

RS·C

ROYAL SOCIETY OF CHEMISTRY
EDUCATION DIVISION - SCOTLAND

MODERN SPECTROSCOPIC TECHNIQUES

SAMPLE SPECTRA

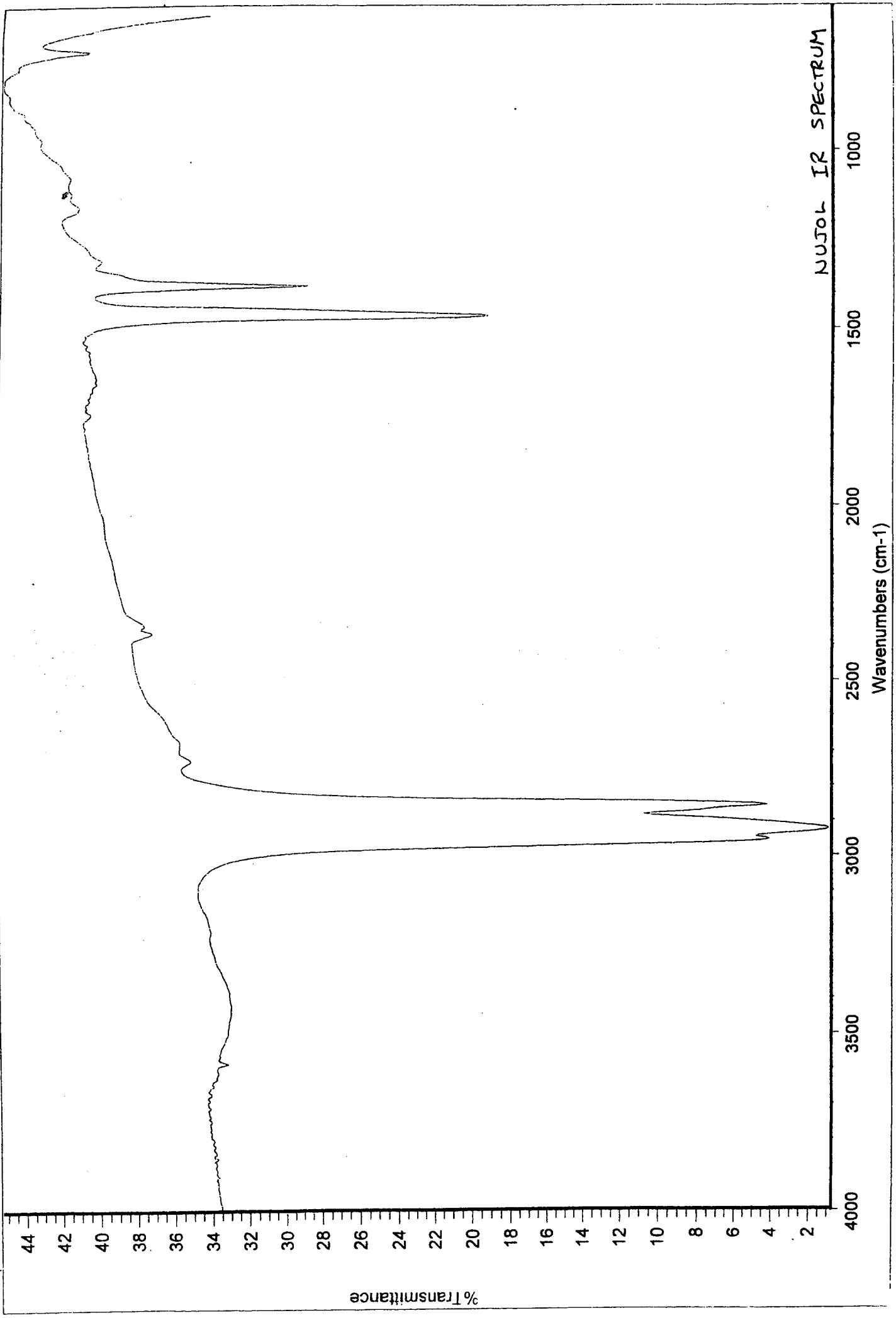
Experimental Details

The assistance of the School of Chemistry of the University of St Andrews in preparing these spectra is gratefully acknowledged.

Infra-red spectra were recorded on a Nicolet Avatar 360 FT-IR spectrophotometer. The samples were prepared as either Nujol mulls or thin films between sodium chloride discs.

NMR spectra were recorded on a Bruker AM 300 f.t. spectrophotometer (^1H , 300 MHz; ^{13}C , 74.76 MHz). All were run in deuterated chloroform as solvent.

Mass spectra were recorded on an A.E.I. MS-902 spectrometer using electron impact (EI) at 70 eV or obtained from its library.



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INFORMATION

The empirical formulae of the unknown compounds are as follows:

Compound 1 is C_2H_6O

Compound 2 is $C_3H_6O_2$

Compounds 3 and 4 are isomers $C_4H_{10}O$

Compounds 5, 6 and 9 are isomers C_2H_4O

(Note: for compound 9 there is also a single proton at δ 12 ppm in the NMR)

Compound 7 is $C_5H_{10}O_2$

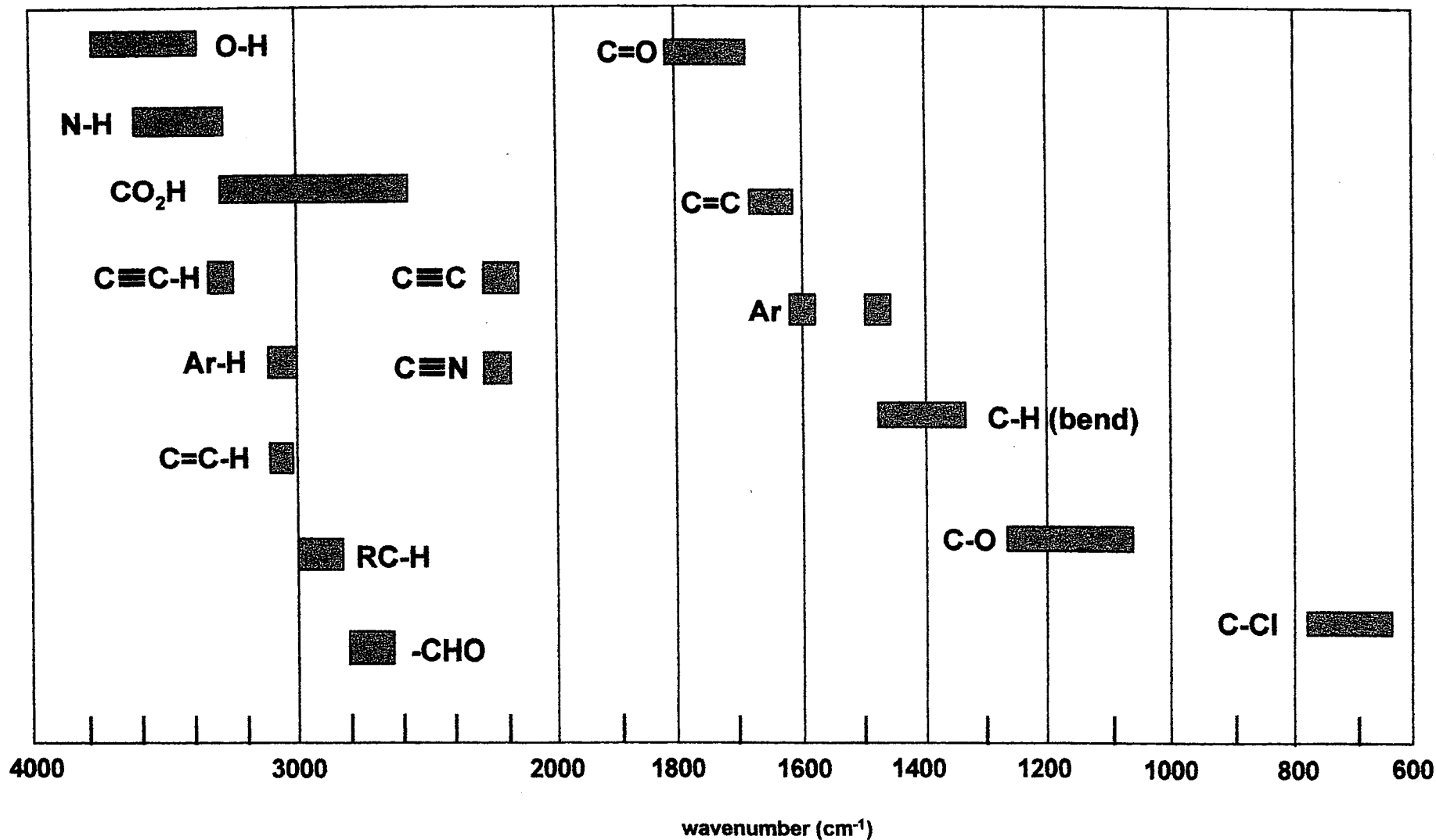
Compound 8 is $C_5H_{10}O$

(Note: in NMR spectrum ratio of peaks should be 3:2:2:2:1)

Compound 10 is C_7H_8

Compound 11 is $C_{10}H_{12}O$

INFRARED ABSORPTION BANDS

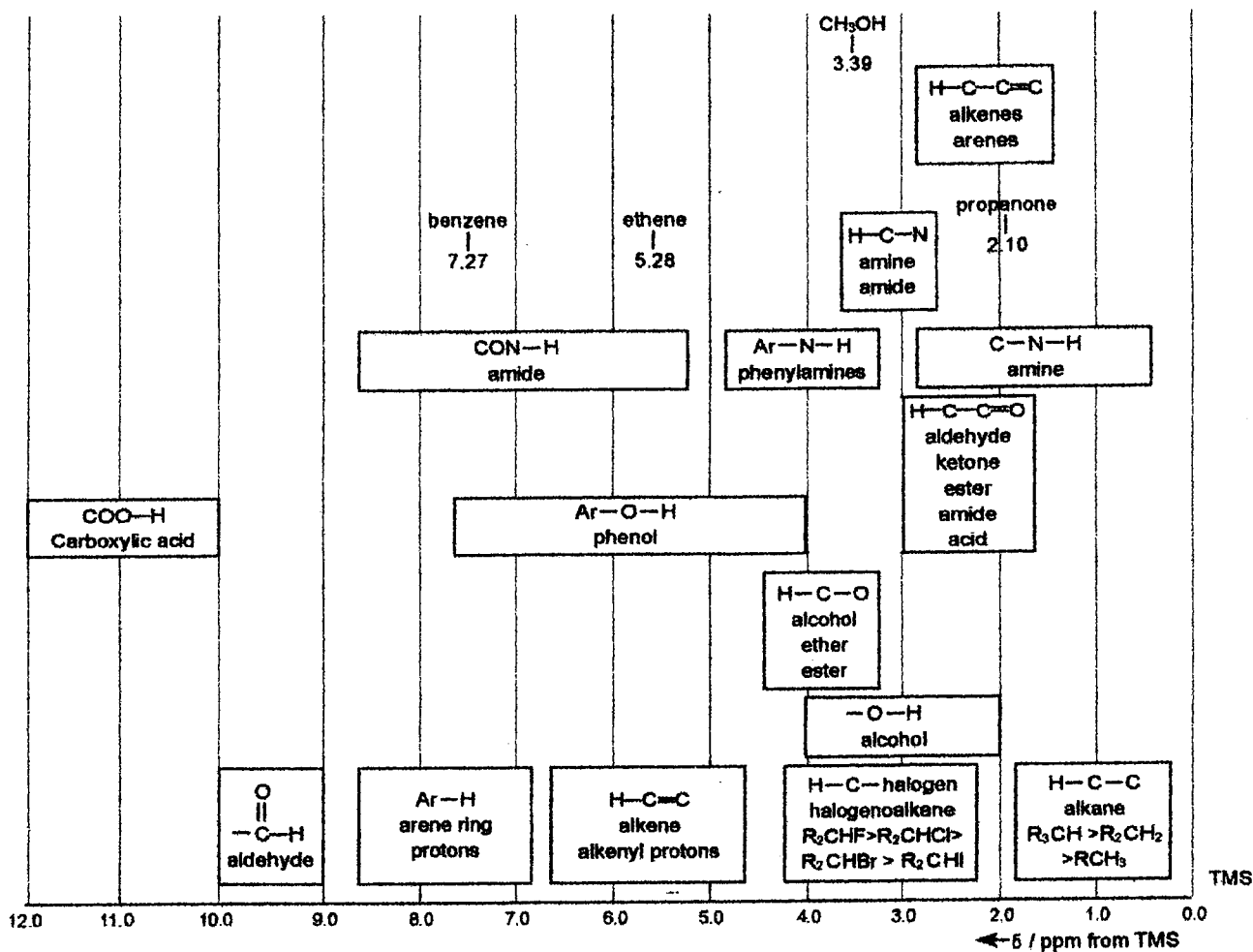


Chemical shifts for hydrogen relative to TMS (tetramethylsilane) and calculated from the relationship

δ / ppm from TMS =

$$\frac{B_{TMS} - B_{sample}}{B_{TMS}} \times 10^6$$

(B is the applied magnetic flux density).



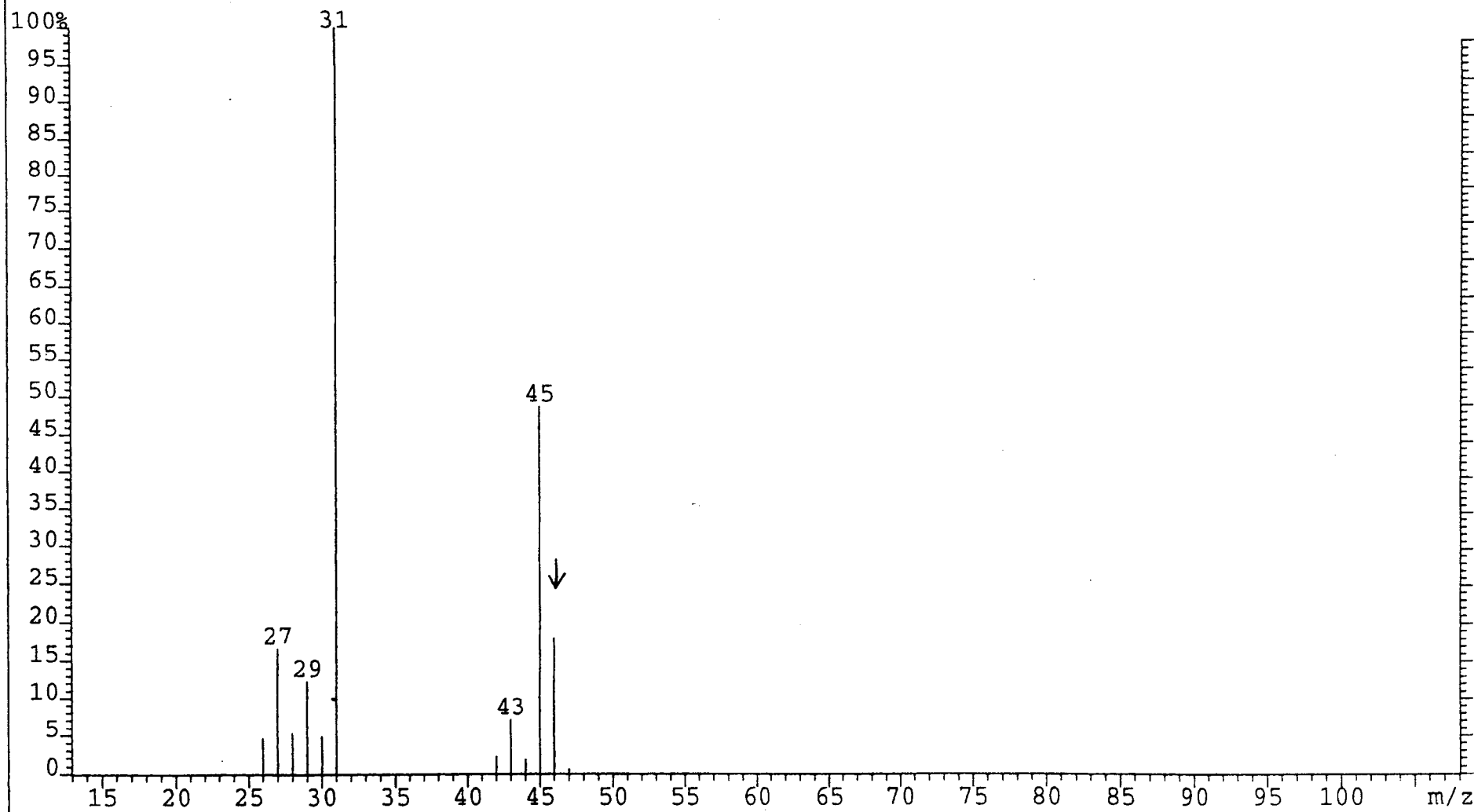
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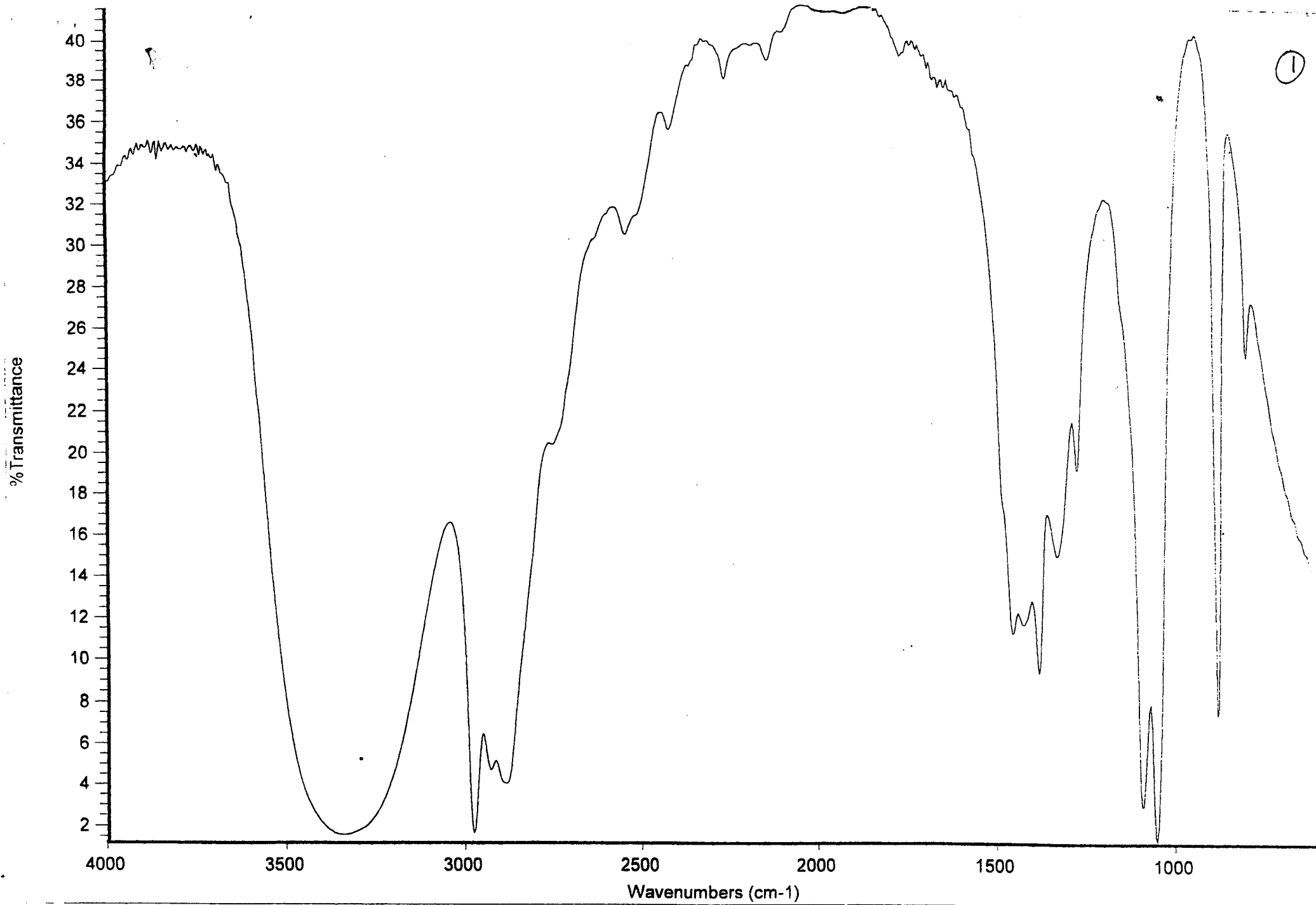
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NIST #49 MF: MW:46 CAS:64-17-5 NIST:61254

