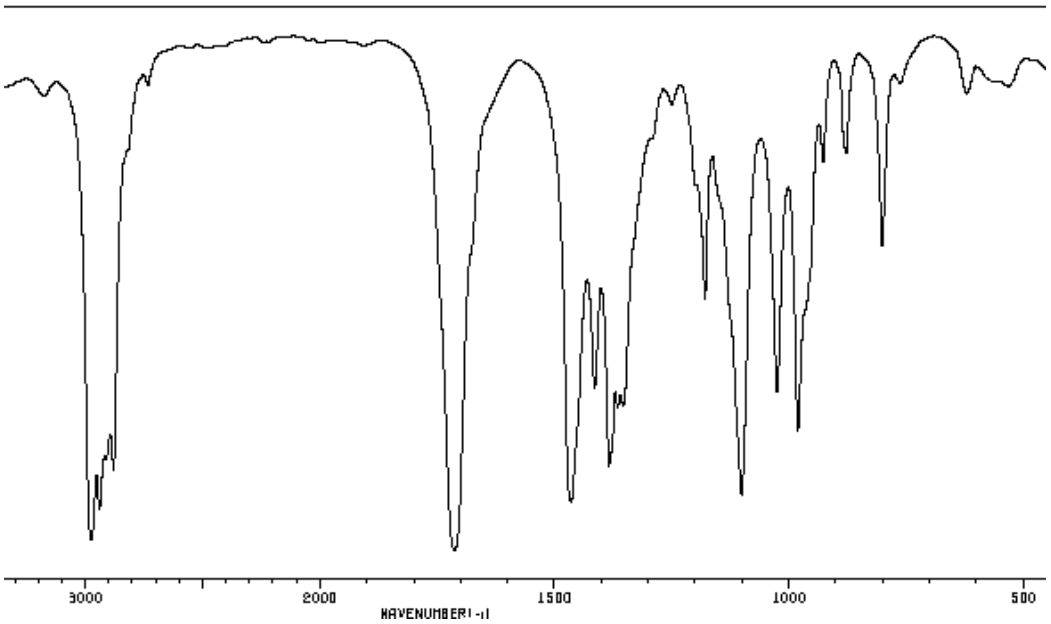
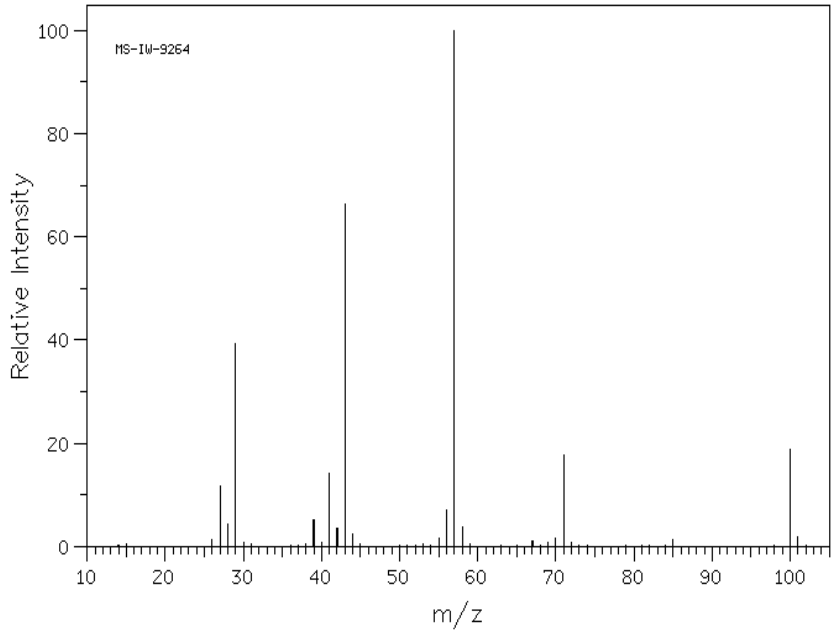
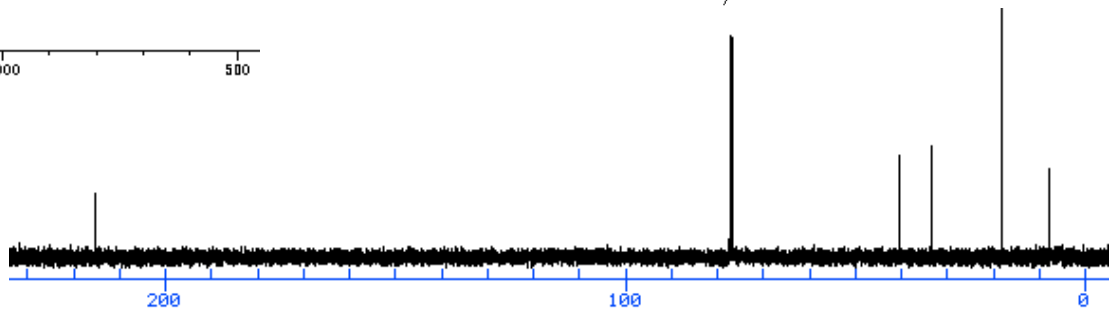
MW to molecular formula

