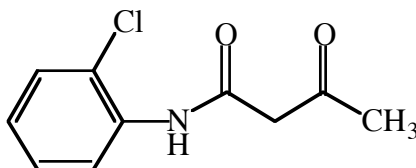


PROBLEM SET #5*Using SciFinder Scholar for Structure and Substructure Searching*

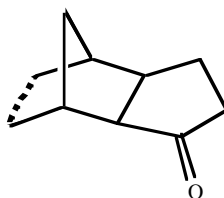
DUE: 8:30 am, 11 October 2005

*Activities on general substances (Work with your partner)***A.** Draw the structure and do an exact/related search for it.

1. How many substances did you find? Group them by categories, e.g. how many were isotopically substituted, charged compounds, polymers, etc. Give estimates if there are too many to count.
2. What is the CA Index Name and Registry Number of the compound shown above? How many different commercial sources are there for this substance?
3. How many references are there to this compound?
4. How many of the references relate to its use in coupling with diazotized aromatic amines?
(a) Refine by Research Topic (b) Refine by Reaction Roles and Chemical Structure

B. As an example of doing a substructure search, redraw the substance in part A but use the X Menu to replace the Cl atom with any halogen. Lock out rings from the ring and chain.

1. Do a Preview search. How many answers are estimated will be found? What percentage of these answers will have X = Cl?
2. List the distribution of real atom attachments at the position ortho to X.
3. Lock out further substitution on the chain atoms. How many answers are projected now? What is the distribution of substituents on the ring carbon that is para to the chain? Choose this substituent to be a Cl atom. How many substances are retrieved for this restriction?

C. Draw the structure below and perform an exact/related structure search on it. Be sure to include the dashed (unspecified) bond as shown.

Examine the substances that are obtained. Analyze by “Ring skeleton with atoms and bonds”. What do you conclude about the role of using the dashed bond in a structure search? Why is the structure with two double bonds included in the group?