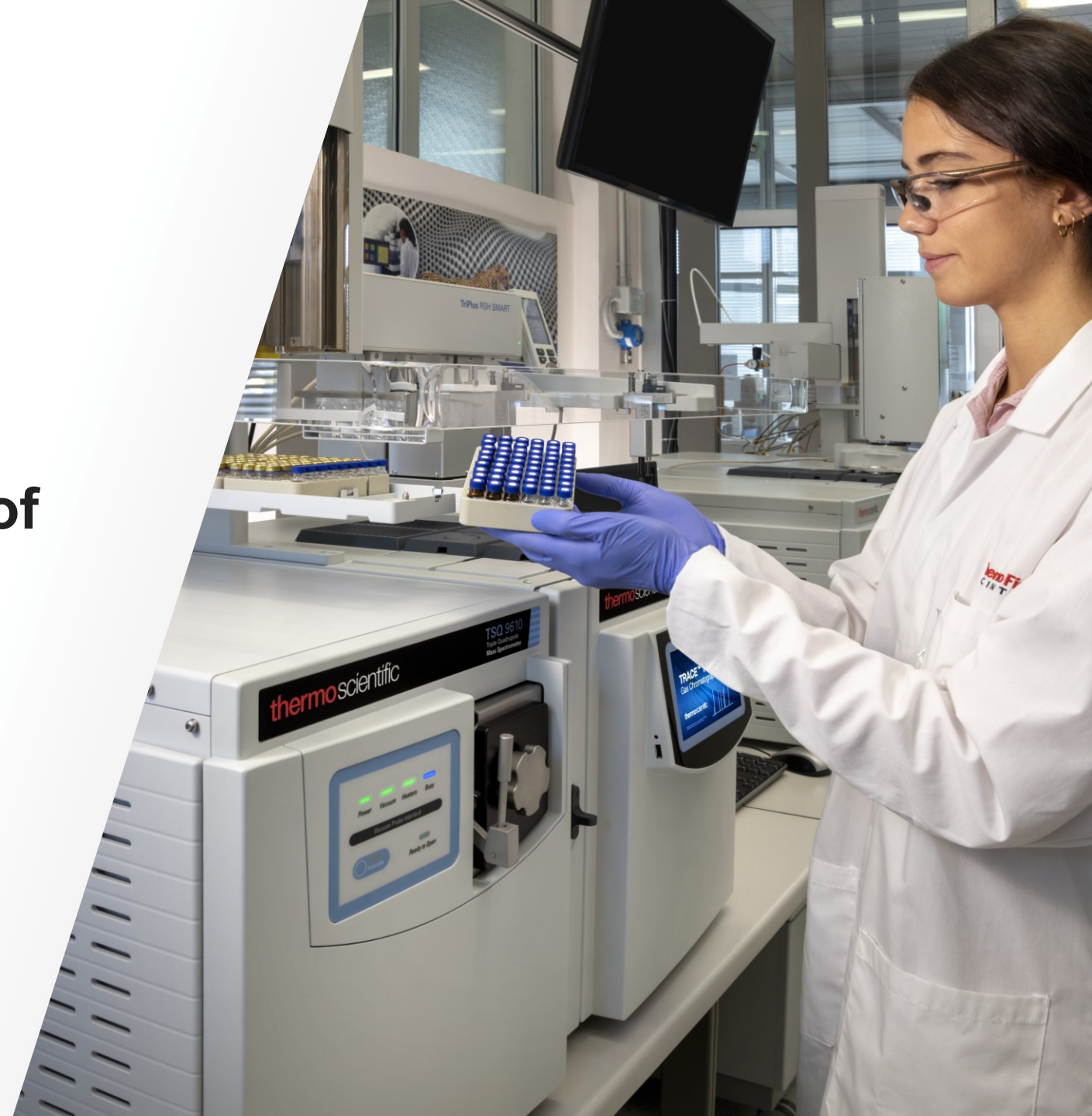# Using GC-MS/MS for analysis of off-flavors in wine