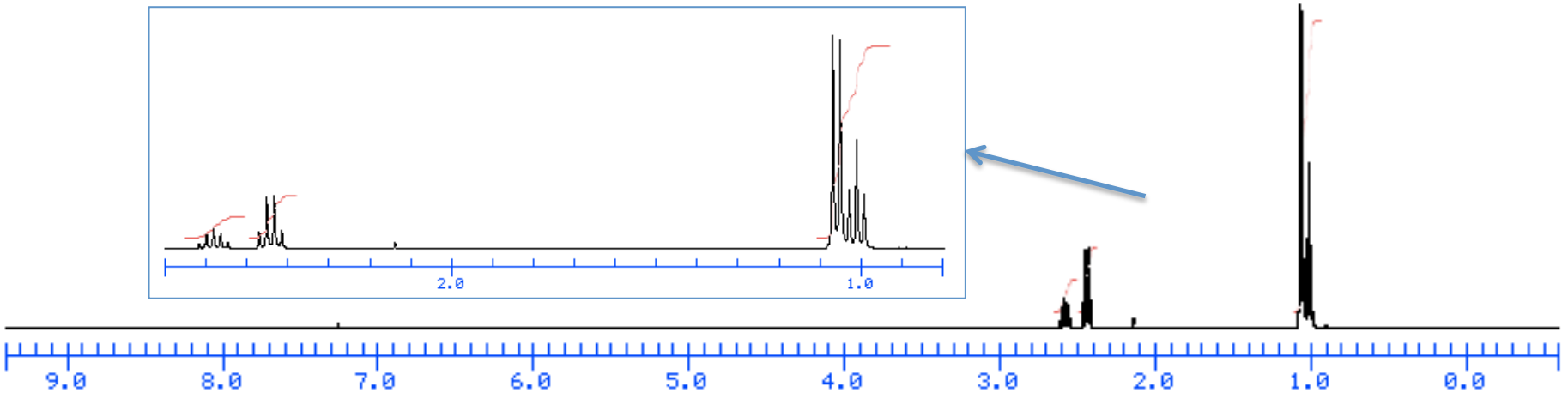
- If even; no halides
  - If hydrocarbon – #C = (mol wt.-2) / 14 (round UP!)
  - Calculate IHD from #C and #H
  - Alternate formulas with O: Add in O, take away CH_4, increase IHD by 1
  - Alt. formulas with 2 N: Add in N_2, take away C_2H_4, increase IHD by 1
  - Alt. formulas with S: Add in S, take away C_2H_8, increase IHD by 2
  - If IHD becomes 7 or more, consider alt. with one fewer C, 12 more H
- If one halide
  - Detect by M+2 peaks (Cl, Br) or M-19 pk (F; may be small) or M-127 (I)
  - Subtract 18, 34, 78 or 126 from M to find wt. if halide replaced by H
- If odd then odd number of nitrogens (1, 3 or 5)
  - Subtract 15, 45 or 75 from M
  - determine formula as above
  - add in NH, N_3H_3 or N_5H_5

