EDITORIAL

Nowhere has computer graphics made more of an impact than in the pharmaceutical industry. The investment both in hardware and in personnel far outstrips that in other industries or in academia. Happily, it seems this expenditure is being justified by results. The feedback from companies suggests that new compounds are being synthesized as a result of computer-aided design techniques and the intelligent synthetic chemist, far from being inhibited, is being stimulated to think in novel directions. A very perceptible momentum has been created in the area of drug design, but we have not reached a stable plateau where there is a concensus on the techniques to be used or on the hardware to be employed.

A few years ago, applying theoretical methods to drug design was considered to be, at the very least, mildly 'dotty'. Now Faculty positions are being created in chemistry and pharmaceutical departments for experts in computer graphics. Belfast has advertized a 'new blood' lectureship in the subject and the University of Minnesota is seeking a specialist in computer-aided drug design who will be equipped with quite stupendous facilities — two Cray 2s, a Cyber 205 and an ETA 10 with a Cray 3 projected, as well as several high resolution colour work stations which will be interfaced to the mainframes.

This worldwide activity is reflected in the large number of meetings on the topic of computer-aided drug design to which this special issue of the Journal of Molecular Graphics is devoted.

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