User manual for

Navmol 2.1

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Navmol is a software built for enhanced browsing and editing of molecular structures by visually impaired users. This document presents a short set of instructions for using the software and the description of the main features implemented in the current version.

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1 Basic description & Introduction

The main window of Navmol is composed of a large visualization area and a small text area placed bellow it. The purpose of the visualization area is to show a large sketch of the molecules loaded in Navmol with two goals in mind. The first is to make a sketch available to people that are not completely blind, and the second is to enhance the interaction between sighted and blind people when using the software together, e.g. in a classroom.

Using the keyboard, the user can browse the molecule and get extra information on atoms; set up bookmarks; browse the history; list functional groups; add/remove atoms and bonds; change atom charge; browse a chemical reaction and perform a wide variety of operations.

2 Software requirements & Installation

Navmol is a Java application and it requires a working Java Runtime Environment to be properly installed. Current version if Java RE can be downloaded from http://www.java.com/getjava.
Current version of Navmol incorporates FreeTTS (http://freetts.sourceforge.net/) sound system and English localization. As an alternative eSpeak (http://espeak.sourceforge.net/) can be used if it is installed on the system with English and Portuguese localization.

3 Single molecule browsing mode

Here we present the main navigation features of Navmol. The items in this section are thought to be presented in a way that allows the user to start by reading about the most frequently used features. Therefore we start by describing the features related to navigation and we will leave the ones related to structure and function analysis more to the end.

3.1 Basic navigation

At start the user will be located in an atom of the molecule. In order to navigate on the molecule the user has to press the arrow keys, **UP**, **DOWN**, **LEFT** and **RIGH**. The directions pointed by these keys are loosely related to the real direction at which the neighbor atoms will be. For example, if the current atom is bonded to another atom that, on the sketch, is above the current atom, then pressing the UP arrow will move the "cursor" to that atom. Furthermore, Navmol uses the **clock coordinate system** to more accurately report on the direction of the neighbor bonded atoms. The current atom, where the cursor is positioned, is located at the center of the clock and the bonds work as if they were the clock pointers. When the cursor is moved to another atom, that atom becomes the center of the clock. Let's say we have the molecule, Cl_2, and, in the sketch, this molecule is drawn horizontally. Let's say, the user starts with the cursor on the atom at the left side. This atom will have only one neighbor, the one at the right side, at 3 o'clock of the current atom. If the user presses the **RIGHT-ARROW** key the cursor will be moved to the atom on the right. Now, there is only on neighbor for this atom, positioned at 9 o'clock, which is the opposite direction to 3 o'clock.

When a move is made, Navmol will give the following information to the user:

1. The atom where the cursor is moving to.
2. The clock coordinates for the direction of the move.
3. The type of bond through which the move is being performed.
4. If this is the first time the atom is visited.

For example, in the case of Cl_2, in the first move, to the right, Navmol would say:

"Moved to atom: Cl2, at 3 o'clock, through a SINGLE bond. First time visited."

The correspondence between the **clock coordinate system** and the arrow keys is made as follows:

- The clock circle is divided in four quadrants corresponding to having an oblique cross superimposed on a circle.
- The TOP quadrant is related to the UP direction (**UP-ARROW** key) and corresponds to the 11, 12 and 1 o'clock coordinates.
- The RIGHT quadrant is related to the RIGHT direction (**RIGHT-ARROW** key) and corresponds to the 2, 3 and 4 o'clock coordinates.
- The BOTTOM quadrant is related to the DOWN direction (**DOWN-ARROW** key) and corresponds to the 5, 6 and 7 o'clock coordinates.

- The LEFT quadrant is related to the LEFT direction (**LEFT-ARROW** key) and corresponds to the 8, 9 and 10 o'clock coordinates.

3.2 Atom information

Atoms, in Navmol, are referenced by their chemical symbol followed by their number I.D. in the molecule. When the user is at an atom, information can be requested for the current atom (where the cursor is positioned) by pressing the **SPACE** key. Navmol will then report the following properties:

1. The chemical symbol and number I.D.
2. Number of bonded neighbors followed by list of all neighbors and respective clock coordinates and type of bonds for each bonded neighbor.
3. Formal charge of this atom, if it is charged.