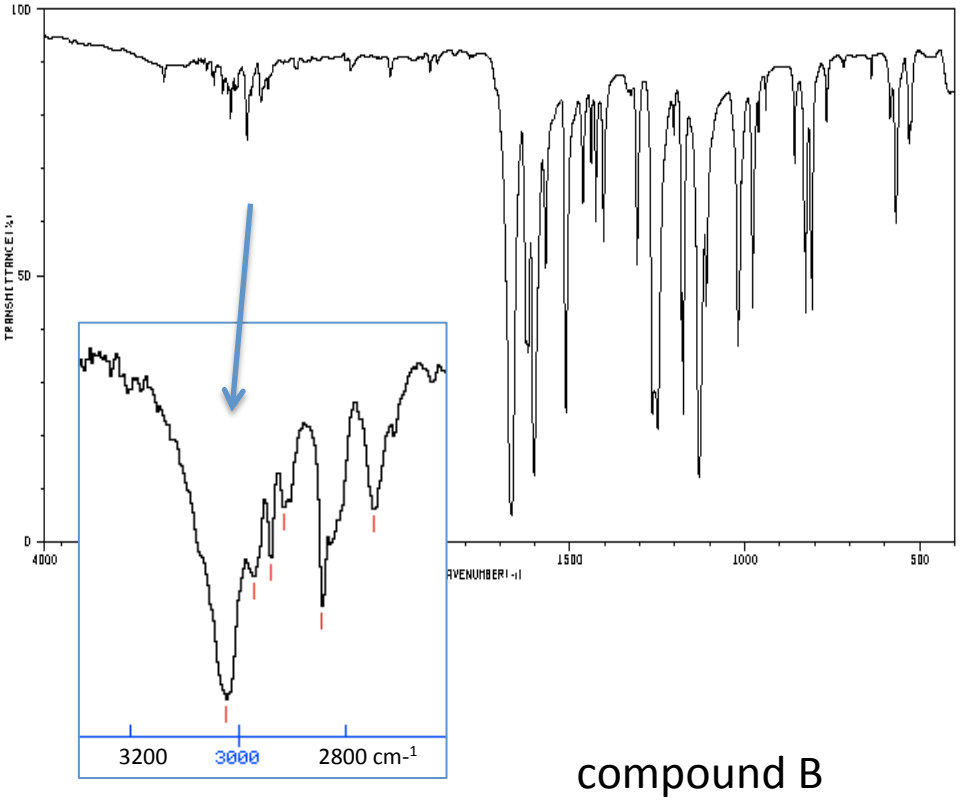

3000
2000
1500
1000
500

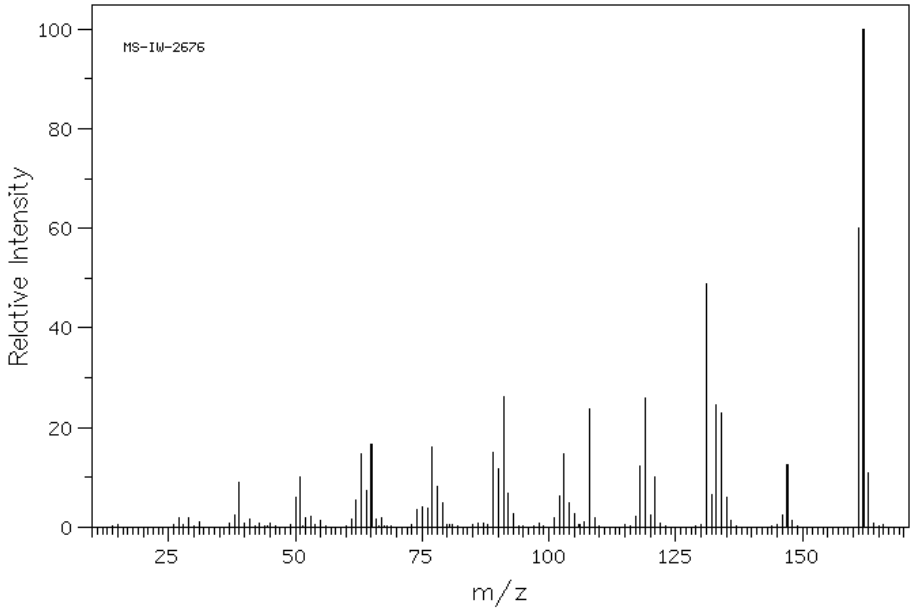

MS-IW-9264
Relative Intensity
100
80
60
40
20
0
10
20
30
40
50
60
70
80
90
100
m/z

