Notes

CHROM. 5545

Computer-generated chromatograms

The computer-guided plotter is a valuable display device between the chromatograph and the digital computer, and is useful, for example, in the analysis of peak shapes and in chromatogram simulation.

Shape-checking

The curves in Figs. 1 and 2 are an example of shape-checking. The computer plot in Fig. 1 was used to check the Gaussian shape of the crude peaks in Fig. 2, obtained by ion-exchange chromatography[1]. When the computer-generated Gaussian peaks, on the original scale delivered by the plotter, are superimposed on the crude chromato-
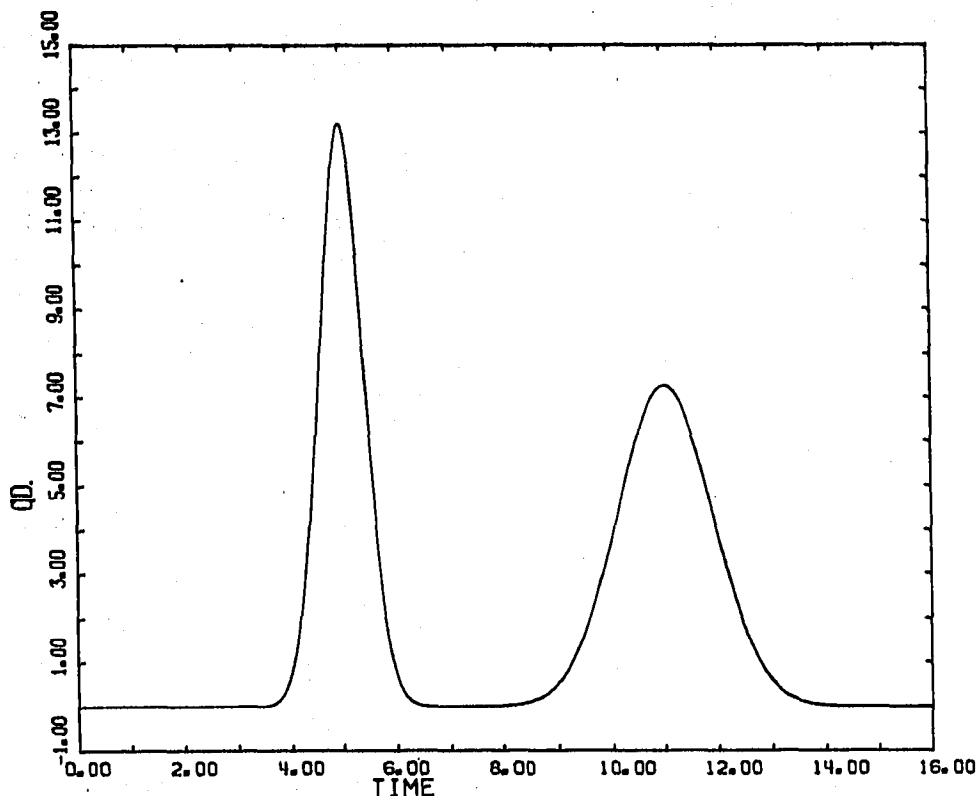

Fig. 1. Computer-generated Gaussian peaks. Original cytosine height (HITE) = 13.21 cm.

gram, the match is so good for the cytosine peak that no difference can be detected with the naked eye, whereas slight asymmetry is visible for the guanine peak.

The computer chromatogram was generated with the Fortran program in Fig. 3a, which shows the Gaussian function used. After first measuring the height and half-width of the crude peaks on the original chart paper, the best match can be obtained after a few attempts. Most computer-plotter libraries contain subroutines
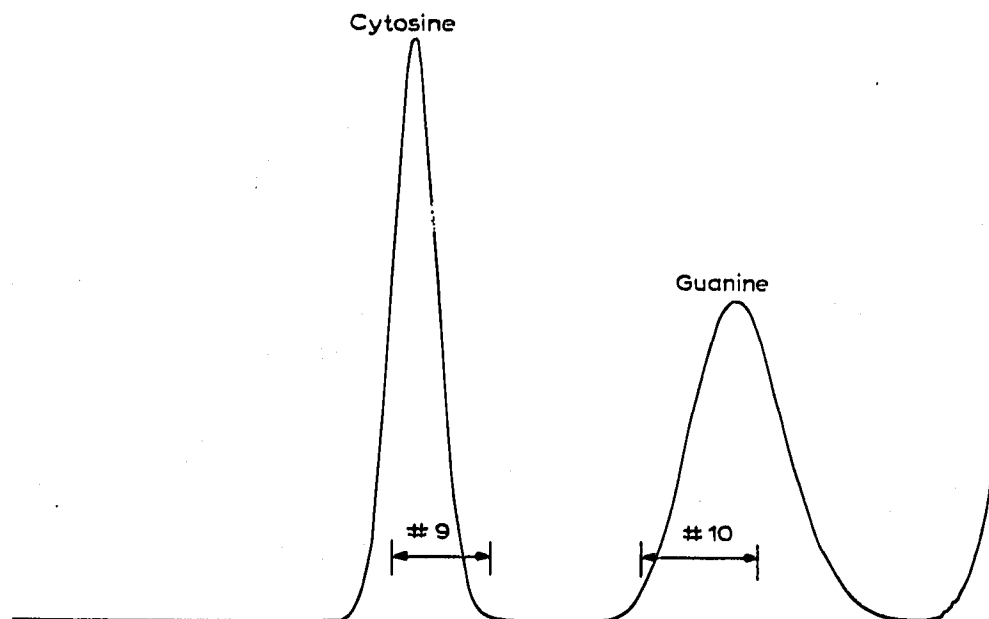
Fig. 2. Crude analogue signal from chromatograph. Original cytosine height = 13.2 cm.

```
      PROGRAM MATCH
C  MATCH GAUSSIAN PEAK WITH REAL PEAK
      DIMENSION  X(801),  Y(801)
C  FUNCTIONS FOLLOW
      S(HW)=  HW**2/ (4.*2.303*0.301)
      CONC(HITE,TIME,SPR,T)=  HITE*EXPF(-(T-TIME)**2/SPR)
      DO 1   I=1,801
2     X(I)=FLOATF(I-1)*16./800.
      Y(I)=  CONC(13.21,5.,S(.98),X(I))  +CONC(7.27,11.02,S(2.08),X(I))
1     CONTINUE
3     CALL PLOTCM(X,Y,801,0,0.,16.,-1.,15.,4HTIME,2HOD)
      END
```

