

**Baeyer-Villiger Oxidation of Substituted Cyclohexanones via Lipase-Mediated Perhydrolysis Utilizing Urea-Hydrogen Peroxide in Ethyl Acetate**

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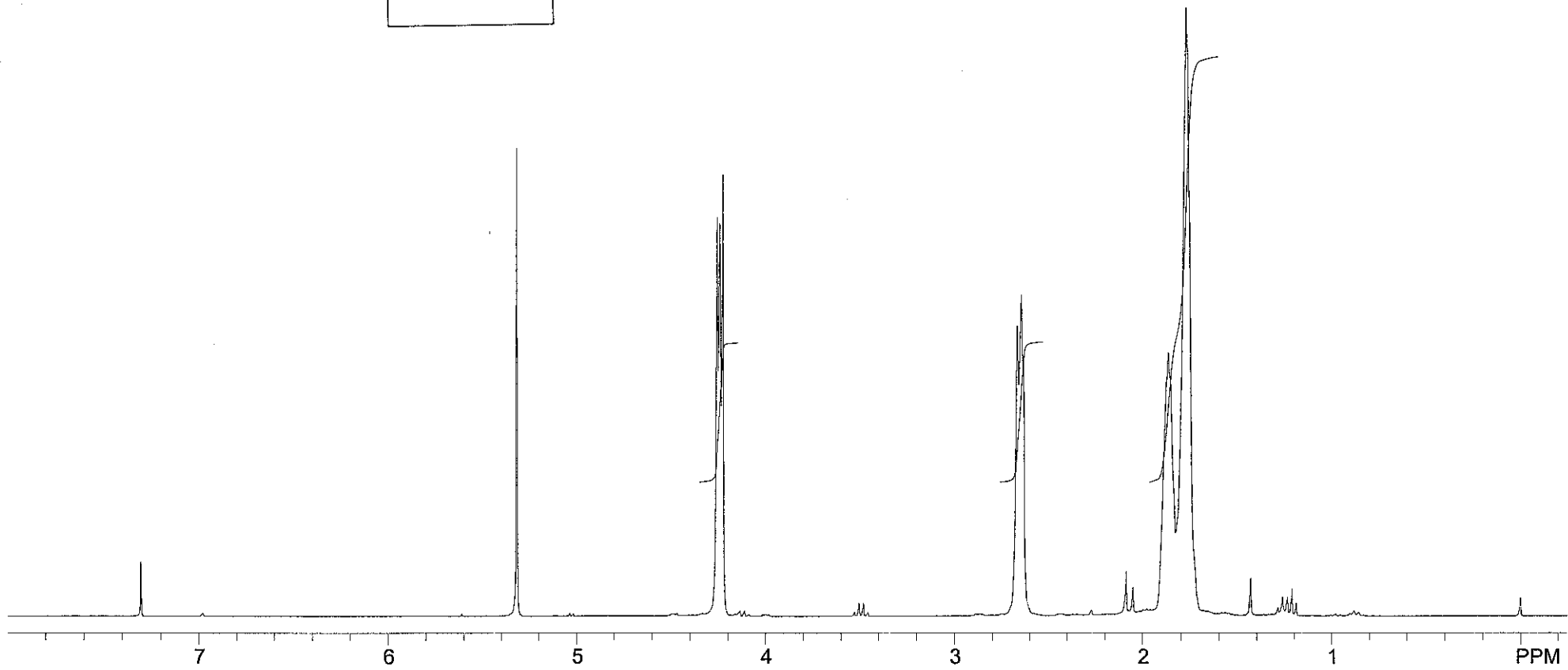
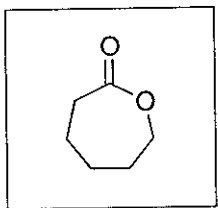
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**Supplementary Material**

<b><math>\epsilon</math>-caprolactone (1)</b>	
<sup>1</sup> H-NMR spectra	S-3
<sup>13</sup> C-NMR spectra	S-4
<b>4-phenyl-<math>\epsilon</math>-caprolactone (2)</b>	
<sup>1</sup> H-NMR spectra	S-5
<sup>13</sup> C-NMR spectra	S-6
<b>6-methyl-<math>\epsilon</math>-caprolactone (3)</b>	
<sup>1</sup> H-NMR spectra	S-7
<sup>13</sup> C-NMR spectra	S-8
<b>6-sec-butyl-<math>\epsilon</math>-caprolactone (4)</b>	
<sup>1</sup> H-NMR spectra	S-9
<sup>13</sup> C-NMR spectra	S-10
<b>6-tert-butyl-<math>\epsilon</math>-caprolactone (5)</b>	
<sup>1</sup> H-NMR spectra	S-11
<sup>13</sup> C-NMR spectra	S-12
<b>6-allyl-<math>\epsilon</math>-caprolactone (6)</b>	
<sup>1</sup> H-NMR spectra	S-13
<sup>13</sup> C-NMR spectra	S-14

<b>6-benzyl-<math>\epsilon</math>-caprolactone (7)</b>	
<sup>1</sup> H-NMR spectra	S-15
<sup>13</sup> C-NMR spectra	S-16
<b>6-phenyl-<math>\epsilon</math>-caprolactone (8)</b>	
<sup>1</sup> H-NMR spectra	S-17
<sup>13</sup> C-NMR spectra	S-18
<b>6,6-dimethyl-<math>\epsilon</math>-caprolactone (9)</b>	
<sup>1</sup> H-NMR spectra	S-19
<sup>13</sup> C-NMR spectra	S-20
<b>4,5-Dihydro-3H-benzo[<i>b</i>]oxepin-2-one (10)</b>	
<sup>1</sup> H-NMR spectra	S-21
<sup>13</sup> C-NMR spectra	S-22



