

# **Supplementary Materials**

## **Synthesis, NMR characterization and antileukemic activity of *N*-nonanoylpiperazinyl- 5 $\alpha$ -androstane-3 $\alpha$ ,17 $\beta$ -diol A-ring derivatives**

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<sup>1</sup> Laboratory of Medicinal Chemistry, Endocrinology and Nephrology Unit, CHU de Québec – Research Center, Québec (Québec), Canada;

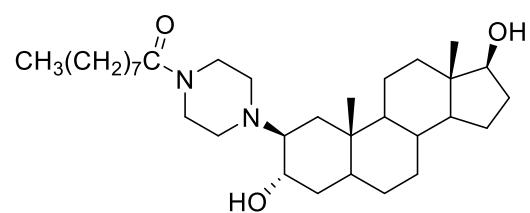
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<sup>1</sup>H NMR, <sup>13</sup>C NMR (APT), NOESY, COSY, HSQC and HMBC spectra  
for compound **1** (IR-542-17-51) in CD<sub>3</sub>OD

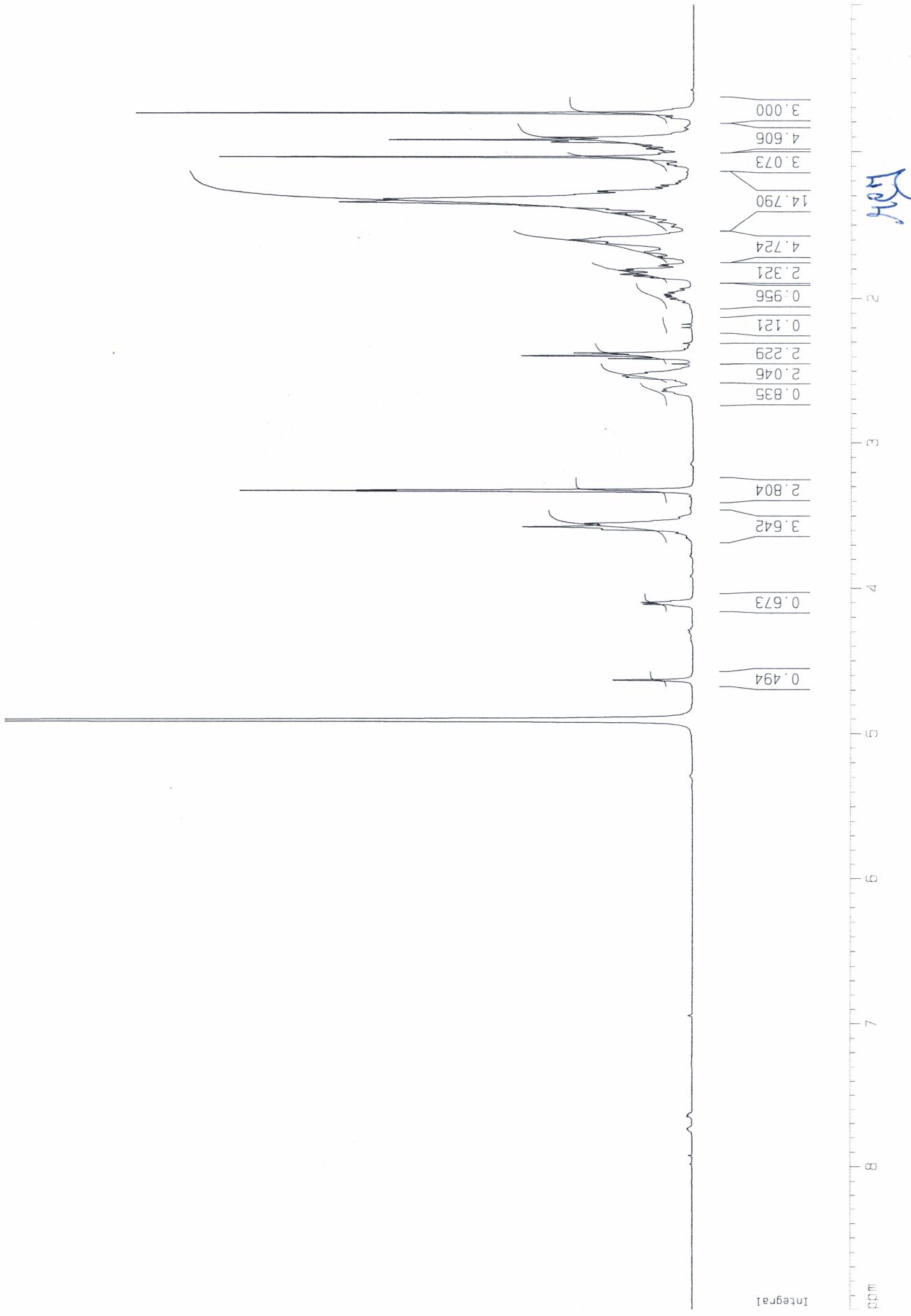


Integral

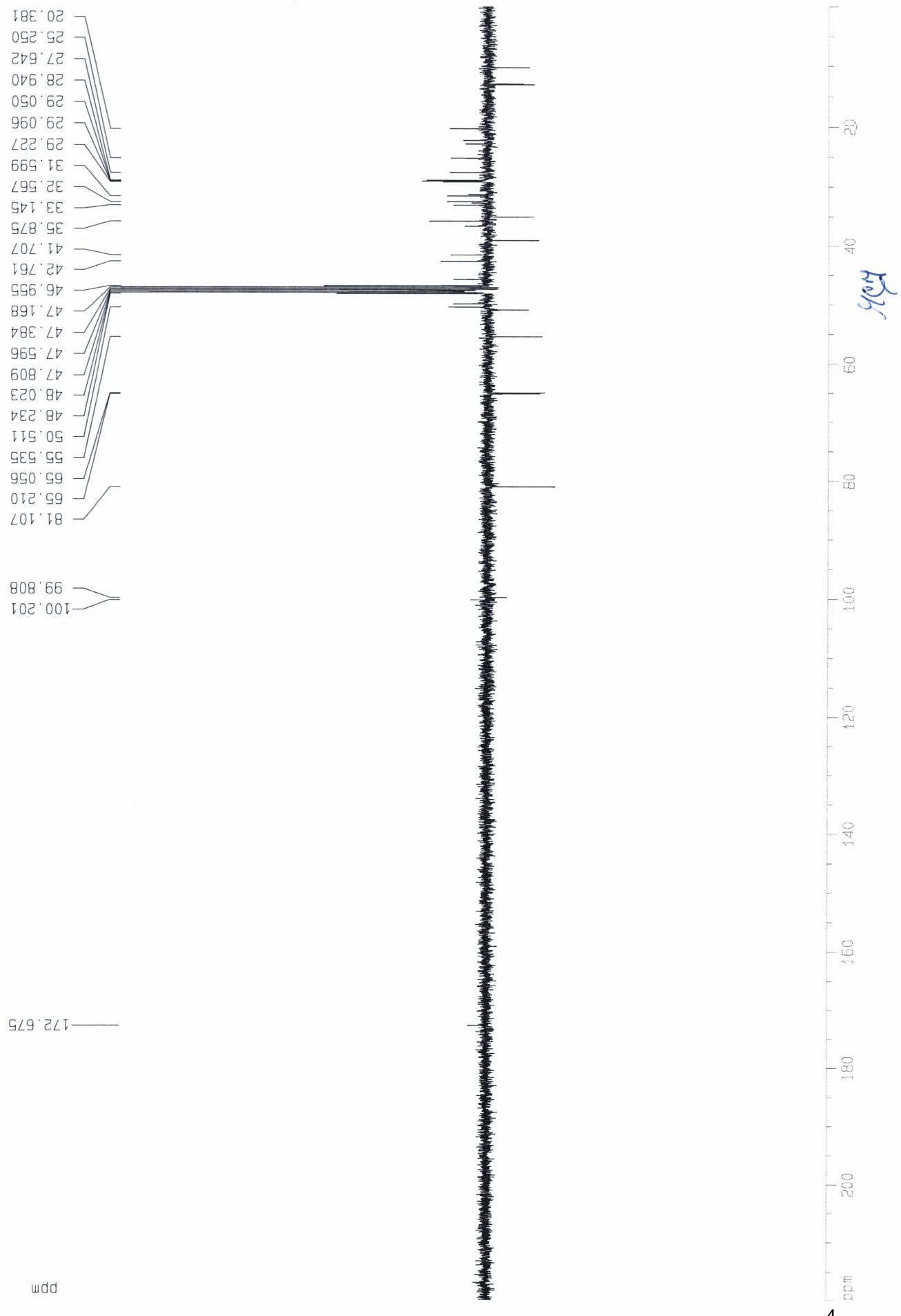
CCS

3

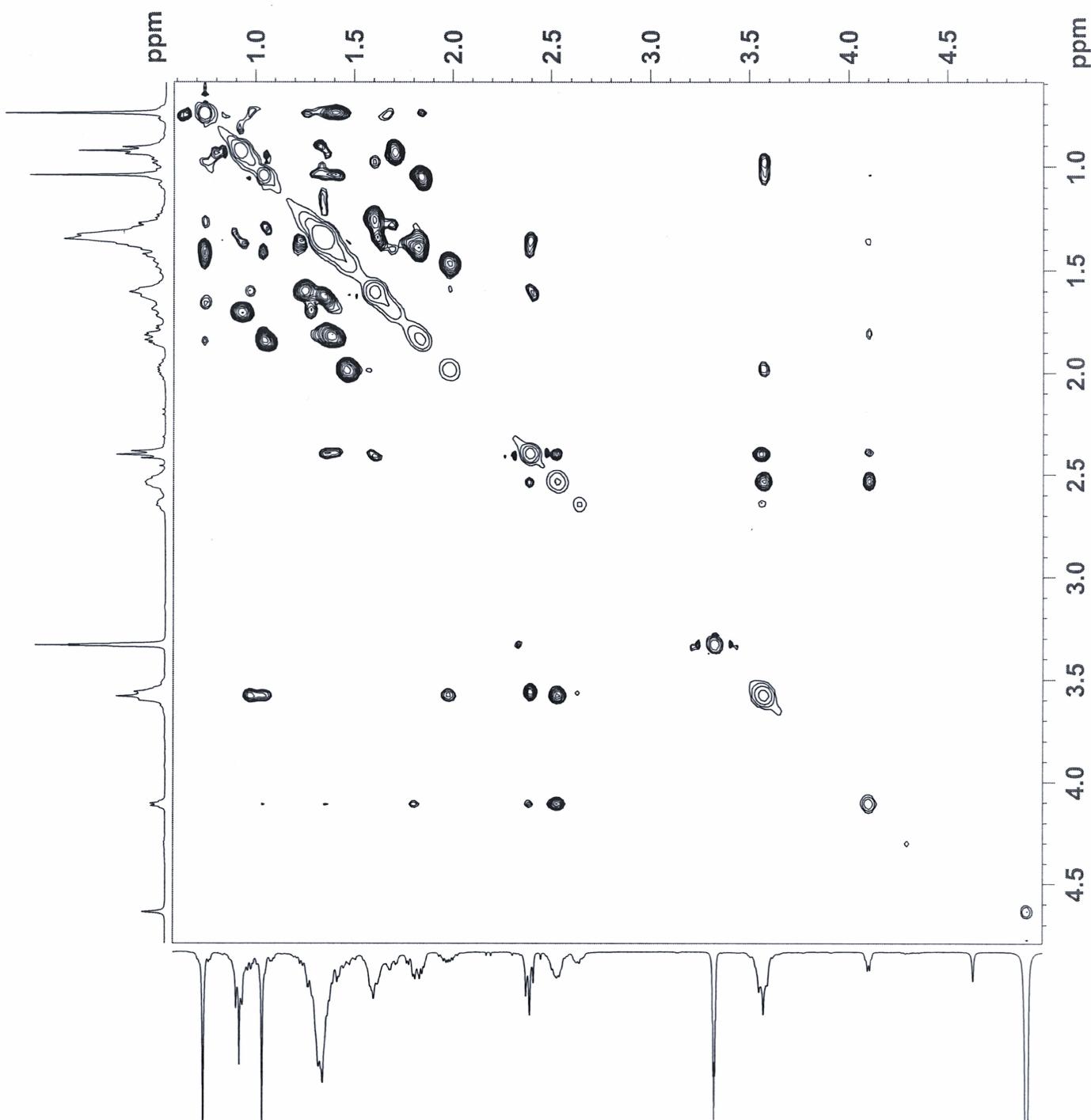
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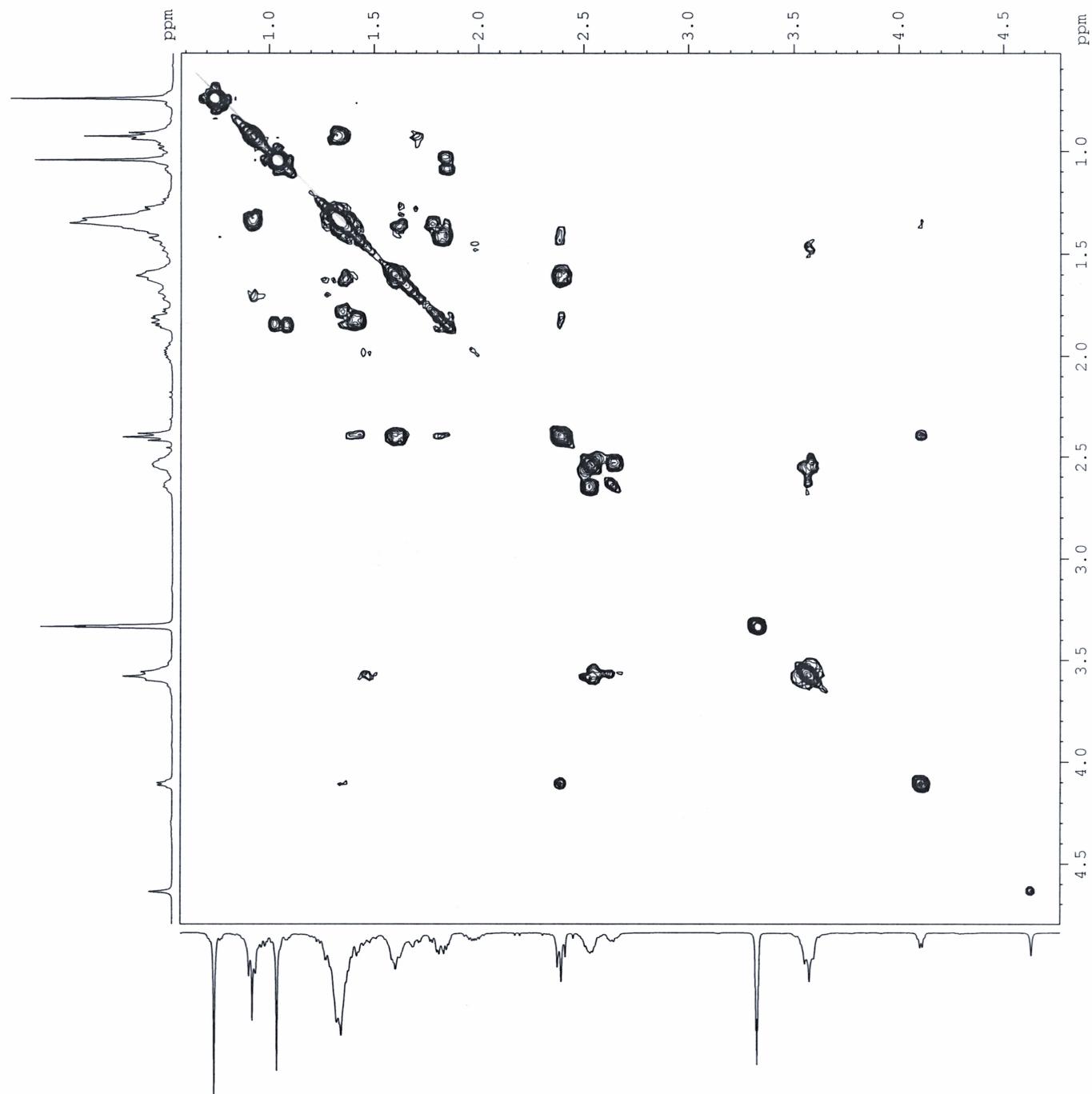
IR-542-17-51  
APT



