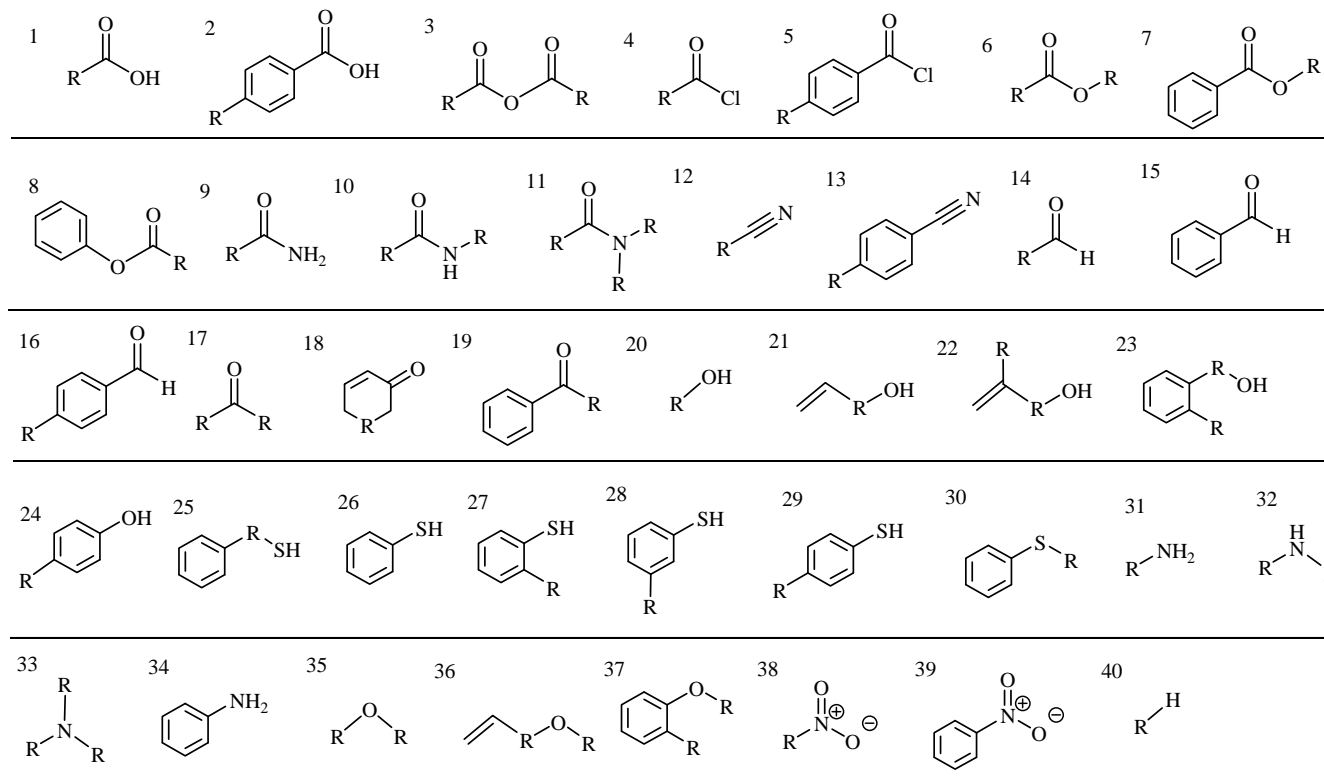
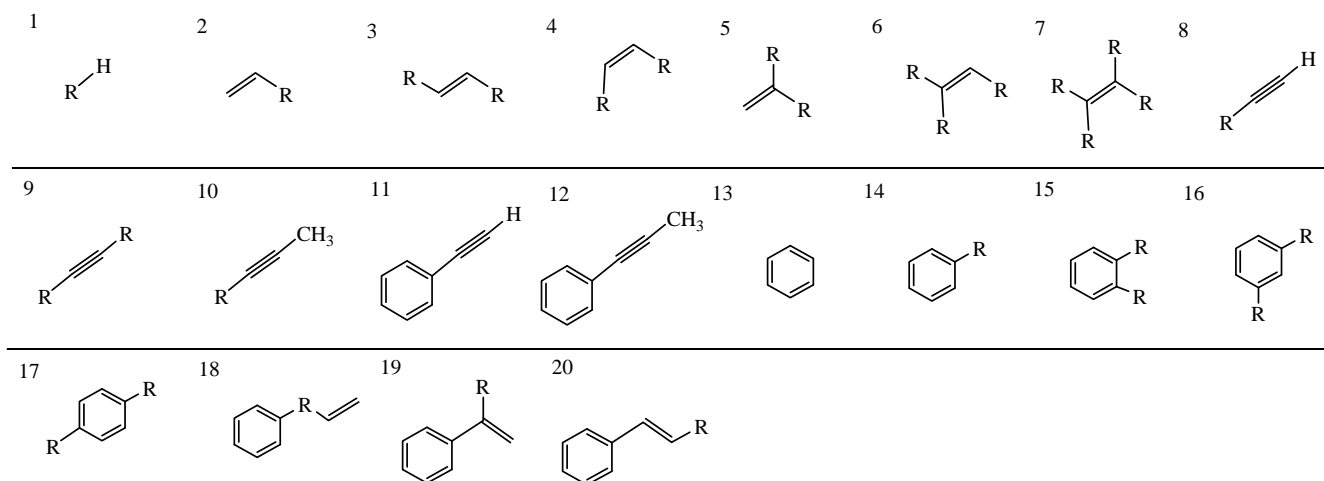


Simulated IR spectra

Group 1 compounds: Functional group patterns are listed below. Match each structure with one of the 40 simulated IR spectra that follow. The wave numbers listed in each spectrum are intended to provide clues as to what the functional group might be. Note your interpretation of what those numbers indicate right on the spectra and write a **structure** (not a number) in the space provided at the right of each IR. Sulfides, tertiary (3o) amines and symmetrical alkynes all lack key diagnostic peaks and can appear similar to one another and similar to simple alkynes. Limited mass spec data is provided to help distinguish these possibilities (M^+ , $M+1$, $M+2$ peaks). Also, watch out for overtone bands ($3200-3400\text{ cm}^{-1}$) in carbonyl compounds ($C=O$). They can be easily mistaken for an amine (N-H) or an alcohol (O-H).

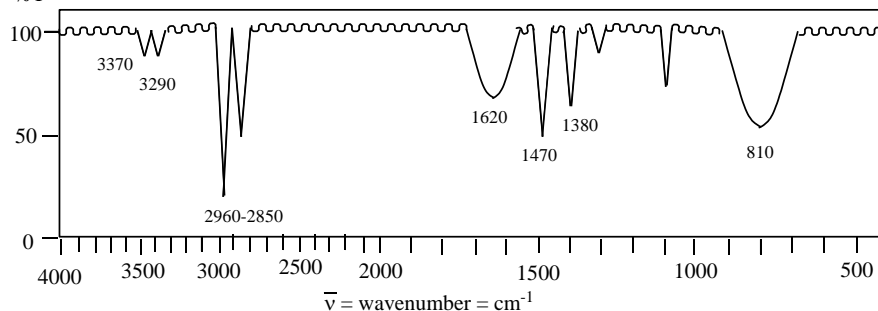


Group 2 compounds: C, H hydrocarbons = alkanyl (=R), alkenyl, alkynyl and aromatic. Answer similarly.



Group 1 compounds: Functional group patterns are listed above (1-40). To the right of each IR draw the structure most consistent with the given IR. Provide a minimal interpretation of the IR bands (e.g. 1° NH₂ stretch, C=O stretch, para substituted aromatic, monosubstituted alkene, etc.) Watch out for carbonyl (C=O) overtone bands.

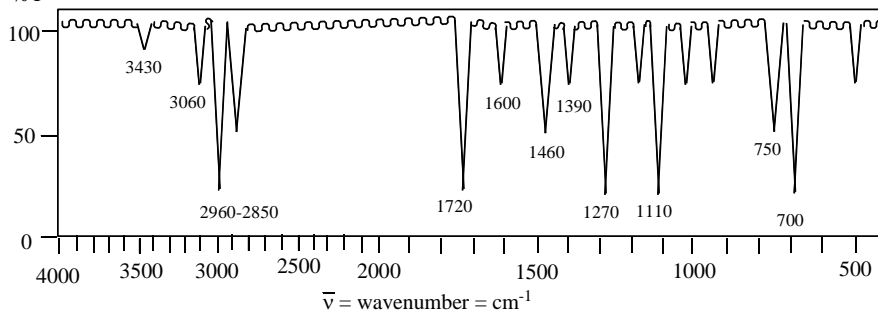
1 %T



Exact Mass: 101.12

M+ = 101.12 (100.0%),
M+1 = 102.12 (6.9%)

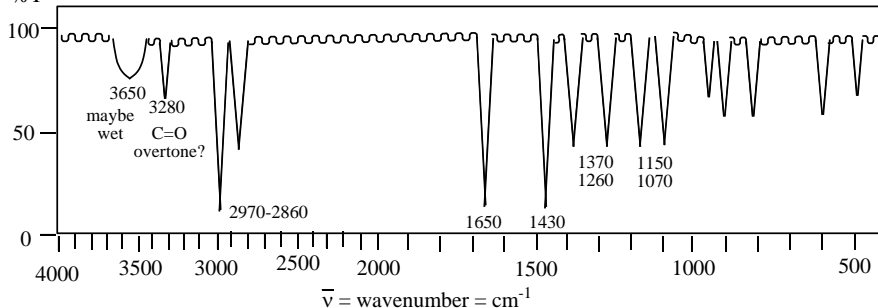
2 %T



Exact Mass: 150.07

M+ = 150.07 (100.0%),
M+1 = 151.07 (9.9%)

