

Trouble-Shooting Tips for Chem 130

	Problem	Cause / Solution
Spectra	Spectral data incomplete in POC	Spectral data isn't present for all compounds. Omit spectra from search. Instead of entering spectral peaks, enter number of Hydrogens in the MF field as well as physical property data.
	Extra Peaks in Spectral Data	Spectral peaks may include solvents or contaminants. Know so you can ignore common peaks for solvents and common contaminants (e.g., water).
	Fewer Peaks in Spectral Data	In POC, when entering NMR data enter only one range for multiplets because POC often treats multiplets as one value.
	Peaks appear at a different place in POC than your spectrum	In POC, do not enter NMR data for ionic hydrogens in carboxylic acids, amines, or alcohols
	Have wrong spectra for compound	If you suspect that this might be the case, consult with TA.

	Problem	Cause / Solution
Physical Property Data	Chemical Test: Error in doing a chemical test or in interpreting chemical test.	Is there some doubt about outcome of a test and can it be interpreted another way? Consult TA.
	MP, BP, and MW data in database doesn't match what you search	Broaden ranges (e.g. standard ranges are MP +/- 5; BP +/- 5; MW +/- 3; try doubling size of ranges). For BP, sometimes database only has data that is at reduced atmospheric pressure.
	Refractive index data in database doesn't match what you search	When entering a Refractive Index use a broad range, such as +/- 0.2. Your data may not be very accurate
	Refractive index missing from record	Instead of refractive index data, drop refractive index and search other information instead.
	Fragrance data missing from record	Consult Ulrich's Flavors and Fragrances catalog on reserve at Swain.

	Problem	Cause / Solution
Substructure Data	Substructure search results don't include your compound.	Structures are not available for all compounds in CCD and POC. Instead of structures, search using molecular formula data.

Closely Related Compounds	Two compounds have almost identical properties	Consult literature for more information.
----------------------------------	--	--