3.3 Bookmarks

Navmol allows for the user to set up a number of bookmarks at different locations on the molecule. This way the user can mark locations, *e.g.* functional groups, on the molecule and then jump between them. Bookmarks are set by pressing the keys **CTRL** plus **1** to **0**, which means the user can set up ten different bookmarks. In order to jump to an atom referenced by a bookmark the user presses one of the 1 to 0 keys. For example, a user could set up the bookmark number 1, by pressing **CTRL+1** keys, at atom 3 of, let’s say, hexane, and then move along to other atoms. If the user wanted to go immediately to atom number 3 again it would have just to press 1 in order to do so.

3.4 Jump to atom

By pressing the key, **J**, the user will be prompted to insert the number I.D. of the atom he/she wants to navigate to (finish by pressing **RETURN** key). This, of course, implies that the user already has some knowledge of the ordering of the atoms on the molecule.

When jumping from one atom to another Navmol will describe the move that was made with the following information:

1. The atom's chemical symbol and number I.D. where the cursor is jumping to.

2. The clock coordinates for the direction of the jump.

3. The number of bonds involved in the jumping.

4. If this is the first time the atom is visited.

3.5 Navigation history

Navmol registers all the navigation actions taken by the user. In order to navigate according to history the user has to press successively the **CTRL + LEFT-ARROW** keys and **CTRL + RIGHT-ARROW** keys to go back and forward in history, respectively. This way the user can remake all steps he/she has done until that point. If the user goes back to a certain point in history and performs any navigation action, from that point on, a new history is started. The previous history is kept but all the steps that were forward to that point are lost.

3.6 Navigation by numerical order

If the user wants to explore the molecule by moving from atom to atom, following the numerical ordering of the atoms in the molecule, he/she can do so by using the keys, **CTRL+UP-ARROW** keys or **CTRL+DOWN-ARROW** keys, in order to go to higher or lower numbered atoms, respectively.

3.7 Functional group search

The identification of the main finctional groups in a molecule is one of the mais tasks, if not the first, when first studying a new molecule.

By pressing the **F** key the user will get a list of the functional groups in the molecule, including the atoms where those groups are found. For example, on ethanol (C-C-O-H), Navmol would report ALCOHOL at atoms 2 and 3 in the following way:

“Functional group: ALCOHOL; Times found: 1; Atom list: 2, 3; “

1. The name of the functional group.
2. The number of times that the functional group is found in the molecule.
3. List of atoms by number I.D. that defined the functional group.

3.8 Molecule information

The user can press **CTRL + SPACE** keys to get general information on the molecule. This information is already reported at the beginning of the Navmol session, when the molecule is first loaded. Navmol will then report the following properties:

1. The chemical symbol and number I.D.
2. Number of bonded neighbors followed by list of all neighbors and respective clock coordinates and type of bonds for each bonded neighbor.
3. Formal charge of this atom, if it is charged.

3.9 Open file with new molecule

To load a new molecule the user can press the **ALT + O** keys. A file selection dialogue will appear for that effect. After selecting a file the current loaded molecule will be lost and a new molecule will be loaded from the file. Currently only SMILES and MDL MOL formats are supported.

4 Single molecule edit mode

All the features implemented for the browsing mode are also available for the edit mode. To enter the edit mode the user must press the key **E** when in browser mode. Pressing the **E** key again will bring the user to browsing mode.

4.1 Add atom

Pressing **A** key in edit mode will bring up a dialog for choosing an atom to be added to the molecule. The atom will be bonded to the current atom. The user can choose de element, the direction and the stereochemical information (up/down).

4.2 Add bond

Pressing **B** key will bring up a dialog for adding a bond to the current atom. The user will be given a list of atoms to which it can be bonded to. The list will be ordered in descending order of geometrical distances to the current atom.

4.3 Remove atom

The option of directly removing an atom does not exist. Instead the user can press **CTRL + A** keys and a dialog will come up to transform the current atom and its respective bonds to dummy objects. The dummy atoms and bonds do not exist in the chemical compound and are only used to connected sets of atoms. After pressing the keys, **CTRL + A**, the user will be prompted to confirm with Y (Yes) or N (No) that he/she wants to transform the current atom and all connected bonds to dummy objects.

4.4 Remove bond

The option to directly remove a bond does not exist. Instead the user can press **CTRL + B** keys and a dialog will come up to transform a bond into a dummy object. The user will be given a list of the bonds connecting to the current atom.

