The code, under GNU license, is named Electron SPIn REsonance Simulation, E-SpiReS and provides a user-friendly, wide-purpose virtual cw-ESR spectrometer, at least for mono and biradicals in solution, with the inclusion of rotational and internal dynamics; it is highly modular and adopts a fully integrated graphical interface; it calls independent software for quantum chemistry calculation creating input files customized automatically and reading output files without any manual intervention from the user.

Efforts are currently being devoted to the integration of E-SpiReS into a general purpose software, called virtual spectroscopy laboratory (VSL), which transparently will guide the user through the tasks setup, calculation and analysis of a number of different spectroscopic observables, both optical and magnetic.

VSL is a new all-in-one application which will provide several tools to facilitate the creation of complicated input files for spectroscopy computations and the understanding of complex output files, and will allow the visualisation of optical electronic, infrared and Raman spectra and electron spin resonance spectra both in solid phase and condensed phase, based on the solution of a multi-body stochastic Liouville equation. VSL will provide an integrated environment for direct comparison between experimental digitised spectra and theoretically estimated spectra in order to correctly interpret complex results, which will be analyzable by different graphical tools. Finally ,an interactive 3D molecule builder will be embedded in VSL to allow the user to build and manipulate complex structures loaded from quantum chemical programme packages.