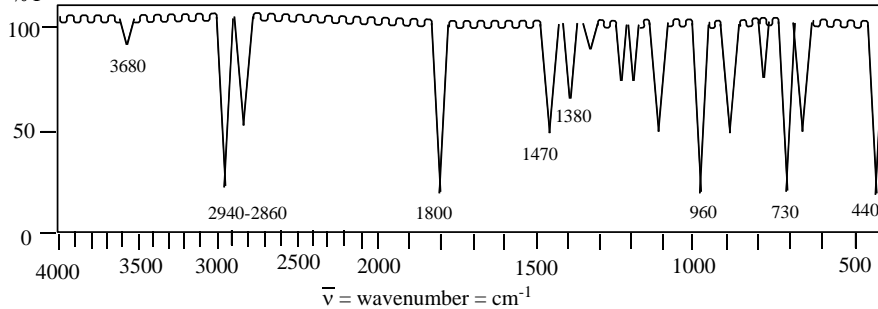
3 %T



Exact Mass: 143.13

M+ = 143.13 (100.0%),
M+1 = 144.13 (9.0%)

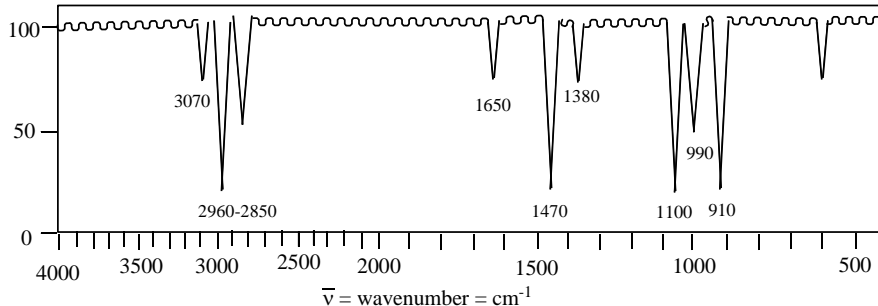
4 %T



Exact Mass: 134.05

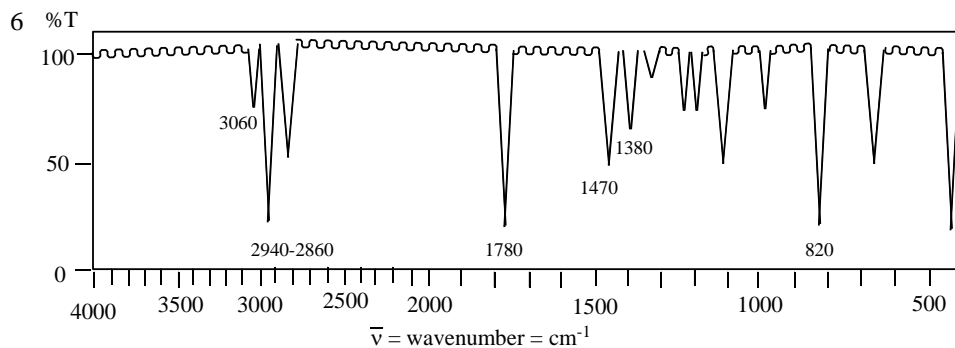
M+ = 134.05 (100.0%),
M+1 = 135.05 (6.5%),
M+2 = 136.05 (32.2%),
M+3 = 137.05 (2.1%)

5 %T

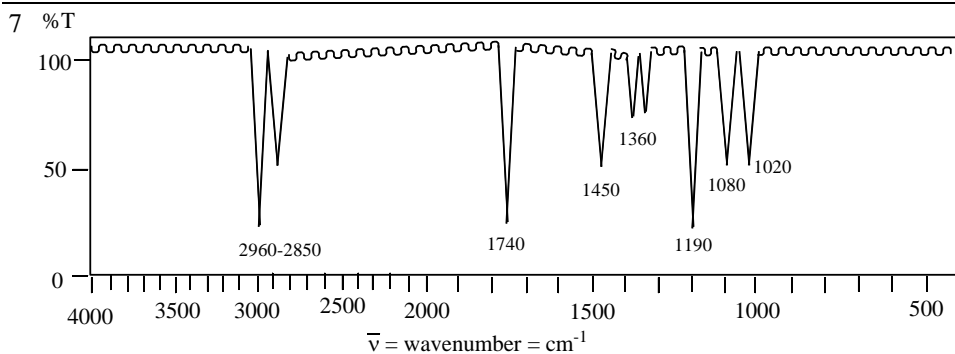


Exact Mass: 114.1

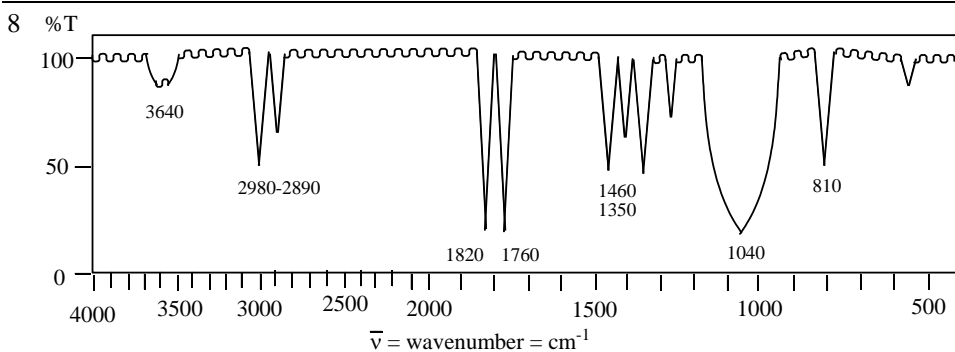
M+ = 114.10 (100.0%),
M+1 = 115.11 (7.8%)



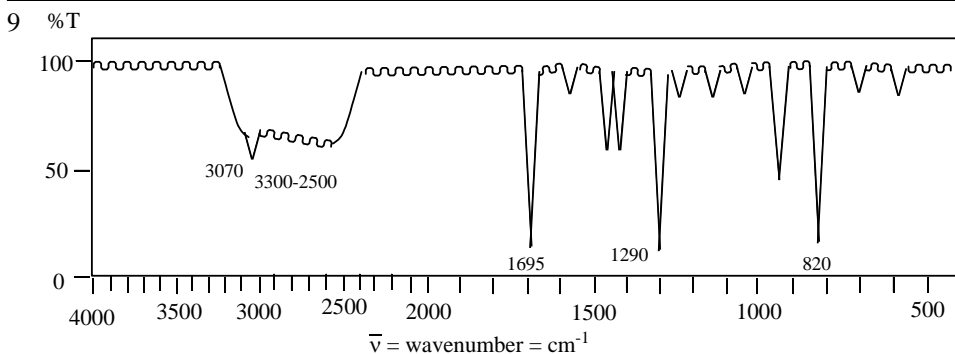
Exact Mass: 154.02
 M+ = 154.02 (100.0%),
 M+1 = 155.02 (8.8%),
 M+2 = 156.02 (32.2%),
 M+3 = 157.02 (2.8%)



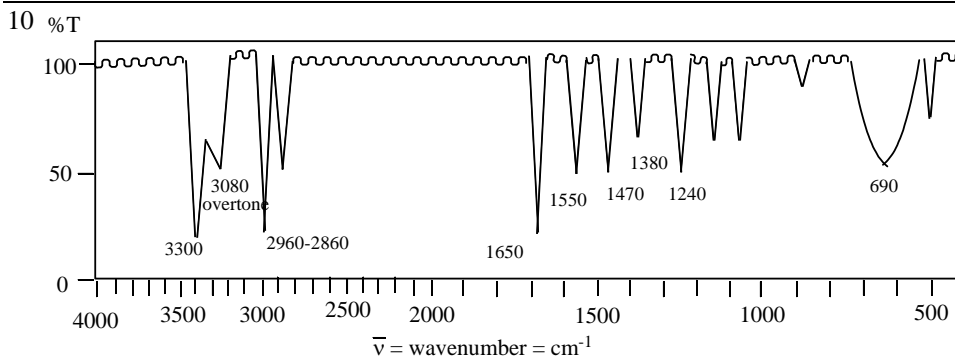
Exact Mass: 144.12
 M+ = 144.12 (100.0%),
 M+1 = 145.12 (8.9%)



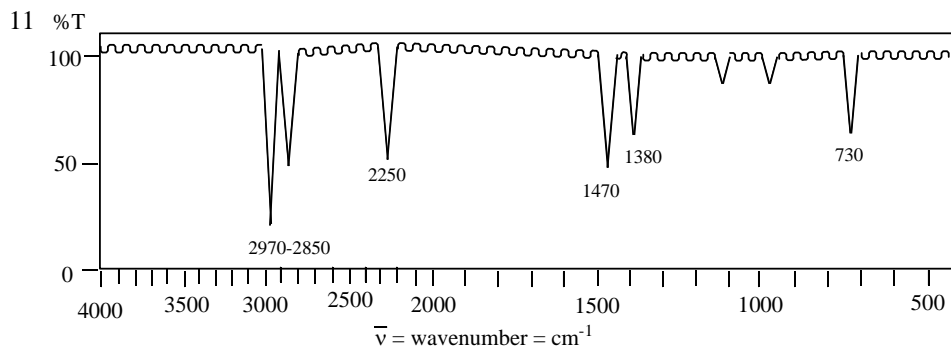
Exact Mass: 158.09
 M+ = 158.09 (100.0%),
 M+1 = 159.10 (8.9%)



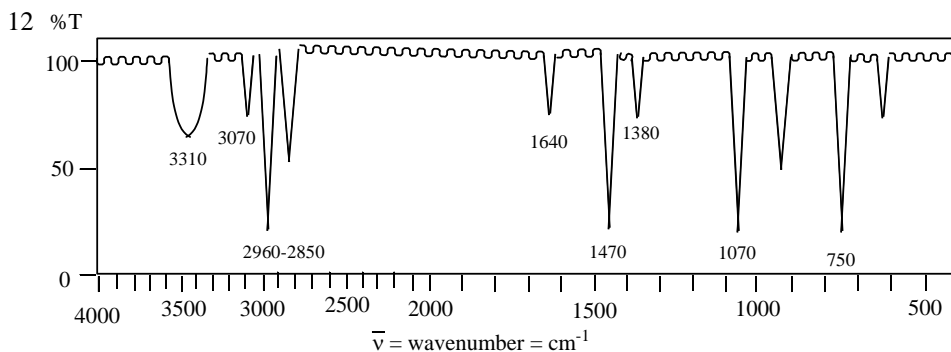
Exact Mass: 136.05
 M+ = 136.05 (100.0%),
 M+1 = 137.06 (8.8%)



