

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)

Accessability:

Package EPRSIM C is a freeware downloadable from
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 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 χ^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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- STRANCAR, Janez, KOKLIC, Tilen, ARSOV, Zoran. Soft picture of lateral heterogeneity in biomembranes. *J Membr Biol*, 2003, vol. 196, 135-146.
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- 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.