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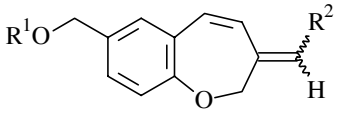
SUPPORTING INFORMATION

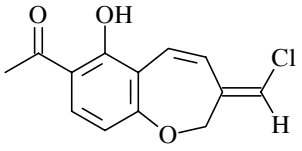
Title: Benzoxepine Esters as Precursors of the Wound-Activated Chemical Defence of *Mycena galopus*

Author(s): Silke Peters, Robert J. R. Jaeger, and Peter Spiteller*

Ref. No.: o200700812

Selected NMR, UV/Vis and mass spectra of *E*-**1,** *E/Z*-**1a**–*E/Z*-**1e, 2**, **2a**–**2e** and **3**.





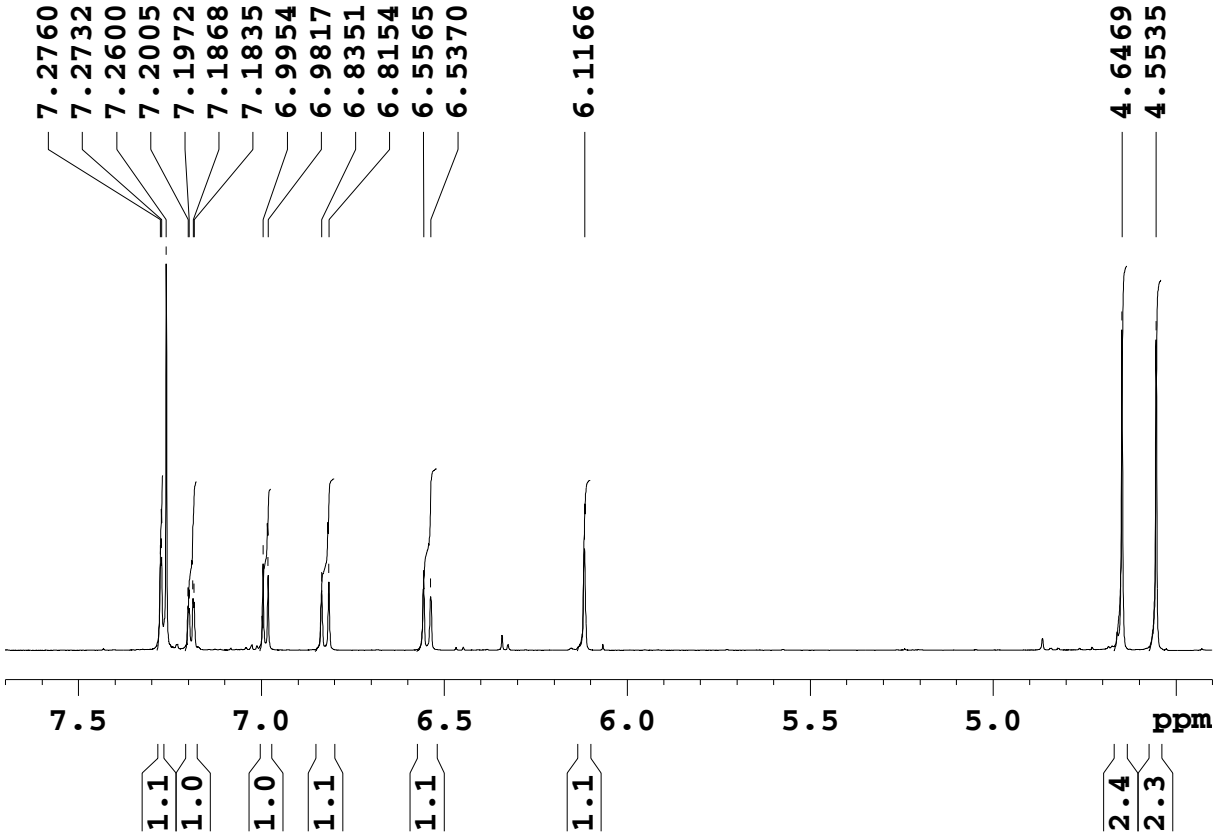
R^1 = H, R^2 = Cl: **1**
R^1 = palmityl, R^2 = Cl: **1a**
R^1 = palmitoleyl, R^2 = Cl: **1b**
R^1 = stearyl, R^2 = Cl: **1c**
R^1 = oleyl, R^2 = Cl: **1d**
R^1 = linoleyl, R^2 = Cl: **1e**

R^1 = H, R^2 = H: **2**
R^1 = palmityl, R^2 = H: **2a**
R^1 = palmitoleyl, R^2 = H: **2b**
R^1 = stearyl, R^2 = H: **2c**
R^1 = oleyl, R^2 = H: **2d**
R^1 = linoleyl, R^2 = H: **2e**

3

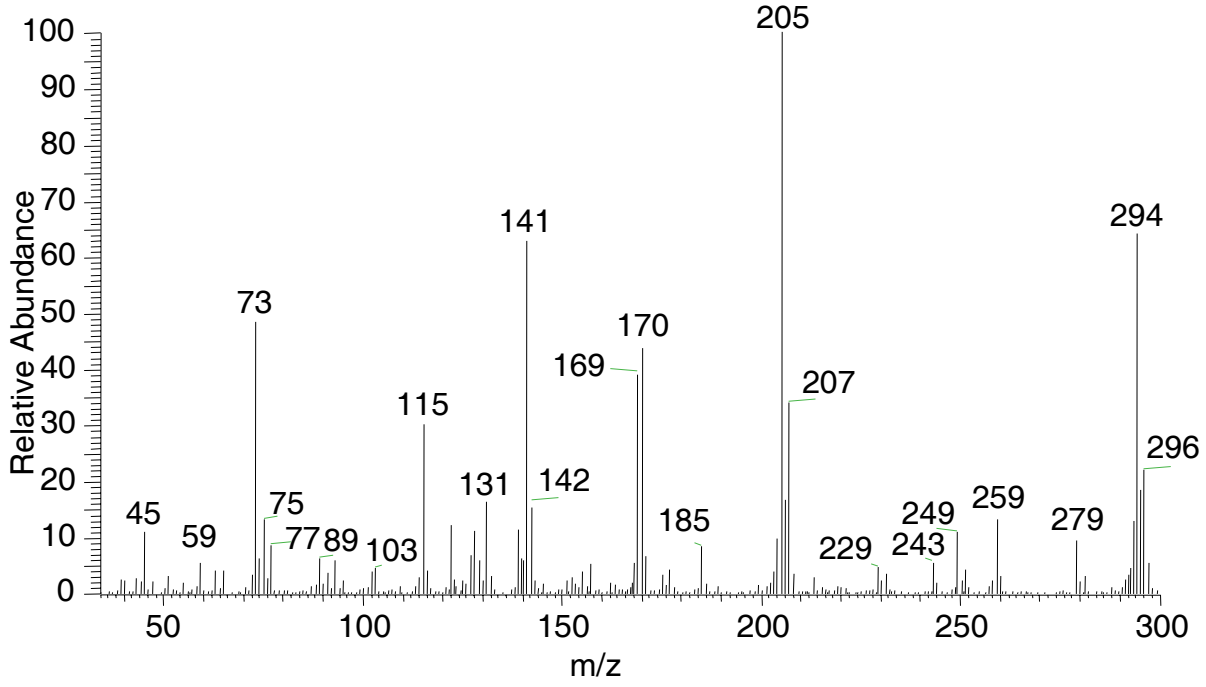
E-3-Chloromethylene-2,3-dihydrobenzo[b]oxepin-7-ylmethanol (*E*-**1**):

^{1}H NMR (600 MHz, $CDCl_3$, 298 K)



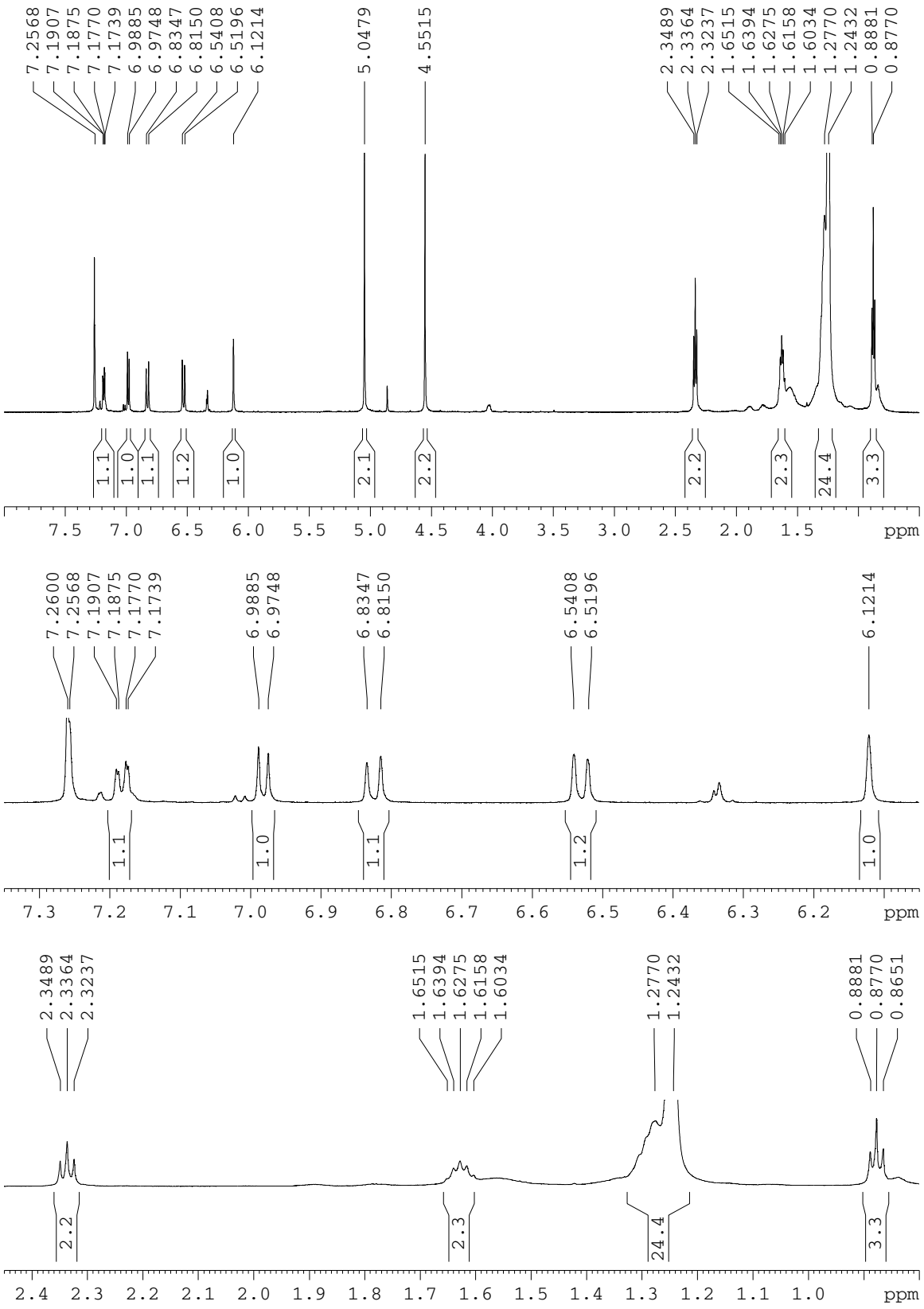
Trimethylsilyl ether of *E*-3-chloromethylene-2,3-dihydrobenzo[b]oxepin-7-ylmethanol (*E*-**1**) and *Z*-**1**:

GC-MS



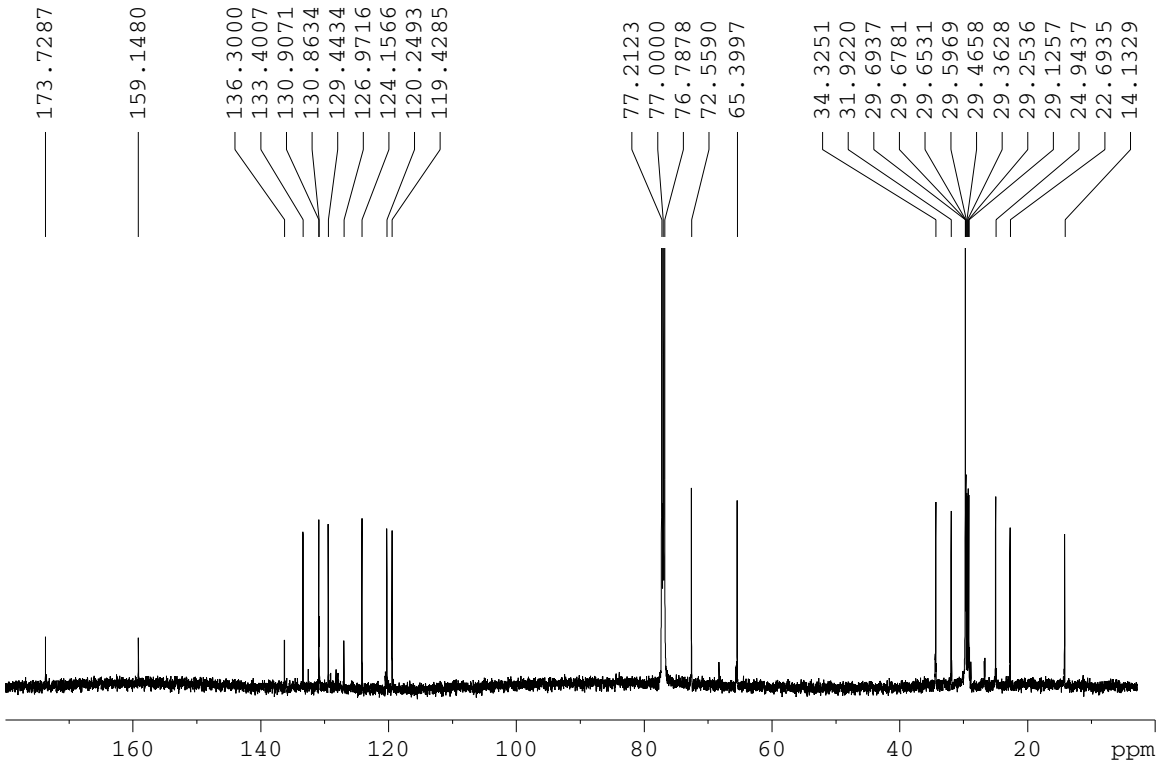
E-3-Chloromethylene-2,3-dihydrobenzo[b]oxepin-7-ylmethyl palmitate (*E*-**1a**):

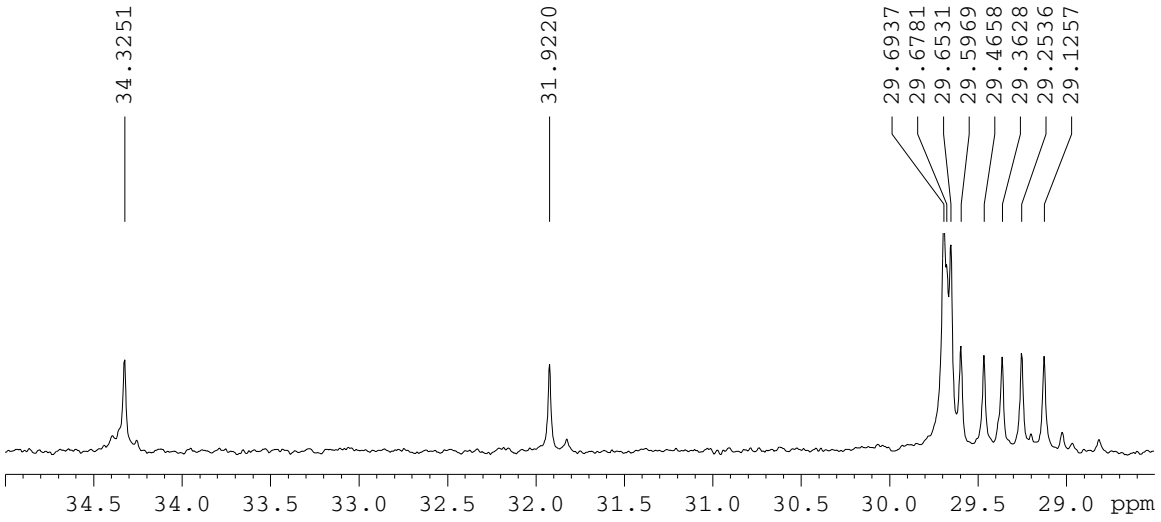
^{1}H NMR (600 MHz, $CDCl_3$, 298 K)



E-3-Chloromethylene-2,3-dihydrobenzo[b]oxepin-7-ylmethyl palmitate (*E*-**1a**):

