thermoscientific

An integrated GC-MS workflow solution for the determination of (semi)volatiles in drinking water and solid waste according to the U.S. EPA guidelines

INTRODUCTION

Worldwide there are many regulatory organizations safeguarding the environment by the issuance of health and environmental standards, such as the United States (U.S.) Environmental Protection Agency (EPA) and the European Committee for Standardization (CEN). These standards include many standardized guidelines for the analysis of hazardous environmental contaminants.

The challenge for today's laboratories is to correctly execute these guidelines, such as those described in the EPA methods, including calculating and assessing the final results. In many labs the chromatographic results generated while executing these methods are transferred to spreadsheets in order to perform the calculations and assess the final results. This process can be time-consuming and transcription errors are a common problem. As a result laboratories may generate results that are hard to compare, are inconsistent, and can even be misleading. In order to establish a system for compliance with the regulatory methodology, environmental laboratories develop internal guidelines, such as standard operating procedures (SOPs), for sequence creation, sample analysis, and result calculation.

Mass spectrometry (MS) is becoming a more common chromatography detection technique in environmental laboratories and is also used in a wide variation of environmental methods. However, MS instruments often use specific software, without the flexibility of a chromatography data system (CDS) which forces users to learn another software package.

This poster will show an integrated GC-MS workflow solution for the determination of volatiles and semi-volatiles in drinking water and solid waste following the U.S. EPA guidelines using one CDS, including all required calculations and assessment of the final result. This solution helps ensure that analysts follow SOPs consistently and accurately, resulting in high quality and reliable results, saving valuable time and ensuring data integrity.

MATERIALS AND METHODS

All experiments were performed with the Thermo Scientific[™] TRACE 1300 Gas Chromatograph in combination with the Thermo Scientific[™] ISQ[™] Series Single Quadrupole GC-MS system. The minimum software version for instrument control, MS data processing, and calculation and reporting of the results with the environmental GC-MS extension pack (Table 1) was Thermo Scientific[™] Chromeleon[™] CDS version 7.2 Service Release 5.

U.S. EPA Method	Scope
524.2, 524.3, 524.4	Volatile organics in Drinking Water
525.1, 525.2, 525.3	Semi-volatile organics in Drinking Water
8260B, 8260C	Volatile organics in Solid Waste
8270C, 8270D	Semi-volatile organics in Solid Waste

Table 1. Overview of methods supported by the environmental GC-MS extension pack

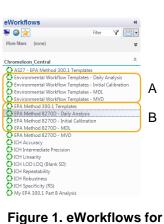
The examples shown are based on U.S. EPA method 8270D¹, for the determination of the concentration of semi-volatile organic compounds in extracts prepared from many types of solid waste matrices, soils, air sampling media and water samples.

Workflow Automation

Even though all steps to execute the U.S. EPA methods are outlined down to the smallest detail, in a typical lab they still have to be executed manually by the analysts, thereby introducing the risk of human-generated errors. Chromeleon CDS solves these problems using built-in eWorkflows[™], a set of rules capturing all the unique aspects of a chromatography workflow, guiding the users through a minimum number of choices needed to create a complete, correct sequence with predefined files and a well-defined structure.

The environmental GC-MS extension pack within Chromeleon CDS provides predefined eWorkflows to execute analysis as defined in U.S. EPA method (Figure 1A). With the available method and report templates, these eWorkflows can be configured to suit any of the U.S. EPA method mentioned in Table 1 and to your laboratories requirements (Figure 1B).

Figure 2 shows the preconfigured sequence layout of the daily analysis (A), including additional custom columns for identification of the analysis type and spike groups, and how this looks for 8 samples (B).



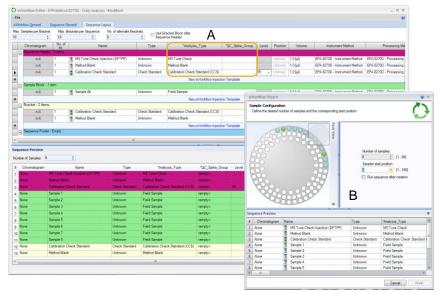


Figure 2. Sequence layout configuration for the daily analysis

RESULTS

environmental GC-MS

analysis

DFTPP Tune Verification

MS instruments are tuned to assure accuracy of masses and maximized intensity. U.S. EPA method 8270 prescribes verification of the MS tune using DFTPP according to the criteria as described in Figure 3. Figure 4 shows a typical mass spectrum of DFTPP.