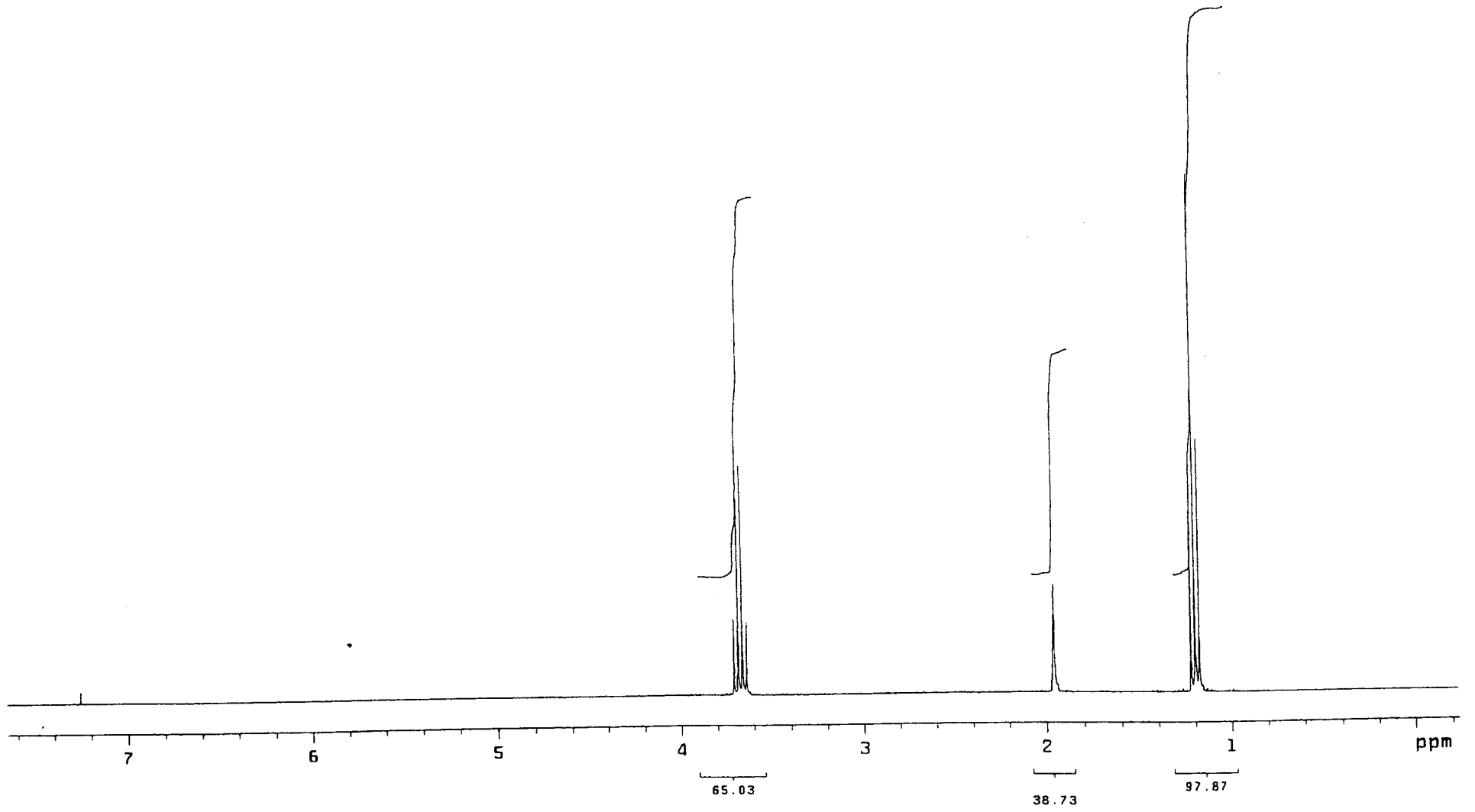
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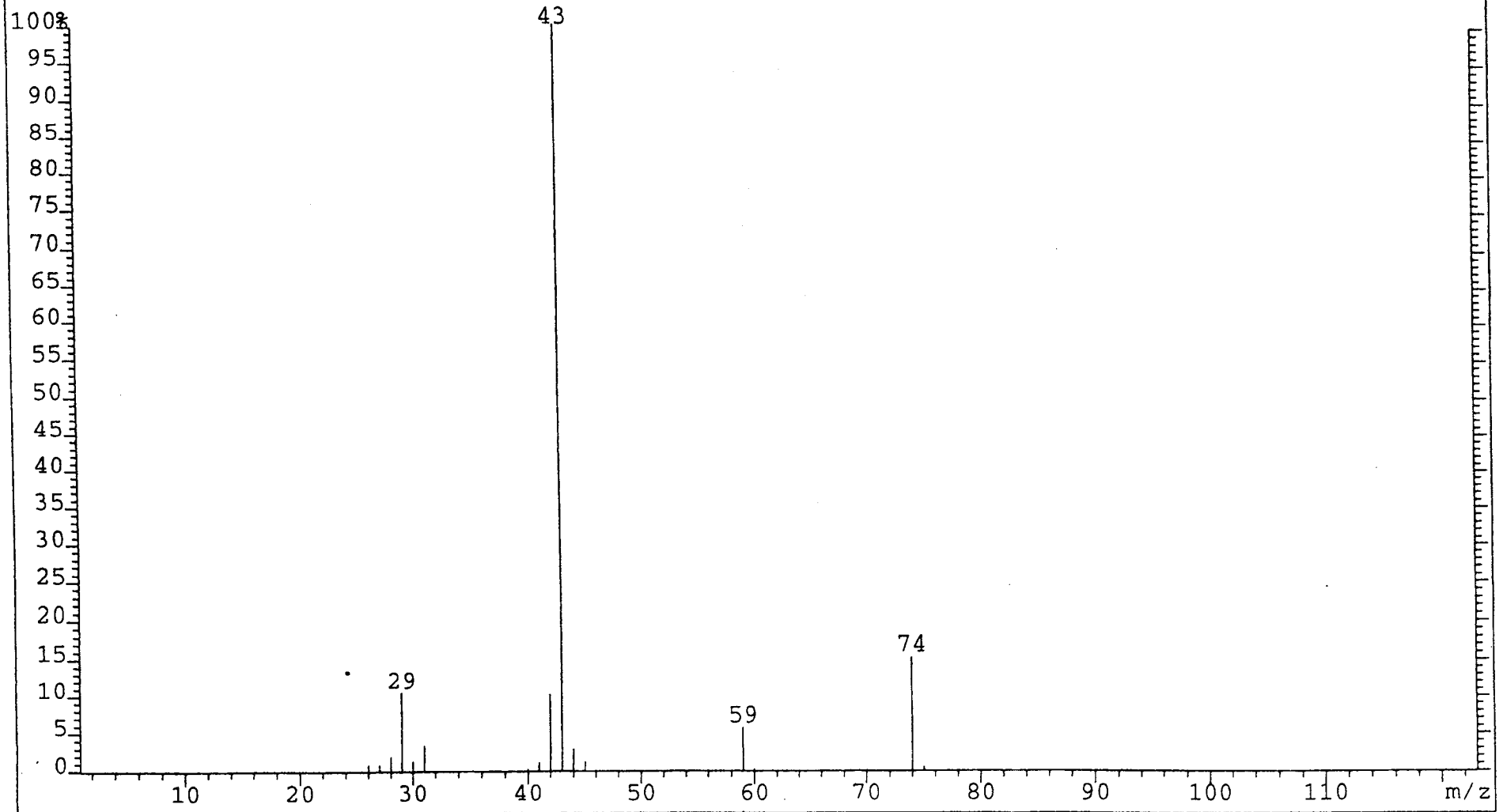
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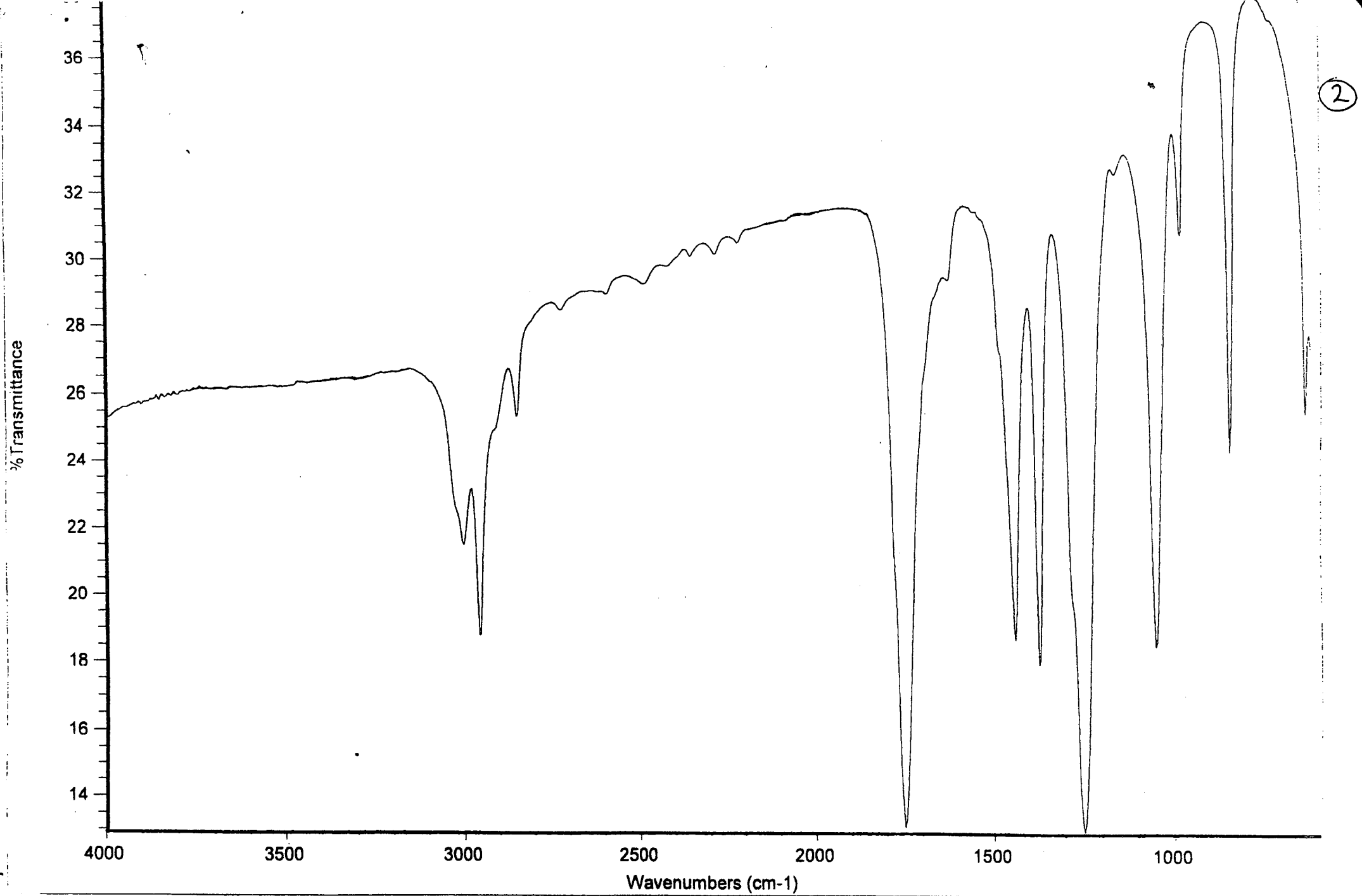
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MW:74 CAS:79-20-9 NIST:19200
| Devoton |