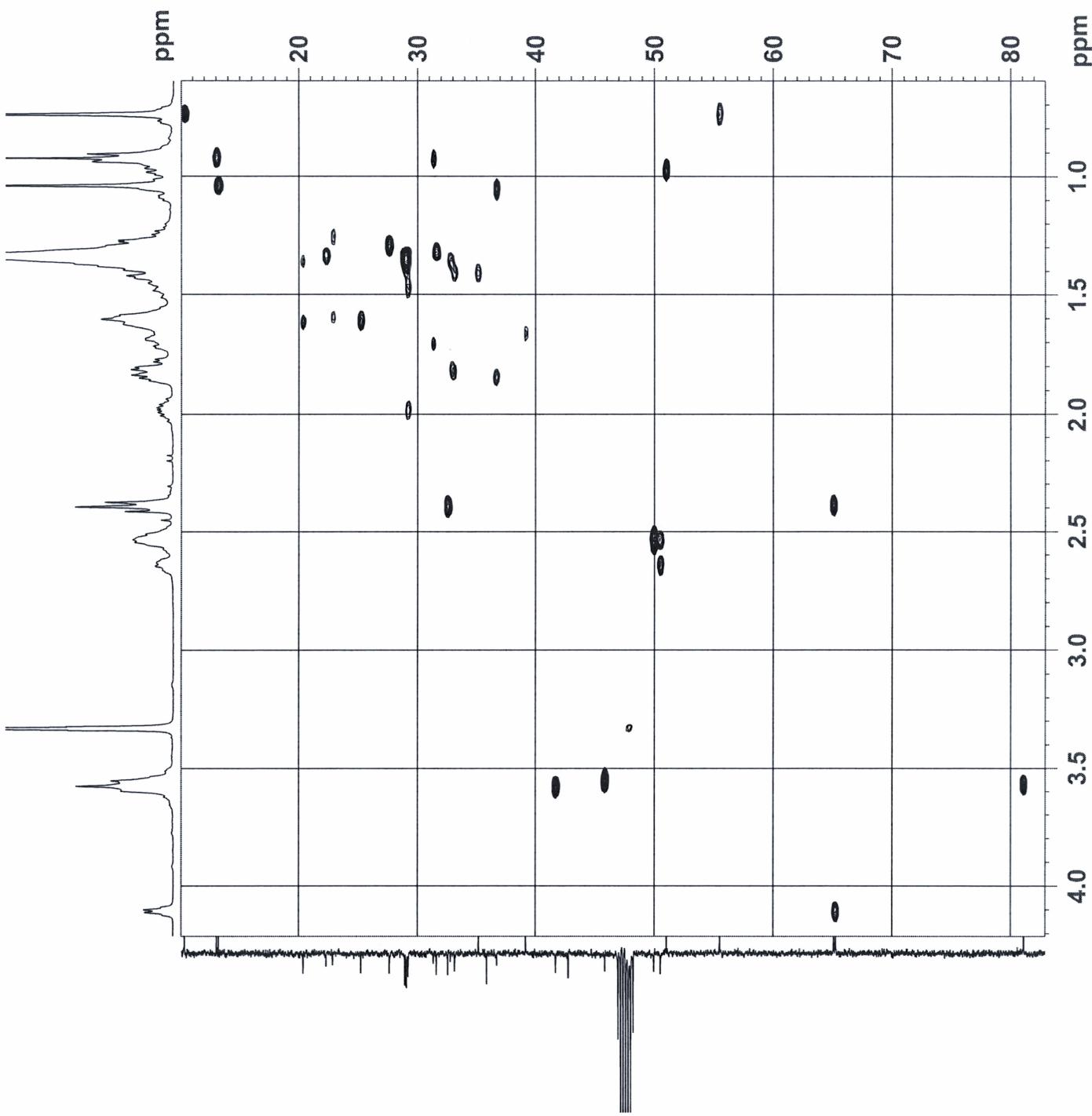
IR-542-17-51  
NOESY



IR-542-17-51  
COSY

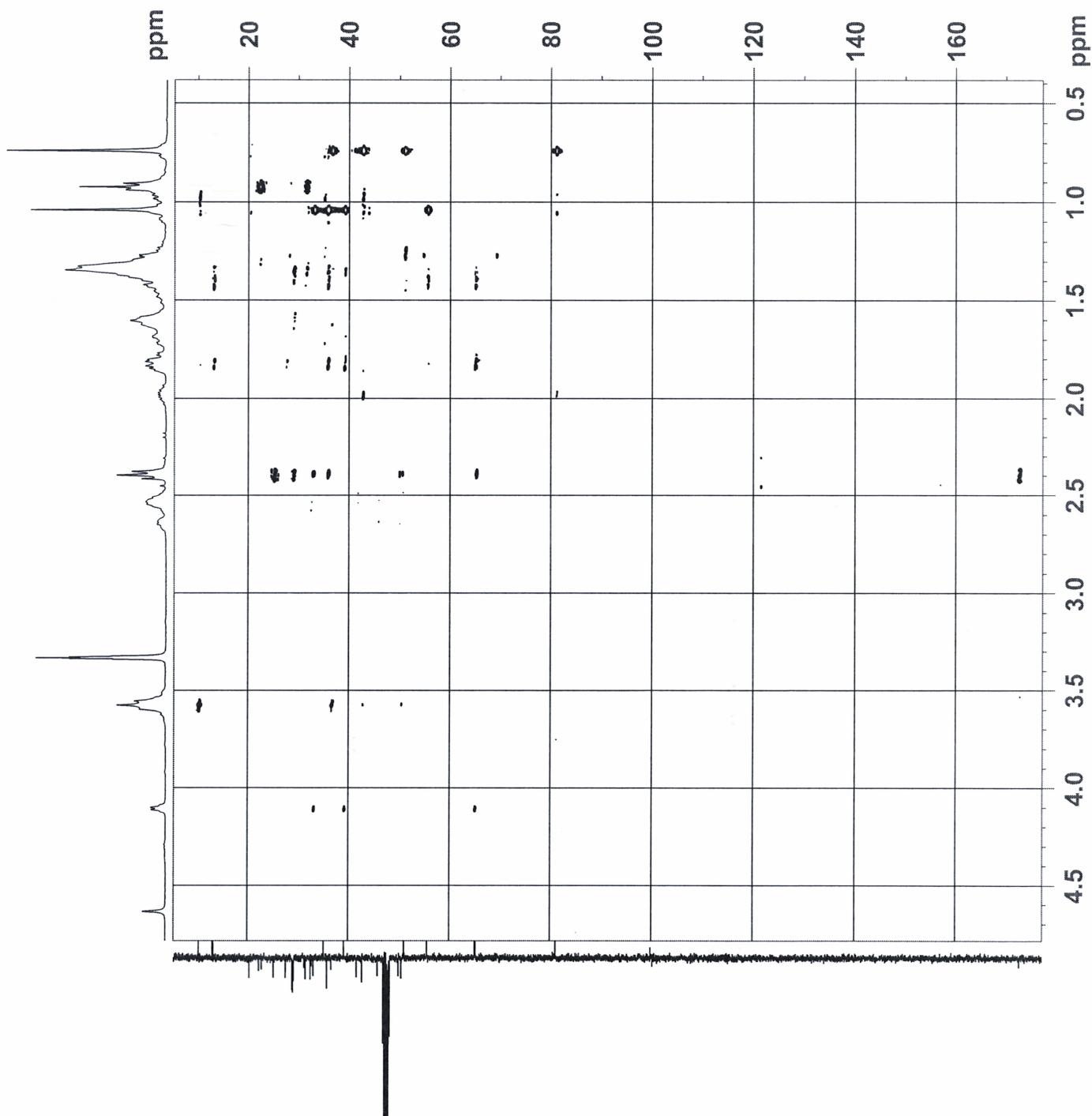


IR-542-17-51  
HSQC

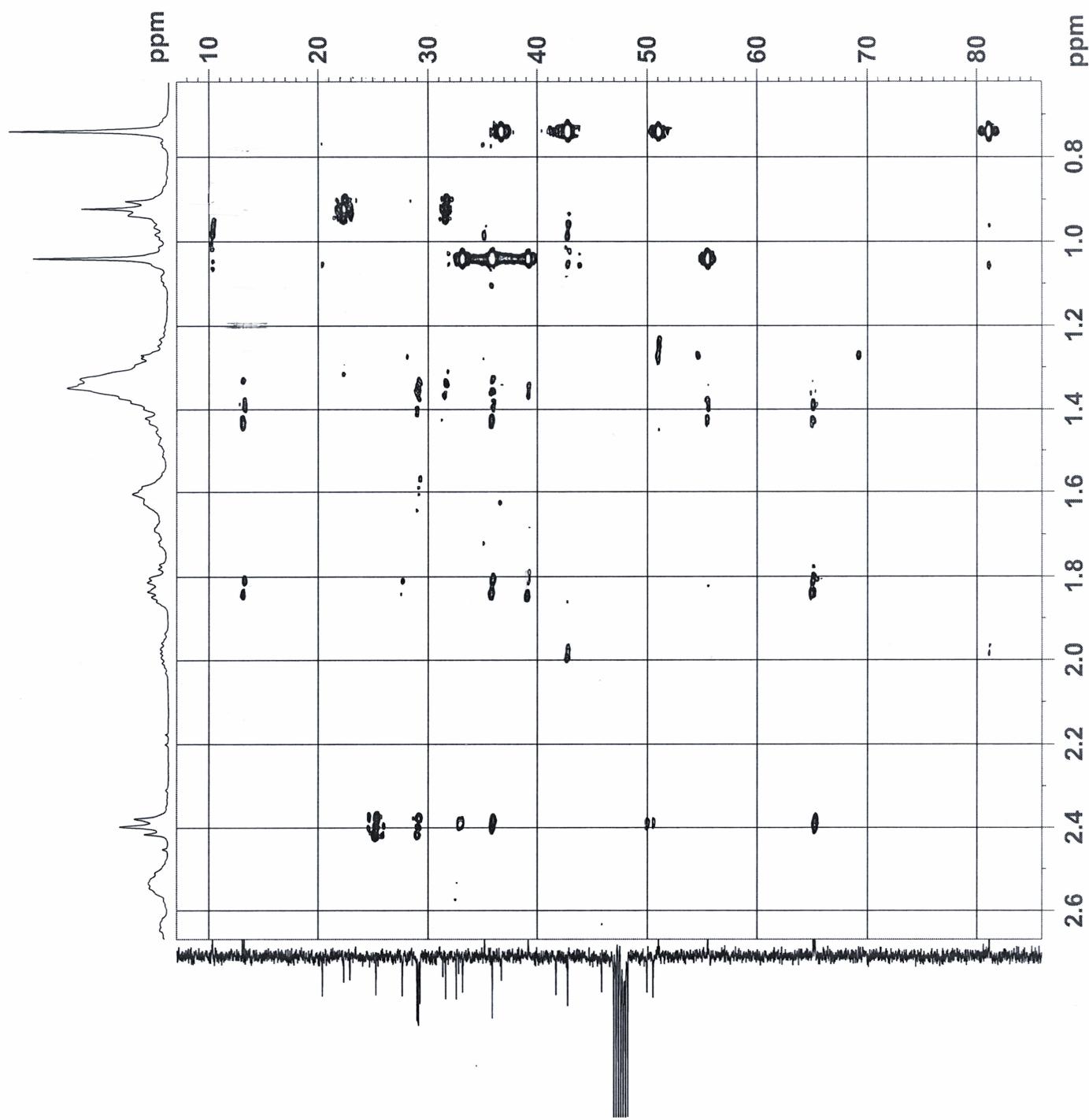


$\text{H}_\text{C}$

IR-542-17-51  
HMBC

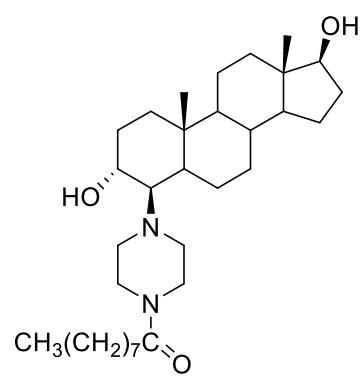


IR-542-17-51  
HMBC



120

<sup>1</sup>H NMR, <sup>13</sup>C NMR (APT), NOESY, COSY, HSQC and HMBC spectra  
for compound **2** (IR-542-17-24) in CD<sub>3</sub>OD