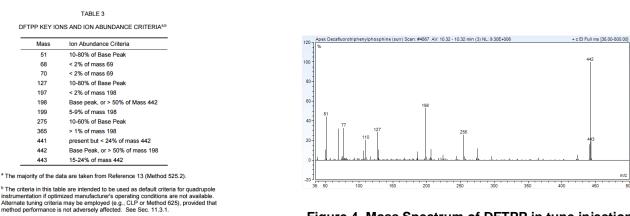


Figure 3. Ion abundance criteria as described in U.S. EPA method 8270

To automate the assessment of these criteria, they can be translated to system suitability tests (SST) in the Chromeleon software (Figure 5). This provides a consistent evaluation of the data and automatic reporting of the results (Figure 6), and allows to setup in-run actions if the test criteria are not met

Group Area Drag a column header here to group by that column.										
#	Name	Eval. Formula	Operator	Ref.Value	Ref.Value	Inj.Condition	Pass	Fail	Peak	
1	m/z 51 - 10 to 80% of the base peak	(peak.mspec.intensity("By Mass",51)/peak.mspec.intensity("By Intensity",1))*100	between	10	80	(injection.customVar("Analysis_Type") ="MS Tune Check")	No Actions	Re-inject, Pause	Decafluorotriphenylphosphine (surr)	
2	m/z 68 - Less than 2% of m/z 69	if(peak.mspec.intensity("By Mass",68)=peak.mspec.intensity("By Mass",69),0, (peak.mspec.intensity("By Mass",68)/peak.mspec.intensity("By Mass",69))*100)	<	2		(injection.customVar("Analysis_Type") ="MS Tune Check")	No Actions	Re-inject, Pause	Decafluorotriphenylphosphine (surr)	
3	m/z 70 - Less than 2% of m/z 69	if(peak.mspec.intensity("By Mass",70)=peak.mspec.intensity("By Mass",69),0, (peak.mspec.intensity("By Mass",70)/peak.mspec.intensity("By Mass",69))*100)	<	2		(injection.customVar("Analysis_Type") ="MS Tune Check")	No Actions	Re-inject, Pause	Decafluorotriphenylphosphine (surr)	
4	m/z 127 - 10 to 80% of the base peak	(peak.mspec.intensity("By Mass", 127)/peak.mspec.intensity("By Intensity", 1))*100	between	10		(injection.customVar("Analysis_Type") ="MS Tune Check")	No Actions	Re-inject, Pause	Decafluorotriphenylphosphine (surr)	
5	m/z 197 - Less than 2% of m/z 198	if(peak.mspec.intensity("By Mass", 197)=peak.mspec.intensity("By Mass", 198).0, (peak.mspec.intensity("By Mass", 197)/peak.mspec.intensity("By Mass", 198))*100)	<	2		(injection.customVar("Analysis_Type") ="MS Tune Check")	No Actions	Re-inject, Pause	Decafluorotriphenylphosphine (surr)	
6	m/z 198 - Greater than 50% of m/z 442	(peak.mspec.intensity("By Mass", 198)/peak.mspec.intensity("By Mass", 442))*100	>	50		(injection.customVar("Analysis_Type") ="MS Tune Check")	No Actions	Re-inject, Pause	Decafluorotriphenylphosphine (surr)	
7	m/z 199 - 5 to 9% of m/z 198	(peak.mspec.intensity("By Mass", 199)/peak.mspec.intensity("By Mass", 198))*100	between	5		(injection.customVar("Analysis_Type") ="MS Tune Check")	No Actions	Re-inject, Pause	Decafluorotriphenylphosphine (surr)	
8	m/z 275 - 10 to 60% of the base peak	(peak.mspec.intensity("By Mass",275)/peak.mspec.intensity("By Intensity",1))*100	between	10	60	(injection.customVar("Analysis_Type") ="MS Tune Check")	No Actions	Re-inject, Pause	Decafluorotriphenylphosphine (surr)	
9	m/z 365 - Greater than 1% of m/z 198	(peak.mspec.intensity("By Mass",365)/peak.mspec.intensity("By Mass",198))*100	>	1		(injection.customVar("Analysis_Type") ="MS Tune Check")	No Actions	Re-inject, Pause	Decafluorotriphenylphosphine (surr)	
10	m/z 441 - Present	peak.mspec.intensity("By Mass",441)	>	0		(injection.customVar("Analysis_Type") ="MS Tune Check")	No Actions	Re-inject, Pause	Decafluorotriphenylphosphine (surr)	
1	m/z 441 - Less than 24% of m/z 442	(peak.mspec.intensity("By Mass",441)/peak.mspec.intensity("By Mass",442))*100	<	24		(injection.customVar("Analysis_Type") ="MS Tune Check")	No Actions	Re-inject, Pause	Decafluorotriphenylphosphine (surr)	
12	m/z 442 - Greater than 50% of m/z 198	(peak.mspec.intensity("By Mass",442)/peak.mspec.intensity("By Mass",198))*100	>	50		(injection.customVar("Analysis_Type") ="MS Tune Check")	No Actions	Re-inject, Pause	Decafluorotriphenylphosphine (surr)	
13	m/z 443 - 15 to 24% of m/z 442	(peak.mspec.intensity("By Mass",443)/peak.mspec.intensity("By Mass",442))*100	between	15	24	(injection.customVar("Analysis_Type") ="MS Tune Check")	No Actions	Re-inject, Pause	Decafluorotriphenylphosphine (surr)	

