E1-06 Accurate calibration of matrix assisted laser desorption/ionization mass spectra

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The technique of matrix assisted laser desorption/ionization (MALDI) mass spectrometry, developed in the recent past, is now well established as a versatile method for studying a variety of large bimolecules. In this approach, a light absorbing low molecular weight compound is mixed with sample molecules to resonantly absorb the laser energy needed for desorption, thereby leading to the ejection of intact molecular ions of large proteins. The time profiles of the ions produced are then recorded and analysed by a suitable data handling system. The usefulness of the technique however, depends essentially on the accuracy with which the corresponding molecular masses can be determined as certain applications require the determination of molecular weights with unit mass precision. As such, calibration of the resulting mass spectra can be identified as a critical step in the mass assignment of molecular compounds.

In this study, we have developed a model for determining accurately the molecular masses of analyte compounds, by employing experimental data previously reported. While internal calibrants, when compared to their external counterparts, have been observed to be the most suitable for overcoming instrumental fluctuations associated with applied voltage, incident laser energy and the homogeneity of the samples, their presence on the target seems to raise the threshold fluence needed to produce analyte ions thereby increasing fragmentation of the molecules. The influence of the chemical structure of the matrix compound and the fluence used for desorption have also been studied.