

# Fast GC–TOF MS for sensitivity and efficiency improvements in the analysis of SVOCs

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## Introduction

The evaluation of semi-volatile organic compounds (SVOCs) in environmental matrices, such as that detailed by US EPA Method 8270, poses many challenges for the analyst, not least the vast number that may be encountered in any given analysis.

In addition, analyte reactivity and the potential for multiple analytes to co-elute can make achieving the required method detection limits quickly and cost-effectively a formidable task – which is especially the case when using quadrupole mass spectrometry (qMS) in 'scan' mode. Selected ion monitoring (SIM) can be used to improve detection limits, but it limits speed of analysis due to SIM window restrictions and prevents retrospective searching of the data for new emerging contaminants.

This study demonstrates improvements to the analysis of SVOCs following US EPA Method 8270, using GC–TOF MS for increased sensitivity, a wide dynamic range and data-rich chromatograms containing high-quality, library-searchable spectra.

# Experimental

- Samples: A 10-point calibration series was prepared from 2–2000 ppb using an 85component standard mix of SVOCs and pesticides.
- Injection: 1 µL pulsed splitless liquid injection.
- Sample throughput: 13 minute injection-toinjection cycle time.
- **MS**: BenchTOF-HD<sup>™</sup> (SepSolve Analytical)
- **Software:** Instrument control and data processing using ChromSpace<sup>®</sup>.



Figure 1: Photograph of the GC-TOF MS used in this study.

# **Results and discussion**

## **DFTPP** tuning criteria

**Table 1:** DFTPP tuning result for GC–TOF MS.

lon ratio	Lower limit	Upper limit	Result	Pass/Fail
51:442	10%	80%	23.60%	Pass
68:69	0%	2%	0.59%	Pass
70:69	0%	2%	1.05%	Pass
127:442	10%	80%	32.00%	Pass
199:198	5%	9%	6.62%	Pass
275:442	10%	60%	22.50%	Pass
365:198	1%	100%	3.08%	Pass
441:442	1%	24%	11.51%	Pass
442:198	50%	200%	172.58%	Pass
443:442	15%	24%	20.03%	Pass

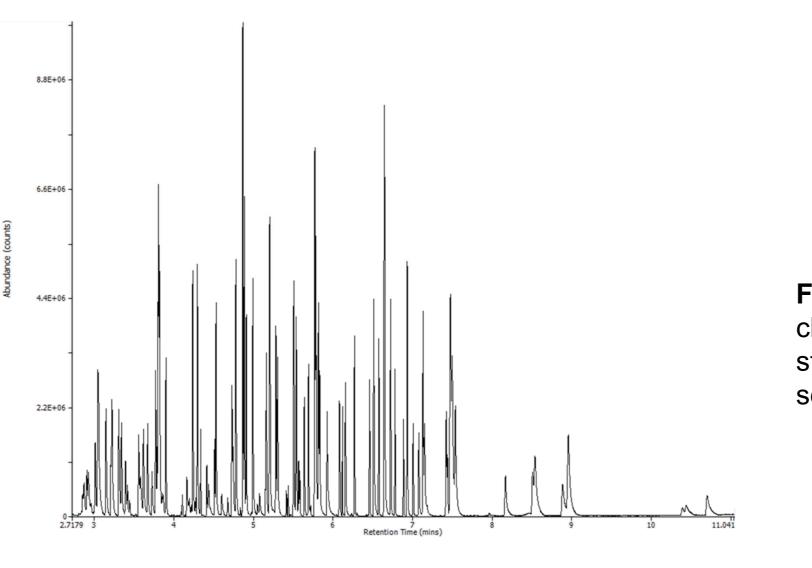
DFTPP tuning was performed at the start of the study to show that all of the instrument tuning and performance criteria for US EPA Method 8270 were met.

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#### Fast GC–TOF MS analysis

Figure 2 shows the separation achieved for fast GC–TOF MS of the 85-component mix, with an injection-to-injection run time of just 13 minutes. The BenchTOF MS used in this study, provides reference-quality spectra, as seen in the examples shown in Figure 3, with excellent matches to the NIST library for confident identification.



