1) Fred Leadhead was given the structural formulae of several compounds, and was asked to name them by the IUPAC system. How many did Fred name correctly? Correct the ones which are incorrect.

Probably the best way to do this is to draw the structures, then look at them and see if there is a better name.

a) 4-bromo-3-pentanol

![Structure](image)

A better name would be: 2-bromo-3-pentanol

b) 2,2-dimethyl-4-ethylheptane

![Structure](image)

This one is fine. ('di' does count in alphabetizing so it would come 1st.

c) 5-methylcyclohexanol

![Structure](image)

d) 3,3-dichlorooctane

![Structure](image)

A better name would be: This one is fine

f) 3,3-dichlorooctane

![Structure](image)

This one is fine.

2) 2,2-dimethyl-4-ethylheptane

![Structure](image)

This one is fine. ('di’ does count in alphabetizing so it would come 1st.

3) 5-ethyl-3-methylhexane

![Structure](image)

Here the longest chain is 7 carbons so we have a heptane, which would therefore be named: 3,5-dimethylheptane

h) 1-bromo-4-pentanol

![Structure](image)

This one is fine.
Numbering is off. Better name is 3-methylcyclohexanol. This name is probably the better one. One could try to argue for 5-bromo-2-pentanol making it a derivative of the alcohol (which takes precedent.)

d) 1,1-dimethyl-2-cyclohexanol

A better name would be: 2,2-dimethylcyclohexanol (the 1 for the alcohol is implied.)

i) 3-isopropyloctane

 Depends on how complicated we want our substituent(s) to be. We could name this one 3-ethyl-2-methyloctane.

e) 5-(2,2-dimethylethyl)nonane

This name is probably fine. One could try To argue for 5-iso-butynonane, and that would probably be fine.

j) 2-methyl-2-isopropylheptane

The longest chain here is octane, and therefore the name should be: 2,3,3-trimethyloctane.

2) Assuming that as alkyl groups get larger, the torsional strain they induce increases (i.e. two ethyl induce more strain than an ethyl and a methyl, which induce more strain than two methyls), draw a qualitative energy diagram for 3,4-dimethylhexane, viewed down the C3,C4 bond. Please use the structure given below.
Need to generate the rotamers (conformational isomers) for this compound, and then make relative energetic guesses. First the conformers; for clarity, the eclipsed are drawn slightly staggered—these are #1, 3, and 5.

![Conformers]

Now we need to realize that: 2 and 6 are the same, as are 3 and 5. It seems to me that 1 is the highest energy, and that 4 is the lowest energy. 2 and 6, being staggered are going to be of lower energy than 3 and 5, which are eclipsed. So we have: 

4<2(=6)<3(=5)<1

3) Generate the molecular orbitals for linear methylene, H-C-H, by combining the appropriate atomic orbitals of carbon with the molecular orbitals of the hydrogen molecule, H₂.

Just a general comment: this is the question which seem to throw most of you! In MO theory, hybridization (usually) does not occur; the molecular orbitals are generated from the unhybridized atomic orbitals, and a bonding diagram comes out.

a) Show clear pictures of the atomic and molecular orbitals you are using.

Here they are:
b) How many MO will linear methylene have?

There are six atomic orbitals above, so linear methylene will also have 6 molecular orbitals. (Number of orbitals is conserved.)

c) Draw pictures of the molecular orbitals for linear methylene.

d) Order these MOs in terms of energy. Place them on a scale relative to the energy of a lone, non-bonding carbon 2p orbital.

These two questions sort of go together. If we generate them out of the orbitals listed above, we get both the picture and the energetic ordering.

e) Place the appropriate number of electrons in the orbitals, being careful to indicate the proper spin quantum numbers by using arrows (↑, ↓).

Using the same diagram we get:
Remember the unused p-orbitals on carbon, in the linear form, are degenerate. (Although beyond the scope of what you were asked to do, we get what is called the triplet state; there will be singlet state which will have a somewhat different orbital diagram.)
4) How would you differentiate between the two compounds in each of the following pairs by $^{13}$C-NMR spectroscopy?

a) 

The first compound would have 4 signals, because it is symmetric; the second, due to no symmetry, would have 8 signals.

b) 

The first compound would have 3 signals; the second, 2 (because of symmetry).

c) 

The first compound, because of symmetry, would have 4 signals; the second would have 8.

5) Go back to question 1. Several of these compounds contain stereogenic carbons. Pick any five of these, and clearly draw and name one enantiomer (Note that naming compounds in which there are no stereogenic centers will earn you no points!)

There are several possibilities. You only needed to do five separate compounds and pick one enantiomer. Here are all of the ones I could find:

a)
(2R, 3S)-2-bromo-3-pentanol  (2S, 3S)-2-bromo-3-pentanol

(2R, 3R)-2-bromo-3-pentanol  (2S, 3R)-2-bromo-3-pentanol

(4S)-2,2-dimethyl-4-ethylheptane  (4R)-2,2-dimethyl-4-ethylheptane

(1R,3S)-3-methyl-cyclohexanol  (1R,3R)-3-methyl-cyclohexanol  (1S,3S)-3-methyl-cyclohexanol  (1S,3R)-3-methyl-cyclohexanol
g) (3S, 5S)-3,5-dimethylheptane
   (3R,5R)-3,5-dimethylheptane
   meso-3,5-dimethylheptane

h) (S)-1-bromo-4-pentanol
   (R)-1-bromo-4-pentanol

i) (R)-3-ethyl-2-methyloctane
   (S)-3-ethyl-2-methyloctane