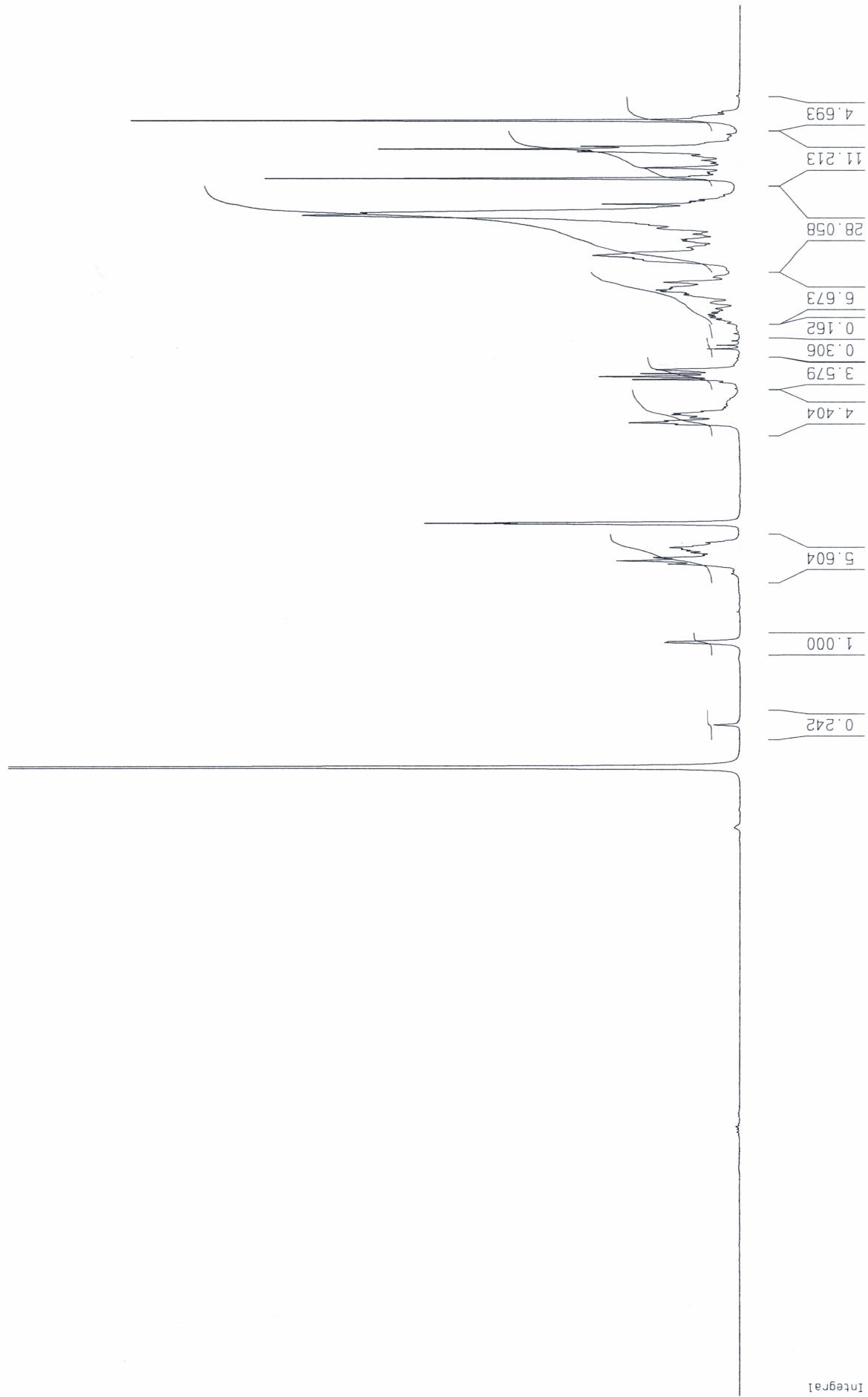


Integral

Total

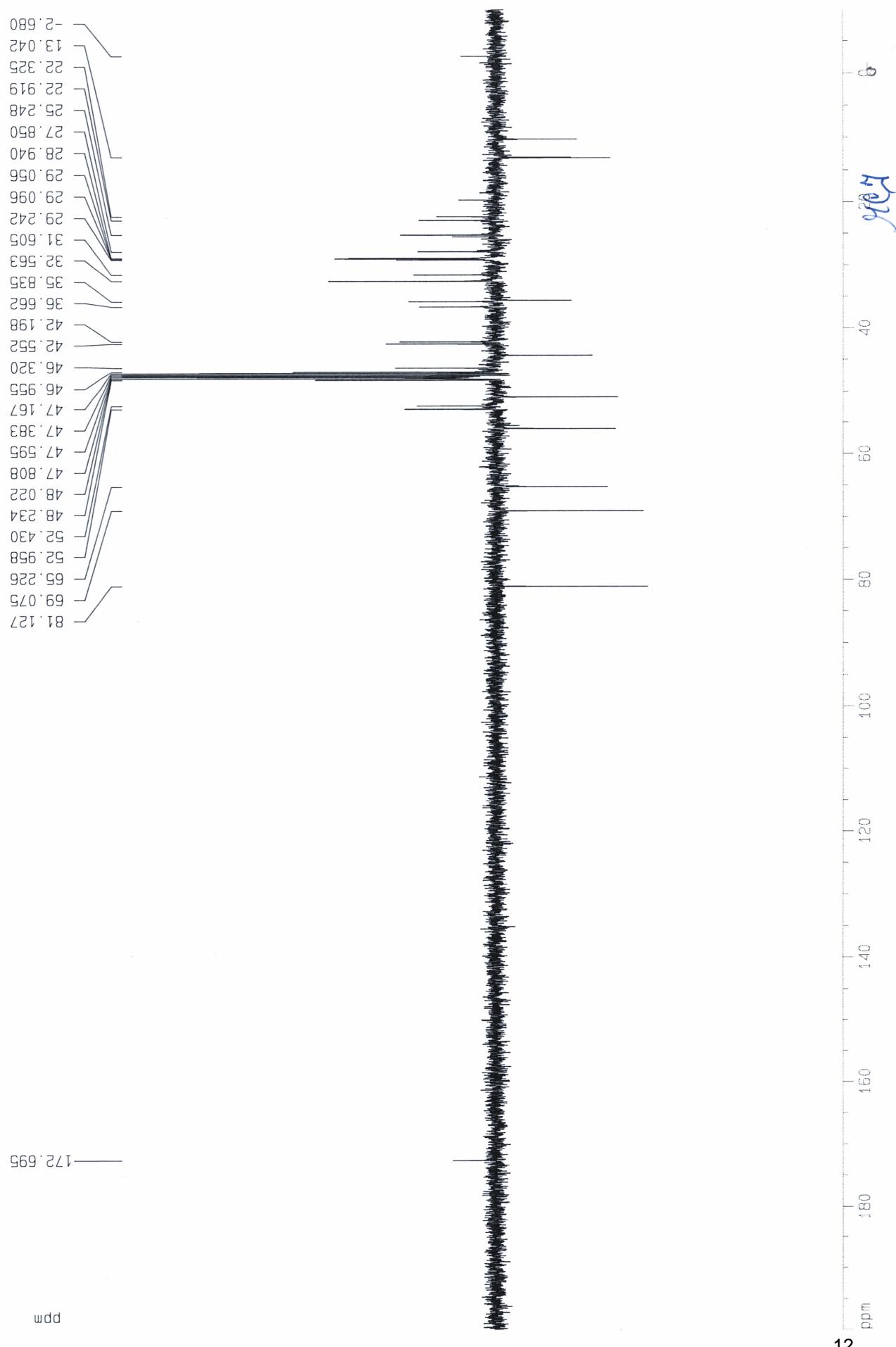
1  
2  
3  
4  
5  
6  
7  
8  
9

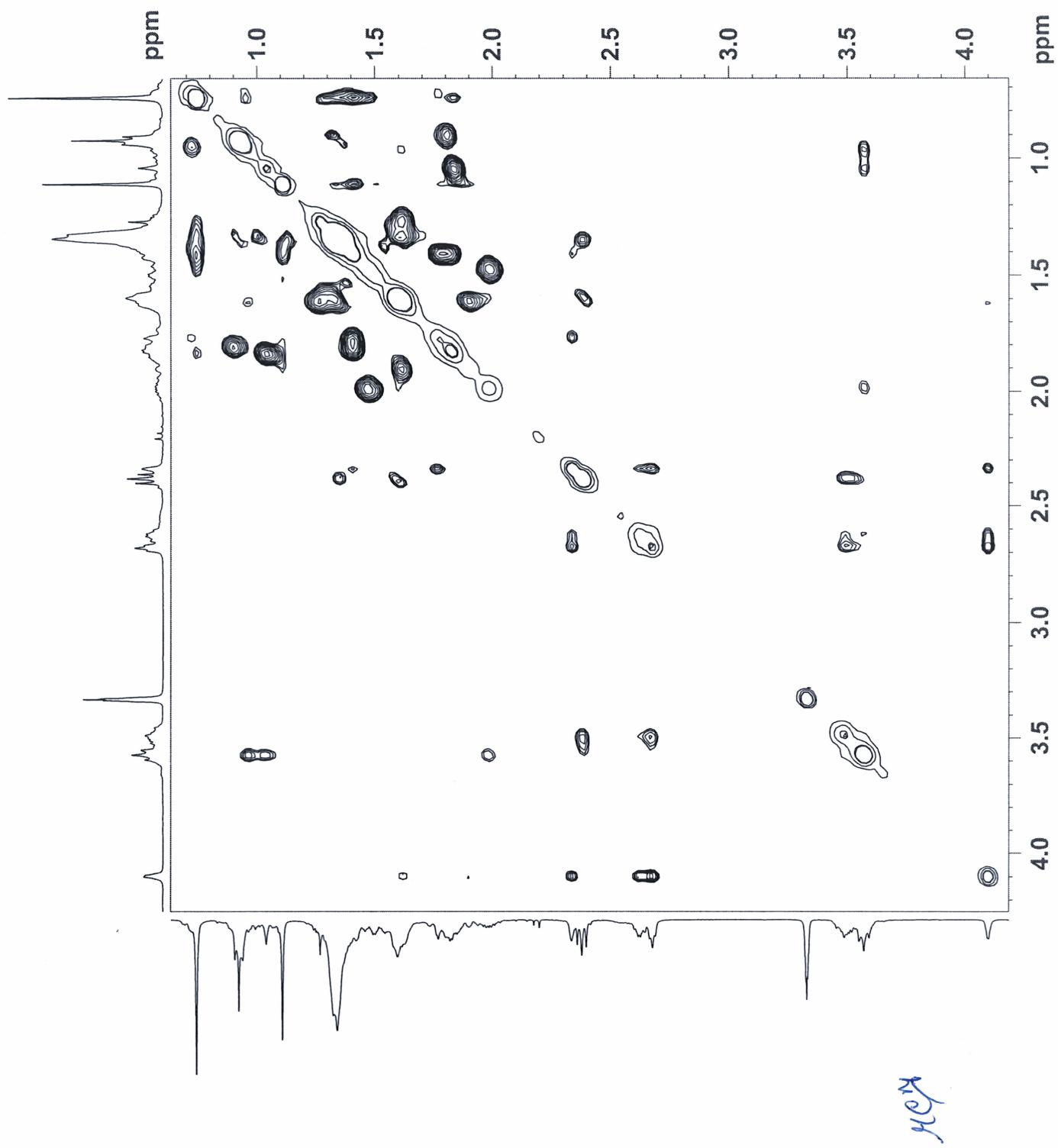
50%



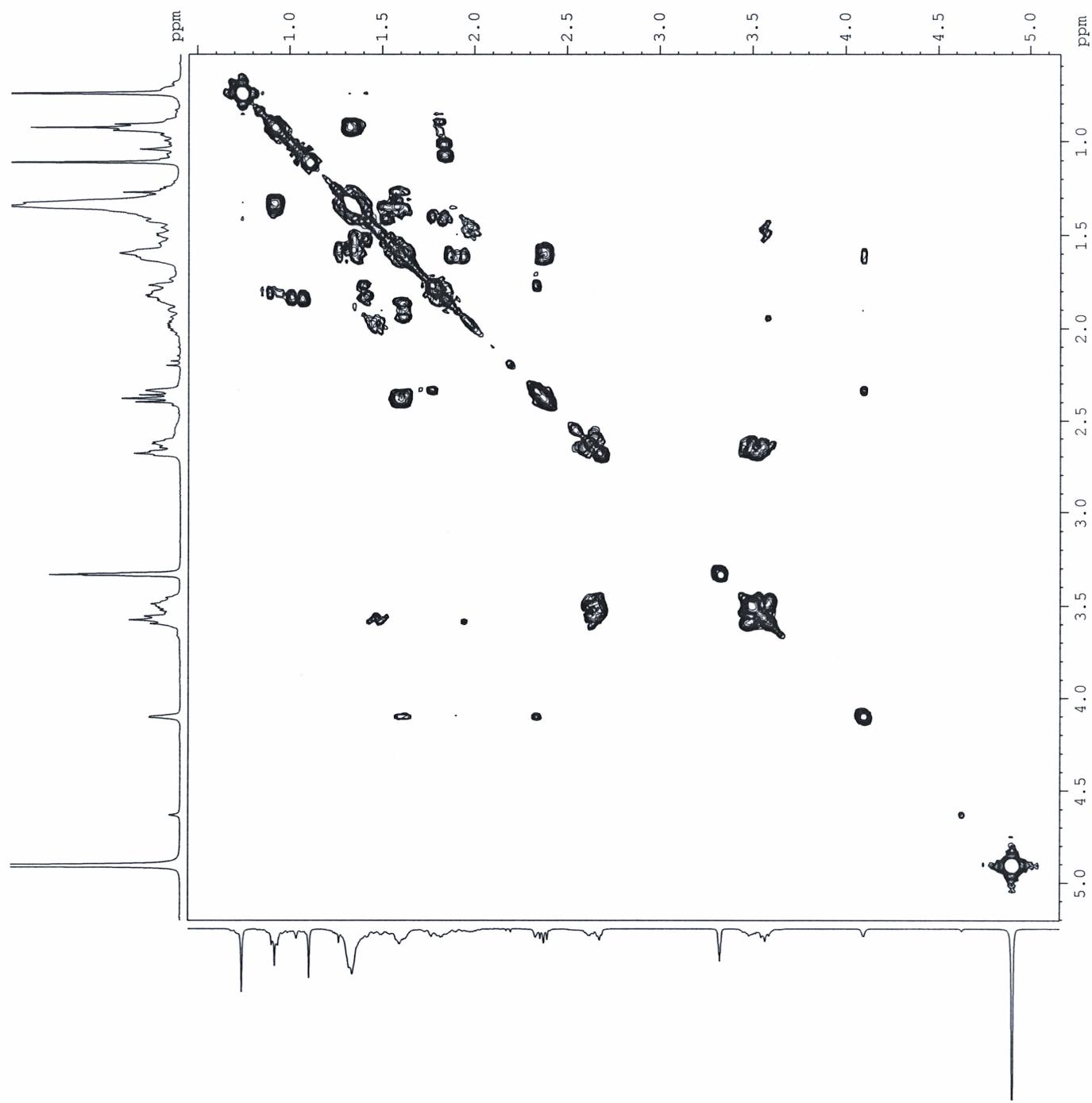
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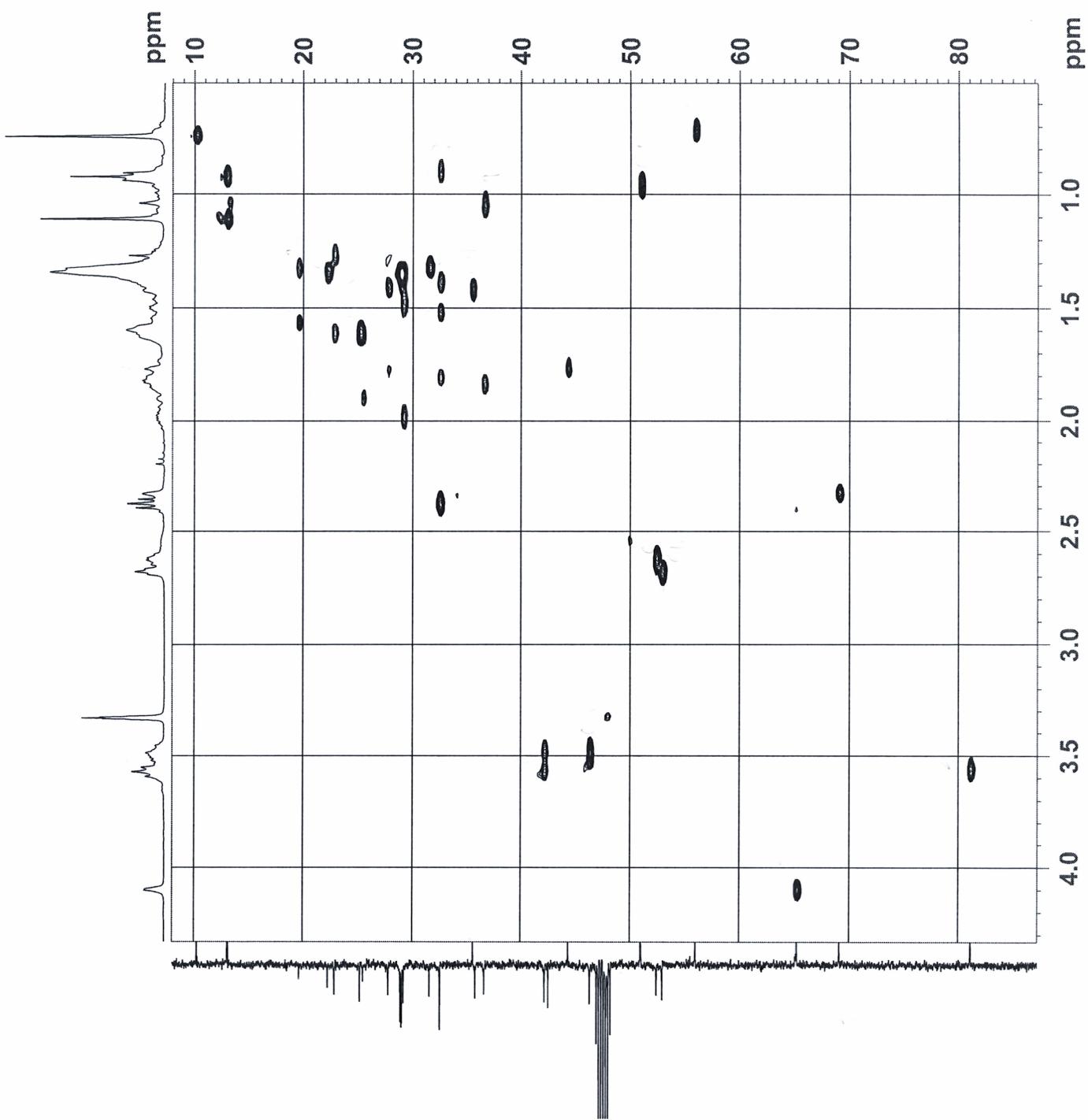
IR-542-17-24  
APT