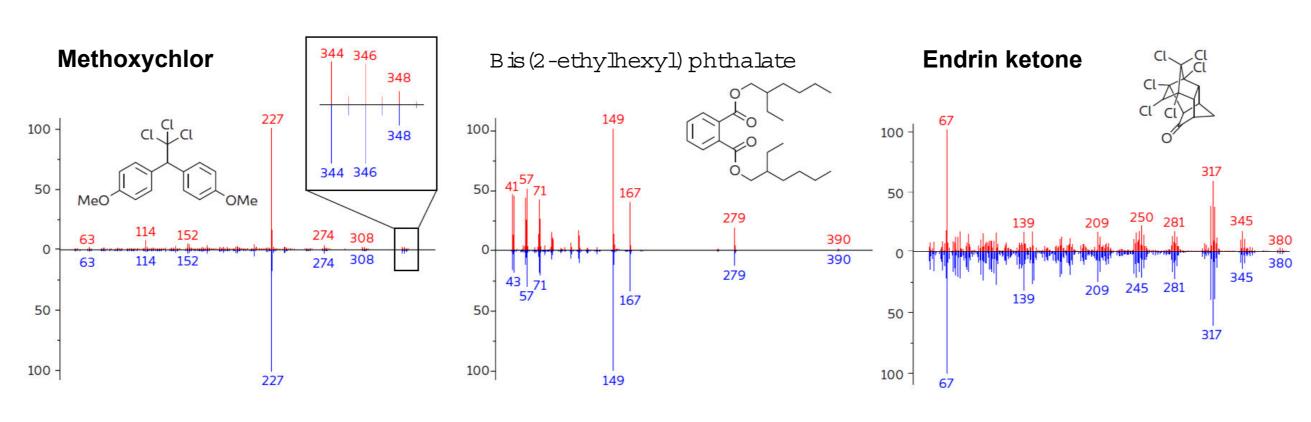


Figure 3: Reference-quality spectra generated by BenchTOF MS for three analytes in the standard.

#### Linearity

Linearities were calculated using a calibration series from 2–2000 ppb (Figure 4). The R<sup>2</sup> values were excellent – all were found to be >0.995. Repeat analysis (n = 5) and quantitation of a mid-point standard gave RSDs <15% for all targets.

Compound	R <sup>2</sup>
Phenol	0.9985
N-Nitroso-n-propylamine	0.9994
Hexachlorobutadiene	0.9997
4-Nitrophenol	0.9959
🛑 β-ВНС	0.9990
Fluorene	0.9996
Heptachlor	0.9978
Di-n-octyl phthalate	0.9996
Dibenz[a,h]anthracene	0.9977

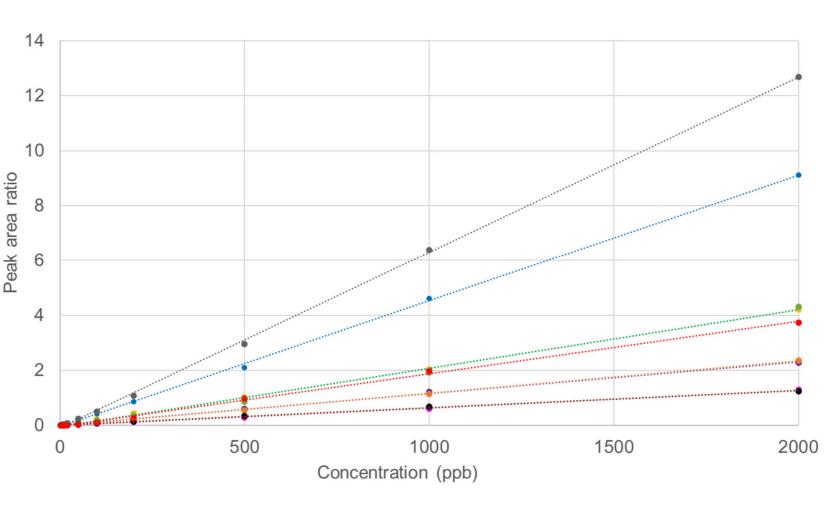
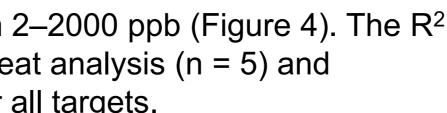


Figure 4: Calibration curves for a selection of compounds in the standard (2-2000 ppb).