S-3

176.664

77.628

77.200

76.781

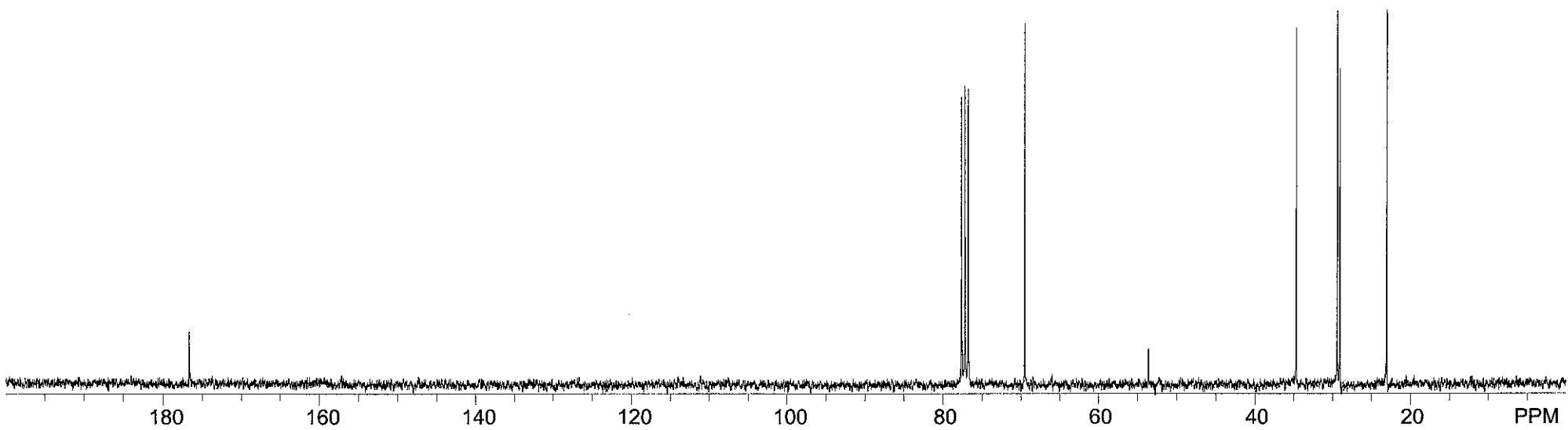
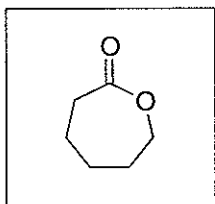
69.500

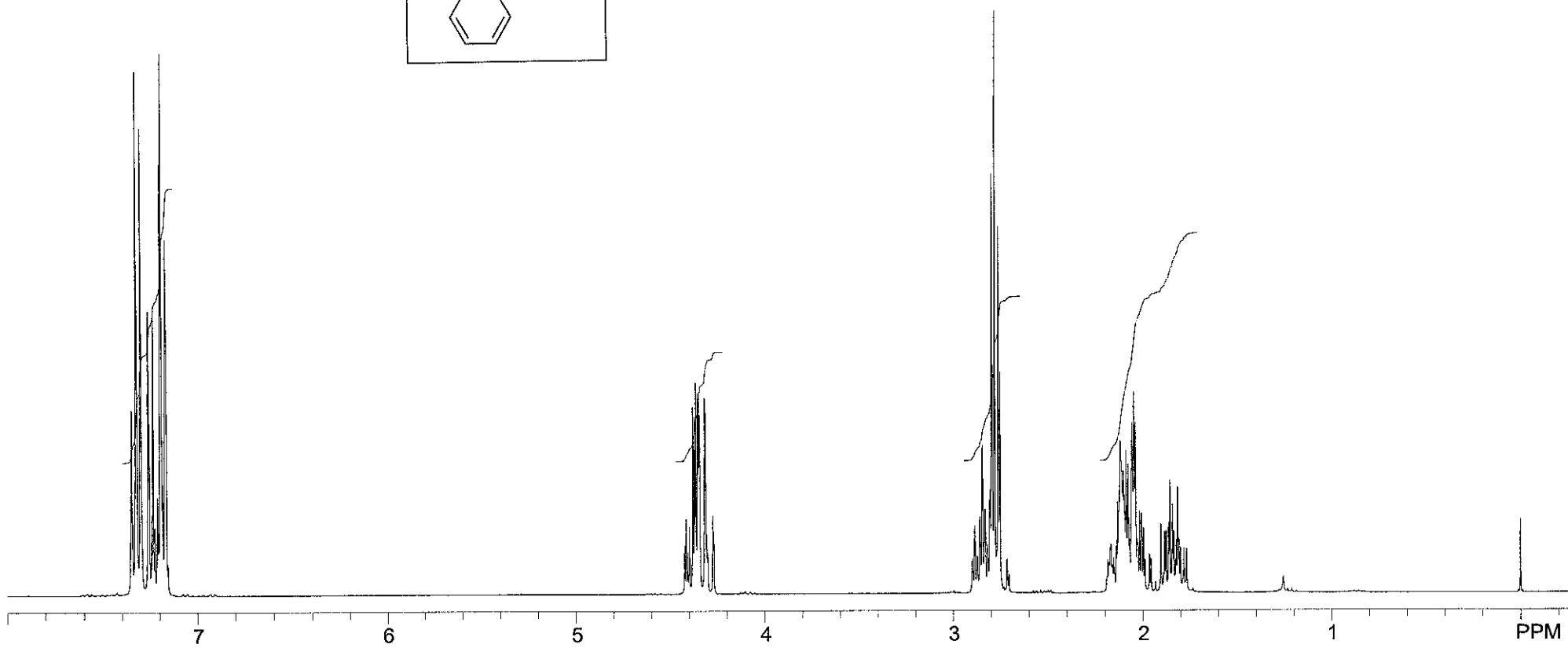
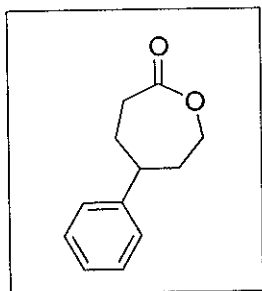
34.644

