

# PocketMol

## A Molecular Visualization Tool for the Pocket PC

Jason R. Gilder  
gilder.2@wright.edu

Dr. Michael Raymer  
michael.raymer@wright.edu

Dr. Travis Doom  
travis.doom@wright.edu

**Bioinformatics Research Group (BiRG)**  
**Computer Science and Engineering**  
**Wright State University**  
**Dayton, OH 45435**

### Abstract

*Molecular visualization programs are available on many platforms. They allow a user to visualize and manipulate molecular structures. PocketMol provides the same functionality on a Pocket PC handheld computer. Using standard protein data bank (pdb) files, the user can move, rotate, and scale a protein to explore its structure and function. The user can choose from a standard backbone view or a simplified view using only alpha carbon atoms. PocketMolGX uses the Microsoft Game API to provide fast animation that is quite smooth. PocketMol is designed as an aid for those wishing to explore or demonstrate protein structures without the availability of a full-size computer.*

### 1.0 Introduction

Recently, palm-sized computing devices, such as Palm Pilots, have become widely available. One such device is the Pocket PC. It provides the functionality of a full-size computer in a fraction of the size, using a touch screen and stylus for input. Molecular visualization programs have been available on many platforms, including Dino [1], RasMol [2], Amber [3], as well as many others [4]. However, the handheld PC market has yet to be supported. PocketMol is a molecular visualization package for the Pocket PC. It comes in two flavors: the standard PocketMol and the graphically accelerated PocketMolGX. The latter only supports the iPaq H3635 Pocket PC, but

provides very fast and smooth animation. PocketMol has the basic functionality of its desktop counterparts, and with some work, will be a suitable alternative for those wishing to explore or demonstrate protein structures on a handheld device.

### 2.0 Background

The Pocket PC is a handheld device that provides the same functionality as a full-size computer. They consist of a touch screen, stylus, and several buttons for input. PocketMol was developed on the Compaq iPaq H3635 (see Figure 1). The iPaq has a 206 Mhz Intel StrongARM processor, a 240 x 320 backlit display with 16-bit color, and 32 megabytes of RAM. The device has no hard drive. All permanent software, including the Windows CE operating system, PocketOffice, and other bundled programs, are stored in 16 megabytes of ROM. The 32 megabytes of RAM is designed for other programs and data storage. The iPaq supports several upgrades including a Compact Flash Expansion sleeve. This allows the addition of Compact Flash memory cards that hold anywhere from four megabytes to one gigabyte of additional memory. The Pocket PC interfaces with a regular PC via a USB or serial connection. The Pocket PC's operating system, Windows CE, is a stripped-down version of Windows 2000 and is fully 32-bit. It retains much of the familiar GUI interface, even including the Start menu. The Pocket PC is a versatile device that is quickly gaining popularity and support.



Figure 1. The iPaq H3635 Pocket PC. Source: <http://www.compaq.com>

### 3.0 Discussion

#### 3.1 Initial development

Development was begun on a desktop PC running Windows 2000. Microsoft provides its eMbedded Visual Studio development suite as a free download on its web site [5]. It contains eMbedded Visual C++ and Visual Basic. These mirror their desktop counterparts in almost every way. The biggest difference is that the user must now select a target processor for the compiled program. Pocket PC manufacturers all use a different processor, so the compiled program is machine-specific. The eMbedded Visual Studio also includes emulation for Pocket PCs and larger handheld PCs. This facilitates quick testing and development.

#### 3.2 The user interface

Pocket PCs replace the menu bar at the top of the screen with a command bar along the bottom. PocketMol follows this standard (see Figure 2). The main controls are text buttons that can be turned on or off. Rotate, Scale, and Move are used to manipulate the protein. The stylus is used to control the rate and direction in each case. The last button, CA, provides a simplified backbone view of only the alpha carbons (see Figure 2). If the Scale, Rotate, or Move buttons are not pressed, the stylus may be used to see information about individual atoms (see Figure 2). Pressing the stylus on an atom will display its number, type, residue number, residue type, and coordinates. The coordinates are measured in pixels to allow the user to quickly establish the relative positions of multiple atoms.