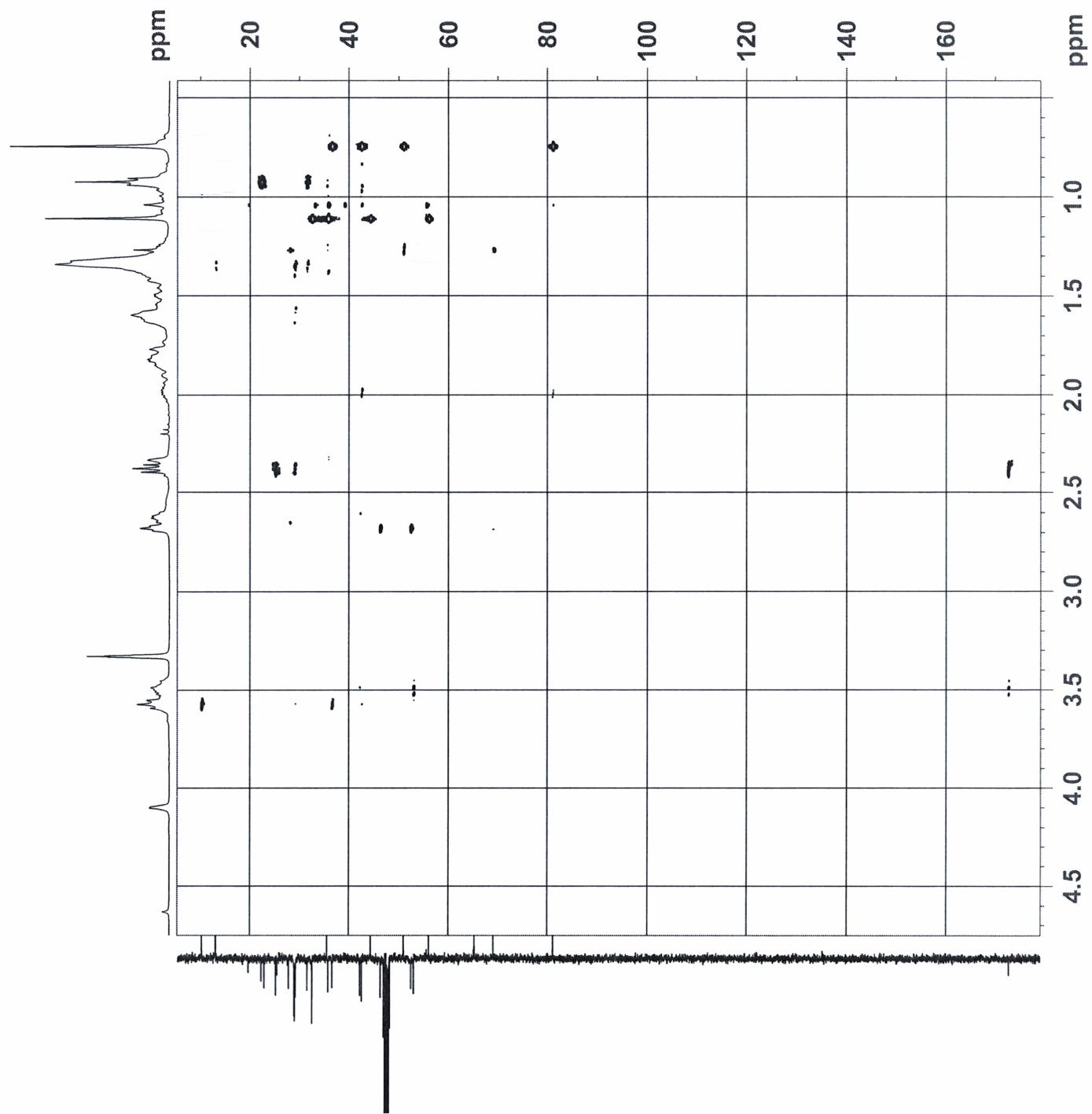
IR-542-17-24  
COSY





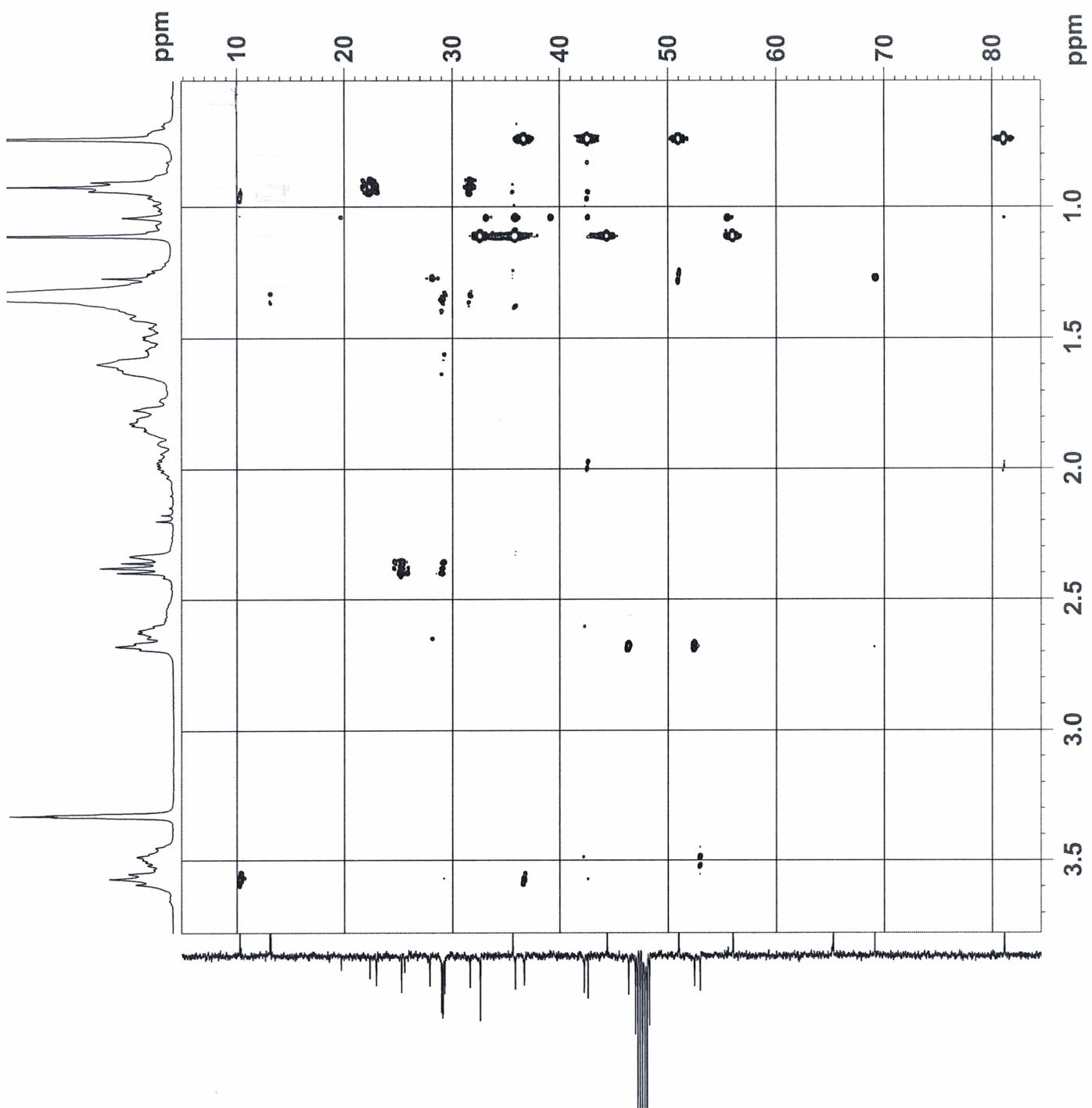
4.0

IR-542-17-24  
HMBC

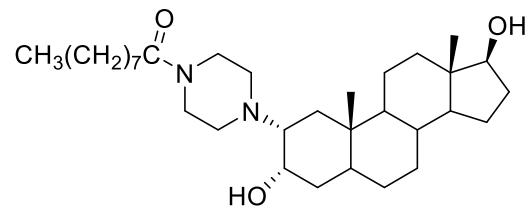


$\mu\text{CH}$

IR-542-17-24  
HMBC



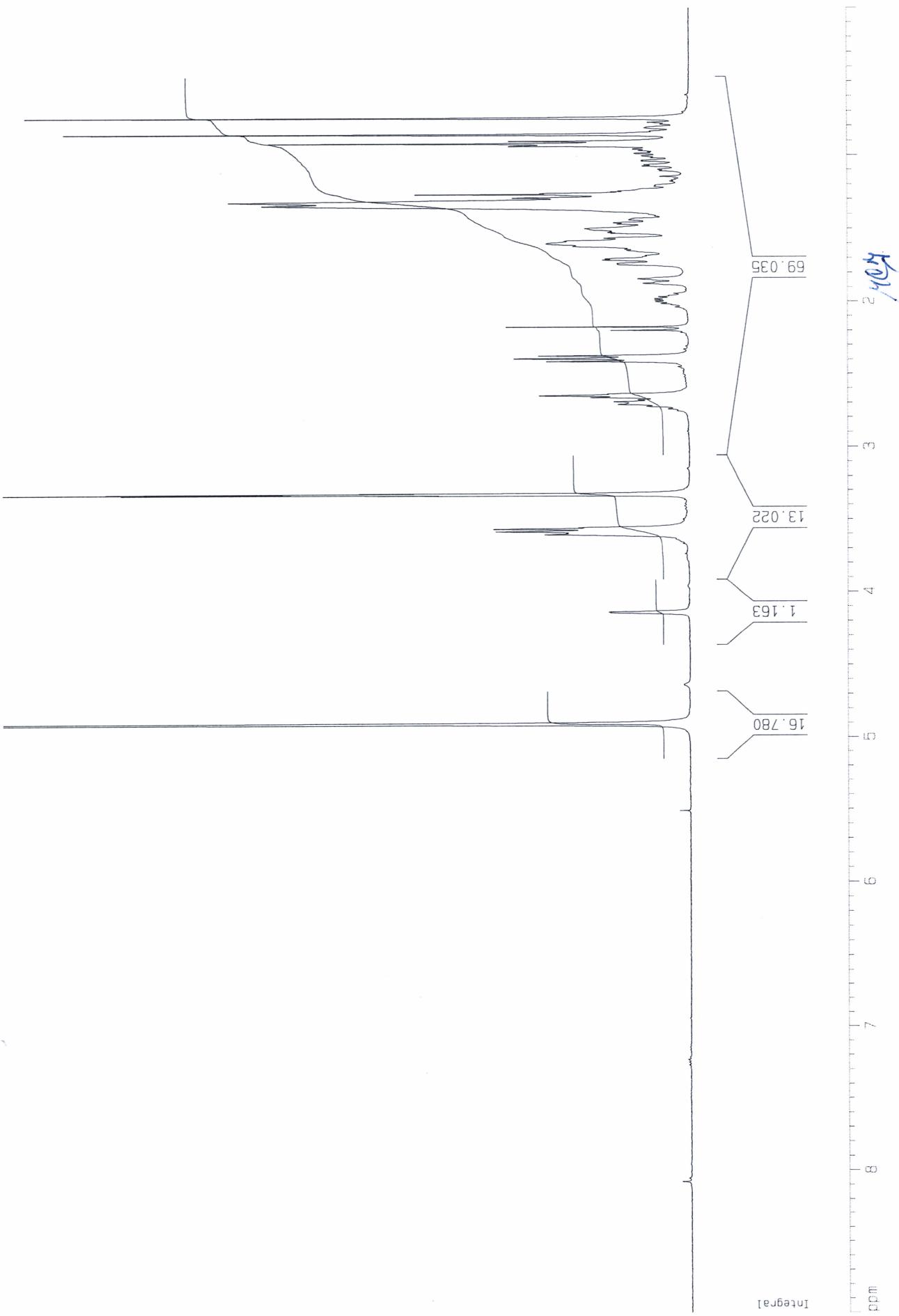
<sup>1</sup>H NMR, <sup>13</sup>C NMR (APT), NOESY, COSY, HSQC and HMBC spectra  
for compound **3** (IR-542-63-30) in CD<sub>3</sub>OD



