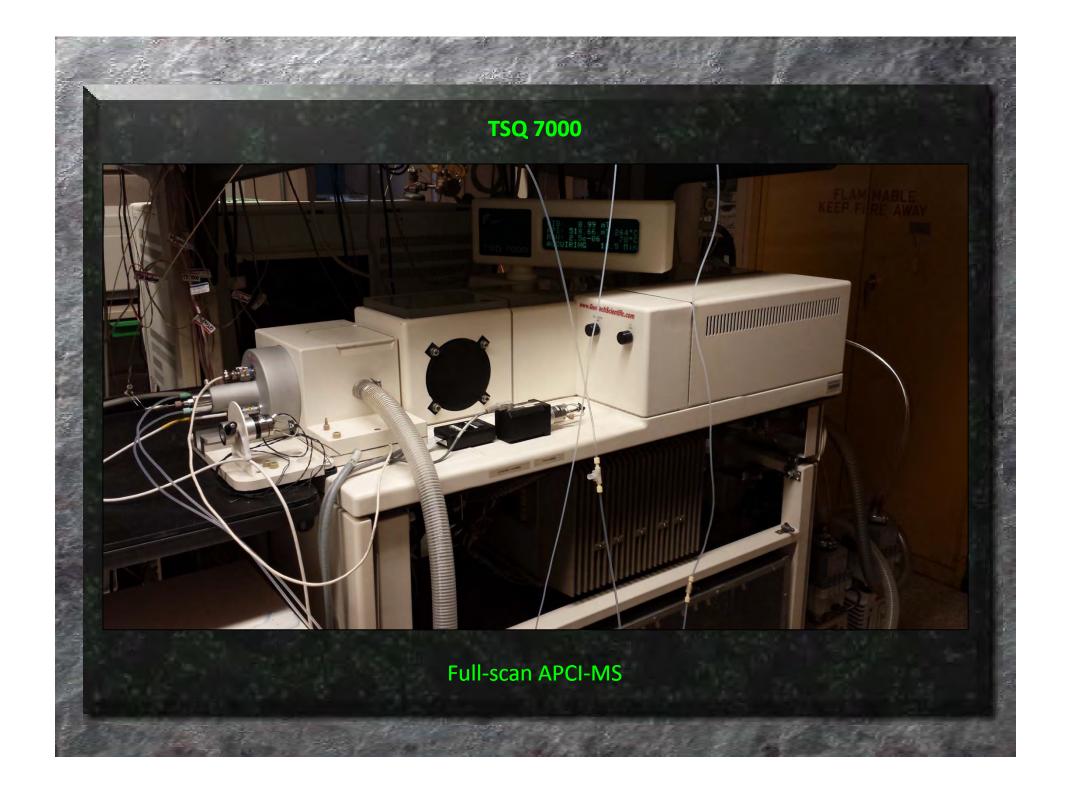
Agilent 1200



Quaternary Pump/Autosampler/Column Thermostat/UV Detector/Corona CAD/ELSD

LCQ Deca XP + TSQ Vantage EMR ESI-MS/MS, w/ NH₄OCOH + APCI-MS (SIM, MRM, Full-scan, MS/MS)





Syringe Pumps and Water wash pump



50 mM NH₄OCOH @ 40 μ L/min for ESI-MS + D.I. H₂O for source wash between runs

Summary, Tips, & Tricks for Parallel MS

- ✓ Multiple Parallel MS can be implemented using simple 'off-the-shelf' components
- ✓ The primary obstacles are preconceptions
- ✓ Simultaneous acquisition using multiple API-MS methods saves time, labor, & resources, plus eliminates run-to-run T_R uncertainties
- ✓ APCI, APPI, and ESI provide different and complementary data
- ✓ Two-dimensional detectors are easily incorporated, and UV detection can be more sensitive than MS
- ✓ Analytical-scale HPLC is more suited to Parallel MS than UHPLC
- ✓ Some API techniques discriminate between molecule classes more than others





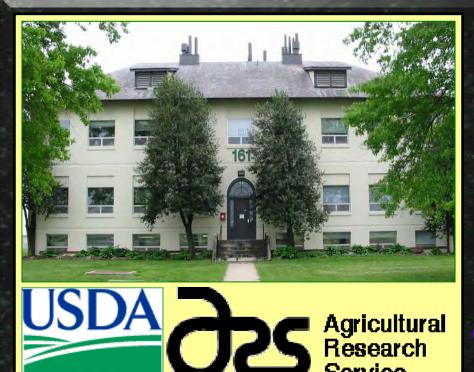
Summary, Tips, & Tricks for Parallel MS

- ✓ Sources from different manufacturers show differences in fragment formation, even for the same API type (differences even from the same manufacturer, and can be affected by tuning/optimization)
- ✓ Keep old instruments online as auxiliary detectors after upgrades (mechanical aptitude helps)
- ✓ Used instruments can be purchased very affordably for use as auxiliary detectors
- ✓ It is helpful to synchronize system clocks on multiple instruments
- ✓ It is helpful to show analysis times in data headers
- ✓ Disadvantage: You accumulate an avalanche of data!





Thank You for Your Attention!



William Craig Byrdwell

USDA, ARS, BHNRC, Food Composition and Methods Development Lab

C.Byrdwell@ars.usda.gov

Byrdwell.com/Ghent2013.ppt



