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Note

Computerized storage of thin-layer and paper chromatographic data

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Data storage of analytical results has always been important for pharmaceutical raw materials, formulations and stability studies. However, this task is becoming very difficult and complicated because of the vast increase in government requirements of supplementary analytical data for the approval of registering a new drug substance.

Application of the computer to store and handle the analytical data has offered a great help in organizing and retrieving stored results. The literature contains many references describing the use of the computer in the analytical laboratory. Some of these applications include selecting and differentiating between chromatographic liquid phases[1], determination of the temperature dependence of the retention index in gas–liquid chromatography[2], on-line interactive data processing for mass spectrometry and gas chromatography[3], acquisition of cyclic voltametric data[4], and data retrieval for assigning of chemical shifts to facilitate interpretation of carbon-13 nuclear magnetic resonance spectra[5].

SYSTEM

In this communication we wish to describe a simple system to report the number of spots, their relative mobilities to the main spot, type of thin-layer adsorbent or paper used, and the R_F value of the compound of interest.

Fig. 1 shows a typical R&D Control Assay form used in our laboratories.

The result section is allocated 5 digits. IBM cards are punched from this form and the data are stored using an IBM-370 computer until needed. The 5 digits of the result section are assigned Positions 1–5.

R & D CONTROL ASSAYS
ELI LILLY AND COMPANY

ITLE _____ DATE SENT

UBMITTER & DEPARTMENT		LOT NO (NOT OVER 10 DIGITS)		(PROJECT NO.)(ITEM CODE) NOT OVER 18 CHARACTERS					
		1		11					
EPORT AS	M	ASSAY FOR (NOT OVER LETTERS)	MAN HOURS (DCML)	NO OF FATAL ANIMALS (DCML)	DEPT. DOING	METHOD NO	CHARGE TO	DATE OUT	
9	36	37	46	50	54	57	60	67	
					ANALYST NO	RESULT (NOT OVER 5 DIGITS)		DISP	
					72	75		80	

Fig. 1. R & D Control Assay form.

Position 1

The first position characterizes whether a spot exists at the point of application (P0A). "0" indicates that there is no material left at the P0A, while "1" indicates that there is a spot at the P0A.

Position 2

The second position is reserved for the number of spots between the P0A and the main spot, *i.e.* the number of the less mobile (more polar) spots.

Position 3

The third position indicates the number of spots between the main spot and the solvent front, *i.e.* the number of more mobile (less polar) spots.

To find the total number of spots, sum the first three positions and add 1 for the main spot. No addition of 1 should be made if the material is only at the P0A.

Position 4

This position is used to indicate the adsorbent type of one of the four commonly used commercially available precoated TLC plates: character S is reserved for silica gel plate, A for alumina plate, C for cellulose plate, and P for polyamide plate. The character W at position 4 indicates paper chromatography on Whatman No. 1 filter paper.

Position 5

The fifth position is reserved for the chromatographic mobility of the main spot reported to the nearest 0.05 R_F unit. Numbers from 0–9 are assigned to the R_F values. 0 indicates that the main spot remains at the P0A, 1 indicates an R_F value of 0.1, 2 is an R_F value of 0.2, etc. To be able to indicate a 0.05 unit of R_F, we use the letters D, E, F, G, H, I, J, K, L, M, where D and E in the fifth position indicate R_F values of 0.05 and of 0.15, respectively. The number or letter chosen in position 5 represents the closest figure to the calculated R_F value.

EXAMPLES

Example 1

A Whatman No. 1 filter paper chromatogram shows a spot at the P0A, two less mobile and three more mobile spots; the R_F value of the main spot is 0.54. The result section is filled as follows:

RESULT (NOT OVER 5 DIGITS)				
1	2	3	W	I
75				

The total number of spots is seven.

Example 2

A silica gel thin-layer chromatogram shows besides the main spot only four

more mobile spots. The main compound has an R_F value of 0.72. The result section is written as follows:

```
RESULT
(NOT OVER 5 DIGITS)
 0  0  4  S  7
75
```

The total number of spots is five.

Example 3

An alumina plate chromatogram shows only one spot at the P0A and nothing else. The result section appears as follows:

```
RESULT
(NOT OVER 5 DIGITS)
 1  0  0  A  0
75
```

The total number of spots is one.

CONCLUSION

Reporting the chromatographic results as shown above offers a means of storing and retrieving the number of spots and all other data mentioned in a useful way. The positions assigned are quite flexible and can be altered to meet the need of different laboratories.

If some of the aforementioned data are not useful, one can report the conditions under which the plate was viewed, *i.e.* short-wave, long-wave UV light, visible light, etc. These data can be assigned numbers or letters and substitute any of the previously assigned positions. Since these R&D Control Assay sheets were designed before the system reported in this paper was established, we were limited to five digits. If one is generating its own form, the result section may be assigned six or more digits. This way more information may be stored.

This system, based on five digits, has been used in our laboratories for the last several years. The numerical characterization of the chromatogram as far as the number of spots, their relative mobilities, type of adsorbent used, and R_F value of the main compound is made easier using solely the computer print-out. The system establishes an effective and simple way of reporting, storing and retrieving the data associated with thin-layer and paper chromatography. This approach saves on photographing and/or tracing of the chromatograms. As a result, the dissemination of the analytical and stability data becomes easier and less bulky.

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