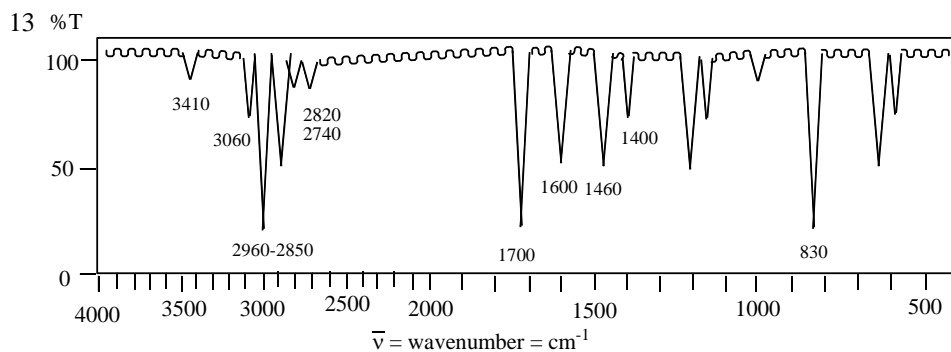
Exact Mass: 129.12
 M+ = 129.12 (100.0%),
 M+1 = 130.12 (7.8%)



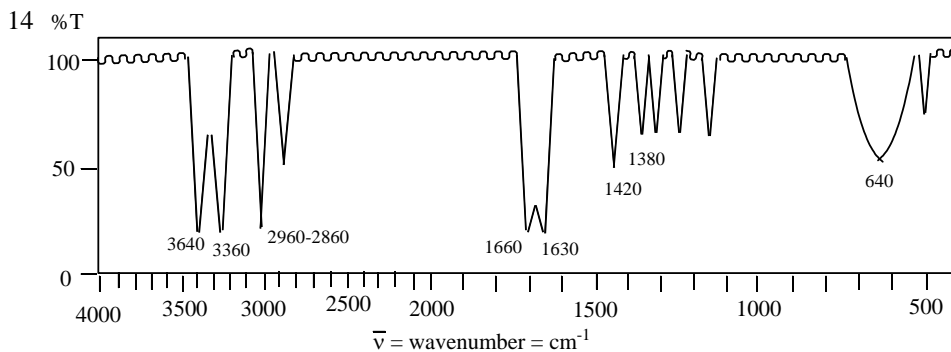
Exact Mass: 97.09
 M+ = 97.09 (100.0%),
 M+1 = 98.09 (6.9%)



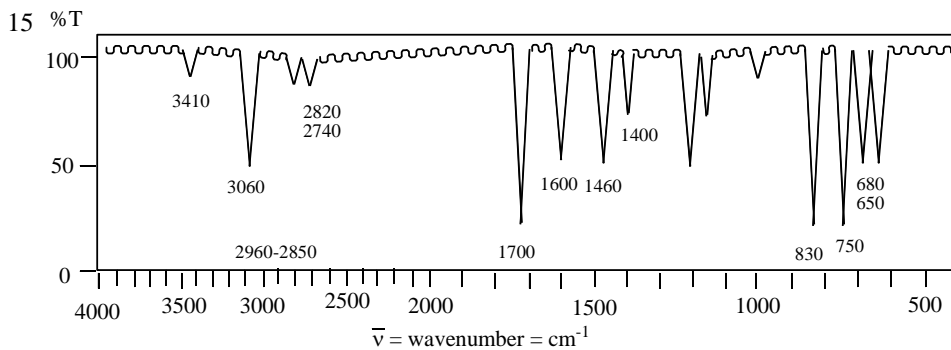
Exact Mass: 136.09
 M+ = 136.09 (100.0%),
 M+1 = 137.09 (9.8%)



Exact Mass: 134.07
 M+ = 134.07 (100.0%),
 M+1 = 135.08 (9.9%)

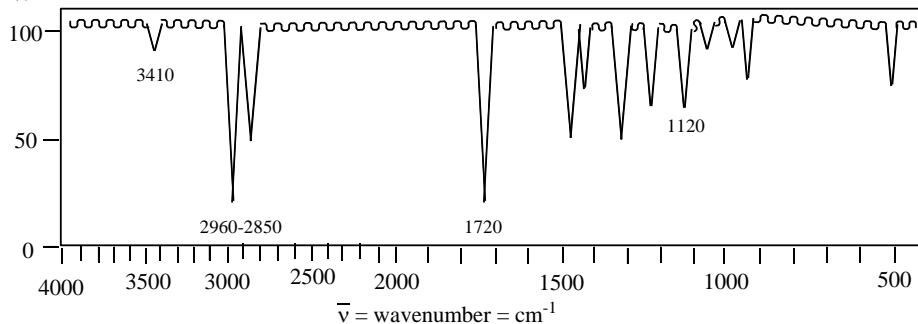


Exact Mass: 115.1
 M+ = 115.10 (100.0%),
 M+1 = 116.10 (6.9%)



Exact Mass: 106.04
 M+ = 106.04 (100.0%),
 M+1 = 107.05 (7.7%)

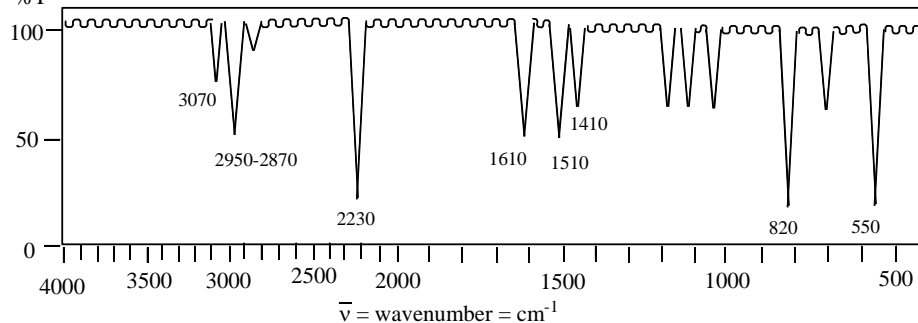
16 %T



Exact Mass: 114.1

$M^+ = 114.10$ (100.0%),
 $M+1 = 115.11$ (7.8%)
 1

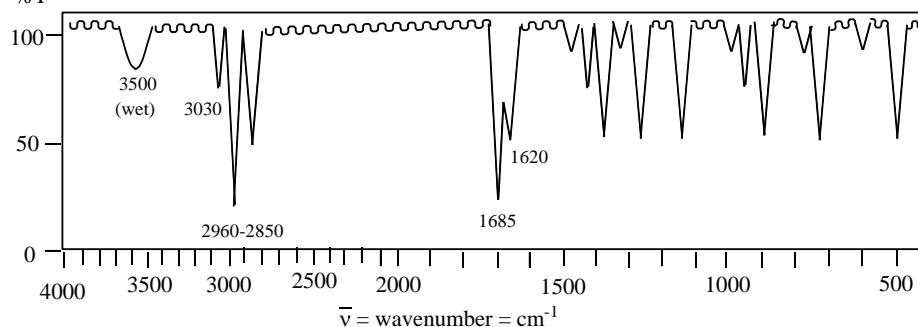
17 %T



Exact Mass: 131.07

$M^+ = 131.07$ (100.0%),
 $M+1 = 132.08$ (9.8%)

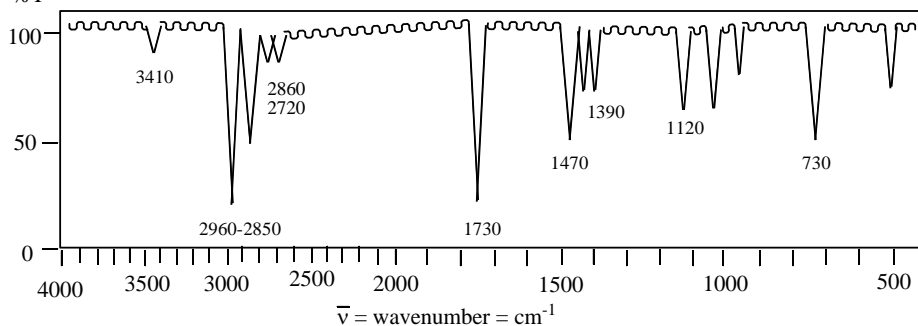
18 %T



Exact Mass: 96.06

$M^+ = 96.06$ (100.0%),
 $M+1 = 97.06$ (6.6%)