Figure 5. Ion abundance criteria translated to SST

No.	Name	Eval. Result	Operator	Ref. Value 1	Ref. Value 2	Result
1	m/z 51 - 10 to 80% of the base peak	48.5	between	10	80	Passed
2	m/z 68 - Less than 2% of m/z 69	0.5	<	2		Passed
3	m/z 70 - Less than 2% of m/z 69	0.4	<	2		Passed
4	m/z 127 - 10 to 80% of the base peak	31.1	between	10	80	Passed
5	m/z 197 - Less than 2% of m/z 198	0.1	<	2		Passed
6	m/z 198 - Greater than 50% of m/z 442	55.0	>	50		Passed
7	m/z 199 - 5 to 9% of m/z 198	5.7	between	5	9	Passed
8	m/z 275 - 10 to 60% of the base peak	11.9	between	10	60	Passed
9	m/z 365 - Greater than 1% of m/z 198	4.3	>	1		Passed
10	m/z 441 - Present	1433459.1	>	0		Passed
11	m/z 441 - Less than 24% of m/z 442	16.2	<	24		Passed
12	m/z 442 - Greater than 50% of m/z 198	181.9	>	50		Passed
13	m/z 443 - 15 to 24% of m/z 442	18.1	between	15	24	Passed
					Overall Result:	Pareod

Figure 6. Reported results of check against ion abundance criteria

B. van Cann¹, W. Liu², T. Albertini³, ¹ Thermo Fisher Scientific, Breda, Netherlands ; ² Thermo Fisher Scientific, Sunnyvale, United States; ³ Thermo Fisher Scientific, Milan, Italy

Figure 4. Mass Spectrum of DFTPP in tune injection

Initial Calibration

To calculate the component amount in a field sample, for each component a calibration is required at a minimum of five levels and is based on the average relative response factor (RRF) or an <u>alternative curve fit</u> if the <u>acceptance criteria for the average RRF</u> are not met. In addition the <u>average RRF must not be below the minimum response factor</u> as specified in the method. This represents a lot of requirements just for the calibration, with an additional need to enter method specific criteria.

The processing method is set up with additional columns to enter the required criteria (Figure 7), such as the minimum response factor or the maximum relative percent difference (RPD). A selection of sheets in the report template provides all calculations and in addition checks the results against the criteria as entered in the processing method.

