

Comparison of Single and Triple Quadrupole GC-MS Instruments for Full Scan Analysis of Semivolatile Organic Compounds

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Key Words

Full Scan Acquisition, LOD, Semivolatile Organic Compounds, Spectral Quality

Introduction

Single quadrupole mass spectrometers, such as the Thermo Scientific™ ISQ™ Series GC-MS system, are a popular choice among analysts using GC-MS for compound identification and quantitation in relatively simple matrices. However, triple quadrupole mass spectrometers such as the Thermo Scientific™ TSQ™ Duo GC-MS/MS and TSQ™ 8000 Evo GC-MS/MS systems have been gaining popularity due to their high selectivity and lower detection limits, especially in complex matrices.

The higher cost of triple quadrupole instruments is one of the main barriers to their adoption by analytical labs, however, the cost differential between single and triple quadrupole mass spectrometers has decreased in recent years such that today, triple quadrupole instruments are a viable alternative to their single quadrupole counterparts.¹

An obvious concern for analysts considering using triple quadrupole GC-MS systems to perform single quadrupole GC-MS workflows is how the full scan performance of the triple quadrupole GC-MS/MS compares to that of the single quadrupole system. In this work, full scan performance of the TSQ Duo GC-MS/MS system is compared to that of the ISQ GC-MS system for full spectrum acquisition of semivolatile organic compounds. Limits of Detection (LOD) and spectral quality (as defined by search-match results of NIST 14 Mass Spectral Library) were chosen as the criteria for comparison.

Goal

To compare the full scan acquisition performance of the TSQ Duo triple quadrupole instrument with that of the ISQ single quadrupole instrument with respect to limits of detection (LOD) and spectral quality of semivolatile organic compounds



Experimental

Sample and sample preparation: Use Restek 8270 MegaMix® as the source of semivolatile organic compounds for analysis. This mixture contains 76 compounds. All but two of these compounds are at 1000 µg/mL concentrations. The other two compounds, 3-methylphenol and 4-methylphenol, are at 500 µg/mL. More details of these compounds can be found at <http://www.restek.com/catalog/view/5744>.

Use dichloromethane (DCM) extract of the soil matrix to dilute the MegaMix® to 1 µg/mL. Use the DCM extract of soil to take advantage of the matrix-induced chromatographic response enhancement phenomena.²

Prepare the extract as follows: Place 10 g of clean loam soil (Fluka mfr. no. CLNLOAM6-100g) in a screw-top vial with a PTFE liner on the cap and add 10 mL DCM.

Shake the vial using a wrist-action shaker (Burrell Scientific Model 75) for 30 minutes. Allow the mixture to settle for 30 minutes, and then remove the DCM extract from the soil using a glass pipette. Add 10 mL DCM to the same soil matrix and repeat the shaking and DCM extract removal process two more times.

Dry the DCM extract over sodium sulfate. Use Thermo Scientific™ eVol™ Sample Dispensing System to dilute MegaMix to 1 µg/mL using the DCM extract prepared above. Store the sample in a refrigerator at 1.5 °C in a National Scientific Target DP® vial (C4000-2W) until it is ready to be injected into the GC-MS.

GC-MS conditions: Use a TSQ Duo GC-MS/MS system and an ISQ GC-MS system, each mated to a Thermo Scientific™ TRACE™ 1310 GC and an AI/AS 1310 autosampler. Table 1 shows the autosampler, GC, and MS parameters used for the experiment.

Perform 10 sample injections on both the TSQ Duo GC-MS/MS and the ISQ GC-MS using the prepared 1 µg/mL MegaMix mixture. Choose a suitable quantitative ion that is unique to the compound and not included in the coeluting compounds. In most cases, the quantitative ion is the base peak for the compound. Calculate the LOD of the compounds by statistical analysis using the two-tailed student t-distribution at a 99% confidence interval for 10 back-to-back injections. Use the Thermo Scientific™ Dionex™ Chromeleon™ 7.2 SR1 CDS software for qualitative and quantitative data analysis.

Table 1. Autosampler, GC, and MS parameters used for the experiment.