compound A

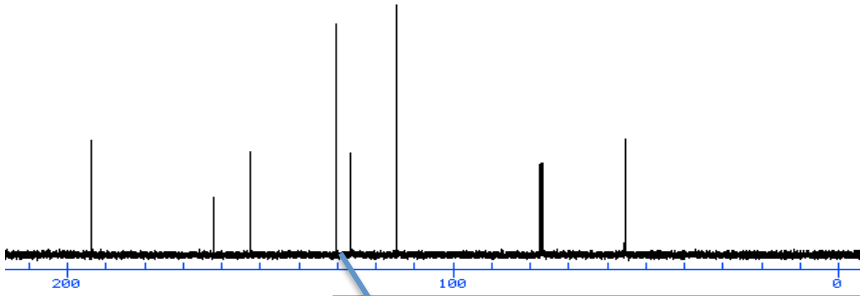

200
100
0

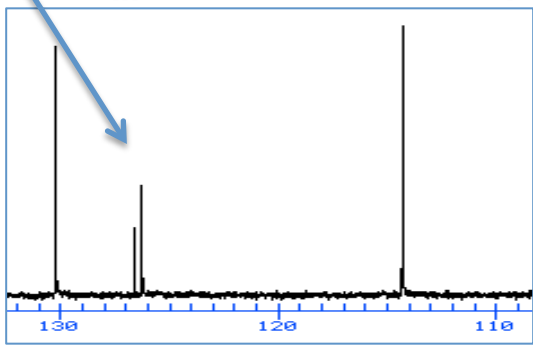

2.0
1.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0


100
50
0
4000
1500
1000
500
3200
3000
2800 cm-1

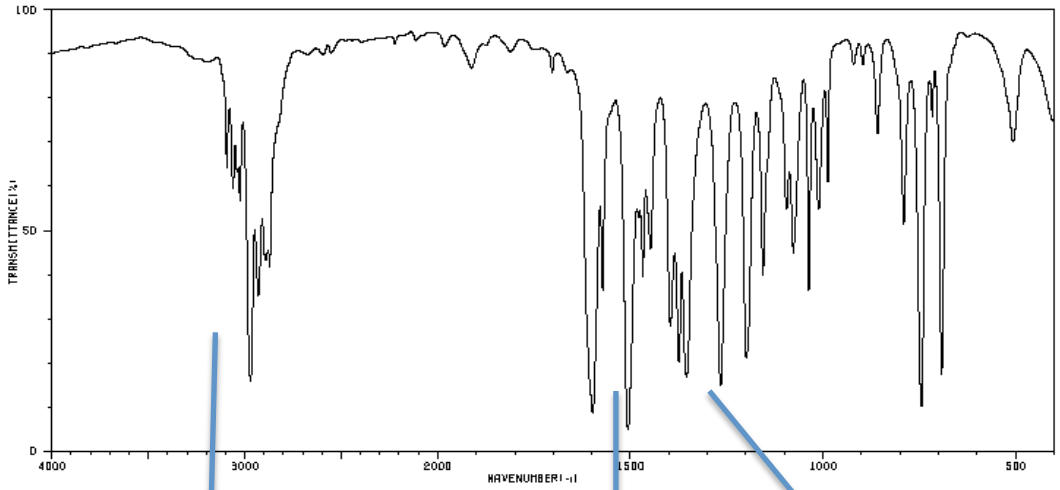

MS-IW-2676
Relative Intensity
100
80
60
40
20
0
25
50
75
100
125
150
m/z

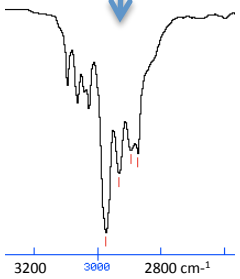
compound B

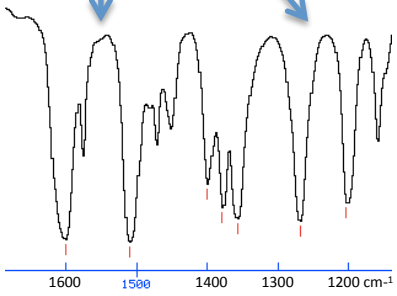

200
100
0

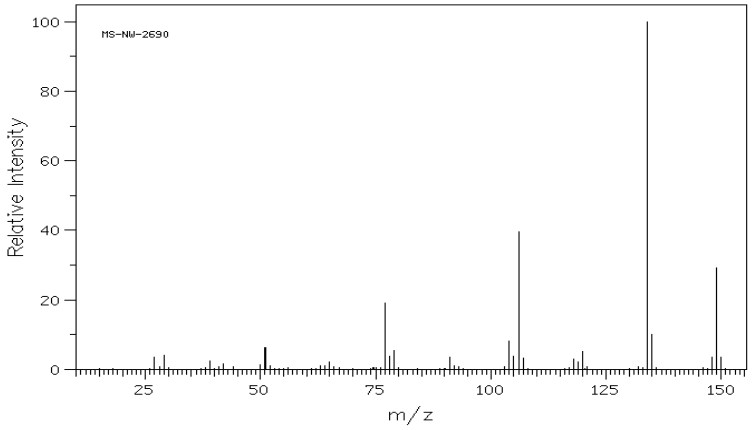

130
120
110

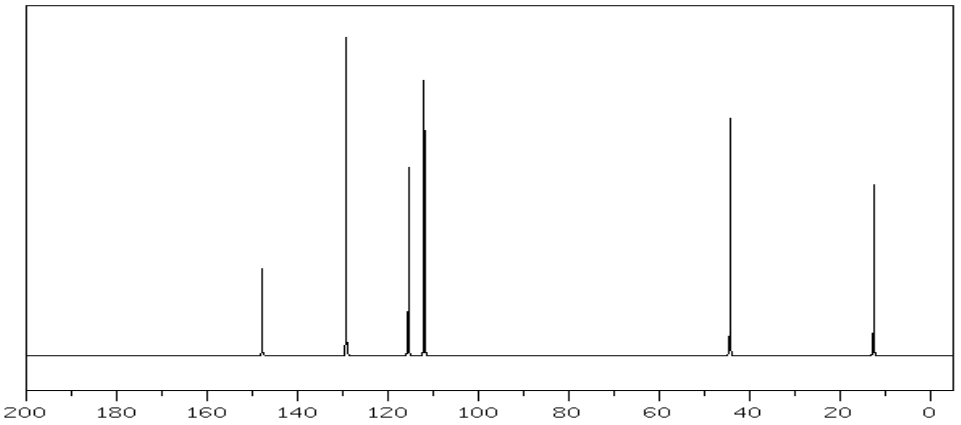
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
