MOBY 1.5

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MOBY 1.5[1] is a molecular modeling program for IBM-PC compatible computers that has been written by a computational organic chemist and offers an extensive range of modeling functions. Some of these features include displaying of up to 2000 centers, of IR and UV/visible spectra, molecular orbitals, and isopotential surfaces for electrostatic potentials, fast 3D graphics, independent manipulation of freely definable fragments, structure and property comparison, force field calculations on up to 150 centers interacting with up to 1850 other centers, Hückel molecular orbital calculations, steepest descent and conjugate gradient geometry optimization (molecular mechanics, MNDO, and AM1), conformational analysis of up to 10 different torsions, and molecular dynamics simulations. MOBY is able to construct and maintain an individual structure library, read standard file formats such as Cambridge Crystallographic Database, Brookhaven Protein Database, MNDO, MOPAC, MACCS II (Molecular Design), and SCHAKAL as well as read non-MOBY data in a freely-definable format.

The program installs very quickly and is not copy protected. Once the software is installed, the manual shows the user how to read in, display, and manipulate a complex structure using MOBY. This reviewer initially found MOBY to have a steeper learning curve when compared to that of HYPERCHEM. After investment of an afternoon of working through the examples in the manual, MOBY was found to be very easy to use.

One particularly nice feature of MOBY is its capability of permitting the user to explore the electronic and spectroscopic properties of a molecule. For example, a structure can be sketched, optimized by using a valence force field, then a quantum mechanical calculation can be performed, and the molecular orbitals or a charge distribution can be visualized. The molecular orbitals are displayed as either a sphere for the s-orbital contribution or two spheres with p-symmetry. The charge distribution can be displayed by color-coding of each atomic center according to charge, as an electrostatic potential color-coded on a van der Waals surface or as isopotential contours. All of these methods are useful in helping to explain the properties of molecules. If the appropriate IR and UV data are available, MOBY can be used to display the spectra. The line spectra can be simultaneously displayed along with the corresponding property change, normal mode vibration for IR, polarization direction, and charge distribution for UV/vis, respectively. This feature is extremely useful in the physical chemistry lecture in helping the students to grasp a deeper appreciation of molecular spectra and its relationship to molecular structure. Somewhat disappointing was that MOBY cannot directly calculate the data necessary to display IR and UV spectra. The IR and UV data must be read from the output of other programs such as MOPAC(QCPE PC version), GAUSSIAN, or VAMP(SCAMP) through the extra program QC4MOBY which converts the appropriate data found in the output file to the MOBY format. QC4MOBY does not come as part of the MOBY distribution. It is not essential to have QC4MOBY since the IR and UV files are ASCII files, and the format of each file is given in the manual.

MOBY is not only capable of performing a variety of calculations and analysis on organic molecules but is able to easily manipulate biological macromolecules. Such calculations and analysis include examining various secondary structures of large macromolecules, conformational analysis of amino acid side chains, molecular mechanics and molecular dynamics of protein fragments, and enzyme–substrate binding and determining the charge distribution of new substrates using semiempirical methods. Another area which MOBY excels in is the ability to manipulate structures. In MOBY the user can make structure comparisons, merge structures, multiply structures, and add hydrogens to the free valences of either all non-carbon atoms or to the free valences of all carbon atoms.

All molecular mechanics and molecular dynamics calculations of MOBY use the "united-atom" AMBER force field.[2] It is possible to carry out these calculations with cutoffs, periodic boundary conditions, and constraints. The user even has control on which terms of the energy function to include in the calculation. During the calculations, monitoring of the energy or forces acting on each atom can be done by color-coding of the centers according to their contributions to the force field energy or the magnitude of the force. MOBY is also able to display unfavorable distances and energy contributions during interactive docking.

The PROTOCOL and DEMO modes of MOBY are easy to use from both instructor and student points of view. The PROTOCOL mode, which only accepts keystroke input, permits an instructor to easily record a demonstration of a concept, while in the DEMO mode the student can replay the recorded session at their own pace. MOBY comes with numerous prerecorded tutorials which illustrate its various features and capabilities.

Output of a structure can be done by printing to an HP LaserJet, NEC P6 and P7 impact printers, and an Epson FX 80 dot matrix printer. Upon registering MOBY, the user receives in the mail a diskette which contains files to convert MOBY files to postscript for printing on a Postscript laser printer. MOBY can also write files in HPGL format.

The latest version of MOBY 1.5, runs on IBM-PC compatible computers and requires the following minimum specifications: 640 KB random access memory (530 KB free random access memory), 80x87 arithmetic coprocessor, graphics adapter (Hercules, EGA, or VGA (1024x768 maximum)), a mouse, and a hard disk is are strongly recommended. MOBY is a DOS program and does not run under WINDOWS. A free demonstration version of MOBY 1.5 is available via anonymous FTP from benny.bsc.mass.edu (or 134.241.41.4).

In summary, this reviewer found MOBY to be a well written program with many capabilities. MOBY's low cost makes it a very attractive program to have and include in an undergraduate biochemistry, organic, and physical chemistry course. I highly recommend this program to those looking for molecular modeling software to use on a PC and in a molecular modeling course.

REFERENCES AND NOTES

(1) *MOBY 1.5 Molecular Modeling on the PC*; Springer-Verlag: Berlin, 1992; ISBN 3-540-14119-7.
(2) Weiner, S. J. *J. Am. Chem. Soc.* **1984**, *106*, 765.