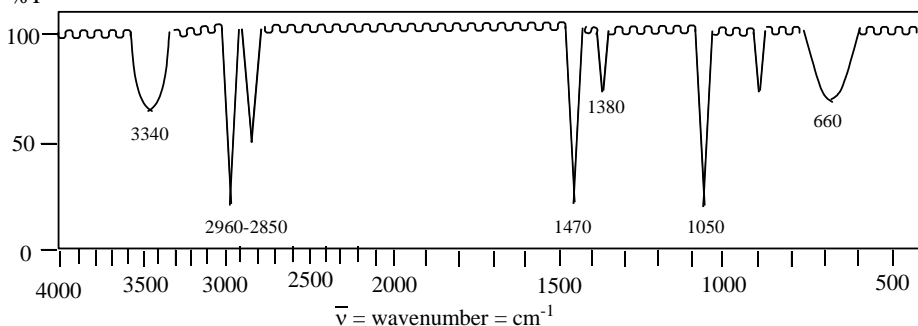
19 %T



Exact Mass: 100.09

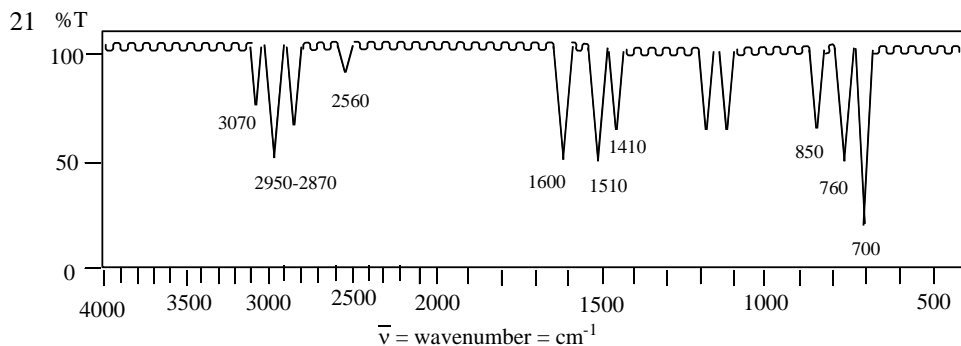
$M^+ = 100.09$ (100.0%),
 $M+1 = 101.09$ (6.5%)

20 %T



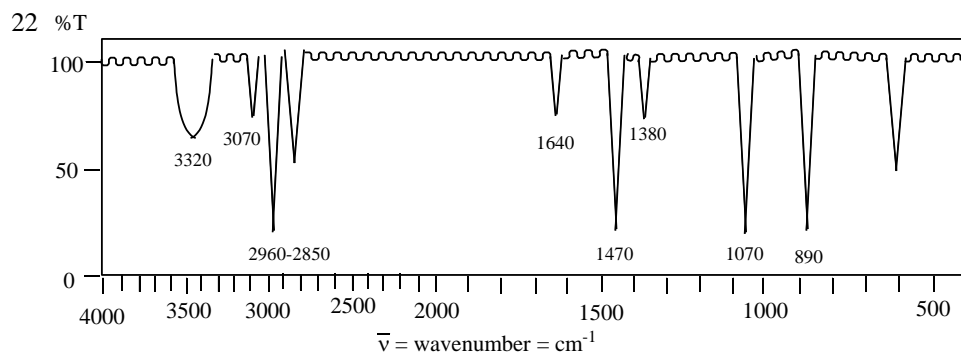
Exact Mass: 100.09

$M^+ = 100.09$ (100.0%),
 $M+1 = 101.09$ (6.5%)



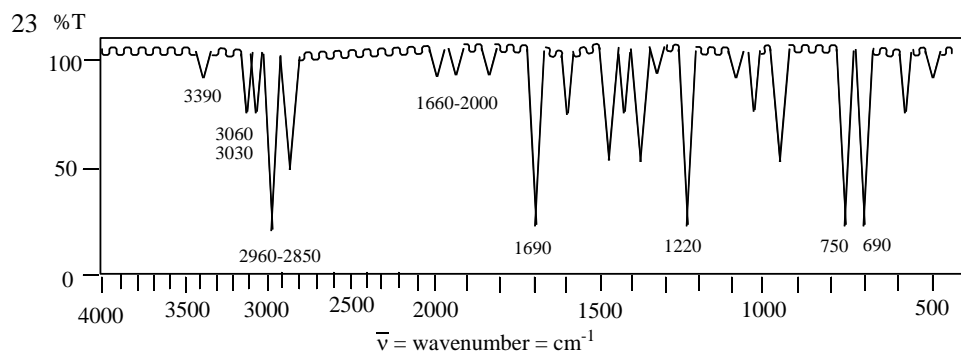
Exact Mass: 152.07

M^+ = 152.07 (100.0%),
 $M+1$ = 153.07 (10.7%),
 $M+2$ = 154.06 (4.5%)



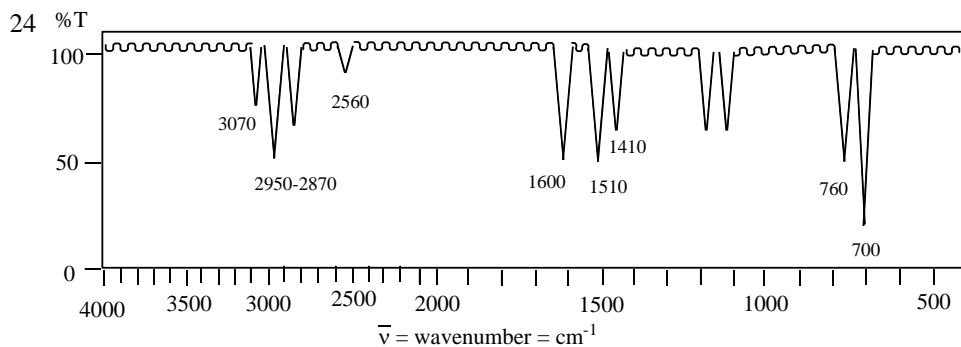
Exact Mass: 100.09

M^+ = 100.09 (100.0%),
 $M+1$ = 101.09 (6.5%)



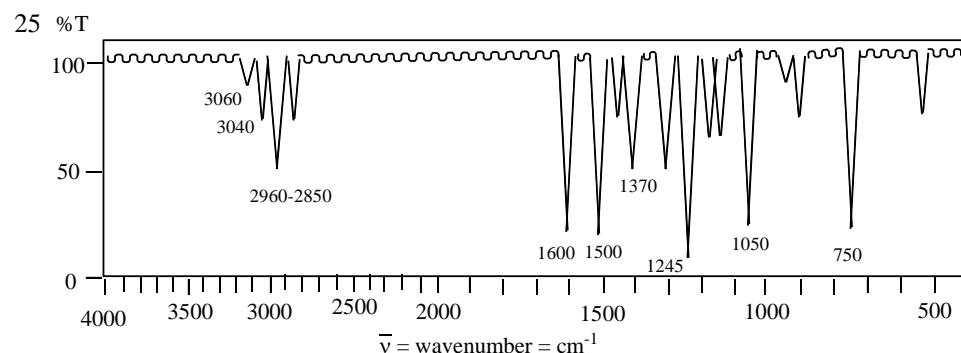
Exact Mass: 134.07

M^+ = 134.07 (100.0%),
 $M+1$ = 135.08 (9.9%)



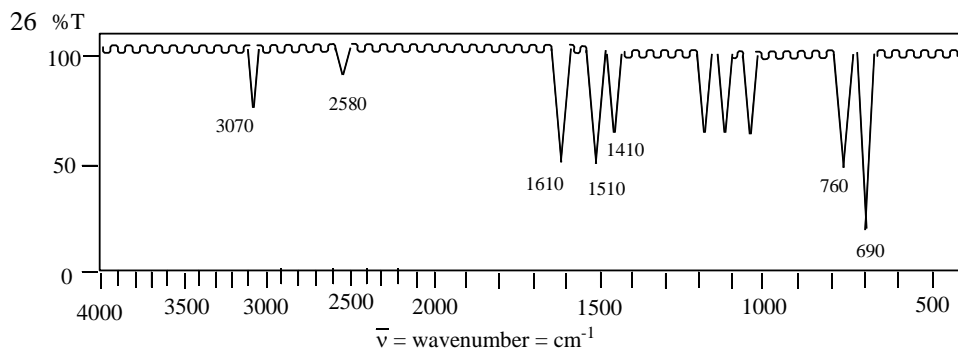
Exact Mass: 152.07

M^+ = 152.07 (100.0%),
 $M+1$ = 153.07 (10.7%),
 $M+2$ = 154.06 (4.5%)



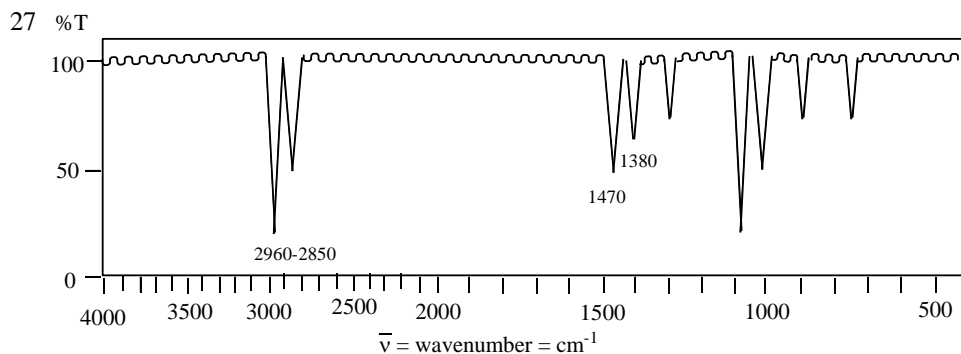
Exact Mass: 136.09

M^+ = 136.09 (100.0%),
 $M+1$ = 137.09 (9.8%)



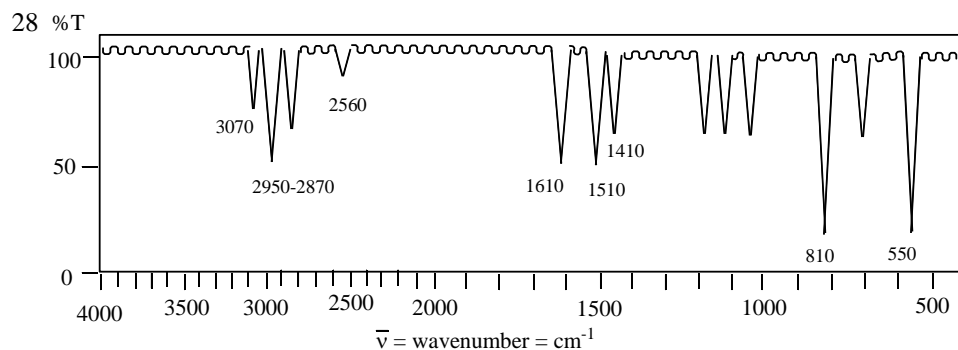
Exact Mass: 110.02

$M^+ = 110.02$ (100.0%),
 $M+1 = 111.02$ (7.3%),
 $M+2 = 112.01$ (4.5%)