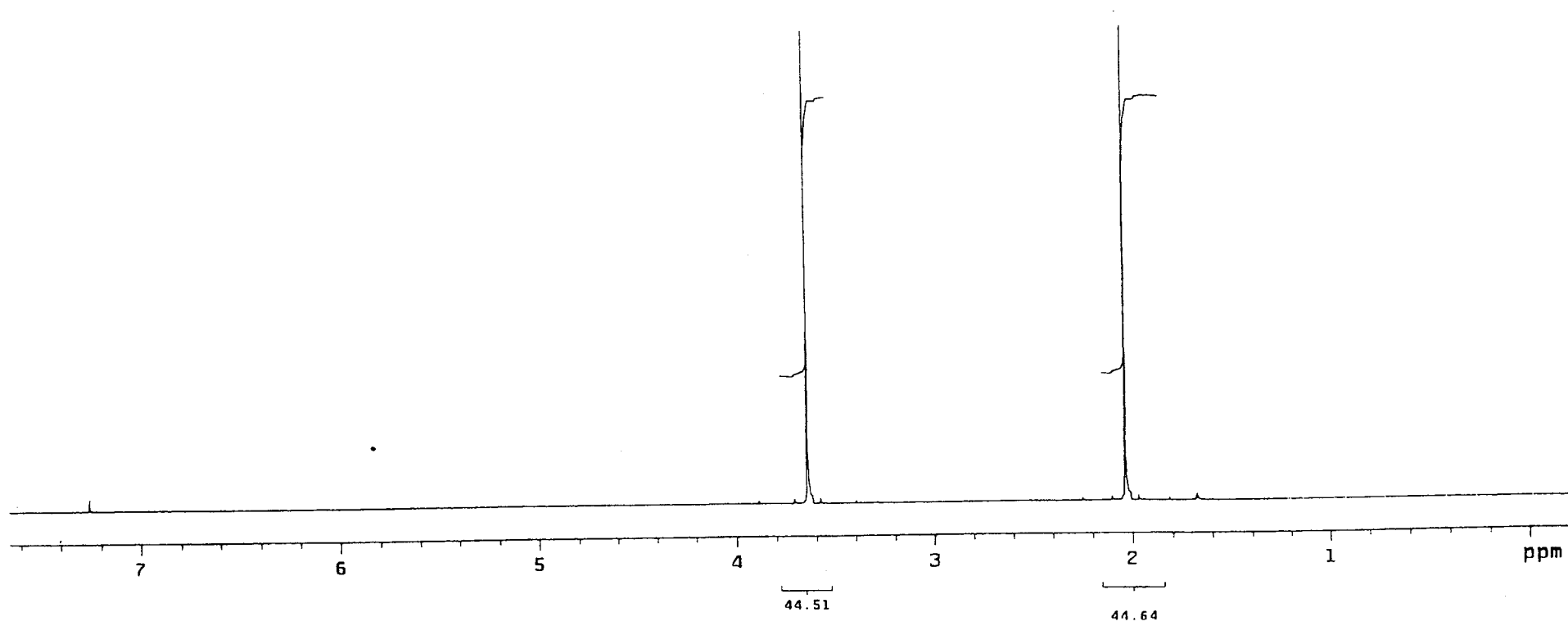
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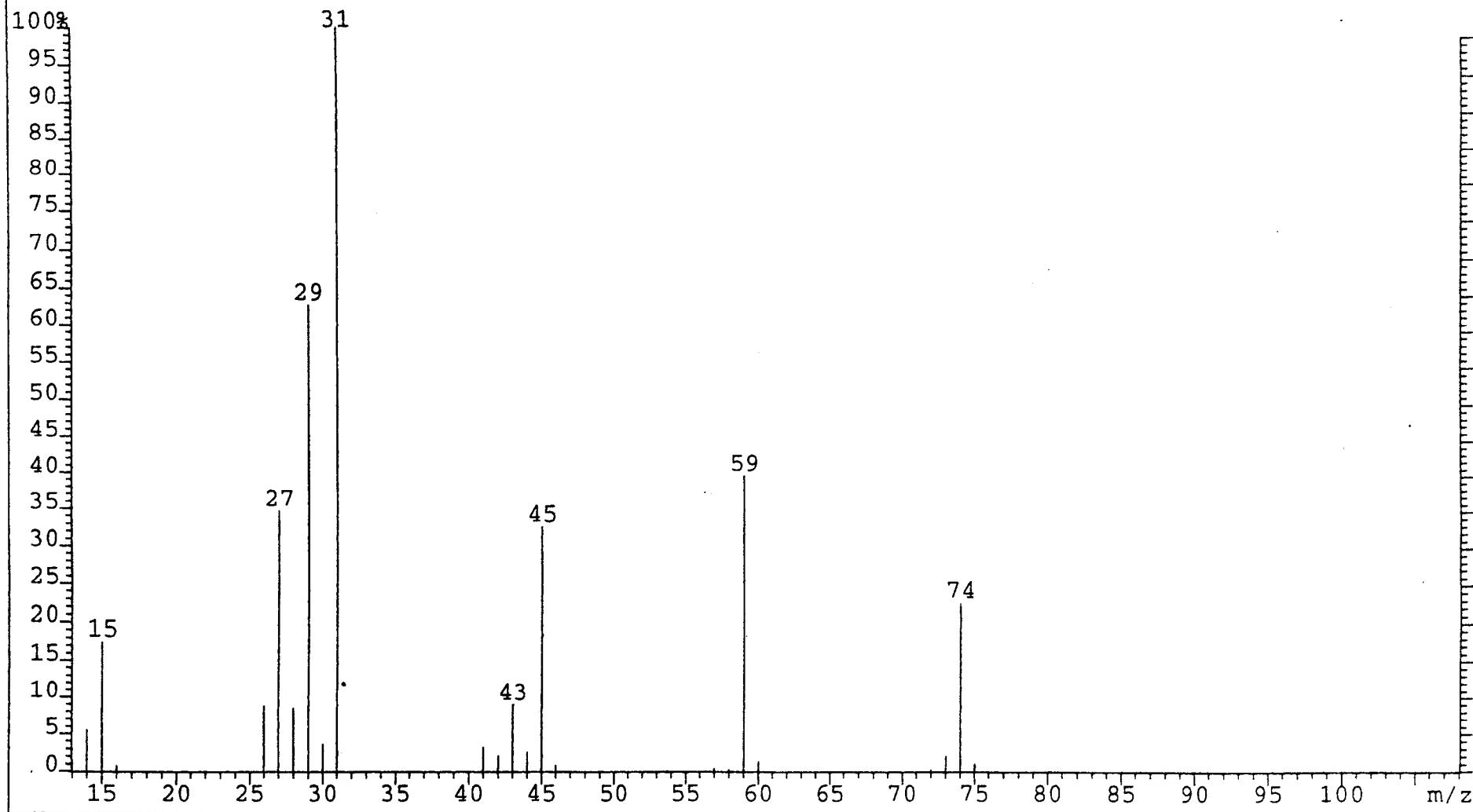


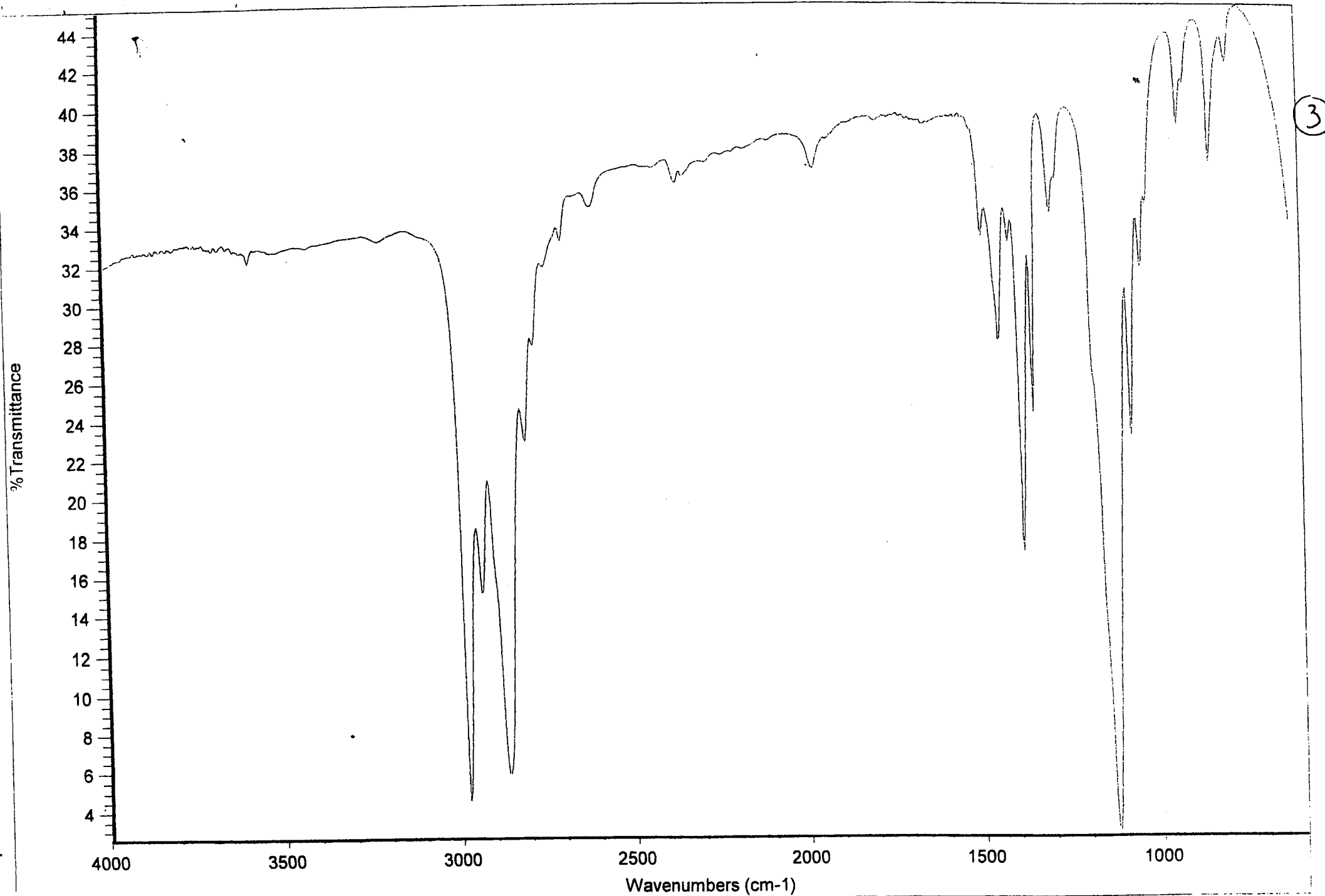
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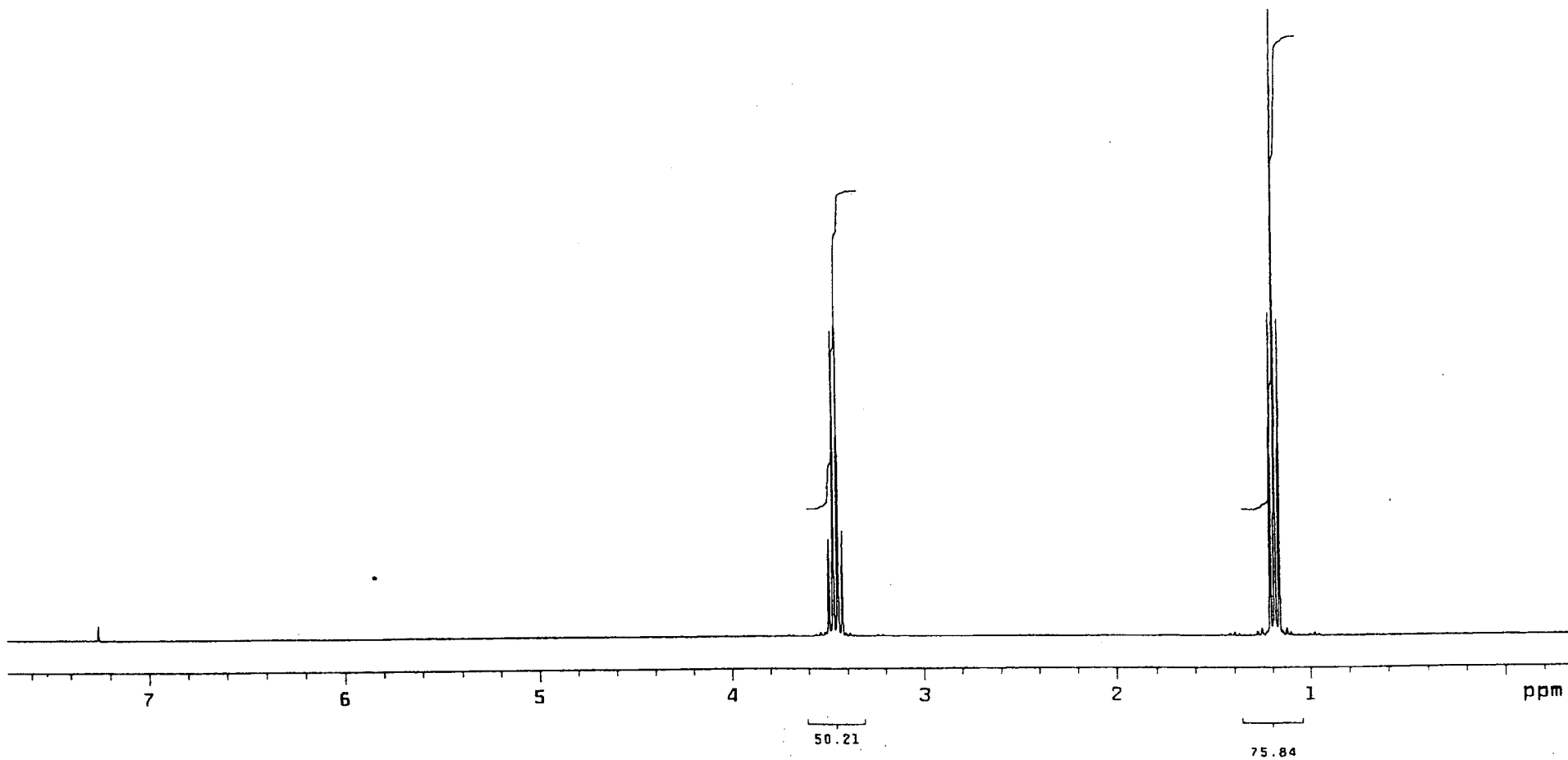
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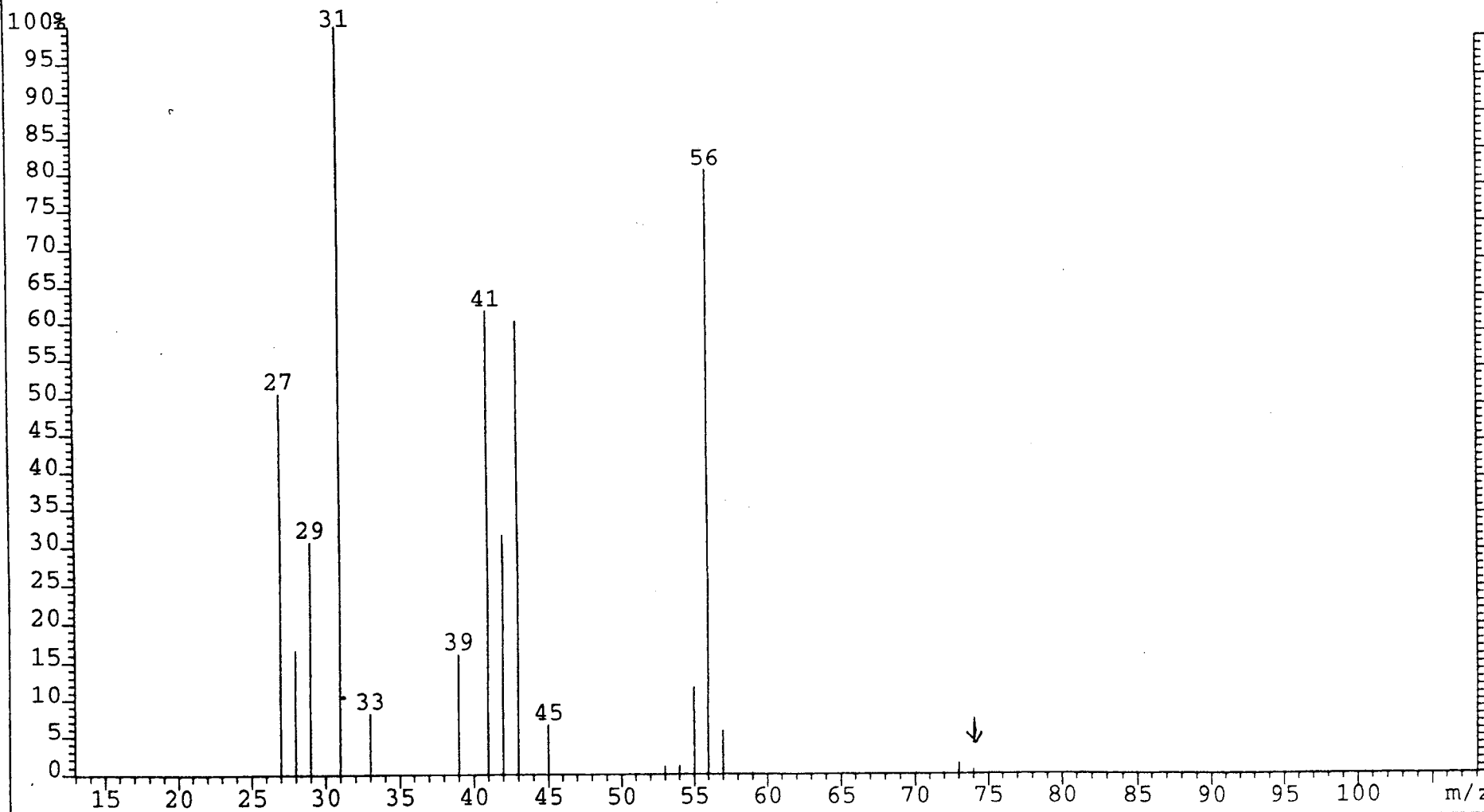


