Waters
Lab Highlights
An Internal Communication of Applications and Techniques
LAH 0413 6/89
AN/ES/PM/IC/HM

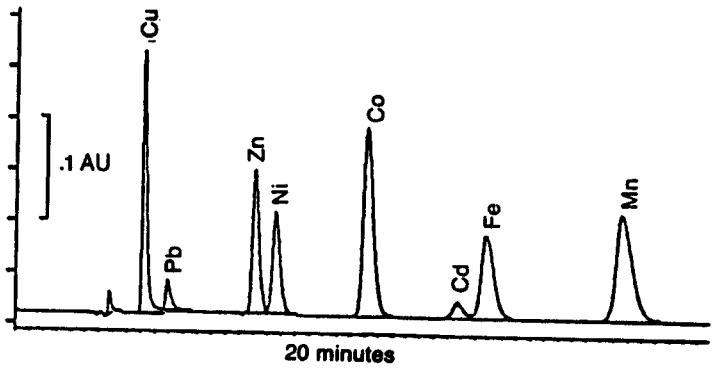
Application of W•I•S•E Software: Optimization of a Tartrate/Citrate Blended Eluent for Transition Metal Analysis

Using a μBondapak™ C_{18} column and an eluent containing tartrate and octanesulfonate, eight divalent transition metal ions can be separated with excellent resolution (see Figure 1). This separation has been discussed in detail in a recent issue of Waters™ Ion Chromatography Notes[1] and has been compared to an ion exchange approach[2]. In actual samples, some of the eight metal ions may either be missing or present at high concentration relative to closely eluting species. Thus, it is useful to be able to manipulate the selectivity of the separation as required.

Figure 1: Divalent transition metal profile for tartrate eluent.

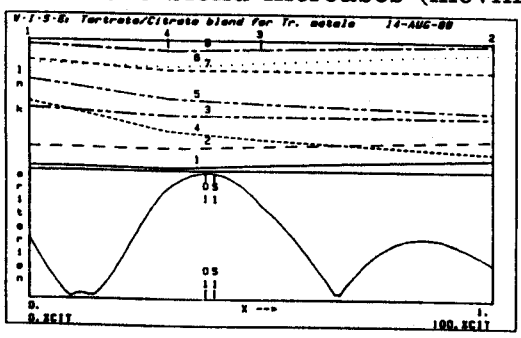
Column:	**μ-Bondapak C_{18} (3.9mm x 30cm)**
Eluent:	**2mM sodium octane sulfonate**
	50mM tartaric acid
	pH 3.4 with NaOH
Flow:	**1ml/min**
Post Column:	**0.2mM PAR at 0.5ml/min**
Detection:	**UV at 520nm**

See reference 1 for additional details.



One approach to selectivity adjustment for this separation is the replacement of tartrate with another organic acid. Alternately, two organic acids may be blended in various proportions to control selectivity. The latter approach is perfectly suited to the capabilities of W•I•S•E software[3-6], and has been studied in our laboratory for optimization of a blend of 50 mM tartrate and 50 mM citrate eluents (both at pH 3.4). Figure 2 presents the Eluent Selection Diagram generated by W•I•S•E software after input of retention times from four experiments, including the starting tartrate and citrate eluents along with two blended eluents. In the upper portion of the diagram, note that several solutes change their elution order as the proportion of citrate eluent in the blend increases (moving from left to right in Figure 2).

Figure 2: Eluent Selection Diagram from W•I•S•E software.



Vince Warren/Jim Krol

For the separation of all eight transition metals, W•I•S•E software predicts a 40/60 citrate/tartrate blend to be optimal. This is confirmed by the actual separation, shown in Figure 3. Overall, peak spacing is improved relative to Figure 1, especially for the Cu/Pb and Zn/Ni peak pairs. Note also that the Zn, Ni, Fe and Cd peaks elute in a different order from that of Figure 1, indicating a change in selectivity.

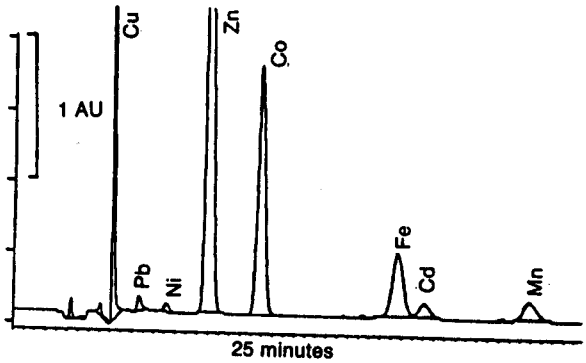


Figure 3: Divalent transition metal profile for tartrate/citrate blend. Conditions as in Figure 1 except eluent contains 30mM tartaric acid and 20mM citric acid.

In addition to optimizing the overall separation, the information provided by W•I•S•E software (Figure 2) can be used to predict the optimal eluent for the separation of any subset of the eight transition metals. Since every sample matrix presents a somewhat unique separation problem (e.g. plating baths vs. polisher condensate), the ability to easily determine the optimal eluent for a subset is significant. As an example, removal of a single transition metal shifts the optimal citrate/tartrate blend as follows:

Missing solute	Optimal blend: (citrate/tartrate)
Cu	38/62
Pb	54/46
Zn	35/65
Ni	58/42
Co	43/57
Cd	28/72
Fe	27/73

As expected, the most dramatic shift in the location of the optimum occurs when either of the least resolved peaks in Figure 3 (Fe or Cd) is removed from the mixture.

References

1 J. Krol, *Ion Chromatography Notes*, **2**, 1.
2 LAH 0393 4/89
3 LAH 0360 2/88
4 LAH 0369 6/88
5 LAH 0384 2/89
6 LAH 0389 2/89

* * *