29.351

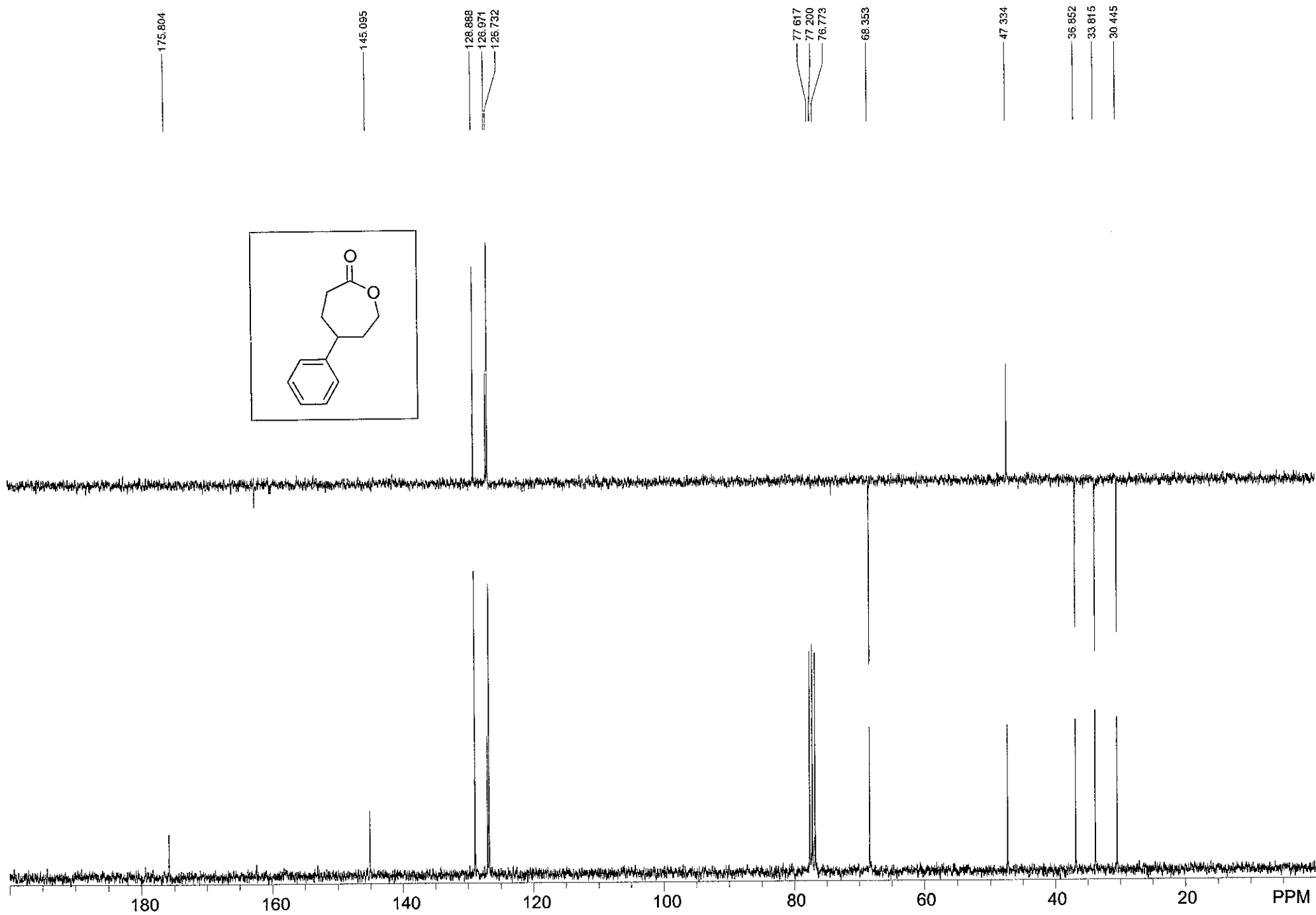
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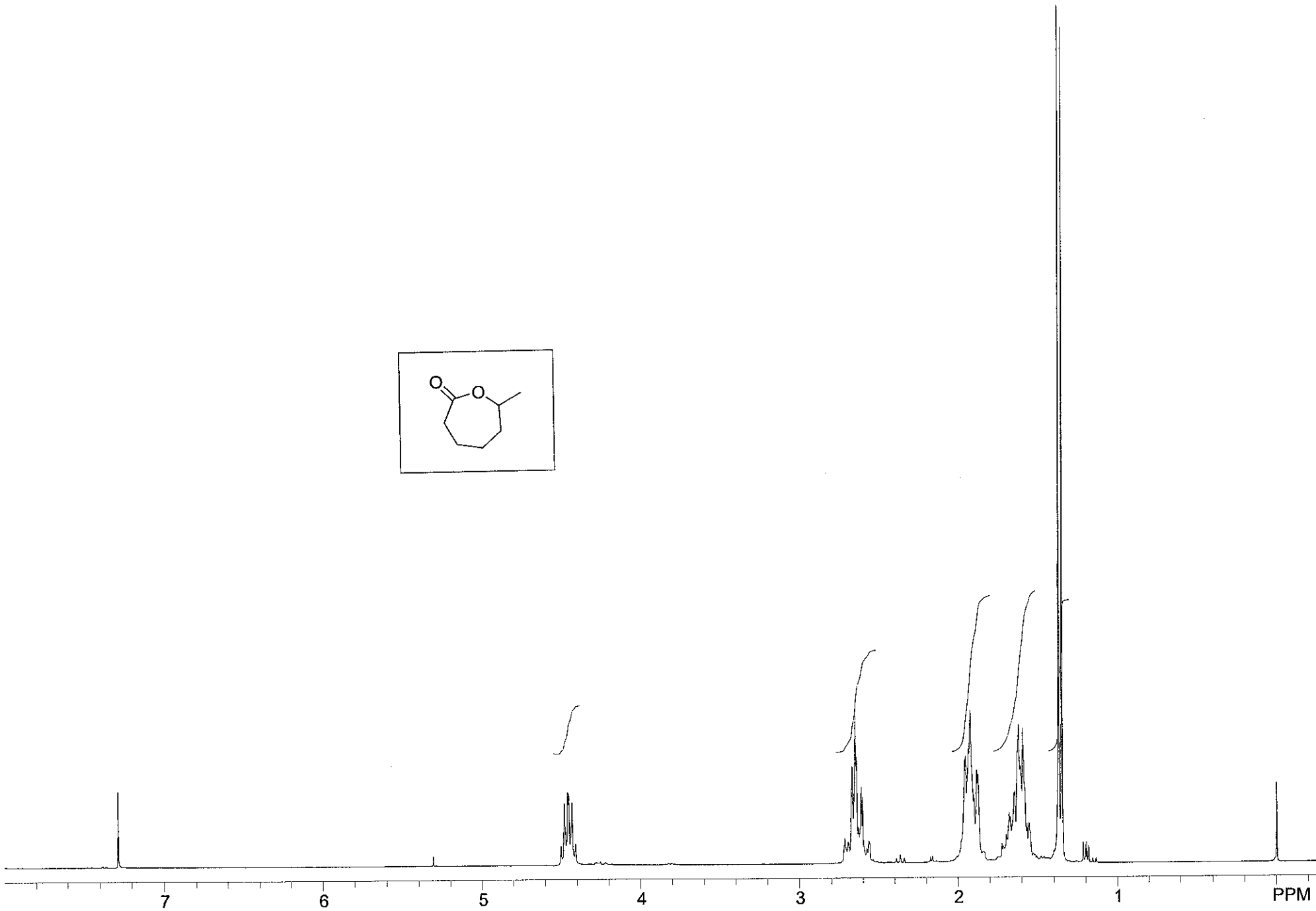
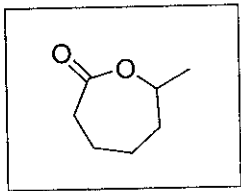
23.007





