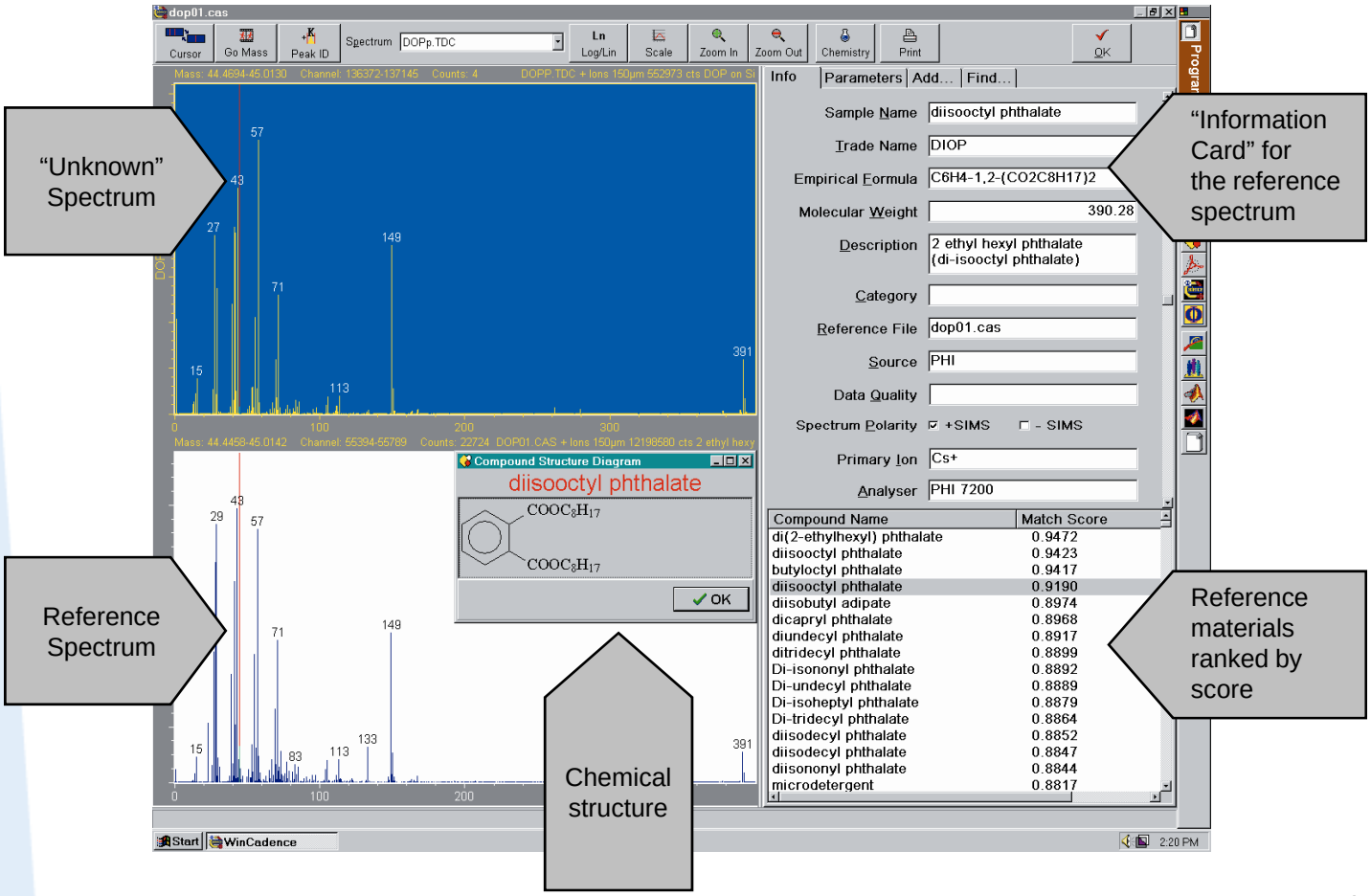
PHYSICAL ELECTRONICS
A DIVISION OF ULVAC-PHI

# *WinCadence*

# Compound Identification Tool

The widespread acceptance of TOF-SIMS has not been limited by instrumentation or technique, but rather by the ability to interpret the complex data. In the past, TOF-SIMS data interpretation required expert knowledge acquired through years of training and experience. Computer software has the potential to transfer this expertise to all analysts.

The *WinCadence* instrument control and data reduction program offers several useful tools to assist in data interpretation, including peak identification by mass and chemistry, isotope markers, and a compound identification tool (Compound ID). Compound ID takes advantage of the high mass resolution information that is available in TOF-SIMS spectra in order to provide the most likely match of the unknown spectrum to a reference spectrum in the spectral database. The high mass resolution of TOF-SIMS can be of assistance in resolving multiple species on the sample surface, which is quite different from data associated with more traditional organic mass spectrometry. Therefore, the spectral matching algorithm takes relative peak intensities and exact mass into account when calculating the “match score” value. The reference spectra with high match scores are useful in identifying the type of material the unknown spectrum represents. Furthermore, the algorithm uses a reverse search, which allows the evaluation of non-pure samples (mixtures).



The library of reference spectra in *WinCadence* represents over 900 spectra. In addition, *WinCadence* is compatible with the electronic data published by SurfaceSpectra (formerly Wiley). The SurfaceSpectra library currently represents over 800 materials and is growing steadily. Together the libraries comprise over 2000 spectra representing a wide variety of materials as shown below.

## Categories of Library Materials

| Organic | Inorganic | Multi-component |
|---|---|---|
| Copolymers | Electronic Materials | Adhesives |
| Coupling agents | Organometallics | Alloys |
| Homopolymers | Oxides | Coatings |
| Lipids | Salts | Formulated Polymers |
| Natural products | Miscellaneous | Miscellaneous |
| Pharmaceuticals | | |
| Polymer additives | | |
| Surfactants | | |

### Useful Compound ID Features

- View the high mass resolution spectrum of every reference compound
- Obtain a “match score” for the unknown spectrum with respect to reference spectra in the library
- Print the unknown spectrum and its “information card” alongside the corresponding reference spectrum
- View the chemical structure of the reference material
- Browse the library of reference spectra
- Search the library using a user-defined list of diagnostic peaks
- Search the library using a material name or name fragment
- Customize the library by adding spectra relevant to your applications

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