4.5 Clear dummy objects

The user must go to a real atom (*i.e.*, a non-dummy atom) and then press **CTRL + C** keys to effectively remove all the dummy objects. The user will be asked to confirm this operation. Navmol will identify any loose fragments and reconnect them with dummy bonds.

4.6 Change atom charge

Pressing **C** key will bring up a dialog for changing the formal charge of the current atom from -8 to +8.

4.7 Replace an atom

Pressing **R** key will bring up a dialog for choosing an atom to replace the current atom. The user can choose de element to be added.

4.8 Change bond order

Pressing **CTRL + SHIFT + B** keys for changing the bond order of the bonds connecting to the current atom. The user will be given a list of the bonds connecting to the current atom. After selecting the bond which bond order will be changed, the user will be prompted to select the new bond order (*i.e.*, single, double, or triple).

4.9 Save file with a new molecule

To save a file with the current molecule the user can press the **ALT + S** keys. A file save dialogue will appear for that effect. After saving the new file the Navmol will inform the user that the file extension .mol will be added to the filename. Currently only MDL MOL formats are supported for saving.

5 Reaction browsing mode

Reaction mode is activated when a reaction file is loaded, in the **.rxn** format. In this mode the user can navigate the individual molecules with all features implemented for the browsing mode and move to the next or previous molecule of reactants (or products) pressing **TAB** key or **SHIFT +TAB** Keys, respectively. The user can as well swap from reactants to products using the mapping key **M** that allows the moving between corresponding atoms in the reactant and product molecules according to the reaction mapping.

6 Summary of keyboard instructions

This is the list of keys and key combinations used to browse a molecule in Navmol. It is also accessible on the program by pressing the **H** key.

List of keys:

- **CTRL + S** keys: select sound system.
- **CTRL + SHIFT + S** keys: turns sound on or off.
- **CTRL + PLUS or MINUS** keys: increases or decreases the rate of speech.
- **CTRL + L** keys: select sound language.

- **CTRL + Q** keys: exit Navmol.
- **H** keys: help menu.
- **UP-ARROW** key: go to a bonded atom at 11, 12 or 1 o'clock.
- **RIGHT-ARROW** key: go to a bonded atom at 2, 3 or 4 o'clock.
- **DOWN-ARROW** key: go to a bonded atom at 5, 6 or 7 o'clock.
- **LEFT-ARROW** key: go to a bonded atom at 8, 9 or 10 o'clock
- **CTRL + UP OR DOWN-ARROW** keys: go to atom next, or previous, following number label.
- **CTRL + LEFT OR RIGHT-ARROW** keys: follow browsing history on forward or backward directions, respectively.
- **J** key: jump to atom labelled by given number.
- **SPACE** key: give information about current atom.
- **CTRL + SPACE** keys: give information about the molecule.
- **F** key: give list of functional groups found on the molecule.
- **CTRL + 0 TO 9** keys: set a bookmark.
- **0 TO 9** keys: go to bookmark.
- **R** keys: give short list of rings.
- **SHIFT + R** keys: give long list of rings.
- **ALT + O** keys: open file with new molecule or reaction.
- **ALT + S** keys: save file with a new molecule.
- **E** key: enter or leave the single molecule editor mode.

The following keys are used only in **editor mode**:

- **A** key: adds a new atom bonded to the current atom.
- **CTRL +A** keys: transform the current atom and all connected bonds to dummy objects.
- **CTRL + B** keys: adds a bond between the current atom and another atom.
- **CTRL + B** keys: transforms a bond of the currently selected atom into a dummy object.
- **CTRL + C** keys: clear dummy objects.
- **CTRL + SHIFT + B** keys: changes the bond order of the current atom with another atom.
- **C** key: changes the atom charge of the current atom.
- **R** key: changes the currently selected atom for a new one.

The following keys are used only in reaction mode:

- **TAB** key: move to the next molecule in the reaction.
- **SHIFT + TAB** keys: move to the previous molecule in the reaction.
- **M** key: moves to the same atom in a different molecule according to the reaction mapping, moving from reactants to products, depending on which is currently chosen.

7 Language selection

Navmol is internationalized and English and Portuguese languages are implemented. The user can switch between them pressing **CTRL+L** keys. Current version of the internal speech engine FreeTTS has English only included. For Portuguese external speech engine like eSpeak is necessary.