

Accurate mass measurements using LC/QTOF-MS and LC/TOF-MS

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Time-of-flight (TOF) mass spectrometry is used for accurate mass measurements so that the elemental composition of compounds can be established. This has become an important method in the pharmaceutical industry for rapid structural elucidation of unknown compounds. Key factors in the use of accurate mass for structural elucidation are the accuracy and precision of such measurements. In our laboratory we apply a standard method for accurate mass measurements. In the present talk, the effect of factors like ion abundances of analyte compounds and mass difference between analyte and reference compounds on the accuracy and precision of the method are presented. Moreover, the accuracy and precision of the method are compared between two standard TOF instruments, i.e. a QTOF-MS and a TOF-MS. In addition, the use of isotope ratio to obtain the correct molecular formula is also discussed.