
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 form 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

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