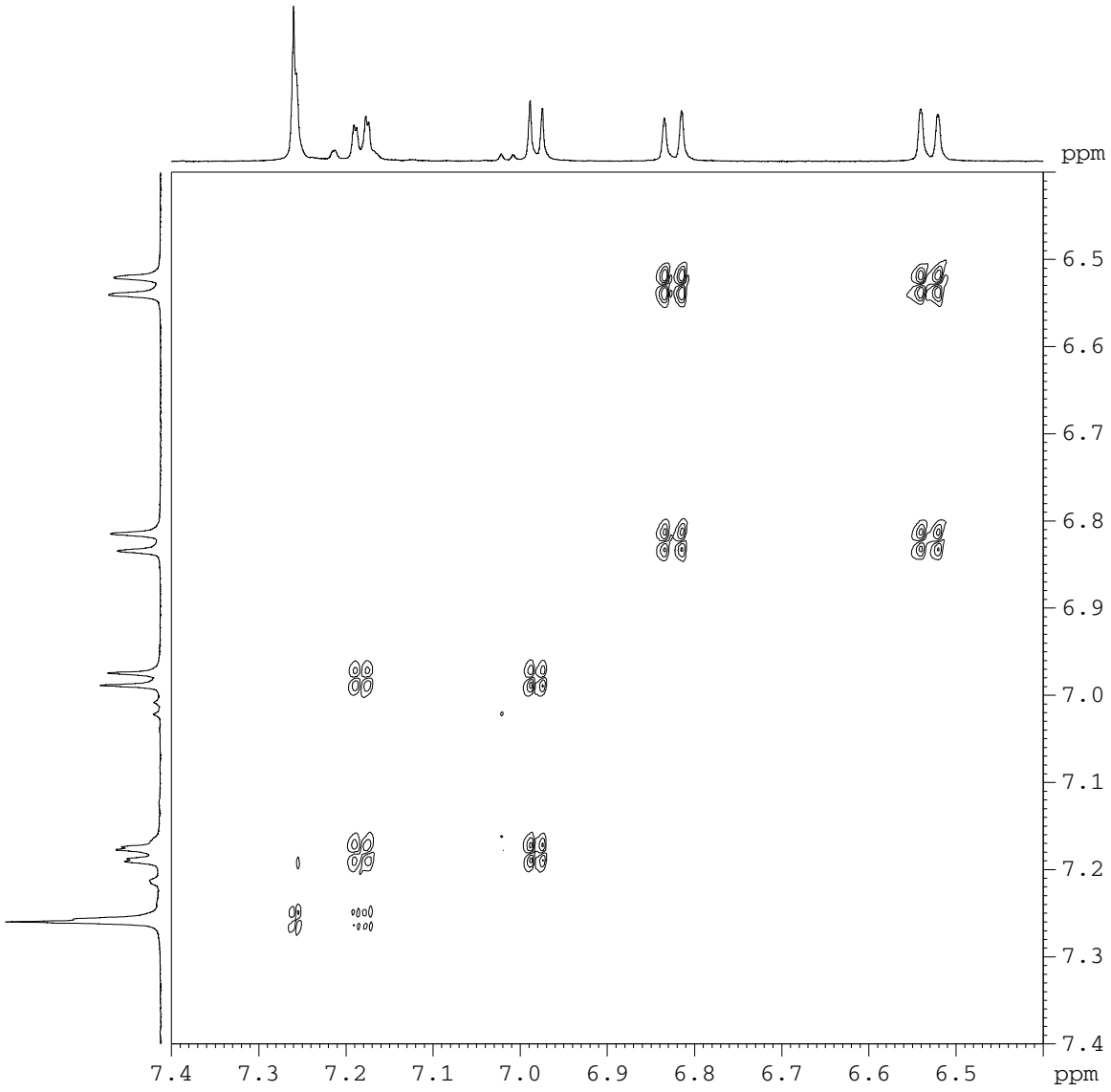
^{13}C NMR (600 MHz, $CDCl_3$, 298 K)





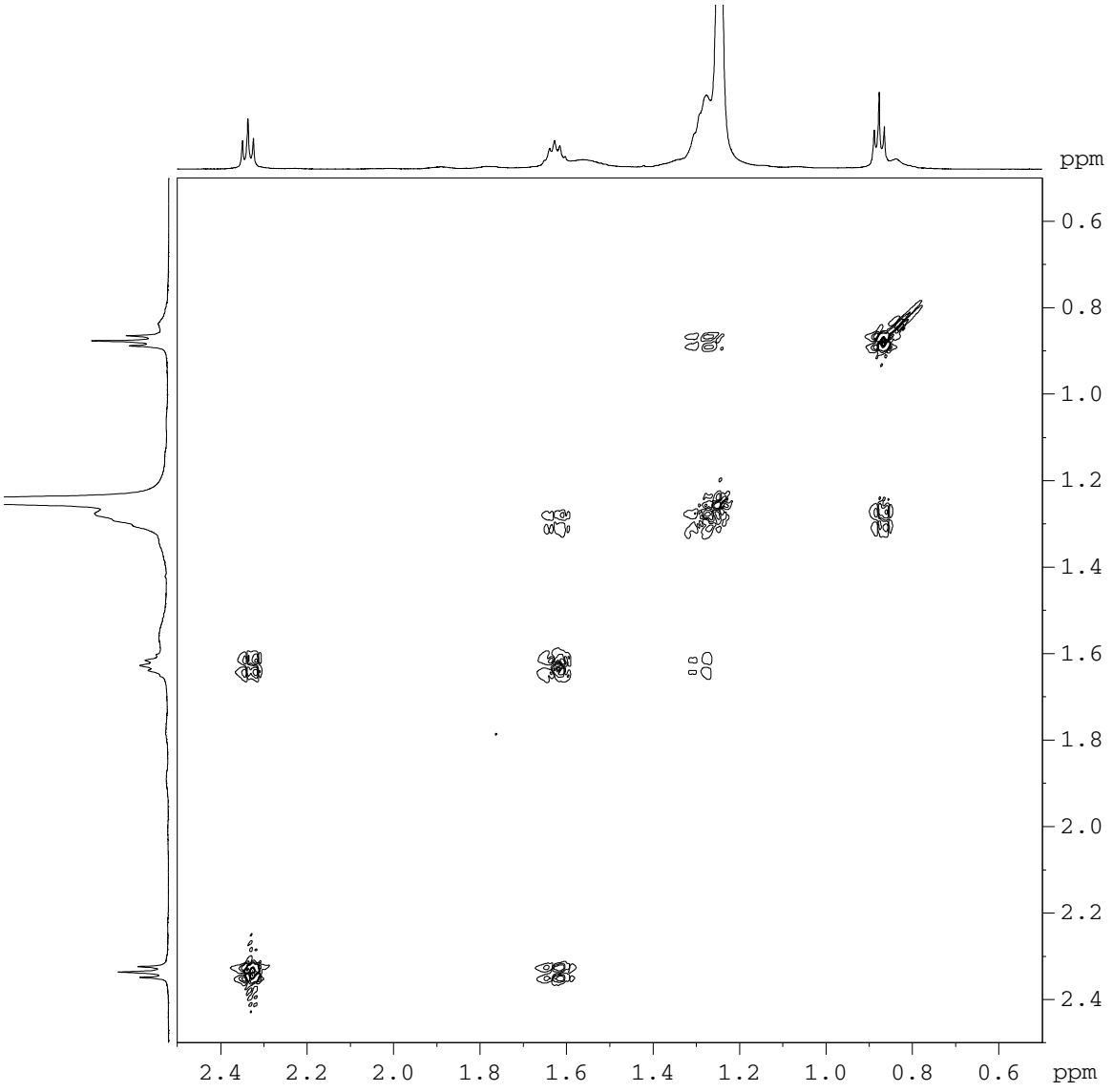
E-3-Chloromethylene-2,3-dihydrobenzo[b]oxepin-7-ylmethyl palmitate (*E*-**1a**):

COSY (600 MHz, $CDCl_3$, 298 K)



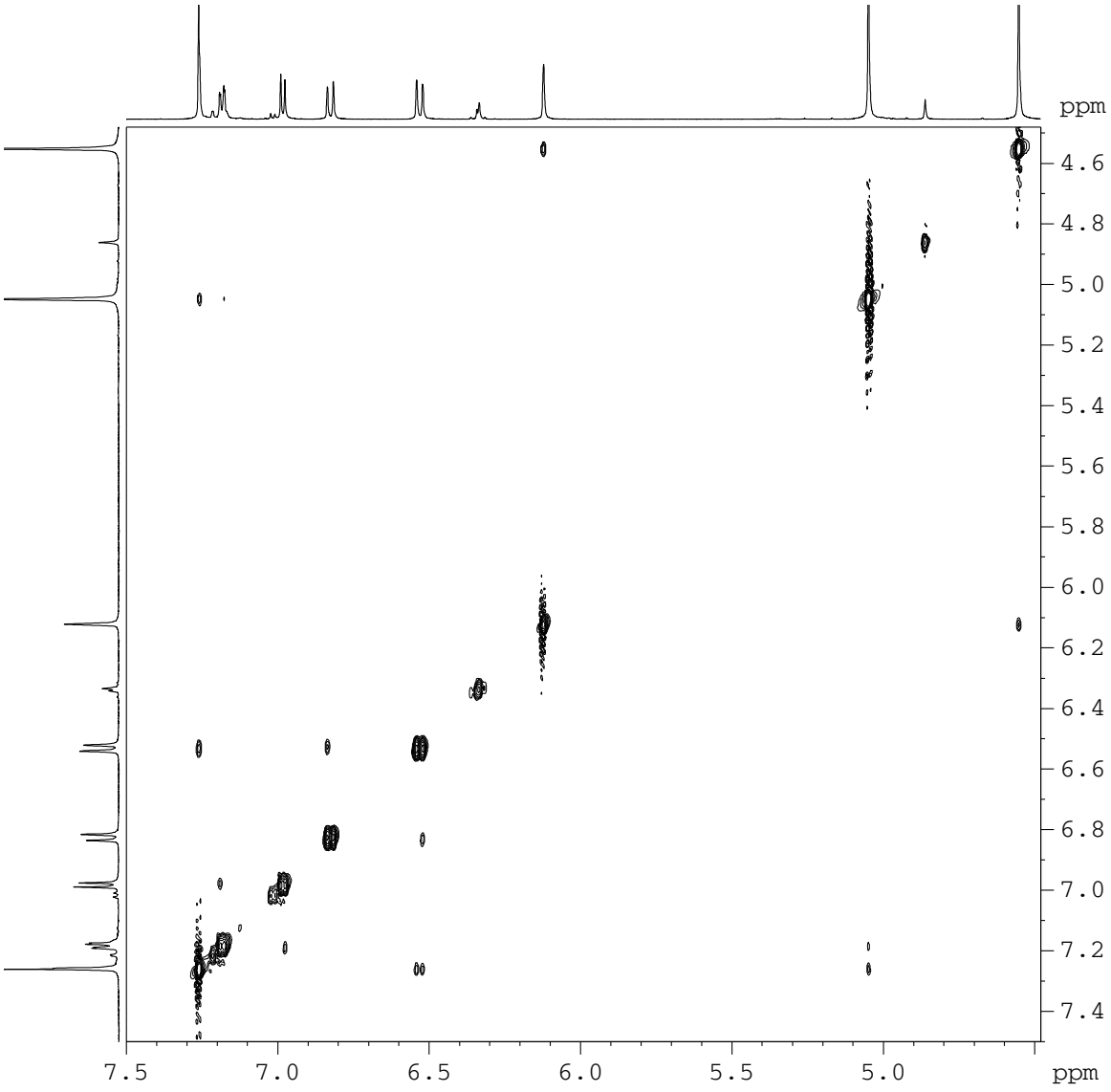
E-3-Chloromethylene-2,3-dihydrobenzo[b]oxepin-7-ylmethyl palmitate (*E*-**1a**):

COSY (600 MHz, $CDCl_3$, 298 K)



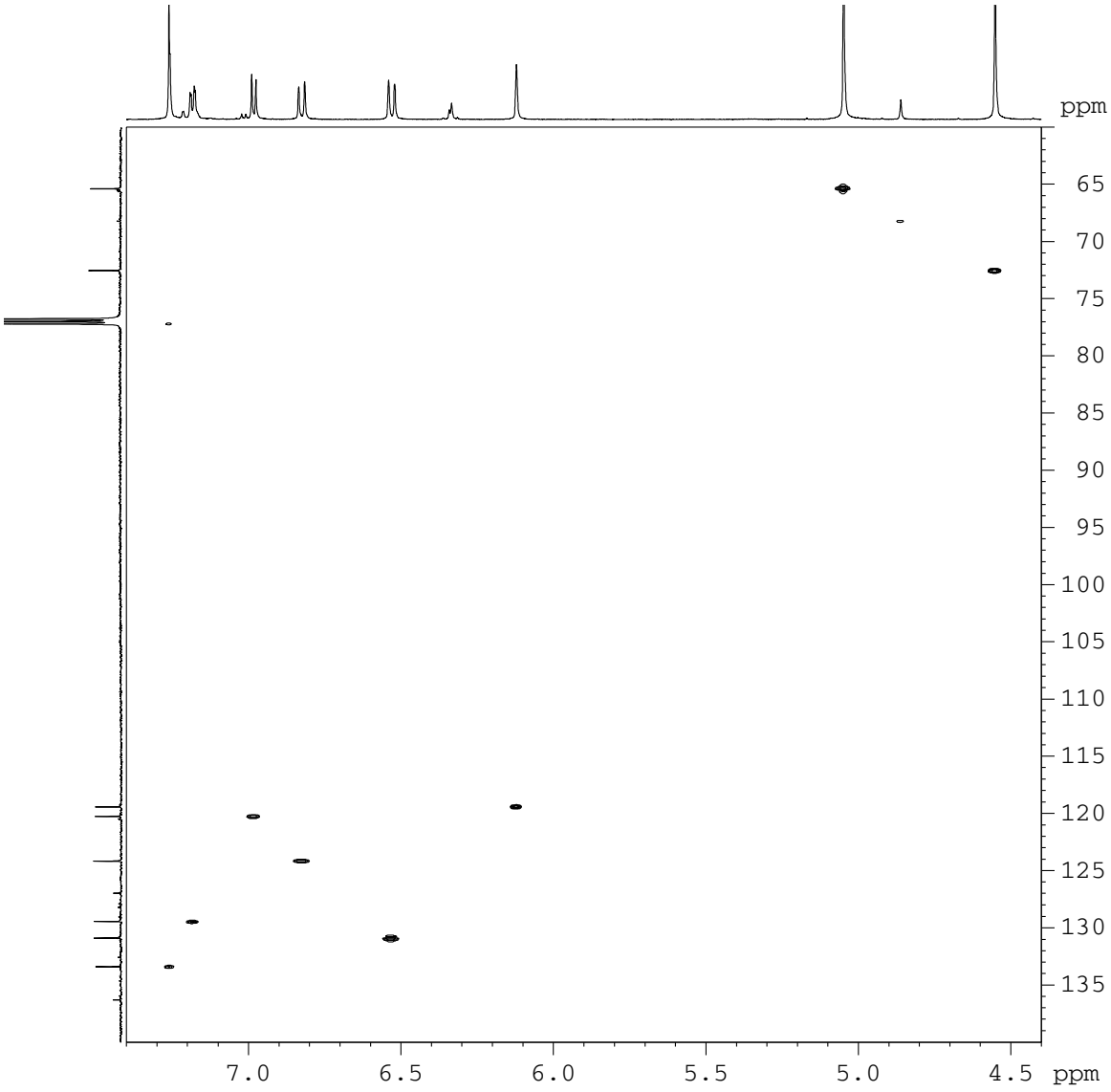
E-3-Chloromethylene-2,3-dihydrobenzo[b]oxepin-7-ylmethyl palmitate (*E*-**1a**):

NOESY (600 MHz, $CDCl_3$, 298 K)



