

## **<sup>1</sup>H/HSQC-Based Automated Structure Verification as tool for Qualifying New Structures for Library Submissions**

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NMR based Computer Assisted Structure Verification has undergone continuous expansion over the past 10 years as many advancements have been made with NMR prediction tools that utilize molecular electrostatic potentials, neural networks, Hierarchical Organization of Spherical Environments (HOSE code), quantum mechanics and the ever growing repository of NMR structural data. The purpose of Computer Assisted Structure Verification software is to use known NMR structural relationships to confirm molecular structures of newly synthesized compounds in a time-efficient manner. The software can assist the chemist with their NMR analyses by assessing the spectroscopic information and attempting to fit the proposed structure to the observed data based on chemical shift correlations, coupling patterns and signal intensities. The automated analysis is facilitated by new cryo-flow probe NMR technology that allows us to rapidly collect 1D and 2D data sets on small quantities of pre-purified samples using automated flow-injection techniques. The NMR data is then processed by ACD's Automated Structure Verification (ASV) software and the results are sent directly to the submitter. The ASV output will help the chemists make better decisions in the structural characterization process and thereby reduce potential sample registration errors in Sample Bank.

### Short Biography

**Steve Hollis** is currently a Scientific Director at Amgen, Inc. in Cambridge MA where he is responsible for the small-molecule molecular structure groups that serve both drug discovery and development efforts across the company. Prior to joining Amgen, Steve spent 14 years at Abbott Laboratories as the head of Structural Chemistry in the Development area of their Pharmaceutical Products Division in North Chicago, IL. Before joining Abbott Steve spent 10 years as a synthetic chemist in the Oncology field and he holds a Ph.D. degree in Bioinorganic Chemistry from Columbia University in NY.