SPECTROSCOPIC DATA TO ASSIST CHEMICAL SYNTHESIS

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Understanding the interdependence of multiple chemical species involved in a multi-step synthesis can be a complicated process involving acquisition and interpretation of several different types of analytical data. Often, several different spectroscopic techniques will be used, generating large, temporal, information-rich datasets. However, it is often difficult to unite the information from the different techniques since each method requires the use of specialized software to process and extract relevant information. Once kinetic and structural information is obtained, it is usually contained within proprietary software and formats and it is often difficult or impossible to collate the results of several different techniques.

Here, we present a unique software tool, Mnova, which has been developed and optimized for working with spectroscopic data acquired from multiple different techniques. The large datasets typically acquired from following chemical reactions using NMR and FT-IR experiments can be simultaneously imported, then processed and kinetic information extracted and displayed quickly and intuitively. Furthermore, the software is not limited to probing datasets restricted to kinetic data – the flexible tools can also be used for confirming or verifying the structures of reaction products or intermediates and even determining the structures of unknown compounds.