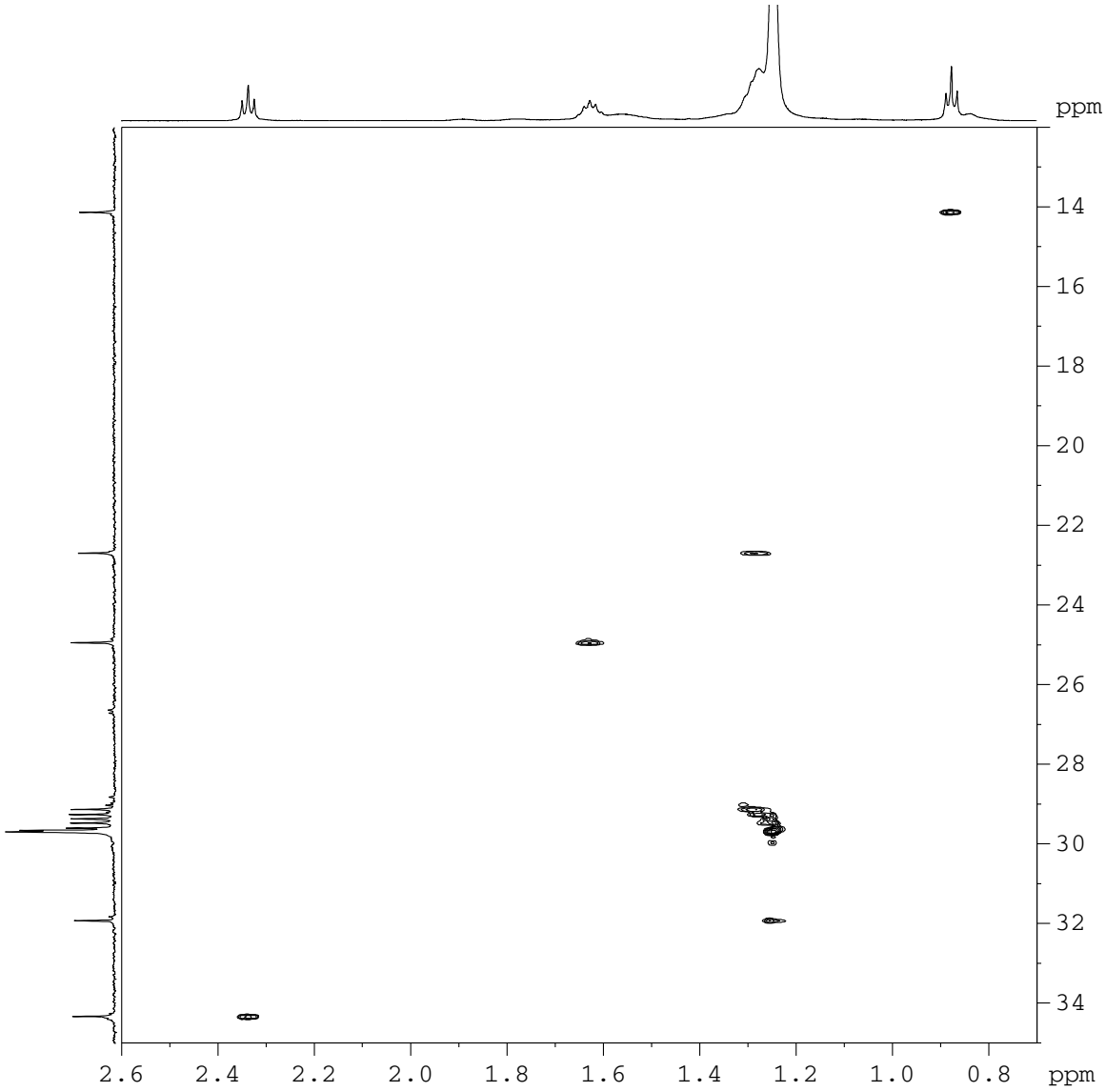
E-3-Chloromethylene-2,3-dihydrobenzo[b]oxepin-7-ylmethyl palmitate (*E*-**1a**):

HSQC (600 MHz, $CDCl_3$, 298 K)



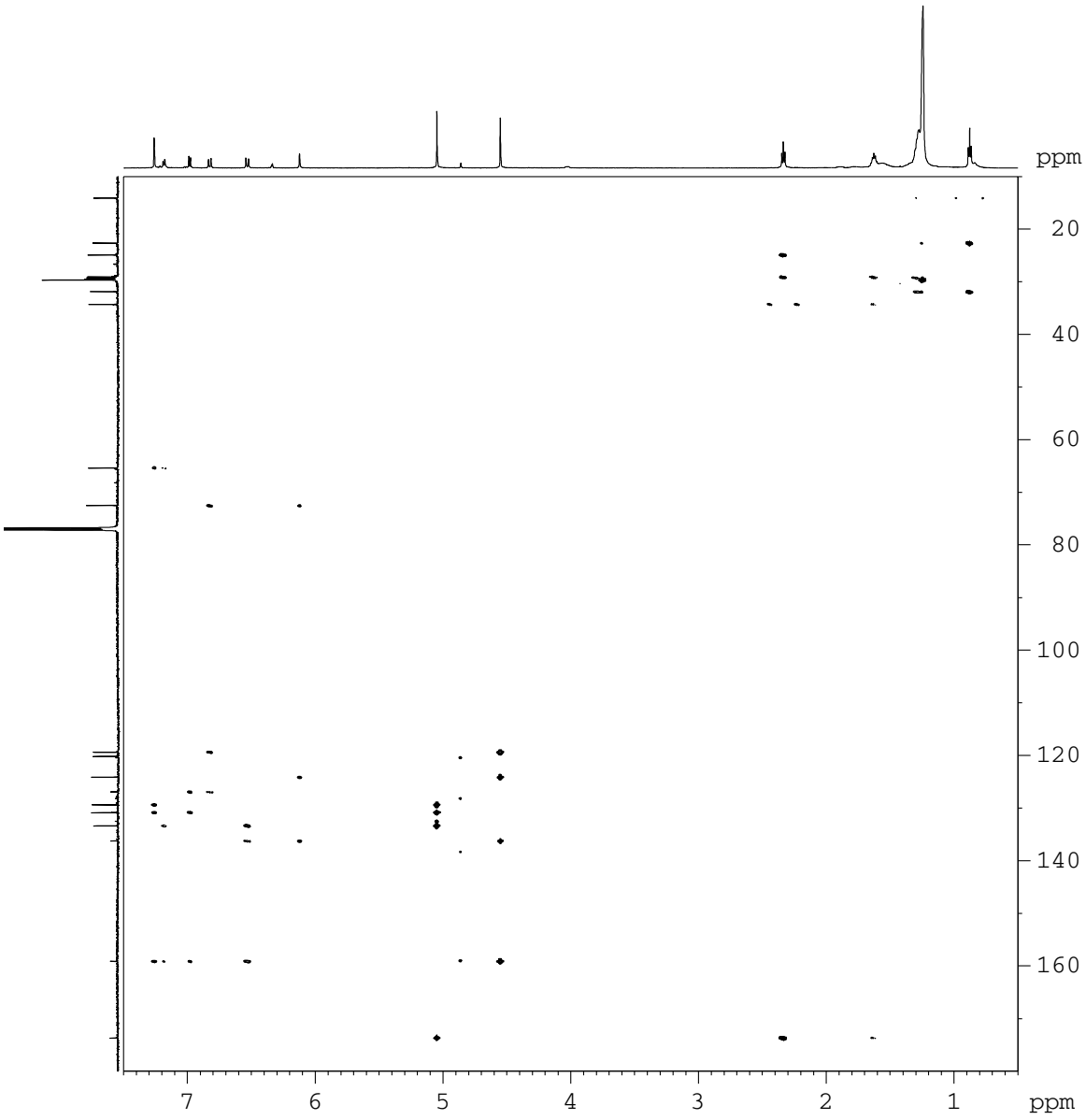
E-3-Chloromethylene-2,3-dihydrobenzo[b]oxepin-7-ylmethyl palmitate (*E*-**1a**):

HSQC (600 MHz, $CDCl_3$, 298 K)



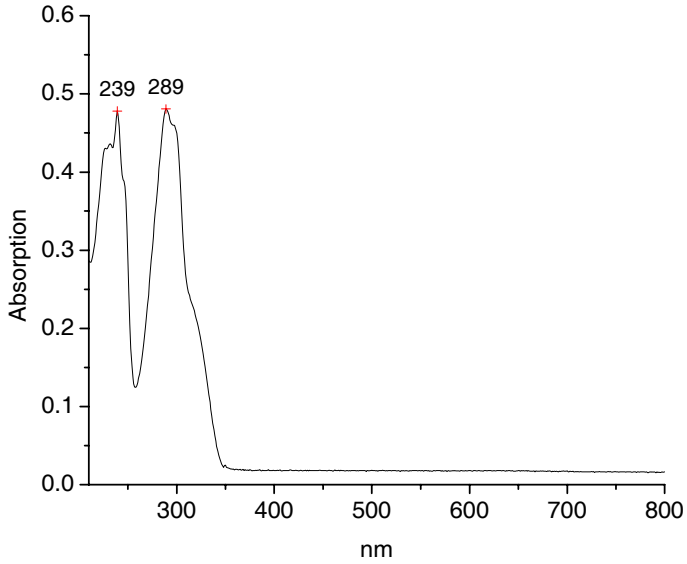
E-3-Chloromethylene-2,3-dihydrobenzo[b]oxepin-7-ylmethyl palmitate (*E*-**1a**):

HMBC (600 MHz, $CDCl_3$, 298 K)



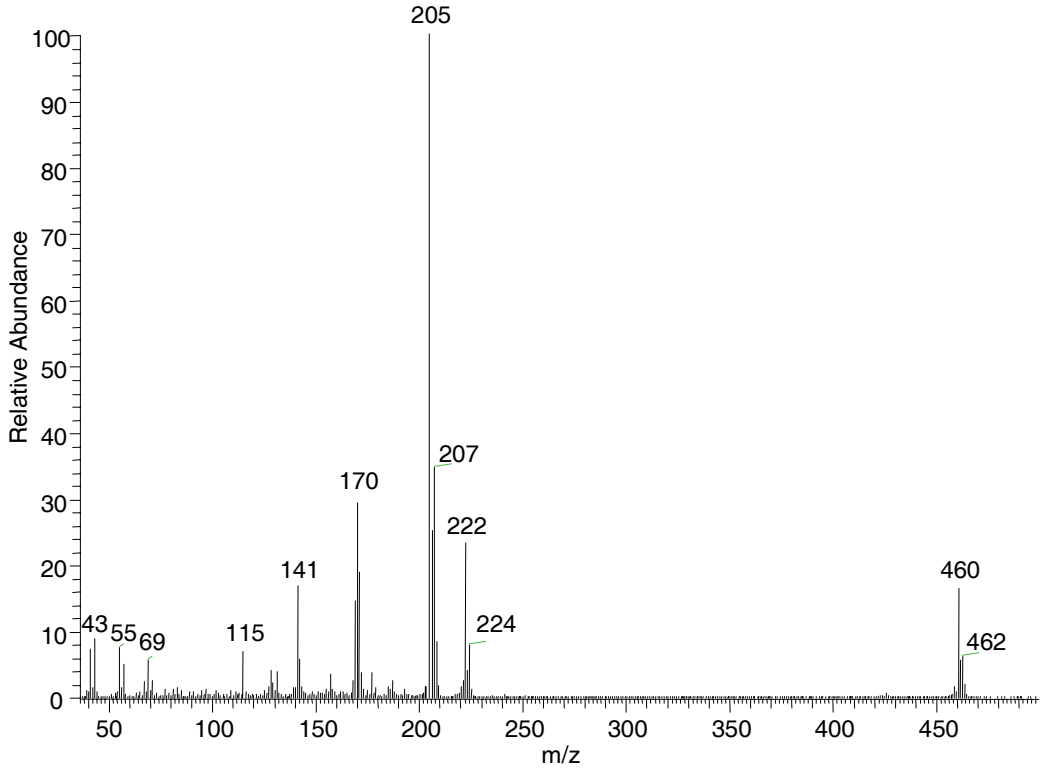
E-3-Chloromethylene-2,3-dihydrobenzo[b]oxepin-7-ylmethyl palmitate (*E*-**1a**):

UV/Vis in MeOH



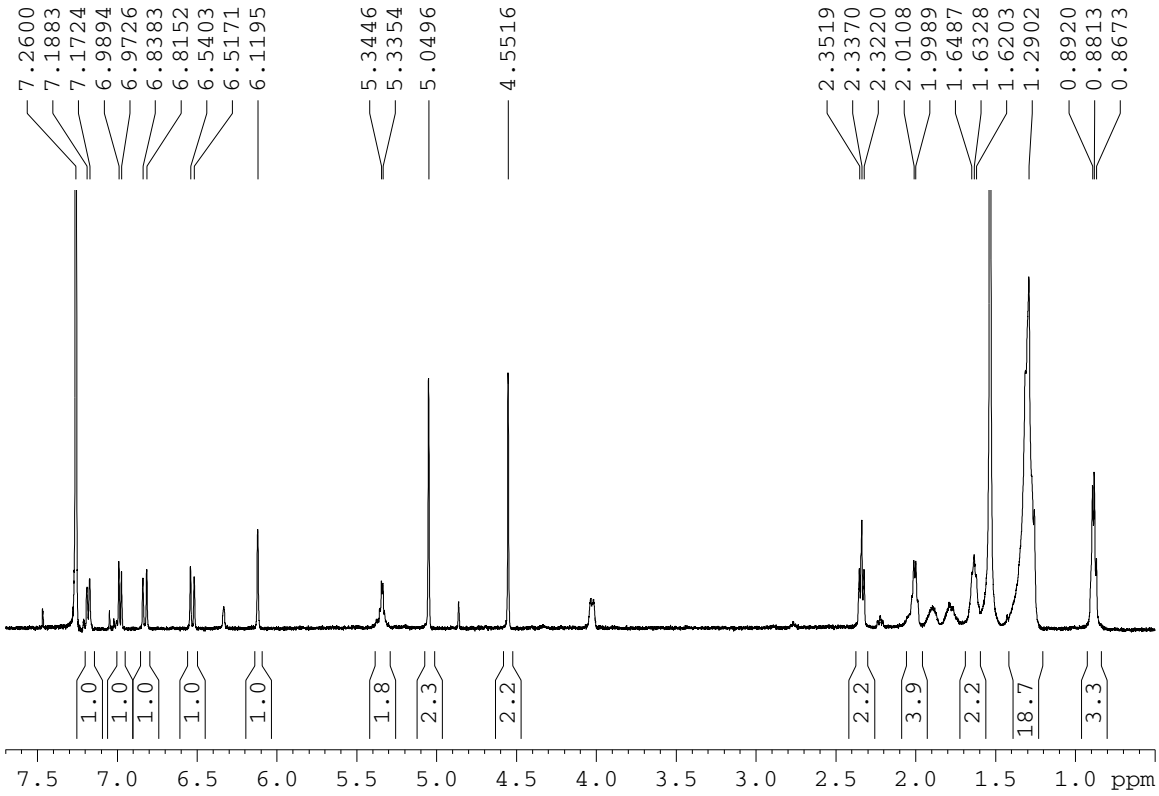
E-3-Chloromethylene-2,3-dihydrobenzo[b]oxepin-7-ylmethyl palmitate (*E*-**1a**) and *Z*-**1a**:

GC-MS



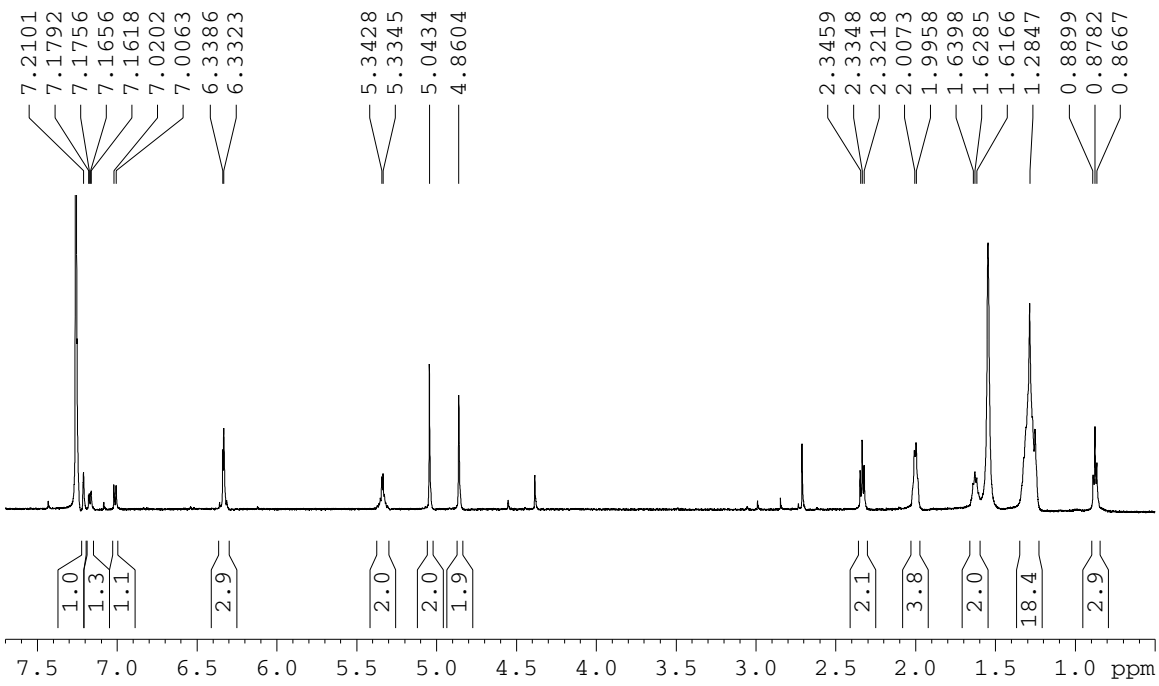
E-3-Chloromethylene-2,3-dihydrobenzo[b]oxepin-7-ylmethyl palmitoleate (*E*-**1b**):

^{1}H NMR (500 MHz, $CDCl_3$, 298 K)