S-5





S-7

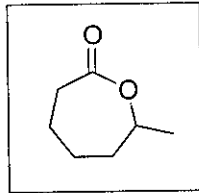
175.591

77.630  
77.200  
76.776

36.216  
34.970

28.211

22.890  
22.555



180

160

140

120

100

80

60

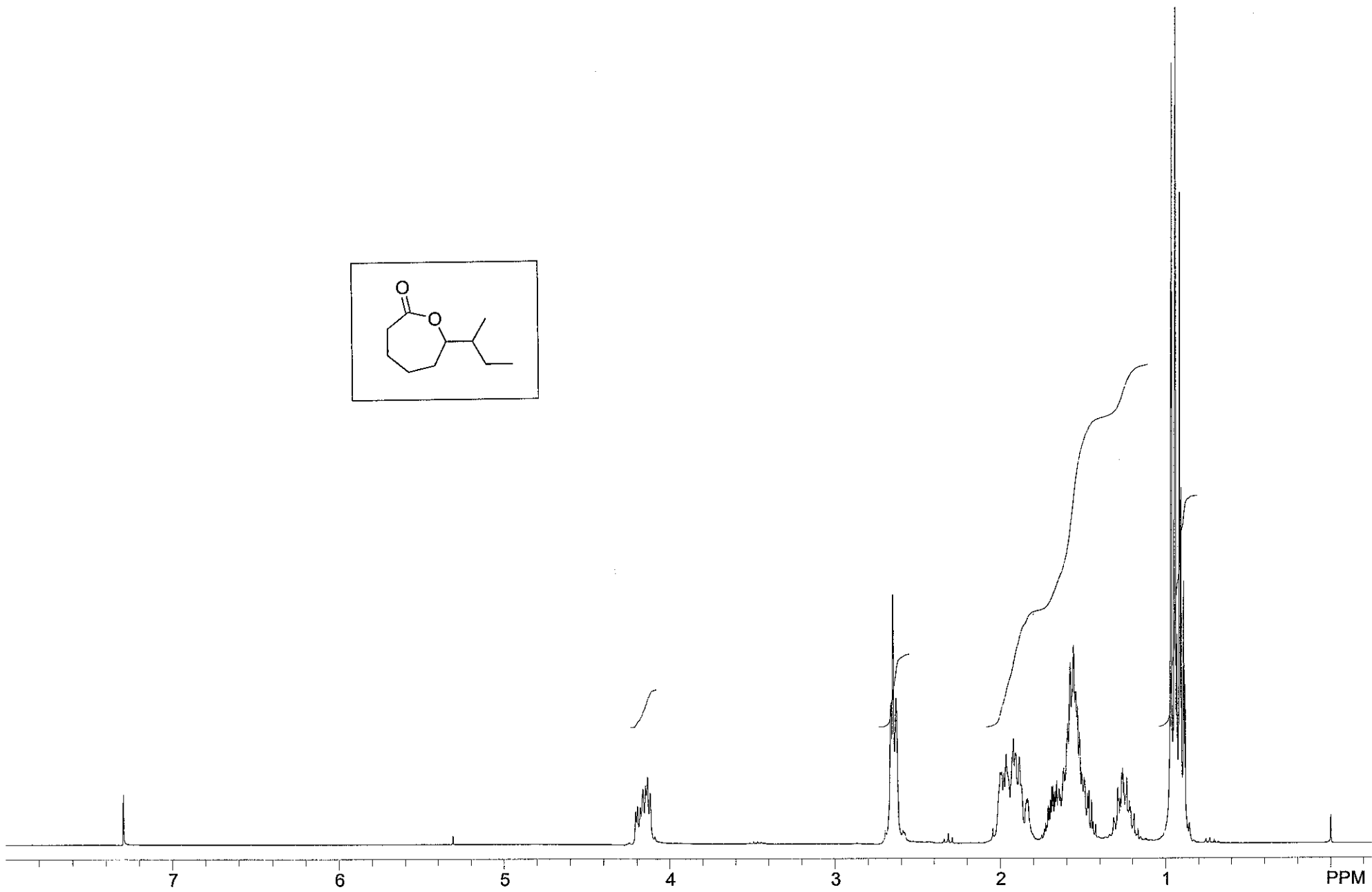
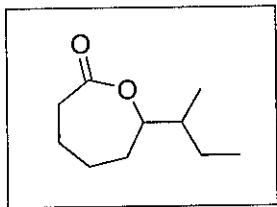
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PPM

