Multispectroscopy: Online Structure Determination Exercises

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We have developed a set of 100 exercises in organic structure determination that we are making freely available online. The program presents students with $^1$H NMR, $^{13}$C NMR, infrared and mass spectra from which they may derive the structure. There are 100 compounds divided into three levels of difficulty. Students may select the level of difficulty and choose an exercise or accept random selections within a difficulty level. When an exercise is begun, the user interface in Figure 1 is shown.

Zoom buttons allow each spectrum to be displayed in full screen, in which case help on the specific compound becomes available, as well as extensive resource material. In the case of infrared spectroscopy, a database can be searched by frequency or functional group. The mass spectral section provides a calculator for obtaining molecular masses from formulas, a table of fragment patterns for different functional groups, and mass tables that include formulas, precise masses, and isotope peak values. The proton NMR section has extensive tables of chemical shifts and a splitting pattern simulator. The carbon NMR section has tables of chemical shifts and several algorithms for estimating shifts.

Interpretation

Although students are expected to enter the solution in the sequence of molecular formula, functional groups, and finally to choose from a set of possible structures, they are not restricted to a particular sequence of analysis of the spectra in making deductions about the compound. Students may work in their own manner and are able to view spectra and consult the databases at any time. If the student enters an incorrect result, an error is indicated, and comments are provided on the spectral features that indicate why this is an error. When the correct answer is given, the system provides comments on each spectrum explaining how the structural information could be deduced from the spectra.

Distribution

The exercises are available in French (1) and English (2). If an instructor wishes to install the program on your college or university system, please contact CDIEC (3).

Acknowledgment

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Literature Cited

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Figure 1. Screen display of the spectra that students use to identify an organic compound.