

POSTER PRESENTATION

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Progress on an open source computer-assisted structure elucidation suite (SENECA)

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We suggested and developed various components for Computer-Assisted Structure Elucidation (CASE) over the years [1,2]. Our current goal is to integrate these into an easy to use and efficient platform for end users, called SENECA. This is based on Bioclipse [3], an integrated software suite for chemo- and bioinformatics providing plugins for file handling and visualisation of compounds and spectra.

The SENECA feature currently comprises the following components and algorithms:

- A deterministic structure generator suitable for small chemical spaces.
- Simulated Annealing and Genetic Algorithm for random structure walks in large spaces.
- Simulation of ¹³C NMR spectra for ranking results.

SENECA is a Bioclipse feature, available via the update site at <http://www.ebi.ac.uk/steinbeck-srv/speclipse/net.bioclipse.seneca-updatesite/>.

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