File:WinHydropro10_54-PUB-Sept-2011.doc

WinHYDROPRO

For HYDROPRO Version 10 (compilation 54)
September 2011

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1. Introduction to WinHYDROPRO

WinHYDROPRO is a graphical user interface for **HYDROPRO** which runs under the Microsoft Windows operating system. It provides an alternative to the input-files based working mode that is the classical – and still most adequate in some instances – form of this program.

Indeed, before using **WinHYDROPRO** we recommend users to take a first look to **HYDROPRO**, reading the User's Manual and trying some executions in the input-files mode. Actually, some of the indications given in this manual refer, for more details to the **HYDROPRO** User's Manual (hereafter, for brevity, HPUM).

2. Entering data

You will first "*Load PDB*", browsing for your file. If yours is a genuine PDB file, some information from the file header will show up. Otherwise the program will detect that such information is not available.

In the box "Molecule data" you have to enter some data of the solvent molecule:

- Molecular weight
- Specific volume

The molecular weight is needed for sedimentation and viscosity. The specific volume is needed for sedimentation. If you ignore any of these values, you still should give some

arbitrary (not absurd, something physically reasonable…) values, and then ignore the results of the property that depend on them.

In the box "Hydrodynamics":

- You will enter the calculation mode, INDMODE (bead or shell, atomic or residue).
- Then, in "*Radius of the atomic elements*" you will see some preset value for this number (AER). We strongly suggest you not too change this value, unless you are doing some special calculations, like those with virtual/dummy elements (section 5 in HPUM).
- In the case of shell elements, the range for the radius for the shell elements (minibeads) must be set. You can mark "Automatic" and then the program itself will find the range during execution. Otherwise, you will give NSIG, SIGMIN and SIGMAX (again, see HPUM).

In the box "Solvent data", you will notice that there are some prefixed values for:

- Solvent viscosity
- Solvent density
- Temperature, centigrade

The prefixed data correspond to 20 degrees in water. You may change any of these values for your own case. Recall that the solvent density is needed only for sedimentation. Solvent viscosity is needed for all the hydrodynamic properties, and temperature needed for all except intrinsic viscosity. Any of these are needed for the conformational properties (distances, scattering). If you ignore any of these values, you still should give some arbitrary (not absurd, something physically reasonable…) values, and then ignore the results of the property that depend on them.

You may provide a generic name for output file. The various output files produced by the program with begin with this name, followed by an appropriate extension.

You can optionally evaluate non-hydrodynamic properties, which would require additional data. You can "Enable" the following calculations:

- Scattering intensities (normalized to unity at zero angle), providing number of values and highest value of the scattering variable.
- Distribution of distances, providing number of intervals and the maximum distance to be considered.
- Covolume, providing the number (typically 100 – 1000) of Monte Carlo trials in the calculation of this property.

You may ignore any of these three calculations by not enabling the corresponding window. For scattering and distances, there is the possibility of asking the program to make an "automatic" choice of data.

Finally, you can enable the calculation of the full 6x6 diffusion tensor of the rigid particle.

3. Calculating and viewing the results

Previously, you can accept a multi-thread calculation, enabled by the number of cores present into your computer, which is detected by the program. This option (which is the default) is strongly recommended, as it will speed-up the calculation extraordinarily. If you unmark this option, it will run on only one core.

Click "*Calculate Hydrodynamics*". You will see a MS/DOS console, produced by the execution of **HYDROPRO**. This console will close itself when the calculation is done. Computing time is now a few seconds (compared to older **HYDROPRO** version, which took several minutes). Please, do not close any window while doing the calculation.

When the calculation is done, a window will pop up with the full list of results (as in the **HYDROPRO** main output, the **-res.txt** file). You may inspect this file for the whole set of results, and/or close this window and look at the main window where most relevant properties will be displayed (translational diffusion and sedimentation coefficient, intrinsic viscosity and radius of gyration).

It is possible to visualize the atomic PDB structure and primary bead model in the results window through the buttons provided for that purpose. Facilities are provided to view the model using RasWin freeware program (provided with **WinHYDROPRO** package, no installation required), that is appropriate for protein models, or getting a VRML image. For the latter case you need a VRML viewer, like for instance the free Cortona plug-in for Internet Explorer or FireFox. More details on installation of this plug-in, and other aspects related to visualizations are given below, or in the VisualBeads User Manual.

Other output files produced by **HYDROPRO** (see HPUM) are also produced by **WinHYDROPRO.**

4. Hints and notes

* This program requires .NET Framework 2.0 or higher.
* All the files needed for the **WinHYDROPRO** calculation (perhaps with the exception of the PDB which can be browsed) must be in the same folder, in which you will find the other output files.
* We recommend viewing atomic and primary models with the RasWin program (instead of VRML viewer). However, if you want show the VRML image, the file path should not be too long or contain special characters (#, @, % and others). In that case, any model cannot be loaded by the Cortona plugin. In recent versions of Internet Explorer you will have to click on the bar that asks for permission for executing the Cortona plugin for VRML image.

5. Release notes

This is the first release of this program.