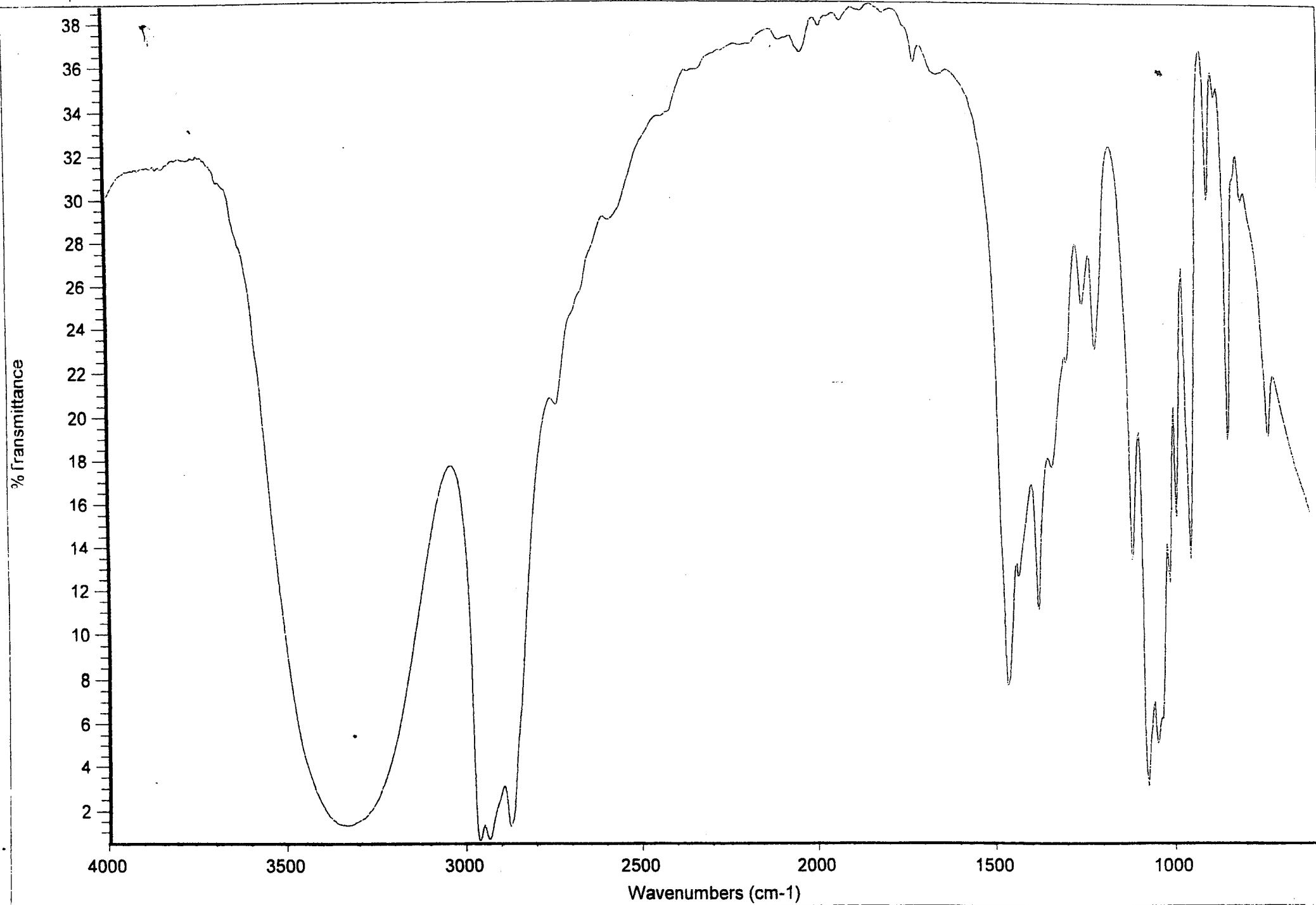
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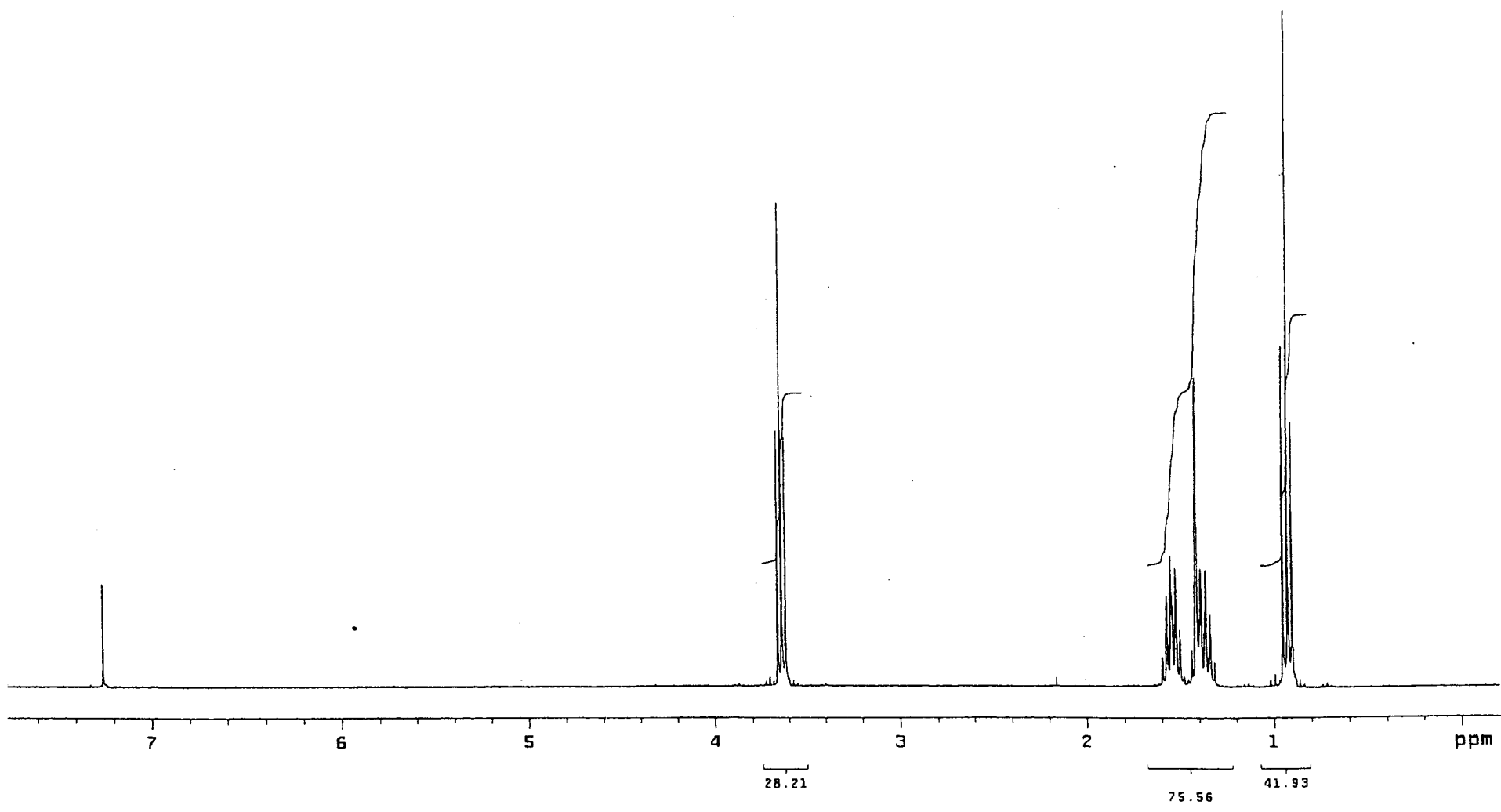
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4



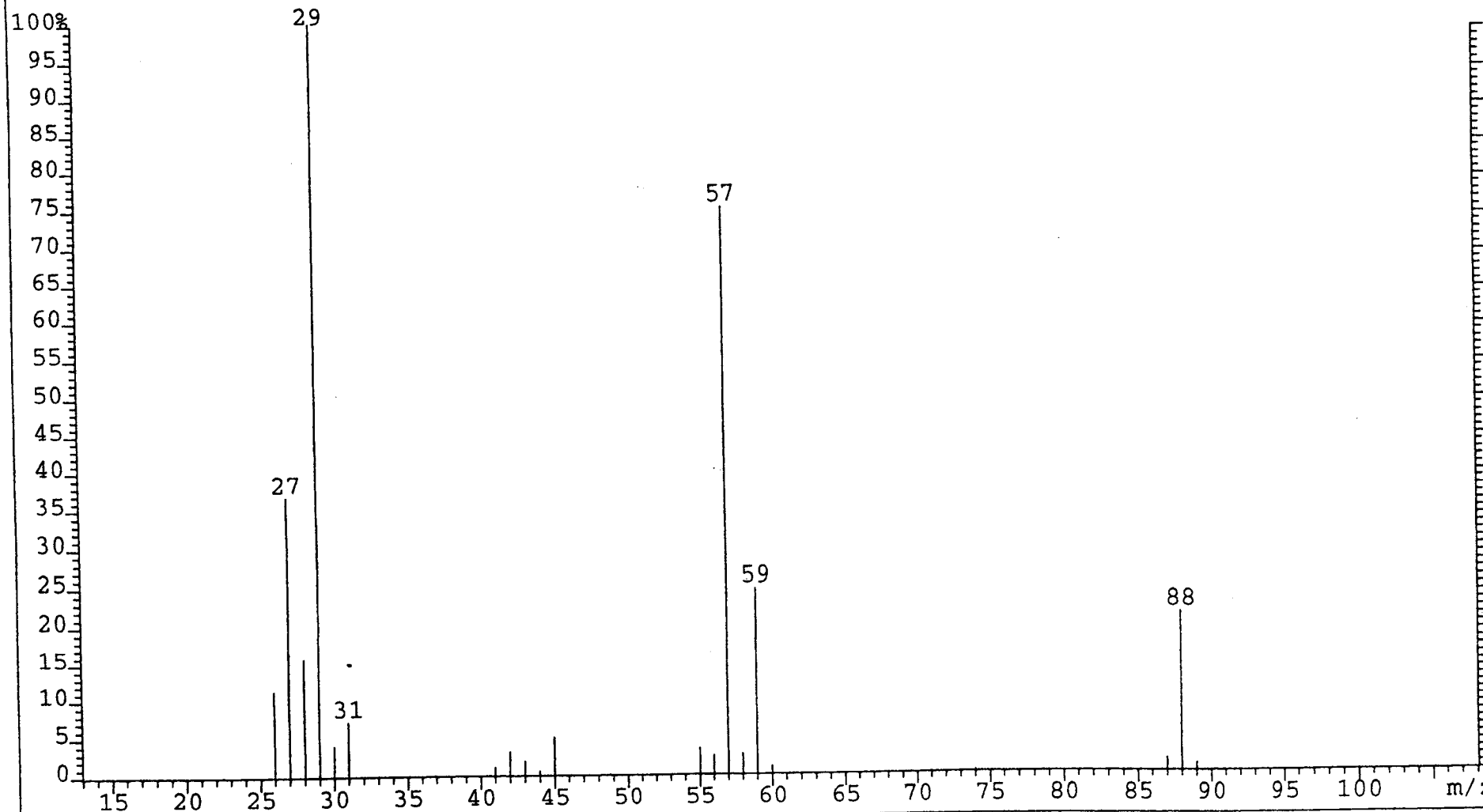
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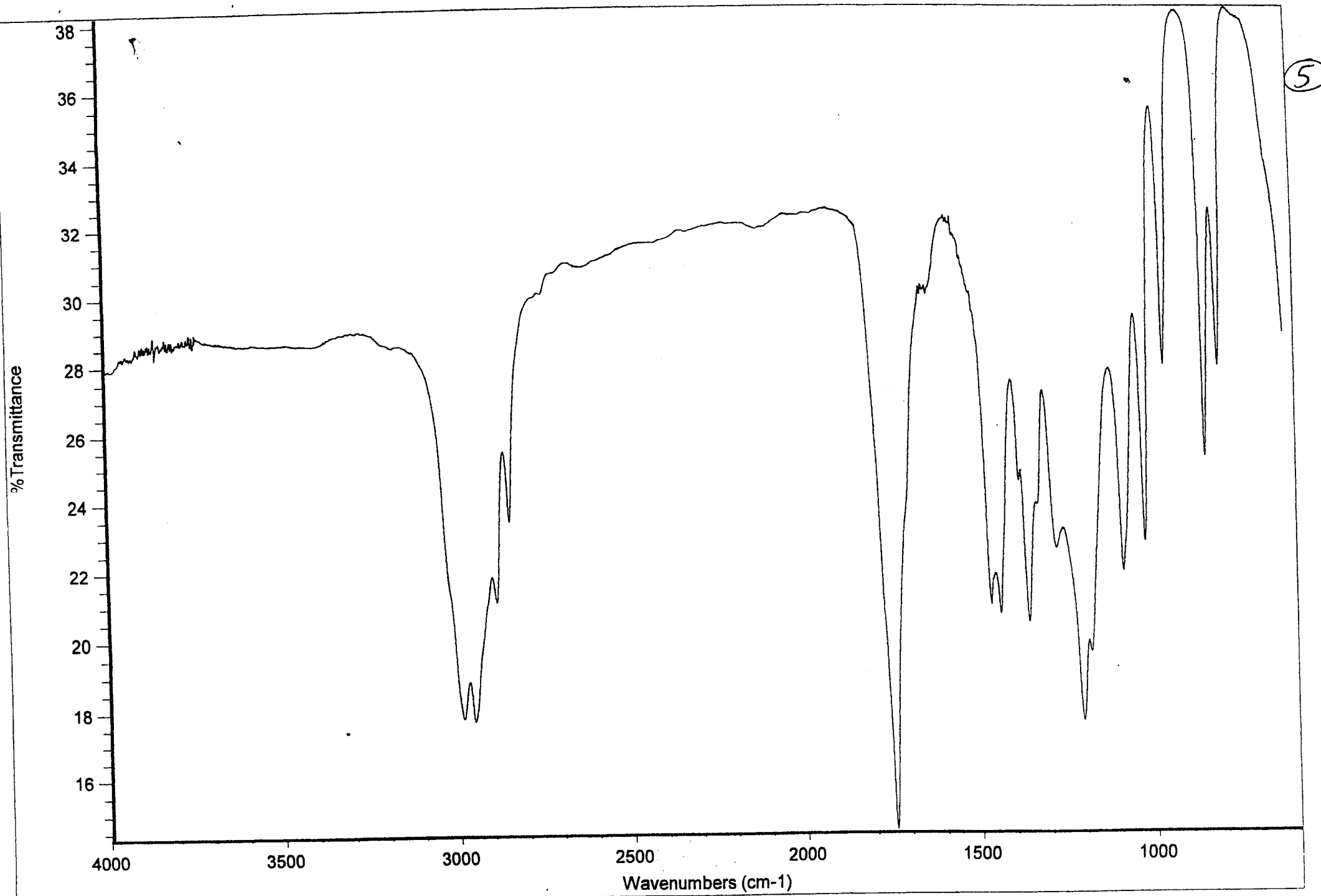
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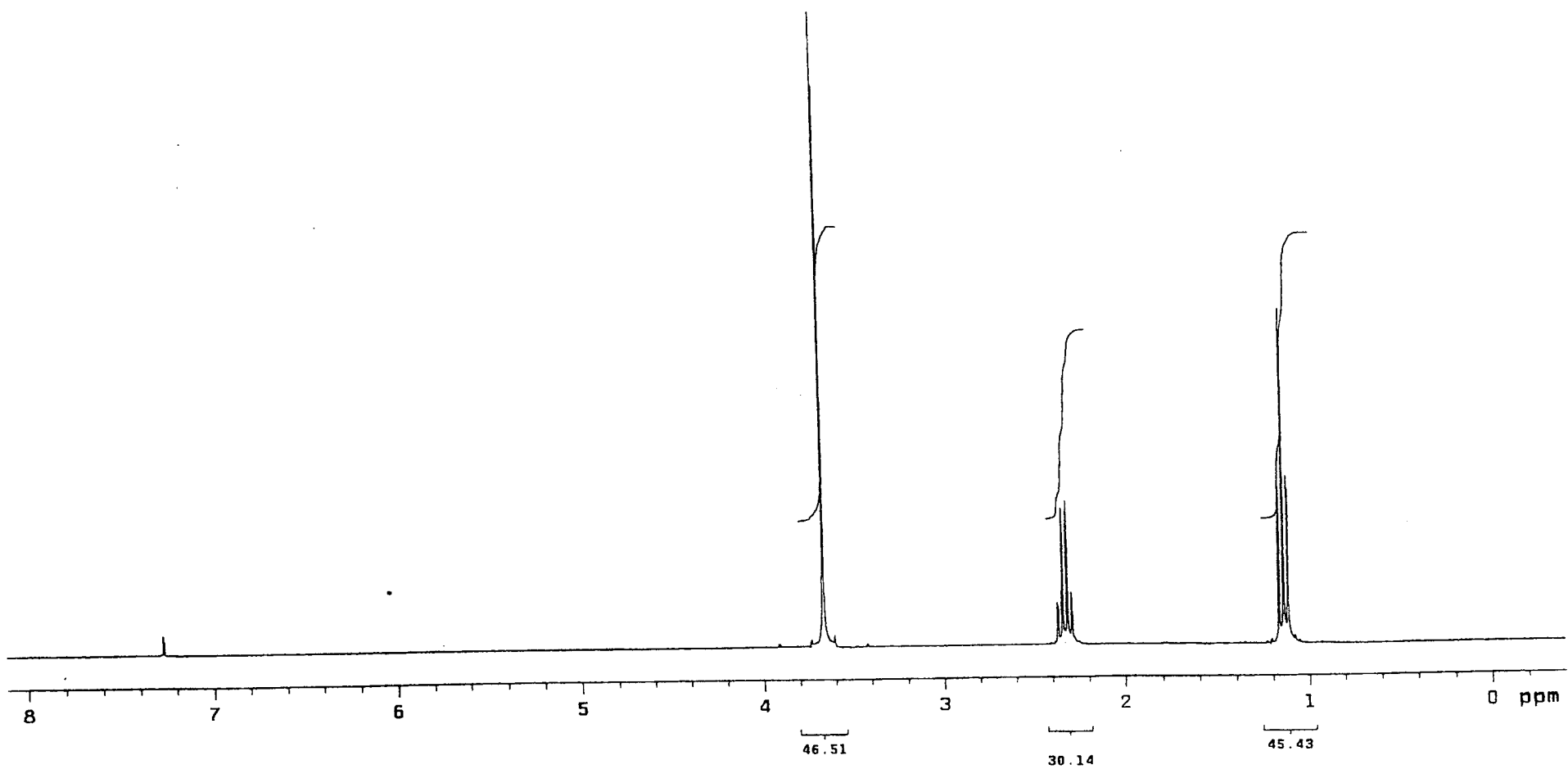
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MW:88 CAS:554-12-1 NIST:678





