

Simplified Flowchart

Student has some or all of following data:
melting &/or boiling point, hetero atoms (you
are given all except C,H,O), chemical tests,
solubility family, IR, C13, H1 NMR

dak 10/30/08

Pick one of the 3 paths shown below (**SDBS**,
POC/DOC, or **Aldrich**). Your unknown may be
in 1, 2, or 3 of them. Choose which you think
is quickest route to unknown. If > ~ 1hr, ->
help.

Use SDBS. Enter C13 &/or
H1 NMR &/or IR peaks, .. and
range for each type of atom,
if known (caution - false
negative if spectrum entered
is not in database)

Do C13, H1 NMR, and IR
spectra match unknown
spectra? If yes, use CAS # in
POC/DOC to verify mp &/or
bp. If no, use **POC** to search
further.

To look up references for
more information about your
unknown, or to look up
information about reactions,
use **Beilstein** or **SciFinder**

Use POC. Enter 1) mp &/or bp, 2) "generic"
molecular formula from hetero atom data (you
must determine if O is present), and 3) #H's
from H1 NMR integrals (if available)

Hit list > ~50? If yes, go to next step. If no,
scan names looking for attributes of unknown,
eg has aromatic ring, is amine, is not alcohol,
does not have acid, ketone, aldehyde, etc.
Examine records which have desired
attributes. Can use **ACD** to confirm C13, H
NMR, if needed. If find match, you're done. If
not, go to **SDBS** or **DOC**.

Enter substructure data (from solubility family,
IR, H1 NMR), &/or HNMR peaks, &/or IR peaks.
Caution: some records have no IR, &/or
HNMR, &/or structure .. can lead to false
negative. If **SDBS** and **POC** did not give
match, search **POC** without structure &/or
spectra, or go to **DOC**.

If find a match, but it does not include spectral
data, use **Sigma Aldrich**, **SDBS**, or **ACD**
to confirm. If no match, use **DOC**, with mp &/or
bp, "generic" molec formula, text, &
substructure, ... or **SDBS** if have not already
tried.

To look up references for more information
about your unknown, or to look up information
about reactions, use **Beilstein** or **SciFinder**

Use Aldrich tables in Swain,
using known chem family
from IR & solub tests. Scan
manually through pages for
match.

Check **Sigma Aldrich** &/or
SDBS for more spectral
info. To look up refs. for
more info about unknown,
or to look up info about
reactions, use **Beilstein**
&/or **SciFinder**