				1 1			-						
4S Detection	on MS Component Table	Cal and Chec	ck Stds QC Checks	Surrogates Calif	oration MS Settings	MS Library Screeni	ng SST/IF	IC					
Compone	omponent Table												
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#	Name	Ret.	*Min_R^2	*Max_RRF_RSD (Calibration)	*Max_RPD_LowStd (Calibration)			*Max_RPD_Low CheckStd	*Max_RPD_ CheckStds	*Max_RRF_%D	Stand.Meth.	Cal.Type	Level "01 🚔
12 2.6-Dir	nitrotoluene	8.710	0.990	20.0 [%]	50 [%]	30 [%]	0.200	50 [%]	30 [%]	25.0 [%]	Internal Acenaphathene-d10 (ISTD)	AvgCalFact	0.500000
3 Acenap	phthylene	8.720	0.990	20.0 [%]	50 [%]	30 [%]	0.900	50 [%]	30 [%]	25.0 [%]	Internal Acenaphathene-d10 (ISTD)	AvgCalFact	0.500000
4 1.2-Dir	nitrobenzene	8.780	0.990	20.0 [%]	50 [%]	30 [%]	0.010	50 [%]	30 [%]	25.0 [%]	Internal Acenaphathene-d10 (ISTD)	AvgCalFact	0.500000
5 Acenar	phathene-d10 (ISTD)	8.840	0.990	20.0 [%]	50 [%]	30 [%]	0.010	50 [%]	30 [%]	25.0 [%]	ISTD Internal	AvgCalFact	5.000000
6 3-Nitro	aniline	8.840	0.990	20.0 [%]	50 (%)	30 [%]	0.010	50 [%]	30 [%]	25.0 [%]	Internal Acenaphathene-d10 (ISTD)	AvgCalFact	0.500000
7 Acenar	phthene	8.870	0.990	20.0 [%]	50 [%]	30 [%]	0.900	50 [%]	30 [%]	25.0 [%]	Internal Acenaphathene-d10 (ISTD)	AvgCalFact	0.500000
8 2,4-Dir	nitroph e nol	8.920	0.990	20.0 [%]	50 [%]	30 [%]	0.010	50 [%]	30 [%]	25.0 [%]	Internal Acenaphathene-d10 (ISTD)	Lin, WithOffset	0.500000
9 4-Nitro	phenol	8.970	0.990	20.0 [%]	50 [%]	30 [%]	0.010	50 [%]	30 [%]	25.0 [%]	Internal Acenaphathene-d10 (ISTD)	Lin, WithOffset	0.500000
0 Dibenz	zofuran	9.000	0.990	20.0 [%]	50 [%]	30 [%]	0.800	50 [%]	30 [%]	25.0 [%]	Internal Acenaphathene-d10 (ISTD)	AvgCalFact	0.500000
1 2,4-Dir	nitrotoluene	9.040	0.990	20.0 [%]	50 [%]	30 [%]	0.200	50 [%]	30 [%]	25.0 [%]	Internal Acenaphathene-d10 (ISTD)	AvgCalFact	0.500000
2 2,3,5,6	-Tetrachlorophenol	9.100	0.990	20.0 [%]	50 [%]	30 [%]	0.010	50 [%]	30 [%]	25.0 [%]	Internal Acenaphathene-d10 (ISTD)	Lin, WithOffset	0.500000
3 2.3.4.6	-Tetrachlorophenol	9.140	0.990	20.0 [%]	50 [%]	30 [%]	0.010	50 [%]	30 [%]	25.0 [%]	Internal Acenaphathene-d10 (ISTD)	Lin, WithOffset	0.500000
Diethyl	I Phthalate	9.220	0.990	20.0 [%]	50 [%]	30 [%]	0.010	50 [%]	30 [%]	25.0 [%]	Internal Acenaphathene-d10 (ISTD)	AvgCalFact	0.500000

Figure 7. Processing Method setup to enter calibration and check standard parameters and acceptance criteria

Figure 8 shows two examples of calibration reports, one for the calibration results and check these results for minimum relative response factor or coefficient of determination (A), the other one checking the relative response factors in all calibration injections against the minimum required response factors.