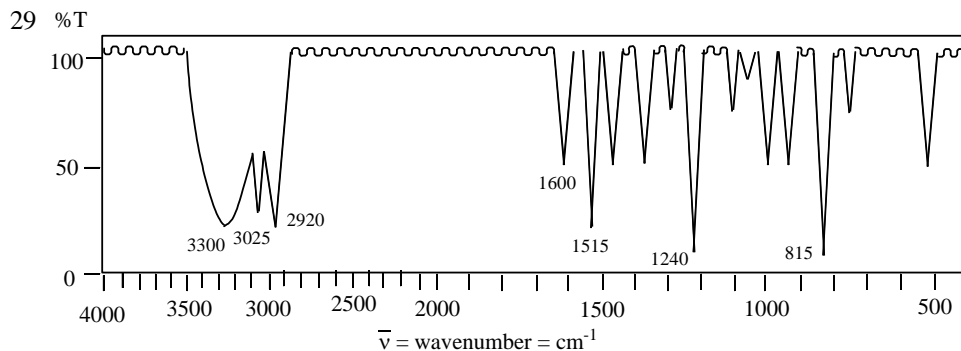
Exact Mass: 129.15

$M^+ = 129.15$ (100.0%),
 $M+1 = 130.16$ (8.9%)



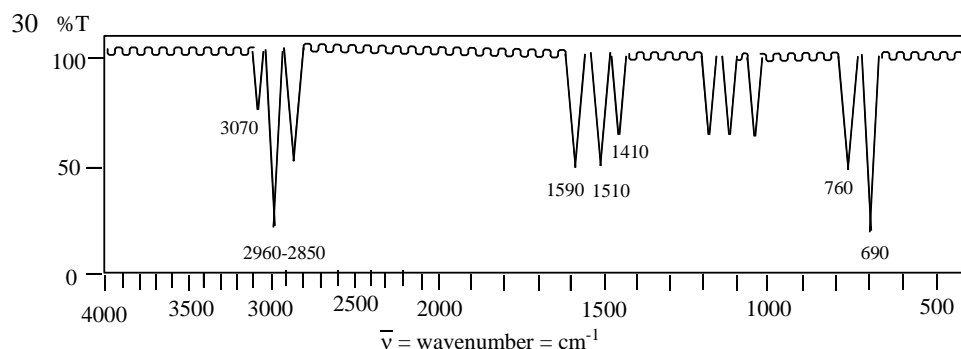
Exact Mass: 138.05

$M^+ = 138.05$ (100.0%),
 $M+1 = 139.05$ (9.5%),
 $M+2 = 140.05$ (4.6%)



Exact Mass: 122.07

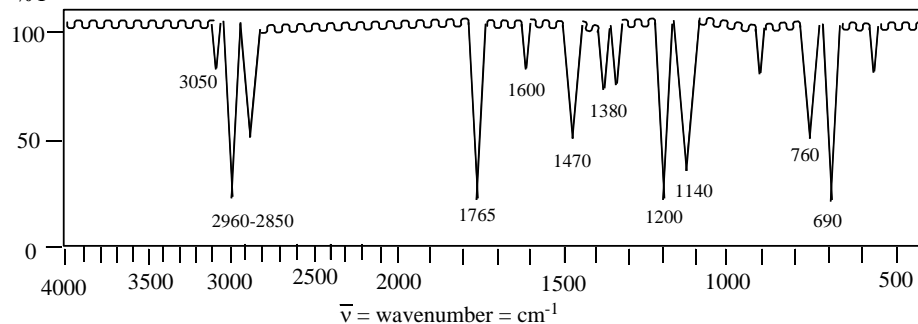
$M^+ = 122.07$ (100.0%),
 $M+1 = 123.08$ (8.8%)



Exact Mass: 152.07

$M^+ = 152.07$ (100.0%),
 $M+1 = 153.07$ (10.7%),
 $M+2 = 154.06$ (4.5%)

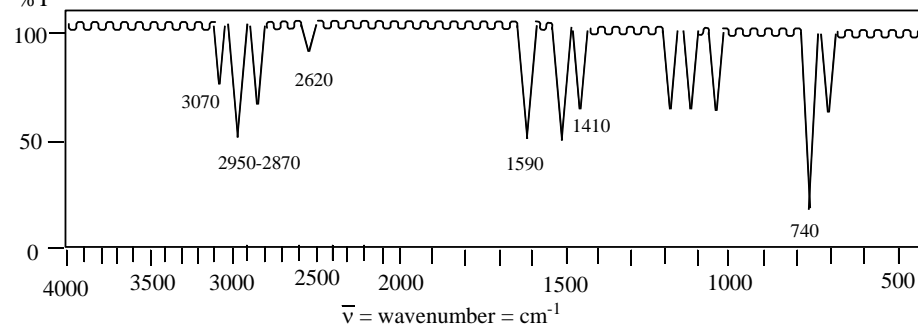
31 %T



Exact Mass: 178.1

M^+ = 178.10 (100.0%),
 $M+1$ = 179.10 (12.0%)

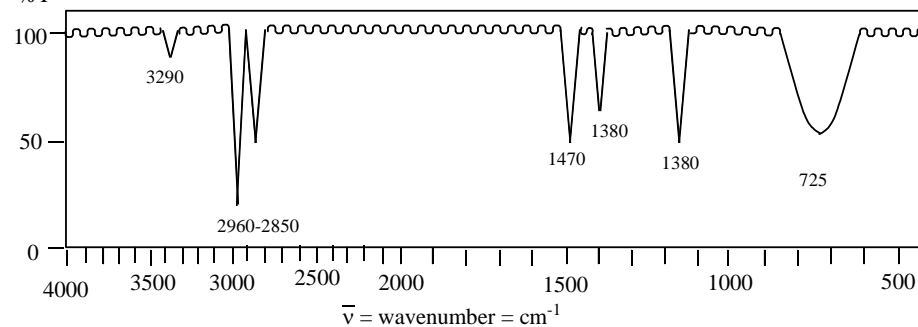
32 %T



Exact Mass: 152.07

M^+ = 152.07 (100.0%),
 $M+1$ = 153.07 (10.7%),
 $M+2$ = 154.06 (4.5%)

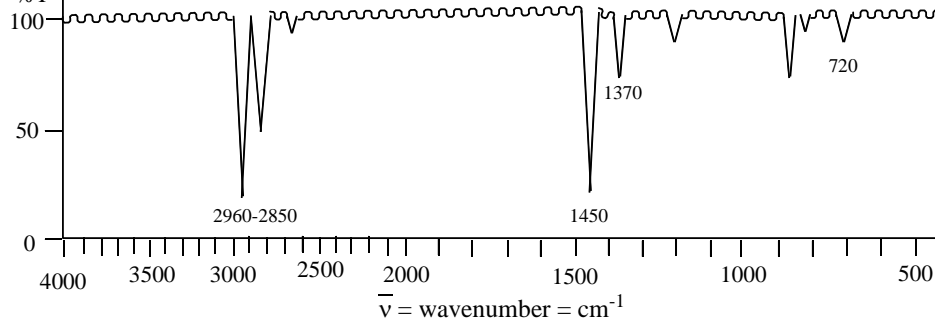
33 %T



Exact Mass: 129.15

M^+ = 129.15 (100.0%),
 $M+1$ = 130.16 (8.9%)

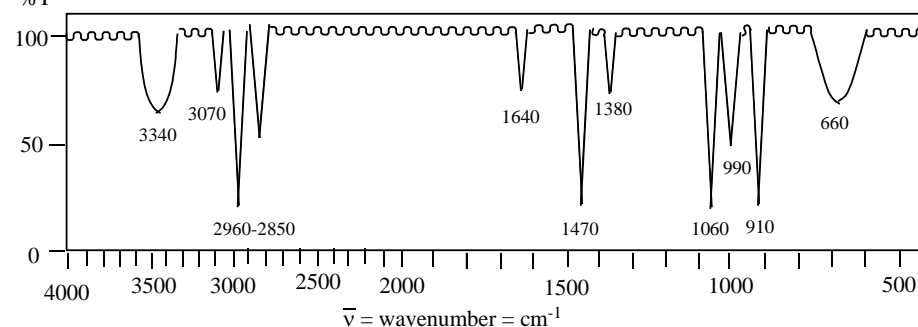
34 %T



Exact Mass: 100.13

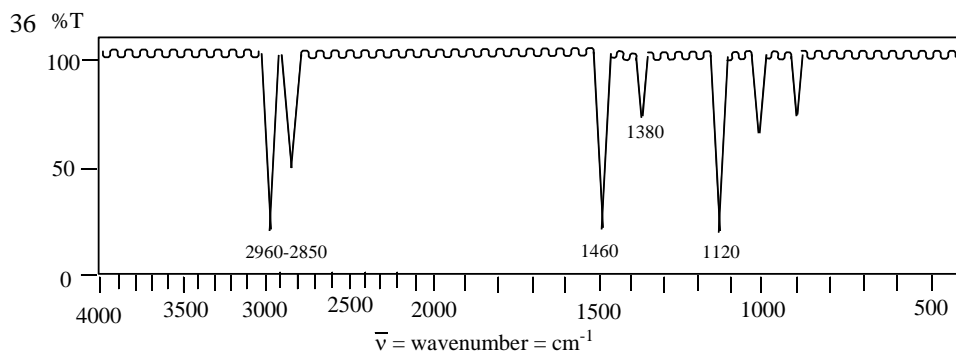
M^+ = 100.13 (100.0%),
 $M+1$ = 101.13 (7.8%)

