

STRUCTURE VERIFICATION OF SMALL MOLECULES

*H. Thiele*¹, *G. McLeod*², *I. Krebs*¹

¹Bruker Daltonik GmbH
(28359 Bremen, Germany; e-mail: ht@bdal.de),

²Bruker Daltonics Ltd.
(Coventry, Englan)

S u m m a r y

The high mass accuracy of the MS and MS/MS data provided by the new generation of ESI-TOF- and ESI-Q-TOF mass spectrometers provides an accurate determination of molecular weight, which is used specifically for the structural verification and purity determination of substances. The high separation of the isotope profile for both MS and MS/MS spectra affords further dimensions of information to achieve precise molecular formula determination.