			ation Repor	t			ŀ	4							
Details															
e Name: It:	20170626-115505 Init Location 1\Lab B1 R1 Chromeleon Central	tial Calibration 43 - QC\Data\EPA Meth	nod 8270D\2017\0	06_June	Created On: Created By: Updated On:	2017/Jun/22 barbara.van.cann 2017/Jul/06	13:09:56								
ections:	13				Updated By:	barbara.van.cann	14:30:31								
n Source:	20170626-115505 Init														
ne	Cal.Type	C0 Average RRF	C1	C2	R^2 RSD (%)	R^2 / %RSD Failed?	Manual Integrate								
titation Jimethylamine	MS Quantitation AvgCalFact	MS Quantitation N 0.604	IS Quantitation	MS Quantitation	MS Quantitation 6.90970	MS Quantitation									
	AvgCalFact	2.185			41.22781	Yes									
henol (surr)	AvpCalFact	2.038			6.16530										
B (sum)	AvgCalFact	2.690			5.67467	1		1							
roethyl) ether	AvgCalFact AvgCalFact	3.071 2.381			6.96609 5.88351	1		1							
henol	AvgCalFact	2.072			7.70399	1									
probenzene	AvgCalFact	2.065			7.18467	1		1							
probenzene	AvgCalFact	2.083			7.85816	I	1								
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roisopropyl) ether	AvgCalFact								Mill RAP Che						
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ene-do (sum) ene	AvgCalFact	No. of Injection	18:	Chromeleo 13	-central									Updated On: Updated By:	06/Jul/17 14:38 barbara.van.ca
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roethoxy) methane prophenol	AvgCalFact AvgCalFact					2.8td2 5	Std2	10 Std2	20 Std2	35 Std2	50 Std2	100 Std2	200 Std2		Failed?
hlorobenzene	AvgCalFact	MS Quantitatio	on	MS Quanti	tation MS	Quantitation MS Q				MS Quantitation	MS Quantitation	MS Quantitation	MS Quantitatio	MS Quantitation	
ene	AvgCalFact	N-Nitrosodimet		AvgCalFac	t	0.596 0	.593	0.574	0.654	0.588	0.608	0.547	0.676	0.010	
niline	AvgCalFact	Pyridine		AvgCalFac			.078	2.141	2.690	2.503	2.825	2.617	3.160	0.010	1
robutadiene 3-methylohenol	AvgCalFact AvgCalFact	2-Fluoropheno Phenol-d8 (sur		AvgCalFac AvgCalFac			.939	1.949 2.646	2.197	1.965	2.157	1.893	2.199	0.010	
3-methylphenol haphthalene	AvgCalFact	Phenol	m)	AvgCalFac			877	3.061	3.391	2.977	3.261	2.781	3.263	0.800	
aphtalene	AvgCalFact	Bis(2-chloroeth	hyl) ether	AvgCalFac			337	2.381	2.576	2.234	2.449	2.145	2.497	0.700	
rocyclopentadiene	Lin, WithOffset	2-Chloropheno		AvgCalFac			.907	2.051	2.293	1.984	2.194	1.882	2.263	0.800	
hlorophenol	AvgCalFact	1,3 Dichlorobe		AvgCalFac			055	2.038	2.274	1.940	2.123	1.789	2.148	0.010	1
hlorophenol	AvgCalFact	1,4-Dichlorobe Benzyl Alcoho		AvgCalFac AvgCalFac			.082	2.079	2.317	1.875	2.169	1.826	2.107	0.010	1
iphenyl (surr) Iaphthalene	AvgCalFact AvgCalFact	1,2-Dichlorobe		AvgCalFac			005	1.902	2.157	1.888	2.048	1.743	1.980	0.010	1
iline	AvgCalFact	2-Methylphend	ol	AvgCalFac	t	1.801 1	.773	1.814	2.028	1.709	1.891	1.637	1.875	0.700	1
obenzene	Lin, WithOffset	Bis(2-chloroiso		AvgCalFac			950	6.050	6.521	5.757	6.314	5.422	6.506	0.300	1
phthalate	AvgCalFact	3Methylphen N-Nitrosodi-n-p		AvgCalFac AvgCalFac			.131 .664	1.133	1.270	1.044	1.152	1.042	1.243	0.010	1
obenzene	Lin, WithOffset	N-Nitrosodi-n-p Hexachloroeth		AvgCalFac			.703	0.767	0.855	0.732	0.845	0.719	2.004	0.500	1
		Nitrobenzene-		AvgCalFac	t	0.471 0	442	0.468	0.516	0.500	0.563	0.514	0.600	0.010	1
		Nitrobenzene		AvgCalFac			467	0.492	0.661	0.531	0.690	0.540	0.678	0.200	1
		Isophorone		AvpCalFac			.994	1.063	1.128	1.031	1.119	1.020	1.225	0.400	1
		2-Nitrophenol 2.4-Dimethylol	henol	AvgCalFac AvgCalFac			.154	0.173	0.200	0.181	0.209	0.199	0.242	0.100	1
