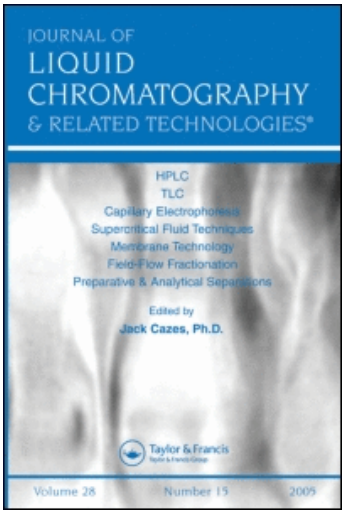

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A review of: "Hyperchem for PC: Windows Version"

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SOFTWARE REVIEW

HYPERCHEM FOR PC: WINDOWS VERSION, Autodesk Corp., 2320 Marinship Way, Sausalito, CA 94965, 1992. Sugg. Retail Price, $3,500; Academic Institutions, $595; Indiv. Acad. Users, $1,875; Fed. Gov't., $2,495; Stae/Local Gov't., $2,995.

This software allows chemists to build, analyze and manipulate 3D molecular structures on desktop computers. Hyperchem runs under Microsoft Windows. Any 3D molecular fragment that one creates on the monitor can be saved in a library file that may be used later as a building block for other, more complex molecules. In addition, one can sequentially select residues from Hyperchem's built-in amino acid and nucleotide libraries to construct proteins and nucleic acids quickly and easily. The software provides a wide choice of analytical tools that help in conceptualizing a deeper understanding of the behavior of molecules and their interactions. The investigation of the reactivities of molecules and the evaluation of chemical pathways and mechanisms is also made possible.

We are currently using Hyperchem to study the transition state of a Diels-Alder addition reaction by using the AM1 semi-empirical method. Thus single point energy calculations and geometrical optimization may be performed by semi-empirical methods such as CNDO, INDO, MINDO3 and AM1. Although the methods that have been mentioned previously may not be sufficiently accurate for predicting optimized geometries, Hyperchem provides a user-friendly environment for performing these calculations for chemists who are, at least, acquainted and experienced with molecular modelling techniques. The fact remains, however, that a desktop molecular modelling alternative is extremely useful for bench chemists, since, in many situations, researchers require only an approximate molecular structure for the analysis of their mechanisms or, perhaps, the end product of a reaction sequence.

In addition, the use of different force fields such as MM+, AMBER, BIO+ and OPLS in molecular mechanics calculations are easily accessible through Hyperchem. These methods provide an extremely useful and powerful technique for studying large molecular fragments. The helical structure of a protein molecular fragment in 3D space can most definitely help drug chemists and pharmacists in designing drug molecules that possess the required functionality. Other features of Hyperchem include plots of the total charge densities, electrostatic potentials and analysis of the effect of solvation on a molecular system.

Being frequent users of low-end, medium-range and high-end molecular packages, the excellent features and the modest price of Hyperchem make it appear as the most attractive molecular modelling support for bench chemists. Although some low-end packages provide graphical manipulation that is sometimes superiorto that of Hyperchem on popular platforms such as IBM 386, Hyperchem remains more versatile and user-friendly. Hyperchem documentation is outstanding as it contains extensive background material for the various methods used by the package. The installation procedure is smooth and the tutorial includes directions for interfacing Hyperchem with Microsoft Excel. Our Windows environment includes CHEMWINDOWS, WORDPERFECT, CHEMEXHIBIT and HYPERCHEM.

Autodesk Corporation is, hereby, duly acknowledged for this excellent contribution to molecular scientists, but should, perhaps, strive to improve the graphical environment of Hyperchem.
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