

## EPRSIM-C Overview

### Package content (Version: 6.2):

- **EPRSIM BBW** release EPRSIM BBW 6.2.5
- **EPRSIM WIZ** release EPRSIM WIZ 6.2.2
- **GHOSTmaker** release GHOSTmaker 3.5.1
- **EPR convert** release EPR convert 2.1.1

### OS environment:

- MS Windows (32 bit)

### General purpose:

- Simulation of nitroxide spectra in fast motion approximation
- Handling EPR experimental data
- EPR-based characterization via automatic HEO/dHEO optimization
- Solution condensation and filtering with GHOST algorithm

### Purpose of individual programs:

- EPRSIM WIZ – handling EPR data, reviewing, collecting or combining EPR experiments
- EPRSIM BBW – fitting, automatic optimization, multithreading, multiple spectra handling, background (resident) calculation, automatic start
- GHOSTmaker – GHOST making, spectral analysis condensation
- EPR convert – converting single or group of SPC / DTA files into single ASCII file(s)

### Accessibility:

- Package EPRSIM-C is a freeware downloadable from web site [http://www.ijs.si/ijs/dept/epr/EPRSIMC\\_overview.htm](http://www.ijs.si/ijs/dept/epr/EPRSIMC_overview.htm) (also check here for the most recent versions).
- Note that the authors can provide further assistance with the EPRSIM-C programs only when the users notify the authors on the usage of the EPRSIM-C programs. Notification should be done via e-mail to [janez.strancar@ijs.si](mailto:janez.strancar@ijs.si) by sending the user's name and affiliation.
- The users can publish the results gained by the EPRSIM-C software only by referring the appropriate papers described below or elsewhere.

### Installation – general hints:

- Copy the EPRSIM-C package to desired location
- Make sure that all the programs and support files are in the same folder
- For usage of the individual programs, see their technical documentation
- Note that all software components of EPRSIM-C can be run over a local network from a single location
- Note that one can submit tasks for EPRSIM BBW running in the stay-resident mode also from a local network
- Note that EPRSIM WIZ needs file »def\_par2.mtp« to create new MTP files; therefore this file should be in the same directory as EPRSIM WIZ
- Note that GHOSTmaker needs EPRSIM BBW to make a spectral-simulation-based weight correction; it is desirable that EPRSIM BBW

and GHOSTmaker are located in the same folder, however you will be asked to locate EPRSIM BBW when running GHOSTmaker for the first time

## Technical documentation (table of contents):

- **EPRSIM WIZ**
  - 1 EPRSIM WIZ user interface
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    - 1.4 Toolbar
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  - 2 EPRSIM WIZ – handling EPR data
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    - 2.3 Saving MTP files
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    - 2.5 Manipulation within MTP data sets
    - 2.6 Optimization control
    - 2.7 Defining goodness of fit (type of  $\chi^2$ )
  - 3 EPRSIM WIZ – user interface to EPR-based characterization
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    - 1.1 EPRSIM BBW Modes
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      - 1.2.3 Examples of program evaluation:
  - 2 EPRSIM BBW input/output
    - 2.1 Input – MTP file format
    - 2.2 Output – MTP file format
    - 2.3 Output – \_POP subdirectory and POP file format
    - 2.4 Additional files
  
- **GHOST maker**
  - 1 GHOST concept
    - 1.1 GHOSTs – 5-dimensional cross-sections
    - 1.2 GHOST condensation algorithm
  - 2 GHOSTmaker usage
    - 2.1 Input files – POP and MTP files
    - 2.2 Output files – WMF and POP files
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    - 2.4 Defining threshold densities by density minimum and density level
  
- **EPRSIM library**
  - 1 Modules for handling files
  - 2 Module for spectral simulation
    - 2.1 1st model = ISO: isotropic tumbling
    - 2.2 2nd model = MEM: anisotropic tumbling with full averaging over long axes
    - 2.3 3rd model = LLE: isotropic spin-exchange label-label
    - 2.4 4th model = LBE: isotropic spin-exchange label-broadening agent

- 2.5 5th model = MES: anisotropic tumbling with partial averaging of all rotations
- 2.6 9th model = TRP: spin trap simulations
- 3 Modules for parameters' optimization
  - 3.1 Simplex downhill optimization (DSO)
  - 3.2 Hybrid evolutionary optimization (HEA = GA hybridized with DS)

- **EPR convert**

- 1 EPR convert usage
  - 1.1 SPC files conversion
  - 1.2 DTA files conversion
  - 1.3 Conversion of multiple spectral files into single file

**References:**

- STRANCAR, Janez, SENTJURC, Marjeta, SCHARA, Milan Valter. Fast and accurate characterization of biological membranes by EPR spectra. *J. Magn. Reson. (San Diego, Calif., 1997: Print)*, 2000, vol. 142, 254-265.
- FILIPIC, Bogdan, STRANCAR, Janez. Tuning EPR spectral parameters with a genetic algorithm. *Applied Soft Computing*, 2001, vol. 1, no. 1, 83-90.
- STRANCAR, Janez, SCHARA, Milan Valter, PECAR, Slavko. New EPR method for cellular surface characterization. *J Membr. Biol.*, 2003, vol. 193, 15-22.
- STRANCAR, Janez, KOKLIC, Tilen, ARSOV, Zoran. Soft picture of lateral heterogeneity in biomembranes. *J Membr. Biol.*, 2003, vol. 196, 135-146.
- STRANCAR, Janez, KOKLIC, Tilen, ARSOV, Zoran, FILIPIČ, Bogdan, STOPAR, David, HEMMINGA, Marcus A. Spin label EPR-based characterization of biosystem complexity. *J. Chem. Inf. Comput. Sci.*, 2005, vol. 45, 394-406.
- FILIPIC, Bogdan, STRANCAR, Janez. Evolutionary computational support for the characterization of biological systems. in: FOGEL, Gary B. (ed.), CORNE, David (ed.). *Evolutionary computation in bioinformatics*. Amsterdam [etc.]: Morgan Kaufmann; Oxford: Elsevier Science, 2003, 279-294.
- KAVALENKA, Aleh A., FILIPIČ, Bogdan, HEMMINGA, Marcus A., ŠTRANCAR, Janez. Speeding up a genetic algorithm for EPR-based spin label characterization of biosystem complexity. *J. Chem. Inf. Mod.*, 2005, vol. 45, no. 6, 1628-1635.
- STOPAR, David, ŠTRANCAR, Janez, SPRUIJT, Ruud B., HEMMINGA, Marcus A. Exploring the local conformational space of a membrane protein by site-directed spin labeling. *J. Chem. Inf. Mod.*, 2005, vol. 45, 1621-1627.