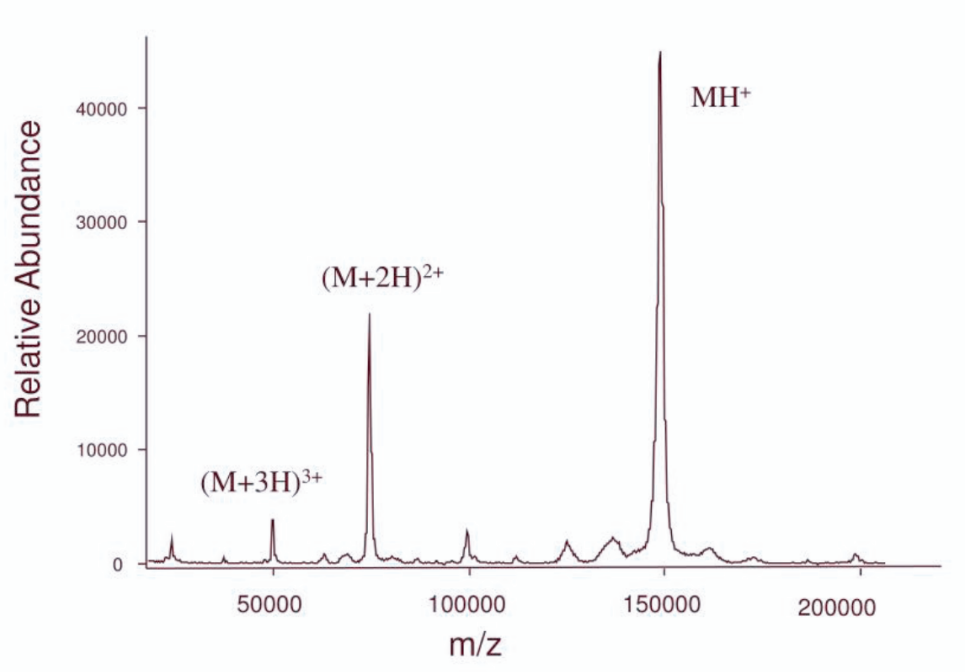
MALDI–TOF
MS Problem Set #3

1. a) Determine the time of flight for an ion of m/z = 800 accelerated across 6.5 kV and allowed to drift through a length of 2 m.

   b) If the instrument used to measure the ion in part (a) has a resolving power of 15,000, what is the expected peak width for that ion?

2. Consider the MALDI–TOF spectrum for immunoglobulin G (IgG), a type of antibody.

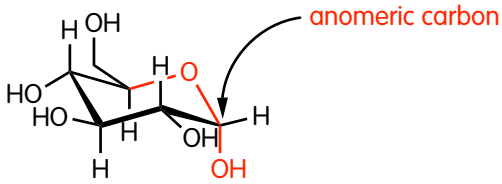


a) According to the spectrum what is the approximate mass of IgG?

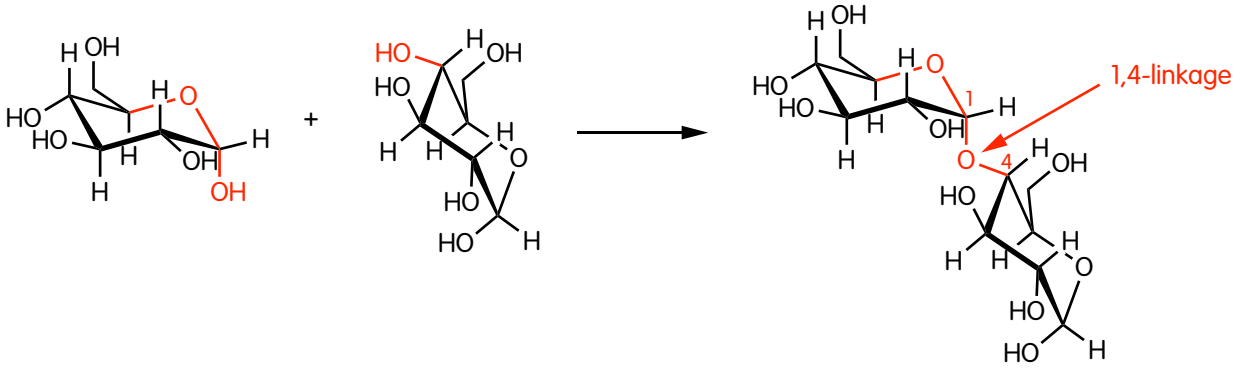
b) The MALDI ionization method results primarily in monocations, but as you can see some amount of di- and tri-cation are produced. How should diprotonation affect the m/z? Does the observed m/z fit with you prediction?

c) How should triprotonation affect the m/z? Does the observed m/z fit with you prediction?

