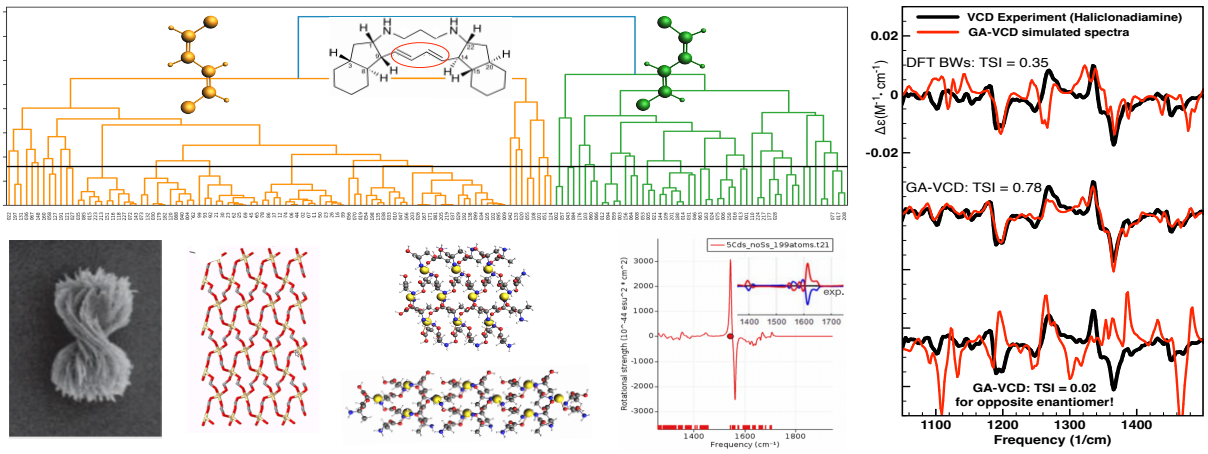
# The Digital Chiroscope
## from AI-assisted spectral analysis to periodic structure simulations

Valentin Paul Nicu[1]

[1]*ProVitam Foundation, Caisului Street 16, Cluj-Napoca, Romania*
*E-mail: vp.nicu@gmail.com*

The widespread availability of quantum mechanical software [1] capable of accurately simulating increasingly large compounds has opened new possibilities for investigating real-world molecular systems with practical applications. While this progress is highly valuable, it also presents the significant challenge of accurately and comprehensively interpreting the vast amounts of experimental and computational data generated — from flexible, diastereomeric biological molecules with many populated conformers at room temperature to nanostructured systems exhibiting exceptionally strong chiroptical signals. To address this challenge, a set of computational tools [2,3] for spectral analysis was recently developed, combining standard genetic algorithms with hierarchical clustering methods. After a brief introduction to the principles of chiroptical spectroscopy, the capabilities of these AI-assisted tools will be demonstrated using several illustrative examples.

In the second part of the talk, I will present a simple yet effective computational protocol for calculating accurate vibrational spectra of large periodic structures using DFT. This protocol is applied to elucidate the origin of the remarkably enhanced vibrational circular dichroism (VCD) signals observed in a “bowtie” nanostructure [4].

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