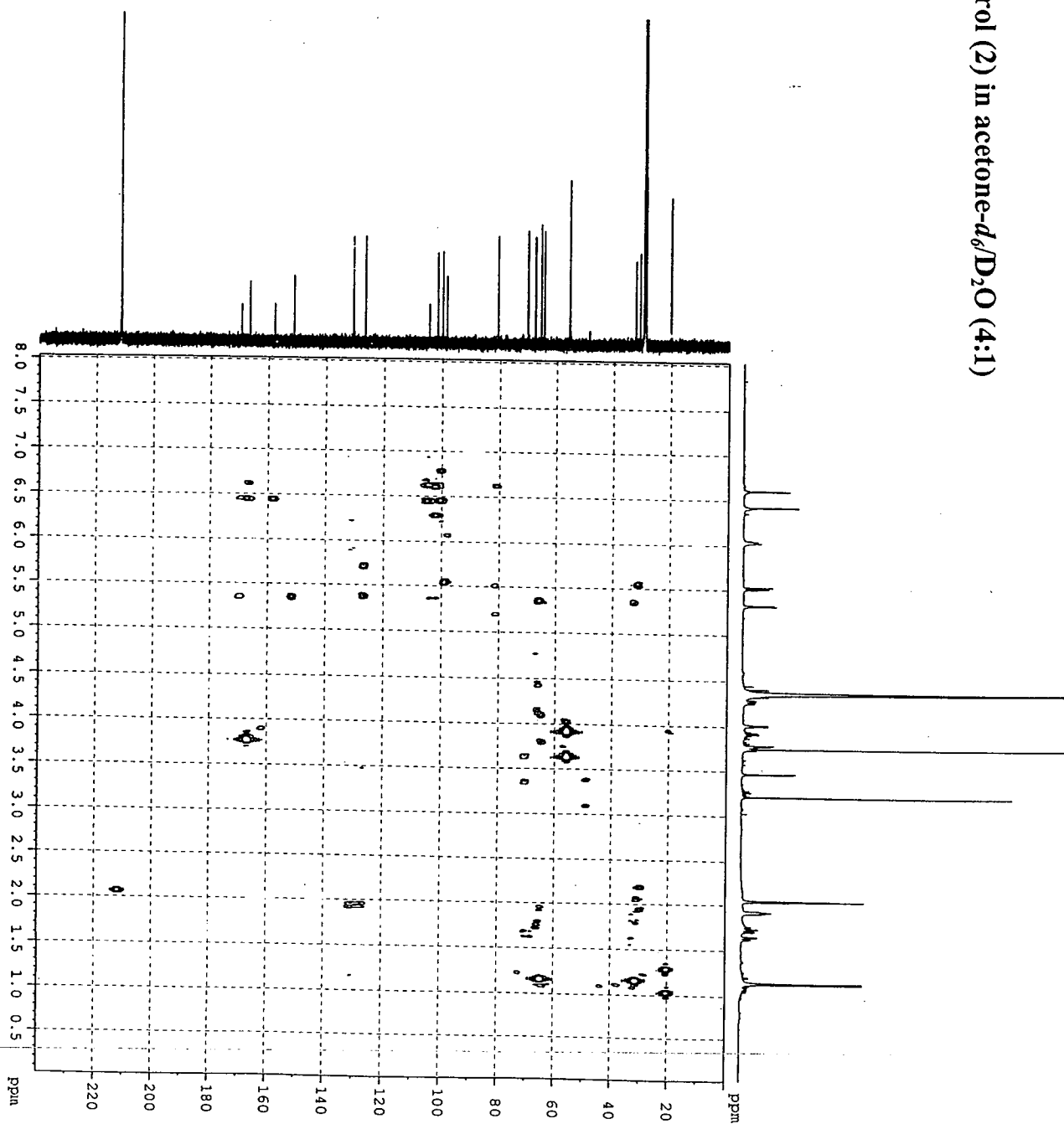
NOESY spectrum (400 MHz) of aigialospirol (2)  
in acetone-*d*<sub>6</sub>/D<sub>2</sub>O (4:1)