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The world leader in serving science

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TSQ™ 9610 GC-MS/MS Overview

Class-leading sensitivity

8 x 1 fg on-column OFN injections with %RSD of 4.1%. IDL is 0.12 fg

NeverVent technology
- Available with ExtractaBrite and AEI
- Increases instrument uptime

Off -axis ion guide pre-filter
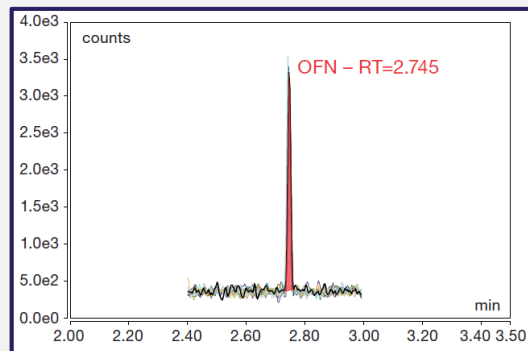- Eliminates the neutral noise

Evo collision cell
- Allows analysis of more compounds
- Shortens runtimes without loss of signal

TRACE™ 1600 GC series
- Unique modular injector and detector design
- Easy-to-use touchscreen with real-time instrument monitoring and video guides

Software productivity tools
- Compliant-ready software
- Instrument health

Advanced automated sampling options
- Robotic autosamplers for sample prep, cleanup, preconcentration, and injection.

XLXR detector as standard
- Extended dynamic range (2X more than previous model)
- Extended lifetime (7X more than previous model)

Volatile phenols in wine by SPME-GC-MS/MS

- ExtractaBrite™ ion source for accurate quantitative analysis

- SPME sampling for minimal sample preparation, maximum ease-of-use, and low impact on environment

Guaiacol

Guaiacol 0.10 µg/L

4-methylguaiacol

4-methylguaiacol 0.10 µg/L
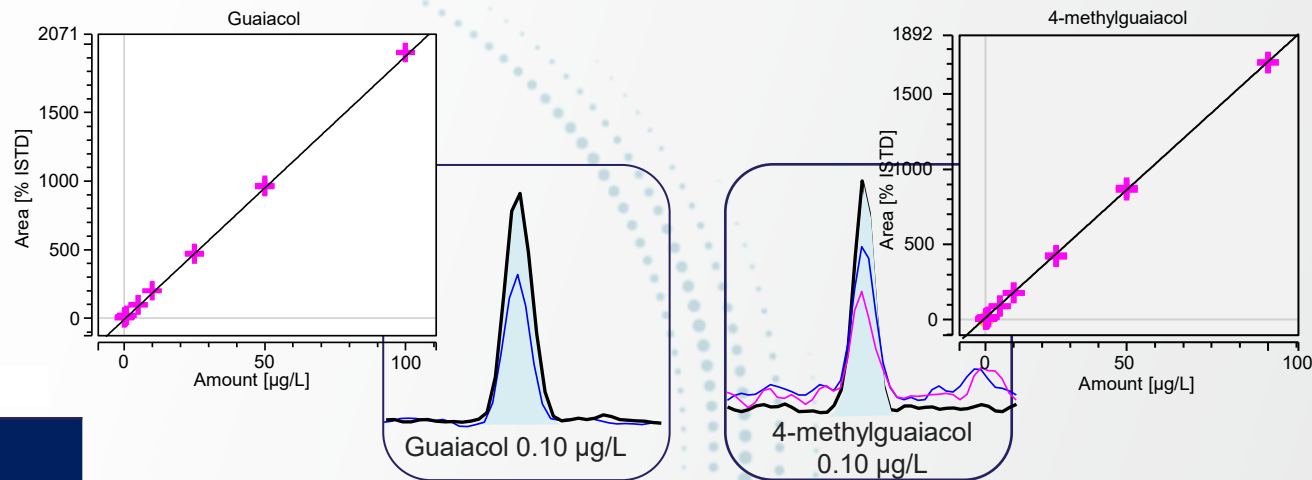
Sample	Form	Average Amount (µg/L)							
		Guaiacol	4-methylguaiacol	o-cresol	4-ethylguaiacol	p-cresol	m-cresol	Eugenol	4-ethylphenol
1 (Merlot)	Free	4.5	1.2	1.6	0.5	1.0	0.9	2.8	0.4
	Total	16.8	6.7	3.0	0.6	4.3	2.6	4.8	1.7
2 (Merlot)	Free	1.7	0.6	0.7	0.5	0.7	0.4	2.6	0.3
	Total	6.1	2.2	1.5	0.6	2.1	1.2	4.9	1.7
3 (Cabernet Sauvignon)	Free	1.9	0.6	1.0	0.5	0.6	0.4	4.3	0.2
	Total	4.8	1.5	1.6	0.6	1.8	1.1	8.8	1.1
4 (Cabernet Franc)	Free	6.0	2.4	1.5	0.7	1.8	0.9	4.8	0.6
	Total	13.7	5.6	2.2	0.8	3.4	1.9	8.5	2.2