35 %T

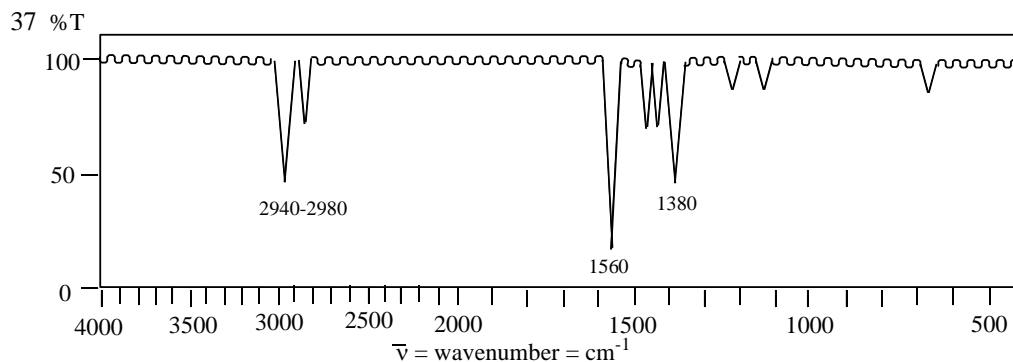


Exact Mass: 100.09

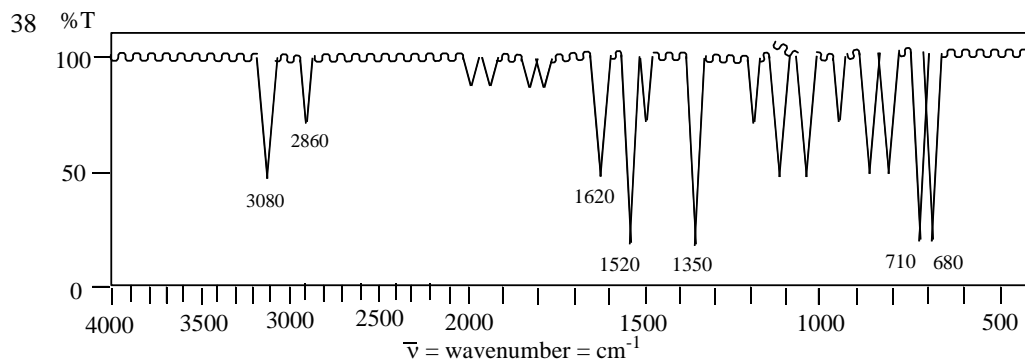
M^+ = 100.09 (100.0%),
 $M+1$ = 101.09 (6.5%)



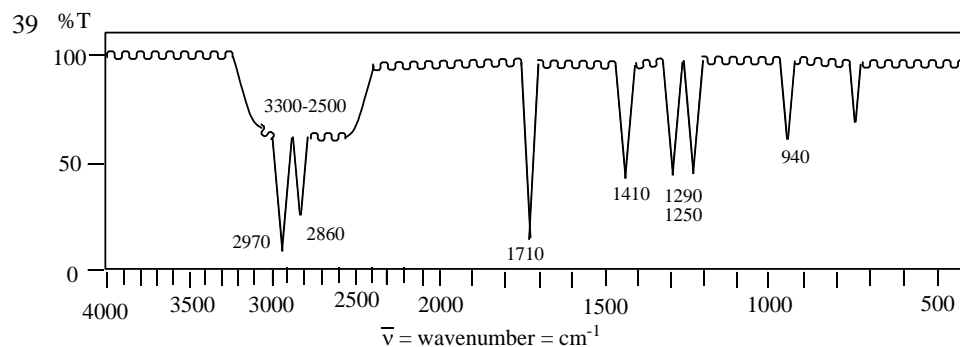
Exact Mass: 130.14
 M+ = 130.14 (100.0%),
 M+1 = 131.14 (8.9%)



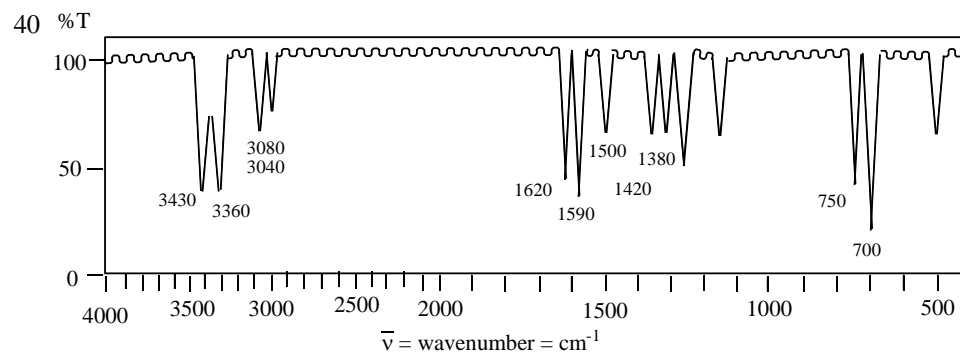
Exact Mass: 117.08
 M+ = 117.08 (100.0%),
 M+1 = 118.08 (5.9%)



Exact Mass: 123.03
 M+ = 123.03 (100.0%),
 M+1 = 124.04 (6.6%)

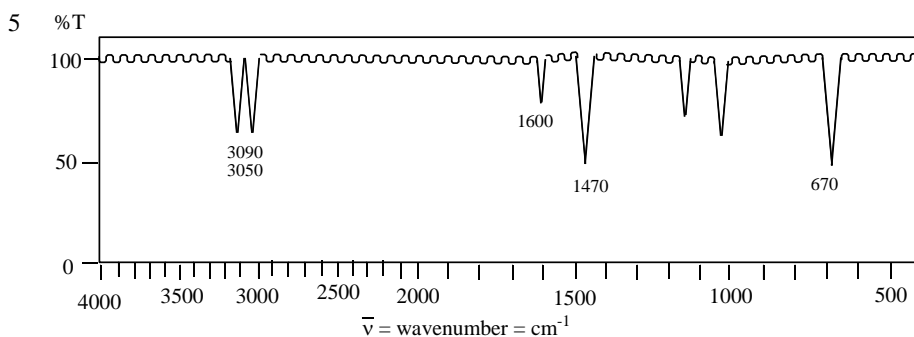
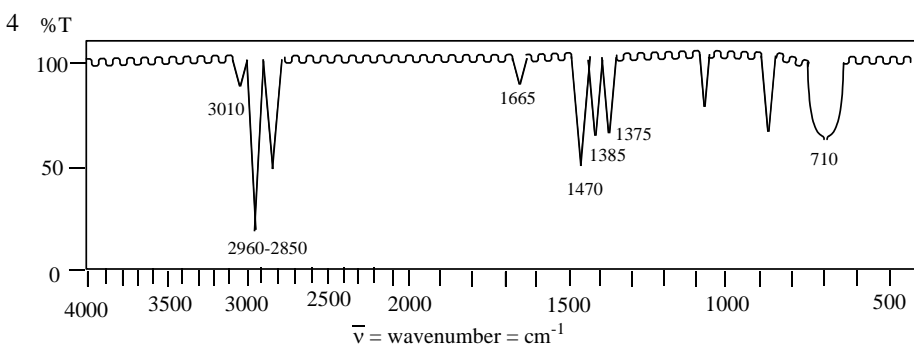
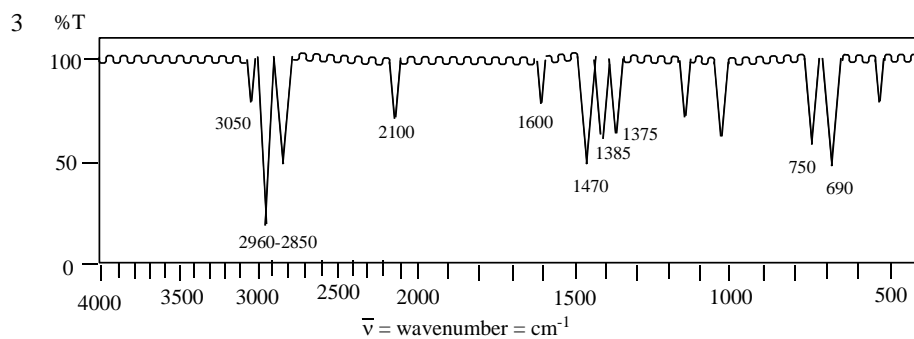
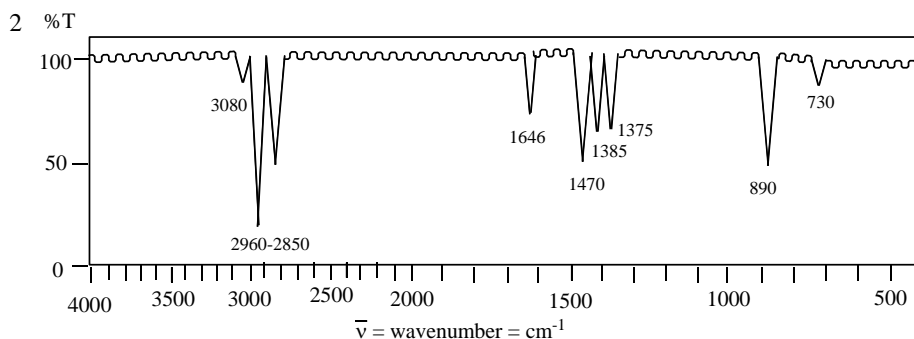
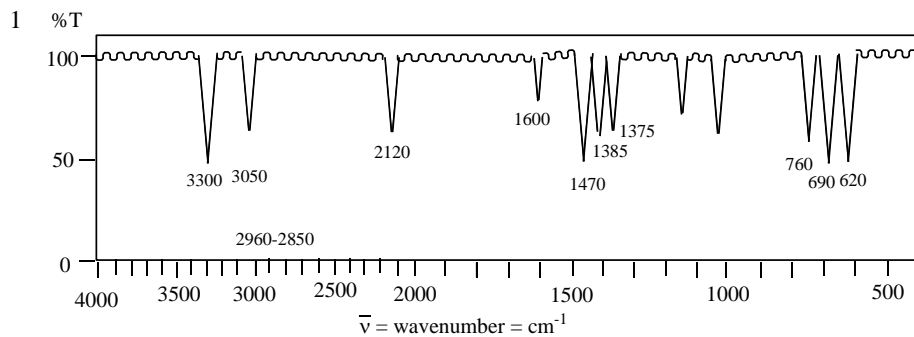


