

Full-scan Analytical Performance

Thermo Scientific Exactive GC and the Thermo Scientific Q Exactive GC Mass Spectrometers

Cristian Cojocariu¹, Dominic Roberts¹ and Paul Silcock¹ ¹ Thermo Fisher Scientific, Runcorn, UK

Goal

The Thermo Scientific™ Exactive™ GC Orbitrap™ GC-MS System and the Thermo Scientific™ Q Exactive™ GC Orbitrap™ GC-MS/MS System have been designed to provide equivalent performance when using full-scan acquisition modes. The objective of this study was to test the analytical performance of the Exactive GC system and the Q Exactive GC system using full-scan acquisition. Both mass spectrometers were evaluated for key analytical parameters such as scan speed, sensitivity, mass accuracy, dynamic range and linearity.

Experimental

In all experiments, a Thermo Scientific Q Exactive GC hybrid quadrupole-Orbitrap mass spectrometer and a Thermo Scientific Exactive GC mass spectrometer were used. Sample injection was performed using a Thermo Scientific™ TriPlus™ RSH™ autosampler, and chromatographic separation of the analytes of interest was obtained using a Thermo Scientific™ TRACE™ 1310 Gas Chromatograph and a Thermo Scientific™ TraceGOLD™ TG-5SiIMS, 30 m × 0.25 mm × 0.25 μm film capillary column (P/N: 26096-1425). The Exactive GC system and the Q Exactive GC system were tuned and calibrated

using PFTBA over exactly the same mass range to achieve mass accuracy of <1.0 ppm. The default ionization mode was electron ionization (EI) and the mass spectrometers were operated using full-scan 60,000 resolution (FWHM, measured at m/z 200) (Table 1). Data acquired was lock-mass corrected using siloxane masses from the GC column bleed. (Table 1)

TRACE 1310 GC System Parameters

Injection Volume (μl):	1.0
Liner	LinerGOLD™, single taper (P/N:453A0344-UI)
Inlet (°C):	250
Inlet Module and Mode:	splitless
Carrier Gas, (mL/min):	He, 1.2
Oven Temperature Program:	
Temperature 1 (°C):	40
Hold Time (min):	1.0
Temperature 2 (°C):	250
Rate (°C/min)	30
Hold Time (min):	0.0
Temperature 3 (°C):	150
Rate (°C/min)	30
Temperature 3 (°C):	320
Rate (°C/min)	2.0

Table 1. Gas chromatography and mass spectrometers analytical parameters.

Mass Spectrometer Parameters

Transfer line (°C):	280
Ionization type:	EI
Ion source (°C):	230
Electron energy (eV):	70
Acquisition Mode:	full-scan
Mass range (Da):	50-450
Mass resolution (FWHM at m/z 200):	60k
	207.03235
Lockmass, column bleed (m/z):	281.05114
	355.06993

Scan speed

The Exactive GC system and the Q Exactive GC system provide the same scan rates when set to the same resolving power. An example is shown in Figure 1, where the same number of data points across a three second

wide peak (extracted ion chromatogram of m/z 179.17923) was obtained. Additional information about the Q Exactive GC system was published before.^{1,2}

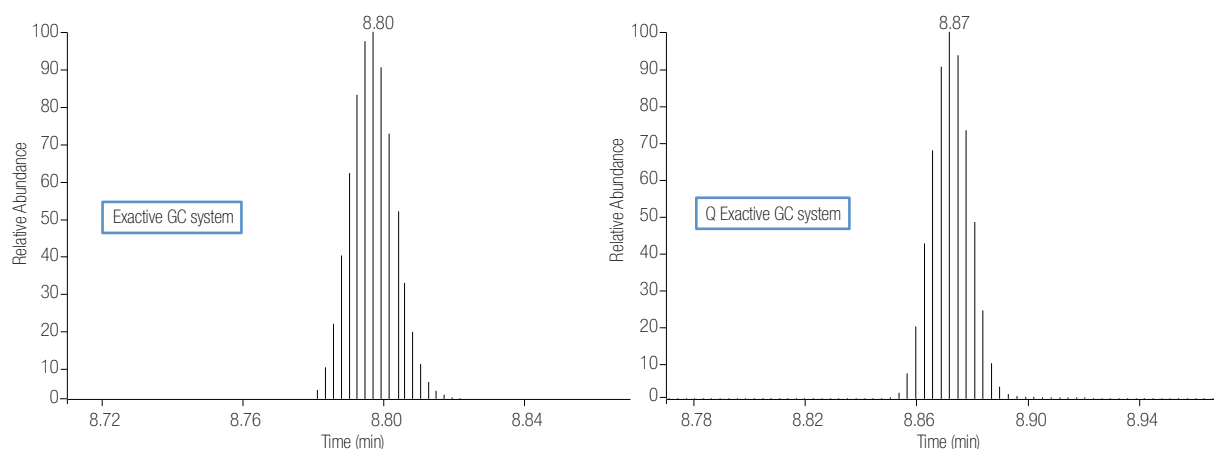


Figure 1. Comparable scan speed demonstrated for 2-butyl-5-hexyloctahydro-1H-Indene measured on the Exactive GC and the Q Exactive GC systems. Both mass spectrometer systems operated in full-scan at 60k resolution (FWHM at m/z 200).

