S343 Unknown Project
Due in lab the week of April 20

One of the requirements for S343 is the identification of an unknown. Some guidelines follow:

1. You must obtain IR, ^{1}H NMR, ^{13}C NMR, MS, and mp data (if applicable) for your compound.
2. Keep in mind that there is not always time during lab to run NMR's, so plan accordingly.
3. Mass Spec Data requests must be submitted to your AI with enough time for them to be run.
4. Requests for some pieces of data (including X-ray crystal structures and DEPT data) will be denied.
5. Melting point analysis should only be used to verify your proposed structure after you have considered all other pieces of data.
6. Informal lab report: 25 points
    a. ChemDraw structure of your proposed unknown structure
    b. Results: data tables
        i. ^{1}H NMR: chemical shifts, coupling constant, integration for each peak, assignment (see iii)
        ii. ^{13}C NMR: chemical shift for each peak and assignments (see iii)
        iii. Lable your chemdraw figure with the protons or carbons labeled a, b, c, etc., then include those letters in your data tables from (i) and (ii)
        iv. IR: List only the relevant absorbancies (you don't have to list anything in the fingerprint region), descriptions (s, m, w, br), and assignments (O-H, N-H, alkane C-H, etc.).
        v. Melting point data (if you have it) including literature values (properly referenced).
        vi. If applicable, mass spec data (include a table listing the molecular ion, base peak, and any other relevant fragments) – also include structures of fragments if you know them.
    c. Discussion: Be thorough—this is how you get partial credit!
        i. Include a detailed analysis of how you interpreted your data and a thorough description of your thought process.
        ii. If you discuss a particular MS fragment, include the structure of that fragment (and a mechanism for how it was formed). If you discuss a particular IR stretch, indicate what specific bond that stretch corresponds to, etc.
    d. Staple copies of all pieces of data to the back of your report