MODIFICATION OF A FINNIGAN ITS 40 TO PERFORM SELECTIVE ISOLATION AND MS/MS FUNCTIONS

S.A. Lammert and M.V. Buchanan
Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831-6120

Historically, ion traps from Finnigan-MAT have been of two main types; the full-functioned ITMS capable of MS/MS , and the ITS-40/Magnum bench-top instruments intended for GC/MS use. Both of these instruments share a common analyzer as well as much of the electronic circuitry and differ only in the amount of electronic and software control provided. The smaller ITS-40/Magnum instruments are considerably less expensive and have a much smaller footprint than the laboratory-based ITMS. As such they are better suited for use as field-deployable or transportable mass spectrometers. In fact, we have used these instruments extensively in direct sampling applications at several locations (Hanford Site, Savannah River Laboratory, Portsmouth Gaseous Diffusion Plant and the TSCA Incinerator Site at Oak Ridge). The ability to perform MS/MS analysis has proven to be valuable in many applications where high selectivity is equal in importance to the high sensitivity already provided by ion traps. Therefore it was desirable to add MS/MS capabilities to our field-deployable direct sampling ion trap mass spectrometers.

The ability to perform MS/MS in ion traps requires both a method of isolation of the precursor ion as well its subsequent fragmentation. The Finnigan-MAT ITMS uses a combination of rf and dc voltages to achieve single ion stability and a frequency generator to resonantly excite the isolated precursor ion. More recently, broadband techniques have been used to activate selected ions in ion traps using white noise. [1] Other methods have been developed for isolation including Stored Waveform Inverse Fourier Transform (SWIFT) [2] and Filtered Noise Fields[3] ; the later of which has been demonstrated on the smaller ITS-40 instruments.[4]

Selective isolation and MS/MS functions are accomplished on the ITS-40/Magnum by using two commercially available accessories. A *Filtered Noise Field (FNF*) waveform generator (Teledyne MEC) is used to apply broadband frequency waveforms to the endcaps of the ion trap. This unit was originally designed as an accessory to the Finnigan-MAT ITMS in order to provide selective ionization and broadband isolation functions to this instrument. For these experiments, the FNF unit is used to generate a broadband waveform to provide selective ion accumulation as well as to apply the resonant frequency of the isolated precursor ion for activation and the axial modulation frequency during the mass scan. Several different waveforms can be stacked and sequentially executed on the FNF. A double TTL trigger executes the first waveform and each subsequent TTL trigger ends that waveform and begins execution of the next waveform in the stack. Place-holding or "dummy" waveforms can be applied between active waveforms. A *DG535 Pulse/Delay Generator* (Stanford Research Systems) is used to coordinate the timing of TTL pulses to the FNF unit. This unit has 4 programmable delay outputs which can be synchronized to an external trigger, in this case the negative-going scan start trigger on the Finnigan ITS-40/Magnum Scan and Acquisition Processor (SAP) board. A home-built circuit was constructed to convert the five "rising edge" outputs of the DG535 to 10 **µ**s TTL pulses to be compatible with the FNF unit. The first of these pulse converters was also designed to generate the double TTL trigger which the FNF unit recognizes as a start trigger. The BNC endcap connections are removed from the SAP board and connected to the two endcap signal leads from the FNF. The full setup is shown below.

The ITS-40 uses a "segmented" rf scan function when operated in the standard electron ionization (EI) mode. This "segmented" scan is not used on the ITMS and is incompatable with the operation of the FNF accessory. The ITS-40 chemical ionization (CI) scan function however is not segmented and can be used

(without adding the CI reagent gas) to produce an EI scan.

The timing of the TTL pulses which control the FNF waveforms was optimized by first coarsely setting their appropriate positions relative to the scan function using an oscilloscope and then fine-tuning each stage of the process using perfluorotributylamine (PFTBA). Both the position of the TTL control pulses, and the frequency components of the FNF waveforms could be adjusted in real-time while observing the effect on the resulting spectrum. The last TTL control pulse was set to occur just prior to the mass scan to activate the 485 KHz FNF waveform which substituted for the axial modulation signal normally provided by the SAP board.

A five-fold increase in ion signal for m/z 264 from PFTBA was observed upon activating the selective ion accumulation waveform. In addition, despite operation at a relatively low q_z-value, the MS/MS efficiency was 83%. Improvements could be expected if two features were added to this arrangement:

1) Longer "filament on" time than the currently allowed 2.5 milliseconds (limited by the CI scan function).
2) Direct control of the rf level during MS/MS. A circuit was designed for this purpose, however has not been tested.

While not necessarily convenient for use as a research instrument, this combination can be easily applied to dedicated, single compound applications for considerably less cost than a research grade instrument (especially for those who already own the ITS-40 instrument). Further enhancements to this instrument were made unnecessary with the announcement by Finnigan-MAT of a retrofit MS/MS accessory for the ITS-40/Magnum ion trap.

REFERENCES

1) McLuckey, S.A., Goeringer, D.E., Glish, G.L., *Anal. Chem.* **64** (1992) 1455-60.
2) Julian, R.K., Jr., Cox, K.A., Cooks, R.G., Proceedings of the 40th ASMS Conference on Mass Spectrometry and Allied Topics, Washington, D.C., (1992) 943-4.
3) Kelley, P.E., U.S. Patent No. 5,134,286, July 28, 1992
4) Van Berkel, G.J. and Goeringer, D.E., *Anal. Chim. Acta.* **277** (1993) 41-54.

Research sponsored by the U.S. Department of Energy Office of Technology Development under U.S. Department of Energy contract DE-AC05-85OR21400 with Martin Marietta Energy Systems