Target Analyte	RT (min)	Calibration range (µg/L)	Coefficient of determination (R^2)	AvCF %RSD	Calculated MDL (µg/L)
Guaiacol	9.52	0.1-100	1.000	1.5	0.03
4-methylguaiacol	9.96	0.1-100	1.000	1.8	0.04
o-cresol	10.13	0.1-100	1.000	1.4	0.03
4-ethylguaiacol	10.32	0.1-100	0.999	2.1	0.03
p-cresol	10.51	0.1-100	0.999	3.0	0.16
m-cresol	10.57	0.1-100	0.999	2.5	0.05
Eugenol	10.92	0.1-100	0.998	5.7	0.04
4-ethylphenol	10.92	0.1-100	0.999	4.1	0.07

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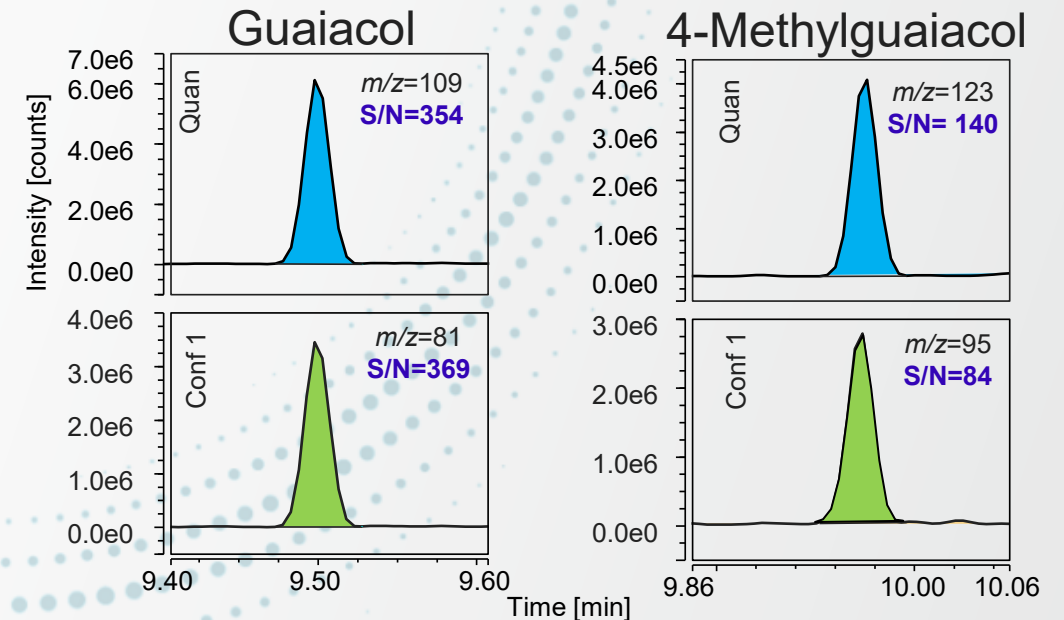
Volatile phenols in wine by SPME-GC-MS/MS