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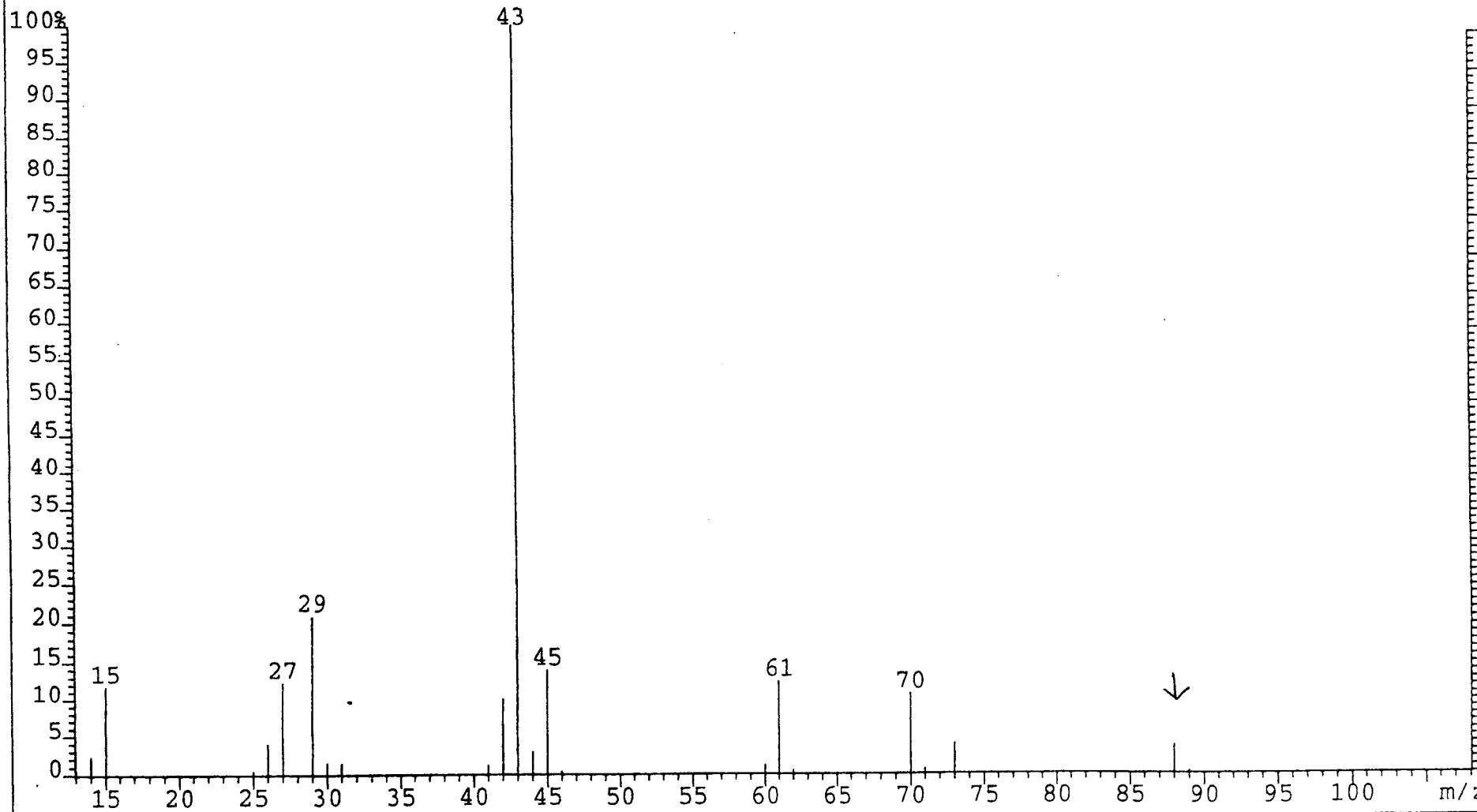
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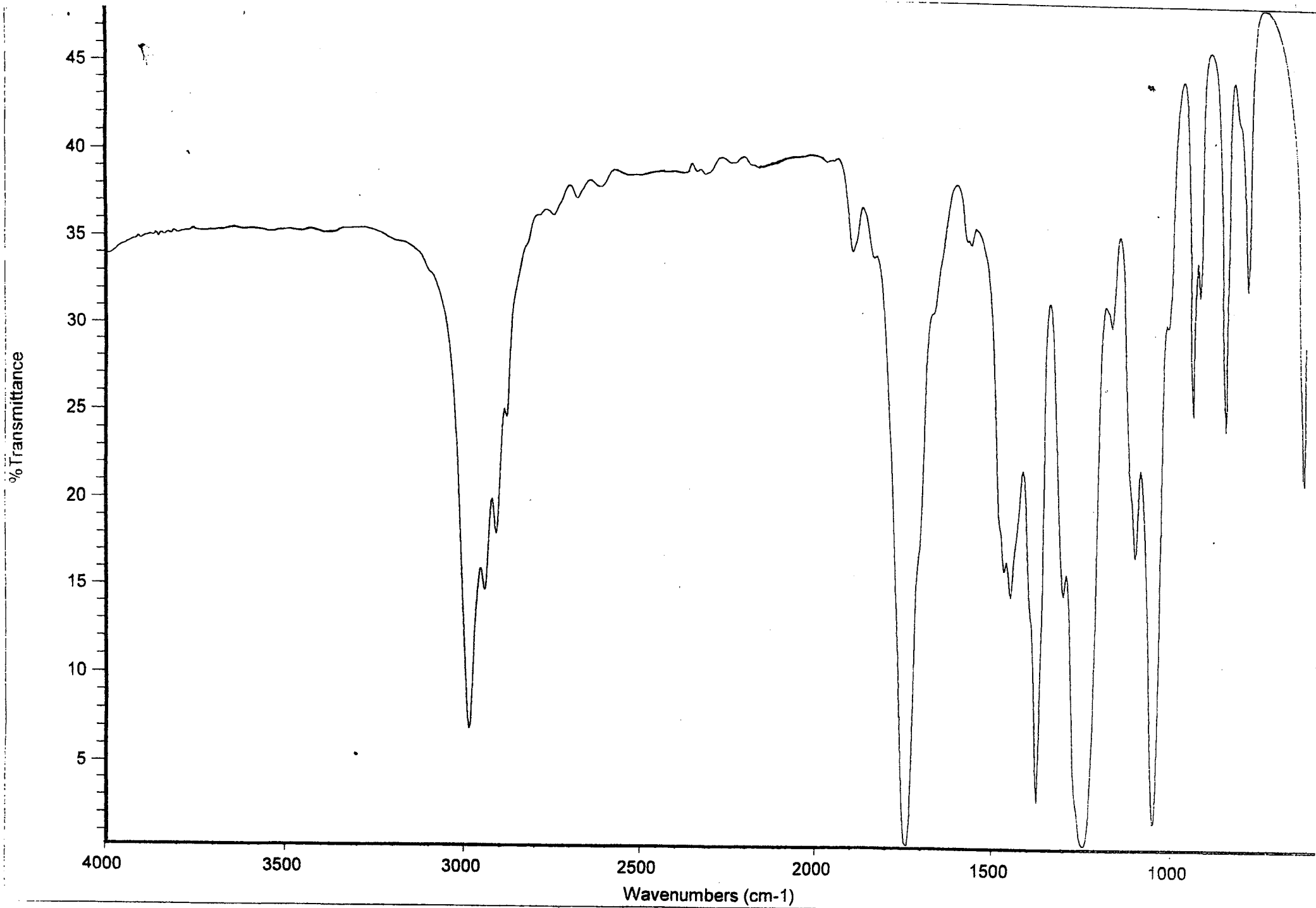
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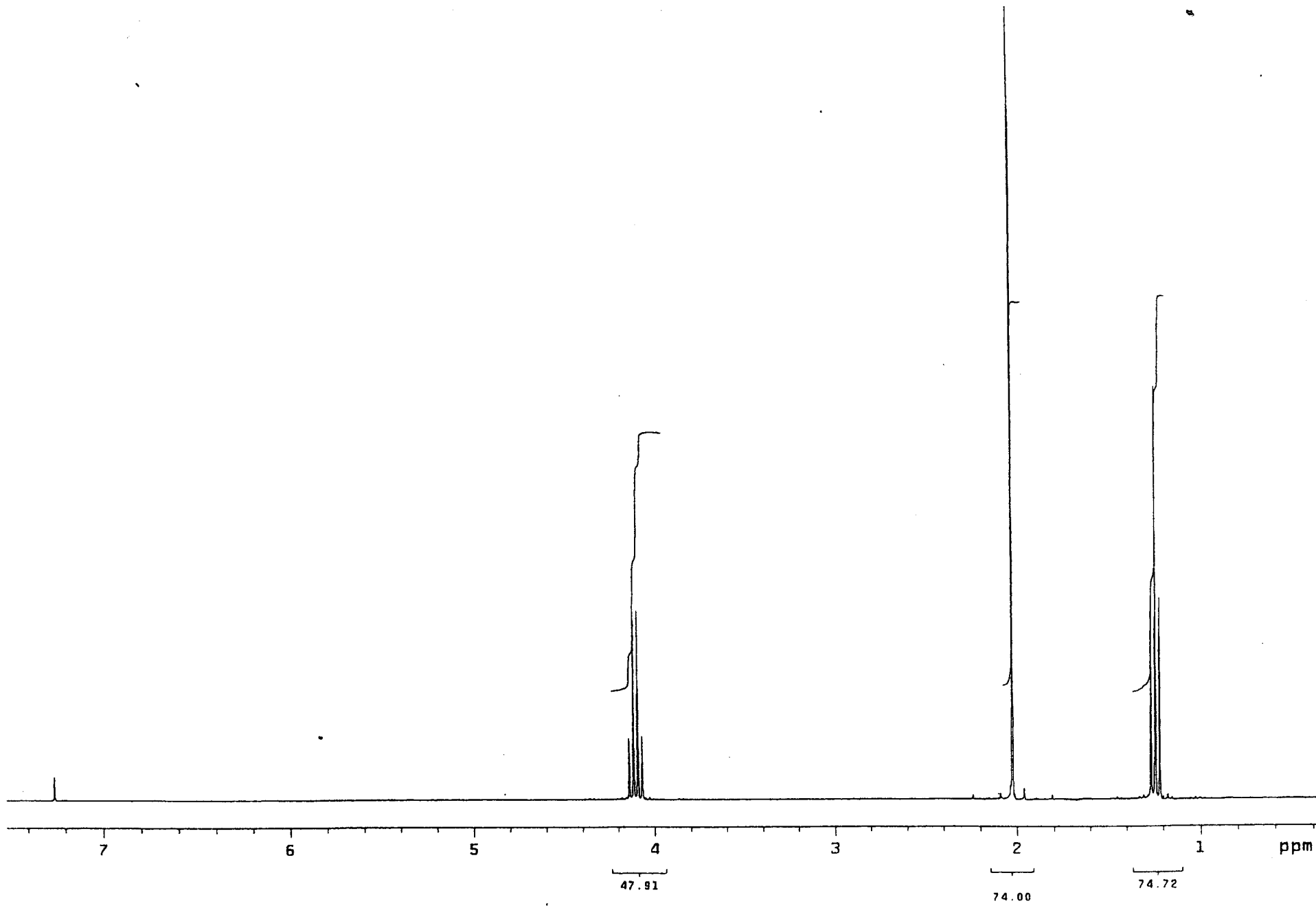
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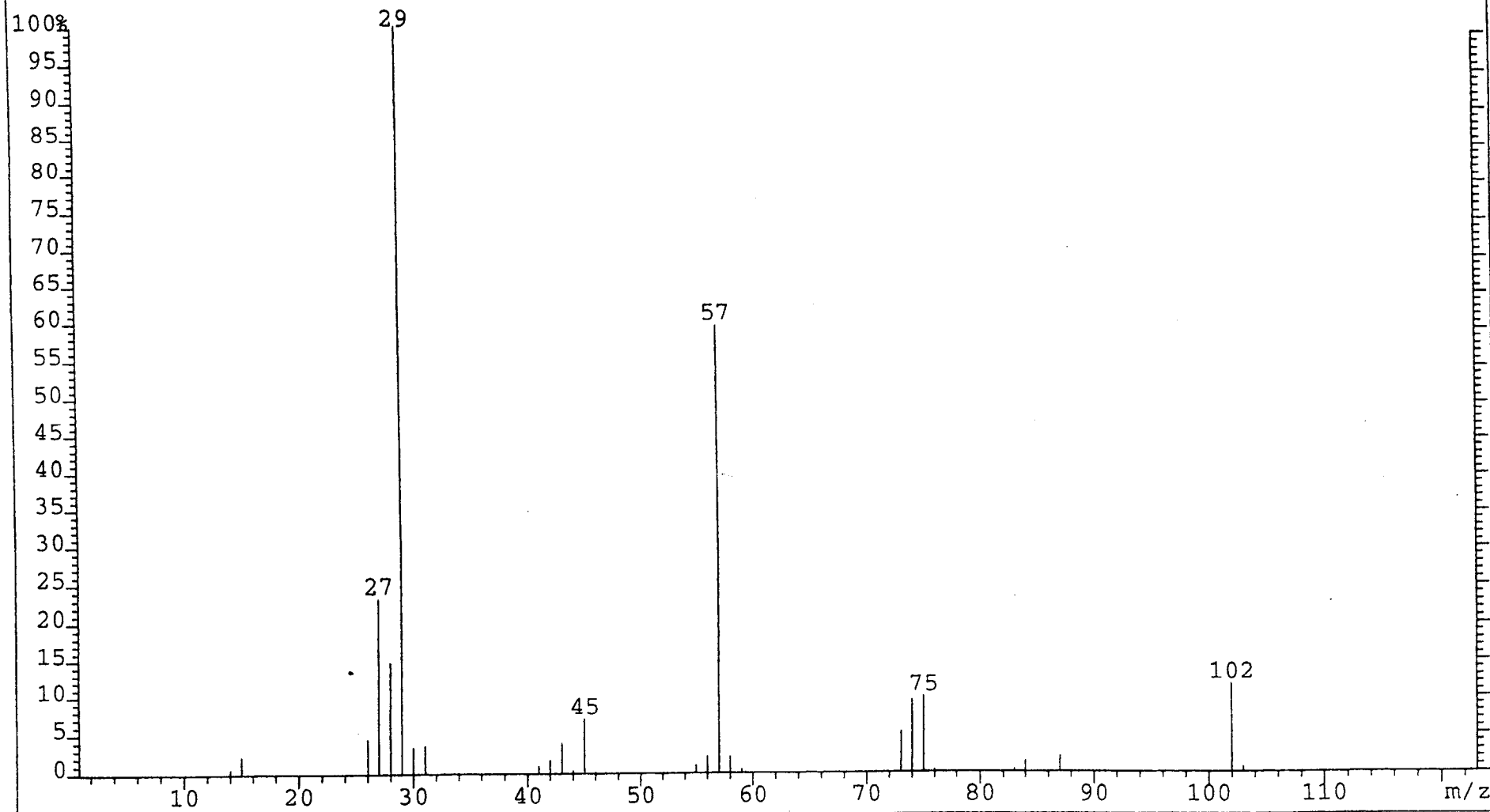