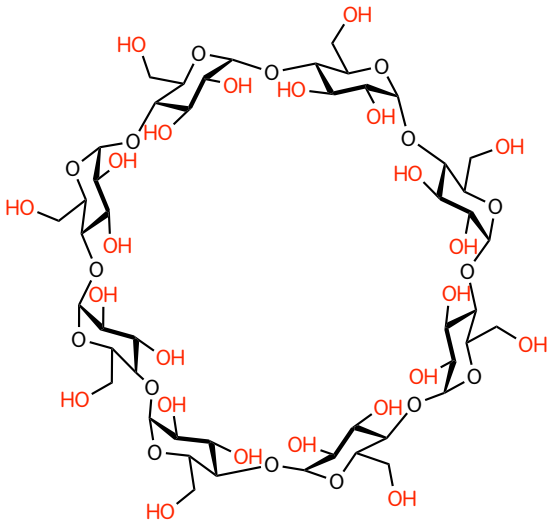
3. Glucose is a familiar example of a hemiacetal - a functional group with its carbon attached to both an ether oxygen and a hydroxy group



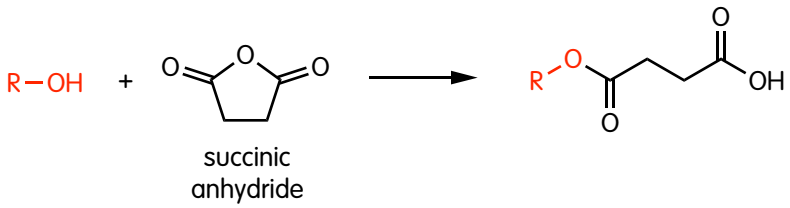

We can create a dimer of glucose by reacting the hemiacetal of one glucose with the alcohol of a second glucose to create an acetal with a new 1,4-glycosidic bond



If we attach many glucose molecules together we create a polymer called amylose, a type of starch. One of the more interesting oligomers of glucose is a cyclic 8-mer known a γ-cyclodextrin.

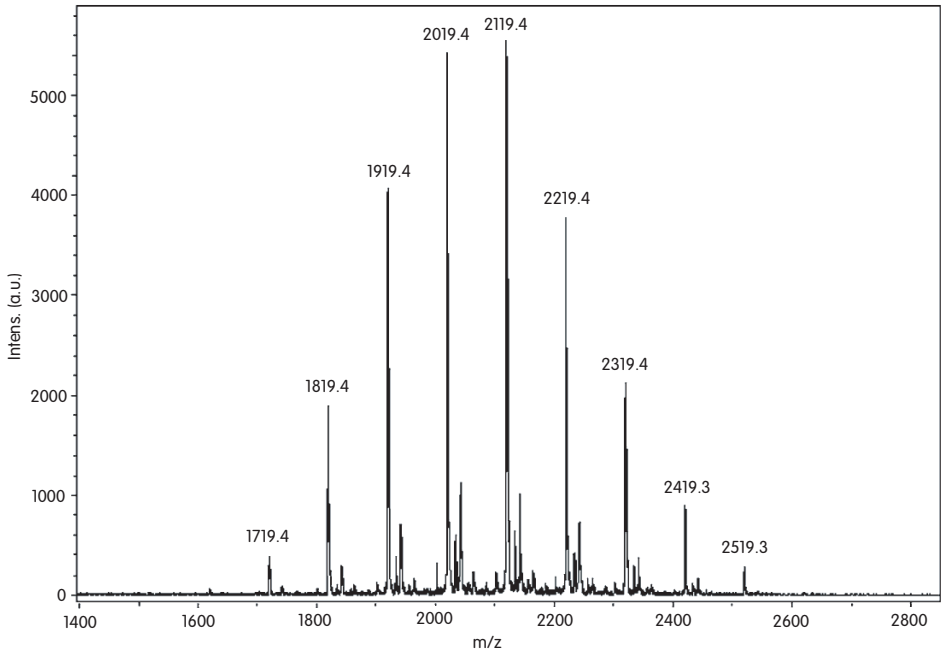


Glucose has a very rich organic chemistry because its many OH groups can be derivatized creating new forms of glucose with interesting properties. One such derivative involves reaction of an OH group with succinic anhydride




(a) How many molecules of succinic anhydride can react with γ-cyclodextrin?

When an excess of succinic anhydride is reacted with γ-cyclodextrin, the following MALDI-TOF spectrum is obtained.



(b) This result already looks different than the MALDI-TOF in problem 2. Why are there so many peaks?

(c) What is the separation between peaks? What molecule might that correspond to?

The experiment run to collect this spectrum is a variation on what we discussed in class. The cationic charge is *not* coming from added protons (from the acidic crystalline matrix), but rather through the addition of Na+ cations.

(d) Write an equation (as you did in the ESI homework) that relates the $(m/z)_{obs}$ to parameters such as MW of cyclodextrin and the various adducts.

(e) Check your equation and see if it gives you the peaks shown in the MALDI-TOF spectrum.