S-8





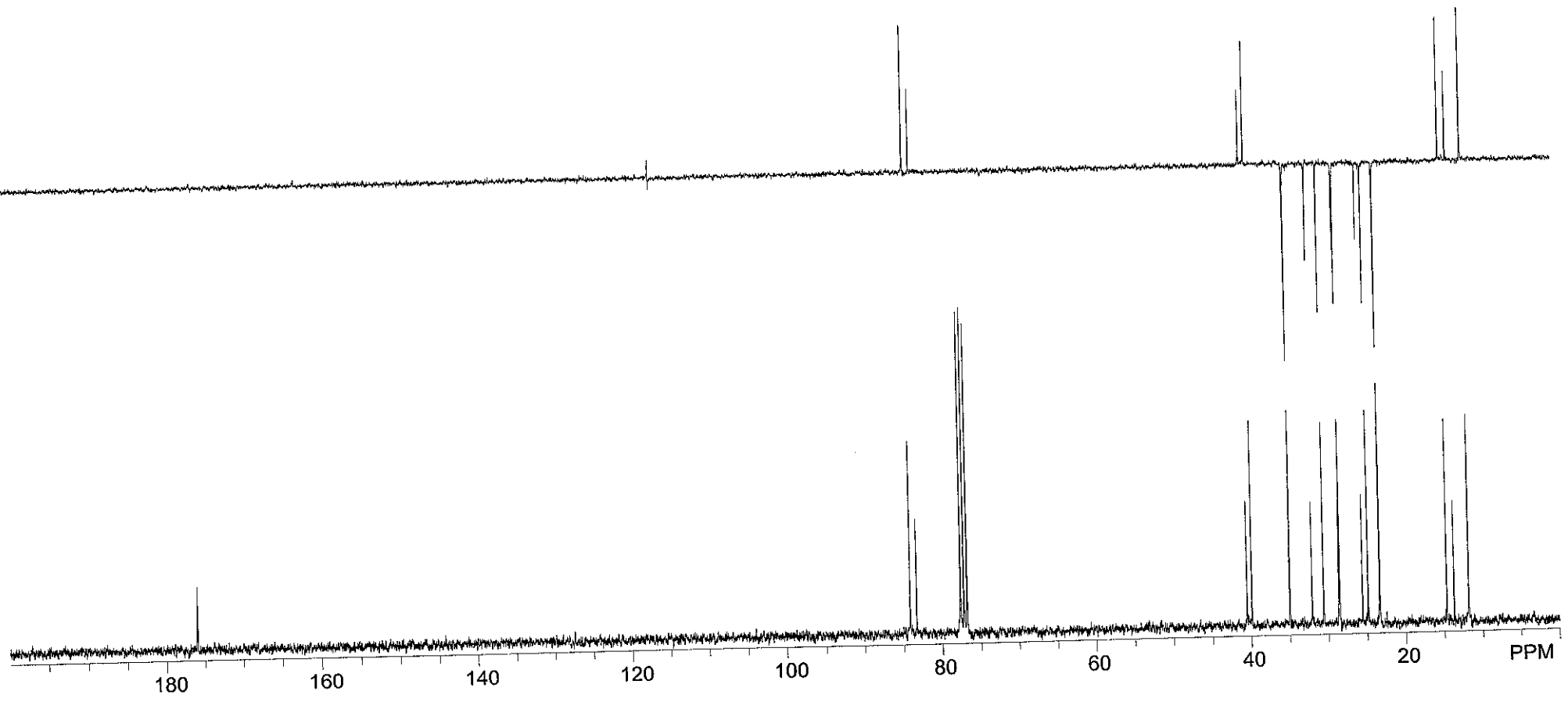
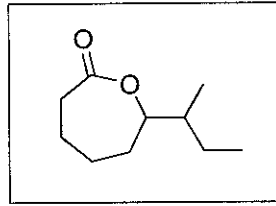
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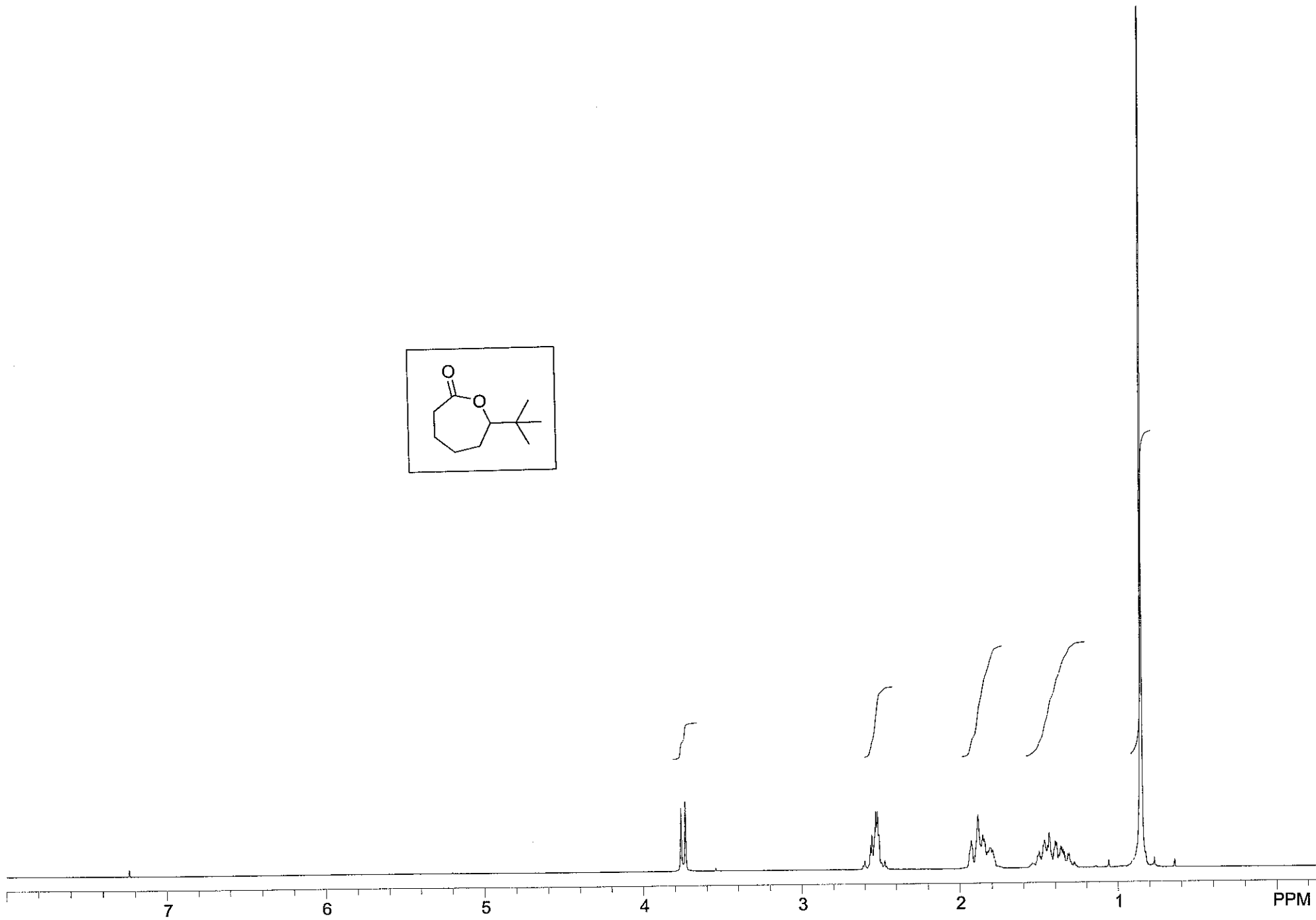
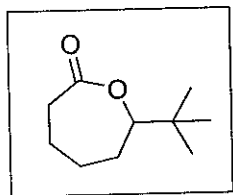
176.028  
175.962

84.152  
83.320  
77.626  
77.200  
76.770

40.511  
39.877  
34.969  
34.931  
32.080  
30.593  
28.610  
28.500  
25.565  
24.836  
23.311