6.5
9.7
9.6
9.5
3.9
3.8
3.7
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0


100
50
0
4000
3000
2000
1500
1000
500

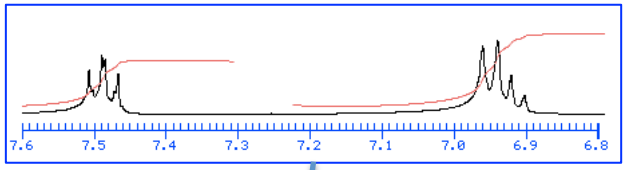

3200
3000
2800 cm-1

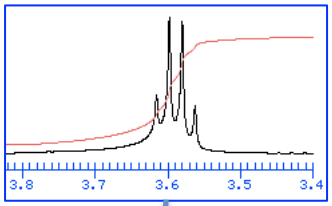

1600
1500
1400
1300
1200 cm-1

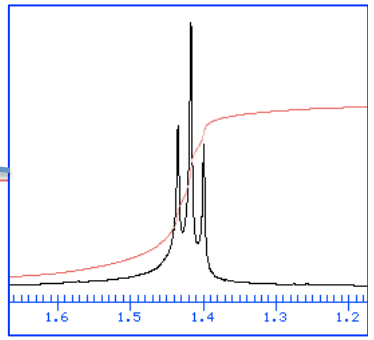

MS-NW-2690
Relative Intensity
100
80
60
40
20
0
25
50
75
100
125
150
m/z


200
180
160
140
120
100
80
60
40
20
0

unknown C


7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8


3.8
3.7
3.6
3.5
3.4


1.6
1.5
1.4
1.3
1.2

9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0