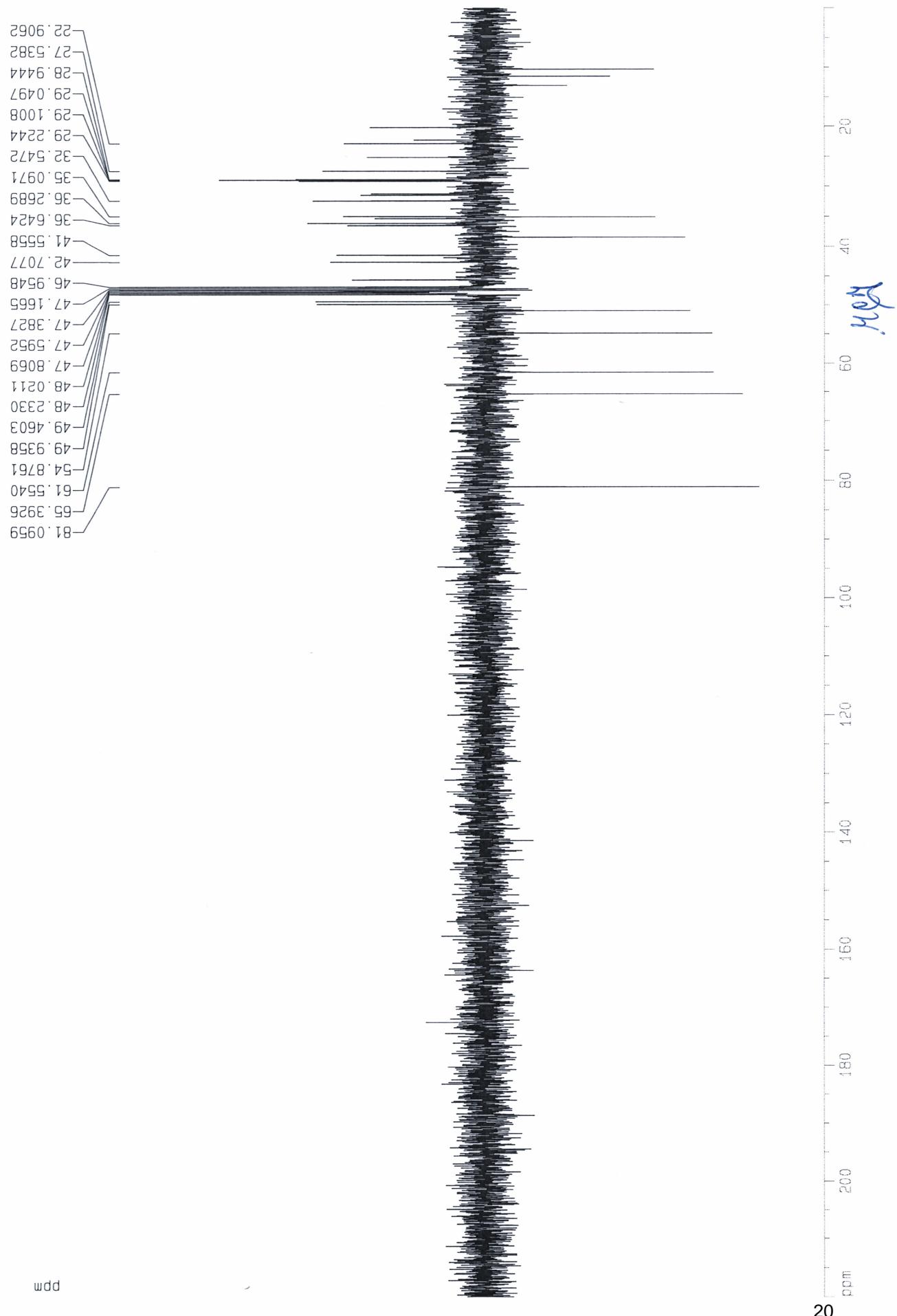
Integral

ppm

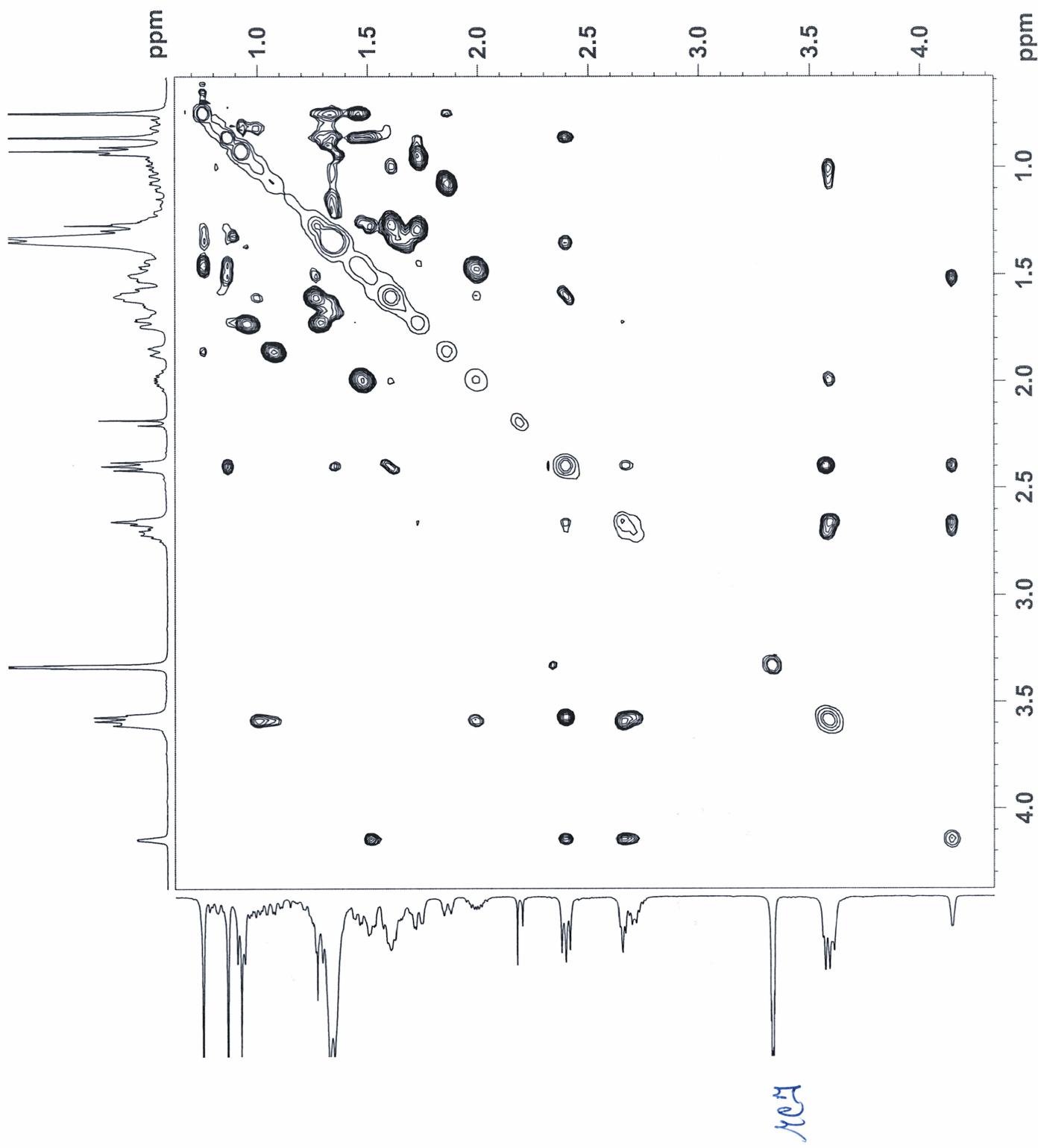
19



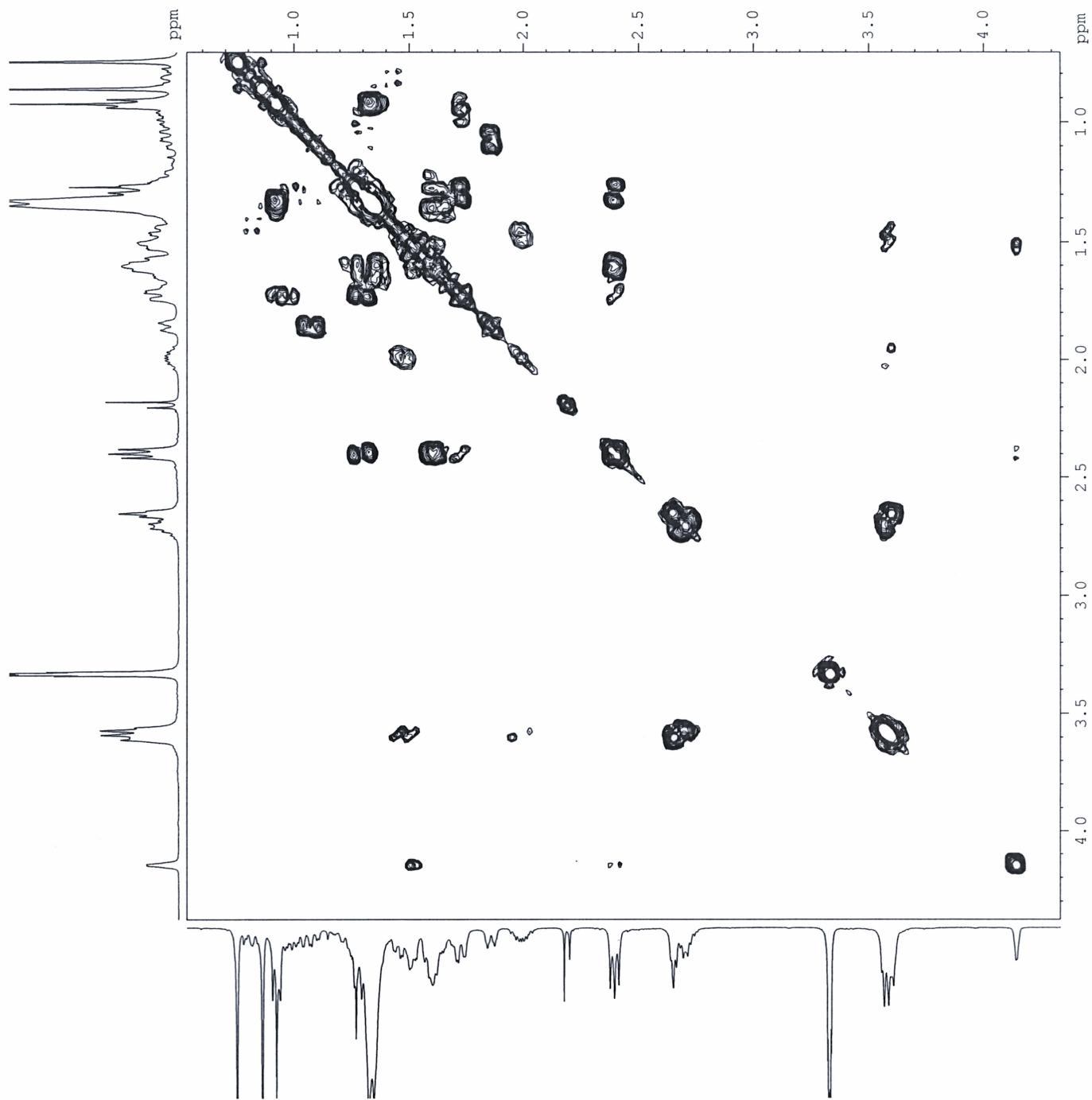
IR-542-65-30



IR-542-65-30  
NOESY

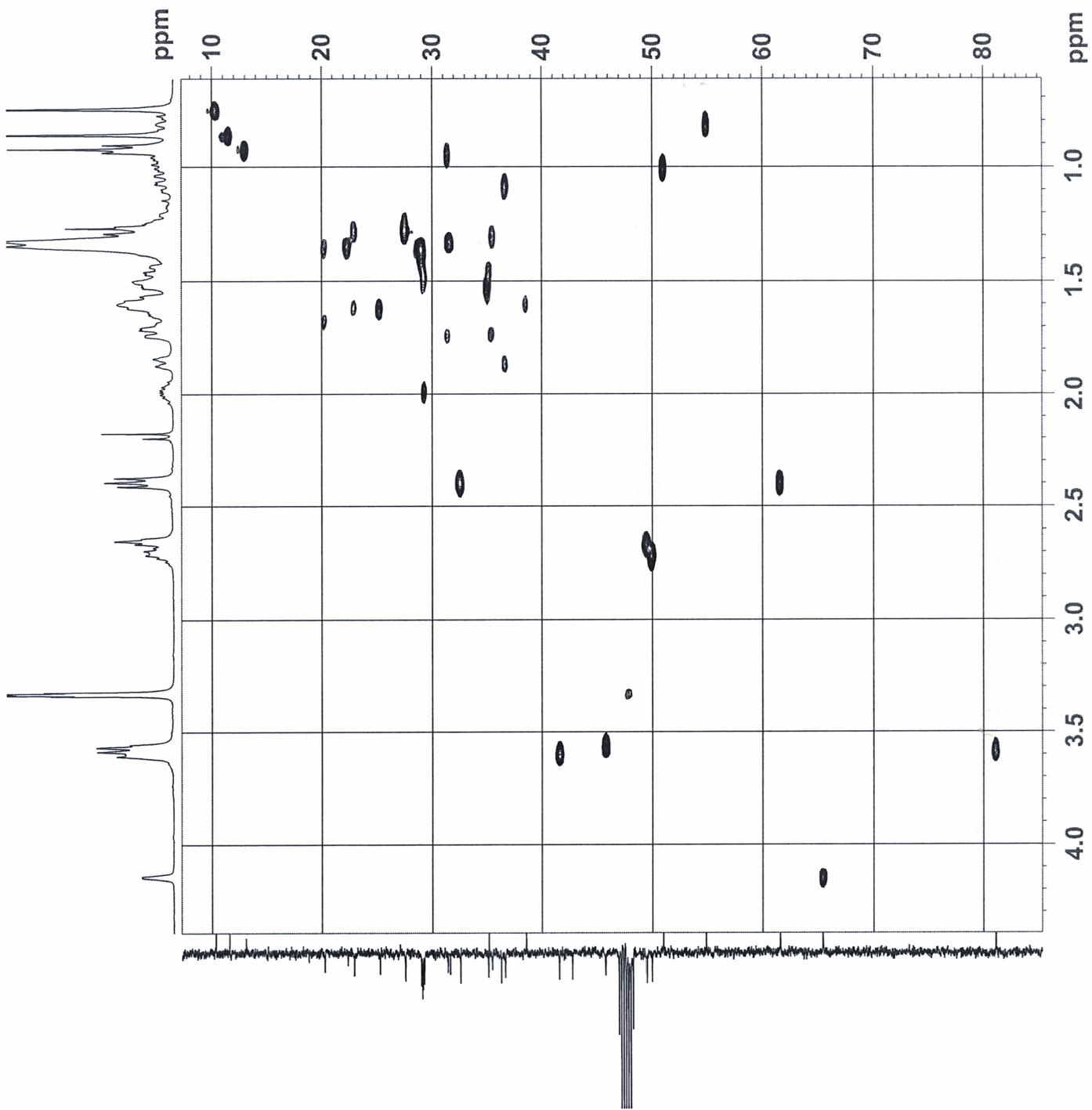


IR-542-65-30  
COSY



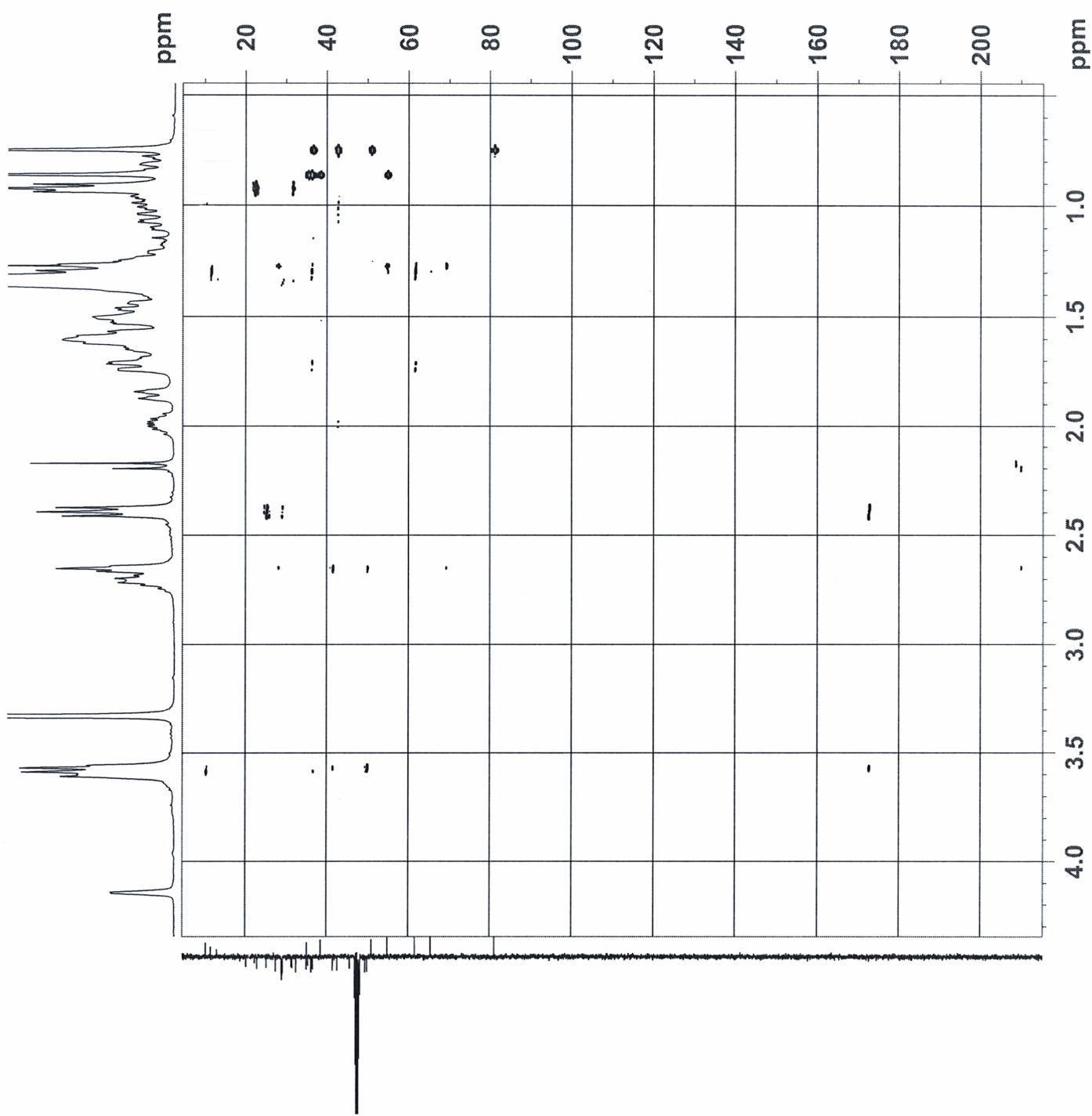
H<sub>CH</sub>

IR-542-65-30  
HSQC



