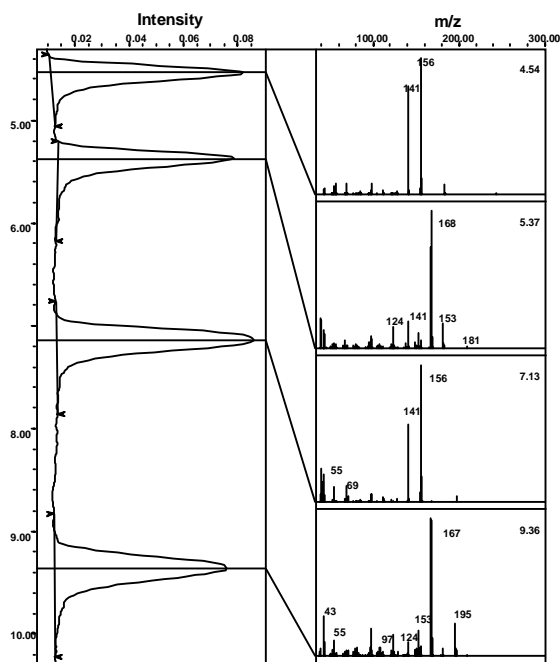### Identifying Barbiturates in Combined Solution

Highlights: Analysis of related compounds with similar UV spectra; confirmation of identity by user-created library matching.

Multiply substituted compounds often produce UV spectra similar enough to each other that positive identification by UV spectra alone can be difficult. Positive identification by LC/MS requires the ability to couple a low dispersion LC system to the mass spectrometer to minimize chromatographic band broadening and enhance sensitivity.
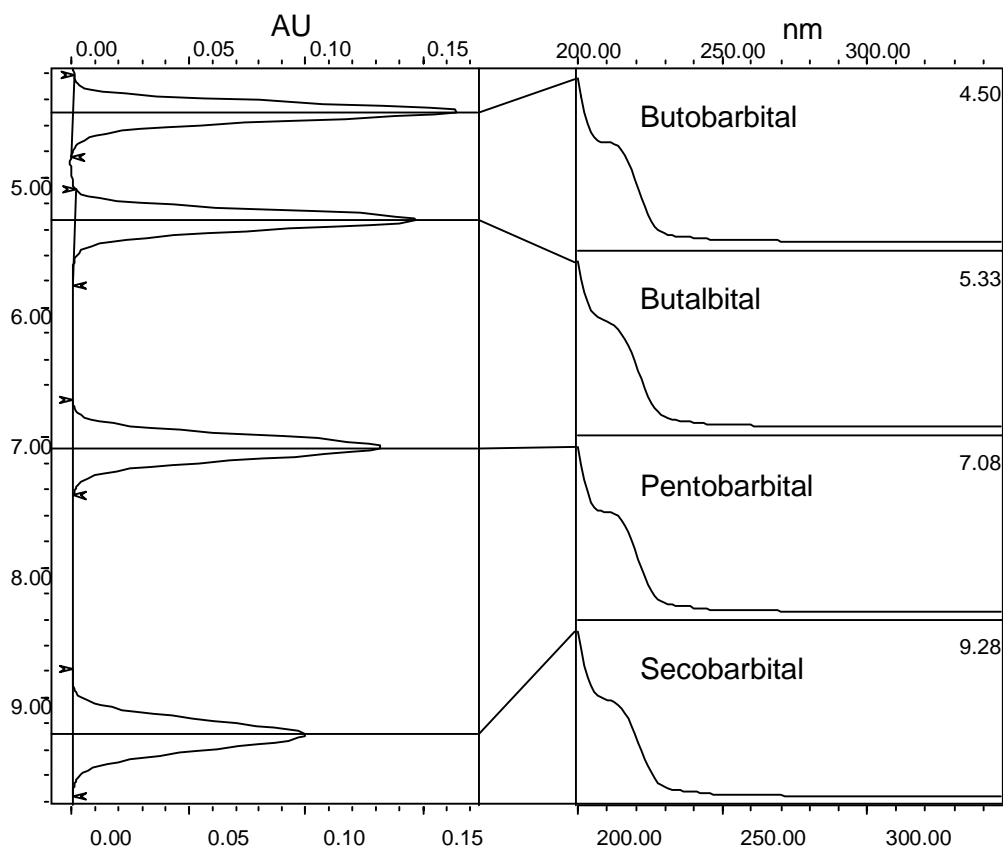

In this example buto-, butal-, and pentobarbital are separated along with secobarbital. The photodiode array spectrum index plot allows comparison of UV spectra for each peak in the chromatogram. These compounds have very similar UV spectral shapes with minimal unique features which makes identification difficult.

Intensity   **m/z**

0.02 0.04 0.06 0.08   100.00   200.00   300.00

Match Plot Peak 4: Unknown RT: 9.36

156
141   4.54

5.00

168   5.37

6.00

124 141 153
181

156   7.13

141

8.00

55
69

167   9.36

9.00

43
195
55 97 124 153

10.00

0.015 **Peak #4**   167

0.010

Intensity
0.005   43
55   97   124   153   195

0.000
50.00   100.00   150.00   200.00   250.00   300.00

0.015 **Match #1 Fit 85 SECOBARBITAL**   168
41

0.010

Intensity
0.005   53   97   124
153   195

0.000
50.00   100.00   150.00   200.00   250.00   300.00

0.01 **Difference**

0.00
Intensity   53   97   124

-0.01
41

50.00   100.00   150.00   200.00   250.00   300.00
m/z

The mass spectrum index plot allows comparison of mass spectra for each peak in the chromatogram. These compounds have unique mass spectra which allow comparison to commercially available reference libraries or user created libraries for compound identification.

A comparison of the retention time and peak shape of peak #4 (secobarbital) in the mass spectrum index plot (on the left) to the photodiode array spectrum index plot (reverse side) illustrates the low dispersion of the Integrity System.
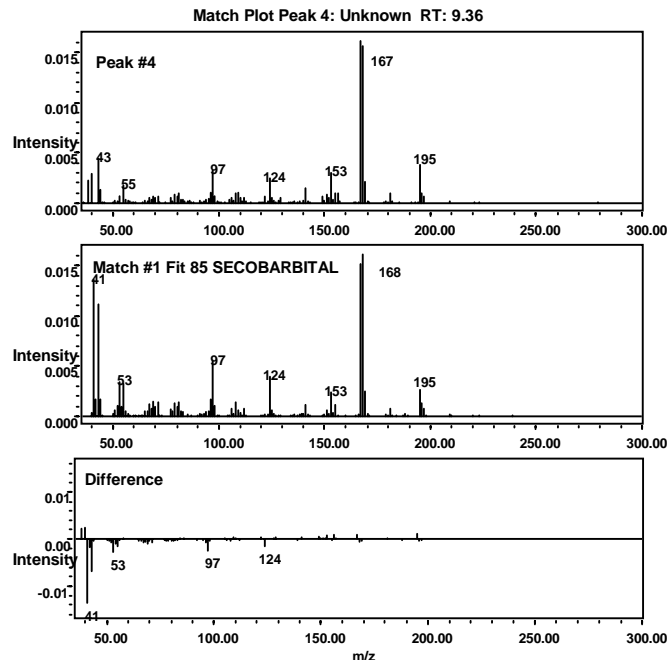
The results of a mass spectral library match on the fourth chromatographic peak are displayed in Triple Plot format (on the right). Triple Plot allows visual comparison of the acquired secobarbital spectrum to the library spectrum and displays the difference between the two. The display reports the probability, or "fit" of the peak, to the library match (in this case a very high probability of 85) and the level of contamination or difference.