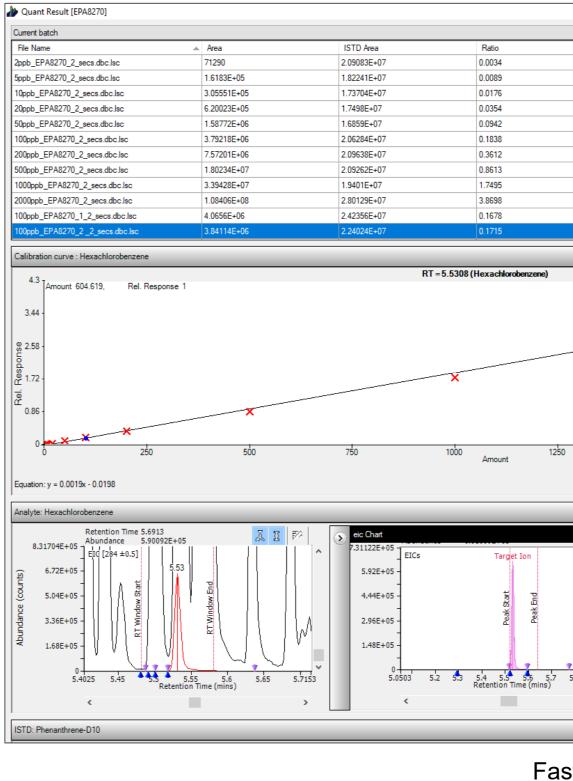
Figure 2: GC–TOF MS (TIC) chromatogram for the 100 ppb standard mix, with all 85 components separated in under 11 minutes.



#### Improved productivity

Not only does the fast injection-to-injection time of 13 minutes increase productivity in this study, software workflows can also provide substantial time savings. ChromSpace software enabled real-time data processing to be employed during analysis. This allowed backgroundsubtraction, integration, identification and quantitation to be performed automatically as part of the acquisition sequence, all while the samples were still being acquired. This means that the results are ready to review and report as soon as the analysis is complete, for improved productivity.

Flagging system shows any issues in identification or suitability parameters



**Figure 5:** Screenshot of quantitative results browser in ChromSpace software, showing calibration results for hexachlorobenzene.

Quantitative results can be reviewed effortlessly in the results browser in ChromSpace – with simple, easy-to-use tools for further time savings (Figure 5).

## Conclusions

- In this poster, we have demonstrated how GC–TOF MS can provide:
- Confident identification using reference-quality spectra from BenchTOF mass spectrometers.
- Excellent reproducibility and linearity across wide-ranging target compounds.
- Streamlined workflows are possible using ChromSpace software, with full instrument control and real-time data processing.

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Export results as a report, to .csv or to LIMS