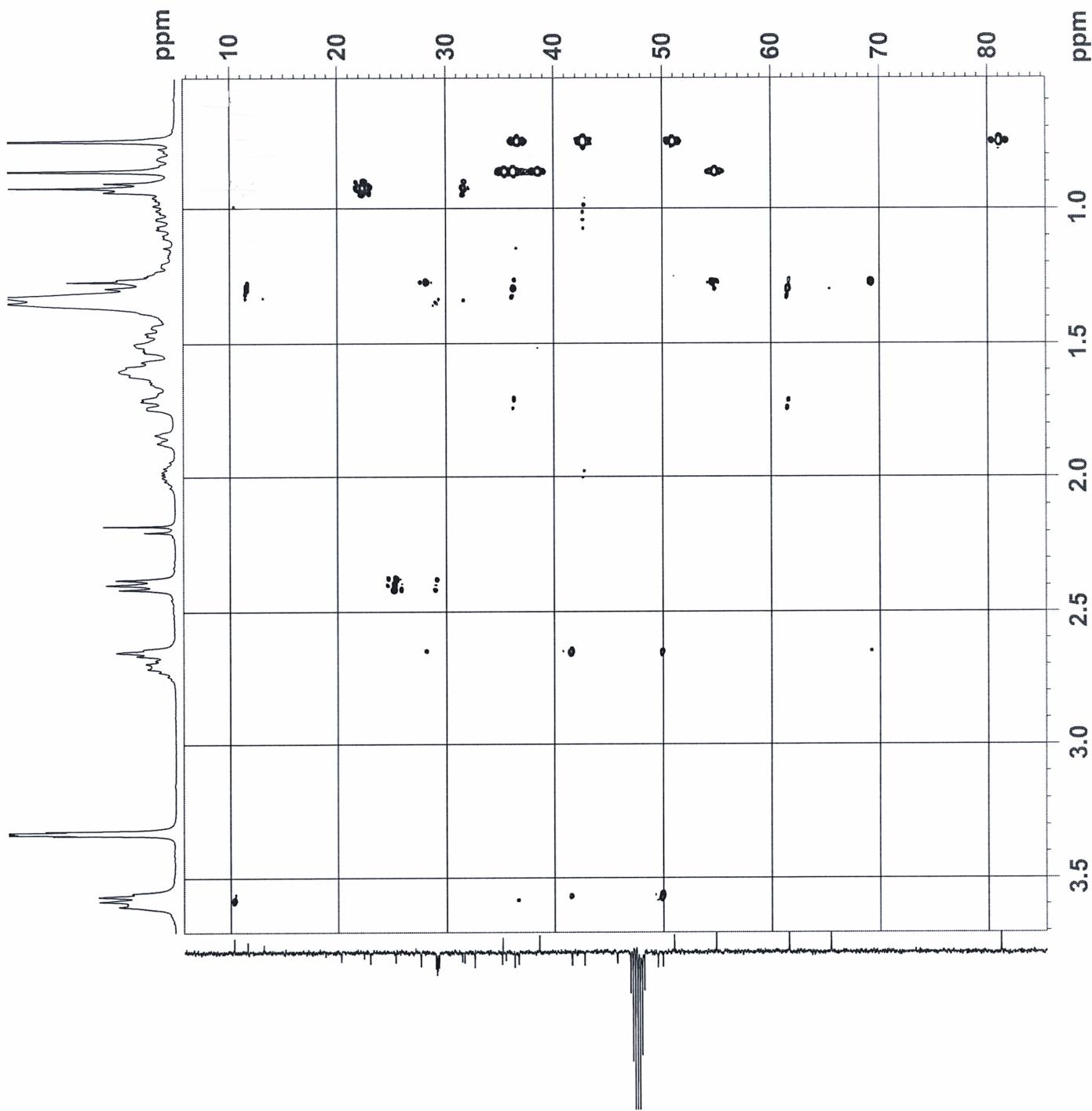
HC<sub>2</sub>

IR-542-65-30  
HMBC



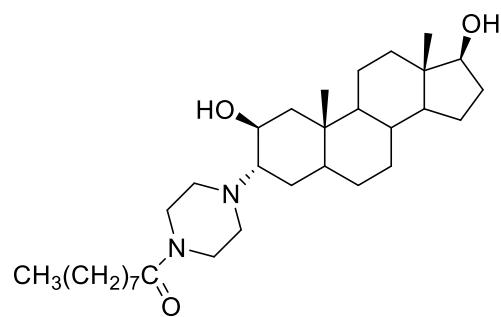
HC

IR-542-65-30  
HMBC

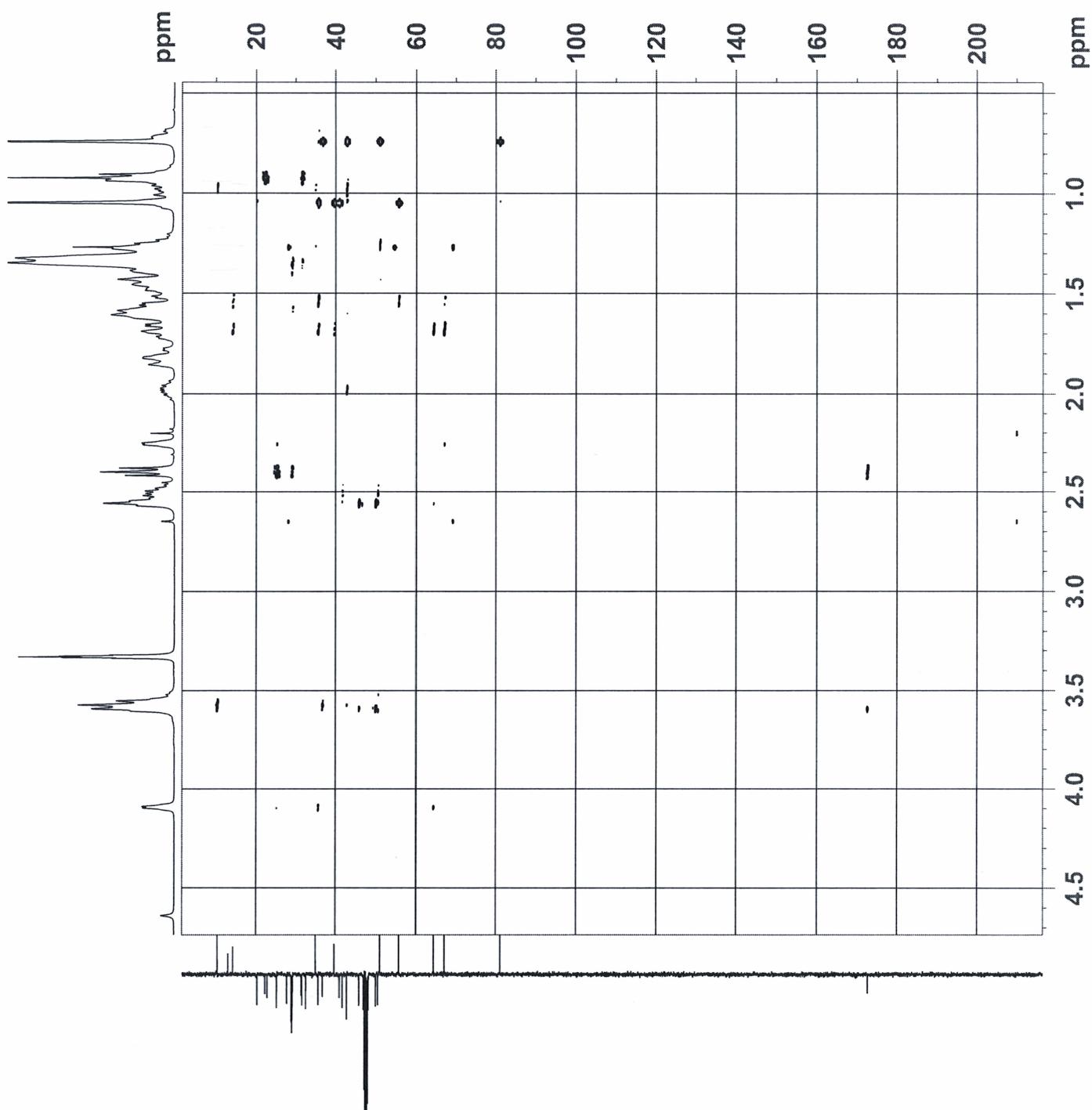


Key

<sup>1</sup>H NMR, <sup>13</sup>C NMR (APT), NOESY, COSY, HSQC and HMBC spectra  
for compound 4 (IR-542-47-27) in CD<sub>3</sub>OD

