Subject: Re: Difference between "selecting" a row and making a row "current"
Posted by thomas on Fri, 08 Nov 2019 20:10:55 GMT
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The 'Current row' (called 'Reference Row' soon) and selected rows serve different purposes in DataWarrior. With selected rows you may, for instance, do these things:
- copy them
- delete them
- create a new row list from them, etc
In graphical views you select rows by moving the mouse to a point, pressing the button, dragging the mouse around some markers and release the button. The surrounded markers change color to indicate that they are selected. In the table or structure view you click (press and release the mouse) one row and then shift-click another one. All rows from the first to the other row are selected indicated by a selection colored background.

The Current row is defined with a single mouse click (press and release) onto a marker (graphical views), structure (structure view) or row number (table view). The row then is drawn in red (graphical views) or with a red frame (table and structure view). The form view always shows the 'Current Row'. This row serves as a reference row, e.g. when a structure similarity is assigned to an axis in a graphical view or used to color markers. In this case, if a current row exists, then the structural similarities are calculated to all other rows and these rows' marker colors adapted to reflect the similarity values. The interesting thing is that this is dynamic: When clicking another marker, then all similarities to the new current row are calculated and all colors are updated (or positions change if similarity is assigned to an axis).
The next update will allow you to automatically superpose a reference conformer (the current row) to others, e.g. to compare docked ligands with the natural inhibitor.

Now comes the tricky answer: Unselecting the current row in the table view is not possible, because there is no unused area to click at. In the structure view you may click ate the gray area after scrolling down (if it exists). But graphical views allow you to click into any empty location to un-set the current row. This also unselects any rows.

This also may be useful: To find the corresponding table row for a given marker in a graphical view: click the marker (make it the current row), then click on the top left button in the table view (the one with the red rectangle). This scrolls the table to the position of the current row.

I hope this explains it...

Thomas