		Bis(2-chloroeth		AvgCalFac			.590	0.627	0.683	0.598	0.649	0.586	0.683	0.010	1
		2,4-Dichloroph	lone	AvgCalFac	t	0.242 0	268	0.291	0.319	0.286	0.320	0.288	0.335	0.200	1
		1,2,4-Trichloro	obenzene	AvgCalFac	t		.314	0.334	0.358	0.305	0.341	0.295	0.330	0.010	
		Naphthalene p-Chloroanilin		AvgCalFac AvgCalFac			.350	1.389	1.459 0.618	1.317	1.409	1.261 0.548	1.368	0.700	
		P-Chloroanilin Hexachlorobut		AvgCalFac			.542	0.569	0.018	0.562	0.000	0.548	0.632	0.010	1
			thylphenol	AvgCalFac			.388	0.455	0.478	0.423	0.476	0.441	0.517	0.200	1
							.809	0.828	0.883	0.788	0.844	0.723	0.798	0.400	
		2-Methylnapht		AvgCalFac				1.129	1.148	0.922	0.994	0.906	1.047	0.010	1
		2-Methylnapht 1-Methylnapht	talene	AvgCalFac	t		.022								
		2-Methylnapht 1-Methylnapht Hexachlorooyd	talene dopentadiene	AvgCalFac Lin, WithO	t ffset	0.041 0	095	0.127	0.209	0.202	0.242	0.322	0.344	0.050	Yes
		2-Methylnapht 1-Methylnapht Hexachlorodyc 2,4,6-Trichloro	talene dopentadiene ophenol	AvgCalFac Lin, WithO AvgCalFac	t ffset t	0.041 0	.095	0.127	0.399	0.332	0.377	0.353	0.344	0.050 0.200	
		2-Methylnapht 1-Methylnapht Hexachlorocyc 2,4,6-Trichloro 2,4,5-Trichloro	talene dopentadiene ophenol ophenol	AvgCalFac Lin, WithO AvgCalFac AvgCalFac	t ffset t	0.041 0 0.295 0 0.186 0	095	0.127					0.344	0.050	Yes Yes
		2-Methylnapht 1-Methylnapht Hexachlorodyc 2,4,6-Trichloro	talene dopentadiene ophenol ophenol nyl (surr)	AvgCalFac Lin, WithO AvgCalFac	t ffset t	0.041 0 0.295 0 0.186 0 1.669 1	.095 .320 .240	0.127 0.348 0.259	0.399	0.332 0.292	0.377 0.341	0.353 0.312	0.344 0.425 0.398	0.050 0.200 0.200	
		2-Methylnapht 1-Methylnapht Hexachlorocyc 2,4,6-Trichloro 2,4,6-Trichloro 2,Fluorobiphei 2-Fluorobiphei 2-Nitroaniline	talene dopentadiene ophenol nyl (surr) thalene	AvgCalFac Lin, WithO AvgCalFac AvgCalFac AvgCalFac AvgCalFac AvgCalFac		0.041 0 0.295 0 0.186 0 1.669 1 1.493 1 0.493 0	.095 .320 .240 .710 .530 .509	0.127 0.348 0.259 1.644 1.552 0.524	0.399 0.331 1.850 1.701 0.629	0.332 0.292 1.523 1.372 0.550	0.377 0.341 1.709 1.558 0.670	0.353 0.312 1.444 1.348 0.609	0.344 0.425 0.398 1.635 1.581 0.767	0.050 0.200 0.200 0.010 0.800 0.010	
		2-Methylnapht 1-Methylnapht Hexachlorocyc 2.4,6-Trichloro 2-Fluorobipher 2-Chloronapht 2-Nitroaniline 1.4-Dinitroben	talene slopentadiene sphenol nyl (surr) ihalene zene	AvgCalFac Lin, WithO AvgCalFac AvgCalFac AvgCalFac AvgCalFac AvgCalFac Lin, WithO	t ffset t t t t	0.041 0 0.295 0 0.186 0 1.669 1 1.493 1 0.493 0 0.144 0	.095 .320 .240 .710 .530 .509 .156	0.127 0.348 0.259 1.644 1.552 0.524 0.162	0.399 0.331 1.850 1.701 0.629 0.204	0.332 0.292 1.523 1.372 0.550 0.168	0.377 0.341 1.709 1.558 0.670 0.203	0.353 0.312 1.444 1.348 0.609 0.196	0.344 0.425 0.398 1.635 1.581 0.767 0.256	0.050 0.200 0.200 0.010 0.800 0.010 0.010	
		2-Methylnapht 1-Methylnapht Hexachlorocyc 2,4,6-Trichloro 2,4,6-Trichloro 2,Fluorobiphei 2-Fluorobiphei 2-Nitroaniline	talene slopentadiene sphenol nyl (sum) shalene zene alate	AvgCalFac Lin, WithO AvgCalFac AvgCalFac AvgCalFac AvgCalFac AvgCalFac	t ffset t t t t t t	0.041 0 0.295 0 0.186 0 1.609 1 1.493 1 0.493 0 0.144 0 0.144 0 1.829 1	.095 .320 .240 .710 .530 .509	0.127 0.348 0.259 1.644 1.552 0.524	0.399 0.331 1.850 1.701 0.629	0.332 0.292 1.523 1.372 0.550	0.377 0.341 1.709 1.558 0.670	0.353 0.312 1.444 1.348 0.609	0.344 0.425 0.398 1.635 1.581 0.767	0.050 0.200 0.200 0.010 0.800 0.010	