- Selectivity for complex matrices

- Evocell collision cell for *t*-SRM for high speed SRM (up to 800 SRM/s) for more transitions and wider acquisition windows


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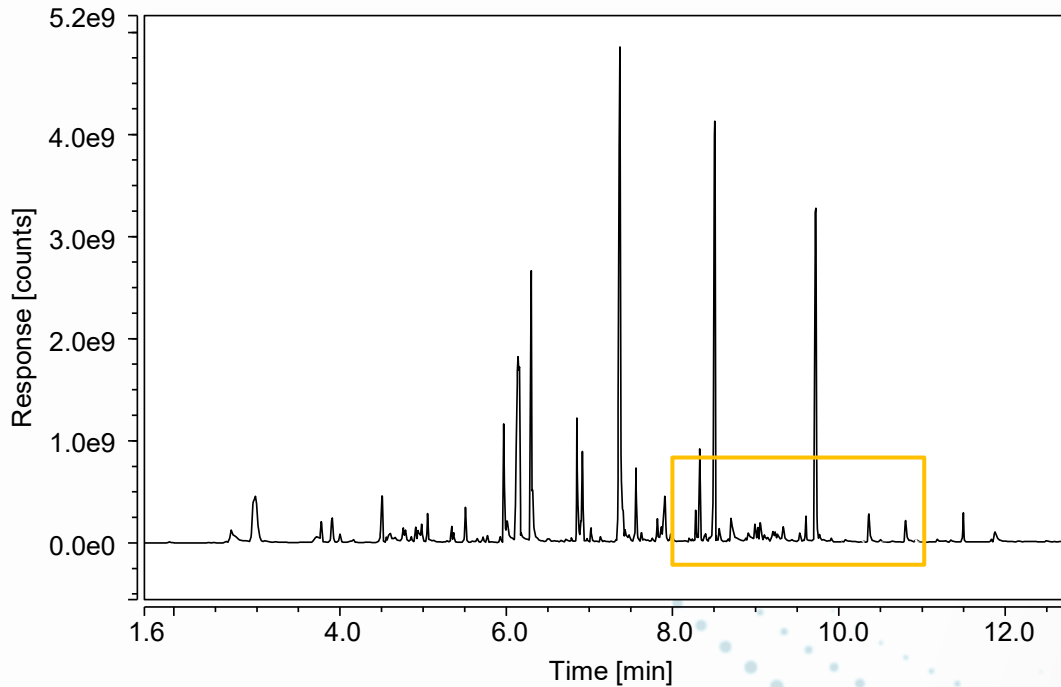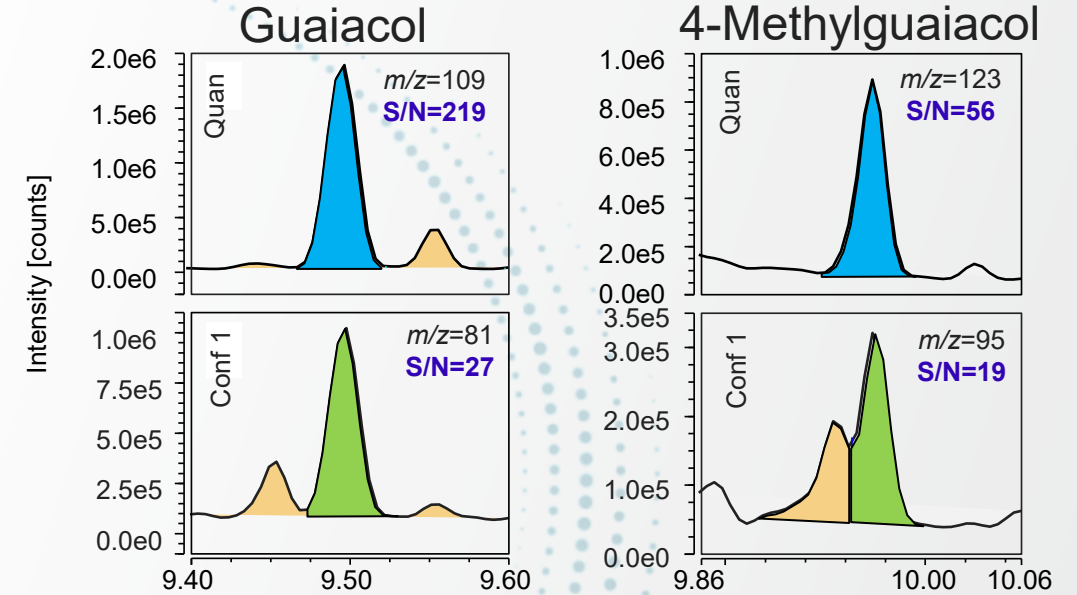
Haloanisoles in wine by SPME Arrow-GC-MS/MS

