# Implementation and validation of a multi-purpose virtual spectrometer for large systems in complex environments

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Despite impressive advances of computational spectroscopy, a robust and user-friendly multi-frequency virtual spectrometer is not yet available. This contribution summarises ongoing efforts in our research group toward the implementation and validation of such a tool with special reference to the building blocks of biomolecules in their natural environment. Our integrated computational tool allows the computation of several kinds of spectra, including vibrational (*e.g.* IR, VCD), electronic (*e.g.* absorption, emission, ECD) as well as magnetic resonance (*e.g.* ESR, NMR) for both closed- and open-shell systems *in vacuo* and in condensed phases, and includes facilities for drawing, comparing, and modifying all the computed spectra. A number of test cases involving a combination of different spectroscopic ranges will be discussed in order to point out strengths, limitations, and ongoing developments of our research plan.

Adres publiczny

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https://www.rsc.org/