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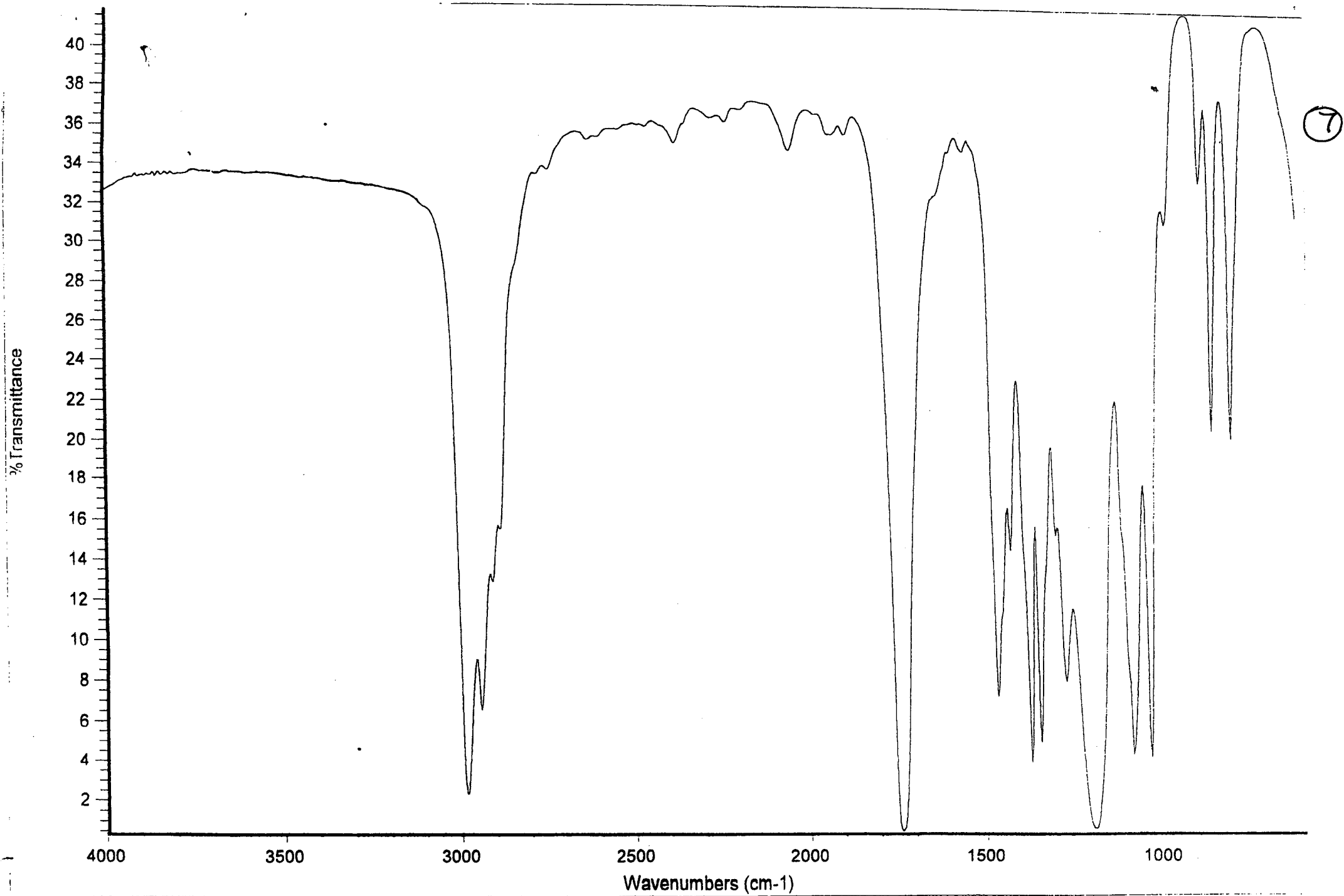
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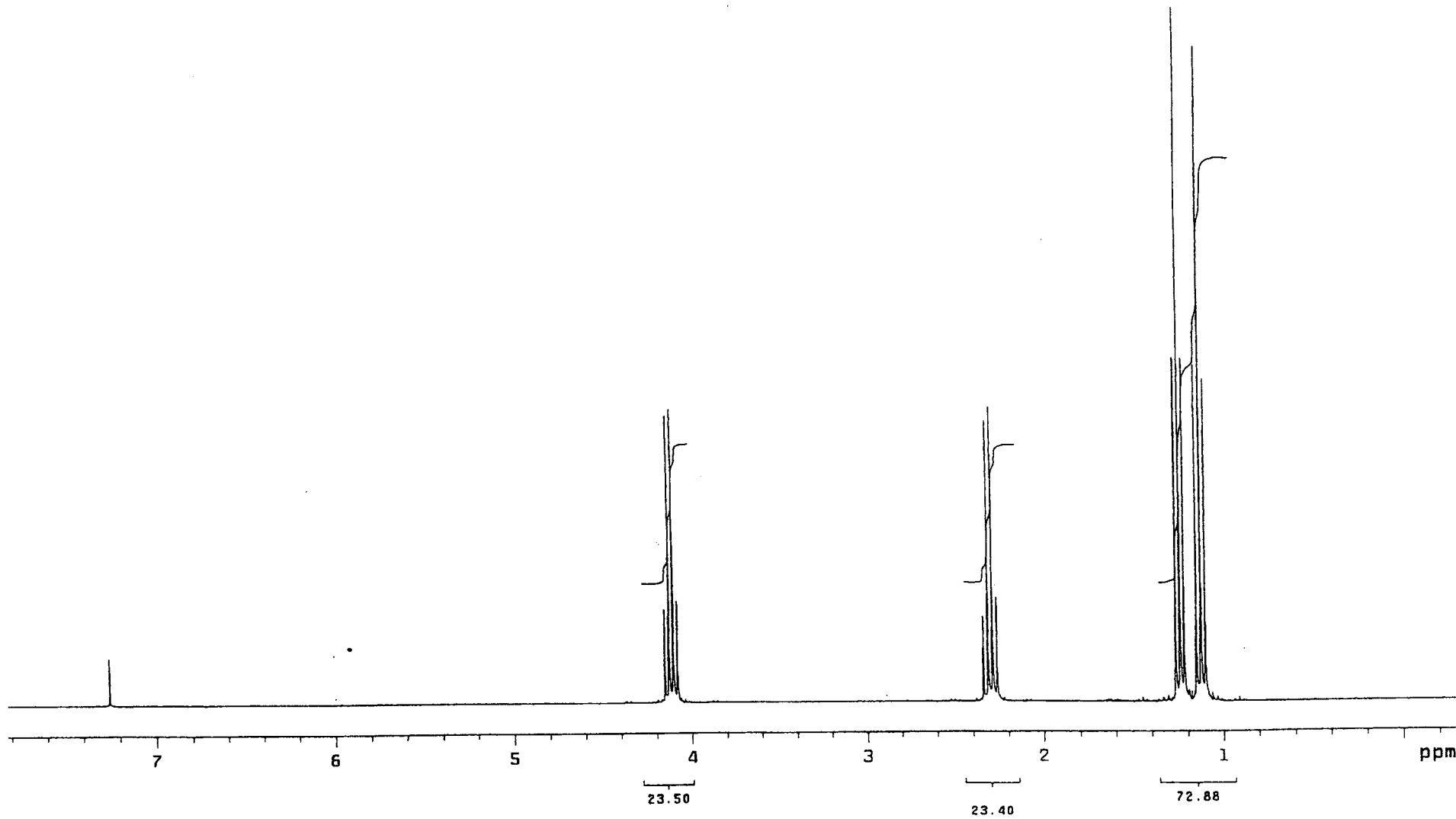
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7



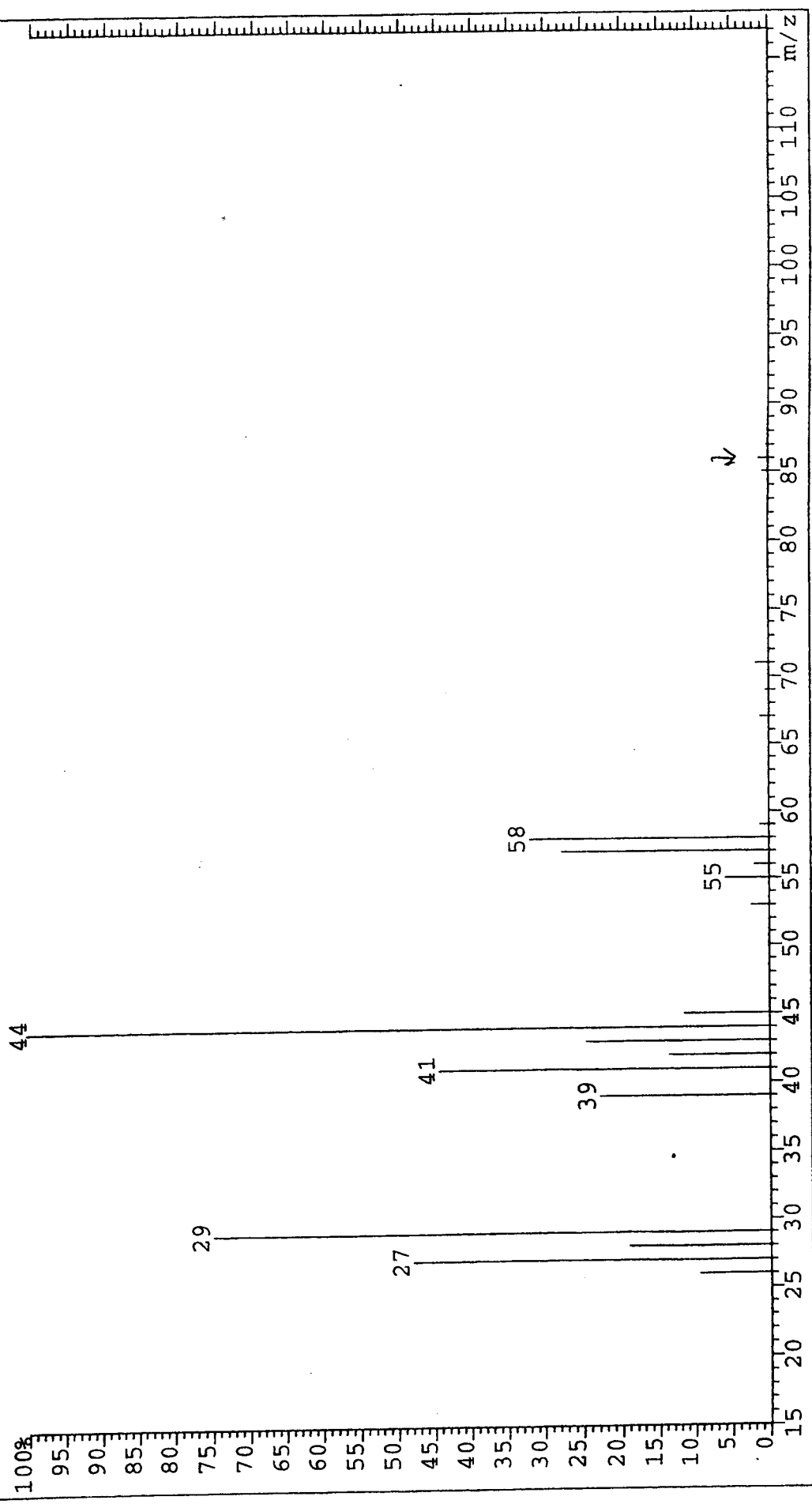
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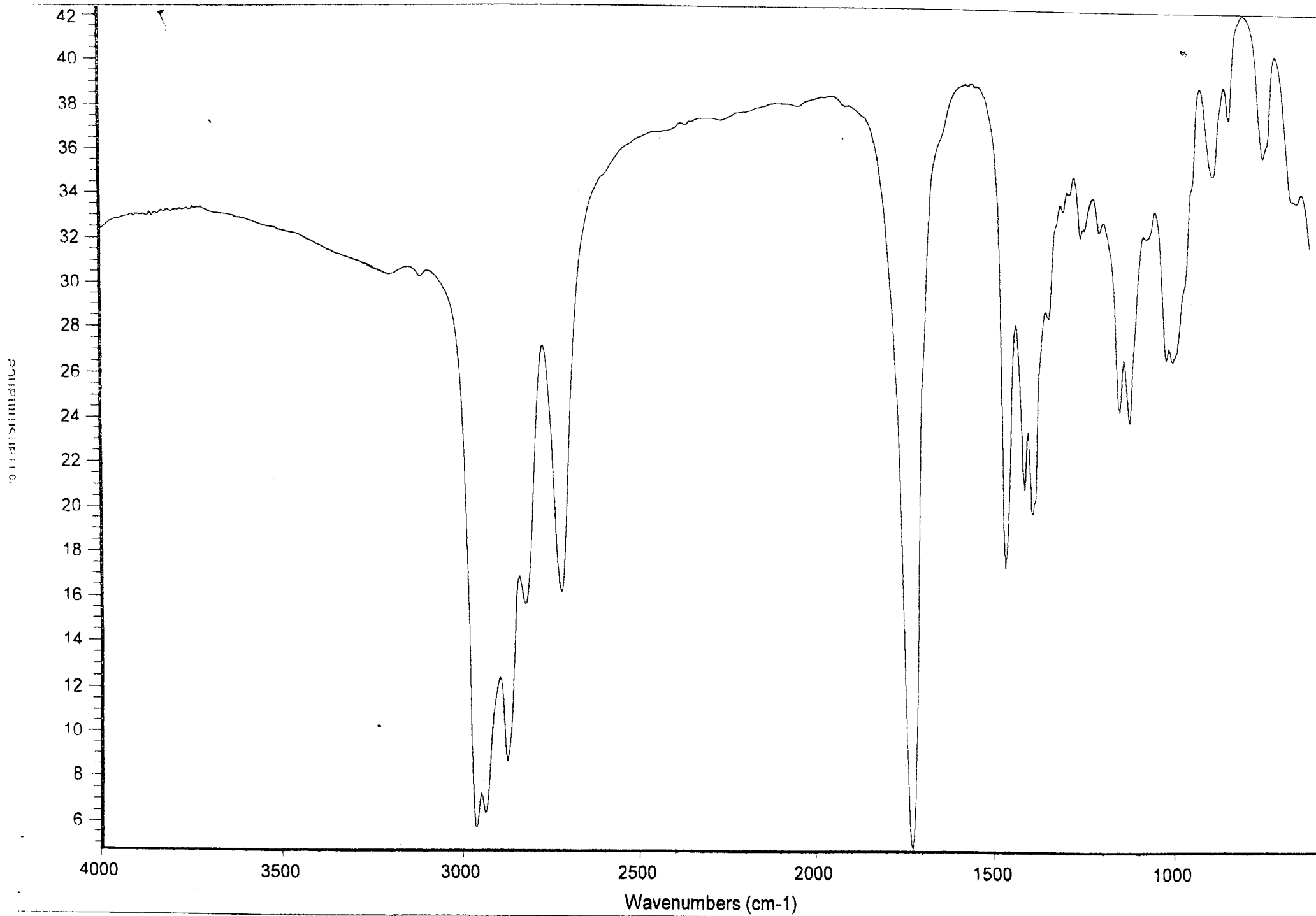


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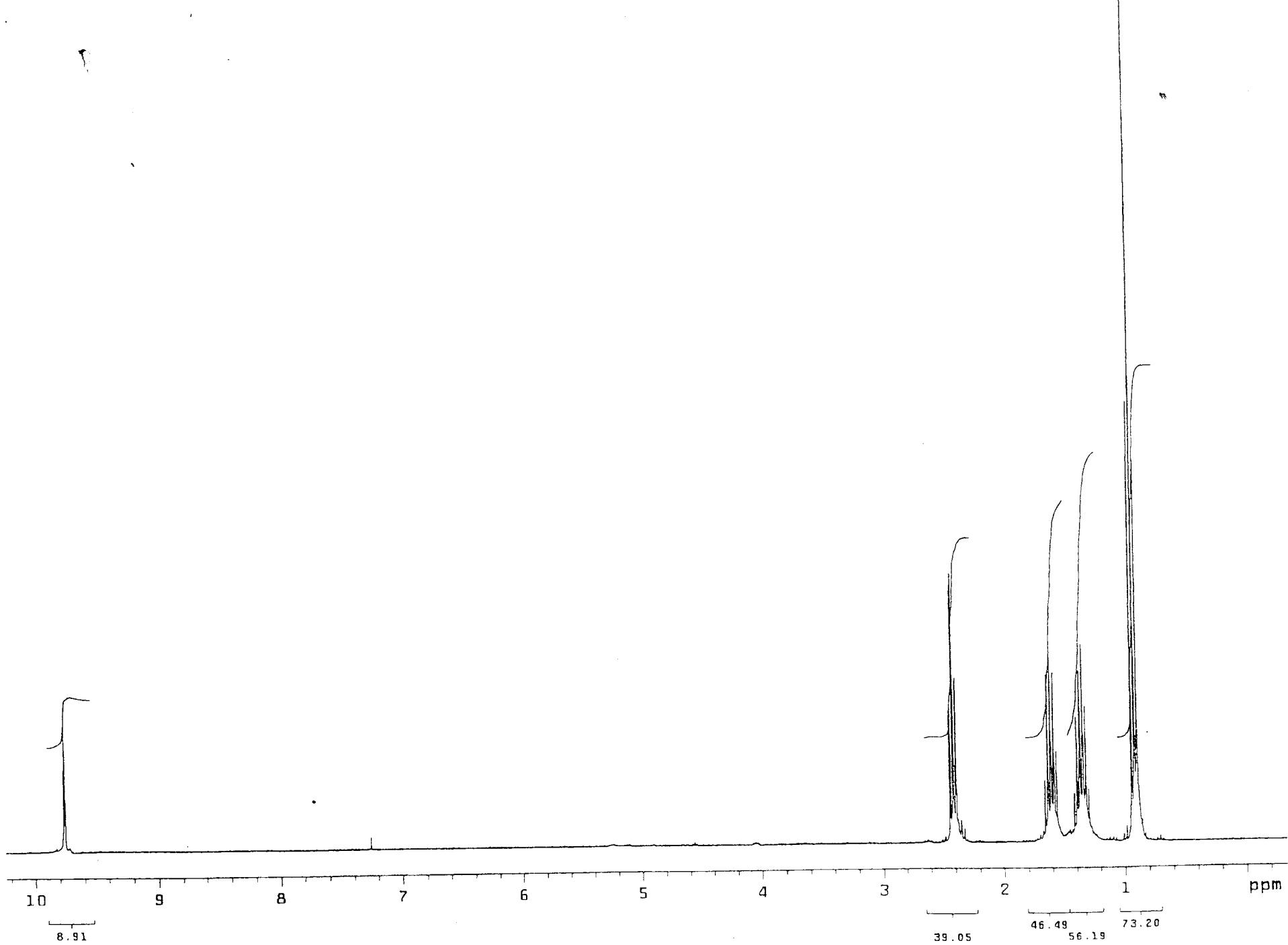
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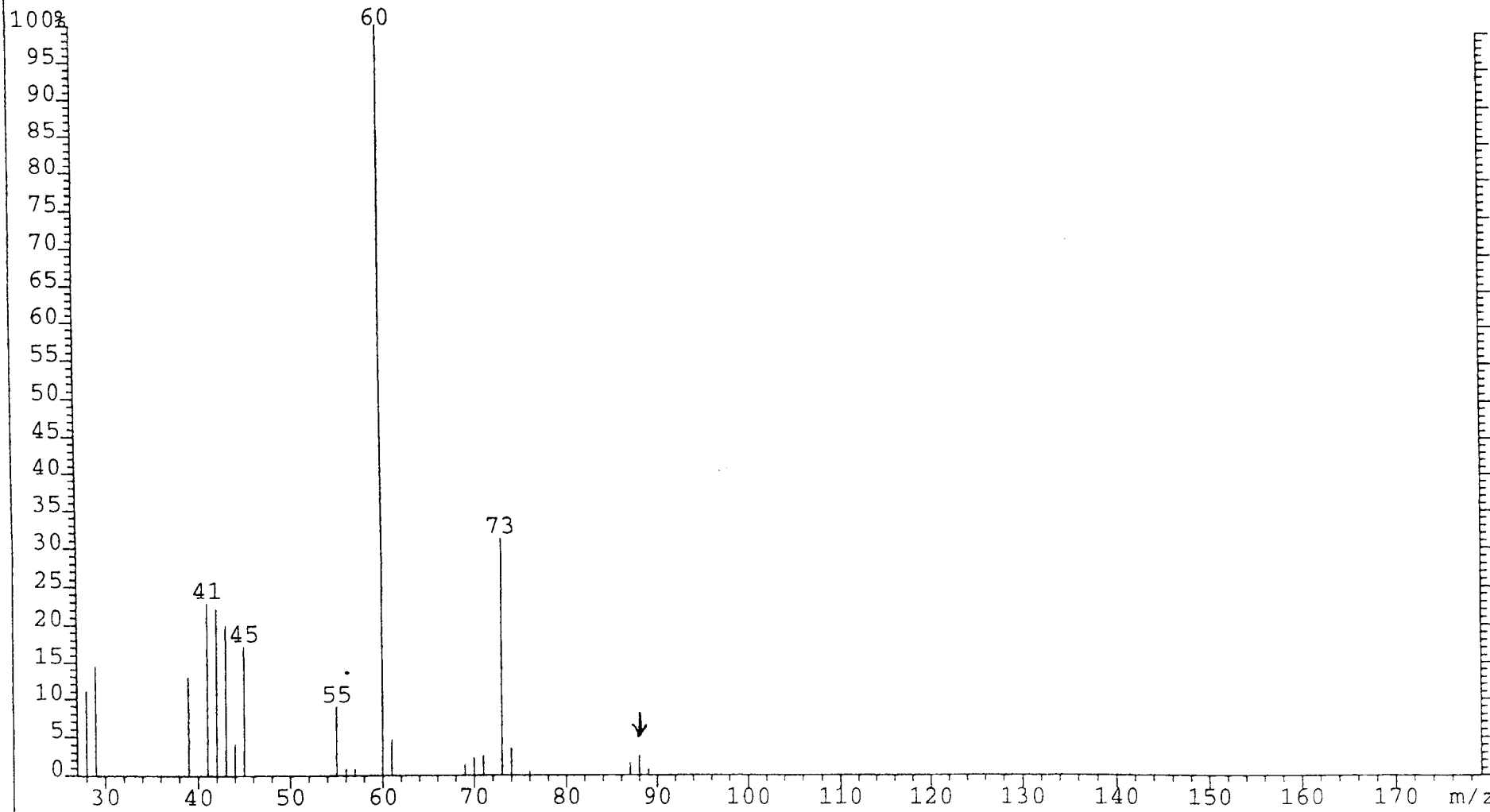


