

## Package name: EPRSIM C - overview

Package content (public domain) - 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 [http://www.ijs.si/ijs/dept/epr/EPRSIMC\\_overview.htm](http://www.ijs.si/ijs/dept/epr/EPRSIMC_overview.htm).

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 directory
- For usage of individual programs see their technical documentation
- Note that all EPRSIM C can be run over the local network from single location
- Note that one can submit the tasks for EPRSIM BBW running in stay-resident mode also from local network
- Note that EPRSIM WIZ needs »def\_par2.mtp« file to create new MTP files therefore the »def\_par2.mtp« needs to be in the same directory as EPRSIM WIZ
- Note that GHOSTmaker needs EPRSIM BBW to make spectral-simulation-based weight correction; it is desired if the 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 content):

- [EPRSIM WIZ](#)
  - 1 EPRSIM WIZ user interface
    - 1.1 Spectral data presentation
    - 1.2 Spectral parameter panel
    - 1.3 Experimental constants panel
    - 1.4 Toolbar
    - 1.5 Status bar
  - 2 EPRSIM WIZ – handling EPR data
    - 2.1 Creating MTP data sets
    - 2.2 Opening existing MTP files
    - 2.3 Saving MTP files
    - 2.4 Printing
    - 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
    - 3.1 Sending optimization task to cluster
    - 3.2 Local optimization
- [EPRSIM BBW](#)
  - 1 EPRSIM BBW usage
    - 1.1 EPRSIM BBW Modes
    - 1.2 EPRSIM BBW switches
      - 1.2.1 Main switches:
      - 1.2.2 Additional switches:
      - 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
    - 2.3 Defining relative uncertainties
    - 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.
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- 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.