

## **ADVANTAGES AND APPLICATIONS OF ELEVATED RESOLUTION AND EXACT MASS ON A BENCHTOP GCTOF MASS SPECTROMETER.**

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This paper discusses the advantages and applications of elevated resolution and exact mass capability on a bench top mass spectrometer. The ease of use of the GCTOF introduces the capabilities of magnetic sector technology to a broader range of the chemical community. We illustrate this with examples from synthetic chemistry, the pharmaceutical and the food and flavour industries.

All experiments were performed on an orthogonal acceleration time of flight mass spectrometer (Micromass, UK, Manchester) coupled to an HP6890 gas chromatograph. The oa TOF produces high quality, full mass spectra with an elevated resolution (~ 7000 FWHM). This elevated resolution reduces mass interferences. Furthermore the precise known relationship between ion arrival time and its mass allows good mass measurement accuracy with only a single internal lock mass.

In the pharmaceutical application we examined the use of GCT in the field of combinatorial chemistry. 'Library' compounds which failed to give an adequate electrospray response, under a commonly used generic method, were submitted to GCT. Preliminary data obtained to date on 0.25mmid and 0.18 mmid DB5 capillary columns indicate that a significant proportion of non polar and intermediate polarity synthetics can be confirmed by GC-MS using EI. Mass measurement accuracy was within 5PPM RMS for the data set examined. Further ongoing work examines the use of 0.53mmid columns coupled with field ionisation.

In the food and flavour industry data is presented on the analysis of complex fragrance mixtures. A fragrance reference was analysed on a 20m x 0.18mmid DB1 column. We demonstrate a high spectral acquisition rate (10 spectra per second), coupled with unskewed spectra and deconvolution of co-eluting chromatographic peaks with confirmation of library search results with elemental composition data. The results indicate the potential errors that can be made when relying on library search ranking alone. Further data presents the selectivity of exact mass chromatograms (20mDa window) for the analysis of trace contaminants in essential oils.

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