

Exam #3

This is an open-book, open notes exam. Show your work, so you can receive credit for correct parts of the final molecule.

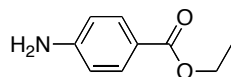
1. (20 points)  $C_9H_{11}NO_2$

**$^{13}C$  NMR**

166.8, s  
150.9, s  
131.5, d (2)  
120.0, s  
113.7, d (2)  
60.3, t  
14.4, q

**$^1H$  NMR**

7.86, d,  $J = 8.8$  Hz, 2H  
6.64, d,  $J = 8.8$  Hz, 2H  
4.32, q,  $J = 7.2$  Hz, 2H  
4.08, bs, 2H, exchanges  
1.37, t,  $J = 7.2$  Hz, 3H



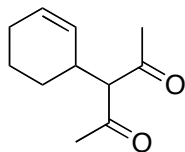
2. (40 points)  $C_{11}H_{16}O_2$

**$^{13}C$  NMR**

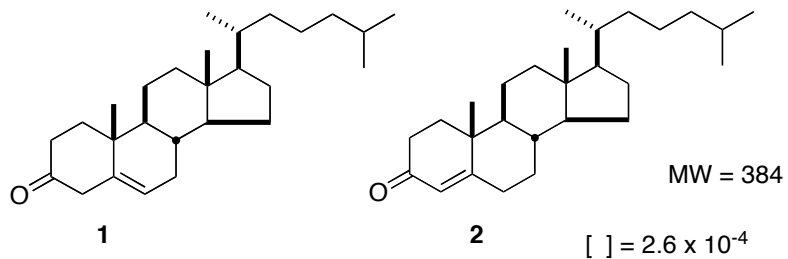
20.4, t  
24.7, t  
26.4, t  
29.9, q (2)  
35.4, d  
74.5, d  
126.9, d  
129.7, d  
203.5, s (2)

**$^1H$  NMR**

1.19-1.22, m, 1H  
1.57-1.59, m, 1H  
1.68-1.74, m, 2H  
1.98-2.00, m, 2H  
2.18, s, 6H  
3.00-3.04, m, 1H  
3.61, d,  $J=10.6$  Hz, 1H  
5.38, dd,  $J=10.2$  Hz, 2.4Hz, 1H  
5.75-5.80, m, 1H



3. (40 points) You have isolated 5-cholestenone **1**. It is crystalline and gives a reasonable melting point, but you are concerned that it might contain a little bit of the more stable isomer **2**. For a 5.0 mg sample in 50 mL of ethanol, you measure  $A = 0.240$  at 280 nm. What % **2** is in the sample?



$\epsilon_{280}$

800

11,200

$$[\mathbf{1}] + [\mathbf{2}] = 2.6 \times 10^{-4}$$

$$800[\mathbf{1}] + 11,200 [\mathbf{2}] = 0.240$$

$$[\mathbf{2}] = 3.1 \times 10^{-6}$$

$$[\mathbf{2}] = 1.2\%$$