AI/AS 1310	
Syringe	10 µL, 25 gauge, 50 mm length, cone tip (P/N 36500525)
Injection Volume	1 µL
Plunger Strokes	3
Viscous Sample	No
Sampling Depth	Bottom
Pre-/Post-Injection Dwell Time	0.0
Pre-Injection Solvent, Cycles	Dichloromethane, 2
Sample Rinses	2
Post-Injection Solvent, Cycles	Dichloromethane, 3

TRACE 1310 GC	
Column	TG-5SILMS 30 m × 0.25 mm × 0.25 µm
Liner	Restek Sky® Inlet liner, splitless single taper gooseneck with wool, 4 mm × 6.5 mm × 76.5 mm
SSL Mode	Splitless with surge
Inlet Temperature	270 °C
Split Flow	100 mL/min
Splitless Time	0.6 min
Surge Pressure	207 kPa
Surge Duration	0.6 min
Septum Purge Flow	Constant flow of 5.0 mL/min
Carrier Flow	Constant He flow of 1.2 mL/min
Oven Program	40 °C (1 min), 25 °C/min to 280 °C, 5 °C/min to 320 °C (1 min)

TSQ Duo GC-MS/MS and ISQ GC-MS	
Method Type	Acquisition – General
MS Transfer Line Temperature	280 °C
Ion Source Temperature	280 °C
Ionization Mode	EI, 70 eV
Emission Current	50 µA
Scan Start	At 2.4 min
Scan Range	35–550 amu
Scan Time	0.2 s
Chrom. Filter Peak Width	1.0 s
Use Last Tuned Detector Gained?	Yes
Tuning Used	EI Standard tune for TSQ Duo GC-MS/MS and EI Full tune for ISQ GC-MS (with 219 intensity set to 20 million)

Results and Discussion

Figure 1 shows the chromatograms for the full scan analyses run on the TSQ Duo GC-MS/MS and the ISQ GC-MS. The chromatograms look similar both in terms of the order of elution of components and their relative intensities. Figure 2 shows the comparison of mass spectra of Benzyl butyl phthalate on the TSQ Duo GC-MS/MS and the ISQ Series instrument. The fragmentation patterns and the relative intensities of the mass fragments are similar on both the systems.

LOD results: Figure 3 compares the results for the LODs for selected semivolatile organic compounds on the TSQ Duo GC-MS/MS and the ISQ GC-MS systems. The LODs for both are similar with 39 compounds showing lower LODs for the TSQ Duo GC-MS/MS than the ISQ GC-MS. The average % RSDs for the quantitative ion areas of 10 consecutive injections for the TSQ Duo system was 4.2% compared to 3.6% for the ISQ instrument.

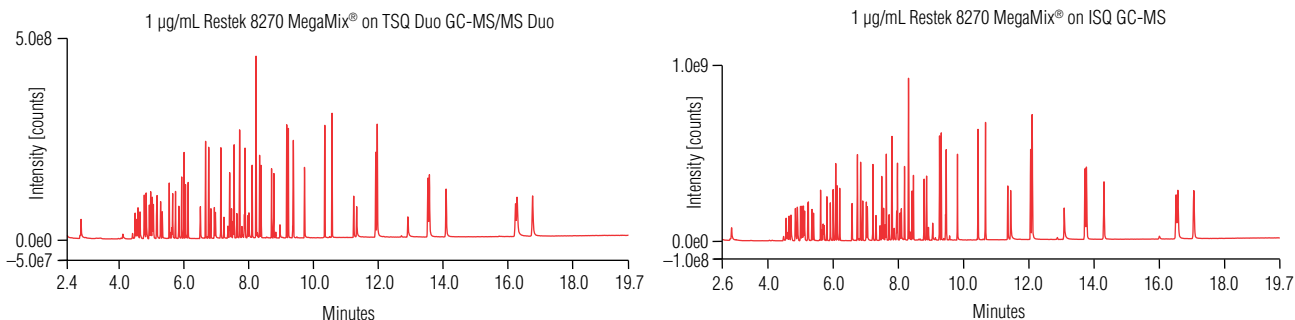


Figure 1. Comparing chromatograms for injections done on the TSQ Duo GC-MS/MS and the ISQ GC-MS.

