

Industry Application



Structure Elucidation at Sequoia Sciences, Inc.

Sequoia Sciences builds novel libraries, from plant-derived biomass, which contain compounds that are structurally diverse and that possess a wide range of potential pharmacological activities. Sequoia has identified compounds that may potentially provide new and alternative treatments for acute and chronic bacterial infections involving bacterial biofilms.

Sequoia collaborates with commercial and academic laboratories to identify active agents in plant-based samples. Once a collaborator finds a compound of interest, Sequoia isolates it and elucidates the structure. The ability to elucidate structures quickly and accurately is important to Sequoia's ability to serve its customers well, so Mark O'Neil-Johnson, Sequoia's Vice President of Analytical Chemistry, looked for a way to make the elucidation process faster and easier. He found it in ACD/Structure Elucidator.

Sequoia's patented library production process involves extensive extraction and purification steps in order to produce a library of samples that are compatible with high-throughput screening regimes. An active sample from Sequoia's library then undergoes a final isolation step, where pure compounds are sent for further study using LC/MS and NMR technologies, followed by structure elucidation.

ACD/Structure Elucidator is a complete software package for the elucidation of unknown structures using NMR data as well as

supporting data from various other analytical techniques (Chrom, IR, Raman and MS) when available. The software provides two paths to elucidation: first, by using 1D and 2D NMR data to generate possible chemical structures that are consistent with the experimental data, and second, by accepting a proposed structure and generating other possibilities based on predicted 1D and 2D spectra. Both approaches drastically reduce data interpretation time.

ACD/Structure Elucidator also facilitates the building of spectral databases, which can be used to enhance the structure elucidation process, by identifying in advance compounds that have been previously studied.

Database searching is an important step for Sequoia's efficiency in structure elucidation and was a key factor in the decision by O'Neil-Johnson to adopt the software. Going forward, new experimental data generated by Sequoia scientists is automatically added to the library, resulting in a knowledge base of legacy information that is complete and highly accessible.

For those compounds that require elucidation from scratch, O'Neil-Johnson and his group frequently use ACD/Structure Elucidator to help facilitate the structure elucidation process, saving days worth of time on each elucidation.



To learn more about how ACD/Structure Elucidator can work in your organization, visit www.acdlabs.com/se or email info@acdlabs.com

Visionary Software



Advancing Research