General Instructions for T6

Please read the detailed instructions in the tutorial appendix of the course manual. You will find sample tables, a marking outline, suggested references, and nmr data for common solvents that will be very helpful in working through your problem and writing your report.

NMR Processing and expansions:
You will need to process your ^{1}H nmr spectra using ACD 1D NMR Processor software available on the University computers (PC only).

The *spectra are available on the SFGClients\\uvic\storage' drive under 'Science' then 'Chemistry' then 'Undergraduate nmr'.* Instructions for using the ACD software are given in T4b.

You may need to process the ^{13}C and/or DEPT-135 depending on whether or not the peak-picking is sufficient in your original output. Do not process spectra unnecessarily - you will be penalized if you choose to process the ^{13}C or DEPT and it wasn't necessary. You do not need to process the 2-dimensional spectra, and you do not have access to these electronic files. You must interpret all spectra.

Report Tables and Calculations:
The sample data tables should be completed as thoroughly as possible, even if you didn't need to use all the spectra to solve your problem. Not all data columns apply to every T6 problem, so eliminate any blank columns when you re-write this information into your report. If your table includes calculations of predicted shift values, please show the full sample calculation in the appropriate cell or below the table: (ie: H^A: δ7.27+0.01(o-Cl)-0.08(p-Cl)-0.10(m-OCH$_3$)=7.10 d).

Structures:
It is recommended that you use a chemistry drawing program to draw your structures. ChemDraw is the most user-friendly option and is available on the University computers in the programs menu under 'ChemBioOffice 2012' then 'ChemDraw Std 13.0'; other options are available as free downloads (details can be found in the manual under "suggested reference sources" in the T6 pages). Neatly drawn hand-written structures are equally acceptable.

Appendices:
Attach all spectra used in your report (originals and processed data) as numbered, labeled appendices (ie: Appendix 1: ^{1}H nmr of Triclosan in CDCl$_3$). It's fine if you have drawn all over these, the interpretation will be marked from your data tables not from the appendices. If you want clean copies for your report a .pdf of your T6 question can be found on the tutorial webpage listed next to your section number.

Academic Integrity:
Each section has been assigned a unique T6 problem; you must complete the problem you were assigned. You may work with others to solve your problem, but the processed spectra and the written report must be an individual effort. A grade of zero will be assigned if cheating is suspected. Under no circumstances should you share an electronic copy of your work with another student - both parties will receive a grade of zero in this case as defined in the department policy on cheating and plagiarism (page C7 in your manual).

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The report is due at the start of your T7 tutorial class.
Need a clean copy of the spectra?
.pdf copies are available on the tutorial webpage.

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Sample tables to help you get started...

Table *x*: ^{1}H and COSY nmr of *xxxxx* in CDCl$_3$ (see appendices *x* - *xx*)

Shift (ppm), multiplicity	Coupling Constant (Hz)	Integration		COSY shows correlation to protons at δ (ppm)	Assignment	Reference Values	
		Actual	Relative			Predicted (manual)	SDBS[1] or Aldrich[2]
ex: 3.46 q	$^3J_{BA} = 7$	0.12	6 H	1.23 (H$_A$)	B	3.4q, J=7 (C-CH$_2$-O-R)	3.34

Table *y*: ^{13}C, DEPT-135 and Hetcor nmr of *yyyyy* in CDCl$_3$ (see appendices *y* - *yy*)

Shift (ppm)	DEPT-135		Hetcor shows correlation to protons at δ (ppm)		Assignment	Reference Values	
	signal	inference	short range	long range		Predicted (manual)	SDBS[1] or Aldrich[2]
ex: 72.4	↓	CH$_2$	3.46 H$_B$	1.12 H$_A$, 6.02 H$_C$ (^{4}J)	b	67-72 ↓ (C-CH$_2$-O-R)	72.352

These may be used to start solving your problem, but must be re-written in your report!