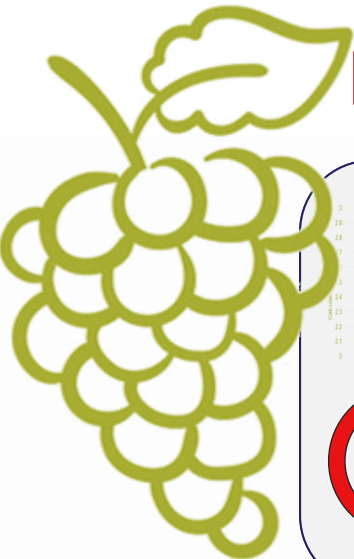**SPME Arrow sampling for fast, high throughput analysis with minimal sample preparation**

AEI ion source for improved detection of trace analytes

TCA 0.1 ng/L

TCA

Target Analyte	RT (min)	Spiked amount (µg/L)	Calculated amount (ng/L)		Recovery (%)	
			Sample 1	Sample 2	Sample 1	Sample 2
TCA	9.24	0.25	0.23	0.23	94	90
		2.5	2.47	2.38	99	95
		5.0	4.90	4.65	98	93
TeCA	10.62	0.25	0.23	0.23	94	91
		2.5	2.47	2.29	99	92
		5.0	4.83	4.66	97	93
TBA	11.56	0.25	0.24	0.25	95	99
		2.5	2.53	2.42	101	97
		5.0	5.00	4.80	100	96
PCA	11.80	0.25	0.26	0.25	105	99
		2.5	2.44	2.35	98	94
		5.0	4.68	4.84	94	97
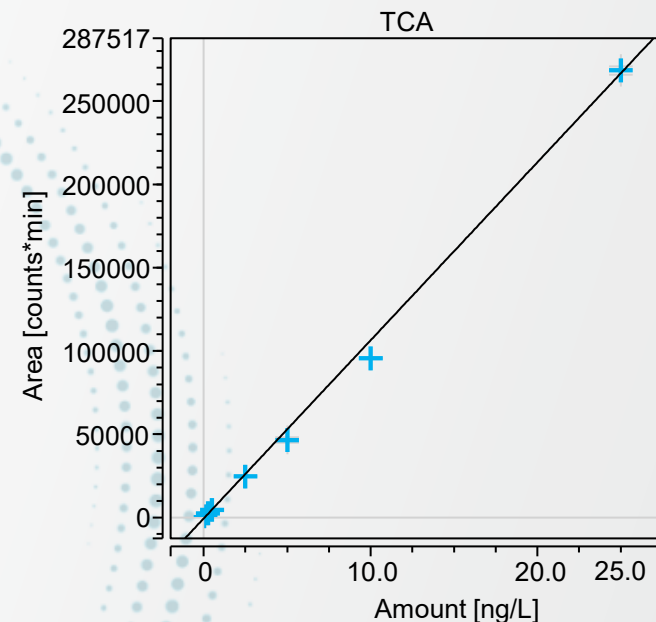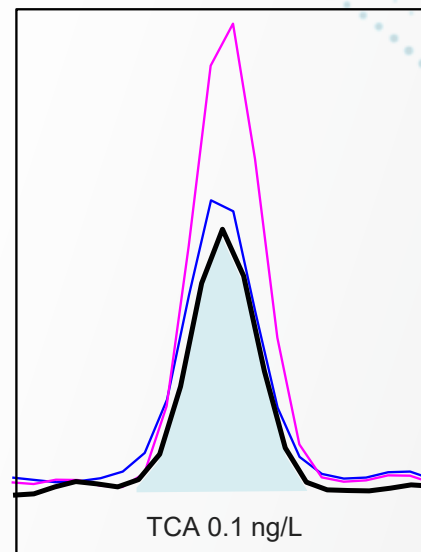
Target analyte	RT (min)	Coefficient of determination (R^2)	AvCF %RSD	Calculated MDL (ng/L)	LOQ (ng/L)
TCA	9.24	0.997	8.2	0.03	0.11
TeCA	10.62	0.998	7.4	0.04	0.14
TBA	11.56	0.998	6.7	0.07	0.23
PCA	11.80	0.998	6.2	0.07	0.24