Sensitivity

To test if the two mass spectrometers have similar sensitivity, an 8270 semivolatle MegaMix[®] working solution (Restek) in dichloromethane was diluted to 1 pg/ μ L (in dichloromethane) and analyzed simultaneously using the Exactive GC and the Q Exactive GC systems. Replicate injections ($n=8$) of this standard were performed on two different days. The instrument detection limits (IDL) of selected chemicals in the mixture were calculated for

each mass spectrometer on both days and the average values are reported in Figure 2. The IDL was calculated taking into account the Student's- t critical values for the corresponding degrees of freedom (99% confidence).² Both systems demonstrated excellent sensitivity with IDL values ranging from 0.04 to 0.17 pg/ μ L. The results of this experiment confirmed that the Exactive GC system and the Q Exactive GC system are able to detect comparable levels of analytes.

Compound	RT (min)	Exactive GC System	Q Exactive GC System
Nitrobenzene	5.53	0.11	0.10
Isoforone	5.75	0.06	0.10
4-Nitroaniline	7.44	0.06	0.10
Acenaphthene	7.93	0.05	0.07
Diphenylamine	8.55	0.04	0.09
Hexachlorobenzene	9.01	0.06	0.13
Phenanthrene	9.40	0.15	0.15
Carbazole	9.61	0.07	0.08

Figure 2. Instrument detection limits (IDLs, as pg on-column) calculated for selected analytes. Data represents repeat injections ($n=8$) of a 1.0 pg on-column 8270 semivolatle solvent standard. Two sets of measurements were acquired in two distinct days using the Exactive GC and the Q Exactive GC systems. Error bars annotated represent one standard deviation calculated from the two sets of measurements. Standard deviation calculated from the two sets of measurements is annotated.

Linear dynamic range

A wide linear dynamic range over which accurate mass measurements are to be made is essential, especially when dealing with applications where the samples analyzed contain a complex and varied chemical background that could potentially interfere with the analytes of interest (ex: routine pesticide screening, metabolomics). To test if

the two mass spectrometers have similar linear dynamic ranges, repeat injections (n=3) of increasing concentration levels (0.1 pg to 10,000 pg on-column) of the 8270 semivolatile mix were performed. An example of compound linearity obtained from both mass spectrometers is shown in Figure 3 for hexachloroethane, the results demonstrating equivalent performance.

