Solutions to Mass Spec sample questions:

(1) 77 is the mass of C6H5 (monosubstituted benzene), so the compound must be (a) or (b). The sharp peak at 1710 cm^{-1} in the IR implies a carbonyl, therefore (a) is the correct structure.

(2) Hard sources break up a molecule (ICP, e^- impact, chemical ionization). The information such a source provides is usually related to the functional groups. Because the molecule breaks up in a predictable way (at weak bonds, or at locations that would provide stable radical cations), the fragments can be traced back to the functional groups the whole molecule once had.

Soft sources (electrospray, MALDI, FAB, field ionization) do not break up the molecule to any great extent. They are usually used for "elemental analysis" – *i.e.*, to confirm the molecular formula of the molecule of interest.

(3) This is straight scribing from the notes – explaining how mass separation takes place in each of these (because the detector proper in any mass spec is mass blind (will register any mass striking it), all mass analyzers must operate to ensure that only 1 mass at a time reaches the detector).

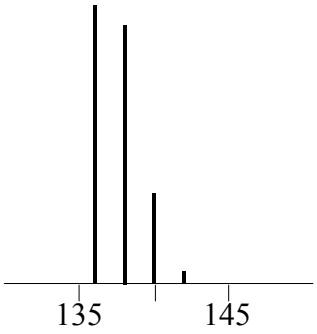
Roughly (for more detail see your notes, none of these quick answers would be worth full marks on the exam!):

Magnetic sector accelerates a mass through a voltage into a curved magnetic field. Depending on the strength of the field only 1 mass will get through.

ToF lets accelerated ions into a drift tube – the lighter, the faster, the sooner they hit the detector.

Quadrupole are 4 poles (two +, two -) that alternate charge to create a kind of charge wave to create a situation where only one mass at a time will have a stable wavelength (and therefore travel through the analyzer to the detector).

(4) (a) This is a relative abundance question. The three masses for the various isotopes would be:
$CF^{35}Cl_3$ *m/z* = 136 amu, abundance $({}^3{}_3C = 1)(0.758)^3(0.242)^0 = 0.436$ (43.6%)
$CF^{35}Cl_2{}^{37}Cl$ *m/z* = 138 amu, abundance $({}^2{}_3C = 3)(0.758)^2(0.242)^1 = 0.417$ (41.7%)
$CF^{35}Cl^{37}Cl_2$ *m/z* = 140 amu, abundance $({}^1{}_3C = 3)(0.758)^1(0.242)^2 = 0.133$ (13.3%)
$CF^{37}Cl_3$ *m/z* = 142 amu, abundance $({}^0{}_3C = 1)(0.758)^0(0.242)^3 = 0.014$ (1.4%)



(b) The biggest peak for the molecular ion should be the one with the most relatively abundant chlorine isotope (^{35}Cl) and carbon (^{12}C), therefore $^{12}C_{12}H_8{}^{35}Cl_2 = 222$.
The other peaks clustered above 222 then:
$^{12}C_{11}{}^{13}CH_8{}^{35}Cl_2 = 223$
$^{12}C_{12}H_8{}^{35}Cl^{37}Cl = 224$ (this peak mostly due to 24% ^{37}Cl)
225 = the 224 peak with one ^{13}C; 226 = two ^{37}Cl

Loss of a Cl from the 222 peak would weigh 187 (one ^{35}Cl left), therefore the peak at 189 would be the same but with a ^{37}Cl attached (these should be in a 3:1 ratio)

152 is loss of both Cl (and all ^{12}C), therefore 153 is the same peak with one ^{13}C

76 is one ring (76 because it was formerly doubly substituted)

(5) Assuming a linear response at the detector, this is a simple ratio question (but you must take into account the diluting effect of adding the Rh solution).

$[^{103}Rh] = (20)(60)/120 = 10$ ppm

10 ppm → 33.61

$[^{75}As] \rightarrow 11.16$

Therefore, crossmultiply to get 3.32 in the diluted MS sample, or (3.32)(120)/100 = 3.98 in the original sample.

Similarly, the $[^{63}Cu] = 12.6$ (diluted) = 15.1 (original solution)

$[^{65}Cu] = 5.64$ (diluted) = 6.76 (original solution)

Total [Cu] = sum of the two = 21.9 ppm