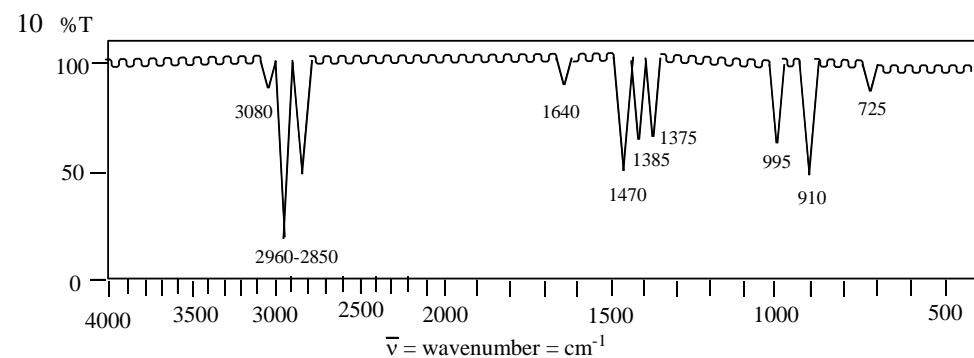
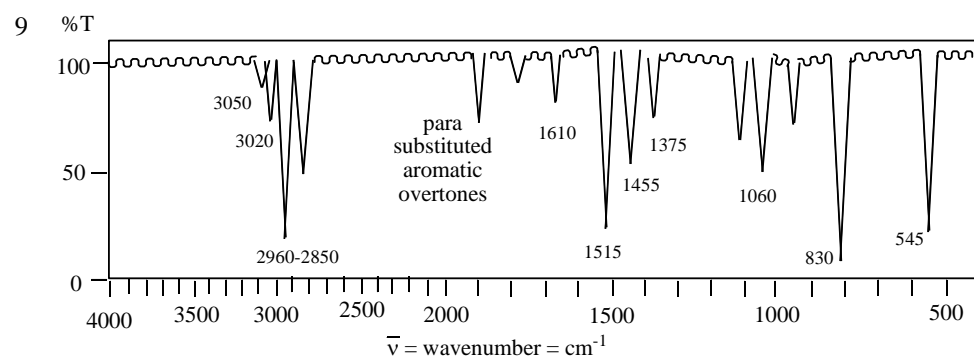
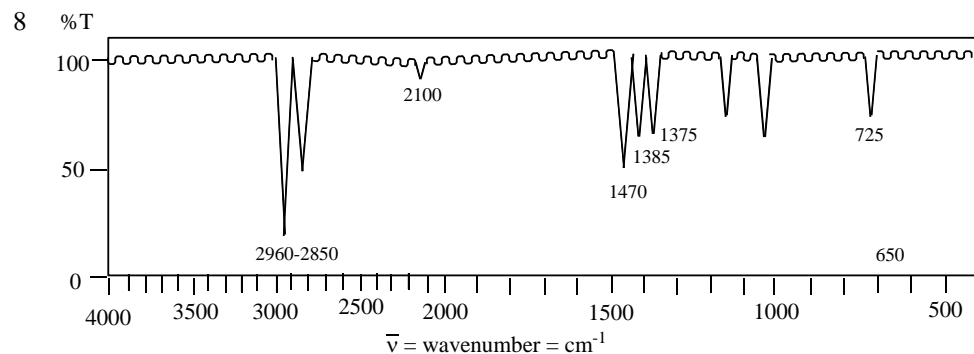
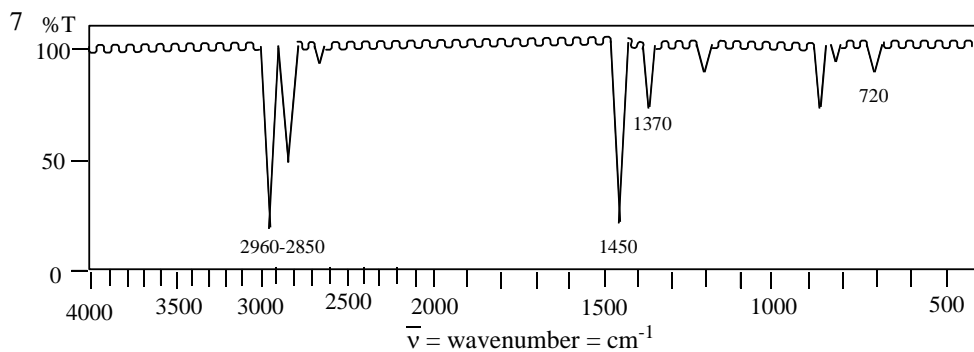
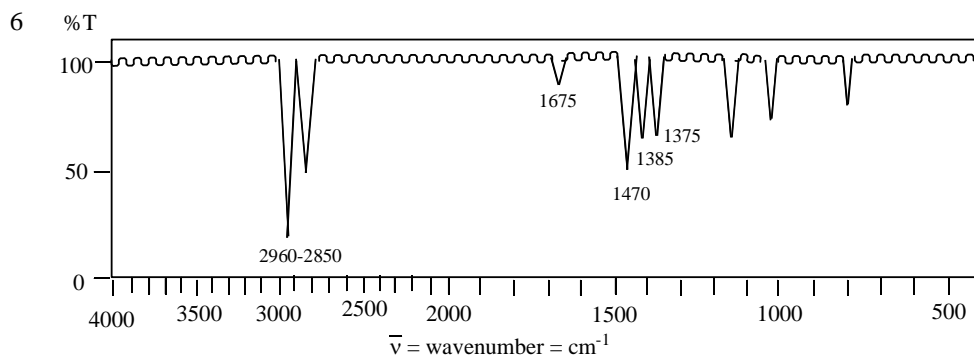
Exact Mass: 116.08
 M+ = 116.08 (100.0%),
 M+1 = 117.09 (6.7%)

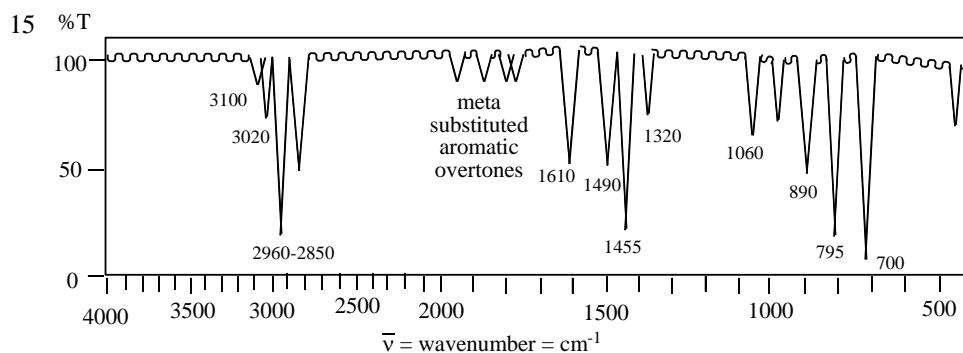
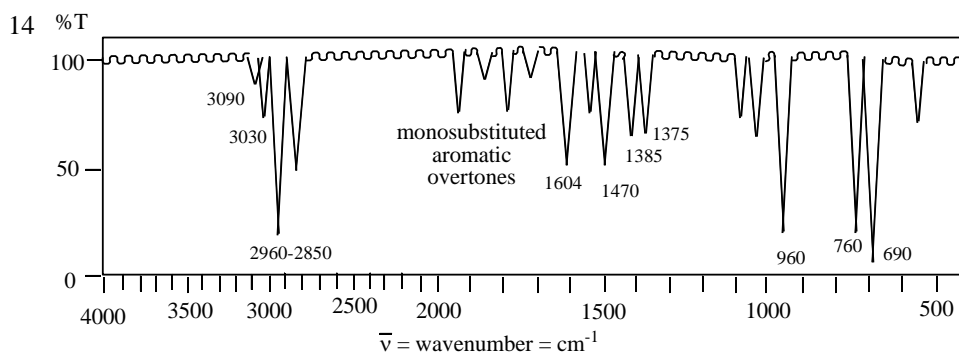
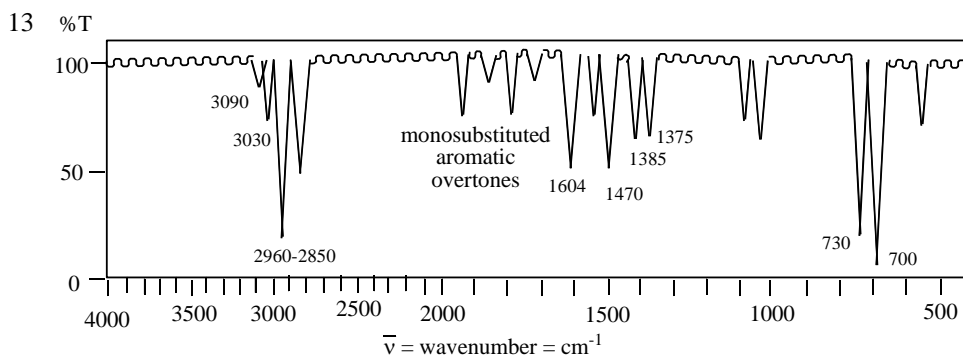
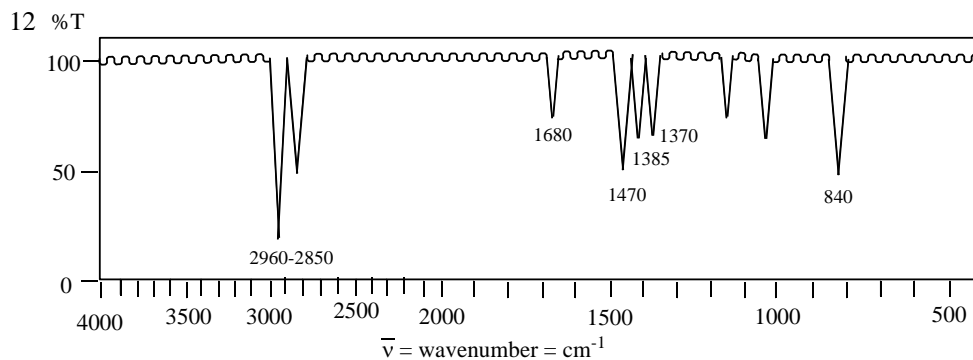
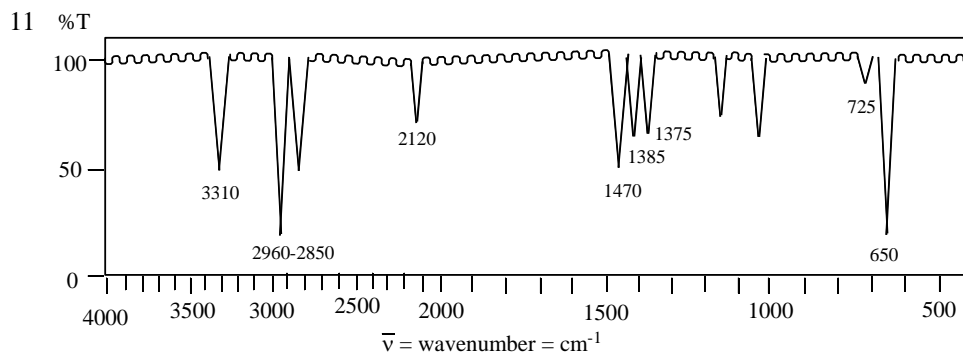