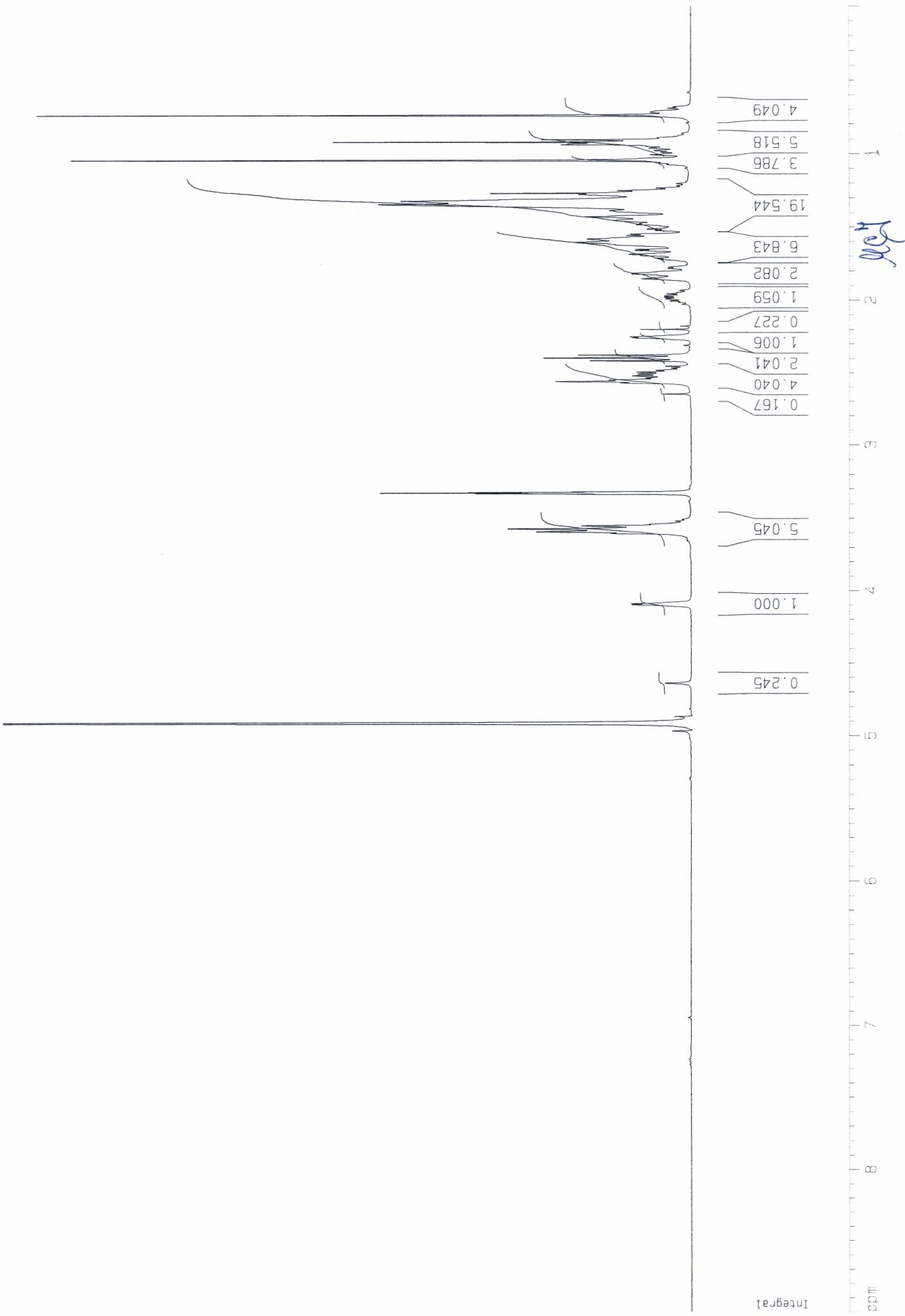


IR-542-47-27  
HMBC



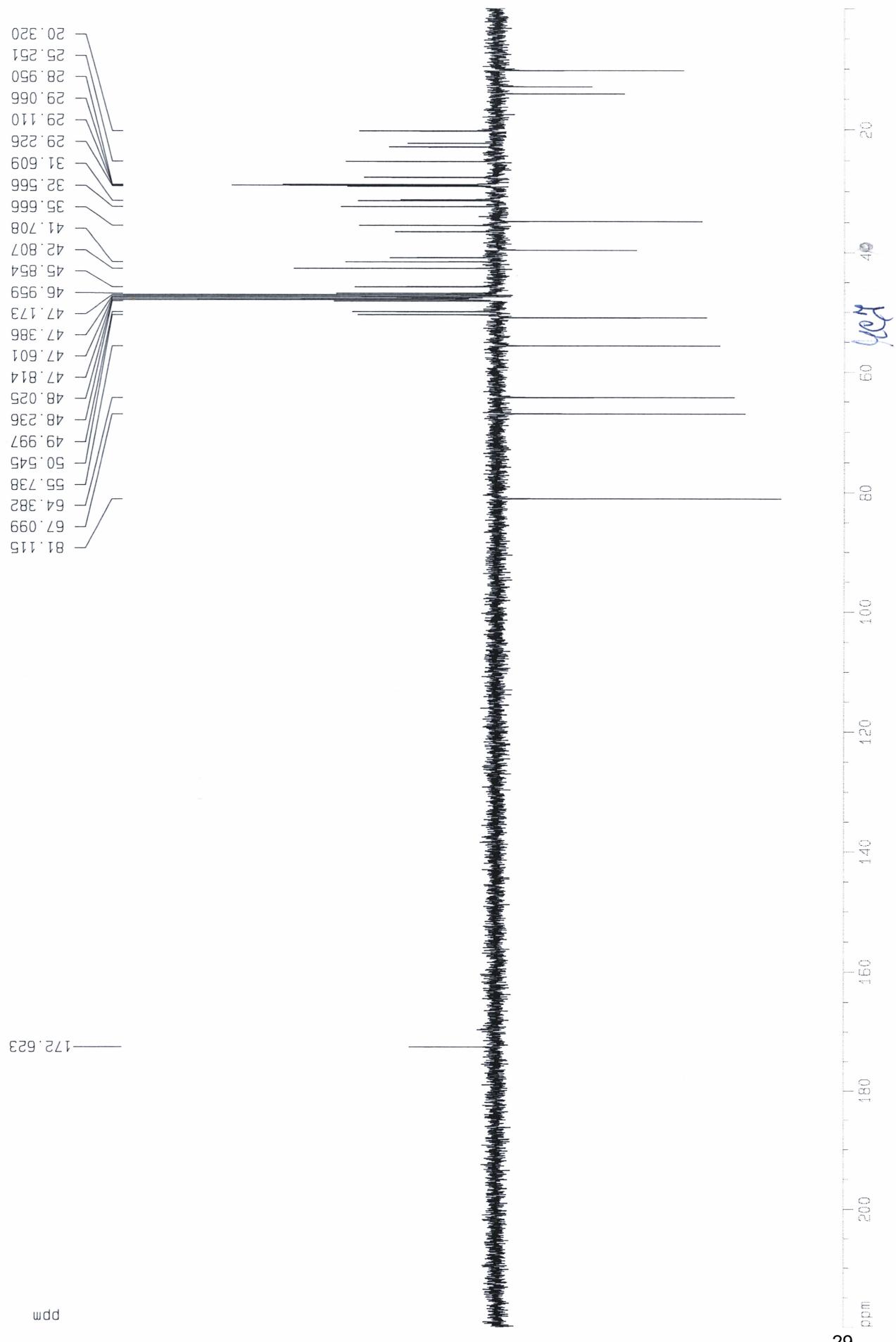
404

Integral  
Add

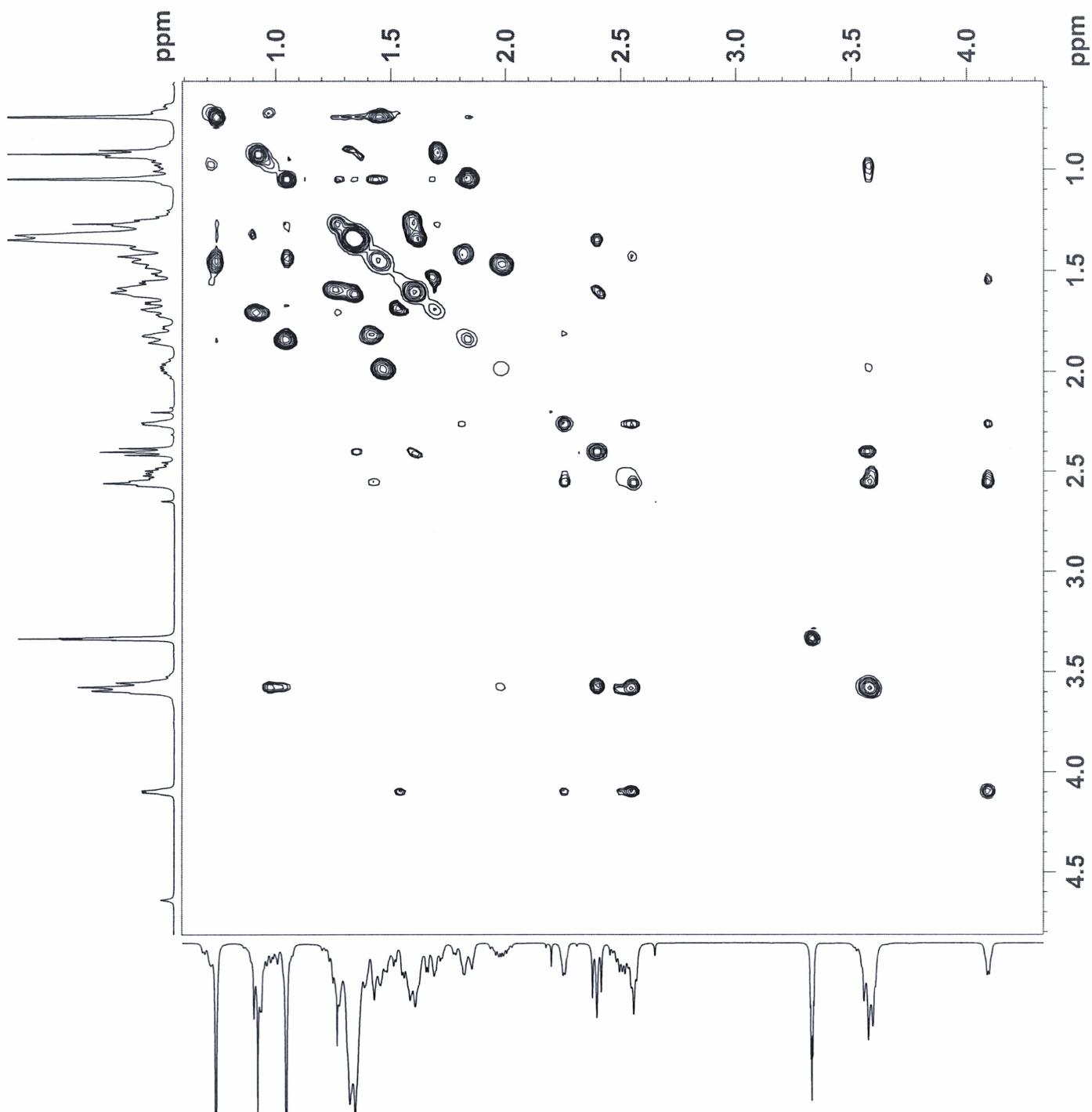


IR-542-47-27

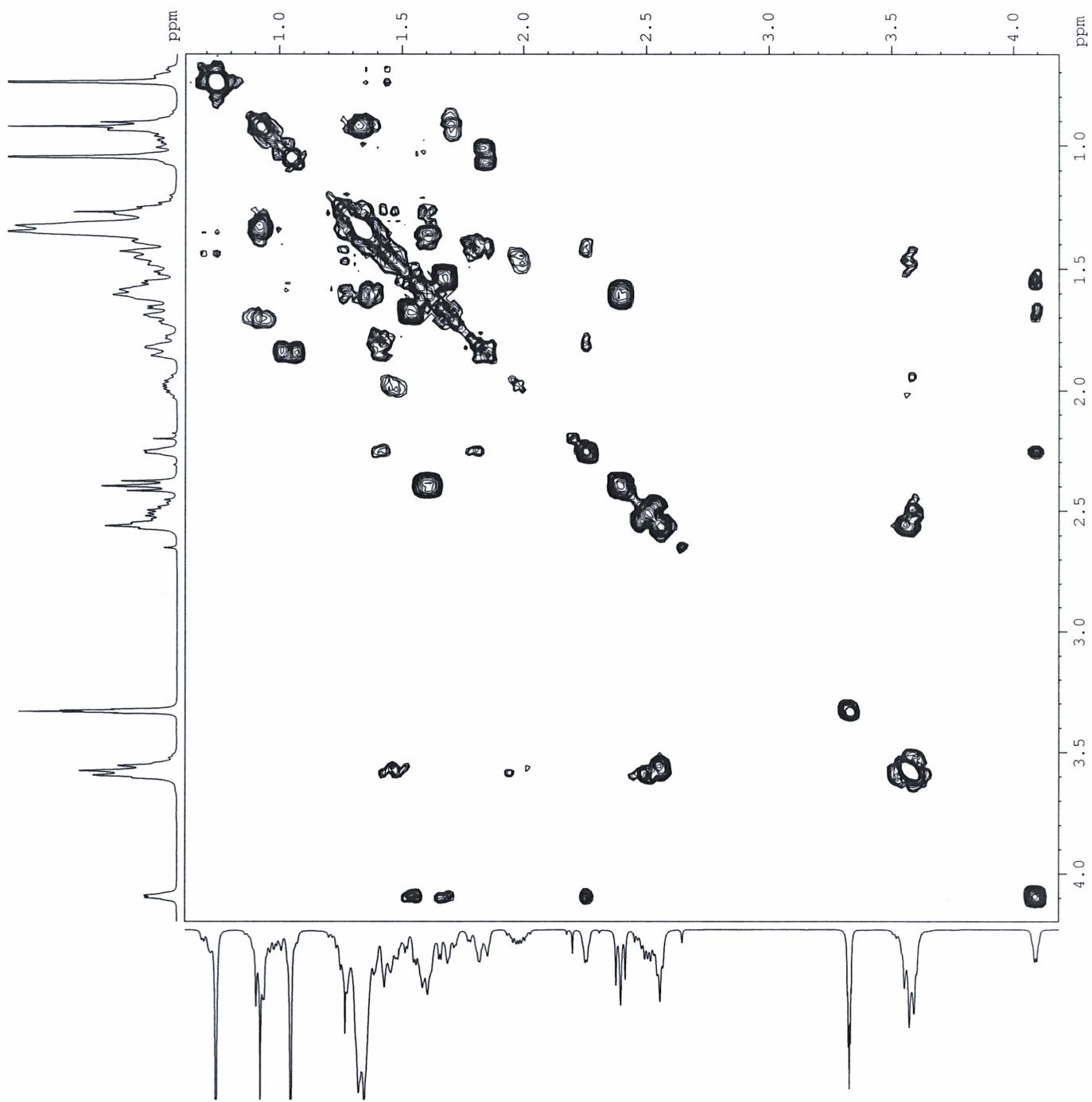
IR-542-47-27  
APT