						-	٥
	✓ Recalculate		S Compounds				
Specified Amount	Calculated Amount	Peak Status \land	Name	Expected RT	Source	Quant lon	Р
2	2			-		-	÷
5	4.9944	✓	4-Chlorophenyl phenyl ether		DBC TIC [204 ±0.5]	EIC	_
10	9.9755	✓	4,6-Dinitro-2-methylphenol		DBC TIC [198 ±0.5]	EIC	+
20	20.0025	✓	4-Nitroaniline		DBC TIC [65 ±0.5]	EIC	+
50	50.2249	✓	Diphenylamine		DBC TIC [169 ±0.5]	EIC	_
100	99.5486	✓	Azobenzene	5.297	DBC TIC [77 ±0.5]	EIC	_
200	199.1081	✓	4-Bromophenyl phenyl ether	5.497	DBC TIC [248 ±0.5]	EIC	
500	496.6851	✓	gamma-BHC (Lindane)	5.5037	DBC TIC [181 ±0.5]	EIC	
1000	1002.3382	✓	Hexachlorobenzene	5.5307	DBC TIC [284 ±0.5]	EIC	
2000	2042.2567	✓	alpha-BHC	5.6337	DBC TIC [181 ±0.5]	EIC	
n/a	98.4812	<ul> <li>✓</li> </ul>	Pentachlorophenol	5.6604	DBC TIC [266 ±0.5]	EIC	
n/a	100.4281	✓ ✓	beta-BHC	5.682	DBC TIC [181 ±0.5]	EIC	
			Phenanthrene-D10	5.7654	DBC TIC [188 ±0.5]	EIC	
		$\odot$	Phenanthrene	5.7787	DBC TIC [178 ±0.5]	EIC	
			Anthracene	5.8087	DBC TIC [178 ±0.5]	EIC	
		V	delta-BHC	5.8254	DBC TIC [183 ±0.5]	EIC	T
		A	Carbazole	5.9154	DBC TIC [167 ±0.5]	EIC	T
			Heptachlor	6.0771	DBC TIC [100 ±0.5]	EIC	T
			Di-n-butyl phthalate	6.1488	DBC TIC [149 ±0.5]	EIC	t
			Aldrin	6.262	DBC TIC [66 ±0.5]	EIC	t
			Heptachlor epoxide	6.4554	DBC TIC [81 ±0.5]	EIC	t
			Fluoranthene	6.5054	DBC TIC [202 ±0.5]	EIC	t
			gamma-Chlordane	6.5688	DBC TIC [373 ±0.5]	EIC	t
			alpha-Chlordane		DBC TIC [373 ±0.5]	EIC	t
			Endosulfan I		DBC TIC [195 ±0.5]	EIC	+
			Pyrene		DBC TIC [202 ±0.5]	EIC	+
1500	1750	2000 2200	4,4'-DDE		DBC TIC [246 ±0.5]	EIC	+
			Dieldrin		DBC TIC [79 ±0.5]	EIC	+
		R <sup>2</sup> : 0.9977	Endrin		DBC TIC [81 ±0.5]	EIC	+
			4.4'-DDD		DBC TIC [235 ±0.5]	EIC	+
		$\sim$	Endosulfan II		DBC TIC [195 ±0.5]	EIC	+
Spectra			Endrin aldehyde		DBC TIC [67 ±0.5]	EIC	+
<b>O</b>			Butyl benzyl phthalate		DBC TIC [149 ±0.5]	EIC	+
7.72951E	+05 -		4,4'-DDT		DBC TIC [145 ±0.5]	EIC	+
	Spectrum	284	4,4-DDT Endosulfan sulfate		DBC TIC [235 ±0.5] DBC TIC [272 ±0.5]	EIC	+
와 6.24E	+05 -	286				EIC	-
0 4.68E	+05 -		Endrin ketone		DBC TIC [317 ±0.5]		+
2C	-	282	Methoxychlor		DBC TIC [227 ±0.5]	EIC	+
· 문 3.12E	142	288	Benzo[a]anthracene		DBC TIC [228 ±0.5]	EIC	+
0 4.68E 20 20 20 20 20 20 20 20 20 20 20 20 20	+05 - 107 144	282 288 249 214 214 214 290	Chrysene-D12		DBC TIC [240 ±0.5]	EIC	_
v 1	/1 108 141 1/9	290	Chrysene		DBC TIC [228 ±0.5]	EIC	_
5.0104	33.7477 <b>1</b> 00 150	200 250 303.7024	Bis(2-ethylhexyl) phthalate		DBC TIC [149 ±0.5]	EIC	_
	33.7477 100 150 2 Mass (m/z)		Di-n-octyl phthalate	8.1688	DBC TIC [149 ±0.5]	EIC	
>		>	Benzo[b]fluoranthene	8.5037	DBC TIC [252 ±0.5]	EIC	
			Benzo[k]fluoranthene	8.5333	DBC TIC [252 ±0.5]	EIC	
		$\odot$	Renzola hyrene	8 8804	DRC TIC [252 +0 5]	FIC	

Fast review of identification and integration

Low detection limits for targets, while also allowing retrospective searching for non-targets.

