

- Electron Impact (EI) mass spectra and infrared (IR) spectra (different phases). These types of spectra are frequently used in computer search systems where a direct comparison between the recorded spectrum and the library spectra is made.
- Gas chromatographic (GC) retention indices and nuclear magnetic resonance (NMR) shifts (³¹P, ¹⁹F). These data are generally single numbers, which could easily be searched.
- ¹H NMR (different field strengths, different solvents) and Chemical Ionization (CI) mass spectra (different reaction gases). These types of spectra are generally not used in computer search systems. NMR spectra are normally interpreted using chemical shift correlation tables and coupling constants. CI mass spectra depend strongly on the type of instrumentation and recording conditions making them less suitable than EI mass spectra for retrieval purposes.
- Standardized thin-layer chromatographic (TLC) RF values. These data are similar in nature as GC retention indices.
- Spectral data such as high resolution mass spectral data, collision activated dissociation (CAD) mass spectra and liquid chromatography-mass spectral data which are produced by instruments which are not generally available.
- ¹³C NMR data. Although very useful for structure elucidation the use of ¹³C NMR spectrometry is limited due to its low sensitivity.
- Spectral data which provide limited additional information, such as originating from ultraviolet (UV), Raman and near-infrared (NIR) spectrometry.

It is not advisable to create a compilation of standardized liquid chromatographic (LC) data in the same way as GC retention indices. Such a system could possibly be effective in one laboratory for a restricted class of compounds. However, due to the variations in column packings and eluents as well as the large variety in nature of the CW agents and their related compounds, a reliable retention index system for LC would be very difficult to achieve at the moment. Although TLC tends to become a forgotten technique, it is in some areas still the method of choice for the screening of polar compounds and could be considered as an alternative for LC data (23). By using coloured or UV-absorbing reference compounds the measured RF values can be converted into standardized data.

4. Distribution of the data

Creating an instrumental data base from existing data obtained from various sources can only be carried out by assembling the data in a central computer system, situated either in the Technical Secretariat or in its central laboratory. However, the best places to actually use the compiled data are the designated laboratories where the analyses are performed. Instead of creating a system such as the Chemical Information System (CIS) (24) where the data are only accessible by a computer network, the relevant verification data should rather be incorporated in the computers used by the laboratories. For this purpose the search/library facilities provided by instrument manufacturers could be used. Nowadays almost every spectrometer manufacturer offers a library search system as a part of their data systems, including a library obtained from NIST (mass spectra) or Sadtler (IR, NMR spectra). Relevant data of the compounds of CW interest from the central computer should be converted into the formats of the various data systems of the designated laboratories using information obtained from the manufacturers about the data format applied. Additional data should be supplied to these laboratories on a regular basis. Finally, despite all these computer systems chemical analysts would still like to have the data in a printed form as well. Therefore the data should also be distributed in the form of atlases.