COMPUTER-AIDED IDENTIFICATION OF HOMOEOPATHIC MOTHER TINCTURES WITHOUT THE USE OF REFERENCE COMPOUNDS

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Thin-layer chromatographic (T-LC) methods for the evaluation of crude drugs monographed in the British and European Pharmacopoeias include details of the layer, solvent system, visualisation technique, reference substances and assessment of the chromatogram. These procedures are possible where the constituents present in the drug are known but, in the case of homoeopathic mother tinctures ($\emptyset$'s) prepared from plant materials the chemical nature of the constituents is not always known thus making it difficult to design T-LC methods for their identification.

The aim of this preliminary work was to establish whether it would be possible to design a single, standard method for T-LC analysis which could be applied to any $\emptyset$ and, being mindful of the number of $\emptyset$'s likely to be involved, to utilise the microcomputer for assessment of results. In addition, the whole procedure was designed to be used by personnel with a minimum of training.

Experimental procedure: A constant load (10 μl) of $\emptyset$ is applied to the base line of the T-LC plate (Silica gel GF_{254}) and developed (10 cm) in each of six solvent systems. Assessment of the developed plates is by monitoring in UV light for quenching of fluorescence (254 nm) and for native fluorescence at (365 nm).

To convert the results into suitable input data for processing by the microcomputer the following procedure is used: a template is made the width of the plate and lines drawn at 1 cm intervals from 0.5-9.5 cm from the starting line. The first and last 0.5 cm are neglected to avoid assessment of any base line fraction and material carried on the solvent front. The nine zones are labelled A-I to represent zones of quenching and J-R for zones of fluorescence. The template is superimposed on the marked plate or tracing and the appropriate zones coded for each solvent system.
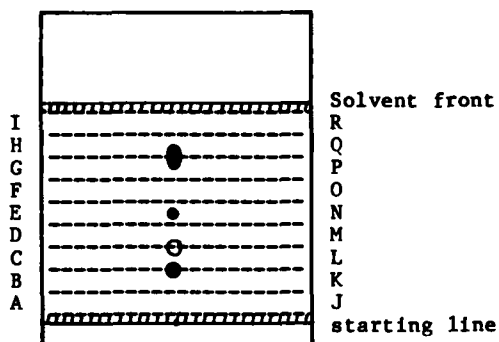
Solvent systems:

1 n-butanol:acetic acid:water
                     (4:1:1)
2 chloroform:methanol   (9:1)
3 methylene dichloride:
   methanol:formamide (3:6:1)
4 chloroform:acetone:ammonia
                  (25:24:1)
5 chloroform:diethylamine (9:1)
6 toluene

A-I:input code for quenching ($\bullet$)
J-R:input code for fluorescence (O)

Example of input code for chromatogram:
     BCEGHLM

Fig.1 Assessment of chromatogram

The program TINCTURE is written in BASIC for the Intertec Superbrain Microcomputer and includes data encoded in such a way that the relevant information is stored in a file. The program calls for the input of the code letters for each solvent system in turn, the results are processed and, by use of a scoring system, the most probable identities are displayed in numerically descending order.

The data bank, consisting of twelve $\emptyset$'s, used in this preliminary work was based on British $\emptyset$'s and, although in some solvent systems the profiles for corresponding French and German tinctures are dissimilar, it is interesting to note that the computer allocated the highest score for the correct tincture in eleven out of twelve cases.