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Applications of UPLC-MS QTOF in structural elucidation of small molecules

The structural elucidation of small molecules by high-resolution mass spectrometry plays important roles in development and quality control of pharmaceuticals and medical devices. Trace amounts of small molecules can be present in forms of impurities, by-products or degradation products, etc. It is often difficult to separate and fractionate enough quantities of these analytes for conventional structural analysis by NMR and FTIR. Recent advances in instrumentation and software of UPLC-MS QTOF with MS/MS fragmentation capability can give structural insight into molecules of interest and in many cases offer structure candidates at high confidence. This presentation will use several practical examples in the analysis of synthetic compounds and identification of impurities associated with pharmaceuticals and medical devices to illustrate the convenience and power of UPLC-QTOF high-resolution mass spectrometry.

Biography

Peng Chen received a Ph.D. in Analytical Chemistry from Indiana University in 1998 and a M.S. in Organic Chemistry from the University of Louisville in 1994. His graduate research includes the introduction of osazones as MALDI matrices for carbohydrate analysis and the structural elucidation of fluorescent aging markers. He has been working in various chemical industry sectors in the fields of chromatography and mass spectrometry. His work in recent years at Chemic Labs Inc. involves structural elucidation of small molecules in pharmaceuticals and medical devices by high-resolution QTOF mass spectrometry.

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