detected. Thus, in a sample, further unknown toxic compounds that affect the test system can be detected, leading to a complete toxicity profile of the sample related to the test system.

III. IDENTIFICATION

In planar chromatography, a substance is identified by comparison with an authentic standard cochromatographed on the same plate. Parameters that are compared are the hR_f value, the analog curve (absorption at a definite wavelength), the color of the zone if the zone is visible or inherently fluorescent, the spectrum, and/or the reaction with a derivatization reagent.

Unknown substances can be detected and identified by a special feature, called a multiwavelength scan (CAMAG TLC Scanner3), with which the plate is automatically scanned at up to 30 different wavelengths. The analog curves at the different wavelengths are overlaid in one graphic (Fig. 7), and the spectral and chromatographic properties are compared to a series of identification standards. Thus, unknown constituents of a sample can be detected and identified over a wide wavelength range.

For fingerprint identification, all samples on one plate are compared to one another at the same time. If necessary, analog curves of samples on different plates are overlaid by a special feature of the CAMAG VideoScan. Thus, for example, in plant analysis the chemical constituent profile is linked to the botanical identity of a plant.

Generally, UV/vis spectra are recorded because they can easily be measured with a conventional TLC scanner. The spectrum can then be compared with a standard cochromatographed on the same plate or with a spectral library. However, if possible, more information is given by recording an FTIR, Raman, or mass spectrum. In former times, zones of interest were recovered by extraction from the adsorbent and were then characterized by FTIR-, Raman, or mass spectrometry. Nowadays, there seems little need to go through time-consuming recovery procedures. FTIR or Raman spectra can be directly recorded on the plate using appropriate instrumentation. Recording of in situ mass spectra is described in detail in Chapter 9, and the detection and identification of radioactively labeled substances in Chapter 12. For identification of very complex mixtures, coupling of separation methods (especially HPTLC with HPLC) is used to cope with difficult separations and to get rid of interfering matrix.

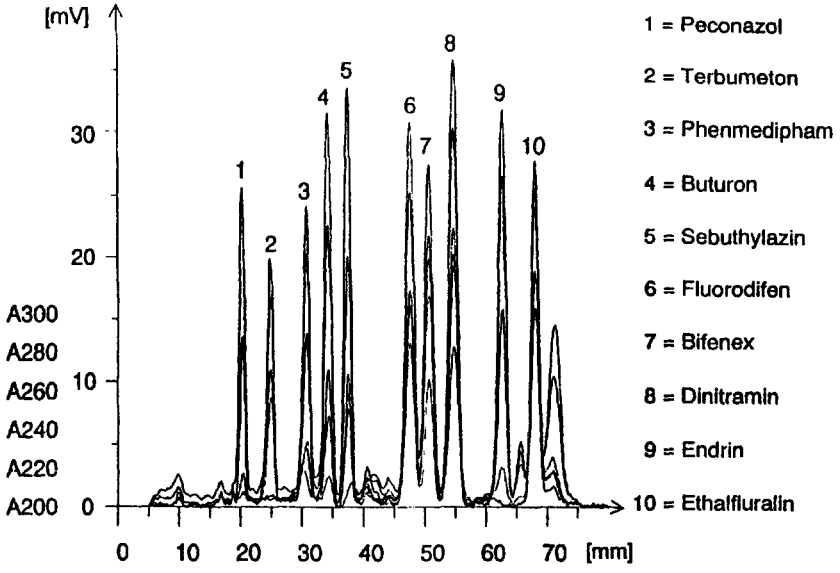

Figure 7 Multiwavelength scan of pesticides recorded at six different wavelengths that are superimposed to get a spectral scan of the track.