Figure 8. Reported results including checks for (A) minimum RRF/r^2 and (B) for minimum ion abundance

Daily Analysis

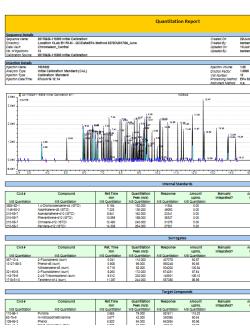
Peak Nam In Quanti NNItrosodi Pridine 2-Fluorobh Bisi2-chiorobh 1-3 Dichorobh 1-3 Dichorobh 1-4 Dichorobh Bisi2-chiorobh 1-4 Dichorobh Bisi2-chiorobh 2-Attertyiph Bisi2-chiorobh NNitrobenze Nitrobenze Nitrobenze S-Nitrobhorone 2-Nitrobhoroh 2

Hexachloro 2,4,6-Trich 2,4,5-Trich 2-Fluorobip 2-Chlorons 2-Nitroanili 1,4-Dinitrot Dimethyl p 1,3-Dinitrot 2 6-Dinitrot

After the initial calibration the daily analysis is a sequence with a fixed structure. Due to the automation delivered via the eWorkflows the correct sequence structure and number of method blanks and calibration check standards are automatically added, depending on the number of samples analyzed.

The report template provides reports for each aspect required in the daily analysis. This results in instant report creation without the need to transfer data to an external spreadsheet, thus eliminating the risk of error due to human data transcription.

Beside the MS Tune Check and calibration reports, the environmental template provides reports for all daily analysis experiments; Sequence overview, breakdown, blanks, check standards, quantitation, tentatively identified peaks, internal standard summaries, surrogate recovery, duplicates and so on. Figure 9 shows some examples of the reports; A is the general quantitation report, B the internal standard summary.



Automated report creation

The data can be automatically reported in order to create the final environmental report of the entire analysis. Chromeleon CDS also supports the creation of an electronic version of the report using the Adobe portable document file format (.pdf) and can be directly integrated with a laboratory information management system (LIMS), making it very easy to distribute the report to all stakeholders.

CONCLUSIONS

Chromeleon CDS offers a fast and simple way to run analyses and create environmental reports according to the extensive requirements as described in the U.S. EPA methods. Benefits include: • Increased reliability of results – eWorkflows ensure that SOPs are followed and transcription errors and errors caused by manual calculations are eliminated.

- calculations.
- reports to be created through three mouse clicks.

REFERENCES

Chromatography/Mass Spectrometry (GC/MS), Revision 5.

TRADEMARKS/LICENSING

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				Internal Standard S	ummary Report	:: 1,4-Dichloro	obenzene-d4	(ISTD)	В
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Yes	Not Confirmed								

 Increased laboratory productivity – users can spend more time running experiments and less time learning different software packages and performing manual data transcription and

Faster creation of environmental reports - the flexible reporting tool enables the environmental

1. U.S. EPA. July 2014. Method 8270D (SW-846): Semivolatile Organic Compounds by Gas