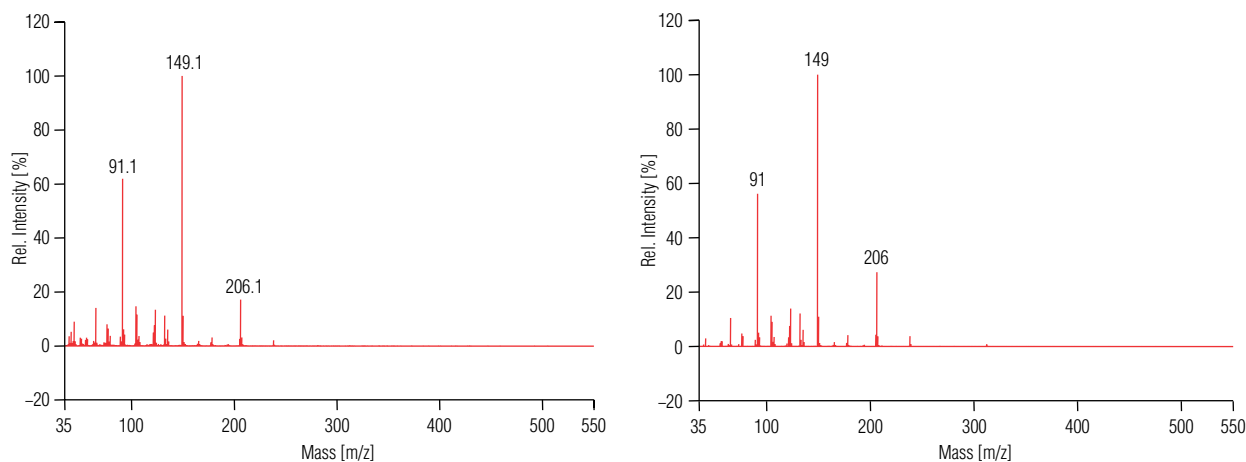


Figure 2. Comparing mass spectra of Benzyl butyl phthalate on the TSQ Duo GC-MS/MS and the ISQ GC-MS.

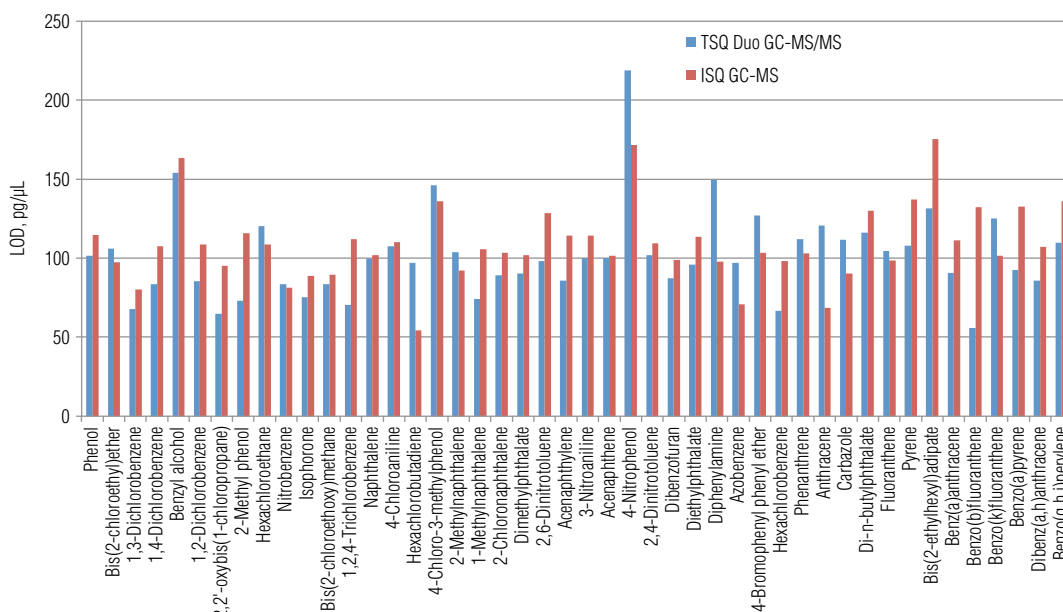


Figure 3. Limits of detection comparison on selected compounds on the TSQ Duo GC-MS/MS and the ISQ GC-MS.

