

How can you improve your confidence to correctly identify an unknown formula?

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Abstract

Identifying an unknown substance can be rather challenging even with Mass Spectrometry. In the past, high resolution sector instruments were used to determine the exact mass of an unknown compound often combined with elemental composition analysis, by combustion technique. Today most people are using NMR combined with accurate mass on TOF instruments for confirming a certain substance. If you have a completely unknown substance what can you do?

At the LSM lab in Sweden we have used DART together with an AccuTOF (Jeol at R=6000) but the results obtained typically give too many possible formulas for an unambiguous identification. We have tried many different software programs but finally we decided to use a program called

MassWorks™. This program can improve results both for quadrupoles and TOF instrument as well as Orbitrap and FT-ICR. A calculation of spectral accuracy (not the same as mass accuracy) is performed by comparing theoretically generated spectra to measured spectra which have been accurately calibrated for spectral line-shape which enables much higher confidence in formula identification.

Examples will be given from different types of MS instruments like TOF and quadrupoles.