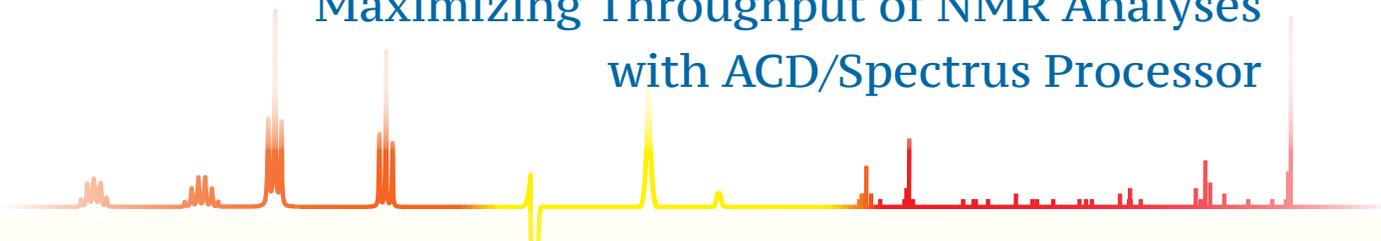


Maximizing Throughput of NMR Analyses with ACD/Spectrus Processor



Victoria, a member of the analytical chemistry team at a global speciality chemicals company, was looking to replace an in-house system for processing and analysis of NMR samples. ACD/Spectrus Processor, was deployed as a solution for processing, analysis, and interpretation of multi-technique analytical data that supported automation of routine analytical tasks.

The analytical chemistry team runs an NMR lab that services 50–100 internal customers. Working primarily with polymers, they routinely carry out compositional analysis using 29Si , ^{19}F , ^{31}P , and ^{13}C NMR spectroscopy. 300 or more samples are run on a weekly basis on four instruments from three instrument vendors. With such a large volume of data, automation of routine tasks is a necessity. Each instrument comes with its own software for data processing and analysis but instrument vendor software has been used for very little other than data acquisition within the organization for over a decade.

“The problem is that we have three different software packages with our four instruments. When you’re trying to automate processing that means it must be done three times in three different ways, leading to a lot of non-uniformity. That doesn’t take into account time wasted in setting up the procedures. There was a major benefit to us for all data processing to be moved to one software package.”

ACD/Spectrus Processor replaced an in-house system that was custom-built to address this need. The motivation to supplant this system was clear:

“The old system was unsupported so we were in the precarious position of being one Windows update away from being unable to work.”

ACD/Spectrus Processor is used to process the data generated from all four instruments. “For routine samples we worked with ACD/Labs to automate standard processing procedures. Integration with our LIMS means results are delivered directly to our internal customers. Research related to non-routine samples for new polymer development usually require more hands-on manual data processing which is also carried out in Spectrus Processor.”

“Spectrus [Processor] is more functional than our old system and I find the software to be far more intuitive. We’ve had very few problems since we deployed the software and technical support at ACD/Labs have been far more responsive than other vendors we’ve worked with to help resolve issues when they arose.”