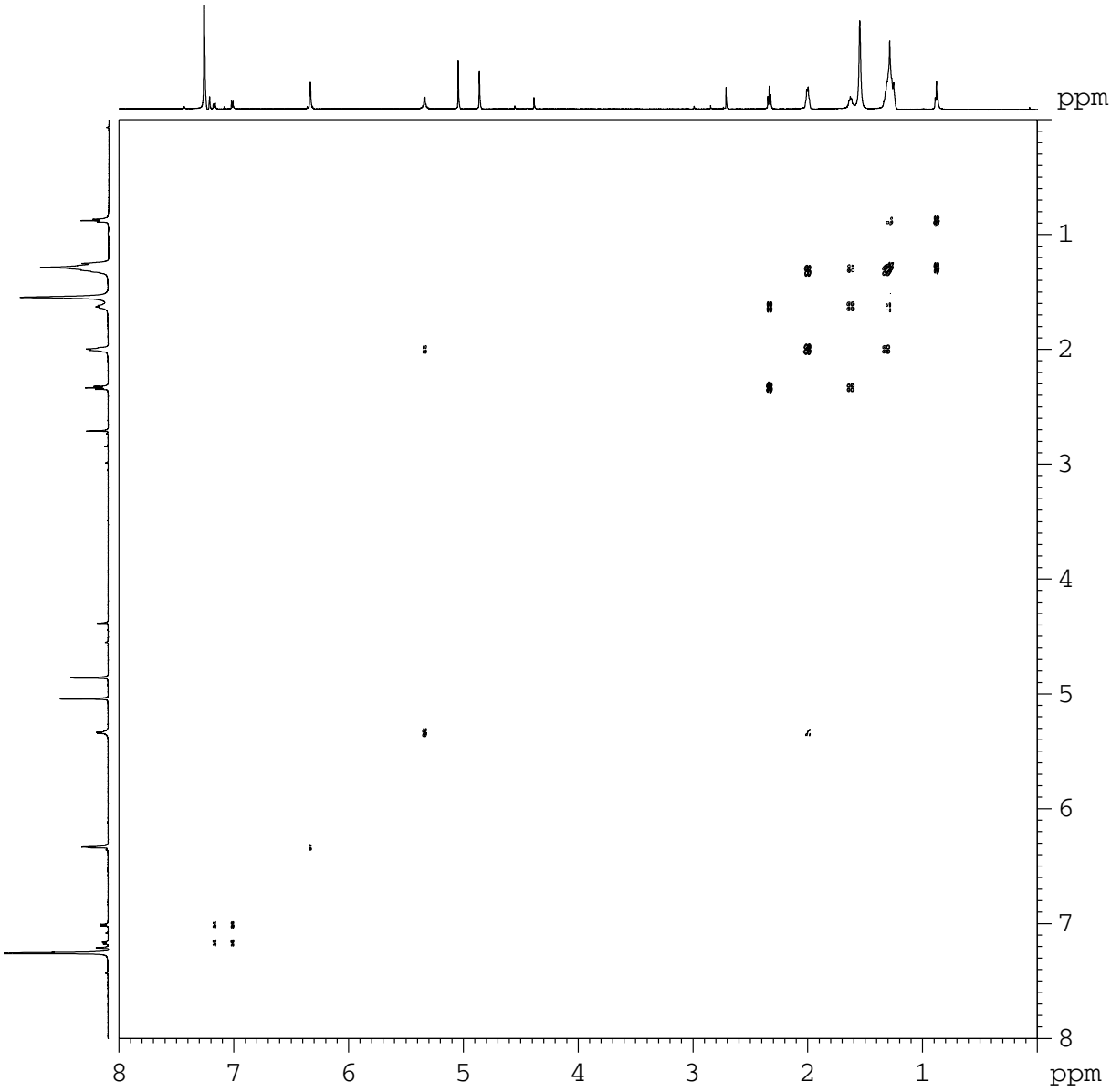
Z-3-Chloromethylene-2,3-dihydrobenzo[b]oxepin-7-ylmethyl palmitoleate (*Z*-**1b**):

^{1}H NMR (600 MHz, $CDCl_3$, 298 K)



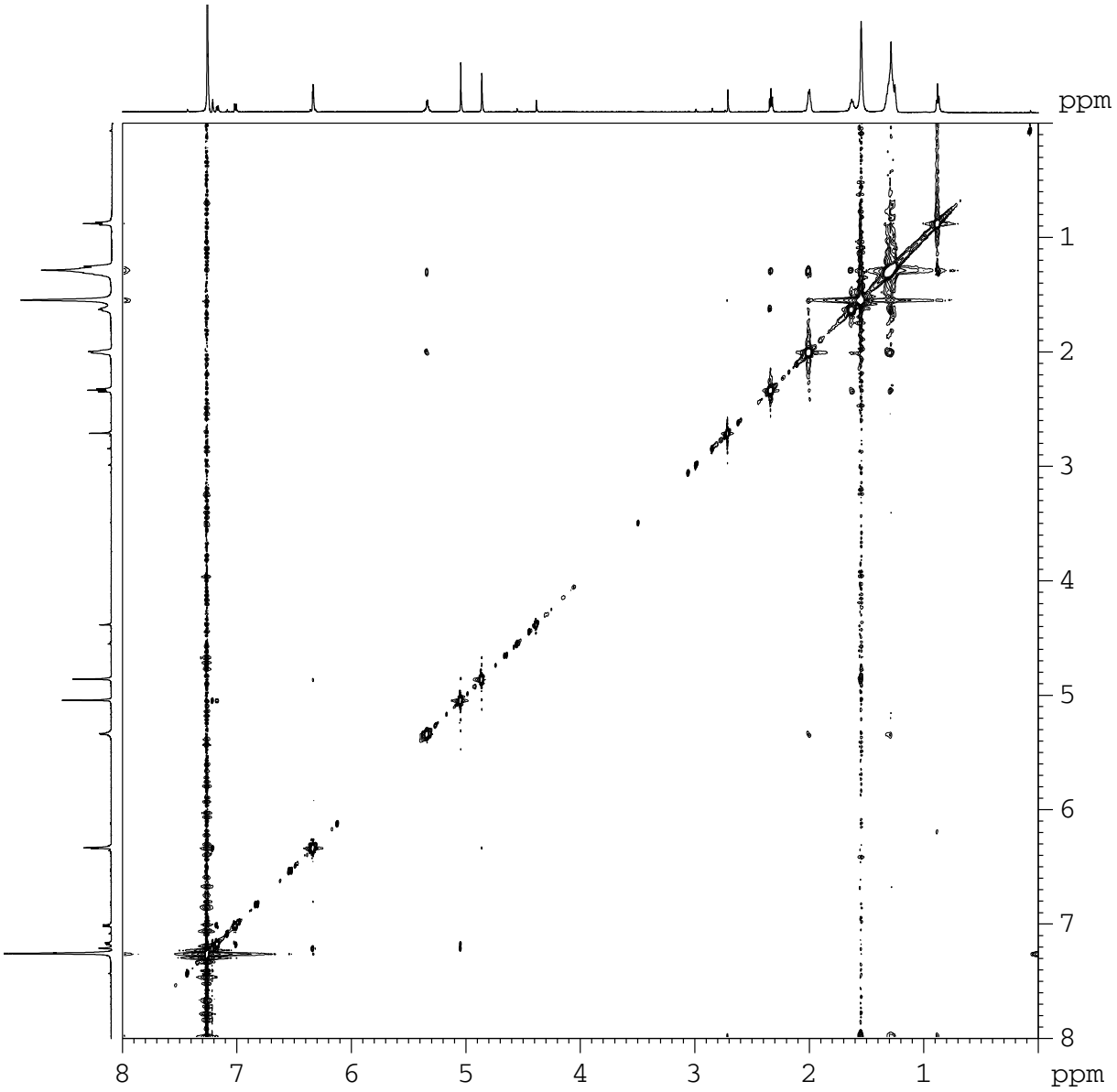
Z-3-Chloromethylene-2,3-dihydrobenzo[b]oxepin-7-ylmethyl palmitoleate (*Z*-**1b**):

COSY (600 MHz, $CDCl_3$, 298 K)



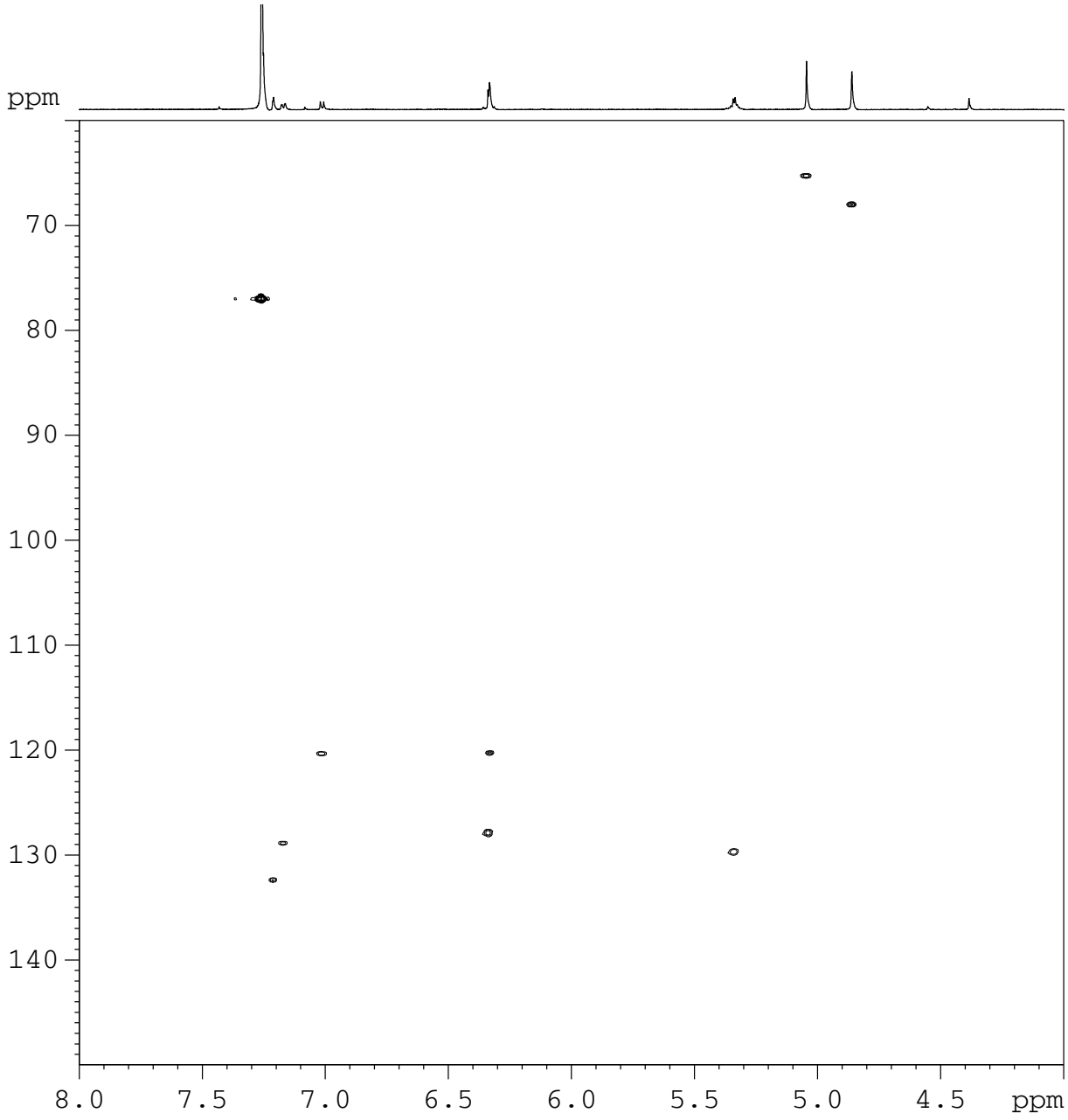
Z-3-Chloromethylene-2,3-dihydrobenzo[b]oxepin-7-ylmethyl palmitoleate (*Z*-**1b**):

NOESY (600 MHz, $CDCl_3$, 298 K)



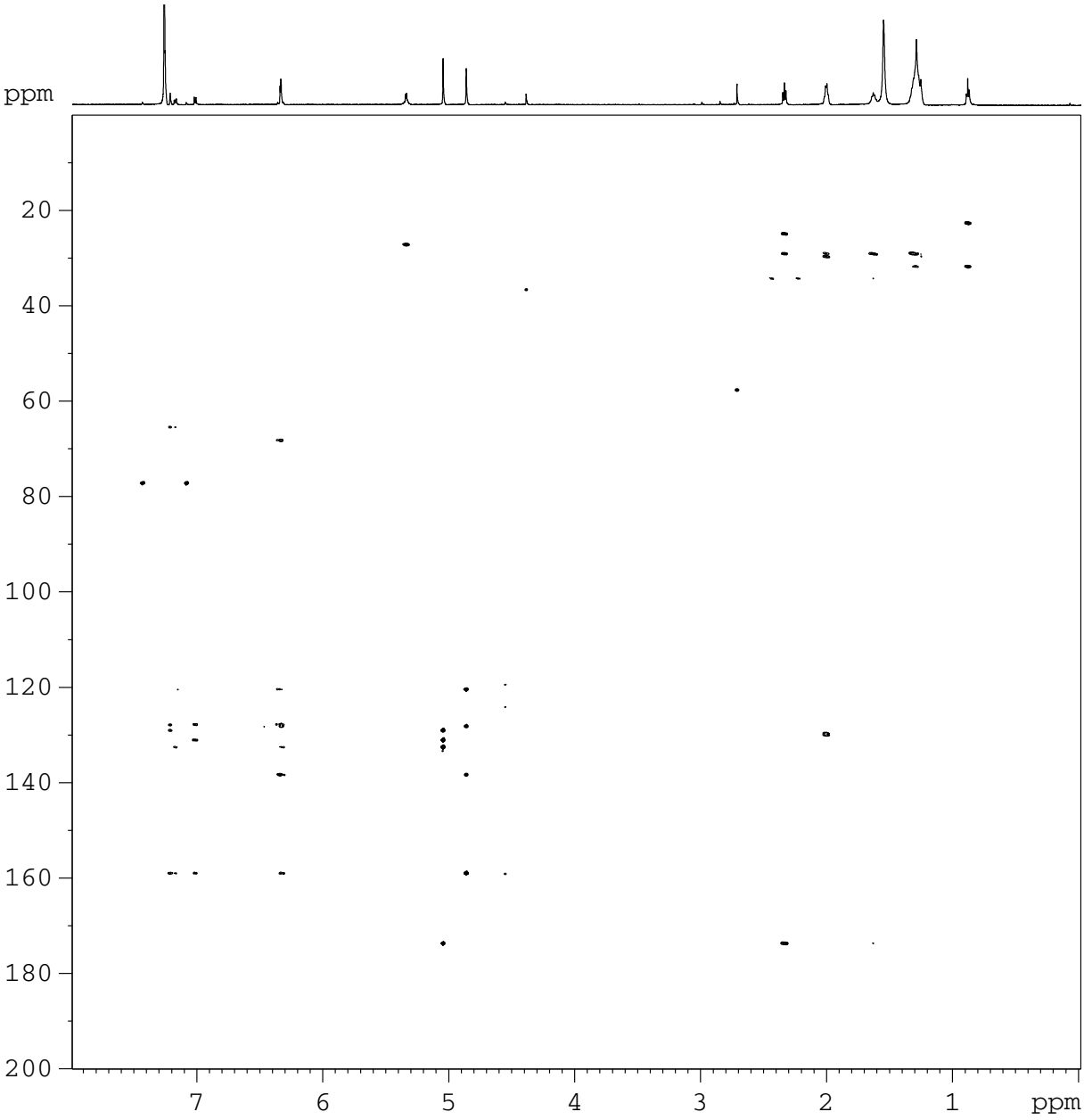
Z-3-Chloromethylene-2,3-dihydrobenzo[b]oxepin-7-ylmethyl palmitoleate (*Z*-**1b**):

HSQC (600 MHz, $CDCl_3$, 298 K)