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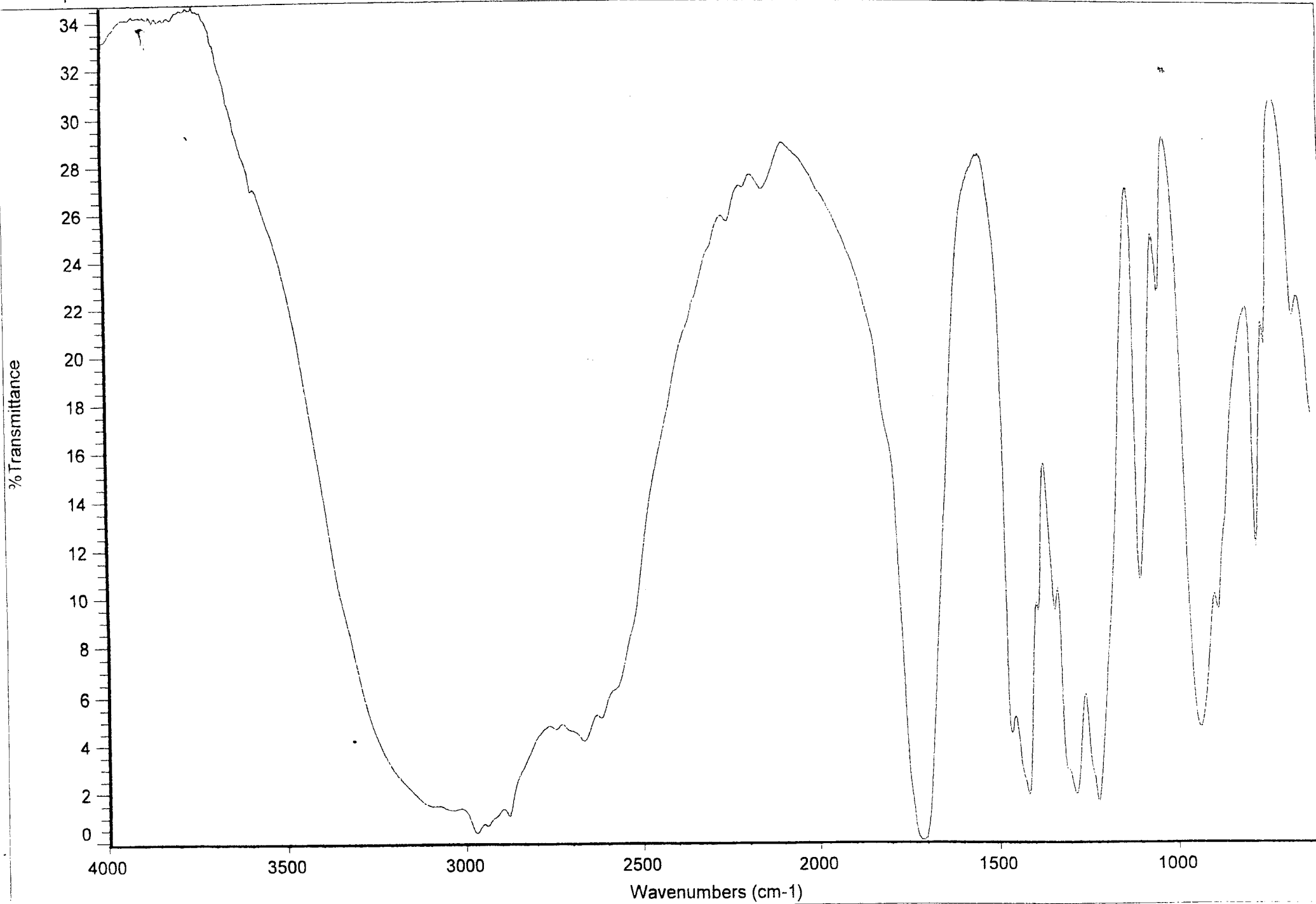
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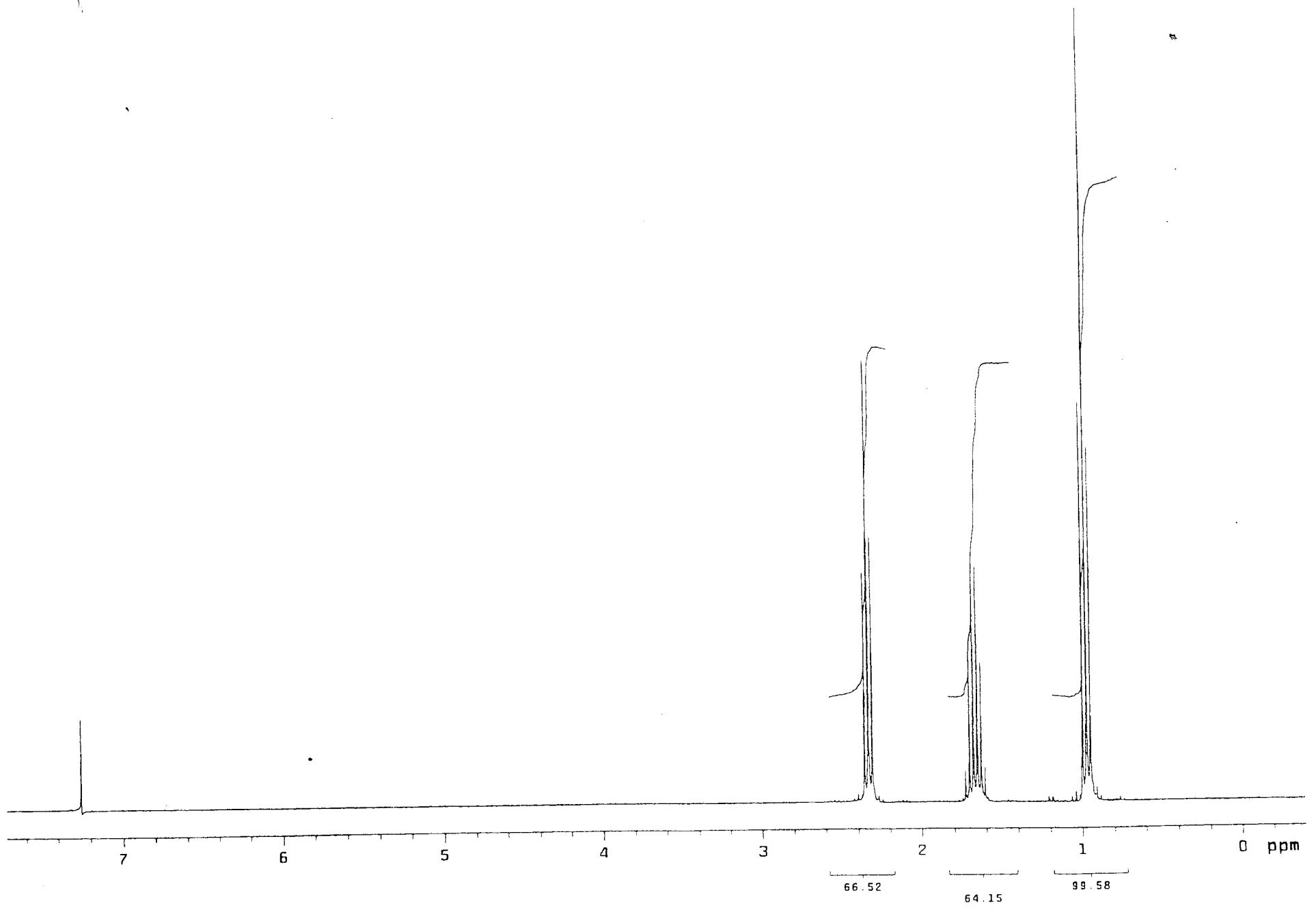


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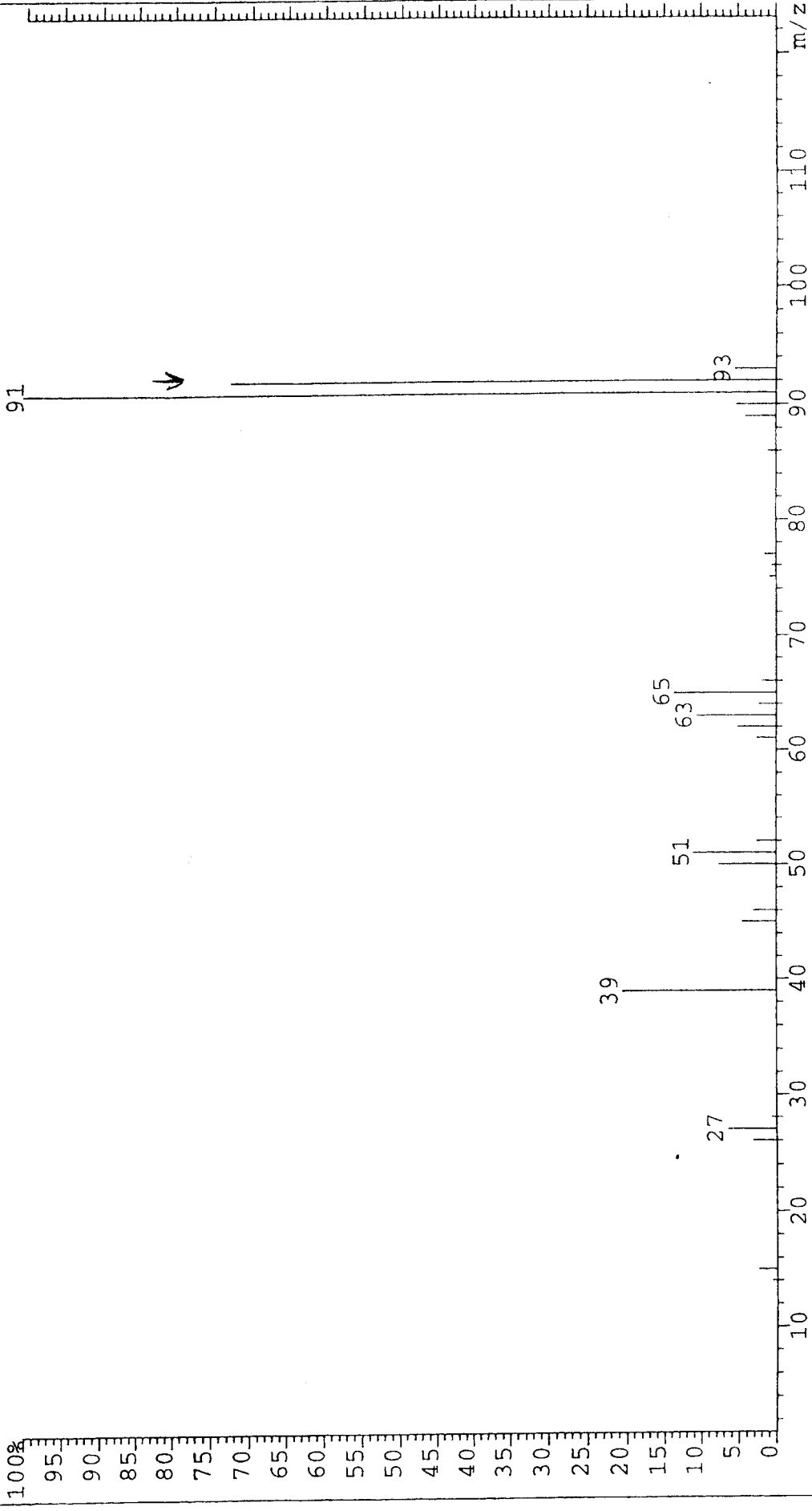