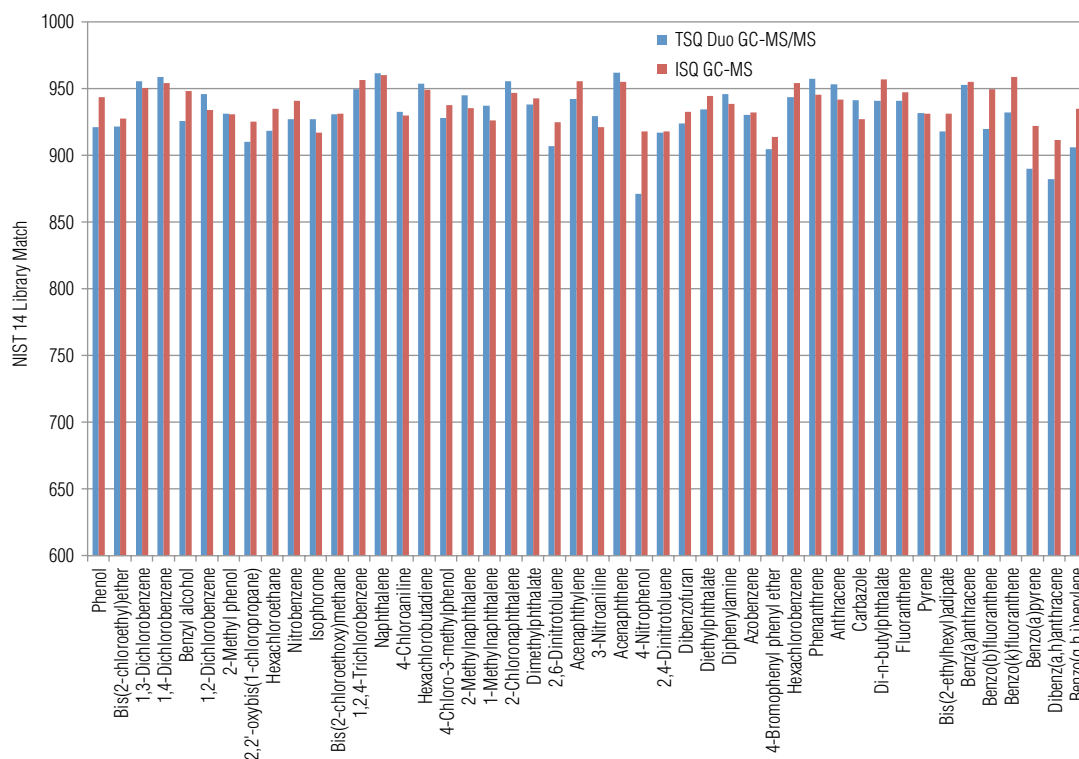


Figure 4. Spectral quality comparison using the NIST 14 library for the TSQ Duo GC-MS/MS and the ISQ GC-MS.

Spectral quality results: Figure 4 shows the results for the search-match for chromatographically resolved components of the mixture with the NIST 14 mass spectral library. The TSQ Duo GC-MS/MS and the ISQ GC-MS have a match factor greater than 900 for 59 and 64 compounds, respectively. Both the TSQ Duo instrument and the ISQ system show 66 number one hits. These results show that the spectral quality for the TSQ Duo and the ISQ system are similar, with both having excellent matching factors with the NIST 14 Mass Spectral Library.

Conclusion

Full scan comparison of the TSQ Duo GC-MS/MS and the ISQ GC-MS systems for 1 µg/mL Restek 8270 MegaMix shows that LODs for both instruments are similar, with 39 compounds having lower LODs on the TSQ Duo system. Additionally, the % RSD on the areas of the quantitative ions for most of the analytes was less than 5%. The spectral quality of the analytes, as measured by matching with NIST 14 Mass Spectral Library, was excellent, with 66 compounds having number one hits on both the TSQ Duo GC-MS/MS system and the ISQ GC-MS system.

References

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