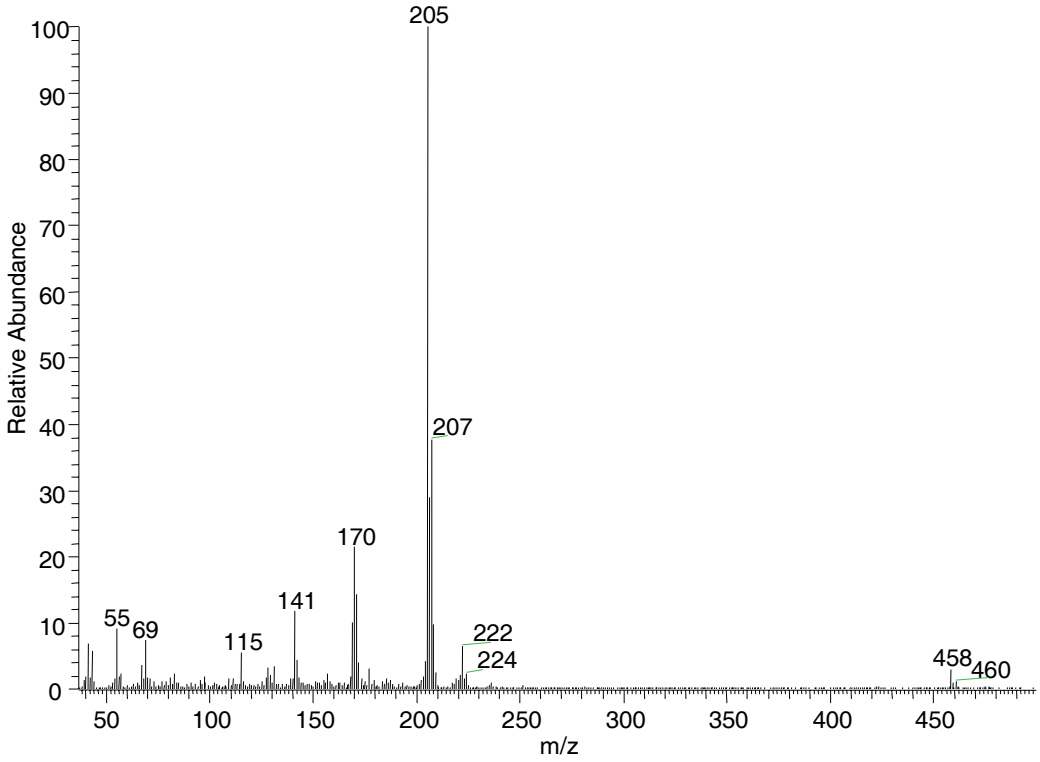
Z-3-Chloromethylene-2,3-dihydrobenzo[b]oxepin-7-ylmethyl palmitoleate (*Z*-**1b**):

HMBC (600 MHz, $CDCl_3$, 298 K)



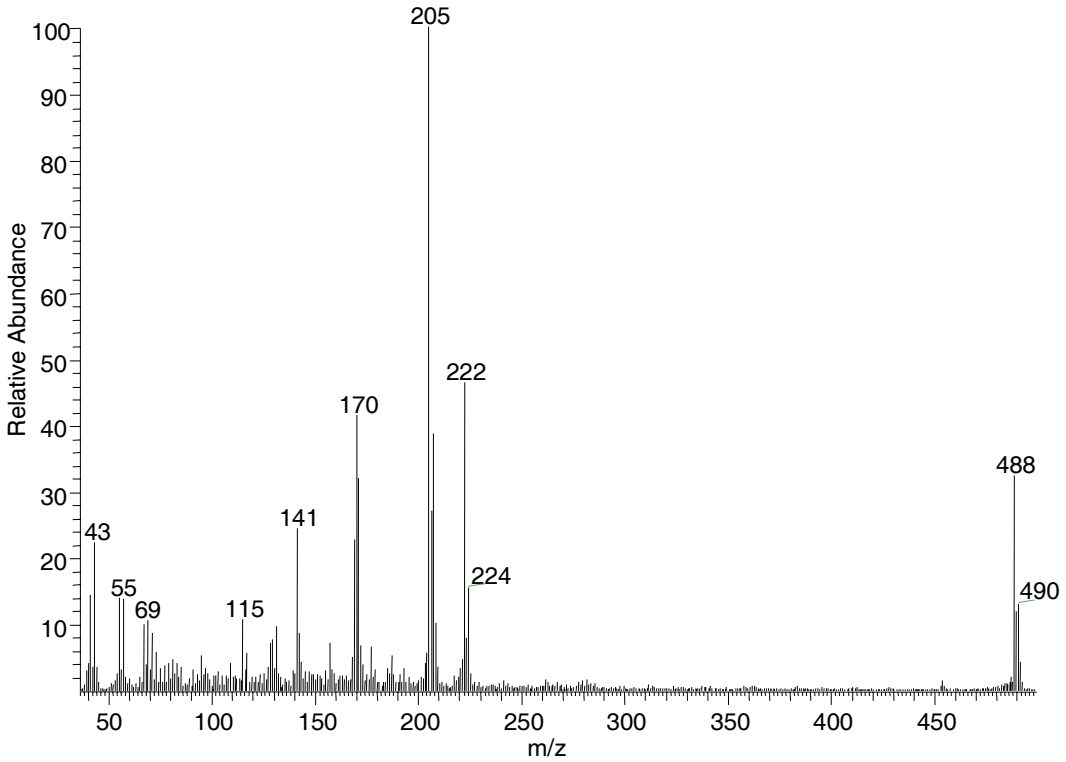
E-3-Chloromethylene-2,3-dihydrobenzo[b]oxepin-7-ylmethyl palmitoleate (*E*-**1b**) and *Z*-**1b**:

GC-MS



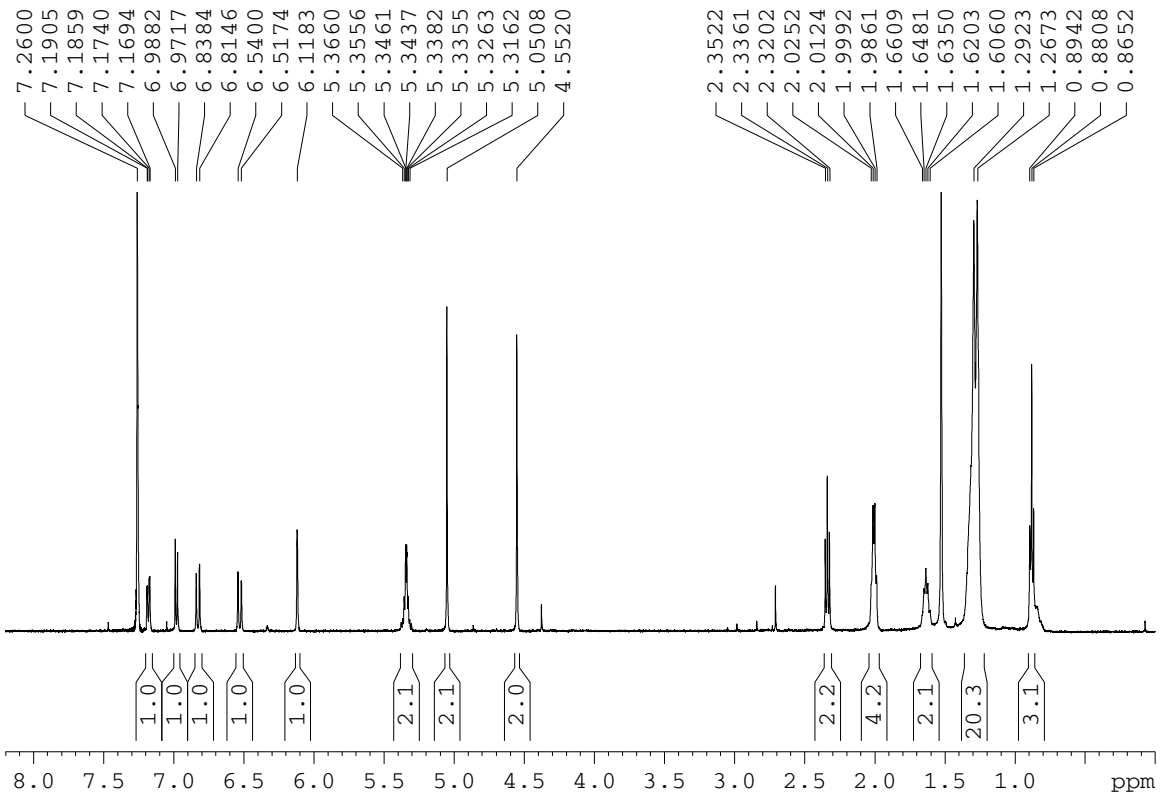
E-3-Chloromethylene-2,3-dihydrobenzo[b]oxepin-7-ylmethyl stearate (*E*-**1c**) and *Z*-**1c**:

GC-MS

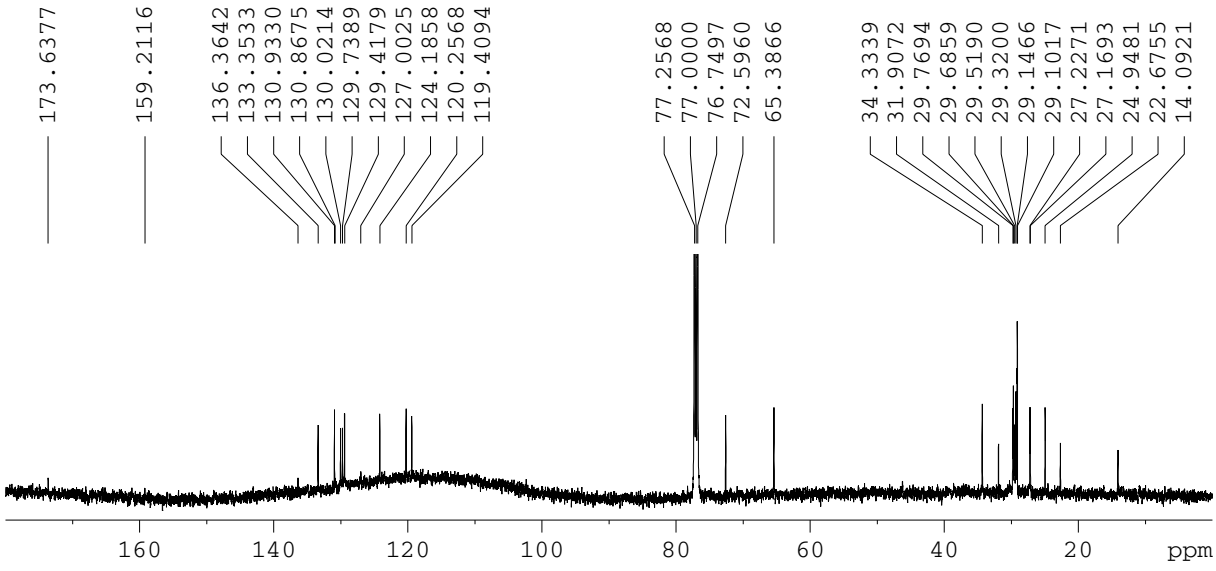


E-3-Chloromethylene-2,3-dihydrobenzo[b]oxepin-7-ylmethyl oleate (*E*-**1d**):

^{1}H NMR (500 MHz, $CDCl_3$, 300 K)

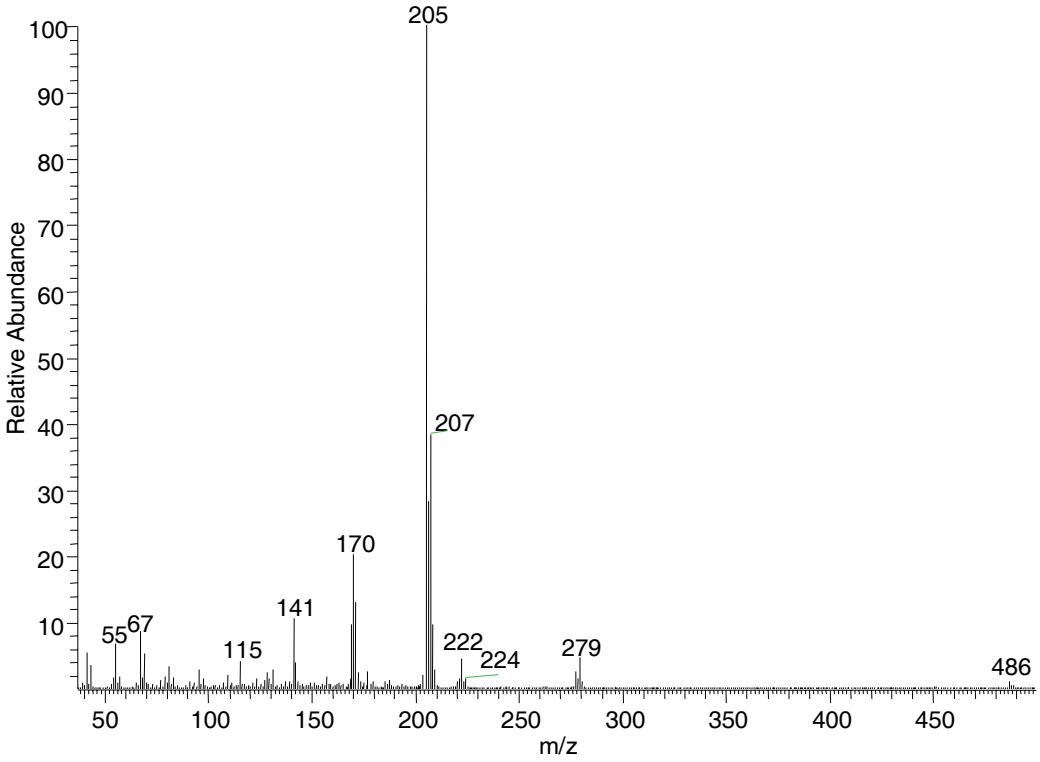


^{13}C NMR (126 MHz, $CDCl_3$, 300 K)



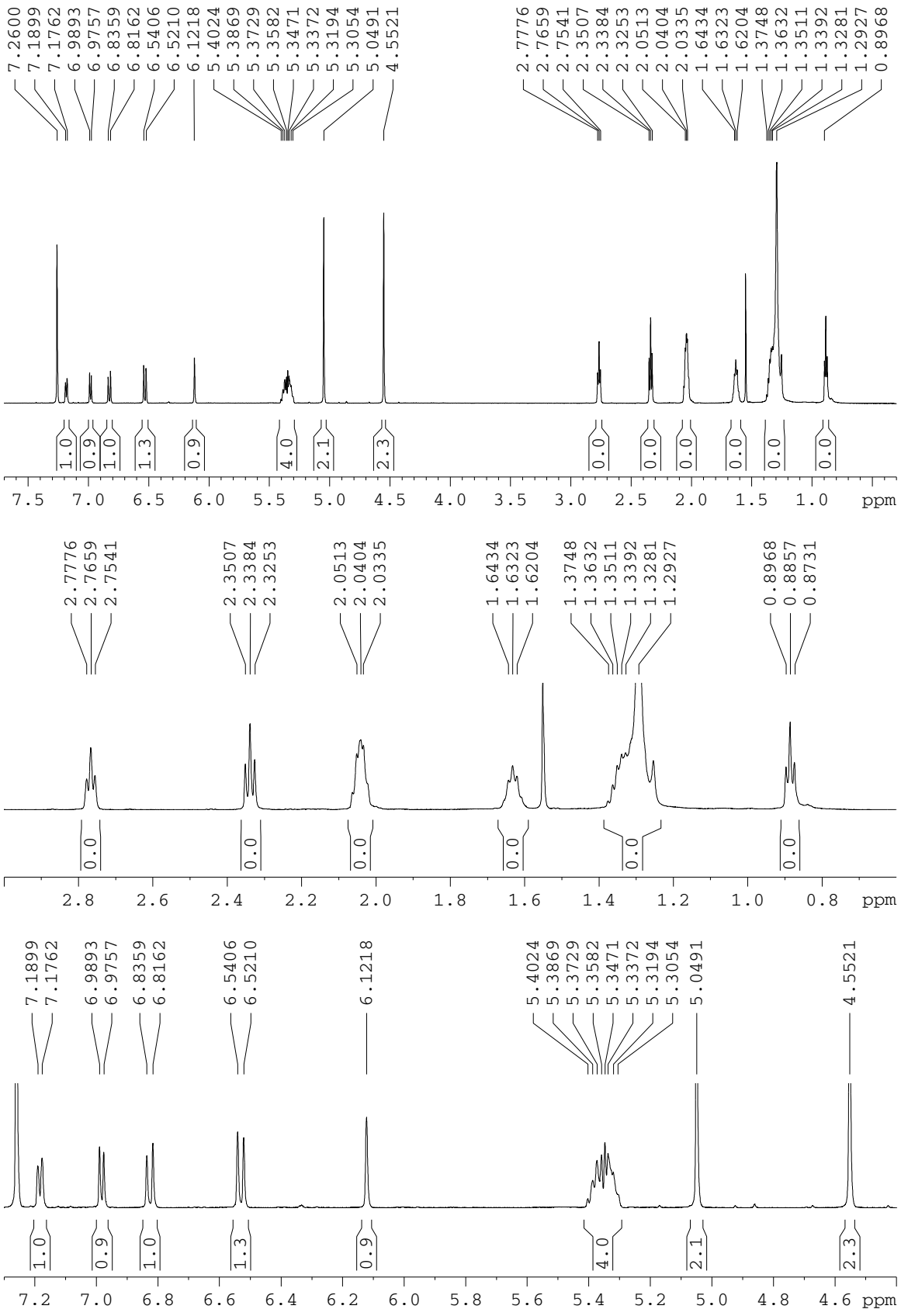
E-3-Chloromethylene-2,3-dihydrobenzo[b]oxepin-7-ylmethyl oleate (*E*-**1d**) and *Z*-**1d**:

GC-MS



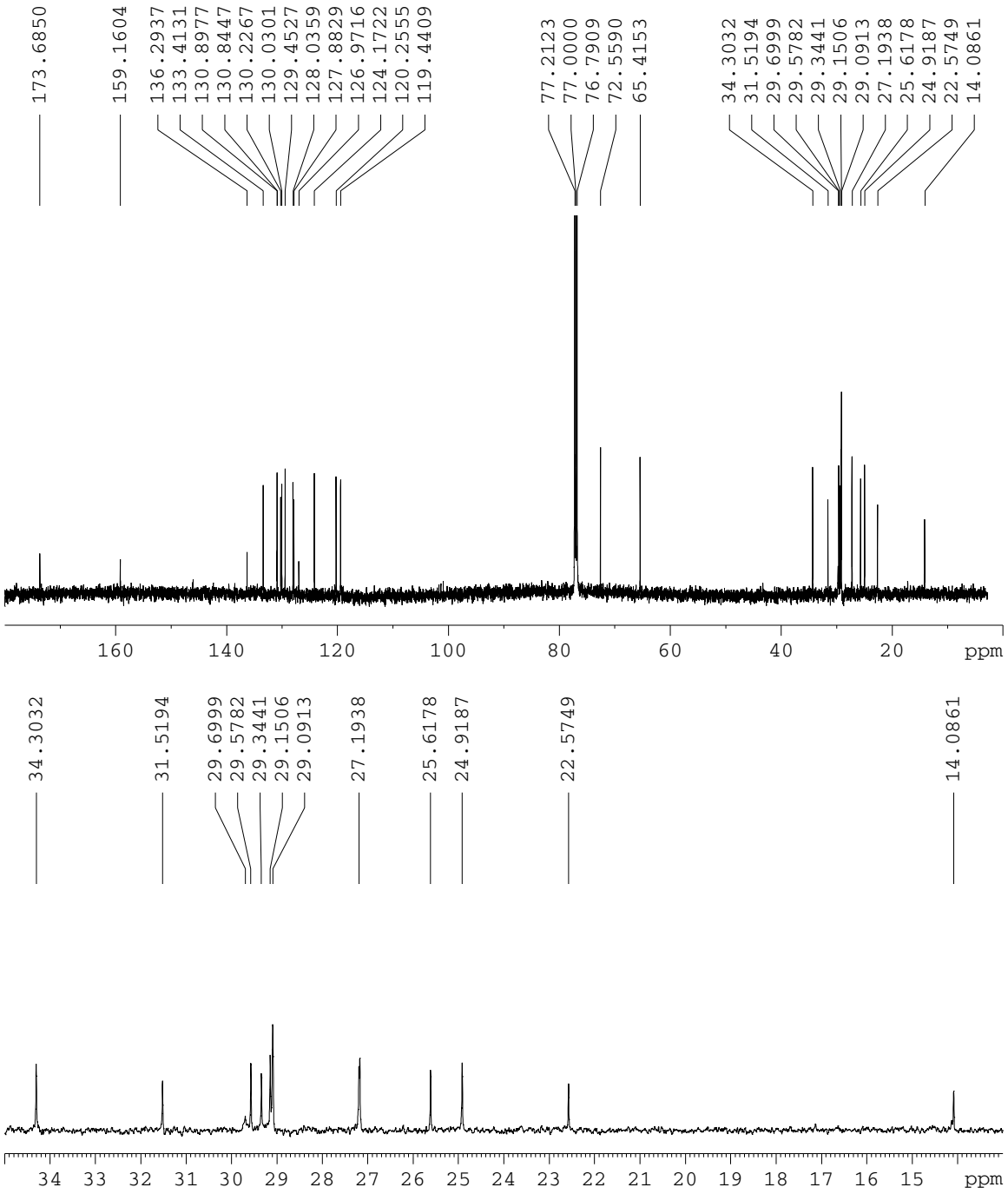
E-3-Chloromethylene-2,3-dihydrobenzo[b]oxepin-7-ylmethyl linoleate (*E*-**1e**):

^{1}H NMR (600 MHz, $CDCl_3$, 298 K)



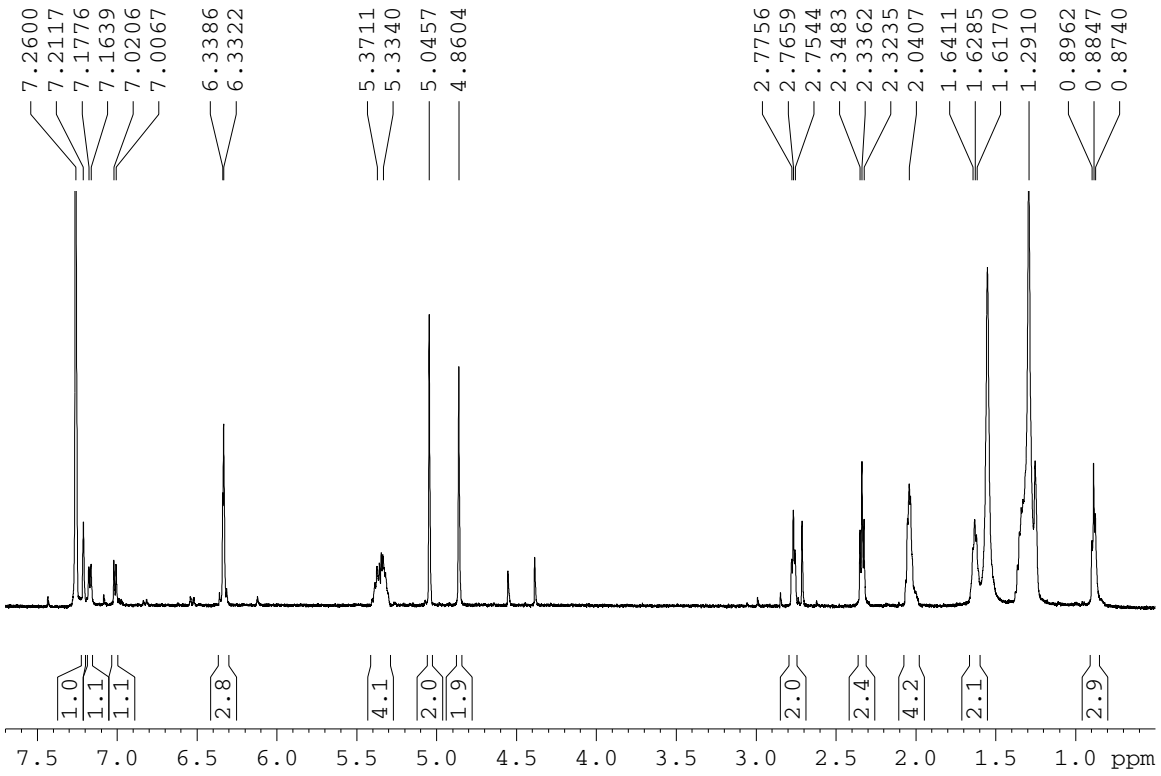
E-3-Chloromethylene-2,3-dihydrobenzo[b]oxepin-7-ylmethyl linoleate (*E*-**1e**):

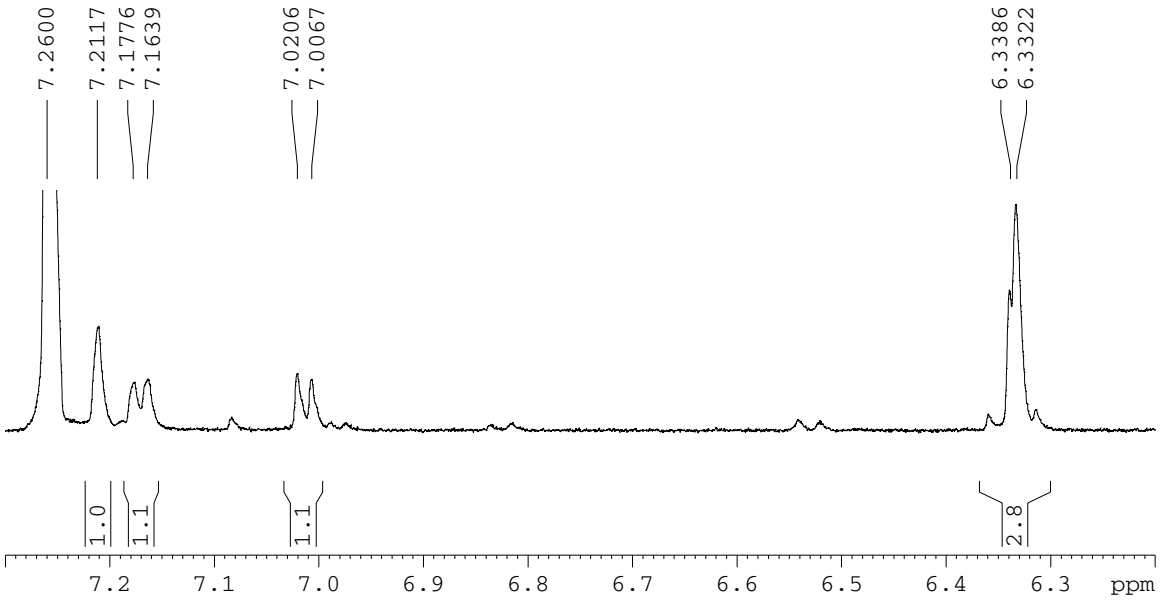
^{13}C NMR (600 MHz, $CDCl_3$, 298 K)



Z-3-Chloromethylene-2,3-dihydrobenzo[b]oxepin-7-ylmethyl linoleate (*Z*-**1e**):

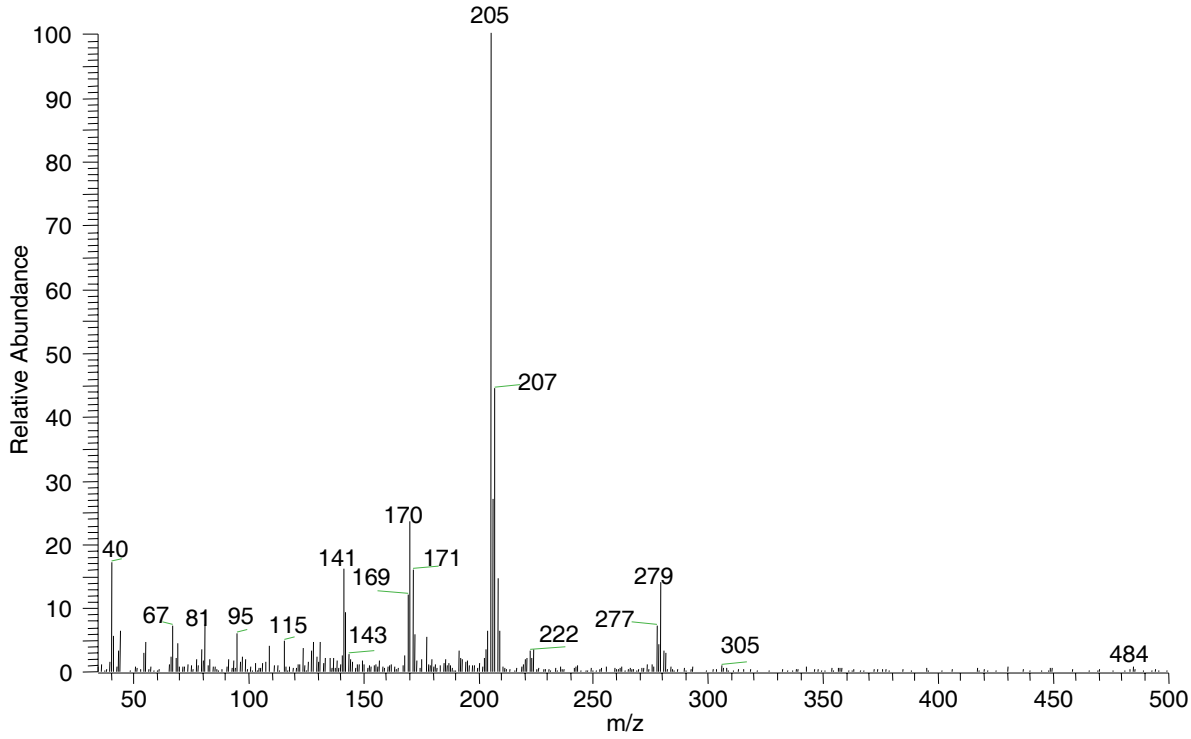
^{1}H NMR (600 MHz, $CDCl_3$, 298 K)





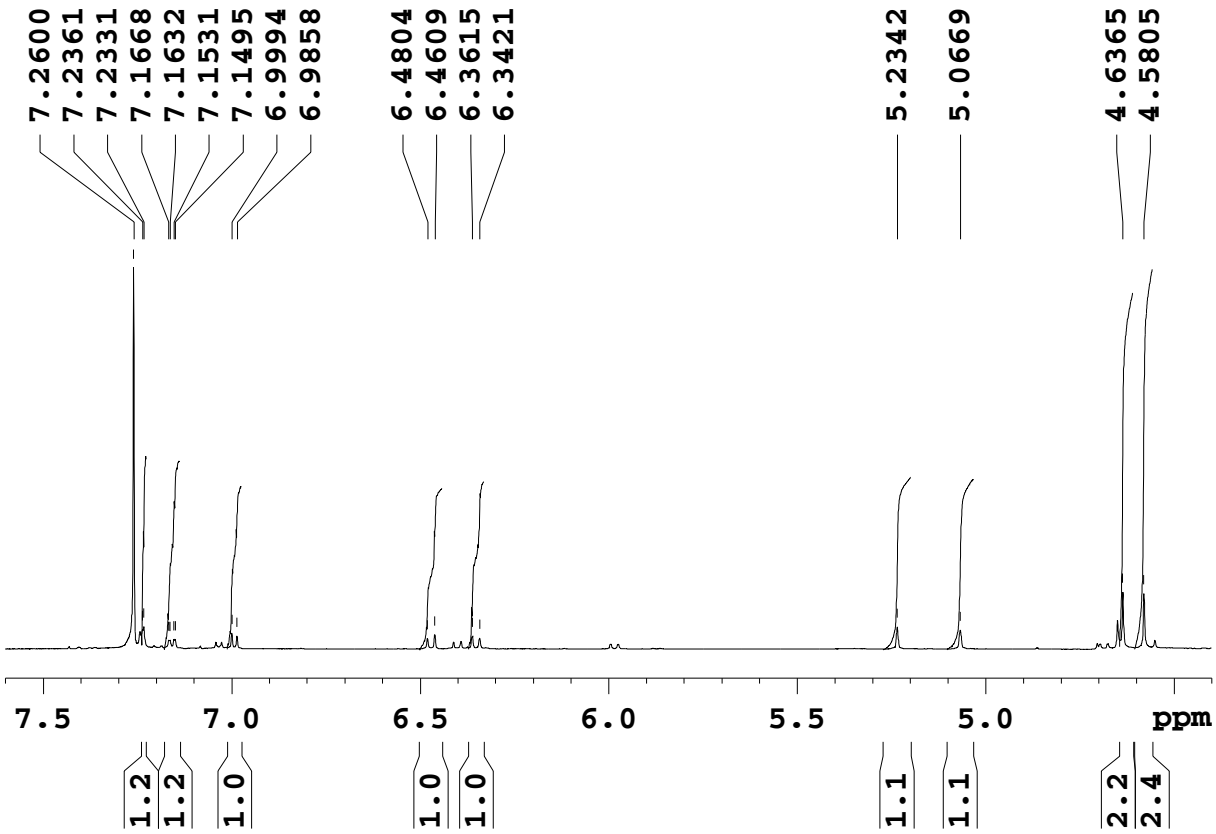
E-3-Chloromethylene-2,3-dihydrobenzo[b]oxepin-7-ylmethyl linoleate (*E*-**1e**) and *Z*-**1e**:

GC-MS



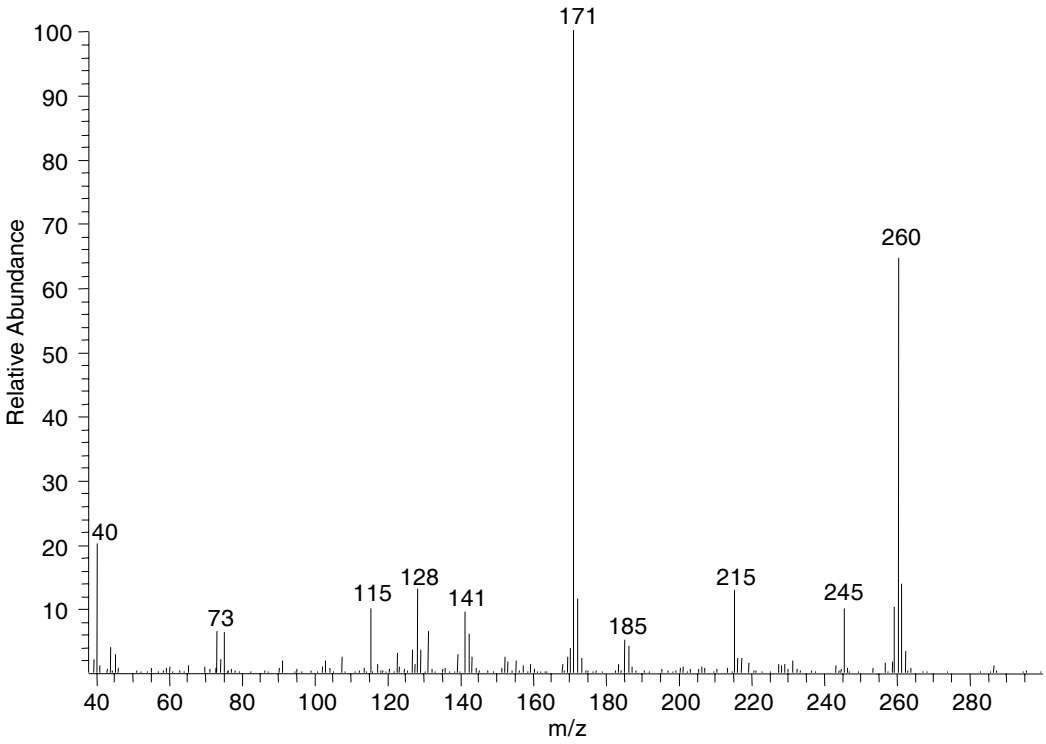
2,3-Dihydrobenzo-3-methylene[b]oxepin-7-ylmethanol (**2**):