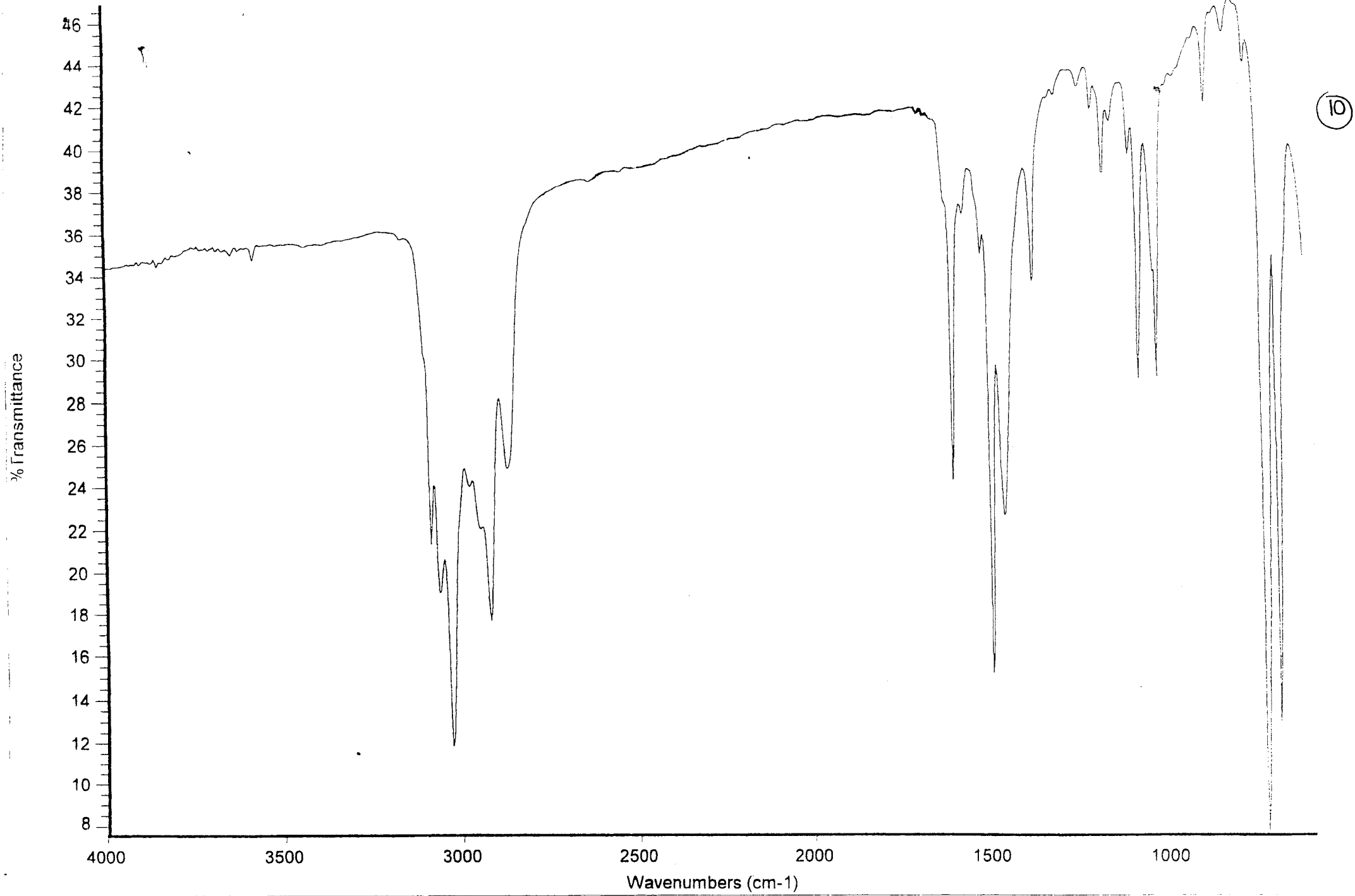
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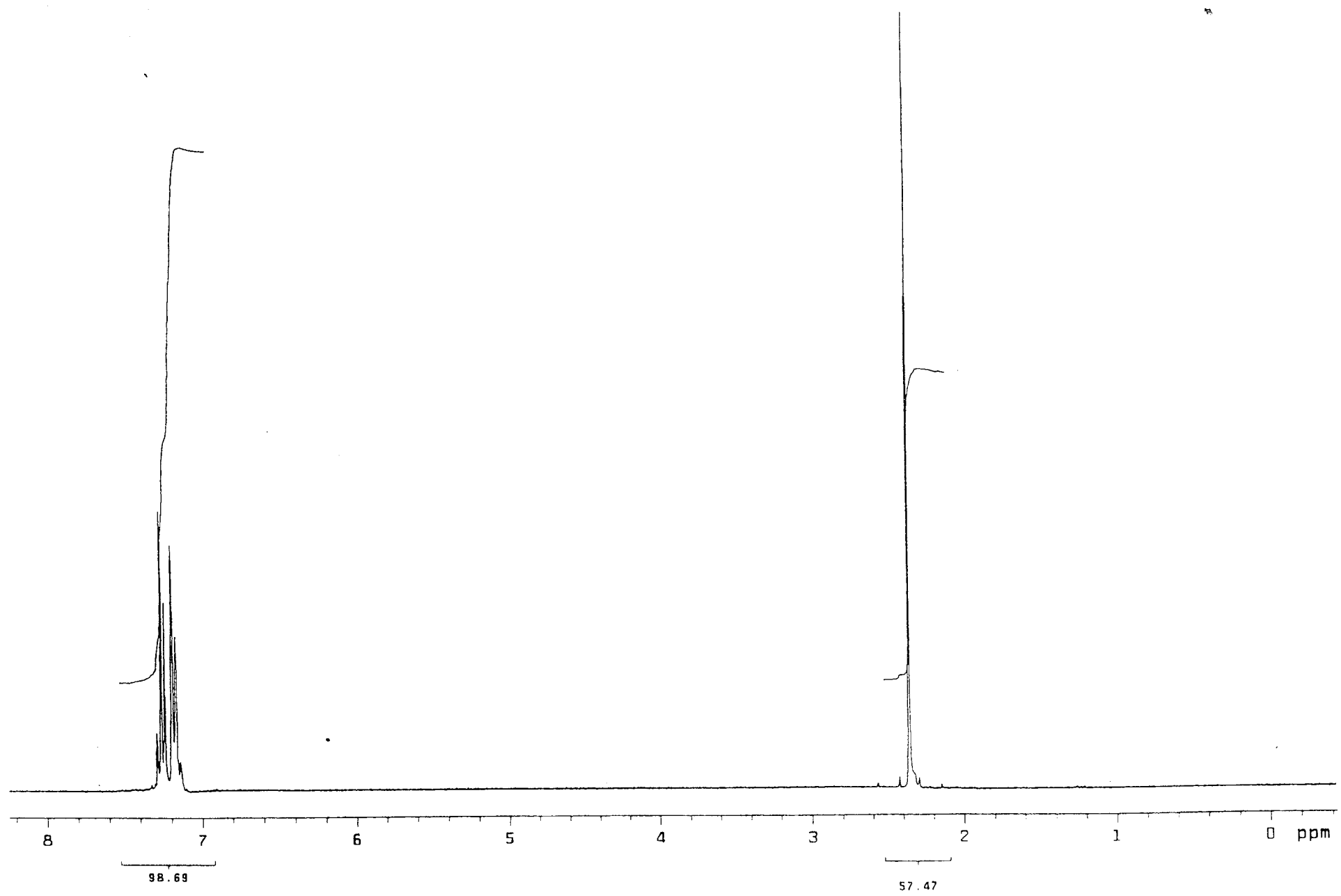
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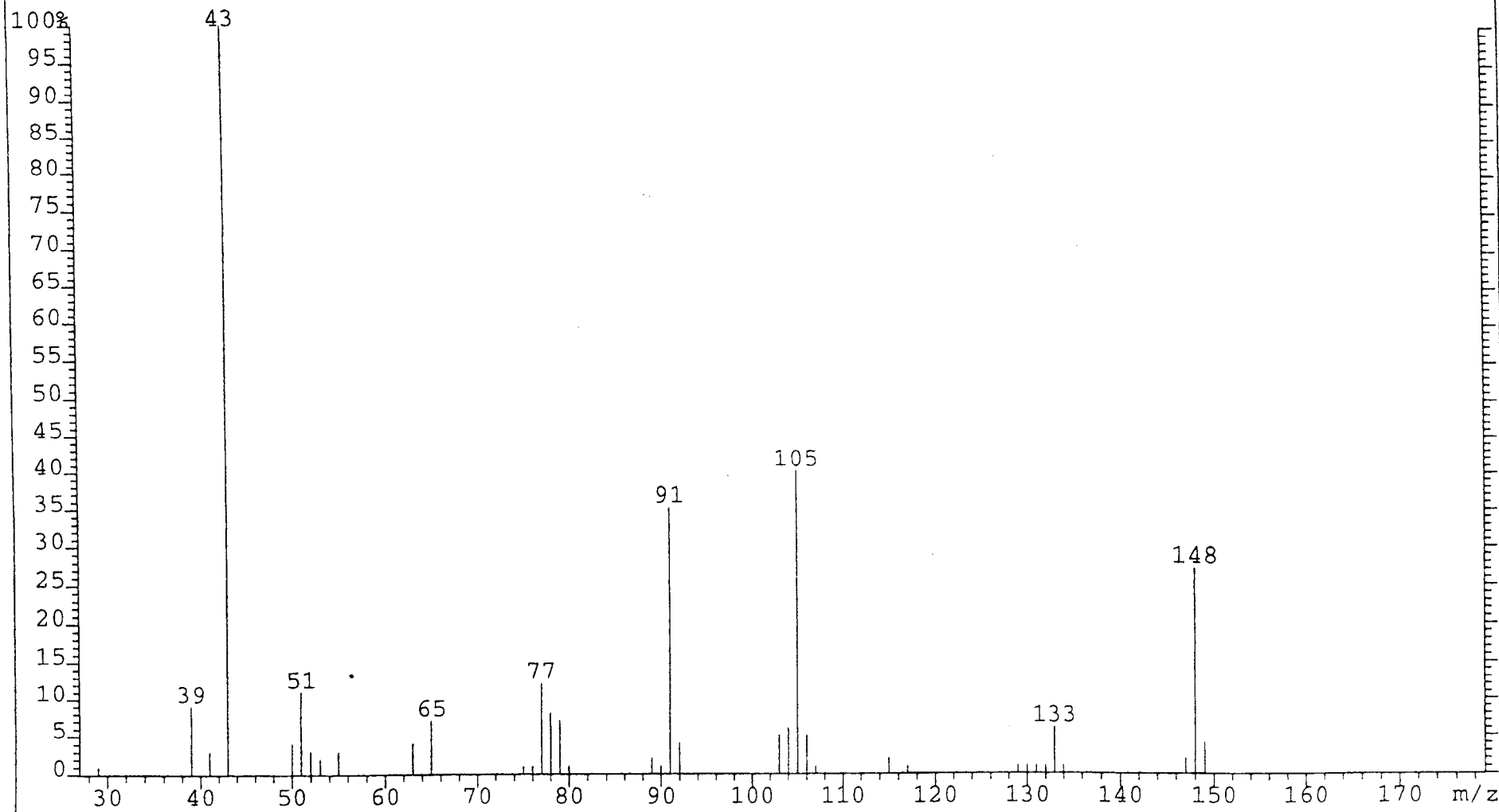
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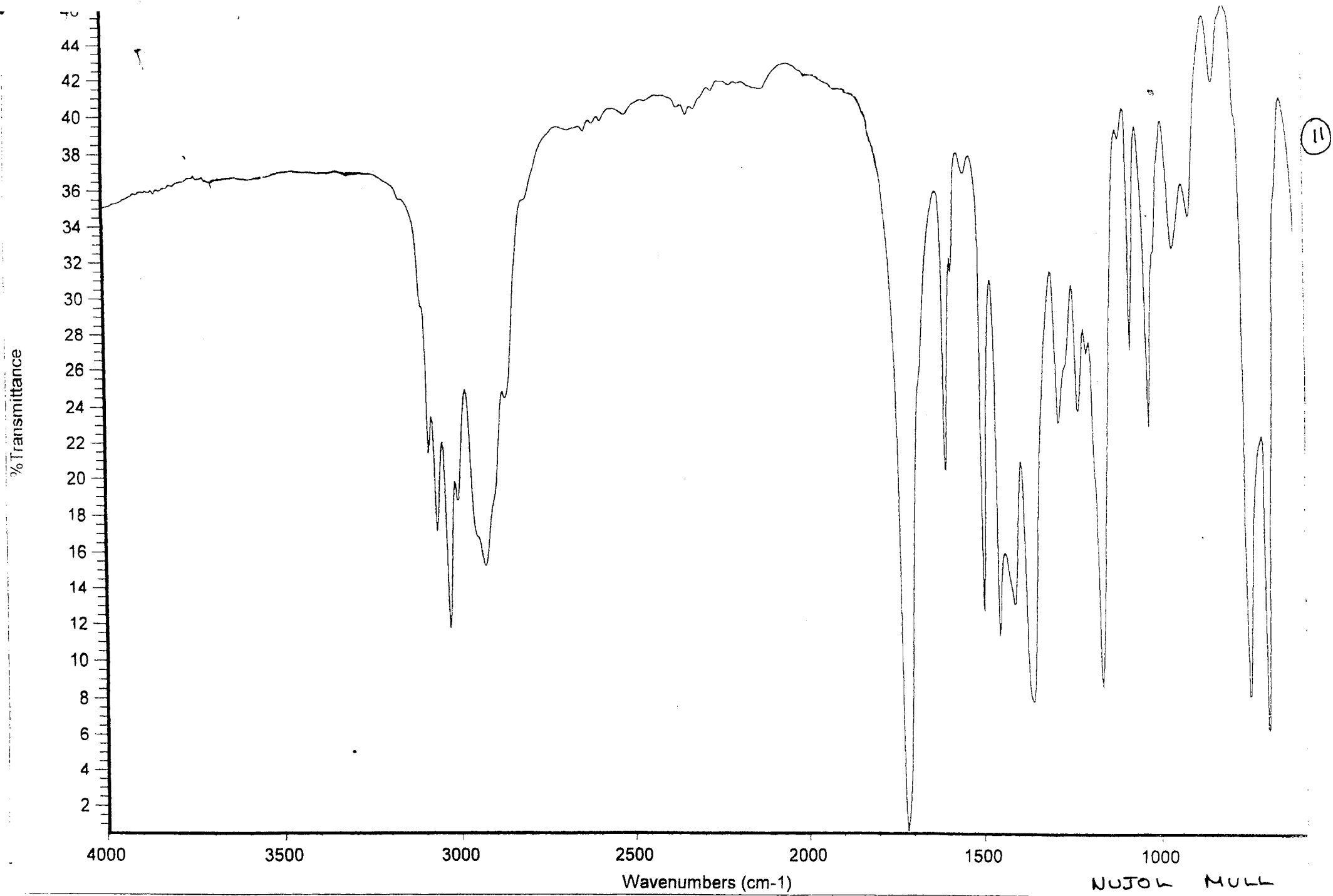
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Name:

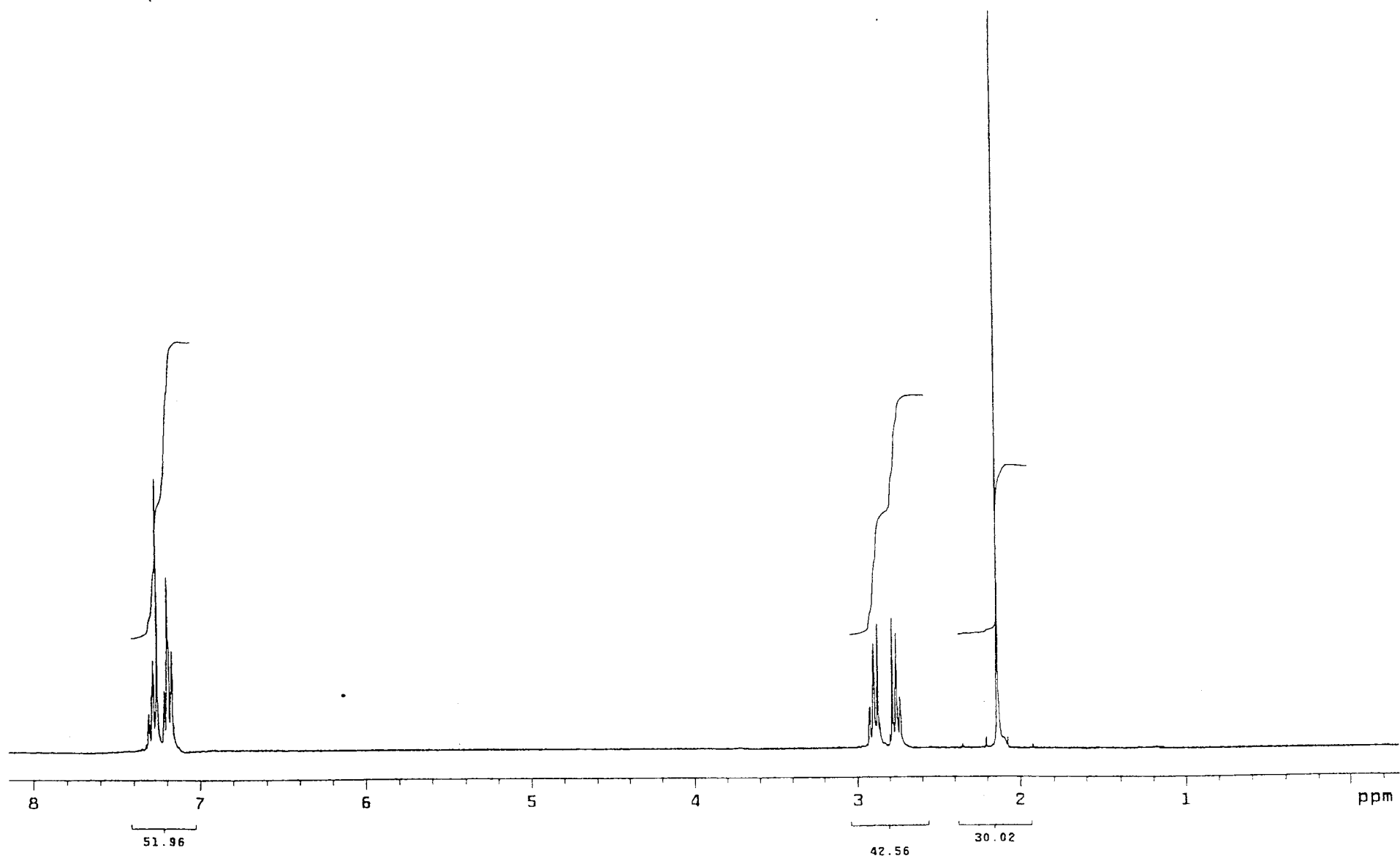


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NUJOL MULL

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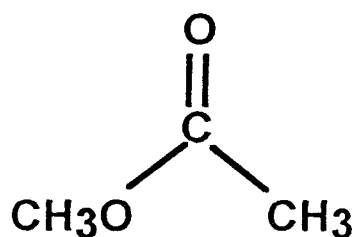
MODERN SPECTROSCOPIC TECHNIQUES

SAMPLE SPECTRA

SOLUTIONS

1 $\text{CH}_3\text{CH}_2\text{OH}$

2



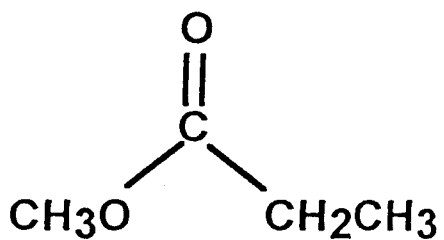
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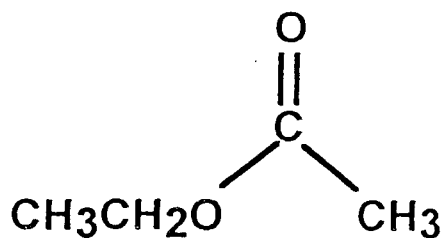
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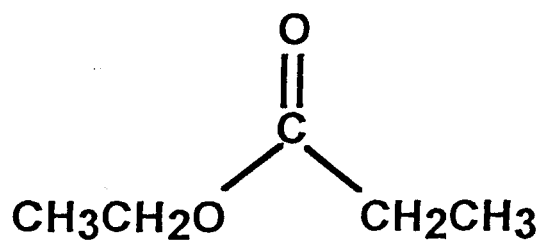
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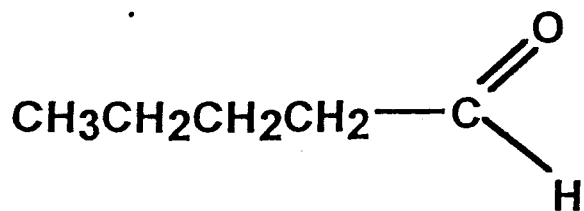
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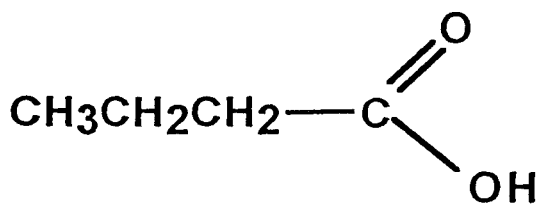
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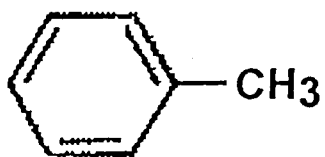
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