Haloanisoles in wine by SPME Arrow-GC-MS/MS

AEI ion source for enhanced sensitivity and precise quantitation of trace analytes

NeverVent technology and AEI ion source for improved robustness and stability

Accuracy for wine samples fortified at 2.5 ng/L

QC absolute peak area %RSD
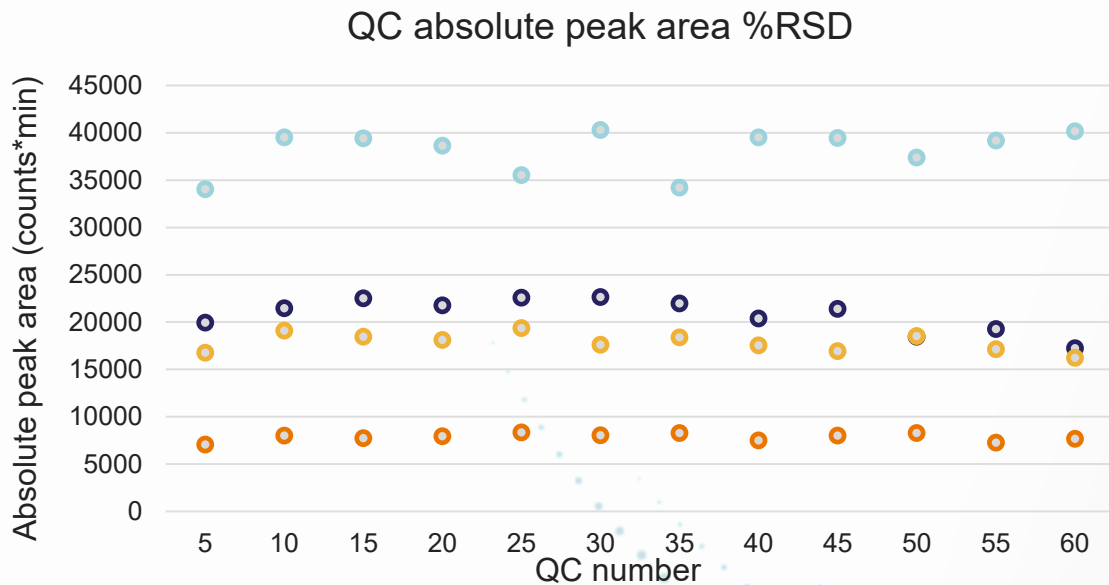
TCA (%RSD=8.5)   TeCA (%RSD=6.0)   TBA (%RSD=5.4)   PCA (%RSD=5.2)
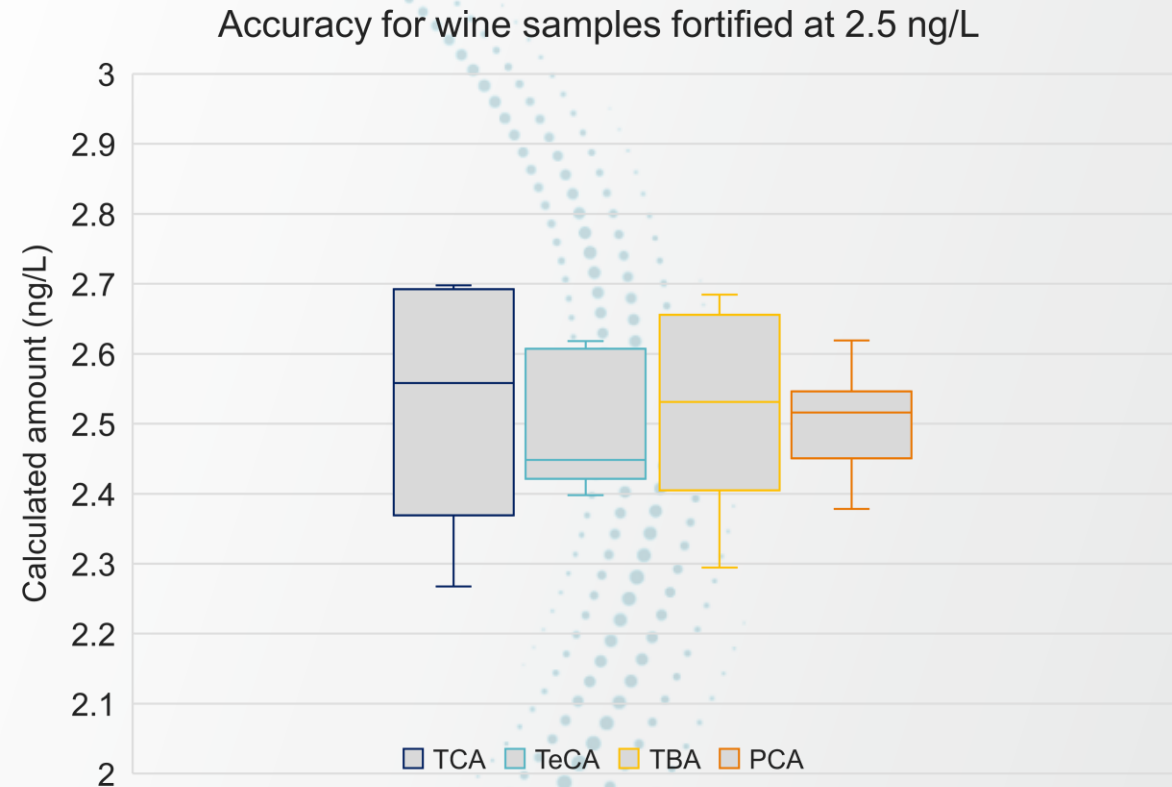
Robust performance running real samples, fortified samples and QCs unattended across 36 hours

Conclusions

- Thermo Scientific™ TSQ™ series GC-MS/MS instruments offer unique features that allow for **increased sensitivity, simplified operation and maintenance, reduced downtime, and a rapid return on investment**.

- Automation of the SPME sampling process offers **increased sensitivity** and **accelerated sample throughput**, well-suited for laboratories with large sample loads and exacting standards

- The data presented here demonstrate applicability of the TSQ series GC-MS/MS towards analysis of **off-flavors** in wine. Including **smoke taint** and associated compounds and **haloanisoles**.

- When analyzing wine samples, extended linearity, long-term stability, and high sensitivity are demonstrated, despite the complexity of sample matrix

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