**MOE Ligand RMSD Calculation Tutorial**

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The following table outlines the steps required to calculate ligand RMSD values when comparing a database of docking results to a reference crystal structure. The ligandrmsd.svl script as well as example files to run the script with can be found in the .zip file available at <https://www.mediafire.com/file/5gpyopq260i6jak/ligand_RMSD_tutorial_files.zip/file>

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| **Step** | **Description** | **Figure** |
| 1 | To begin, you should ensure that both the reference crystal structure (saved as a .moe or .pdb file) and database containing docking results (ending in .mdb) are contained within the same folder. In MOE, navigate to this folder and set your current working directory with the *CWD* button. |  |
| 2 | Click *File* 🡪 *Open* and navigate to where you have downloaded the ligandrmsd.svl script file. Click the filename and then click *Edit.* Do not click *OK* as this will result in an error. |  |
| 3 | A new window with the ligandrmsd.svl script loaded into the MOE text editor will appear. From the text editor, click *SVL* 🡪 *Save and Load*. This will load the script’s functions into MOE and allow you to call them from the SVL Commands window.  Here, you should also take note of the main function of the script titled ligandRMSD and its arguments reference\_file, database\_file, database\_field1, and database\_field2. |  |

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| 4 | Open the SVL Commands window by clicking the *SVL* button at the top right of the main MOE window. From here, you should be able to use the ligandRMSD function with the reference structure and docking output files in your current working directory. The function can be called with the following command:  ligandRMSD [reference\_file, database\_file, database\_field1, database\_field2]  where:  reference\_file: .pdb or .moe file containing your crystal structure  database\_file: .mdb with docked ligand poses  database\_field1: .mdb column containing your ligand poses, most likely 'mol'  database\_field2: .mdb column containing you receptor poses, most likely 'receptor'  For example, let’s apply this function to the filenames found in the screenshot from step 1. In this case, the command to calculate ligand RMSD values would be:  ligandRMSD ['reference\_structure.moe', 'dock\_output.mdb', 'mol', 'receptor']  Once the calculation is complete (usually instantly), a ligand RMSD value for each docked ligand pose entry can be found in the output database in a field titled ‘Ligand RMSD’. | SVL button:    Example command:    Output: |