Chem 333
Fall 2012
Exam #4
December 3, 2012 Name_____Key_____

1. (30 points) Deduce the structure of **A**.

A $C_9H_9NO_2$

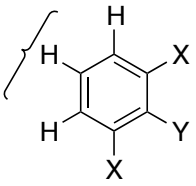
^{1}H NMR:
7.43, t, J = 8.4 Hz, 1H
6.55, d, J = 8.4 Hz, 2H
3.93, s, 6H

^{13}C NMR:
162.6, s (2)
134.8, d
114.2, s
103.4, d (2)
91.2, s
56.2, q (2)

1. IHD = 6 no OH, NH

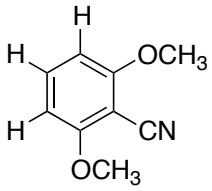
2. Benzene ring with three substituents, ortho to each other

note *ortho* coupling constants



162.6, s (2) says O directly atteched to ring
56.2, q says that these are Me ethers

That leaves CN for the substituent, 114.2, s



2. (30 points) Deduce the structure of B.

B $C_{15}H_{20}O_2$ MS: 232 (90), 163 (100), 115 (45)

^{1}H NMR:	**^{13}C NMR:**
0.89, s, 3H	209.6, s
0.96, s, 3H	158.8, s
1.8, m, 2H	136.5, s
2.0, m, 2H	128.3, d
245, m, 2H	123.7, d
3.48, s, 1H	117.3, d
3.82, s, 3H	111.9, d
6.8, m, 3H	67.4, d
7.25, t, J = 7.8 Hz, 1H	55.2, q
	41.5, t
	40.8, s
	22.5, t
	30.6, t
	22.3, q
	17.3, q

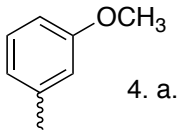
1. IHD = 6 no OH

2. carbonyl 209.6, s is a ketone from chemical shift cyclohexanone or acyclic

benzene is disubstituted, not symmetrical

from ^{1}H NMR carbonyl is not directly attached to ring (from chemical shift of carbonyl also)

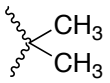
From 158.8, s, O directly atttached to benzene ring
from 55.2, q this is OCH3
from 111.9, d 117.3, d methoxy group has CH ortho to it.
no symmetry

so: 

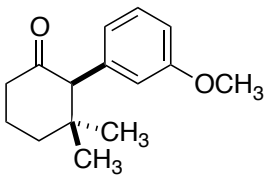
4. a. two methyl groups attached to same carbon, no H's on that carbon, but no symmetry

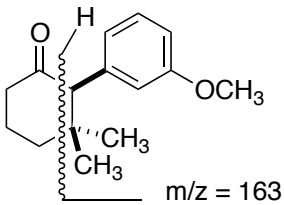
one more ring

b. 3.48, s, 1H a C-H with no C-H neighbors



c. no extra CH2's, so must be cyclohexanone





m/z = 163

3. (40 points) Deduce the structure of C.

C $C_{14}H_{28}O_2$

MS: 228 (40), 171 (100), 130 (35)

IR: 2920, 2870, 1756 cm^{-1}

^{1}H NMR:

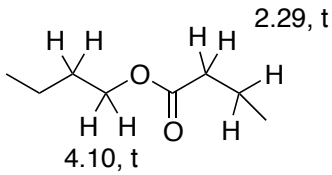
0.95, t, J = 7.2 Hz, 3H
0.98, d, J = 6.9 Hz, 6H
1.3-1.7, m, 15 H
2.29, t, J = 7.4 Hz, 2H
4.10, t, J = 7.3 Hz, 2H

^{13}C NMR:

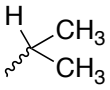
173.9, s
62.9, t
37.4, t
34.4, t
31.9, t
29.3, t
29.2, t
29.1, t
25.1, d
25.0, t
22.7, t
22.5, q (2)
14.1, q

1. IHD = 1 no OH

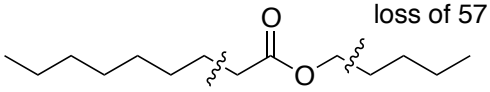
2. 173.9, s ester 1756 cm-1 also



4. a. Branching methyls at one end attached carbon has an H



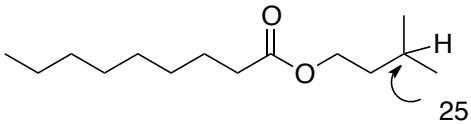
From MS,



loss of 57

loss of 98
= McLafferty

but which end has the branching methyls?



25.1, d must be gamma shifted