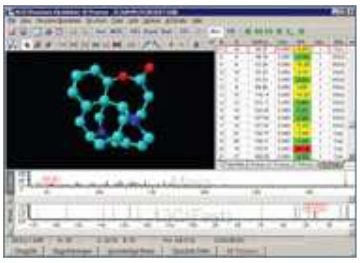
Biosciences

CSIR acquires state-of-the-art software to streamline bioresearch



Structural elucidator software combines several analytical data types in one package, enabling spectroscopists to use several techniques at once to investigate the chemical structure of a compound

Until recently the analytical science research group at CSIR Biosciences, led by Dr Paul Steenkamp, had to make use of a difficult and time-consuming process to elucidate the chemical structure of potentially lucrative compounds. Steenkamp and his team use structure elucidation as an integral tool in characterising compounds derived from indigenous resources and other technologies used.

Until now they have relied on several analytical techniques such as nuclear magnetic resonance (NMR) spectroscopy, mass spectroscopy (MS), ultraviolet visible spectroscopy (UV-Vis) and chromatography, combining multiple data formats to piece together the puzzle of a chemical's structure. To streamline their research process the team recently purchased state-of-art structural elucidator software - thought to be the first of its kind in South Africa.

The highly-sophisticated structural elucidator manufactured by Advanced Chemistry Development, Inc (ACD/Labs) in Canada provides spectroscopists with the ability to combine and manage NMR and other analytical data types from various sources in one software package. According to ACD/Labs the structure elucidator software contains sophisticated algorithms that can complement a spectroscopist's work flow and greatly accelerate the structure elucidation process by automating many of the routine processing, analysis and interpretation steps. "A fringe benefit of this software is that it provides a means of organising and storing chemical data and knowledge in a central, searchable database," said the company in a statement.

"We needed to streamline the structure elucidation process and make it as efficient as possible. The structure elucidator is compatible with most of our instrument and software platforms, and fits well with the planned expansion of our NMR facility," says Steenkamp.

"As an added benefit, we will be able to combine our NMR data with all the other analytical data and process, predict and create our own database. The ability to create a comprehensive database with this software provides the opportunity for us to build our own library using our own experimental data - a valuable tool in compound identification."

More information on the structure elucidation software is available at www.acdlabs.com/elucidator