IR-542-47-27  
NOESY

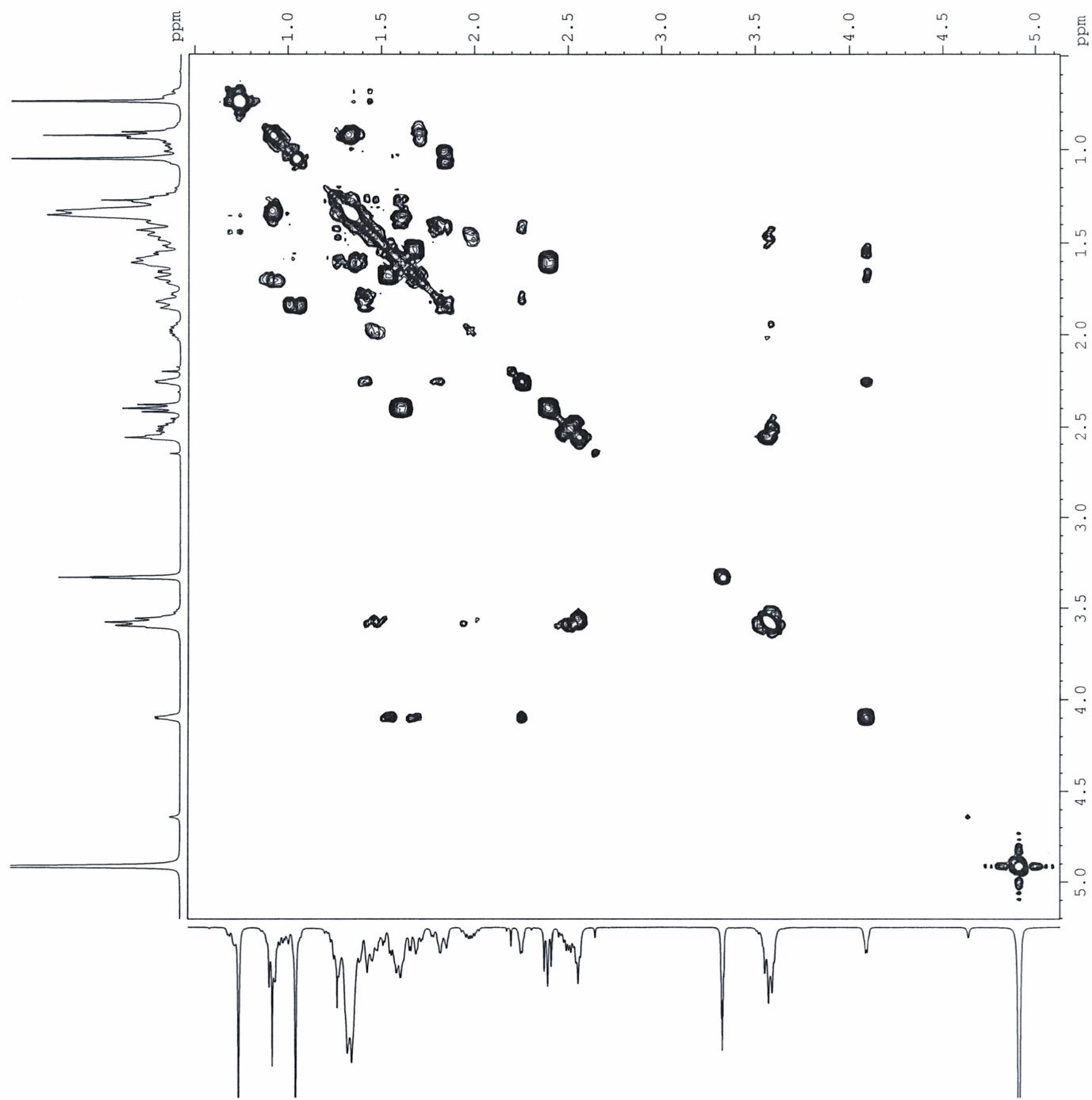


IR-542-47-27  
COSY

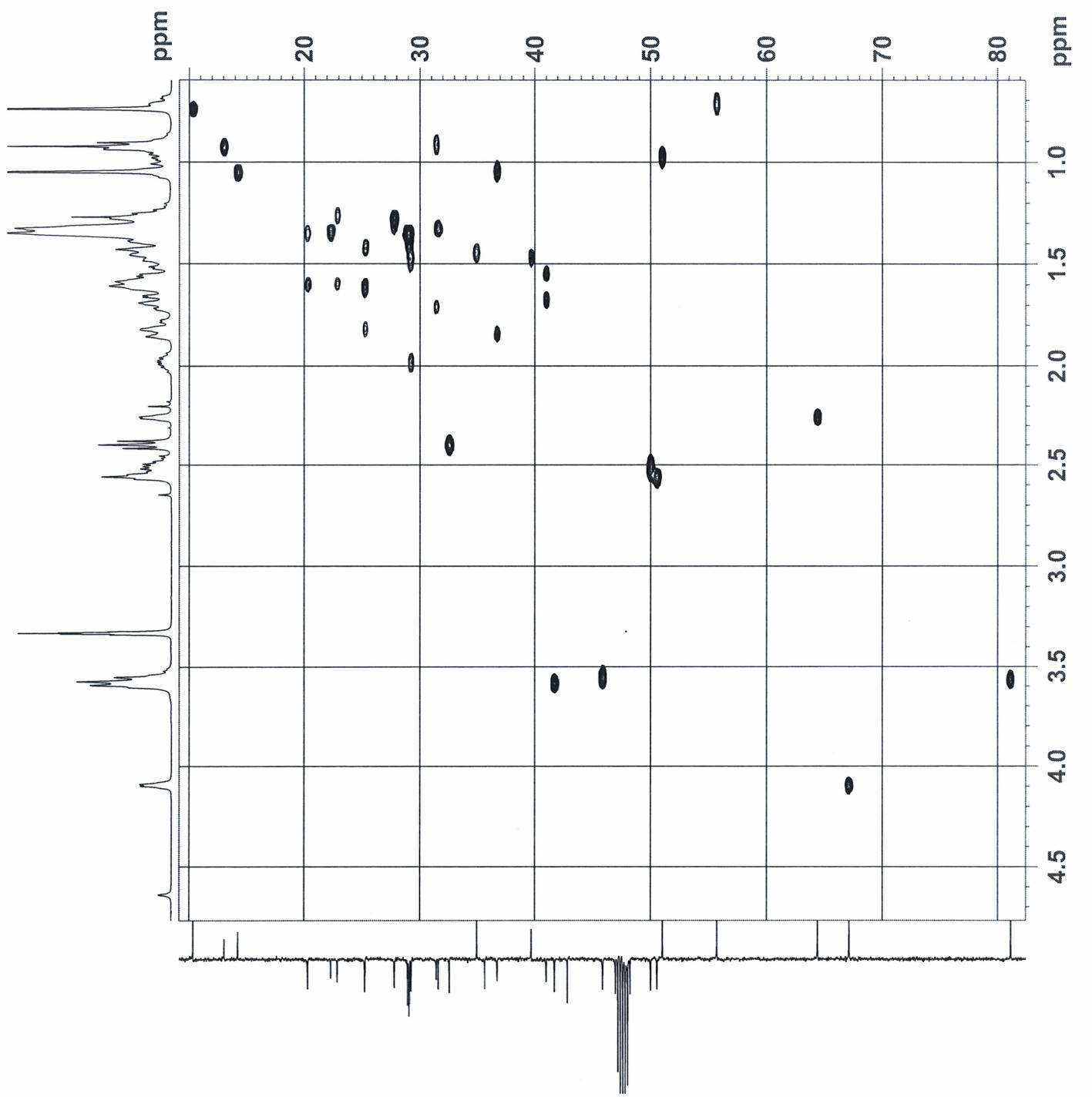


IR

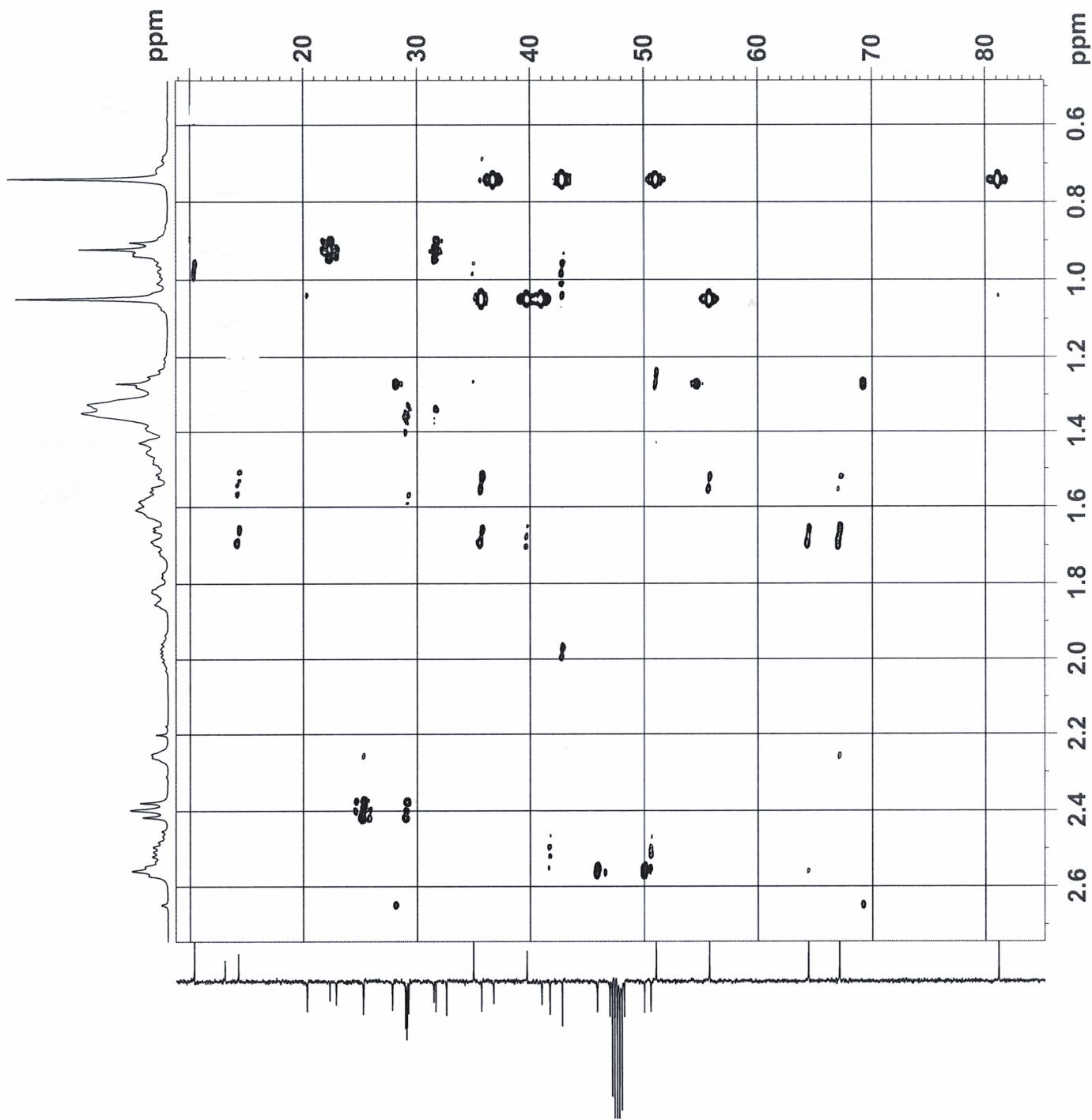
IR-542-47-27  
COSY



IR-542-47-27  
HSQC



$\text{H}_\alpha$



HC