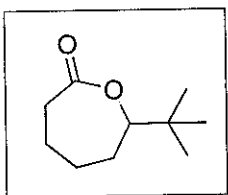
14.658  
13.711  
11.820  
11.792





S-11

175.889



87.983

77.627  
77.200  
76.777

34.752  
34.606

29.277  
28.367

25.697

23.276

180

160

140

120

100

80

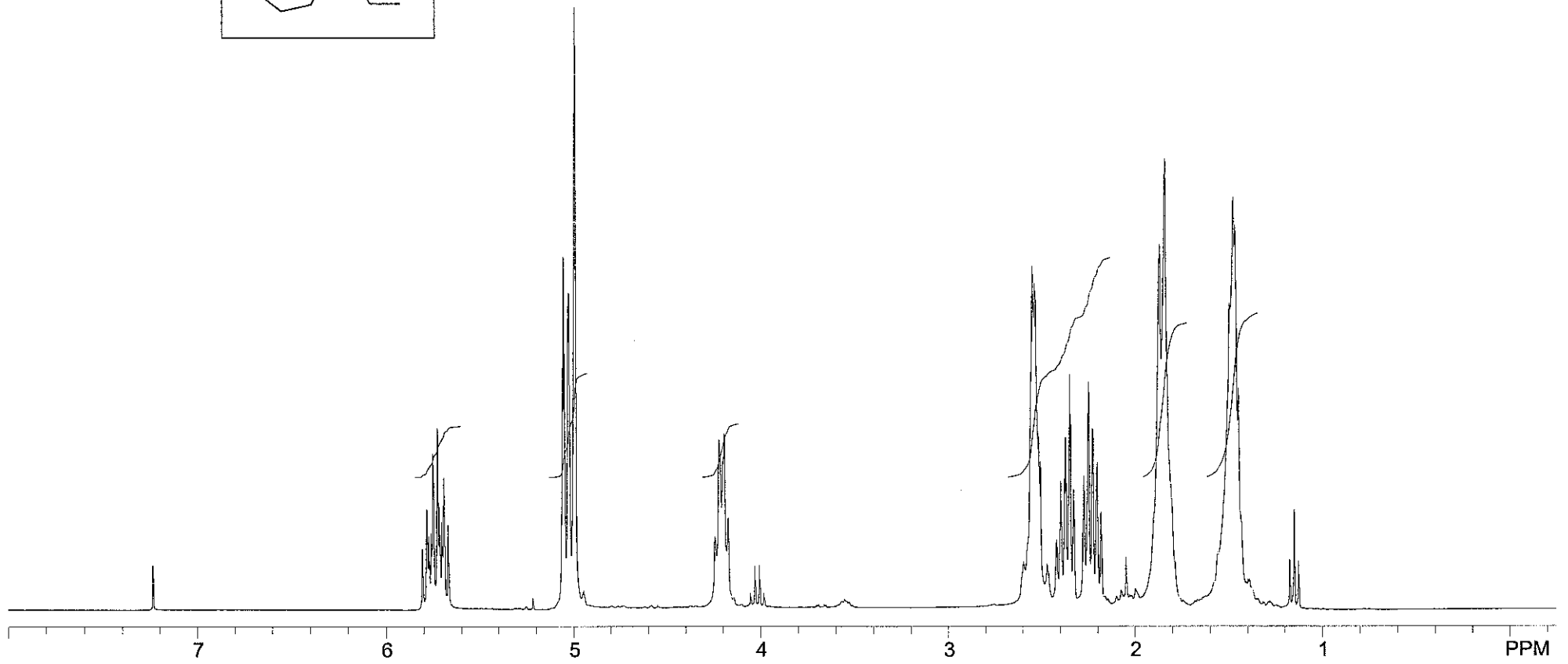
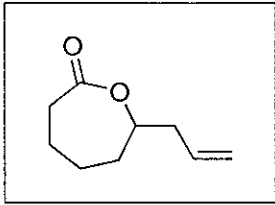
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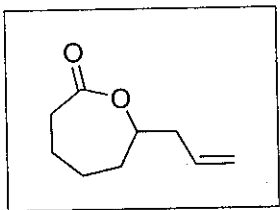
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PPM

S-12



S-13



175.455

133.448

118.149

79.803

77.815

77.200

76.771

40.568

34.855

33.812

28.150

22.949

180

160

140

120

100

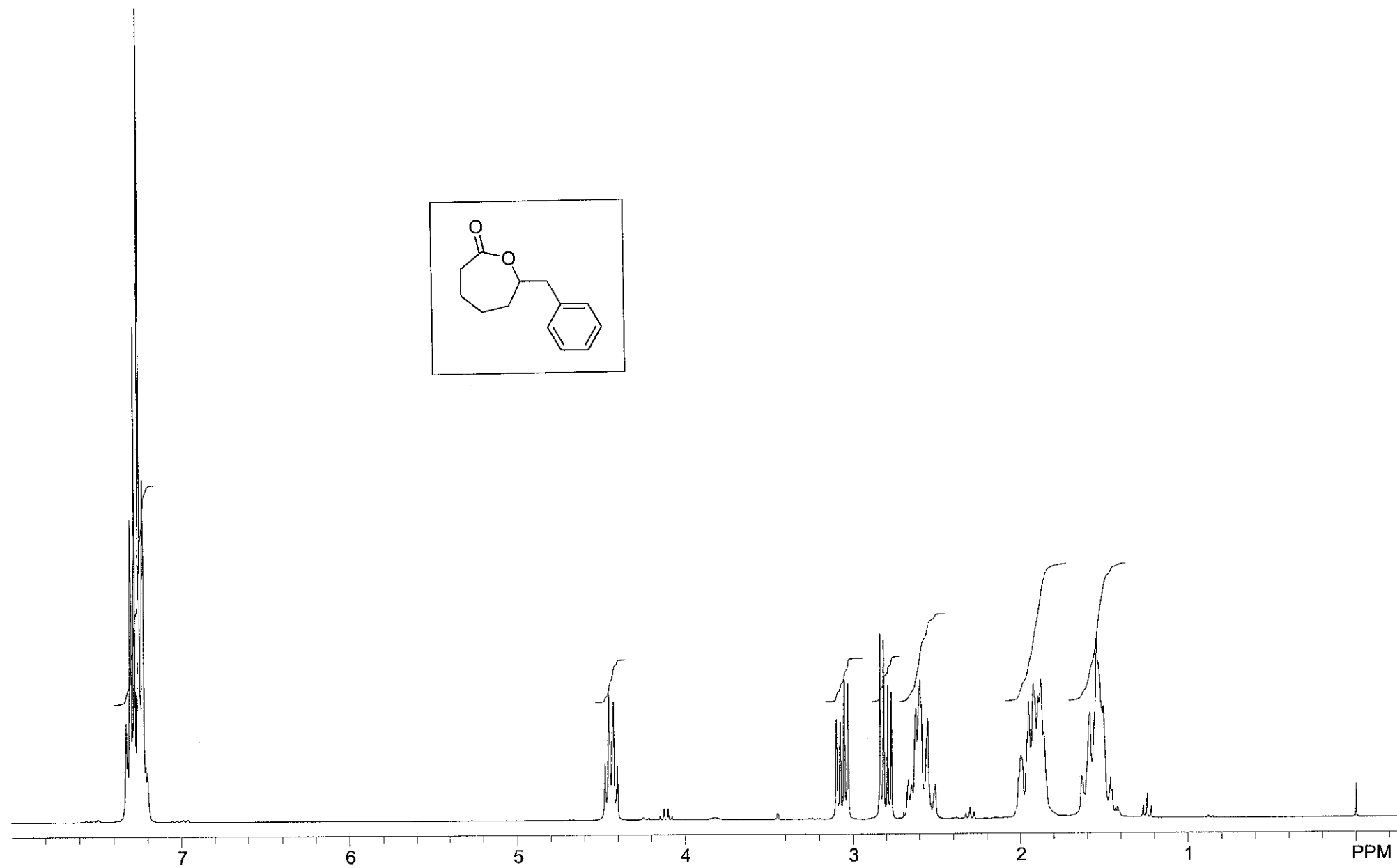
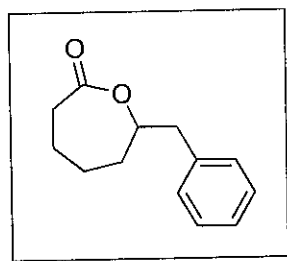
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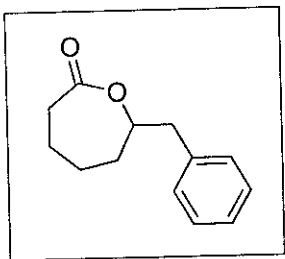
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PPM



