

## Editorial: Accurate Mass Measurements in Identification of Metabolites

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### Editorial

Identification of metabolites is an important aspect in the drug discovery and development process [1,2]. For better understanding the drug efficiency and safety profiles, it is essential to study the drug metabolism in animals or humans and to identify the reactive and toxic metabolites [3,4]. The information generated in the identification of metabolites can be used to identify lead compounds and adverse metabolic products followed by optimization of pharmacokinetic and safety profiles. Identification of metabolites is usually carried out in *in vitro* and *in vivo* models and liquid chromatography-mass spectrometry (LC-MS) [5-9] is a powerful technique that can use in identification of metabolites. In particular, Q-TOF can be efficiently used to perform LC/MS and MS/MS experiments with better resolution and good mass accuracy for both molecular and fragment ions [6-9]. Accurate mass data of the metabolites that were acquired on a Q-TOF-MS provides additional supporting information on their identification. The predicted formulas observed and calculated masses ( $m/z$  value) and mass errors (ppm) help in structural characterization of each unknown metabolite. The application of accurate mass measurements (HRMS data with error in ppm) is very important in identification of metabolites for distinguishing isobaric molecular ions and assigning fragment ions to elucidate the fragmentation mechanisms [8]. Knowing the accurate mass can confirm the molecular formula of the entity under investigation. Further, the trace level metabolites can also be verified by extracting the accurate masses of metabolites to confirm their elemental compositions in structure elucidation. Accurate masses of the elemental compositions of metabolites and their fragment ions that are confirmed by HRMS are within  $\pm 5$  ppm of calculated exact masses. Interpretation of the product ion spectra obtained from Q-TOF may help to confirm the structure of each fragment ion [6-9]. The structure elucidation of metabolites can be effectively achieved with the help of HR-MS/MS spectra when compared to MS/MS spectra obtained from low resolution instruments. Thus, with help of accurate mass measurements performed on Q-TOF, unambiguous metabolite

identification [6-9], which can be very useful in the early stages of drug discovery, can be achieved without the use of large scale preparation for NMR or other analytical characterizations.

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