(a)

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      PROGRAM ELUTE
C  CHROMATOGRAM SIMULATION BY DIGITAL PLOTTING
      DIMENSION  X(961),  Y(961),  ABS(50),PATH(50),ELTIME(50),HW(50)
C  PEAK PARAMETERS FOLLOW
      DATA(ELTIME=40.,70.,90.,130.,140.,180.,190.,230.,260.,290.)
      DATA(ABS=1.5,1.,.5,.4,1.,.75,.65,.25,.5,.25)
      DATA(HW=3.,6.,9.,7.,6.,6.,8.,14.,9.,20.)
      DATA(PATH=50(1.))
C  FUNCTIONS FOLLOW
4     CONC(POS,SPREAD,T)=  EXPF(-(T-POS)**2/SPREAD)
8     SPR(Q)=  Q**2/(4.*2.303*0.301)
      NO=10
      DO 2   J=1,961
5     X(J)=FLOATF(J-1)*320./960.
      SUM=0.
      DO 3   I=1,NO
6     SUM= SUM  +  ABS(I)*PATH(I)*CONC(ELTIME(I),SPR(HW(I)),X(J))
3     CONTINUE
      Y(J)=SUM
2     CONTINUE
7     CALL PLOTCM(X,Y,961,0,0.,320.,-1.,7.,8HTIME MIN,2HOD)
      END
```

(b)

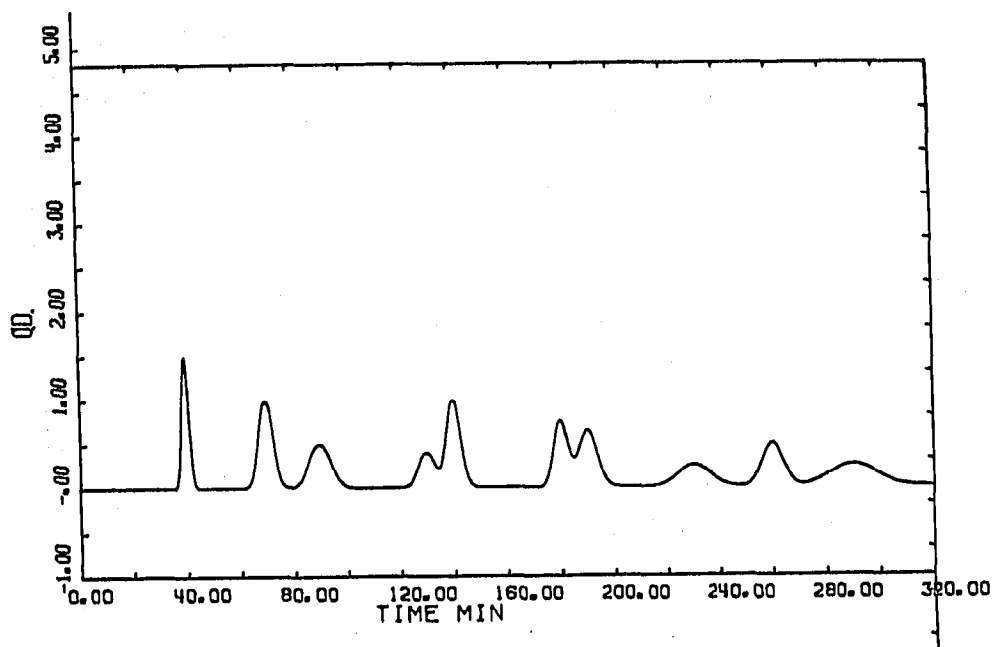Fig. 3. Fortran programs for shape-checking (a) and chromatogram simulation (b).

Fig. 4. Computer-generated chromatogram of multicomponent mixture.

of varying complexity, including a subroutine such as PLOTCM used here, which plots the contents of two arrays, X and Y, inside a tailor-made box provided with graduated coordinates. In PLOTCM, the first two arguments are the x and y coordinates of the points, and the third argument shows that 801 points are to be plotted.

Chromatogram simulation

The simulated chromatogram in Fig. 4 was generated with the Fortran program in Fig. 3b. This type of computer-generated chromatogram suggests the way in which real peaks, stored in the on-line computer during the chromatography of single-component solutions, may be displayed on the plotter in order to predict rapidly the composite chromatogram of a multicomponent mixture.

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1 B. E. BONNELYCKE, K. DUS AND S. L. MILLER, *Anal. Biochem.*, 27 (1969) 262.

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