S-15



175.387

137.311

129.634

128.511

126.735

81.169

77.627

77.200

76.772

42.563

34.931

33.654

28.244

22.930

200

150

100

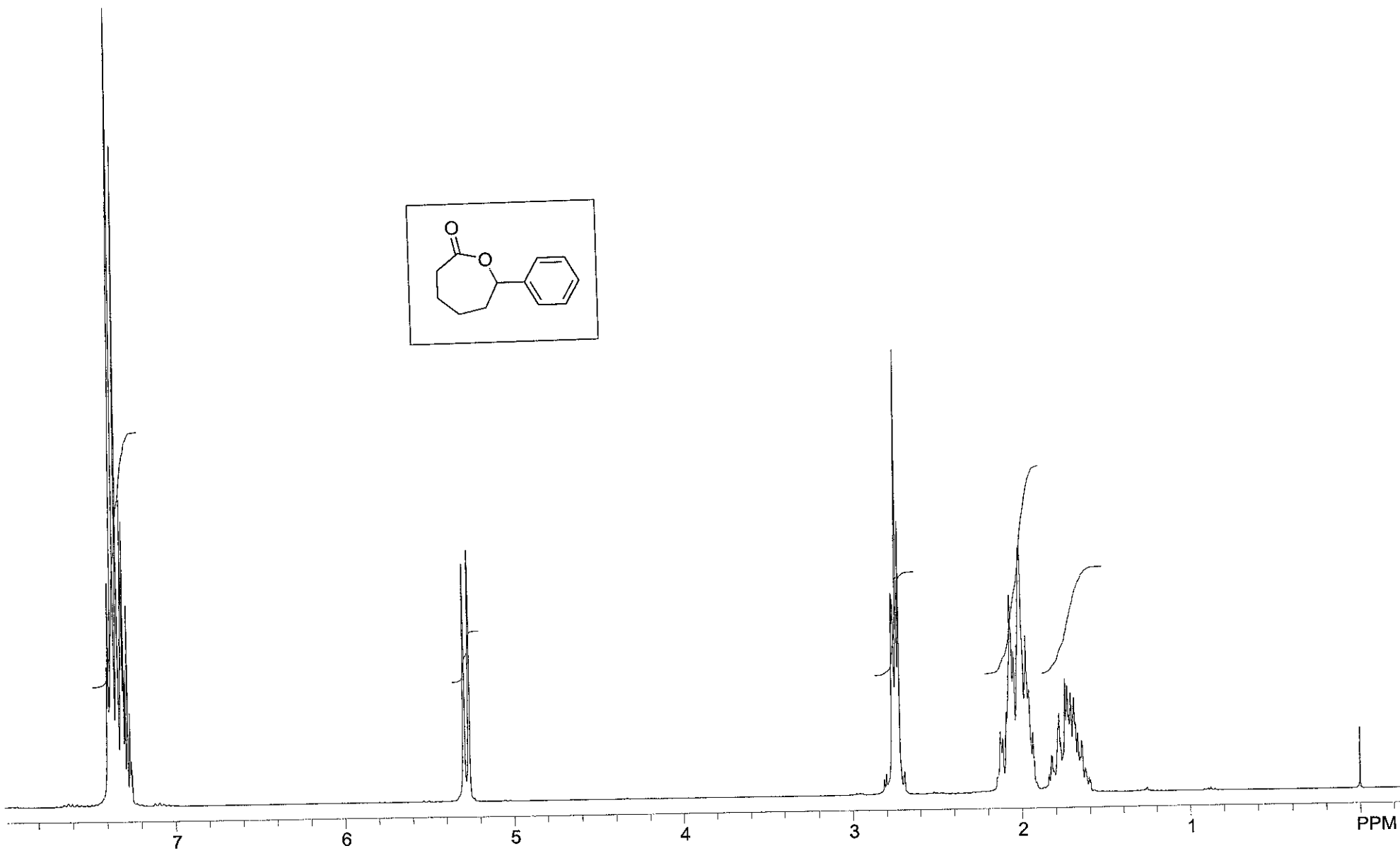
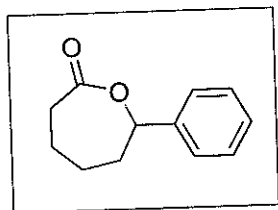
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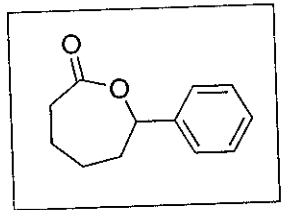
PPM

