Exam 1 Specific Objectives

1. Be able to quickly determine the following from a low resolution MS: molecular weight, whether an odd number of N atoms is present in the sample, whether there are Cl’s, Br’s or S’s present and, if so, how many.

2. Given a low-resolution mass spectrum of a compound, be able to determine plausible molecular formulas; be able to calculate IHD values for proposed (and other) molecular formulas, as well.

3. Given a high-resolution mass spectrum, be able to determine the correct molecular formula from appropriate tables.

4. Be able to distinguish between fragmentation and rearrangement peaks in a mass spectrum.

5. Be able to predict the outcome of the principal rearrangement reactions for a particular molecular ion (McClafferty; tropylium; loss of water, HX, NO; retro-Diels Alder).

6. Given the structure of a compound and its mass spectrum, be able to account reasonably for all of the major peaks. The presence of peaks such as M-1, M-15, M-18, M-27, M-28, M-29, M-46, m/z 91, m/a 60, which are clues to the presence or absence of specific functional groups, should also be determined.

7. Know the general theory and principals of IR and UV spectroscopy.

8. Be able to quickly determine from an IR spectrum whether or not the following functional groups are present: alcohols/amines, vinyl/aromatic hydrogens, carbonyls, alkenes, aromatic rings, nitro groups, aldehydes, alkynes, nitriles, methyl groups.

9. Be able to determine the substitution pattern of aromatic from the IR spectrum.

10. Be able to suggest a reasonable structure for a compound, given its mass spectrum, IR and UV spectra. Be able to explain how you arrived at your conclusion(s).