^{1}H NMR (600 MHz, $CDCl_3$, 298 K)



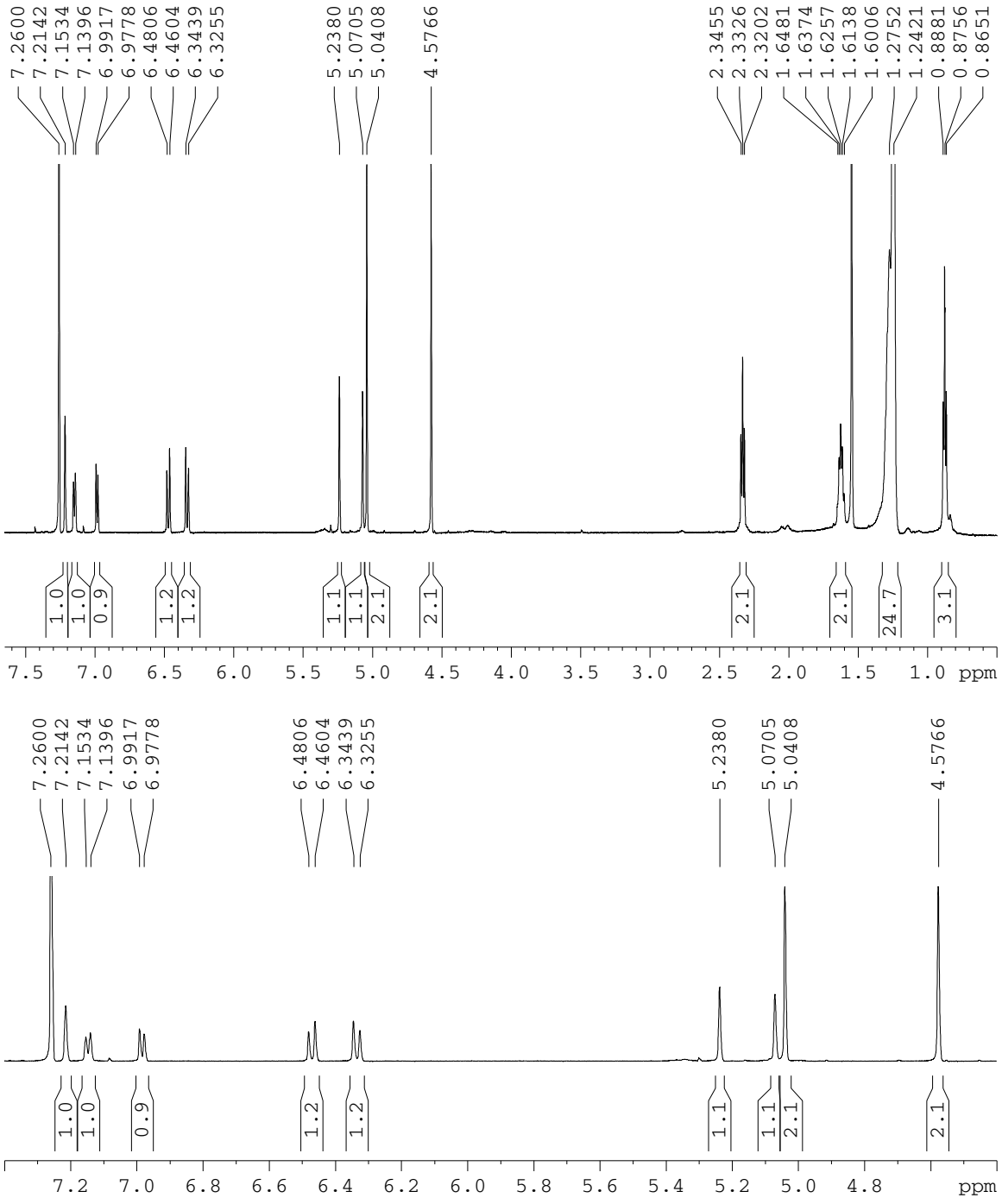
Trimethylsilyl ether of 2,3-dihydrobenzo-3-methylene[b]oxepin-7-ylmethanol (**2**):

GC-MS



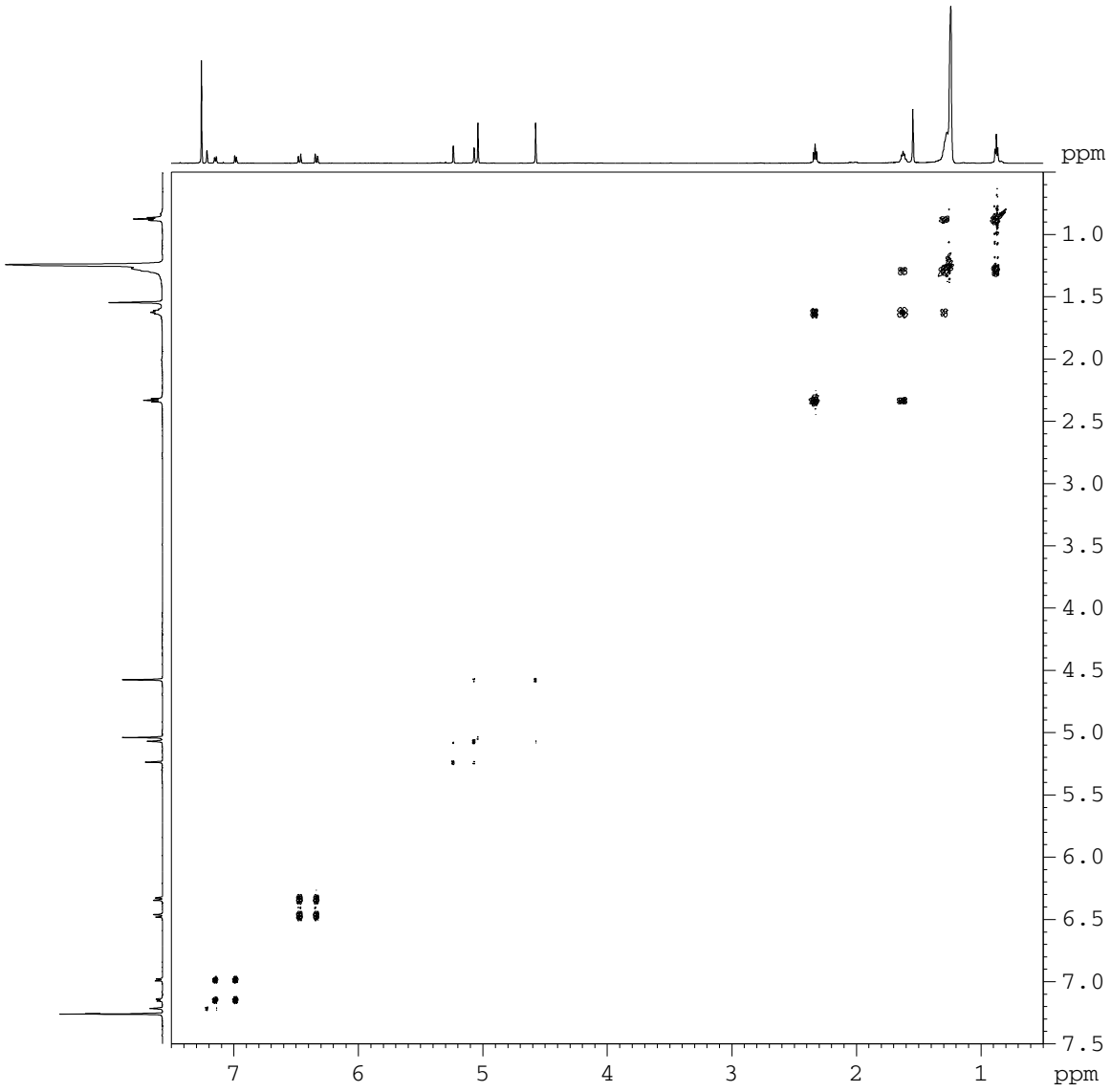
2,3-Dihydrobenzo-3-methylene[b]oxepin-7-ylmethyl palmitate (**2a**):

^{1}H NMR (600 MHz, $CDCl_3$, 298 K)



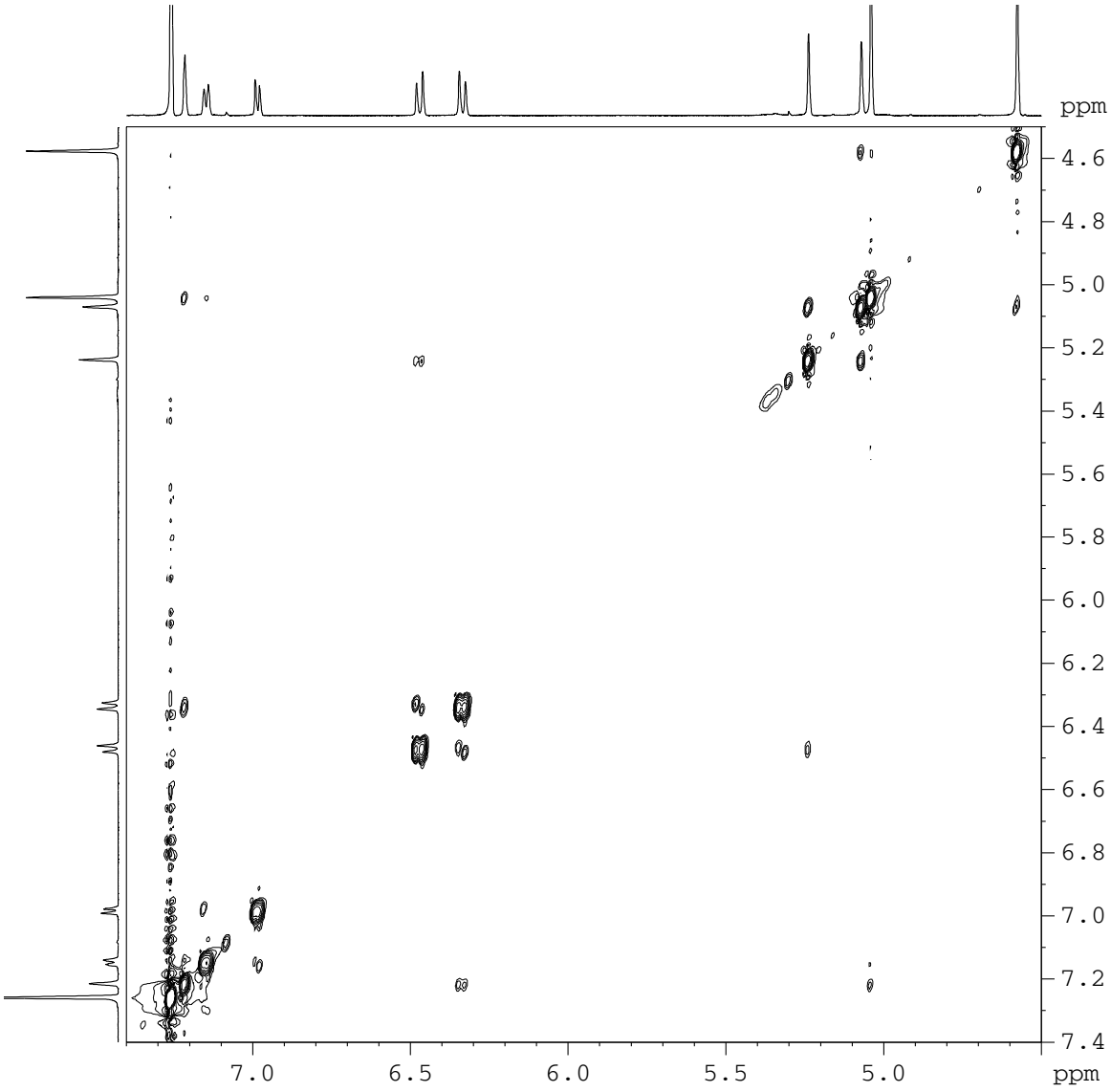
2,3-Dihydrobenzo-3-methylene[b]oxepin-7-ylmethyl palmitate (**2a**):

COSY (600 MHz, $CDCl_3$, 298 K)



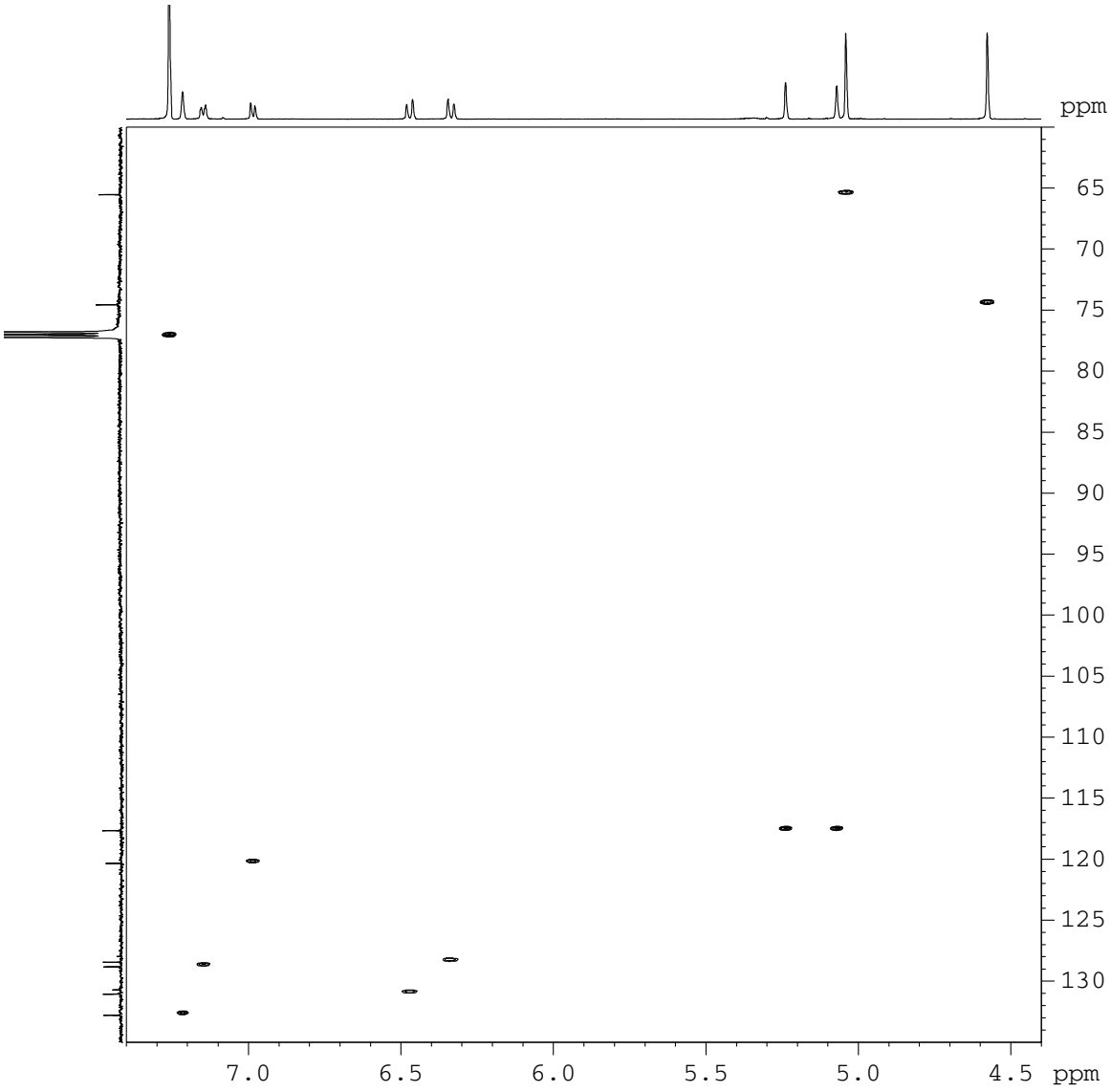
2,3-Dihydrobenzo-3-methylene[b]oxepin-7-ylmethyl palmitate (**2a**):

NOESY (600 MHz, $CDCl_3$, 298 K)