S-16





S-17



174.959

146.897

128.591

128.107

125.910

82.083

77.634

77.200

76.782

37.482

34.976

28.590

22.869

180

160

140

120

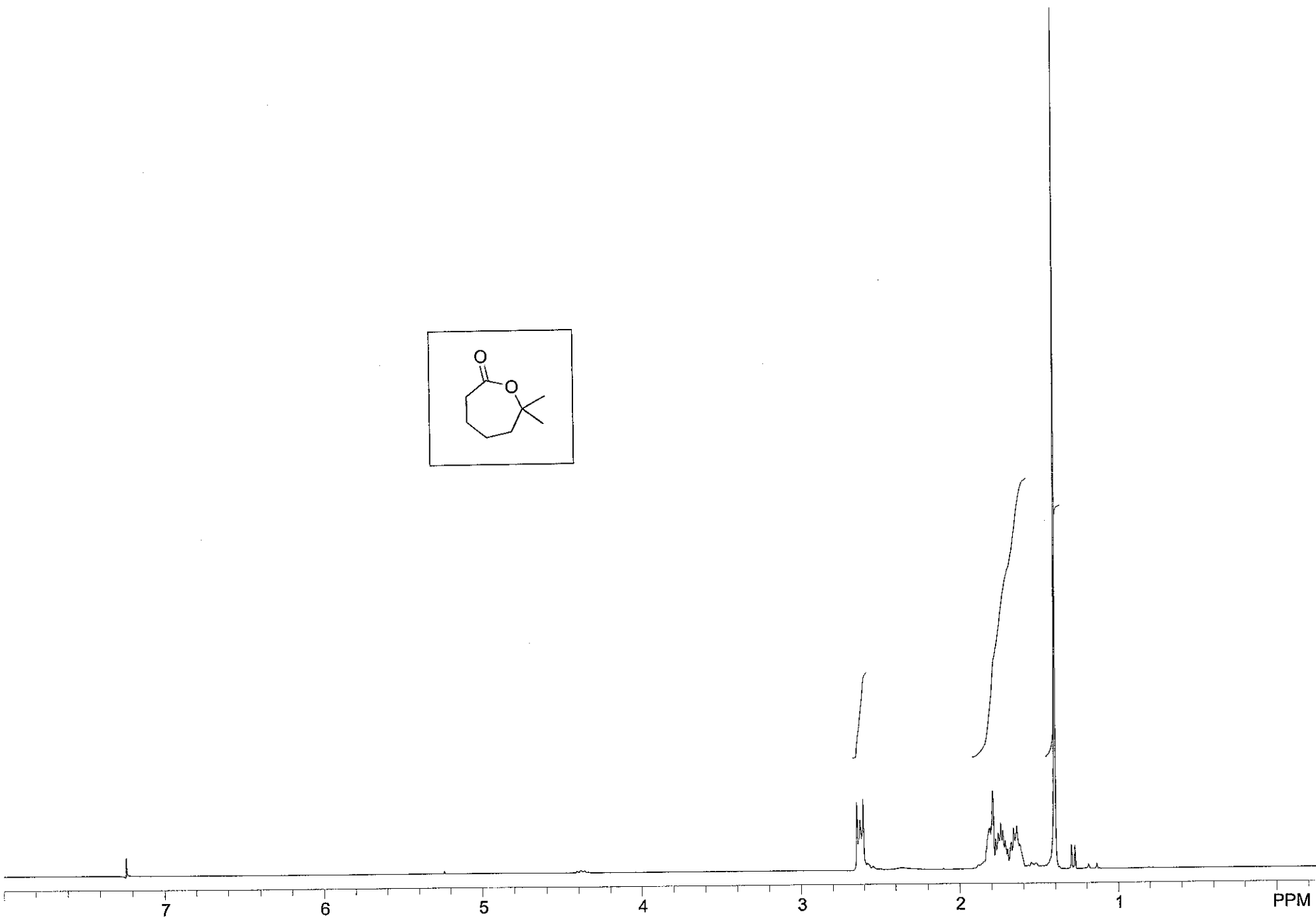
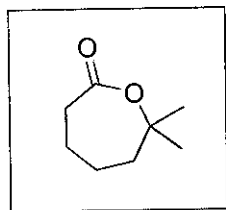
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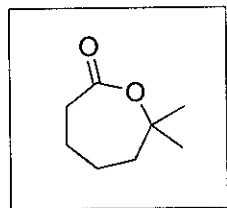
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PPM



S-19



175.043

81.491  
77.616  
77.200  
76.775

40.385  
37.315

28.632  
24.376  
23.511

200

150

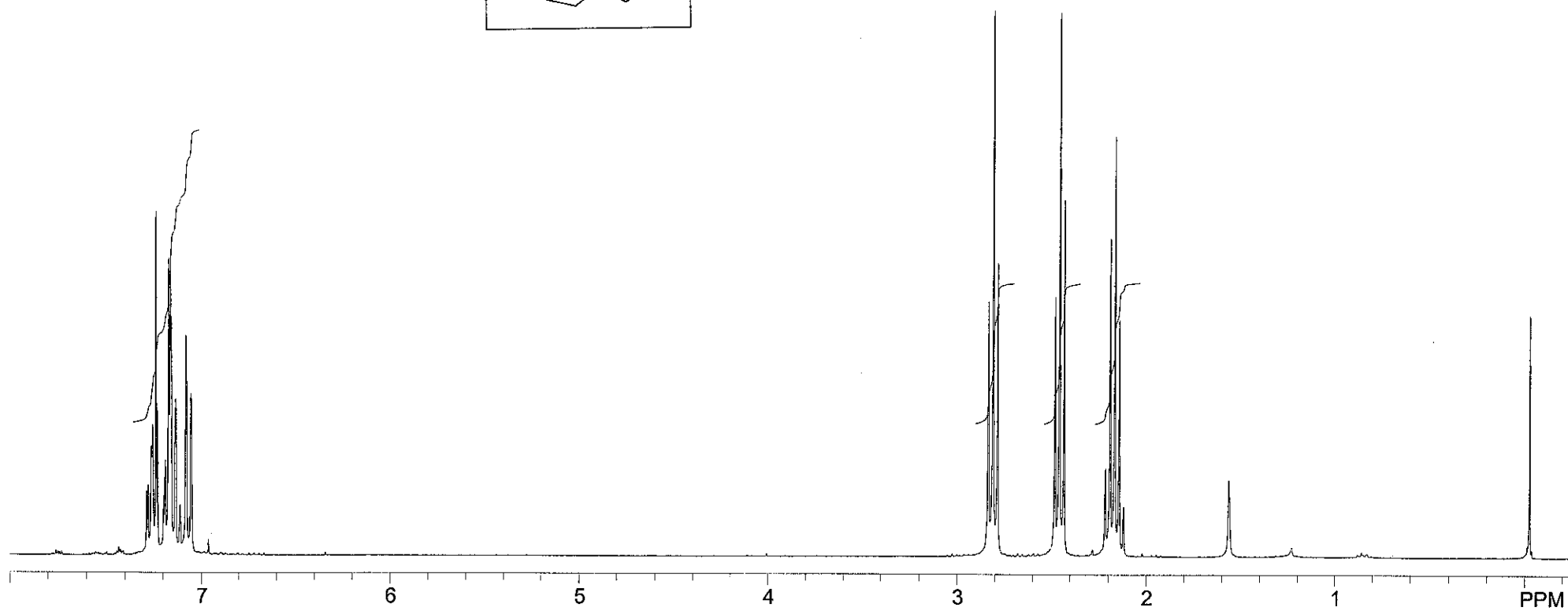
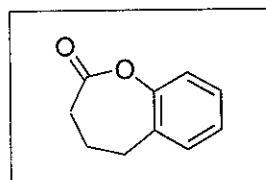
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50

0

PPM

S-20



171.832

151.954

130.210

129.794

128.449

126.041

119.447

77.626

77.200

76.773

31.230

26.387

26.685

