

RASMOL AB — New functionalities in the program for structure analysis

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For many years RasMol was one of the most used programs for molecular visualization. It was an excellent tool due to its simplicity and its low demand of computer power. Today it is replaced by OpenGL programs, which have excellent graphics that new computers can additionally handle. Molecular graphics is one of the best tools for the analysis of biomolecular data. With high efficiency and a low demand of computer power, RasMol can still be used as a quick and handy tool used for the analysis of biomolecular structures with good results. In this paper, we describe modifications to the RasMol program, as implemented on the base of RasMol AB 2. We introduced several new functions, namely: the identification of histidine isomers, and advanced structural selection and macro capabilities (as implemented in the point-click menu), which result in an increase in the speed and accuracy of structural analyses.

The program can be downloaded from the project page: <http://etoh.chem.univ.gda.pl/rasmol/>

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INTRODUCTION

RasMol is one of the best known programs for molecular graphics, since Sayle and Milner-White (1995) introduced it to the world. With a very low demand for computer power and a relatively high quality of graphics, it became the most commonly used tool for the analysis of molecular structures, and for the creation of publication quality pictures. With the evolution of computer technology, it became replaced by programs with rendering capabilities that use OpenGL (opengl.org), like MOLMOL by Koradi, Billeter and Wüthrich (1996), PyMOL by DeLano, UCSF Chimera by Pettersen and coworkers (2004), and many others Johansson and coworkers (2012), Sanchez-Ferrer and coworkers (1995), Gu and Bourne (2009).

The standard menu of RasMol possess a lot of useful functions, as it is described by Goodsel (2005). However, many functions of the program are hidden, and are available only from the command line (rasmol.org). In the work presented herein, we extended the standard menu of RasMol to get more of its useful features, as was implemented in the program from its point-and-click menu.

Many versions of RasMol are available on the internet, with the program developing three supervised by H. J. Bernstein (2000). The work presented here com-

brates two versions of RasMol (2.6ab 2 and the current version, RasMol 2.7), with additional code improvements and functionalities.

RESULTS

Code modification

The code of the RasMol program was originally written in C language. GTK+ library was used to generate user interface. In the work presented here, we modified `rasmol.c` file to add supporting functions as they can be called from the point-and-click menu with the selected arguments. The additional buttons as visible in RasMol AB, were created by the modification of the following files: `x11win.c`, `actionmenu.gtk` and `gtkwin.c`. To add the recognition of the non-standard residues, we modified: `molecule.c`, `molecule.h` and `abstree.c`.

New functions of the program

We extended the standard menu of the RasMol program by adding features previously available only from the command line. This modification made the program easier and more effective to use. The major modification is the addition of user predefined macros, which are now available as a separate option in the menu.

Sel AA — this menu allows the user to select a specific residue by name. Users can select any one of the 20 standard residues. In addition, we added some non-standard residues to the menu: selenocysteine — SEC (CSH), selenomethionine - MSE (used for labeling in the x-ray crystallography as described by Strub *et al.* (2003)), and pyrrolysine — PYL (PYH). To make further additions much easier, we made some improvements to the source code. The program is now capable of recognizing some residue synonyms and correctly displaying their C α trace, what was a common problem in earlier versions. Abbreviations of the following residues for describing the different protonation states were therefore implemented: aspartic and glutamic acids [ASP/ASH and GLU/GLH], histidine [HIS/(HID, HIE, HIP)], lysine [LYS/LYN], and cysteine (as involved in the formation of the disulfide bridge [CYX]); all of which are commonly used in the AMBER forcefield by Pearlman *et al.* (1995).

Sel AA Group — this menu allows the user to select a specific residue by type. All logical relations between

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Abbreviations:

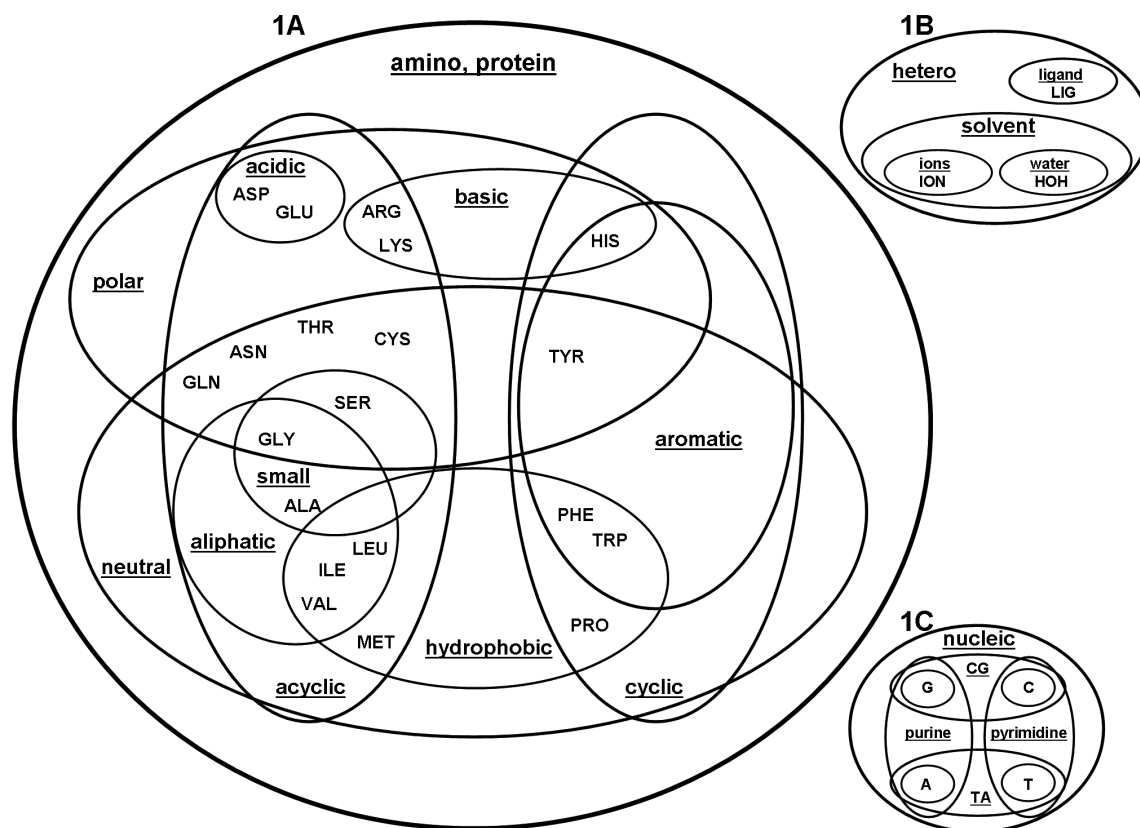


Figure 1. Venn diagram of the applied selection logic in the Sel AA Group (1A) and Sel Other (1B and 1C) menu. All underlined words are available as menu options.

residues and the selection menu can be well described by Taylor (1986) by using a Venn (1880) diagram, as was first drawn by K. Giles (umass.edu) (see Fig. 1A). We added two new selection types to this menu. The first selection group allows the user to select a secondary structure: helix, sheet, or turn. To make this selection positive, one of the following requirements must be fulfilled: information regarding the secondary structure, as present in a pdb file, or the protein at hand must conform to the expected Ramachandran map conformations as described in Crieghton (1992). The second selection group enables the user to highlight structural elements as per the following criteria: $C\alpha$, backbone, and/or side chain.

Sel Other — this menu allow the user to select a non-protein part of the examined structure (see Fig. 1B and 1C). Most of the options in this menu work if the atoms in the pdb file are marked as HETATM. Water molecules have to be marked as HOH. Additionally, we added the abbreviation LIG and ION as ligand and ion markers, respectively.

Sel Colour — this menu allows the selection of one of the fourteen predefined colors. The selected color will be applied to the current selection.

Macros — this is one of the most useful options in the program, especially when multiple analyses are to be made. It allows the user to create user-specific macros with a set of commands. The first line is started with the “#” symbol and contains the macro name, which will then be dynamically incorporated into the menu during the initialization of the program. All such accepted RasMol commands can then be placed in the macro file line

by line. The macro file must be named “macroX.scr”, where X is a number between 1 and 20. The program is capable of reading up to 20 macros. RasMol AB looks for macros in the directory specified by the system variable RASMOLMACROPATH, or in the local directory.

CONCLUSIONS

The goal of this project was to increase the functionality and simplicity of the RasMol program by pulling out powerful functions from the point-and-click menu, and by creating a dynamic user-specific macro system. Similar macro implementations have worked with success in programs such as MOLMOL or PyMOL, however, our implementation is much more user friendly. The necessary macro file can even be created by users without programming skills; from a research perspective, such a macro can be attached to published biomolecular structures as a supplement. About 20 years ago, Sayle and Milner-White (1995) wrote: “In the future, RASMOL will have to work hard to provide the many extra facilities that are going to be needed for molecular graphics while maintaining the simple interface that makes the program attractive to new users.” With this work, we tried to continue this spirit.

Availability and requirements

Project name: RasMol AB

Project home page: <http://etoh.chem.univ.gda.pl/ras-mol/>

Operating system(s): Microsoft Windows and Linux

Programming language: ANSI C

Other requirements: None

License: The program is protected by the RasMol GPL license (rasmol.org).

Competing interests

The authors declare that they have no competing interests.

Authors' contributions

MP transformed the code to produce the new program. AG was the project supervisor, and wrote this manuscript. All authors have read and approved the final manuscript.

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