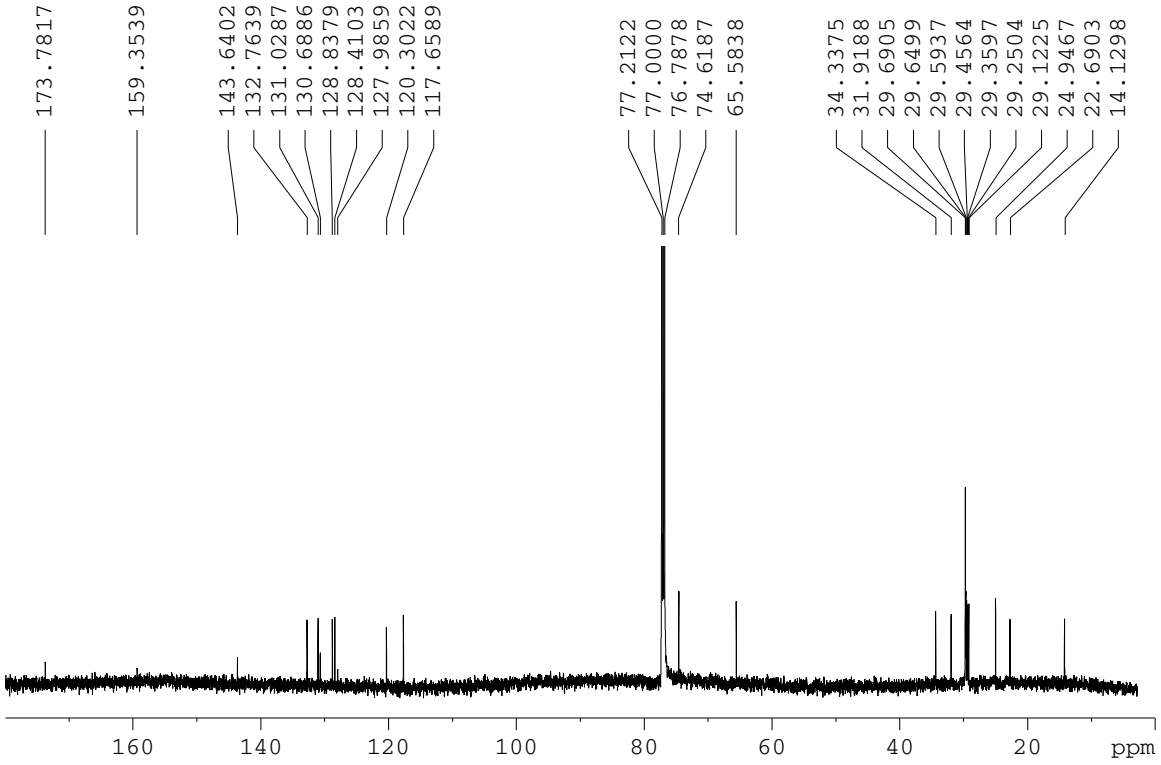
2,3-Dihydrobenzo-3-methylene[b]oxepin-7-ylmethyl palmitate (**2a**):

HSQC (600 MHz, $CDCl_3$, 298 K)



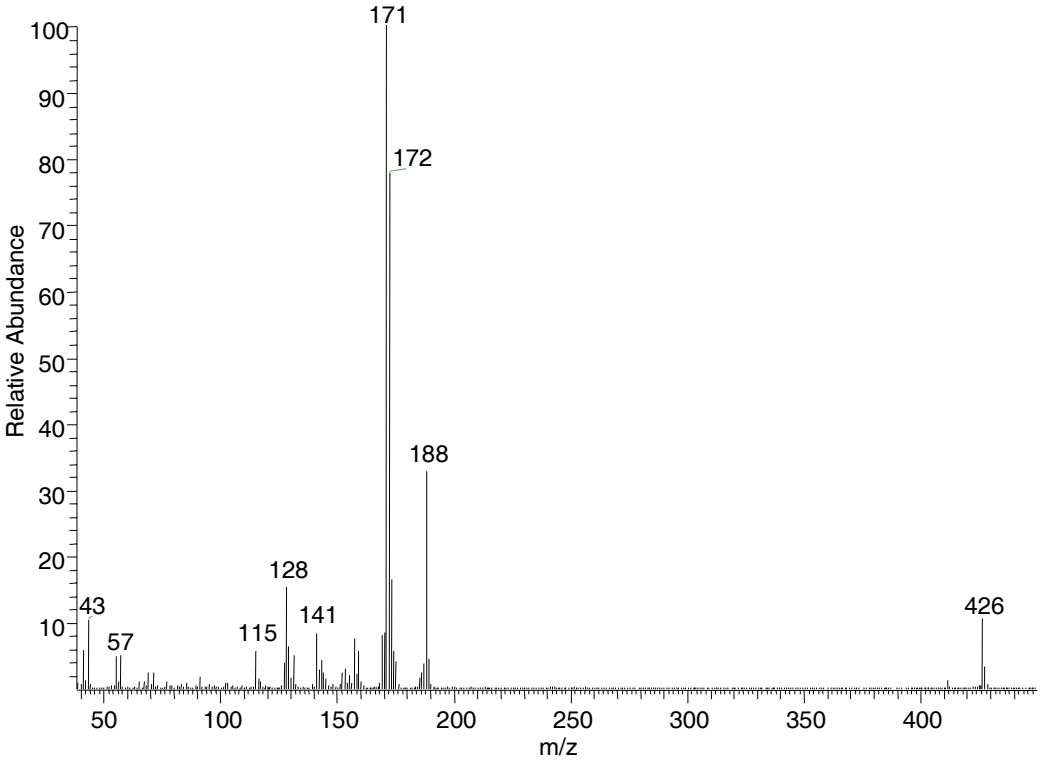
2,3-Dihydrobenzo-3-methylene[b]oxepin-7-ylmethyl palmitate (**2a**):

^{13}C NMR (600 MHz, $CDCl_3$, 298 K)



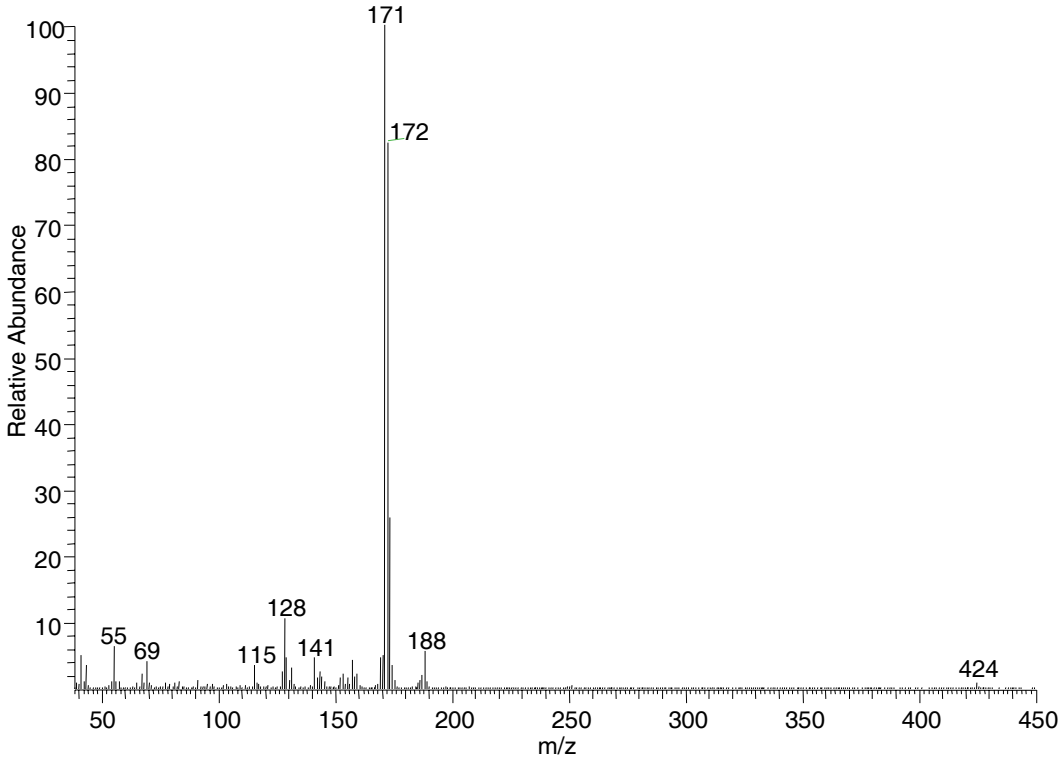
2,3-Dihydrobenzo-3-methylene[b]oxepin-7-ylmethyl palmitate (**2a**):

GC-MS



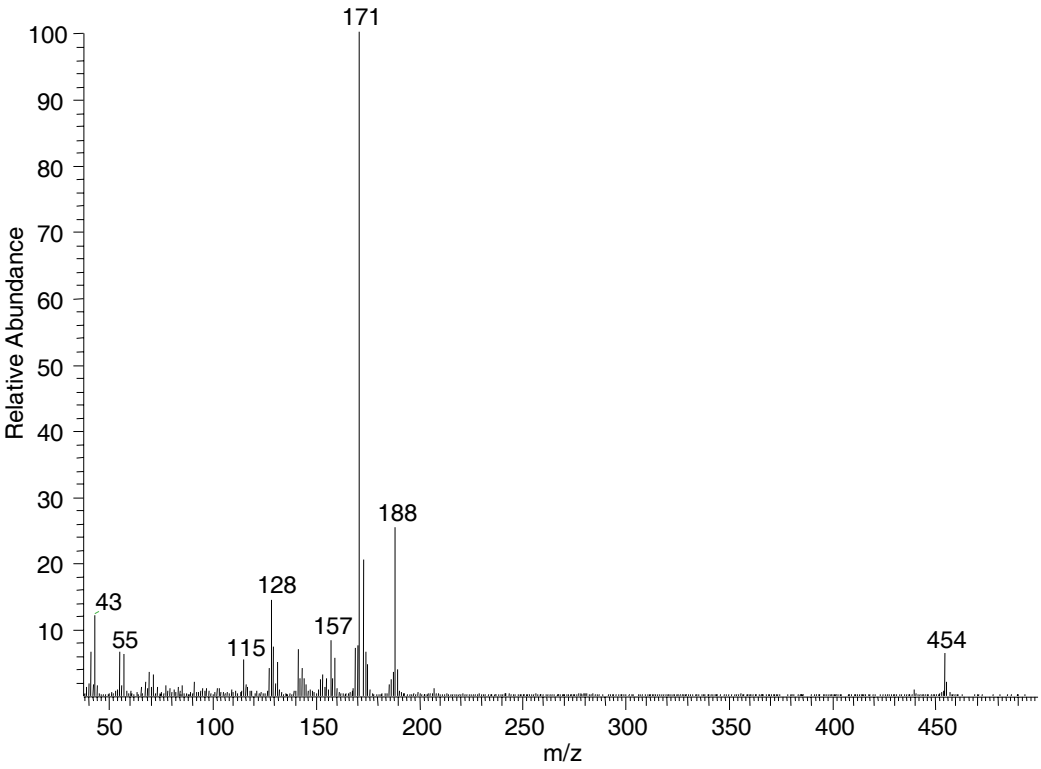
2,3-Dihydrobenzo-3-methylene[b]oxepin-7-ylmethyl palmitoleate (**2b**):

GC-MS



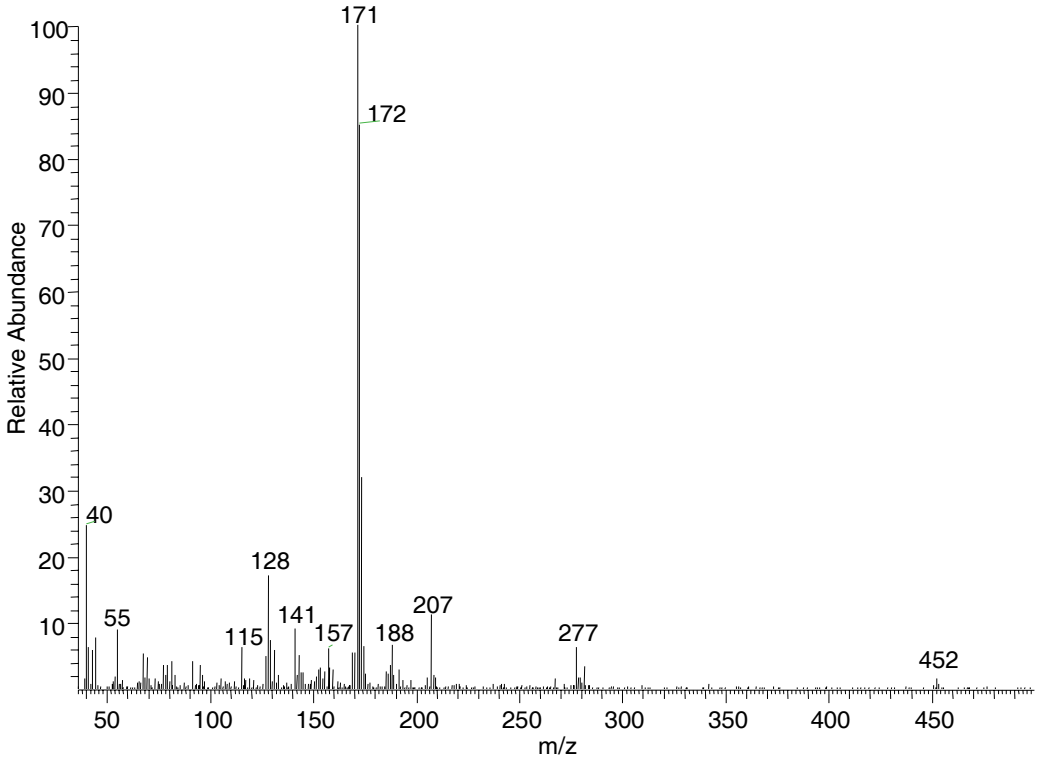
2,3-Dihydrobenzo-3-methylene[b]oxepin-7-ylmethyl stearate (**2c**):

GC-MS



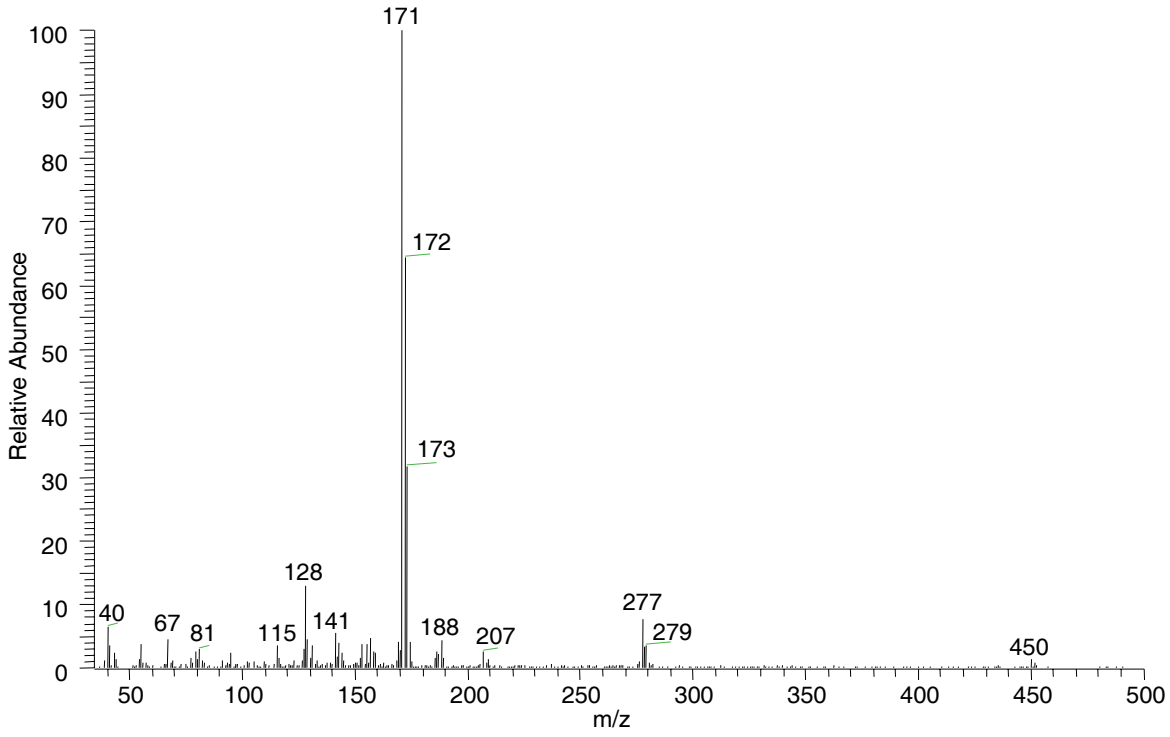
2,3-Dihydrobenzo-3-methylene[b]oxepin-7-ylmethyl oleate (**2d**):

GC-MS



2,3-Dihydrobenzo-3-methylene[b]oxepin-7-ylmethyl linoleate (**2e**):

GC-MS



1-(3-Chloromethylene-2,3-dihydro-6-hydroxybenzo[b]oxepin-7-yl)-ethanone (**3**):

GC-MS