# HMOC spectrum of aigialospirol (2) in acetone- $d_6$ /D $_2$ O (4:1)

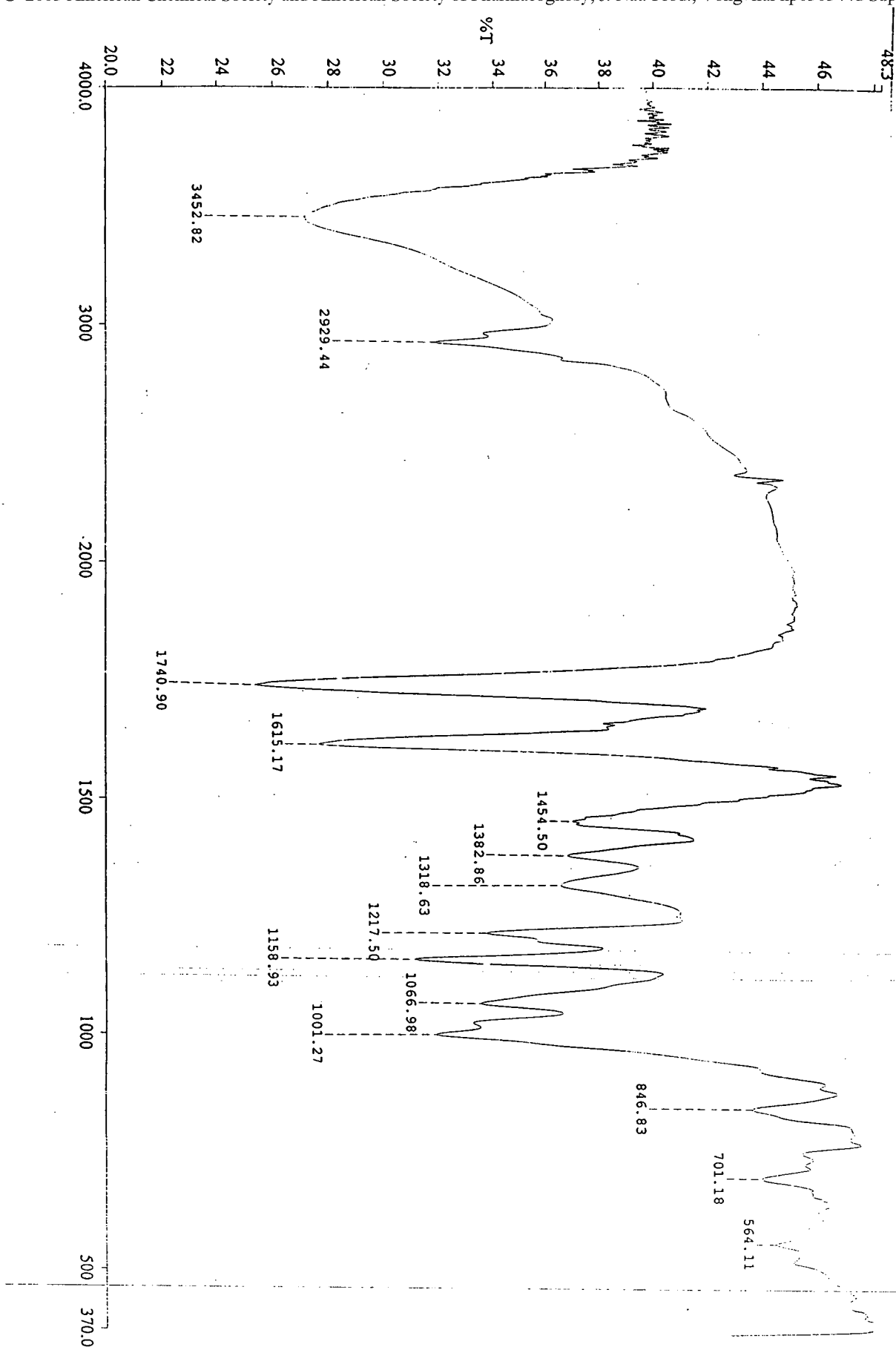


HMBC spectrum of aigialospirol (2) in acetone-*d*<sub>6</sub>/D<sub>2</sub>O (4:1)