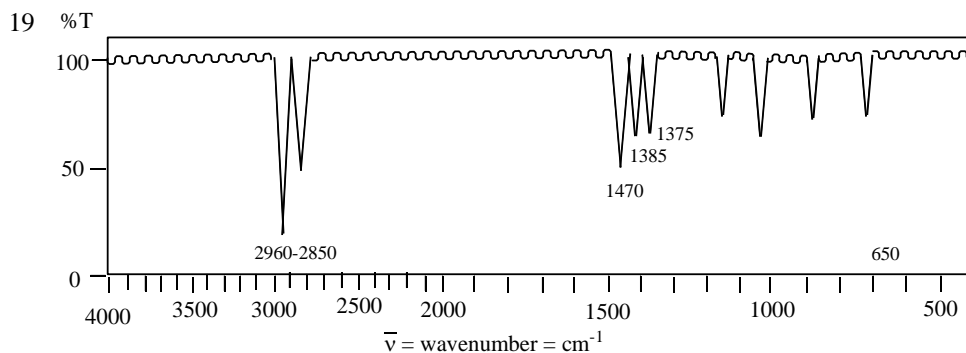
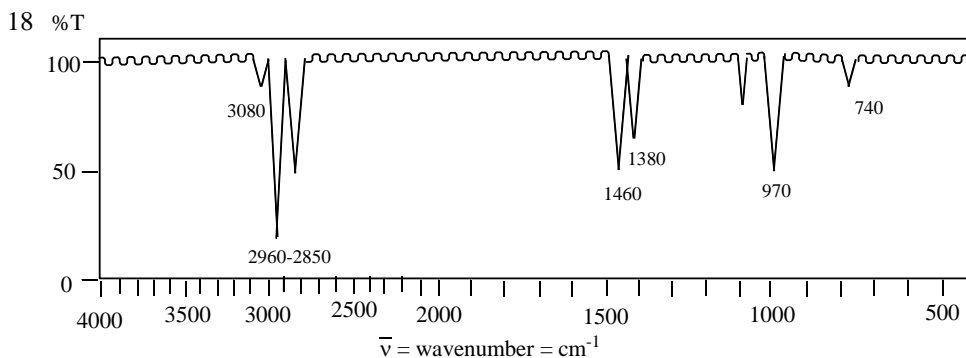
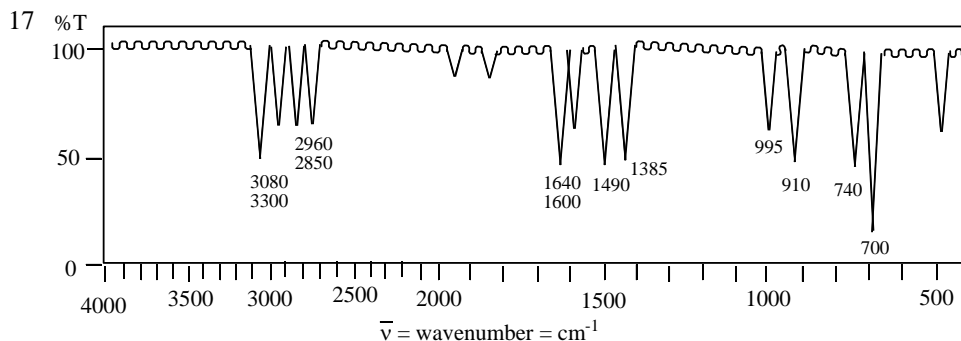
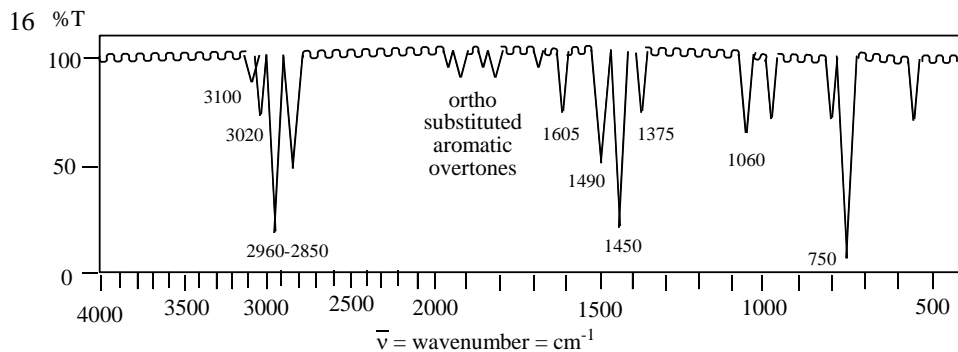
Exact Mass: 93.06
 M+ = 93.06 (100.0%),
 M+1 = 94.06 (6.6%)

Group 2 compounds: C, H hydrocarbons = alkanyl (=R), alkenyl, alkynyl and aromatic patterns are listed above (1-20). To the right of each IR draw the structure most consistent with the given IR. Provide a minimal interpretation of the IR bands (e.g. para substituted aromatic, monosubstituted alkene, etc.)

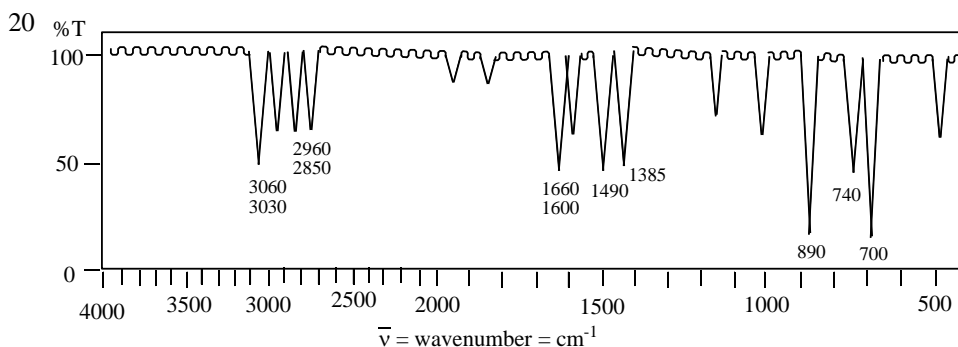








Exact Mass: 96.09
 M^+ = 96.09 (100.0%),
 $M+1$ = 97.10 (7.7%)



Formula problem 1

Exact Mass: 277.01

$M^+ = 277.01$ (100.0%),
 $M+1 = 278.01$ (14.5%),
 $M+2 = 279.01$ (97.5%),
 $M+3 = 280.01$ (14.2%),
 $M+4 = 281.01$ (1.1%)

Hints:

1. What does the odd mass tell you?
2. What does the $M+1$ tell you?
3. What does the $M+2$ tell you?
4. There are 12 H in the proton NMR.
5. There are 13 C in the C-13 NMR.
6. There are 5 pi bonds in the C-13 NMR.

Questions:

What is the molecular formula?
How many degrees of unsaturation are there?
How many rings and pi bonds are there?

Formula problem 2

Exact Mass: 330.08

$M^+ = 330.08$ (100.0%),
 $M+1 = 331.09$ (20.8%),
 $M+2 = 332.08$ (38.9%),
 $M+3 = 333.08$ (7.8%),
 $M+4 = 334.08$ (1.5%)

Hints:

1. What does the even mass tell you?
2. What does the $M+1$ tell you?
3. What does the $M+2$ tell you?
4. There are 19 H in the proton NMR.
5. There are 19 C in the C-13 NMR.
6. There are 6 pi bonds in the C-13 NMR.

Questions:

What is the molecular formula?
How many degrees of unsaturation are there?
How many rings and pi bonds are there?

Formula problem 3

Exact Mass: 262.14

$M^+ = 262.14$ (100.0%),
 $M+1 = 263.14$ (12.3%),
 $M+2 = 264.13$ (6.0%),
 $M+3 = 263.13$ (1.5%),

Hints:

1. What does the even mass tell you?
2. What does the $M+1$ tell you?
3. What does the $M+2$ tell you?
4. There are 22 H in the proton NMR.
5. There are 11 C in the C-13 NMR.
6. There is 1 pi bonds in the C-13 NMR.

Questions:

What is the molecular formula?
How many degrees of unsaturation are there?
How many rings and pi bonds are there?