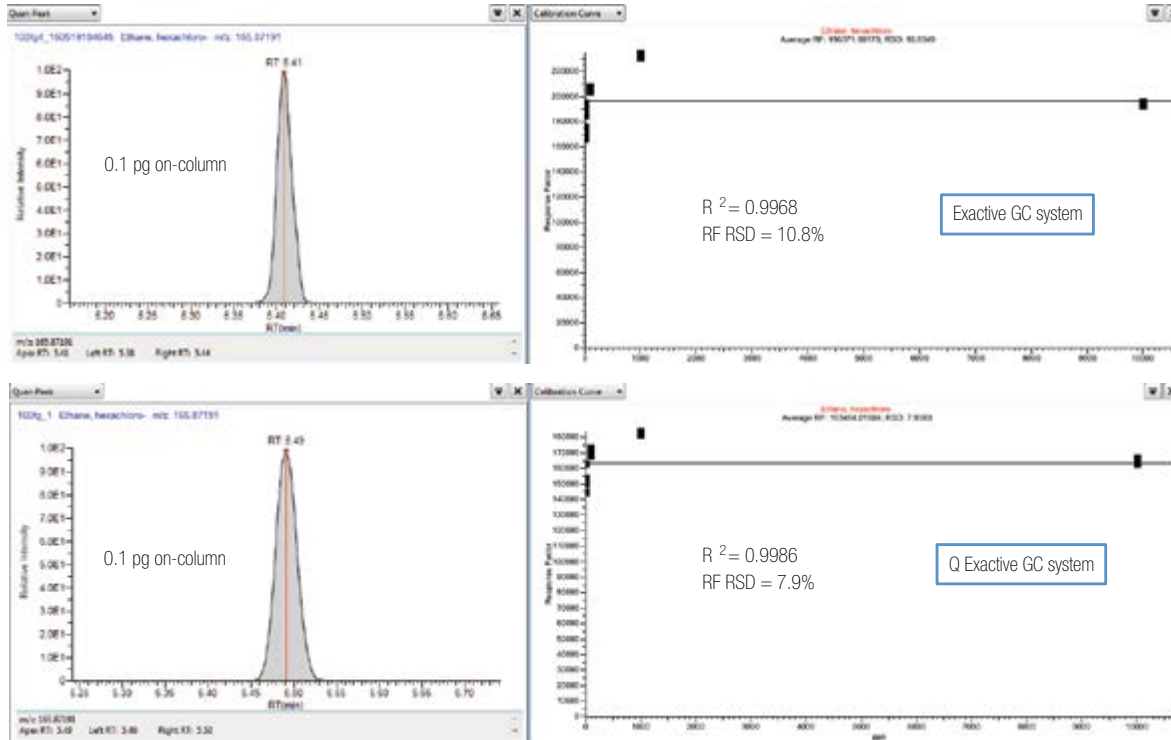


Figure 3. Linear dynamic range of the Exactive GC system and the Q Exactive GC system demonstrated using hexachloroethane solvent standards injected over six orders of magnitude. Extracted ion chromatogram (m/z 165.87191) corresponding to hexachloroethane at 0.1 pg on-column is shown together with the coefficient of determination (R^2) and the RF %RSD values determined over a concentration range of 0.1-10,000 pg on-column.

Moreover, excellent peak area repeatability (n=3 injections) was obtained on both mass spectrometers at each concentration level as demonstrated for hexachloroethane in Table 2 which shows %RSD ranged from 0.6-6.9% across the six orders of magnitude.

Hexachloroethane concentration (pg on-column)	Exactive GC system %CV (n=3)	Q Exactive GC system %CV (n=3)
10000	0.8	1.7
1000	0.6	0.6
100	0.9	1.6
10	1.4	1.2
1	0.8	2.1
0.1	6.9	3.6

Table 2. Calculated % CV from n=3 repeat injections of hexachloroethane solvent standard at various on-column concentrations. Data from the Exactive GC system and the Q Exactive GC system is shown.

Maintaining sub-ppm mass accuracy irrespective of compound concentration

Sub-ppm mass accuracy was maintained across compound concentrations on both mass spectrometers as exemplified below for hexachloroethane. In all cases, irrespective of the m/z and concentration level, <1ppm

mass accuracy was obtained on both the Exactive GC and the Q Exactive GC systems. This is essential as any compromise in accuracy of mass measurements can result in false identification and non detection of compounds of concern, such as pesticides in a screening experiment.¹

Level	EGC	QEGC	EGC	QEGC	EGC	QEGC	EGC	QEGC	EGC	QEGC
ppb on-column	m/z	m/z	m/z	m/z	m/z	m/z	m/z	m/z	m/z	m/z
	118.90306	118.90306	116.90601	116.90601	120.90011	120.90011	165.87191	165.87191	202.83781	202.83781
0.1	0.6	0.1	0.8	0.1	0.5	0.2	0.3	0.2	0.7	0.1
1	0.7	0.1	0.5	0.2	0.4	0.1	0.1	0.7	0.4	0.8
10	0.4	0.1	0.3	0.0	0.3	0.1	0.4	0.7	0.5	0.9
100	0.2	0.1	0.1	0.1	0.3	0.2	0.8	0.7	1.0	1.0
1000	0.8	0.4	0.5	0.2	0.4	0.1	0.7	0.4	0.9	0.7
10000	0.5	0.4	0.5	0.3	0.5	0.2	0.6	0.3	1.0	0.7
average Δ ppm	0.5	0.2	0.4	0.2	0.4	0.1	0.5	0.5	0.7	0.7

Figure 4. Comparative mass accuracy (Δ ppm) measurements for several hexachloroethane ions over > 5 orders of magnitude using the Exactive GC (EGC) and the Q Exactive GC (QEGC) systems. Average mass accuracy (Δ ppm) value for each ion is also indicated.

Conclusions

Overall, the experimental data shown here demonstrate that the Exactive GC and the Q Exactive GC mass spectrometers deliver comparable high-quality analytical performance using full-scan acquisition.

Both systems have the same fast scan speed, allowing the analyst to obtain sufficient data points across narrow chromatographic peaks, to accurately describe the peak area and to ensure signal reproducibility.

The sensitivity of the Exactive GC system and the Q Exactive GC system used for this study is also very similar and this was demonstrated from the IDL values obtained for the test compounds.

The linear dynamic range was also comparable on both systems, extending to six orders of magnitude (0.1-10,000 pg on-column) as demonstrated for selected compounds.

Mass accuracy was consistently maintained on both mass spectrometers at sub-ppm levels irrespective of compound concentration.

References

1. The Power of High Resolution Accurate Mass Using Orbitrap Based GC-MS. Thermo Scientific White Paper 10456, May 2015. [Online] <https://tools.thermofisher.com/content/sfs/brochures/WP-10456-GC-MS-Orbitrap-High-Resolution-Accurate-Mass-WP10456-EN.pdf>.
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