**File: solpro11.doc**

# SOLPRO Version 11

**(February 2002)**

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## 1. Introduction to SOLPRO

The HYDRO family of program provides the basic solution properties, including hydrodynamic coefficients, radius of gyration and covolume, scattering-related properties, etc. SOLPRO is an ancillary program intended for the calculation of two other classes of solution properties

- Time dependent properties, including (1) Fluorescence anisotropy decay; (2) Electric birefringence and electric dichroism decay (3) Decay of the function <P2(t)> for a particle-fixed vector, <P2(t)> being a shorthand notation for the time-dependent function $<(3\cos^2(\vartheta)-1)/2>$, where is $\vartheta$ the angle subtended by two orientations of that vector separated by time t.

- Shape-dependent, size-independent quantities, like the Perrin parameter P (also known as $f/f_0$ ), the viscosity increment (Einstein-Shima parameter), the Flory parameters for translational diffusion and intrinsic viscosity, and many, many others.

## 2. Literature

If you employ SOLPRO in your published work, the proper references to be cited are:


[1] J. Garcia de la Torre, B. Carrasco and S.E. Harding. "SOLPRO: theory and computer program for the prediction of SOLution PROperties of rigid macromolecules and bioparticles". Eur. Biophys. J. 25, 361-372 (1997)

and, eventually,

[2] J. Garcia de la Torre, S.E. Harding and B. Carrasco. "Calculation of NMR relaxation, covolume and scattering of properties of bead models using the SOLPRO computer program". Eur. Biophys. J. 28, 119-132 (1999)

Reference [1] contains a description of the rotational relaxation of a rigid particle, applied to the electric birefringence and dichroism decay, and to the decay of fluorescence anisotropy. In the second part of this paper, the size-independent parameters are defined and formulated.

Reference [2] contains a description of the rotational relaxation of a particle-fixed in terms of the <P2(t)> function . This was applied to the prediction of NMR but this calculation is no longer done in SOLPRO but in a program, HYDRONMR, that is specific for thus purpose. This paper also described the calculation of the distribution of distances and the scattering functions, but these two things are no longer part of SOLPRO; they are now included in some of the HYDRO family of programs.

## 3. Running SOLPRO. Input data files

SOLPRO needs a set of basic solution properties that are calculated running first the one of the HYDRO family of programs (HYDROPRO, HYDROSUB, HYDROPIX, etc), which will be generate a file named `xxxxxx.sol`, where xxxxxx is a user-supplied name. You also have to supply another input data file, named `solpro.dat`, which will contain the specific data for SOLPRO. The contents (and the FORTRAN data types) of the `solpro.dat` file is as follows

- SOLPROFILE `(character*30)` is the name of the file previously generated by the HYDRO programs, i.e., what we called `xxxxxx.sol`

- SOLPROOUTPUT `(character*30)` is the name of a file that will contain the output from this program

- IUNIV `(integer)` is a flag. Set IUNIV=1 if you wish the calculation of the shape-dependent parameters

- IFLU `(integer)` is a flag. Set IFLU=1 if you wish the calculation of the fluorescence anisotropy decay
- Optionally, if IFLU=1, you have to supply two additional lines:
  (1) The three components `(real),` separated by spaces or commas of the unitary (direction cosines) absorbing dipole,$\phi$
  (2) The three components `(real),` separated by spaces or commas of the unitary (direction cosines) emitting dipole, $\omega$

- IBIR `(integer)` is a flag. Set IBIR=1 if you wish the calculation of the birefringence decay
- Optionally, if IBIR=1, you have to supply six additional lines
  (1) The three components of the first row of the optical polarizability tensor, $\alpha$
  (2) The three components of the second row of the optical polarizability tensor, $\alpha$
  (3) The three components of the third row of the optical polarizability tensor, $\alpha$
  (4) The three components of the first row of the electrical alignment tensor, $\chi$

(5) The three components of the second row of the electrical alignment tensor, $\chi$
(6) The three components of the third row of the electrical alignment tensor, $\chi$
In the six lines, the component are `real,` separated by spaces or commas.

- IP2 `(integer)` is a flag. Set IP2=1 if you wish the calculation of the <P2(t)> function
- Optionally, if IP2=1, you have to supply one additional line with the three components `(real),` separated by spaces or commas of the unitary (direction cosines) of the particle-fixed vector for which you want the <P2(t)> function

Any number of cases can be included in a single execution; their data will be following each other, all in the same `solpro.dat` file. Finally:

- An asterisk (followed by 29 spaces), in place of a new SOLPROFILE, indicates the end of this input file

## 4. Output files

For each case included in the run, you will get one output file, with the name given in SOLPROOUTPUT.

## 5. Notes and hints

- The electrical alignment tensor and the optical polarizability tensor may be given in arbitary units; in such case the values obtained for the absolute birefrigence will be useless, but the results for the normalized birefringence [value(t)/value(t=0)] will be valid

- According to their definition, the shape functions only depend on the shape of the particle, but not on the size. Two particles of the same shape and different size are obtained one from the other by uniform expansion, and their shape functions are identical. Of course, the shape functions do not depend on the unit of length, molecular weight, specific volume and the solution density. In the previous calculation with one of the HYDRO programs, you can give arbitrary values to this quantities, if you are just interested in the shape functions.

- However, the other SOLPRO results, i.e., the time-dependent functions, depend on the rotational diffusion tensor, and requires the use of true quantities for temperature and the solvent viscosity. However, the molecular weight, specific volume of the solvent and solution density do not enter in the calculation of these time functions, so that they can, again, be given arbitary values.

## 6. Release notes

The previously released version of this program was SOLPRO10. The main changes introduced in this new version are:

- The calculation of the shape-functions is now optional.
- The program reads a data file calculated by one of the programs of the HYDRO family (HYDRO, HYDROPRO, HYDROPIX, HYDROMIC or HYDROSUB).
- The calculation of the covolume, distribution of distances and scattering function are now done by the programs of the HYDRO family.
- For the NMR relaxation calculations, the proper tool is now HYDRONMR. Thus, the calculation of spectral densities has been removed. Still this version contains the calculation of the <P2(t)> function for a user-supplied vector.

This program has been developed in a Windows PC using Microsoft Developer Studio 97 with the FORTRAN compiler DIGITAL-Compaq Visual Fortran 5.0. The MS DOS/Windows executable can be started from Windows, but we advise to open a MS DOS session in a window for program execution, while doing the other tasks (editing, visualization, etc) as usually in Windows.

Executables of this program are also available for other platforms: Linux, Silicon Graphics and Compaq-DEC Alpha.