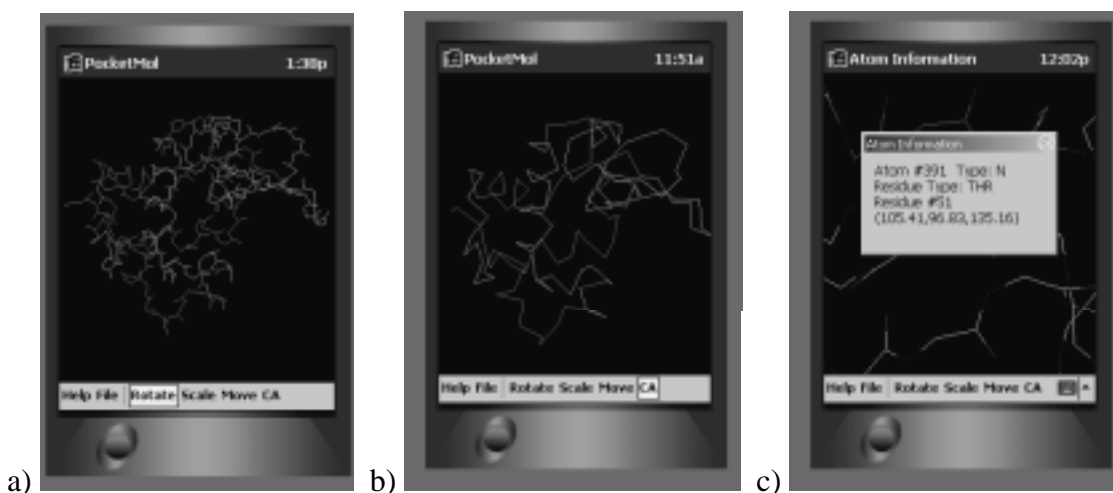


Figure 2. a) PocketMol interface b) a simplified alpha carbon view c) atom information screen

### 3.3 Reading PDB files

PocketMol reads a standard protein data bank (pdb) file. The RCSB Protein Data Bank [6] is a worldwide repository for all known protein structures. PDB files are formatted ASCII text files containing all of the structural information of a protein. PocketMol looks for all records beginning with "ATOM" and stores the data in an array. A display array is created afterwards containing only the atoms that will be displayed. If the Alpha Carbon button is pushed, only the CA atoms will be stored in the display array. Otherwise, the backbone atoms (N-CA-C=O) will be stored. PocketMol uses the residue number to ensure that all atoms are read and stored in their proper order.

### 3.4 Displaying the protein

Once the display array has been created, the protein may be displayed on the screen. There are two versions of PocketMol: PocketMol and PocketMolGX. The former uses the standard Windows Graphics Device Interface (GDI) drawing functions [7]. These are compatible with all Pocket PC and Windows CE devices. Unfortunately, the Pocket PC does not contain any dedicated display hardware, so GDI commands are very slow. Double buffering is used to make the animation smooth and flicker free. All drawing is done on a blank bitmap object, and that object is copied to the main display. Performance should increase as the second generation of Pocket PCs are introduced.

PocketMolGX is a graphically accelerated version of PocketMol that uses the Microsoft Game API (GAPI) [7]. GAPI allows a program to directly access video memory without dealing with the cumbersome GDI interface. Unfortunately, there are no display routines built in to GAPI, so all drawing routines must be developed. PocketMolGX uses a pseudo-double buffering technique by storing all display information in an array that is copied directly to memory. The result

is a very fast, smooth, and flicker-free image at the cost of requiring a system-dependent binary. PocketPC devices each contain different display hardware, so their video memory structure is also different. The initial version of PocketMolGX supports the iPaq H3635. Other Pocket PC systems may be supported in future releases.

### 3.5 Colors and shading

Color helps the user understand the structure of a protein at a glance. PocketMol uses the standard color scheme for atoms shared by most molecular viewers: oxygen is red, carbon is gray, and nitrogen is blue. Connections are colored by atom type, and each half of the connection is colored for the connecting atoms. Therefore, when a nitrogen atom is connected to an alpha carbon, half of the connection line will be blue while the remaining half is gray.

Shading is accomplished with a basic depth cueing method. Each color has three intensities: light, medium, and dark. The color is selected depending on its depth (z position) relative to the rest of the protein. Each connection is compared to the coordinates of all of the other atoms in the protein to determine its final color.

### 4.0 Future enhancements

In its current form, PocketMol is a basic visualization program. Several visual options will be added in the near future. Ribbons will be the first addition using wire-frame bezier curves. Solid shaded ribbons will be added by the final release. The addition of spheres is a bit more complicated because it requires many calculations, especially if the spheres are shaded. Regardless of what is completed, the framework has been established for anyone to expand PocketMol to a fully functional modeling program.

## 5.0 Conclusion

Biologists and computer scientists alike use molecular visualization programs to examine molecular structures to determine their shape and function. PocketMol expands molecular visualization to the realm of the Pocket PC. PocketMol provides the basic functionality to explore protein structures during conferences, lab meetings, workshops, brain-storming sessions, or even over lunch – anywhere where access to a desktop computer is unavailable.

## References

- [1] “Dino Homepage.”<http://www.bioz.unibas.ch/~xray/dino/> (August 17, 2001).
- [2] “RasMol Homepage.”<http://www.bernstein-plus-sons.com/software/rasmol/> (August 17, 2001).
- [3] “Amber Homepage.”<http://www.amber-ucsf.edu/amber/amber.html> (August 17, 2001).
- [4] “Linux4Chemistry.”<http://zeus.polsl.gliwice.pl/~nikodem/linux4chemistry.html> (August 17, 2001).
- [5] “Microsoft Embedded Visual Tools 3.0.”<http://www.microsoft.com/mobile/downloads/emvt30.asp> (August 17, 2001).
- [6] “The RCSB Protein Data Bank.”  
<http://www.rcsb.org/pdb/> (August 17, 2001).
- [7] Harbour, Jonathan S. Pocket PC Game Programming: Using the Windows CE Game API. Roseville, CA: Prima Publishing, 2001.