050

# IR spectrum of aigalospinol (2) (KBr)



**Figure S1.** X-ray crystal structure of aigialone (1).

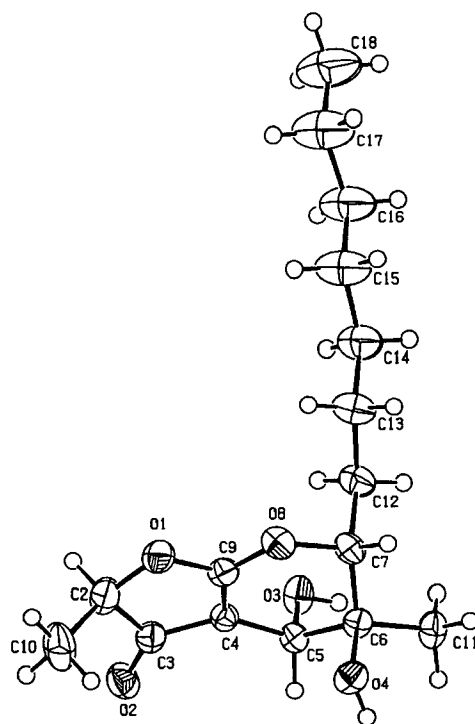


Table S1. Crystal Data and Structure Refinement of Aigialone (1)

**Experimental***Crystal data* $C_{16}H_{26}O_5$  $M_r = 298.379$ 

Monoclinic

 $P2_1$  $a = 5.4952 (2) \text{ \AA}$  $b = 8.6872 (4) \text{ \AA}$  $c = 17.1402 (8) \text{ \AA}$  $\alpha = 90.00^\circ$  $\beta = 93.979 (2)^\circ$  $\gamma = 90.00^\circ$  $V = 816.27 (6) \text{ \AA}^3$  $Z = 2$  $D_x = 1.214 \text{ Mg m}^{-3}$ 

fine-focus sealed tube

Mo  $K\alpha$  radiation $\lambda = 0.71073$ 

Cell parameters from 1,028 reflections

 $\mu = 0.089 \text{ mm}^{-1}$  $T = 298 \text{ K}$ 

plate

Colourless

Crystal source: *Aigialus parvus* BCC 5311*Data collection*

KappaCCD

Absorption correction: none

19048 measured reflections

2028 independent reflections

1882 observed reflections

Criterion:  $>2\sigma(I)$  $\theta_{\max} = 28.17^\circ$  $h = 0 \rightarrow 7$  $k = 0 \rightarrow 11$  $l = -22 \rightarrow 21$ *Refinement*Refinement on  $F^2$ 

Full-matrix least-squares refinement

 $R(\text{all}) = 0.0438$  $R(\text{gt}) = 0.0392$  $wR(\text{ref}) = 0.1001$  $wR(\text{gt}) = 0.0968$  $S(\text{ref}) = 1.020$ 

2028 reflections

191 parameters

Calculated weights calc

 $\Delta/\sigma_{\max} = 0.000$  $\Delta\rho_{\max} = 0.186 \text{ e \AA}^{-3}$  $\Delta\rho_{\min} = -0.162 \text{ e \AA}^{-3}$ Extinction correction: *SHELXL* $F_c^* = kF_c [1 + 0.001 \times F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$ 

Extinction coefficient = 0.034 (15)

Atomic scattering factors from International

Tables Vol C Tables 4.2.6.8 and 6.1.1.4

Data collection: KappaCCD

Cell refinement: HKL Scalepack (Otwinowski &amp; Minor 1997)

Data reduction: Denzo and Scalepak (Otwinowski &amp; Minor, 1997)

Program(s) used to refine structure: *SHELXL-97* (Sheldrick, 1997)